



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:08 PM UTC

PDB ID : 7QSN / pdb_00007qsn
EMDB ID : EMD-14139
Title : Bovine complex I in lipid nanodisc, Deactive-apo
Authors : Chung, I.; Bridges, H.R.; Hirst, J.
Deposited on : 2022-01-13
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

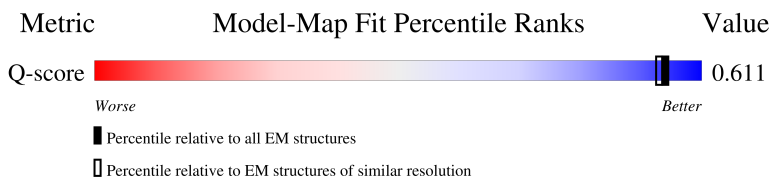
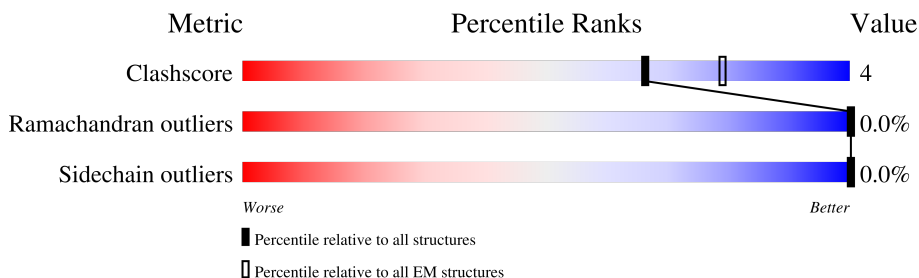
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 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.



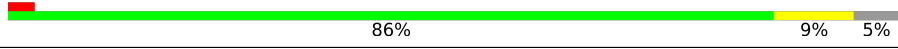
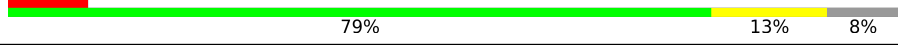
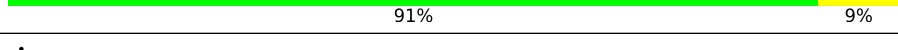
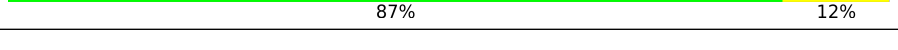
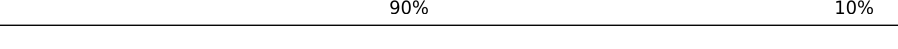
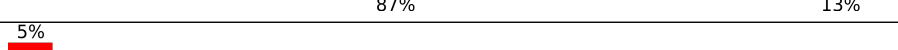
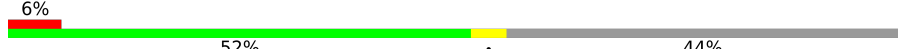
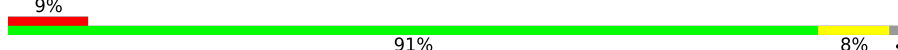
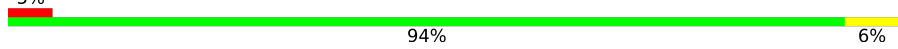
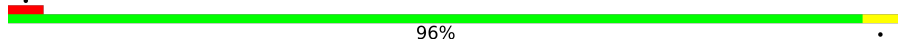
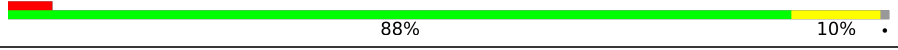
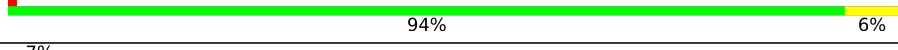
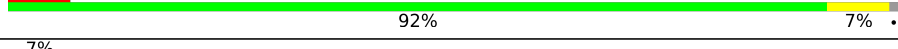
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	18% 73% 19% 8%
2	B	216	62% 10% 28%
3	C	266	71% 7% 22%
4	D	463	81% 7% 13%

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

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	127	
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 59 unique types of molecules in this entry. The entry contains 69319 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	106	Total	C	N	O	S	0	0
			852	578	124	145	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	404	Total	C	N	O	S	0	0
			3262	2083	560	595	24		

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	1	0
			3336	2102	597	617	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	291	Total	C	N	O	S	1	0
			2316	1555	357	381	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	327	Total	C	N	O	S	0	0
			2623	1695	464	459	5		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			688	444	101	138	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			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	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	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	1	0
			1498	958	276	257	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	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		

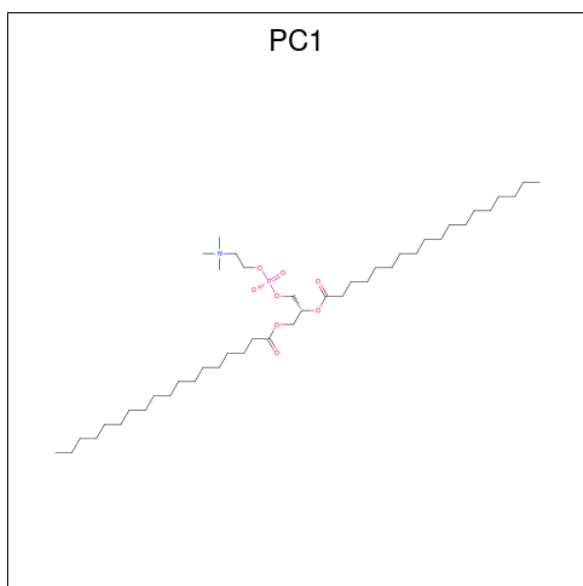
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

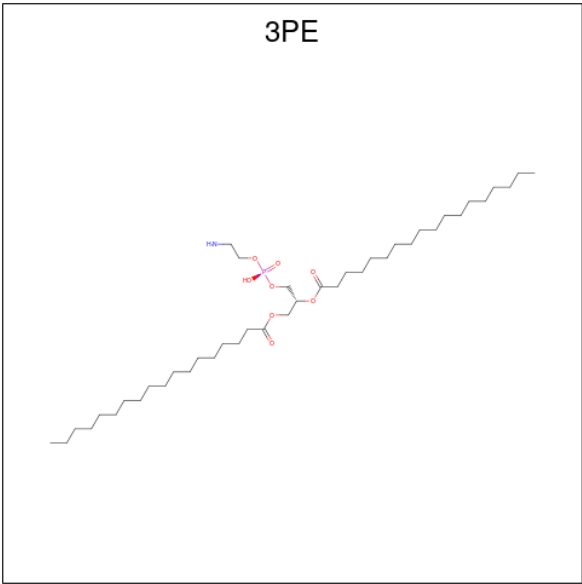
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	N	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	d	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



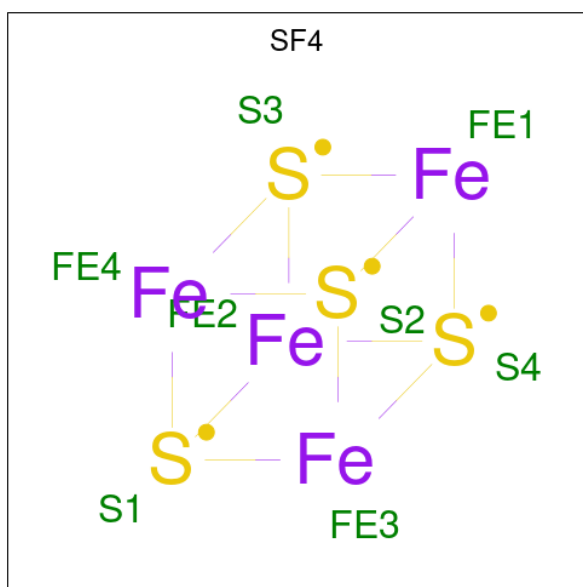
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	L	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

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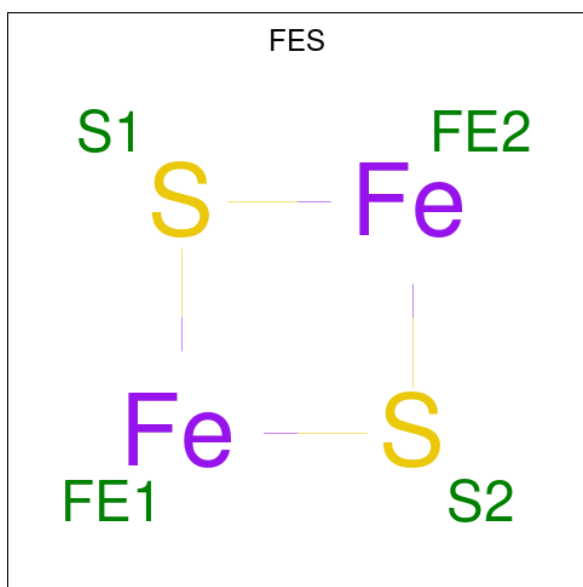
Mol	Chain	Residues	Atoms					AltConf
46	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	O	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	Y	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	b	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	d	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	f	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	g	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	h	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	m	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



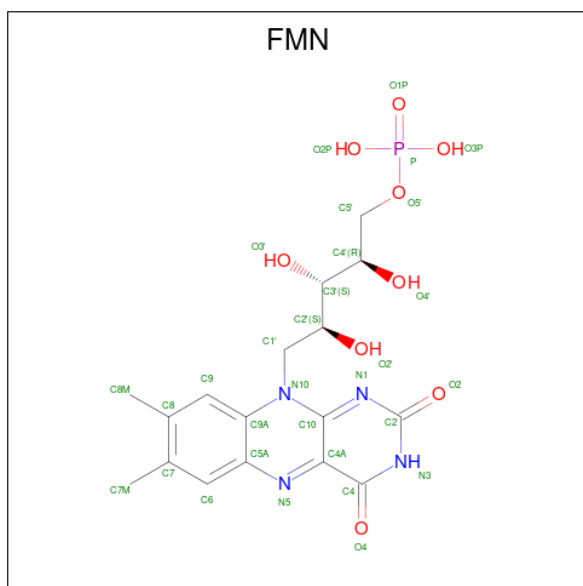
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

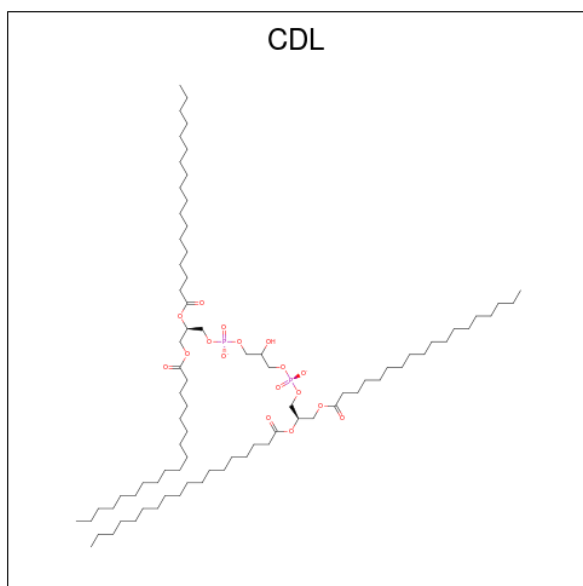


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

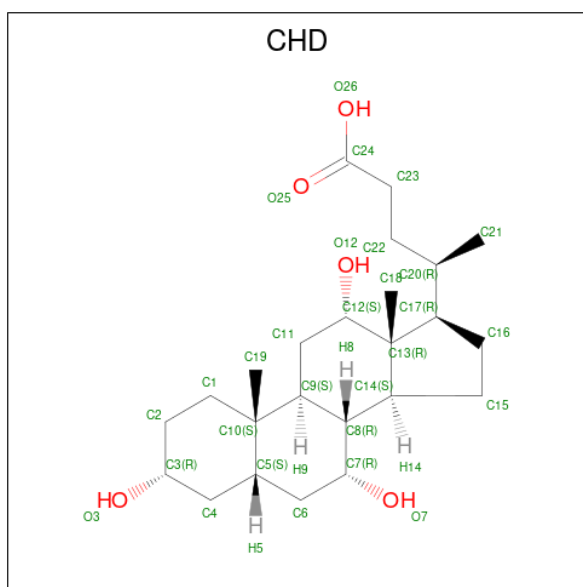
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



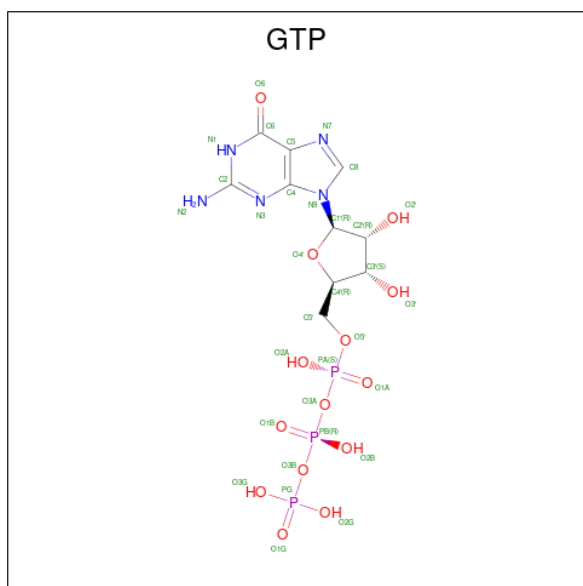
Mol	Chain	Residues	Atoms				AltConf
51	L	1	Total	C	O	P	0
			79	60	17	2	
51	N	1	Total	C	O	P	0
			85	66	17	2	
51	X	1	Total	C	O	P	0
			86	67	17	2	
51	d	1	Total	C	O	P	0
			65	46	17	2	
51	h	1	Total	C	O	P	0
			68	49	17	2	
51	r	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 52 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
52	L	1	Total	C	O	0
			29	24	5	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

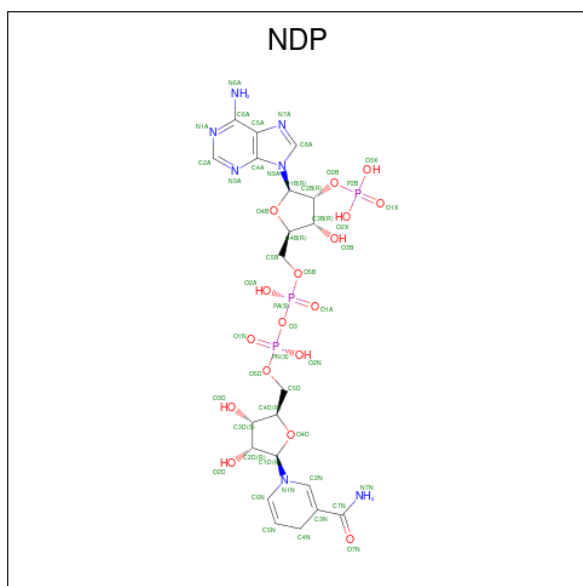


Mol	Chain	Residues	Atoms					AltConf
53	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

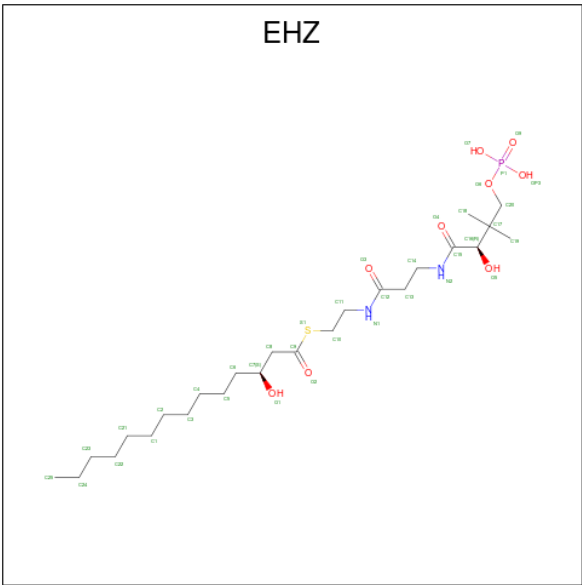


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

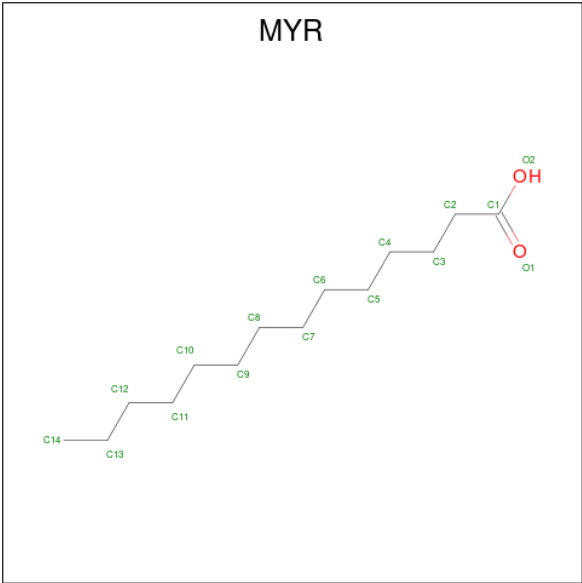
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



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

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	A	5	Total 5	O 5	0
59	B	37	Total 37	O 37	0
59	C	58	Total 58	O 58	0
59	D	113	Total 113	O 113	0
59	E	8	Total 8	O 8	0
59	F	30	Total 30	O 30	0
59	G	157	Total 157	O 157	0
59	H	39	Total 39	O 39	0
59	I	65	Total 65	O 65	0
59	J	18	Total 18	O 18	0
59	K	10	Total 10	O 10	0
59	L	64	Total 64	O 64	0
59	M	80	Total 80	O 80	0
59	N	48	Total 48	O 48	0
59	O	8	Total 8	O 8	0
59	P	29	Total 29	O 29	0
59	Q	63	Total 63	O 63	0
59	R	12	Total 12	O 12	0
59	S	1	Total 1	O 1	0
59	U	8	Total 8	O 8	0
59	V	5	Total 5	O 5	0
59	W	3	Total 3	O 3	0

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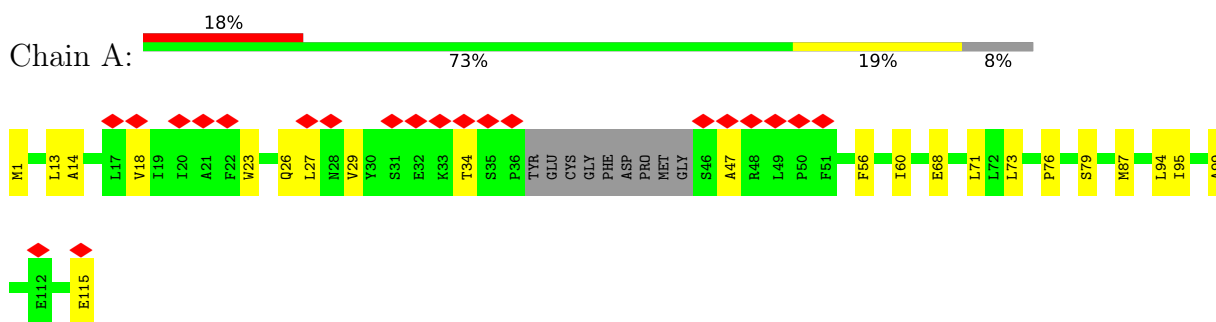
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Mol	Chain	Residues	Atoms		AltConf
59	X	13	Total 13	O 13	0
59	Y	1	Total 1	O 1	0
59	Z	23	Total 23	O 23	0
59	a	13	Total 13	O 13	0
59	b	2	Total 2	O 2	0
59	c	1	Total 1	O 1	0
59	d	16	Total 16	O 16	0
59	e	14	Total 14	O 14	0
59	f	1	Total 1	O 1	0
59	g	12	Total 12	O 12	0
59	h	26	Total 26	O 26	0
59	i	5	Total 5	O 5	0
59	j	2	Total 2	O 2	0
59	l	13	Total 13	O 13	0
59	m	10	Total 10	O 10	0
59	n	23	Total 23	O 23	0
59	o	3	Total 3	O 3	0
59	p	22	Total 22	O 22	0
59	q	19	Total 19	O 19	0
59	r	14	Total 14	O 14	0
59	s	2	Total 2	O 2	0

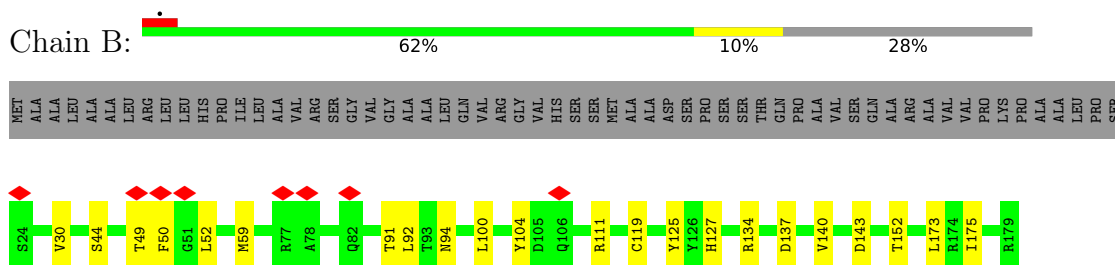
3 Residue-property plots [i](#)

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

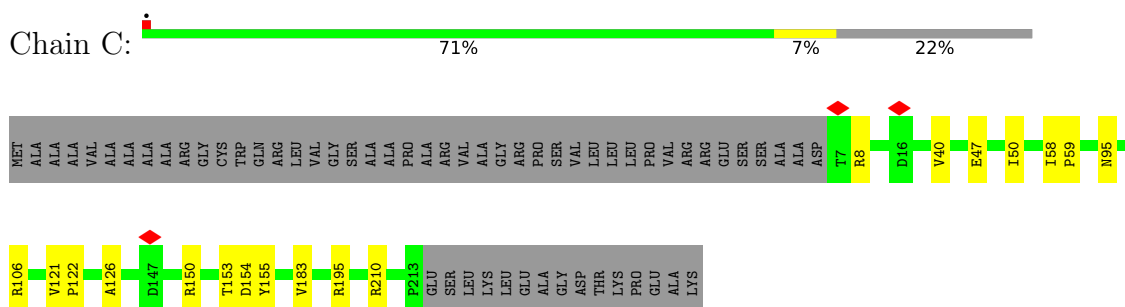
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



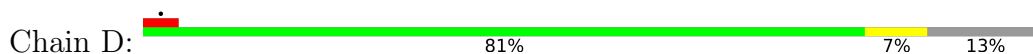
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

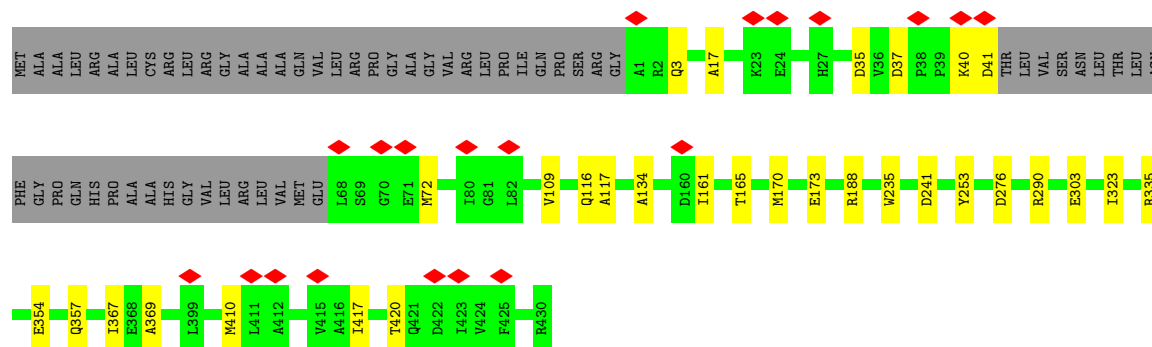


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

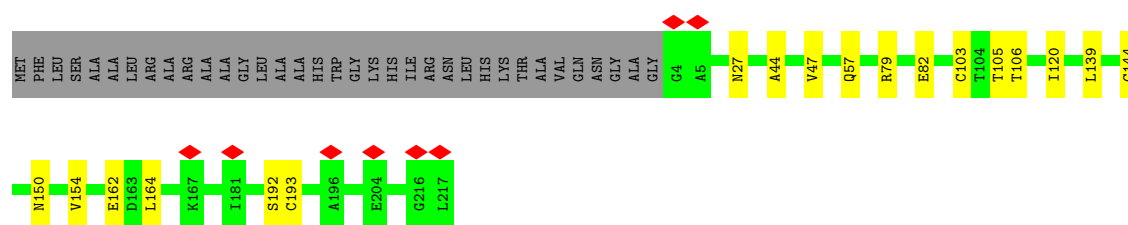
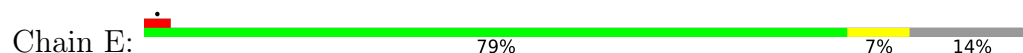


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

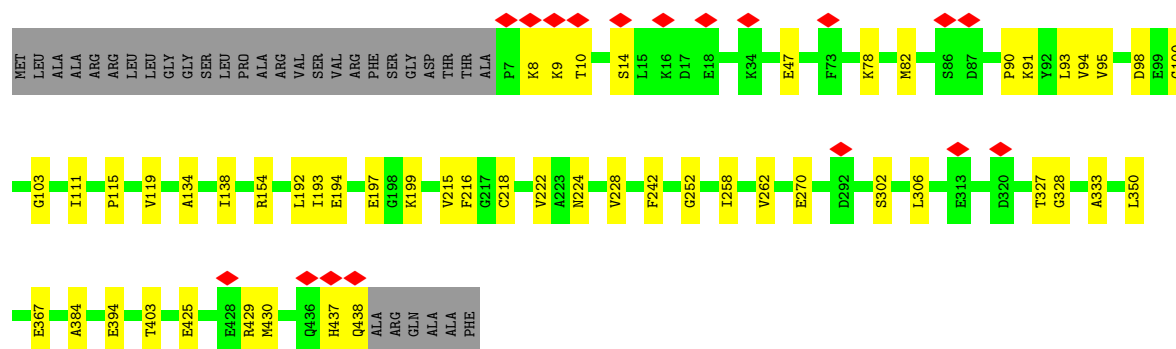
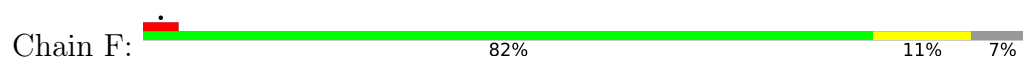




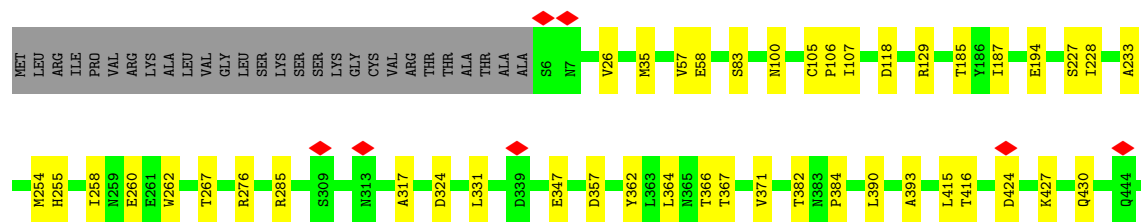
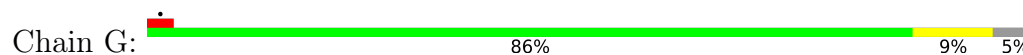
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

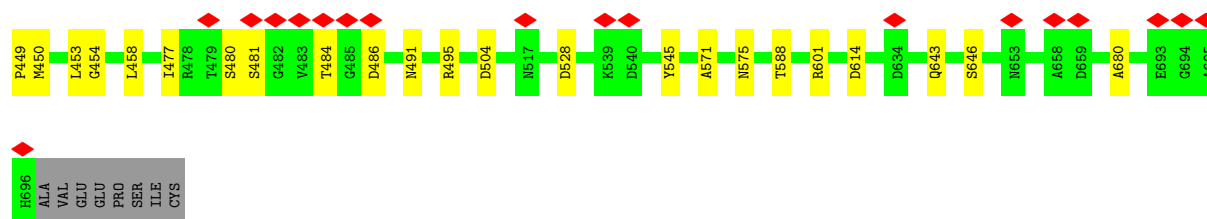


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

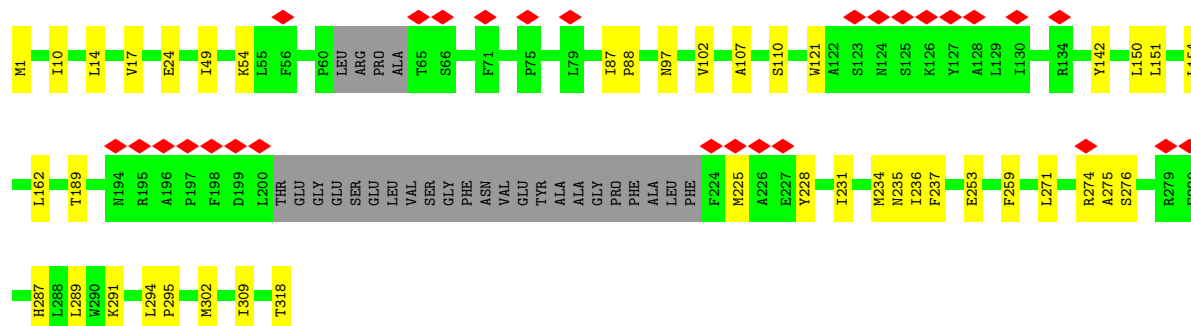
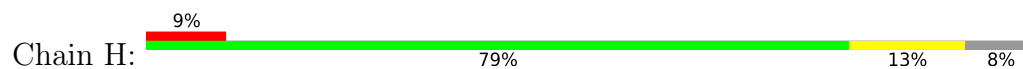


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

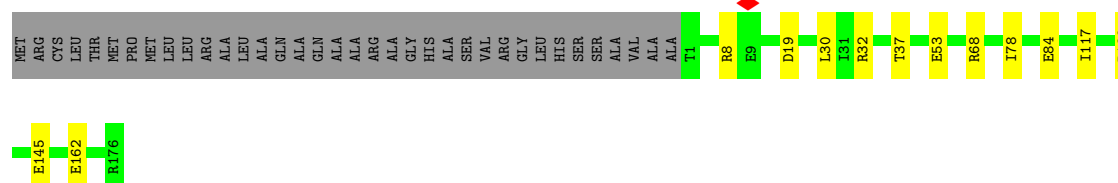




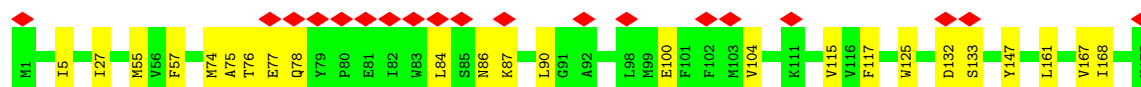
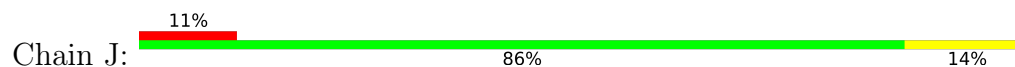
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



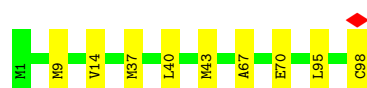
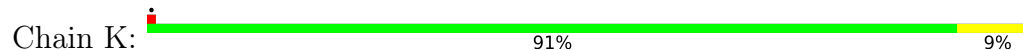
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



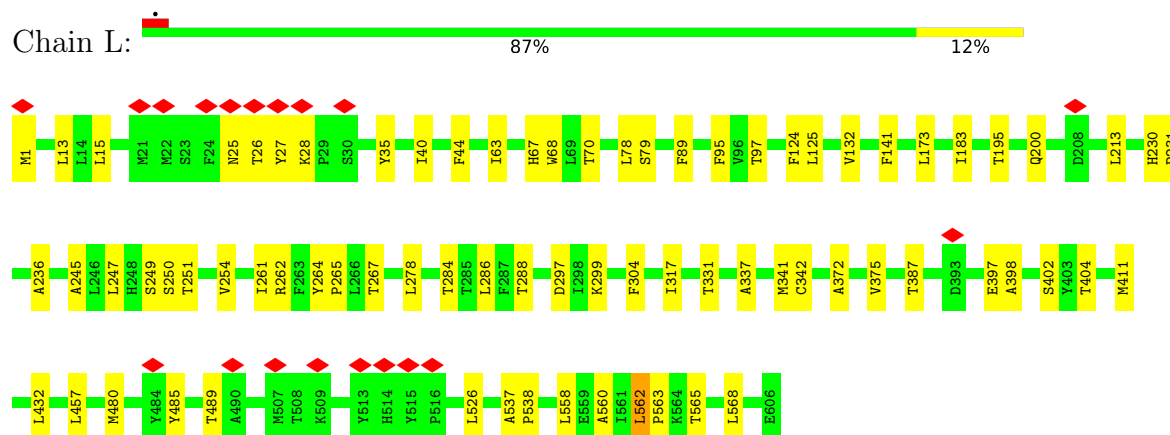
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



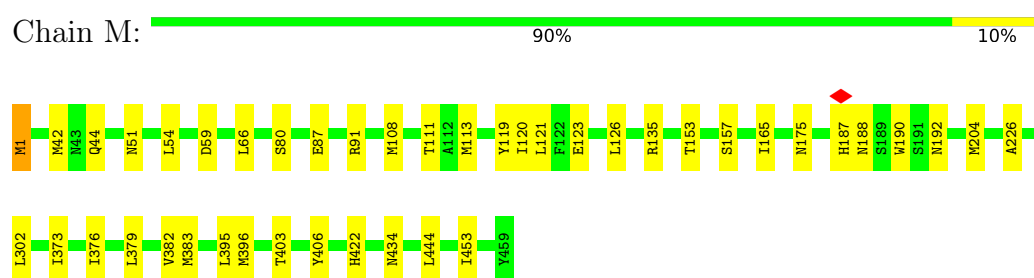
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



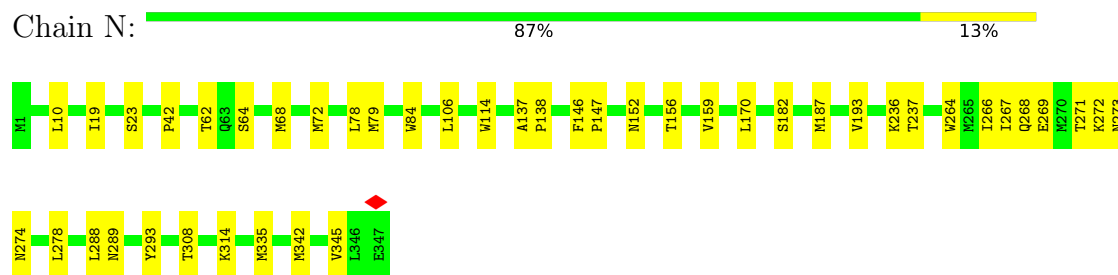
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



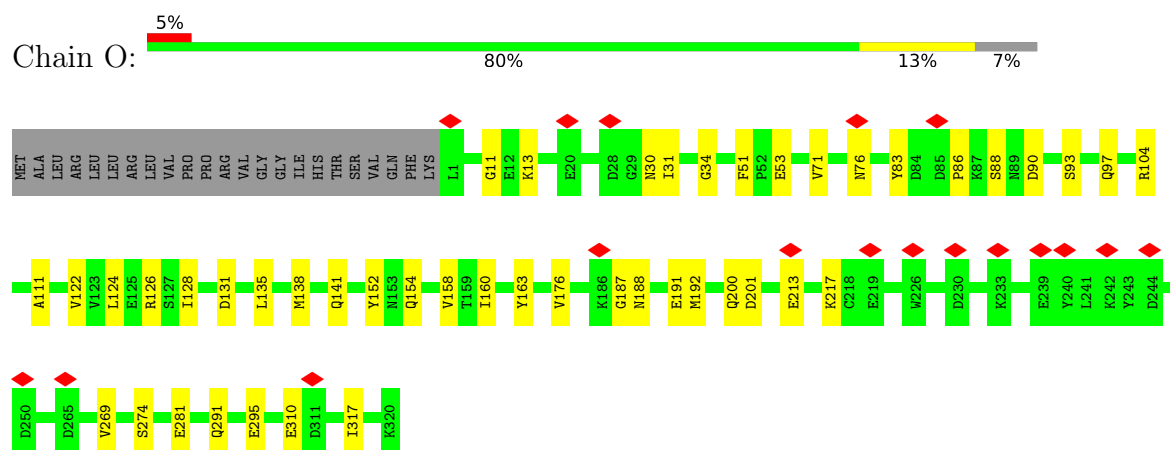
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



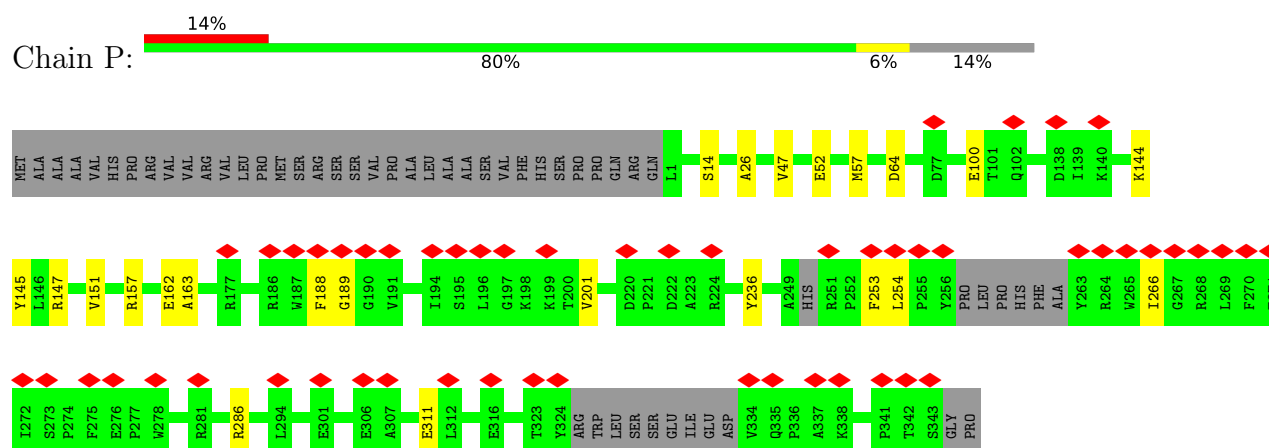
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



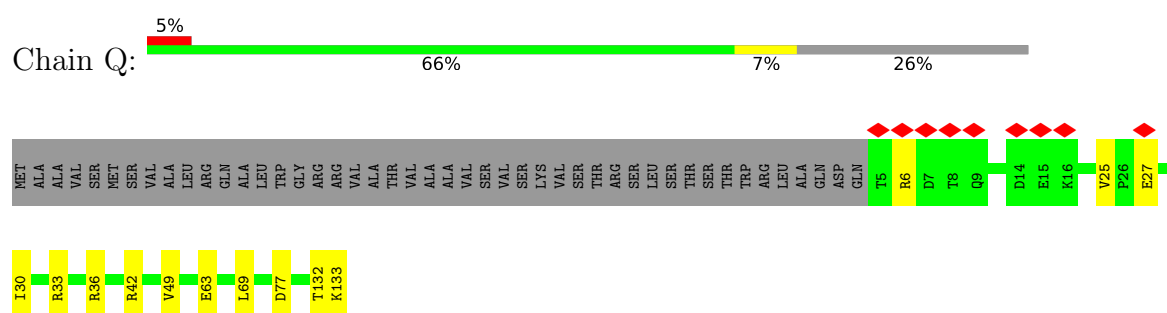
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



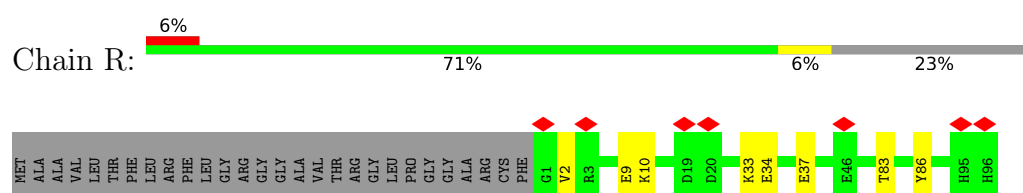
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



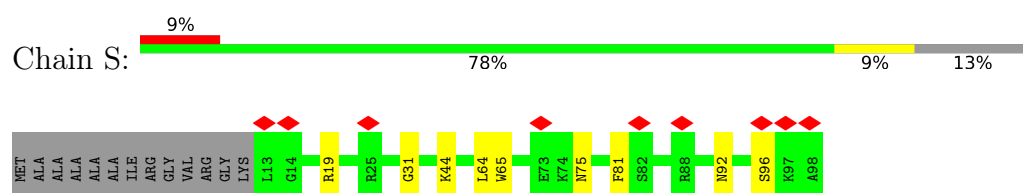
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



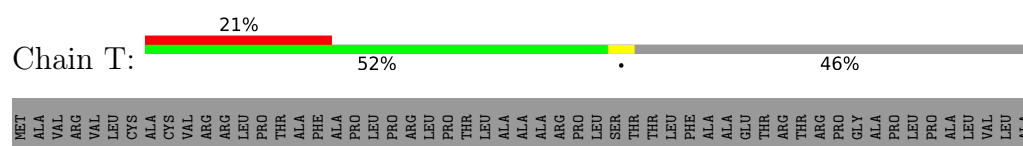
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

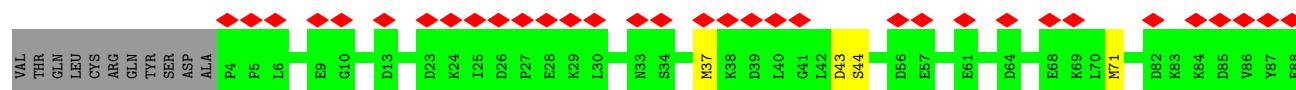


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

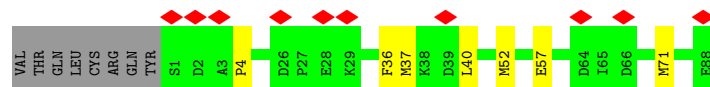


- Molecule 20: Acyl carrier protein, mitochondrial

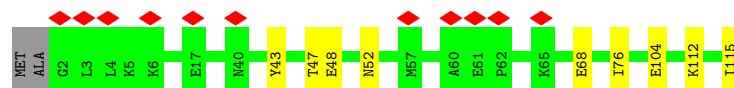




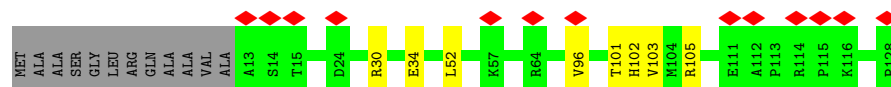
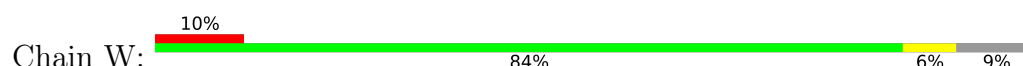
- Molecule 20: Acyl carrier protein, mitochondrial



