



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:37 AM UTC

PDB ID : 7R4G / pdb_00007r4g
EMDB ID : EMD-14307
Title : Bovine complex I in the presence of IM1761092, slack class ii (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.50 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

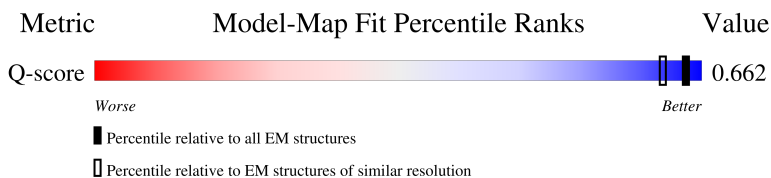
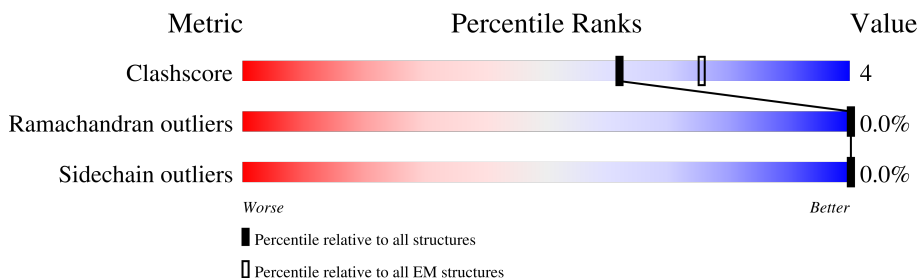
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



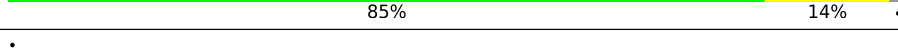
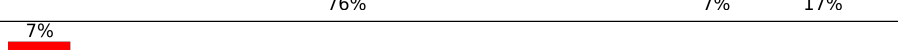
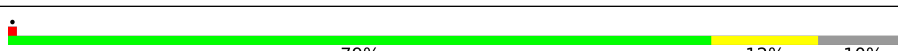
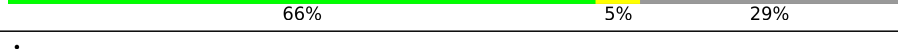
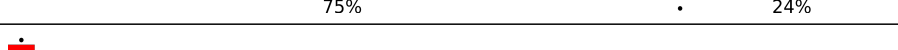
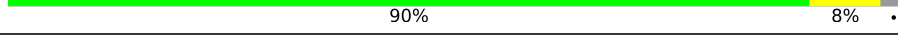
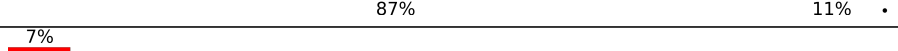
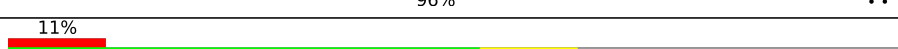
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	 6% 60% 21% 19%
2	B	216	 63% 8% 29%
3	C	266	 73% 5% 23%
4	D	463	 75% 8% 17%

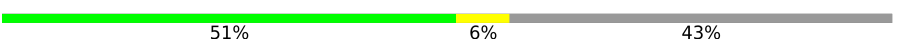
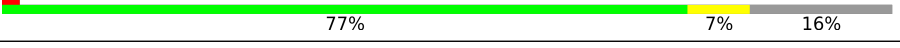
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

There are 60 unique types of molecules in this entry. The entry contains 65153 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	93	Total	C	N	O	S	0	0
			748	513	108	122	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	154	Total	C	N	O	S	0	0
			1230	786	220	210	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1714	1107	295	309	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	386	Total	C	N	O	S	0	0
			3095	1973	536	562	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	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3310	2085	591	614	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	313	Total	C	N	O	S	0	0
			2468	1655	379	411	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	127	Total	C	N	O	S	0	0
			946	635	135	167	9		

- 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	547	Total	C	N	O	S	0	0
			4318	2869	665	743	41		

- 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
			3632	2424	565	604	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	288	Total	C	N	O	S	0	0
			2289	1464	413	407	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			663	416	124	121	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	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	20	Total	C	N	O	S	0	0
			154	102	25	26	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	140	Total	C	N	O	S	0	0
			1145	736	200	200	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	69	Total	C	N	O	S	0	0
			561	361	103	92	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	48	Total	C	N	O	0	0
			405	268	69	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	112	Total	C	N	O	S	0	0
			934	613	157	161	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	95	Total	C	N	O	S	0	0
			799	506	150	137	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			451	296	79	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	88	Total	C	N	O	S	0	0
			733	474	122	133	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	104	Total	C	N	O	S	0	0
			892	588	151	152	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	79	Total	C	N	O	S	0	0
			638	418	107	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	108	Total	C	N	O	S	0	0
			908	580	161	167			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1435	900	265	262	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	768	214	206	4		

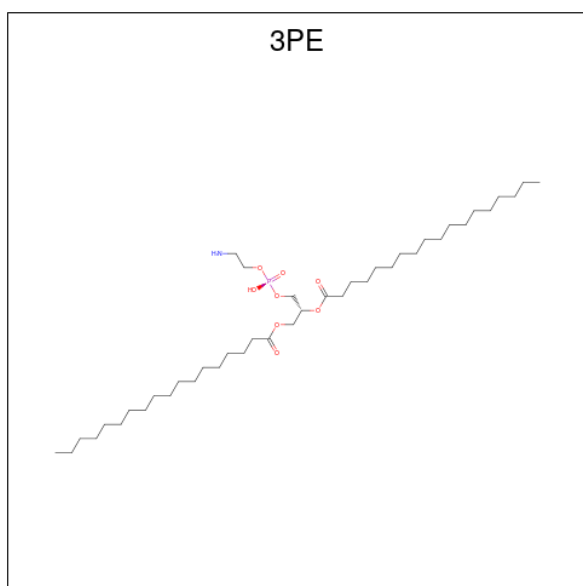
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	43	Total	C	N	O	S	0	0
			364	228	65	70	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



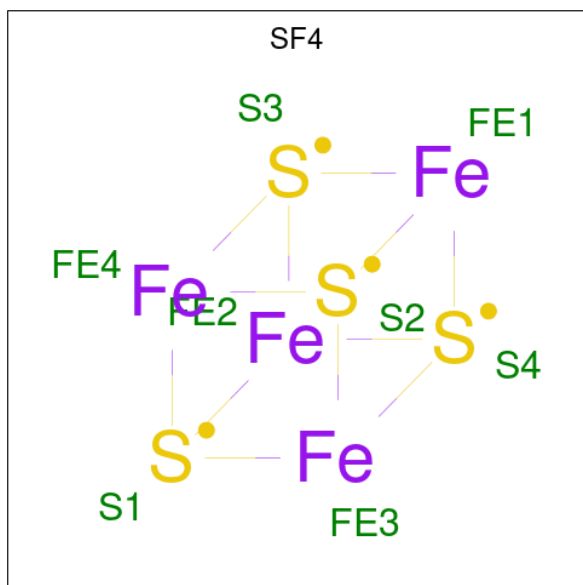
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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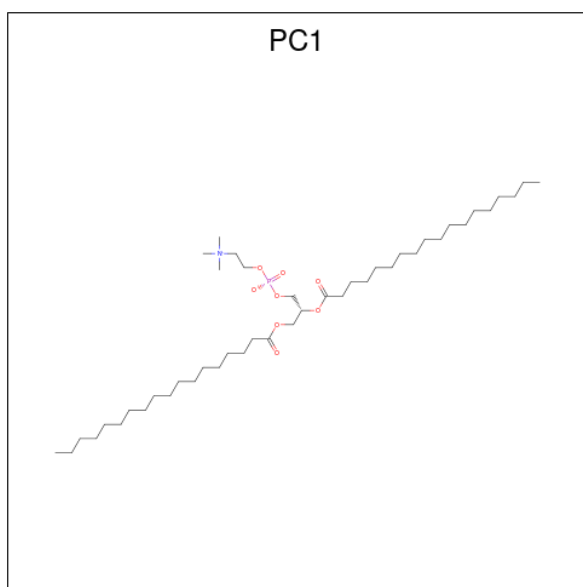
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	O	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



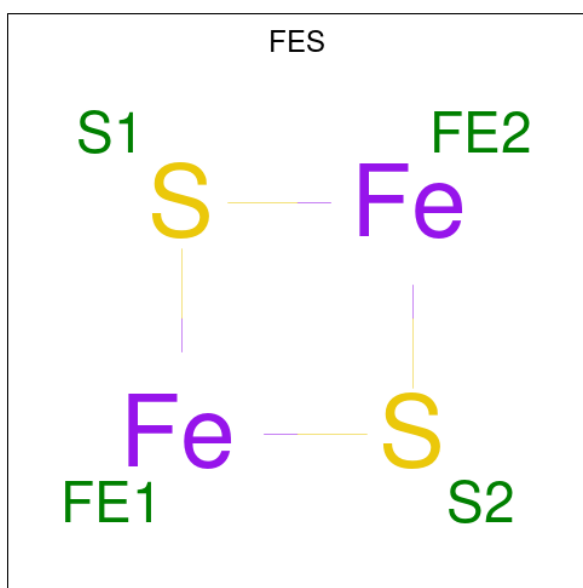
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$).



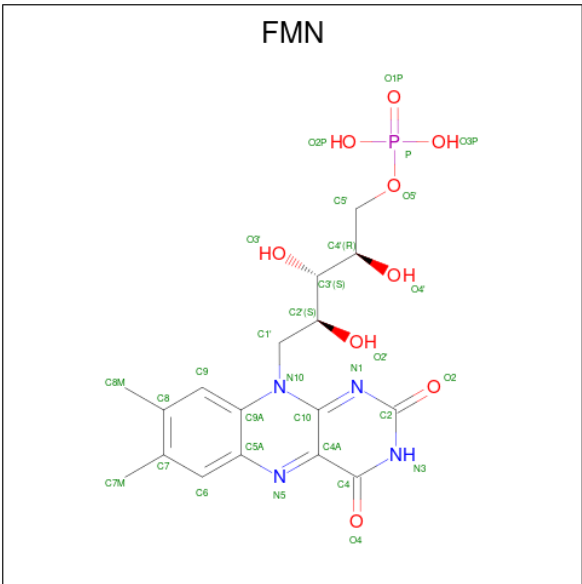
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	M	1	Total	C	N	O	P	0
			49	39	1	8	1	

- 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: C₁₇H₂₁N₄O₉P).

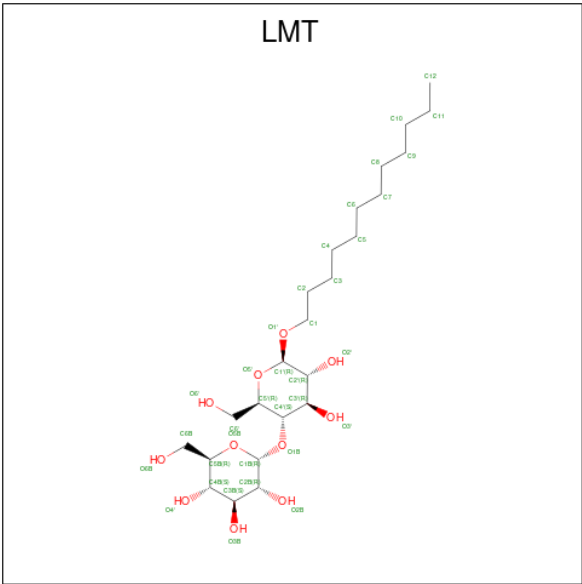


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

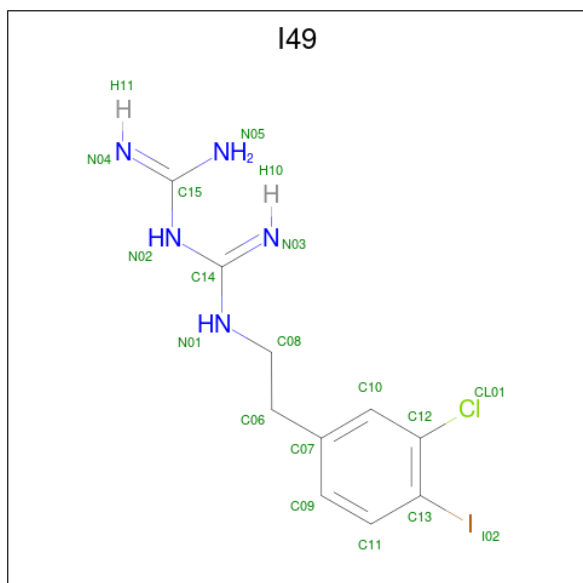
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			35	24	11	
51	J	1	Total	C	O	0
			35	24	11	
51	K	1	Total	C	O	0
			35	24	11	
51	L	1	Total	C	O	0
			35	24	11	
51	N	1	Total	C	O	0
			35	24	11	
51	b	1	Total	C	O	0
			35	24	11	
51	g	1	Total	C	O	0
			35	24	11	
51	h	1	Total	C	O	0
			35	24	11	
51	l	1	Total	C	O	0
			35	24	11	
51	p	1	Total	C	O	0
			35	24	11	

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (CCD ID: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



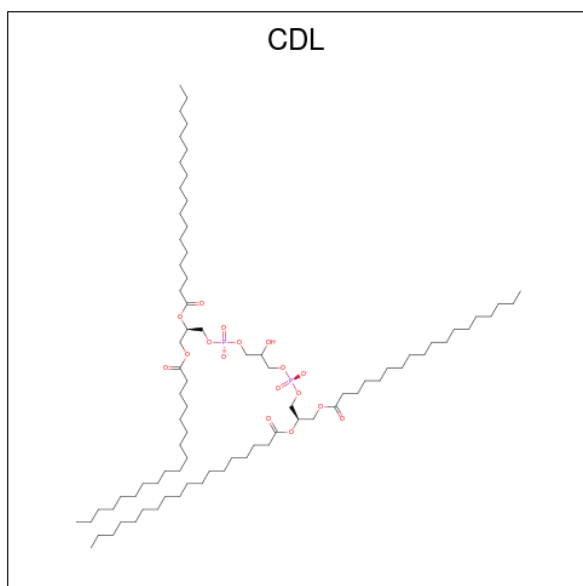
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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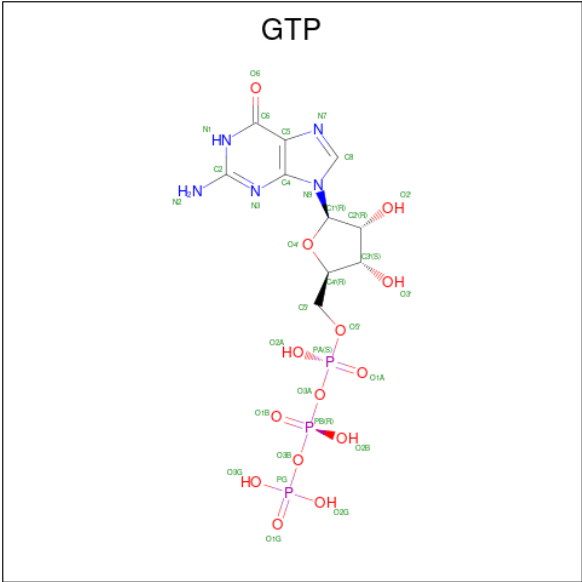
Mol	Chain	Residues	Atoms					AltConf
52	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			69	50	17	2	
53	N	1	Total	C	O	P	0
			67	48	17	2	
53	N	1	Total	C	O	P	0
			65	46	17	2	
53	X	1	Total	C	O	P	0
			52	33	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

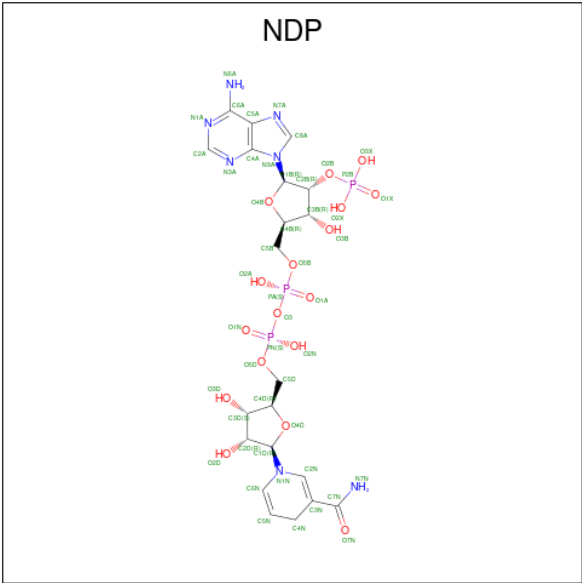


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

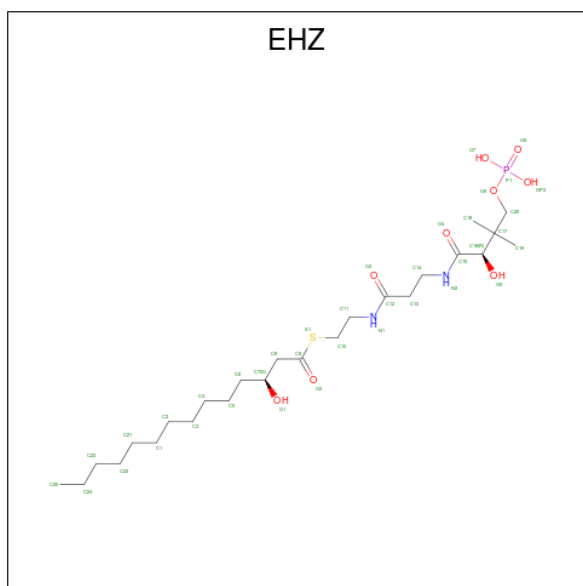


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

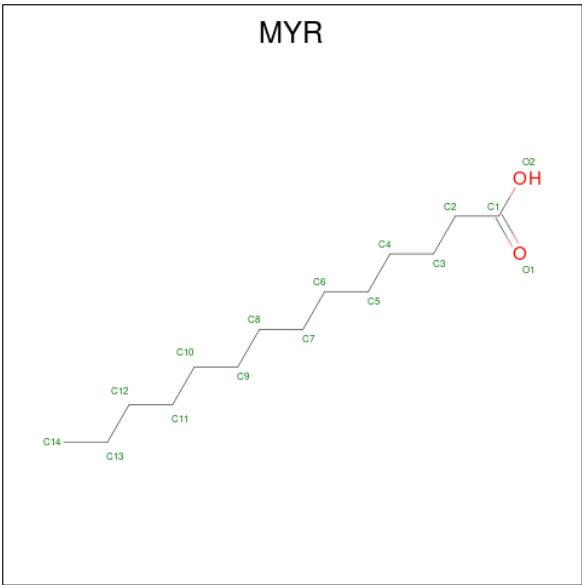
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

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



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

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	6	Total	O	0
			6	6	
60	B	36	Total	O	0
			36	36	
60	C	55	Total	O	0
			55	55	
60	D	104	Total	O	0
			104	104	
60	E	8	Total	O	0
			8	8	
60	F	38	Total	O	0
			38	38	
60	G	139	Total	O	0
			139	139	
60	H	25	Total	O	0
			25	25	
60	I	76	Total	O	0
			76	76	
60	J	1	Total	O	0
			1	1	
60	K	1	Total	O	0
			1	1	

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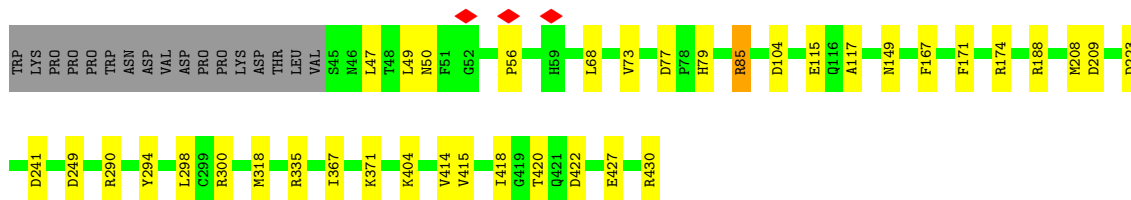
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Mol	Chain	Residues	Atoms		AltConf
60	L	32	Total 32	O 32	0
60	M	25	Total 25	O 25	0
60	N	7	Total 7	O 7	0
60	P	25	Total 25	O 25	0
60	Q	54	Total 54	O 54	0
60	R	25	Total 25	O 25	0
60	U	5	Total 5	O 5	0
60	V	3	Total 3	O 3	0
60	W	7	Total 7	O 7	0
60	X	12	Total 12	O 12	0
60	Y	1	Total 1	O 1	0
60	Z	13	Total 13	O 13	0
60	a	4	Total 4	O 4	0
60	b	5	Total 5	O 5	0
60	d	2	Total 2	O 2	0
60	e	4	Total 4	O 4	0
60	f	6	Total 6	O 6	0
60	g	5	Total 5	O 5	0
60	h	9	Total 9	O 9	0
60	i	1	Total 1	O 1	0
60	j	3	Total 3	O 3	0

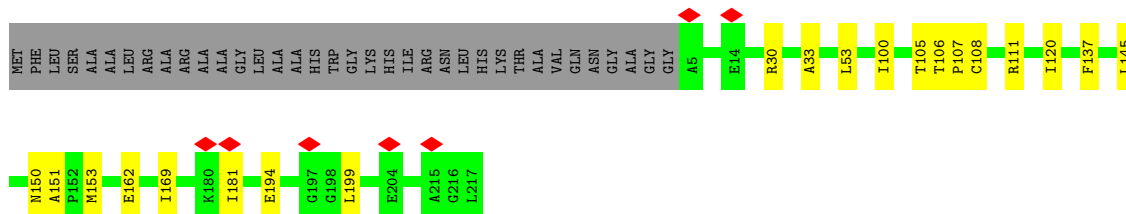
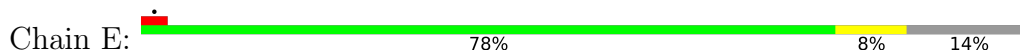
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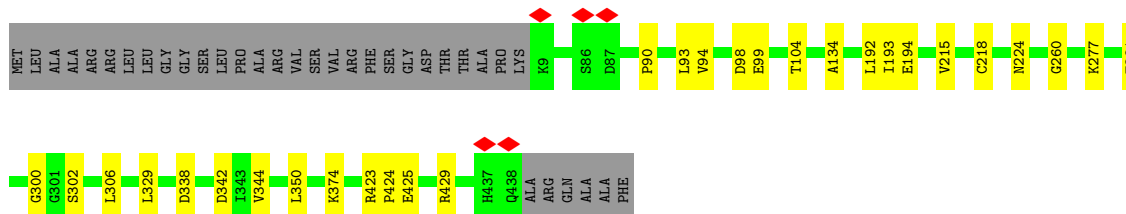
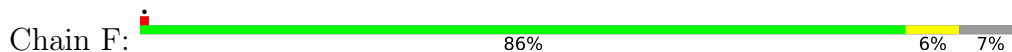
Mol	Chain	Residues	Atoms		AltConf
60	k	4	Total 4	O 4	0
60	l	11	Total 11	O 11	0
60	m	9	Total 9	O 9	0
60	n	16	Total 16	O 16	0
60	o	5	Total 5	O 5	0
60	p	18	Total 18	O 18	0
60	q	22	Total 22	O 22	0
60	r	26	Total 26	O 26	0
60	s	3	Total 3	O 3	0



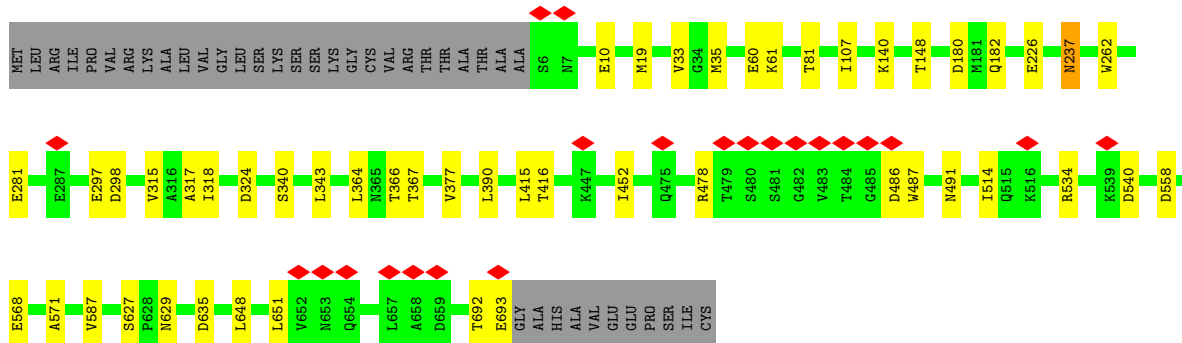
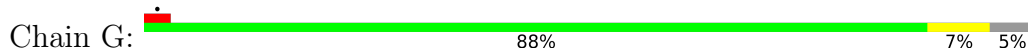
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



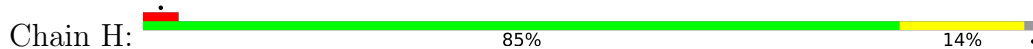
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

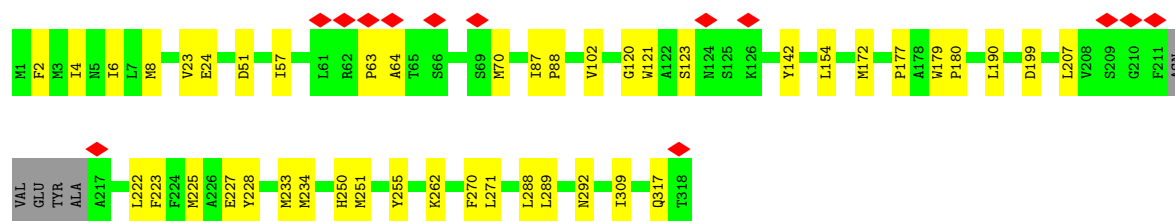


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

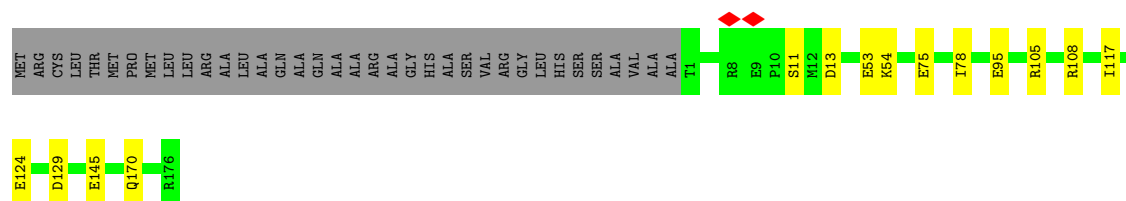
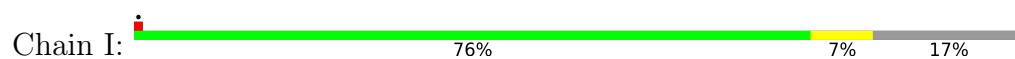


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

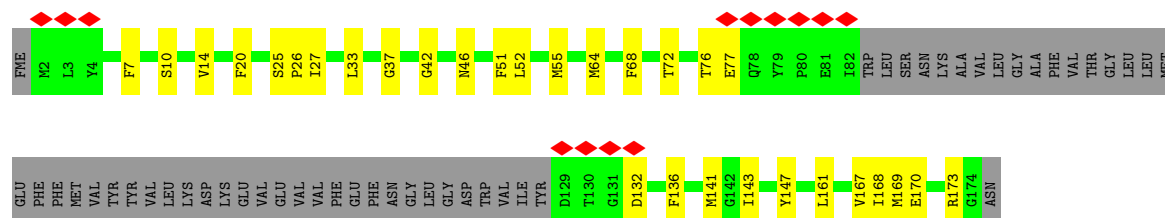




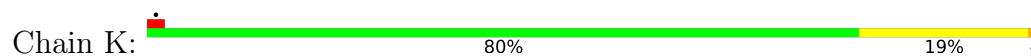
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



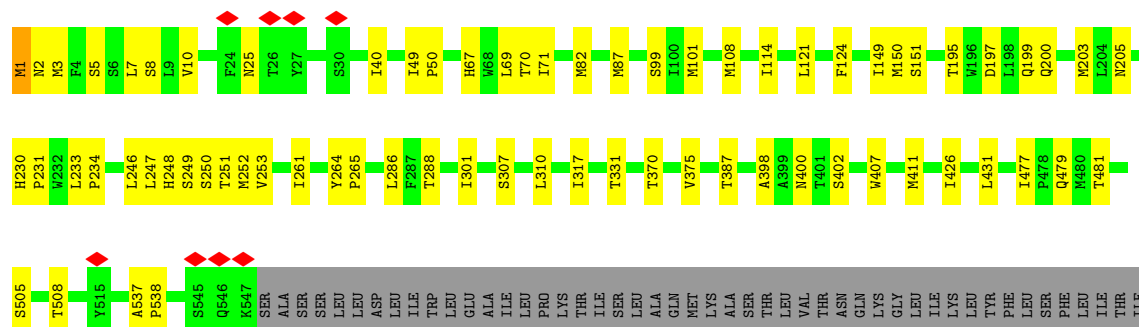
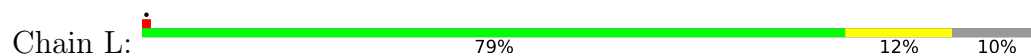
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



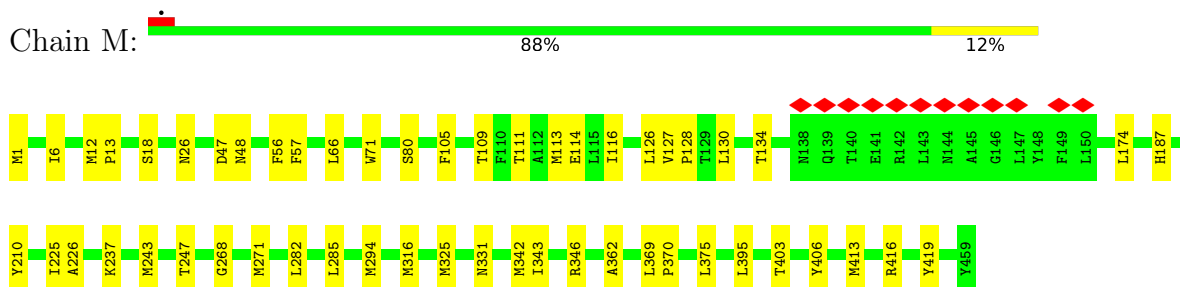
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



LEU
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LEU
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GLU

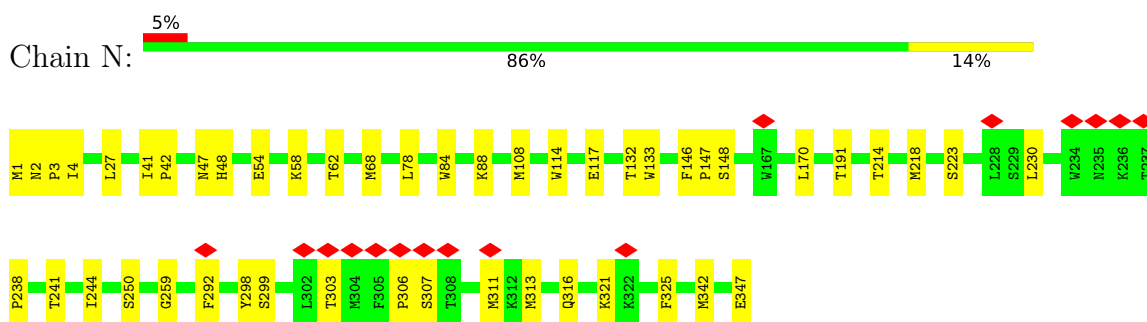
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



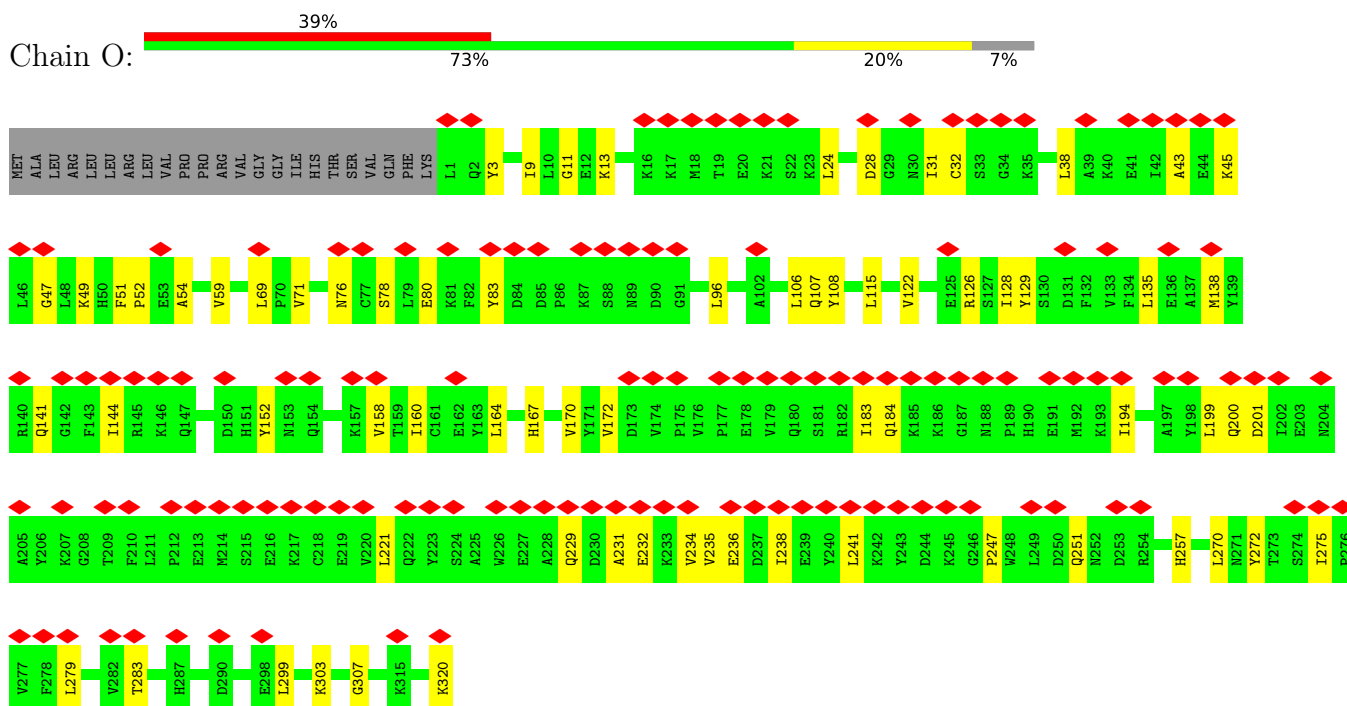
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



