Full wwPDB EM Validation Report

Sep 8, 2026 – 09:49 pm BST

PDB ID	:	8RGR / pdb_00008rgr
EMDB ID	:	EMD-19147
Title	:	Closed Complex I from murine liver
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2023-12-14
Resolution	:	2.90 Å(reported)
Based on initial model	:	6g2j

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:

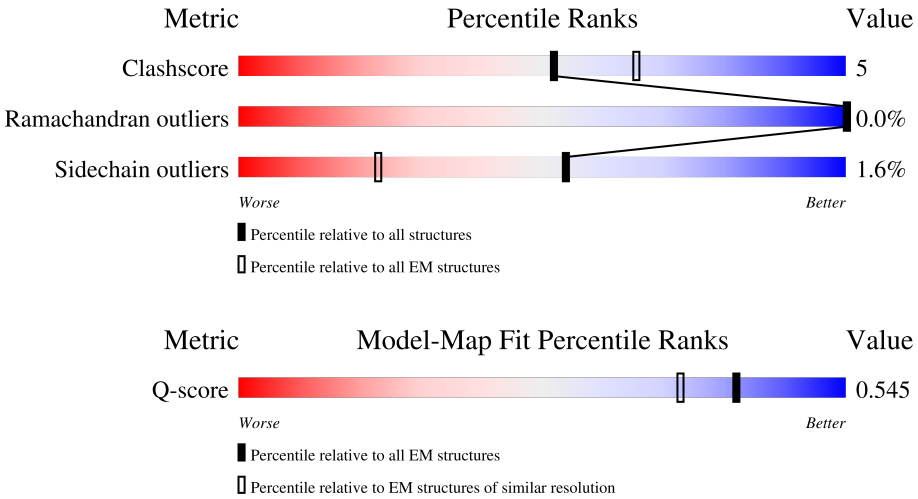
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the 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)	:	2.50

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 2.90 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	13054 (2.40 - 3.40)

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 <=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	6	224	55% 14% 30%
2	C	263	67% 12% 21%
3	D	463	5% 76% 16% • 7%
4	2	248	72% 14% 14%

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Mol	Chain	Length	Quality of chain
5	1	464	78% 14% 7%
6	3	727	81% 13% 5%
7	9	212	71% 12% 16%
8	P	377	74% 16% 9%
9	Q	175	62% 10% 28%
10	7	116	76% 7% 17%
11	S	99	69% 16% 15%
12	T	156	40% 10% 49%
12	U	156	45% 12% 44%
13	V	116	88% 9%
14	W	131	79% 8% 13%
15	q	145	88% 12%
16	r	113	78% 10% 12%
17	s	104	33% 8% 60%
18	A	115	83% 17%
19	H	318	78% 21%
20	J	172	12% 85% 15%
21	K	98	87% 12%
22	L	607	81% 18%
23	M	459	81% 18%
24	N	345	81% 17%
25	O	355	80% 10% 10%
26	X	172	81% 19%
27	Y	141	86% 13%
28	Z	144	87% 10%

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Mol	Chain	Length	Quality of chain
29	a	70	90% 9%
30	b	84	92% 7%
31	c	76	58% 5% 37%
32	d	120	88% 12%
33	e	106	88% 11%
34	f	57	5% 86% 7% 7%
35	g	151	62% 5% 33%
36	h	189	59% 15% 26%
37	i	128	9% 67% 16% 17%
38	j	105	53% 9% 38%
39	k	104	66% 8% 26%
40	l	186	74% 11% 16%
41	m	129	5% 87% 11%
42	n	179	88% 12%
43	o	137	76% 10% 14%
44	p	176	87% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	9	201	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 68141 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 dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	157	1258	802	227	215	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	208	1730	1116	297	314	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	430	3464	2215	595	630	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	214	1660	1056	279	314	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	430	3321	2092	596	611	22	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	79	Total	C	N	O	S	0	0
			637	410	95	127	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	s	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	115	Total	C	N	O	S	0	0
			932	633	132	160	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

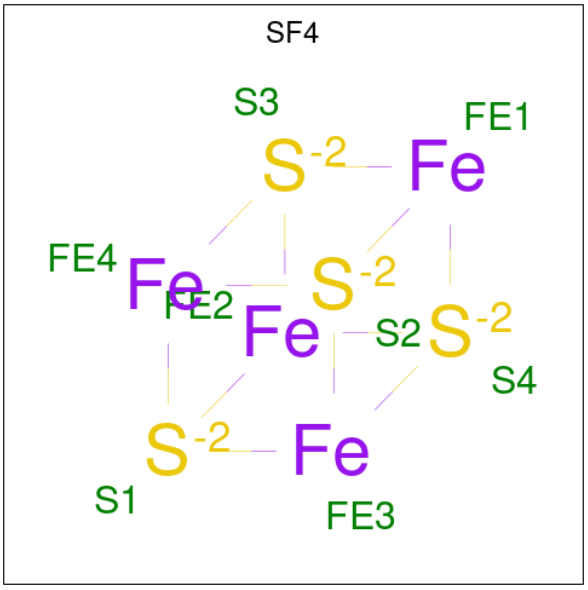
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

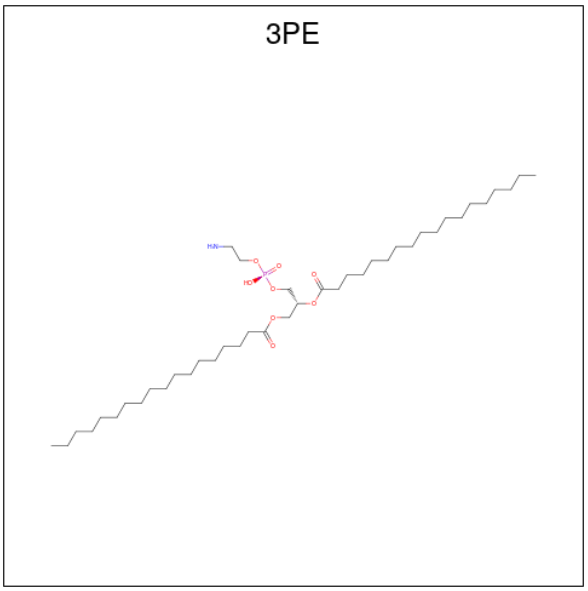
Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
45	6	1	Total	Fe	S	0
			8	4	4	
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



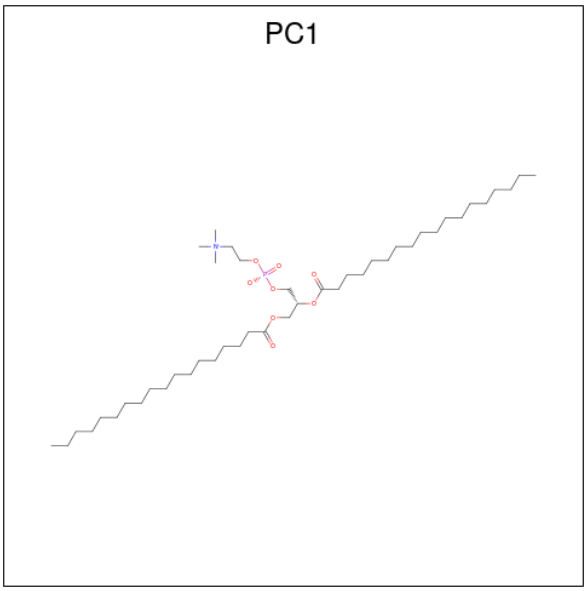
Mol	Chain	Residues	Atoms					AltConf
46	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	r	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	Y	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	d	1	Total	C	N	O	P	0
			31	21	1	8	1	

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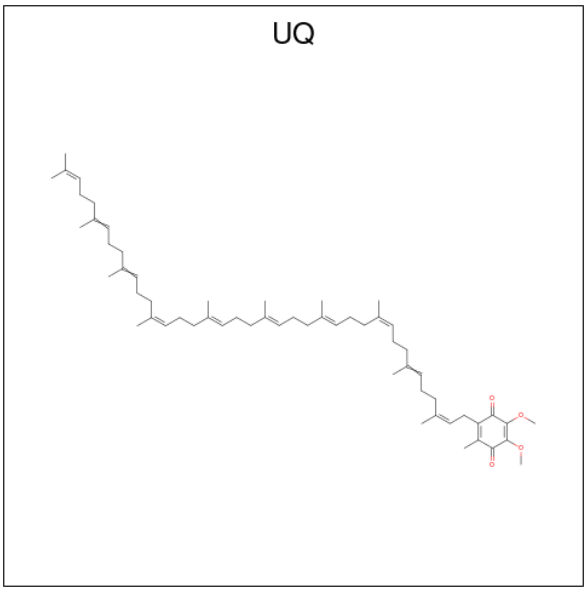
Mol	Chain	Residues	Atoms					AltConf
46	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	m	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



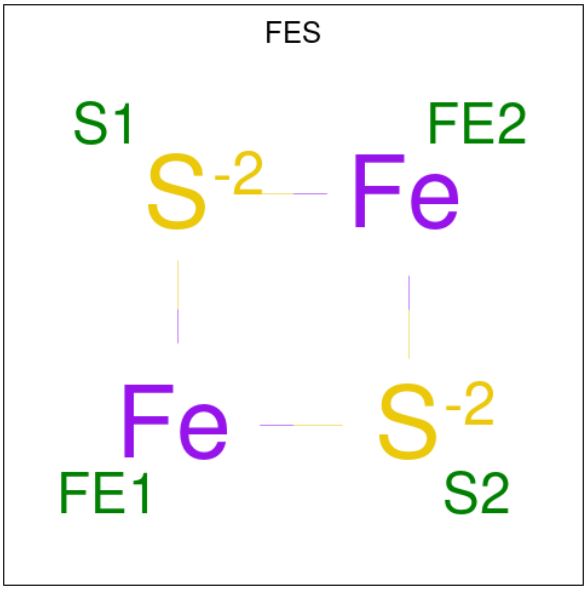
Mol	Chain	Residues	Atoms					AltConf
47	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	N	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 48 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$).



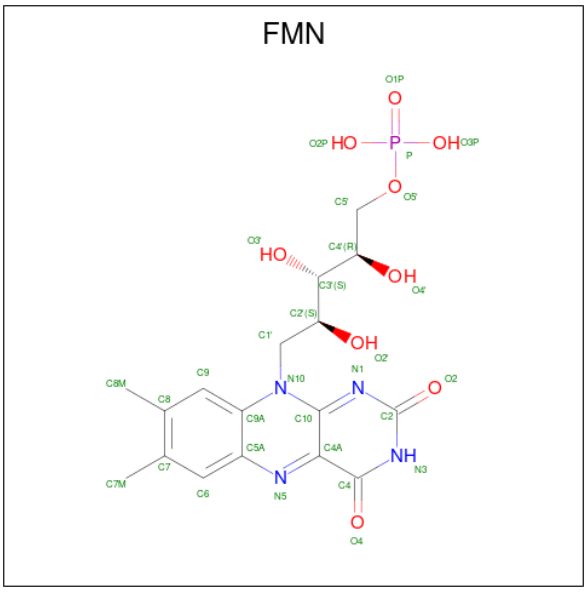
Mol	Chain	Residues	Atoms			AltConf
48	D	1	Total	C	O	0
			63	59	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
49	2	1	Total	Fe	S	0
			4	2	2	
49	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

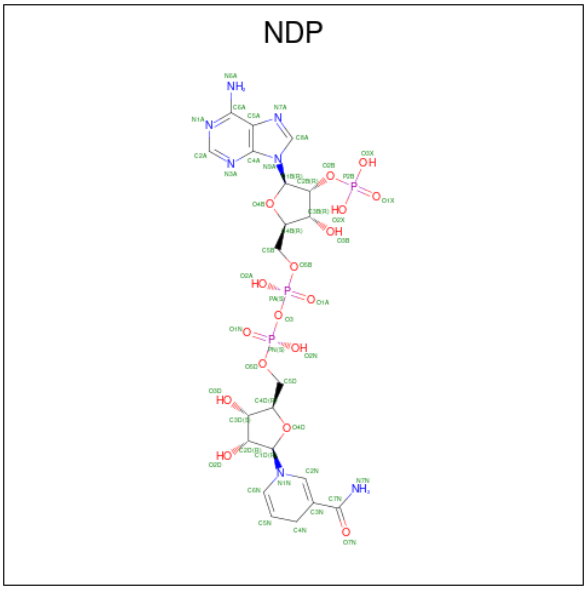


Mol	Chain	Residues	Atoms					AltConf
50	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

Mol	Chain	Residues	Atoms		AltConf
51	3	1	Total	K	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

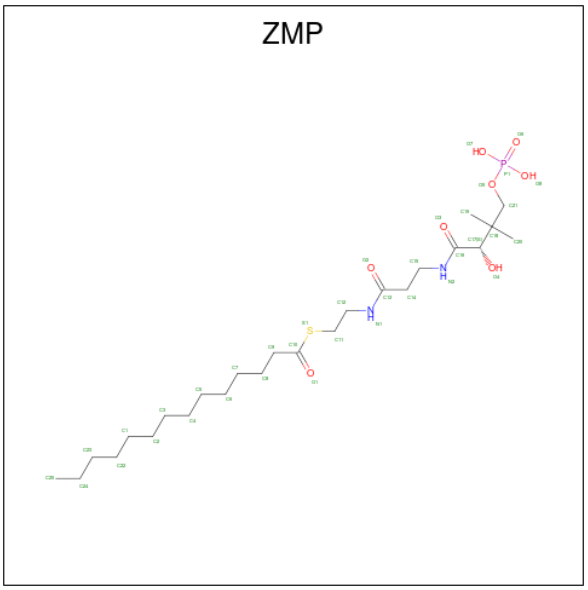


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

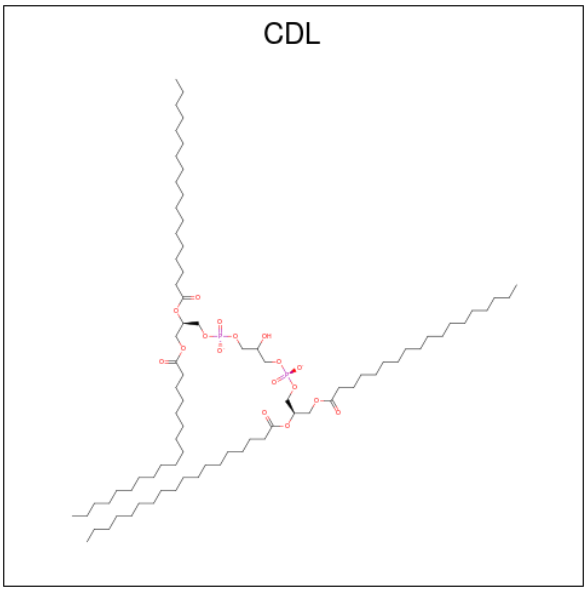
Mol	Chain	Residues	Atoms		AltConf
53	7	1	Total	Zn	0
			1	1	

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



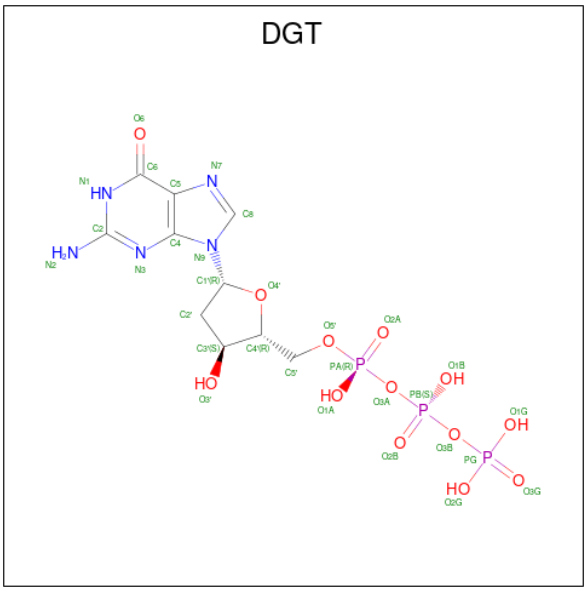
Mol	Chain	Residues	Atoms						AltConf
54	W	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
54	n	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
55	r	1	Total 57	C 38	O 17	P 2	0
55	H	1	Total 51	C 33	O 16	P 2	0
55	L	1	Total 78	C 59	O 17	P 2	0
55	L	1	Total 46	C 27	O 17	P 2	0
55	N	1	Total 90	C 71	O 17	P 2	0
55	Y	1	Total 94	C 75	O 17	P 2	0
55	Y	1	Total 57	C 38	O 17	P 2	0
55	d	1	Total 67	C 48	O 17	P 2	0
55	h	1	Total 70	C 51	O 17	P 2	0
55	m	1	Total 72	C 53	O 17	P 2	0

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

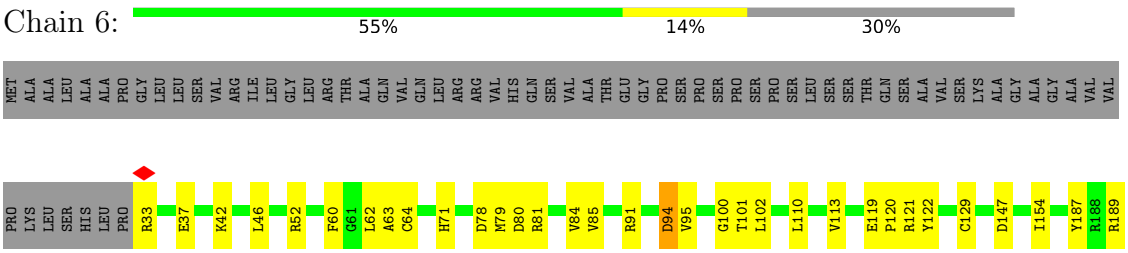
Mol	Chain	Residues	Atoms		AltConf
57	O	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

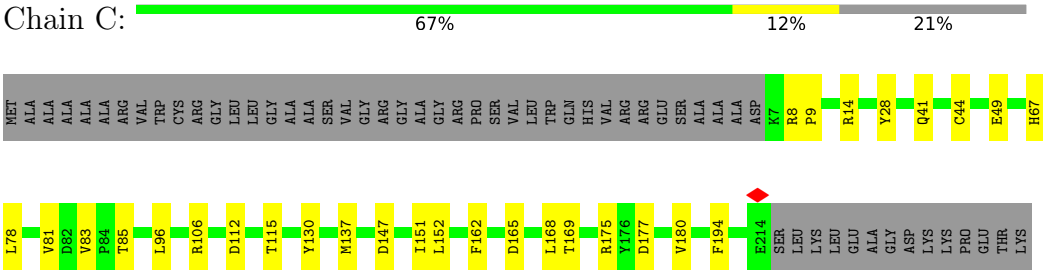
• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:



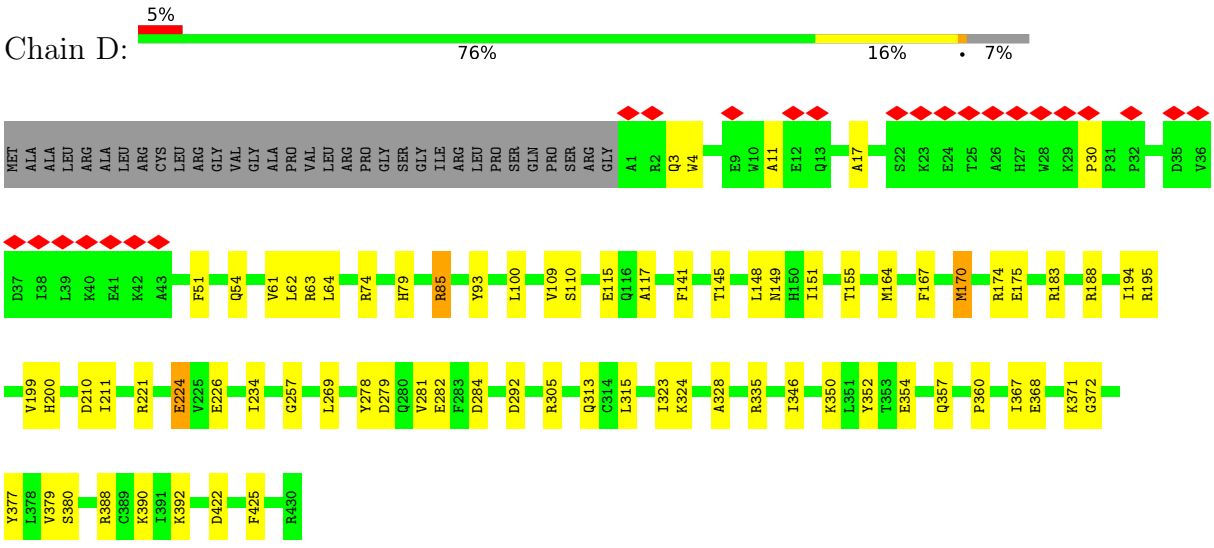
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



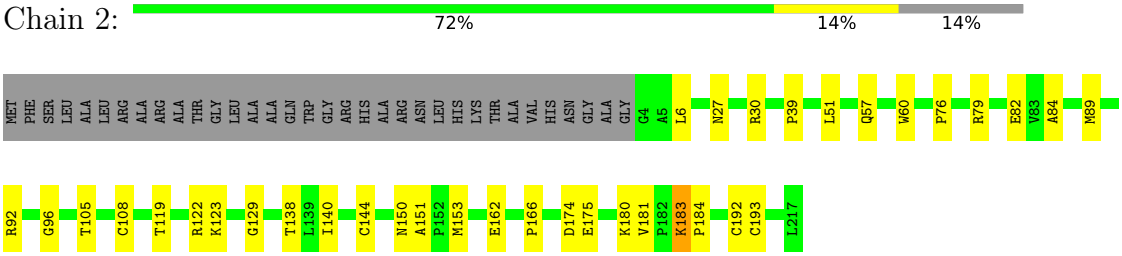
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



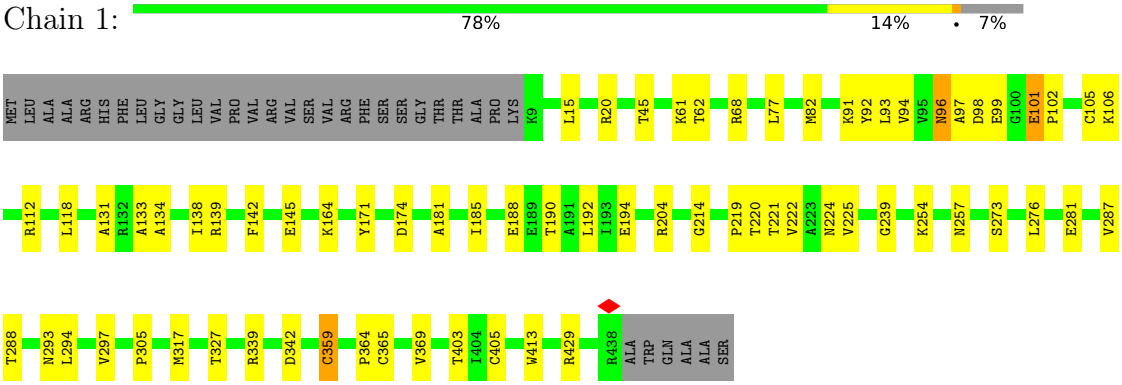
• Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:



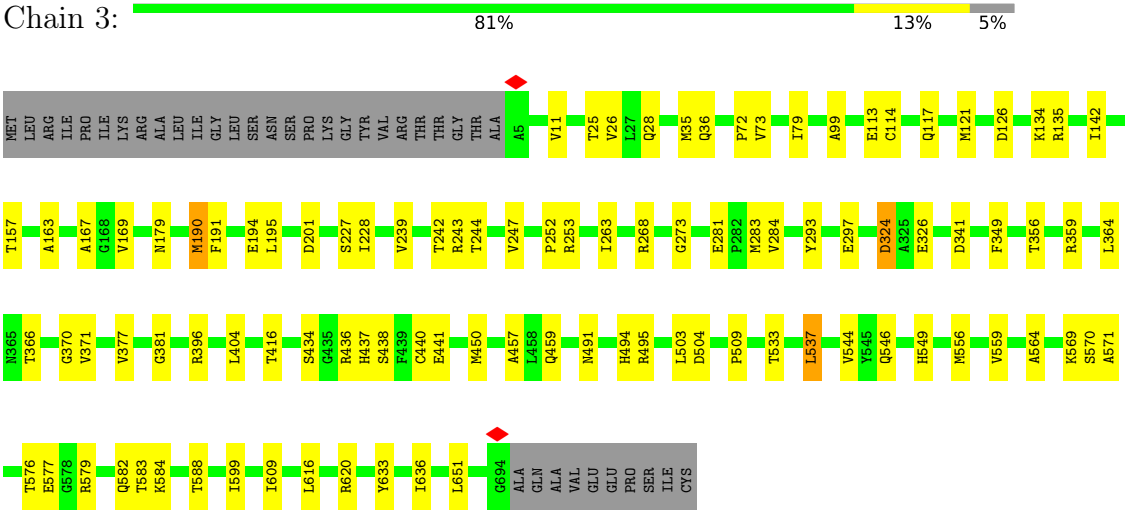
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:



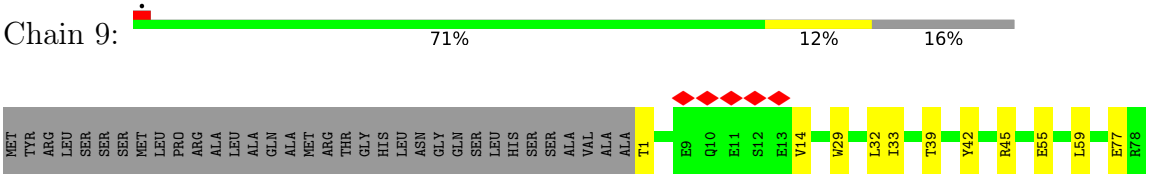
• Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

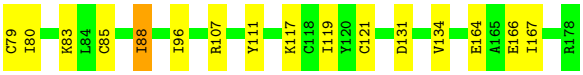
Chain 3:



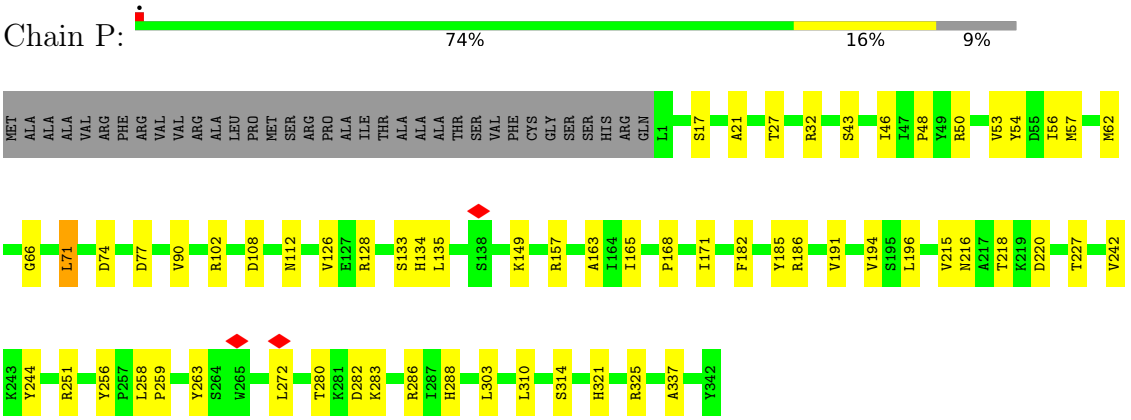
• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:

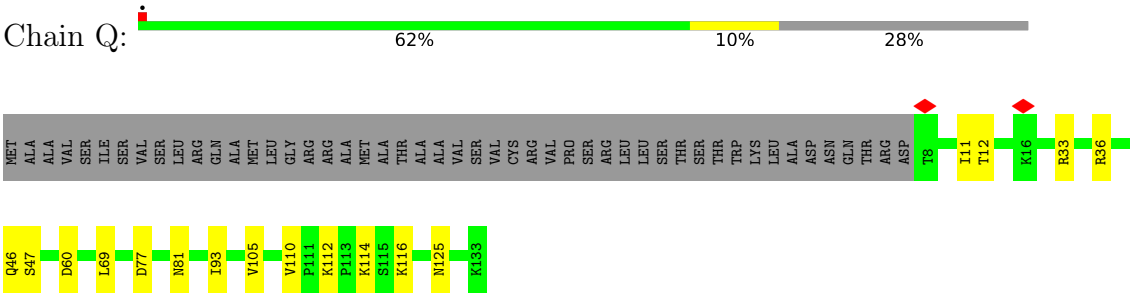




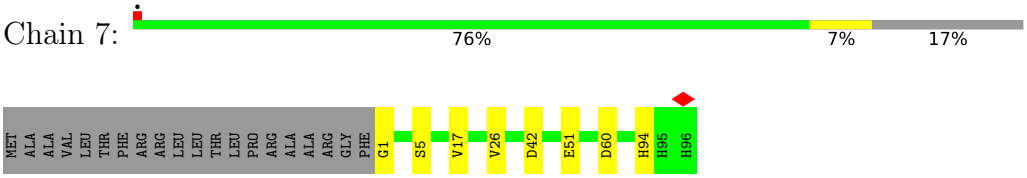
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



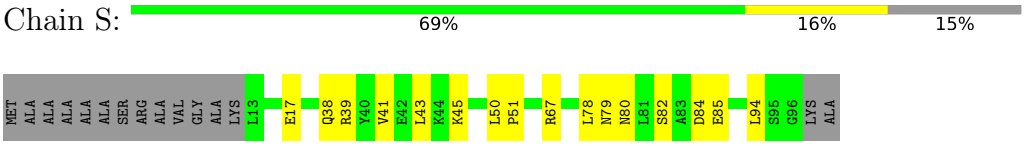
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



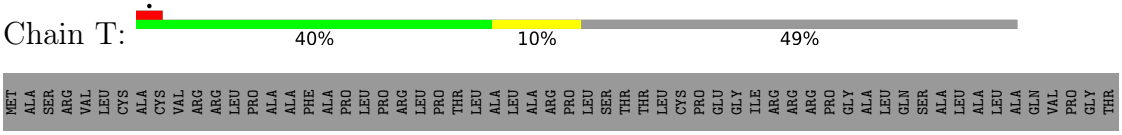
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

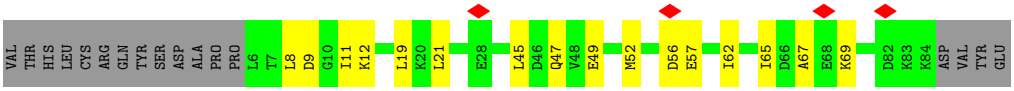


• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



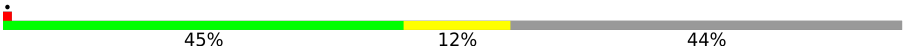
• Molecule 12: Acyl carrier protein, mitochondrial



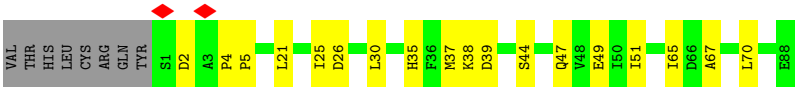


• Molecule 12: Acyl carrier protein, mitochondrial

Chain U:



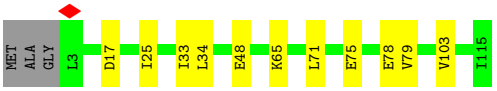




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:

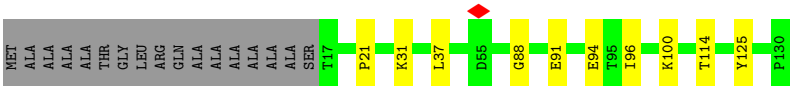




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

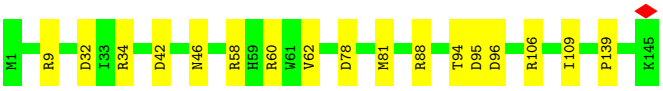




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

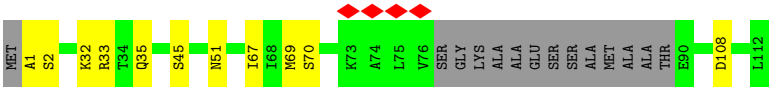




• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



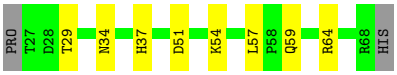


• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

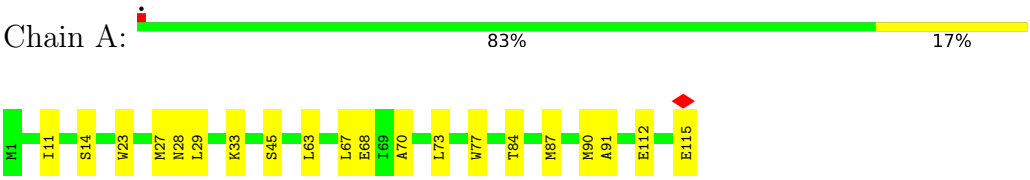
Chain s:



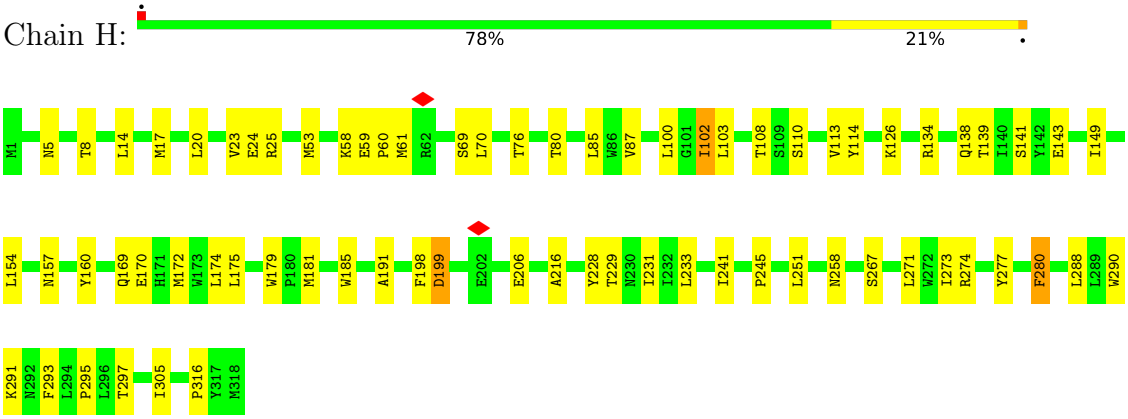




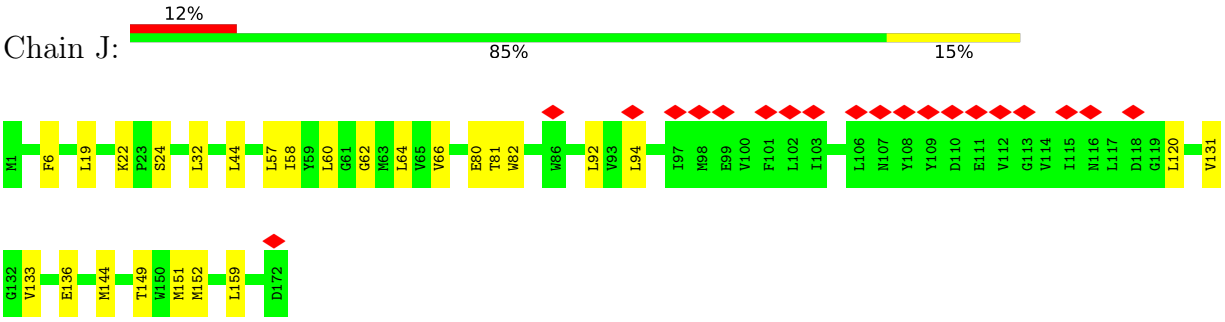
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3



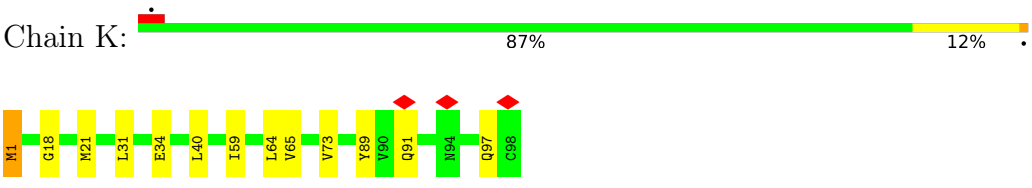
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1



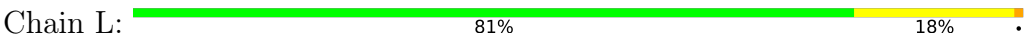
• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

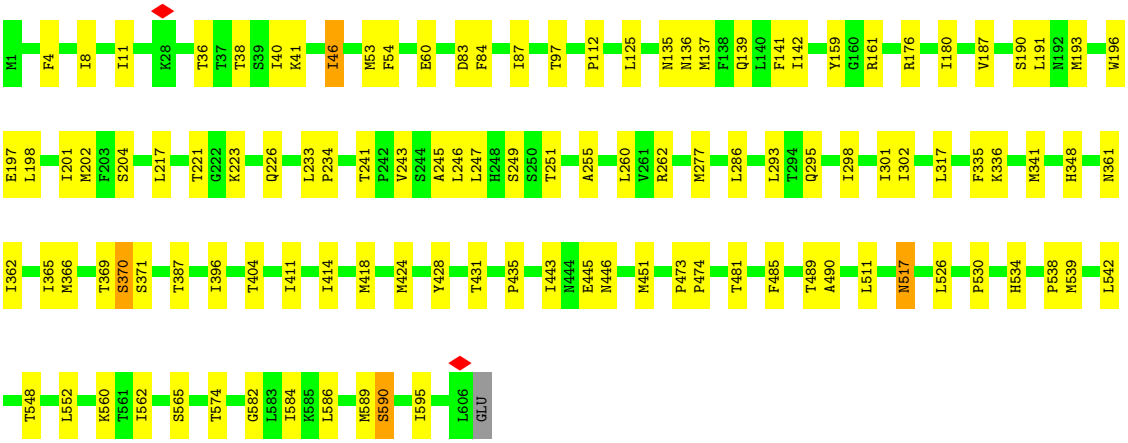


• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

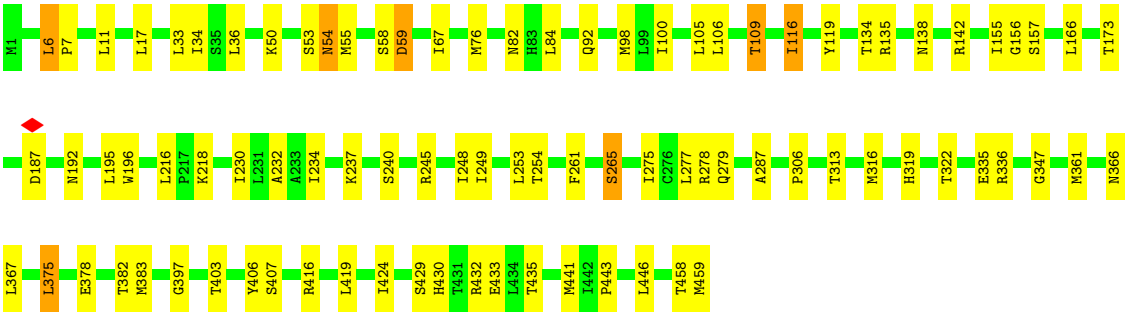




• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain M:

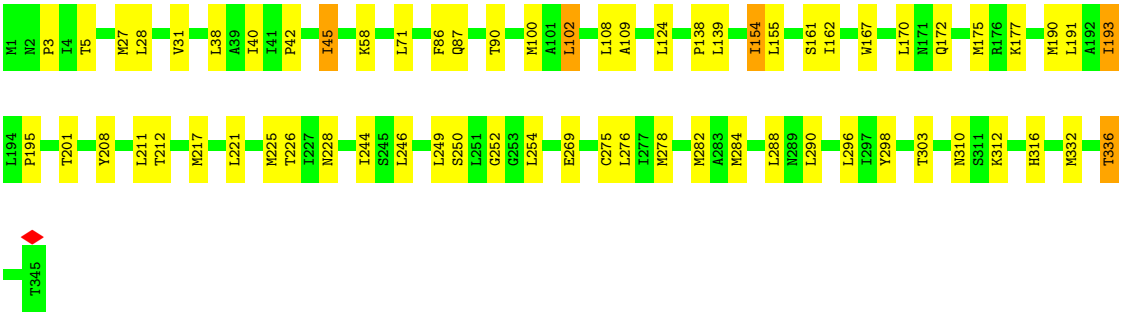




• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain N:

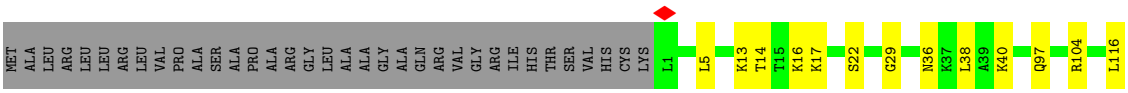


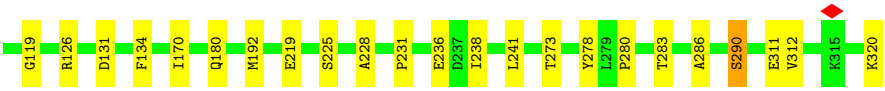


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



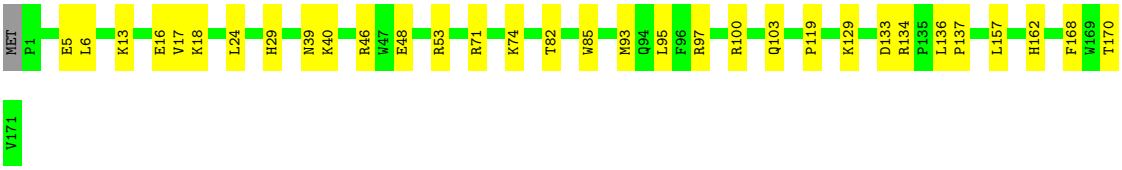




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

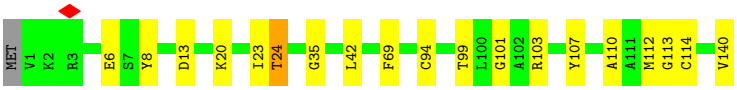




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

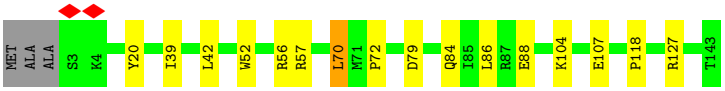




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

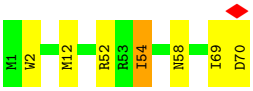




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:

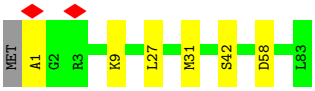




• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:

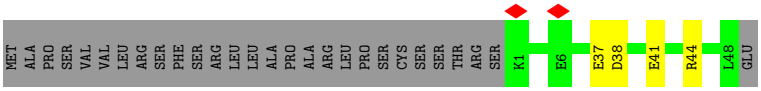




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:

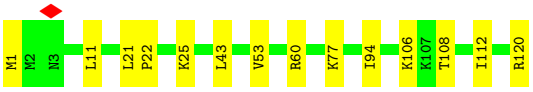




• Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:

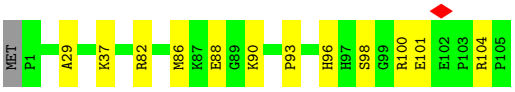




• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:

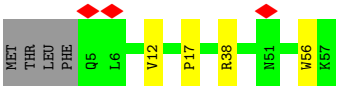




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

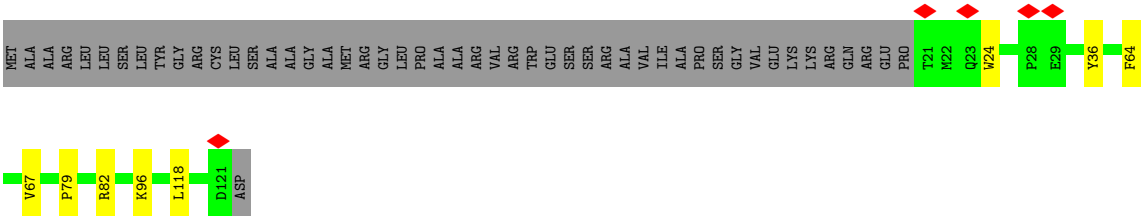




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:

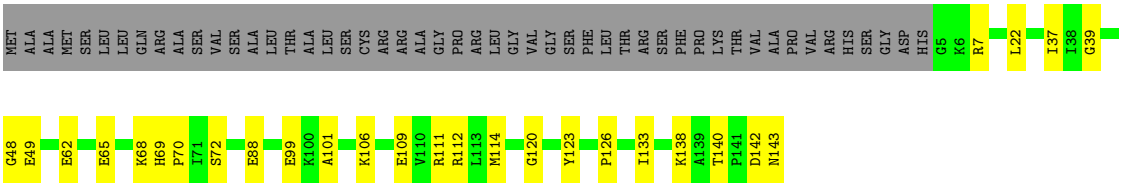




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

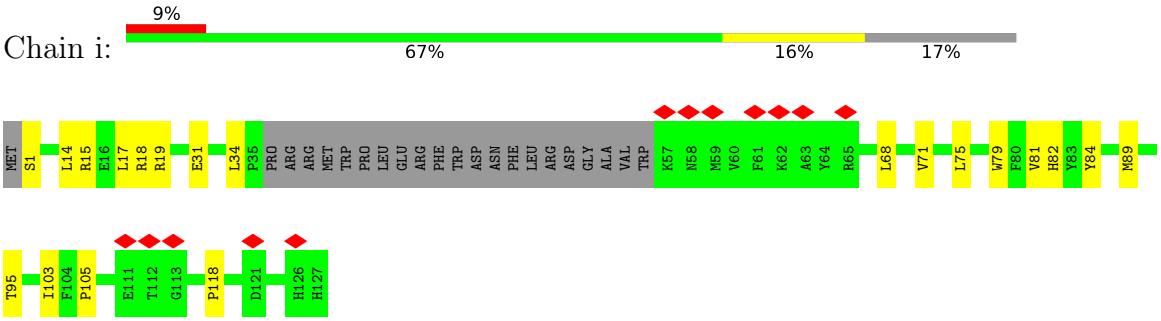
Chain h:





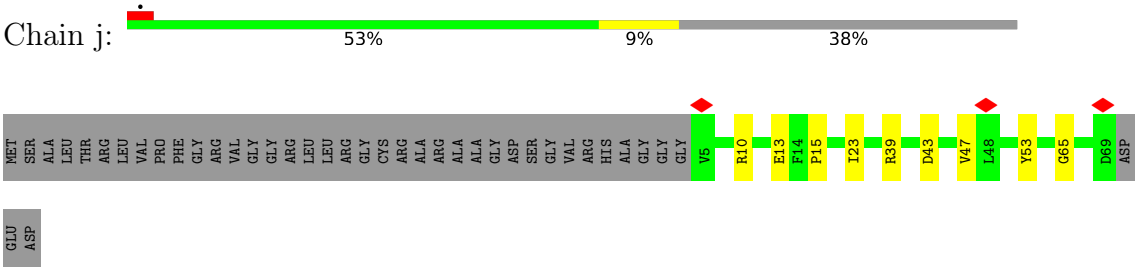
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



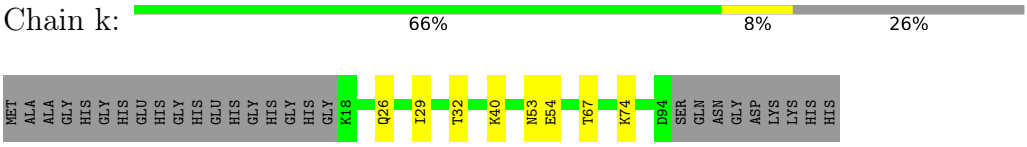
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



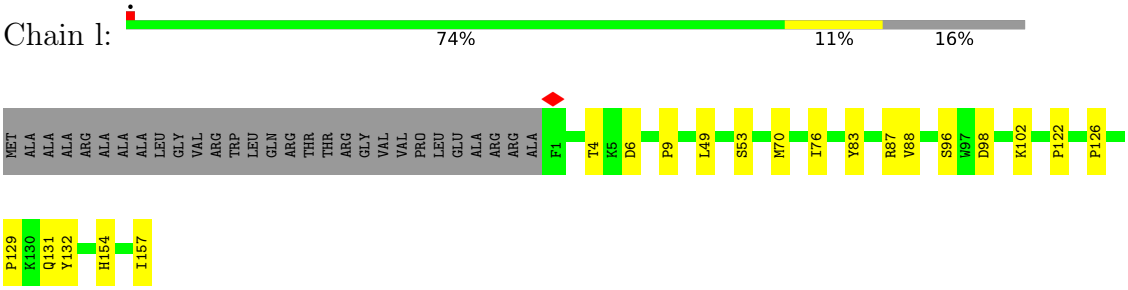
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



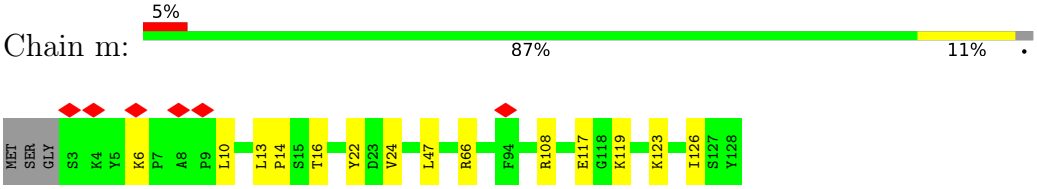
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



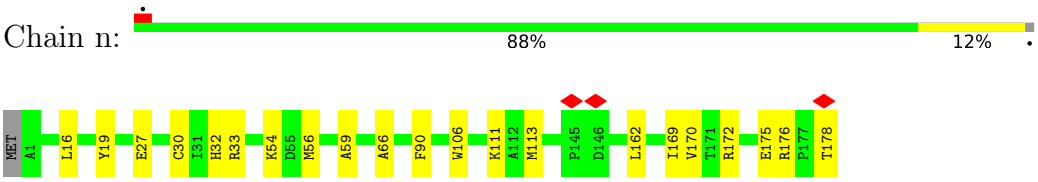
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



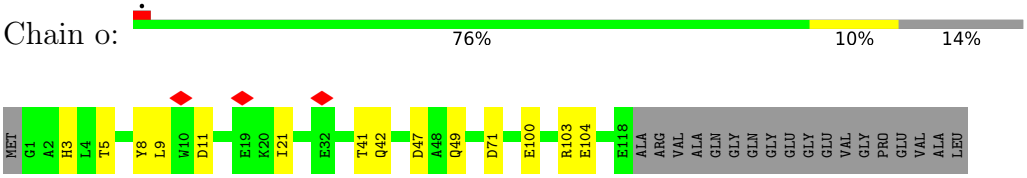
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



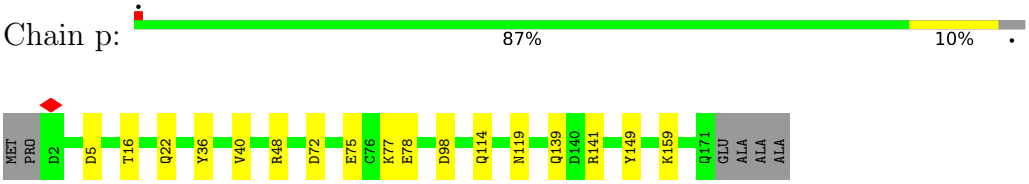
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	604185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	226.83998, 213.05998, 203.51999	wwPDB
Map dimensions	214, 201, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	6	0.25	0/1289	0.43	1/1744 (0.1%)
2	C	0.22	0/1780	0.36	0/2424
3	D	0.24	0/3540	0.38	0/4795
4	2	0.25	0/1700	0.40	0/2316
5	1	0.27	0/3396	0.48	3/4586 (0.1%)
6	3	0.25	0/5392	0.39	0/7305
7	9	0.25	0/1461	0.37	0/1974
8	P	0.22	0/2823	0.39	0/3828
9	Q	0.24	0/1045	0.32	0/1411
10	7	0.23	0/773	0.33	0/1041
11	S	0.22	0/682	0.38	0/920
12	T	0.17	0/646	0.44	0/869
12	U	0.18	0/718	0.36	0/970
13	V	0.20	0/945	0.33	0/1281
14	W	0.20	0/993	0.34	0/1335
15	q	0.21	0/1251	0.34	0/1702
16	r	0.21	0/806	0.30	0/1090
17	s	0.20	0/360	0.37	0/489
18	A	0.23	0/948	0.41	0/1295
19	H	0.28	0/2607	0.48	0/3564
20	J	0.21	0/1330	0.38	0/1810
21	K	0.24	0/738	0.41	0/1002
22	L	0.24	0/4913	0.46	0/6686
23	M	0.25	0/3709	0.42	0/5052
24	N	0.24	0/2755	0.44	0/3751
25	O	0.20	0/2674	0.37	0/3626
26	X	0.18	0/1434	0.35	0/1937
27	Y	0.16	0/1061	0.30	0/1439
28	Z	0.19	0/1198	0.31	0/1616
29	a	0.21	0/585	0.36	0/788
30	b	0.18	0/666	0.35	0/914
31	c	0.16	0/409	0.28	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.18	0/1028	0.35	0/1387
33	e	0.17	0/900	0.35	0/1199
34	f	0.16	0/468	0.30	0/630
35	g	0.17	0/878	0.36	0/1196
36	h	0.20	0/1201	0.36	0/1626
37	i	0.19	0/917	0.36	0/1243
38	j	0.16	0/587	0.35	0/804
39	k	0.18	0/646	0.28	0/873
40	l	0.19	0/1379	0.34	0/1882
41	m	0.19	0/1079	0.34	0/1463
42	n	0.21	0/1596	0.35	0/2162
43	o	0.18	0/1039	0.33	0/1394
44	p	0.18	0/1471	0.30	0/1988
All	All	0.22	0/67816	0.39	4/91962 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	96	ASN	N-CA-C	-7.60	96.89	108.67
5	1	101	GLU	CA-C-N	5.26	125.20	119.78
5	1	101	GLU	C-N-CA	5.26	125.20	119.78
1	6	63	ALA	N-CA-C	5.11	114.78	108.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1258	0	1268	29	0
2	C	1730	0	1686	20	0
3	D	3464	0	3416	58	0
4	2	1660	0	1653	21	0
5	1	3321	0	3278	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3	5305	0	5330	62	0
7	9	1431	0	1383	22	0
8	P	2748	0	2768	42	0
9	Q	1022	0	1023	14	0
10	7	758	0	731	5	0
11	S	671	0	688	9	0
12	T	637	0	640	5	0
12	U	706	0	699	12	0
13	V	923	0	965	6	0
14	W	970	0	991	5	0
15	q	1209	0	1170	11	0
16	r	796	0	831	7	0
17	s	351	0	331	4	0
18	A	932	0	967	17	0
19	H	2540	0	2626	55	0
20	J	1308	0	1319	21	0
21	K	737	0	768	15	0
22	L	4800	0	4985	72	0
23	M	3632	0	3853	61	0
24	N	2703	0	2902	44	0
25	O	2607	0	2566	22	0
26	X	1396	0	1385	24	0
27	Y	1037	0	1025	12	0
28	Z	1167	0	1166	13	0
29	a	572	0	583	7	0
30	b	651	0	653	4	0
31	c	398	0	401	2	0
32	d	996	0	1001	11	0
33	e	877	0	871	9	0
34	f	456	0	452	3	0
35	g	850	0	783	7	0
36	h	1166	0	1166	23	0
37	i	897	0	902	13	0
38	j	562	0	515	7	0
39	k	626	0	620	5	0
40	l	1323	0	1216	15	0
41	m	1050	0	1061	10	0
42	n	1541	0	1473	16	0
43	o	1014	0	1002	12	0
44	p	1438	0	1404	15	0
45	1	8	0	0	0	0
45	3	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	6	8	0	0	1	0
45	9	16	0	0	2	0
46	6	32	0	38	1	0
46	A	43	0	60	1	0
46	D	51	0	82	5	0
46	K	41	0	59	2	0
46	L	51	0	82	2	0
46	M	138	0	210	7	0
46	N	38	0	50	2	0
46	Y	70	0	88	2	0
46	Z	51	0	82	0	0
46	d	63	0	74	1	0
46	i	42	0	61	2	0
46	m	30	0	34	0	0
46	r	46	0	66	0	0
47	6	43	0	63	0	0
47	9	101	0	159	4	0
47	A	31	0	36	1	0
47	N	54	0	88	7	0
48	D	63	0	90	3	0
49	2	4	0	0	0	0
49	3	4	0	0	0	0
50	1	31	0	19	2	0
51	3	1	0	0	0	0
52	P	48	0	26	7	0
53	7	1	0	0	0	0
54	W	34	0	40	2	0
54	n	32	0	36	2	0
55	H	51	0	52	3	0
55	L	124	0	136	2	0
55	N	90	0	133	7	0
55	Y	151	0	199	3	0
55	d	67	0	81	5	0
55	h	70	0	87	4	0
55	m	72	0	91	1	0
55	r	57	0	58	3	0
56	O	31	0	12	1	0
57	O	1	0	0	0	0
All	All	68141	0	68908	746	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 5.