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



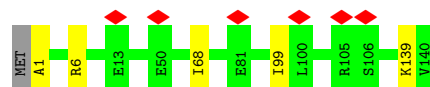
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

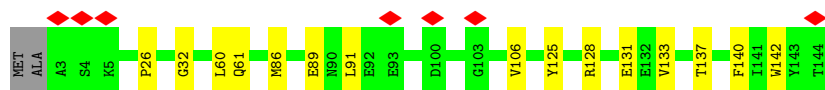


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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

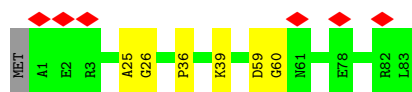




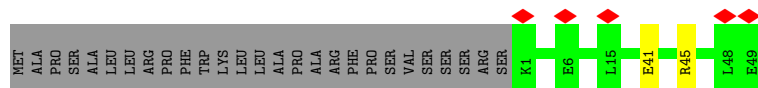
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



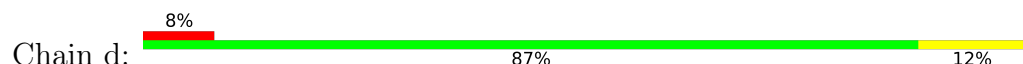
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



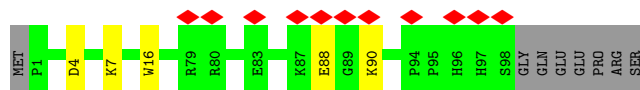
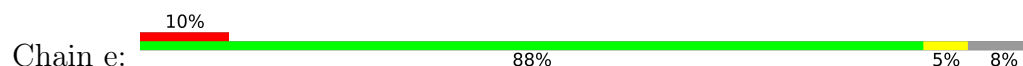
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



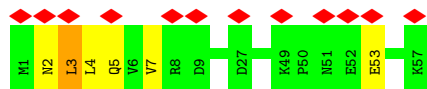
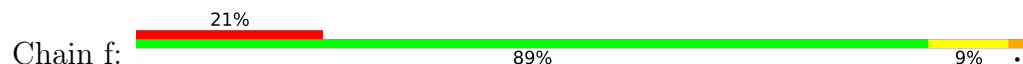
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



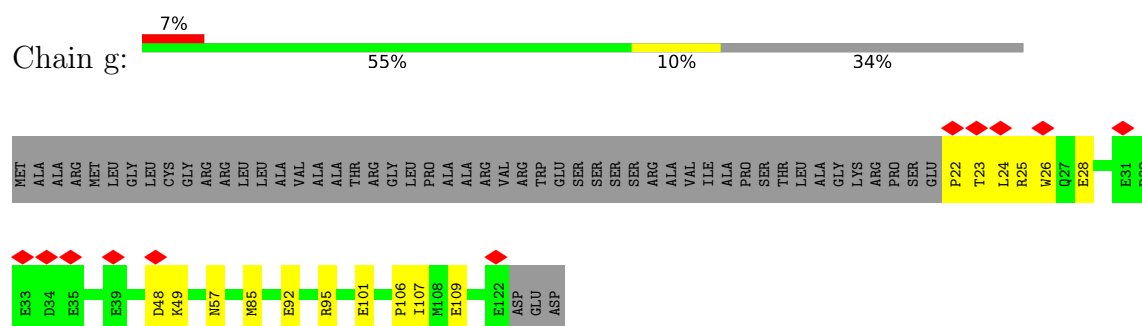
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



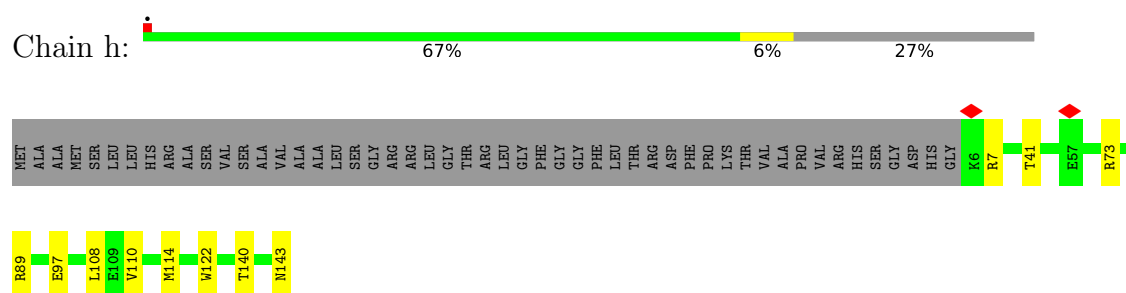
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



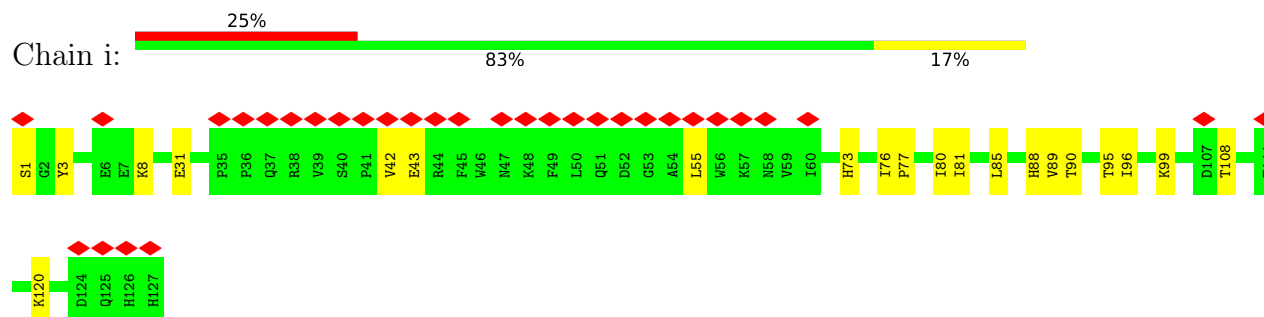
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



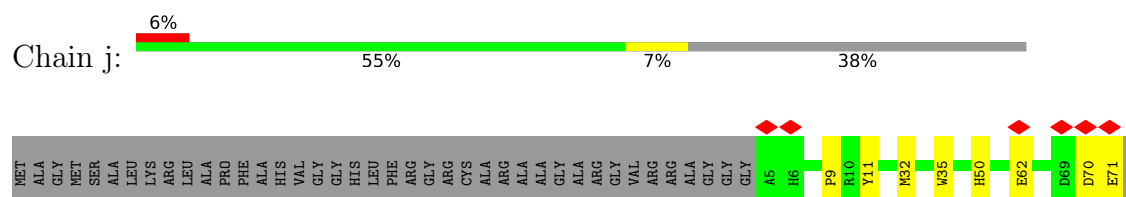
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



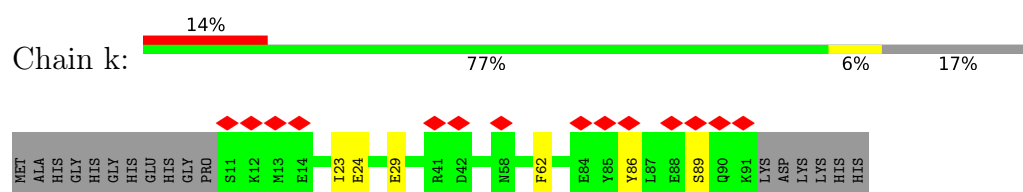
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



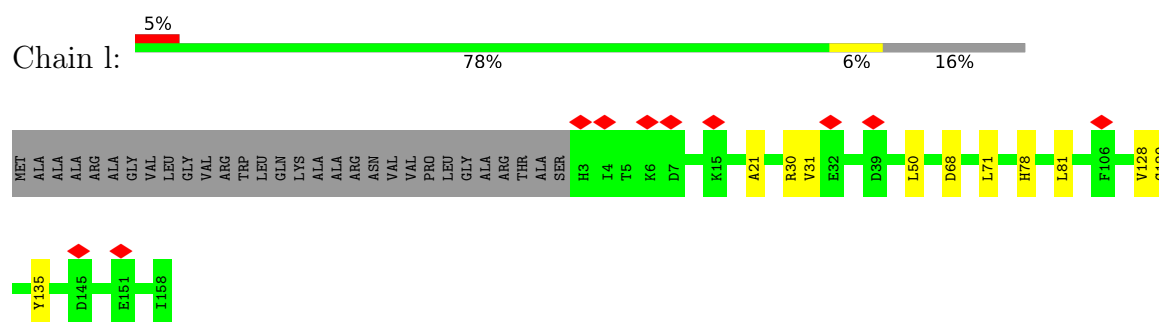
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



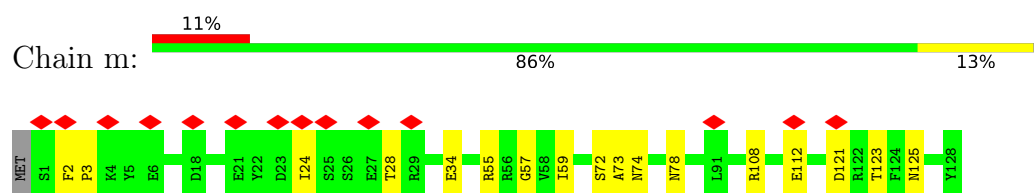
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



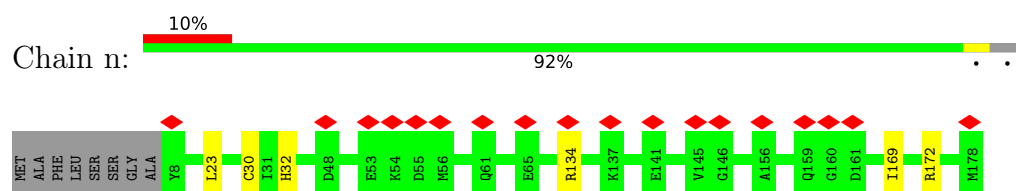
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



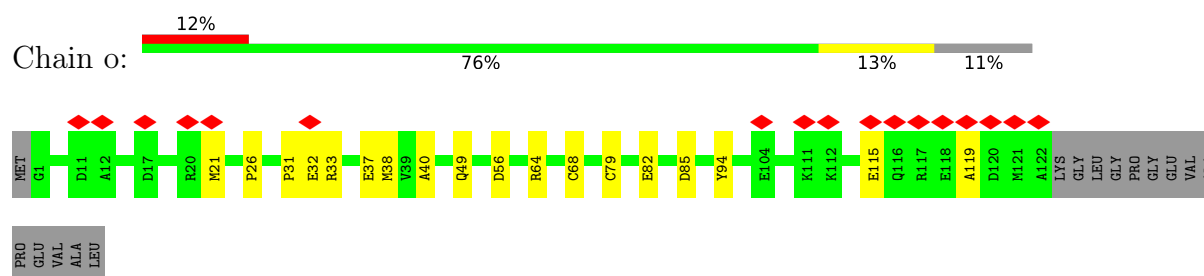
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



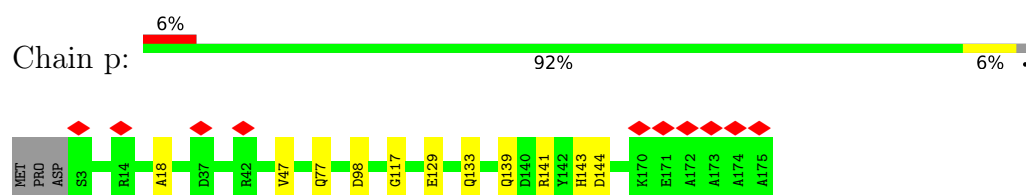
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



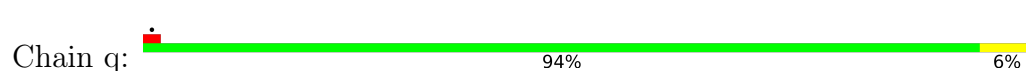
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

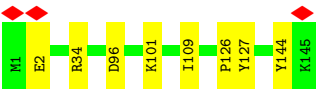


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

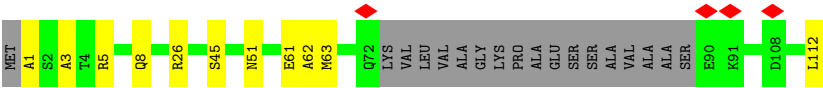


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

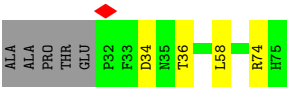
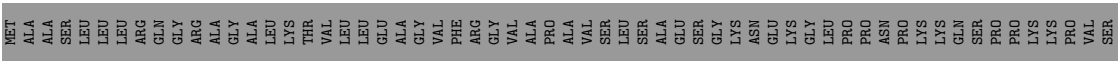




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23583	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	29.852	Depositor
Minimum map value	-10.648	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.943	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	479.744, 479.744, 479.744	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7496, 0.7496, 0.7496	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/863	0.31	0/1181
2	B	0.31	0/1278	0.39	0/1728
3	C	0.29	0/1772	0.35	0/2413
4	D	0.29	0/3334	0.33	0/4514
5	E	0.26	0/1699	0.34	0/2312
6	F	0.28	0/3412	0.36	0/4610
7	G	0.27	0/5387	0.34	0/7301
8	H	0.26	0/2371	0.33	0/3237
9	I	0.30	0/1445	0.37	0/1956
10	J	0.26	0/1370	0.33	0/1859
11	K	0.27	0/745	0.30	0/1008
12	L	0.27	0/4920	0.33	0/6694
13	M	0.28	0/3738	0.32	0/5097
14	N	0.28	0/2792	0.32	0/3800
15	O	0.26	0/2651	0.32	0/3587
16	P	0.25	0/2690	0.37	0/3642
17	Q	0.27	0/1072	0.32	0/1449
18	R	0.28	0/753	0.31	0/1014
19	S	0.24	0/702	0.36	0/945
20	T	0.22	0/700	0.42	0/944
20	U	0.27	0/719	0.33	0/971
21	V	0.24	0/943	0.30	0/1277
22	W	0.26	0/1006	0.34	0/1352
23	X	0.27	0/1439	0.34	0/1942
24	Y	0.25	0/1042	0.28	0/1414
25	Z	0.27	0/1186	0.29	0/1599
26	a	0.27	0/584	0.33	0/786
27	b	0.26	0/672	0.33	0/923
28	c	0.26	0/427	0.27	0/579
29	d	0.30	0/1018	0.33	0/1375
30	e	0.27	0/846	0.32	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.26	0/505	0.40	0/681
32	g	0.26	0/873	0.38	0/1186
33	h	0.29	0/1188	0.37	0/1607
34	i	0.25	0/1127	0.41	0/1534
35	j	0.26	0/607	0.36	0/833
36	k	0.25	0/672	0.31	0/906
37	l	0.26	0/1369	0.32	0/1873
38	m	0.26	0/1094	0.34	0/1480
39	n	0.26	0/1551	0.35	0/2099
40	o	0.29	0/1073	0.40	0/1437
41	p	0.27	0/1483	0.34	0/2000
42	q	0.27	0/1250	0.32	0/1698
43	r	0.27	0/789	0.32	0/1068
44	s	0.24	0/383	0.33	0/518
All	All	0.27	0/67540	0.34	0/91560

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	852	0	896	20	0
2	B	1247	0	1256	14	0
3	C	1721	0	1675	13	0
4	D	3262	0	3201	23	0
5	E	1659	0	1664	11	0
6	F	3336	0	3288	34	0
7	G	5298	0	5316	47	0
8	H	2316	0	2435	34	0
9	I	1414	0	1370	16	0
10	J	1345	0	1352	23	0
11	K	745	0	785	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	51	0
13	M	3654	0	3852	38	0
14	N	2733	0	2912	35	0
15	O	2589	0	2566	28	0
16	P	2623	0	2651	15	0
17	Q	1049	0	1045	10	0
18	R	740	0	714	6	0
19	S	691	0	706	5	0
20	T	688	0	684	2	0
20	U	707	0	700	6	0
21	V	923	0	964	5	0
22	W	982	0	999	6	0
23	X	1402	0	1381	7	0
24	Y	1030	0	1039	3	0
25	Z	1157	0	1156	12	0
26	a	569	0	568	3	0
27	b	651	0	662	4	0
28	c	414	0	415	1	0
29	d	999	0	988	17	0
30	e	825	0	826	4	0
31	f	492	0	501	5	0
32	g	846	0	798	12	0
33	h	1154	0	1168	12	0
34	i	1097	0	1108	18	0
35	j	580	0	519	8	0
36	k	653	0	639	4	0
37	l	1314	0	1210	8	0
38	m	1067	0	1067	12	0
39	n	1498	0	1445	4	0
40	o	1048	0	1018	13	0
41	p	1450	0	1426	9	0
42	q	1209	0	1182	7	0
43	r	776	0	782	7	0
44	s	371	0	344	3	0
45	A	50	0	77	0	0
45	B	51	0	79	1	0
45	J	46	0	69	3	0
45	M	95	0	144	4	0
45	N	30	0	34	0	0
45	d	40	0	54	1	0
46	A	47	0	71	0	0
46	H	36	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	I	102	0	164	2	0
46	K	43	0	60	1	0
46	L	121	0	170	4	0
46	M	145	0	224	6	0
46	N	90	0	137	2	0
46	O	36	0	46	0	0
46	Y	211	0	304	1	0
46	Z	43	0	63	0	0
46	b	88	0	130	4	0
46	d	90	0	131	1	0
46	f	31	0	36	0	0
46	g	36	0	46	0	0
46	h	39	0	52	1	0
46	m	40	0	57	1	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	L	79	0	108	2	0
51	N	85	0	117	1	0
51	X	86	0	125	2	0
51	d	65	0	77	2	0
51	h	68	0	80	5	0
51	r	64	0	72	0	0
52	L	29	0	37	2	0
53	O	32	0	12	4	0
54	O	1	0	0	0	0
55	P	48	0	26	0	0
56	R	1	0	0	0	0
57	T	37	0	0	1	0
57	U	37	0	0	0	0
58	o	15	0	27	0	0
59	A	5	0	0	0	0
59	B	37	0	0	1	0
59	C	58	0	0	3	0
59	D	113	0	0	5	0
59	E	8	0	0	0	0
59	F	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	G	157	0	0	5	0
59	H	39	0	0	1	0
59	I	65	0	0	1	0
59	J	18	0	0	0	0
59	K	10	0	0	0	0
59	L	64	0	0	3	0
59	M	80	0	0	4	0
59	N	48	0	0	3	0
59	O	8	0	0	1	0
59	P	29	0	0	2	0
59	Q	63	0	0	3	0
59	R	12	0	0	1	0
59	S	1	0	0	0	0
59	U	8	0	0	0	0
59	V	5	0	0	0	0
59	W	3	0	0	0	0
59	X	13	0	0	0	0
59	Y	1	0	0	0	0
59	Z	23	0	0	0	0
59	a	13	0	0	0	0
59	b	2	0	0	0	0
59	c	1	0	0	0	0
59	d	16	0	0	1	0
59	e	14	0	0	0	0
59	f	1	0	0	0	0
59	g	12	0	0	1	0
59	h	26	0	0	0	0
59	i	5	0	0	0	0
59	j	2	0	0	0	0
59	l	13	0	0	0	0
59	m	10	0	0	1	0
59	n	23	0	0	0	0
59	o	3	0	0	0	0
59	p	22	0	0	0	0
59	q	19	0	0	0	0
59	r	14	0	0	1	0
59	s	2	0	0	1	0
All	All	69319	0	69130	535	0

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

All (535) 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)
17:Q:133:LYS:O	59:Q:201:HOH:O	1.87	0.93
6:F:98:ASP:OD2	59:F:601:HOH:O	1.90	0.89
7:G:484:THR:OG1	7:G:486:ASP:OD1	1.92	0.87
15:O:83:TYR:OH	53:O:401:GTP:O2'	1.92	0.86
13:M:44:GLN:OE1	59:M:701:HOH:O	1.94	0.86
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.10	0.84
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.11	0.83
4:D:369:ALA:O	59:D:501:HOH:O	1.96	0.83
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.61	0.83
1:A:71:LEU:O	10:J:147:TYR:OH	1.96	0.83
32:g:85:MET:SD	59:g:311:HOH:O	2.37	0.81
46:M:601:3PE:O14	14:N:274:ASN:ND2	2.14	0.81
7:G:393:ALA:O	59:G:901:HOH:O	2.00	0.80
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.15	0.80
34:i:99:LYS:NZ	40:o:49:GLN:OE1	2.14	0.80
7:G:324:ASP:OD1	59:G:902:HOH:O	2.01	0.79
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.16	0.79
3:C:95:ASN:OD1	59:C:301:HOH:O	2.01	0.78
43:r:26:ARG:NH1	59:r:301:HOH:O	2.17	0.78
4:D:170:MET:SD	59:D:561:HOH:O	2.41	0.78
15:O:128:ILE:O	59:O:501:HOH:O	2.02	0.78
14:N:289:ASN:OD1	59:N:1001:HOH:O	2.00	0.78
19:S:92:ASN:O	19:S:96:SER:OG	2.02	0.77
14:N:19:ILE:O	14:N:23:SER:OG	2.01	0.77
8:H:318:THR:OG1	25:Z:61:GLN:OE1	2.02	0.77
4:D:303:GLU:OE1	59:D:502:HOH:O	2.02	0.77
30:e:88:GLU:OE2	30:e:90:LYS:NZ	2.12	0.77
8:H:253:GLU:OE2	26:a:25:ARG:NH1	2.19	0.76
35:j:62:GLU:OE1	35:j:62:GLU:N	2.18	0.76
6:F:199:LYS:NZ	59:F:603:HOH:O	2.16	0.76
12:L:236:ALA:O	59:L:801:HOH:O	2.03	0.76
18:R:83:THR:O	59:R:301:HOH:O	2.04	0.76
9:I:19:ASP:OD1	25:Z:32:GLY:N	2.20	0.75
11:K:70:GLU:OE2	14:N:64:SER:OG	2.02	0.75
41:p:129:GLU:OE2	41:p:133:GLN:NE2	2.19	0.75
6:F:82:MET:O	6:F:91:LYS:NZ	2.18	0.74
12:L:397:GLU:OE1	59:L:802:HOH:O	2.04	0.74
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.20	0.74
2:B:94:ASN:OD1	59:B:301:HOH:O	2.05	0.74
14:N:269:GLU:OE2	59:N:1002:HOH:O	2.06	0.73
15:O:187:GLY:HA2	15:O:192:MET:HE2	1.69	0.73
13:M:108:MET:HE1	51:X:201:CDL:H221	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.70	0.73
13:M:382:VAL:HG22	13:M:396:MET:HE3	1.71	0.72
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.71	0.72
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.70	0.71
14:N:308:THR:O	59:N:1003:HOH:O	2.08	0.71
33:h:41:THR:OG1	51:h:201:CDL:OB9	2.01	0.71
45:J:201:PC1:H142	25:Z:140:PHE:O	1.90	0.70
14:N:314:LYS:NZ	15:O:274:SER:OG	2.24	0.70
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.23	0.69
46:M:604:3PE:N	45:M:605:PC1:O32	2.23	0.69
7:G:366:THR:O	7:G:367:THR:OG1	2.10	0.69
46:M:601:3PE:H2E2	46:N:901:3PE:H3I1	1.73	0.69
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.74	0.69
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.22	0.69
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.23	0.69
44:s:34:ASP:OD1	44:s:36:THR:OG1	2.07	0.69
23:X:21:SER:OG	26:a:51:ASP:OD1	2.09	0.69
40:o:82:GLU:N	40:o:82:GLU:OE1	2.26	0.68
6:F:47:GLU:N	6:F:47:GLU:OE1	2.26	0.68
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.74	0.68
4:D:165:THR:OG1	8:H:275:ALA:O	2.08	0.67
13:M:135:ARG:O	59:M:703:HOH:O	2.12	0.67
46:M:601:3PE:C2E	46:N:901:3PE:H3I1	2.25	0.67
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.28	0.67
15:O:34:GLY:N	53:O:401:GTP:O3G	2.28	0.66
14:N:273:ASN:O	24:Y:139:LYS:NZ	2.29	0.66
6:F:100:GLY:O	59:F:602:HOH:O	2.14	0.66
9:I:68:ARG:O	59:I:301:HOH:O	2.13	0.66
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.25	0.65
40:o:64:ARG:NH1	40:o:85:ASP:OD2	2.29	0.65
1:A:14:ALA:O	1:A:18:VAL:HG23	1.96	0.65
13:M:271:MET:HE2	13:M:271:MET:HA	1.78	0.65
29:d:120:ARG:O	38:m:108:ARG:NH2	2.30	0.64
4:D:173:GLU:OE2	59:D:503:HOH:O	2.13	0.64
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.32	0.64
15:O:53:GLU:OE2	15:O:126:ARG:NH2	2.29	0.64
10:J:75:ALA:O	10:J:76:THR:OG1	2.13	0.64
38:m:72:SER:O	59:m:301:HOH:O	2.15	0.64
22:W:30:ARG:NH2	22:W:34:GLU:OE1	2.30	0.64
31:f:53:GLU:N	31:f:53:GLU:OE1	2.30	0.64
15:O:88:SER:OG	15:O:90:ASP:OD1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:LEU:HD21	14:N:72:MET:HE2	1.79	0.63
13:M:59:ASP:OD2	59:M:704:HOH:O	2.16	0.63
2:B:104:TYR:O	2:B:111:ARG:NH2	2.30	0.63
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.81	0.63
12:L:485:TYR:O	12:L:489:THR:OG1	2.16	0.63
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.81	0.63
5:E:105:THR:HG22	5:E:106:THR:H	1.64	0.63
16:P:64:ASP:OD2	59:P:602:HOH:O	2.16	0.63
27:b:59:ASP:OD2	27:b:60:GLY:N	2.33	0.62
29:d:63:LEU:HD23	51:d:204:CDL:OA9	1.99	0.62
52:L:705:CHD:H12	52:L:705:CHD:H212	1.82	0.62
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.81	0.62
22:W:96:VAL:HG12	22:W:96:VAL:O	1.99	0.62
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.80	0.62
29:d:1:AME:HE2	33:h:122:TRP:CD2	2.35	0.61
29:d:2:MET:HG2	33:h:122:TRP:CD1	2.36	0.61
16:P:311:GLU:OE1	16:P:311:GLU:N	2.33	0.61
3:C:210:ARG:NH2	7:G:35:MET:SD	2.74	0.61
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.81	0.61
20:U:37:MET:HE3	20:U:71:MET:HE1	1.83	0.61
7:G:588:THR:O	59:G:903:HOH:O	2.16	0.61
32:g:22:PRO:O	32:g:23:THR:OG1	2.16	0.61
40:o:115:GLU:O	40:o:119:ALA:N	2.26	0.61
8:H:97:ASN:ND2	59:H:702:HOH:O	2.33	0.60
31:f:2:ASN:O	31:f:4:LEU:N	2.34	0.60
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.83	0.60
15:O:104:ARG:NE	15:O:131:ASP:OD2	2.33	0.60
17:Q:6:ARG:NH1	21:V:104:GLU:OE1	2.34	0.60
1:A:34:THR:HG23	1:A:34:THR:O	2.01	0.60
6:F:425:GLU:OE1	6:F:429:ARG:NH1	2.35	0.60
8:H:162:LEU:HD21	8:H:237:PHE:HE1	1.66	0.60
25:Z:131:GLU:N	25:Z:131:GLU:OE1	2.34	0.60
1:A:99:ALA:HB1	46:b:102:3PE:H2B1	1.84	0.59
23:X:104:ALA:O	23:X:108:GLU:OE1	2.20	0.59
33:h:73:ARG:NH2	46:h:202:3PE:O14	2.33	0.59
13:M:87:GLU:OE2	13:M:91:ARG:NE	2.31	0.59
12:L:95:PHE:O	59:L:803:HOH:O	2.16	0.59
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.33	0.59
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.31	0.59
13:M:42:MET:HE1	13:M:453:ILE:HB	1.84	0.59
15:O:30:ASN:OD1	15:O:31:ILE:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:ARG:NH2	43:r:112:LEU:O	2.36	0.58
21:V:68:GLU:OE1	21:V:76:ILE:N	2.35	0.58
1:A:47:ALA:HB1	10:J:77:GLU:H	1.69	0.58
5:E:120:ILE:HG21	5:E:139:LEU:HD13	1.86	0.58
9:I:30:LEU:HD13	46:I:201:3PE:H262	1.86	0.58
11:K:9:MET:HE3	14:N:79:MET:HE1	1.86	0.58
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.84	0.58
17:Q:36:ARG:NH1	59:Q:205:HOH:O	2.37	0.58
13:M:434:ASN:ND2	59:M:707:HOH:O	2.30	0.57
17:Q:27:GLU:N	17:Q:27:GLU:OE1	2.35	0.57
45:B:202:PC1:H143	45:B:202:PC1:O13	2.03	0.57
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.85	0.57
16:P:14:SER:OG	59:P:601:HOH:O	2.05	0.57
2:B:152:THR:HG22	4:D:188:ARG:HD3	1.86	0.57
7:G:449:PRO:HG3	7:G:477:ILE:HG21	1.86	0.57
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.18	0.57
7:G:194:GLU:OE1	7:G:194:GLU:N	2.35	0.56
20:U:52:MET:HE1	39:n:23:LEU:CB	2.34	0.56
34:i:55:LEU:O	34:i:55:LEU:HD23	2.05	0.56
38:m:121:ASP:OD2	38:m:123:THR:OG1	2.18	0.56
1:A:115:GLU:N	1:A:115:GLU:OE1	2.38	0.56
4:D:35:ASP:OD1	59:D:506:HOH:O	2.18	0.56
12:L:132:VAL:O	12:L:262:ARG:NH1	2.33	0.56
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.87	0.56
4:D:37:ASP:OD2	11:K:95:LEU:HD13	2.05	0.56
12:L:25:ASN:OD1	12:L:26:THR:N	2.39	0.56
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.37	0.56
15:O:281:GLU:N	15:O:281:GLU:OE1	2.38	0.56
6:F:384:ALA:HB3	6:F:430:MET:HE2	1.88	0.55
33:h:110:VAL:CG1	33:h:114:MET:HE3	2.36	0.55
5:E:154:VAL:HG13	5:E:164:LEU:HD12	1.88	0.55
8:H:231:ILE:O	8:H:235:ASN:ND2	2.39	0.55
12:L:284:THR:O	12:L:288:THR:OG1	2.20	0.55
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.41	0.55
21:V:112:LYS:NZ	21:V:115:ILE:O	2.39	0.55
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.40	0.55
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.88	0.55
9:I:145:GLU:OE1	9:I:145:GLU:N	2.40	0.55
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.42	0.55
43:r:62:ALA:O	43:r:63:MET:HE2	2.06	0.55
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:9:GLU:OE2	18:R:33:LYS:NZ	2.39	0.54
16:P:100:GLU:OE2	16:P:144:LYS:NZ	2.28	0.54
16:P:157:ARG:NH2	16:P:163:ALA:O	2.39	0.54
8:H:14:LEU:HD22	8:H:225:MET:SD	2.47	0.54
51:h:201:CDL:OB3	34:i:88:HIS:NE2	2.39	0.54
7:G:357:ASP:OD2	19:S:44:LYS:NZ	2.31	0.54
13:M:296:LEU:CD2	13:M:396:MET:HE1	2.38	0.54
36:k:24:GLU:OE1	36:k:24:GLU:N	2.40	0.54
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.42	0.54
15:O:86:PRO:O	15:O:93:SER:OG	2.25	0.54
34:i:89:VAL:O	34:i:95:THR:OG1	2.25	0.54
26:a:43:TYR:CZ	26:a:47:LEU:HD11	2.43	0.54
29:d:2:MET:HG2	33:h:122:TRP:NE1	2.23	0.54
3:C:154:ASP:OD2	59:C:302:HOH:O	2.18	0.53
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.44	0.53
7:G:643:GLN:O	7:G:646:SER:OG	2.20	0.53
43:r:3:ALA:O	43:r:8:GLN:NE2	2.42	0.53
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.38	0.53
21:V:48:GLU:O	21:V:52:ASN:ND2	2.40	0.53
12:L:398:ALA:O	12:L:402:SER:OG	2.20	0.53
1:A:27:LEU:O	1:A:29:VAL:HG23	2.09	0.53
2:B:143:ASP:OD1	16:P:57:MET:HE2	2.08	0.53
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.41	0.53
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.91	0.52
29:d:63:LEU:HD23	51:d:204:CDL:HA62	1.92	0.52
7:G:185:THR:O	7:G:187:ILE:N	2.42	0.52
11:K:43:MET:HE1	14:N:72:MET:HE1	1.91	0.52
8:H:121:TRP:CH2	10:J:78:GLN:HA	2.44	0.52
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.92	0.52
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.92	0.51
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.42	0.51
12:L:13:LEU:HD23	34:i:81:ILE:HD11	1.92	0.51
13:M:187:HIS:O	13:M:192:ASN:ND2	2.43	0.51
11:K:40:LEU:CD2	14:N:72:MET:HE2	2.40	0.51
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.75	0.51
12:L:27:TYR:CE2	52:L:705:CHD:H5	2.44	0.51
2:B:50:PHE:CE2	2:B:52:LEU:HD21	2.45	0.51
7:G:415:LEU:O	7:G:416:THR:OG1	2.27	0.51
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.38	0.51
16:P:147:ARG:O	16:P:151:VAL:HG23	2.10	0.51
1:A:68:GLU:CG	10:J:161:LEU:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.38	0.51
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.93	0.51
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.92	0.51
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.45	0.51
15:O:291:GLN:NE2	15:O:295:GLU:OE1	2.41	0.51
1:A:23:TRP:HA	1:A:26:GLN:OE1	2.11	0.51
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.93	0.51
12:L:560:ALA:O	12:L:565:THR:HG23	2.10	0.51
12:L:251:THR:O	12:L:254:VAL:HG22	2.10	0.51
10:J:100:GLU:O	10:J:104:VAL:HG23	2.11	0.51
12:L:286:LEU:HD13	12:L:411:MET:SD	2.51	0.51
32:g:57:ASN:ND2	32:g:57:ASN:O	2.44	0.50
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.93	0.50
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.46	0.50
1:A:79:SER:HA	1:A:87:MET:HE2	1.93	0.50
13:M:54:LEU:HD22	33:h:97:GLU:OE2	2.11	0.50
13:M:270:ILE:CD1	13:M:395:LEU:HD22	2.40	0.50
33:h:7:ARG:NH1	34:i:31:GLU:O	2.44	0.50
38:m:72:SER:OG	38:m:73:ALA:N	2.45	0.50
3:C:126:ALA:HB2	4:D:253:TYR:C	2.37	0.50
8:H:17:VAL:HG13	8:H:228:TYR:HB3	1.94	0.50
36:k:86:TYR:O	36:k:89:SER:OG	2.16	0.50
18:R:34:GLU:O	42:q:127:TYR:OH	2.28	0.50
32:g:25:ARG:HE	32:g:26:TRP:H	1.60	0.50
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.94	0.50
11:K:14:VAL:HG22	46:K:101:3PE:H3C1	1.94	0.49
29:d:8:ARG:NH2	45:d:203:PC1:O14	2.42	0.49
15:O:83:TYR:HH	53:O:401:GTP:HO2'	1.42	0.49
40:o:38:MET:HE1	40:o:56:ASP:O	2.11	0.49
14:N:182:SER:OG	14:N:293:TYR:OH	2.29	0.49
32:g:92:GLU:OE2	32:g:95:ARG:NH2	2.39	0.49
1:A:94:LEU:HD12	10:J:147:TYR:HE1	1.76	0.49
9:I:78:ILE:HD13	18:R:86:TYR:CD1	2.47	0.49
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.43	0.49
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.13	0.49
29:d:1:AME:HE1	29:d:2:MET:HG3	1.95	0.49
11:K:37:MET:HG3	11:K:67:ALA:CB	2.42	0.49
25:Z:89:GLU:OE1	25:Z:128:ARG:NH2	2.46	0.49
29:d:13:PHE:O	29:d:78:ARG:NH1	2.44	0.49
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.94	0.49
7:G:58:GLU:OE2	7:G:83:SER:OG	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.95	0.49
45:J:201:PC1:O13	45:J:201:PC1:H133	2.12	0.49
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.95	0.49
7:G:424:ASP:OD1	7:G:424:ASP:N	2.44	0.49
34:i:1:SAC:H2A1	34:i:1:SAC:C	2.43	0.49
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.94	0.48
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.94	0.48
6:F:78:LYS:NZ	6:F:222:VAL:O	2.42	0.48
7:G:480:SER:OG	7:G:481:SER:N	2.44	0.48
8:H:87:ILE:N	8:H:88:PRO:CD	2.77	0.48
13:M:119:TYR:O	13:M:123:GLU:OE1	2.31	0.48
16:P:26:ALA:HB3	16:P:47:VAL:HG13	1.95	0.48
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.95	0.48
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.30	0.48
38:m:55:ARG:NH2	38:m:57:GLY:O	2.46	0.48
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.95	0.48
12:L:89:PHE:CD2	12:L:132:VAL:HG21	2.49	0.48
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.95	0.48
28:c:41:GLU:OE1	28:c:45:ARG:NE	2.44	0.48
51:h:201:CDL:H581	41:p:47:VAL:HG21	1.95	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.95	0.48
12:L:261:ILE:HG13	12:L:317:ILE:HD11	1.95	0.48
38:m:24:ILE:CD1	38:m:28:THR:HG21	2.44	0.48
13:M:204:MET:HE1	13:M:302:LEU:HD11	1.96	0.48
35:j:70:ASP:O	35:j:71:GLU:HB3	2.14	0.48
2:B:175:ILE:HD12	16:P:52:GLU:OE1	2.13	0.48
5:E:44:ALA:O	5:E:47:VAL:HG23	2.13	0.48
6:F:103:GLY:O	6:F:333:ALA:HB1	2.14	0.48
18:R:2:VAL:HG21	18:R:37:GLU:HG3	1.95	0.48
43:r:45:SER:O	43:r:51:ASN:ND2	2.42	0.48
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.44	0.47
10:J:86:ASN:OD1	10:J:87:LYS:N	2.47	0.47
6:F:111:ILE:HD13	6:F:138:ILE:HD12	1.96	0.47
6:F:302:SER:CB	6:F:350:LEU:HD22	2.44	0.47
8:H:107:ALA:O	8:H:110:SER:OG	2.26	0.47
8:H:121:TRP:CZ2	10:J:27:ILE:HG12	2.49	0.47
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.96	0.47
46:L:704:3PE:H222	35:j:35:TRP:CH2	2.50	0.47
37:l:129:GLY:HA2	40:o:21:MET:HE3	1.96	0.47
12:L:141:PHE:CZ	12:L:183:ILE:HD11	2.49	0.47
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:189:THR:HG22	8:H:234:MET:CE	2.44	0.47
10:J:77:GLU:O	10:J:78:GLN:HB2	2.14	0.47
15:O:138:MET:CE	53:O:401:GTP:HN21	2.27	0.47
16:P:253:PHE:C	16:P:254:LEU:HD22	2.40	0.47
7:G:267:THR:O	59:G:904:HOH:O	2.20	0.47
9:I:30:LEU:HD13	46:I:201:3PE:C26	2.45	0.47
39:n:169:ILE:O	39:n:172:ARG:NH1	2.47	0.47
6:F:194:GLU:OE1	6:F:199:LYS:NZ	2.47	0.47
13:M:66:LEU:HD11	13:M:111:THR:HG23	1.96	0.47
32:g:48:ASP:OD1	32:g:49:LYS:N	2.48	0.47
34:i:108:THR:O	41:p:18:ALA:N	2.44	0.47
37:l:135:TYR:OH	40:o:40:ALA:O	2.32	0.47
1:A:13:LEU:CD2	8:H:10:ILE:HG21	2.45	0.46
5:E:192:SER:OG	5:E:193:CYS:N	2.49	0.46
12:L:15:LEU:HD22	12:L:40:ILE:CD1	2.45	0.46
13:M:190:TRP:CE2	45:M:605:PC1:H132	2.49	0.46
3:C:183:VAL:O	22:W:101:THR:OG1	2.33	0.46
5:E:105:THR:HG22	5:E:106:THR:N	2.30	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.46
20:T:37:MET:HE2	20:T:71:MET:HE1	1.96	0.46
6:F:403:THR:HB	47:F:502:SF4:S4	2.54	0.46
12:L:78:LEU:HD11	51:L:702:CDL:H673	1.98	0.46
13:M:113:MET:HG2	13:M:175:ASN:OD1	2.16	0.46
15:O:310:GLU:HG2	15:O:317:ILE:HD12	1.97	0.46
2:B:91:THR:HA	2:B:119:CYS:HB3	1.98	0.46
6:F:10:THR:HG22	6:F:10:THR:O	2.15	0.46
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.49	0.46
7:G:382:THR:HB	7:G:454:GLY:HA3	1.97	0.46
10:J:132:ASP:OD1	10:J:133:SER:N	2.49	0.46
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.96	0.46
39:n:30:CYS:O	39:n:32:HIS:N	2.48	0.46
10:J:57:PHE:CZ	45:J:201:PC1:H352	2.50	0.46
32:g:26:TRP:CZ3	32:g:28:GLU:HB2	2.51	0.46
51:h:201:CDL:C58	41:p:47:VAL:HG21	2.46	0.46
6:F:115:PRO:O	6:F:119:VAL:HG23	2.16	0.46
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.51	0.46
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.96	0.46
7:G:382:THR:HG23	7:G:384:PRO:HD3	1.97	0.46
15:O:213:GLU:OE2	15:O:217:LYS:NZ	2.35	0.46
29:d:10:THR:HG22	30:e:4:ASP:HB3	1.97	0.46
42:q:2:GLU:OE2	43:r:5:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.97	0.45
7:G:486:ASP:OD1	7:G:486:ASP:N	2.49	0.45
12:L:297:ASP:OD2	12:L:299:LYS:N	2.49	0.45
12:L:558:LEU:HD21	46:m:201:3PE:H2I2	1.96	0.45
25:Z:86:MET:HE1	25:Z:125:TYR:CE2	2.52	0.45
29:d:106:LYS:HZ2	41:p:77:GLN:CD	2.24	0.45
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.97	0.45
29:d:120:ARG:NH1	38:m:112:GLU:OE1	2.40	0.45
3:C:195:ARG:NH1	9:I:84:GLU:OE2	2.49	0.45
16:P:162:GLU:OE2	16:P:162:GLU:N	2.46	0.45
19:S:64:LEU:O	19:S:75:ASN:HA	2.16	0.45
27:b:25:ALA:HB1	46:b:102:3PE:H2I2	1.99	0.45
22:W:52:LEU:HD11	22:W:103:VAL:HG11	1.98	0.45
41:p:143:HIS:O	41:p:144:ASP:HB2	2.16	0.45
6:F:197:GLU:OE2	6:F:216:PHE:N	2.49	0.45
12:L:15:LEU:HD22	12:L:40:ILE:HD13	1.97	0.45
46:M:602:3PE:H3I2	14:N:335:MET:HB3	1.98	0.45
14:N:342:MET:HB3	46:d:202:3PE:H2I2	1.98	0.45
5:E:103:CYS:SG	5:E:144:CYS:HA	2.57	0.45
7:G:285:ARG:NE	42:q:144:TYR:OH	2.50	0.45
10:J:5:ILE:HG21	25:Z:142:TRP:HZ2	1.82	0.45
10:J:76:THR:O	10:J:78:GLN:N	2.39	0.45
17:Q:132:THR:OG1	59:Q:202:HOH:O	2.21	0.45
22:W:101:THR:O	22:W:105:ARG:HG3	2.17	0.45
25:Z:91:LEU:HD11	25:Z:106:VAL:HG12	1.99	0.45
29:d:109:TYR:HA	29:d:112:VAL:HG22	1.98	0.45
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.31	0.45
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.98	0.45
20:U:36:PHE:HD1	20:U:40:LEU:HD12	1.82	0.45
4:D:72:MET:HE2	4:D:410:MET:HG2	1.99	0.45
12:L:250:SER:OG	12:L:337:ALA:HB2	2.16	0.45
19:S:19:ARG:HB2	19:S:65:TRP:HB2	1.99	0.45
4:D:417:ILE:O	4:D:420:THR:HG22	2.17	0.44
46:L:703:3PE:H291	34:i:80:ILE:HG23	1.98	0.44
4:D:3:GLN:NE2	13:M:135:ARG:O	2.51	0.44
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.44
12:L:264:TYR:N	12:L:265:PRO:CD	2.80	0.44
13:M:80:SER:OG	13:M:226:ALA:HB2	2.18	0.44
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.99	0.44
3:C:150:ARG:NH1	3:C:153:THR:OG1	2.50	0.44
8:H:17:VAL:HG13	8:H:228:TYR:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1:AME:HG1	33:h:122:TRP:HB3	2.00	0.44
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.40	0.44
37:l:21:ALA:HA	37:l:31:VAL:HG23	2.00	0.44
10:J:84:LEU:HB3	10:J:90:LEU:HD13	1.98	0.44
12:L:124:PHE:CE2	12:L:247:LEU:HD22	2.53	0.44
13:M:188:ASN:OD1	45:M:605:PC1:H151	2.18	0.44
14:N:10:LEU:HD13	51:N:902:CDL:H721	2.00	0.44
14:N:159:VAL:CG2	14:N:278:LEU:HD11	2.47	0.44
8:H:287[A]:HIS:CD2	8:H:291:LYS:HD2	2.52	0.44
12:L:44:PHE:CZ	46:L:704:3PE:H2F1	2.53	0.44
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.53	0.44
12:L:213:LEU:HD22	12:L:267:THR:HG22	2.00	0.43
30:e:4:ASP:OD2	30:e:7:LYS:HB3	2.18	0.43
37:l:68:ASP:N	37:l:68:ASP:OD1	2.49	0.43
42:q:96:ASP:OD2	42:q:101:LYS:HG3	2.19	0.43
12:L:245:ALA:O	12:L:249:SER:OG	2.36	0.43
14:N:272:LYS:HD3	33:h:108:LEU:HD21	2.00	0.43
16:P:201:VAL:HA	16:P:236:TYR:O	2.18	0.43
34:i:76:ILE:HB	34:i:77:PRO:HD3	1.99	0.43
14:N:170:LEU:HD11	14:N:288:LEU:HD22	1.99	0.43
15:O:176:VAL:HG21	15:O:200:GLN:OE1	2.18	0.43
23:X:97:ARG:HD3	25:Z:60:LEU:HD13	2.00	0.43
34:i:42:VAL:HG23	34:i:43:GLU:OE1	2.18	0.43
3:C:121:VAL:N	3:C:122:PRO:CD	2.82	0.43
29:d:9:ALA:HB3	29:d:15:PRO:HB3	2.01	0.43
6:F:437:HIS:O	6:F:438:GLN:C	2.60	0.43
46:M:604:3PE:H3I1	46:M:604:3PE:H2H1	2.00	0.43
29:d:108:THR:OG1	29:d:111:GLU:OE2	2.33	0.43
2:B:127:HIS:O	2:B:134:ARG:NH1	2.49	0.43
12:L:341:MET:SD	12:L:457:LEU:HD12	2.59	0.43
12:L:562:LEU:CB	12:L:563:PRO:CD	2.97	0.43
14:N:193:VAL:O	14:N:193:VAL:HG22	2.17	0.43
31:f:3:LEU:O	31:f:7:VAL:N	2.45	0.43
31:f:4:LEU:O	31:f:5:GLN:HB3	2.18	0.43
2:B:30:VAL:HG13	2:B:173:LEU:HB3	1.99	0.43
2:B:137:ASP:HA	2:B:140:VAL:O	2.19	0.43
7:G:366:THR:HB	7:G:450:MET:HE3	2.00	0.43
51:L:702:CDL:H473	51:h:201:CDL:H751	2.01	0.43
12:L:63:ILE:O	12:L:79:SER:HA	2.19	0.43
15:O:154:GLN:O	15:O:158:VAL:HG22	2.19	0.43
23:X:136:LEU:HD12	23:X:137:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.49	0.43
2:B:92:LEU:HD13	2:B:100:LEU:HD12	2.01	0.43
4:D:40:LYS:O	4:D:41:ASP:C	2.62	0.43
12:L:278:LEU:HD21	12:L:404:THR:OG1	2.18	0.43
6:F:14:SER:N	6:F:270:GLU:OE2	2.52	0.42
12:L:375:VAL:HG22	35:j:32:MET:SD	2.59	0.42
14:N:342:MET:O	14:N:345:VAL:HG22	2.19	0.42
19:S:31:GLY:HA3	19:S:81:PHE:O	2.19	0.42
21:V:43:TYR:O	21:V:47:THR:OG1	2.26	0.42
32:g:25:ARG:O	32:g:26:TRP:C	2.62	0.42
12:L:27:TYR:O	12:L:28:LYS:HB2	2.19	0.42
1:A:76:PRO:HD3	8:H:151:LEU:HD11	2.02	0.42
7:G:105:CYS:HB2	7:G:106:PRO:HD3	2.00	0.42
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.55	0.42
34:i:85:LEU:O	34:i:90:THR:HG23	2.19	0.42
6:F:93:LEU:O	6:F:134:ALA:HA	2.19	0.42
10:J:115:VAL:O	10:J:117:PHE:N	2.51	0.42
13:M:403:THR:HA	13:M:406:TYR:CE1	2.55	0.42
29:d:79:GLN:NE2	59:d:301:HOH:O	2.38	0.42
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.02	0.42
9:I:162:GLU:HB3	42:q:109:ILE:HG12	2.01	0.42
12:L:173:LEU:C	12:L:173:LEU:HD23	2.44	0.42
14:N:152:ASN:O	14:N:156:THR:OG1	2.20	0.42
16:P:188:PHE:O	16:P:189:GLY:C	2.63	0.42
40:o:38:MET:HE3	40:o:40:ALA:HB3	2.01	0.42
3:C:47:GLU:OE1	3:C:106:ARG:NH2	2.41	0.42
7:G:588:THR:HG21	17:Q:63:GLU:HA	2.02	0.42
9:I:32:ARG:NH2	25:Z:26:PRO:O	2.44	0.42
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.54	0.42
7:G:427:LYS:O	7:G:430:GLN:N	2.51	0.42
14:N:68:MET:HE2	14:N:68:MET:HA	2.01	0.42
15:O:128:ILE:HD12	15:O:160:ILE:HG13	2.02	0.42
3:C:40:VAL:HG13	3:C:50:ILE:HD13	2.00	0.42
12:L:480:MET:HE2	35:j:50:HIS:CG	2.55	0.42
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.50	0.42
13:M:123:GLU:OE2	13:M:157:SER:HB2	2.18	0.42
17:Q:69:LEU:HD11	42:q:126:PRO:HG2	2.02	0.42
33:h:140:THR:OG1	33:h:143:ASN:ND2	2.52	0.42
40:o:26:PRO:O	40:o:33:ARG:NH1	2.50	0.42
2:B:44:SER:O	8:H:54:LYS:HE2	2.20	0.42
12:L:331:THR:HB	12:L:387:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:605:PC1:O31	45:M:605:PC1:H342	2.19	0.42
15:O:51:PHE:HB2	15:O:124:LEU:HD23	2.02	0.42
4:D:134:ALA:HB2	4:D:323:ILE:O	2.20	0.41
10:J:125:TRP:HB2	25:Z:137:THR:HG21	2.02	0.41
13:M:108:MET:HE1	51:X:201:CDL:C22	2.45	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.41
17:Q:42:ARG:HD3	17:Q:49:VAL:HG12	2.01	0.41
34:i:120:LYS:NZ	40:o:37:GLU:OE2	2.50	0.41
7:G:227:SER:OG	7:G:228:ILE:N	2.43	0.41
27:b:36:PRO:O	27:b:39:LYS:NZ	2.49	0.41
37:l:30:ARG:HD2	38:m:34:GLU:HB2	2.02	0.41
6:F:90:PRO:O	6:F:218:CYS:HB3	2.19	0.41
8:H:49:ILE:HD12	8:H:49:ILE:H	1.86	0.41
12:L:183:ILE:HG21	13:M:382:VAL:HG11	2.02	0.41
7:G:254:MET:HA	7:G:260:GLU:O	2.20	0.41
7:G:276:ARG:NH1	7:G:680:ALA:O	2.49	0.41
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.53	0.41
20:T:43:ASP:O	20:T:44:SER:C	2.63	0.41
6:F:306:LEU:C	6:F:306:LEU:HD12	2.45	0.41
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.03	0.41
13:M:379:LEU:O	13:M:383:MET:HG2	2.20	0.41
32:g:24:LEU:O	32:g:25:ARG:HB3	2.20	0.41
34:i:90:THR:HG22	34:i:96:ILE:HD12	2.02	0.41
40:o:31:PRO:O	40:o:32:GLU:C	2.64	0.41
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.45	0.41
6:F:394:GLU:OE2	7:G:129:ARG:NH1	2.52	0.41
7:G:118:ASP:OD2	59:G:905:HOH:O	2.22	0.41
13:M:51:ASN:O	33:h:89:ARG:NE	2.54	0.41
14:N:193:VAL:HB	14:N:266:ILE:HG23	2.03	0.41
23:X:44:LEU:HD22	23:X:130:VAL:HG11	2.00	0.41
24:Y:68:ILE:HG13	24:Y:99:ILE:HG13	2.03	0.41
34:i:3:TYR:O	34:i:8:LYS:NZ	2.53	0.41
38:m:125:ASN:O	41:p:139:GLN:NE2	2.53	0.41
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.03	0.41
11:K:43:MET:CE	14:N:72:MET:HE1	2.49	0.41
40:o:68:CYS:C	40:o:79:CYS:SG	3.04	0.41
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.02	0.41
16:P:266:ILE:HD12	16:P:266:ILE:H	1.86	0.41
22:W:101:THR:HG23	22:W:102:HIS:N	2.36	0.41
23:X:8:SER:OG	23:X:10:GLU:HG2	2.20	0.41
36:k:23:ILE:O	36:k:29:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:2:PHE:HB3	38:m:3:PRO:HD2	2.03	0.41
2:B:49:THR:CG2	2:B:59:MET:HE3	2.51	0.41
4:D:117:ALA:HB2	4:D:367:ILE:HG12	2.02	0.41
7:G:26:VAL:HG11	7:G:57:VAL:HG11	2.01	0.41
7:G:233:ALA:O	7:G:575:ASN:HB2	2.21	0.41
12:L:68:TRP:HH2	13:M:376:ILE:HD11	1.86	0.41
14:N:267:ILE:O	14:N:271:THR:HG23	2.20	0.41
18:R:2:VAL:HG11	18:R:10:LYS:HD2	2.03	0.41
32:g:28:GLU:OE1	32:g:28:GLU:HA	2.21	0.41
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.60	0.41
6:F:8:LYS:O	6:F:9:LYS:C	2.64	0.41
7:G:371:VAL:HG22	7:G:450:MET:HE1	2.03	0.41
7:G:528:ASP:OD2	7:G:545:TYR:OH	2.40	0.41
8:H:295:PRO:HB3	46:b:102:3PE:H2A2	2.03	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.35	0.41
15:O:11:GLY:O	15:O:13:LYS:N	2.54	0.41
20:U:4:PRO:HG3	35:j:9:PRO:HG3	2.02	0.41
31:f:3:LEU:O	31:f:7:VAL:HG23	2.21	0.41
4:D:109:VAL:O	4:D:109:VAL:HG12	2.21	0.40
6:F:95:VAL:HG22	6:F:228:VAL:HG21	2.03	0.40
7:G:347:GLU:OE1	7:G:495:ARG:NE	2.47	0.40
8:H:276:SER:HB3	9:I:37:THR:HG21	2.02	0.40
13:M:1:FME:HE3	13:M:111:THR:HG21	2.03	0.40
13:M:373:ILE:HD11	13:M:444:LEU:CD1	2.50	0.40
24:Y:6:ARG:HA	24:Y:6:ARG:HE	1.86	0.40
12:L:432:LEU:HD11	36:k:62:PHE:HA	2.03	0.40
13:M:373:ILE:HD11	13:M:444:LEU:HD12	2.03	0.40
15:O:188:ASN:OD1	15:O:191:GLU:N	2.47	0.40
44:s:74:ARG:NE	59:s:101:HOH:O	2.55	0.40
3:C:155:TYR:O	59:C:303:HOH:O	2.22	0.40
46:L:704:3PE:H222	35:j:35:TRP:HH2	1.85	0.40
32:g:106:PRO:HG2	32:g:109:GLU:OE2	2.21	0.40
12:L:568:LEU:HD23	46:Y:205:3PE:O22	2.20	0.40
30:e:16:TRP:CD1	30:e:16:TRP:H	2.39	0.40
37:l:50:LEU:HD12	37:l:78:HIS:HA	2.02	0.40
38:m:74:ASN:OD1	38:m:78:ASN:ND2	2.54	0.40
6:F:192:LEU:HD23	6:F:192:LEU:C	2.46	0.40
6:F:258:ILE:HG22	6:F:262:VAL:HG21	2.02	0.40
12:L:13:LEU:CD2	34:i:81:ILE:HD11	2.51	0.40
12:L:342:CYS:SG	12:L:372:ALA:HB3	2.62	0.40
27:b:26:GLY:HA3	46:b:102:3PE:H3H1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:99:LYS:HZ3	41:p:117:GLY:HA3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/115 (89%)	101 (99%)	1 (1%)	0	100	100
2	B	154/216 (71%)	148 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	198 (97%)	7 (3%)	0	100	100
4	D	399/463 (86%)	382 (96%)	17 (4%)	0	100	100
5	E	212/249 (85%)	205 (97%)	7 (3%)	0	100	100
6	F	431/464 (93%)	416 (96%)	15 (4%)	0	100	100
7	G	689/727 (95%)	664 (96%)	25 (4%)	0	100	100
8	H	286/318 (90%)	277 (97%)	9 (3%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	572 (95%)	31 (5%)	1 (0%)	43	71
13	M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	319/380 (84%)	304 (95%)	15 (5%)	0	100	100
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
19	S	84/99 (85%)	80 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	114/128 (89%)	110 (96%)	4 (4%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	6	22
32	g	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	n	170/179 (95%)	167 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	87 (96%)	4 (4%)	0	100	100
44	s	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
All	All	8097/9212 (88%)	7827 (97%)	268 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
31	f	3	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	93/100 (93%)	93 (100%)	0	100	100
2	B	132/175 (75%)	132 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	348/392 (89%)	348 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	347/368 (94%)	347 (100%)	0	100	100
7	G	579/608 (95%)	579 (100%)	0	100	100
8	H	255/274 (93%)	255 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	141/141 (100%)	141 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
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%)	283 (100%)	0	100	100
16	P	282/327 (86%)	282 (100%)	0	100	100
17	Q	116/153 (76%)	116 (100%)	0	100	100
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	79/135 (58%)	79 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	105 (100%)	0	100	100
30	e	89/96 (93%)	89 (100%)	0	100	100
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	92/131 (70%)	92 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	120/120 (100%)	120 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	63/76 (83%)	63 (100%)	0	100	100
37	l	140/159 (88%)	140 (100%)	0	100	100
38	m	114/115 (99%)	114 (100%)	0	100	100
39	n	157/161 (98%)	155 (99%)	2 (1%)	61	85
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7156/7892 (91%)	7154 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	n	134[A]	ARG
39	n	134[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
3	C	39	GLN
3	C	192	GLN
4	D	150	HIS