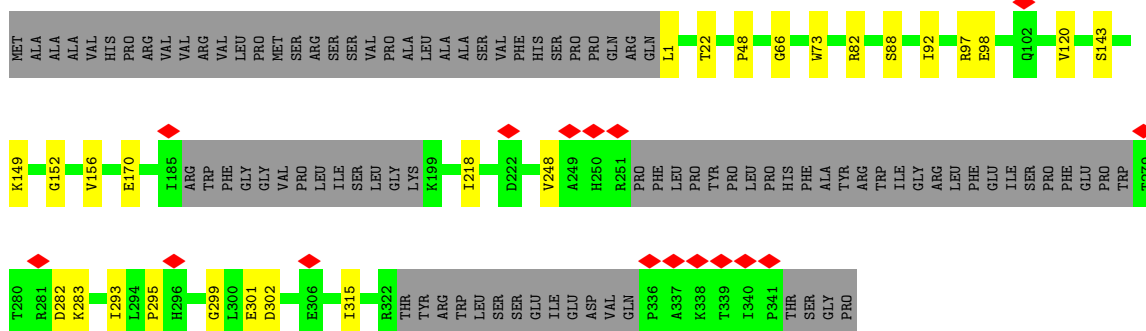
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



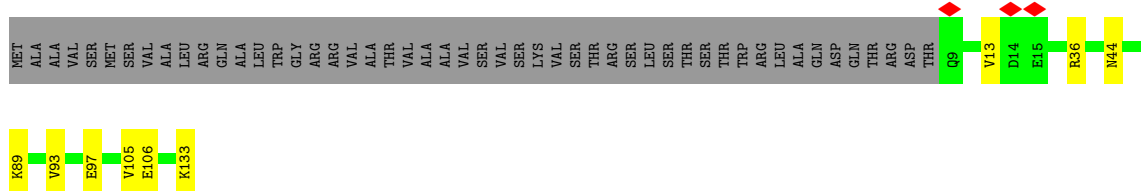
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 69% 7% 24%

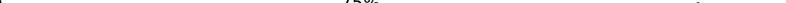


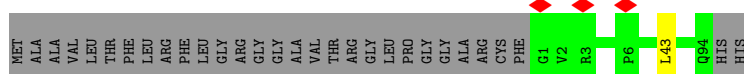
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  66% 5% 29%



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

Chain R:  75% 24%



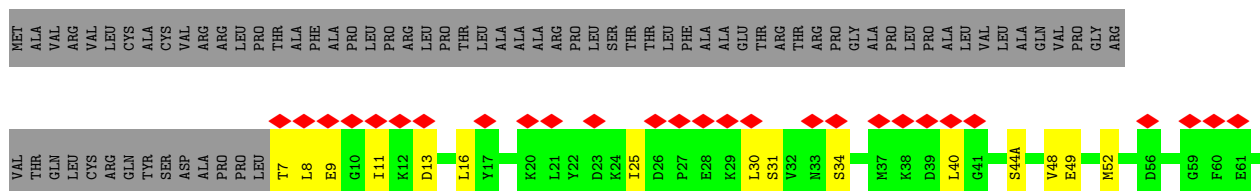
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

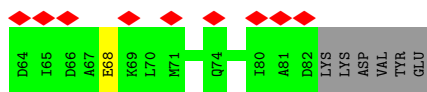
Chain S: 81% 17%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain T: 





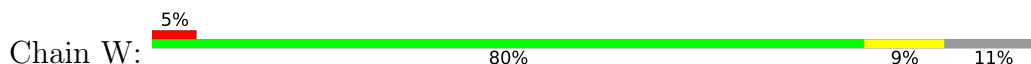
- Molecule 20: Acyl carrier protein, mitochondrial



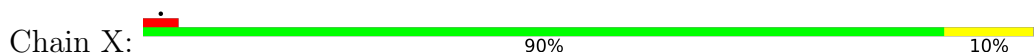
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



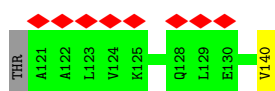
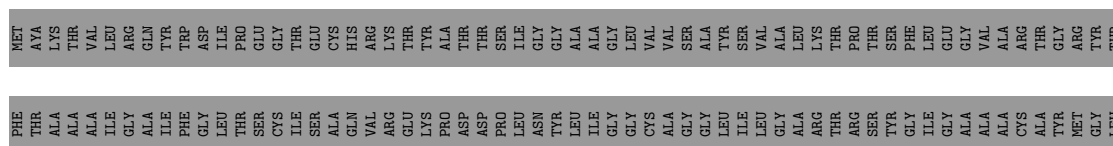
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



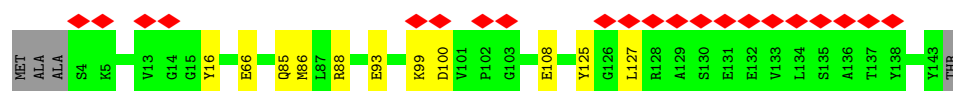
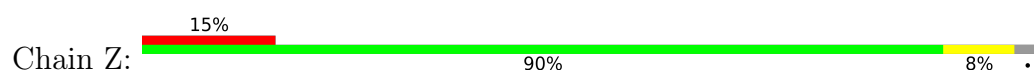
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



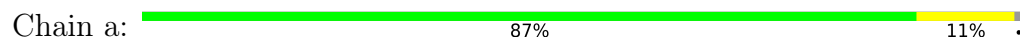
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



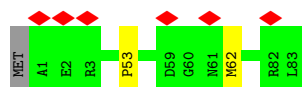
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



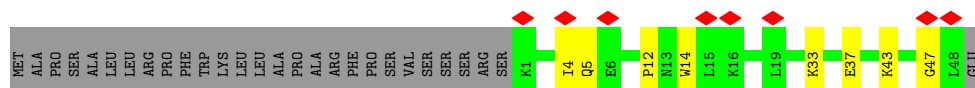
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



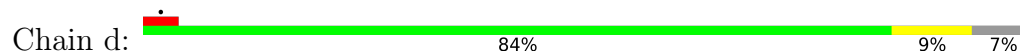
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



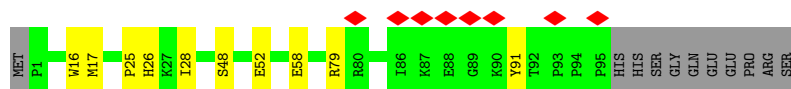
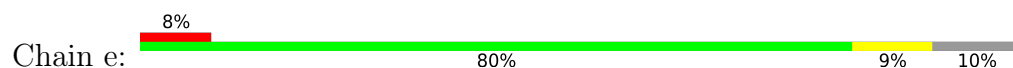
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



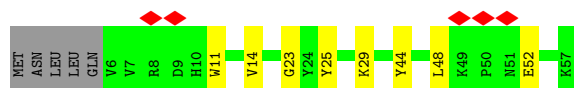
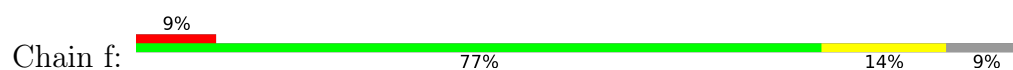
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



- 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

Chain g:  51% 6% 43%

MET ALA ALA ARG MET LEU GLY LEU CYS ARG ARG LEU LEU ALA VAL ALA ALA THR ARG GLY LEU PRO PRO ALA ARG VAL ARG TRP GLY SER SER SER ARG ALA VAL ILE ALA PRO SER THR LEU ALA GLY LYS ARG PRO SER SER GLU PRO THR LEU ARG TRP GLN GLU ASP PRO GLU

PRO GLU ASP E35 D54 N57 F66 V69 L70 V71 M85 E101 T107 N111 E122 ASP GLU ASP

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

Chain h:  70% 27%

MET ALA ALA MET SER LEU HIS ALA ARG VAL SER ALA VAL VAL ALA ALA LEU SER GLY THR ARG LEU LEU PHE GLY PHE LEU THR ASP PHE PRO LYS THR VAL ALA PRO VAL ARG HIS SER GLY ASP HIS GLY R6 T34 P35 E51 K106 E107

R115 N143

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

Chain i:  5% 80% 18%

S1 P35 GLN ARG VAL SER PRO VAL ARG ARG PHE TRP ASN LYS PHE LEU LEU ASP GLY ALA LEU TRP LYS N58 V59 I60 Y61 K62 R65 E98 E111 D124 Q125 HIS HIS

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

Chain j:  60% 38%

MET ALA GLY MET SER ALA LEU LYS ARG LEU ALA ALA PRO PHE ALA HIS VAL VAL GLY HIS LEU PHE ARG GLY ARG CYS ALA ARG ALA LYS ASP LYS ALA ARG GLY VAL ARG ARG ALA GLY GLY GLY A5 R12 M32 D70 E71 ASP

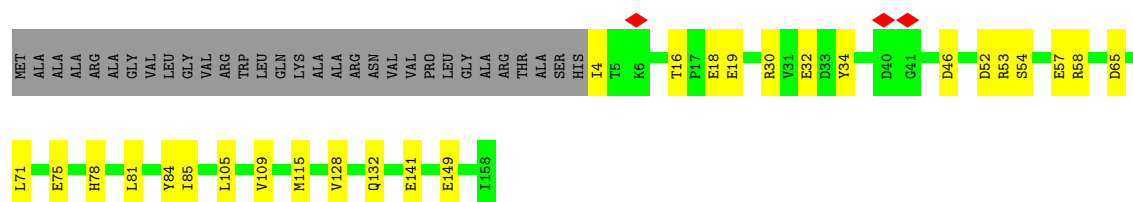
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:  74% 6% 19%

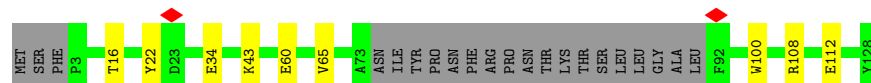
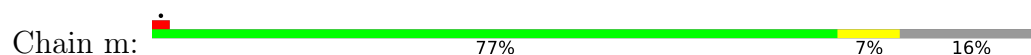
MET ALA HIS GLY HIS GLY HIS HIS GLY PRO SER K12 D17 Y18 E24 P27 N47 Y52 Q99 LYS LYS ASP LYS HIS HIS

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

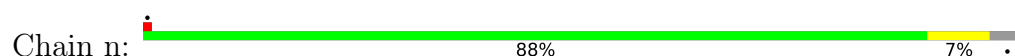
Chain l:  69% 15% 17%



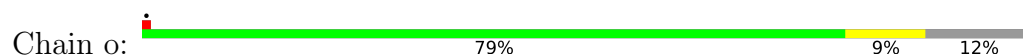
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



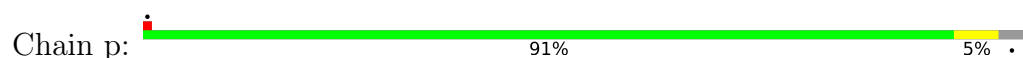
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



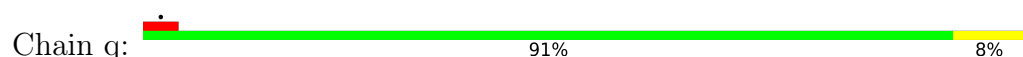
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



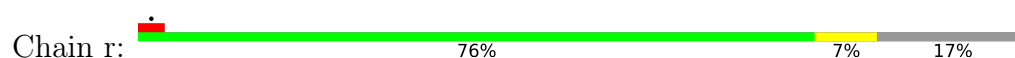
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

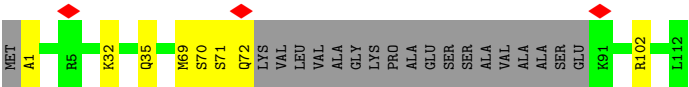


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

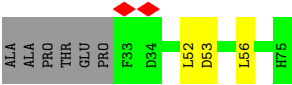
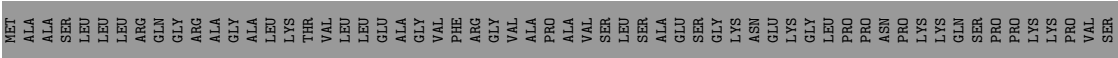


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40154	Depositor
Resolution determination method	OTHER	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	33.163	Depositor
Minimum map value	-13.512	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.066	Depositor
Recommended contour level	6	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I49, FES, GTP, FME, K, FMN, EHZ, LMT, 2MR, SF4, MG, CDL, MYR, AYA, PC1, ZN, 3PE, SAC, NDP

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	0.26	0/756	0.30	0/1034
2	B	0.30	0/1261	0.41	0/1706
3	C	0.27	0/1765	0.35	0/2403
4	D	0.27	0/3155	0.33	0/4264
5	E	0.22	0/1695	0.29	0/2307
6	F	0.24	0/3384	0.32	0/4573
7	G	0.24	0/5367	0.32	0/7274
8	H	0.27	0/2528	0.34	0/3452
9	I	0.28	0/1445	0.33	0/1956
10	J	0.26	0/968	0.33	0/1311
11	K	0.25	0/745	0.29	0/1008
12	L	0.30	0/4426	0.31	0/6025
13	M	0.29	0/3716	0.32	0/5069
14	N	0.25	0/2792	0.30	0/3800
15	O	0.17	0/2651	0.30	0/3587
16	P	0.23	0/2339	0.33	0/3159
17	Q	0.25	0/1039	0.30	0/1404
18	R	0.24	0/731	0.29	0/984
19	S	0.21	0/674	0.30	0/908
20	T	0.18	0/621	0.27	0/837
20	U	0.33	0/692	0.30	0/932
21	V	0.21	0/931	0.27	0/1261
22	W	0.22	0/995	0.31	0/1337
23	X	0.24	0/1439	0.32	0/1942
24	Y	0.14	0/157	0.23	0/211
25	Z	0.24	0/1174	0.32	0/1582
26	a	0.26	0/576	0.29	0/775
27	b	0.23	0/672	0.28	0/923
28	c	0.19	0/418	0.26	0/567
29	d	0.23	0/964	0.29	0/1305
30	e	0.24	0/818	0.35	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.26	0/464	0.31	0/626
32	g	0.28	0/755	0.28	0/1023
33	h	0.26	0/1188	0.29	0/1607
34	i	0.29	0/912	0.33	0/1241
35	j	0.28	0/607	0.28	0/833
36	k	0.29	0/657	0.31	0/887
37	l	0.28	0/1358	0.30	0/1858
38	m	0.27	0/929	0.30	0/1252
39	n	0.31	0/1540	0.33	0/2085
40	o	0.33	0/1060	0.37	0/1420
41	p	0.30	0/1468	0.29	0/1979
42	q	0.22	0/1233	0.31	0/1676
43	r	0.24	0/780	0.34	0/1056
44	s	0.20	0/375	0.27	0/507
All	All	0.26	0/64220	0.32	0/87039