All (746) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:99:GLU:OE2	5:1:105:CYS:HA	1.68	0.91
5:1:99:GLU:OE2	5:1:105:CYS:CA	2.25	0.84
43:o:5:THR:O	43:o:9:LEU:HB2	1.86	0.74
5:1:93:LEU:O	5:1:134:ALA:HA	1.90	0.72
6:3:570:SER:HA	6:3:583:THR:O	1.91	0.71
4:2:144:CYS:O	5:1:139:ARG:NH2	2.26	0.69
4:2:119:THR:HG21	4:2:166:PRO:HB3	1.76	0.67
3:D:269:LEU:HB2	3:D:368:GLU:HB2	1.77	0.67
23:M:98:MET:HE1	55:N:402:CDL:H801	1.77	0.67
3:D:328:ALA:HB3	6:3:126:ASP:HB2	1.78	0.66
23:M:33:LEU:HD23	46:M:502:3PE:H2F2	1.77	0.66
4:2:150:ASN:HB3	4:2:162:GLU:HB3	1.78	0.66
20:J:144:MET:HG2	20:J:152:MET:HG2	1.77	0.65
8:P:216:ASN:O	8:P:220:ASP:HB2	1.97	0.65
27:Y:107:TYR:HB2	55:m:201:CDL:HB62	1.79	0.65
1:6:62:LEU:HB2	1:6:100:GLY:HA3	1.78	0.65
1:6:91:ARG:HD2	19:H:61:MET:HG3	1.80	0.64
15:q:60:ARG:HH22	15:q:95:ASP:HA	1.63	0.64
22:L:221:THR:HG23	22:L:226:GLN:HB2	1.80	0.63
3:D:4:TRP:O	23:M:142:ARG:NH2	2.31	0.63
24:N:162:ILE:HD12	24:N:282:MET:HG2	1.81	0.62
24:N:249:LEU:HD22	24:N:254:LEU:HD12	1.81	0.62
19:H:24:GLU:HG3	19:H:271:LEU:HD22	1.80	0.62
37:i:82:HIS:HD1	44:p:36:TYR:HH	1.45	0.62
5:1:190:THR:HB	5:1:204:ARG:HG2	1.82	0.62
19:H:114:TYR:OH	20:J:60:LEU:O	2.13	0.61
23:M:7:PRO:HB2	23:M:34:ILE:HD11	1.81	0.61
3:D:51:PHE:HB3	3:D:64:LEU:HB3	1.82	0.61
25:O:286:ALA:O	25:O:290:SER:OG	2.18	0.61
22:L:161:ARG:NH1	42:n:90:PHE:O	2.33	0.61
23:M:187:ASP:OD1	23:M:192:ASN:ND2	2.34	0.61
8:P:17:SER:HG	8:P:43:SER:HG	1.48	0.61
22:L:60:GLU:HG3	44:p:114:GLN:HE22	1.66	0.60
23:M:232:ALA:O	23:M:237:LYS:NZ	2.34	0.60
24:N:175:MET:HE1	24:N:296:LEU:HD21	1.83	0.60
22:L:362:ILE:HB	22:L:431:THR:HA	1.84	0.60
3:D:110:SER:OG	3:D:149:ASN:ND2	2.34	0.60
5:1:112:ARG:HB3	5:1:145:GLU:HG3	1.82	0.60
37:i:103:ILE:HB	43:o:47:ASP:HB3	1.83	0.60
1:6:119:GLU:O	8:P:54:TYR:OH	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:O:170:ILE:HD11	25:O:238:ILE:HD11	1.84	0.60
1:6:79:MET:HB2	1:6:84:VAL:HB	1.83	0.60
3:D:352:TYR:HD1	7:9:88:ILE:HG12	1.65	0.60
8:P:251:ARG:NH2	8:P:321:HIS:O	2.35	0.60
22:L:137:MET:HB2	22:L:196:TRP:HB3	1.84	0.59
23:M:50:LYS:HB2	23:M:58:SER:HB3	1.85	0.59
23:M:105:LEU:O	23:M:109:THR:OG1	2.20	0.59
19:H:110:SER:HB2	20:J:60:LEU:HD13	1.85	0.59
24:N:276:LEU:HD22	47:N:401:PC1:H2	1.85	0.59
5:1:287:VAL:HG21	5:1:294:LEU:HB2	1.84	0.59
6:3:324:ASP:HB3	6:3:571:ALA:HB1	1.85	0.59
11:S:82:SER:OG	11:S:84:ASP:OD1	2.20	0.59
46:A:602:3PE:H381	19:H:295:PRO:HB3	1.84	0.59
24:N:102:LEU:HD12	24:N:138:PRO:HB3	1.83	0.59
6:3:396:ARG:NH1	6:3:416:THR:O	2.35	0.59
18:A:23:TRP:HB3	47:A:601:PC1:H321	1.85	0.59
24:N:193:ILE:HD11	24:N:269:GLU:HB3	1.85	0.59
2:C:77:ASP:HB3	3:D:392:LYS:HG3	1.85	0.59
6:3:243:ARG:HG2	6:3:244:THR:HG23	1.84	0.59
20:J:66:VAL:HG11	21:K:31:LEU:HD21	1.85	0.59
3:D:199:VAL:HG23	3:D:323:ILE:HG23	1.83	0.58
22:L:584:ILE:HD12	24:N:58:LYS:HG2	1.86	0.58
28:Z:84:GLN:OE1	33:e:104:ARG:NH1	2.36	0.58
46:D:502:3PE:H3E1	47:N:401:PC1:H3H1	1.85	0.58
27:Y:8:TYR:HB2	27:Y:23:ILE:HG21	1.86	0.58
46:D:502:3PE:H2C2	24:N:284:MET:HB3	1.85	0.58
24:N:217:MET:HE2	46:N:403:3PE:H221	1.86	0.58
5:1:98:ASP:O	5:1:139:ARG:HB2	2.04	0.58
22:L:560:LYS:HE3	46:Y:403:3PE:H221	1.85	0.58
24:N:252:GLY:HA3	24:N:290:LEU:HD13	1.85	0.58
47:9:203:PC1:H2D1	28:Z:39:ILE:HD11	1.86	0.57
3:D:175:GLU:OE2	3:D:188:ARG:NH1	2.36	0.57
6:3:114:CYS:HB3	6:3:117:GLN:HB2	1.85	0.57
19:H:24:GLU:OE2	19:H:274:ARG:NH1	2.36	0.57
20:J:144:MET:HE3	20:J:152:MET:HE2	1.85	0.57
22:L:517:ASN:OD1	22:L:517:ASN:N	2.35	0.57
19:H:175:LEU:O	19:H:179:TRP:HB3	2.03	0.57
20:J:19:LEU:HD11	21:K:31:LEU:HB3	1.86	0.57
25:O:104:ARG:NH2	56:O:401:DGT:N7	2.53	0.57
3:D:226:GLU:OE1	3:D:305:ARG:NH2	2.38	0.57
19:H:169:GLN:NE2	19:H:241:ILE:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:37:LYS:HG3	36:h:133:ILE:HG21	1.86	0.57
37:i:84:TYR:HB2	46:i:201:3PE:H272	1.85	0.57
2:C:151:ILE:HG23	2:C:152:LEU:HG	1.86	0.57
4:2:89:MET:HE2	5:1:181:ALA:HA	1.86	0.57
5:1:99:GLU:HG2	5:1:99:GLU:O	2.03	0.57
22:L:135:ASN:ND2	22:L:197:GLU:OE1	2.37	0.57
4:2:6:LEU:O	4:2:92:ARG:NH2	2.37	0.57
22:L:361:ASN:HD22	22:L:435:PRO:HD3	1.69	0.57
36:h:140:THR:O	36:h:143:ASN:ND2	2.38	0.57
26:X:18:LYS:HA	29:a:54:ILE:HD12	1.87	0.57
8:P:310:LEU:O	8:P:314:SER:HB2	2.05	0.56
22:L:249:SER:HB3	22:L:336:LYS:HB3	1.85	0.56
33:e:88:GLU:HG3	33:e:90:LYS:HG2	1.87	0.56
41:m:117:GLU:HG3	41:m:119:LYS:HD3	1.86	0.56
5:1:224:ASN:ND2	50:1:501:FMN:O2	2.34	0.56
23:M:336:ARG:NH1	23:M:433:GLU:OE2	2.38	0.56
1:6:187:TYR:O	8:P:102:ARG:NH2	2.38	0.56
7:9:55:GLU:OE2	15:q:34:ARG:NH2	2.38	0.56
6:3:569:LYS:HG3	6:3:571:ALA:HB2	1.88	0.56
47:9:204:PC1:H2E2	19:H:175:LEU:HD21	1.86	0.56
6:3:324:ASP:OD1	6:3:324:ASP:N	2.32	0.56
18:A:68:GLU:HG2	20:J:159:LEU:HD13	1.87	0.56
23:M:36:LEU:HB2	35:g:67:VAL:HG22	1.88	0.56
5:1:91:LYS:HG2	5:1:219:PRO:HG2	1.86	0.56
6:3:364:LEU:HD12	6:3:491:ASN:HB3	1.88	0.56
23:M:134:THR:O	23:M:142:ARG:NH1	2.37	0.56
32:d:108:THR:HA	44:p:77:LYS:HA	1.88	0.56
3:D:11:ALA:O	24:N:228:ASN:ND2	2.34	0.56
18:A:28:ASN:O	18:A:33:LYS:NZ	2.37	0.56
15:q:32:ASP:OD2	15:q:58:ARG:NH2	2.39	0.56
12:U:35:HIS:HB3	12:U:38:LYS:HB2	1.86	0.56
23:M:261:PHE:O	23:M:265:SER:OG	2.21	0.55
34:f:56:TRP:NE1	36:h:88:GLU:OE1	2.34	0.55
4:2:27:ASN:ND2	4:2:57:GLN:OE1	2.39	0.55
55:L:703:CDL:H311	55:L:703:CDL:H152	1.89	0.55
3:D:224:GLU:OE2	7:9:45:ARG:NH2	2.39	0.55
6:3:25:THR:HA	6:3:72:PRO:HA	1.89	0.55
18:A:11:ILE:HD13	19:H:80:THR:HG21	1.87	0.55
13:V:71:LEU:HD13	13:V:79:VAL:HG11	1.88	0.55
19:H:199:ASP:OD1	19:H:199:ASP:N	2.38	0.55
22:L:539:MET:HG3	41:m:10:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:142:PHE:HB3	5:1:145:GLU:HB2	1.89	0.55
9:Q:33:ARG:NH1	9:Q:60:ASP:OD1	2.39	0.55
22:L:485:PHE:O	22:L:489:THR:OG1	2.25	0.55
26:X:129:LYS:HB2	30:b:58:ASP:HB2	1.87	0.55
42:n:106:TRP:O	42:n:111:LYS:NZ	2.40	0.55
6:3:239:VAL:HG23	6:3:253:ARG:HG3	1.88	0.54
32:d:106:LYS:HE3	44:p:78:GLU:HG3	1.89	0.54
25:O:13:LYS:HB2	25:O:16:LYS:HB2	1.89	0.54
6:3:620:ARG:NH1	6:3:633:TYR:OH	2.40	0.54
15:q:78:ASP:HB3	15:q:81:MET:HG3	1.87	0.54
24:N:298:TYR:O	24:N:303:THR:OG1	2.25	0.54
1:6:94:ASP:O	1:6:121:ARG:HA	2.07	0.54
14:W:94:GLU:OE1	14:W:100:LYS:NZ	2.40	0.54
19:H:293:PHE:O	19:H:297:THR:OG1	2.24	0.54
24:N:170:LEU:HD22	24:N:288:LEU:HD11	1.88	0.54
6:3:135:ARG:NH1	6:3:179:ASN:OD1	2.41	0.54
8:P:325:ARG:O	8:P:325:ARG:NH1	2.38	0.54
22:L:190:SER:HB3	22:L:196:TRP:HE1	1.72	0.54
4:2:192:CYS:SG	4:2:193:CYS:N	2.80	0.54
9:Q:33:ARG:NH2	9:Q:77:ASP:OD2	2.40	0.54
14:W:31:LYS:NZ	54:W:201:ZMP:O3	2.40	0.54
3:D:141:PHE:O	3:D:145:THR:OG1	2.26	0.54
5:1:99:GLU:OE2	5:1:105:CYS:C	2.50	0.54
8:P:251:ARG:NH1	55:H:401:CDL:OB3	2.38	0.54
8:P:108:ASP:OD1	8:P:112:ASN:ND2	2.39	0.54
18:A:27:MET:HE1	19:H:60:PRO:HD2	1.90	0.54
21:K:97:GLN:HB3	22:L:582:GLY:HA3	1.90	0.54
22:L:83:ASP:OD2	22:L:262:ARG:NH1	2.41	0.54
23:M:84:LEU:O	23:M:92:GLN:NE2	2.40	0.54
23:M:458:THR:O	44:p:149:TYR:OH	2.25	0.54
37:i:82:HIS:ND1	44:p:36:TYR:OH	2.38	0.54
38:j:43:ASP:OD1	38:j:43:ASP:N	2.40	0.54
5:1:96:ASN:O	5:1:225:VAL:HG23	2.08	0.53
16:r:45:SER:O	16:r:51:ASN:ND2	2.41	0.53
18:A:90:MET:HE3	20:J:149:THR:HB	1.91	0.53
20:J:22:LYS:NZ	21:K:18:GLY:O	2.41	0.53
15:q:9:ARG:HH21	55:r:202:CDL:HA22	1.73	0.53
24:N:86:PHE:HB3	24:N:90:THR:HG21	1.89	0.53
3:D:3:GLN:NE2	23:M:135:ARG:O	2.34	0.53
9:Q:93:ILE:HD11	9:Q:105:VAL:HG21	1.90	0.53
12:T:65:ILE:O	12:T:69:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:82:ASN:ND2	23:M:335:GLU:OE1	2.39	0.53
1:6:71:HIS:CE1	3:D:174:ARG:HE	2.27	0.53
15:q:106:ARG:HB2	15:q:109:ILE:HG13	1.89	0.53
18:A:45:SER:O	19:H:126:LYS:NZ	2.42	0.53
25:O:320:LYS:O	32:d:60:ARG:NH2	2.42	0.53
2:C:14:ARG:NH1	2:C:44:CYS:O	2.42	0.53
6:3:142:ILE:HB	6:3:191:PHE:HB3	1.89	0.53
6:3:252:PRO:HB3	6:3:263:ILE:HG23	1.91	0.53
6:3:434:SER:OG	6:3:436:ARG:NH1	2.41	0.53
6:3:577:GLU:OE1	6:3:579:ARG:NH1	2.41	0.53
40:l:53:SER:HA	40:l:83:TYR:HB3	1.91	0.53
24:N:109:ALA:HB3	24:N:161:SER:HA	1.89	0.53
25:O:225:SER:O	25:O:228:ALA:C	2.52	0.53
48:D:501:UQ:H502	19:H:14:LEU:HB3	1.91	0.53
5:1:188:GLU:O	5:1:192:LEU:HB2	2.07	0.53
8:P:149:LYS:NZ	52:P:501:NDP:O2D	2.41	0.53
22:L:193:MET:HG3	22:L:204:SER:HB2	1.91	0.53
1:6:95:VAL:HG23	1:6:122:TYR:HB2	1.90	0.52
26:X:168:PHE:HE2	55:d:201:CDL:H542	1.74	0.52
36:h:114:MET:HE2	36:h:120:GLY:HA3	1.92	0.52
7:9:29:TRP:HB3	7:9:32:LEU:HD12	1.92	0.52
22:L:424:MET:HE3	22:L:428:TYR:HB2	1.90	0.52
11:S:79:ASN:ND2	11:S:80:ASN:OD1	2.42	0.52
18:A:77:TRP:NE1	20:J:136:GLU:OE2	2.43	0.52
40:l:131:GLN:OE1	40:l:154:HIS:ND1	2.43	0.52
23:M:240:SER:OG	23:M:316:MET:SD	2.61	0.52
6:3:28:GLN:NE2	9:Q:114:LYS:O	2.43	0.52
1:6:85:VAL:HG11	48:D:501:UQ:H352	1.91	0.52
1:6:101:THR:OG1	1:6:129:CYS:SG	2.65	0.52
52:P:501:NDP:N7N	52:P:501:NDP:O2N	2.43	0.52
6:3:366:THR:HG22	6:3:370:GLY:HA3	1.91	0.52
7:9:79:CYS:O	7:9:107:ARG:NH1	2.42	0.52
8:P:50:ARG:NH2	52:P:501:NDP:O2X	2.38	0.52
26:X:16:GLU:OE2	33:e:104:ARG:NH2	2.43	0.52
5:1:68:ARG:HD2	5:1:254:LYS:HE2	1.91	0.52
19:H:245:PRO:HB3	19:H:258:ASN:HB3	1.90	0.52
46:M:502:3PE:H3I1	36:h:39:GLY:HA3	1.91	0.52
6:3:533:THR:HA	6:3:556:MET:HE1	1.91	0.52
18:A:70:ALA:HB2	20:J:58:ILE:HD11	1.92	0.52
23:M:430:HIS:HD2	23:M:432:ARG:HH21	1.58	0.52
1:6:102:LEU:HD13	1:6:110:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:46:ARG:NH2	36:h:142:ASP:OD1	2.43	0.51
2:C:78:LEU:HB3	2:C:130:TYR:HB3	1.90	0.51
22:L:159:TYR:HB2	23:M:416:ARG:HD2	1.93	0.51
12:U:39:ASP:OD1	12:U:39:ASP:N	2.38	0.51
32:d:11:LEU:HD23	46:d:202:3PE:H11	1.91	0.51
33:e:86:MET:HE2	33:e:93:PRO:HG3	1.93	0.51
18:A:73:LEU:O	19:H:160:TYR:OH	2.28	0.51
26:X:29:HIS:HB3	26:X:119:PRO:HD2	1.92	0.51
32:d:112:ILE:O	44:p:159:LYS:NZ	2.42	0.51
35:g:96:LYS:NZ	44:p:5:ASP:OD2	2.40	0.51
3:D:74:ARG:NH2	18:A:115:GLU:OE1	2.43	0.51
4:2:51:LEU:HD21	4:2:84:ALA:HB2	1.93	0.51
1:6:52:ARG:NH2	46:6:202:3PE:O32	2.44	0.51
3:D:335:ARG:NH2	7:9:131:ASP:OD1	2.41	0.51
6:3:341:ASP:OD1	11:S:67:ARG:NH2	2.43	0.51
25:O:29:GLY:O	25:O:126:ARG:NH2	2.44	0.51
32:d:120:ARG:O	41:m:108:ARG:NH2	2.43	0.51
3:D:115:GLU:OE1	3:D:194:ILE:N	2.43	0.51
8:P:53:VAL:HA	8:P:56:ILE:HG12	1.91	0.51
26:X:5:GLU:O	26:X:53:ARG:NH1	2.44	0.51
6:3:201:ASP:OD2	6:3:268:ARG:NH2	2.35	0.51
12:T:8:LEU:HD13	12:T:11:ILE:HD11	1.92	0.51
26:X:136:LEU:HD12	26:X:137:PRO:HD2	1.93	0.51
27:Y:103:ARG:NH1	55:Y:404:CDL:OA7	2.44	0.51
6:3:283:MET:HE1	15:q:139:PRO:HG3	1.93	0.51
37:i:18:ARG:NH1	42:n:170:VAL:O	2.38	0.51
1:6:189:ARG:NH1	52:P:501:NDP:O2X	2.43	0.50
6:3:349:PHE:H	6:3:509:PRO:HB2	1.77	0.50
21:K:59:ILE:HG23	24:N:27:MET:HG2	1.93	0.50
22:L:348:HIS:NE2	12:U:2:ASP:OD2	2.44	0.50
22:L:526:LEU:HD12	22:L:530:PRO:HG2	1.92	0.50
23:M:11:LEU:HB3	23:M:100:ILE:HD13	1.93	0.50
35:g:24:TRP:H	35:g:24:TRP:CD1	2.29	0.50
6:3:571:ALA:O	6:3:582:GLN:HA	2.10	0.50
28:Z:88:GLU:OE2	28:Z:127:ARG:NH2	2.42	0.50
40:l:4:THR:OG1	40:l:6:ASP:OD1	2.28	0.50
19:H:114:TYR:OH	20:J:64:LEU:N	2.45	0.50
20:J:81:THR:OG1	20:J:82:TRP:N	2.45	0.50
42:n:66:ALA:HB1	54:n:201:ZMP:H7	1.93	0.50
11:S:38:GLN:HE22	11:S:39:ARG:HH21	1.59	0.50
3:D:117:ALA:HA	3:D:367:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:119:TYR:HE1	23:M:157:SER:HB2	1.76	0.50
32:d:94:ILE:HD13	36:h:106:LYS:HE3	1.94	0.50
5:1:194:GLU:OE2	5:1:204:ARG:NH2	2.31	0.49
6:3:227:SER:OG	6:3:228:ILE:N	2.44	0.49
8:P:157:ARG:NH1	8:P:163:ALA:O	2.45	0.49
19:H:138:GLN:NE2	19:H:191:ALA:O	2.45	0.49
12:U:47:GLN:NE2	12:U:70:LEU:O	2.43	0.49
33:e:29:ALA:HB2	36:h:138:LYS:HD3	1.94	0.49
34:f:38:ARG:NH1	34:f:56:TRP:O	2.45	0.49
38:j:10:ARG:HG3	38:j:15:PRO:HA	1.94	0.49
1:6:119:GLU:H	19:H:59:GLU:HG2	1.77	0.49
22:L:295:GLN:HB2	22:L:301:ILE:HG12	1.94	0.49
3:D:200:HIS:O	3:D:324:LYS:NZ	2.41	0.49
22:L:190:SER:HB3	22:L:196:TRP:NE1	2.27	0.49
23:M:59:ASP:OD2	23:M:245:ARG:NH2	2.44	0.49
24:N:87:GLN:NE2	36:h:126:PRO:O	2.45	0.49
40:l:98:ASP:OD1	40:l:98:ASP:N	2.46	0.49
7:9:14:VAL:HG22	30:b:9:LYS:HE2	1.93	0.49
22:L:548:THR:O	22:L:552:LEU:HB3	2.12	0.49
3:D:346:ILE:HG23	6:3:117:GLN:HG2	1.93	0.49
8:P:171:ILE:HG13	52:P:501:NDP:H42N	1.94	0.49
8:P:186:ARG:HD2	8:P:251:ARG:HG2	1.95	0.49
10:7:1:GLY:N	10:7:42:ASP:OD2	2.46	0.49
37:i:14:LEU:HD13	42:n:169:ILE:HG21	1.94	0.49
43:o:71:ASP:HB3	44:p:22:GLN:HG2	1.94	0.49
28:Z:86:LEU:HD11	28:Z:118:PRO:HG3	1.94	0.49
2:C:81:VAL:HG22	3:D:388:ARG:HG2	1.95	0.49
19:H:316:PRO:HG3	28:Z:56:ARG:HB3	1.95	0.49
23:M:106:LEU:HD13	23:M:234:ILE:HG21	1.95	0.49
26:X:39:ASN:HB3	28:Z:72:PRO:HG2	1.94	0.49
36:h:37:ILE:HG23	55:h:201:CDL:H552	1.94	0.49
12:T:49:GLU:HA	12:T:52:MET:HE3	1.95	0.49
22:L:11:ILE:HG13	22:L:46:ILE:HG22	1.94	0.49
22:L:534:HIS:HB3	46:L:701:3PE:H2	1.94	0.49
32:d:43:LEU:HG	32:d:53:VAL:HG12	1.94	0.49
19:H:134:ARG:NH1	19:H:206:GLU:OE1	2.45	0.48
22:L:371:SER:HG	39:k:74:LYS:HZ3	1.57	0.48
22:L:446:ASN:HA	22:L:451:MET:HE3	1.95	0.48
6:3:113:GLU:HA	9:Q:46:GLN:HE21	1.78	0.48
8:P:282:ASP:OD2	8:P:286:ARG:NH1	2.45	0.48
37:i:79:TRP:HD1	44:p:40:VAL:HG13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:7:5:SER:HB2	10:7:17:VAL:HG21	1.94	0.48
20:J:94:LEU:HD21	46:K:201:3PE:H2F1	1.96	0.48
22:L:187:VAL:HG22	23:M:383:MET:HG3	1.95	0.48
22:L:542:LEU:HB3	23:M:278:ARG:HD3	1.94	0.48
2:C:137:MET:HB3	2:C:162:PHE:HB2	1.94	0.48
22:L:538:PRO:HB2	40:l:88:VAL:HG22	1.95	0.48
36:h:48:GLY:HA3	36:h:70:PRO:HG3	1.96	0.48
18:A:112:GLU:OE2	19:H:291:LYS:NZ	2.45	0.48
19:H:24:GLU:HA	19:H:271:LEU:HD13	1.96	0.48
24:N:124:LEU:HG	24:N:225:MET:HE1	1.95	0.48
28:Z:104:LYS:HB2	28:Z:107:GLU:HB2	1.96	0.48
36:h:109:GLU:OE2	36:h:112:ARG:NH2	2.37	0.48
3:D:110:SER:HG	3:D:149:ASN:ND2	2.11	0.48
46:D:502:3PE:H372	23:M:155:ILE:HD12	1.95	0.48
6:3:194:GLU:HG2	6:3:195:LEU:HG	1.96	0.48
8:P:244:TYR:HB2	8:P:337:ALA:HB2	1.96	0.48
22:L:97:THR:HG21	22:L:125:LEU:HD22	1.95	0.48
44:p:98:ASP:OD2	44:p:141:ARG:NH1	2.45	0.48
6:3:36:GLN:NE2	9:Q:47:SER:O	2.43	0.48
8:P:258:LEU:HD12	8:P:259:PRO:HD2	1.95	0.48
12:U:21:LEU:HD13	39:k:53:ASN:HA	1.96	0.48
4:2:39:PRO:HA	17:s:59:GLN:HB3	1.96	0.48
9:Q:112:LYS:O	9:Q:114:LYS:NZ	2.46	0.48
19:H:169:GLN:HE21	19:H:174:LEU:H	1.62	0.48
23:M:403:THR:HA	23:M:406:TYR:CE2	2.48	0.47
25:O:38:LEU:HD12	25:O:231:PRO:HB3	1.95	0.47
25:O:97:GLN:NE2	25:O:131:ASP:OD2	2.47	0.47
25:O:104:ARG:NE	25:O:131:ASP:OD1	2.44	0.47
2:C:28:TYR:OH	2:C:67:HIS:NE2	2.39	0.47
4:2:27:ASN:OD1	4:2:30:ARG:NH1	2.47	0.47
5:1:185:ILE:HG12	5:1:359:CYS:HB3	1.95	0.47
8:P:74:ASP:HB3	8:P:77:ASP:HB2	1.97	0.47
23:M:443:PRO:HB3	46:M:501:3PE:H3C1	1.95	0.47
11:S:50:LEU:HD12	11:S:51:PRO:HD2	1.96	0.47
22:L:530:PRO:O	22:L:534:HIS:HB2	2.14	0.47
24:N:208:TYR:O	24:N:212:THR:OG1	2.32	0.47
3:D:279:ASP:OD1	3:D:279:ASP:N	2.47	0.47
3:D:379:VAL:HB	3:D:388:ARG:HB3	1.95	0.47
26:X:74:LYS:NZ	29:a:69:ILE:O	2.40	0.47
37:i:15:ARG:O	37:i:19:ARG:HG2	2.15	0.47
8:P:182:PHE:HA	8:P:185:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:269:GLU:OE2	36:h:111:ARG:NH2	2.47	0.47
40:l:96:SER:HB3	41:m:6:LYS:H	1.79	0.47
11:S:84:ASP:OD1	11:S:84:ASP:N	2.46	0.47
20:J:32:LEU:HD21	21:K:34:GLU:HB3	1.96	0.47
43:o:49:GLN:OE1	44:p:119:ASN:ND2	2.48	0.47
1:6:101:THR:HA	1:6:129:CYS:HB3	1.95	0.47
3:D:148:LEU:HD23	3:D:174:ARG:HG2	1.97	0.47
5:1:276:LEU:HD21	5:1:297:VAL:HG11	1.95	0.47
8:P:48:PRO:HA	8:P:71:LEU:O	2.14	0.47
23:M:173:THR:HB	36:h:101:ALA:HB2	1.95	0.47
24:N:3:PRO:HG3	25:O:5:LEU:HD11	1.95	0.47
40:l:102:LYS:HA	40:l:102:LYS:HD3	1.69	0.47
5:1:15:LEU:O	5:1:20:ARG:NH1	2.46	0.47
7:9:83:LYS:NZ	7:9:96:ILE:O	2.48	0.47
9:Q:125:ASN:O	17:s:64:ARG:NE	2.42	0.47
23:M:53:SER:OG	23:M:54:ASN:N	2.47	0.47
2:C:147:ASP:N	2:C:147:ASP:OD1	2.47	0.47
4:2:108:CYS:HA	4:2:151:ALA:HB1	1.97	0.47
5:1:98:ASP:O	5:1:139:ARG:HD2	2.15	0.47
8:P:191:VAL:HG11	8:P:242:VAL:HG11	1.96	0.47
22:L:8:ILE:HA	22:L:11:ILE:HD12	1.97	0.47
23:M:429:SER:O	35:g:36:TYR:OH	2.29	0.47
43:o:21:ILE:HG23	43:o:104:GLU:HG2	1.97	0.47
3:D:282:GLU:O	3:D:313:GLN:NE2	2.34	0.47
23:M:17:LEU:HD11	55:N:402:CDL:H141	1.96	0.47
2:C:75:LEU:HA	2:C:96:LEU:HD23	1.97	0.46
21:K:1:FME:HB2	21:K:1:FME:HE3	1.70	0.46
22:L:414:ILE:HG22	22:L:418:MET:HE2	1.97	0.46
23:M:156:GLY:HA2	47:N:401:PC1:H3I2	1.96	0.46
4:2:129:GLY:HA2	4:2:140:ILE:HG22	1.96	0.46
6:3:35:MET:HE2	6:3:35:MET:HB2	1.73	0.46
19:H:113:VAL:HG11	19:H:139:THR:HG21	1.96	0.46
22:L:136:ASN:HD21	55:h:201:CDL:H261	1.80	0.46
22:L:246:LEU:O	22:L:251:THR:OG1	2.26	0.46
43:o:11:ASP:OD1	43:o:11:ASP:N	2.49	0.46
4:2:76:PRO:HB2	4:2:79:ARG:HG2	1.95	0.46
50:1:501:FMN:N1	50:1:501:FMN:O3'	2.37	0.46
17:s:34:ASN:O	17:s:37:HIS:ND1	2.41	0.46
8:P:128:ARG:NH1	8:P:220:ASP:O	2.48	0.46
20:J:6:PHE:HB2	20:J:120:LEU:HD11	1.98	0.46
22:L:223:LYS:HG2	22:L:255:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:341:MET:HE3	22:L:341:MET:HB2	1.87	0.46
29:a:52:ARG:NH1	29:a:58:ASN:OD1	2.43	0.46
40:l:9:PRO:HD3	41:m:66:ARG:HG2	1.98	0.46
3:D:257:GLY:HA3	3:D:372:GLY:HA2	1.97	0.46
4:2:119:THR:HG22	4:2:122:ARG:HH12	1.80	0.46
24:N:155:LEU:HB3	24:N:278:MET:HE2	1.97	0.46
3:D:377:TYR:HB3	3:D:390:LYS:HB3	1.98	0.46
4:2:123:LYS:NZ	4:2:174:ASP:OD1	2.39	0.46
13:V:65:LYS:HA	13:V:65:LYS:HD3	1.79	0.46
36:h:49:GLU:HG3	36:h:68:LYS:HZ1	1.80	0.46
40:l:70:MET:HE1	40:l:76:ILE:HA	1.96	0.46
2:C:112:ASP:OD1	2:C:115:THR:OG1	2.27	0.46
46:D:502:3PE:H3A1	47:N:401:PC1:H3I3	1.98	0.46
6:3:494:HIS:HB2	6:3:576:THR:HG22	1.97	0.46
7:9:59:LEU:O	16:r:33:ARG:NH2	2.47	0.46
54:W:201:ZMP:O2	54:W:201:ZMP:N2	2.46	0.46
22:L:176:ARG:HH12	23:M:367:LEU:HD13	1.81	0.46
22:L:243:VAL:O	22:L:247:LEU:HB2	2.16	0.46
22:L:574:THR:OG1	24:N:167:TRP:O	2.27	0.46
23:M:275:ILE:O	23:M:279:GLN:HB2	2.14	0.46
36:h:69:HIS:NE2	55:h:201:CDL:OA3	2.48	0.46
43:o:41:THR:OG1	43:o:42:GLN:N	2.48	0.46
8:P:46:ILE:HG12	10:7:26:VAL:HG21	1.98	0.46
26:X:82:THR:HA	26:X:85:TRP:CD1	2.51	0.46
54:n:201:ZMP:H15	54:n:201:ZMP:H17	1.66	0.46
3:D:354:GLU:OE2	3:D:357:GLN:NE2	2.47	0.46
19:H:181:MET:HE2	19:H:181:MET:HB3	1.85	0.46
20:J:57:LEU:HA	20:J:60:LEU:HD12	1.97	0.46
46:M:502:3PE:H2H1	34:f:17:PRO:HG3	1.97	0.46
24:N:28:LEU:HA	24:N:31:VAL:HG22	1.98	0.46
55:N:402:CDL:H861	55:d:201:CDL:H651	1.96	0.46
6:3:546:GLN:HE21	6:3:599:ILE:HD12	1.81	0.46
24:N:332:MET:O	24:N:336:THR:OG1	2.32	0.46
27:Y:24:THR:HG21	27:Y:69:PHE:HD2	1.81	0.46
31:c:41:GLU:OE2	31:c:44:ARG:NH2	2.49	0.46
37:i:89:MET:HB3	37:i:95:THR:HG21	1.98	0.46
22:L:245:ALA:O	22:L:249:SER:HB2	2.15	0.45
55:h:201:CDL:OB4	44:p:48:ARG:NH1	2.49	0.45
3:D:183:ARG:NH1	3:D:210:ASP:OD2	2.34	0.45
6:3:371:VAL:HG22	6:3:450:MET:HE1	1.98	0.45
16:r:69:MET:HE2	16:r:69:MET:HB2	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:77:GLU:O	7:9:107:ARG:NH1	2.49	0.45
7:9:164:GLU:HB3	15:q:109:ILE:HG12	1.99	0.45
14:W:37:LEU:HD21	14:W:88:GLY:HA3	1.98	0.45
17:s:51:ASP:OD1	17:s:54:LYS:NZ	2.49	0.45
48:D:501:UQ:H451	48:D:501:UQ:H471	1.73	0.45
19:H:85:LEU:HB3	19:H:233:LEU:HD21	1.98	0.45
20:J:151:MET:HE2	20:J:151:MET:HB2	1.81	0.45
1:6:33:ARG:HG3	1:6:37:GLU:HG2	1.99	0.45
3:D:155:THR:HB	3:D:167:PHE:HA	1.98	0.45
4:2:175:GLU:OE1	4:2:180:LYS:NZ	2.48	0.45
8:P:185:TYR:HH	8:P:263:TYR:HH	1.55	0.45
55:H:401:CDL:H162	20:J:92:LEU:HD21	1.98	0.45
31:c:38:ASP:OD2	32:d:77:LYS:NZ	2.40	0.45
40:l:157:ILE:HG21	43:o:100:GLU:HG2	1.98	0.45
6:3:228:ILE:HB	6:3:583:THR:HG22	1.98	0.45
19:H:172:MET:HE2	19:H:172:MET:HB3	1.82	0.45
20:J:24:SER:N	20:J:80:GLU:O	2.36	0.45
22:L:365:ILE:HG13	22:L:366:MET:HG3	1.98	0.45
22:L:562:ILE:HG23	47:N:401:PC1:H2I1	1.98	0.45
23:M:361:MET:HE2	23:M:441:MET:HG3	1.99	0.45
23:M:446:LEU:HB3	46:M:501:3PE:H342	1.99	0.45
26:X:100:ARG:NH1	26:X:103:GLN:OE1	2.46	0.45
40:l:132:TYR:O	40:l:154:HIS:NE2	2.49	0.45
3:D:350:LYS:HG3	6:3:121:MET:HG3	1.98	0.45
8:P:134:HIS:HD2	52:P:501:NDP:H5N	1.80	0.45
23:M:67:ILE:HG22	46:M:501:3PE:H3D1	1.98	0.45
6:3:537:LEU:HD12	6:3:537:LEU:HA	1.83	0.45
25:O:126:ARG:HD3	25:O:134:PHE:HE2	1.81	0.45
27:Y:94:CYS:HA	27:Y:114:CYS:HA	1.99	0.45
3:D:371:LYS:NZ	3:D:422:ASP:OD1	2.48	0.45
5:1:364:PRO:HG2	5:1:403:THR:HG22	1.98	0.45
16:r:108:ASP:OD2	28:Z:20:TYR:OH	2.30	0.45
18:A:87:MET:HE3	18:A:87:MET:HB3	1.84	0.45
12:U:44:SER:HB3	42:n:16:LEU:HD11	1.99	0.45
42:n:175:GLU:HG2	42:n:176:ARG:HG2	1.98	0.45
2:C:165:ASP:N	2:C:165:ASP:OD1	2.42	0.45
5:1:214:GLY:HA3	5:1:220:THR:HG22	1.99	0.45
6:3:377:VAL:HG22	6:3:450:MET:HE2	1.99	0.45
38:j:39:ARG:NH2	38:j:43:ASP:OD2	2.50	0.45
6:3:169:VAL:HG21	6:3:191:PHE:HE1	1.82	0.44
7:9:85:CYS:SG	7:9:111:TYR:OH	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:166:GLU:HG3	15:q:88:ARG:HD3	1.99	0.44
8:P:90:VAL:HG11	8:P:218:THR:HG22	1.99	0.44
22:L:369:THR:OG1	22:L:445:GLU:OE1	2.31	0.44
25:O:14:THR:HA	25:O:17:LYS:HG2	1.99	0.44
36:h:62:GLU:O	36:h:65:GLU:HB2	2.17	0.44
3:D:360:PRO:HA	3:D:380:SER:O	2.17	0.44
19:H:149:ILE:HG21	19:H:185:TRP:HB2	2.00	0.44
22:L:473:PRO:HA	22:L:474:PRO:HD3	1.89	0.44
27:Y:113:GLY:HA2	46:Y:403:3PE:H371	1.99	0.44
40:l:122:PRO:O	43:o:8:TYR:OH	2.35	0.44
1:6:46:LEU:HG	19:H:53:MET:HE1	1.99	0.44
1:6:100:GLY:HA2	45:6:201:SF4:S4	2.57	0.44
3:D:17:ALA:HB2	3:D:30:PRO:HA	2.00	0.44
47:9:203:PC1:H32	19:H:288:LEU:HD11	2.00	0.44
23:M:196:TRP:HE1	23:M:254:THR:HB	1.82	0.44
3:D:221:ARG:NH2	7:9:45:ARG:HH12	2.15	0.44
5:1:106:LYS:HG2	5:1:257:ASN:HD21	1.82	0.44
5:1:276:LEU:HD13	5:1:317:MET:HE3	1.98	0.44
8:P:134:HIS:ND1	8:P:135:LEU:O	2.51	0.44
8:P:194:VAL:H	8:P:288:HIS:CE1	2.35	0.44
12:T:47:GLN:NE2	12:T:67:ALA:O	2.49	0.44
23:M:166:LEU:HD23	23:M:195:LEU:HD13	1.98	0.44
27:Y:101:GLY:HA3	27:Y:110:ALA:HB2	1.99	0.44
2:C:49:GLU:OE2	2:C:106:ARG:NH1	2.50	0.44
3:D:151:ILE:HG23	3:D:170:MET:HB3	1.99	0.44
6:3:297:GLU:HG3	14:W:125:TYR:CZ	2.52	0.44
13:V:25:ILE:HD12	25:O:236:GLU:HB3	1.98	0.44
23:M:319:HIS:HA	23:M:322:THR:HG22	2.00	0.44
6:3:26:VAL:HG13	6:3:79:ILE:HD13	1.99	0.44
8:P:215:VAL:O	8:P:218:THR:OG1	2.27	0.44
18:A:67:LEU:HD12	21:K:65:VAL:HG22	2.00	0.44
22:L:36:THR:O	22:L:40:ILE:HG12	2.18	0.44
1:6:79:MET:HE3	1:6:84:VAL:HG12	1.99	0.44
3:D:292:ASP:OD1	3:D:292:ASP:N	2.51	0.44
9:Q:11:ILE:HD13	14:W:21:PRO:HB3	2.00	0.44
18:A:63:LEU:HD21	20:J:62:GLY:HA2	2.00	0.44
19:H:70:LEU:HD23	19:H:70:LEU:HA	1.85	0.44
22:L:198:LEU:O	22:L:202:MET:HG2	2.18	0.44
30:b:27:LEU:O	30:b:31:MET:HB2	2.18	0.44
2:C:175:ARG:NH2	2:C:177:ASP:OD2	2.50	0.43
3:D:62:LEU:HB2	3:D:425:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2:183:LYS:HA	4:2:184:PRO:HD3	1.83	0.43
22:L:481:THR:HG22	38:j:53:TYR:HD1	1.82	0.43
23:M:116:ILE:HD13	23:M:116:ILE:HA	1.84	0.43
23:M:459:MET:O	35:g:82:ARG:NH1	2.50	0.43
24:N:172:GLN:HG3	24:N:177:LYS:HB3	2.00	0.43
55:N:402:CDL:H652	55:d:201:CDL:H652	2.00	0.43
25:O:14:THR:HG21	25:O:116:LEU:HD22	2.00	0.43
3:D:100:LEU:HD11	3:D:195:ARG:HA	2.00	0.43
6:3:356:THR:HG21	6:3:503:LEU:HD22	1.99	0.43
6:3:584:LYS:HE2	9:Q:36:ARG:HD2	2.00	0.43
19:H:17:MET:HE3	19:H:17:MET:HB3	1.76	0.43
22:L:298:ILE:O	22:L:302:ILE:HG12	2.17	0.43
23:M:435:THR:HG23	35:g:64:PHE:HE1	1.83	0.43
24:N:211:LEU:HD21	24:N:250:SER:HB3	2.00	0.43
47:N:401:PC1:H2B2	47:N:401:PC1:H3F1	2.00	0.43
26:X:24:LEU:HD22	28:Z:70:LEU:HD11	2.00	0.43
6:3:381:GLY:HA3	6:3:457:ALA:HB2	2.00	0.43
46:M:501:3PE:H3A1	46:M:501:3PE:H372	1.82	0.43
3:D:155:THR:HG21	3:D:170:MET:HB2	2.00	0.43
15:q:42:ASP:OD1	15:q:46:ASN:N	2.51	0.43
18:A:84:THR:OG1	30:b:42:SER:OG	2.35	0.43
19:H:69:SER:HA	55:H:401:CDL:H711	2.01	0.43
27:Y:35:GLY:HA2	55:Y:401:CDL:H322	1.99	0.43
40:l:129:PRO:HD3	43:o:21:ILE:HB	1.99	0.43
1:6:91:ARG:HB3	19:H:216:ALA:HB2	2.00	0.43
3:D:278:TYR:HA	3:D:281:VAL:HG22	2.01	0.43
5:1:101:GLU:HA	5:1:102:PRO:HD3	1.83	0.43
22:L:586:LEU:O	22:L:590:SER:OG	2.36	0.43
23:M:248:ILE:HG23	23:M:249:ILE:HG23	2.01	0.43
27:Y:13:ASP:HA	27:Y:20:LYS:HE3	2.00	0.43
29:a:12:MET:HE2	29:a:12:MET:HB3	1.96	0.43
40:l:126:PRO:HD3	43:o:3:HIS:CE1	2.53	0.43
6:3:99:ALA:O	6:3:134:LYS:NZ	2.46	0.43
7:9:33:ILE:HD12	47:9:204:PC1:H3A2	2.00	0.43
8:P:280:THR:H	8:P:283:LYS:HB3	1.82	0.43
19:H:5:ASN:HA	19:H:8:THR:HG22	2.00	0.43
22:L:38:THR:HA	22:L:41:LYS:HG2	1.99	0.43
55:L:702:CDL:HA62	36:h:22:LEU:HD13	2.00	0.43
46:N:403:3PE:H351	46:N:403:3PE:H251	2.00	0.43
5:1:92:TYR:O	5:1:220:THR:HA	2.18	0.43
8:P:32:ARG:HB2	8:P:62:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:q:96:ASP:OD1	15:q:96:ASP:N	2.44	0.43
21:K:89:TYR:HB3	21:K:91:GLN:HG2	2.00	0.43
46:L:701:3PE:H222	40:l:87:ARG:HA	1.99	0.43
32:d:1:MET:SD	36:h:111:ARG:NH1	2.92	0.43
38:j:23:ILE:HD13	38:j:23:ILE:HA	1.91	0.43
42:n:30:CYS:O	42:n:32:HIS:N	2.50	0.43
1:6:147:ASP:N	1:6:147:ASP:OD1	2.52	0.43
5:1:118:LEU:HD13	5:1:225:VAL:HG13	1.99	0.43
10:7:51:GLU:HG3	10:7:94:HIS:HB2	2.01	0.43
13:V:75:GLU:HB2	13:V:78:GLU:HG3	2.01	0.43
19:H:170:GLU:OE1	26:X:97:ARG:NH2	2.41	0.43
22:L:141:PHE:HE2	23:M:375:LEU:HD11	1.84	0.43
23:M:378:GLU:O	23:M:382:THR:OG1	2.37	0.43
24:N:154:ILE:HD12	24:N:195:PRO:HG3	2.01	0.43
5:1:62:THR:HG23	5:1:239:GLY:HA3	2.01	0.43
23:M:306:PRO:HA	23:M:458:THR:HG21	2.00	0.43
24:N:312:LYS:O	24:N:316:HIS:ND1	2.32	0.43
3:D:115:GLU:HB3	3:D:194:ILE:HB	2.01	0.43
5:1:164:LYS:HE3	5:1:164:LYS:HB3	1.67	0.43
7:9:88:ILE:HD12	7:9:88:ILE:HA	1.90	0.43
26:X:93:MET:HB2	26:X:95:LEU:HG	2.00	0.43
6:3:273:GLY:O	6:3:549:HIS:NE2	2.44	0.42
6:3:564:ALA:HB3	6:3:569:LYS:HD3	2.02	0.42
7:9:134:VAL:HG21	7:9:167:ILE:HG21	2.00	0.42
16:r:2:SER:O	55:r:202:CDL:O1	2.28	0.42
38:j:65:GLY:O	43:o:103:ARG:NH1	2.52	0.42
44:p:72:ASP:N	44:p:75:GLU:OE2	2.52	0.42
6:3:242:THR:HG22	6:3:247:VAL:HA	2.00	0.42
24:N:284:MET:HE3	47:N:401:PC1:H2C1	2.00	0.42
26:X:13:LYS:HE3	26:X:13:LYS:HB2	1.81	0.42
28:Z:57:ARG:HA	28:Z:57:ARG:HD2	1.82	0.42
36:h:7:ARG:NH2	37:i:31:GLU:O	2.47	0.42
38:j:13:GLU:OE2	39:k:26:GLN:NE2	2.50	0.42
5:1:94:VAL:O	5:1:222:VAL:HA	2.19	0.42
23:M:76:MET:SD	23:M:230:ILE:HB	2.59	0.42
2:C:8:ARG:HA	2:C:9:PRO:HD3	1.95	0.42
2:C:41:GLN:NE2	2:C:49:GLU:OE1	2.43	0.42
11:S:43:LEU:HD11	11:S:94:LEU:HD11	2.02	0.42
12:T:9:ASP:HA	12:T:12:LYS:HG2	2.00	0.42
22:L:366:MET:O	22:L:370:SER:OG	2.26	0.42
12:U:25:ILE:HG21	12:U:30:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:ASN:HD21	3:D:371:LYS:HG3	1.85	0.42
6:3:11:VAL:HG11	6:3:73:VAL:HB	2.01	0.42
9:Q:60:ASP:OD1	9:Q:60:ASP:N	2.49	0.42
10:7:60:ASP:OD1	10:7:60:ASP:N	2.51	0.42
18:A:91:ALA:HB1	19:H:305:ILE:HD13	2.01	0.42
42:n:54:LYS:HD2	42:n:54:LYS:HA	1.79	0.42
3:D:224:GLU:HG2	7:9:42:TYR:HE2	1.85	0.42
5:1:97:ALA:HB3	5:1:138:ILE:HA	2.01	0.42
55:r:202:CDL:OB4	29:a:2:TRP:NE1	2.47	0.42
19:H:229:THR:O	19:H:233:LEU:HB2	2.19	0.42
23:M:55:MET:HE3	26:X:170:THR:HG23	2.02	0.42
39:k:54:GLU:OE2	42:n:33:ARG:NH2	2.50	0.42
6:3:190:MET:HB3	6:3:190:MET:HE3	1.73	0.42
8:P:165:ILE:O	8:P:227:THR:HA	2.19	0.42
13:V:17:ASP:OD1	13:V:17:ASP:N	2.52	0.42
22:L:112:PRO:HG3	42:n:178:THR:HG21	2.02	0.42
55:N:402:CDL:H671	55:d:201:CDL:H672	2.01	0.42
32:d:21:LEU:HD13	32:d:22:PRO:HD2	2.02	0.42
3:D:211:ILE:HG22	3:D:315:LEU:HD11	2.01	0.42
4:2:79:ARG:NH1	4:2:82:GLU:OE2	2.52	0.42
6:3:163:ALA:HA	6:3:167:ALA:HB3	2.02	0.42
6:3:359:ARG:HE	6:3:504:ASP:CG	2.27	0.42
19:H:20:LEU:HA	19:H:23:VAL:HG12	2.02	0.42
19:H:139:THR:O	19:H:143:GLU:HB2	2.20	0.42
19:H:228:TYR:HA	19:H:231:ILE:HD12	2.01	0.42
21:K:21:MET:HE1	46:K:201:3PE:H332	2.02	0.42
24:N:42:PRO:HA	24:N:45:ILE:HG22	2.01	0.42
24:N:244:ILE:HD13	24:N:244:ILE:HA	1.92	0.42
24:N:246:LEU:HD21	55:N:402:CDL:H792	2.02	0.42
41:m:16:THR:O	41:m:22:TYR:OH	2.27	0.42
3:D:151:ILE:HG21	3:D:174:ARG:HG3	2.02	0.42
4:2:60:TRP:CD1	4:2:60:TRP:H	2.37	0.42
6:3:326:GLU:OE2	6:3:620:ARG:NE	2.53	0.42
6:3:377:VAL:HG23	6:3:404:LEU:HD11	2.02	0.42
19:H:154:LEU:HA	19:H:157:ASN:HB3	2.01	0.42
22:L:139:GLN:HA	22:L:142:ILE:HD12	2.01	0.42
24:N:310:ASN:ND2	25:O:273:THR:O	2.44	0.42
26:X:46:ARG:NH1	28:Z:79:ASP:OD2	2.53	0.42
33:e:98:SER:OG	33:e:100:ARG:NH1	2.53	0.42
41:m:123:LYS:HE2	41:m:123:LYS:HB2	1.93	0.42
6:3:157:THR:N	45:3:802:SF4:S4	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:54:TYR:HA	8:P:57:MET:HG2	2.02	0.42
8:P:66:GLY:HA3	9:Q:69:LEU:HD13	2.01	0.42
23:M:313:THR:HA	23:M:316:MET:HE3	2.02	0.42
2:C:168:LEU:HD22	3:D:93:TYR:HD2	1.85	0.41
3:D:164:MET:SD	3:D:164:MET:N	2.92	0.41
3:D:234:ILE:HG12	19:H:280:PHE:HE1	1.84	0.41
4:2:153:MET:HE2	4:2:153:MET:HB2	1.88	0.41
6:3:577:GLU:HB3	6:3:636:ILE:HD11	2.02	0.41
19:H:138:GLN:NE2	19:H:198:PHE:O	2.53	0.41
21:K:64:LEU:HD23	21:K:64:LEU:HA	1.88	0.41
22:L:565:SER:HB2	27:Y:112:MET:HE1	2.02	0.41
12:U:49:GLU:OE2	42:n:19:TYR:OH	2.38	0.41
46:D:502:3PE:H291	23:M:155:ILE:HD11	2.02	0.41
5:1:133:ALA:HA	5:1:174:ASP:O	2.19	0.41
24:N:193:ILE:HA	24:N:193:ILE:HD12	1.82	0.41
26:X:133:ASP:OD1	26:X:133:ASP:N	2.46	0.41
39:k:40:LYS:HE2	39:k:40:LYS:HB3	1.86	0.41
1:6:42:LYS:HD3	1:6:42:LYS:HA	1.73	0.41
19:H:85:LEU:HB2	19:H:233:LEU:HD11	2.01	0.41
22:L:180:ILE:HD12	23:M:397:GLY:HA2	2.02	0.41
22:L:217:LEU:HD13	22:L:277:MET:HG2	2.02	0.41
24:N:190:MET:HB3	24:N:201:THR:HG23	2.02	0.41
25:O:36:ASN:OD1	25:O:40:LYS:NZ	2.52	0.41
25:O:219:GLU:HG2	25:O:241:LEU:HD22	2.02	0.41
25:O:311:GLU:HG2	25:O:312:VAL:HG13	2.02	0.41
12:U:51:ILE:HG21	12:U:67:ALA:HB1	2.01	0.41
37:i:105:PRO:HB3	37:i:118:PRO:HA	2.01	0.41
41:m:126:ILE:HG22	44:p:139:GLN:HG3	2.02	0.41
1:6:71:HIS:HE1	3:D:174:ARG:HE	1.66	0.41
1:6:120:PRO:HD2	19:H:58:LYS:HG3	2.02	0.41
2:C:112:ASP:OD1	2:C:112:ASP:N	2.52	0.41
22:L:260:LEU:HB2	22:L:317:LEU:HD13	2.01	0.41
33:e:82:ARG:HG2	33:e:86:MET:HE3	2.03	0.41
1:6:80:ASP:OD1	19:H:25:ARG:NE	2.43	0.41
1:6:101:THR:HG21	3:D:85:2MR:HG3	2.00	0.41
6:3:438:SER:O	6:3:441:GLU:HG2	2.20	0.41
11:S:41:VAL:O	11:S:45:LYS:HG2	2.20	0.41
19:H:100:LEU:HB3	19:H:103:LEU:HD12	2.02	0.41
22:L:197:GLU:O	22:L:201:ILE:HG12	2.20	0.41
55:N:402:CDL:H552	55:N:402:CDL:H312	2.01	0.41
12:U:26:ASP:OD1	12:U:26:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:96:HIS:HA	33:e:101:GLU:HB3	2.02	0.41
37:i:81:VAL:HG22	46:i:201:3PE:H2A1	2.02	0.41
3:D:11:ALA:HB1	25:O:278:TYR:CZ	2.56	0.41
3:D:63:ARG:HB3	3:D:79:HIS:HB2	2.02	0.41
6:3:281:GLU:HB2	6:3:293:TYR:HD1	1.85	0.41
6:3:616:LEU:O	6:3:620:ARG:HG2	2.21	0.41
11:S:17:GLU:HB3	11:S:67:ARG:HB3	2.01	0.41
16:r:32:LYS:O	16:r:35:GLN:NE2	2.51	0.41
21:K:73:VAL:HG21	24:N:38:LEU:HD22	2.02	0.41
22:L:396:ILE:HG21	22:L:490:ALA:HB2	2.03	0.41
22:L:595:ILE:HG12	24:N:100:MET:SD	2.61	0.41
23:M:218:LYS:HB3	23:M:218:LYS:HE2	1.80	0.41
25:O:22:SER:OG	25:O:119:GLY:O	2.37	0.41
26:X:48:GLU:OE1	26:X:134:ARG:NH2	2.39	0.41
29:a:54:ILE:HD13	29:a:54:ILE:HA	1.84	0.41
2:C:194:PHE:O	9:Q:81:ASN:ND2	2.52	0.41
5:1:305:PRO:HD3	5:1:413:TRP:HB3	2.02	0.41
5:1:365:CYS:O	5:1:369:VAL:HB	2.21	0.41
6:3:284:VAL:HG12	6:3:559:VAL:HG22	2.03	0.41
6:3:459:GLN:HG3	6:3:495:ARG:HH21	1.84	0.41
9:Q:116:LYS:HA	9:Q:116:LYS:HD3	1.84	0.41
19:H:273:ILE:HG23	19:H:277:TYR:HD2	1.86	0.41
22:L:53:MET:HE2	22:L:53:MET:HB3	1.98	0.41
22:L:335:PHE:HE1	22:L:387:THR:HB	1.84	0.41
23:M:347:GLY:HA3	23:M:419:LEU:HA	2.02	0.41
26:X:40:LYS:HD3	26:X:40:LYS:HA	1.88	0.41
27:Y:140:VAL:O	36:h:123:TYR:OH	2.29	0.41
5:1:61:LYS:HE2	5:1:77:LEU:HD23	2.03	0.41
5:1:293:ASN:O	5:1:339:ARG:HG2	2.20	0.41
7:9:117:LYS:HB2	7:9:117:LYS:HE3	1.86	0.41
13:V:34:LEU:HD13	13:V:48:GLU:HG3	2.03	0.41
22:L:191:LEU:HD23	22:L:191:LEU:HA	1.93	0.41
23:M:187:ASP:OD1	23:M:187:ASP:N	2.45	0.41
27:Y:99:THR:HG23	55:Y:404:CDL:H322	2.02	0.41
42:n:113:MET:HE2	42:n:113:MET:HB3	1.89	0.41
1:6:113:VAL:HG11	3:D:54:GLN:HG3	2.03	0.41
2:C:83:VAL:HG12	2:C:85:THR:HG22	2.03	0.41
5:1:82:MET:SD	5:1:221:THR:OG1	2.69	0.41
7:9:121:CYS:N	45:9:201:SF4:S4	2.92	0.41
8:P:134:HIS:HB2	8:P:149:LYS:HE2	2.02	0.41
8:P:303:LEU:HD23	8:P:303:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:102:ILE:HG13	19:H:103:LEU:N	2.35	0.41
19:H:179:TRP:HE1	28:Z:42:LEU:HG	1.86	0.41
21:K:40:LEU:HD13	24:N:71:LEU:HD23	2.02	0.41
22:L:54:PHE:CZ	22:L:84:PHE:HB2	2.56	0.41
24:N:254:LEU:HD23	24:N:254:LEU:HA	1.87	0.41
25:O:280:PRO:HA	25:O:283:THR:HG22	2.03	0.41
35:g:79:PRO:HG3	36:h:72:SER:HB3	2.03	0.41
8:P:196:LEU:HD12	8:P:196:LEU:HA	1.94	0.41
19:H:267:SER:O	19:H:271:LEU:HG	2.21	0.41
21:K:21:MET:HE3	22:L:589:MET:HE1	2.03	0.41
22:L:286:LEU:HD13	22:L:411:ILE:HB	2.03	0.41
23:M:277:LEU:HD23	23:M:277:LEU:HA	1.87	0.41
24:N:139:LEU:HD23	24:N:139:LEU:HA	1.94	0.41
12:U:35:HIS:HE1	12:U:37:MET:HE2	1.86	0.41
26:X:157:LEU:HD12	26:X:157:LEU:HA	1.93	0.41
1:6:60:PHE:HD1	3:D:54:GLN:HG2	1.86	0.40
4:2:96:GLY:H	4:2:138:THR:HG1	1.65	0.40
5:1:342:ASP:OD1	5:1:429:ARG:NH2	2.46	0.40
22:L:4:PHE:HZ	22:L:87:ILE:HD11	1.86	0.40
22:L:233:LEU:HB3	22:L:234:PRO:HD3	2.02	0.40
24:N:71:LEU:HD12	24:N:71:LEU:HA	1.91	0.40
41:m:13:LEU:HD12	41:m:14:PRO:HD2	2.03	0.40
3:D:284:ASP:OD1	7:9:1:THR:OG1	2.37	0.40
5:1:131:ALA:O	5:1:171:TYR:OH	2.34	0.40
8:P:256:TYR:HE2	8:P:258:LEU:HD13	1.87	0.40
19:H:141:SER:HA	19:H:290:TRP:HE1	1.87	0.40
23:M:6:LEU:HD13	23:M:6:LEU:HA	1.94	0.40
23:M:216:LEU:HD23	23:M:287:ALA:HB1	2.03	0.40
24:N:102:LEU:HD13	24:N:102:LEU:HA	1.86	0.40
37:i:17:LEU:HD11	42:n:162:LEU:HD22	2.03	0.40
42:n:169:ILE:O	42:n:172:ARG:NH1	2.52	0.40
6:3:437:HIS:HB3	6:3:440:CYS:H	1.86	0.40
8:P:21:ALA:HA	8:P:90:VAL:O	2.21	0.40
21:K:59:ILE:HD12	24:N:27:MET:HG2	2.03	0.40
23:M:366:ASN:ND2	23:M:407:SER:OG	2.54	0.40
26:X:162:HIS:NE2	36:h:99:GLU:OE1	2.48	0.40
28:Z:52:TRP:NE1	28:Z:56:ARG:HD2	2.37	0.40
42:n:56:MET:HA	42:n:59:ALA:HB3	2.03	0.40
2:C:177:ASP:HB3	2:C:180:VAL:HG22	2.04	0.40
5:1:288:THR:O	5:1:293:ASN:ND2	2.41	0.40
8:P:27:THR:OG1	52:P:501:NDP:O3B	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:105:LEU:HD21	55:d:201:CDL:H673	2.04	0.40
1:6:78:ASP:HB3	1:6:81:ARG:HB3	2.03	0.40
5:1:403:THR:OG1	5:1:405:CYS:O	2.37	0.40
7:9:119:ILE:HG12	45:9:201:SF4:S3	2.62	0.40
8:P:133:SER:O	8:P:168:PRO:HD2	2.22	0.40
16:r:67:ILE:HG21	16:r:70:SER:HB2	2.04	0.40
12:U:4:PRO:HA	12:U:5:PRO:HD3	1.89	0.40
26:X:71:ARG:NH1	29:a:70:ASP:OD1	2.46	0.40
41:m:47:LEU:HD23	41:m:47:LEU:HA	1.96	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	6	155/224 (69%)	149 (96%)	6 (4%)	0	100	100
2	C	206/263 (78%)	199 (97%)	7 (3%)	0	100	100
3	D	427/463 (92%)	414 (97%)	13 (3%)	0	100	100
4	2	212/248 (86%)	201 (95%)	10 (5%)	1 (0%)	24	54
5	1	428/464 (92%)	411 (96%)	17 (4%)	0	100	100
6	3	688/727 (95%)	662 (96%)	26 (4%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	340/377 (90%)	327 (96%)	13 (4%)	0	100	100
9	Q	124/175 (71%)	120 (97%)	4 (3%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
12	T	77/156 (49%)	77 (100%)	0	0	100	100
12	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	V	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
14	W	112/131 (86%)	109 (97%)	3 (3%)	0	100	100
15	q	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
16	r	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
19	H	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
20	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	L	604/607 (100%)	574 (95%)	30 (5%)	0	100	100
23	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
24	N	343/345 (99%)	333 (97%)	10 (3%)	0	100	100
25	O	318/355 (90%)	298 (94%)	20 (6%)	0	100	100
26	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
27	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
29	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	c	46/76 (60%)	46 (100%)	0	0	100	100
32	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
33	e	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	60 (95%)	3 (5%)	0	100	100
39	k	75/104 (72%)	74 (99%)	1 (1%)	0	100	100
40	l	155/186 (83%)	154 (99%)	1 (1%)	0	100	100
41	m	124/129 (96%)	123 (99%)	1 (1%)	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	107 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	p	168/176 (96%)	167 (99%)	1 (1%)	0	100	100
All	All	8141/9212 (88%)	7858 (96%)	282 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS