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Mol	Chain	Res	Type
4	D	200	HIS
4	D	231	ASN
6	F	373	ASN
6	F	421	HIS
6	F	432	GLN
7	G	155	GLN
7	G	308	GLN
7	G	402	ASN
7	G	644	GLN
8	H	99	ASN
8	H	138	GLN
12	L	56	HIS
12	L	115	ASN
12	L	170	GLN
12	L	296	ASN
13	M	184	GLN
13	M	366	ASN
13	M	415	GLN
14	N	36	ASN
14	N	48	HIS
14	N	134	GLN
14	N	274	ASN
14	N	289	ASN
15	O	50	HIS
15	O	251	GLN
16	P	49	HIS
16	P	103	ASN
18	R	94	GLN
21	V	75	GLN
23	X	76	HIS
23	X	105	GLN
24	Y	133	GLN
25	Z	85	GLN
28	c	46	ASN
30	e	26	HIS
30	e	69	GLN
31	f	30	ASN
34	i	25	GLN
34	i	125	GLN
34	i	127	HIS
37	l	56	GLN
39	n	123	GLN

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Mol	Chain	Res	Type
41	p	58	ASN
41	p	133	GLN
42	q	91	HIS
42	q	135	GLN
44	s	43	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z > 2$
34	SAC	i	1	34	7,8,9	1.03	0	7,9,11	1.19	0
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	1.00	0
11	FME	K	1	11	8,9,10	0.89	0	8,9,11	1.11	0
24	AYA	Y	1	24	6,7,8	1.25	1 (16%)	6,8,10	1.15	1 (16%)
10	FME	J	1	10	8,9,10	0.99	0	8,9,11	0.85	0
43	AYA	r	1	43	6,7,8	1.28	1 (16%)	6,8,10	1.09	1 (16%)
13	FME	M	1	13	8,9,10	1.05	1 (12%)	8,9,11	0.99	0
4	2MR	D	85	4	10,12,13	0.39	0	5,13,15	1.08	0
8	FME	H	1	8	8,9,10	1.08	1 (12%)	8,9,11	0.75	0
12	FME	L	1	12	8,9,10	0.96	0	8,9,11	1.08	1 (12%)
29	AME	d	1	29	9,10,11	1.49	1 (11%)	9,11,13	1.43	2 (22%)
1	FME	A	1	1	8,9,10	1.06	1 (12%)	8,9,11	0.83	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
34	SAC	i	1	34	-	6/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
24	AYA	Y	1	24	-	3/5/6/8	-
10	FME	J	1	10	-	2/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
13	FME	M	1	13	-	1/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
8	FME	H	1	8	-	4/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
29	AME	d	1	29	-	2/9/10/12	-
1	FME	A	1	1	-	0/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	d	1	AME	CT1-N	3.38	1.45	1.34
43	r	1	AYA	CA-N	-2.61	1.43	1.46
24	Y	1	AYA	CA-N	-2.51	1.43	1.46
8	H	1	FME	CA-N	-2.34	1.43	1.46
1	A	1	FME	CA-N	-2.27	1.43	1.46
13	M	1	FME	CA-N	-2.21	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	1	AYA	CB-CA-N	2.45	112.44	109.68
29	d	1	AME	CG-CB-CA	-2.30	105.84	112.87
43	r	1	AYA	CB-CA-N	2.21	112.17	109.68
12	L	1	FME	C-CA-N	2.17	113.69	109.50
29	d	1	AME	CE-SD-CG	2.05	110.93	100.32

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
24	Y	1	AYA	O-C-CA-CB
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
11	K	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CA-N-CT1
34	i	1	SAC	CB-CA-N-C1A
29	d	1	AME	CB-CG-SD-CE
24	Y	1	AYA	C-CA-N-CT
34	i	1	SAC	C-CA-N-C1A
11	K	1	FME	C-CA-CB-CG
24	Y	1	AYA	CB-CA-N-CT

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	i	1	SAC	1	0
13	M	1	FME	1	0
29	d	1	AME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
49	FMN	F	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.23	6 (12%)
53	GTP	O	401	54	33,34,34	3.24	14 (42%)	50,54,54	1.86	15 (30%)
46	3PE	N	904	-	38,38,50	1.00	3 (7%)	41,43,55	1.14	2 (4%)
46	3PE	L	703	-	42,42,50	0.93	3 (7%)	45,47,55	1.13	2 (4%)
46	3PE	H	601	-	35,35,50	1.02	4 (11%)	38,40,55	1.14	2 (5%)
46	3PE	g	201	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
46	3PE	L	704	-	38,38,50	0.99	4 (10%)	41,43,55	1.17	2 (4%)
55	NDP	P	501	-	51,52,52	2.24	8 (15%)	71,80,80	1.55	16 (22%)
45	PC1	B	202	-	50,50,53	0.98	4 (8%)	56,58,61	1.04	2 (3%)
46	3PE	I	201	-	50,50,50	0.88	4 (8%)	53,55,55	1.03	2 (3%)
46	3PE	Y	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)
46	3PE	d	202	-	48,48,50	0.89	3 (6%)	51,53,55	1.06	2 (3%)
46	3PE	I	204	-	50,50,50	0.87	4 (8%)	53,55,55	0.95	2 (3%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
46	3PE	m	201	-	39,39,50	0.97	4 (10%)	42,44,55	1.06	2 (4%)
46	3PE	f	101	-	30,30,50	1.13	4 (13%)	33,35,55	1.15	2 (6%)
45	PC1	M	603	-	45,45,53	1.05	3 (6%)	51,53,61	1.00	2 (3%)
51	CDL	N	902	-	84,84,99	0.96	8 (9%)	90,96,111	1.09	5 (5%)
45	PC1	J	201	-	45,45,53	0.40	0	51,53,61	0.39	0
51	CDL	h	201	-	67,67,99	1.07	7 (10%)	73,79,111	1.23	4 (5%)
46	3PE	Y	203	-	38,38,50	1.02	4 (10%)	41,43,55	1.15	2 (4%)
46	3PE	d	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.15	2 (4%)
52	CHD	L	705	-	32,32,32	3.26	10 (31%)	51,51,51	2.87	25 (49%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
46	3PE	O	403	-	35,35,50	1.04	4 (11%)	38,40,55	1.19	2 (5%)
46	3PE	Y	202	-	43,43,50	0.94	4 (9%)	46,48,55	1.05	2 (4%)
45	PC1	A	301	-	49,49,53	1.01	4 (8%)	55,57,61	1.03	2 (3%)
57	EHZ	U	101	20	31,36,37	1.53	5 (16%)	36,44,47	1.45	3 (8%)
46	3PE	M	601	-	42,42,50	0.94	3 (7%)	45,47,55	1.16	2 (4%)
45	PC1	N	903	-	29,29,53	1.23	3 (10%)	35,37,61	1.05	1 (2%)
46	3PE	N	901	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	Z	201	-	42,42,50	0.96	4 (9%)	45,47,55	1.04	2 (4%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PC1	d	203	-	39,39,53	1.13	4 (10%)	45,47,61	1.09	2 (4%)
51	CDL	L	702	-	78,78,99	0.99	6 (7%)	84,90,111	1.15	4 (4%)
46	3PE	b	102	-	50,50,50	0.89	4 (8%)	53,55,55	1.03	2 (3%)
57	EHZ	T	101	20	31,36,37	1.54	4 (12%)	36,44,47	1.56	3 (8%)
46	3PE	M	602	-	50,50,50	0.88	3 (6%)	53,55,55	1.08	2 (3%)
46	3PE	M	604	-	50,50,50	0.88	4 (8%)	53,55,55	0.99	2 (3%)
46	3PE	K	101	-	42,42,50	0.92	4 (9%)	45,47,55	1.16	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
51	CDL	d	204	-	64,64,99	1.09	8 (12%)	70,76,111	1.08	4 (5%)
45	PC1	M	605	-	48,48,53	1.03	4 (8%)	54,56,61	1.03	3 (5%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
46	3PE	L	701	-	38,38,50	0.98	2 (5%)	41,43,55	1.12	2 (4%)
46	3PE	Y	205	-	44,44,50	0.93	3 (6%)	47,49,55	1.04	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
58	MYR	o	201	40	13,14,15	0.91	0	12,13,15	0.57	0
46	3PE	h	202	-	38,38,50	0.99	4 (10%)	41,43,55	1.07	2 (4%)
51	CDL	X	201	-	85,85,99	0.95	6 (7%)	91,97,111	1.10	4 (4%)
46	3PE	A	302	-	46,46,50	0.90	4 (8%)	49,51,55	1.00	2 (4%)
51	CDL	r	201	-	63,63,99	1.11	7 (11%)	69,75,111	1.16	4 (5%)
46	3PE	Y	204	-	31,31,50	1.09	4 (12%)	34,36,55	1.12	2 (5%)
46	3PE	b	101	-	36,36,50	1.04	4 (11%)	39,41,55	1.12	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
47	SF4	B	201	2	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FMN	F	501	-	-	4/18/18/18	0/3/3/3
53	GTP	O	401	54	-	3/22/38/38	0/3/3/3
46	3PE	N	904	-	-	21/42/42/54	-
46	3PE	L	703	-	-	23/46/46/54	-
46	3PE	H	601	-	-	20/39/39/54	-
46	3PE	g	201	-	-	17/39/39/54	-
46	3PE	L	704	-	-	16/42/42/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	NDP	P	501	-	-	11/34/77/77	0/5/5/5
45	PC1	B	202	-	-	18/54/54/57	-
46	3PE	I	201	-	-	24/54/54/54	-
46	3PE	Y	201	-	-	22/54/54/54	-
46	3PE	d	202	-	-	21/52/52/54	-
46	3PE	I	204	-	-	24/54/54/54	-
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	m	201	-	-	21/43/43/54	-
46	3PE	f	101	-	-	16/34/34/54	-
45	PC1	M	603	-	-	18/49/49/57	-
51	CDL	N	902	-	-	43/95/95/110	-
45	PC1	J	201	-	-	5/49/49/57	-
51	CDL	h	201	-	-	36/78/78/110	-
46	3PE	Y	203	-	-	20/42/42/54	-
46	3PE	d	201	-	-	15/44/44/54	-
52	CHD	L	705	-	-	3/9/74/74	0/4/4/4
48	FES	G	803	7	-	-	0/1/1/1
46	3PE	O	403	-	-	20/39/39/54	-
46	3PE	Y	202	-	-	18/47/47/54	-
45	PC1	A	301	-	-	19/53/53/57	-
57	EHZ	U	101	20	-	6/42/44/45	-
46	3PE	M	601	-	-	24/46/46/54	-
45	PC1	N	903	-	-	15/32/32/57	-
46	3PE	N	901	-	-	16/54/54/54	-
46	3PE	Z	201	-	-	19/46/46/54	-
51	CDL	L	702	-	-	35/89/89/110	-
45	PC1	d	203	-	-	18/43/43/57	-
57	EHZ	T	101	20	-	10/42/44/45	-
46	3PE	b	102	-	-	23/54/54/54	-
47	SF4	I	203	9	-	-	0/6/5/5
46	3PE	M	602	-	-	28/54/54/54	-
46	3PE	M	604	-	-	25/54/54/54	-
46	3PE	K	101	-	-	21/46/46/54	-
47	SF4	G	801	7	-	-	0/6/5/5
51	CDL	d	204	-	-	33/75/75/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PC1	M	605	-	-	17/52/52/57	-
48	FES	E	301	5	-	-	0/1/1/1
46	3PE	L	701	-	-	16/42/42/54	-
46	3PE	Y	205	-	-	28/48/48/54	-
58	MYR	o	201	40	-	4/12/12/13	-
47	SF4	I	202	9	-	-	0/6/5/5
46	3PE	h	202	-	-	21/42/42/54	-
51	CDL	X	201	-	-	48/96/96/110	-
46	3PE	A	302	-	-	19/50/50/54	-
51	CDL	r	201	-	-	27/74/74/110	-
46	3PE	Y	204	-	-	20/35/35/54	-
46	3PE	b	101	-	-	18/40/40/54	-
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	B	201	2	-	-	0/6/5/5

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	P2B-O2B	12.70	1.81	1.59
52	L	705	CHD	C11-C12	8.64	1.67	1.53
53	O	401	GTP	O6-C6	8.61	1.39	1.23
52	L	705	CHD	C16-C15	6.89	1.72	1.54
53	O	401	GTP	C5-N7	6.68	1.52	1.39
52	L	705	CHD	C8-C9	5.96	1.65	1.53
52	L	705	CHD	C13-C17	5.86	1.65	1.55
52	L	705	CHD	C20-C17	-5.61	1.44	1.54
52	L	705	CHD	O12-C12	-5.36	1.34	1.43
52	L	705	CHD	C6-C5	5.28	1.62	1.53
57	T	101	EHZ	C15-N2	4.91	1.45	1.33
57	U	101	EHZ	C12-N1	4.88	1.44	1.33
53	O	401	GTP	PB-O3B	4.86	1.64	1.59
57	T	101	EHZ	C12-N1	4.85	1.44	1.33
53	O	401	GTP	C2-N1	4.80	1.49	1.37
57	U	101	EHZ	C15-N2	4.80	1.44	1.33
53	O	401	GTP	PB-O3A	4.65	1.64	1.59
53	O	401	GTP	C2-N2	4.64	1.45	1.34
53	O	401	GTP	C2-N3	4.62	1.44	1.33
53	O	401	GTP	PA-O3A	4.61	1.64	1.59
53	O	401	GTP	C8-N9	-4.36	1.27	1.37
55	P	501	NDP	PA-O3	3.96	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	705	CHD	C15-C14	3.89	1.62	1.54
53	O	401	GTP	C4-N9	-3.87	1.28	1.38
52	L	705	CHD	C6-C7	3.58	1.59	1.52
55	P	501	NDP	O2B-C2B	-3.53	1.32	1.44
55	P	501	NDP	PN-O5D	3.29	1.72	1.59
49	F	501	FMN	C4A-N5	3.20	1.37	1.30
51	h	201	CDL	OA6-CA4	-3.03	1.39	1.46
51	r	201	CDL	OB6-CB4	-3.01	1.39	1.46
46	M	602	3PE	O21-C2	-2.99	1.39	1.46
51	L	702	CDL	OA6-CA4	-2.95	1.39	1.46
46	M	601	3PE	O21-C2	-2.93	1.39	1.46
51	X	201	CDL	OB6-CB4	-2.87	1.39	1.46
46	L	701	3PE	O21-C2	-2.86	1.39	1.46
53	O	401	GTP	O4'-C1'	2.83	1.48	1.42
46	Y	205	3PE	O21-C2	-2.83	1.39	1.46
45	M	603	PC1	O21-C2	-2.83	1.39	1.46
51	r	201	CDL	OA6-CA4	-2.80	1.40	1.46
46	Y	204	3PE	O21-C2	-2.80	1.40	1.46
46	L	703	3PE	O21-C2	-2.80	1.40	1.46
46	b	102	3PE	O21-C2	-2.80	1.40	1.46
51	h	201	CDL	OB6-CB4	-2.79	1.40	1.46
46	I	201	3PE	O21-C2	-2.79	1.40	1.46
51	N	902	CDL	OA6-CA4	-2.79	1.40	1.46
46	h	202	3PE	O21-C2	-2.78	1.40	1.46
46	d	201	3PE	O21-C2	-2.78	1.40	1.46
46	d	202	3PE	O21-C2	-2.78	1.40	1.46
46	I	204	3PE	O21-C2	-2.78	1.40	1.46
45	M	605	PC1	O21-C2	-2.76	1.40	1.46
46	L	704	3PE	O21-C2	-2.75	1.40	1.46
46	Y	202	3PE	O21-C2	-2.75	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.75	1.40	1.46
51	d	204	CDL	OA6-CA4	-2.73	1.40	1.46
45	B	202	PC1	O21-C2	-2.73	1.40	1.46
51	L	702	CDL	OB6-CB4	-2.73	1.40	1.46
46	Y	203	3PE	O21-C2	-2.71	1.40	1.46
46	N	904	3PE	O21-C2	-2.70	1.40	1.46
45	A	301	PC1	O21-C2	-2.69	1.40	1.46
46	N	901	3PE	O21-C2	-2.69	1.40	1.46
51	N	902	CDL	OB6-CB4	-2.68	1.40	1.46
46	g	201	3PE	O21-C2	-2.66	1.40	1.46
45	N	903	PC1	O21-C2	-2.66	1.40	1.46
45	d	203	PC1	O21-C2	-2.65	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	m	201	3PE	O21-C2	-2.65	1.40	1.46
46	H	601	3PE	O21-C2	-2.64	1.40	1.46
51	d	204	CDL	OB6-CB4	-2.64	1.40	1.46
46	Z	201	3PE	O21-C2	-2.63	1.40	1.46
46	O	403	3PE	O21-C2	-2.62	1.40	1.46
57	U	101	EHZ	O4-C15	-2.61	1.18	1.23
46	M	604	3PE	O21-C2	-2.59	1.40	1.46
51	X	201	CDL	OA8-CA7	2.59	1.40	1.33
57	T	101	EHZ	O4-C15	-2.58	1.18	1.23
46	A	302	3PE	O21-C2	-2.57	1.40	1.46
53	O	401	GTP	C2'-C3'	-2.56	1.46	1.53
46	f	101	3PE	O21-C2	-2.55	1.40	1.46
46	L	701	3PE	O31-C3	-2.55	1.39	1.45
45	M	605	PC1	O31-C31	2.54	1.40	1.33
51	L	702	CDL	OA8-CA7	2.53	1.40	1.33
46	Y	201	3PE	O21-C2	-2.52	1.40	1.46
46	f	101	3PE	O31-C31	2.51	1.40	1.33
45	A	301	PC1	O31-C3	-2.51	1.39	1.45
46	b	101	3PE	O21-C2	-2.51	1.40	1.46
46	M	602	3PE	O31-C3	-2.50	1.39	1.45
51	X	201	CDL	OB8-CB7	2.48	1.40	1.33
55	P	501	NDP	O5D-C5D	-2.47	1.35	1.44
46	b	101	3PE	O31-C31	2.45	1.40	1.33
45	d	203	PC1	O31-C31	2.45	1.40	1.33
46	Y	201	3PE	O31-C31	2.45	1.40	1.33
46	b	102	3PE	O31-C31	2.45	1.40	1.33
51	r	201	CDL	OA8-CA6	-2.45	1.39	1.45
51	L	702	CDL	OB8-CB7	2.45	1.40	1.33
46	H	601	3PE	O31-C3	-2.44	1.39	1.45
57	T	101	EHZ	O3-C12	-2.43	1.18	1.23
46	L	704	3PE	O31-C31	2.43	1.40	1.33
46	I	201	3PE	O31-C3	-2.42	1.39	1.45
46	Y	203	3PE	O31-C31	2.42	1.40	1.33
46	Y	205	3PE	O31-C31	2.42	1.40	1.33
51	d	204	CDL	OA8-CA7	2.41	1.40	1.33
46	K	101	3PE	O21-C2	-2.40	1.41	1.46
46	d	202	3PE	O31-C31	2.40	1.40	1.33
51	N	902	CDL	OA8-CA7	2.40	1.40	1.33
57	U	101	EHZ	O3-C12	-2.39	1.18	1.23
46	Z	201	3PE	O31-C31	2.39	1.40	1.33
51	d	204	CDL	OB8-CB7	2.39	1.40	1.33
51	r	201	CDL	OB8-CB7	2.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	h	201	CDL	OA8-CA7	2.38	1.40	1.33
46	A	302	3PE	O31-C3	-2.38	1.39	1.45
46	O	403	3PE	O31-C31	2.38	1.40	1.33
46	Y	202	3PE	O31-C31	2.38	1.40	1.33
45	B	202	PC1	O31-C3	-2.37	1.39	1.45
53	O	401	GTP	PG-O3G	-2.37	1.46	1.54
51	r	201	CDL	OA8-CA7	2.37	1.40	1.33
46	K	101	3PE	O31-C3	-2.35	1.39	1.45
51	N	902	CDL	OB8-CB7	2.35	1.40	1.33
46	h	202	3PE	O31-C31	2.35	1.40	1.33
46	M	604	3PE	O31-C31	2.35	1.40	1.33
46	g	201	3PE	O31-C31	2.34	1.40	1.33
45	M	603	PC1	O31-C31	2.34	1.40	1.33
46	m	201	3PE	O31-C31	2.33	1.40	1.33
46	d	201	3PE	O31-C3	-2.33	1.40	1.45
46	N	904	3PE	O31-C3	-2.33	1.40	1.45
46	b	101	3PE	O21-C21	2.31	1.40	1.34
51	d	204	CDL	OA8-CA6	-2.31	1.40	1.45
46	d	201	3PE	O31-C31	2.31	1.40	1.33
46	I	201	3PE	O31-C31	2.30	1.40	1.33
52	L	705	CHD	C13-C12	-2.30	1.51	1.54
46	M	601	3PE	O31-C3	-2.29	1.40	1.45
46	M	602	3PE	O31-C31	2.29	1.40	1.33
46	N	904	3PE	O31-C31	2.29	1.40	1.33
45	M	603	PC1	O31-C3	-2.29	1.40	1.45
46	M	604	3PE	O31-C3	-2.29	1.40	1.45
53	O	401	GTP	PG-O2G	-2.28	1.46	1.54
51	r	201	CDL	OB8-CB6	-2.27	1.40	1.45
46	K	101	3PE	O31-C31	2.27	1.40	1.33
45	d	203	PC1	O31-C3	-2.26	1.40	1.45
46	N	901	3PE	O31-C31	2.26	1.40	1.33
46	I	204	3PE	O31-C3	-2.26	1.40	1.45
46	Y	204	3PE	O31-C31	2.26	1.39	1.33
51	h	201	CDL	OB8-CB7	2.25	1.39	1.33
51	N	902	CDL	OB8-CB6	-2.25	1.40	1.45
51	N	902	CDL	OB6-CB5	2.25	1.40	1.34
46	N	901	3PE	O31-C3	-2.25	1.40	1.45
51	h	201	CDL	OB8-CB6	-2.25	1.40	1.45
46	I	204	3PE	O31-C31	2.25	1.39	1.33
46	L	703	3PE	O31-C3	-2.25	1.40	1.45
46	A	302	3PE	O31-C31	2.24	1.39	1.33
51	d	204	CDL	OA6-CA5	2.24	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	601	3PE	O31-C31	2.24	1.39	1.33
46	Z	201	3PE	O21-C21	2.24	1.40	1.34
46	f	101	3PE	O21-C21	2.24	1.40	1.34
46	m	201	3PE	O31-C3	-2.23	1.40	1.45
46	O	403	3PE	O21-C21	2.23	1.40	1.34
49	F	501	FMN	C10-N1	2.23	1.37	1.33
51	h	201	CDL	OB6-CB5	2.23	1.40	1.34
46	f	101	3PE	O31-C3	-2.22	1.40	1.45
46	L	703	3PE	O31-C31	2.22	1.39	1.33
45	M	605	PC1	O31-C3	-2.22	1.40	1.45
51	d	204	CDL	OB8-CB6	-2.22	1.40	1.45
46	g	201	3PE	O31-C3	-2.21	1.40	1.45
45	N	903	PC1	O31-C3	-2.21	1.40	1.45
55	P	501	NDP	O2D-C2D	-2.21	1.37	1.43
46	K	101	3PE	O21-C21	2.20	1.40	1.34
51	N	902	CDL	OA8-CA6	-2.20	1.40	1.45
46	H	601	3PE	O31-C31	2.20	1.39	1.33
46	Y	204	3PE	O31-C3	-2.20	1.40	1.45
51	N	902	CDL	OA6-CA5	2.19	1.40	1.34
46	b	102	3PE	O31-C3	-2.19	1.40	1.45
51	d	204	CDL	OB6-CB5	2.19	1.40	1.34
46	Z	201	3PE	O31-C3	-2.19	1.40	1.45
46	g	201	3PE	O21-C21	2.18	1.40	1.34
45	A	301	PC1	O21-C21	2.18	1.40	1.34
46	O	403	3PE	O31-C3	-2.18	1.40	1.45
46	h	202	3PE	O31-C3	-2.18	1.40	1.45
45	A	301	PC1	O31-C31	2.17	1.39	1.33
46	b	101	3PE	O31-C3	-2.17	1.40	1.45
51	X	201	CDL	OB8-CB6	-2.17	1.40	1.45
46	A	302	3PE	O21-C21	2.16	1.40	1.34
46	H	601	3PE	O21-C21	2.14	1.40	1.34
46	Y	201	3PE	O31-C3	-2.14	1.40	1.45
46	M	604	3PE	O21-C21	2.13	1.40	1.34
46	m	201	3PE	O21-C21	2.13	1.40	1.34
51	h	201	CDL	OA8-CA6	-2.13	1.40	1.45
55	P	501	NDP	O5B-C5B	-2.12	1.36	1.44
46	Y	205	3PE	O31-C3	-2.12	1.40	1.45
46	d	202	3PE	O31-C3	-2.12	1.40	1.45
46	Y	203	3PE	O21-C21	2.11	1.40	1.34
45	M	605	PC1	O21-C21	2.11	1.40	1.34
45	d	203	PC1	O21-C21	2.11	1.40	1.34
46	Y	201	3PE	O21-C21	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	L	702	CDL	OA8-CA6	-2.10	1.40	1.45
46	Y	202	3PE	O31-C3	-2.10	1.40	1.45
51	X	201	CDL	OA6-CA5	2.09	1.40	1.34
46	Y	204	3PE	O21-C21	2.09	1.40	1.34
45	B	202	PC1	O31-C31	2.08	1.39	1.33
46	I	204	3PE	O21-C21	2.08	1.40	1.34
57	U	101	EHZ	C9-S1	2.08	1.81	1.76
45	N	903	PC1	O21-C21	2.07	1.40	1.34
46	I	201	3PE	O21-C21	2.07	1.40	1.34
46	Y	203	3PE	O31-C3	-2.06	1.40	1.45
51	r	201	CDL	OA6-CA5	2.06	1.40	1.34
46	Y	202	3PE	O21-C21	2.05	1.40	1.34
46	h	202	3PE	O21-C21	2.05	1.40	1.34
51	L	702	CDL	OB6-CB5	2.05	1.40	1.34
46	L	704	3PE	O21-C21	2.04	1.40	1.34
46	N	901	3PE	O21-C21	2.04	1.40	1.34
55	P	501	NDP	O3D-C3D	-2.04	1.37	1.43
46	d	201	3PE	O21-C21	2.03	1.40	1.34
45	B	202	PC1	O21-C21	2.02	1.40	1.34
46	b	102	3PE	O21-C21	2.02	1.40	1.34
46	L	704	3PE	O31-C3	-2.01	1.40	1.45