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
34	i	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
34	i	1	SAC	Mainchain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	748	0	797	19	0
2	B	1230	0	1238	17	0
3	C	1714	0	1668	10	0
4	D	3095	0	3068	28	0
5	E	1655	0	1661	13	0
6	F	3310	0	3261	20	0
7	G	5279	0	5301	37	0
8	H	2468	0	2585	34	0
9	I	1414	0	1370	14	0
10	J	946	0	958	32	0
11	K	745	0	785	18	0
12	L	4318	0	4424	54	0
13	M	3632	0	3813	37	0
14	N	2733	0	2912	32	0
15	O	2589	0	2566	51	0
16	P	2289	0	2323	18	0
17	Q	1016	0	1014	8	0
18	R	720	0	700	1	0
19	S	663	0	672	1	0
20	T	612	0	604	11	0
20	U	681	0	677	6	0
21	V	911	0	950	7	0
22	W	971	0	989	10	0
23	X	1402	0	1381	16	0
24	Y	154	0	158	1	0
25	Z	1145	0	1144	10	0
26	a	561	0	564	7	0
27	b	651	0	662	2	0
28	c	405	0	409	4	0
29	d	934	0	919	11	0
30	e	799	0	807	10	0
31	f	451	0	453	6	0
32	g	733	0	701	7	0
33	h	1154	0	1168	5	0
34	i	892	0	911	2	0
35	j	580	0	519	2	0
36	k	638	0	621	4	0
37	l	1304	0	1203	20	0
38	m	908	0	903	8	0
39	n	1487	0	1433	9	0
40	o	1035	0	1003	8	0
41	p	1435	0	1411	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	q	1192	0	1164	9	0
43	r	767	0	776	5	0
44	s	364	0	336	3	0
45	A	92	0	138	4	0
45	H	34	0	47	1	0
45	I	84	0	122	0	0
45	L	94	0	142	2	0
45	M	43	0	63	0	0
45	N	51	0	82	1	0
45	O	51	0	82	2	0
46	B	8	0	0	0	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	B	35	0	44	1	0
47	M	49	0	75	2	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	H	35	0	46	2	0
51	J	35	0	46	0	0
51	K	35	0	46	0	0
51	L	35	0	46	1	0
51	N	35	0	46	0	0
51	b	35	0	46	0	0
51	g	35	0	46	1	0
51	h	35	0	46	0	0
51	l	35	0	46	1	0
51	p	35	0	46	0	0
52	H	17	0	0	0	0
52	N	17	0	0	3	0
53	L	69	0	82	0	0
53	N	132	0	158	3	0
53	X	52	0	48	0	0
53	h	67	0	81	1	0
53	q	76	0	96	0	0
54	O	32	0	12	3	0
55	O	1	0	0	0	0
56	P	48	0	26	2	0
57	R	1	0	0	0	0
58	T	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	U	37	0	0	2	0
59	o	15	0	27	2	0
60	A	6	0	0	1	0
60	B	36	0	0	1	0
60	C	55	0	0	3	0
60	D	104	0	0	3	0
60	E	8	0	0	0	0
60	F	38	0	0	1	0
60	G	139	0	0	5	0
60	H	25	0	0	0	0
60	I	76	0	0	4	0
60	J	1	0	0	0	0
60	K	1	0	0	0	0
60	L	32	0	0	5	0
60	M	25	0	0	3	0
60	N	7	0	0	1	0
60	P	25	0	0	1	0
60	Q	54	0	0	2	0
60	R	25	0	0	0	0
60	U	5	0	0	0	0
60	V	3	0	0	1	0
60	W	7	0	0	0	0
60	X	12	0	0	0	0
60	Y	1	0	0	0	0
60	Z	13	0	0	0	0
60	a	4	0	0	0	0
60	b	5	0	0	1	0
60	d	2	0	0	0	0
60	e	4	0	0	0	0
60	f	6	0	0	1	0
60	g	5	0	0	1	0
60	h	9	0	0	1	0
60	i	1	0	0	0	0
60	j	3	0	0	1	0
60	k	4	0	0	1	0
60	l	11	0	0	1	0
60	m	9	0	0	0	0
60	n	16	0	0	2	0
60	o	5	0	0	0	0
60	p	18	0	0	0	0
60	q	22	0	0	1	0
60	r	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	s	3	0	0	0	0
All	All	65153	0	64786	550	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 (550) 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)
9:I:75:GLU:OE2	60:I:301:HOH:O	1.91	0.86
37:l:132:GLN:O	60:l:301:HOH:O	1.93	0.86
3:C:201:SER:O	60:C:301:HOH:O	1.94	0.85
25:Z:93:GLU:OE1	30:e:91:TYR:OH	1.95	0.84
12:L:479:GLN:NE2	12:L:481:THR:O	2.10	0.83
15:O:108:TYR:OH	15:O:164:LEU:O	1.95	0.83
15:O:307:GLY:O	15:O:320:LYS:NZ	2.10	0.83
32:g:54:ASP:OD2	60:g:1201:HOH:O	1.96	0.82
42:q:13:GLN:OE1	60:q:301:HOH:O	1.96	0.82
1:A:71:LEU:O	10:J:147:TYR:OH	1.96	0.82
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.59	0.82
2:B:49:THR:HG21	2:B:59:MET:HE2	1.59	0.82
6:F:342:ASP:OD1	6:F:429:ARG:NH1	2.12	0.82
1:A:112:GLU:OE1	60:A:1001:HOH:O	1.98	0.80
34:i:98:GLU:OE1	41:p:14:ARG:NH1	2.13	0.80
27:b:53:PRO:O	60:b:401:HOH:O	2.00	0.80
14:N:1:FME:O	60:N:1401:HOH:O	1.99	0.79
16:P:170:GLU:OE2	60:P:601:HOH:O	2.01	0.79
40:o:23:THR:OG1	40:o:104:GLU:OE2	2.02	0.77
37:l:32:GLU:N	37:l:32:GLU:OE2	2.18	0.77
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.67	0.77
38:m:16:THR:O	38:m:22:TYR:OH	2.00	0.77
17:Q:44:ASN:OD1	60:Q:201:HOH:O	2.02	0.77
33:h:107:GLU:OE1	60:h:1101:HOH:O	2.01	0.76
3:C:145:HIS:O	60:C:302:HOH:O	2.03	0.76
12:L:505:SER:O	12:L:508:THR:OG1	2.03	0.76
15:O:126:ARG:NH1	54:O:1202:GTP:O1A	2.20	0.75
7:G:692:THR:OG1	7:G:693:GLU:OE1	2.01	0.75
40:o:105:ARG:NH2	40:o:109:GLN:OE1	2.20	0.74
12:L:400:ASN:O	60:L:802:HOH:O	2.04	0.74
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.20	0.74
6:F:194:GLU:OE2	17:Q:133:LYS:NZ	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:197:ASP:OD2	41:p:110:LYS:NZ	2.17	0.74
7:G:180:ASP:OD1	60:G:901:HOH:O	2.06	0.73
7:G:478:ARG:NH2	7:G:487:TRP:O	2.22	0.73
4:D:427:GLU:OE2	60:D:501:HOH:O	2.06	0.73
29:d:108:THR:OG1	29:d:111:GLU:OE1	2.04	0.72
14:N:307:SER:OG	14:N:311:MET:SD	2.47	0.72
4:D:249:ASP:OD1	4:D:404:LYS:NZ	2.22	0.72
15:O:200:GLN:O	15:O:200:GLN:NE2	2.23	0.72
4:D:415:VAL:CG2	8:H:207:LEU:HD11	2.20	0.71
12:L:205:ASN:OD1	60:L:803:HOH:O	2.07	0.71
7:G:226:GLU:OE1	60:G:902:HOH:O	2.07	0.71
7:G:693:GLU:OE1	7:G:693:GLU:N	2.23	0.71
20:T:48:VAL:HG12	20:T:52:MET:HE2	1.72	0.71
20:U:49:GLU:OE2	39:n:44:ARG:NH1	2.23	0.71
52:N:1305:I49:I02	29:d:86:ARG:HB2	2.61	0.70
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.24	0.70
7:G:140:LYS:O	7:G:148:THR:OG1	2.10	0.70
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.73	0.70
12:L:199:GLN:OE1	60:L:804:HOH:O	2.10	0.70
9:I:11:SER:OG	9:I:13:ASP:OD1	2.09	0.70
21:V:110:GLN:OE1	60:V:201:HOH:O	2.09	0.70
14:N:347:GLU:HG3	52:N:1305:I49:I02	2.62	0.69
37:l:53:ARG:NE	37:l:57:GLU:OE1	2.25	0.69
12:L:87:MET:HA	12:L:87:MET:HE2	1.74	0.69
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.26	0.69
14:N:214:THR:HG22	14:N:218:MET:HE2	1.75	0.69
22:W:96:VAL:HG12	22:W:96:VAL:O	1.93	0.69
39:n:31:ILE:O	60:n:201:HOH:O	2.10	0.68
39:n:104:ASP:OD1	60:n:202:HOH:O	2.12	0.68
30:e:58:GLU:OE2	30:e:58:GLU:N	2.26	0.67
12:L:199:GLN:NE2	60:L:805:HOH:O	2.23	0.67
14:N:342:MET:HE1	53:N:1304:CDL:H473	1.75	0.67
3:C:91:GLU:OE2	60:C:303:HOH:O	2.12	0.67
8:H:57:ILE:O	51:H:401:LMT:O6'	2.12	0.67
51:l:201:LMT:O1'	51:l:201:LMT:O6'	2.12	0.67
14:N:342:MET:HE1	53:N:1304:CDL:C47	2.25	0.66
20:T:49:GLU:OE2	22:W:64:ARG:NH1	2.27	0.66
2:B:138:ARG:NH1	60:B:301:HOH:O	2.24	0.66
15:O:279:LEU:O	15:O:283:THR:OG1	2.06	0.66
15:O:52:PRO:O	15:O:107:GLN:NE2	2.27	0.66
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:194:ILE:HD12	15:O:199:LEU:HD11	1.77	0.65
15:O:49:LYS:HB3	15:O:122:VAL:HG12	1.79	0.65
10:J:167:VAL:HG13	14:N:42:PRO:HG3	1.79	0.65
20:T:25:ILE:HG23	20:T:40:LEU:HD22	1.77	0.65
11:K:59:MET:HG2	14:N:27:LEU:HD22	1.79	0.65
7:G:366:THR:O	7:G:367:THR:OG1	2.11	0.64
4:D:422:ASP:OD2	60:D:502:HOH:O	2.14	0.64
4:D:209:ASP:OD1	25:Z:16:TYR:OH	2.14	0.64
7:G:635:ASP:O	60:G:903:HOH:O	2.14	0.64
12:L:286:LEU:HD22	12:L:411:MET:SD	2.38	0.64
37:l:4:ILE:HD11	38:m:60:GLU:OE2	1.98	0.64
29:d:120:ARG:O	38:m:108:ARG:NH2	2.31	0.64
15:O:3:TYR:HH	15:O:257:HIS:HD1	1.45	0.63
17:Q:133:LYS:NZ	60:Q:203:HOH:O	2.29	0.63
10:J:27:ILE:HD11	10:J:77:GLU:O	1.96	0.63
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.80	0.63
36:k:47:ASN:O	60:k:101:HOH:O	2.15	0.63
2:B:44:SER:OG	8:H:51:ASP:OD1	2.15	0.63
14:N:170:LEU:HD23	14:N:292:PHE:HB2	1.80	0.62
14:N:325:PHE:N	53:N:1304:CDL:OB3	2.30	0.62
12:L:108:MET:O	12:L:114:ILE:HD13	1.99	0.62
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.33	0.62
37:l:18:GLU:N	37:l:18:GLU:OE1	2.33	0.62
23:X:129:LYS:NZ	27:b:62:MET:O	2.31	0.61
33:h:51:GLU:OE1	41:p:59:LYS:NZ	2.31	0.61
12:L:251:THR:HG22	12:L:252:MET:N	2.14	0.61
23:X:30:HIS:O	23:X:32:GLY:N	2.32	0.61
1:A:68:GLU:OE1	1:A:98:LEU:HD13	1.99	0.61
31:f:44:TYR:O	60:f:101:HOH:O	2.16	0.61
12:L:151:SER:OG	12:L:252:MET:SD	2.47	0.61
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.33	0.61
16:P:301:GLU:OE1	16:P:301:GLU:N	2.32	0.60
12:L:2:ASN:OD1	12:L:3:MET:N	2.35	0.60
12:L:121:LEU:HD22	12:L:246:LEU:HD12	1.83	0.60
14:N:238:PRO:O	14:N:241:THR:OG1	2.19	0.60
39:n:139:LEU:O	39:n:143:THR:OG1	2.16	0.60
5:E:181:ILE:HG23	5:E:181:ILE:O	2.01	0.60
6:F:99:GLU:OE2	6:F:104:THR:HG22	2.02	0.59
23:X:6:LEU:O	25:Z:88:ARG:NH2	2.35	0.59
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.37	0.59
13:M:343:ILE:O	13:M:346:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:261:ILE:HG13	12:L:317:ILE:HD11	1.84	0.59
19:S:57:CYS:O	19:S:60:VAL:HG22	2.02	0.59
14:N:3:PRO:HB2	15:O:9:ILE:HD11	1.85	0.58
23:X:43:MET:HE3	23:X:47:TRP:CZ3	2.38	0.58
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.32	0.58
13:M:57:PHE:HD1	13:M:113:MET:HG2	1.67	0.58
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.38	0.58
39:n:131:SER:OG	39:n:135:GLU:OE2	2.12	0.58
12:L:288:THR:HG21	12:L:307:SER:HB3	1.84	0.58
15:O:128:ILE:HD12	15:O:160:ILE:HD12	1.86	0.58
15:O:54:ALA:HB2	15:O:107:GLN:OE1	2.04	0.58
10:J:42:GLY:O	10:J:46:ASN:ND2	2.37	0.58
4:D:223:ASP:OD2	60:D:503:HOH:O	2.17	0.58
15:O:78:SER:O	15:O:96:LEU:HD22	2.04	0.58
4:D:68:LEU:HD23	4:D:73:VAL:HA	1.86	0.57
10:J:52:LEU:HD23	11:K:61:ILE:HD11	1.86	0.57
15:O:232:GLU:O	15:O:236:GLU:N	2.34	0.57
8:H:262:LYS:NZ	45:H:402:3PE:O14	2.38	0.57
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.87	0.57
13:M:419:TYR:OH	60:M:701:HOH:O	2.02	0.57
37:l:16:THR:HG23	37:l:19:GLU:H	1.70	0.57
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.35	0.57
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.87	0.56
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.37	0.56
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.11	0.56
31:f:11:TRP:O	31:f:14:VAL:HG22	2.05	0.56
13:M:187:HIS:ND1	60:M:704:HOH:O	2.32	0.56
37:l:149:GLU:OE1	37:l:149:GLU:N	2.38	0.56
2:B:165:LYS:NZ	42:q:77:VAL:O	2.38	0.56
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.88	0.56
45:L:703:3PE:H2	45:L:703:3PE:O32	2.06	0.56
15:O:272:TYR:HA	15:O:275:ILE:HG23	1.87	0.56
1:A:93:PHE:CZ	1:A:97:LEU:HD11	2.41	0.55
13:M:105:PHE:O	13:M:109:THR:OG1	2.17	0.55
13:M:282:LEU:HD21	13:M:342:MET:HG3	1.89	0.55
15:O:129:TYR:CE2	15:O:160:ILE:HD11	2.42	0.55
10:J:25:SER:OG	10:J:77:GLU:OE2	2.18	0.55
20:U:68:GLU:O	20:U:71:MET:HE2	2.07	0.55
14:N:313:MET:HE2	15:O:59:VAL:HG21	1.89	0.55
4:D:415:VAL:HG21	8:H:207:LEU:HD11	1.87	0.55
7:G:237:ASN:N	7:G:237:ASN:HD22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M:602:PC1:O13	47:M:602:PC1:H152	2.06	0.55
11:K:42:VAL:O	11:K:46:LEU:HD13	2.07	0.54
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.38	0.54
13:M:114:GLU:HG2	23:X:168:PHE:HB3	1.90	0.54
23:X:43:MET:HE3	23:X:47:TRP:HZ3	1.73	0.54
8:H:4:ILE:HG22	8:H:8:MET:HE2	1.89	0.54
15:O:11:GLY:O	15:O:13:LYS:N	2.40	0.54
20:T:7:THR:O	20:T:7:THR:HG23	2.07	0.54
58:U:101:EHZ:O5	58:U:101:EHZ:O6	2.26	0.54
20:T:8:LEU:C	20:T:8:LEU:HD23	2.33	0.54
14:N:88:LYS:HG2	14:N:148:SER:HB3	1.90	0.54
11:K:37:MET:HB2	14:N:68:MET:HE1	1.89	0.53
52:N:1305:I49:I02	29:d:82:MET:O	2.95	0.53
31:f:48:LEU:HD22	31:f:52:GLU:HG2	1.90	0.53
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.89	0.53
8:H:222:LEU:HD23	8:H:225:MET:CE	2.39	0.53
9:I:170:GLN:NE2	60:I:304:HOH:O	2.26	0.53
10:J:170:GLU:OE1	10:J:173:ARG:NH1	2.42	0.53
20:U:11:ILE:O	20:U:15:VAL:HG23	2.08	0.53
4:D:414:VAL:O	4:D:418:ILE:HD12	2.08	0.53
43:r:32:LYS:O	43:r:35:GLN:NE2	2.41	0.53
15:O:115:LEU:O	15:O:115:LEU:HD23	2.09	0.53
16:P:82:ARG:HG2	16:P:120:VAL:HG13	1.91	0.53
5:E:105:THR:HG22	5:E:106:THR:H	1.74	0.53
13:M:271:MET:HE2	13:M:271:MET:HA	1.91	0.53
20:U:68:GLU:OE1	39:n:17:ARG:NH1	2.34	0.52
4:D:49:LEU:HD23	4:D:50:ASN:O	2.09	0.52
7:G:297:GLU:OE2	22:W:123:TYR:CE2	2.62	0.52
8:H:120:GLY:O	8:H:123:SER:OG	2.22	0.52
47:M:602:PC1:H143	53:h:1001:CDL:OA3	2.08	0.52
16:P:293:ILE:HG22	16:P:295:PRO:HD3	1.91	0.52
32:g:66:PHE:O	32:g:71:VAL:HG23	2.08	0.52
2:B:78:ALA:O	2:B:79:SER:CB	2.58	0.52
23:X:122:GLY:N	25:Z:66:GLU:OE2	2.43	0.52
15:O:303:LYS:O	29:d:50:ARG:NH2	2.42	0.52
37:l:128:VAL:HG12	40:o:98:MET:HG3	1.92	0.52
8:H:233:MET:HE1	8:H:234:MET:HE3	1.92	0.51
32:g:57:ASN:ND2	32:g:57:ASN:O	2.43	0.51
7:G:648:LEU:HA	7:G:651:LEU:HD23	1.92	0.51
13:M:114:GLU:OE2	13:M:174:LEU:HB2	2.11	0.51
12:L:7:LEU:HA	12:L:10:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:316:GLN:OE1	15:O:59:VAL:HG12	2.09	0.51
10:J:76:THR:HG22	10:J:77:GLU:H	1.74	0.51
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.93	0.51
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.44	0.51
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.92	0.51
1:A:79:SER:HA	1:A:87:MET:HE2	1.93	0.51
10:J:141:MET:HE1	30:e:26:HIS:ND1	2.26	0.51
12:L:301:ILE:CG2	12:L:426:ILE:HD11	2.40	0.51
29:d:94:ILE:HD13	33:h:106:LYS:HD3	1.92	0.51
23:X:4:VAL:HG13	23:X:4:VAL:O	2.10	0.51
13:M:18:SER:OG	13:M:26:ASN:ND2	2.43	0.51
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.92	0.51
23:X:30:HIS:O	23:X:31:TYR:HB3	2.09	0.50
1:A:80:GLN:HG3	8:H:317:GLN:HG3	1.92	0.50
2:B:51:GLY:HA2	2:B:56:ALA:HB2	1.93	0.50
26:a:49:GLU:OE1	26:a:52:ARG:NH2	2.39	0.50
7:G:627:SER:OG	7:G:629:ASN:OD1	2.28	0.50
8:H:121:TRP:CE2	10:J:27:ILE:HD12	2.46	0.50
2:B:59:MET:HE1	4:D:56:PRO:CB	2.41	0.50
13:M:416:ARG:NH2	60:M:705:HOH:O	2.45	0.50
13:M:413:MET:HE1	37:l:85:ILE:HD13	1.94	0.50
7:G:415:LEU:O	7:G:416:THR:OG1	2.14	0.50
15:O:138:MET:HE2	15:O:144:ILE:HG21	1.94	0.50
21:V:65:LYS:O	21:V:69:GLU:OE1	2.28	0.50
25:Z:86:MET:HE1	25:Z:125:TYR:CE1	2.47	0.50
6:F:306:LEU:C	6:F:306:LEU:HD12	2.37	0.50
8:H:70:MET:HE1	8:H:121:TRP:CE3	2.47	0.50
16:P:22:THR:OG1	16:P:88:SER:OG	2.20	0.50
21:V:20:HIS:NE2	21:V:61:GLU:O	2.43	0.50
5:E:111:ARG:NH1	6:F:260:GLY:O	2.45	0.49
10:J:20:PHE:CE1	10:J:33:LEU:HB2	2.47	0.49
14:N:132:THR:OG1	14:N:133:TRP:N	2.44	0.49
10:J:68:PHE:O	10:J:72:THR:OG1	2.24	0.49
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.95	0.49
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.47	0.49
13:M:127:VAL:HB	13:M:128:PRO:HD3	1.94	0.49
16:P:98:GLU:OE1	16:P:283:LYS:NZ	2.37	0.49
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.30	0.49
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.48	0.49
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.94	0.49
12:L:288:THR:HG21	12:L:307:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:182:GLN:NE2	60:G:912:HOH:O	2.39	0.49
10:J:136:PHE:CE2	10:J:141:MET:SD	3.06	0.49
14:N:2:ASN:OD1	14:N:4:ILE:N	2.43	0.49
15:O:69:LEU:HD22	15:O:299:LEU:HD23	1.95	0.49
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.93	0.48
15:O:247:PRO:O	15:O:251:GLN:NE2	2.38	0.48
5:E:120:ILE:HD11	5:E:169:ILE:HG12	1.95	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.48
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.49	0.48
20:T:31:SER:O	20:T:34:SER:N	2.39	0.48
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.94	0.48
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.47	0.48
15:O:172:VAL:HG13	15:O:172:VAL:O	2.14	0.48
34:i:111:GLU:OE1	41:p:16:THR:HG22	2.13	0.48
7:G:534:ARG:NH2	7:G:558:ASP:OD1	2.46	0.48
9:I:54:LYS:O	60:I:302:HOH:O	2.20	0.48
16:P:248:VAL:HG13	16:P:315:ILE:HD13	1.96	0.48
3:C:32:ILE:HG22	3:C:33:LEU:HD22	1.96	0.48
8:H:199:ASP:OD1	8:H:199:ASP:N	2.47	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.96	0.48
43:r:71:SER:O	43:r:72:GLN:C	2.57	0.48
8:H:63:PRO:O	8:H:64:ALA:HB3	2.14	0.48
11:K:1:FME:HE3	11:K:4:VAL:HG11	1.96	0.48
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.46	0.48
14:N:108:MET:SD	14:N:191:THR:HG21	2.53	0.48
38:m:60:GLU:OE2	38:m:65:VAL:HG21	2.14	0.48
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.49	0.48
25:Z:99:LYS:O	25:Z:100:ASP:HB2	2.14	0.48
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.31	0.47
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.96	0.47
2:B:172:ARG:NH1	51:H:401:LMT:O2'	2.46	0.47
3:C:58:ILE:HD11	3:C:119:SER:O	2.15	0.47
25:Z:127:LEU:O	30:e:79:ARG:NH1	2.47	0.47
1:A:57:LEU:O	1:A:61:THR:OG1	2.16	0.47
41:p:16:THR:HG23	41:p:16:THR:O	2.13	0.47
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.48	0.47
37:l:65:ASP:OD1	38:m:43:LYS:NZ	2.46	0.47
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.41	0.47
17:Q:13:VAL:HG23	17:Q:13:VAL:O	2.14	0.47
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.45	0.47
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:172:MET:HE3	8:H:177:PRO:HD3	1.97	0.47
13:M:285:LEU:HD23	13:M:285:LEU:O	2.14	0.47
15:O:45:LYS:NZ	15:O:232:GLU:OE2	2.41	0.47
15:O:128:ILE:CD1	15:O:160:ILE:HD12	2.45	0.47
12:L:331:THR:HB	12:L:387:THR:HG22	1.97	0.47
15:O:24:LEU:O	15:O:167:HIS:N	2.48	0.47
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	1.97	0.47
8:H:233:MET:SD	8:H:234:MET:HE2	2.54	0.47
23:X:98:ARG:HG2	23:X:98:ARG:HH11	1.80	0.47
13:M:285:LEU:HD23	13:M:285:LEU:C	2.40	0.47
23:X:120:ASP:OD1	23:X:121:LEU:N	2.48	0.47
33:h:34:ILE:HB	33:h:35:PRO:HD3	1.97	0.47
14:N:306:PRO:O	14:N:307:SER:CB	2.63	0.46
15:O:38:LEU:HD11	15:O:234:VAL:HG21	1.95	0.46
30:e:48:SER:O	30:e:52:GLU:HG3	2.15	0.46
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.97	0.46
9:I:95:GLU:OE2	42:q:130:THR:HG21	2.14	0.46
13:M:403:THR:HA	13:M:406:TYR:CE1	2.50	0.46
37:l:141:GLU:N	37:l:141:GLU:OE1	2.48	0.46
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.45	0.46
12:L:124:PHE:HD1	12:L:150:MET:HB2	1.81	0.46
20:T:8:LEU:O	20:T:11:ILE:N	2.48	0.46
7:G:540:ASP:OD1	7:G:540:ASP:N	2.46	0.46
11:K:37:MET:HG3	11:K:67:ALA:CB	2.45	0.46
12:L:233:LEU:HD11	12:L:248:HIS:NE2	2.30	0.46
13:M:325:MET:SD	13:M:362:ALA:HB2	2.56	0.46
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.97	0.46
10:J:132:ASP:OD2	10:J:132:ASP:N	2.48	0.46
10:J:136:PHE:CE2	30:e:28:ILE:HD11	2.50	0.46
11:K:9:MET:CG	11:K:43:MET:HE1	2.46	0.46
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.98	0.46
8:H:8:MET:CE	26:a:26:ILE:HD11	2.45	0.46
8:H:179:TRP:N	8:H:180:PRO:CD	2.79	0.46
10:J:76:THR:HG22	10:J:77:GLU:N	2.31	0.46
12:L:301:ILE:HG21	12:L:426:ILE:HD11	1.96	0.46
12:L:375:VAL:HG22	35:j:32:MET:SD	2.54	0.46
14:N:230:LEU:HD11	14:N:244:ILE:HG21	1.98	0.46
12:L:124:PHE:CE2	12:L:251:THR:HG21	2.50	0.46
13:M:370:PRO:HB3	13:M:375:LEU:CD2	2.46	0.46
15:O:106:LEU:HD13	15:O:270:LEU:HD21	1.97	0.46
2:B:59:MET:SD	4:D:56:PRO:HB3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:33:VAL:HG22	7:G:33:VAL:O	2.14	0.46
6:F:192:LEU:HD23	6:F:192:LEU:O	2.16	0.46
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.44	0.46
12:L:69:LEU:HD21	12:L:71:ILE:HD11	1.97	0.46
23:X:21:SER:HG	26:a:51:ASP:CG	2.23	0.46
23:X:21:SER:OG	26:a:51:ASP:OD1	2.34	0.46
10:J:141:MET:CE	30:e:26:HIS:ND1	2.79	0.45
15:O:229:GLN:O	15:O:231:ALA:N	2.49	0.45
29:d:103:GLU:OE1	29:d:103:GLU:N	2.48	0.45
2:B:30:VAL:HG11	2:B:174:ARG:HA	1.99	0.45
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.46	0.45
45:A:901:3PE:H3C2	45:A:901:3PE:H3G1	1.98	0.45
2:B:91:THR:HA	2:B:119:CYS:HB3	1.97	0.45
3:C:37:VAL:HG12	43:r:69:MET:CE	2.47	0.45
13:M:243:MET:O	13:M:247:THR:HG23	2.16	0.45
14:N:146:PHE:N	14:N:147:PRO:CD	2.79	0.45
14:N:223:SER:OG	14:N:321:LYS:NZ	2.50	0.45
45:O:1201:3PE:H321	29:d:53:VAL:HG21	1.97	0.45
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.99	0.45
5:E:108:CYS:HA	5:E:151:ALA:HB1	1.98	0.45
9:I:124:GLU:OE2	60:I:303:HOH:O	2.21	0.45
12:L:82:MET:HE3	12:L:87:MET:HE1	1.99	0.45
22:W:50:PHE:O	22:W:100:ARG:NH1	2.50	0.45
32:g:85:MET:O	32:g:85:MET:HG2	2.17	0.45
4:D:208:MET:HE1	4:D:318:MET:HB2	1.98	0.45
21:V:43:TYR:O	21:V:47:THR:OG1	2.27	0.45
36:k:24:GLU:OE1	36:k:24:GLU:N	2.45	0.45
37:l:34:TYR:OH	37:l:46:ASP:O	2.19	0.45
7:G:486:ASP:N	7:G:486:ASP:OD2	2.50	0.45
15:O:51:PHE:HB3	15:O:107:GLN:HE21	1.82	0.45
37:l:115:MET:CE	59:o:201:MYR:H142	2.47	0.45
10:J:20:PHE:CZ	11:K:31:LEU:HB3	2.52	0.45
15:O:221:LEU:HD21	15:O:241:LEU:HD21	1.98	0.45
12:L:1:FME:O	12:L:5:SER:OG	2.32	0.45
12:L:398:ALA:O	12:L:402:SER:OG	2.28	0.45
12:L:477:ILE:HD11	40:o:54:GLN:HA	1.98	0.45
16:P:143:SER:OG	16:P:282:ASP:OD1	2.34	0.45
20:T:68:GLU:OE2	22:W:33:ARG:NE	2.50	0.45
37:l:71:LEU:HD11	37:l:81:LEU:CD1	2.39	0.45
42:q:144:TYR:O	42:q:145:LYS:C	2.59	0.45
4:D:427:GLU:O	4:D:430:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:315:VAL:O	7:G:340:SER:OG	2.26	0.44
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.44
15:O:115:LEU:HD23	15:O:115:LEU:C	2.42	0.44
23:X:1:PRO:N	25:Z:108:GLU:OE1	2.50	0.44
6:F:98:ASP:O	6:F:99:GLU:C	2.61	0.44
7:G:324:ASP:OD2	60:G:904:HOH:O	2.21	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.80	0.44
11:K:1:FME:HE3	11:K:4:VAL:CG1	2.46	0.44
13:M:56:PHE:HA	13:M:111:THR:O	2.17	0.44
37:l:30:ARG:NE	38:m:34:GLU:OE2	2.50	0.44
1:A:68:GLU:CG	10:J:161:LEU:HD13	2.47	0.44
15:O:158:VAL:HG22	15:O:158:VAL:O	2.17	0.44
23:X:12:LEU:HD13	25:Z:85:GLN:HG3	1.99	0.44
30:e:16:TRP:CE3	30:e:17:MET:HB2	2.52	0.44
10:J:51:PHE:CD1	10:J:143:ILE:HD13	2.51	0.44
15:O:31:ILE:HD12	15:O:31:ILE:H	1.82	0.44
16:P:149:LYS:NZ	56:P:501:NDP:O2D	2.39	0.44
7:G:281:GLU:OE1	16:P:1:LEU:N	2.38	0.44
8:H:255:TYR:CD2	8:H:255:TYR:C	2.96	0.44
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.47	0.44
29:d:106:LYS:HD2	41:p:78:GLU:HB2	1.99	0.44
2:B:50:PHE:HZ	2:B:103:VAL:HG21	1.83	0.44
4:D:77:ASP:OD2	4:D:79:HIS:NE2	2.50	0.44
4:D:171:PHE:CD1	4:D:174:ARG:HD3	2.53	0.44
10:J:136:PHE:CD2	10:J:141:MET:SD	3.11	0.44
11:K:73:LEU:HD21	14:N:41:ILE:HG13	2.00	0.44
12:L:25:ASN:O	51:L:704:LMT:O2'	2.35	0.44
13:M:47:ASP:OD1	13:M:48:ASN:N	2.49	0.44
40:o:27:ASP:OD1	40:o:27:ASP:N	2.48	0.44
43:r:102:ARG:HG3	43:r:102:ARG:HH11	1.82	0.44
6:F:423:ARG:N	6:F:424:PRO:HD2	2.33	0.44
13:M:6:ILE:HD12	31:f:23:GLY:CA	2.47	0.44
5:E:194:GLU:HB2	5:E:199:LEU:HD23	1.99	0.44
8:H:223:PHE:O	8:H:227:GLU:HG3	2.18	0.44
12:L:99:SER:OG	60:L:801:HOH:O	2.00	0.44
40:o:117:ARG:NH2	40:o:118:GLU:OE1	2.50	0.44
13:M:294:MET:HE2	13:M:294:MET:HA	2.00	0.44
36:k:17:ASP:OD1	36:k:18:TYR:N	2.51	0.44
37:l:58:ARG:NH2	37:l:75:GLU:OE2	2.51	0.44
42:q:78:ASP:OD2	42:q:80:SER:OG	2.31	0.44
13:M:126:LEU:O	13:M:130:LEU:HD23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:250:HIS:O	8:H:251:MET:HE2	2.18	0.43
9:I:108:ARG:HB2	42:q:130:THR:HG23	2.00	0.43
9:I:145:GLU:OE2	16:P:66:GLY:N	2.48	0.43
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.99	0.43
1:A:104:TYR:O	1:A:108:GLN:HG2	2.17	0.43
12:L:124:PHE:CZ	12:L:251:THR:HG21	2.53	0.43
31:f:25:TYR:CE2	31:f:29:LYS:HD2	2.53	0.43
7:G:60:GLU:O	7:G:61:LYS:HB2	2.18	0.43
10:J:26:PRO:HG3	10:J:76:THR:HG21	2.01	0.43
22:W:96:VAL:O	22:W:96:VAL:CG1	2.64	0.43
28:c:12:PRO:O	28:c:14:TRP:N	2.52	0.43
40:o:32:GLU:N	40:o:32:GLU:OE1	2.52	0.43
4:D:300:ARG:NH2	4:D:420:THR:O	2.50	0.43
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.99	0.43
6:F:192:LEU:HD23	6:F:192:LEU:C	2.42	0.43
22:W:51:GLN:C	22:W:100:ARG:HH12	2.27	0.43
6:F:344:VAL:HG23	6:F:425:GLU:OE1	2.18	0.43
8:H:23:VAL:HG21	26:a:12:MET:HE2	2.00	0.43
14:N:250:SER:O	14:N:259:GLY:HA3	2.18	0.43
18:R:43:LEU:HD22	42:q:107:LYS:HE2	2.00	0.43
10:J:7:PHE:O	10:J:10:SER:OG	2.30	0.43
13:M:57:PHE:CD1	13:M:113:MET:HG2	2.49	0.43
3:C:121:VAL:N	3:C:122:PRO:CD	2.82	0.43
11:K:59:MET:HB3	11:K:60:PRO:HD3	2.00	0.43
12:L:203:MET:HG2	41:p:109:LEU:HD11	2.01	0.43
13:M:116:ILE:HG12	13:M:174:LEU:HD13	1.99	0.43
16:P:97:ARG:HE	56:P:501:NDP:H8A	1.83	0.43
16:P:248:VAL:HG13	16:P:315:ILE:CD1	2.49	0.43
7:G:10:GLU:HG3	7:G:19:MET:HE2	2.00	0.43
15:O:43:ALA:O	15:O:47:GLY:N	2.52	0.43
15:O:183:ILE:HG13	15:O:184:GLN:N	2.34	0.43
22:W:42:GLU:OE1	22:W:45:ASN:HB2	2.19	0.43
23:X:28:ALA:O	23:X:30:HIS:O	2.37	0.43
15:O:83:TYR:CE2	15:O:194:ILE:CG2	3.01	0.42
12:L:407:TRP:HB2	59:o:201:MYR:H143	2.00	0.42
16:P:248:VAL:CG1	16:P:315:ILE:HD13	2.49	0.42
21:V:77:GLU:OE2	21:V:77:GLU:N	2.45	0.42
6:F:90:PRO:O	6:F:218:CYS:HB3	2.19	0.42
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.00	0.42
12:L:40:ILE:HG13	12:L:101:MET:SD	2.59	0.42
12:L:230:HIS:H	12:L:231:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:MET:HE1	4:D:56:PRO:HB2	2.01	0.42
12:L:82:MET:HE3	12:L:87:MET:CE	2.49	0.42
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.55	0.42
45:N:1301:3PE:H2I3	45:O:1201:3PE:H2F1	2.01	0.42
12:L:264:TYR:N	12:L:265:PRO:CD	2.82	0.42
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.55	0.42
13:M:80:SER:OG	13:M:226:ALA:HB2	2.19	0.42
3:C:33:LEU:HD13	21:V:98:PRO:CB	2.49	0.42
16:P:299:GLY:N	16:P:302:ASP:OD2	2.47	0.42
47:B:202:PC1:O13	47:B:202:PC1:C14	2.68	0.42
11:K:56:ALA:HA	30:e:17:MET:HE3	2.02	0.42
15:O:194:ILE:CD1	15:O:199:LEU:HD11	2.48	0.42
15:O:231:ALA:O	15:O:235:VAL:HG23	2.19	0.42
1:A:102:LEU:HD23	45:A:901:3PE:H2A1	2.02	0.42
4:D:167:PHE:CE1	4:D:171:PHE:CE2	3.08	0.42
39:n:12:GLN:NE2	39:n:16:LEU:HD11	2.35	0.42
1:A:22:PHE:HB3	1:A:23:TRP:HD1	1.84	0.42
1:A:46:SER:HA	10:J:77:GLU:HA	2.02	0.42
1:A:109:LYS:HE2	1:A:109:LYS:HA	2.02	0.42
4:D:47:LEU:HD12	4:D:68:LEU:HD11	2.00	0.42
15:O:138:MET:HE2	15:O:144:ILE:CG2	2.50	0.42
37:l:52:ASP:OD2	37:l:78:HIS:NE2	2.51	0.42
37:l:54:SER:HA	37:l:84:TYR:HB3	2.02	0.42
9:I:75:GLU:O	9:I:105:ARG:NH1	2.52	0.42
10:J:14:VAL:HG22	11:K:7:ASN:O	2.20	0.42
15:O:28:ASP:N	15:O:170:VAL:O	2.50	0.42
15:O:238:ILE:HA	15:O:241:LEU:HG	2.02	0.42
26:a:59:ARG:HD2	26:a:61:TYR:OH	2.20	0.42
14:N:299:SER:O	14:N:303:THR:HB	2.20	0.41
15:O:32:CYS:N	54:O:1202:GTP:O2B	2.44	0.41
40:o:30:PHE:HB3	40:o:33:ARG:HG3	2.01	0.41
7:G:298:ASP:OD2	7:G:298:ASP:C	2.61	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.41
12:L:247:LEU:HD22	12:L:248:HIS:CD2	2.56	0.41
42:q:12:GLN:OE1	42:q:15:SER:OG	2.38	0.41
1:A:99:ALA:HB1	45:A:901:3PE:H2B1	2.01	0.41
7:G:318:ILE:HD11	7:G:514:ILE:HD13	2.02	0.41
25:Z:86:MET:HE1	25:Z:125:TYR:CZ	2.55	0.41
29:d:10:THR:O	29:d:10:THR:HG23	2.20	0.41
45:A:902:3PE:O31	45:A:902:3PE:O22	2.38	0.41
4:D:117:ALA:HB2	4:D:367:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:83:TYR:OH	54:O:1202:GTP:O2'	2.38	0.41
1:A:105:GLU:HG2	10:J:169:MET:SD	2.60	0.41
8:H:233:MET:HE3	8:H:233:MET:HB3	1.92	0.41
17:Q:44:ASN:OD1	17:Q:44:ASN:O	2.38	0.41
38:m:112:GLU:OE2	38:m:112:GLU:HA	2.21	0.41
12:L:8:SER:HB3	12:L:82:MET:HE2	2.02	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.41
36:k:27:PRO:HG2	36:k:52:TYR:CE1	2.56	0.41
37:l:105:LEU:O	37:l:109:VAL:HG23	2.21	0.41
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.03	0.41
3:C:148:LEU:O	22:W:88:MET:HE2	2.21	0.41
6:F:374:LYS:NZ	60:F:607:HOH:O	2.49	0.41
8:H:102:VAL:HG11	8:H:154:LEU:HD11	2.03	0.41
2:B:49:THR:CG2	2:B:59:MET:HE2	2.39	0.41
2:B:59:MET:SD	4:D:56:PRO:CB	3.09	0.41
17:Q:93:VAL:O	17:Q:97:GLU:HG2	2.21	0.41
28:c:4:ILE:HG23	28:c:5:GLN:HG3	2.03	0.41
5:E:33:ALA:HB2	44:s:56:LEU:HD12	2.03	0.41
6:F:93:LEU:O	6:F:134:ALA:HA	2.21	0.41
6:F:338:ASP:OD1	6:F:338:ASP:C	2.62	0.41
10:J:64:MET:HE2	11:K:68:ALA:HA	2.02	0.41
10:J:141:MET:HE2	30:e:25:PRO:HB2	2.02	0.41
12:L:233:LEU:HD11	12:L:248:HIS:CE1	2.56	0.41
13:M:210:TYR:CG	13:M:268:GLY:HA3	2.56	0.41
20:T:16:LEU:HD12	20:T:30:LEU:HD21	2.02	0.41
20:U:52:MET:HE1	39:n:23:LEU:HB3	2.03	0.41
28:c:33:LYS:O	28:c:37:GLU:HG3	2.20	0.41
29:d:103:GLU:N	29:d:103:GLU:CD	2.79	0.41
39:n:70:PHE:O	39:n:74:GLN:N	2.54	0.41
43:r:69:MET:SD	43:r:70:SER:N	2.94	0.41
4:D:104:ASP:OD1	4:D:115:GLU:OE2	2.38	0.41
7:G:35:MET:SD	7:G:81:THR:CB	3.09	0.41
10:J:37:GLY:HA2	11:K:38:LEU:HD21	2.03	0.41
16:P:48:PRO:HB2	16:P:73:TRP:CD1	2.56	0.41
7:G:377:VAL:HG13	7:G:452:ILE:CD1	2.51	0.40
7:G:568:GLU:HA	7:G:587:VAL:O	2.21	0.40
8:H:4:ILE:CG2	8:H:8:MET:HE2	2.50	0.40
8:H:288:LEU:O	8:H:292:ASN:HB2	2.20	0.40
10:J:51:PHE:O	10:J:55:MET:HG2	2.20	0.40
11:K:95:LEU:HB2	14:N:54:GLU:OE1	2.21	0.40
12:L:253:VAL:HB	12:L:310:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:47:ASN:O	14:N:48:HIS:HB2	2.20	0.40
28:c:43:LYS:O	28:c:47:GLY:N	2.54	0.40
51:g:1101:LMT:O5B	51:g:1101:LMT:H3'	2.21	0.40
8:H:70:MET:HE3	8:H:121:TRP:HB2	2.04	0.40
15:O:78:SER:OG	15:O:80:GLU:N	2.53	0.40
21:V:71:LEU:HD13	21:V:79:VAL:HG11	2.03	0.40
12:L:67:HIS:HB3	45:L:703:3PE:H112	2.03	0.40
15:O:129:TYR:CZ	15:O:160:ILE:HD11	2.56	0.40
16:P:152:GLY:O	16:P:156:VAL:HG23	2.21	0.40
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.56	0.40
5:E:106:THR:HB	5:E:107:PRO:HD3	2.02	0.40
5:E:145:LEU:HD12	5:E:153:MET:SD	2.62	0.40
6:F:277:LYS:O	6:F:281:GLU:HG2	2.21	0.40
6:F:300:GLY:HA3	6:F:329:LEU:O	2.22	0.40
7:G:317:ALA:HB3	7:G:343:LEU:HD13	2.03	0.40
11:K:24:SER:O	11:K:90:VAL:HG22	2.20	0.40
12:L:249:SER:OG	12:L:250:SER:N	2.55	0.40
13:M:134:THR:HG21	14:N:298:TYR:HE1	1.87	0.40
13:M:237:LYS:HB3	13:M:316:MET:HE2	2.04	0.40
20:U:51:ILE:HG21	20:U:67:ALA:HB1	2.04	0.40
35:j:12:ARG:NH1	60:j:101:HOH:O	2.48	0.40
7:G:35:MET:SD	7:G:81:THR:HB	2.61	0.40
11:K:9:MET:HG2	11:K:43:MET:HE1	2.04	0.40
20:T:9:GLU:O	20:T:13:ASP:OD2	2.39	0.40
20:T:25:ILE:HG21	20:T:30:LEU:HD12	2.03	0.40
22:W:42:GLU:OE2	22:W:94:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/115 (77%)	87 (98%)	2 (2%)	0	100	100
2	B	152/216 (70%)	140 (92%)	11 (7%)	1 (1%)	18	34
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	383/463 (83%)	370 (97%)	13 (3%)	0	100	100
5	E	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
6	F	428/464 (92%)	411 (96%)	17 (4%)	0	100	100
7	G	686/727 (94%)	663 (97%)	23 (3%)	0	100	100
8	H	309/318 (97%)	294 (95%)	15 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	123/175 (70%)	115 (94%)	8 (6%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	545/606 (90%)	522 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	O	318/343 (93%)	302 (95%)	16 (5%)	0	100	100
16	P	280/380 (74%)	276 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	92/124 (74%)	89 (97%)	3 (3%)	0	100	100
19	S	80/99 (81%)	79 (99%)	1 (1%)	0	100	100
20	T	74/156 (47%)	71 (96%)	3 (4%)	0	100	100
20	U	82/156 (53%)	81 (99%)	1 (1%)	0	100	100
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	18/141 (13%)	16 (89%)	2 (11%)	0	100	100
25	Z	138/144 (96%)	129 (94%)	9 (6%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	43 (94%)	3 (6%)	0	100	100
29	d	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	86/154 (56%)	83 (96%)	3 (4%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	63 (97%)	2 (3%)	0	100	100
36	k	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
38	m	104/129 (81%)	100 (96%)	4 (4%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	118/137 (86%)	112 (95%)	6 (5%)	0	100	100
41	p	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
42	q	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	39 (95%)	2 (5%)	0	100	100
All	All	7693/9212 (84%)	7447 (97%)	245 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	79	SER

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	80/100 (80%)	80 (100%)	0	100	100
2	B	130/175 (74%)	130 (100%)	0	100	100
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	332/392 (85%)	332 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	344/368 (94%)	344 (100%)	0	100	100
7	G	578/608 (95%)	577 (100%)	1 (0%)	87	95
8	H	270/274 (98%)	270 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	100/141 (71%)	100 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	475/533 (89%)	475 (100%)	0	100	100
13	M	406/412 (98%)	406 (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	247/327 (76%)	247 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	69 (99%)	1 (1%)	59	81
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	15/102 (15%)	15 (100%)	0	100	100
25	Z	119/121 (98%)	119 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100
31	f	49/54 (91%)	49 (100%)	0	100	100
32	g	79/131 (60%)	79 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	99/120 (82%)	99 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	96/115 (84%)	96 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	6809/7892 (86%)	6807 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
7	G	237	ASN
20	T	44(A)	SER

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

Mol	Chain	Res	Type
2	B	82	GLN
3	C	39	GLN
3	C	69	ASN
3	C	192	GLN
4	D	55	HIS
4	D	201	GLN
4	D	231	ASN
6	F	29	HIS
6	F	200	GLN
6	F	356	HIS
6	F	421	HIS
6	F	437	HIS
7	G	155	GLN
7	G	237	ASN
7	G	401	HIS
7	G	402	ASN
7	G	517	ASN
7	G	581	GLN

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Mol	Chain	Res	Type
7	G	665	GLN
8	H	47	GLN
12	L	199	GLN
12	L	296	ASN
12	L	348	HIS
12	L	447	ASN
12	L	514	HIS
13	M	44	GLN
13	M	103	GLN
13	M	138	ASN
13	M	180	GLN
14	N	91	ASN
14	N	150	ASN
14	N	222	ASN
15	O	167	HIS
16	P	8	HIS
16	P	93	ASN
18	R	51	GLN
19	S	80	ASN
20	T	74	GLN
22	W	99	GLN
23	X	29	HIS
27	b	10	ASN
28	c	9	HIS
30	e	76	HIS
32	g	86	GLN
33	h	124	HIS
35	j	58	GLN
37	l	28	ASN
37	l	126	GLN
37	l	147	ASN
37	l	155	HIS
38	m	125	ASN
39	n	32	HIS
39	n	74	GLN
39	n	159	GLN
41	p	143	HIS
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	2MR	D	85	4	10,12,13	2.77	4 (40%)	5,13,15	1.03	0
13	FME	M	1	13	8,9,10	1.02	1 (12%)	8,9,11	0.97	1 (12%)
12	FME	L	1	12	8,9,10	1.01	1 (12%)	8,9,11	0.73	0
11	FME	K	1	11	8,9,10	0.98	0	8,9,11	1.02	1 (12%)
43	AYA	r	1	43	6,7,8	1.89	2 (33%)	6,8,10	1.38	1 (16%)
8	FME	H	1	8	8,9,10	1.00	0	8,9,11	1.07	0
1	FME	A	1	1	8,9,10	0.95	0	8,9,11	1.10	1 (12%)
34	SAC	i	1	34	7,8,9	1.93	1 (14%)	7,9,11	2.13	1 (14%)
14	FME	N	1	14	8,9,10	1.01	0	8,9,11	0.86	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
4	2MR	D	85	4	-	0/10/13/15	-
13	FME	M	1	13	-	1/7/9/11	-
12	FME	L	1	12	-	5/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
8	FME	H	1	8	-	0/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
34	SAC	i	1	34	-	5/7/8/10	-
14	FME	N	1	14	-	2/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.44	1.44	1.33
4	D	85	2MR	CZ-NE	4.68	1.44	1.34
34	i	1	SAC	O-C	4.44	1.36	1.20
4	D	85	2MR	O-C	4.16	1.35	1.20
43	r	1	AYA	CT-N	3.48	1.45	1.34
43	r	1	AYA	OT-CT	-2.15	1.18	1.23
13	M	1	FME	CA-N	-2.13	1.43	1.46
12	L	1	FME	CA-N	-2.08	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.02	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.76	112.53	124.77
43	r	1	AYA	CM-CT-N	2.46	120.19	116.12
1	A	1	FME	C-CA-N	2.41	114.16	109.50
13	M	1	FME	C-CA-N	2.12	113.59	109.50
11	K	1	FME	C-CA-N	2.04	113.43	109.50

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
34	i	1	SAC	O-C-CA-CB
34	i	1	SAC	C-CA-CB-OG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
34	i	1	SAC	N-CA-CB-OG
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
13	M	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	1	0
11	K	1	FME	2	0
14	N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 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
46	SF4	B	201	2	0,12,12	-	-	-		
51	LMT	H	401	-	36,36,36	1.24	4 (11%)	47,47,47	1.04	2 (4%)
46	SF4	G	801	7	0,12,12	-	-	-		
45	3PE	I	201	-	50,50,50	0.88	4 (8%)	53,55,55	1.08	2 (3%)
51	LMT	K	901	-	36,36,36	1.15	2 (5%)	47,47,47	1.12	4 (8%)
51	LMT	g	1101	-	36,36,36	1.22	3 (8%)	47,47,47	0.86	0
52	I49	H	403	-	15,17,17	0.90	1 (6%)	17,22,22	1.92	6 (35%)
53	CDL	q	201	-	75,75,99	1.01	8 (10%)	81,87,111	1.13	4 (4%)
58	EHZ	U	101	20	31,36,37	1.53	4 (12%)	36,44,47	1.54	4 (11%)
48	FES	G	803	7	0,4,4	-	-	-		
53	CDL	X	201	-	51,51,99	1.19	7 (13%)	57,63,111	1.32	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	M	601	-	42,42,50	0.93	4 (9%)	45,47,55	1.03	2 (4%)
59	MYR	o	201	40	13,14,15	0.91	0	12,13,15	0.57	0
52	I49	N	1305	-	15,17,17	0.85	1 (6%)	17,22,22	1.83	4 (23%)
45	3PE	L	701	-	48,48,50	0.89	3 (6%)	51,53,55	1.17	3 (5%)
53	CDL	N	1304	-	64,64,99	1.07	8 (12%)	70,76,111	1.13	4 (5%)
51	LMT	p	201	-	36,36,36	1.17	3 (8%)	47,47,47	1.13	5 (10%)
49	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.25	6 (12%)
45	3PE	L	703	-	44,44,50	0.92	3 (6%)	47,49,55	1.26	4 (8%)
51	LMT	b	301	-	36,36,36	1.21	2 (5%)	47,47,47	0.96	1 (2%)
45	3PE	N	1301	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
51	LMT	N	1303	-	36,36,36	1.19	3 (8%)	47,47,47	1.06	4 (8%)
51	LMT	L	704	-	36,36,36	1.22	2 (5%)	47,47,47	0.81	1 (2%)
56	NDP	P	501	-	51,52,52	2.23	7 (13%)	71,80,80	1.49	14 (19%)
53	CDL	h	1001	-	66,66,99	1.08	8 (12%)	72,78,111	1.20	4 (5%)
45	3PE	A	901	-	47,47,50	0.89	4 (8%)	50,52,55	1.21	3 (6%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
46	SF4	I	203	9	0,12,12	-	-	-	-	-
45	3PE	O	1201	-	50,50,50	0.88	4 (8%)	53,55,55	1.05	2 (3%)
45	3PE	I	204	-	32,32,50	1.08	4 (12%)	35,37,55	1.09	2 (5%)
47	PC1	M	602	-	48,48,53	1.02	3 (6%)	54,56,61	1.02	2 (3%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
51	LMT	J	201	-	36,36,36	1.18	3 (8%)	47,47,47	0.94	1 (2%)
51	LMT	l	201	-	36,36,36	1.23	3 (8%)	47,47,47	0.90	0
53	CDL	L	702	-	68,68,99	1.05	7 (10%)	74,80,111	1.10	4 (5%)
54	GTP	O	1202	55	33,34,34	3.29	16 (48%)	50,54,54	1.93	15 (30%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
51	LMT	h	1002	-	36,36,36	1.14	2 (5%)	47,47,47	1.30	9 (19%)
46	SF4	I	202	9	0,12,12	-	-	-	-	-
58	EHZ	T	101	20	31,36,37	1.66	5 (16%)	36,44,47	1.83	7 (19%)
45	3PE	A	902	-	43,43,50	0.94	4 (9%)	46,48,55	1.13	2 (4%)
47	PC1	B	202	-	34,34,53	1.18	4 (11%)	40,42,61	1.11	2 (5%)
53	CDL	N	1302	-	66,66,99	1.06	7 (10%)	72,78,111	1.16	4 (5%)
45	3PE	H	402	-	33,33,50	1.28	4 (12%)	34,37,55	1.23	2 (5%)