5.3.2 Protein sidechains (i)

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	6	133/185 (72%)	130 (98%)	3 (2%)	44	76
2	C	190/227 (84%)	189 (100%)	1 (0%)	81	93
3	D	370/394 (94%)	366 (99%)	4 (1%)	65	88
4	2	184/206 (89%)	182 (99%)	2 (1%)	65	88
5	1	345/370 (93%)	340 (99%)	5 (1%)	59	85
6	3	580/610 (95%)	573 (99%)	7 (1%)	63	86
7	9	152/178 (85%)	149 (98%)	3 (2%)	48	78
8	P	299/325 (92%)	296 (99%)	3 (1%)	68	89
9	Q	113/153 (74%)	111 (98%)	2 (2%)	51	80
10	7	81/96 (84%)	81 (100%)	0	100	100
11	S	74/80 (92%)	72 (97%)	2 (3%)	39	73
12	T	73/135 (54%)	67 (92%)	6 (8%)	10	32
12	U	81/135 (60%)	80 (99%)	1 (1%)	63	86
13	V	101/102 (99%)	99 (98%)	2 (2%)	48	78
14	W	108/114 (95%)	105 (97%)	3 (3%)	38	72
15	q	131/131 (100%)	129 (98%)	2 (2%)	57	84
16	r	88/96 (92%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	s	41/95 (43%)	39 (95%)	2 (5%)	22 54
18	A	103/103 (100%)	101 (98%)	2 (2%)	50 79
19	H	279/279 (100%)	272 (98%)	7 (2%)	42 74
20	J	137/137 (100%)	134 (98%)	3 (2%)	45 77
21	K	87/87 (100%)	87 (100%)	0	100 100
22	L	548/549 (100%)	539 (98%)	9 (2%)	55 83
23	M	414/414 (100%)	404 (98%)	10 (2%)	43 75
24	N	307/307 (100%)	295 (96%)	12 (4%)	28 63
25	O	284/309 (92%)	281 (99%)	3 (1%)	65 88
26	X	153/154 (99%)	151 (99%)	2 (1%)	61 86
27	Y	105/106 (99%)	102 (97%)	3 (3%)	37 71
28	Z	122/123 (99%)	121 (99%)	1 (1%)	73 90
29	a	60/60 (100%)	59 (98%)	1 (2%)	53 82
30	b	72/73 (99%)	72 (100%)	0	100 100
31	c	42/67 (63%)	41 (98%)	1 (2%)	43 75
32	d	107/107 (100%)	106 (99%)	1 (1%)	70 90
33	e	93/94 (99%)	93 (100%)	0	100 100
34	f	49/53 (92%)	48 (98%)	1 (2%)	48 78
35	g	92/129 (71%)	91 (99%)	1 (1%)	65 88
36	h	123/162 (76%)	123 (100%)	0	100 100
37	i	99/119 (83%)	95 (96%)	4 (4%)	28 62
38	j	61/87 (70%)	60 (98%)	1 (2%)	55 83
39	k	60/78 (77%)	57 (95%)	3 (5%)	22 53
40	l	142/161 (88%)	141 (99%)	1 (1%)	76 92
41	m	112/114 (98%)	111 (99%)	1 (1%)	70 90
42	n	163/164 (99%)	162 (99%)	1 (1%)	78 93
43	o	109/121 (90%)	109 (100%)	0	100 100
44	p	155/158 (98%)	154 (99%)	1 (1%)	78 93
All	All	7222/7947 (91%)	7105 (98%)	117 (2%)	54 83

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	64	CYS
1	6	94	ASP
1	6	154	ILE
2	C	169	THR
3	D	61	VAL
3	D	109	VAL
3	D	170	MET
3	D	224	GLU
4	2	105	THR
4	2	181	VAL
5	1	45	THR
5	1	273	SER
5	1	281	GLU
5	1	327	THR
5	1	359	CYS
6	3	190	MET
6	3	324	ASP
6	3	537	LEU
6	3	544	VAL
6	3	588	THR
6	3	609	ILE
6	3	651	LEU
7	9	39	THR
7	9	80	ILE
7	9	88	ILE
8	P	71	LEU
8	P	126	VAL
8	P	272	LEU
9	Q	12	THR
9	Q	110	VAL
11	S	78	LEU
11	S	85	GLU
12	T	19	LEU
12	T	21	LEU
12	T	45	LEU
12	T	56	ASP
12	T	57	GLU
12	T	62	ILE
13	V	33	ILE
13	V	103	VAL
14	W	91	GLU
14	W	96	ILE
14	W	114	THR

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Mol	Chain	Res	Type
15	q	62	VAL
15	q	94	THR
17	s	29	THR
17	s	57	LEU
18	A	14	SER
18	A	29	LEU
19	H	76	THR
19	H	87	VAL
19	H	102	ILE
19	H	108	THR
19	H	199	ASP
19	H	251	LEU
19	H	280	PHE
20	J	44	LEU
20	J	131	VAL
20	J	133	VAL
22	L	46	ILE
22	L	241	THR
22	L	293	LEU
22	L	370	SER
22	L	404	THR
22	L	443	ILE
22	L	511	LEU
22	L	517	ASN
22	L	590	SER
23	M	6	LEU
23	M	54	ASN
23	M	59	ASP
23	M	109	THR
23	M	116	ILE
23	M	138	ASN
23	M	253	LEU
23	M	265	SER
23	M	375	LEU
23	M	424	ILE
24	N	5	THR
24	N	40	ILE
24	N	45	ILE
24	N	102	LEU
24	N	108	LEU
24	N	154	ILE
24	N	191	LEU

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Mol	Chain	Res	Type
24	N	193	ILE
24	N	221	LEU
24	N	226	THR
24	N	275	CYS
24	N	336	THR
25	O	180	GLN
25	O	192	MET
25	O	290	SER
12	U	65	ILE
26	X	6	LEU
26	X	17	VAL
27	Y	6	GLU
27	Y	24	THR
27	Y	42	LEU
28	Z	70	LEU
29	a	54	ILE
31	c	37	GLU
32	d	25	LYS
34	f	12	VAL
35	g	118	LEU
37	i	34	LEU
37	i	68	LEU
37	i	71	VAL
37	i	75	LEU
38	j	47	VAL
39	k	29	ILE
39	k	32	THR
39	k	67	THR
40	l	49	LEU
41	m	24	VAL
42	n	27	GLU
44	p	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	2	37	ASN
4	2	42	HIS
4	2	58	ASN
5	1	421	HIS
6	3	259	ASN
6	3	402	ASN

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Mol	Chain	Res	Type
6	3	581	GLN
6	3	640	ASN
8	P	36	ASN
8	P	58	HIS
8	P	216	ASN
9	Q	46	GLN
10	7	47	GLN
10	7	50	ASN
11	S	47	HIS
11	S	61	GLN
11	S	79	ASN
12	T	74	GLN
14	W	50	HIS
14	W	60	GLN
15	q	112	ASN
19	H	47	GLN
19	H	169	GLN
19	H	194	ASN
19	H	235	ASN
21	K	97	GLN
22	L	29	HIS
22	L	136	ASN
22	L	505	ASN
22	L	506	ASN
22	L	572	ASN
23	M	51	ASN
23	M	83	HIS
23	M	193	ASN
24	N	171	ASN
24	N	174	GLN
24	N	309	ASN
25	O	140	ASN
25	O	180	GLN
25	O	251	GLN
25	O	271	ASN
27	Y	16	GLN
28	Z	75	GLN
30	b	61	ASN
31	c	9	ASN
32	d	88	HIS
32	d	117	HIS
33	e	33	HIS

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Mol	Chain	Res	Type
33	e	96	HIS
35	g	23	GLN
35	g	25	GLN
35	g	101	ASN
36	h	143	ASN
38	j	21	GLN
40	l	54	GLN
43	o	43	GLN
44	p	22	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

11 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	$\#\|Z\|>2$
16	AYA	r	1	16	6,7,8	1.37	1 (16%)	5,8,10	1.25	1 (20%)
18	FME	A	1	18	8,9,10	0.95	0	7,9,11	0.86	0
24	FME	N	1	24	8,9,10	0.96	0	7,9,11	0.93	0
22	FME	L	1	22	8,9,10	0.92	0	7,9,11	0.98	0
21	FME	K	1	21	8,9,10	0.91	0	7,9,11	1.94	2 (28%)
3	2MR	D	85	3	10,12,13	2.54	2 (20%)	5,13,15	2.55	2 (40%)
37	SAC	i	1	37	7,8,9	1.03	0	8,9,11	0.93	1 (12%)
20	FME	J	1	20	8,9,10	0.92	0	7,9,11	0.73	0
19	FME	H	1	19	8,9,10	0.92	0	7,9,11	1.01	0
23	FME	M	1	23	8,9,10	0.98	0	7,9,11	0.65	0
30	AYA	b	1	30	6,7,8	1.27	1 (16%)	5,8,10	1.36	1 (20%)

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
16	AYA	r	1	16	-	0/4/6/8	-
18	FME	A	1	18	-	1/7/9/11	-
24	FME	N	1	24	-	1/7/9/11	-
22	FME	L	1	22	-	4/7/9/11	-
21	FME	K	1	21	-	3/7/9/11	-
3	2MR	D	85	3	-	3/10/13/15	-
37	SAC	i	1	37	-	0/7/8/10	-
20	FME	J	1	20	-	1/7/9/11	-
19	FME	H	1	19	-	1/7/9/11	-
23	FME	M	1	23	-	2/7/9/11	-
30	AYA	b	1	30	-	0/4/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.80	1.46	1.34
3	D	85	2MR	CZ-NH2	4.93	1.44	1.33
16	r	1	AYA	CA-N	-2.88	1.43	1.46
30	b	1	AYA	CA-N	-2.35	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	1	FME	C-CA-N	4.34	117.56	109.73
3	D	85	2MR	CD-NE-CZ	4.30	131.47	123.41
3	D	85	2MR	NE-CZ-NH2	-3.09	116.64	119.48
30	b	1	AYA	CB-CA-N	2.78	112.70	109.61
16	r	1	AYA	CB-CA-N	2.64	112.55	109.61
37	i	1	SAC	OG-CB-CA	-2.23	105.29	110.97
21	K	1	FME	O-C-CA	-2.20	119.00	124.78

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	O-C-CA-CB
19	H	1	FME	N-CA-CB-CG
21	K	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
22	L	1	FME	N-CA-CB-CG
3	D	85	2MR	NE-CD-CG-CB
21	K	1	FME	N-CA-CB-CG
23	M	1	FME	N-CA-CB-CG
21	K	1	FME	CA-CB-CG-SD
22	L	1	FME	CB-CG-SD-CE
3	D	85	2MR	CA-CB-CG-CD
18	A	1	FME	N-CA-CB-CG
20	J	1	FME	C-CA-CB-CG
22	L	1	FME	C-CA-CB-CG
24	N	1	FME	CA-CB-CG-SD
22	L	1	FME	CB-CA-N-CN
23	M	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	1	FME	1	0
3	D	85	2MR	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 3 are monoatomic - leaving 46 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	3PE	M	502	-	50,50,50	0.29	0	53,55,55	0.29	0
54	ZMP	W	201	-	27,33,36	0.61	0	32,40,45	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	3PE	d	202	-	30,30,50	0.38	0	33,35,55	0.34	0
46	3PE	m	202	-	29,29,50	0.38	0	32,34,55	0.33	0
55	CDL	h	201	-	69,69,99	0.36	0	75,81,111	0.44	0
54	ZMP	n	201	-	25,31,36	0.76	1 (4%)	30,38,45	0.90	1 (3%)
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.47	0
55	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.33	0
55	CDL	Y	401	-	93,93,99	0.31	0	99,105,111	0.29	0
55	CDL	Y	404	-	56,56,99	0.39	0	62,68,111	0.46	1 (1%)
48	UQ	D	501	-	63,63,63	0.32	0	76,79,79	0.75	2 (2%)
47	PC1	N	401	-	53,53,53	0.29	0	59,61,61	0.36	0
49	FES	2	301	4	0,4,4	-	-	-		
49	FES	3	803	6	0,4,4	-	-	-		
47	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.44	0
50	FMN	1	501	-	33,33,33	0.38	0	48,50,50	0.53	1 (2%)
46	3PE	A	602	-	42,42,50	0.33	0	45,47,55	0.32	0
46	3PE	Y	402	-	27,27,50	0.40	0	30,32,55	0.35	0
46	3PE	N	403	-	37,37,50	0.34	0	40,42,55	0.33	0
45	SF4	6	201	1	0,12,12	-	-	-		
45	SF4	1	502	5	0,12,12	-	-	-		
45	SF4	9	202	7	0,12,12	-	-	-		
52	NDP	P	501	-	49,52,52	0.39	0	66,80,80	0.44	0
55	CDL	N	402	-	89,89,99	0.32	0	95,101,111	0.40	0
56	DGT	O	401	57	29,33,33	0.32	0	44,52,52	0.30	0
47	PC1	A	601	-	30,30,53	0.40	0	36,38,61	0.56	0
46	3PE	D	502	-	50,50,50	0.31	0	53,55,55	0.30	0
46	3PE	M	501	-	50,50,50	0.30	0	53,55,55	0.32	0
55	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.30	0
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.49	0
46	3PE	Y	403	-	41,41,50	0.33	0	44,46,55	0.33	0
45	SF4	3	801	6	0,12,12	-	-	-		
55	CDL	r	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
45	SF4	9	201	7	0,12,12	-	-	-		
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.31	0
46	3PE	M	503	-	35,35,50	0.36	0	38,40,55	0.31	0
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.35	0
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.34	0
46	3PE	r	201	-	45,45,50	0.32	0	48,50,55	0.29	0
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.32	0
55	CDL	m	201	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)
45	SF4	3	802	6	0,12,12	-	-	-		
47	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.32	0
55	CDL	L	703	-	45,45,99	0.43	0	51,57,111	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	CDL	H	401	-	50,50,99	0.42	0	55,61,111	0.38	0
46	3PE	Z	401	-	50,50,50	0.31	0	53,55,55	0.48	1 (1%)

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
46	3PE	M	502	-	-	10/54/54/54	-
54	ZMP	W	201	-	-	3/38/40/43	-
46	3PE	d	202	-	-	9/34/34/54	-
46	3PE	m	202	-	-	7/33/33/54	-
55	CDL	h	201	-	-	23/80/80/110	-
54	ZMP	n	201	-	-	15/36/38/43	-
46	3PE	L	701	-	-	7/54/54/54	-
55	CDL	d	201	-	-	14/77/77/110	-
55	CDL	Y	401	-	-	13/104/104/110	-
55	CDL	Y	404	-	-	17/67/67/110	-
48	UQ	D	501	-	-	13/63/87/87	0/1/1/1
47	PC1	N	401	-	-	12/57/57/57	-
49	FES	2	301	4	-	-	0/1/1/1
49	FES	3	803	6	-	-	0/1/1/1
47	PC1	9	203	-	-	12/57/57/57	-
50	FMN	1	501	-	-	6/18/18/18	0/3/3/3
46	3PE	A	602	-	-	12/46/46/54	-
46	3PE	Y	402	-	-	7/31/31/54	-
46	3PE	N	403	-	-	11/41/41/54	-
45	SF4	6	201	1	-	-	0/6/5/5
55	CDL	N	402	-	-	16/100/100/110	-
45	SF4	1	502	5	-	-	0/6/5/5
52	NDP	P	501	-	-	8/34/77/77	0/5/5/5
45	SF4	9	202	7	-	-	0/6/5/5
56	DGT	O	401	57	-	6/22/34/34	0/3/3/3
47	PC1	A	601	-	-	12/34/34/57	-
46	3PE	D	502	-	-	8/54/54/54	-
46	3PE	M	501	-	-	14/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	L	702	-	-	19/88/88/110	-
47	PC1	6	203	-	-	10/46/46/57	-
46	3PE	Y	403	-	-	7/45/45/54	-
55	CDL	r	202	-	-	14/67/67/110	-
45	SF4	3	801	6	-	-	0/6/5/5
45	SF4	9	201	7	-	-	0/6/5/5
46	3PE	K	201	-	-	10/44/44/54	-
46	3PE	M	503	-	-	10/39/39/54	-
46	3PE	d	203	-	-	6/35/35/54	-
46	3PE	6	202	-	-	4/35/35/54	-
46	3PE	r	201	-	-	6/49/49/54	-
46	3PE	i	201	-	-	5/45/45/54	-
55	CDL	m	201	-	-	18/82/82/110	-
45	SF4	3	802	6	-	-	0/6/5/5
47	PC1	9	204	-	-	10/50/50/57	-
55	CDL	L	703	-	-	12/56/56/110	-
55	CDL	H	401	-	-	14/59/59/110	-
46	3PE	Z	401	-	-	10/54/54/54	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	n	201	ZMP	C9-C10	2.53	1.53	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	D	501	UQ	C37-C36-C34	-2.81	103.72	112.98
54	W	201	ZMP	O1-C10-C9	-2.75	120.74	123.99
48	D	501	UQ	C7-C6-C1	-2.65	115.29	118.48
54	W	201	ZMP	C15-C14-C13	-2.65	107.95	112.36
50	1	501	FMN	P-O5'-C5'	2.50	125.18	118.30
54	n	201	ZMP	O1-C10-C9	-2.37	121.19	123.99
46	Z	401	3PE	C2-O21-C21	2.07	122.89	117.79
55	m	201	CDL	CA4-OA6-CA5	2.02	122.77	117.79
55	r	202	CDL	CA4-OA6-CA5	2.02	122.76	117.79
55	Y	404	CDL	CA4-OA6-CA5	2.01	122.73	117.79

There are no chirality outliers.