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	L	705	CHD	C4-C5-C10	9.30	122.56	112.66
53	O	401	GTP	C8-N9-C4	7.46	120.01	106.03
52	L	705	CHD	C11-C9-C8	6.36	120.31	110.89
57	T	101	EHZ	C8-C9-S1	6.11	121.27	113.56
52	L	705	CHD	C11-C9-C10	5.73	119.52	113.70
57	U	101	EHZ	C8-C9-S1	5.50	120.50	113.56
52	L	705	CHD	C17-C13-C12	4.92	122.09	117.67
52	L	705	CHD	C4-C3-C2	4.77	116.44	110.62
52	L	705	CHD	C14-C13-C12	4.72	111.73	107.42
51	h	201	CDL	OB6-CB5-C51	4.59	121.41	111.48
46	O	403	3PE	O21-C21-C22	4.47	121.15	111.48
46	f	101	3PE	O21-C21-C22	4.47	121.15	111.48
51	N	902	CDL	OB6-CB5-C51	4.45	121.10	111.48
45	d	203	PC1	O21-C21-C22	4.33	120.84	111.48
52	L	705	CHD	C10-C9-C8	4.31	116.64	111.84
52	L	705	CHD	C6-C5-C4	4.31	116.15	111.23
52	L	705	CHD	C6-C5-C10	4.26	117.20	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	L	702	CDL	OB6-CB5-C51	4.17	120.50	111.48
46	L	704	3PE	O21-C21-C22	4.17	120.50	111.48
51	r	201	CDL	OA6-CA5-C11	4.15	120.46	111.48
46	g	201	3PE	O21-C21-C22	4.14	120.43	111.48
45	B	202	PC1	O21-C21-C22	4.13	120.41	111.48
46	b	101	3PE	O21-C21-C22	4.13	120.41	111.48
46	M	601	3PE	O21-C21-C22	4.11	120.38	111.48
55	P	501	NDP	P2B-O2B-C2B	-4.09	112.50	123.43
46	N	904	3PE	O21-C21-C22	4.04	120.22	111.48
51	X	201	CDL	OB6-CB5-C51	4.03	120.20	111.48
46	Y	201	3PE	O21-C21-C22	4.02	120.19	111.48
46	L	703	3PE	O21-C21-C22	4.02	120.18	111.48
46	K	101	3PE	O21-C21-C22	4.00	120.14	111.48
45	N	903	PC1	O21-C21-C22	3.96	120.04	111.48
46	H	601	3PE	O21-C21-C22	3.94	120.00	111.48
46	d	201	3PE	O21-C21-C22	3.94	120.00	111.48
46	b	102	3PE	O21-C21-C22	3.92	119.97	111.48
55	P	501	NDP	O2B-P2B-O1X	-3.92	95.36	109.33
51	L	702	CDL	OA6-CA5-C11	3.91	119.95	111.48
45	M	605	PC1	O31-C31-C32	3.90	123.74	111.83
51	h	201	CDL	OA6-CA5-C11	3.90	119.92	111.48
46	L	701	3PE	O21-C21-C22	3.89	119.89	111.48
46	d	202	3PE	O21-C21-C22	3.88	119.89	111.48
46	m	201	3PE	O21-C21-C22	3.88	119.87	111.48
45	A	301	PC1	O21-C21-C22	3.86	119.84	111.48
46	Y	205	3PE	O21-C21-C22	3.85	119.81	111.48
46	I	201	3PE	O21-C21-C22	3.83	119.77	111.48
46	N	901	3PE	O21-C21-C22	3.82	119.75	111.48
51	X	201	CDL	OA6-CA5-C11	3.81	119.71	111.48
51	d	204	CDL	OA6-CA5-C11	3.80	119.69	111.48
46	h	202	3PE	O21-C21-C22	3.77	119.65	111.48
52	L	705	CHD	C18-C13-C12	-3.77	105.28	109.06
51	r	201	CDL	OB6-CB5-C51	3.76	119.62	111.48
45	M	603	PC1	O21-C21-C22	3.76	119.61	111.48
51	N	902	CDL	OA6-CA5-C11	3.72	119.53	111.48
46	Y	203	3PE	O31-C31-C32	3.71	123.16	111.83
46	Z	201	3PE	O21-C21-C22	3.66	119.40	111.48
45	M	605	PC1	O21-C21-C22	3.65	119.37	111.48
46	M	602	3PE	O21-C21-C22	3.64	119.36	111.48
46	Y	203	3PE	O21-C21-C22	3.60	119.26	111.48
46	A	302	3PE	O21-C21-C22	3.57	119.20	111.48
46	Y	202	3PE	O21-C21-C22	3.56	119.19	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	L	705	CHD	C14-C8-C9	3.55	114.71	109.75
55	P	501	NDP	O3-PA-O1A	-3.52	100.12	110.70
46	Y	204	3PE	O21-C21-C22	3.46	118.97	111.48
46	I	204	3PE	O21-C21-C22	3.45	118.94	111.48
52	L	705	CHD	C17-C13-C14	3.33	103.45	100.11
46	M	604	3PE	O21-C21-C22	3.28	118.58	111.48
49	F	501	FMN	C4-N3-C2	-3.25	119.86	125.64
53	O	401	GTP	C2-N1-C6	-3.23	119.25	125.11
46	d	201	3PE	O31-C31-C32	3.07	121.20	111.83
55	P	501	NDP	PA-O5B-C5B	-3.06	103.82	121.35
46	Y	204	3PE	O31-C31-C32	3.04	121.11	111.83
46	H	601	3PE	O31-C31-C32	3.03	120.35	111.15
46	d	202	3PE	O31-C31-C32	3.01	121.02	111.83
49	F	501	FMN	C4A-C10-N10	2.99	120.76	116.48
46	N	904	3PE	O31-C31-C32	2.99	120.94	111.83
52	L	705	CHD	C18-C13-C17	-2.95	106.58	111.20
46	M	601	3PE	O31-C31-C32	2.94	120.81	111.83
46	L	704	3PE	O31-C31-C32	2.94	120.80	111.83
51	h	201	CDL	OA8-CA7-C31	2.94	120.80	111.83
46	b	102	3PE	O31-C31-C32	2.93	120.78	111.83
57	T	101	EHZ	O2-C9-S1	-2.93	118.96	122.68
51	L	702	CDL	OB8-CB7-C71	2.90	120.69	111.83
51	h	201	CDL	OB8-CB7-C71	2.87	120.59	111.83
51	d	204	CDL	OA8-CA7-C31	2.87	120.57	111.83
51	L	702	CDL	OA8-CA7-C31	2.86	120.56	111.83
46	O	403	3PE	O31-C31-C32	2.83	120.48	111.83
46	M	602	3PE	O31-C31-C32	2.80	120.37	111.83
45	B	202	PC1	O31-C31-C32	2.80	120.36	111.83
52	L	705	CHD	C18-C13-C14	-2.79	106.82	111.20
52	L	705	CHD	C16-C17-C20	-2.77	107.98	112.18
51	r	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
46	Z	201	3PE	O31-C31-C32	2.73	120.16	111.83
53	O	401	GTP	O2G-PG-O3B	2.73	113.78	104.64
53	O	401	GTP	O3G-PG-O3B	2.71	113.74	104.64
45	A	301	PC1	O31-C31-C32	2.70	120.06	111.83
45	M	603	PC1	O31-C31-C32	2.67	119.99	111.83
46	L	703	3PE	O31-C31-C32	2.67	119.97	111.83
46	Y	202	3PE	O31-C31-C32	2.67	119.97	111.83
55	P	501	NDP	C2A-N1A-C6A	-2.65	114.38	118.73
51	N	902	CDL	OA8-CA7-C31	2.65	119.91	111.83
46	Y	205	3PE	O31-C31-C32	2.64	119.88	111.83
45	d	203	PC1	O31-C31-C32	2.64	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	b	101	3PE	O31-C31-C32	2.64	119.88	111.83
51	X	201	CDL	OA8-CA7-C31	2.64	119.87	111.83
46	K	101	3PE	O31-C31-C32	2.63	119.87	111.83
49	F	501	FMN	C4A-C4-N3	2.63	119.94	113.25
46	h	202	3PE	O31-C31-C32	2.61	119.80	111.83
51	X	201	CDL	OB8-CB7-C71	2.60	119.75	111.83
46	g	201	3PE	O31-C31-C32	2.59	119.75	111.83
46	N	901	3PE	O31-C31-C32	2.59	119.75	111.83
51	r	201	CDL	OA8-CA7-C31	2.59	119.72	111.83
52	L	705	CHD	C11-C12-C13	2.57	113.88	111.26
55	P	501	NDP	O3X-P2B-O2X	2.57	117.44	107.80
51	d	204	CDL	OB8-CB7-C71	2.55	119.60	111.83
52	L	705	CHD	C1-C2-C3	2.54	113.85	110.48
46	M	604	3PE	O31-C31-C32	2.54	119.58	111.83
46	f	101	3PE	O31-C31-C32	2.53	119.55	111.83
52	L	705	CHD	C5-C4-C3	2.53	116.52	112.71
53	O	401	GTP	C5-C6-N1	2.53	119.69	113.25
57	T	101	EHZ	O2-C9-C8	-2.53	119.77	123.74
55	P	501	NDP	N3A-C4A-N9A	2.52	131.45	127.17
55	P	501	NDP	O2N-PN-O3	2.51	114.07	107.27
57	U	101	EHZ	O2-C9-S1	-2.49	119.52	122.68
53	O	401	GTP	O2A-PA-O1A	-2.48	100.92	112.44
46	I	201	3PE	O31-C31-C32	2.48	119.39	111.83
51	N	902	CDL	OB8-CB7-C71	2.45	119.29	111.83
49	F	501	FMN	O4-C4-C4A	-2.44	120.08	126.53
55	P	501	NDP	PN-O5D-C5D	-2.44	107.39	121.35
51	d	204	CDL	OB6-CB5-C51	2.43	119.87	110.93
55	P	501	NDP	C5B-C4B-C3B	-2.43	106.46	115.21
46	A	302	3PE	O31-C31-C32	2.42	119.21	111.83
49	F	501	FMN	C10-C4A-N5	-2.41	119.88	124.81
57	U	101	EHZ	O2-C9-C8	-2.38	119.99	123.74
53	O	401	GTP	O6-C6-C5	-2.38	120.25	126.53
46	m	201	3PE	O31-C31-C32	2.38	119.09	111.83
46	L	701	3PE	O31-C31-C32	2.38	119.08	111.83
46	Y	201	3PE	O31-C31-C32	2.36	119.02	111.83
53	O	401	GTP	C1'-N9-C8	-2.35	120.05	126.73
55	P	501	NDP	C5A-C4A-N3A	-2.34	123.49	126.72
55	P	501	NDP	O4B-C4B-C3B	2.34	109.79	105.15
46	I	204	3PE	O31-C31-C32	2.33	118.95	111.83
52	L	705	CHD	C21-C20-C22	-2.31	106.77	110.34
55	P	501	NDP	C2B-C1B-N9A	-2.30	109.97	113.75
53	O	401	GTP	O2B-PB-O1B	-2.29	101.77	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	501	NDP	O2N-PN-O1N	2.29	123.08	112.44
55	P	501	NDP	O7N-C7N-N7N	-2.27	117.81	122.89
53	O	401	GTP	C3'-C2'-C1'	2.27	105.75	101.46
53	O	401	GTP	C5-C4-N9	-2.25	101.63	105.66
53	O	401	GTP	C1'-N9-C4	-2.22	119.94	126.49
53	O	401	GTP	C2'-C3'-C4'	2.19	106.85	102.61
52	L	705	CHD	C13-C17-C20	-2.19	116.83	119.48
52	L	705	CHD	C13-C14-C8	2.18	117.48	114.72
52	L	705	CHD	C23-C22-C20	-2.10	110.54	114.46
52	L	705	CHD	C5-C6-C7	-2.10	111.91	114.40
53	O	401	GTP	C8-N7-C5	-2.08	100.55	104.26
53	O	401	GTP	N9-C8-N7	-2.07	109.56	113.40
52	L	705	CHD	O26-C24-C23	2.07	120.53	114.00
52	L	705	CHD	C1-C10-C5	2.02	110.65	107.75
55	P	501	NDP	C5D-C4D-C3D	-2.02	107.93	115.21
49	F	501	FMN	C4A-C10-N1	-2.00	119.69	124.59
45	M	605	PC1	O31-C31-O32	-2.00	118.62	123.63
51	N	902	CDL	OB6-CB5-OB7	-2.00	119.03	123.70

There are no chirality outliers.

All (949) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	PC1	O21-C2-C3-O31
45	B	202	PC1	C22-C21-O21-C2
45	M	603	PC1	C11-O13-P-O12
45	M	603	PC1	C11-O13-P-O14
45	M	603	PC1	C11-O13-P-O11
45	M	603	PC1	C2-C1-O11-P
45	M	605	PC1	C11-O13-P-O12
45	M	605	PC1	C11-O13-P-O11
45	N	903	PC1	C1-O11-P-O12
45	N	903	PC1	C1-O11-P-O13
45	d	203	PC1	C11-O13-P-O12
45	d	203	PC1	C11-O13-P-O14
45	d	203	PC1	C11-O13-P-O11
45	d	203	PC1	C1-O11-P-O14
46	A	302	3PE	O13-C11-C12-N
46	A	302	3PE	C22-C21-O21-C2
46	H	601	3PE	C1-O11-P-O13
46	I	201	3PE	C1-O11-P-O13
46	I	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	I	201	3PE	C11-O13-P-O12
46	I	204	3PE	C1-O11-P-O13
46	I	204	3PE	C11-O13-P-O11
46	I	204	3PE	C11-O13-P-O12
46	K	101	3PE	C1-O11-P-O12
46	K	101	3PE	O13-C11-C12-N
46	K	101	3PE	C22-C21-O21-C2
46	L	701	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O14
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O14
46	L	703	3PE	O13-C11-C12-N
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C1-O11-P-O13
46	M	601	3PE	O13-C11-C12-N
46	M	602	3PE	O13-C11-C12-N
46	M	604	3PE	C11-O13-P-O12
46	M	604	3PE	O13-C11-C12-N
46	N	901	3PE	C11-O13-P-O11
46	N	901	3PE	O11-C1-C2-O21
46	N	904	3PE	C1-O11-P-O13
46	N	904	3PE	C1-O11-P-O14
46	N	904	3PE	C11-O13-P-O11
46	N	904	3PE	C11-O13-P-O12
46	N	904	3PE	C11-O13-P-O14
46	N	904	3PE	O13-C11-C12-N
46	N	904	3PE	O22-C21-O21-C2
46	N	904	3PE	C22-C21-O21-C2
46	O	403	3PE	O13-C11-C12-N
46	O	403	3PE	O22-C21-O21-C2
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	O11-C1-C2-O21
46	Y	201	3PE	O22-C21-O21-C2
46	Y	202	3PE	C12-C11-O13-P
46	Y	202	3PE	O13-C11-C12-N
46	Y	203	3PE	C11-O13-P-O11
46	Y	203	3PE	C11-O13-P-O12
46	Y	203	3PE	C11-O13-P-O14
46	Y	203	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
46	Y	204	3PE	C1-O11-P-O13
46	Y	204	3PE	O22-C21-O21-C2
46	Y	205	3PE	C11-O13-P-O11
46	Y	205	3PE	C11-O13-P-O14
46	Y	205	3PE	O13-C11-C12-N
46	Y	205	3PE	O22-C21-O21-C2
46	Y	205	3PE	C22-C21-O21-C2
46	Z	201	3PE	C1-O11-P-O13
46	Z	201	3PE	C1-O11-P-O14
46	Z	201	3PE	C11-O13-P-O11
46	Z	201	3PE	C11-O13-P-O12
46	Z	201	3PE	C11-O13-P-O14
46	b	101	3PE	C11-O13-P-O11
46	b	101	3PE	C11-O13-P-O12
46	d	201	3PE	C1-O11-P-O14
46	d	201	3PE	O13-C11-C12-N
46	d	201	3PE	O22-C21-O21-C2
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O14
46	d	202	3PE	O13-C11-C12-N
46	f	101	3PE	O13-C11-C12-N
46	g	201	3PE	C11-O13-P-O11
46	g	201	3PE	C11-O13-P-O14
46	h	202	3PE	C1-O11-P-O12
46	h	202	3PE	C1-O11-P-O13
46	h	202	3PE	C1-O11-P-O14
46	h	202	3PE	O13-C11-C12-N
46	m	201	3PE	C1-O11-P-O13
46	m	201	3PE	C1-O11-P-O14
46	m	201	3PE	C11-O13-P-O14
46	m	201	3PE	C22-C21-O21-C2
49	F	501	FMN	C5'-O5'-P-O1P
49	F	501	FMN	C5'-O5'-P-O2P
51	L	702	CDL	OA5-CA3-CA4-OA6
51	L	702	CDL	CB2-OB2-PB2-OB3
51	L	702	CDL	CB3-OB5-PB2-OB2
51	L	702	CDL	CB3-OB5-PB2-OB4
51	N	902	CDL	CA2-OA2-PA1-OA3
51	N	902	CDL	CA2-OA2-PA1-OA4
51	N	902	CDL	CA2-OA2-PA1-OA5
51	N	902	CDL	CB2-OB2-PB2-OB4
51	N	902	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
51	N	902	CDL	OB7-CB5-OB6-CB4
51	N	902	CDL	C51-CB5-OB6-CB4
51	X	201	CDL	O1-C1-CB2-OB2
51	X	201	CDL	CA3-OA5-PA1-OA2
51	X	201	CDL	CA3-OA5-PA1-OA3
51	X	201	CDL	OB7-CB5-OB6-CB4
51	d	204	CDL	CA2-OA2-PA1-OA4
51	d	204	CDL	CA2-OA2-PA1-OA5
51	d	204	CDL	CA3-OA5-PA1-OA2
51	d	204	CDL	CA3-OA5-PA1-OA4
51	d	204	CDL	CB2-OB2-PB2-OB3
51	d	204	CDL	CB2-OB2-PB2-OB4
51	d	204	CDL	CB3-OB5-PB2-OB2
51	d	204	CDL	CB3-OB5-PB2-OB3
51	h	201	CDL	CA3-OA5-PA1-OA2
51	h	201	CDL	CA3-OA5-PA1-OA3
51	h	201	CDL	CA3-OA5-PA1-OA4
51	h	201	CDL	C11-CA5-OA6-CA4
51	h	201	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	CB2-OB2-PB2-OB4
51	h	201	CDL	CB2-OB2-PB2-OB5
51	h	201	CDL	CB3-OB5-PB2-OB2
51	h	201	CDL	CB3-OB5-PB2-OB3
51	h	201	CDL	OB5-CB3-CB4-OB6
51	h	201	CDL	C51-CB5-OB6-CB4
51	r	201	CDL	CA3-OA5-PA1-OA2
51	r	201	CDL	CA3-OA5-PA1-OA3
51	r	201	CDL	CA3-OA5-PA1-OA4
55	P	501	NDP	C5B-O5B-PA-O2A
55	P	501	NDP	C5B-O5B-PA-O3
55	P	501	NDP	C5D-O5D-PN-O3
55	P	501	NDP	C5D-O5D-PN-O1N
57	T	101	EHZ	C11-C10-S1-C9
57	T	101	EHZ	N2-C15-C16-O5
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
46	M	604	3PE	O32-C31-O31-C3
46	d	201	3PE	O32-C31-O31-C3
46	d	202	3PE	O32-C31-O31-C3
46	g	201	3PE	O32-C31-O31-C3
46	d	201	3PE	C32-C31-O31-C3
45	N	903	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	M	605	PC1	O32-C31-O31-C3
45	d	203	PC1	O32-C31-O31-C3
46	M	602	3PE	O32-C31-O31-C3
46	Y	202	3PE	O32-C31-O31-C3
51	L	702	CDL	OA9-CA7-OA8-CA6
46	O	403	3PE	O32-C31-O31-C3
45	B	202	PC1	O22-C21-O21-C2
46	K	101	3PE	O22-C21-O21-C2
46	b	101	3PE	O22-C21-O21-C2
46	m	201	3PE	O22-C21-O21-C2
51	h	201	CDL	OA7-CA5-OA6-CA4
51	h	201	CDL	OB7-CB5-OB6-CB4
45	M	605	PC1	C32-C31-O31-C3
45	d	203	PC1	C32-C31-O31-C3
46	H	601	3PE	C32-C31-O31-C3
46	M	602	3PE	C32-C31-O31-C3
46	M	604	3PE	C32-C31-O31-C3
46	d	202	3PE	C32-C31-O31-C3
46	g	201	3PE	C32-C31-O31-C3
51	L	702	CDL	C31-CA7-OA8-CA6
51	X	201	CDL	C71-CB7-OB8-CB6
51	h	201	CDL	C31-CA7-OA8-CA6
46	O	403	3PE	C22-C21-O21-C2
46	Y	201	3PE	C22-C21-O21-C2
46	Y	204	3PE	C22-C21-O21-C2
46	b	101	3PE	C22-C21-O21-C2
46	d	201	3PE	C22-C21-O21-C2
51	X	201	CDL	C51-CB5-OB6-CB4
45	N	903	PC1	O32-C31-O31-C3
46	L	704	3PE	C32-C31-O31-C3
46	N	904	3PE	C32-C31-O31-C3
46	O	403	3PE	C32-C31-O31-C3
46	Y	202	3PE	C32-C31-O31-C3
51	d	204	CDL	C71-CB7-OB8-CB6
51	r	201	CDL	C71-CB7-OB8-CB6
46	N	904	3PE	O32-C31-O31-C3
46	Z	201	3PE	O32-C31-O31-C3
51	d	204	CDL	OB9-CB7-OB8-CB6
51	h	201	CDL	OA9-CA7-OA8-CA6
51	r	201	CDL	OB9-CB7-OB8-CB6
46	A	302	3PE	O22-C21-O21-C2
46	N	901	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	Z	201	3PE	C32-C31-O31-C3
51	N	902	CDL	C71-CB7-OB8-CB6
46	H	601	3PE	O32-C31-O31-C3
51	N	902	CDL	OB9-CB7-OB8-CB6
51	X	201	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	C22-C21-O21-C2
55	P	501	NDP	C3B-C4B-C5B-O5B
46	L	704	3PE	O32-C31-O31-C3
46	N	901	3PE	O32-C31-O31-C3
51	r	201	CDL	C31-CA7-OA8-CA6
51	r	201	CDL	OA9-CA7-OA8-CA6
46	L	701	3PE	O22-C21-O21-C2
51	X	201	CDL	CA2-C1-CB2-OB2
45	A	301	PC1	C32-C31-O31-C3
45	M	603	PC1	C32-C31-O31-C3
46	h	202	3PE	C32-C31-O31-C3
58	o	201	MYR	C2-C3-C4-C5
45	A	301	PC1	O32-C31-O31-C3
46	Z	201	3PE	O21-C2-C3-O31
46	Y	204	3PE	C32-C31-O31-C3
46	b	101	3PE	C32-C31-O31-C3
51	h	201	CDL	CA5-C11-C12-C13
55	P	501	NDP	O4B-C4B-C5B-O5B
46	M	601	3PE	C31-C32-C33-C34
46	Y	201	3PE	C31-C32-C33-C34
46	Y	204	3PE	C21-C22-C23-C24
46	h	202	3PE	C21-C22-C23-C24
51	L	702	CDL	CA7-C31-C32-C33
46	L	701	3PE	C31-C32-C33-C34
46	b	102	3PE	C21-C22-C23-C24
51	h	201	CDL	CB5-C51-C52-C53
45	M	603	PC1	O32-C31-O31-C3
45	d	203	PC1	C21-C22-C23-C24
46	A	302	3PE	C21-C22-C23-C24
46	Y	202	3PE	C31-C32-C33-C34
46	Y	204	3PE	C31-C32-C33-C34
51	h	201	CDL	CB7-C71-C72-C73
46	h	202	3PE	O32-C31-O31-C3
51	d	204	CDL	CA5-C11-C12-C13
46	Y	204	3PE	O32-C31-O31-C3
46	b	101	3PE	O32-C31-O31-C3
46	d	201	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
51	d	204	CDL	C31-CA7-OA8-CA6
46	K	101	3PE	C31-C32-C33-C34
46	m	201	3PE	C31-C32-C33-C34
45	d	203	PC1	C36-C37-C38-C39
46	m	201	3PE	C32-C31-O31-C3
46	I	201	3PE	C22-C21-O21-C2
46	I	204	3PE	C22-C21-O21-C2
46	L	703	3PE	C22-C21-O21-C2
46	M	601	3PE	C22-C21-O21-C2
46	Y	203	3PE	C32-C33-C34-C35
46	I	201	3PE	O22-C21-O21-C2
51	d	204	CDL	OA9-CA7-OA8-CA6
46	K	101	3PE	C1-C2-O21-C21
46	M	601	3PE	C26-C27-C28-C29
46	H	601	3PE	C2E-C2F-C2G-C2H
46	h	202	3PE	C2C-C2D-C2E-C2F
51	d	204	CDL	C42-C43-C44-C45
45	B	202	PC1	C32-C33-C34-C35
46	K	101	3PE	C39-C3A-C3B-C3C
46	b	102	3PE	C29-C2A-C2B-C2C
51	X	201	CDL	C15-C16-C17-C18
51	r	201	CDL	C51-C52-C53-C54
45	B	202	PC1	C22-C23-C24-C25
45	J	201	PC1	C24-C25-C26-C27
46	Z	201	3PE	C3A-C3B-C3C-C3D
46	d	201	3PE	C33-C34-C35-C36
51	X	201	CDL	C35-C36-C37-C38
51	X	201	CDL	C42-C43-C44-C45
46	I	204	3PE	O22-C21-O21-C2
46	L	703	3PE	O22-C21-O21-C2
46	M	601	3PE	O22-C21-O21-C2
46	L	703	3PE	C3A-C3B-C3C-C3D
46	N	904	3PE	C23-C24-C25-C26
46	Y	202	3PE	C24-C25-C26-C27
51	N	902	CDL	C12-C13-C14-C15
52	L	705	CHD	C21-C20-C22-C23
46	I	204	3PE	C31-C32-C33-C34
46	b	102	3PE	C31-C32-C33-C34
45	N	903	PC1	C22-C21-O21-C2
57	T	101	EHZ	C5-C6-C7-C8
46	I	204	3PE	C2D-C2E-C2F-C2G
45	A	301	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
46	N	904	3PE	C32-C33-C34-C35
46	h	202	3PE	C27-C28-C29-C2A
51	X	201	CDL	C34-C35-C36-C37
51	N	902	CDL	CB7-C71-C72-C73
51	L	702	CDL	C62-C63-C64-C65
51	h	201	CDL	C57-C58-C59-C60
46	Y	201	3PE	C32-C31-O31-C3
45	M	603	PC1	C26-C27-C28-C29
45	d	203	PC1	C3A-C3B-C3C-C3D
46	m	201	3PE	C33-C34-C35-C36
51	L	702	CDL	C57-C58-C59-C60
51	d	204	CDL	C33-C34-C35-C36
51	h	201	CDL	C56-C57-C58-C59
51	r	201	CDL	C12-C13-C14-C15
46	I	204	3PE	C26-C27-C28-C29
46	N	904	3PE	C24-C25-C26-C27
46	b	101	3PE	C32-C33-C34-C35
46	b	102	3PE	C24-C25-C26-C27
46	g	201	3PE	C32-C33-C34-C35
51	X	201	CDL	C54-C55-C56-C57
51	X	201	CDL	C56-C57-C58-C59
46	m	201	3PE	O32-C31-O31-C3
46	L	701	3PE	C38-C39-C3A-C3B
46	N	904	3PE	C29-C2A-C2B-C2C
46	b	102	3PE	C32-C33-C34-C35
46	f	101	3PE	C22-C23-C24-C25
51	X	201	CDL	C31-C32-C33-C34
51	d	204	CDL	C72-C73-C74-C75
57	U	101	EHZ	C3-C4-C5-C6
45	B	202	PC1	C38-C39-C3A-C3B
45	M	603	PC1	C2A-C2B-C2C-C2D
46	I	201	3PE	C3A-C3B-C3C-C3D
46	O	403	3PE	C33-C34-C35-C36
45	M	603	PC1	C31-C32-C33-C34
45	M	603	PC1	C32-C33-C34-C35
46	A	302	3PE	C39-C3A-C3B-C3C
46	Z	201	3PE	C3D-C3E-C3F-C3G
46	b	102	3PE	C2C-C2D-C2E-C2F
46	M	601	3PE	C23-C24-C25-C26
46	N	901	3PE	C37-C38-C39-C3A
51	X	201	CDL	C51-C52-C53-C54
46	A	302	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
46	f	101	3PE	C23-C24-C25-C26
51	N	902	CDL	C14-C15-C16-C17
46	I	201	3PE	C21-C22-C23-C24
45	M	603	PC1	C2C-C2D-C2E-C2F
46	Y	201	3PE	C3E-C3F-C3G-C3H
46	m	201	3PE	C2E-C2F-C2G-C2H
46	A	302	3PE	C23-C24-C25-C26
45	N	903	PC1	O22-C21-O21-C2
46	Y	203	3PE	O22-C21-O21-C2
46	L	701	3PE	C36-C37-C38-C39
46	Y	204	3PE	C34-C35-C36-C37
45	A	301	PC1	C36-C37-C38-C39
46	b	102	3PE	C2E-C2F-C2G-C2H
46	d	202	3PE	C26-C27-C28-C29
46	I	201	3PE	C31-C32-C33-C34
46	N	904	3PE	C31-C32-C33-C34
46	I	201	3PE	C33-C34-C35-C36
46	Y	205	3PE	C38-C39-C3A-C3B
51	X	201	CDL	C22-C23-C24-C25
52	L	705	CHD	C17-C20-C22-C23
45	M	603	PC1	C23-C24-C25-C26
46	b	102	3PE	C3D-C3E-C3F-C3G
45	B	202	PC1	C3E-C3F-C3G-C3H
46	Z	201	3PE	C25-C26-C27-C28
46	b	102	3PE	C3B-C3C-C3D-C3E
46	O	403	3PE	C35-C36-C37-C38
46	d	202	3PE	C35-C36-C37-C38
46	M	602	3PE	C22-C21-O21-C2
46	M	604	3PE	C22-C21-O21-C2
46	Y	203	3PE	C22-C21-O21-C2
46	f	101	3PE	C22-C21-O21-C2
46	h	202	3PE	C22-C21-O21-C2
51	N	902	CDL	C11-CA5-OA6-CA4
51	X	201	CDL	C11-CA5-OA6-CA4
51	d	204	CDL	C51-CB5-OB6-CB4
46	O	403	3PE	C31-C32-C33-C34
46	f	101	3PE	O22-C21-O21-C2
51	N	902	CDL	OA7-CA5-OA6-CA4
51	d	204	CDL	OB7-CB5-OB6-CB4
46	Y	201	3PE	C2A-C2B-C2C-C2D
46	g	201	3PE	C29-C2A-C2B-C2C
55	P	501	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
51	N	902	CDL	C71-C72-C73-C74
46	Z	201	3PE	C35-C36-C37-C38
46	b	102	3PE	C26-C27-C28-C29
46	d	202	3PE	C24-C25-C26-C27
46	M	602	3PE	C36-C37-C38-C39
46	M	604	3PE	C26-C27-C28-C29
46	h	202	3PE	C2A-C2B-C2C-C2D
51	h	201	CDL	C54-C55-C56-C57
51	L	702	CDL	C15-C16-C17-C18
46	Y	201	3PE	O32-C31-O31-C3
51	N	902	CDL	C16-C17-C18-C19
46	L	701	3PE	C21-C22-C23-C24
46	Y	205	3PE	C31-C32-C33-C34
46	Y	205	3PE	C21-C22-C23-C24
46	M	604	3PE	O22-C21-O21-C2
51	X	201	CDL	OA7-CA5-OA6-CA4
46	M	601	3PE	O11-C1-C2-O21
46	M	602	3PE	O11-C1-C2-O21
46	b	101	3PE	O11-C1-C2-O21
51	X	201	CDL	OA5-CA3-CA4-OA6
46	N	901	3PE	C2D-C2E-C2F-C2G
51	N	902	CDL	C32-C33-C34-C35
46	d	202	3PE	C31-C32-C33-C34
45	N	903	PC1	C26-C27-C28-C29
46	N	901	3PE	C23-C24-C25-C26
46	Y	201	3PE	C22-C23-C24-C25
45	M	603	PC1	O21-C2-C3-O31
46	O	403	3PE	O21-C2-C3-O31
46	b	102	3PE	O21-C2-C3-O31
51	L	702	CDL	C71-CB7-OB8-CB6
46	L	704	3PE	C28-C29-C2A-C2B
46	M	602	3PE	C2E-C2F-C2G-C2H
46	M	602	3PE	C22-C23-C24-C25
46	Y	201	3PE	C2B-C2C-C2D-C2E
46	Y	205	3PE	C2C-C2D-C2E-C2F
51	L	702	CDL	C39-C40-C41-C42
46	K	101	3PE	C35-C36-C37-C38
46	L	701	3PE	C34-C35-C36-C37
46	M	604	3PE	C34-C35-C36-C37
46	M	604	3PE	C2A-C2B-C2C-C2D
51	N	902	CDL	C51-C52-C53-C54
45	B	202	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C22-C23-C24-C25
46	h	202	3PE	O22-C21-O21-C2
46	M	602	3PE	C3D-C3E-C3F-C3G
46	d	202	3PE	C3A-C3B-C3C-C3D
46	I	201	3PE	C28-C29-C2A-C2B
46	Y	205	3PE	C35-C36-C37-C38
51	X	201	CDL	C59-C60-C61-C62
46	I	201	3PE	C2E-C2F-C2G-C2H
51	L	702	CDL	C38-C39-C40-C41
51	N	902	CDL	C60-C61-C62-C63
57	T	101	EHZ	O4-C15-C16-O5
51	N	902	CDL	CA5-C11-C12-C13
45	A	301	PC1	C3E-C3F-C3G-C3H
46	H	601	3PE	C24-C25-C26-C27
46	I	204	3PE	C28-C29-C2A-C2B
46	N	901	3PE	C3D-C3E-C3F-C3G
46	d	201	3PE	C35-C36-C37-C38
46	M	602	3PE	O11-C1-C2-C3
46	N	901	3PE	O11-C1-C2-C3
46	O	403	3PE	O11-C1-C2-C3
46	Y	204	3PE	O11-C1-C2-C3
51	L	702	CDL	OA5-CA3-CA4-CA6
46	M	602	3PE	O22-C21-O21-C2
46	H	601	3PE	C22-C23-C24-C25
51	N	902	CDL	CA4-CA6-OA8-CA7
46	m	201	3PE	C21-C22-C23-C24
46	K	101	3PE	C3A-C3B-C3C-C3D
46	g	201	3PE	C23-C24-C25-C26
51	X	201	CDL	CB7-C71-C72-C73
45	M	605	PC1	C22-C21-O21-C2
46	Y	202	3PE	C2A-C2B-C2C-C2D
46	m	201	3PE	C2D-C2E-C2F-C2G
55	P	501	NDP	O4D-C1D-N1N-C6N
51	X	201	CDL	C60-C61-C62-C63
45	A	301	PC1	C1-C2-C3-O31
46	L	703	3PE	C1-C2-C3-O31
46	L	704	3PE	C1-C2-C3-O31
46	M	604	3PE	C1-C2-C3-O31
46	Z	201	3PE	C1-C2-C3-O31
46	b	101	3PE	C1-C2-C3-O31
46	d	202	3PE	C1-C2-C3-O31
46	h	202	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
51	d	204	CDL	CB3-CB4-CB6-OB8
51	h	201	CDL	CA3-CA4-CA6-OA8
51	r	201	CDL	CA3-CA4-CA6-OA8
51	r	201	CDL	CB3-CB4-CB6-OB8
45	A	301	PC1	C34-C35-C36-C37
45	M	605	PC1	C3B-C3C-C3D-C3E
46	A	302	3PE	C2E-C2F-C2G-C2H
46	I	204	3PE	C37-C38-C39-C3A
46	M	602	3PE	C3C-C3D-C3E-C3F
46	Y	202	3PE	C33-C34-C35-C36
46	I	204	3PE	C36-C37-C38-C39
46	L	701	3PE	C28-C29-C2A-C2B
45	d	203	PC1	C33-C34-C35-C36
46	I	201	3PE	C3E-C3F-C3G-C3H
51	X	201	CDL	C1-CB2-OB2-PB2
51	d	204	CDL	C1-CB2-OB2-PB2
51	X	201	CDL	C39-C40-C41-C42
51	L	702	CDL	OB9-CB7-OB8-CB6
45	M	605	PC1	C36-C37-C38-C39
45	M	603	PC1	C36-C37-C38-C39
46	I	201	3PE	C26-C27-C28-C29
46	H	601	3PE	C28-C29-C2A-C2B
57	T	101	EHZ	C5-C6-C7-O1
46	M	602	3PE	C38-C39-C3A-C3B
46	N	901	3PE	C3A-C3B-C3C-C3D
46	Y	201	3PE	C3B-C3C-C3D-C3E
46	d	201	3PE	C36-C37-C38-C39
46	I	204	3PE	C33-C34-C35-C36
51	h	201	CDL	C31-C32-C33-C34
46	d	202	3PE	C2B-C2C-C2D-C2E
46	b	101	3PE	C21-C22-C23-C24
51	d	204	CDL	C31-C32-C33-C34
51	d	204	CDL	OB5-CB3-CB4-OB6
46	Y	201	3PE	C2E-C2F-C2G-C2H
46	I	204	3PE	C32-C31-O31-C3
46	m	201	3PE	C34-C35-C36-C37
46	Y	204	3PE	C35-C36-C37-C38
46	Y	202	3PE	C34-C35-C36-C37
45	M	603	PC1	C34-C35-C36-C37
46	L	703	3PE	C35-C36-C37-C38
51	L	702	CDL	C58-C59-C60-C61
46	d	202	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	A	301	PC1	C22-C23-C24-C25
46	Y	203	3PE	C25-C26-C27-C28
46	O	403	3PE	C23-C24-C25-C26
46	I	204	3PE	C39-C3A-C3B-C3C
46	M	602	3PE	C3A-C3B-C3C-C3D
46	d	202	3PE	C39-C3A-C3B-C3C
51	X	201	CDL	C24-C25-C26-C27
46	N	904	3PE	C33-C34-C35-C36
46	b	101	3PE	C36-C37-C38-C39
46	H	601	3PE	C29-C2A-C2B-C2C
46	g	201	3PE	C25-C26-C27-C28
51	N	902	CDL	C31-C32-C33-C34
46	f	101	3PE	C34-C35-C36-C37
46	Y	203	3PE	C28-C29-C2A-C2B
57	T	101	EHZ	O4-C15-C16-C17
46	m	201	3PE	C2C-C2D-C2E-C2F
45	B	202	PC1	C32-C31-O31-C3
51	N	902	CDL	C38-C39-C40-C41
46	Y	203	3PE	C26-C27-C28-C29
46	O	403	3PE	C2-C1-O11-P
51	X	201	CDL	C19-C20-C21-C22
46	M	604	3PE	C33-C34-C35-C36
46	M	601	3PE	O11-C1-C2-C3
46	Y	203	3PE	O11-C1-C2-C3
46	b	101	3PE	O11-C1-C2-C3
51	L	702	CDL	OB5-CB3-CB4-CB6
46	L	704	3PE	C21-C22-C23-C24
45	M	603	PC1	C2F-C2G-C2H-C2I
45	M	605	PC1	C33-C34-C35-C36
46	Y	205	3PE	C28-C29-C2A-C2B
45	M	605	PC1	C31-C32-C33-C34
46	M	604	3PE	C22-C23-C24-C25
46	A	302	3PE	C1-C2-C3-O31
46	O	403	3PE	C1-C2-C3-O31
46	b	102	3PE	C1-C2-C3-O31
46	N	901	3PE	C31-C32-C33-C34
51	d	204	CDL	CA7-C31-C32-C33
46	I	201	3PE	C2B-C2C-C2D-C2E
46	f	101	3PE	O21-C21-C22-C23
46	I	204	3PE	C3B-C3C-C3D-C3E
46	f	101	3PE	C2-C1-O11-P
51	L	702	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
51	N	902	CDL	C1-CA2-OA2-PA1
57	T	101	EHZ	O1-C7-C8-C9
45	N	903	PC1	C23-C24-C25-C26
51	L	702	CDL	C42-C43-C44-C45
46	M	601	3PE	C32-C33-C34-C35
46	A	302	3PE	O21-C2-C3-O31
46	g	201	3PE	O21-C2-C3-O31
45	M	605	PC1	O22-C21-O21-C2
45	M	605	PC1	C23-C24-C25-C26
46	L	704	3PE	C32-C33-C34-C35
46	d	202	3PE	C21-C22-C23-C24
51	X	201	CDL	CA5-C11-C12-C13
46	I	201	3PE	C3B-C3C-C3D-C3E
46	g	201	3PE	C34-C35-C36-C37
46	L	703	3PE	C32-C31-O31-C3
46	Y	204	3PE	C23-C24-C25-C26
57	T	101	EHZ	C6-C7-C8-C9
51	d	204	CDL	C77-C78-C79-C80
46	A	302	3PE	C2C-C2D-C2E-C2F
46	K	101	3PE	C27-C28-C29-C2A
51	L	702	CDL	C44-C45-C46-C47
51	N	902	CDL	C31-CA7-OA8-CA6
46	d	201	3PE	C37-C38-C39-C3A
46	Y	201	3PE	C3D-C3E-C3F-C3G
46	d	201	3PE	C29-C2A-C2B-C2C
46	I	204	3PE	O32-C31-O31-C3
46	f	101	3PE	C32-C31-O31-C3
46	M	601	3PE	C2B-C2C-C2D-C2E
45	A	301	PC1	O11-C1-C2-C3
46	H	601	3PE	O11-C1-C2-C3
46	I	201	3PE	O11-C1-C2-C3
46	Y	201	3PE	O11-C1-C2-C3
46	d	202	3PE	C33-C34-C35-C36
51	h	201	CDL	C52-C53-C54-C55
58	o	201	MYR	C7-C8-C9-C10
46	Y	205	3PE	C39-C3A-C3B-C3C
49	F	501	FMN	C5'-O5'-P-O3P
51	h	201	CDL	C36-C37-C38-C39
51	h	201	CDL	C74-C75-C76-C77
46	M	601	3PE	O21-C21-C22-C23
45	B	202	PC1	O32-C31-O31-C3
46	b	102	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
51	N	902	CDL	C59-C60-C61-C62
46	M	604	3PE	C3-C2-O21-C21
46	I	204	3PE	C38-C39-C3A-C3B
45	A	301	PC1	O11-C1-C2-O21
46	I	201	3PE	C37-C38-C39-C3A
46	b	101	3PE	C28-C29-C2A-C2B
51	N	902	CDL	C36-C37-C38-C39
46	K	101	3PE	C23-C24-C25-C26
45	M	603	PC1	C1-C2-C3-O31
51	N	902	CDL	OA9-CA7-OA8-CA6
45	B	202	PC1	C2B-C2C-C2D-C2E
46	Y	205	3PE	C25-C26-C27-C28
46	M	601	3PE	C12-C11-O13-P
46	N	904	3PE	C12-C11-O13-P
46	O	403	3PE	C12-C11-O13-P
46	Y	203	3PE	C12-C11-O13-P
46	Y	204	3PE	C12-C11-O13-P
46	f	101	3PE	C12-C11-O13-P
46	g	201	3PE	C12-C11-O13-P
46	K	101	3PE	C28-C29-C2A-C2B
46	Y	201	3PE	C33-C34-C35-C36
46	L	703	3PE	O21-C2-C3-O31
46	L	704	3PE	O21-C2-C3-O31
46	M	604	3PE	O21-C2-C3-O31
46	b	101	3PE	O21-C2-C3-O31
51	d	204	CDL	OB6-CB4-CB6-OB8
51	r	201	CDL	OB6-CB4-CB6-OB8
46	Y	203	3PE	C35-C36-C37-C38
46	M	602	3PE	C34-C35-C36-C37
46	L	703	3PE	O32-C31-O31-C3
46	f	101	3PE	O32-C31-O31-C3
46	N	904	3PE	C2F-C2G-C2H-C2I
46	d	202	3PE	C34-C35-C36-C37
46	H	601	3PE	C25-C26-C27-C28
45	A	301	PC1	O13-C11-C12-N
51	X	201	CDL	C11-C12-C13-C14
46	Y	205	3PE	C37-C38-C39-C3A
46	A	302	3PE	C27-C28-C29-C2A
46	Y	202	3PE	C2F-C2G-C2H-C2I
46	Y	205	3PE	C33-C34-C35-C36
46	L	703	3PE	O11-C1-C2-C3
51	X	201	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
51	d	204	CDL	OB5-CB3-CB4-CB6
51	h	201	CDL	OB5-CB3-CB4-CB6
51	X	201	CDL	C18-C19-C20-C21
49	F	501	FMN	N10-C1'-C2'-O2'
46	I	201	3PE	C34-C35-C36-C37
46	b	102	3PE	C3E-C3F-C3G-C3H
46	L	704	3PE	C23-C24-C25-C26
46	H	601	3PE	C2-C1-O11-P
46	M	604	3PE	C2-C1-O11-P
46	Y	202	3PE	C2-C1-O11-P
46	Y	203	3PE	C2-C1-O11-P
46	h	202	3PE	C2-C1-O11-P
51	L	702	CDL	CA4-CA3-OA5-PA1
46	Y	205	3PE	C27-C28-C29-C2A
46	H	601	3PE	O11-C1-C2-O21
46	I	201	3PE	O11-C1-C2-O21
46	O	403	3PE	O11-C1-C2-O21
46	Y	205	3PE	O11-C1-C2-O21
51	L	702	CDL	OB5-CB3-CB4-OB6
51	X	201	CDL	OB5-CB3-CB4-OB6
51	d	204	CDL	OA5-CA3-CA4-OA6
51	L	702	CDL	C51-CB5-OB6-CB4
46	M	601	3PE	C2A-C2B-C2C-C2D
46	g	201	3PE	C26-C27-C28-C29
46	M	604	3PE	C25-C26-C27-C28
46	N	901	3PE	C28-C29-C2A-C2B
46	Y	205	3PE	C22-C23-C24-C25
46	g	201	3PE	C2A-C2B-C2C-C2D
46	N	901	3PE	C35-C36-C37-C38
46	h	202	3PE	O21-C2-C3-O31
46	Z	201	3PE	C39-C3A-C3B-C3C
46	I	204	3PE	C1-C2-C3-O31
46	K	101	3PE	C32-C33-C34-C35
46	I	204	3PE	C2C-C2D-C2E-C2F
46	A	302	3PE	C32-C33-C34-C35
46	I	204	3PE	C29-C2A-C2B-C2C
46	Y	201	3PE	C27-C28-C29-C2A
45	d	203	PC1	C34-C35-C36-C37
45	M	605	PC1	C11-O13-P-O14
45	N	903	PC1	C11-O13-P-O12
45	N	903	PC1	C11-O13-P-O14
45	N	903	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	N	903	PC1	C1-O11-P-O14
45	d	203	PC1	C1-O11-P-O12
45	d	203	PC1	C1-O11-P-O13
46	H	601	3PE	C1-O11-P-O14
46	H	601	3PE	C11-O13-P-O12
46	I	201	3PE	C1-O11-P-O14
46	I	204	3PE	C1-O11-P-O12
46	I	204	3PE	C11-O13-P-O14
46	K	101	3PE	C1-O11-P-O13
46	K	101	3PE	C1-O11-P-O14
46	L	701	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	C1-O11-P-O14
46	L	704	3PE	C1-O11-P-O14
46	L	704	3PE	O13-C11-C12-N
46	M	601	3PE	C11-O13-P-O11
46	M	601	3PE	C11-O13-P-O14
46	M	602	3PE	C1-O11-P-O12
46	M	602	3PE	C1-O11-P-O13
46	M	602	3PE	C1-O11-P-O14
46	M	602	3PE	C11-O13-P-O11
46	M	602	3PE	C11-O13-P-O14
46	M	604	3PE	C1-O11-P-O12
46	M	604	3PE	C11-O13-P-O11
46	N	901	3PE	O13-C11-C12-N
46	Y	202	3PE	C11-O13-P-O12
46	Y	203	3PE	C1-O11-P-O14
46	Y	203	3PE	O13-C11-C12-N
46	Z	201	3PE	C1-O11-P-O12
46	b	102	3PE	C11-O13-P-O11
46	b	102	3PE	C11-O13-P-O12
46	d	202	3PE	C11-O13-P-O12
46	f	101	3PE	C11-O13-P-O11
46	h	202	3PE	C11-O13-P-O11
46	h	202	3PE	C11-O13-P-O12
46	h	202	3PE	C11-O13-P-O14
46	m	201	3PE	C1-O11-P-O12
51	L	702	CDL	CB3-OB5-PB2-OB3
51	N	902	CDL	CA3-OA5-PA1-OA2
51	N	902	CDL	CA3-OA5-PA1-OA3
51	N	902	CDL	CA3-OA5-PA1-OA4
51	N	902	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	CA3-OA5-PA1-OA4
51	X	201	CDL	CB3-OB5-PB2-OB3
51	d	204	CDL	CA3-OA5-PA1-OA3
51	d	204	CDL	CB2-OB2-PB2-OB5
51	d	204	CDL	CB3-OB5-PB2-OB4
51	r	201	CDL	CB3-OB5-PB2-OB3
53	O	401	GTP	C5'-O5'-PA-O3A
53	O	401	GTP	C5'-O5'-PA-O1A
53	O	401	GTP	C5'-O5'-PA-O2A
55	P	501	NDP	C5D-O5D-PN-O2N
51	h	201	CDL	OB9-CB7-OB8-CB6
46	H	601	3PE	O31-C31-C32-C33
51	N	902	CDL	C37-C38-C39-C40
46	L	704	3PE	C2-C1-O11-P
46	N	901	3PE	C2-C1-O11-P
46	Y	201	3PE	C2-C1-O11-P
51	L	702	CDL	CB4-CB3-OB5-PB2
46	d	202	3PE	C29-C2A-C2B-C2C
46	K	101	3PE	C36-C37-C38-C39
51	N	902	CDL	C33-C34-C35-C36
51	d	204	CDL	C73-C74-C75-C76
51	h	201	CDL	C71-CB7-OB8-CB6
46	O	403	3PE	C3-C2-O21-C21
46	H	601	3PE	C2A-C2B-C2C-C2D
46	L	703	3PE	C39-C3A-C3B-C3C
46	M	604	3PE	C3D-C3E-C3F-C3G
58	o	201	MYR	C5-C6-C7-C8
46	M	601	3PE	C33-C34-C35-C36
46	K	101	3PE	C3C-C3D-C3E-C3F
45	B	202	PC1	C3C-C3D-C3E-C3F
51	r	201	CDL	C16-C17-C18-C19
46	m	201	3PE	O11-C1-C2-C3
51	X	201	CDL	OB5-CB3-CB4-CB6
45	A	301	PC1	C3B-C3C-C3D-C3E
51	N	902	CDL	CB5-C51-C52-C53
46	Y	204	3PE	O11-C1-C2-O21
46	m	201	3PE	O11-C1-C2-O21
51	N	902	CDL	C54-C55-C56-C57
46	M	601	3PE	C34-C35-C36-C37
46	A	302	3PE	C38-C39-C3A-C3B
46	M	604	3PE	C2C-C2D-C2E-C2F
46	Y	202	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	r	201	CDL	C71-C72-C73-C74
45	J	201	PC1	O22-C21-O21-C2
51	X	201	CDL	CA4-CA3-OA5-PA1
51	h	201	CDL	OA6-CA4-CA6-OA8
51	r	201	CDL	OA6-CA4-CA6-OA8
46	L	704	3PE	C33-C34-C35-C36
46	L	703	3PE	C22-C23-C24-C25
46	Z	201	3PE	C33-C34-C35-C36
51	N	902	CDL	C76-C77-C78-C79
45	J	201	PC1	C22-C21-O21-C2
46	M	602	3PE	C2F-C2G-C2H-C2I
46	O	403	3PE	C36-C37-C38-C39
46	M	604	3PE	C3F-C3G-C3H-C3I
46	m	201	3PE	C27-C28-C29-C2A
51	L	702	CDL	OB7-CB5-OB6-CB4
46	f	101	3PE	C31-C32-C33-C34
46	Y	203	3PE	C39-C3A-C3B-C3C
45	A	301	PC1	C2B-C2C-C2D-C2E
51	r	201	CDL	C32-C33-C34-C35
46	I	201	3PE	C2A-C2B-C2C-C2D
46	L	704	3PE	C22-C23-C24-C25
46	M	602	3PE	C3E-C3F-C3G-C3H
46	M	601	3PE	C38-C39-C3A-C3B
51	h	201	CDL	C34-C35-C36-C37
46	I	204	3PE	C3A-C3B-C3C-C3D
46	M	601	3PE	C28-C29-C2A-C2B
51	r	201	CDL	C31-C32-C33-C34
46	M	602	3PE	C29-C2A-C2B-C2C
51	L	702	CDL	C34-C35-C36-C37
51	r	201	CDL	C55-C56-C57-C58
57	T	101	EHZ	N2-C15-C16-C17
46	Y	204	3PE	O21-C2-C3-O31
51	N	902	CDL	C73-C74-C75-C76
46	M	602	3PE	C26-C27-C28-C29
51	N	902	CDL	C75-C76-C77-C78
51	r	201	CDL	CB4-CB6-OB8-CB7
57	U	101	EHZ	C1-C2-C3-C4
45	M	605	PC1	C39-C3A-C3B-C3C
45	d	203	PC1	C3C-C3D-C3E-C3F
46	h	202	3PE	C32-C33-C34-C35
46	b	102	3PE	C39-C3A-C3B-C3C
51	X	201	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
46	A	302	3PE	C32-C31-O31-C3
46	Y	205	3PE	C26-C27-C28-C29
45	A	301	PC1	C27-C28-C29-C2A
46	N	904	3PE	C2B-C2C-C2D-C2E
45	M	605	PC1	C28-C29-C2A-C2B
46	L	703	3PE	C24-C25-C26-C27
45	M	605	PC1	O31-C31-C32-C33
51	L	702	CDL	CA3-CA4-OA6-CA5
51	L	702	CDL	CA6-CA4-OA6-CA5
51	h	201	CDL	C55-C56-C57-C58
46	Y	202	3PE	C21-C22-C23-C24
51	X	201	CDL	C32-C33-C34-C35
46	A	302	3PE	O32-C31-O31-C3
52	L	705	CHD	C16-C17-C20-C22
51	N	902	CDL	C39-C40-C41-C42
46	M	601	3PE	C29-C2A-C2B-C2C
51	X	201	CDL	C37-C38-C39-C40
46	f	101	3PE	C24-C25-C26-C27
51	X	201	CDL	C20-C21-C22-C23
51	r	201	CDL	C14-C15-C16-C17
46	H	601	3PE	O32-C31-C32-C33
51	d	204	CDL	OA5-CA3-CA4-CA6
46	N	901	3PE	C38-C39-C3A-C3B
46	N	904	3PE	C26-C27-C28-C29
57	U	101	EHZ	C21-C1-C2-C3
46	Y	205	3PE	C2A-C2B-C2C-C2D
46	L	701	3PE	C26-C27-C28-C29
45	M	605	PC1	C29-C2A-C2B-C2C
51	L	702	CDL	C13-C14-C15-C16
45	B	202	PC1	C2A-C2B-C2C-C2D
46	d	202	3PE	C23-C24-C25-C26
46	A	302	3PE	C37-C38-C39-C3A
45	N	903	PC1	C24-C25-C26-C27
46	Y	204	3PE	C2-C1-O11-P
46	b	101	3PE	C2-C1-O11-P
46	d	201	3PE	C2-C1-O11-P
46	g	201	3PE	C2-C1-O11-P
57	T	101	EHZ	C1-C21-C22-C23
51	L	702	CDL	C52-C53-C54-C55
46	Y	201	3PE	C2D-C2E-C2F-C2G
46	Y	202	3PE	C1-C2-C3-O31
46	g	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
51	N	902	CDL	CA3-CA4-CA6-OA8
46	Y	204	3PE	C32-C33-C34-C35
46	L	703	3PE	O21-C21-C22-C23
51	d	204	CDL	C36-C37-C38-C39
46	Y	204	3PE	C26-C27-C28-C29
46	L	703	3PE	O11-C1-C2-O21
46	M	602	3PE	C2D-C2E-C2F-C2G
46	A	302	3PE	C22-C23-C24-C25
46	b	101	3PE	C2A-C2B-C2C-C2D
46	L	704	3PE	O11-C1-C2-C3
51	X	201	CDL	C33-C34-C35-C36
46	Z	201	3PE	C38-C39-C3A-C3B
58	o	201	MYR	C11-C12-C13-C14
51	X	201	CDL	C12-C13-C14-C15
46	I	201	3PE	C23-C24-C25-C26
46	L	703	3PE	C25-C26-C27-C28
51	X	201	CDL	C53-C54-C55-C56
46	f	101	3PE	O22-C21-C22-C23
51	r	201	CDL	C11-C12-C13-C14
46	M	604	3PE	C24-C25-C26-C27
51	L	702	CDL	C12-C13-C14-C15
46	L	701	3PE	C1-C2-C3-O31
46	M	602	3PE	C2A-C2B-C2C-C2D
46	m	201	3PE	C25-C26-C27-C28
46	h	202	3PE	C31-C32-C33-C34
46	A	302	3PE	C33-C34-C35-C36
51	X	201	CDL	C14-C15-C16-C17
51	X	201	CDL	C64-C65-C66-C67
51	r	201	CDL	CA7-C31-C32-C33
46	K	101	3PE	O21-C21-C22-C23
46	d	201	3PE	C22-C23-C24-C25
46	I	204	3PE	O21-C2-C3-O31
46	b	102	3PE	C2B-C2C-C2D-C2E
46	Y	202	3PE	C37-C38-C39-C3A
46	Y	205	3PE	O11-C1-C2-C3
46	d	202	3PE	C36-C37-C38-C39
46	O	403	3PE	O31-C31-C32-C33
46	M	602	3PE	C23-C24-C25-C26
51	N	902	CDL	C19-C20-C21-C22
46	Y	204	3PE	O31-C31-C32-C33
46	Y	205	3PE	O21-C21-C22-C23
51	L	702	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	A	301	PC1	C3C-C3D-C3E-C3F
45	B	202	PC1	C2-C1-O11-P
46	Y	205	3PE	C2-C1-O11-P
46	N	904	3PE	C28-C29-C2A-C2B
46	L	701	3PE	C32-C33-C34-C35
46	b	102	3PE	O21-C21-C22-C23
46	H	601	3PE	C2F-C2G-C2H-C2I
46	I	201	3PE	C32-C31-O31-C3
46	M	601	3PE	C36-C37-C38-C39
51	h	201	CDL	C35-C36-C37-C38
46	H	601	3PE	O21-C21-C22-C23
51	r	201	CDL	OA7-CA5-OA6-CA4
46	L	701	3PE	C35-C36-C37-C38
45	B	202	PC1	C37-C38-C39-C3A
46	M	601	3PE	C35-C36-C37-C38
46	Y	205	3PE	C2E-C2F-C2G-C2H
46	K	101	3PE	O31-C31-C32-C33
45	N	903	PC1	O21-C21-C22-C23
45	d	203	PC1	O21-C21-C22-C23
46	Y	205	3PE	C29-C2A-C2B-C2C
46	M	604	3PE	C2B-C2C-C2D-C2E
51	r	201	CDL	C1-CB2-OB2-PB2
46	Z	201	3PE	C23-C24-C25-C26
46	I	201	3PE	O32-C31-O31-C3
51	X	201	CDL	C41-C42-C43-C44
45	B	202	PC1	O31-C31-C32-C33
45	d	203	PC1	O31-C31-C32-C33
51	N	902	CDL	C72-C73-C74-C75
46	h	202	3PE	C25-C26-C27-C28
51	r	201	CDL	C52-C51-CB5-OB6
46	Y	203	3PE	C34-C35-C36-C37
46	L	703	3PE	C38-C39-C3A-C3B
46	d	201	3PE	C26-C27-C28-C29
46	M	604	3PE	C35-C36-C37-C38
45	A	301	PC1	C24-C25-C26-C27
46	M	601	3PE	O22-C21-C22-C23
51	L	702	CDL	C11-CA5-OA6-CA4
46	b	102	3PE	C23-C24-C25-C26
46	Z	201	3PE	C27-C28-C29-C2A
45	B	202	PC1	O21-C21-C22-C23
46	O	403	3PE	O21-C21-C22-C23
46	Y	205	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	CA6-CA4-OA6-CA5
51	h	201	CDL	C71-C72-C73-C74
46	Y	205	3PE	C2F-C2G-C2H-C2I
45	A	301	PC1	O21-C21-C22-C23
46	b	102	3PE	O31-C31-C32-C33
46	m	201	3PE	O21-C21-C22-C23
46	O	403	3PE	O32-C31-C32-C33
46	H	601	3PE	O22-C21-C22-C23
46	M	602	3PE	O21-C21-C22-C23
45	d	203	PC1	O22-C21-C22-C23
46	Y	202	3PE	O11-C1-C2-O21
51	h	201	CDL	C12-C11-CA5-OA6
46	K	101	3PE	O22-C21-C22-C23
45	J	201	PC1	C2B-C2C-C2D-C2E
46	Y	205	3PE	O22-C21-C22-C23
57	U	101	EHZ	C4-C5-C6-C7
46	Y	201	3PE	C3A-C3B-C3C-C3D
46	f	101	3PE	C32-C33-C34-C35
46	K	101	3PE	O32-C31-C32-C33
46	b	102	3PE	O22-C21-C22-C23
51	X	201	CDL	C36-C37-C38-C39
45	B	202	PC1	O32-C31-C32-C33
46	Y	204	3PE	C1-C2-C3-O31
46	g	201	3PE	C22-C23-C24-C25
46	b	102	3PE	O32-C31-C32-C33
46	Y	202	3PE	O21-C21-C22-C23
51	L	702	CDL	C72-C71-CB7-OB8
46	Y	204	3PE	C25-C26-C27-C28
45	N	903	PC1	O22-C21-C22-C23
46	m	201	3PE	O22-C21-C22-C23
51	r	201	CDL	C52-C51-CB5-OB7
46	g	201	3PE	C31-C32-C33-C34
46	L	703	3PE	C27-C28-C29-C2A
45	M	603	PC1	C2D-C2E-C2F-C2G
45	J	201	PC1	O21-C21-C22-C23
45	M	605	PC1	C21-C22-C23-C24
46	M	604	3PE	C3E-C3F-C3G-C3H
46	b	101	3PE	O31-C31-C32-C33
45	d	203	PC1	O32-C31-C32-C33
46	M	601	3PE	O31-C31-C32-C33
55	P	501	NDP	PA-O3-PN-O2N
45	B	202	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	b	101	3PE	C26-C27-C28-C29
46	Y	201	3PE	C36-C37-C38-C39
55	P	501	NDP	C3D-C4D-C5D-O5D
46	Y	203	3PE	O31-C31-C32-C33
51	h	201	CDL	C32-C31-CA7-OA8
45	A	301	PC1	O22-C21-C22-C23