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
51	LMT	H	401	-	-	9/21/61/61	0/2/2/2
46	SF4	B	201	2	-	-	0/6/5/5
46	SF4	G	801	7	-	-	0/6/5/5
45	3PE	I	201	-	-	18/54/54/54	-
51	LMT	K	901	-	-	7/21/61/61	0/2/2/2
51	LMT	g	1101	-	-	6/21/61/61	0/2/2/2
52	I49	H	403	-	-	5/10/10/10	0/1/1/1
53	CDL	q	201	-	-	41/86/86/110	-
58	EHZ	U	101	20	-	14/42/44/45	-
53	CDL	X	201	-	-	18/61/61/110	-
48	FES	G	803	7	-	-	0/1/1/1
45	3PE	M	601	-	-	18/46/46/54	-
59	MYR	o	201	40	-	7/12/12/13	-
52	I49	N	1305	-	-	4/10/10/10	0/1/1/1
45	3PE	L	701	-	-	22/52/52/54	-
53	CDL	N	1304	-	-	28/75/75/110	-
51	LMT	p	201	-	-	10/21/61/61	0/2/2/2
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
45	3PE	L	703	-	-	18/48/48/54	-
51	LMT	b	301	-	-	7/21/61/61	0/2/2/2
45	3PE	N	1301	-	-	18/54/54/54	-
51	LMT	N	1303	-	-	3/21/61/61	0/2/2/2
51	LMT	L	704	-	-	8/21/61/61	0/2/2/2
56	NDP	P	501	-	-	7/34/77/77	0/5/5/5
53	CDL	h	1001	-	-	35/77/77/110	-
45	3PE	A	901	-	-	25/51/51/54	-
46	SF4	F	502	6	-	-	0/6/5/5
46	SF4	I	203	9	-	-	0/6/5/5
45	3PE	O	1201	-	-	28/54/54/54	-
45	3PE	I	204	-	-	16/36/36/54	-
47	PC1	M	602	-	-	25/52/52/57	-
51	LMT	l	201	-	-	9/21/61/61	0/2/2/2
51	LMT	J	201	-	-	7/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
53	CDL	L	702	-	-	20/79/79/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	GTP	O	1202	55	-	5/22/38/38	0/3/3/3
46	SF4	G	802	7	-	-	0/6/5/5
51	LMT	h	1002	-	-	4/21/61/61	0/2/2/2
58	EHZ	T	101	20	-	15/42/44/45	-
46	SF4	I	202	9	-	-	0/6/5/5
45	3PE	A	902	-	-	23/47/47/54	-
47	PC1	B	202	-	-	20/38/38/57	-
53	CDL	N	1302	-	-	39/77/77/110	-
45	3PE	H	402	-	-	19/36/36/54	-

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.65	1.81	1.59
54	O	1202	GTP	O6-C6	8.70	1.40	1.23
54	O	1202	GTP	C5-N7	6.67	1.52	1.39
58	T	101	EHZ	C15-N2	5.53	1.46	1.33
58	T	101	EHZ	C12-N1	5.13	1.45	1.33
54	O	1202	GTP	PA-O3A	5.13	1.65	1.59
54	O	1202	GTP	PB-O3A	5.11	1.65	1.59
54	O	1202	GTP	C2-N1	4.85	1.49	1.37
54	O	1202	GTP	C2-N3	4.73	1.44	1.33
58	U	101	EHZ	C12-N1	4.73	1.44	1.33
54	O	1202	GTP	PB-O3B	4.72	1.64	1.59
58	U	101	EHZ	C15-N2	4.71	1.44	1.33
54	O	1202	GTP	C2-N2	4.68	1.45	1.34
54	O	1202	GTP	C8-N9	-4.48	1.27	1.37
45	H	402	3PE	O21-C2	-4.44	1.40	1.46
56	P	501	NDP	PA-O3	3.97	1.63	1.59
54	O	1202	GTP	C4-N9	-3.85	1.28	1.38
51	l	201	LMT	O5B-C1B	3.70	1.51	1.41
51	H	401	LMT	O5B-C1B	3.58	1.51	1.41
51	g	1101	LMT	O5B-C1B	3.55	1.51	1.41
56	P	501	NDP	PN-O5D	3.54	1.73	1.59
51	N	1303	LMT	O5B-C1B	3.48	1.50	1.41
51	p	201	LMT	O5B-C1B	3.44	1.50	1.41
51	b	301	LMT	O5B-C1B	3.40	1.50	1.41
51	h	1002	LMT	O5B-C1B	3.34	1.50	1.41
51	L	704	LMT	O5'-C1'	3.33	1.50	1.41
51	L	704	LMT	O5B-C1B	3.29	1.50	1.41
51	g	1101	LMT	O5'-C1'	3.24	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O2B-C2B	-3.22	1.33	1.44
51	J	201	LMT	O5B-C1B	3.19	1.50	1.41
51	J	201	LMT	O5'-C1'	3.15	1.50	1.41
49	F	501	FMN	C4A-N5	3.13	1.37	1.30
51	b	301	LMT	O5'-C1'	3.13	1.49	1.41
51	H	401	LMT	O5'-C1'	3.11	1.49	1.41
45	H	402	3PE	O21-C21	3.09	1.40	1.33
51	l	201	LMT	O5'-C1'	3.03	1.49	1.41
51	K	901	LMT	O5B-C1B	2.93	1.49	1.41
45	L	701	3PE	O21-C2	-2.88	1.39	1.46
53	q	201	CDL	OB6-CB4	-2.86	1.39	1.46
51	K	901	LMT	O5'-C1'	2.86	1.49	1.41
53	L	702	CDL	OA6-CA4	-2.85	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.83	1.39	1.46
53	h	1001	CDL	OB6-CB4	-2.82	1.40	1.46
53	L	702	CDL	OB6-CB4	-2.82	1.40	1.46
53	h	1001	CDL	OA6-CA4	-2.81	1.40	1.46
45	O	1201	3PE	O21-C2	-2.80	1.40	1.46
51	h	1002	LMT	O5'-C1'	2.80	1.49	1.41
58	U	101	EHZ	O4-C15	-2.78	1.18	1.23
54	O	1202	GTP	O4'-C1'	2.78	1.48	1.42
51	p	201	LMT	O5'-C1'	2.77	1.49	1.41
47	M	602	PC1	O21-C2	-2.77	1.40	1.46
45	L	703	3PE	O21-C2	-2.76	1.40	1.46
51	N	1303	LMT	O5'-C1'	2.75	1.48	1.41
53	X	201	CDL	OB6-CB4	-2.73	1.40	1.46
45	I	201	3PE	O21-C2	-2.71	1.40	1.46
53	X	201	CDL	OA6-CA4	-2.71	1.40	1.46
53	N	1302	CDL	OA6-CA4	-2.70	1.40	1.46
58	T	101	EHZ	O4-C15	-2.65	1.18	1.23
53	N	1304	CDL	OA6-CA4	-2.65	1.40	1.46
53	q	201	CDL	OB8-CB7	2.58	1.40	1.33
47	B	202	PC1	O21-C2	-2.58	1.40	1.46
53	N	1302	CDL	OB6-CB4	-2.58	1.40	1.46
45	N	1301	3PE	O21-C2	-2.57	1.40	1.46
45	M	601	3PE	O21-C2	-2.57	1.40	1.46
45	I	204	3PE	O21-C2	-2.56	1.40	1.46
58	U	101	EHZ	O3-C12	-2.52	1.18	1.23
45	L	703	3PE	O31-C31	2.51	1.40	1.33
53	N	1304	CDL	OB6-CB4	-2.49	1.40	1.46
58	T	101	EHZ	O3-C12	-2.49	1.18	1.23
45	A	902	3PE	O31-C31	2.48	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	H	403	I49	C15-N02	-2.45	1.31	1.36
47	M	602	PC1	O31-C31	2.41	1.40	1.33
45	A	901	3PE	O21-C2	-2.41	1.40	1.46
45	A	902	3PE	O21-C21	2.40	1.41	1.34
53	q	201	CDL	OA8-CA6	-2.39	1.39	1.45
47	M	602	PC1	O31-C3	-2.39	1.39	1.45
53	N	1304	CDL	OB8-CB7	2.38	1.40	1.33
53	N	1302	CDL	OB8-CB7	2.38	1.40	1.33
53	X	201	CDL	OB8-CB7	2.38	1.40	1.33
53	N	1302	CDL	OA8-CA7	2.38	1.40	1.33
45	I	201	3PE	O31-C3	-2.36	1.39	1.45
45	N	1301	3PE	O31-C31	2.36	1.40	1.33
45	A	901	3PE	O21-C21	2.35	1.40	1.34
54	O	1202	GTP	PG-O2G	-2.35	1.46	1.54
53	h	1001	CDL	OB8-CB6	-2.35	1.39	1.45
45	I	204	3PE	O31-C31	2.34	1.40	1.33
52	N	1305	I49	C15-N02	-2.34	1.31	1.36
45	L	701	3PE	O31-C31	2.34	1.40	1.33
51	p	201	LMT	O5B-C5B	2.33	1.50	1.44
45	O	1201	3PE	O31-C31	2.33	1.40	1.33
45	H	402	3PE	O31-C31	2.33	1.40	1.33
45	L	701	3PE	O31-C3	-2.33	1.40	1.45
53	L	702	CDL	OB8-CB6	-2.32	1.40	1.45
53	h	1001	CDL	OA8-CA6	-2.32	1.40	1.45
53	h	1001	CDL	OA8-CA7	2.32	1.40	1.33
53	L	702	CDL	OA8-CA6	-2.31	1.40	1.45
45	A	901	3PE	O31-C31	2.31	1.40	1.33
53	X	201	CDL	OA8-CA6	-2.31	1.40	1.45
45	M	601	3PE	O31-C31	2.31	1.40	1.33
47	B	202	PC1	O31-C31	2.29	1.40	1.33
45	I	201	3PE	O31-C31	2.29	1.40	1.33
47	B	202	PC1	O21-C21	2.29	1.40	1.34
53	N	1304	CDL	OB8-CB6	-2.28	1.40	1.45
54	O	1202	GTP	PG-O3G	-2.28	1.46	1.54
45	O	1201	3PE	O31-C3	-2.28	1.40	1.45
53	X	201	CDL	OA8-CA7	2.27	1.40	1.33
53	N	1304	CDL	OA8-CA6	-2.27	1.40	1.45
51	l	201	LMT	O5B-C5B	2.27	1.49	1.44
45	A	901	3PE	O31-C3	-2.27	1.40	1.45
54	O	1202	GTP	C2'-C3'	-2.26	1.47	1.53
53	N	1304	CDL	OA8-CA7	2.26	1.39	1.33
45	I	204	3PE	O31-C3	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	L	702	CDL	OB8-CB7	2.26	1.39	1.33
47	B	202	PC1	O31-C3	-2.26	1.40	1.45
45	I	204	3PE	O21-C21	2.25	1.40	1.34
53	N	1302	CDL	OB6-CB5	2.25	1.40	1.34
53	L	702	CDL	OA8-CA7	2.23	1.39	1.33
45	H	402	3PE	O31-C3	-2.23	1.40	1.45
49	F	501	FMN	C10-N1	2.22	1.37	1.33
53	q	201	CDL	OA8-CA7	2.22	1.39	1.33
56	P	501	NDP	O4B-C4B	-2.21	1.40	1.45
53	N	1302	CDL	OB8-CB6	-2.21	1.40	1.45
53	X	201	CDL	OB8-CB6	-2.20	1.40	1.45
53	h	1001	CDL	OB6-CB5	2.20	1.40	1.34
51	g	1101	LMT	O1B-C4'	2.20	1.49	1.43
53	h	1001	CDL	OB8-CB7	2.19	1.39	1.33
45	A	902	3PE	O31-C3	-2.19	1.40	1.45
45	I	201	3PE	O21-C21	2.18	1.40	1.34
45	M	601	3PE	O21-C21	2.18	1.40	1.34
56	P	501	NDP	O5D-C5D	-2.17	1.36	1.44
53	N	1304	CDL	OB6-CB5	2.16	1.40	1.34
51	H	401	LMT	O1B-C4'	2.16	1.49	1.43
58	T	101	EHZ	C9-S1	2.15	1.81	1.76
51	N	1303	LMT	O5B-C5B	2.15	1.49	1.44
45	N	1301	3PE	O31-C3	-2.12	1.40	1.45
45	L	703	3PE	O31-C3	-2.12	1.40	1.45
53	X	201	CDL	OA6-CA5	2.11	1.39	1.35
53	N	1304	CDL	OA6-CA5	2.10	1.40	1.34
45	M	601	3PE	O31-C3	-2.10	1.40	1.45
53	N	1302	CDL	OA8-CA6	-2.10	1.40	1.45
45	O	1201	3PE	O21-C21	2.08	1.40	1.34
53	q	201	CDL	OB6-CB5	2.07	1.40	1.34
45	A	902	3PE	O21-C2	-2.07	1.41	1.46
53	L	702	CDL	OB6-CB5	2.07	1.40	1.34
45	N	1301	3PE	O21-C21	2.06	1.40	1.34
53	q	201	CDL	OA6-CA5	2.05	1.40	1.34
54	O	1202	GTP	C4-N3	2.05	1.38	1.34
51	J	201	LMT	O5'-C5'	2.04	1.49	1.44
53	q	201	CDL	OB8-CB6	-2.02	1.40	1.45
54	O	1202	GTP	C1'-N9	-2.02	1.41	1.47
53	h	1001	CDL	OA6-CA5	2.01	1.40	1.34
56	P	501	NDP	C2A-N1A	2.01	1.37	1.33
51	H	401	LMT	O5'-C5'	2.00	1.49	1.44

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	1202	GTP	C8-N9-C4	7.70	120.46	106.03
58	U	101	EHZ	C8-C9-S1	6.11	121.27	113.56
58	T	101	EHZ	C16-C15-N2	5.90	127.68	116.48
58	T	101	EHZ	C8-C9-S1	5.33	120.28	113.56
53	X	201	CDL	OA6-CA5-C11	5.05	120.09	111.09
45	A	901	3PE	O21-C21-C22	4.97	122.22	111.48
45	H	402	3PE	O21-C21-O22	-4.83	119.51	125.70
53	h	1001	CDL	OB6-CB5-C51	4.82	121.91	111.48
45	L	703	3PE	O21-C21-C22	4.65	121.55	111.48
47	B	202	PC1	O21-C21-C22	4.45	121.10	111.48
45	L	701	3PE	O21-C21-C22	4.43	121.06	111.48
53	X	201	CDL	OB6-CB5-C51	4.27	120.72	111.48
52	N	1305	I49	N01-C14-N03	4.26	128.11	120.26
45	N	1301	3PE	O21-C21-C22	4.24	120.65	111.48
52	H	403	I49	N01-C14-N03	4.14	127.89	120.26
45	I	201	3PE	O21-C21-C22	4.11	120.36	111.48
53	h	1001	CDL	OA6-CA5-C11	4.06	120.27	111.48
53	N	1302	CDL	OB6-CB5-C51	4.06	120.27	111.48
47	M	602	PC1	O21-C21-C22	4.03	120.20	111.48
53	q	201	CDL	OA6-CA5-C11	4.02	120.17	111.48
53	q	201	CDL	OB6-CB5-C51	3.94	119.99	111.48
53	L	702	CDL	OA6-CA5-C11	3.91	119.94	111.48
53	N	1302	CDL	OA6-CA5-C11	3.85	119.82	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.85	95.62	109.33
45	A	902	3PE	O21-C21-C22	3.84	119.79	111.48
45	O	1201	3PE	O21-C21-C22	3.84	119.79	111.48
45	I	204	3PE	O21-C21-C22	3.83	119.76	111.48
53	N	1304	CDL	OA6-CA5-C11	3.78	119.67	111.48
45	M	601	3PE	O21-C21-C22	3.60	119.28	111.48
56	P	501	NDP	P2B-O2B-C2B	-3.56	113.92	123.43
58	T	101	EHZ	O4-C15-N2	-3.55	115.48	122.98
49	F	501	FMN	C4-N3-C2	-3.45	119.51	125.64
53	L	702	CDL	OB6-CB5-C51	3.41	118.85	111.48
53	N	1304	CDL	OB8-CB7-C71	3.31	121.93	111.83
51	h	1002	LMT	C1'-O5'-C5'	-3.28	107.31	113.72
56	P	501	NDP	O3-PA-O1A	-3.21	101.04	110.70
51	K	901	LMT	C3B-C4B-C5B	3.14	115.93	110.23
45	A	902	3PE	O31-C31-C32	3.14	121.40	111.83
58	U	101	EHZ	O2-C9-C8	-3.13	118.81	123.74
54	O	1202	GTP	O2G-PG-O3B	3.06	114.90	104.64
45	L	703	3PE	O31-C31-C32	3.04	121.12	111.83
45	L	701	3PE	O31-C31-C32	3.02	121.04	111.83
53	q	201	CDL	OA8-CA7-C31	3.00	120.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	1202	GTP	C2-N1-C6	-2.99	119.68	125.11
45	N	1301	3PE	O31-C31-C32	2.96	120.85	111.83
51	p	201	LMT	O1'-C1'-C2'	2.95	112.76	108.27
53	h	1001	CDL	OA8-CA7-C31	2.95	120.83	111.83
49	F	501	FMN	C4A-C10-N10	2.92	120.66	116.48
56	P	501	NDP	PA-O5B-C5B	-2.88	104.87	121.35
45	H	402	3PE	O31-C31-C32	2.87	120.58	111.83
52	H	403	I49	N05-C15-N04	-2.85	111.96	120.07
45	A	901	3PE	O31-C31-C32	2.85	120.52	111.83
53	N	1302	CDL	OB8-CB7-C71	2.84	120.51	111.83
52	N	1305	I49	N05-C15-N04	-2.81	112.09	120.07
53	h	1001	CDL	OB8-CB7-C71	2.81	120.39	111.83
53	N	1304	CDL	OA8-CA7-C31	2.80	120.36	111.83
45	I	204	3PE	O31-C31-C32	2.78	120.30	111.83
53	N	1302	CDL	OA8-CA7-C31	2.76	120.25	111.83
45	I	201	3PE	O31-C31-C32	2.75	120.21	111.83
49	F	501	FMN	C4A-C4-N3	2.74	120.23	113.25
54	O	1202	GTP	O3G-PG-O3B	2.73	113.78	104.64
53	L	702	CDL	OB8-CB7-C71	2.72	120.12	111.83
53	q	201	CDL	OB8-CB7-C71	2.70	120.07	111.83
53	X	201	CDL	OB8-CB7-C71	2.69	120.05	111.83
54	O	1202	GTP	C3'-C2'-C1'	2.69	106.55	101.46
56	P	501	NDP	PN-O5D-C5D	-2.68	106.01	121.35
45	O	1201	3PE	O31-C31-C32	2.65	119.92	111.83
54	O	1202	GTP	C1'-N9-C8	-2.64	119.22	126.73
51	H	401	LMT	C1B-C2B-C3B	2.63	115.55	110.01
53	X	201	CDL	OA8-CA7-C31	2.63	119.85	111.83
45	M	601	3PE	O31-C31-C32	2.62	119.83	111.83
56	P	501	NDP	O2N-PN-O3	2.58	114.25	107.27
52	N	1305	I49	N05-C15-N02	2.57	126.98	117.97
52	H	403	I49	N05-C15-N02	2.56	126.96	117.97
45	L	703	3PE	C2-O21-C21	-2.56	111.66	117.80
58	T	101	EHZ	C10-S1-C9	2.55	109.37	101.84
56	P	501	NDP	O3X-P2B-O2X	2.55	117.35	107.80
51	h	1002	LMT	C1'-C2'-C3'	2.53	115.34	110.01
54	O	1202	GTP	C5-C4-N9	-2.53	101.12	105.66
47	M	602	PC1	O31-C31-C32	2.52	119.51	111.83
51	h	1002	LMT	O5B-C5B-C4B	2.49	114.19	109.70
56	P	501	NDP	C2A-N1A-C6A	-2.48	114.65	118.73
47	B	202	PC1	O31-C31-C32	2.48	119.39	111.83
56	P	501	NDP	O5D-PN-O1N	-2.47	99.13	108.94
51	K	901	LMT	O5B-C5B-C4B	2.46	114.14	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	1202	GTP	O2B-PB-O1B	-2.46	101.00	112.44
53	N	1304	CDL	OB6-CB5-C51	2.46	119.97	110.93
54	O	1202	GTP	C2'-C3'-C4'	2.45	107.35	102.61
52	N	1305	I49	C08-N01-C14	-2.44	118.98	123.46
49	F	501	FMN	O4-C4-C4A	-2.44	120.08	126.53
54	O	1202	GTP	C5-C6-N1	2.43	119.44	113.25
53	L	702	CDL	OA8-CA7-C31	2.43	119.23	111.83
54	O	1202	GTP	O2A-PA-O1A	-2.42	101.18	112.44
56	P	501	NDP	O4B-C4B-C3B	2.42	109.96	105.15
51	N	1303	LMT	C2'-C3'-C4'	2.42	115.17	109.68
56	P	501	NDP	N3A-C4A-N9A	2.41	131.27	127.17
54	O	1202	GTP	O6-C6-C5	-2.40	120.20	126.53
56	P	501	NDP	O2N-PN-O1N	2.40	123.61	112.44
58	T	101	EHZ	O2-C9-C8	-2.39	119.98	123.74
49	F	501	FMN	C10-C4A-N5	-2.38	119.95	124.81
51	H	401	LMT	O5B-C1B-C2B	2.38	115.25	110.37
56	P	501	NDP	O7N-C7N-N7N	-2.33	117.66	122.89
51	L	704	LMT	C1B-O1B-C4'	-2.32	112.47	117.98
51	J	201	LMT	C1B-O1B-C4'	-2.32	112.49	117.98
58	T	101	EHZ	O2-C9-S1	-2.31	119.74	122.68
51	h	1002	LMT	C3B-C4B-C5B	2.30	114.40	110.23
52	H	403	I49	C12-C10-C07	-2.30	118.98	120.46
52	H	403	I49	C08-N01-C14	-2.29	119.26	123.46
51	N	1303	LMT	O5B-C5B-C4B	2.26	113.77	109.70
51	p	201	LMT	O5B-C5B-C4B	2.26	113.77	109.70
51	K	901	LMT	C1B-O5B-C5B	-2.21	109.41	113.72
51	h	1002	LMT	C2'-C3'-C4'	2.20	114.68	109.68
58	U	101	EHZ	O2-C9-S1	-2.17	119.92	122.68
51	N	1303	LMT	C6B-C5B-C4B	-2.17	107.69	113.02
45	A	901	3PE	O21-C21-O22	-2.16	118.64	123.70
51	p	201	LMT	C1-O1'-C1'	-2.15	110.01	113.68
54	O	1202	GTP	N9-C8-N7	-2.14	109.43	113.40
45	L	701	3PE	C2-O21-C21	-2.12	112.73	117.80
54	O	1202	GTP	C8-N7-C5	-2.12	100.49	104.26
51	p	201	LMT	O5'-C5'-C4'	2.11	114.09	109.72
51	h	1002	LMT	O1'-C1'-C2'	2.11	111.48	108.27
51	h	1002	LMT	C1-O1'-C1'	2.09	117.25	113.68
51	h	1002	LMT	C1B-O1B-C4'	-2.09	113.03	117.98
54	O	1202	GTP	C1'-N9-C4	-2.09	120.32	126.49
51	p	201	LMT	C1'-O5'-C5'	-2.08	109.65	113.72
52	H	403	I49	C09-C07-C10	2.08	121.41	118.55
51	K	901	LMT	C6B-C5B-C4B	-2.07	107.93	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	C5A-C4A-N3A	-2.07	123.86	126.72
58	T	101	EHZ	C14-N2-C15	2.07	126.27	122.55
49	F	501	FMN	C4A-C10-N1	-2.06	119.55	124.59
58	U	101	EHZ	C7-C8-C9	-2.05	109.28	113.86
51	N	1303	LMT	C1'-O5'-C5'	-2.04	109.73	113.72
45	L	703	3PE	O21-C21-O22	-2.04	118.93	123.70
51	h	1002	LMT	C4B-C3B-C2B	2.02	114.38	110.83
51	b	301	LMT	C6B-C5B-C4B	-2.02	108.07	113.02

There are no chirality outliers.