All (410) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N
46	D	502	3PE	C1-O11-P-O12
46	D	502	3PE	O13-C11-C12-N
46	r	201	3PE	C11-O13-P-O14
46	A	602	3PE	C11-O13-P-O11
46	A	602	3PE	C11-O13-P-O12
46	A	602	3PE	C11-O13-P-O14
46	K	201	3PE	C1-O11-P-O12
46	K	201	3PE	C1-O11-P-O13
46	K	201	3PE	C1-O11-P-O14
46	K	201	3PE	O13-C11-C12-N
46	L	701	3PE	C1-O11-P-O14
46	L	701	3PE	O13-C11-C12-N
46	M	501	3PE	C1-O11-P-O12
46	M	501	3PE	C11-O13-P-O12
46	M	501	3PE	C12-C11-O13-P
46	M	501	3PE	O13-C11-C12-N
46	M	502	3PE	C11-O13-P-O12
46	M	502	3PE	C11-O13-P-O14
46	M	502	3PE	O13-C11-C12-N
46	M	503	3PE	C1-O11-P-O12
46	M	503	3PE	C1-O11-P-O13
46	M	503	3PE	C1-O11-P-O14
46	M	503	3PE	C11-O13-P-O12
46	N	403	3PE	C1-O11-P-O12
46	N	403	3PE	C11-O13-P-O11
46	N	403	3PE	C11-O13-P-O12
46	N	403	3PE	C11-O13-P-O14
46	N	403	3PE	O13-C11-C12-N
46	Y	402	3PE	C1-O11-P-O14
46	Y	402	3PE	O13-C11-C12-N
46	Y	403	3PE	C11-O13-P-O11
46	Y	403	3PE	C11-O13-P-O12
46	Y	403	3PE	C11-O13-P-O14
46	Y	403	3PE	O13-C11-C12-N
46	Z	401	3PE	O13-C11-C12-N
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C11-O13-P-O12
46	d	202	3PE	C11-O13-P-O14
46	d	202	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	d	203	3PE	C1-O11-P-O12
46	d	203	3PE	C1-O11-P-O13
46	d	203	3PE	C1-O11-P-O14
46	d	203	3PE	O13-C11-C12-N
46	m	202	3PE	C1-O11-P-O14
46	m	202	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O12
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O13-C11-C12-N
47	6	203	PC1	C11-O13-P-O12
47	6	203	PC1	C11-O13-P-O14
47	6	203	PC1	C11-O13-P-O11
47	6	203	PC1	C1-O11-P-O12
47	6	203	PC1	C1-O11-P-O14
47	9	203	PC1	C11-O13-P-O11
47	9	203	PC1	C1-O11-P-O12
47	9	203	PC1	C1-O11-P-O14
47	9	203	PC1	C1-O11-P-O13
47	A	601	PC1	C11-O13-P-O12
47	A	601	PC1	C11-O13-P-O14
47	A	601	PC1	C11-O13-P-O11
47	A	601	PC1	C1-O11-P-O12
47	A	601	PC1	C1-O11-P-O13
47	N	401	PC1	C11-O13-P-O12
47	N	401	PC1	C11-O13-P-O14
47	N	401	PC1	C11-O13-P-O11
48	D	501	UQ	C14-C16-C17-C18
48	D	501	UQ	C43-C44-C46-C47
48	D	501	UQ	C45-C44-C46-C47
50	1	501	FMN	N10-C1'-C2'-O2'
50	1	501	FMN	N10-C1'-C2'-C3'
50	1	501	FMN	C3'-C4'-C5'-O5'
50	1	501	FMN	O4'-C4'-C5'-O5'
50	1	501	FMN	C5'-O5'-P-O1P
50	1	501	FMN	C5'-O5'-P-O2P
52	P	501	NDP	C5B-O5B-PA-O3
54	W	201	ZMP	S1-C11-C12-N1
54	W	201	ZMP	O1-C10-S1-C11
54	W	201	ZMP	C9-C10-S1-C11
54	n	201	ZMP	C17-C18-C21-O5
54	n	201	ZMP	C16-C17-C18-C21
54	n	201	ZMP	O3-C16-C17-O4

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Mol	Chain	Res	Type	Atoms
54	n	201	ZMP	C17-C16-N2-C15
55	r	202	CDL	CA2-OA2-PA1-OA3
55	r	202	CDL	CA2-OA2-PA1-OA4
55	r	202	CDL	CA2-OA2-PA1-OA5
55	H	401	CDL	CA2-OA2-PA1-OA3
55	H	401	CDL	CB2-OB2-PB2-OB3
55	H	401	CDL	CB2-OB2-PB2-OB4
55	H	401	CDL	CB3-OB5-PB2-OB3
55	L	702	CDL	CA2-OA2-PA1-OA3
55	L	702	CDL	CA2-OA2-PA1-OA4
55	L	702	CDL	CA2-OA2-PA1-OA5
55	L	702	CDL	CA3-OA5-PA1-OA3
55	L	702	CDL	CB2-OB2-PB2-OB3
55	L	702	CDL	CB2-OB2-PB2-OB4
55	L	702	CDL	CB3-OB5-PB2-OB2
55	L	702	CDL	CB3-OB5-PB2-OB4
55	L	703	CDL	CA2-OA2-PA1-OA4
55	L	703	CDL	CA3-OA5-PA1-OA3
55	L	703	CDL	CB2-OB2-PB2-OB3
55	L	703	CDL	CB2-OB2-PB2-OB5
55	N	402	CDL	OA6-CA4-CA6-OA8
55	N	402	CDL	CB2-OB2-PB2-OB3
55	N	402	CDL	CB2-OB2-PB2-OB4
55	N	402	CDL	CB2-OB2-PB2-OB5
55	Y	401	CDL	CA2-OA2-PA1-OA3
55	Y	401	CDL	CA2-OA2-PA1-OA4
55	Y	401	CDL	CB3-OB5-PB2-OB2
55	Y	404	CDL	CA3-OA5-PA1-OA2
55	d	201	CDL	CA3-OA5-PA1-OA3
55	h	201	CDL	CA2-OA2-PA1-OA3
55	h	201	CDL	CB2-OB2-PB2-OB4
55	h	201	CDL	CB3-OB5-PB2-OB2
55	h	201	CDL	CB3-OB5-PB2-OB3
55	h	201	CDL	CB3-OB5-PB2-OB4
55	m	201	CDL	CB2-OB2-PB2-OB3
55	m	201	CDL	CB2-OB2-PB2-OB4
55	m	201	CDL	CB3-OB5-PB2-OB2
55	m	201	CDL	CB3-OB5-PB2-OB3
55	m	201	CDL	CB3-OB5-PB2-OB4
56	O	401	DGT	PB-O3B-PG-O1G
56	O	401	DGT	C5'-O5'-PA-O3A
54	n	201	ZMP	O3-C16-N2-C15

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Mol	Chain	Res	Type	Atoms
48	D	501	UQ	C9-C11-C12-C13
48	D	501	UQ	C34-C36-C37-C38
48	D	501	UQ	C49-C51-C52-C53
47	9	204	PC1	C11-C12-N-C13
47	9	204	PC1	C11-C12-N-C15
55	m	201	CDL	OB5-CB3-CB4-OB6
47	A	601	PC1	C21-C22-C23-C24
46	L	701	3PE	C21-C22-C23-C24
55	L	702	CDL	CA5-C11-C12-C13
47	6	203	PC1	C11-C12-N-C14
48	D	501	UQ	C24-C26-C27-C28
46	D	502	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O13
46	M	501	3PE	C11-O13-P-O11
46	M	502	3PE	C11-O13-P-O11
46	Y	402	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O13
46	d	202	3PE	C11-O13-P-O11
47	6	203	PC1	C1-O11-P-O13
55	r	202	CDL	CA3-OA5-PA1-OA2
55	H	401	CDL	CA2-OA2-PA1-OA5
55	H	401	CDL	CB2-OB2-PB2-OB5
55	L	702	CDL	CB2-OB2-PB2-OB5
55	L	703	CDL	CA3-OA5-PA1-OA2
55	N	402	CDL	CA2-OA2-PA1-OA5
55	Y	401	CDL	CA2-OA2-PA1-OA5
55	Y	404	CDL	CB2-OB2-PB2-OB5
55	Y	404	CDL	CB3-OB5-PB2-OB2
55	d	201	CDL	CB2-OB2-PB2-OB5
55	h	201	CDL	CA2-OA2-PA1-OA5
55	h	201	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	CA2-OA2-PA1-OA5
55	m	201	CDL	CA3-OA5-PA1-OA2
55	m	201	CDL	CB2-OB2-PB2-OB5
47	6	203	PC1	C11-C12-N-C13
46	D	502	3PE	C38-C39-C3A-C3B
46	M	502	3PE	C2A-C2B-C2C-C2D
55	N	402	CDL	C81-C82-C83-C84
54	n	201	ZMP	C6-C7-C8-C9
46	M	501	3PE	C36-C37-C38-C39
46	M	502	3PE	C28-C29-C2A-C2B
48	D	501	UQ	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
46	M	503	3PE	O13-C11-C12-N
46	N	403	3PE	C36-C37-C38-C39
46	Z	401	3PE	C21-C22-C23-C24
47	9	204	PC1	C2A-C2B-C2C-C2D
55	Y	401	CDL	C73-C74-C75-C76
46	M	501	3PE	C23-C24-C25-C26
47	9	204	PC1	C11-C12-N-C14
47	A	601	PC1	C11-C12-N-C15
47	N	401	PC1	C37-C38-C39-C3A
55	d	201	CDL	C55-C56-C57-C58
46	D	502	3PE	C31-C32-C33-C34
55	d	201	CDL	C63-C64-C65-C66
55	d	201	CDL	OB5-CB3-CB4-OB6
47	6	203	PC1	C11-C12-N-C15
46	D	502	3PE	C32-C33-C34-C35
47	9	204	PC1	C34-C35-C36-C37
46	r	201	3PE	C1-O11-P-O13
46	N	403	3PE	C1-O11-P-O13
55	L	702	CDL	CA3-OA5-PA1-OA2
55	d	201	CDL	CA2-OA2-PA1-OA5
47	9	204	PC1	C21-C22-C23-C24
54	n	201	ZMP	C19-C18-C21-O5
46	d	203	3PE	C21-C22-C23-C24
55	h	201	CDL	OB6-CB4-CB6-OB8
55	Y	401	CDL	C82-C83-C84-C85
46	M	502	3PE	O11-C1-C2-C3
55	d	201	CDL	OB5-CB3-CB4-CB6
55	m	201	CDL	OB5-CB3-CB4-CB6
55	H	401	CDL	C1-CB2-OB2-PB2
55	N	402	CDL	CA3-CA4-CA6-OA8
55	m	201	CDL	CB3-CB4-CB6-OB8
48	D	501	UQ	C50-C49-C51-C52
47	A	601	PC1	C11-C12-N-C14
46	M	503	3PE	C11-O13-P-O11
46	Y	402	3PE	C11-O13-P-O11
46	m	202	3PE	C1-O11-P-O13
46	Z	401	3PE	O11-C1-C2-O21
47	N	401	PC1	C3B-C3C-C3D-C3E
46	M	503	3PE	C2-C1-O11-P
55	N	402	CDL	C1-CA2-OA2-PA1
55	Y	404	CDL	C31-C32-C33-C34
54	n	201	ZMP	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
46	M	501	3PE	C37-C38-C39-C3A
46	K	201	3PE	C2-C1-O11-P
46	N	403	3PE	C1-C2-C3-O31
55	Y	401	CDL	CB3-CB4-CB6-OB8
46	M	502	3PE	O11-C1-C2-O21
47	9	204	PC1	C35-C36-C37-C38
46	N	403	3PE	O21-C2-C3-O31
55	m	201	CDL	OB6-CB4-CB6-OB8
56	O	401	DGT	PB-O3A-PA-O1A
46	A	602	3PE	C3A-C3B-C3C-C3D
46	r	201	3PE	C11-O13-P-O11
46	M	502	3PE	C1-O11-P-O13
46	i	201	3PE	C11-O13-P-O11
55	H	401	CDL	CB3-OB5-PB2-OB2
55	L	703	CDL	CA2-OA2-PA1-OA5
55	d	201	CDL	CA3-OA5-PA1-OA2
46	A	602	3PE	C2-C1-O11-P
55	H	401	CDL	C1-CA2-OA2-PA1
55	h	201	CDL	CA4-CA3-OA5-PA1
48	D	501	UQ	C48-C49-C51-C52
46	r	201	3PE	C1-O11-P-O12
46	r	201	3PE	C1-O11-P-O14
46	L	701	3PE	C1-O11-P-O12
46	M	503	3PE	C11-O13-P-O14
46	N	403	3PE	C1-O11-P-O14
46	Y	402	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O14
47	9	203	PC1	C11-O13-P-O12
47	A	601	PC1	C1-O11-P-O14
52	P	501	NDP	C5B-O5B-PA-O2A
55	r	202	CDL	CA3-OA5-PA1-OA3
55	r	202	CDL	CA3-OA5-PA1-OA4
55	H	401	CDL	CA2-OA2-PA1-OA4
55	L	702	CDL	CA3-OA5-PA1-OA4
55	L	702	CDL	CB3-OB5-PB2-OB3
55	L	703	CDL	CA2-OA2-PA1-OA3
55	L	703	CDL	CA3-OA5-PA1-OA4
55	N	402	CDL	CA2-OA2-PA1-OA3
55	N	402	CDL	CA2-OA2-PA1-OA4
55	Y	401	CDL	CB3-OB5-PB2-OB3
55	Y	404	CDL	CA3-OA5-PA1-OA3
55	Y	404	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
55	Y	404	CDL	CB2-OB2-PB2-OB3
55	Y	404	CDL	CB3-OB5-PB2-OB4
55	d	201	CDL	CB2-OB2-PB2-OB3
55	h	201	CDL	CA2-OA2-PA1-OA4
55	m	201	CDL	CA2-OA2-PA1-OA3
55	m	201	CDL	CA3-OA5-PA1-OA3
46	Z	401	3PE	O11-C1-C2-C3
55	L	702	CDL	OB5-CB3-CB4-CB6
46	A	602	3PE	C39-C3A-C3B-C3C
47	N	401	PC1	O11-C1-C2-O21
55	L	702	CDL	OB5-CB3-CB4-OB6
55	h	201	CDL	OB5-CB3-CB4-OB6
47	A	601	PC1	C11-C12-N-C13
46	Y	403	3PE	C1-C2-C3-O31
47	9	203	PC1	O13-C11-C12-N
47	N	401	PC1	O13-C11-C12-N
46	Y	403	3PE	O21-C2-C3-O31
46	L	701	3PE	C2-C1-O11-P
55	r	202	CDL	C1-CB2-OB2-PB2
55	Y	404	CDL	C1-CB2-OB2-PB2
55	h	201	CDL	C1-CA2-OA2-PA1
52	P	501	NDP	C2D-C1D-N1N-C6N
55	H	401	CDL	C13-C14-C15-C16
55	h	201	CDL	OB5-CB3-CB4-CB6
46	A	602	3PE	C35-C36-C37-C38
47	9	203	PC1	C37-C38-C39-C3A
46	M	502	3PE	C2-C1-O11-P
46	Y	402	3PE	C2-C1-O11-P
55	N	402	CDL	C51-C52-C53-C54
46	D	502	3PE	O21-C21-C22-C23
52	P	501	NDP	O4D-C1D-N1N-C6N
55	L	702	CDL	CA7-C31-C32-C33
55	Y	401	CDL	OB6-CB4-CB6-OB8
47	N	401	PC1	C28-C29-C2A-C2B
46	K	201	3PE	C11-O13-P-O11
55	r	202	CDL	CB2-OB2-PB2-OB5
55	r	202	CDL	CB3-OB5-PB2-OB2
55	N	402	CDL	CA3-OA5-PA1-OA2
48	D	501	UQ	C35-C34-C36-C37
48	D	501	UQ	C33-C34-C36-C37
52	P	501	NDP	PN-O3-PA-O2A
55	H	401	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
46	d	203	3PE	O21-C21-C22-C23
54	n	201	ZMP	C13-C14-C15-N2
55	L	703	CDL	OB5-CB3-CB4-CB6
55	L	703	CDL	OB5-CB3-CB4-OB6
55	d	201	CDL	C11-C12-C13-C14
47	N	401	PC1	C21-C22-C23-C24
55	H	401	CDL	C15-C16-C17-C18
47	9	204	PC1	C2B-C2C-C2D-C2E
46	A	602	3PE	C1-C2-C3-O31
54	n	201	ZMP	C20-C18-C21-O5
46	Z	401	3PE	C3-C2-O21-C21
47	9	203	PC1	C3-C2-O21-C21
46	M	501	3PE	C3D-C3E-C3F-C3G
46	Z	401	3PE	C31-C32-C33-C34
55	Y	404	CDL	OA5-CA3-CA4-OA6
46	Z	401	3PE	C2C-C2D-C2E-C2F
54	n	201	ZMP	C12-C11-S1-C10
47	N	401	PC1	O21-C2-C3-O31
46	Z	401	3PE	C2A-C2B-C2C-C2D
55	L	703	CDL	O1-C1-CB2-OB2
46	r	201	3PE	O31-C31-C32-C33
47	A	601	PC1	O21-C21-C22-C23
54	n	201	ZMP	O1-C10-S1-C11
55	r	202	CDL	C52-C51-CB5-OB6
46	i	201	3PE	C24-C25-C26-C27
47	N	401	PC1	O11-C1-C2-C3
54	n	201	ZMP	C7-C8-C9-C10
46	A	602	3PE	O21-C2-C3-O31
46	Y	403	3PE	C23-C24-C25-C26
55	d	201	CDL	C57-C58-C59-C60
54	n	201	ZMP	N2-C16-C17-O4
56	O	401	DGT	PB-O3B-PG-O3G
55	Y	404	CDL	C32-C31-CA7-OA8
47	9	204	PC1	O31-C31-C32-C33
55	Y	404	CDL	C72-C71-CB7-OB8
46	L	701	3PE	C3-C2-O21-C21
47	6	203	PC1	C3-C2-O21-C21
46	K	201	3PE	O31-C31-C32-C33
55	h	201	CDL	C72-C71-CB7-OB8
46	K	201	3PE	O21-C21-C22-C23
55	h	201	CDL	CB3-CB4-CB6-OB8
55	m	201	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
55	d	201	CDL	C59-C60-C61-C62
46	M	501	3PE	O31-C31-C32-C33
54	n	201	ZMP	C16-C17-C18-C20
48	D	501	UQ	C15-C14-C16-C17
52	P	501	NDP	O4D-C1D-N1N-C2N
55	Y	401	CDL	C81-C82-C83-C84
46	A	602	3PE	O31-C31-C32-C33
46	d	202	3PE	O31-C31-C32-C33
55	L	702	CDL	C72-C71-CB7-OB8
55	Y	401	CDL	C23-C24-C25-C26
46	M	501	3PE	O21-C21-C22-C23
46	M	503	3PE	O21-C21-C22-C23
55	Y	404	CDL	C52-C51-CB5-OB6
46	Z	401	3PE	C2-C1-O11-P
55	h	201	CDL	C52-C51-CB5-OB6
52	P	501	NDP	C2D-C1D-N1N-C2N
52	P	501	NDP	PN-O3-PA-O1A
56	O	401	DGT	PB-O3A-PA-O2A
47	9	203	PC1	C22-C23-C24-C25
55	h	201	CDL	C32-C31-CA7-OA8
55	d	201	CDL	C14-C15-C16-C17
55	Y	404	CDL	C32-C31-CA7-OA9
46	d	202	3PE	O32-C31-C32-C33
55	h	201	CDL	C12-C11-CA5-OA6
46	K	201	3PE	O22-C21-C22-C23
55	L	703	CDL	C1-CA2-OA2-PA1
55	m	201	CDL	C1-CB2-OB2-PB2
47	9	204	PC1	O32-C31-C32-C33
55	L	702	CDL	C72-C71-CB7-OB9
46	i	201	3PE	C2B-C2C-C2D-C2E
46	6	202	3PE	C1-O11-P-O14
46	M	501	3PE	C1-O11-P-O14
46	i	201	3PE	C11-O13-P-O12
55	r	202	CDL	CB2-OB2-PB2-OB3
55	r	202	CDL	CB3-OB5-PB2-OB3
55	N	402	CDL	CA3-OA5-PA1-OA3
55	N	402	CDL	CB3-OB5-PB2-OB3
55	d	201	CDL	CA2-OA2-PA1-OA3
56	O	401	DGT	C5'-O5'-PA-O2A
55	Y	401	CDL	C32-C31-CA7-OA8
47	9	203	PC1	C3C-C3D-C3E-C3F
55	Y	404	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
46	Z	401	3PE	C23-C24-C25-C26
46	K	201	3PE	O32-C31-C32-C33
46	M	503	3PE	O22-C21-C22-C23
46	M	501	3PE	O32-C31-C32-C33
55	h	201	CDL	C32-C31-CA7-OA9
55	h	201	CDL	C72-C71-CB7-OB9
47	N	401	PC1	C23-C24-C25-C26
46	D	502	3PE	C12-C11-O13-P
46	A	602	3PE	C12-C11-O13-P
47	9	203	PC1	C12-C11-O13-P
47	A	601	PC1	C1-C2-O21-C21
55	r	202	CDL	CA3-CA4-OA6-CA5
55	N	402	CDL	CB3-CB4-OB6-CB5
55	N	402	CDL	CB6-CB4-OB6-CB5
55	Y	404	CDL	CA3-CA4-OA6-CA5
55	h	201	CDL	CB3-CB4-OB6-CB5
55	h	201	CDL	CB6-CB4-OB6-CB5
55	m	201	CDL	CA6-CA4-OA6-CA5
55	h	201	CDL	C52-C51-CB5-OB7
47	9	203	PC1	C29-C2A-C2B-C2C
46	Y	402	3PE	O31-C31-C32-C33
46	i	201	3PE	O31-C31-C32-C33
55	r	202	CDL	C17-C18-C19-C20
46	M	501	3PE	O22-C21-C22-C23
55	H	401	CDL	CB4-CB3-OB5-PB2
55	L	702	CDL	C1-CA2-OA2-PA1
46	N	403	3PE	O21-C21-C22-C23
55	Y	404	CDL	C52-C51-CB5-OB7
46	m	202	3PE	O31-C31-C32-C33
46	A	602	3PE	O32-C31-C32-C33
55	Y	401	CDL	C32-C31-CA7-OA9
55	m	201	CDL	C12-C11-CA5-OA6

There are no ring outliers.

34 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	M	502	3PE	3	0
54	W	201	ZMP	2	0
46	d	202	3PE	1	0
55	h	201	CDL	4	0
54	n	201	ZMP	2	0

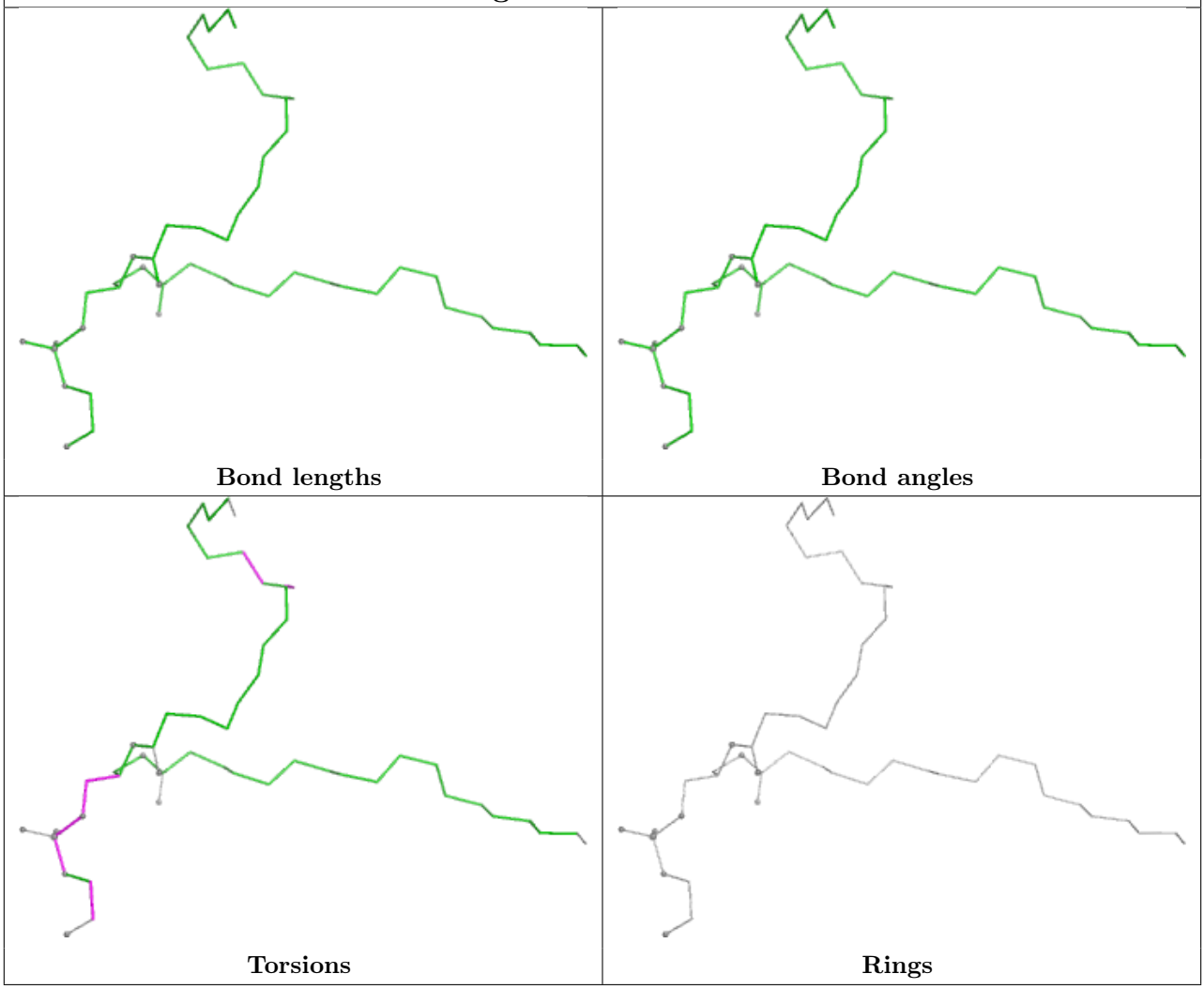
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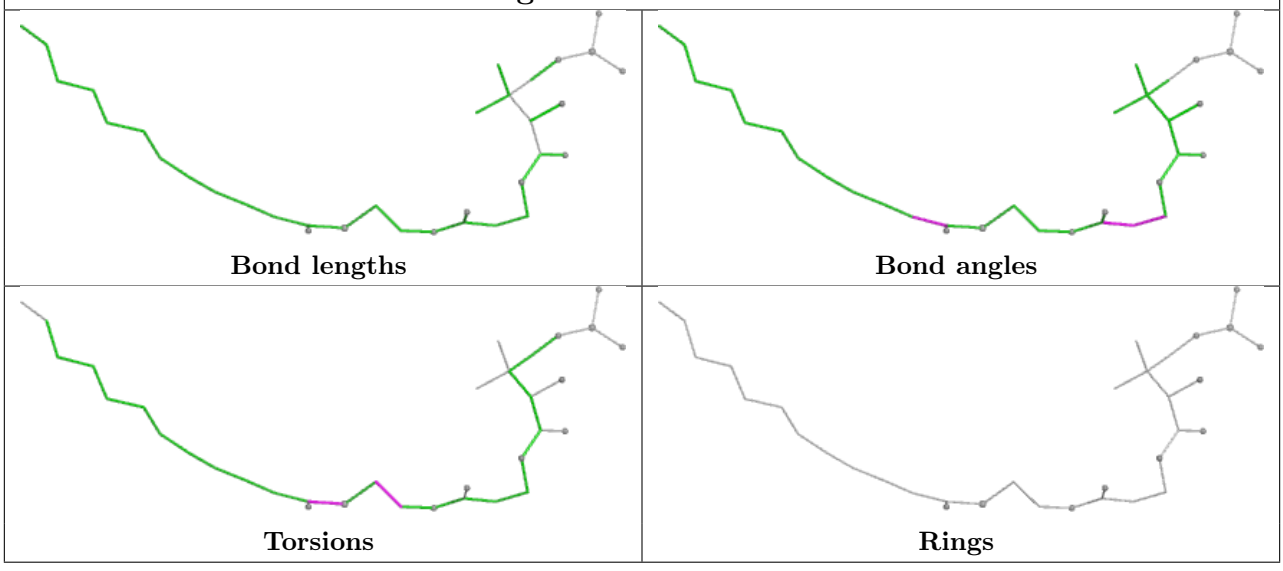
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	L	701	3PE	2	0
55	d	201	CDL	5	0
55	Y	401	CDL	1	0
55	Y	404	CDL	2	0
48	D	501	UQ	3	0
47	N	401	PC1	7	0
47	9	203	PC1	2	0
50	1	501	FMN	2	0
46	A	602	3PE	1	0
46	N	403	3PE	2	0
45	6	201	SF4	1	0
52	P	501	NDP	7	0
55	N	402	CDL	7	0
56	O	401	DGT	1	0
47	A	601	PC1	1	0
46	D	502	3PE	5	0
46	M	501	3PE	4	0
55	L	702	CDL	1	0
46	Y	403	3PE	2	0
55	r	202	CDL	3	0
45	9	201	SF4	2	0
46	K	201	3PE	2	0
46	6	202	3PE	1	0
46	i	201	3PE	2	0
55	m	201	CDL	1	0
45	3	802	SF4	1	0
47	9	204	PC1	2	0
55	L	703	CDL	1	0
55	H	401	CDL	3	0