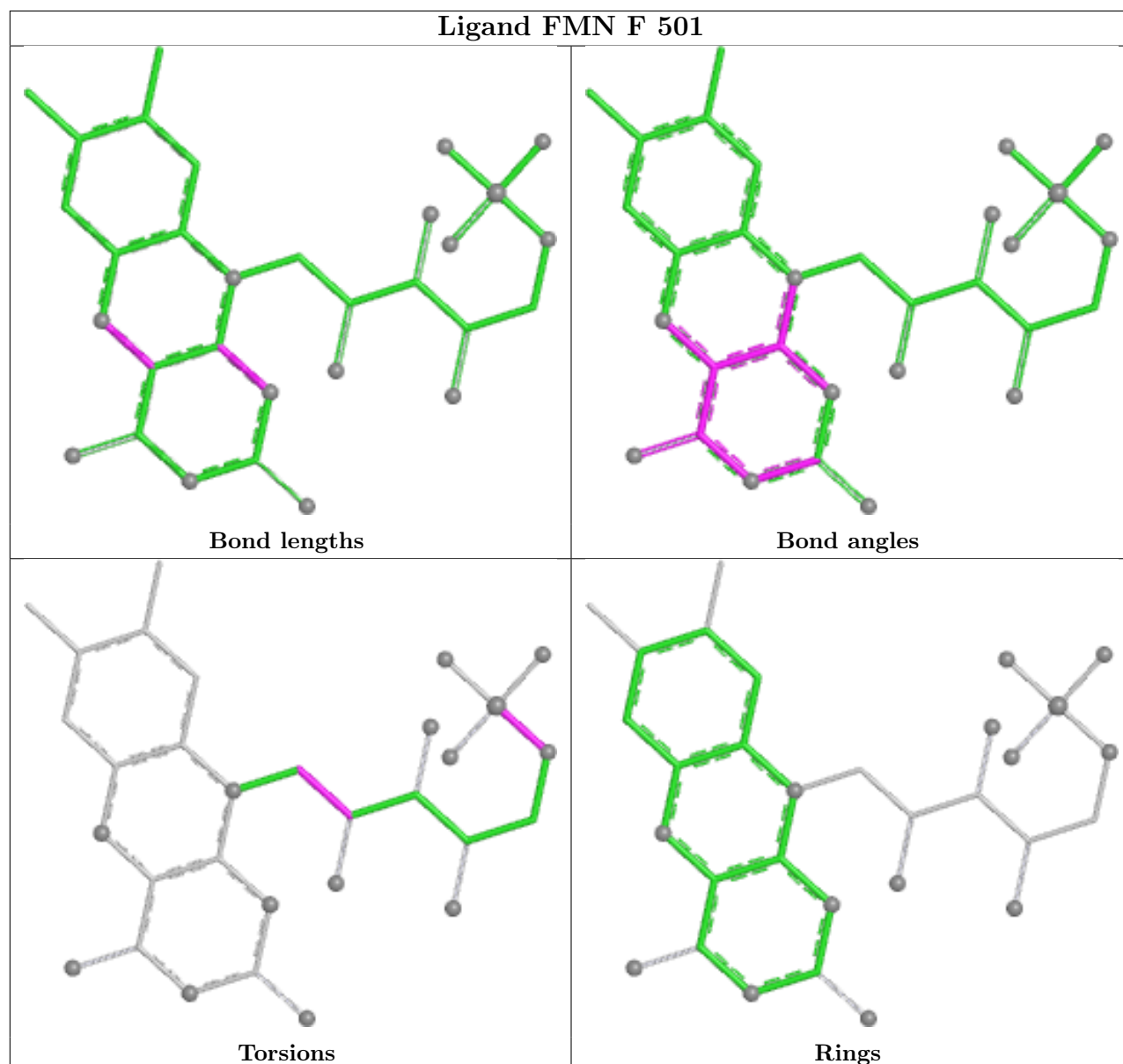
There are no ring outliers.

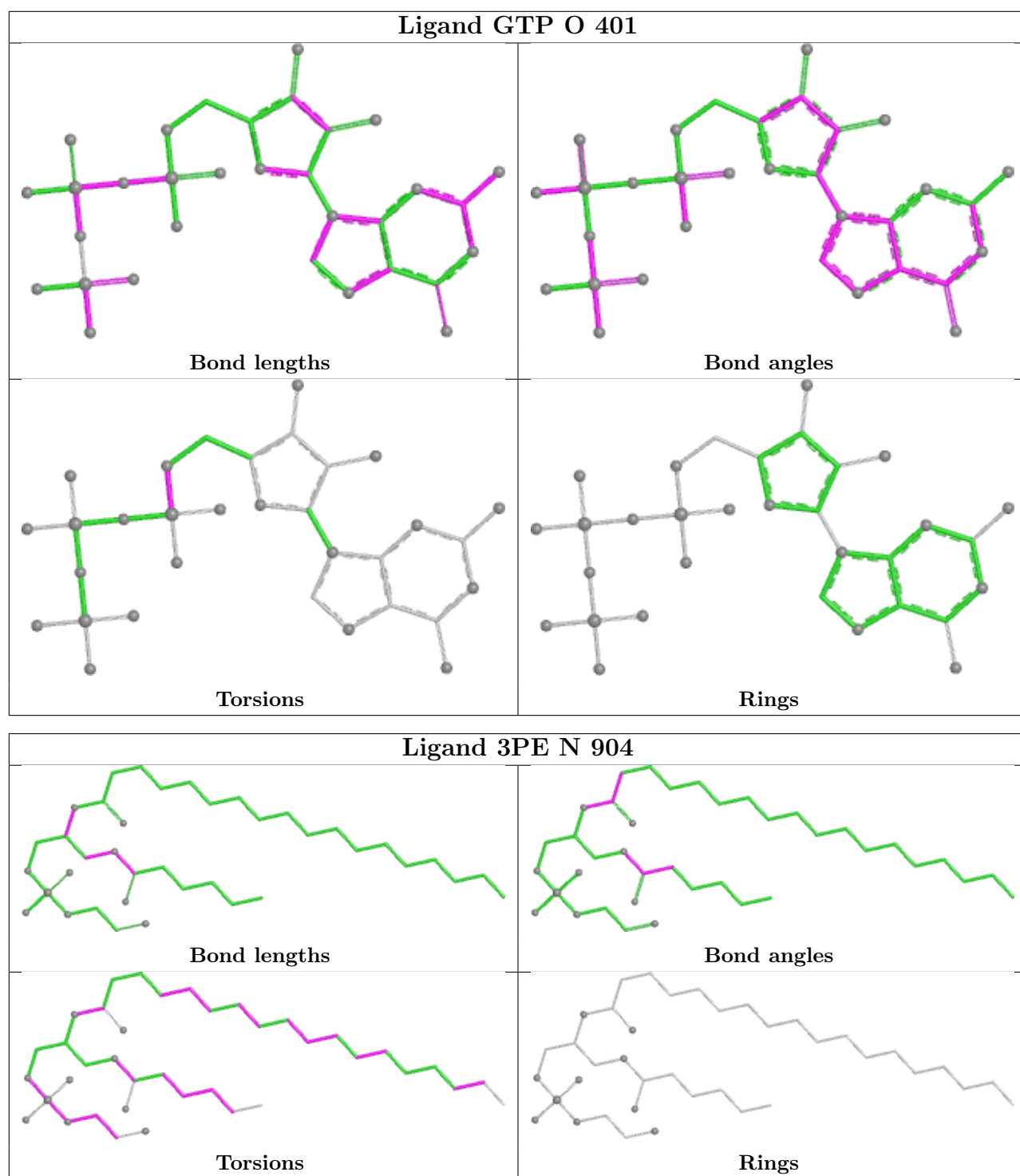
27 monomers are involved in 49 short contacts:

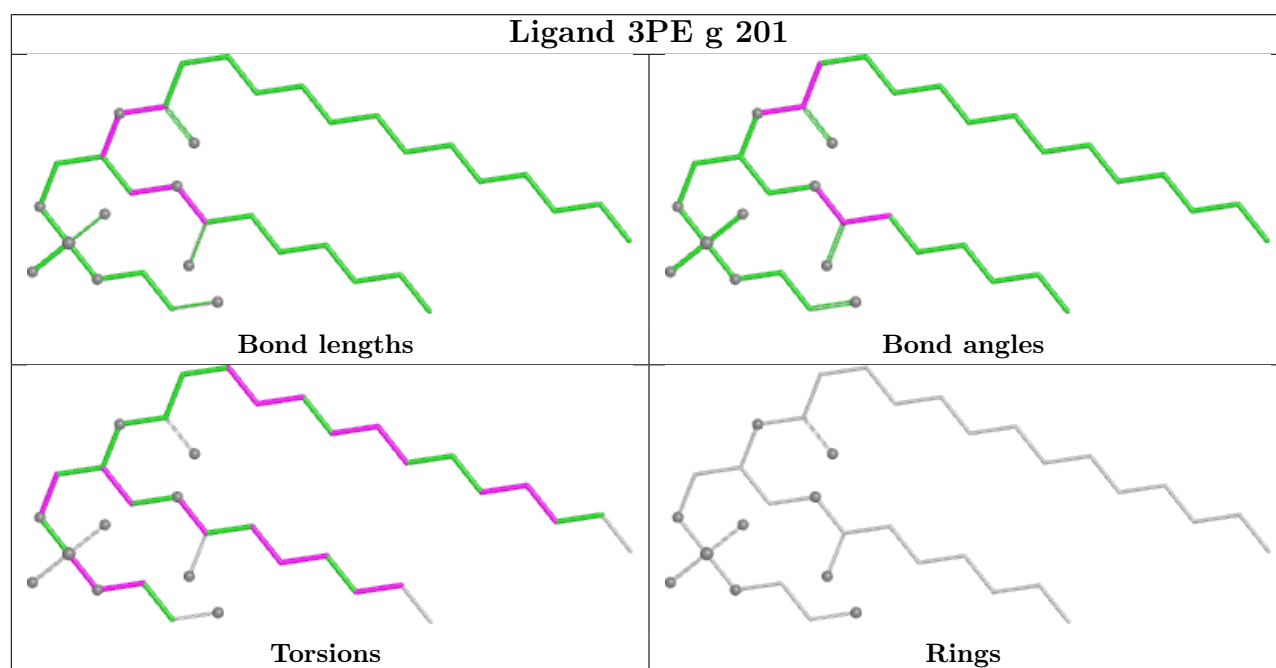
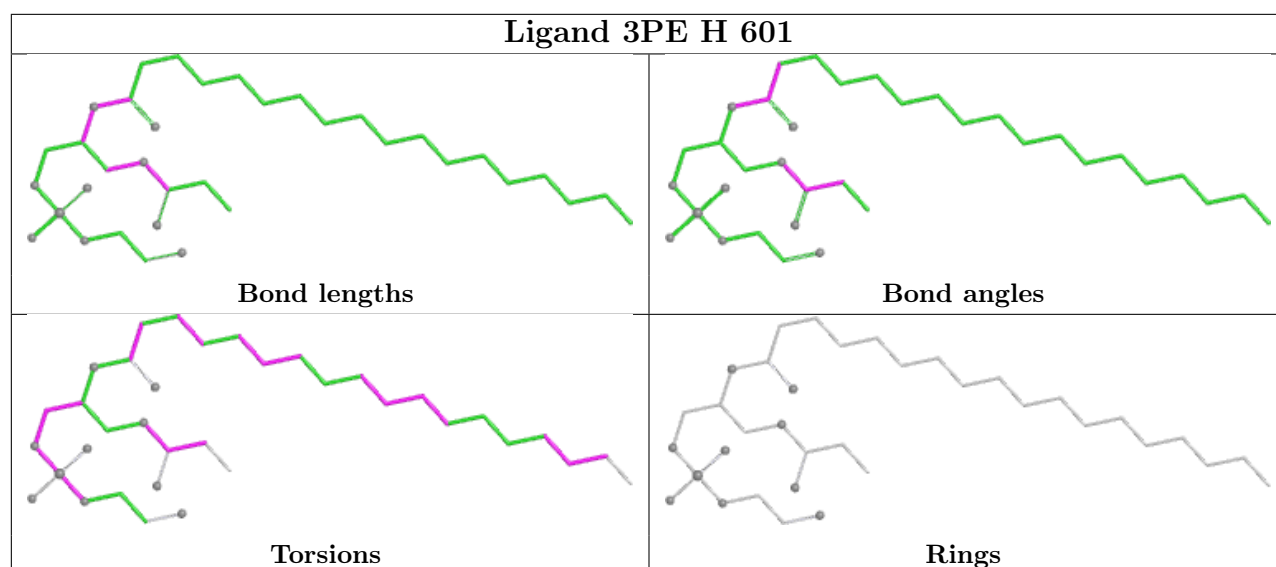
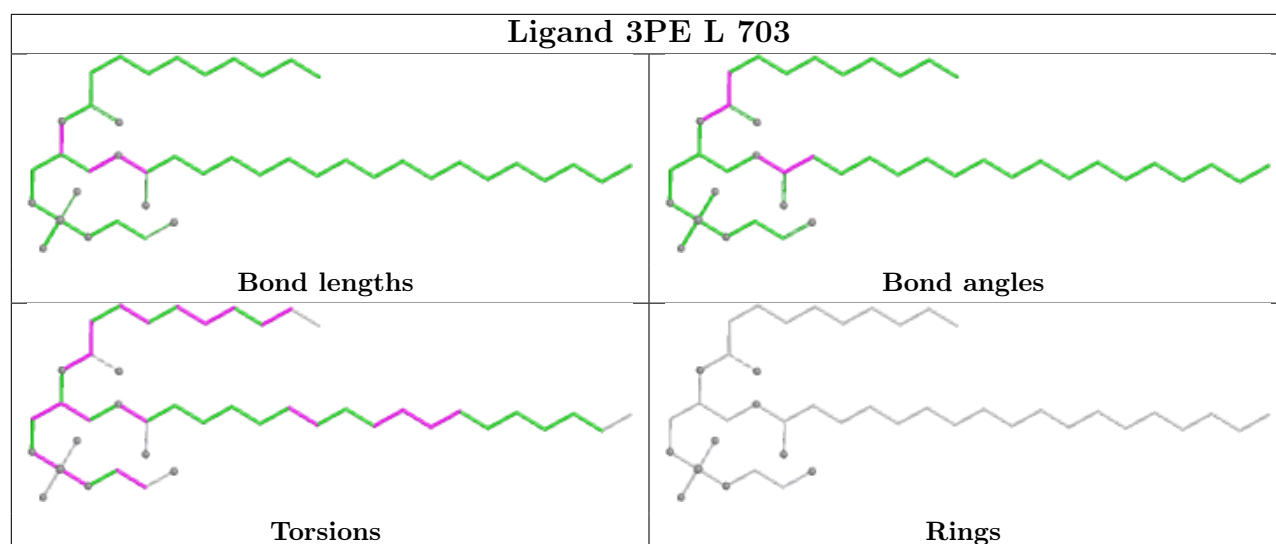
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	F	501	FMN	1	0
53	O	401	GTP	4	0
46	L	703	3PE	1	0
46	L	704	3PE	3	0
45	B	202	PC1	1	0
46	I	201	3PE	2	0
46	d	202	3PE	1	0
47	F	502	SF4	1	0
46	m	201	3PE	1	0
51	N	902	CDL	1	0
45	J	201	PC1	3	0
51	h	201	CDL	5	0
52	L	705	CHD	2	0
46	M	601	3PE	3	0
46	N	901	3PE	2	0
45	d	203	PC1	1	0
51	L	702	CDL	2	0
46	b	102	3PE	4	0
57	T	101	EHZ	1	0
46	M	602	3PE	1	0
46	M	604	3PE	2	0
46	K	101	3PE	1	0
51	d	204	CDL	2	0
45	M	605	PC1	4	0
46	Y	205	3PE	1	0
46	h	202	3PE	1	0
51	X	201	CDL	2	0

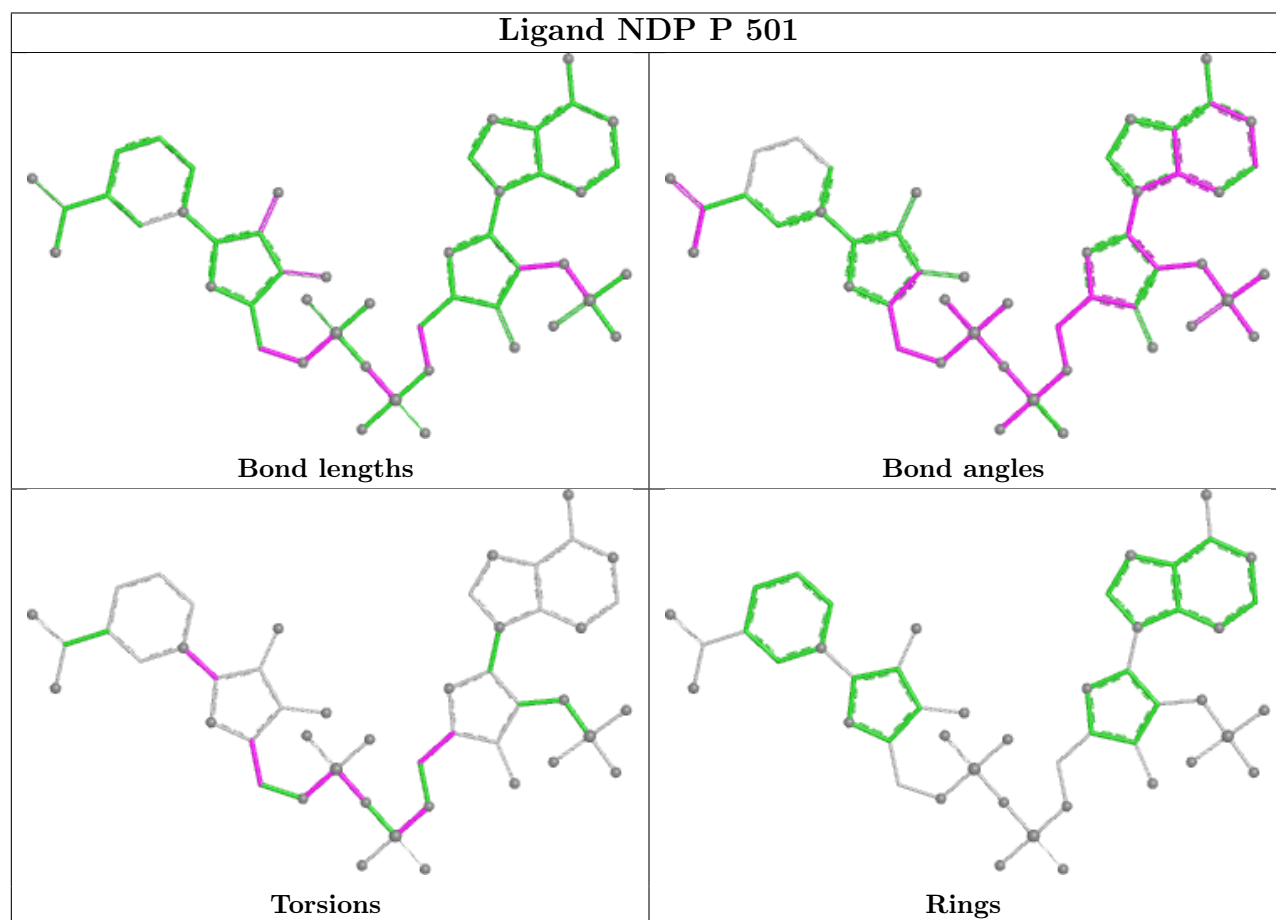
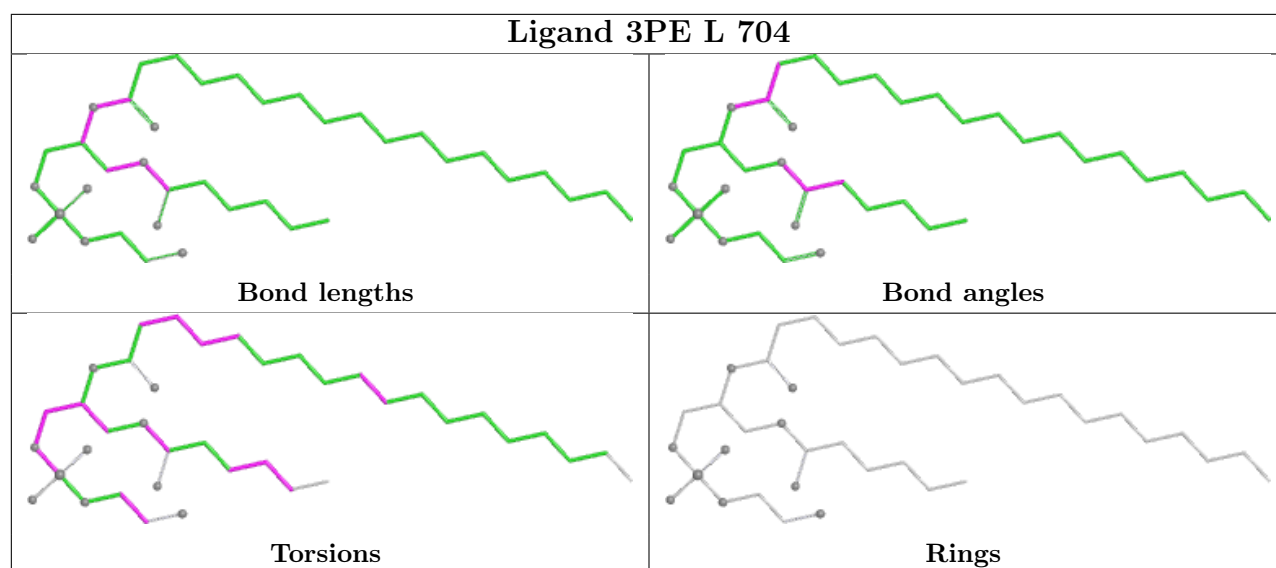
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