All (561) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	901	3PE	C11-O13-P-O11
45	A	901	3PE	C11-O13-P-O14
45	A	901	3PE	C12-C11-O13-P
45	A	901	3PE	O13-C11-C12-N
45	A	901	3PE	O22-C21-O21-C2
45	A	902	3PE	C1-O11-P-O12
45	A	902	3PE	C1-O11-P-O13
45	A	902	3PE	C1-O11-P-O14
45	A	902	3PE	O13-C11-C12-N
45	H	402	3PE	C11-O13-P-O11
45	H	402	3PE	C11-O13-P-O12
45	H	402	3PE	C11-O13-P-O14
45	H	402	3PE	O13-C11-C12-N
45	H	402	3PE	C3-C2-O21-C21
45	H	402	3PE	O22-C21-O21-C2
45	I	201	3PE	C11-O13-P-O11
45	I	201	3PE	C11-O13-P-O12
45	I	204	3PE	C1-O11-P-O13
45	I	204	3PE	C1-O11-P-O14
45	I	204	3PE	O11-C1-C2-O21
45	L	701	3PE	C11-O13-P-O11
45	L	701	3PE	C11-O13-P-O12
45	L	701	3PE	C11-O13-P-O14
45	L	701	3PE	O13-C11-C12-N
45	L	703	3PE	C1-O11-P-O13
45	L	703	3PE	C1-O11-P-O14
45	L	703	3PE	O13-C11-C12-N
45	M	601	3PE	O13-C11-C12-N
45	N	1301	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	N	1301	3PE	O11-C1-C2-O21
45	N	1301	3PE	O22-C21-O21-C2
45	O	1201	3PE	C1-O11-P-O12
45	O	1201	3PE	C1-O11-P-O13
45	O	1201	3PE	C1-O11-P-O14
45	O	1201	3PE	C11-O13-P-O14
45	O	1201	3PE	O13-C11-C12-N
45	O	1201	3PE	O22-C21-O21-C2
47	B	202	PC1	C11-O13-P-O14
47	B	202	PC1	C11-O13-P-O11
47	B	202	PC1	C1-O11-P-O14
47	M	602	PC1	C1-O11-P-O12
47	M	602	PC1	C1-O11-P-O14
47	M	602	PC1	C1-O11-P-O13
47	M	602	PC1	O13-C11-C12-N
49	F	501	FMN	C5'-O5'-P-O1P
51	H	401	LMT	O5'-C1'-O1'-C1
51	K	901	LMT	C2-C1-O1'-C1'
51	g	1101	LMT	O5'-C1'-O1'-C1
51	l	201	LMT	C2'-C1'-O1'-C1
51	l	201	LMT	O5'-C1'-O1'-C1
52	H	403	I49	C07-C06-C08-N01
52	H	403	I49	N05-C15-N02-C14
52	N	1305	I49	C07-C06-C08-N01
52	N	1305	I49	N04-C15-N02-C14
52	N	1305	I49	N05-C15-N02-C14
53	L	702	CDL	CB3-OB5-PB2-OB2
53	L	702	CDL	CB3-OB5-PB2-OB3
53	L	702	CDL	CB3-OB5-PB2-OB4
53	N	1302	CDL	CB2-C1-CA2-OA2
53	N	1302	CDL	CA3-OA5-PA1-OA4
53	N	1302	CDL	CB2-OB2-PB2-OB3
53	N	1302	CDL	CB2-OB2-PB2-OB5
53	N	1302	CDL	CB3-OB5-PB2-OB2
53	N	1302	CDL	CB3-OB5-PB2-OB3
53	N	1302	CDL	CB3-OB5-PB2-OB4
53	N	1304	CDL	CA3-OA5-PA1-OA2
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CA2-OA2-PA1-OA5
53	X	201	CDL	OA7-CA5-OA6-CA4
53	X	201	CDL	C11-CA5-OA6-CA4
53	X	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
53	X	201	CDL	CB3-OB5-PB2-OB3
53	X	201	CDL	CB3-OB5-PB2-OB4
53	h	1001	CDL	O1-C1-CB2-OB2
53	h	1001	CDL	CA2-C1-CB2-OB2
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB2-OB2-PB2-OB4
53	h	1001	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	CB3-OB5-PB2-OB2
53	h	1001	CDL	CB3-OB5-PB2-OB3
53	h	1001	CDL	CB3-OB5-PB2-OB4
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	h	1001	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB2-OB2-PB2-OB3
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CB3-OB5-PB2-OB3
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C16-C15-N2-C14
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
51	l	201	LMT	O5B-C1B-O1B-C4'
53	N	1304	CDL	OB9-CB7-OB8-CB6
45	A	902	3PE	O32-C31-O31-C3
45	H	402	3PE	O32-C31-O31-C3
45	I	204	3PE	O32-C31-O31-C3
53	L	702	CDL	OB9-CB7-OB8-CB6
53	X	201	CDL	OA9-CA7-OA8-CA6
45	O	1201	3PE	O32-C31-O31-C3
47	B	202	PC1	O22-C21-O21-C2
53	q	201	CDL	OA7-CA5-OA6-CA4
45	A	902	3PE	C32-C31-O31-C3
45	H	402	3PE	C32-C31-O31-C3
47	M	602	PC1	C32-C31-O31-C3
53	N	1304	CDL	C71-CB7-OB8-CB6
53	X	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	C71-CB7-OB8-CB6
45	A	901	3PE	C22-C21-O21-C2
45	N	1301	3PE	C22-C21-O21-C2
45	O	1201	3PE	C22-C21-O21-C2
47	B	202	PC1	C22-C21-O21-C2
51	p	201	LMT	O5B-C5B-C6B-O6B
45	A	901	3PE	C32-C31-O31-C3
45	I	204	3PE	C32-C31-O31-C3
45	L	701	3PE	C32-C31-O31-C3
45	O	1201	3PE	C32-C31-O31-C3
53	L	702	CDL	C71-CB7-OB8-CB6
53	N	1302	CDL	C71-CB7-OB8-CB6
51	b	301	LMT	O5'-C5'-C6'-O6'
51	H	401	LMT	C3'-C4'-O1B-C1B
51	H	401	LMT	O5'-C5'-C6'-O6'
45	A	901	3PE	O32-C31-O31-C3
45	L	701	3PE	O32-C31-O31-C3
53	N	1302	CDL	OB9-CB7-OB8-CB6
53	h	1001	CDL	OA9-CA7-OA8-CA6
53	h	1001	CDL	OB9-CB7-OB8-CB6
51	b	301	LMT	C3'-C4'-O1B-C1B
53	q	201	CDL	O1-C1-CA2-OA2
53	q	201	CDL	C31-CA7-OA8-CA6
51	l	201	LMT	O5'-C5'-C6'-O6'
47	M	602	PC1	O32-C31-O31-C3
58	T	101	EHZ	O4-C15-N2-C14
51	H	401	LMT	O5B-C5B-C6B-O6B
51	J	201	LMT	O5'-C5'-C6'-O6'
51	H	401	LMT	C4'-C5'-C6'-O6'
53	L	702	CDL	C11-CA5-OA6-CA4
53	q	201	CDL	C11-CA5-OA6-CA4
51	p	201	LMT	C4B-C5B-C6B-O6B
56	P	501	NDP	O4D-C4D-C5D-O5D
53	h	1001	CDL	C31-CA7-OA8-CA6
53	q	201	CDL	OA9-CA7-OA8-CA6
51	L	704	LMT	O5B-C5B-C6B-O6B
51	H	401	LMT	C4B-C5B-C6B-O6B
51	b	301	LMT	C4'-C5'-C6'-O6'
51	l	201	LMT	C4'-C5'-C6'-O6'
53	X	201	CDL	C71-CB7-OB8-CB6
51	b	301	LMT	C2-C3-C4-C5
51	J	201	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	OA7-CA5-OA6-CA4
53	N	1302	CDL	C31-CA7-OA8-CA6
45	A	902	3PE	C21-C22-C23-C24
45	H	402	3PE	C31-C32-C33-C34
53	h	1001	CDL	CA7-C31-C32-C33
53	X	201	CDL	OB9-CB7-OB8-CB6
51	L	704	LMT	C4B-C5B-C6B-O6B
47	M	602	PC1	C21-C22-C23-C24
53	N	1304	CDL	C11-CA5-OA6-CA4
53	N	1302	CDL	OA9-CA7-OA8-CA6
51	p	201	LMT	O5B-C1B-O1B-C4'
53	N	1304	CDL	OA7-CA5-OA6-CA4
45	I	201	3PE	C32-C31-O31-C3
51	K	901	LMT	C4'-C5'-C6'-O6'
51	g	1101	LMT	C5'-C4'-O1B-C1B
45	L	703	3PE	C32-C31-O31-C3
51	b	301	LMT	C2'-C1'-O1'-C1
53	N	1302	CDL	CB7-C71-C72-C73
53	X	201	CDL	CB5-C51-C52-C53
53	N	1302	CDL	O1-C1-CA2-OA2
53	q	201	CDL	O1-C1-CB2-OB2
51	J	201	LMT	C4B-C5B-C6B-O6B
45	A	902	3PE	C3B-C3C-C3D-C3E
45	O	1201	3PE	C3E-C3F-C3G-C3H
47	B	202	PC1	C34-C35-C36-C37
45	A	901	3PE	C2A-C2B-C2C-C2D
51	g	1101	LMT	C3'-C4'-O1B-C1B
45	L	703	3PE	C27-C28-C29-C2A
51	K	901	LMT	O1'-C1-C2-C3
45	H	402	3PE	C3C-C3D-C3E-C3F
45	I	201	3PE	C33-C34-C35-C36
45	I	201	3PE	C2B-C2C-C2D-C2E
45	N	1301	3PE	C2D-C2E-C2F-C2G
47	M	602	PC1	C25-C26-C27-C28
47	M	602	PC1	C36-C37-C38-C39
53	h	1001	CDL	C11-C12-C13-C14
53	h	1001	CDL	C18-C19-C20-C21
47	B	202	PC1	C24-C25-C26-C27
47	M	602	PC1	C26-C27-C28-C29
45	I	201	3PE	C22-C21-O21-C2
58	T	101	EHZ	C5-C6-C7-C8
45	M	601	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
56	P	501	NDP	C3D-C4D-C5D-O5D
45	A	901	3PE	C28-C29-C2A-C2B
45	N	1301	3PE	C25-C26-C27-C28
53	L	702	CDL	C53-C54-C55-C56
45	I	201	3PE	O32-C31-O31-C3
53	N	1304	CDL	C72-C73-C74-C75
51	p	201	LMT	C5-C6-C7-C8
45	L	703	3PE	O32-C31-O31-C3
47	M	602	PC1	C2C-C2D-C2E-C2F
53	N	1302	CDL	C72-C73-C74-C75
45	L	703	3PE	C33-C34-C35-C36
53	N	1304	CDL	C33-C34-C35-C36
53	q	201	CDL	C57-C58-C59-C60
45	M	601	3PE	C23-C24-C25-C26
53	N	1302	CDL	C61-C62-C63-C64
51	L	704	LMT	C3-C4-C5-C6
51	l	201	LMT	C4-C5-C6-C7
47	B	202	PC1	C21-C22-C23-C24
53	N	1302	CDL	C11-CA5-OA6-CA4
52	H	403	I49	N04-C15-N02-C14
45	M	601	3PE	C2C-C2D-C2E-C2F
53	N	1302	CDL	C76-C77-C78-C79
45	A	902	3PE	C3D-C3E-C3F-C3G
45	L	701	3PE	C27-C28-C29-C2A
45	N	1301	3PE	C29-C2A-C2B-C2C
45	M	601	3PE	C32-C33-C34-C35
47	M	602	PC1	C39-C3A-C3B-C3C
45	L	703	3PE	C21-C22-C23-C24
45	A	901	3PE	C3C-C3D-C3E-C3F
45	O	1201	3PE	C2B-C2C-C2D-C2E
51	H	401	LMT	C3-C4-C5-C6
56	P	501	NDP	O4D-C1D-N1N-C6N
51	h	1002	LMT	C2'-C1'-O1'-C1
45	N	1301	3PE	C35-C36-C37-C38
53	h	1001	CDL	C72-C73-C74-C75
47	M	602	PC1	C22-C21-O21-C2
53	N	1302	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	C11-CA5-OA6-CA4
58	T	101	EHZ	C12-C13-C14-N2
45	I	201	3PE	O22-C21-O21-C2
47	M	602	PC1	O22-C21-O21-C2
53	N	1302	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C38-C39-C3A-C3B
45	M	601	3PE	C33-C34-C35-C36
51	J	201	LMT	O5B-C5B-C6B-O6B
51	L	704	LMT	C5-C6-C7-C8
53	X	201	CDL	C72-C73-C74-C75
53	q	201	CDL	C71-C72-C73-C74
58	U	101	EHZ	C5-C6-C7-O1
45	I	201	3PE	O11-C1-C2-O21
45	A	902	3PE	C33-C34-C35-C36
53	q	201	CDL	C13-C14-C15-C16
45	A	901	3PE	O21-C2-C3-O31
53	N	1304	CDL	OB6-CB4-CB6-OB8
45	A	901	3PE	C26-C27-C28-C29
45	M	601	3PE	C2D-C2E-C2F-C2G
53	L	702	CDL	C55-C56-C57-C58
53	h	1001	CDL	C19-C20-C21-C22
47	M	602	PC1	C33-C34-C35-C36
53	q	201	CDL	C16-C17-C18-C19
45	H	402	3PE	C2-C1-O11-P
51	l	201	LMT	C3'-C4'-O1B-C1B
53	q	201	CDL	CA2-C1-CB2-OB2
45	L	701	3PE	C22-C21-O21-C2
45	M	601	3PE	C22-C23-C24-C25
45	O	1201	3PE	C3A-C3B-C3C-C3D
58	U	101	EHZ	C2-C1-C21-C22
51	l	201	LMT	C5'-C4'-O1B-C1B
45	A	901	3PE	C2C-C2D-C2E-C2F
45	A	901	3PE	O11-C1-C2-C3
45	I	204	3PE	O11-C1-C2-C3
45	N	1301	3PE	O11-C1-C2-C3
53	X	201	CDL	OA5-CA3-CA4-CA6
53	N	1302	CDL	OA7-CA5-OA6-CA4
53	h	1001	CDL	OA7-CA5-OA6-CA4
53	L	702	CDL	C52-C53-C54-C55
53	q	201	CDL	C51-C52-C53-C54
51	p	201	LMT	C2-C3-C4-C5
45	I	204	3PE	C22-C21-O21-C2
45	L	701	3PE	C38-C39-C3A-C3B
45	N	1301	3PE	C33-C34-C35-C36
59	o	201	MYR	C2-C3-C4-C5
45	A	901	3PE	C1-C2-C3-O31
45	H	402	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	N	1302	CDL	CA3-CA4-CA6-OA8
53	q	201	CDL	C38-C39-C40-C41
45	O	1201	3PE	C34-C35-C36-C37
45	I	201	3PE	C39-C3A-C3B-C3C
45	O	1201	3PE	C32-C33-C34-C35
45	O	1201	3PE	C2D-C2E-C2F-C2G
51	L	704	LMT	O5'-C5'-C6'-O6'
51	b	301	LMT	O1'-C1-C2-C3
53	L	702	CDL	C11-C12-C13-C14
53	q	201	CDL	C15-C16-C17-C18
45	I	204	3PE	C25-C26-C27-C28
51	p	201	LMT	O5'-C5'-C6'-O6'
53	q	201	CDL	CA7-C31-C32-C33
51	h	1002	LMT	C5'-C4'-O1B-C1B
58	T	101	EHZ	C5-C6-C7-O1
45	I	201	3PE	C24-C25-C26-C27
45	A	901	3PE	C37-C38-C39-C3A
58	U	101	EHZ	C2-C3-C4-C5
51	K	901	LMT	O5'-C5'-C6'-O6'
45	M	601	3PE	O11-C1-C2-O21
53	N	1302	CDL	OA5-CA3-CA4-OA6
53	q	201	CDL	OB5-CB3-CB4-OB6
45	I	204	3PE	C28-C29-C2A-C2B
53	N	1302	CDL	C53-C54-C55-C56
58	T	101	EHZ	C1-C21-C22-C23
53	q	201	CDL	C54-C55-C56-C57
53	N	1304	CDL	C77-C78-C79-C80
45	I	201	3PE	C29-C2A-C2B-C2C
45	N	1301	3PE	C2B-C2C-C2D-C2E
47	M	602	PC1	O21-C2-C3-O31
53	N	1302	CDL	OB6-CB4-CB6-OB8
45	M	601	3PE	C25-C26-C27-C28
51	h	1002	LMT	C3'-C4'-O1B-C1B
45	L	701	3PE	C35-C36-C37-C38
53	h	1001	CDL	C52-C53-C54-C55
45	O	1201	3PE	C29-C2A-C2B-C2C
53	N	1302	CDL	C59-C60-C61-C62
45	L	701	3PE	C23-C24-C25-C26
53	N	1302	CDL	C71-C72-C73-C74
45	L	703	3PE	C29-C2A-C2B-C2C
45	L	701	3PE	C2B-C2C-C2D-C2E
51	b	301	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
45	O	1201	3PE	C2-C1-O11-P
45	I	201	3PE	O11-C1-C2-C3
53	N	1304	CDL	OB5-CB3-CB4-CB6
45	N	1301	3PE	C3A-C3B-C3C-C3D
53	X	201	CDL	O1-C1-CB2-OB2
45	A	901	3PE	C27-C28-C29-C2A
51	g	1101	LMT	O1'-C1-C2-C3
53	N	1302	CDL	CA5-C11-C12-C13
53	h	1001	CDL	C51-C52-C53-C54
45	L	703	3PE	C35-C36-C37-C38
53	N	1304	CDL	CA3-CA4-CA6-OA8
53	N	1304	CDL	CB3-CB4-CB6-OB8
45	O	1201	3PE	C31-C32-C33-C34
58	T	101	EHZ	C21-C22-C23-C24
45	H	402	3PE	C35-C36-C37-C38
53	X	201	CDL	OA5-CA3-CA4-OA6
51	p	201	LMT	C3'-C4'-O1B-C1B
53	N	1302	CDL	CA4-CA3-OA5-PA1
58	T	101	EHZ	O1-C7-C8-C9
45	A	902	3PE	C24-C25-C26-C27
53	h	1001	CDL	C24-C25-C26-C27
45	L	703	3PE	C39-C3A-C3B-C3C
47	B	202	PC1	O21-C2-C3-O31
53	N	1304	CDL	OA6-CA4-CA6-OA8
47	B	202	PC1	C23-C24-C25-C26
51	g	1101	LMT	C2-C3-C4-C5
59	o	201	MYR	C7-C8-C9-C10
45	N	1301	3PE	C24-C25-C26-C27
53	q	201	CDL	C36-C37-C38-C39
45	L	701	3PE	C2F-C2G-C2H-C2I
45	L	703	3PE	C32-C33-C34-C35
45	O	1201	3PE	C22-C23-C24-C25
53	N	1304	CDL	CA5-C11-C12-C13
47	B	202	PC1	C32-C31-O31-C3
45	L	701	3PE	C24-C25-C26-C27
53	q	201	CDL	CB2-C1-CA2-OA2
53	h	1001	CDL	C20-C21-C22-C23
45	L	701	3PE	C3D-C3E-C3F-C3G
51	p	201	LMT	C5'-C4'-O1B-C1B
51	H	401	LMT	C5'-C4'-O1B-C1B
45	L	701	3PE	C32-C33-C34-C35
47	M	602	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
49	F	501	FMN	C5'-O5'-P-O2P
51	J	201	LMT	C2B-C1B-O1B-C4'
45	I	204	3PE	O22-C21-O21-C2
45	L	701	3PE	O22-C21-O21-C2
45	A	901	3PE	C1-C2-O21-C21
45	O	1201	3PE	C35-C36-C37-C38
47	M	602	PC1	C28-C29-C2A-C2B
45	L	701	3PE	C3C-C3D-C3E-C3F
45	A	901	3PE	C33-C34-C35-C36
53	h	1001	CDL	C33-C34-C35-C36
53	N	1304	CDL	OB5-CB3-CB4-OB6
58	U	101	EHZ	C21-C1-C2-C3
47	B	202	PC1	C1-C2-C3-O31
45	A	901	3PE	C22-C23-C24-C25
45	I	204	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
45	N	1301	3PE	C12-C11-O13-P
53	N	1302	CDL	OA6-CA4-CA6-OA8
53	N	1304	CDL	C31-C32-C33-C34
51	H	401	LMT	C5-C6-C7-C8
53	L	702	CDL	C32-C33-C34-C35
47	B	202	PC1	O32-C31-O31-C3
51	J	201	LMT	O5B-C1B-O1B-C4'
47	M	602	PC1	C11-C12-N-C14
45	I	201	3PE	C3B-C3C-C3D-C3E
53	h	1001	CDL	C22-C23-C24-C25
51	L	704	LMT	C2'-C1'-O1'-C1
47	M	602	PC1	C2-C1-O11-P
45	M	601	3PE	C26-C27-C28-C29
45	A	901	3PE	C34-C35-C36-C37
58	U	101	EHZ	C21-C22-C23-C24
47	M	602	PC1	C11-C12-N-C15
53	h	1001	CDL	C13-C14-C15-C16
45	N	1301	3PE	C3B-C3C-C3D-C3E
45	M	601	3PE	O11-C1-C2-C3
53	N	1302	CDL	OA5-CA3-CA4-CA6
45	A	902	3PE	C39-C3A-C3B-C3C
45	L	701	3PE	C39-C3A-C3B-C3C
53	N	1304	CDL	C32-C33-C34-C35
53	h	1001	CDL	C34-C35-C36-C37
45	A	901	3PE	O11-C1-C2-O21
53	q	201	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
52	H	403	I49	N01-C14-N02-C15
45	H	402	3PE	O21-C2-C3-O31
53	h	1001	CDL	OA6-CA4-CA6-OA8
47	M	602	PC1	C1-C2-C3-O31
53	L	702	CDL	CA3-CA4-CA6-OA8
53	N	1302	CDL	CB3-CB4-CB6-OB8
47	M	602	PC1	C2A-C2B-C2C-C2D
45	H	402	3PE	C3F-C3G-C3H-C3I
45	I	204	3PE	C33-C34-C35-C36
45	A	902	3PE	C35-C36-C37-C38
45	I	201	3PE	C11-O13-P-O14
45	I	204	3PE	C1-O11-P-O12
45	M	601	3PE	C11-O13-P-O11
45	M	601	3PE	C11-O13-P-O12
45	M	601	3PE	C11-O13-P-O14
47	B	202	PC1	C1-O11-P-O12
47	B	202	PC1	C1-O11-P-O13
53	N	1302	CDL	CA2-OA2-PA1-OA4
53	N	1302	CDL	CA3-OA5-PA1-OA2
53	N	1304	CDL	CA2-OA2-PA1-OA3
53	N	1304	CDL	CA2-OA2-PA1-OA4
53	N	1304	CDL	CA2-OA2-PA1-OA5
53	N	1304	CDL	CA3-OA5-PA1-OA3
53	N	1304	CDL	CA3-OA5-PA1-OA4
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CB3-OB5-PB2-OB2
45	A	902	3PE	C2-C1-O11-P
53	N	1304	CDL	C38-C39-C40-C41
53	N	1304	CDL	C43-C44-C45-C46
53	q	201	CDL	C72-C73-C74-C75
53	N	1304	CDL	C11-C12-C13-C14
51	N	1303	LMT	O1'-C1-C2-C3
45	L	703	3PE	C3C-C3D-C3E-C3F
51	N	1303	LMT	C4'-C5'-C6'-O6'
53	N	1302	CDL	CA6-CA4-OA6-CA5
53	q	201	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	C39-C40-C41-C42
53	L	702	CDL	C59-C60-C61-C62
45	A	901	3PE	C3F-C3G-C3H-C3I
51	K	901	LMT	C2-C3-C4-C5
53	h	1001	CDL	C17-C18-C19-C20
45	I	204	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	C38-C39-C40-C41
58	U	101	EHZ	C12-C13-C14-N2
45	H	402	3PE	C33-C34-C35-C36
45	H	402	3PE	C32-C33-C34-C35
53	N	1304	CDL	C40-C41-C42-C43
53	h	1001	CDL	CA3-CA4-CA6-OA8
54	O	1202	GTP	PB-O3A-PA-O1A
56	P	501	NDP	PN-O3-PA-O1A
59	o	201	MYR	C5-C6-C7-C8
45	O	1201	3PE	C38-C39-C3A-C3B
47	M	602	PC1	C11-C12-N-C13
53	q	201	CDL	C1-CB2-OB2-PB2
45	A	902	3PE	C22-C23-C24-C25
51	p	201	LMT	C4-C5-C6-C7
53	q	201	CDL	C59-C60-C61-C62
53	L	702	CDL	C32-C31-CA7-OA8
47	B	202	PC1	O11-C1-C2-O21
45	O	1201	3PE	C23-C24-C25-C26
53	L	702	CDL	C13-C14-C15-C16
51	h	1002	LMT	O5'-C5'-C6'-O6'
45	H	402	3PE	C37-C38-C39-C3A
58	T	101	EHZ	C1-C2-C3-C4
53	L	702	CDL	OA6-CA4-CA6-OA8
53	X	201	CDL	C51-C52-C53-C54
53	q	201	CDL	CA5-C11-C12-C13
47	B	202	PC1	C32-C33-C34-C35
45	A	902	3PE	C37-C38-C39-C3A
51	K	901	LMT	C5-C6-C7-C8
45	N	1301	3PE	C3E-C3F-C3G-C3H
45	A	902	3PE	C1-C2-O21-C21
51	l	201	LMT	C11-C10-C9-C8
45	I	201	3PE	C2D-C2E-C2F-C2G
54	O	1202	GTP	PG-O3B-PB-O3A
53	q	201	CDL	OB9-CB7-OB8-CB6
47	B	202	PC1	C2-C1-O11-P
51	p	201	LMT	O1'-C1-C2-C3
53	N	1302	CDL	C57-C58-C59-C60
58	U	101	EHZ	O1-C7-C8-C9
59	o	201	MYR	C11-C10-C9-C8
45	A	902	3PE	O11-C1-C2-C3
45	A	902	3PE	C32-C33-C34-C35
45	L	701	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	OA6-CA4-CA6-OA8
58	T	101	EHZ	C3-C4-C5-C6
56	P	501	NDP	C2B-O2B-P2B-O1X
45	A	902	3PE	C3E-C3F-C3G-C3H
54	O	1202	GTP	PA-O3A-PB-O2B
56	P	501	NDP	PN-O3-PA-O2A
45	L	703	3PE	C2-C3-O31-C31
51	g	1101	LMT	C4-C5-C6-C7
53	L	702	CDL	C33-C34-C35-C36
47	M	602	PC1	C24-C25-C26-C27
45	L	703	3PE	C2-C1-O11-P
53	N	1302	CDL	CB4-CB3-OB5-PB2
45	I	204	3PE	C27-C28-C29-C2A
52	H	403	I49	N03-C14-N02-C15
52	N	1305	I49	N03-C14-N02-C15
59	o	201	MYR	C6-C7-C8-C9
58	U	101	EHZ	C3-C4-C5-C6
51	L	704	LMT	C1-C2-C3-C4
45	L	701	3PE	O21-C21-C22-C23
53	q	201	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	OB5-CB3-CB4-CB6
53	N	1304	CDL	C76-C77-C78-C79
53	q	201	CDL	C40-C41-C42-C43
53	q	201	CDL	C19-C20-C21-C22
53	h	1001	CDL	C16-C17-C18-C19
45	I	201	3PE	C25-C26-C27-C28
51	K	901	LMT	C3-C4-C5-C6
45	H	402	3PE	C1-C2-O21-C21
58	U	101	EHZ	C22-C23-C24-C25
53	N	1304	CDL	C74-C75-C76-C77
53	N	1302	CDL	C55-C56-C57-C58
51	L	704	LMT	O5'-C1'-O1'-C1
45	O	1201	3PE	C37-C38-C39-C3A
59	o	201	MYR	C4-C5-C6-C7
45	M	601	3PE	C27-C28-C29-C2A
45	N	1301	3PE	O21-C21-C22-C23
51	J	201	LMT	C7-C8-C9-C10
58	U	101	EHZ	C5-C6-C7-C8
45	O	1201	3PE	C3D-C3E-C3F-C3G
56	P	501	NDP	O4B-C4B-C5B-O5B
45	A	902	3PE	O31-C31-C32-C33
51	N	1303	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	C72-C71-CB7-OB8
45	O	1201	3PE	C36-C37-C38-C39
45	L	703	3PE	C22-C23-C24-C25
54	O	1202	GTP	C4'-C5'-O5'-PA
53	L	702	CDL	C12-C13-C14-C15
59	o	201	MYR	C3-C4-C5-C6
47	B	202	PC1	O21-C21-C22-C23
45	O	1201	3PE	O21-C21-C22-C23
45	A	901	3PE	C2B-C2C-C2D-C2E
53	N	1302	CDL	C72-C71-CB7-OB8
49	F	501	FMN	N10-C1'-C2'-O2'
45	M	601	3PE	O21-C21-C22-C23
45	L	701	3PE	C22-C23-C24-C25
45	I	204	3PE	C24-C25-C26-C27
47	B	202	PC1	O22-C21-C22-C23
45	I	201	3PE	C3C-C3D-C3E-C3F
53	X	201	CDL	C32-C31-CA7-OA8
45	A	902	3PE	O32-C31-C32-C33
45	N	1301	3PE	O22-C21-C22-C23
53	N	1302	CDL	C72-C71-CB7-OB9
45	A	902	3PE	C1-C2-C3-O31
58	T	101	EHZ	C10-C11-N1-C12
53	h	1001	CDL	C14-C15-C16-C17
45	O	1201	3PE	C21-C22-C23-C24
45	O	1201	3PE	O22-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA8
54	O	1202	GTP	PG-O3B-PB-O1B
45	M	601	3PE	O22-C21-C22-C23

There are no ring outliers.

20 monomers are involved in 33 short contacts:

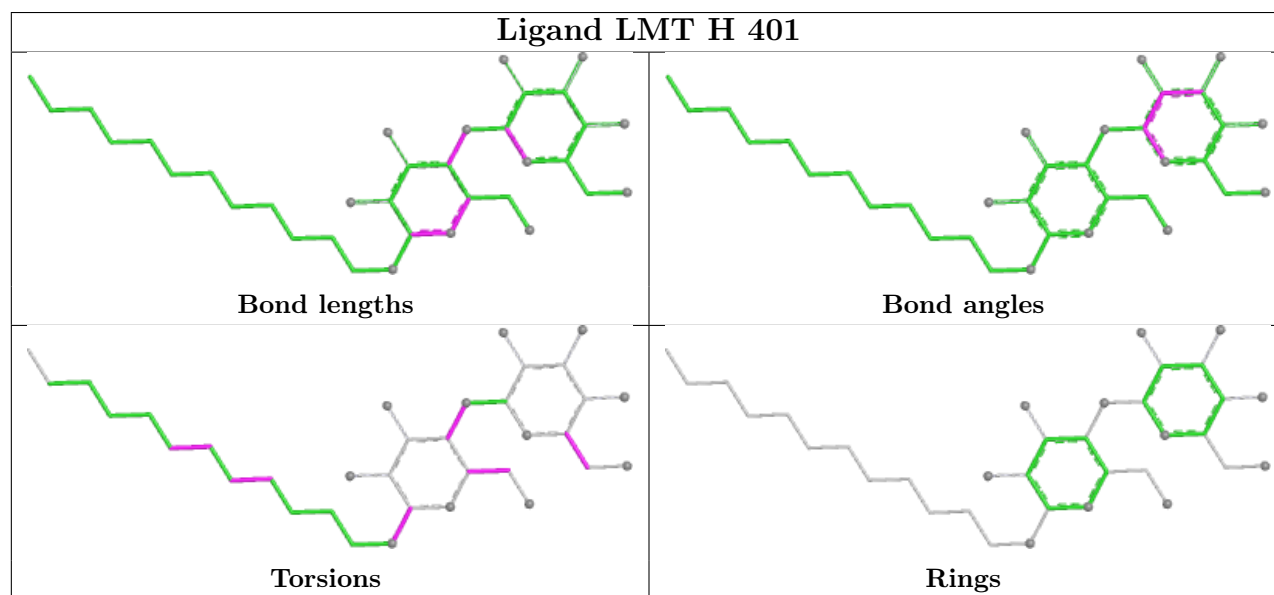
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	H	401	LMT	2	0
51	g	1101	LMT	1	0
58	U	101	EHZ	2	0
59	o	201	MYR	2	0
52	N	1305	I49	3	0
53	N	1304	CDL	3	0
49	F	501	FMN	1	0
45	L	703	3PE	2	0
45	N	1301	3PE	1	0

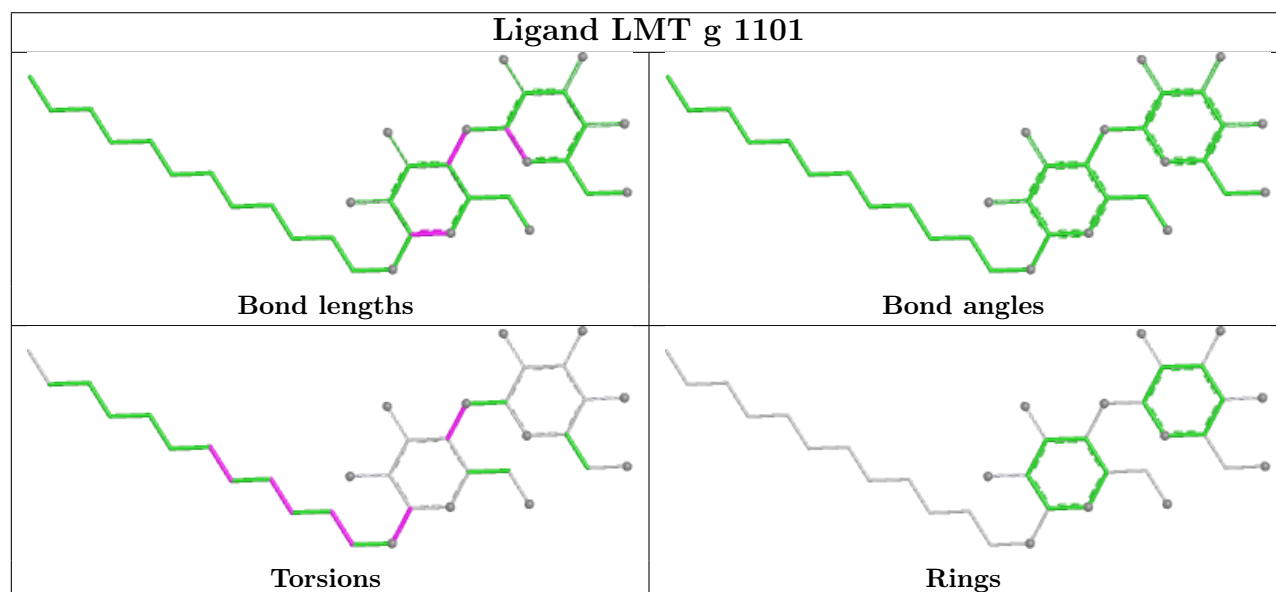
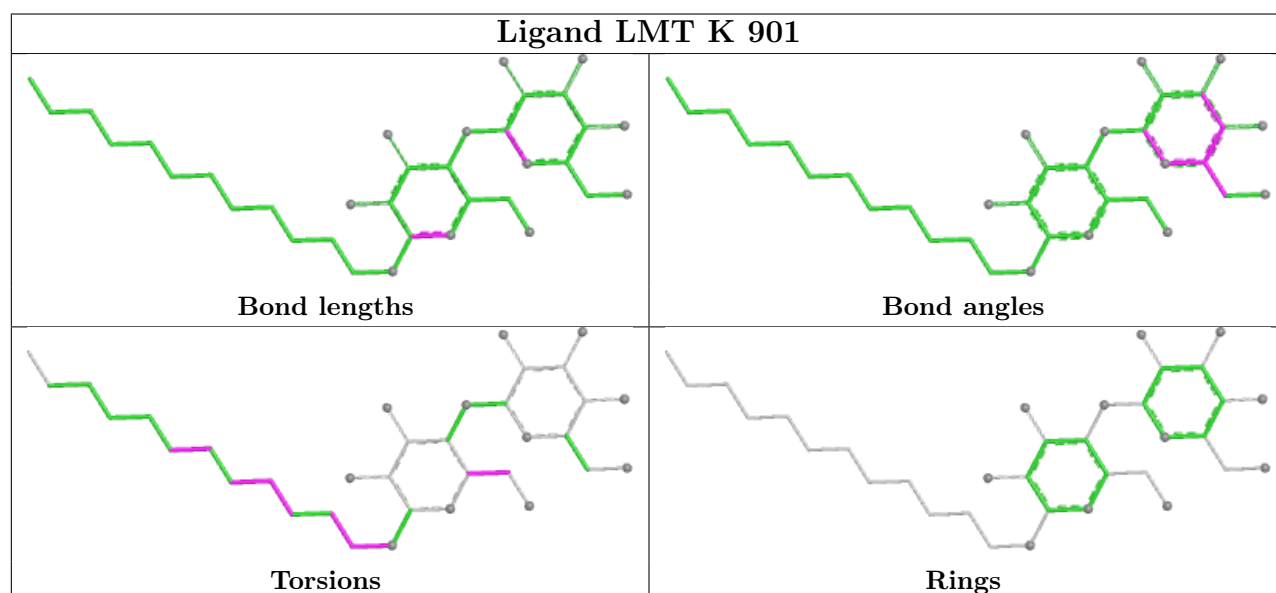
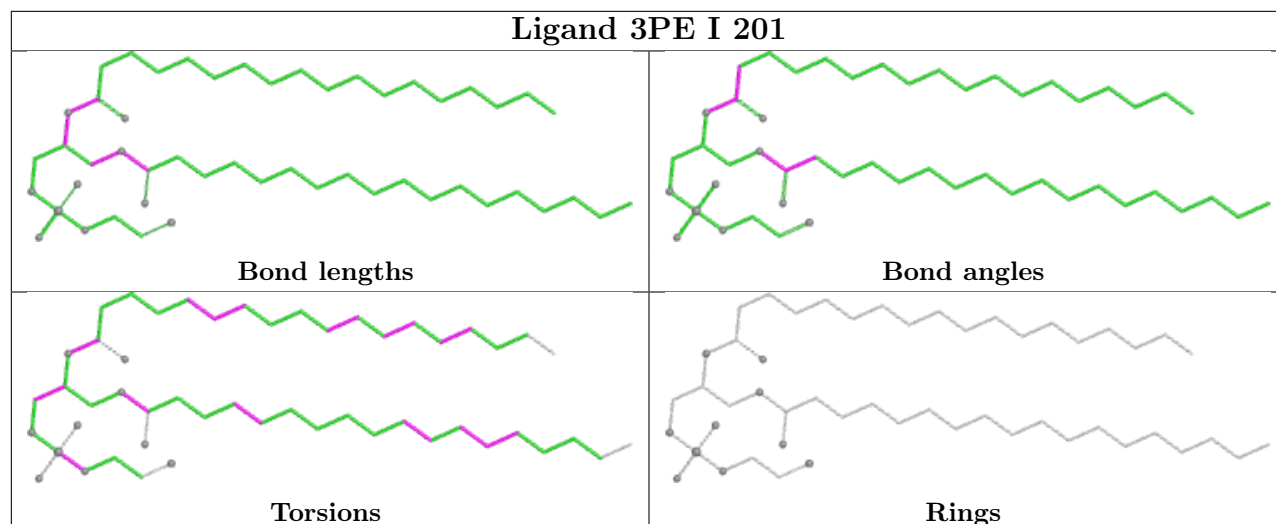
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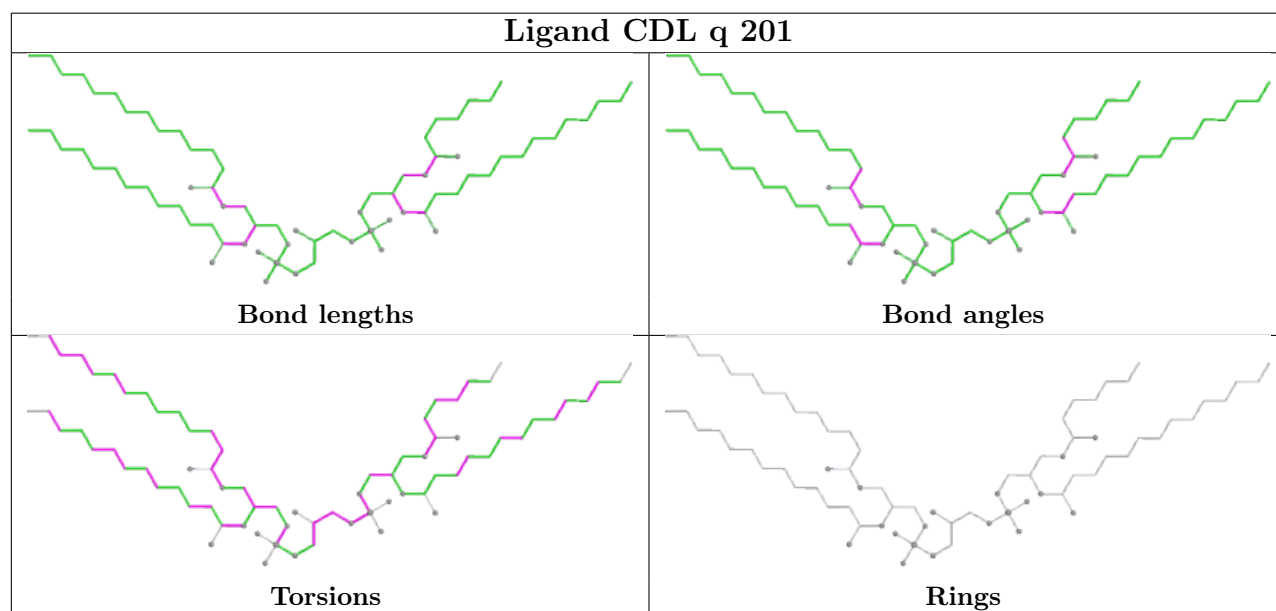
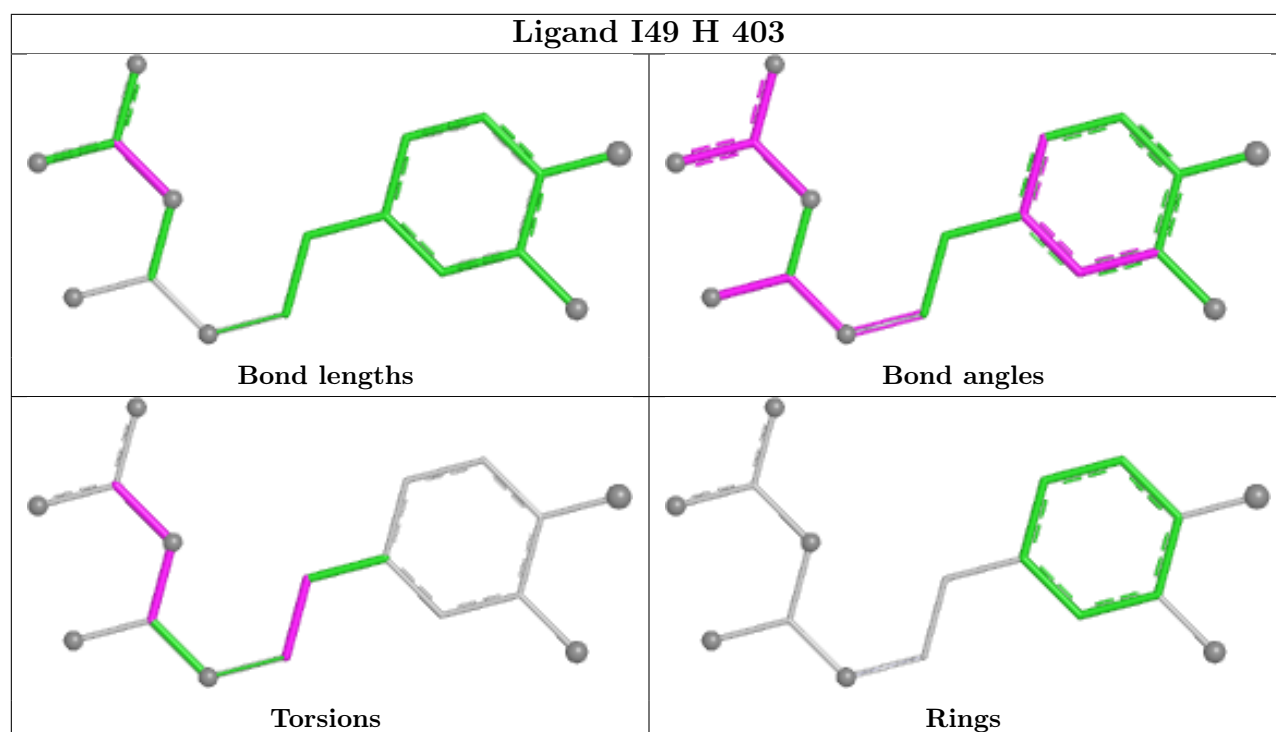
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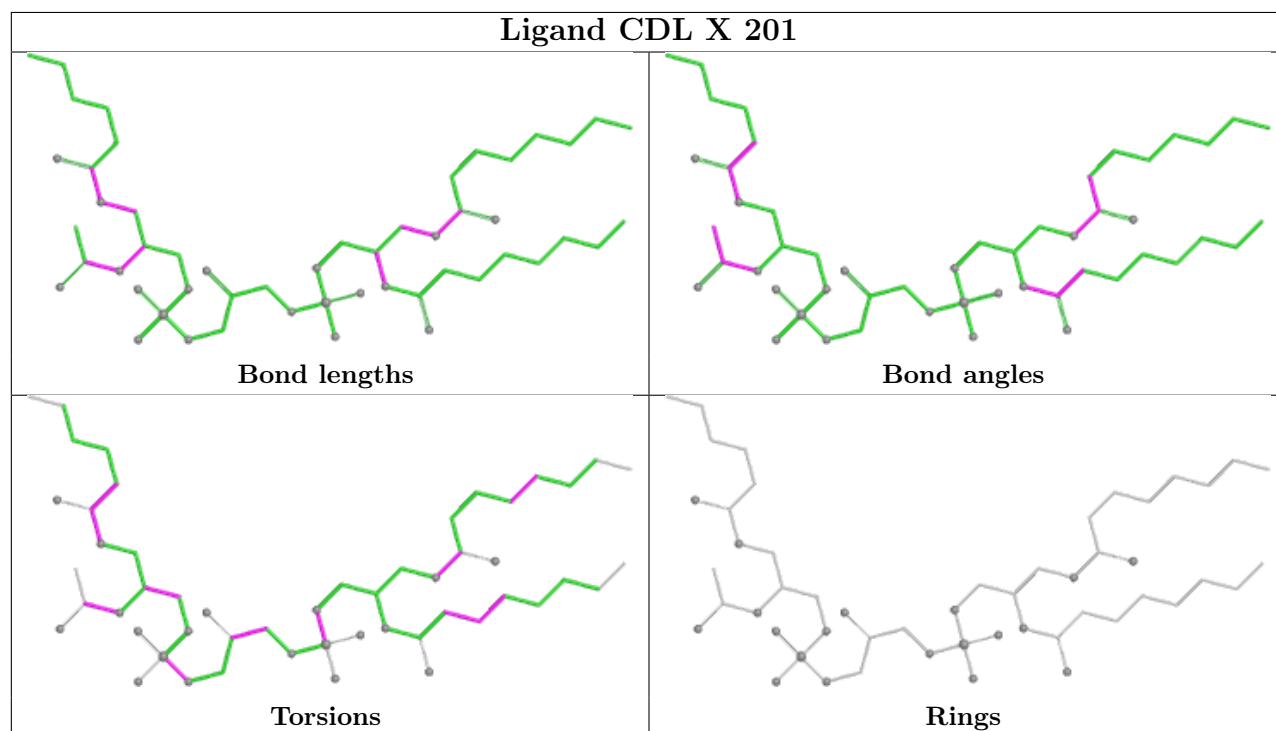
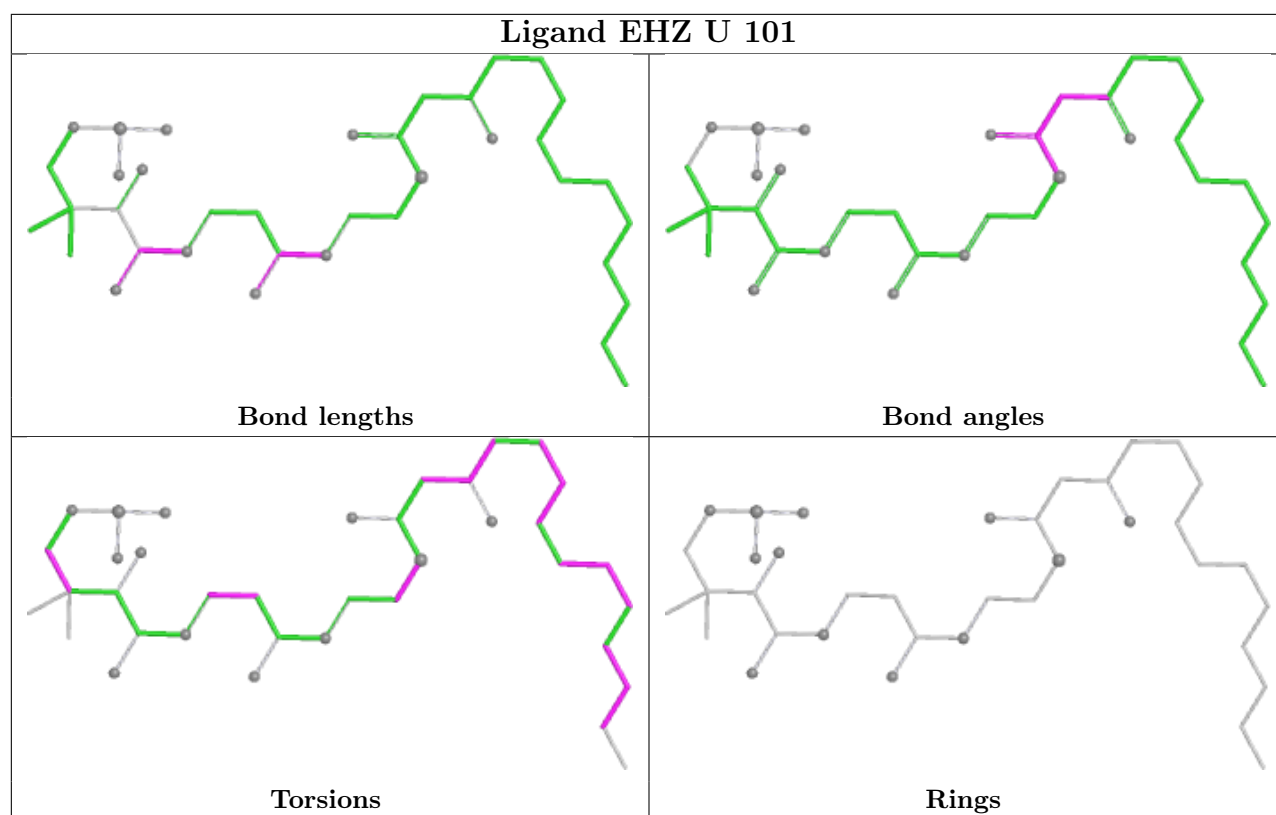
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	L	704	LMT	1	0
56	P	501	NDP	2	0
53	h	1001	CDL	1	0
45	A	901	3PE	3	0
45	O	1201	3PE	2	0
47	M	602	PC1	2	0
51	l	201	LMT	1	0
54	O	1202	GTP	3	0
45	A	902	3PE	1	0
47	B	202	PC1	1	0
45	H	402	3PE	1	0