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

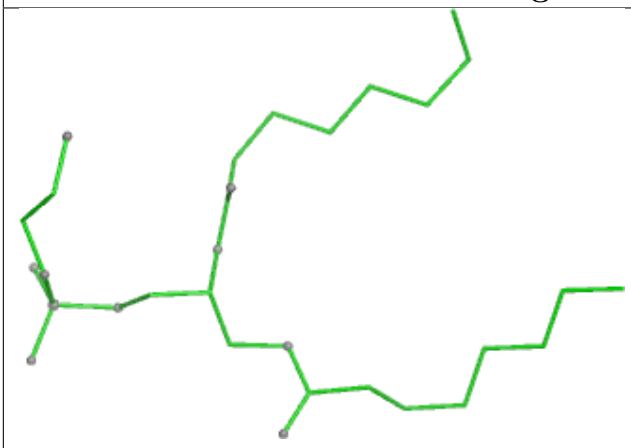
Ligand 3PE M 502



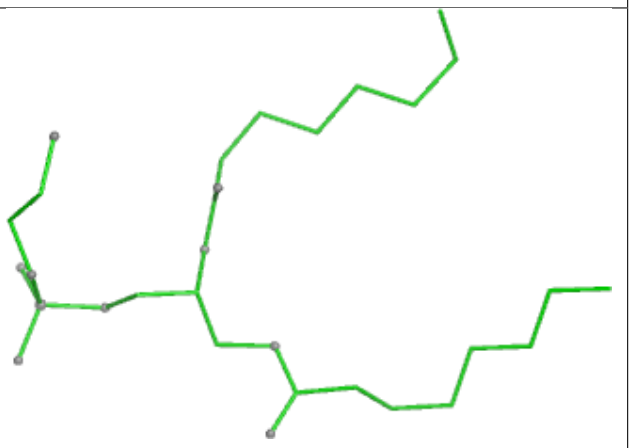
Ligand ZMP W 201



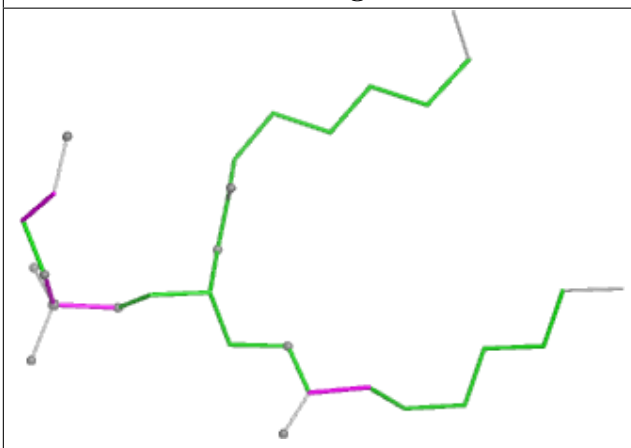
Ligand 3PE d 202



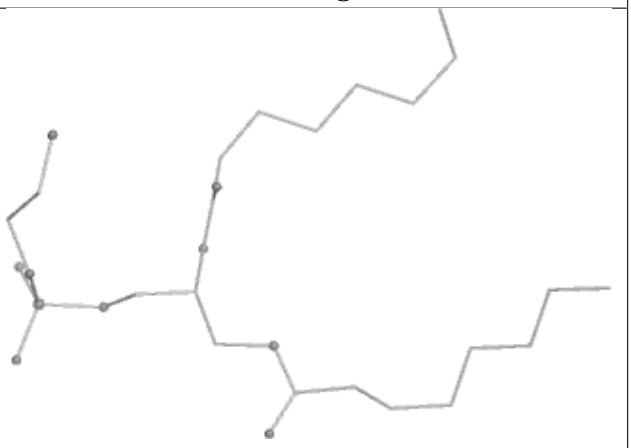
Bond lengths



Bond angles

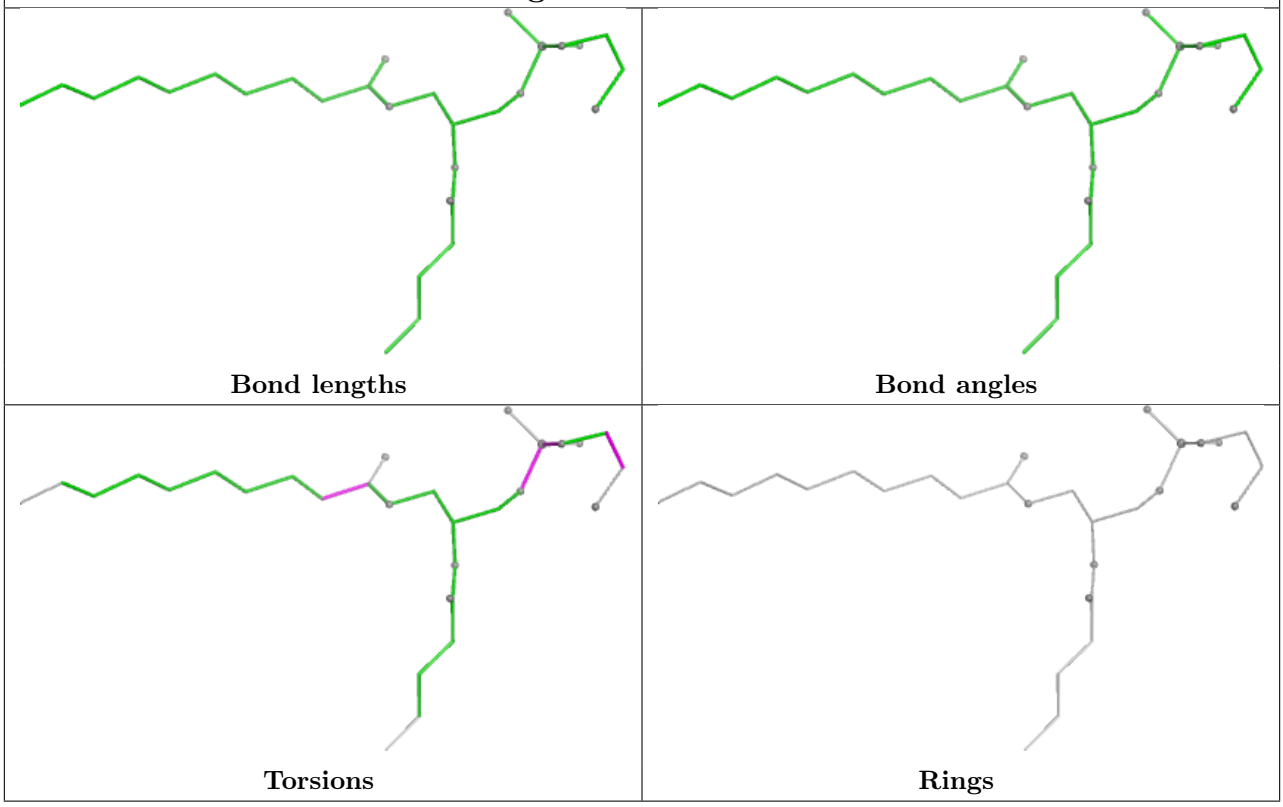


Torsions

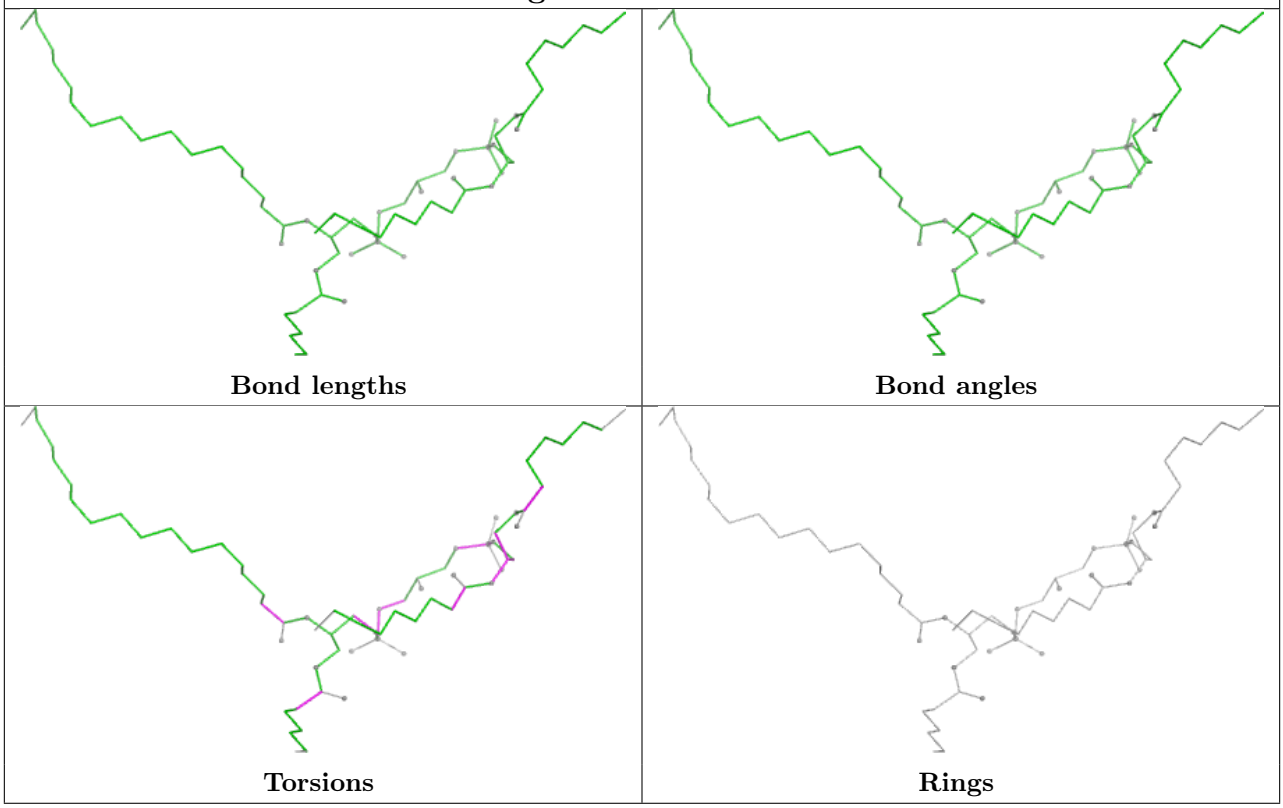


Rings

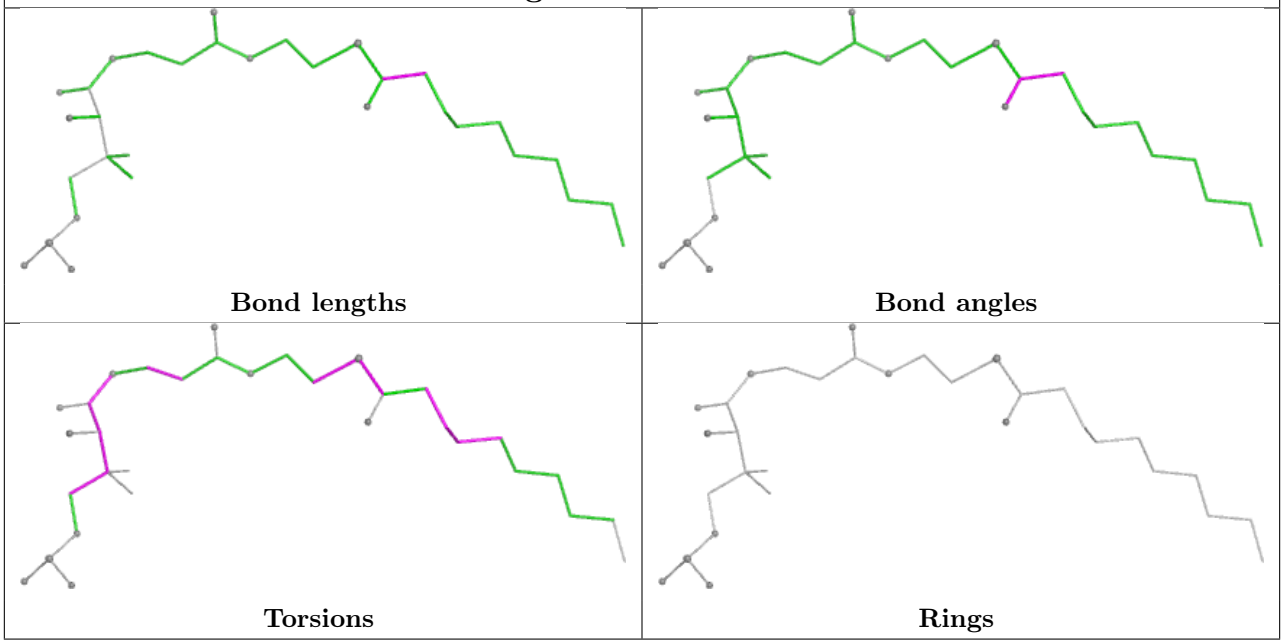
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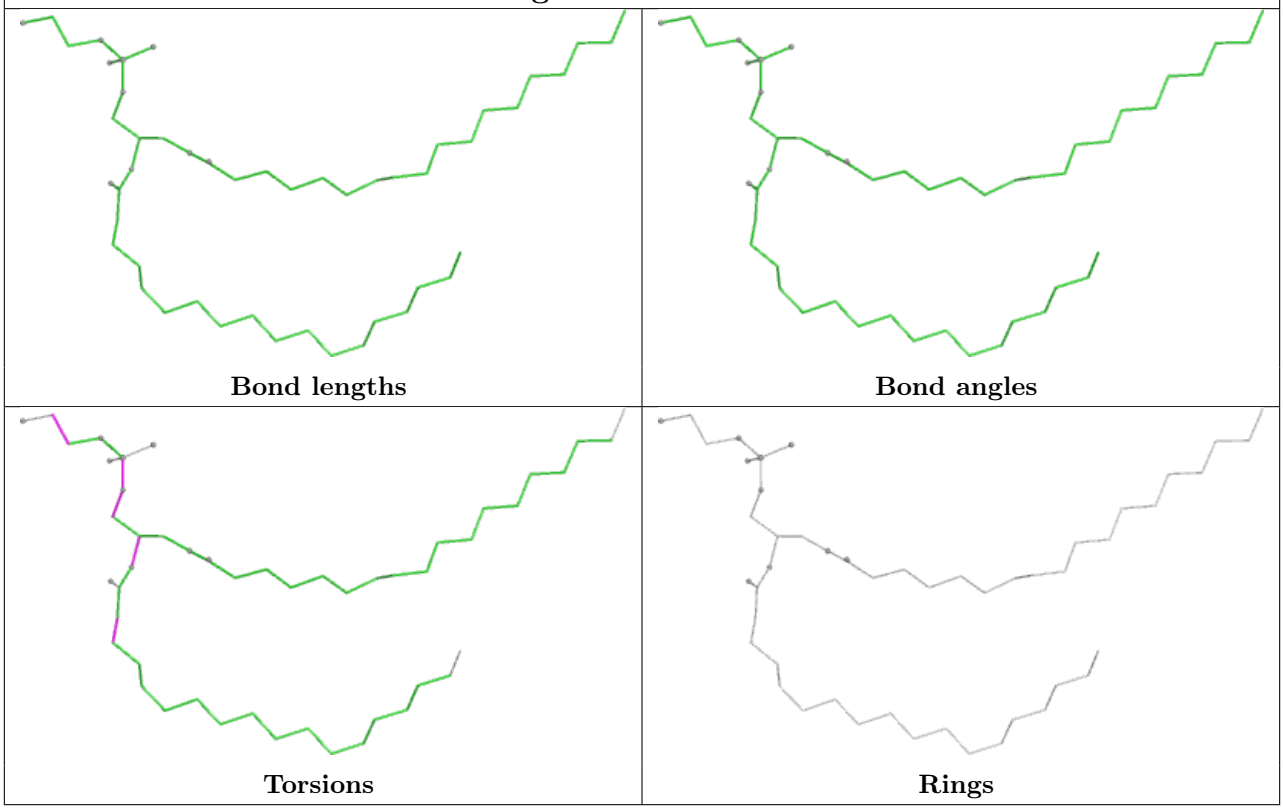
Ligand CDL h 201



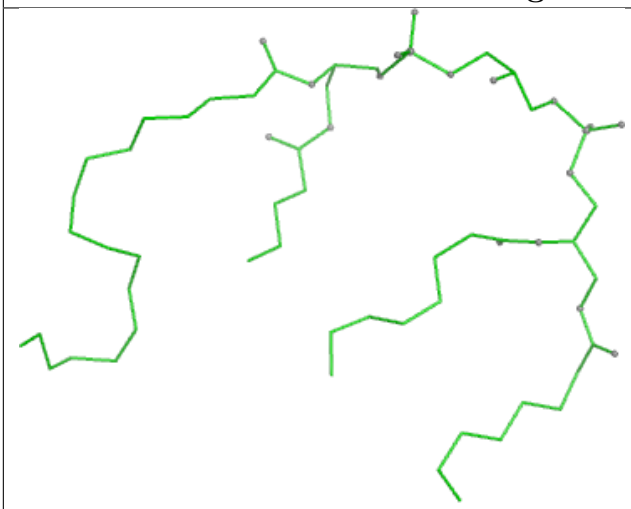
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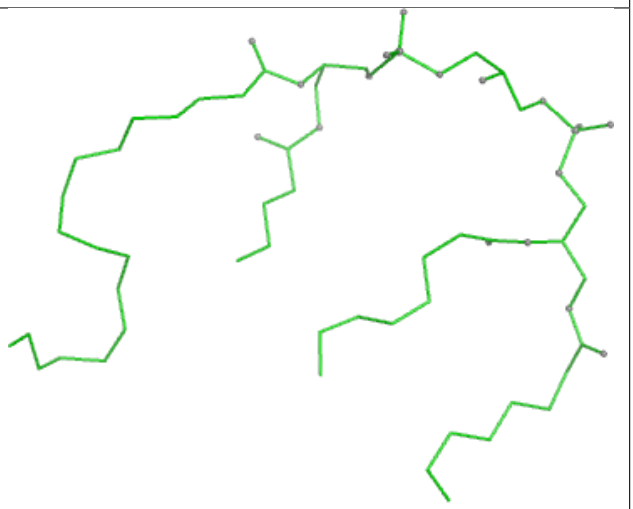
Ligand 3PE L 701



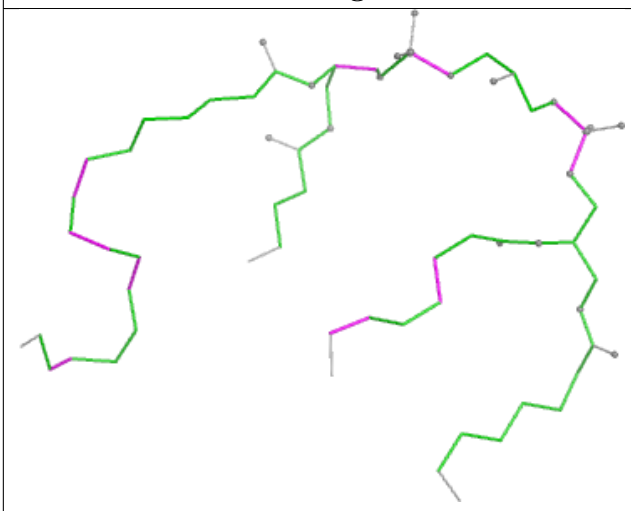
Ligand CDL d 201



Bond lengths



Bond angles

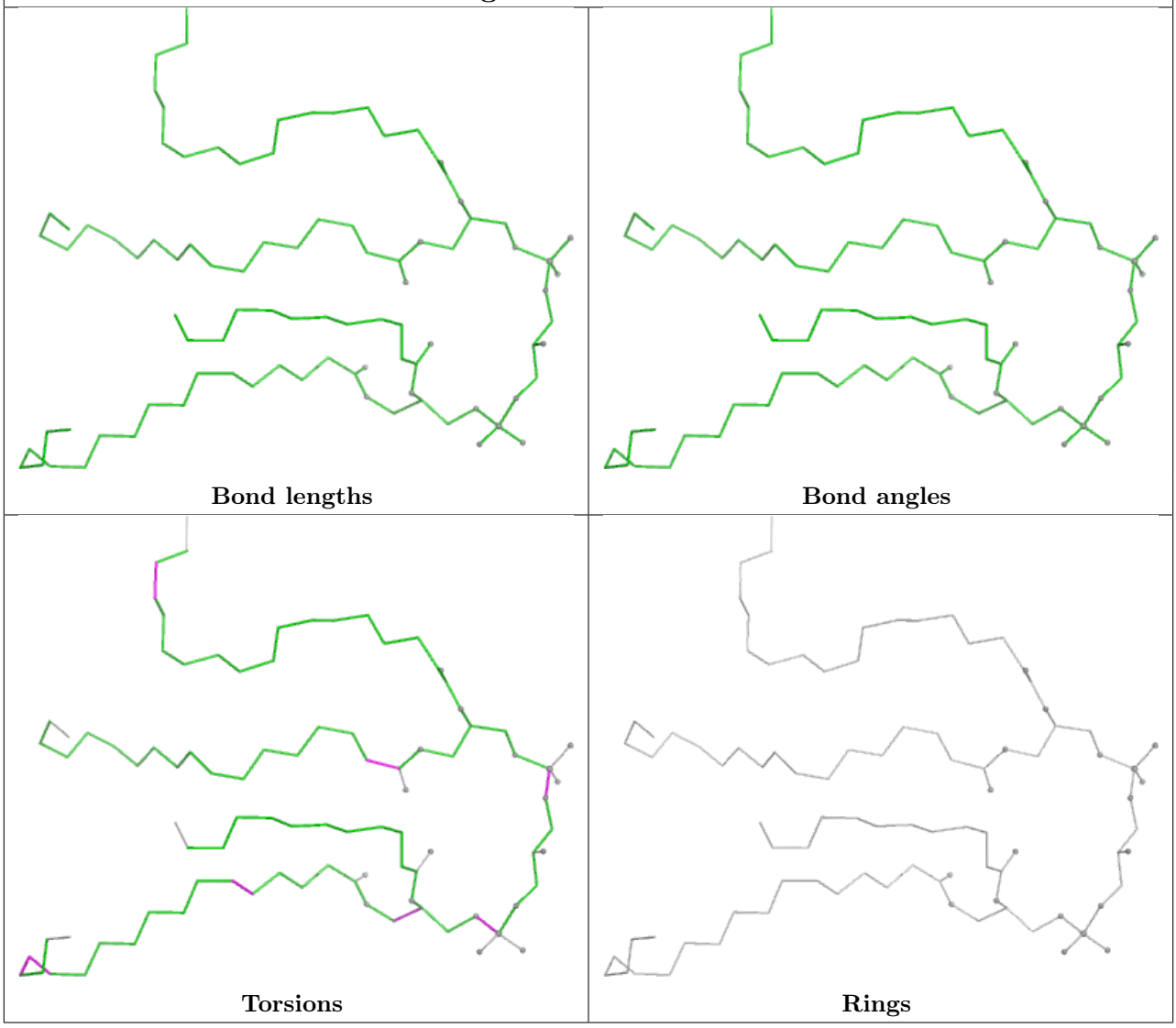


Torsions



Rings

Ligand CDL Y 401



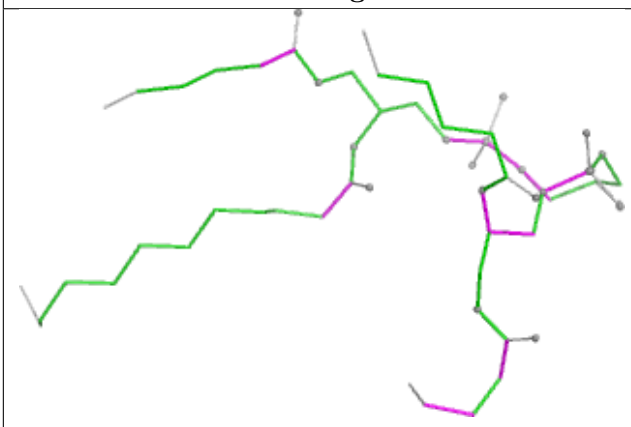
Ligand CDL Y 404



Bond lengths



Bond angles

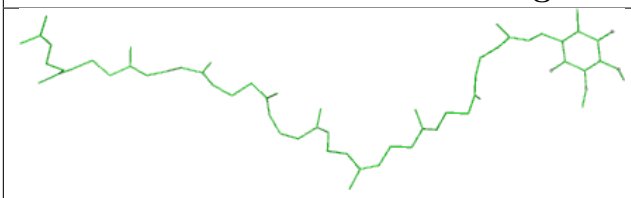


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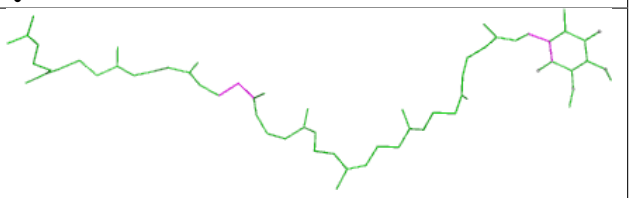


Rings

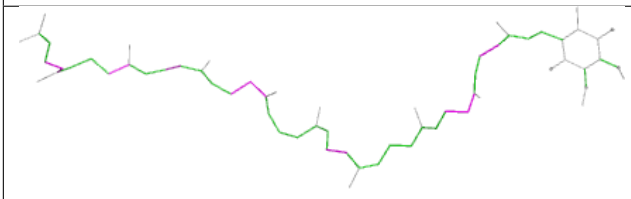
Ligand UQ D 501



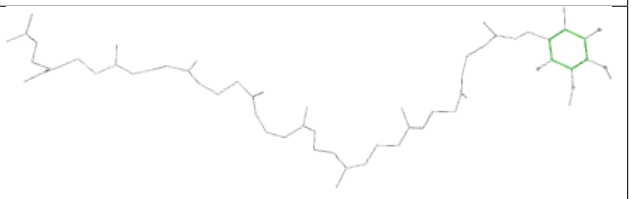
Bond lengths



Bond angles

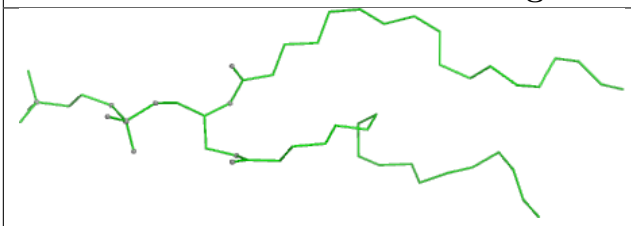


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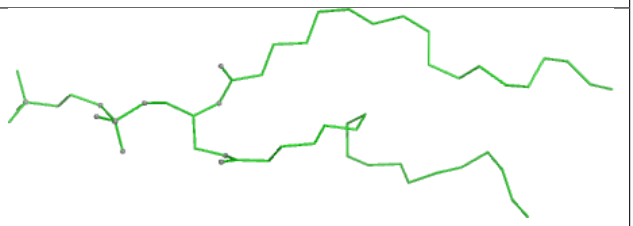


Rings

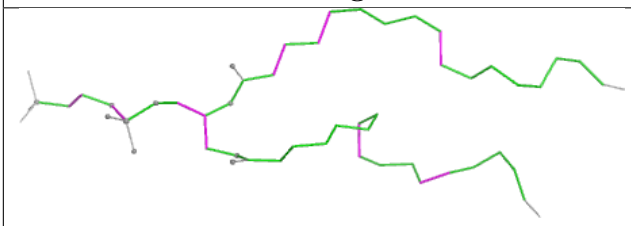
Ligand PC1 N 401



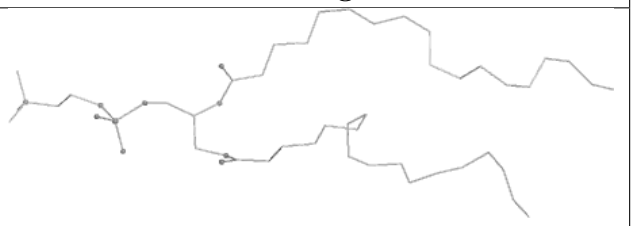
Bond lengths



Bond angles

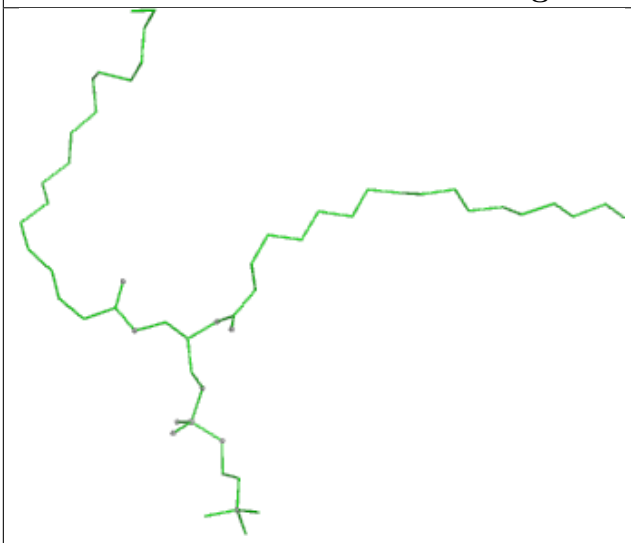


Torsions



Rings

Ligand PC1 9 203



Bond lengths



Bond angles

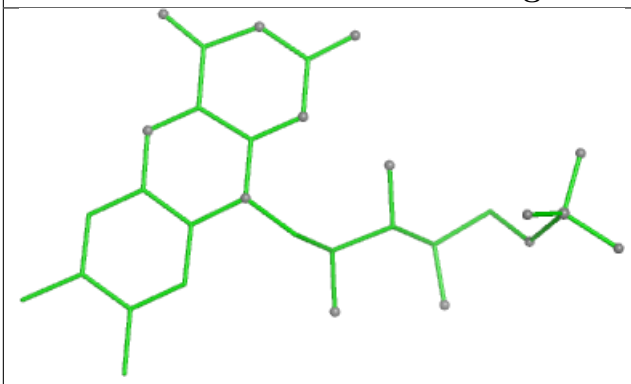


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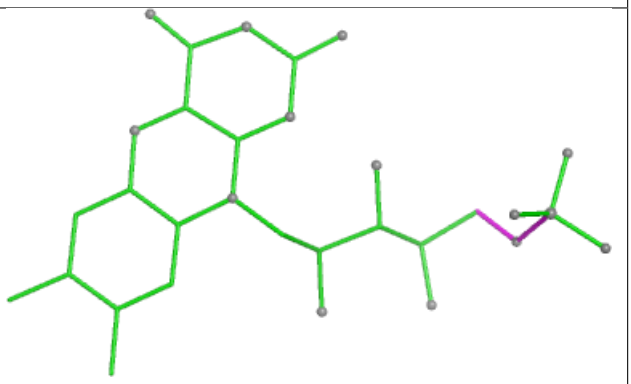


Rings

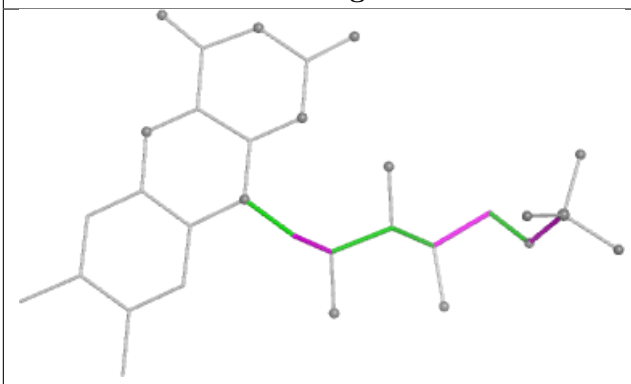
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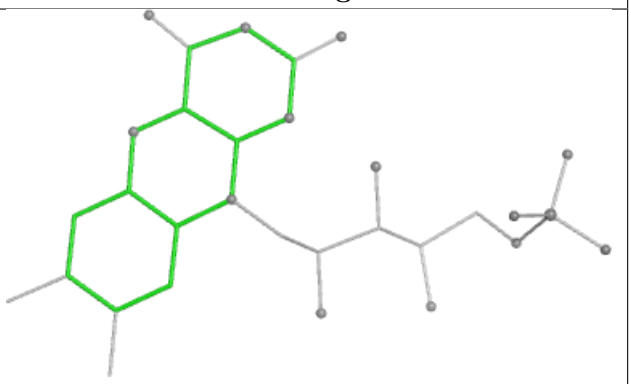
Bond lengths



Bond angles

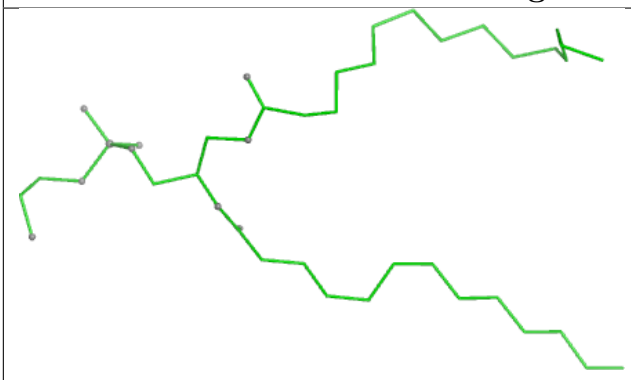


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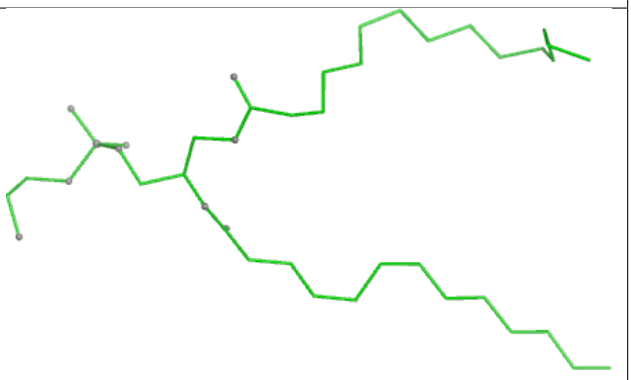