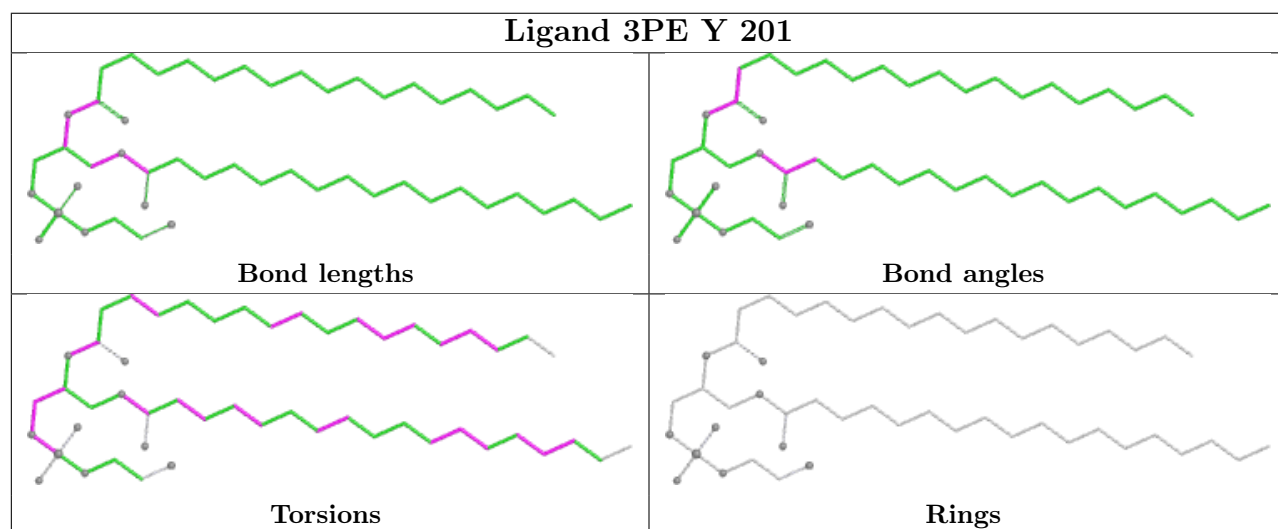
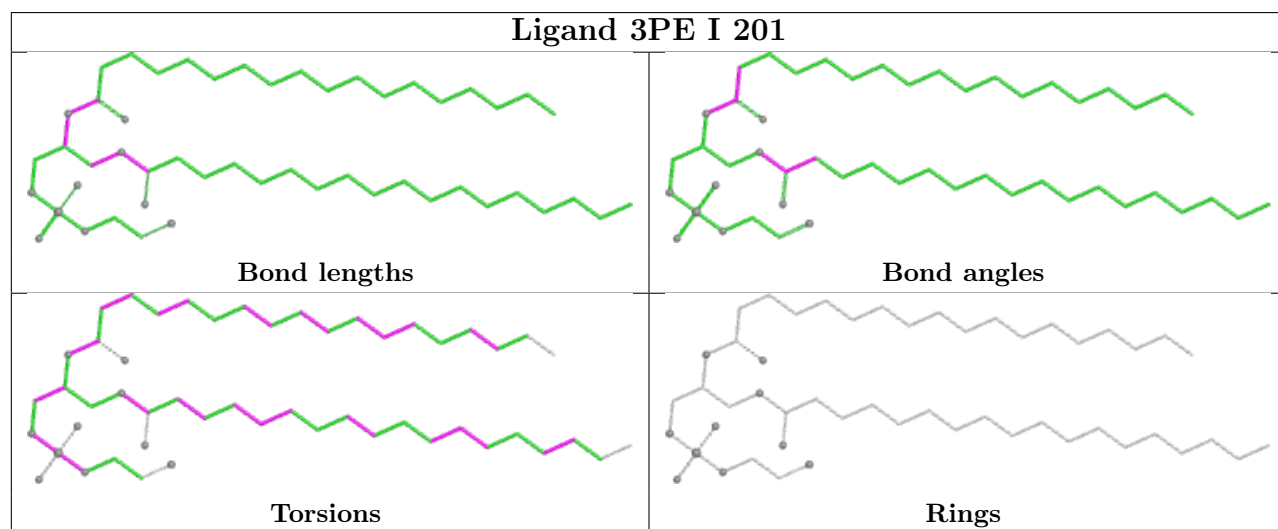
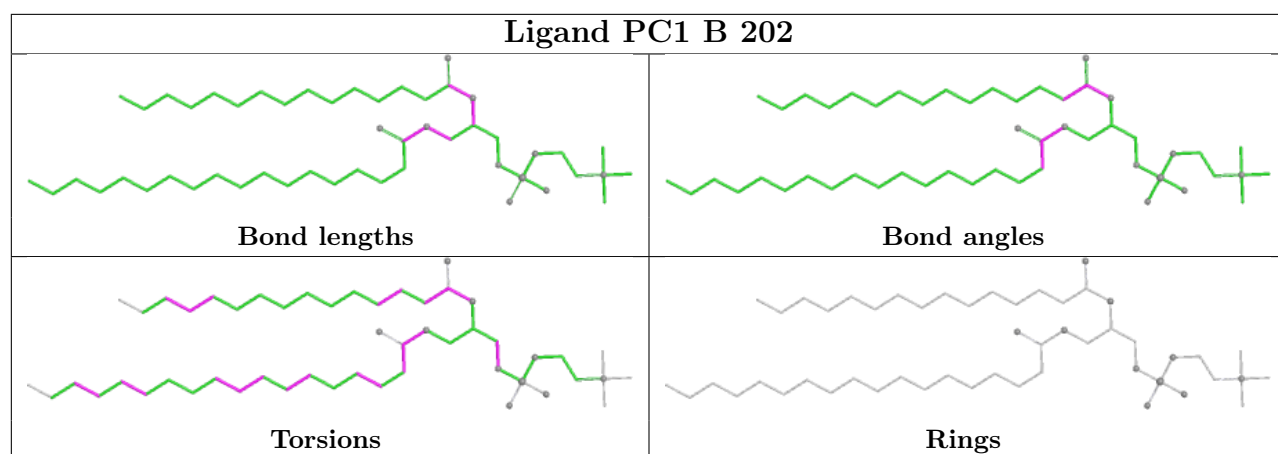
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

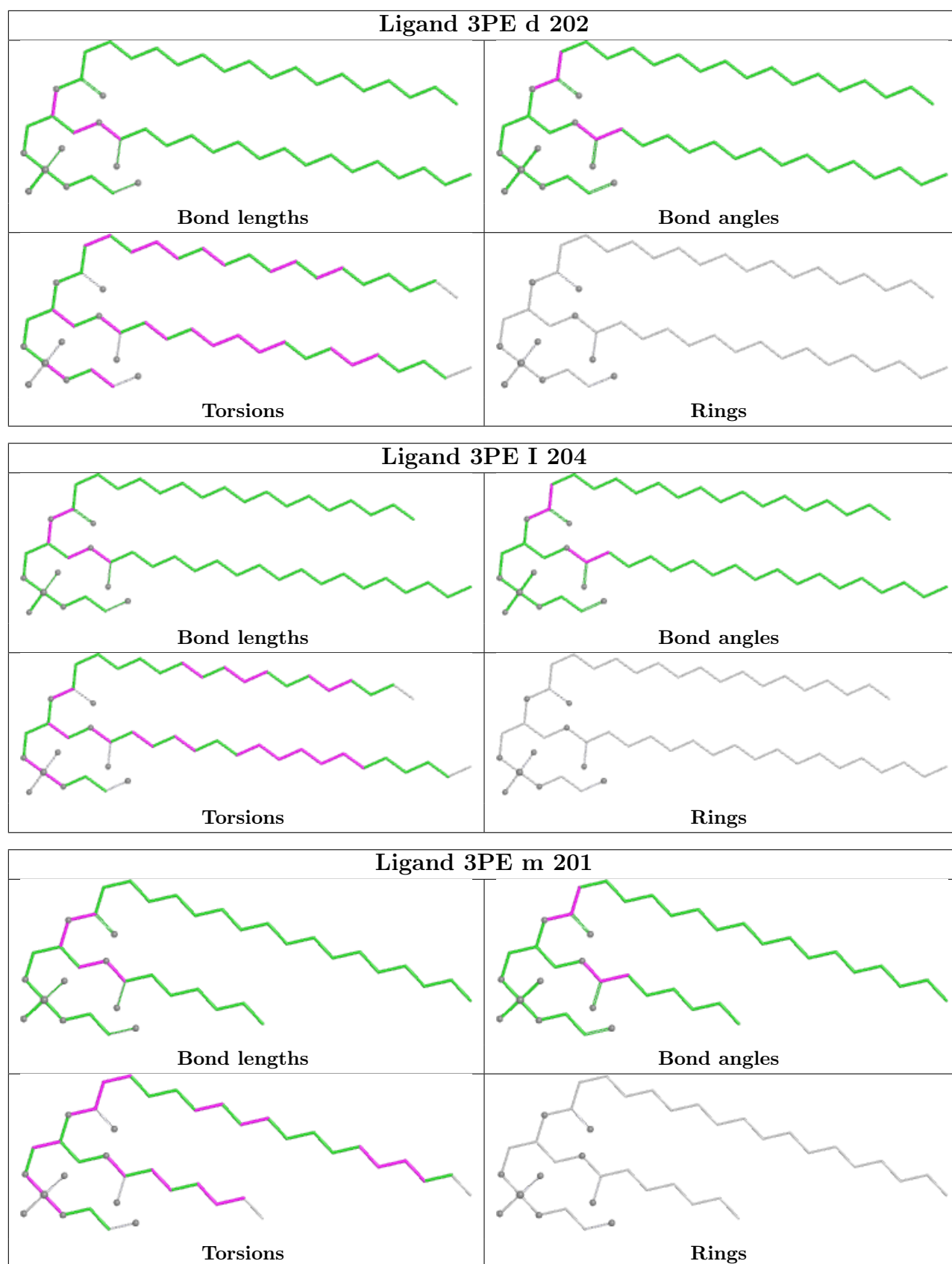




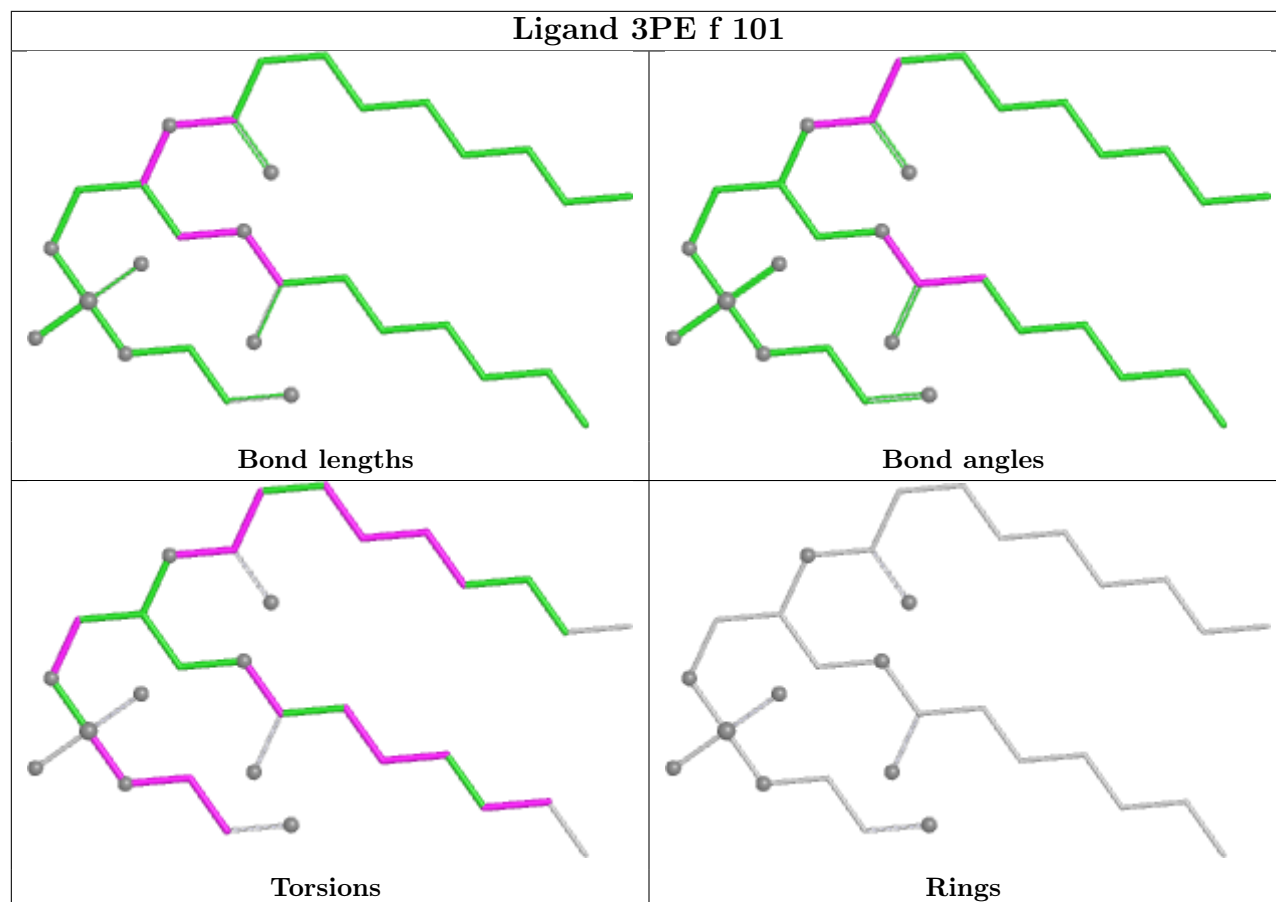




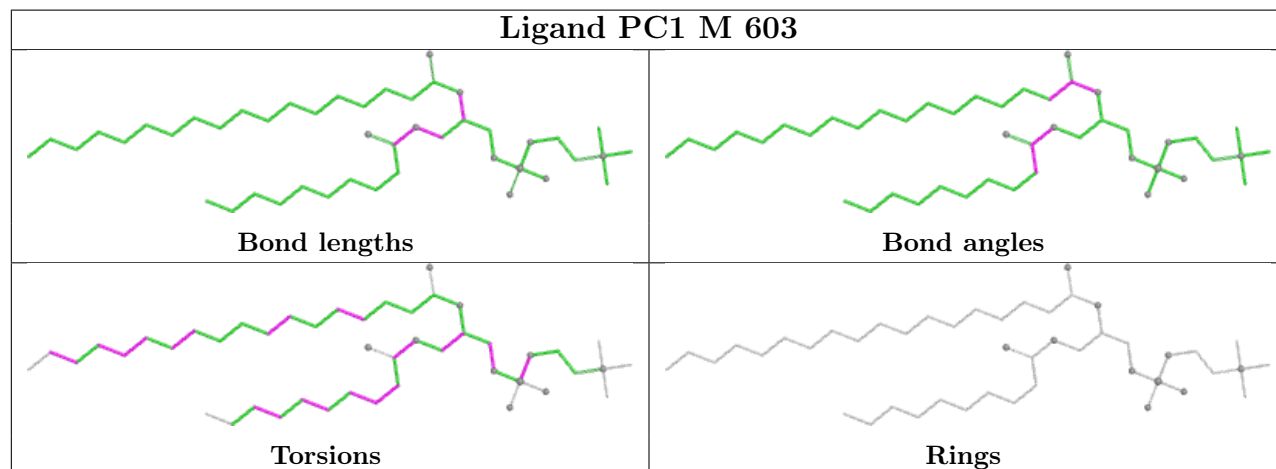


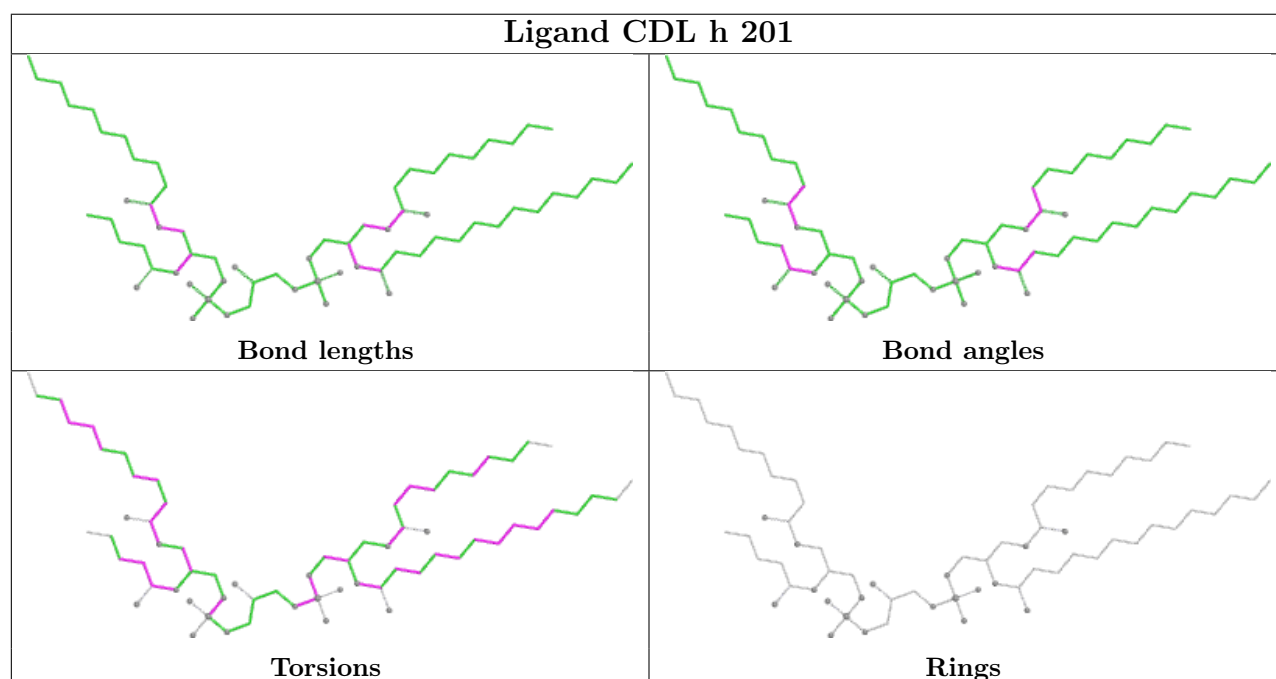
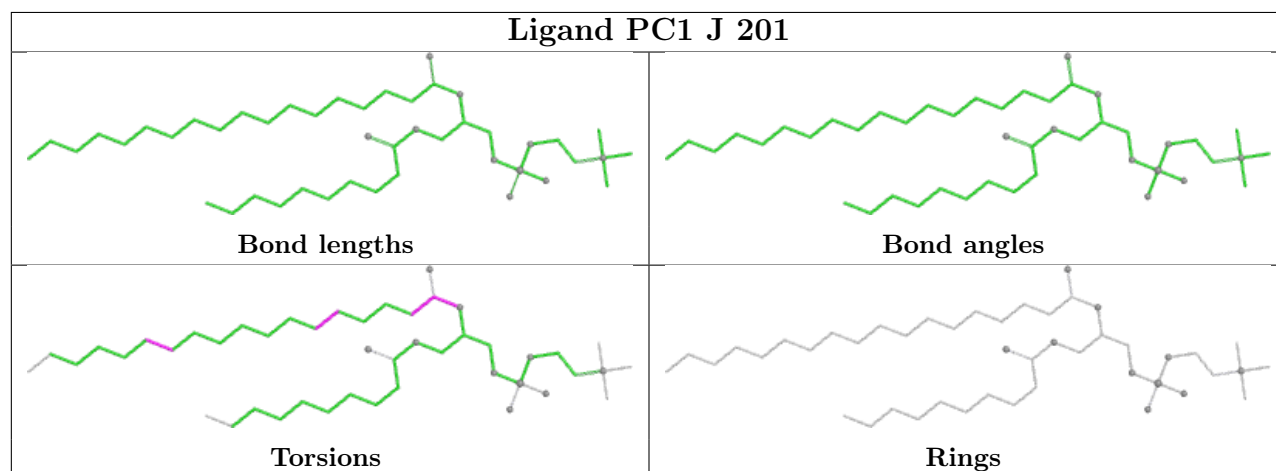
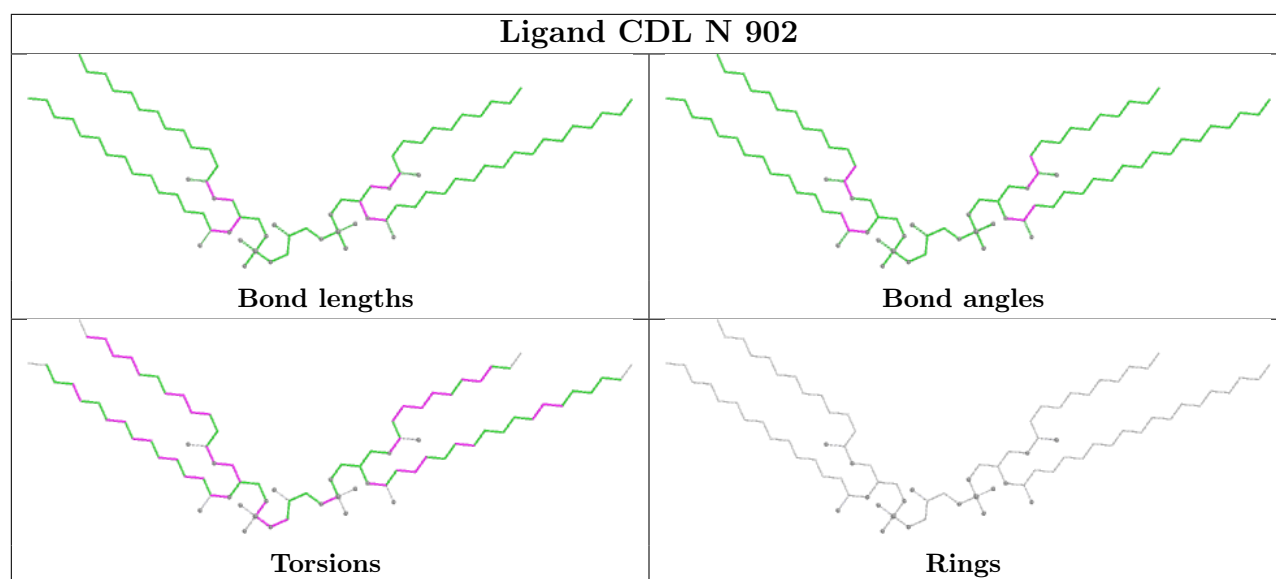


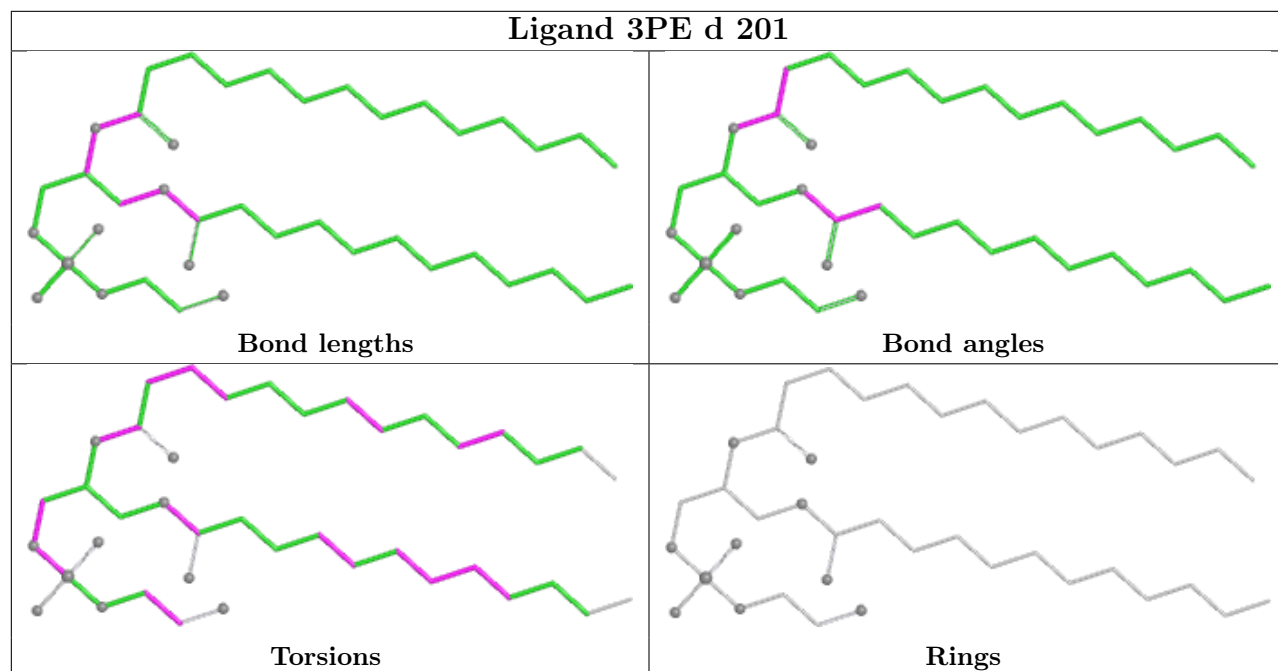
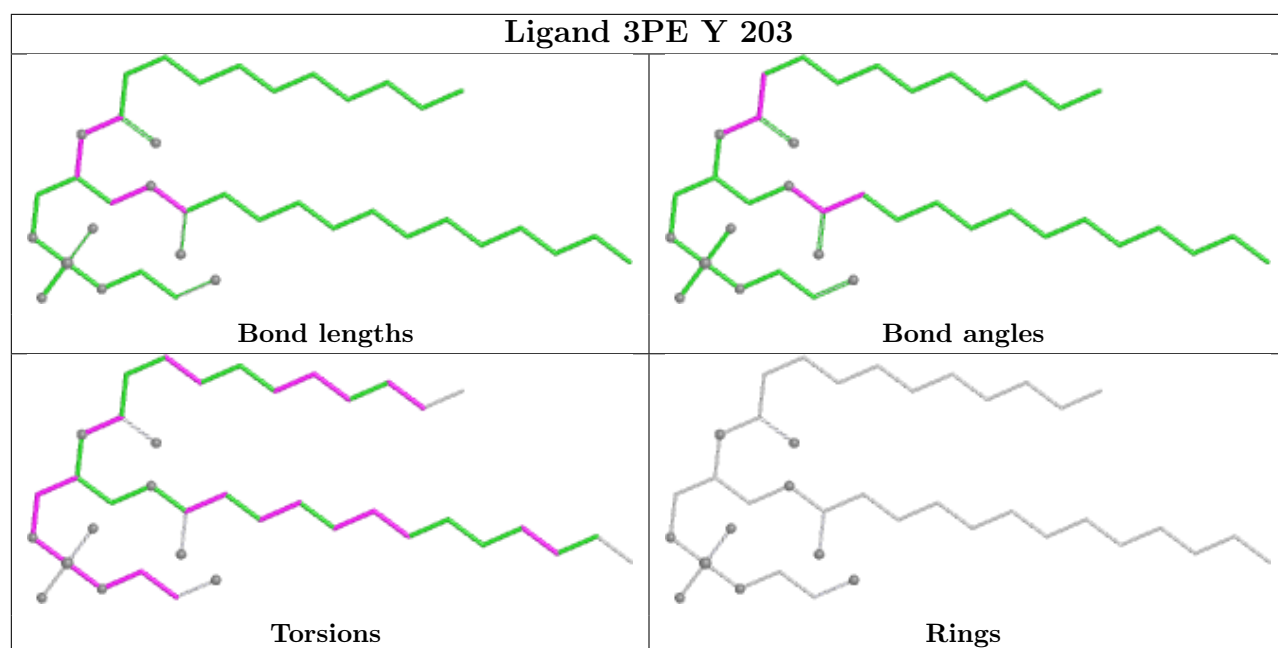
Ligand 3PE f 101

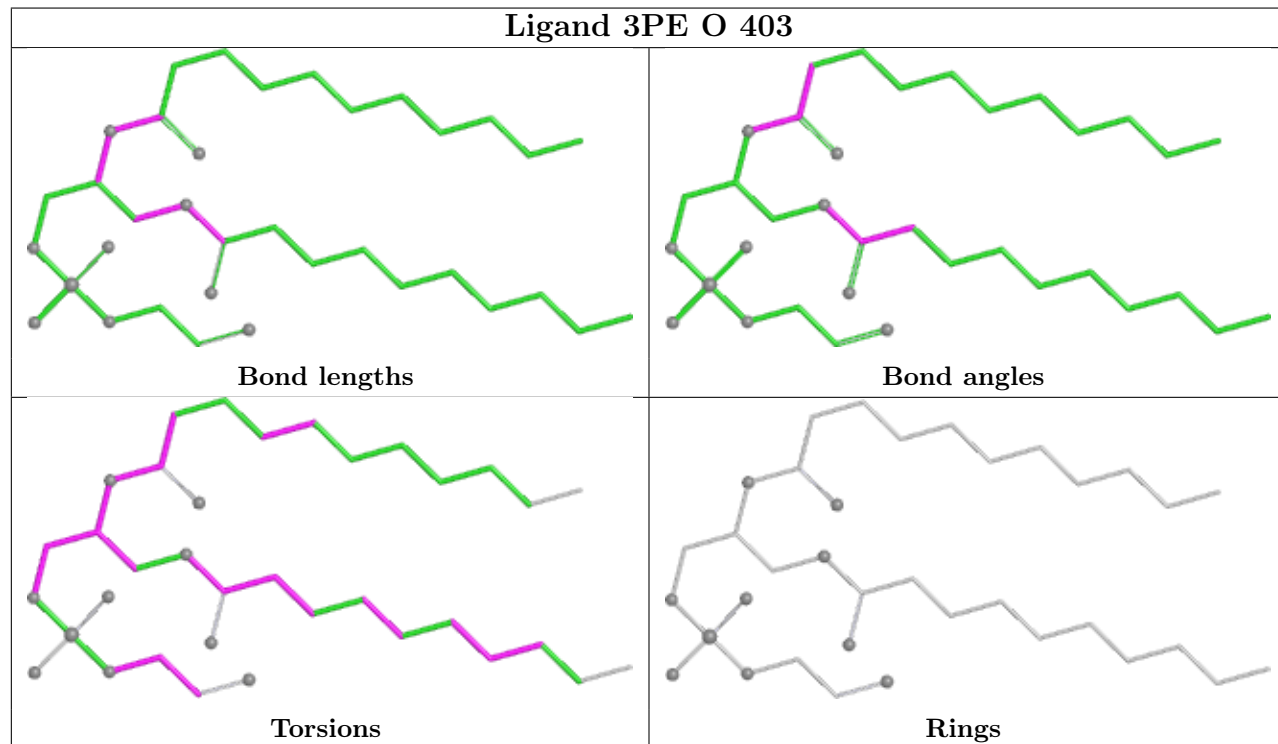
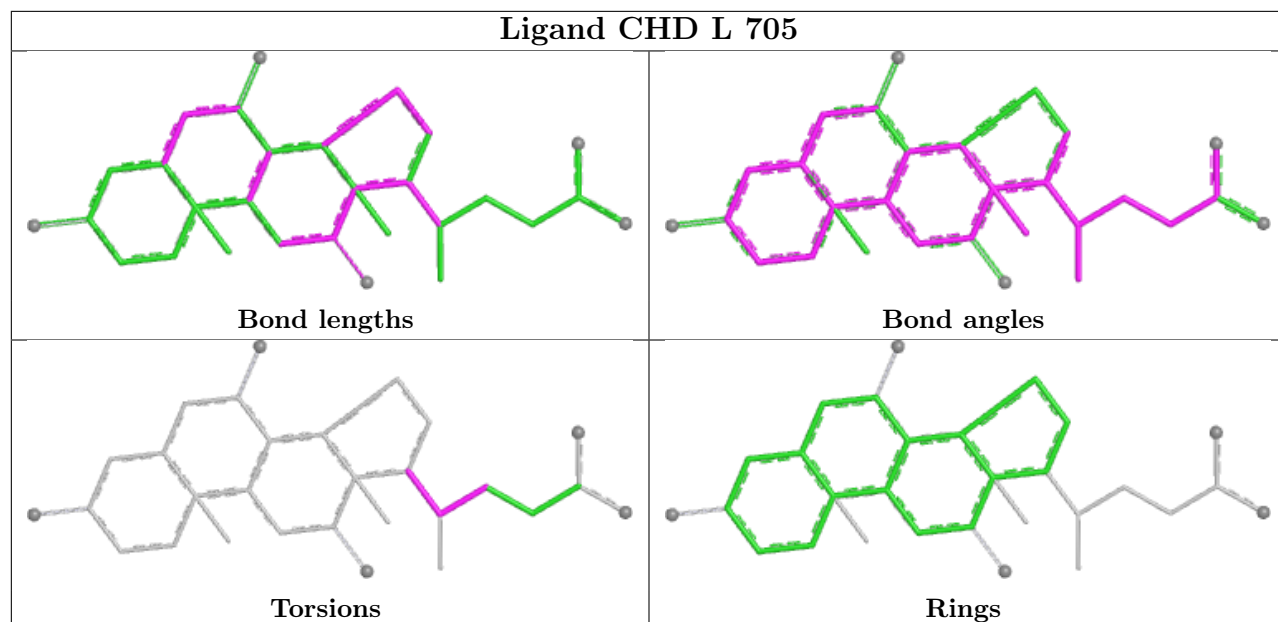


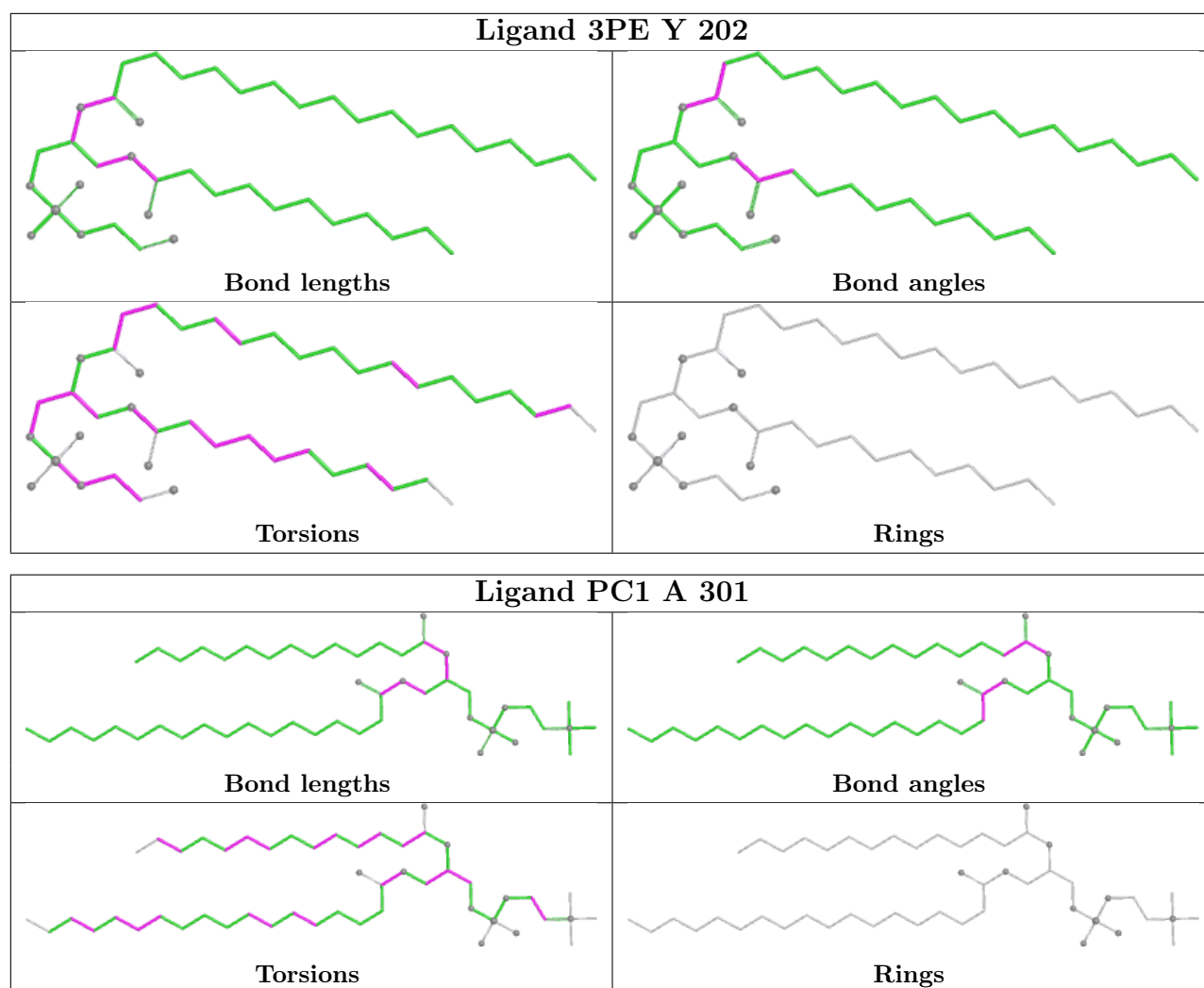
Ligand PC1 M 603

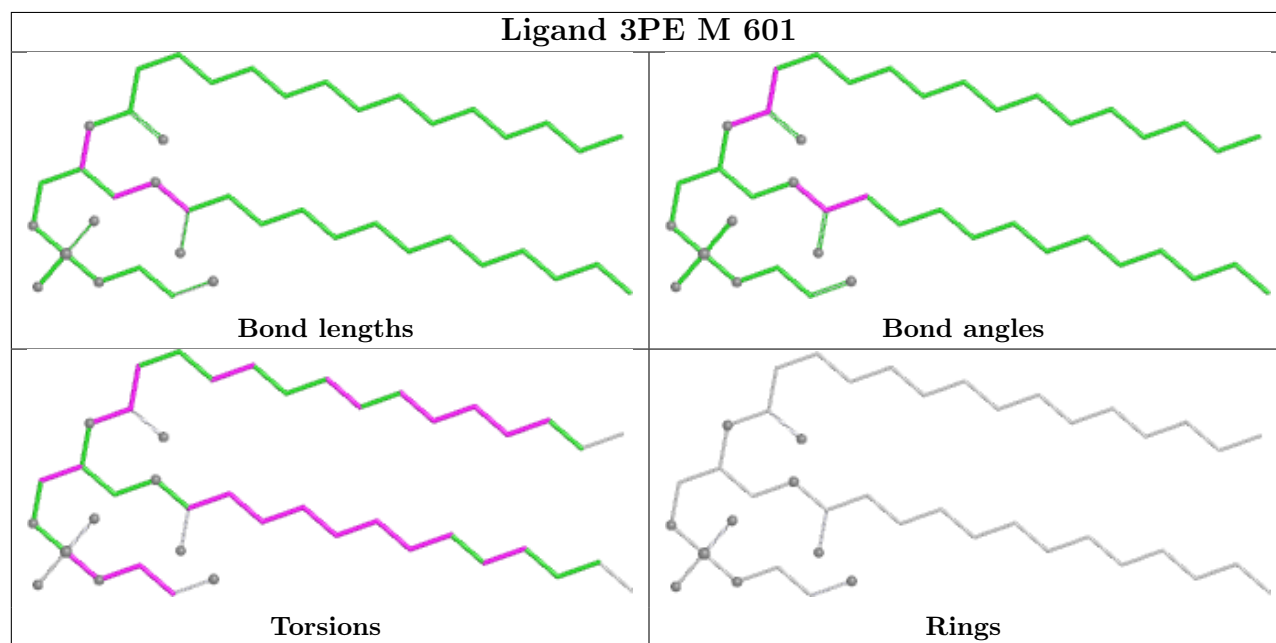
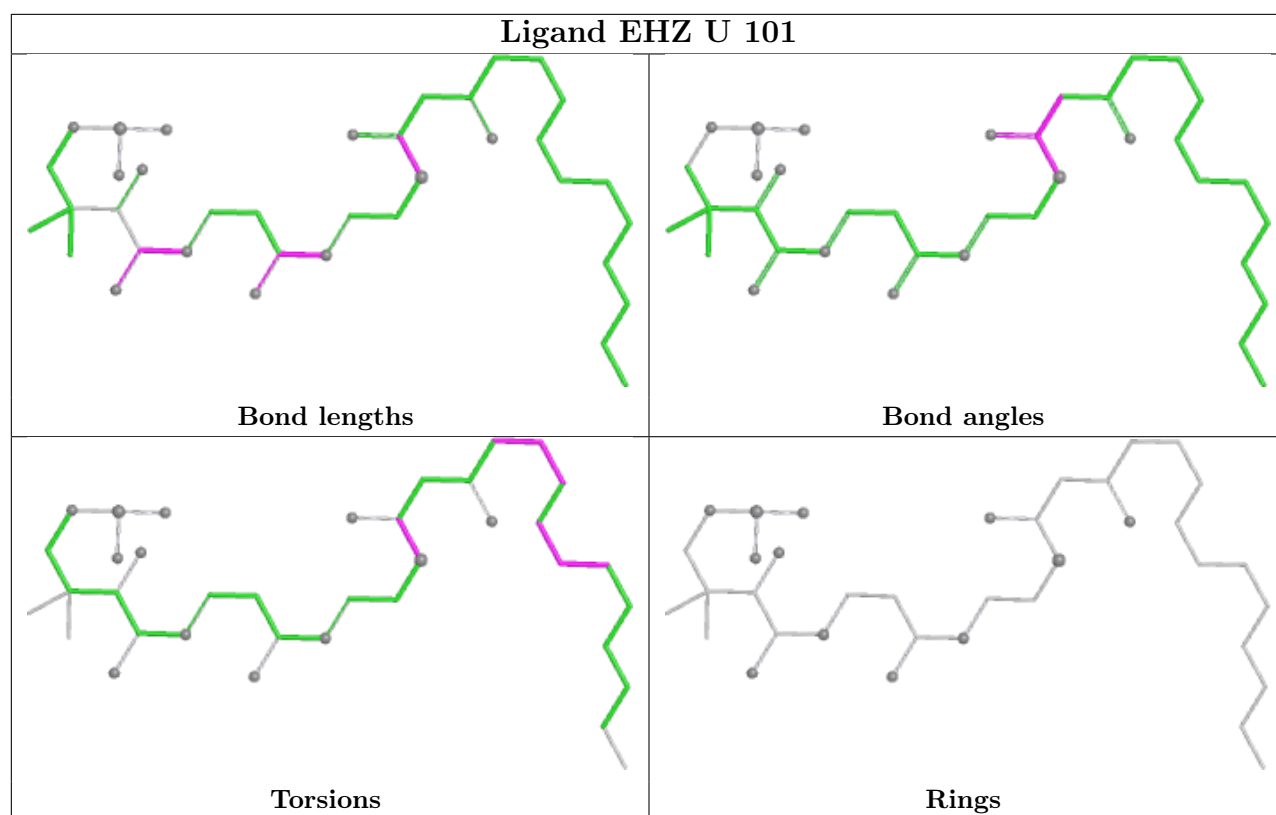