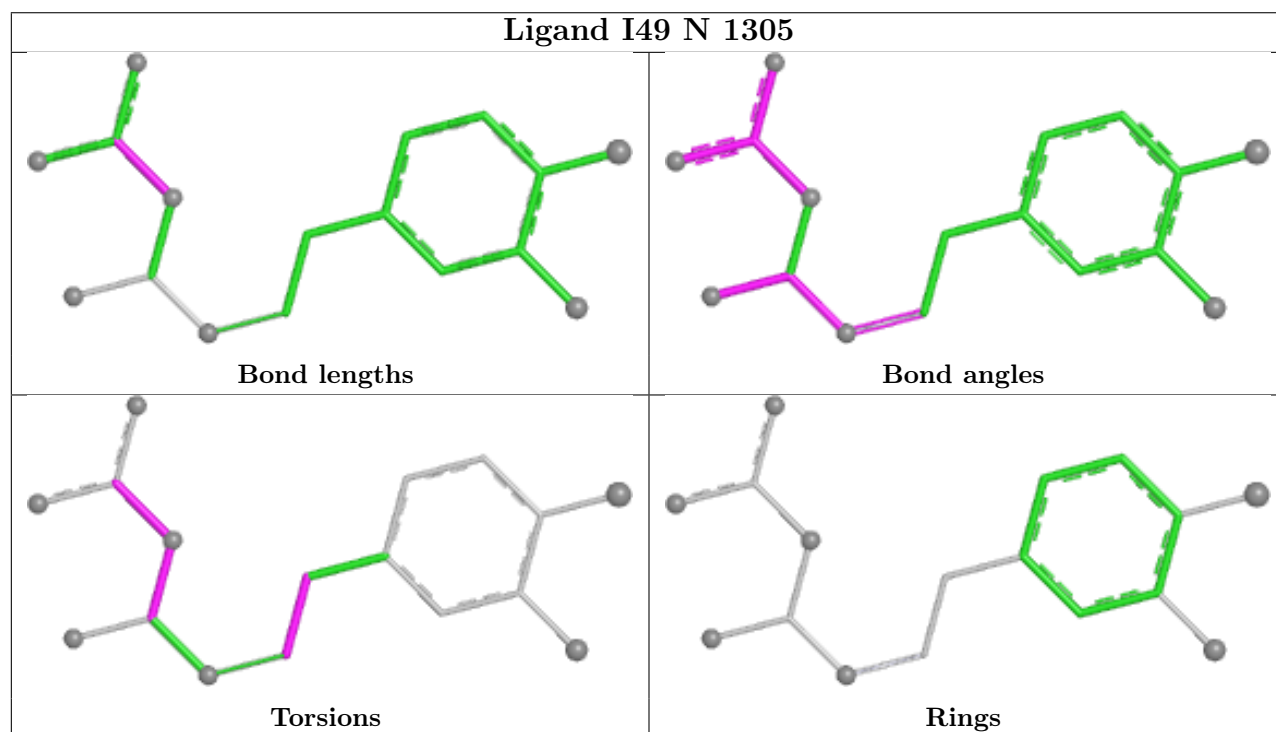
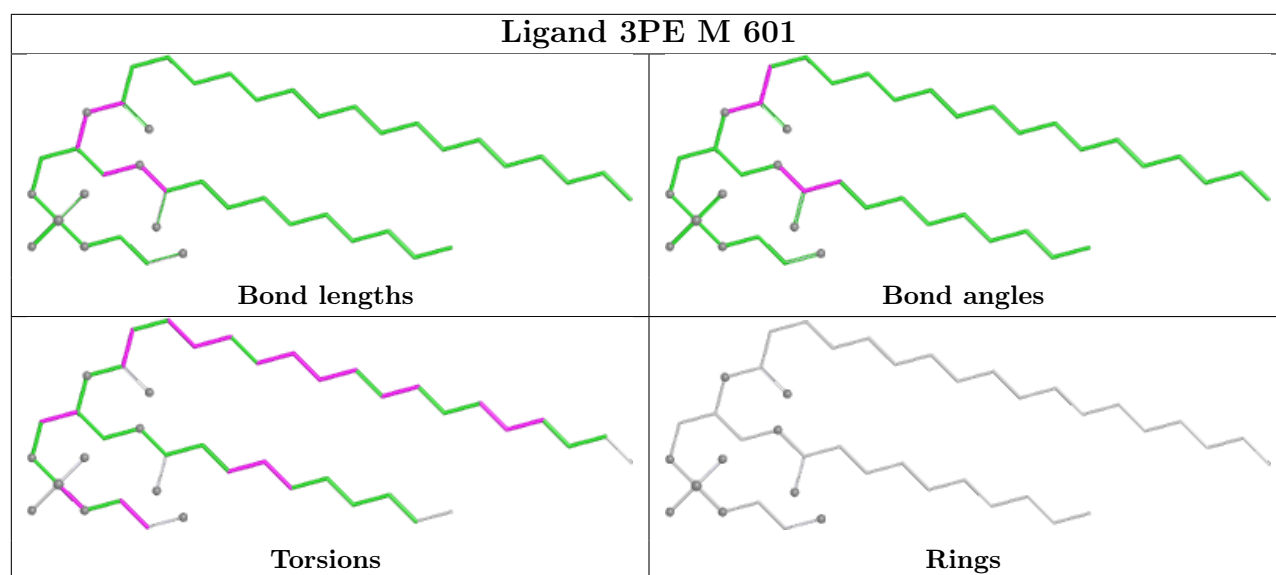
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

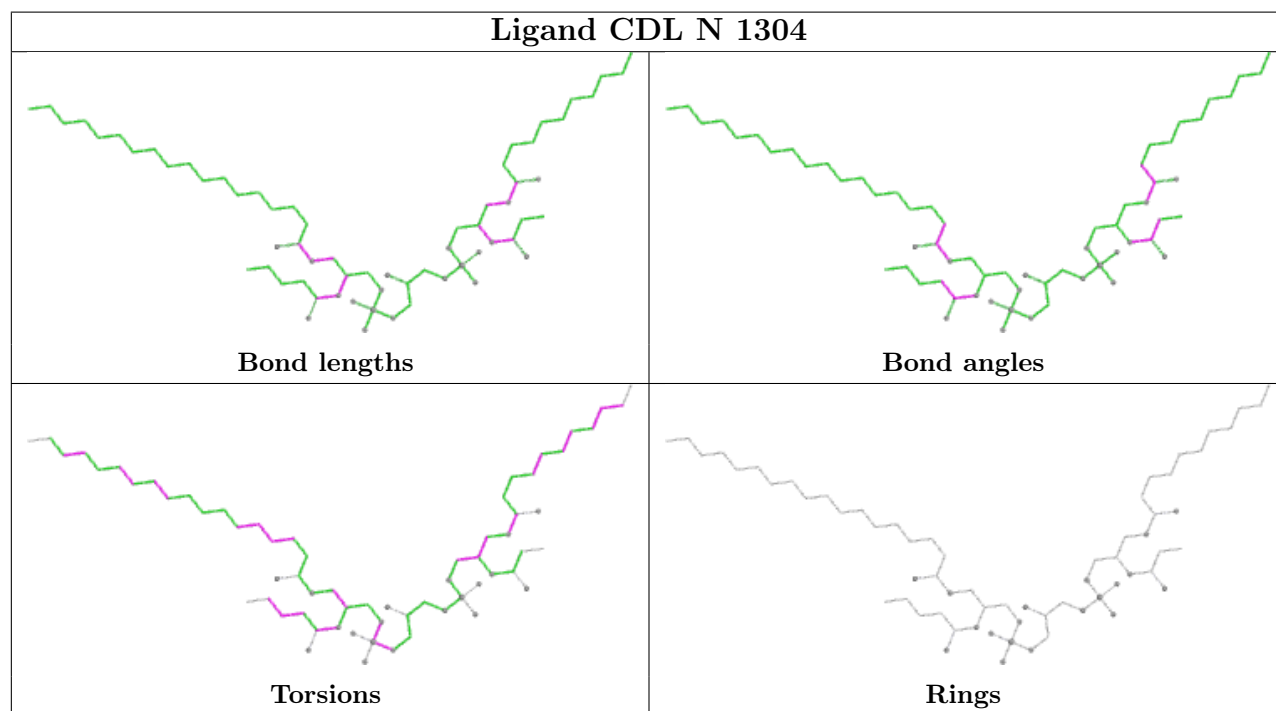
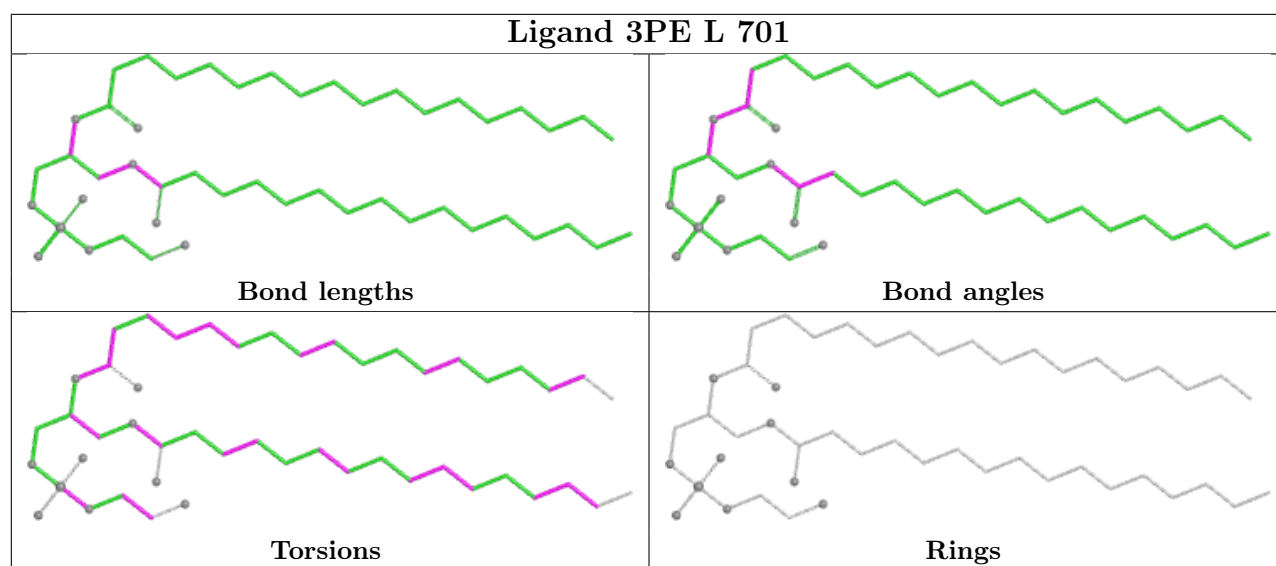


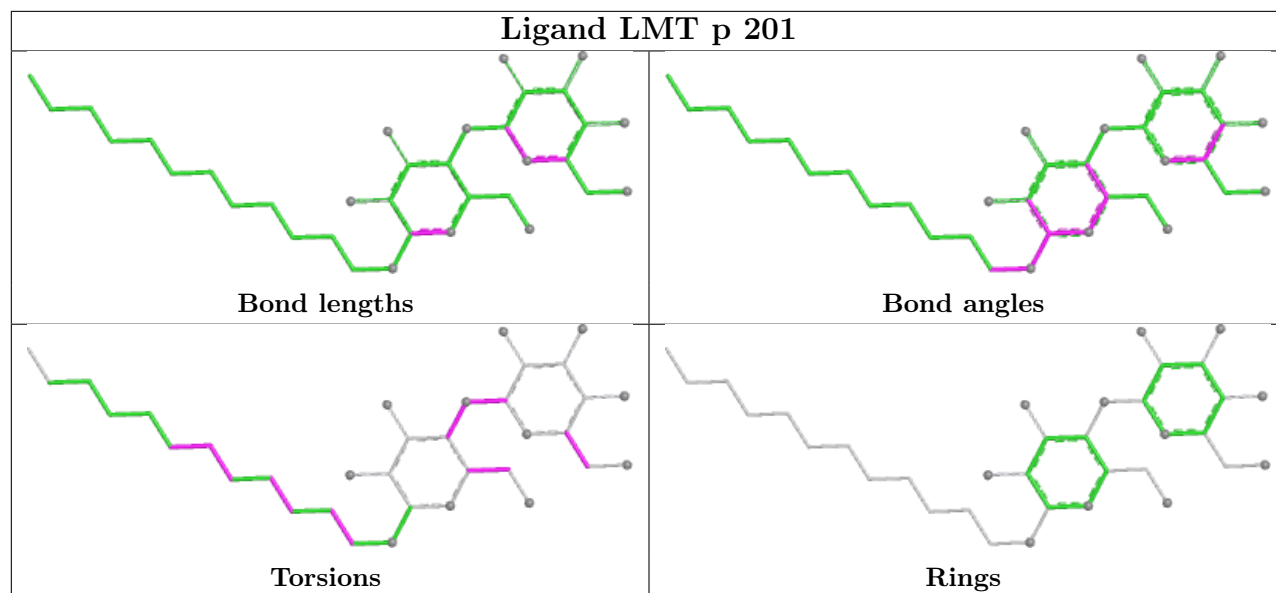


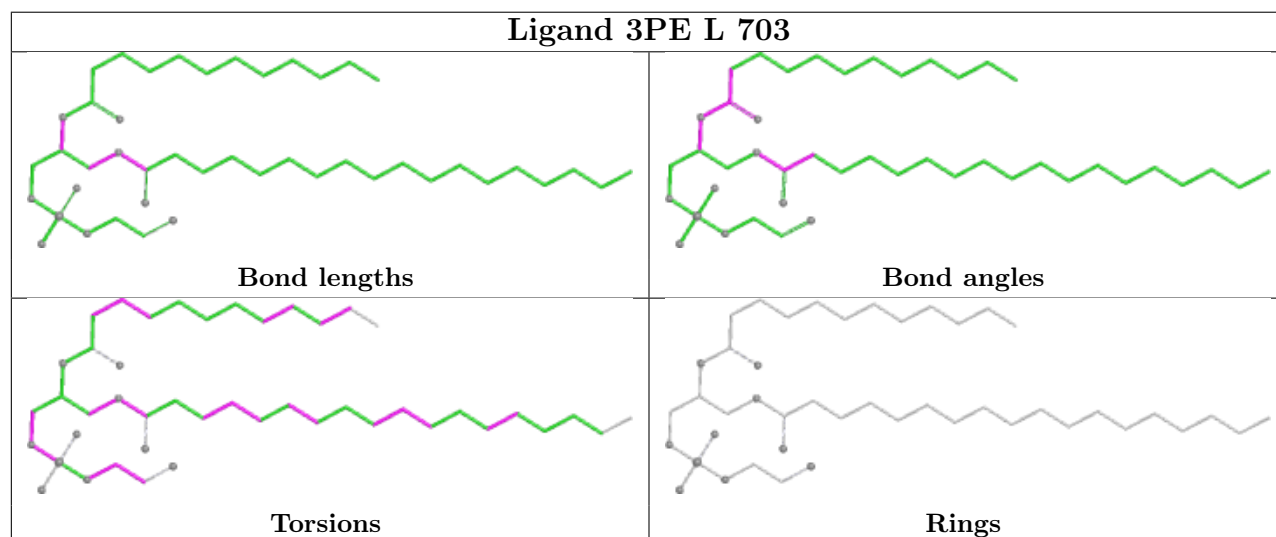
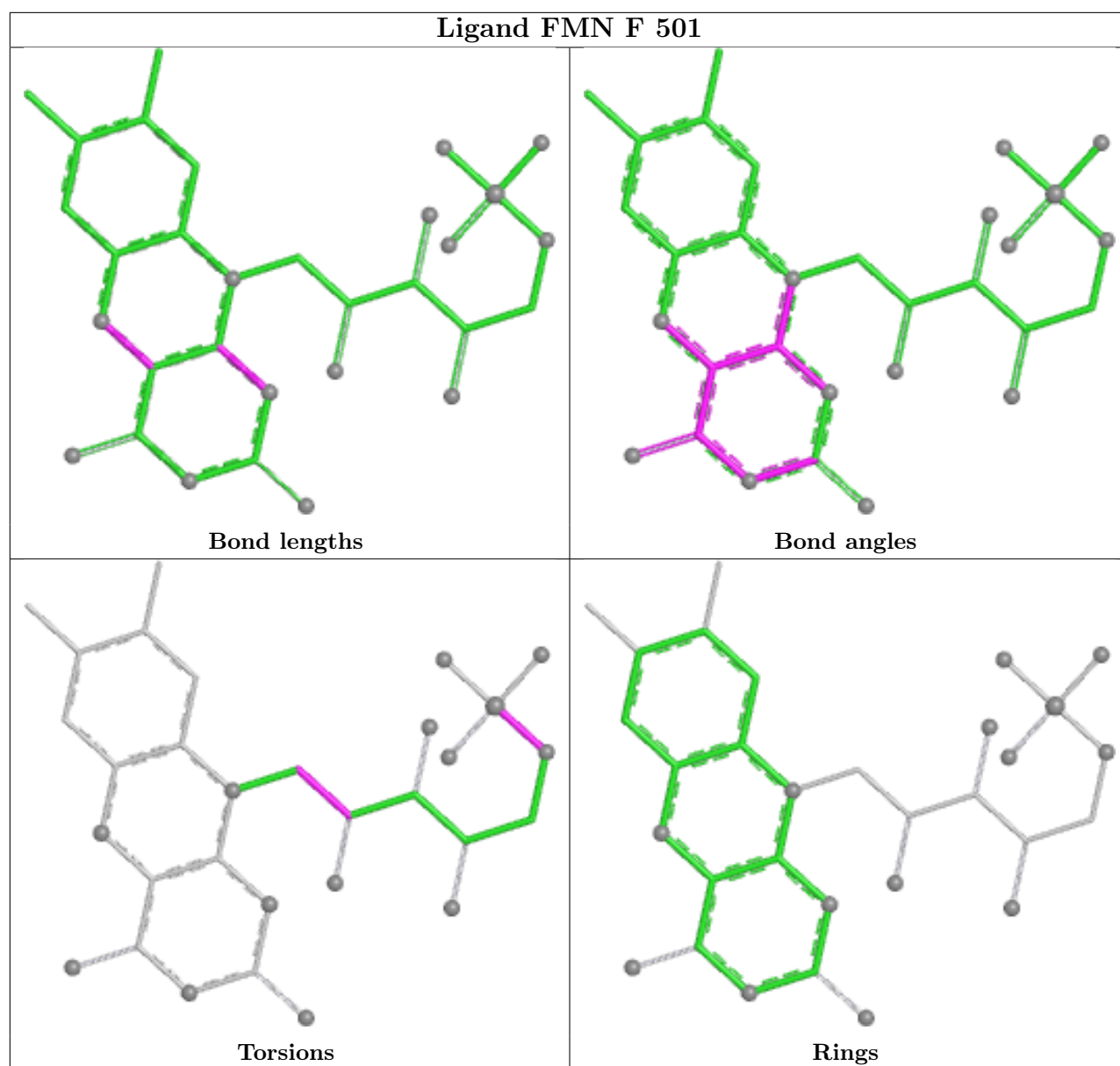


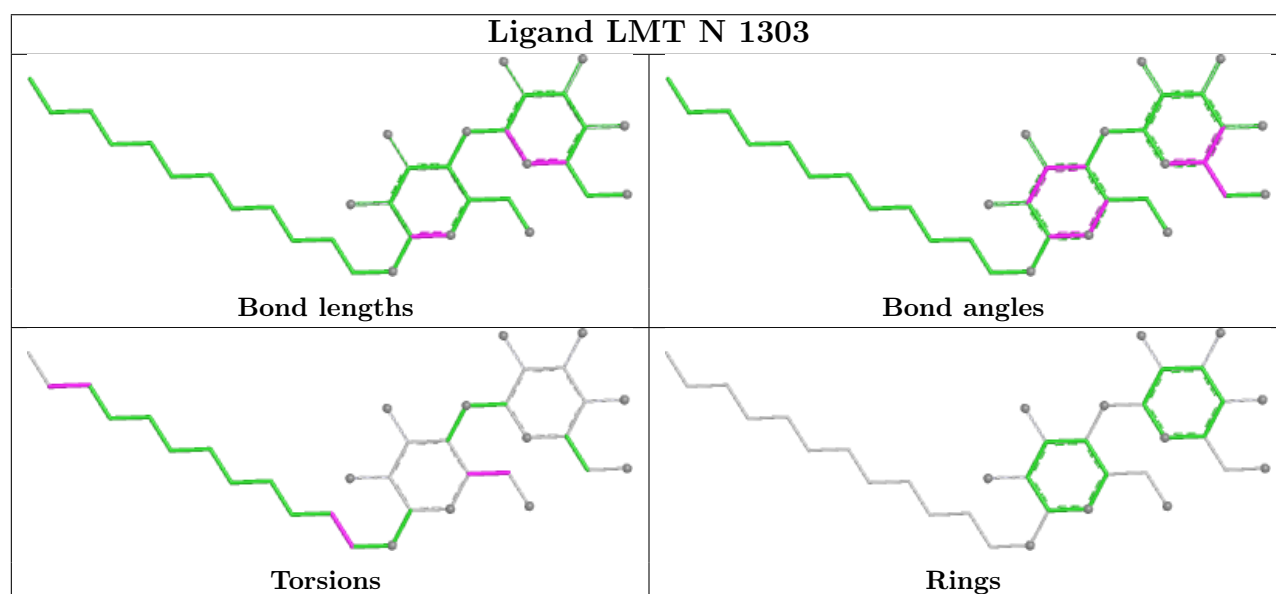
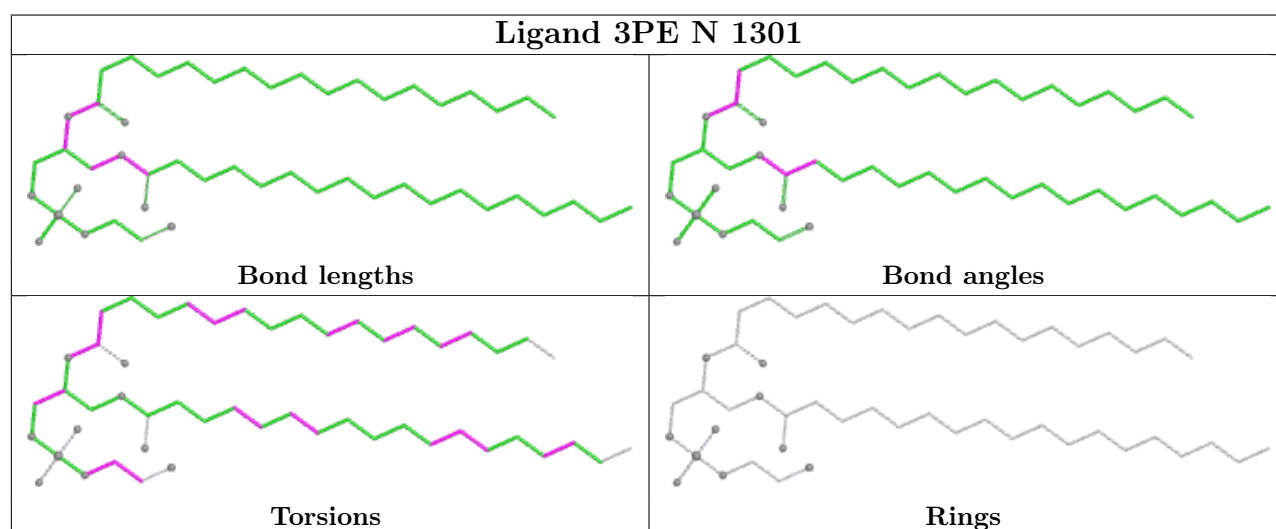
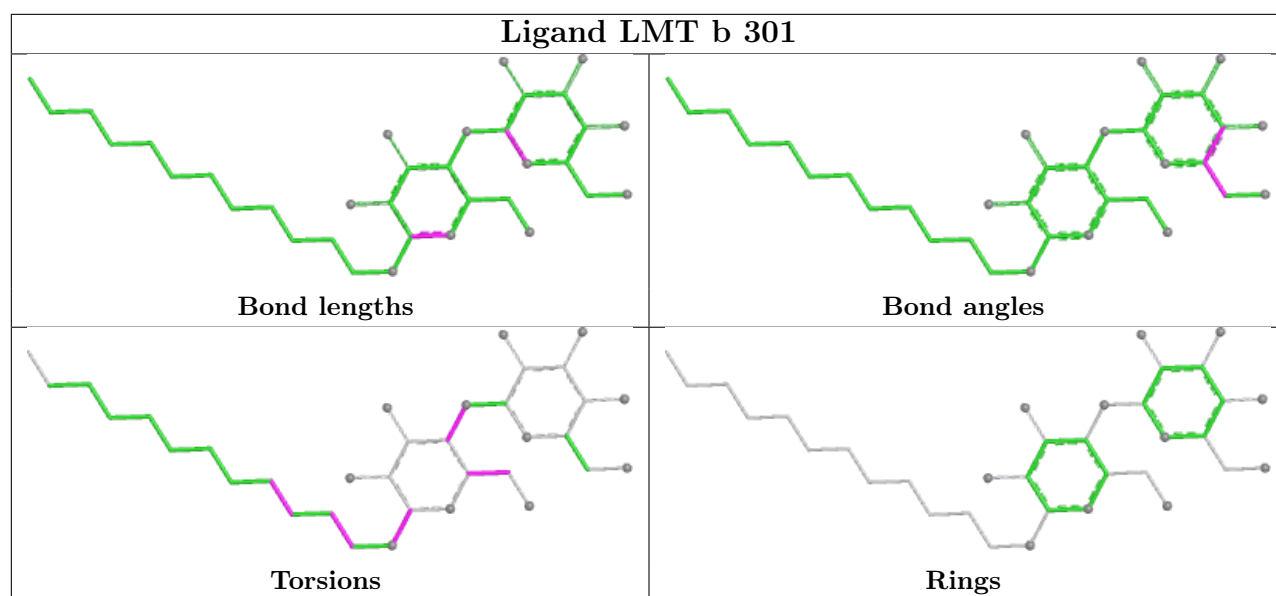