Rings

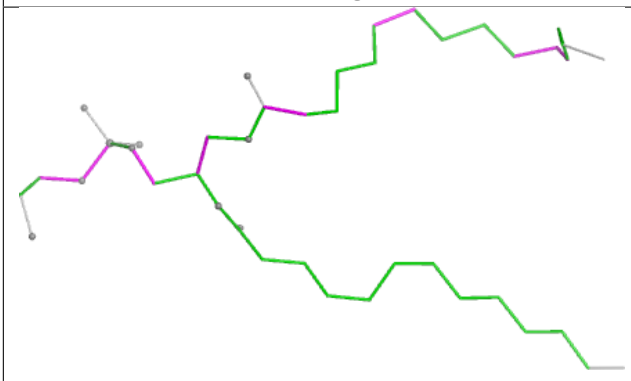
Ligand 3PE A 602



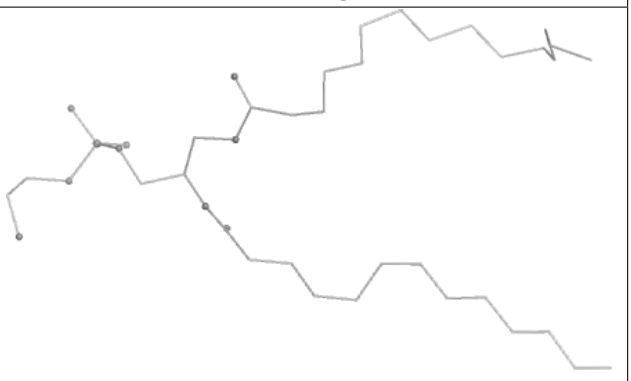
Bond lengths



Bond angles

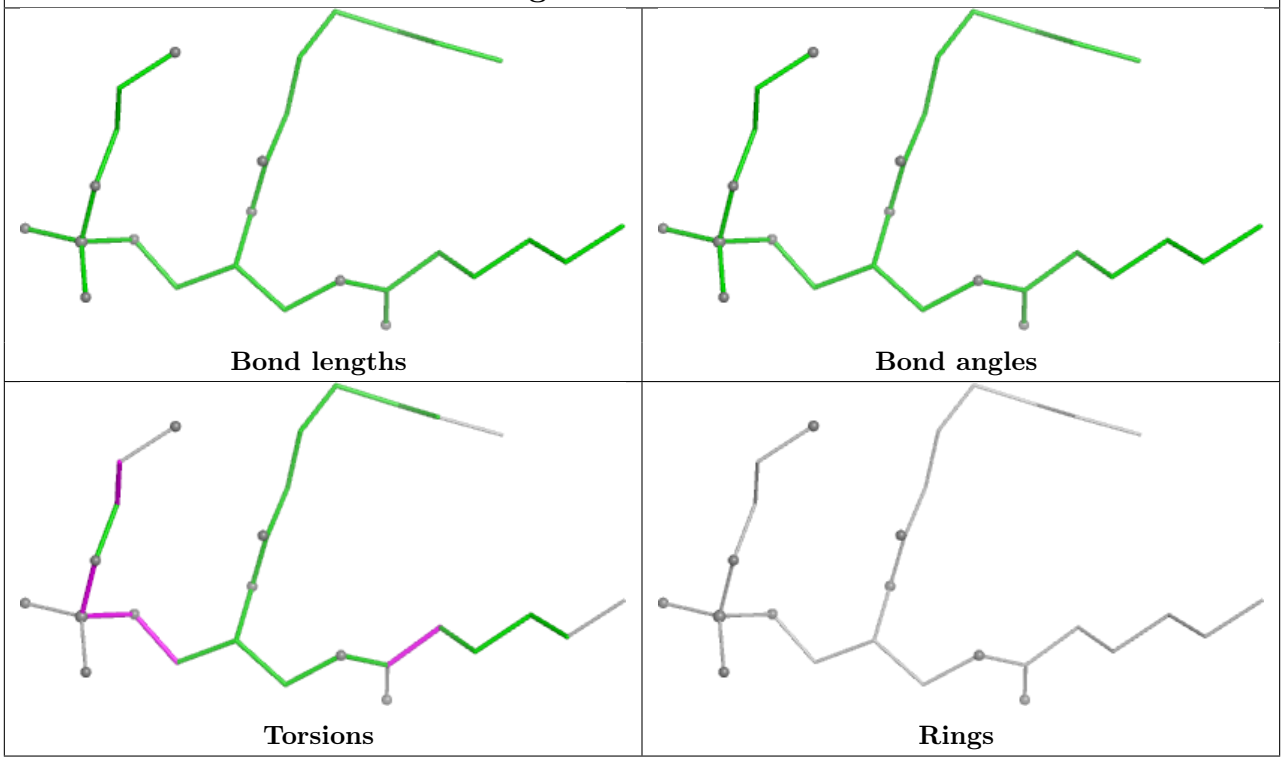


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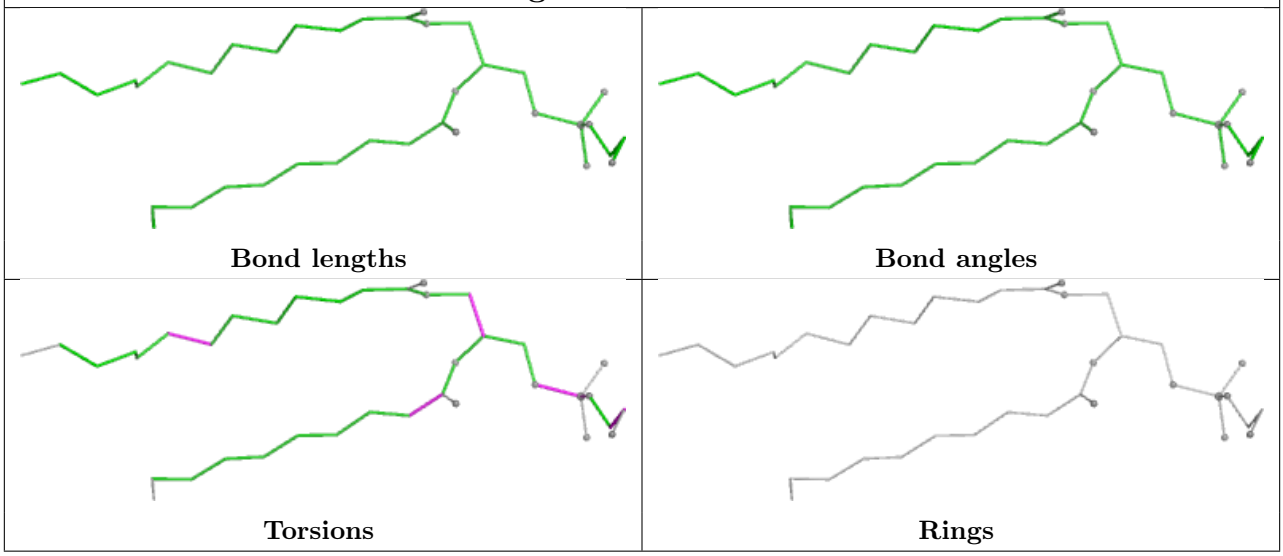


Rings

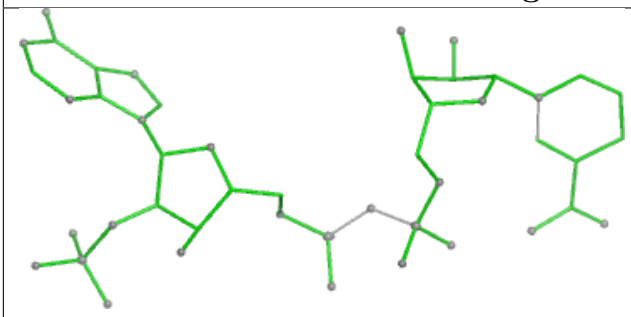
Ligand 3PE Y 402



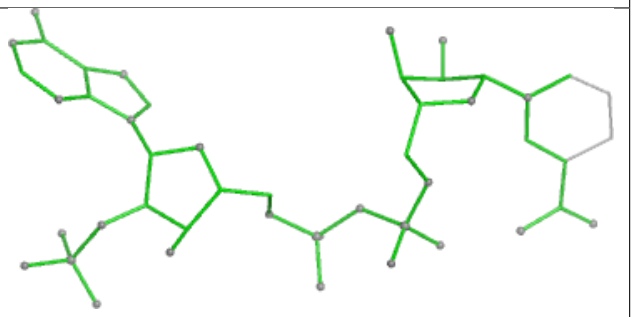
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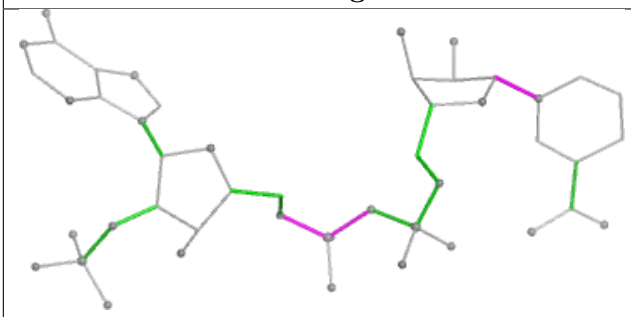
Ligand NDP P 501



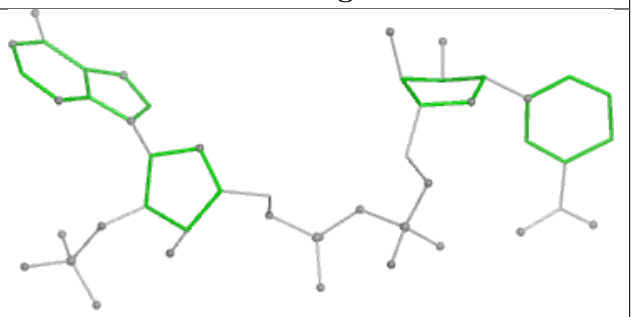
Bond lengths



Bond angles

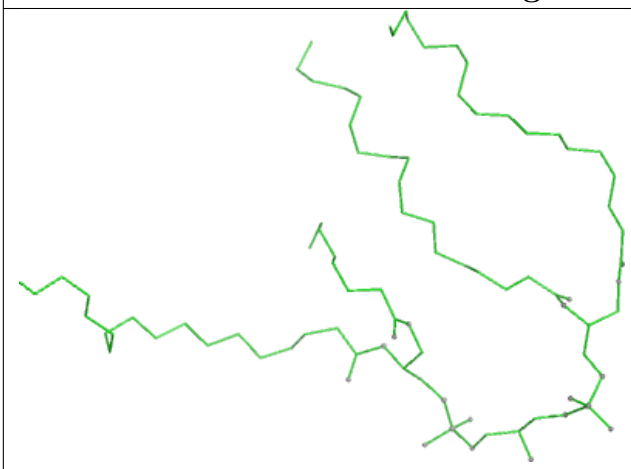


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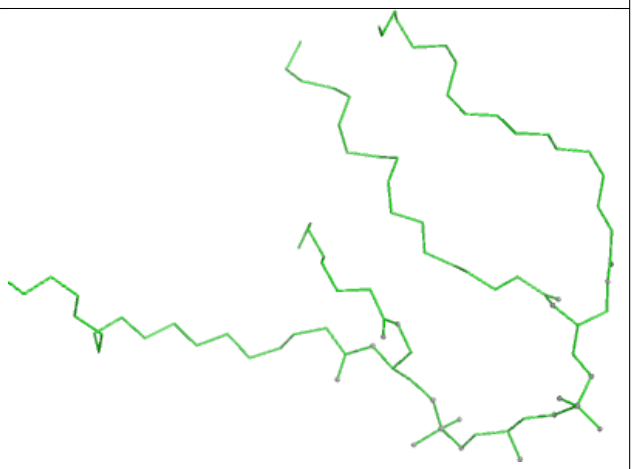


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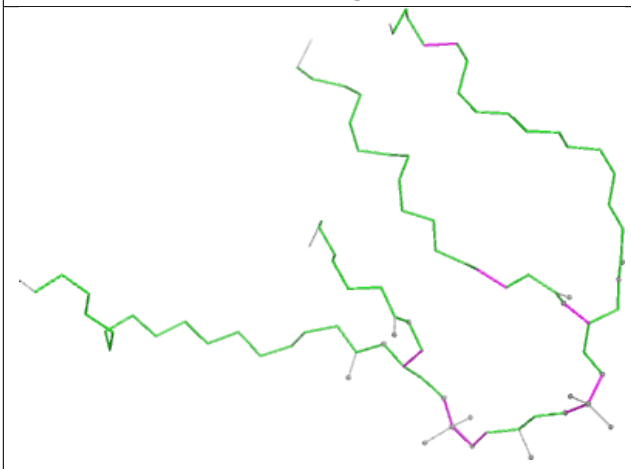
Ligand CDL N 402



Bond lengths



Bond angles

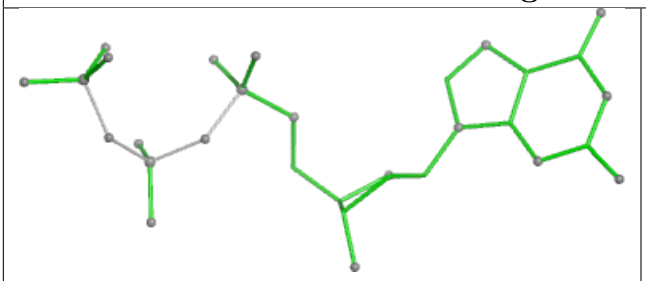


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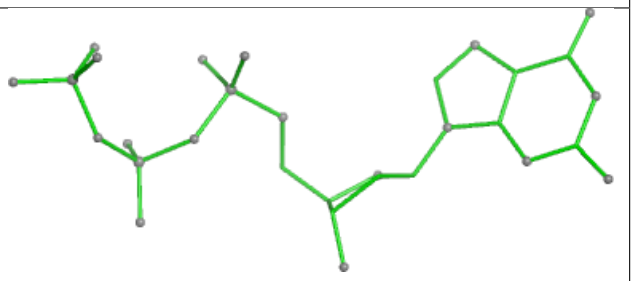


Rings

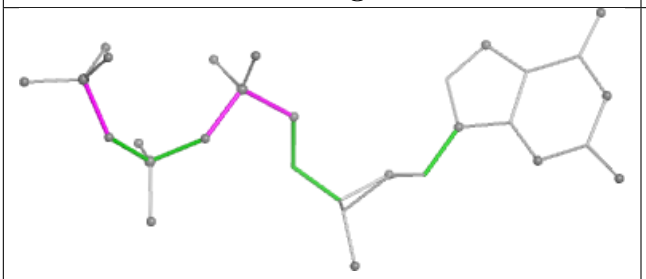
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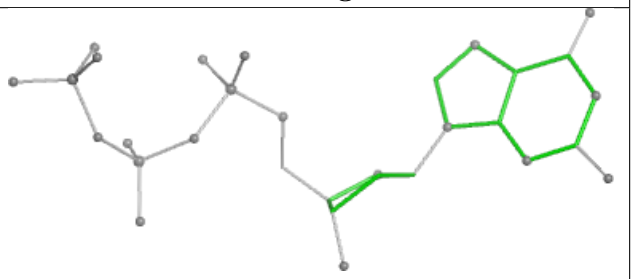
Bond lengths



Bond angles



Torsions

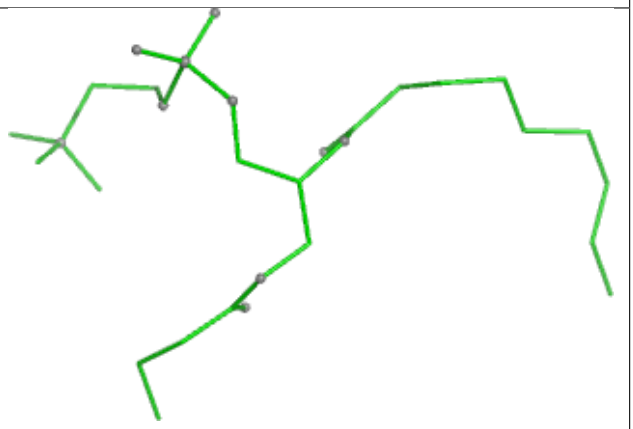


Rings

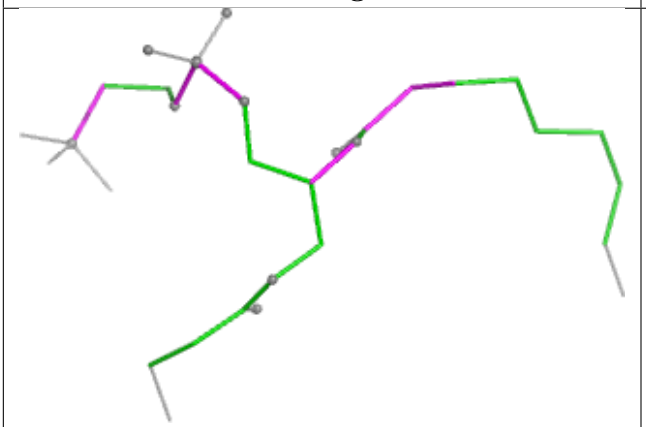
Ligand PC1 A 601



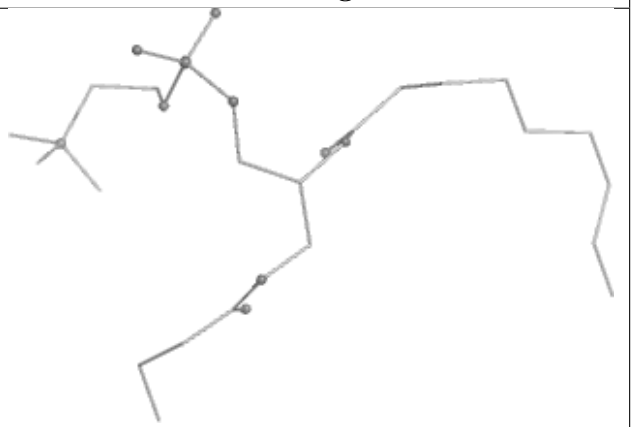
Bond lengths



Bond angles

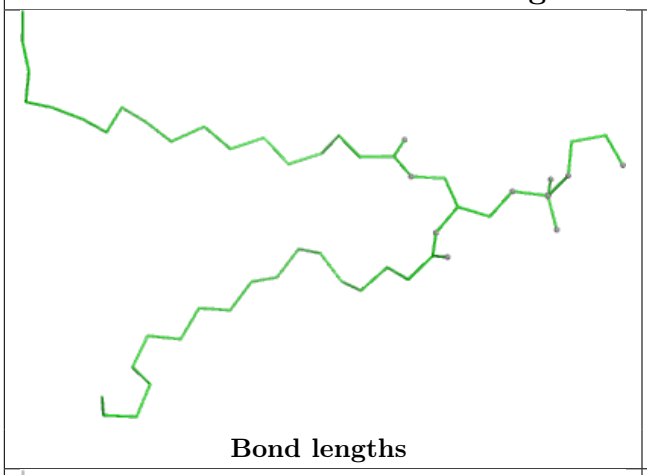


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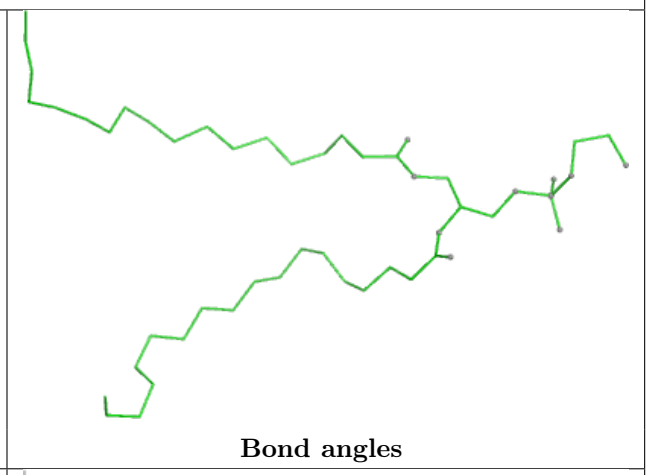


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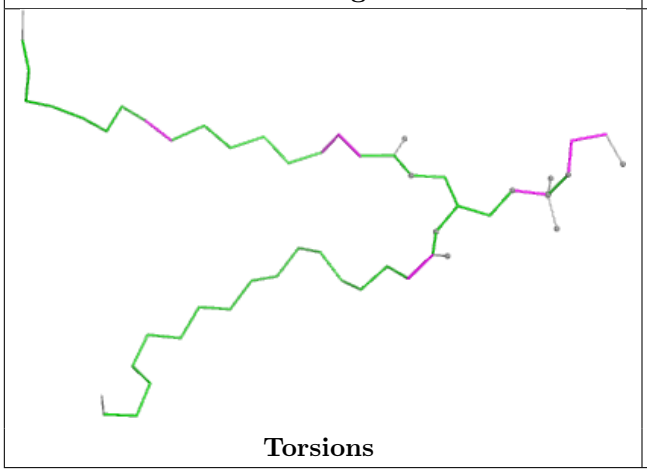
Ligand 3PE D 502



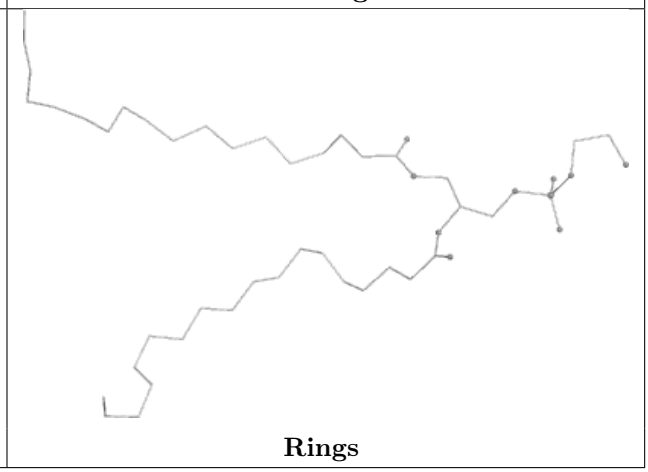
Bond lengths



Bond angles

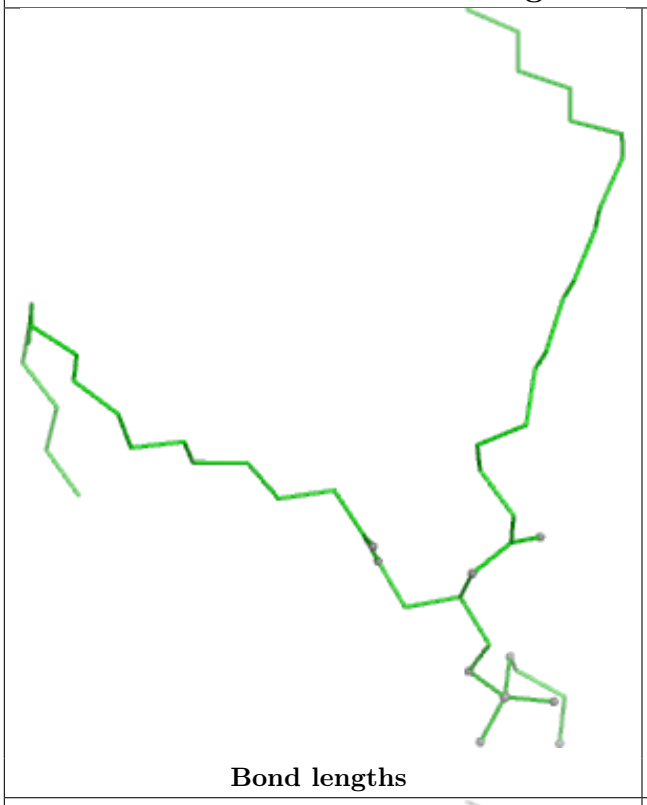


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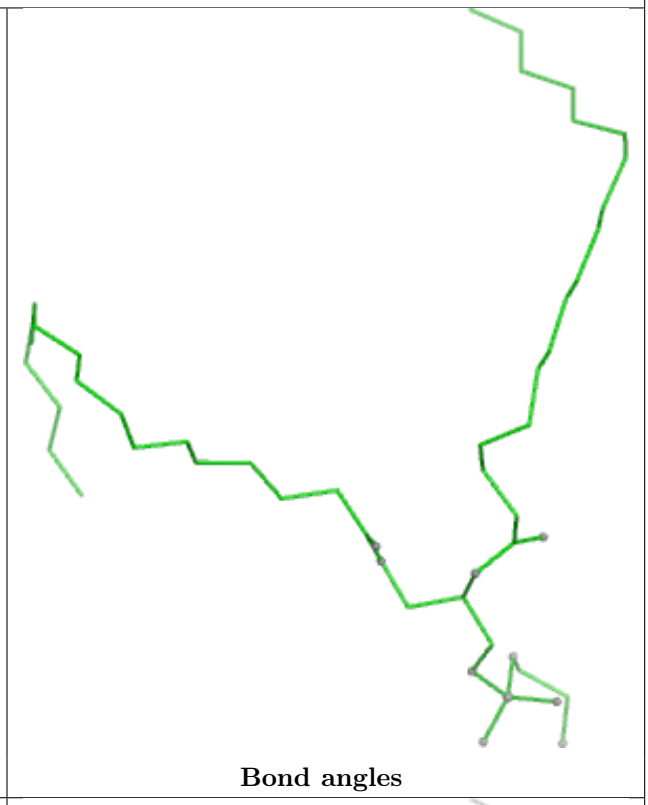


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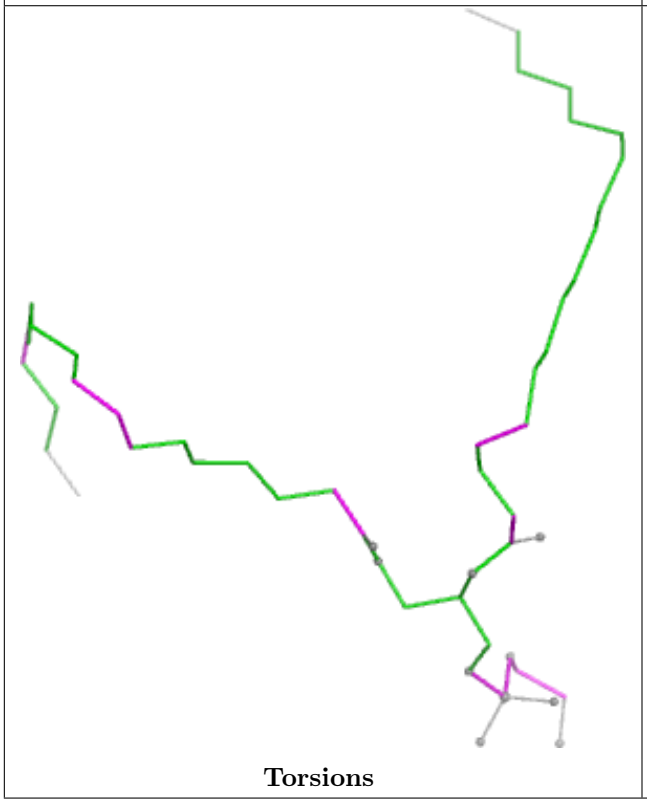
Ligand 3PE M 501



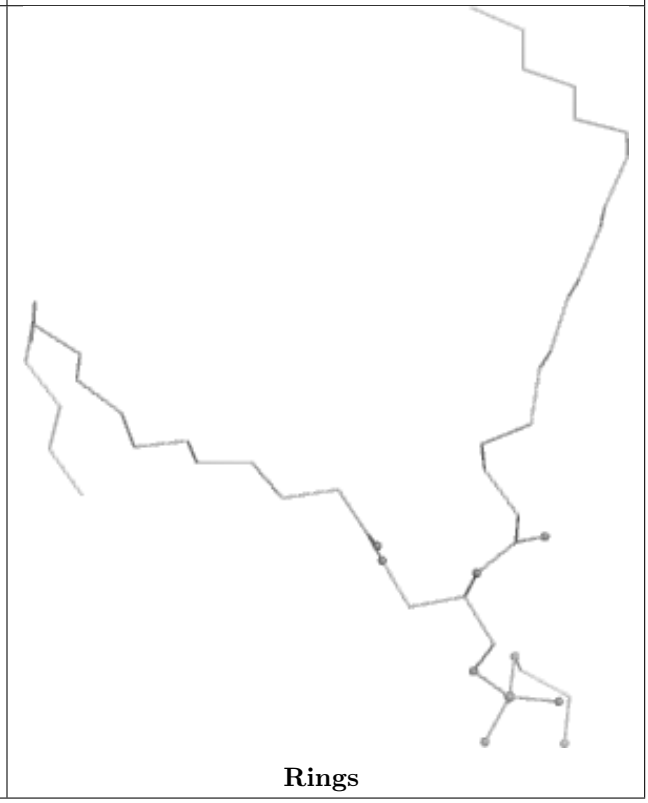
Bond lengths



Bond angles

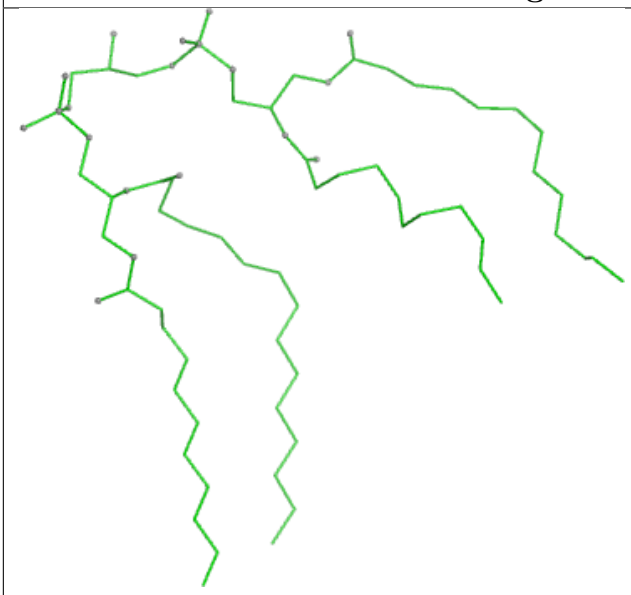


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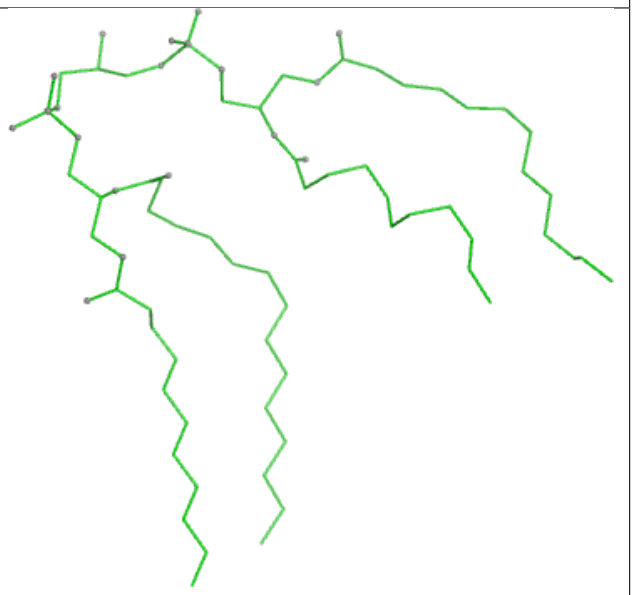


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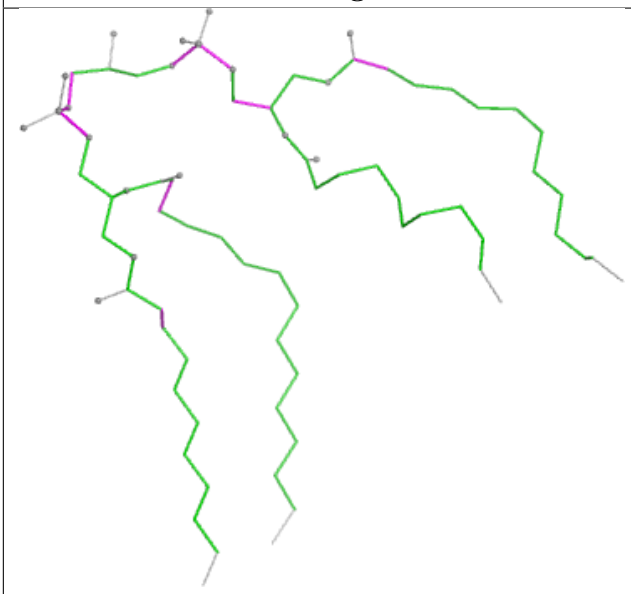
Ligand CDL L 702