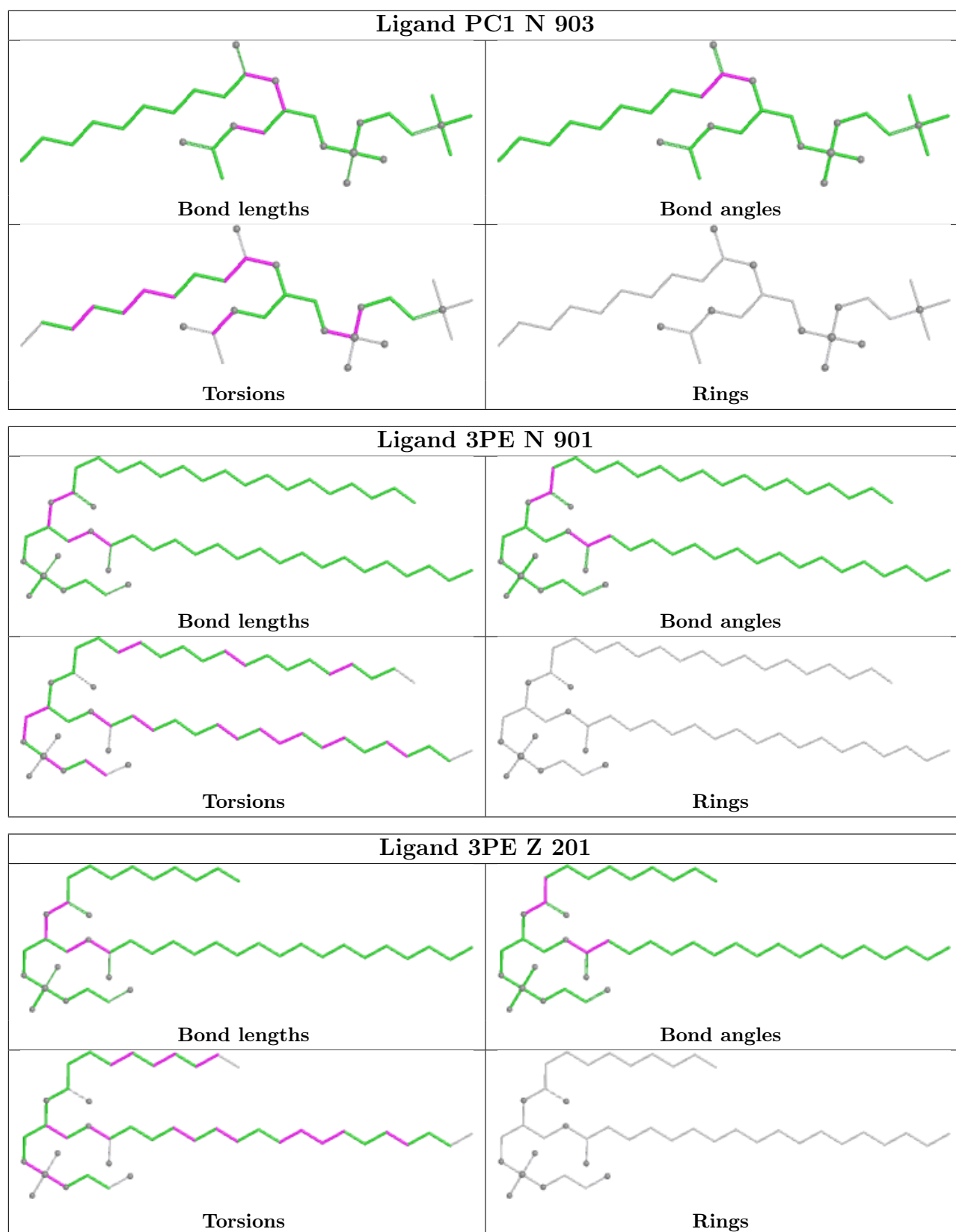


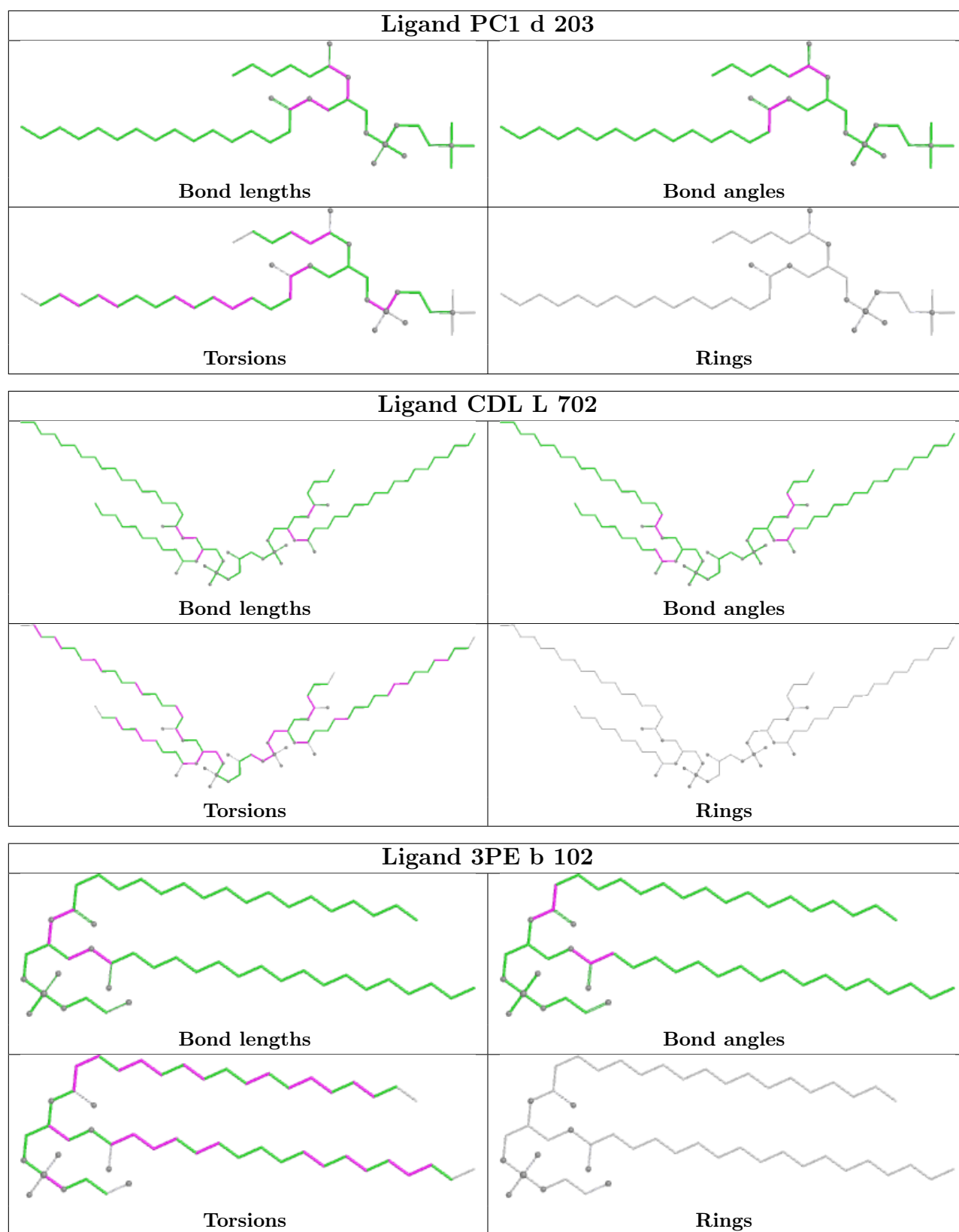


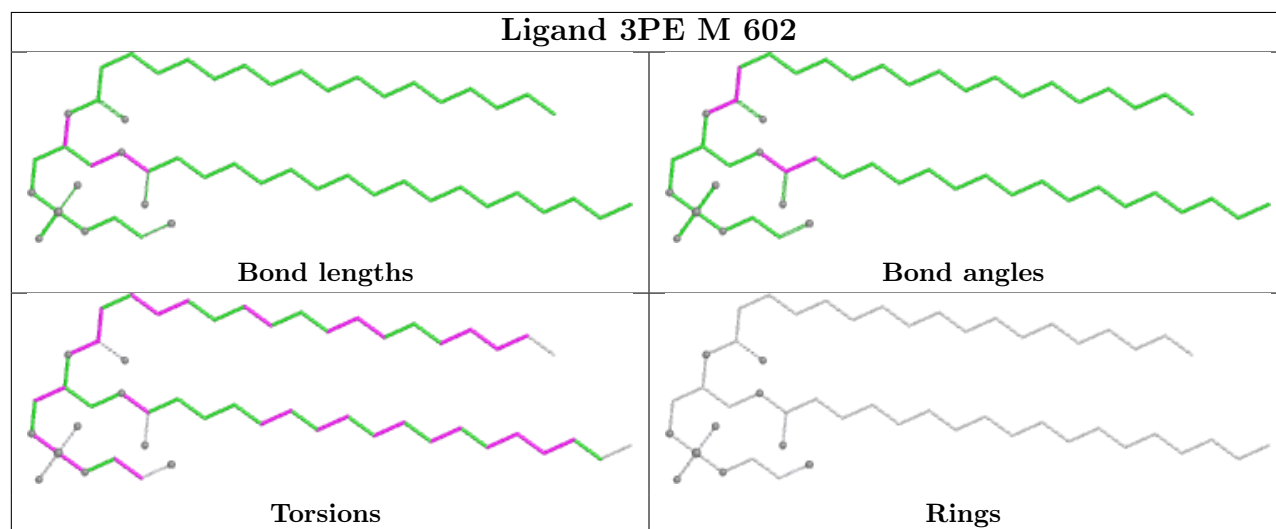
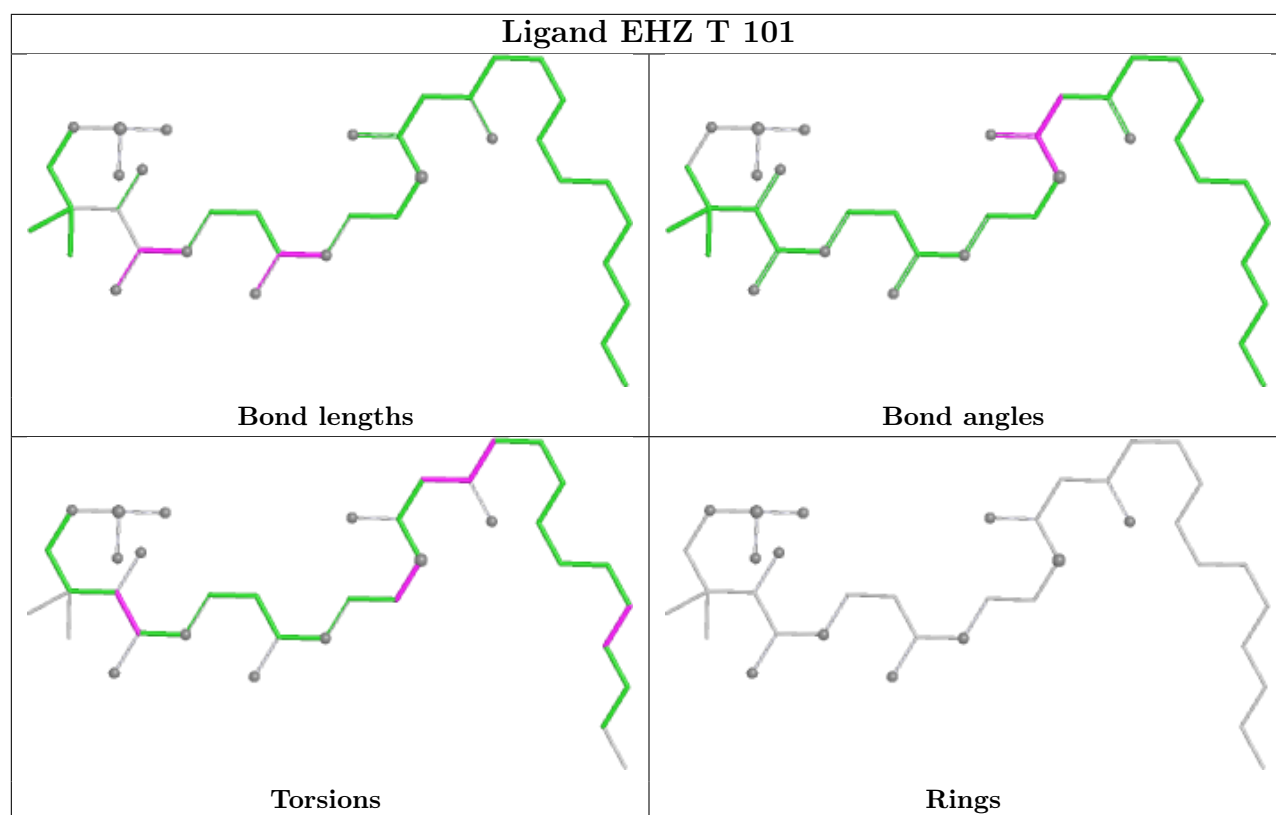


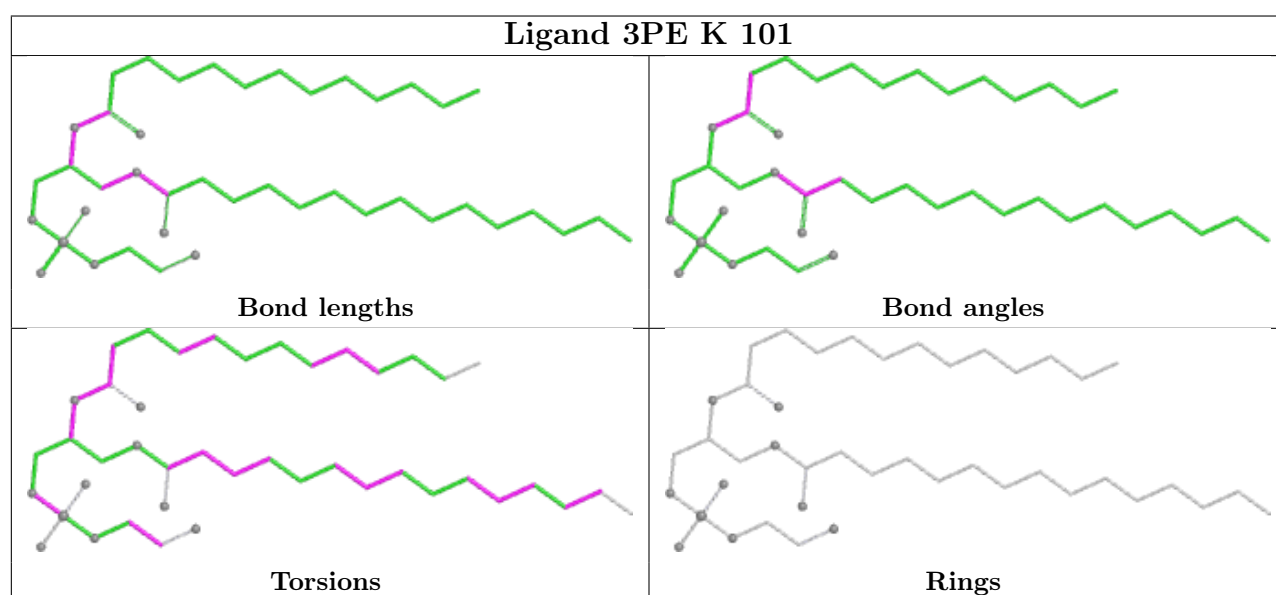
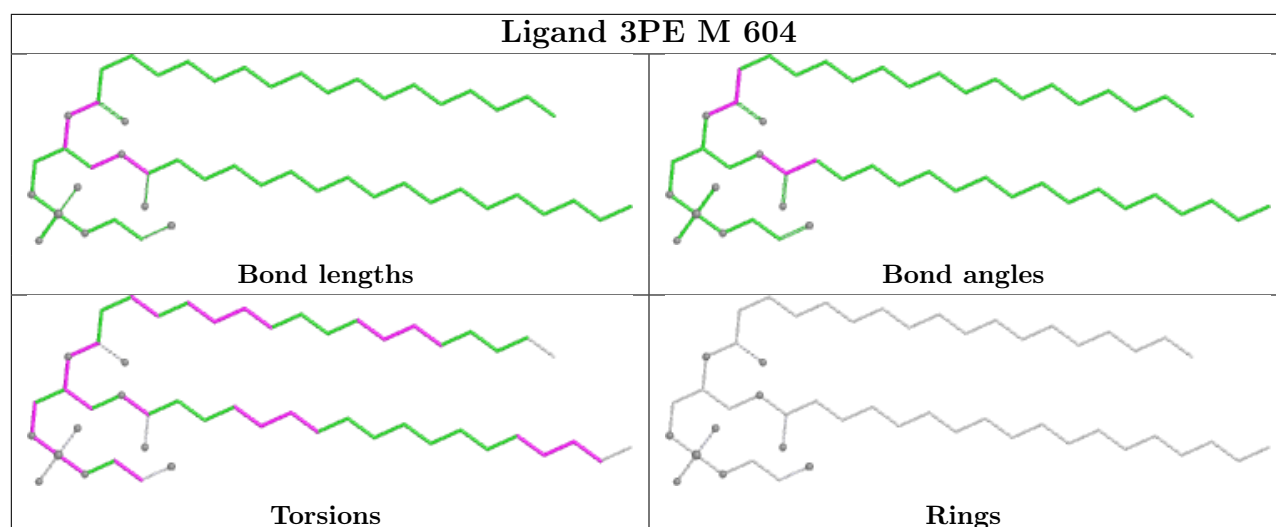


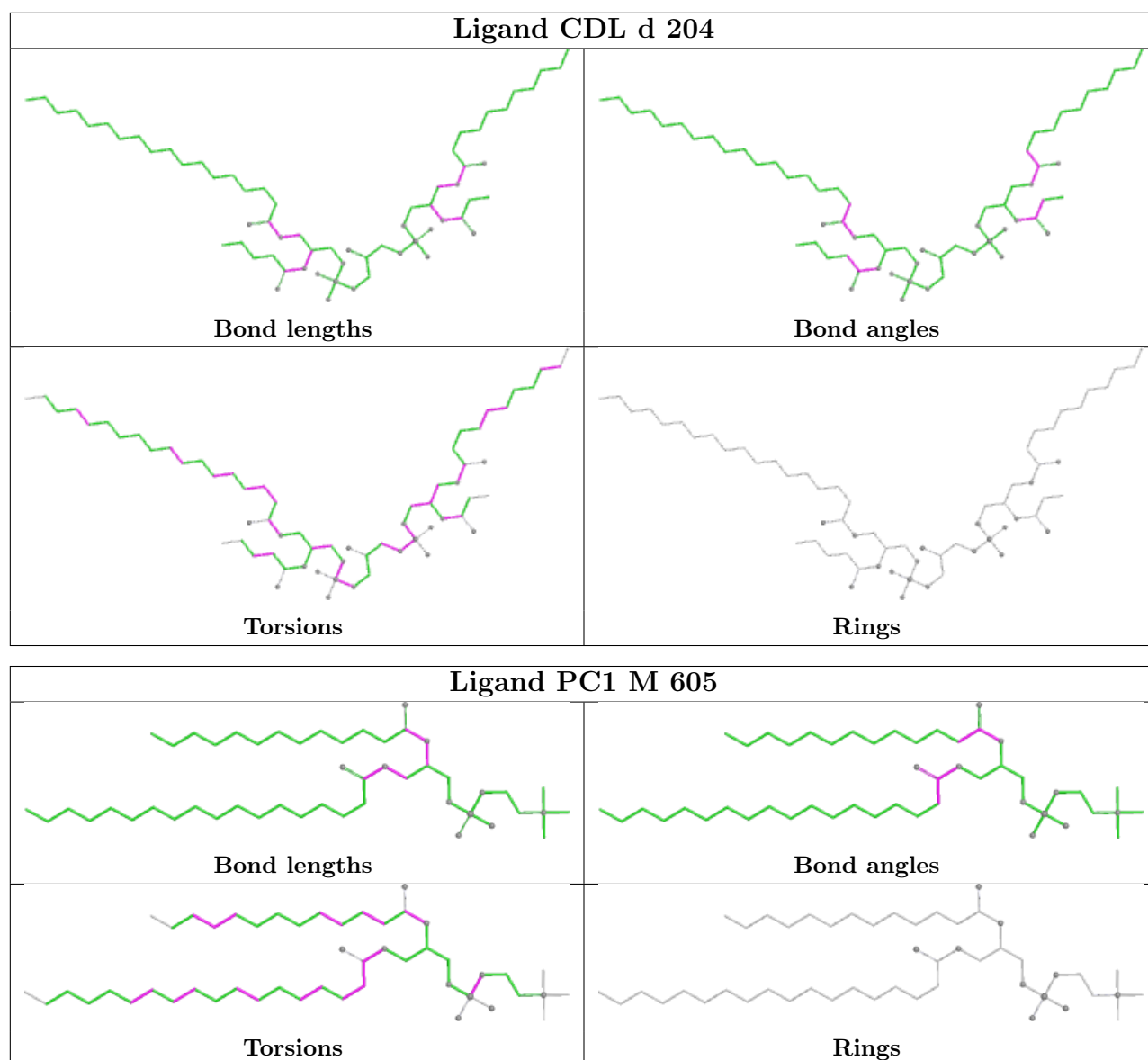


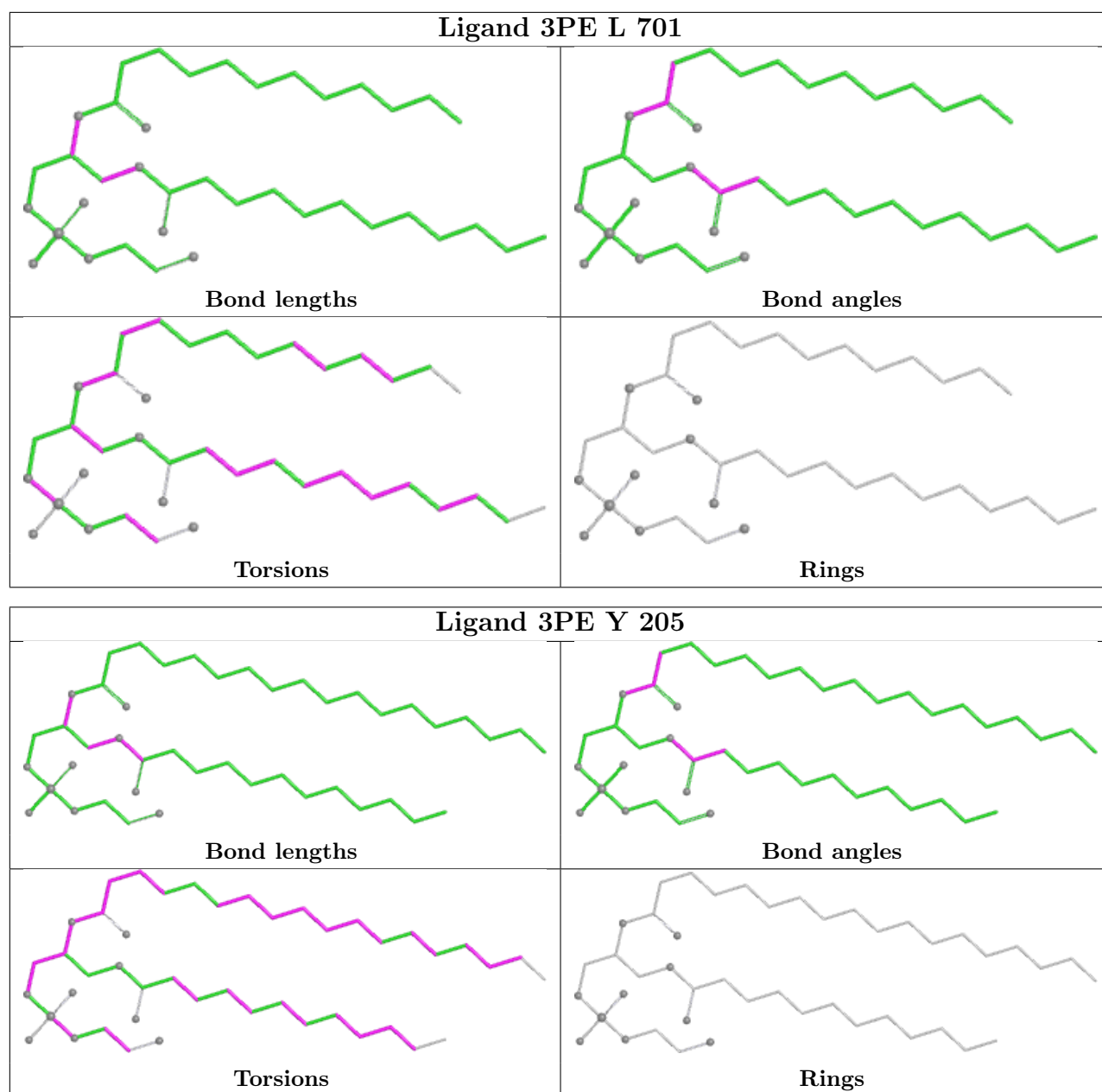


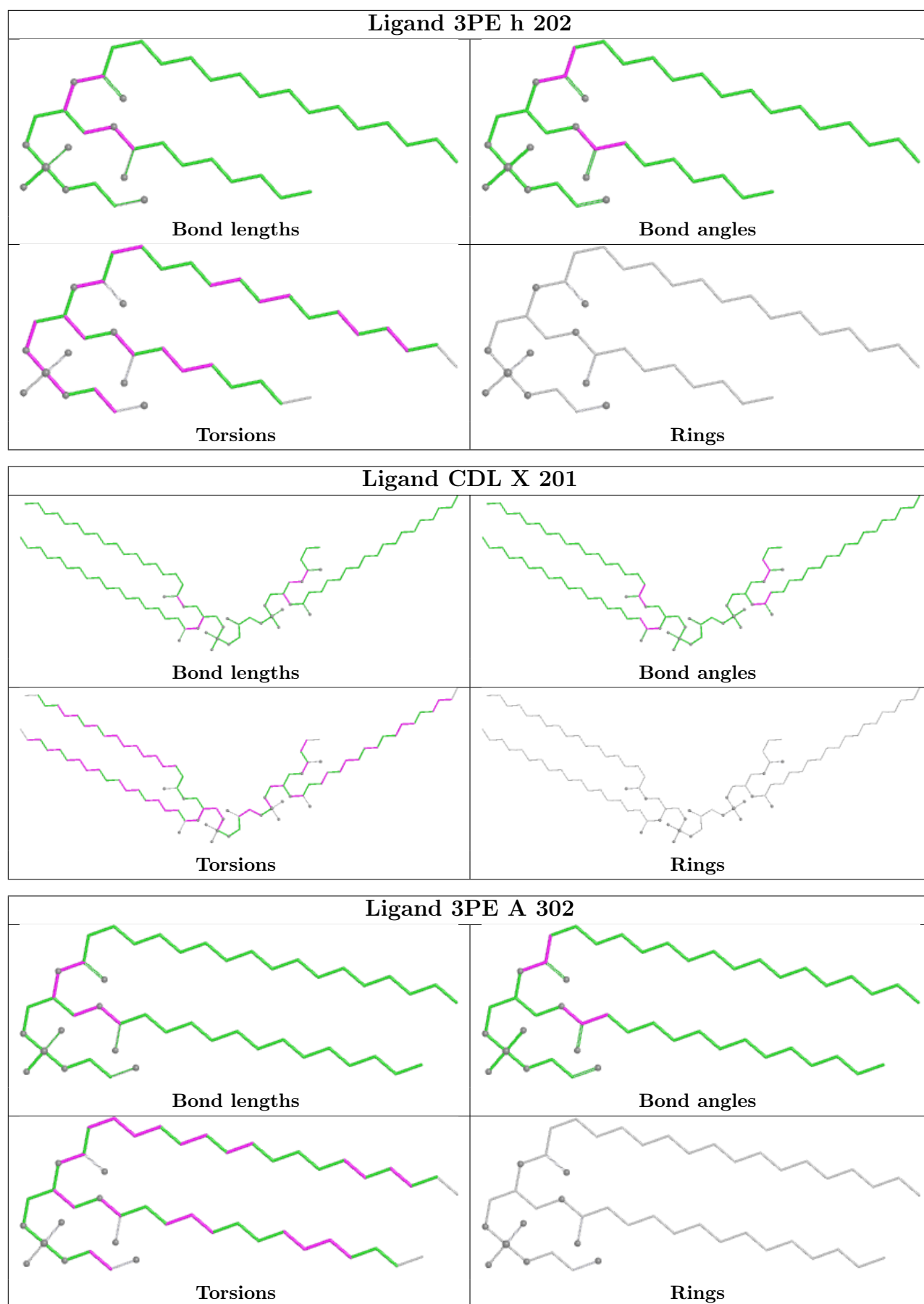


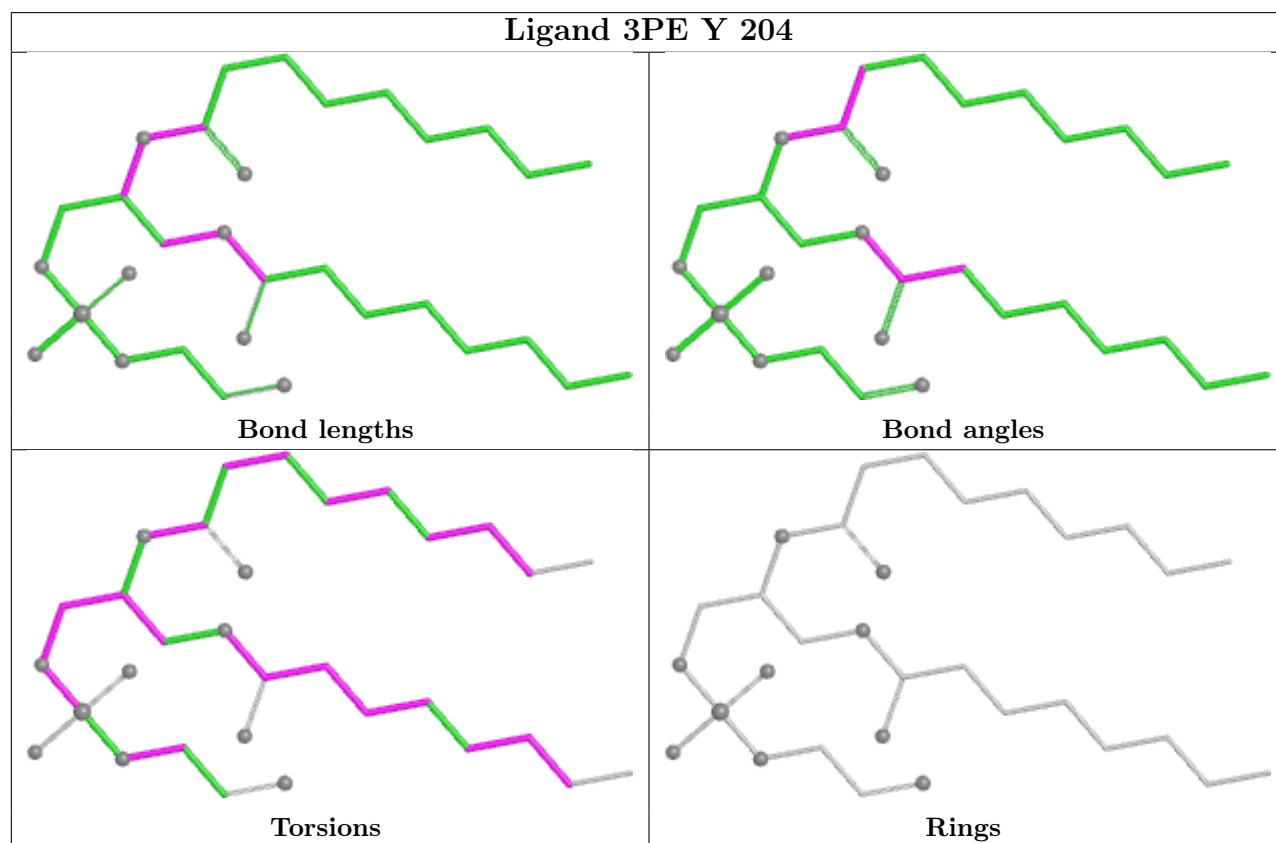
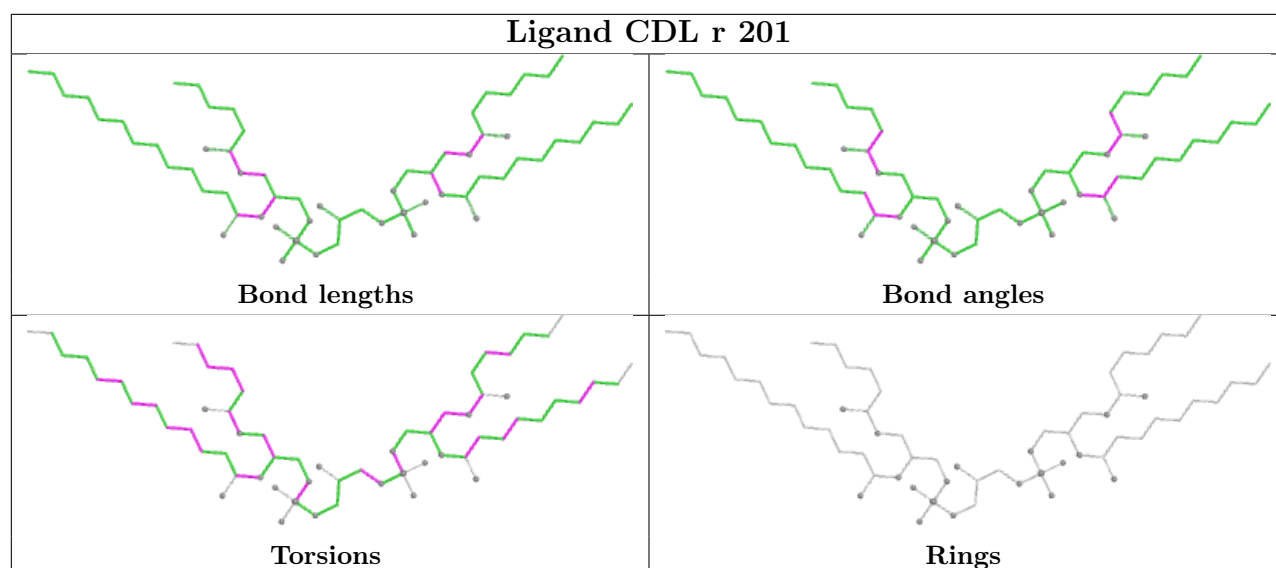


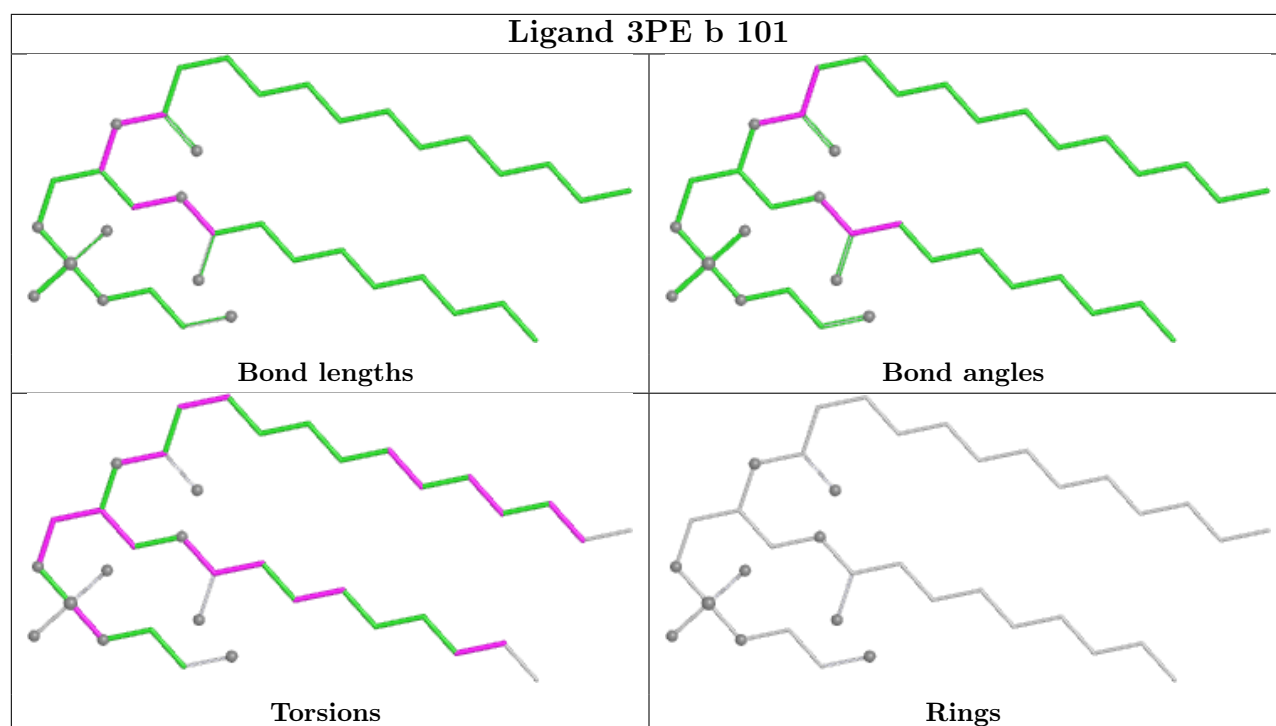












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

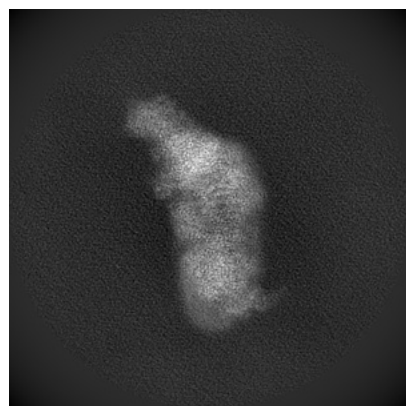
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14139. These allow visual inspection of the internal detail of the map and identification of artifacts.