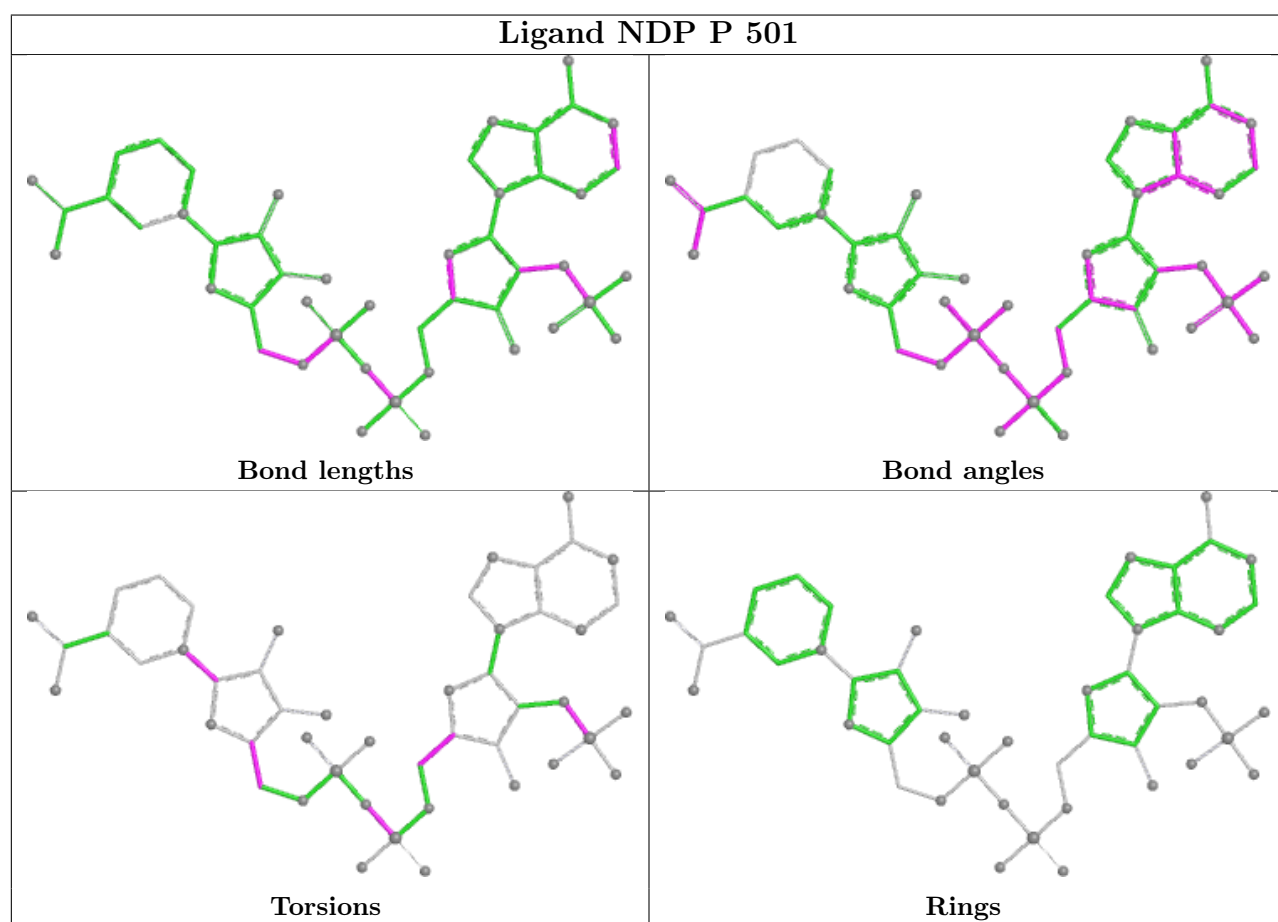
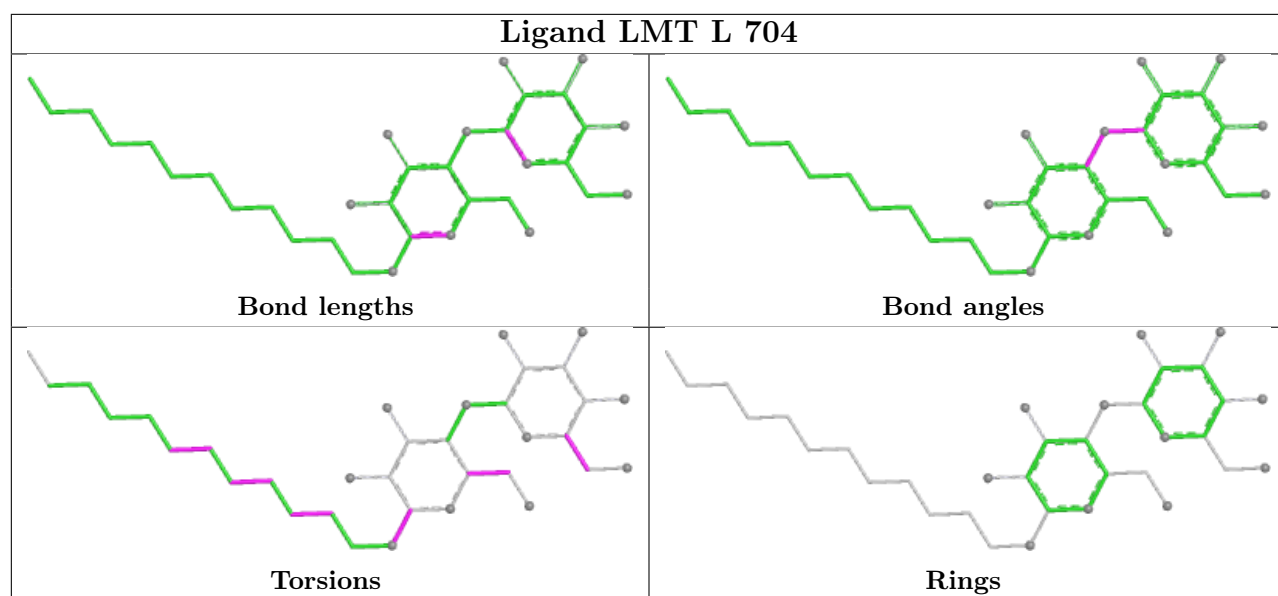


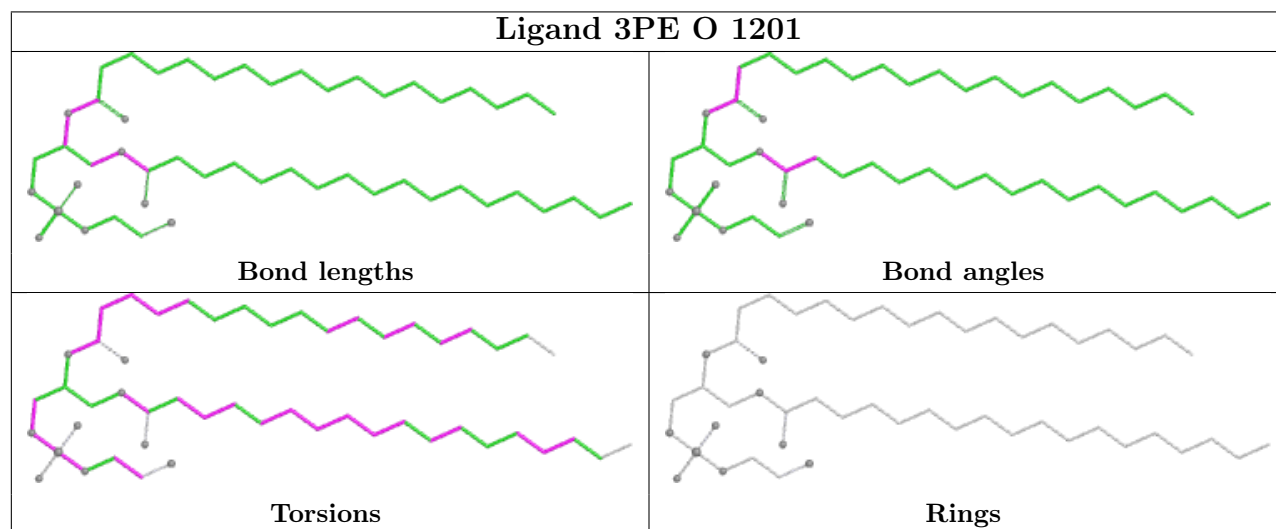
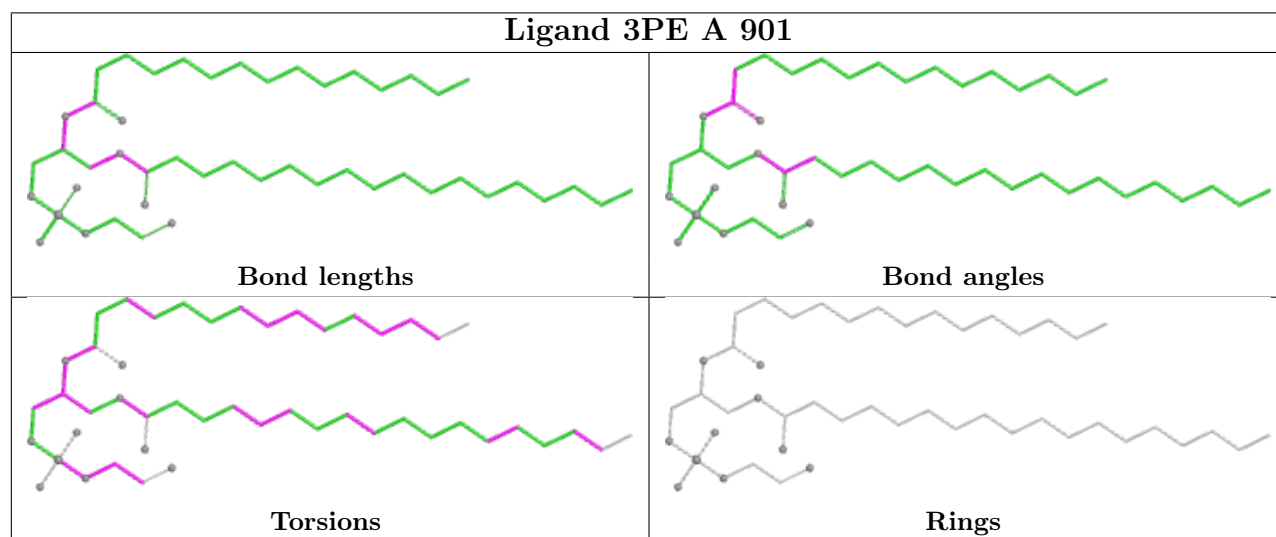
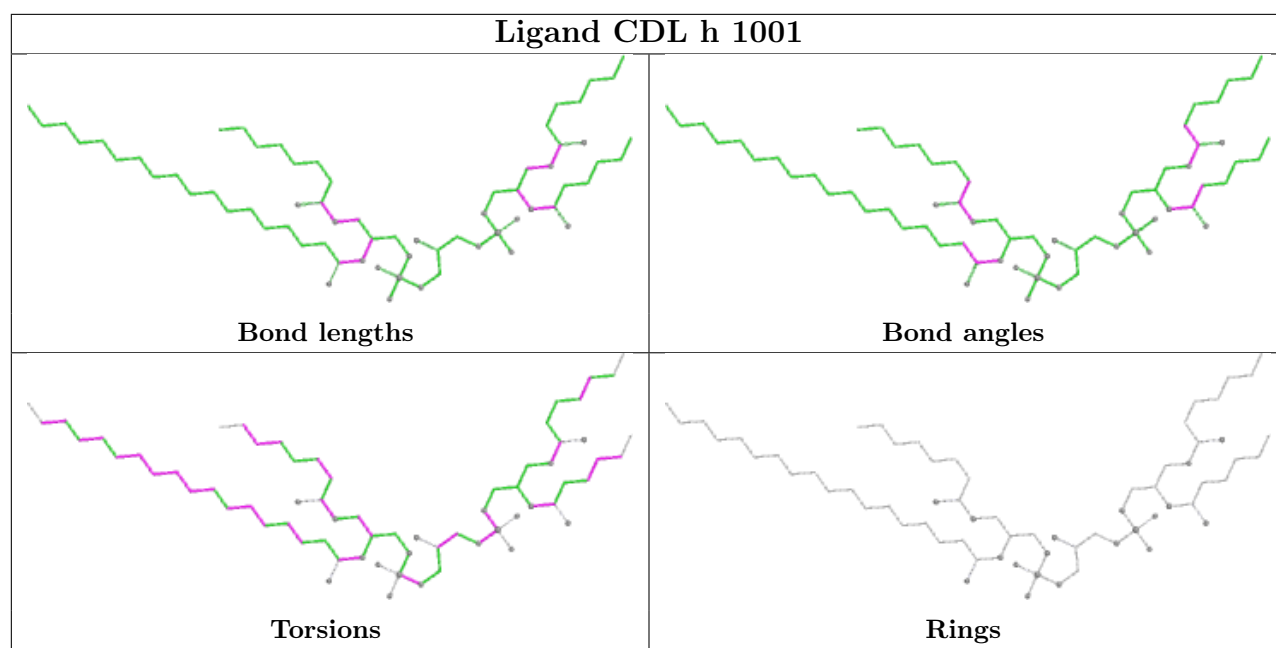


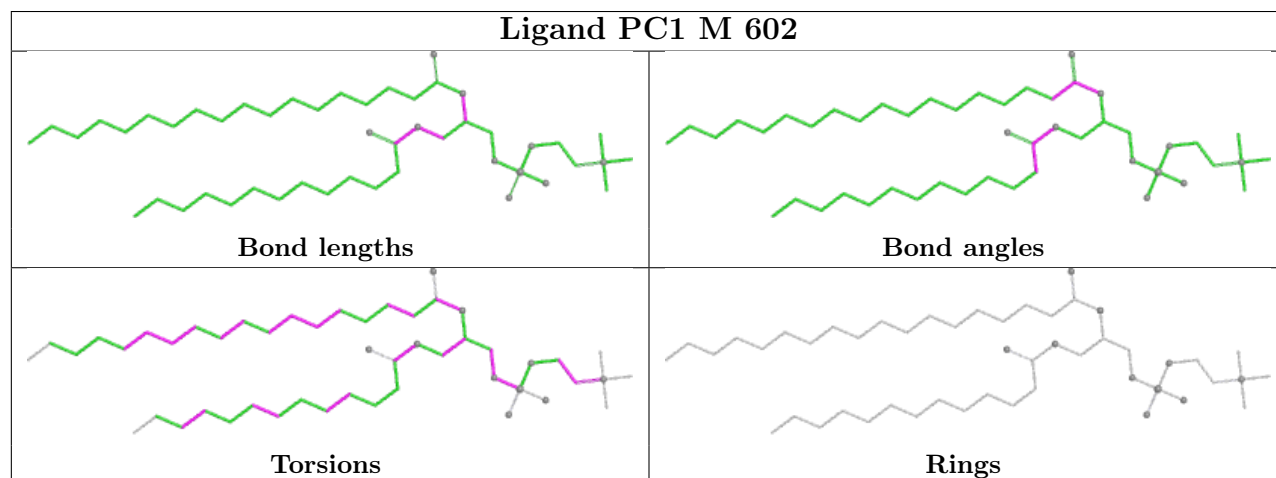
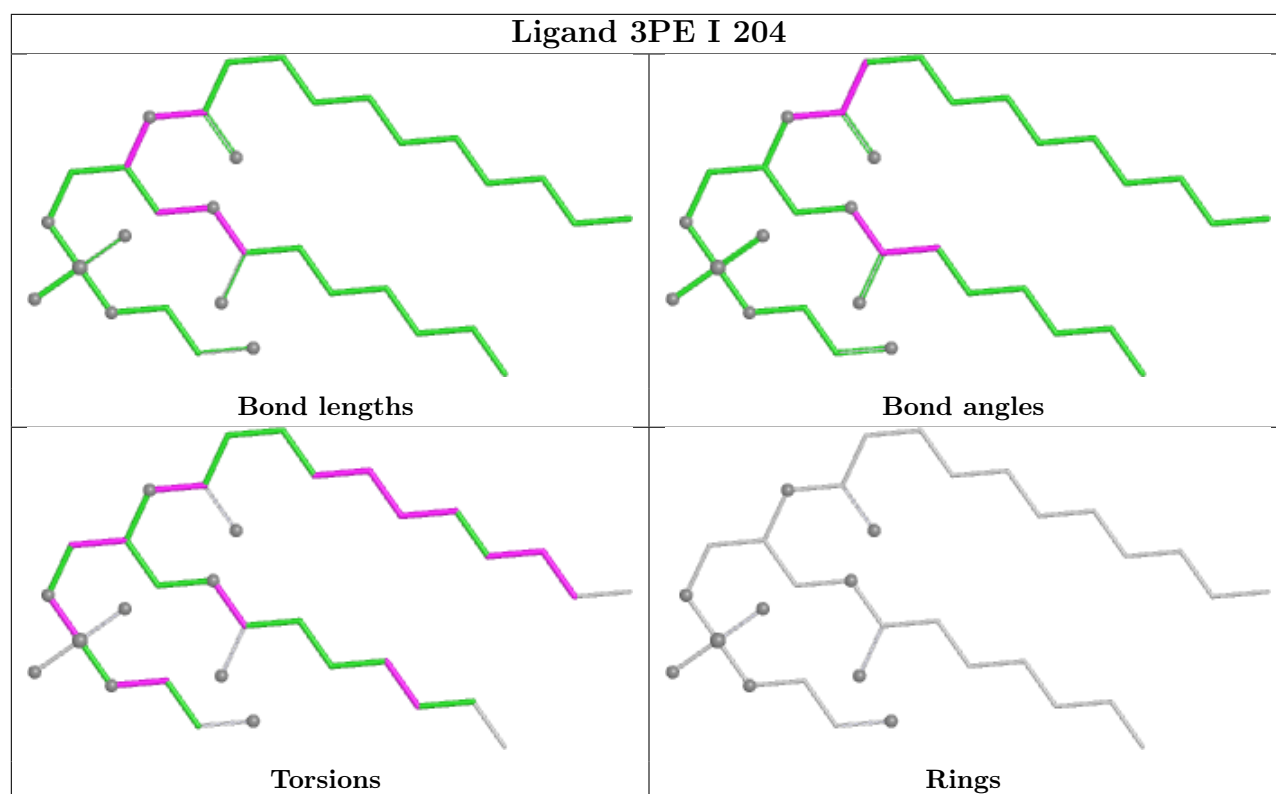


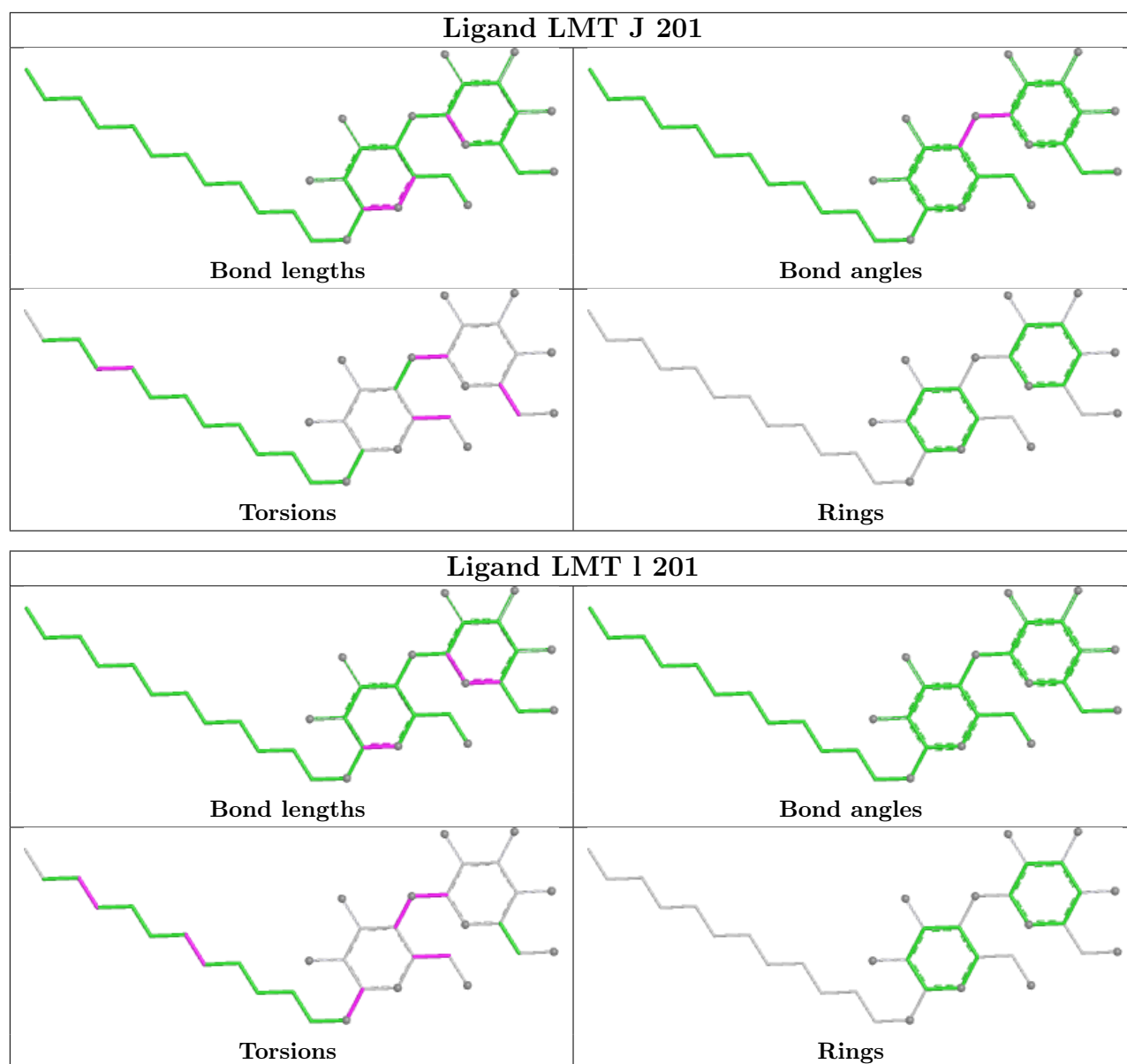


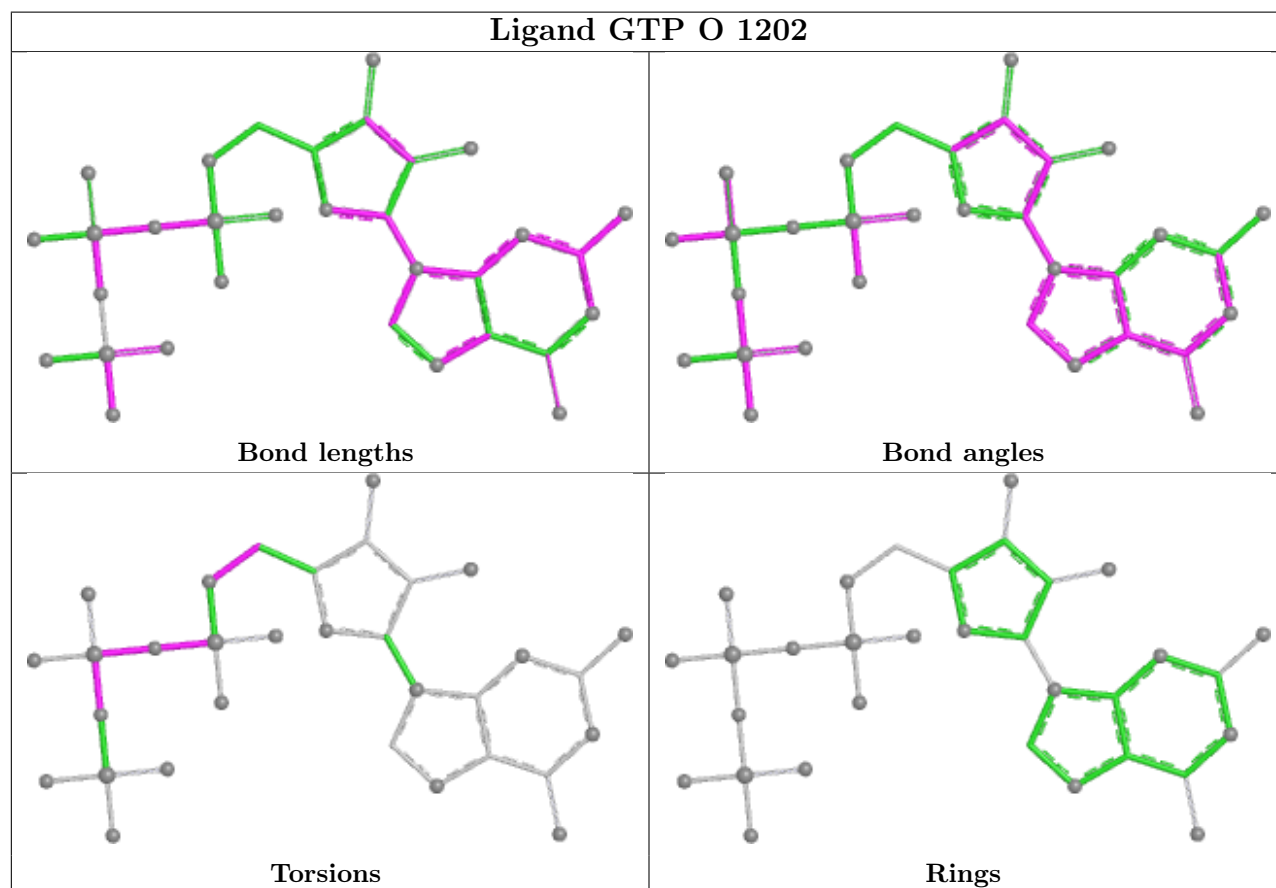
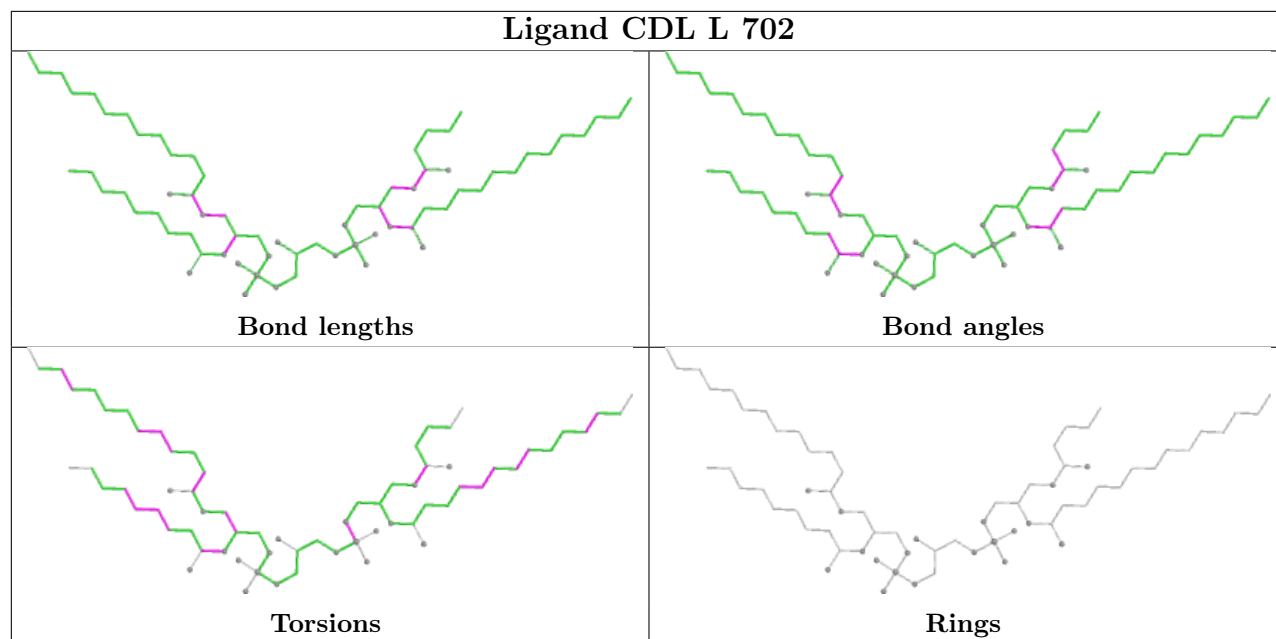


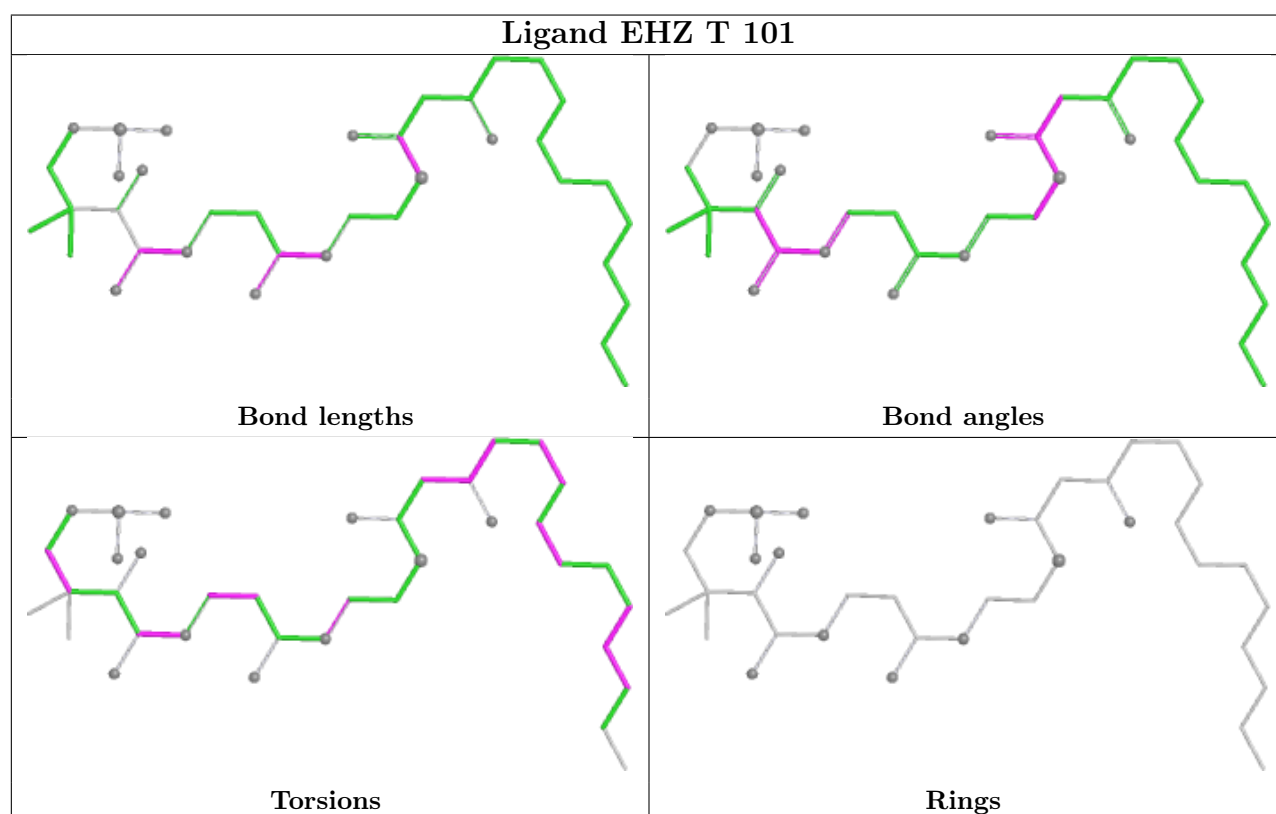
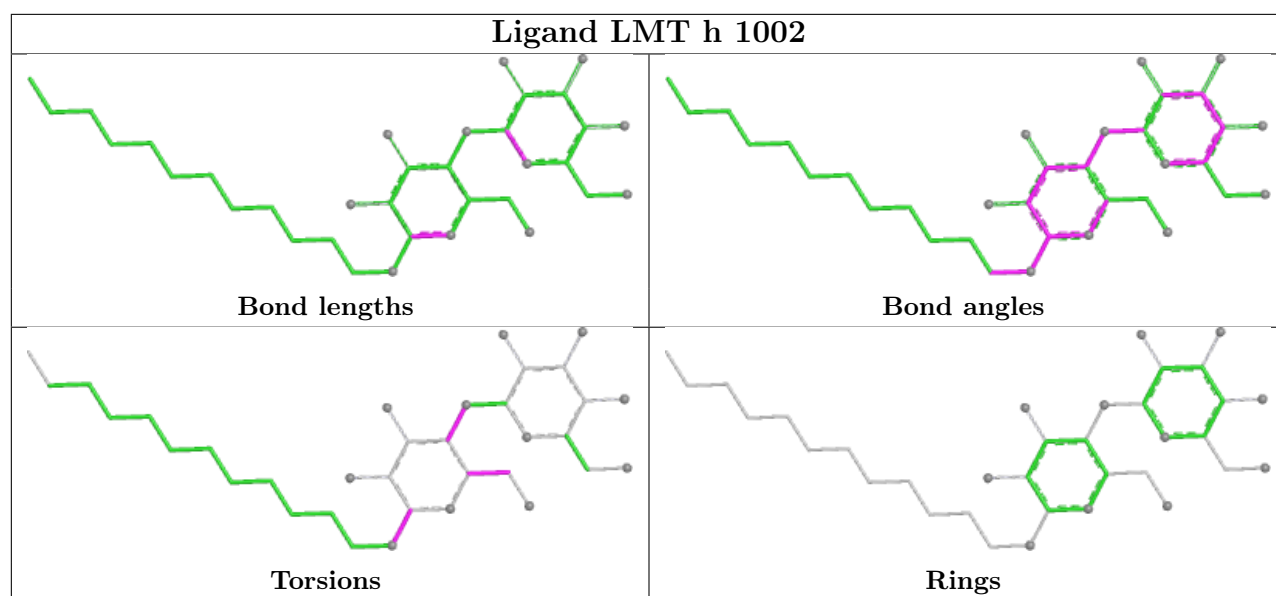


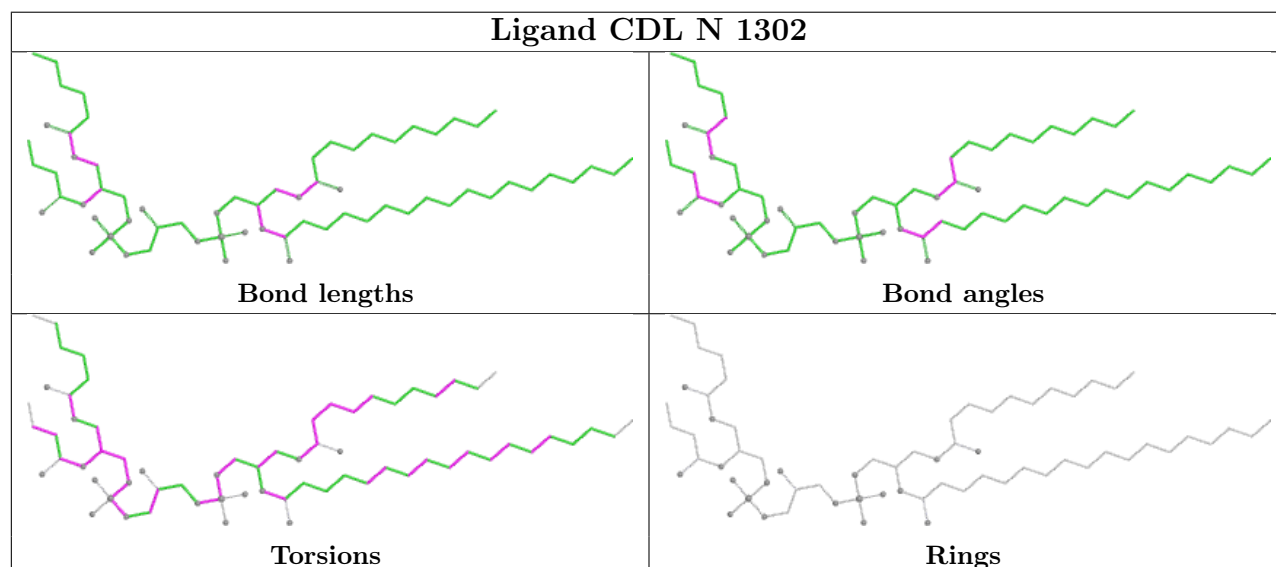
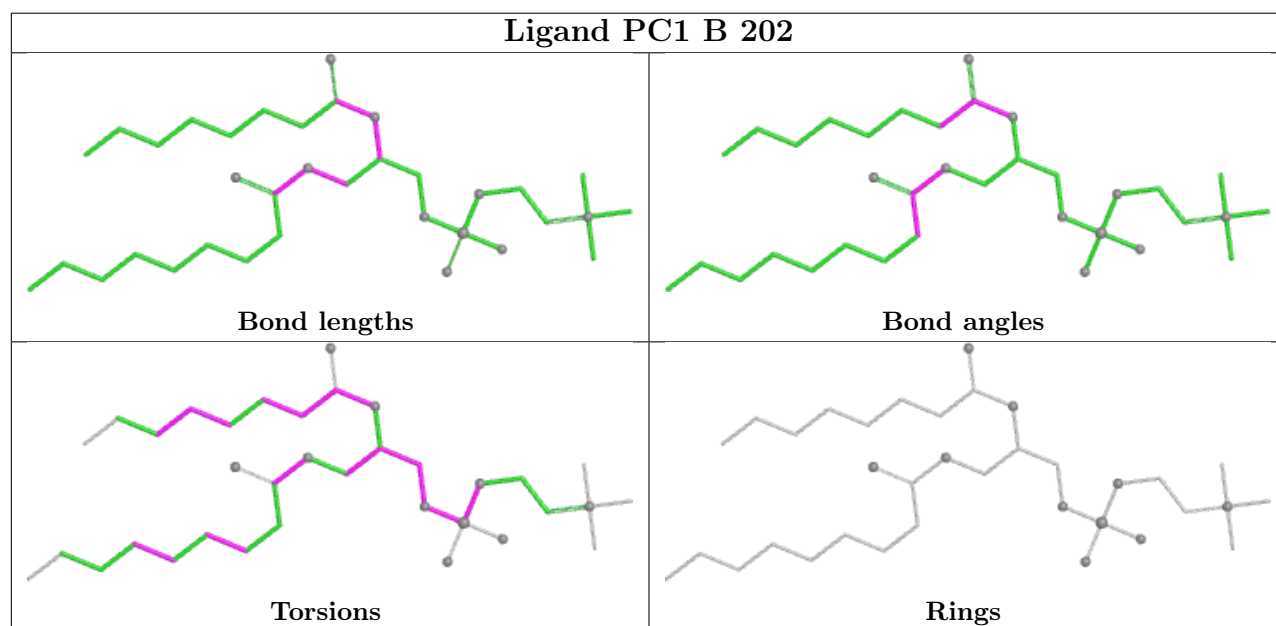
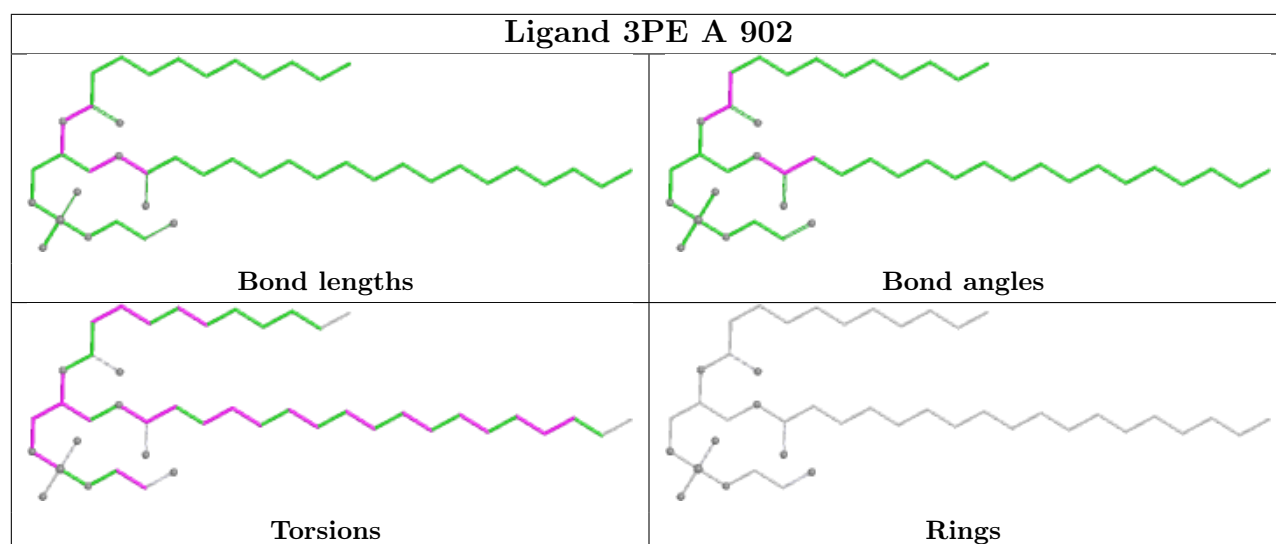


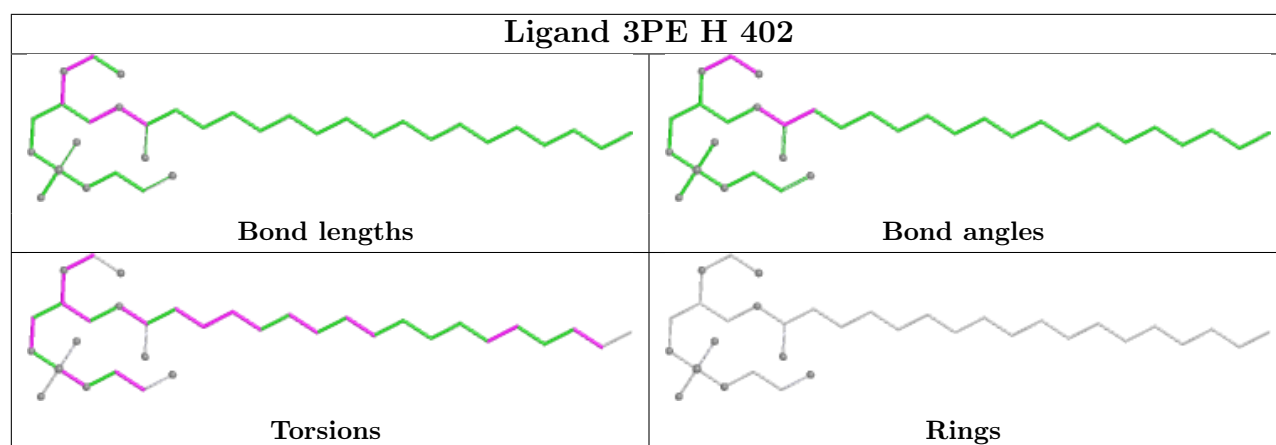












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

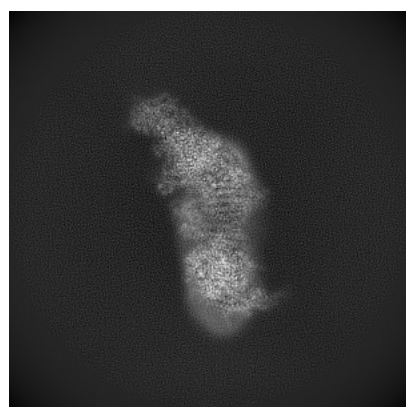
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14307. These allow visual inspection of the internal detail of the map and identification of artifacts.

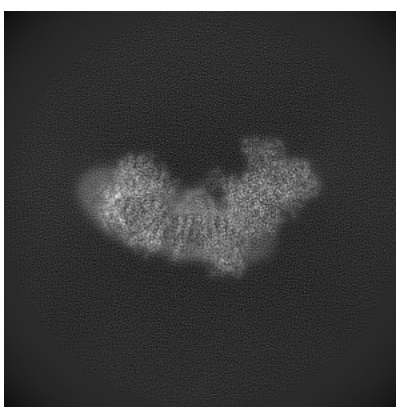
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

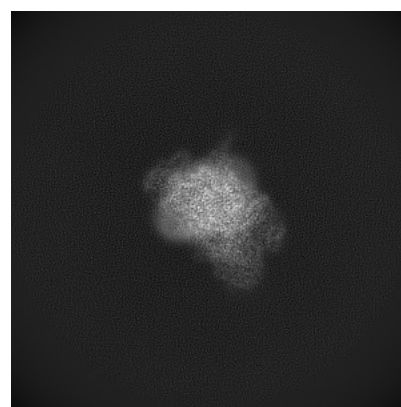
6.1.1 Primary map



X



Y

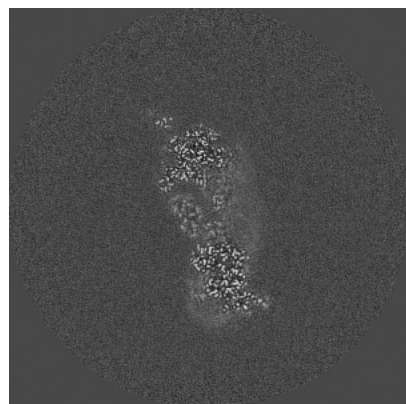


Z

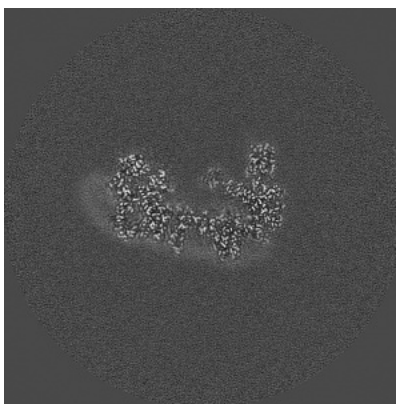
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

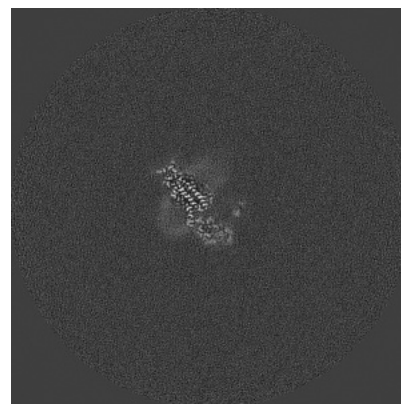
6.2.1 Primary map



X Index: 330



Y Index: 330

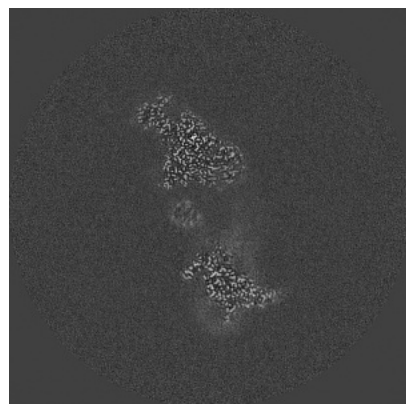


Z Index: 330

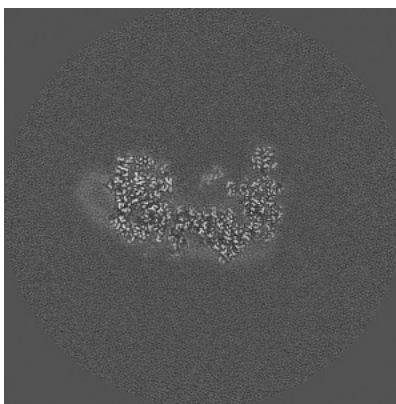
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

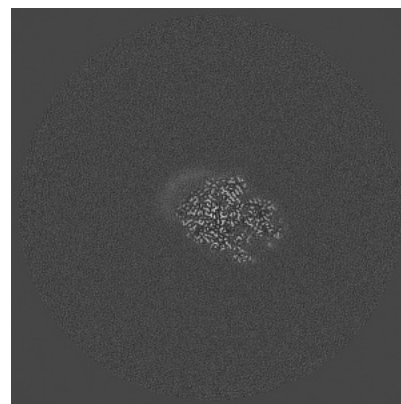
6.3.1 Primary map



X Index: 353



Y Index: 337

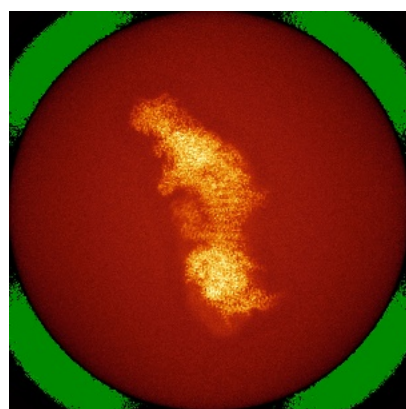


Z Index: 423

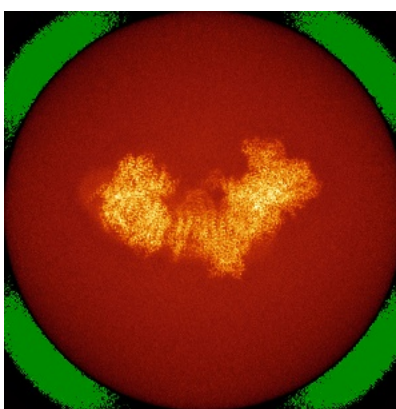
The images above show the largest variance slices of the map in three orthogonal directions.

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

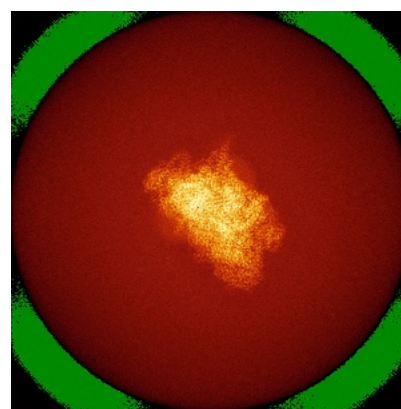
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

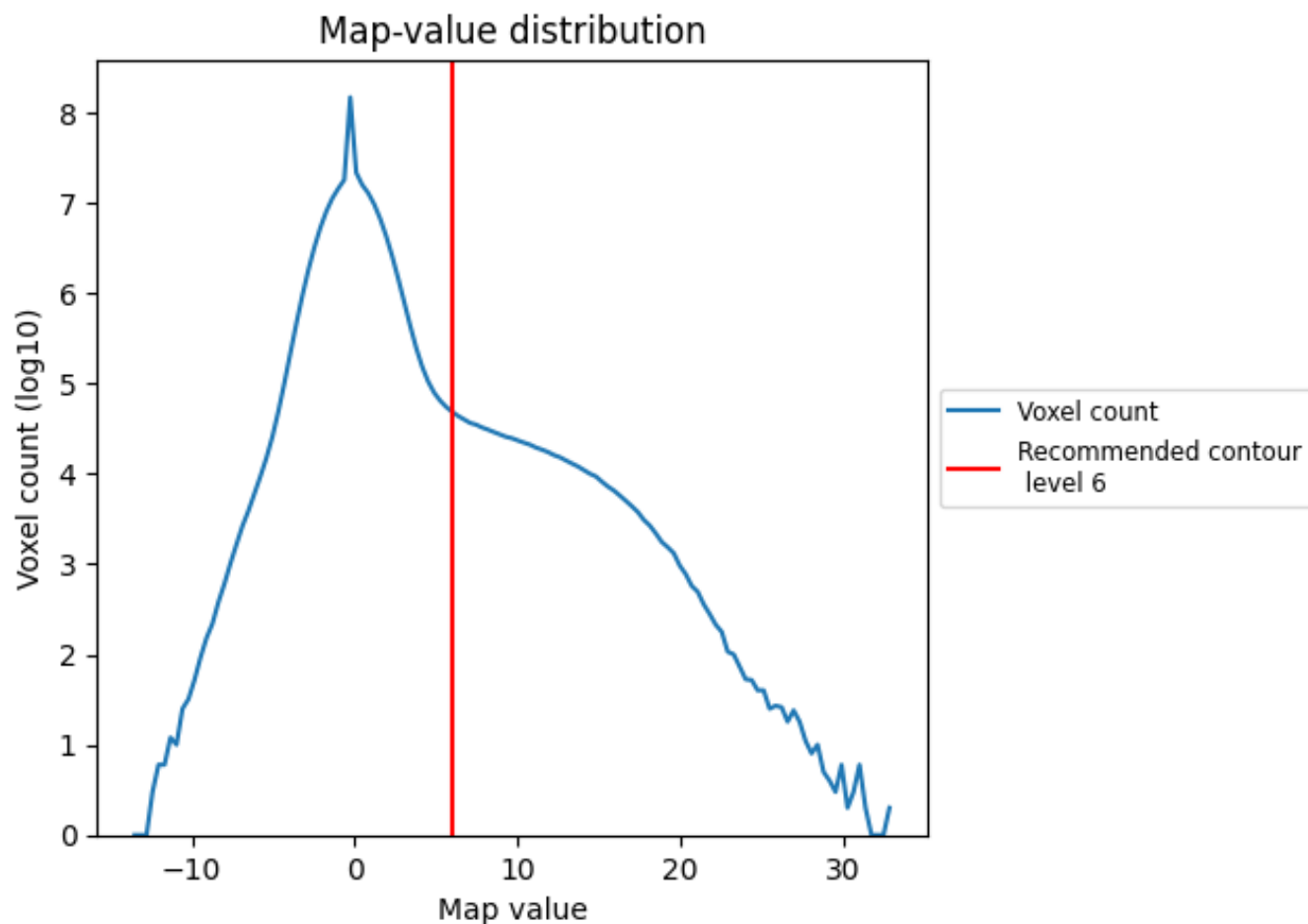
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

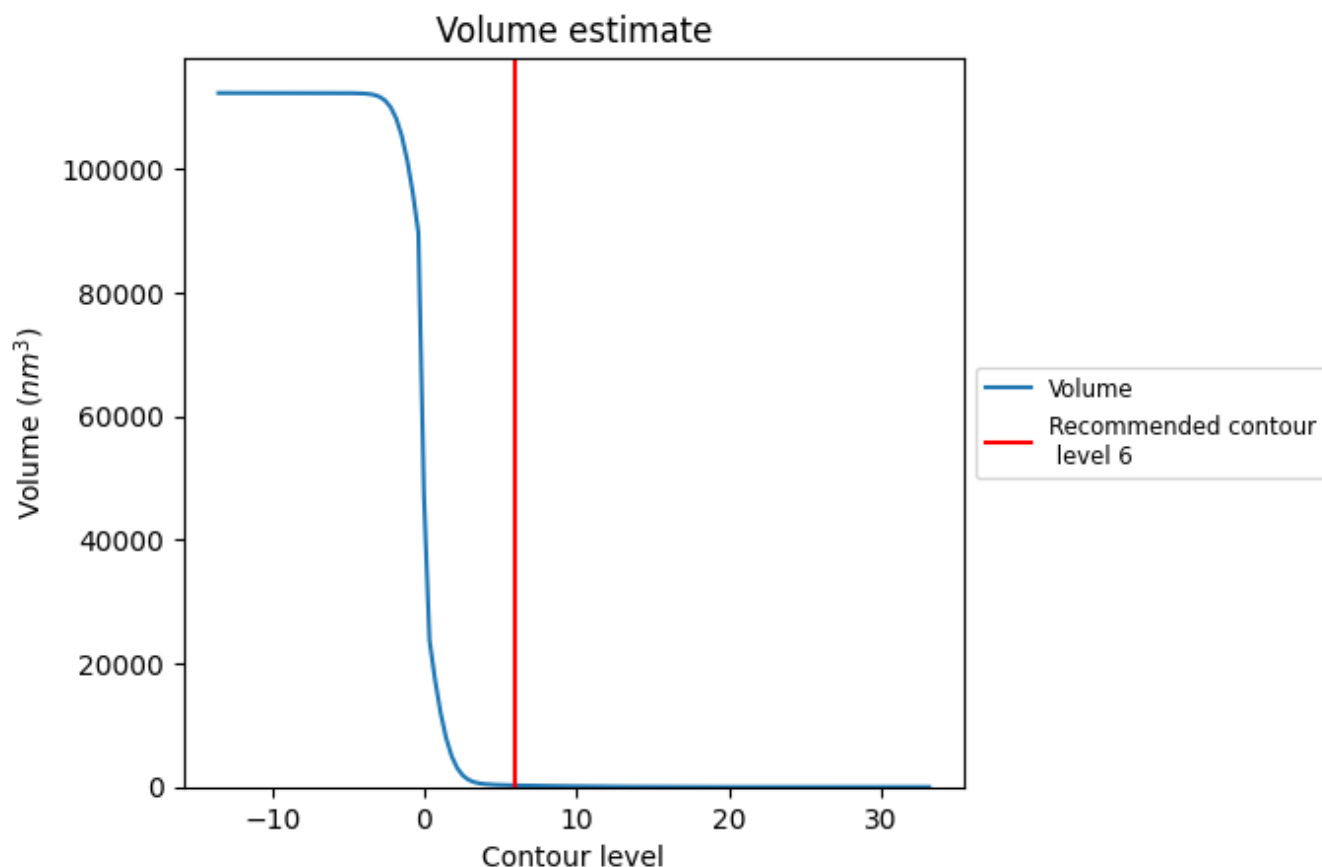
This section contains the results of statistical analysis of the map.

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.

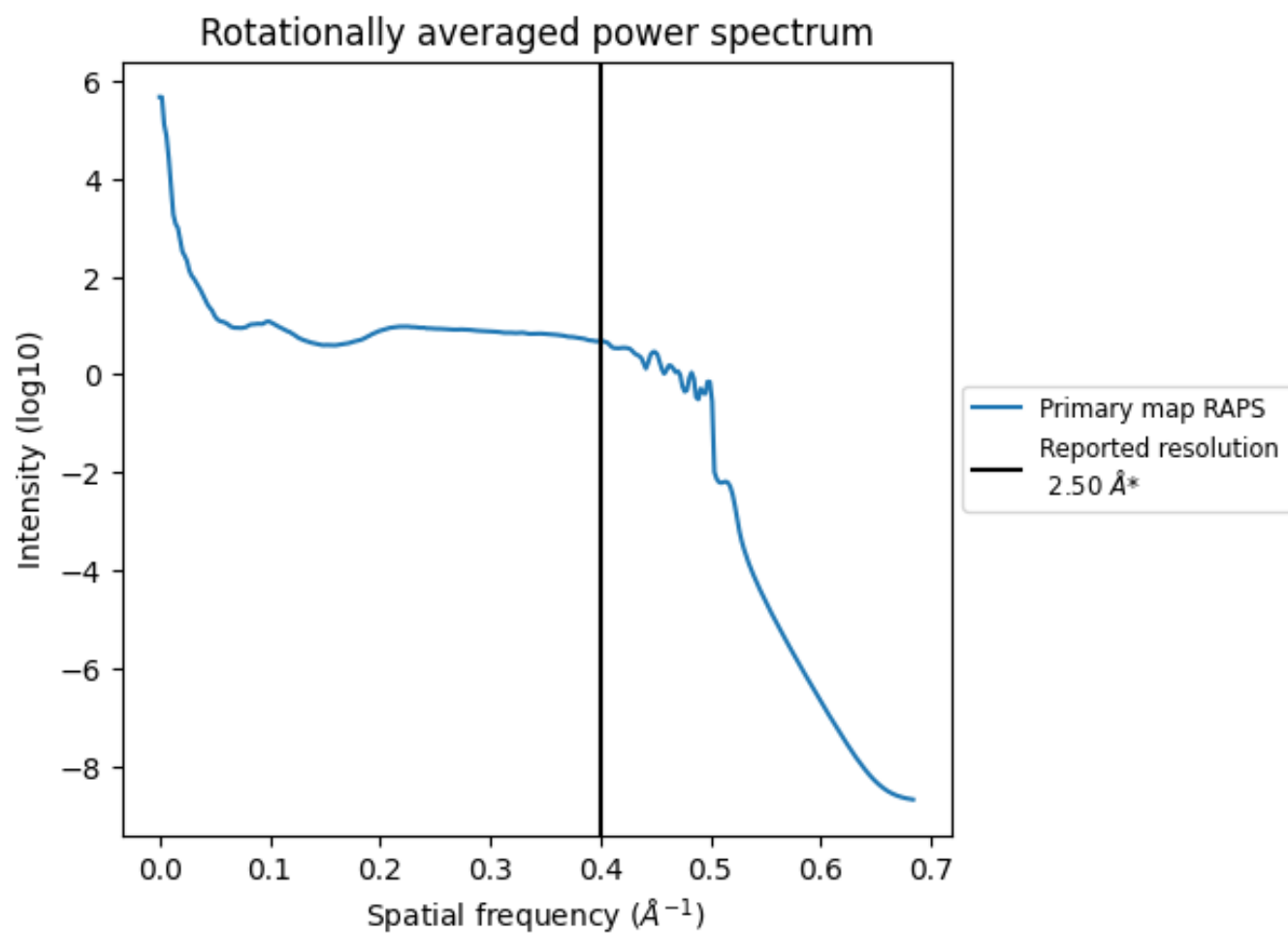
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm^3 ; this corresponds to an approximate mass of 229 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 0.400 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

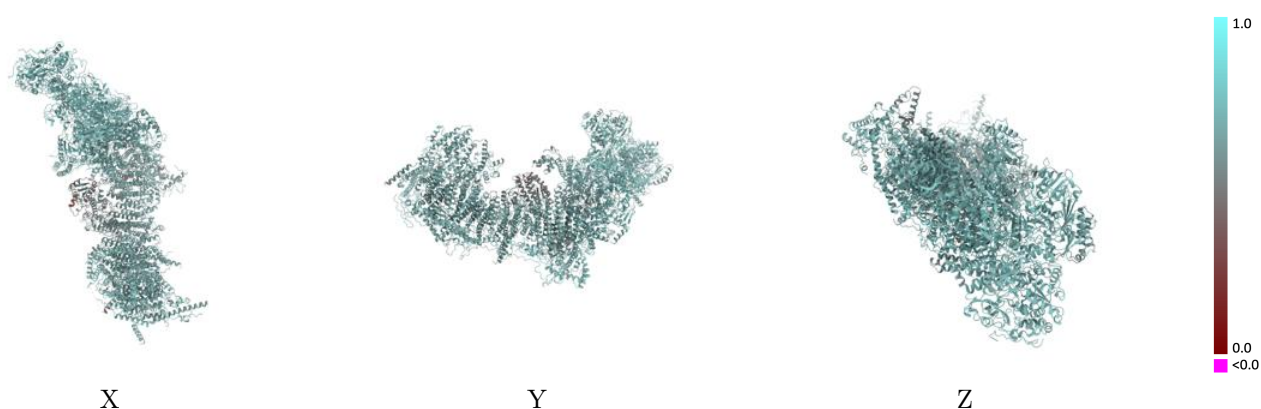
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14307 and PDB model 7R4G. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

This section was not generated.

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

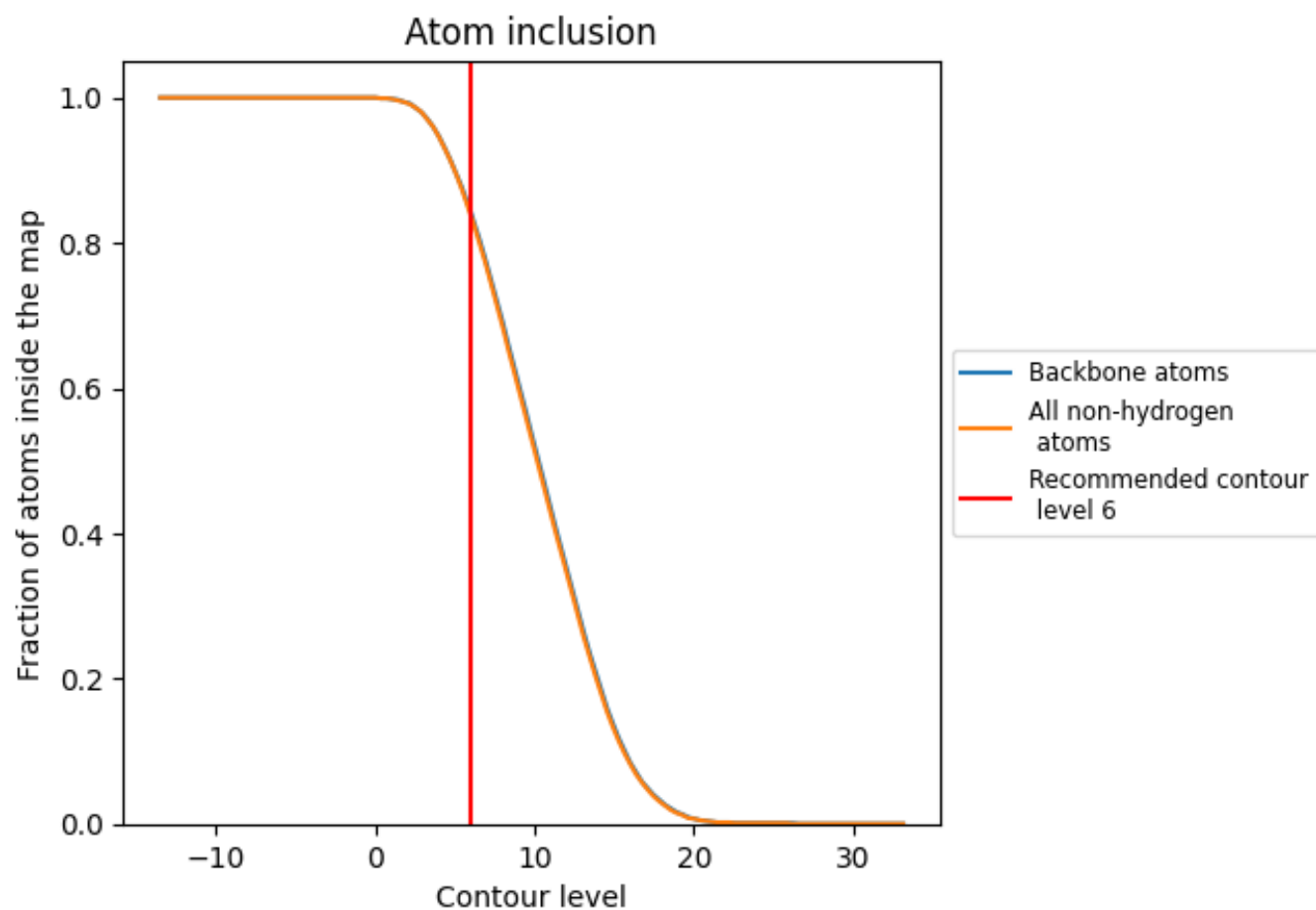


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.6620
A	 0.7560	 0.6400
B	 0.8930	 0.6960
C	 0.9360	 0.7150
D	 0.9320	 0.7110
E	 0.8340	 0.6700
F	 0.8830	 0.6820
G	 0.8800	 0.6920
H	 0.8800	 0.6760
I	 0.9250	 0.7160
J	 0.7600	 0.6340
K	 0.8400	 0.6620
L	 0.9200	 0.6550
M	 0.9170	 0.6680
N	 0.8050	 0.6520
O	 0.4660	 0.5290
P	 0.8150	 0.6640
Q	 0.8800	 0.6990
R	 0.8880	 0.7000
S	 0.7840	 0.6600
T	 0.4880	 0.5850
U	 0.9140	 0.6530
V	 0.8060	 0.6730
W	 0.8090	 0.6770
X	 0.8010	 0.6520
Y	 0.4970	 0.6310
Z	 0.7470	 0.6380
a	 0.8850	 0.6740
b	 0.7690	 0.6390
c	 0.6160	 0.5970
d	 0.7830	 0.6510
e	 0.7670	 0.6460
f	 0.8150	 0.6310
g	 0.8940	 0.6530
h	 0.8750	 0.6620



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Chain	Atom inclusion	Q-score
i	 0.8620	 0.6330
j	 0.8850	 0.6330
k	 0.8790	 0.6280
l	 0.8600	 0.6380
m	 0.8540	 0.6430
n	 0.8990	 0.6510
o	 0.8730	 0.6340
p	 0.8810	 0.6510
q	 0.8000	 0.6830
r	 0.8530	 0.6950
s	 0.8200	 0.6780