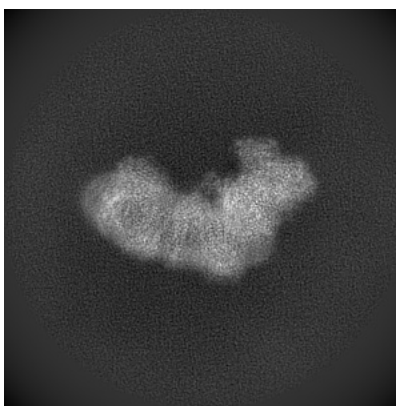
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

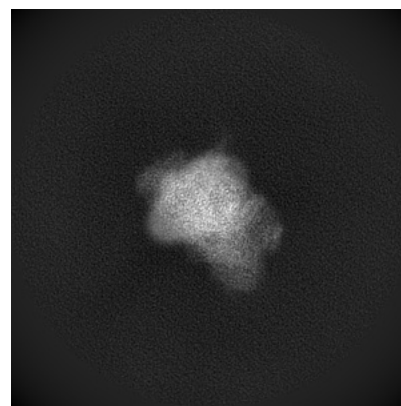
6.1.1 Primary map



X

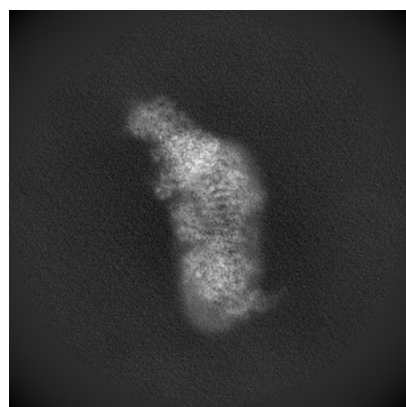


Y

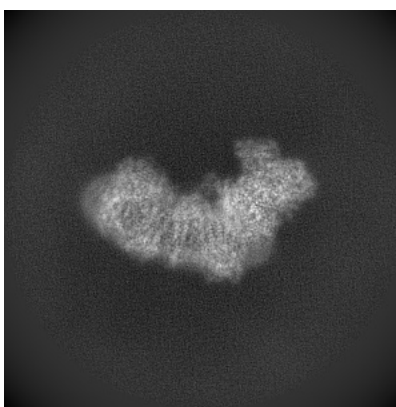


Z

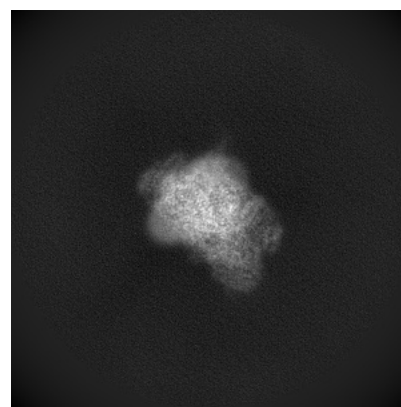
6.1.2 Raw map



X



Y

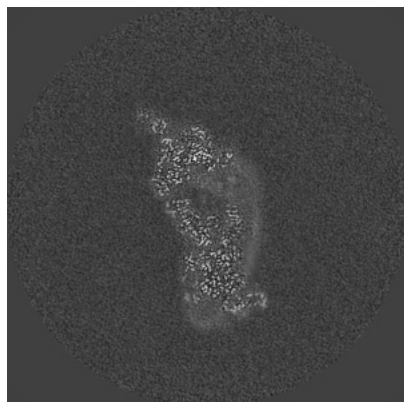


Z

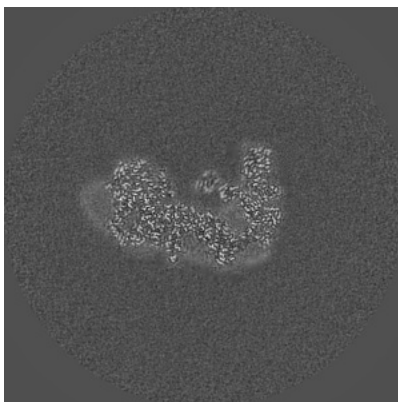
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

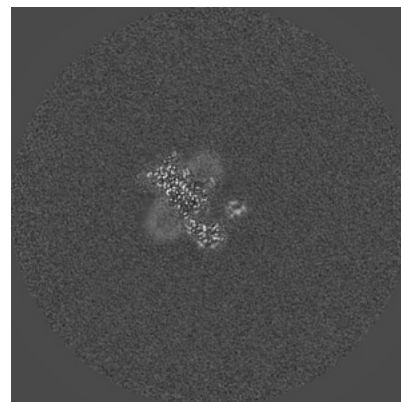
6.2.1 Primary map



X Index: 320

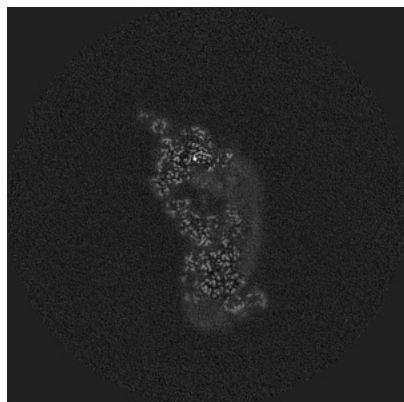


Y Index: 320

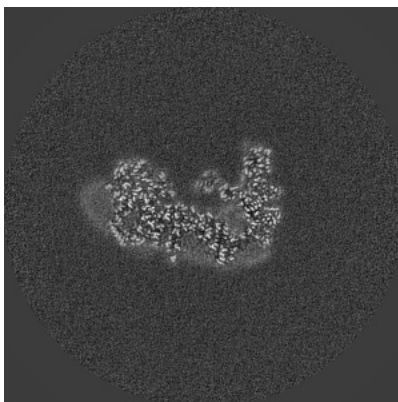


Z Index: 320

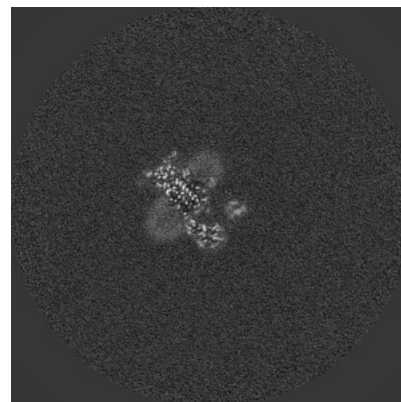
6.2.2 Raw map



X Index: 320



Y Index: 320

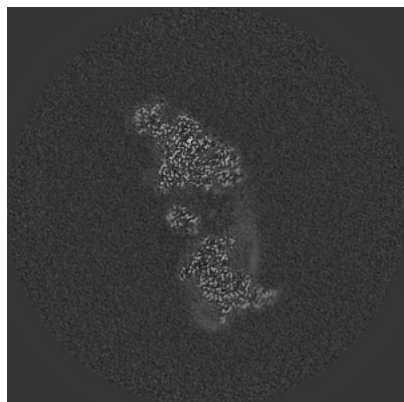


Z Index: 320

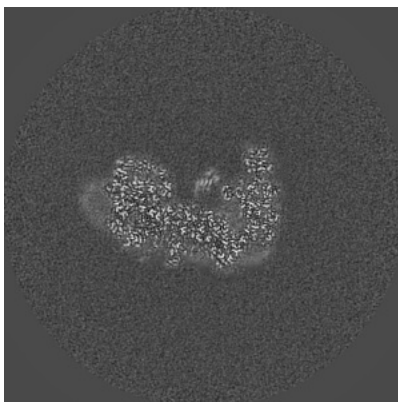
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

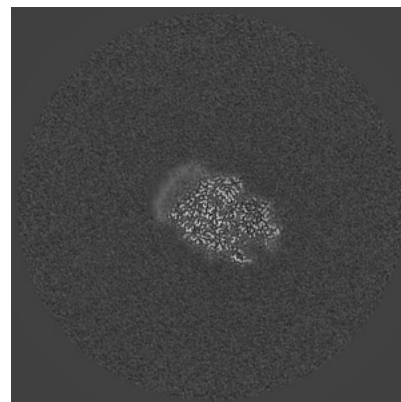
6.3.1 Primary map



X Index: 337

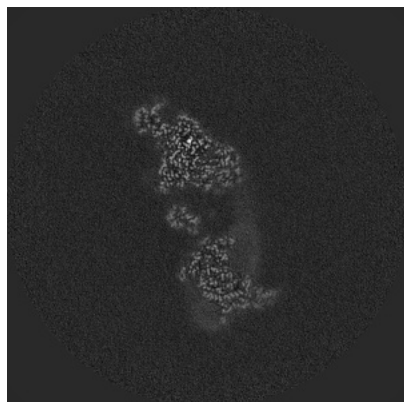


Y Index: 324

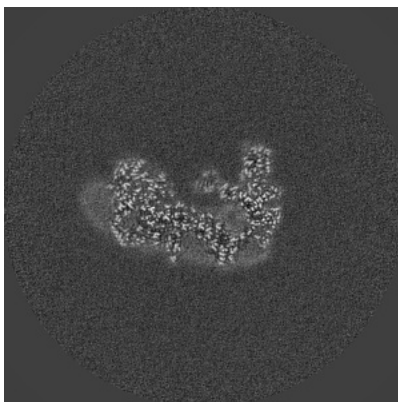


Z Index: 404

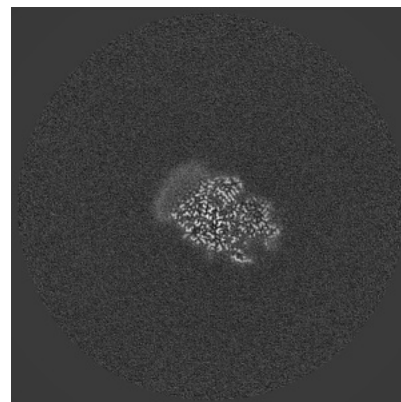
6.3.2 Raw map



X Index: 337



Y Index: 319

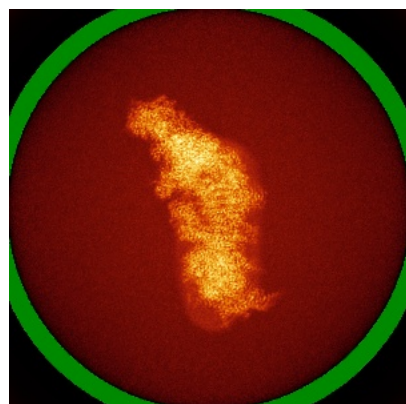


Z Index: 404

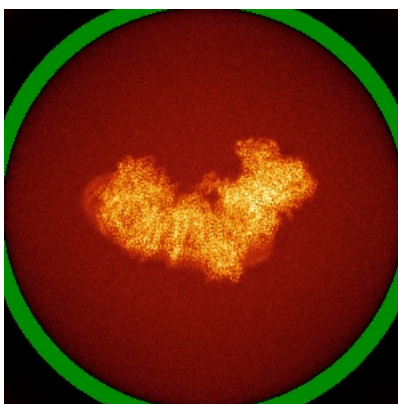
The images above show the largest variance slices of the map in three orthogonal directions.

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

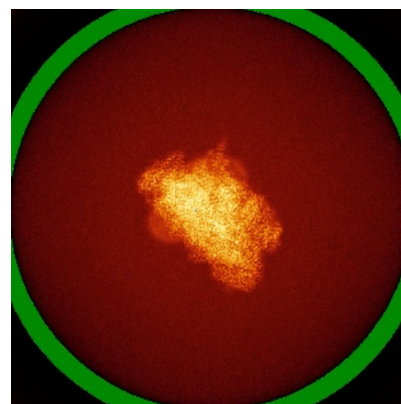
6.4.1 Primary map



X

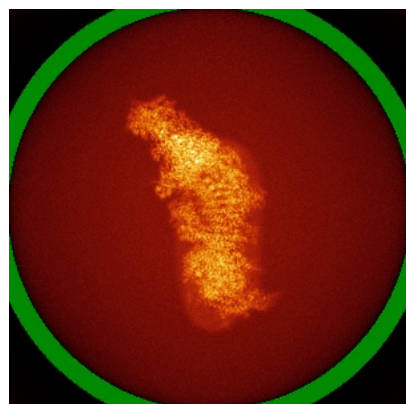


Y

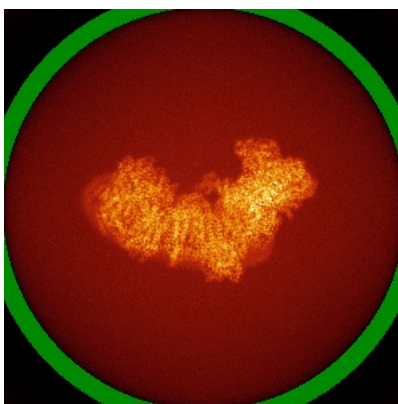


Z

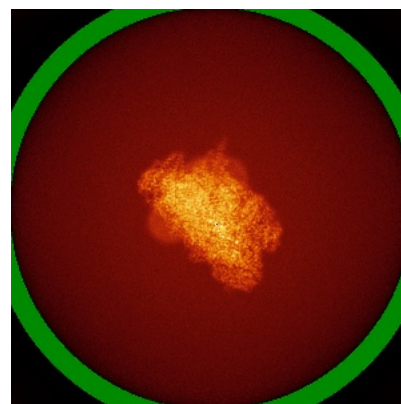
6.4.2 Raw map



X



Y

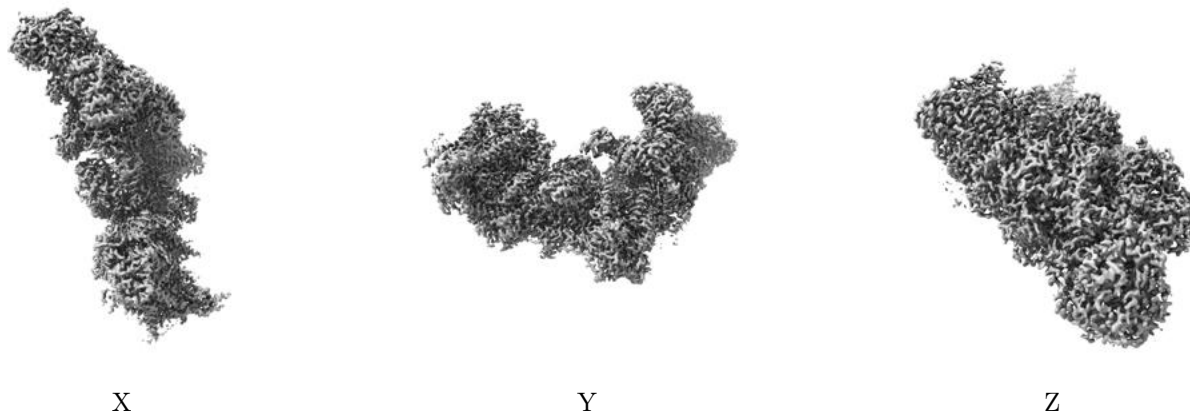


Z

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.

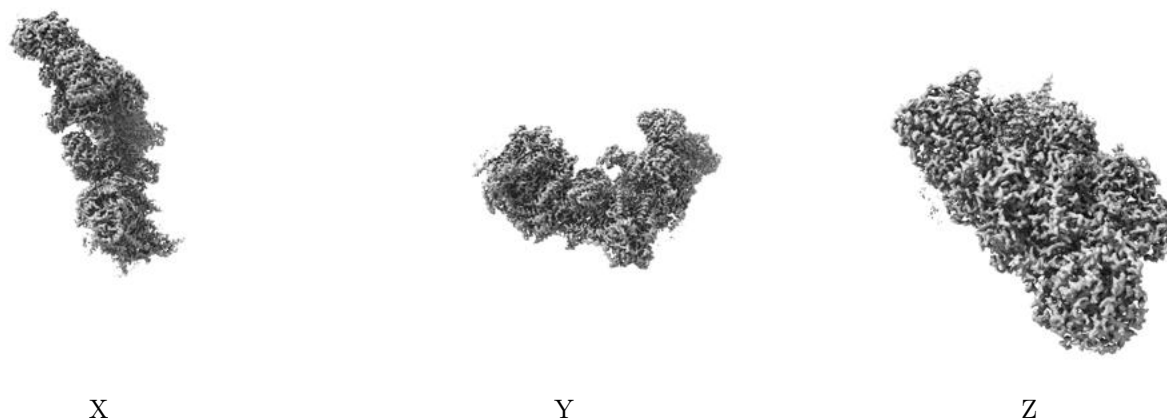
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.5. 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.

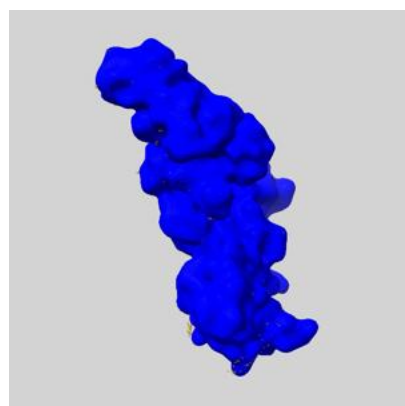
6.6 Mask visualisation [i](#)

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

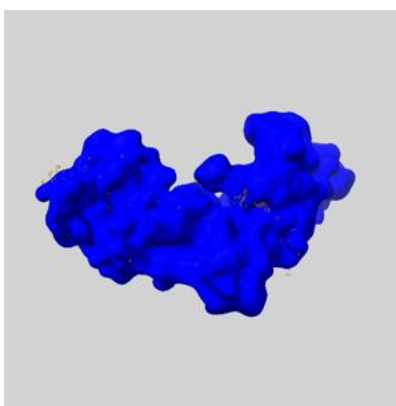
A mask typically either:

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

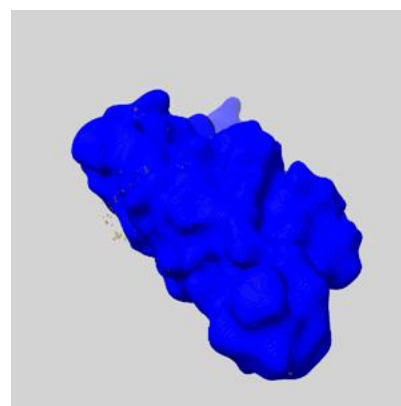
6.6.1 emd_14139_msk_1.map [i](#)



X



Y

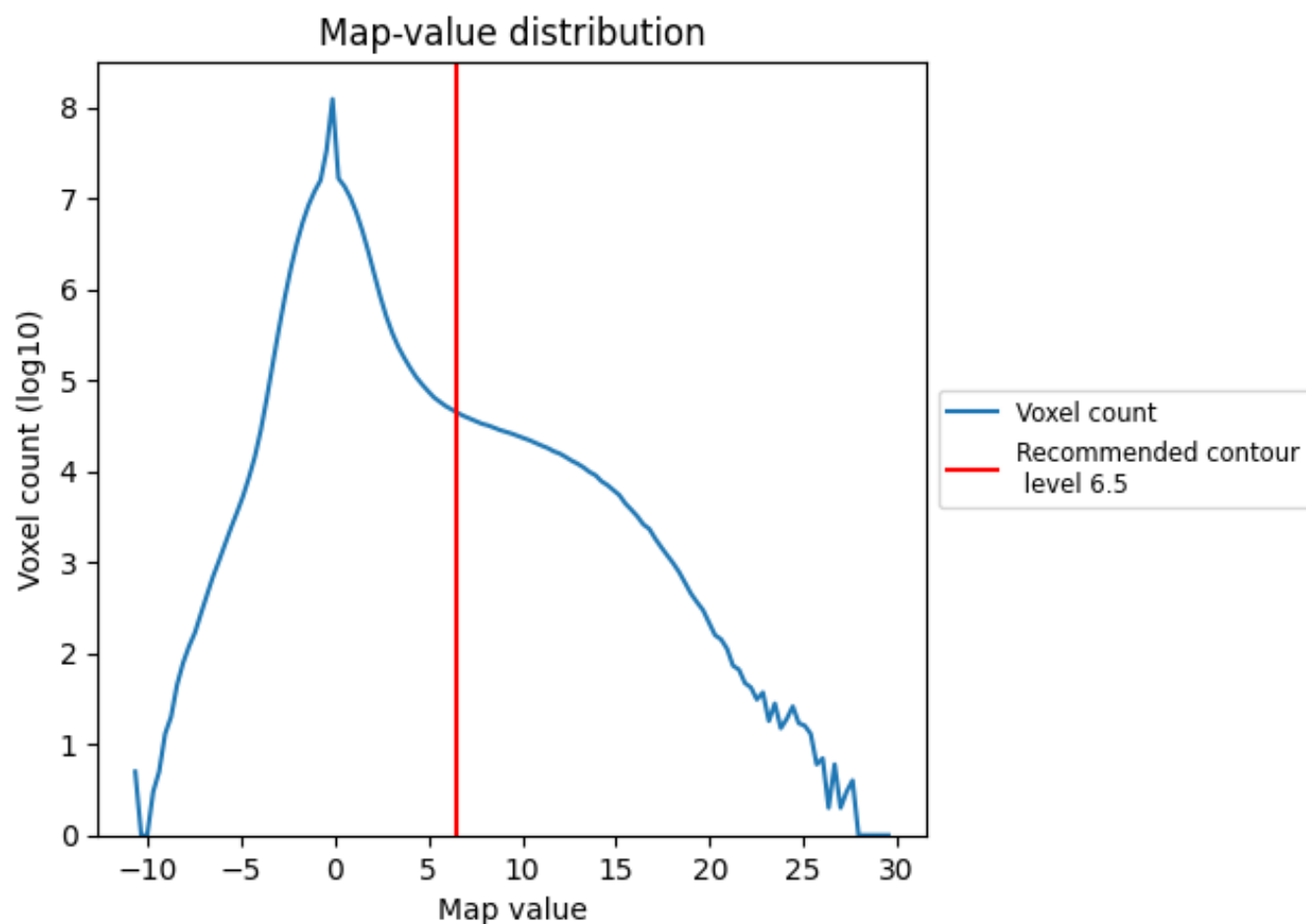


Z

7 Map analysis [i](#)

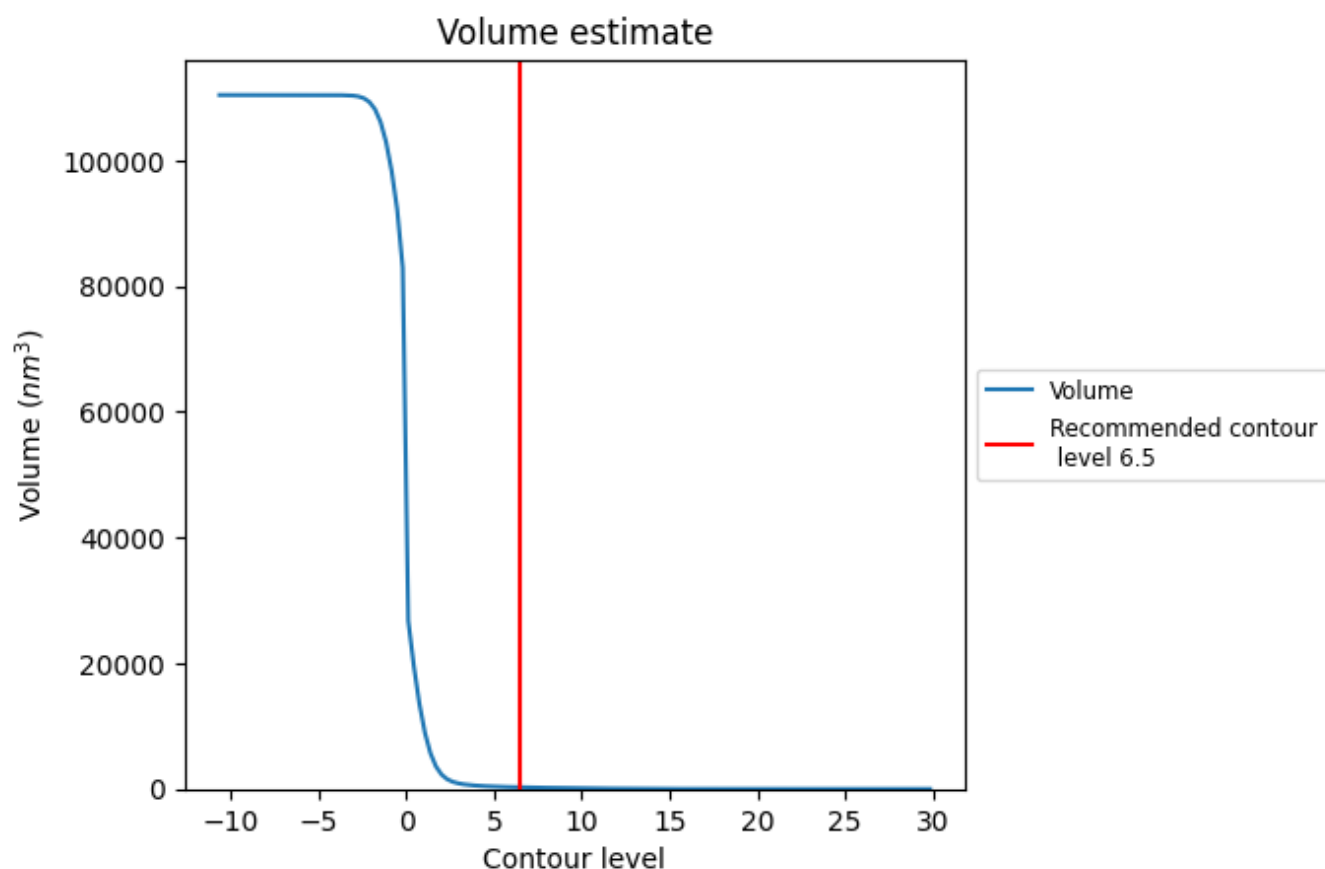
This section contains the results of statistical analysis of the map.

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.

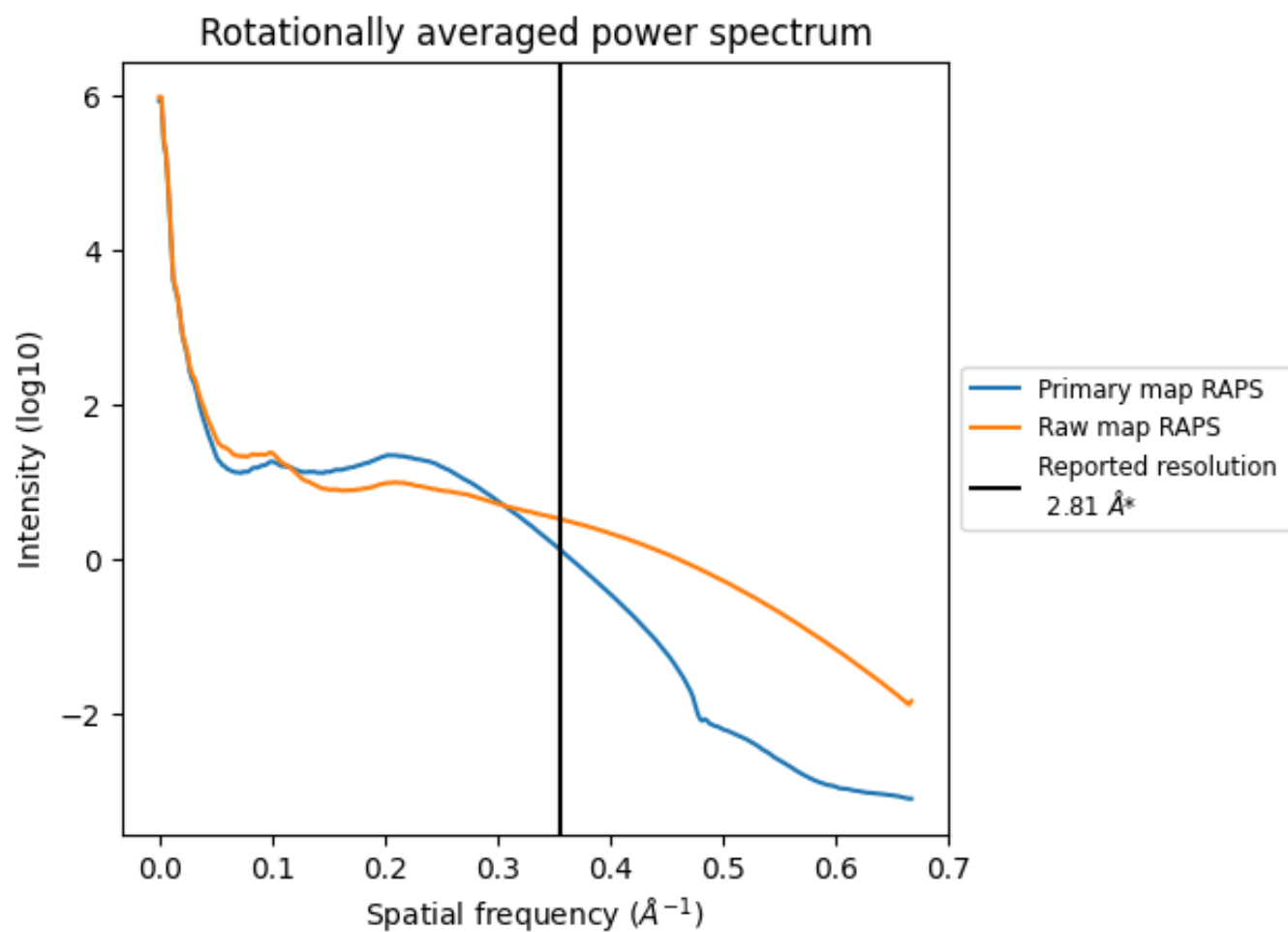
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm³; this corresponds to an approximate mass of 237 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 ⓘ

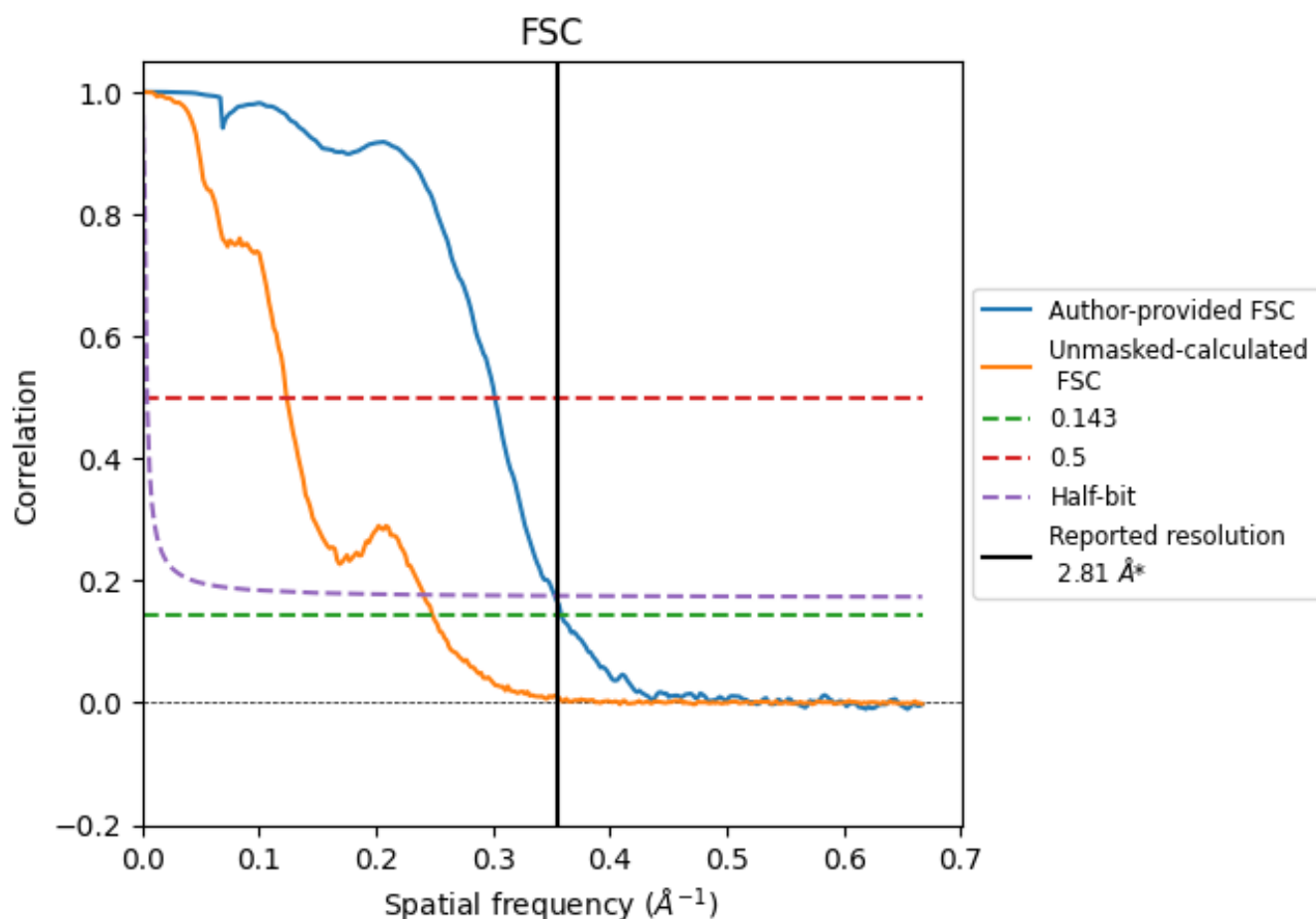


*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.356 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

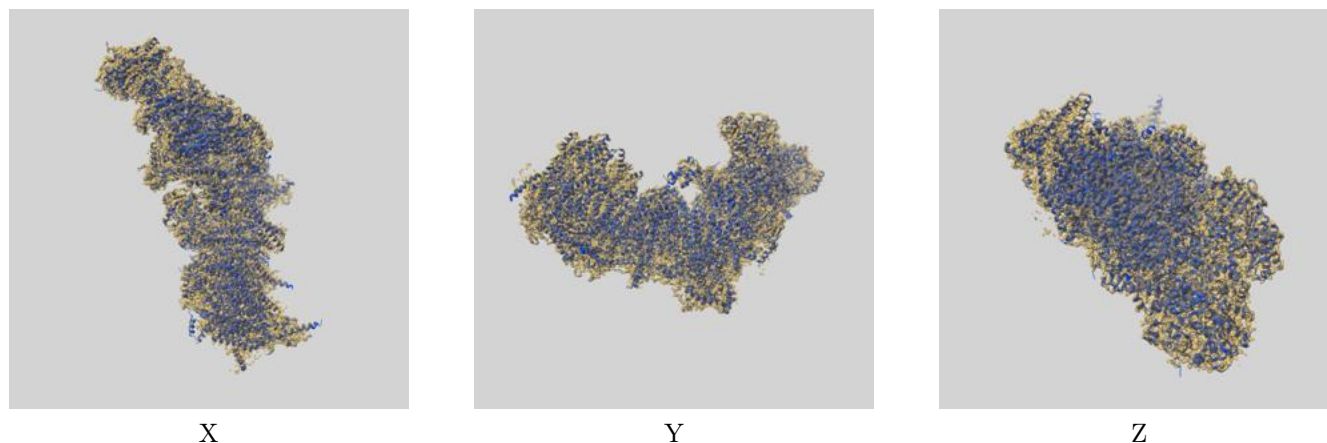
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.32	2.84
Unmasked-calculated*	4.03	8.10	4.15

*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 4.03 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

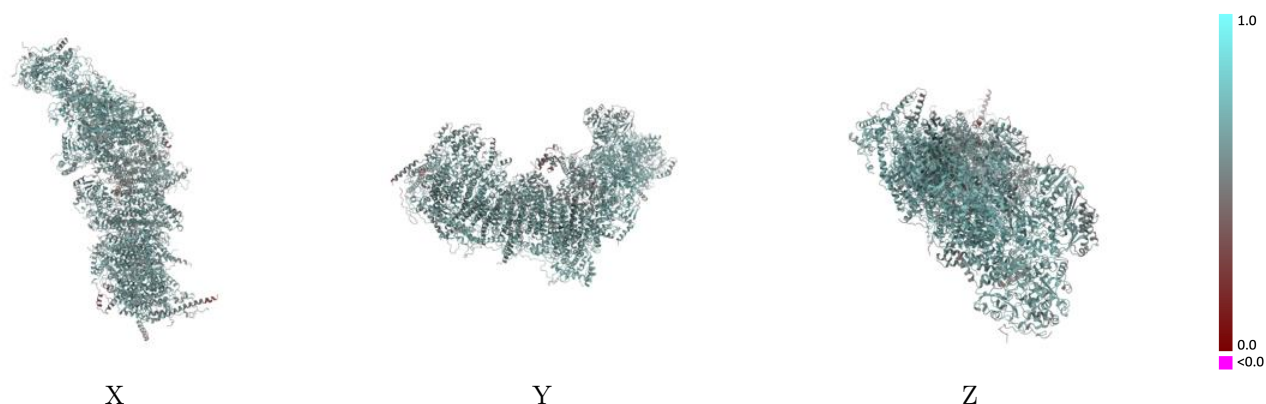
This section contains information regarding the fit between EMDB map EMD-14139 and PDB model 7QSN. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



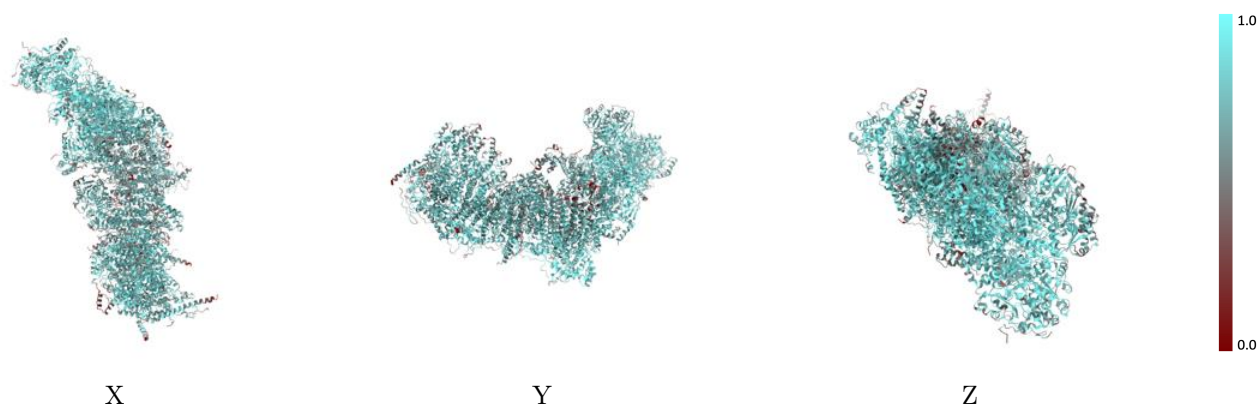
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



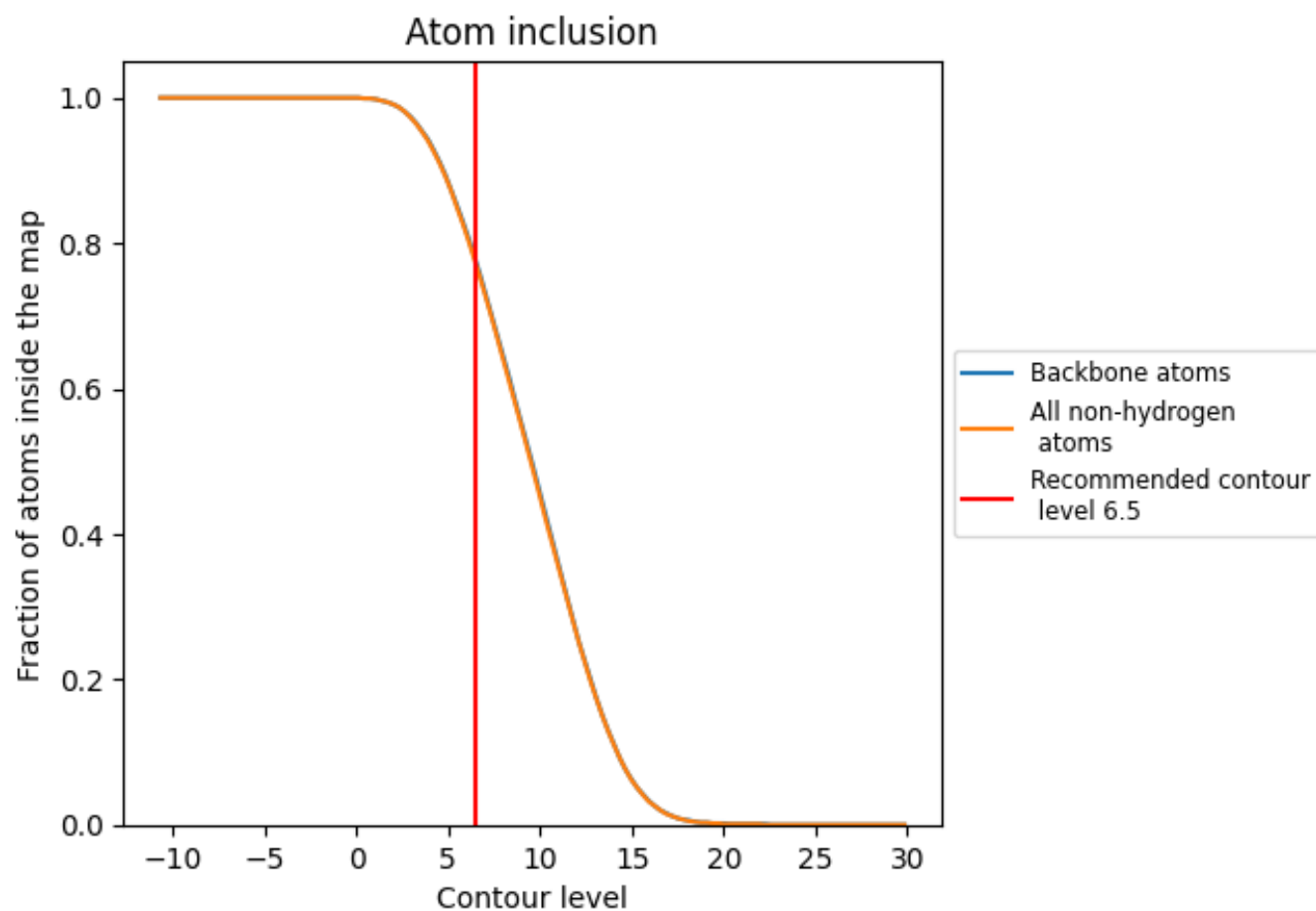
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.6110
A	 0.6420	 0.5930
B	 0.8330	 0.6460
C	 0.9030	 0.6640
D	 0.8640	 0.6580
E	 0.7860	 0.5890
F	 0.8150	 0.6100
G	 0.8160	 0.6220
H	 0.7710	 0.6390
I	 0.9000	 0.6770
J	 0.7230	 0.6010
K	 0.8390	 0.6470
L	 0.8000	 0.6210
M	 0.8860	 0.6570
N	 0.8630	 0.6570
O	 0.7340	 0.5900
P	 0.6840	 0.5630
Q	 0.8060	 0.6310
R	 0.8080	 0.6340
S	 0.6790	 0.5380
T	 0.4920	 0.4480
U	 0.6720	 0.5570
V	 0.6980	 0.5890
W	 0.7070	 0.5780
X	 0.7750	 0.6090
Y	 0.6380	 0.5790
Z	 0.8030	 0.6200
a	 0.8530	 0.6230
b	 0.7070	 0.5890
c	 0.6790	 0.5720
d	 0.7380	 0.6080
e	 0.7590	 0.6130
f	 0.5980	 0.5490
g	 0.7210	 0.5950
h	 0.8050	 0.6260



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Chain	Atom inclusion	Q-score
i	 0.6050	 0.5220
j	 0.6850	 0.5470
k	 0.6580	 0.5380
l	 0.7420	 0.5920
m	 0.7280	 0.6050
n	 0.7440	 0.5870
o	 0.6640	 0.5180
p	 0.7740	 0.5970
q	 0.8340	 0.6350
r	 0.7830	 0.6290
s	 0.7650	 0.5860