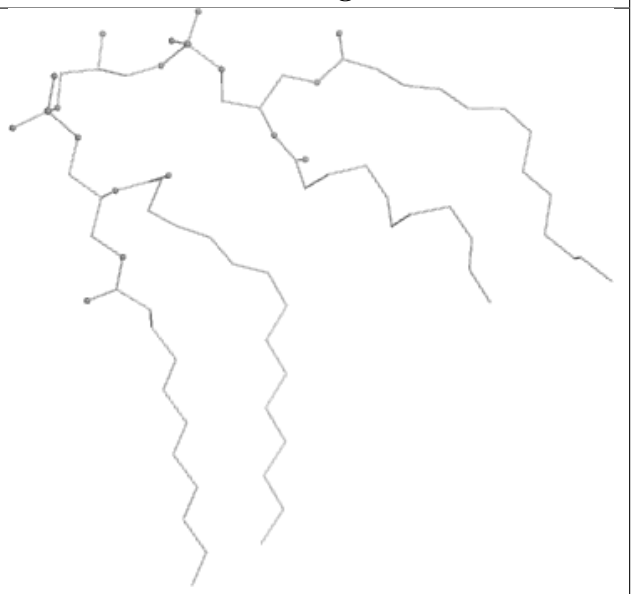
Bond lengths



Bond angles

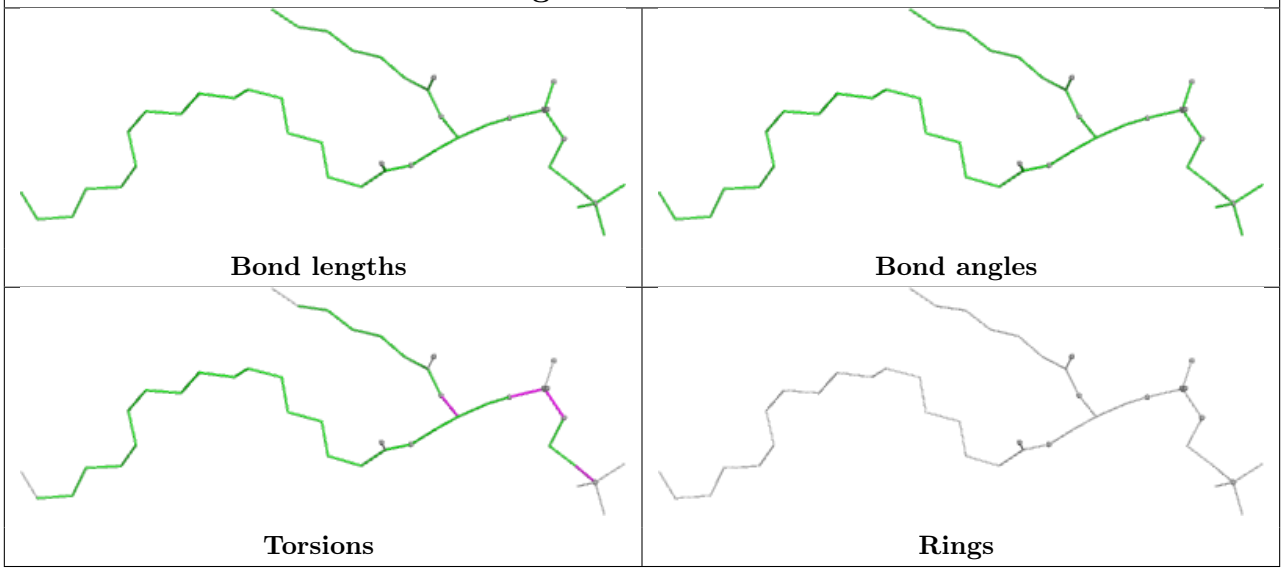


Torsions

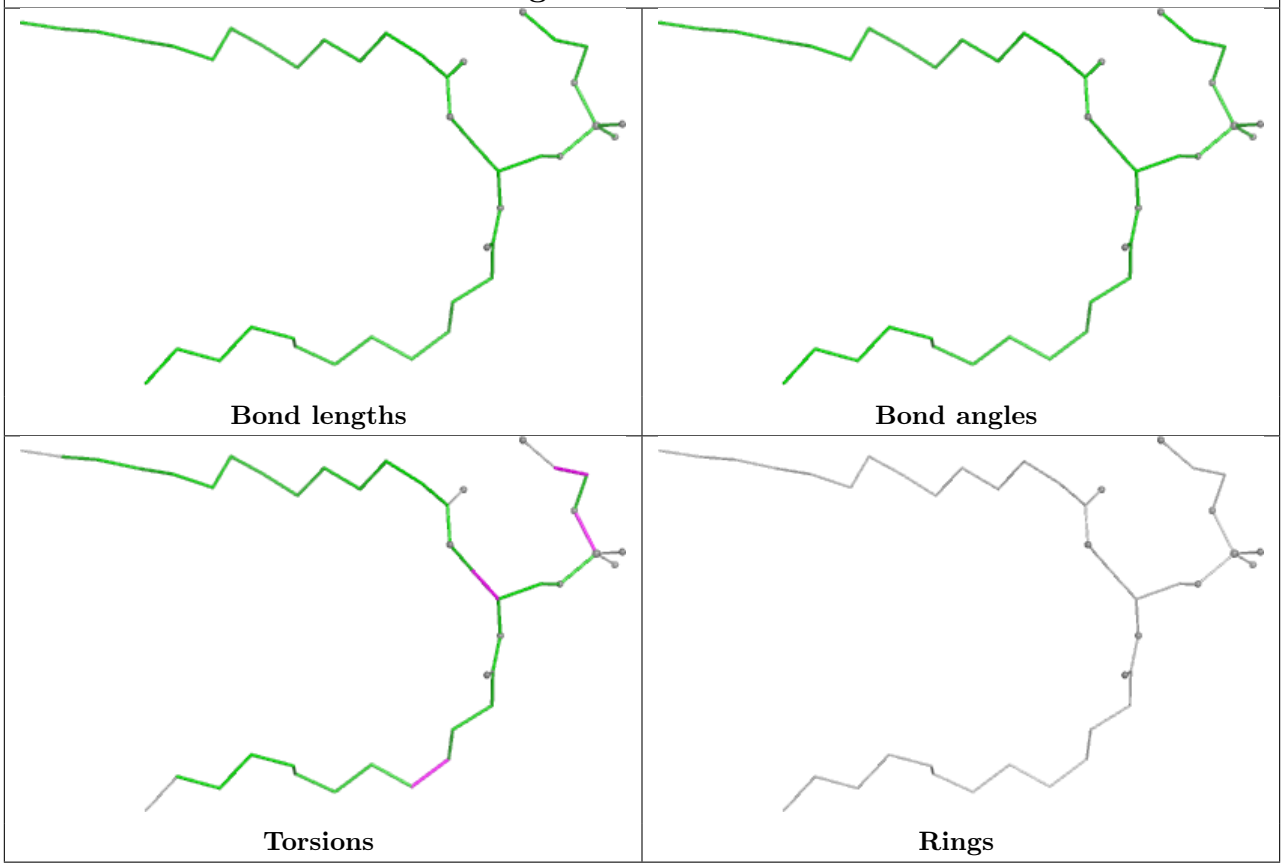


Rings

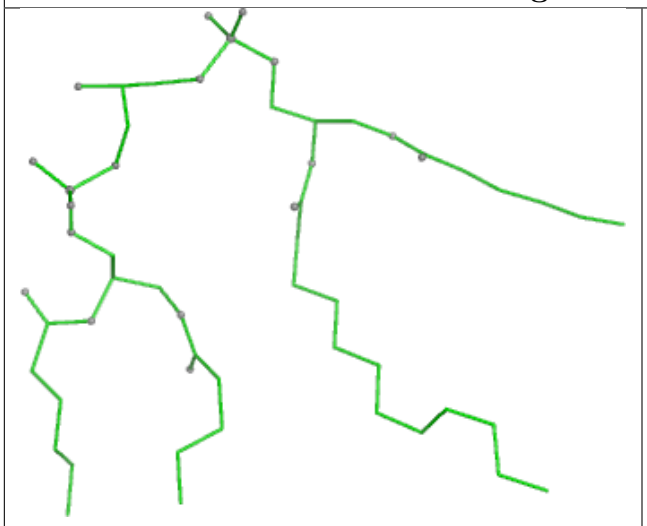
Ligand PC1 6 203



Ligand 3PE Y 403



Ligand CDL r 202



Bond lengths



Bond angles

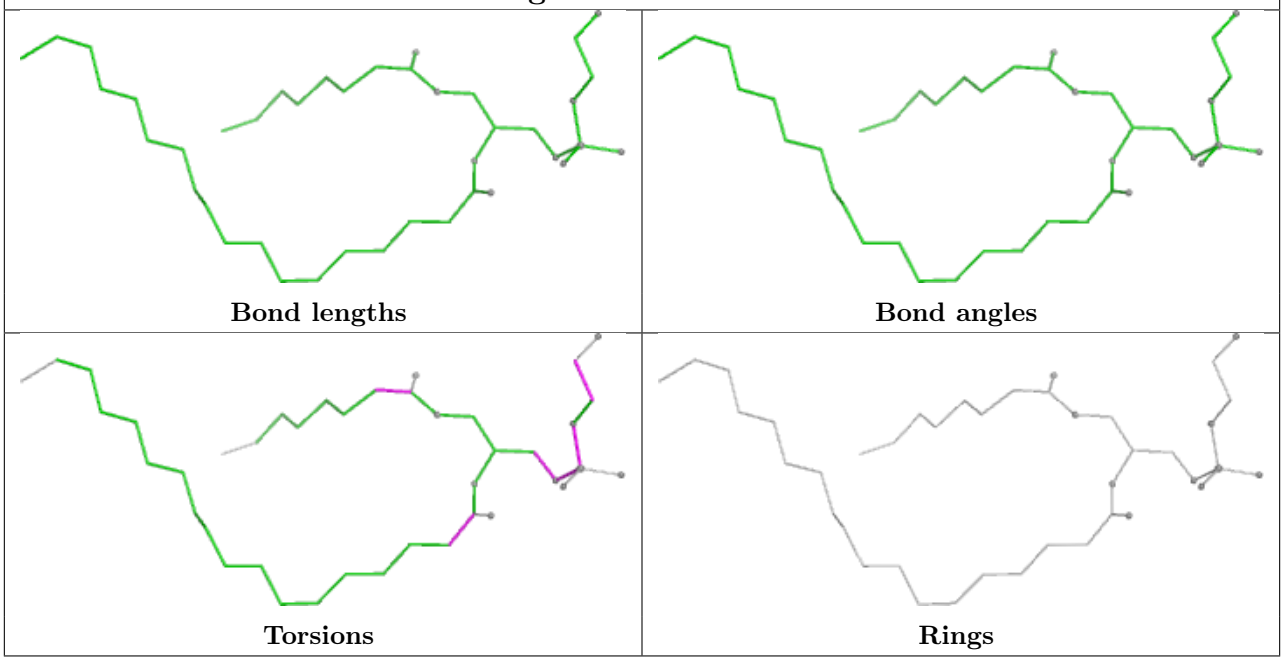


Torsions

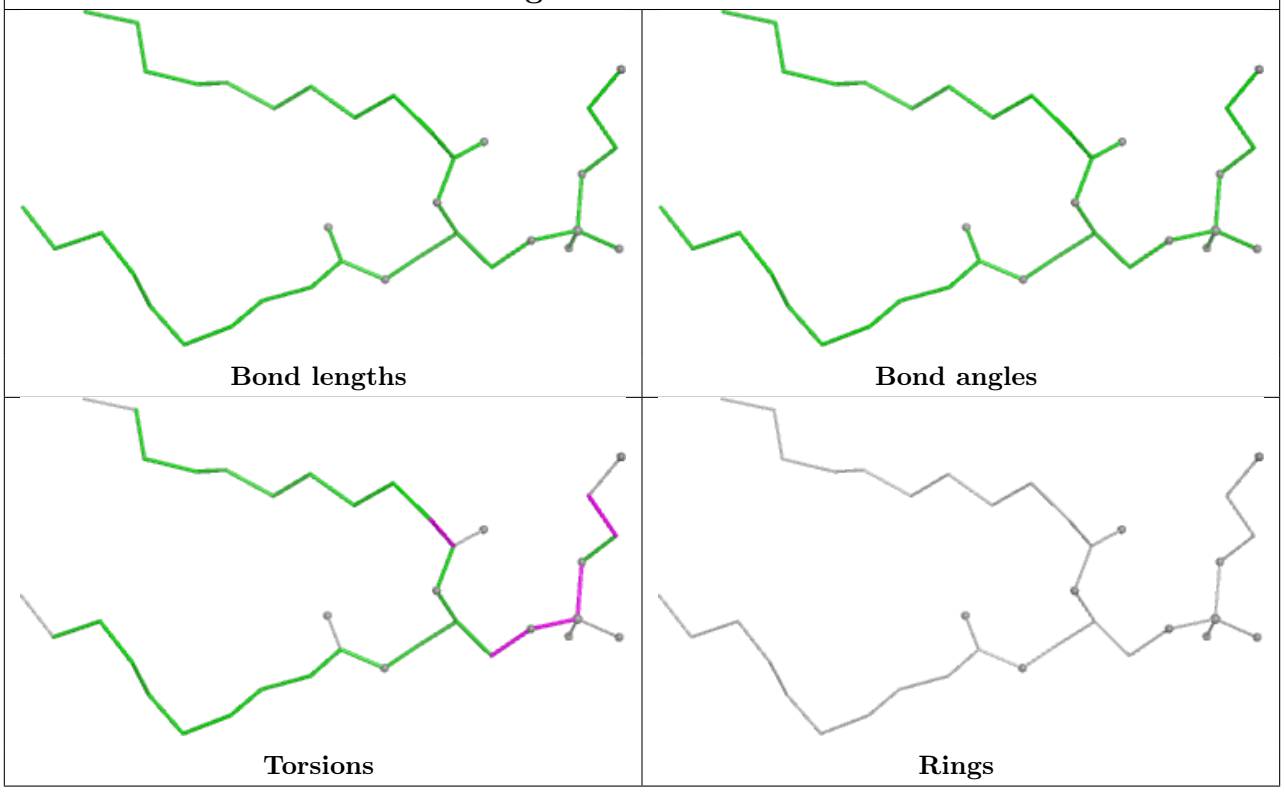


Rings

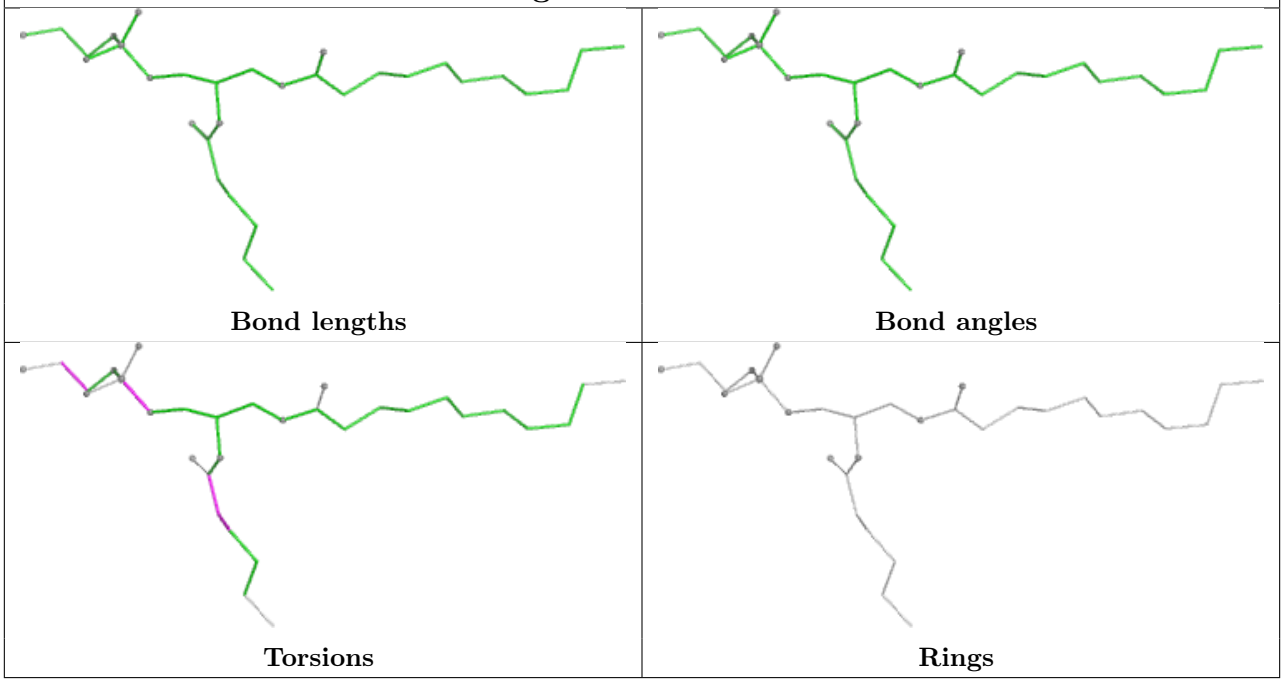
Ligand 3PE K 201



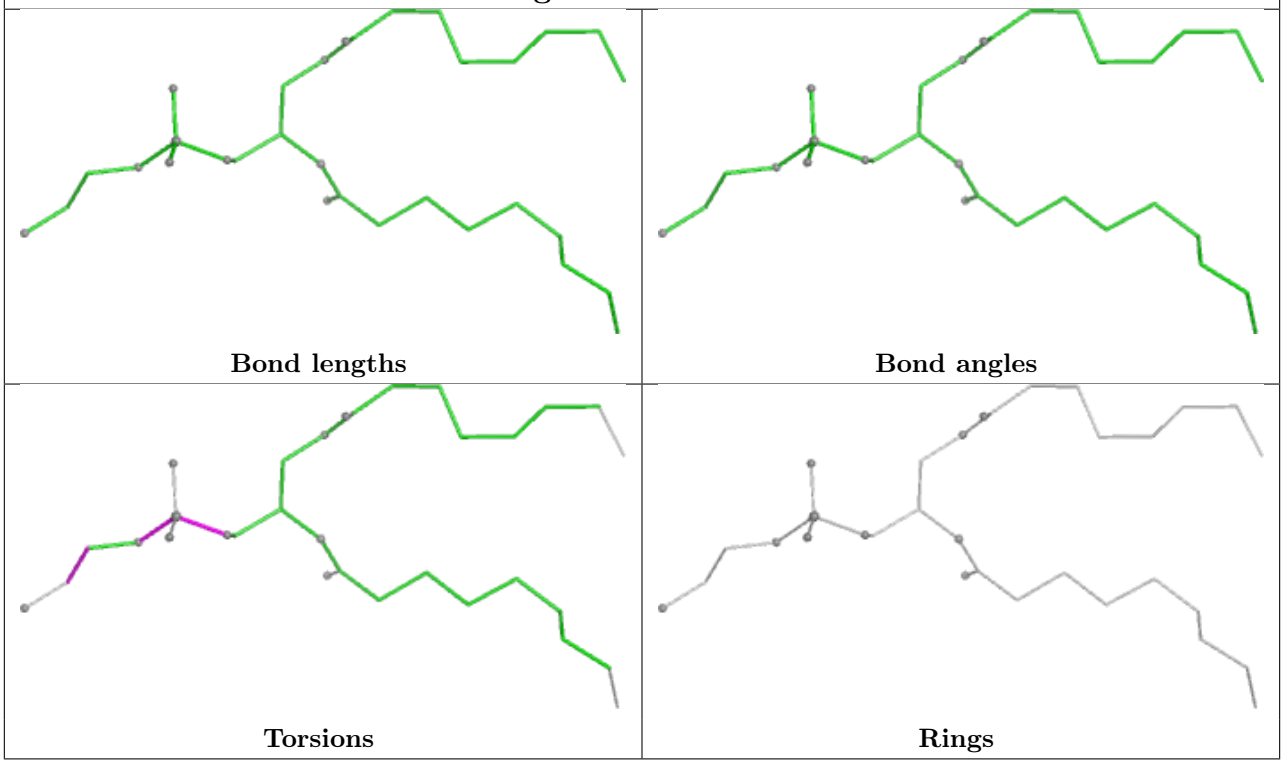
Ligand 3PE M 503



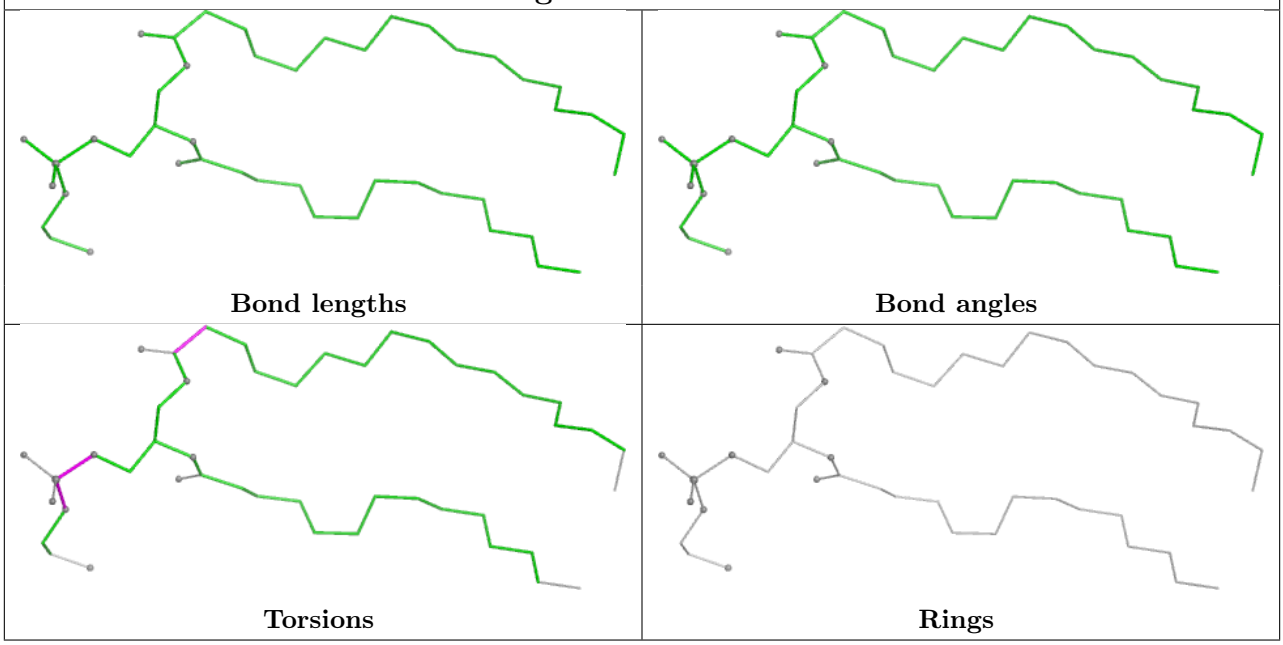
Ligand 3PE d 203



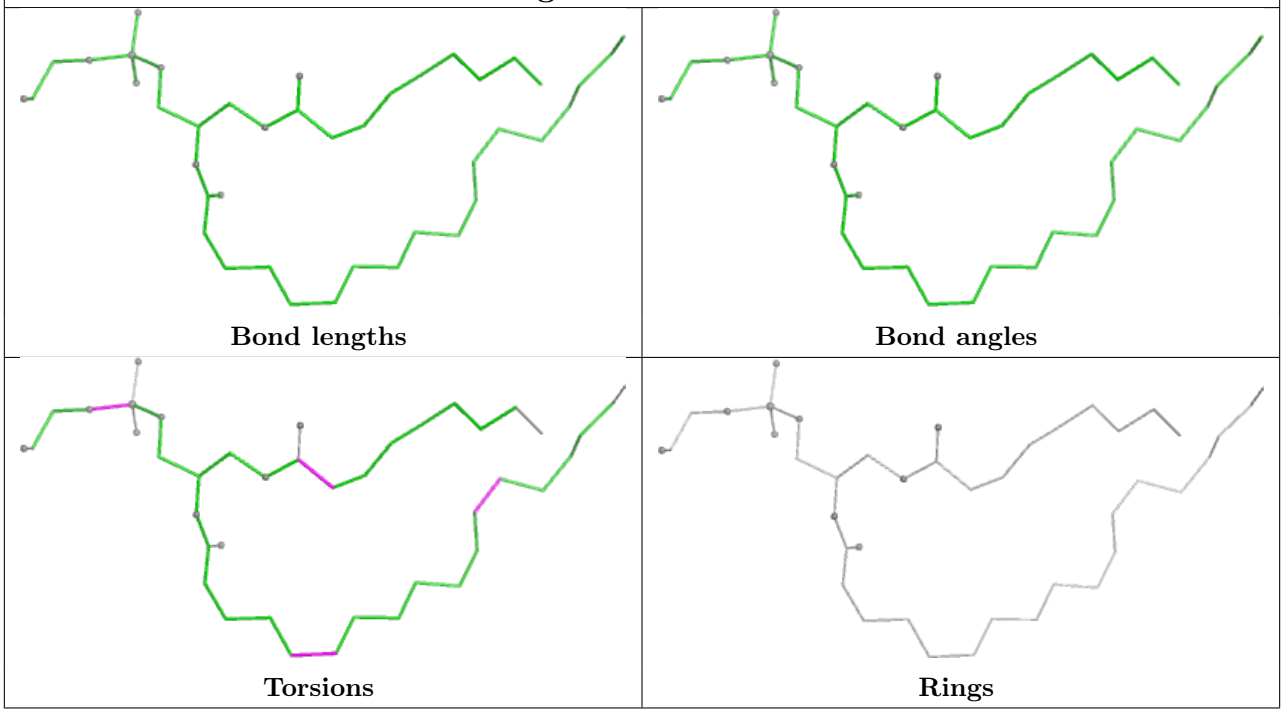
Ligand 3PE 6 202



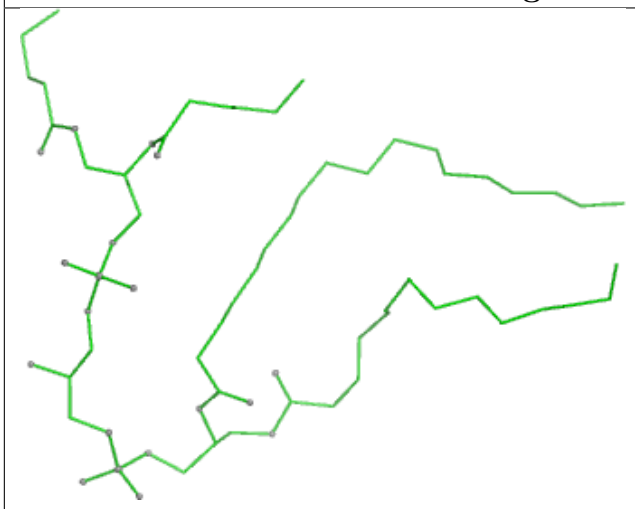
Ligand 3PE r 201



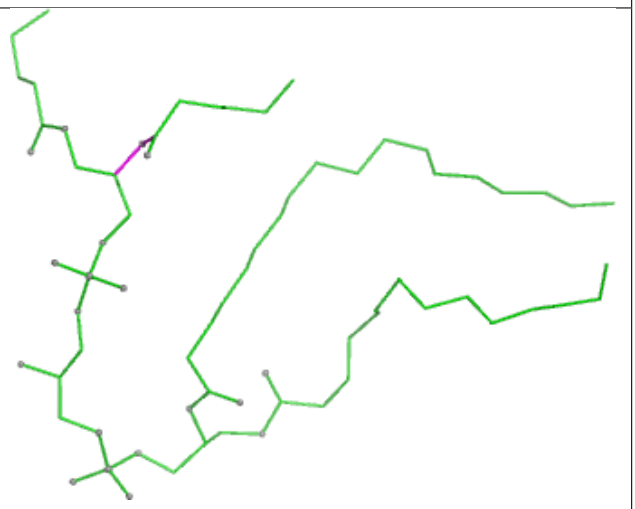
Ligand 3PE i 201



Ligand CDL m 201



Bond lengths



Bond angles

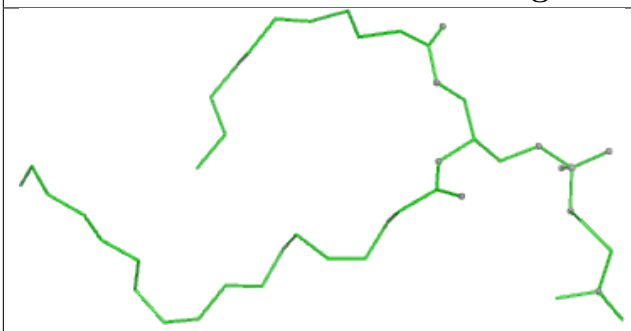


Torsions

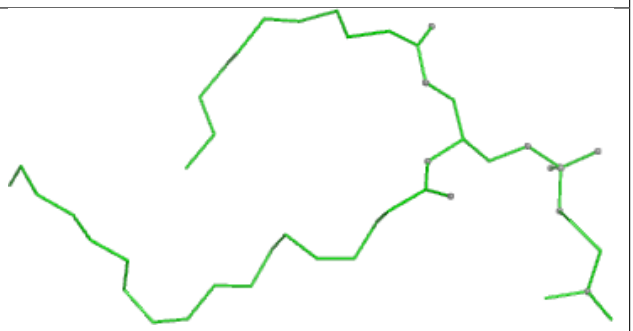


Rings

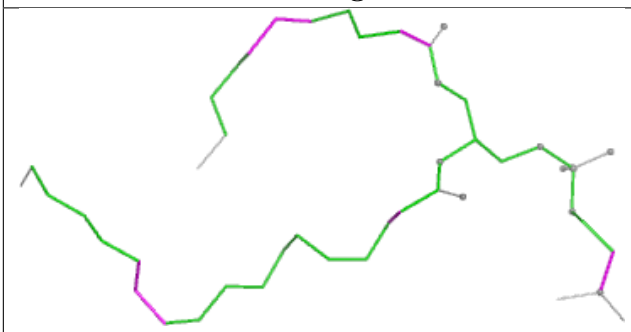
Ligand PC1 9 204



Bond lengths



Bond angles

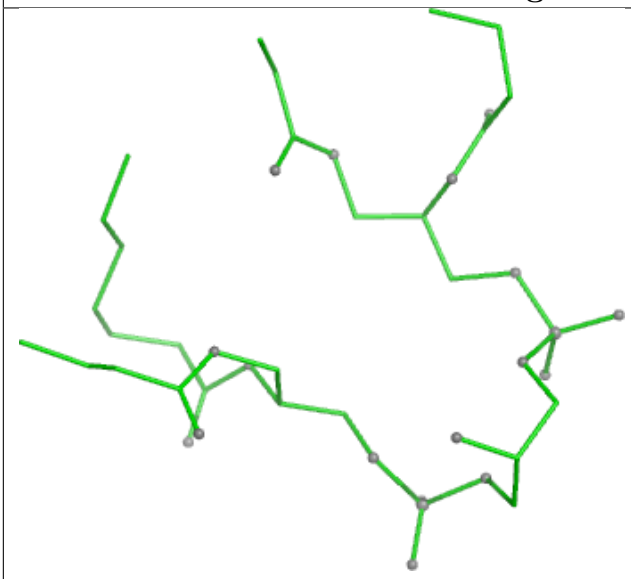


Torsions

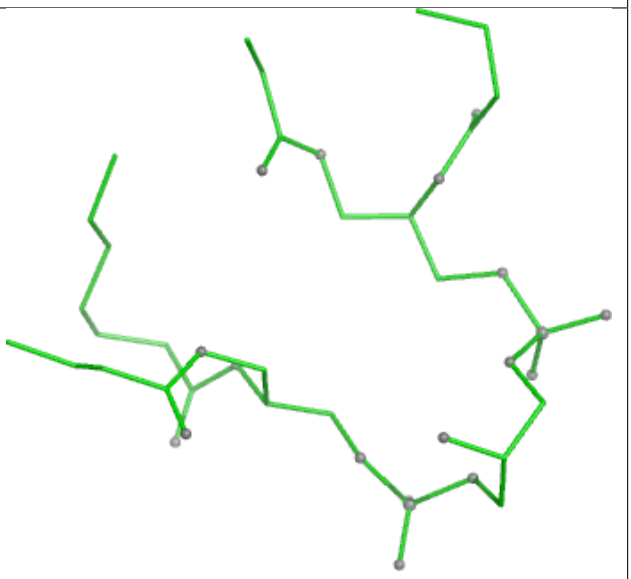


Rings

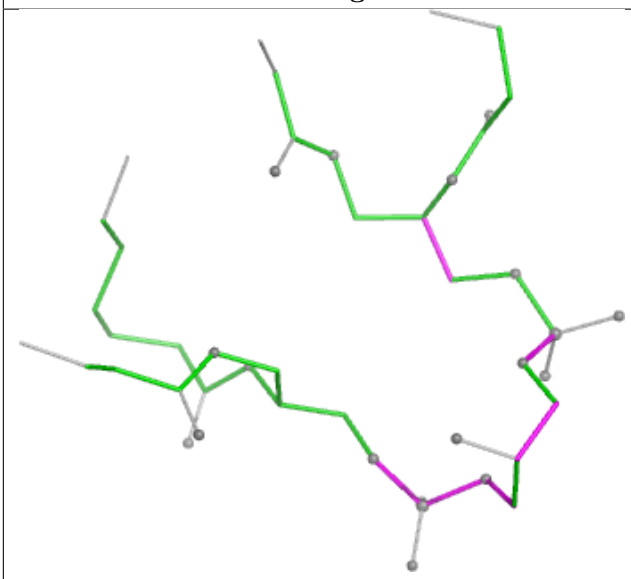
Ligand CDL L 703



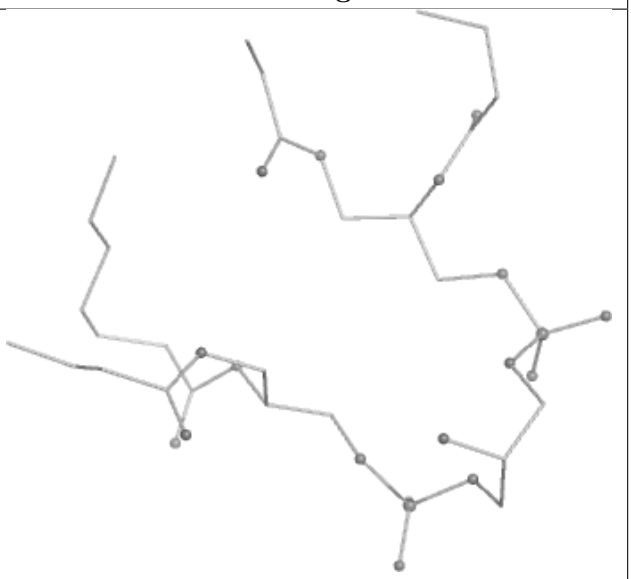
Bond lengths



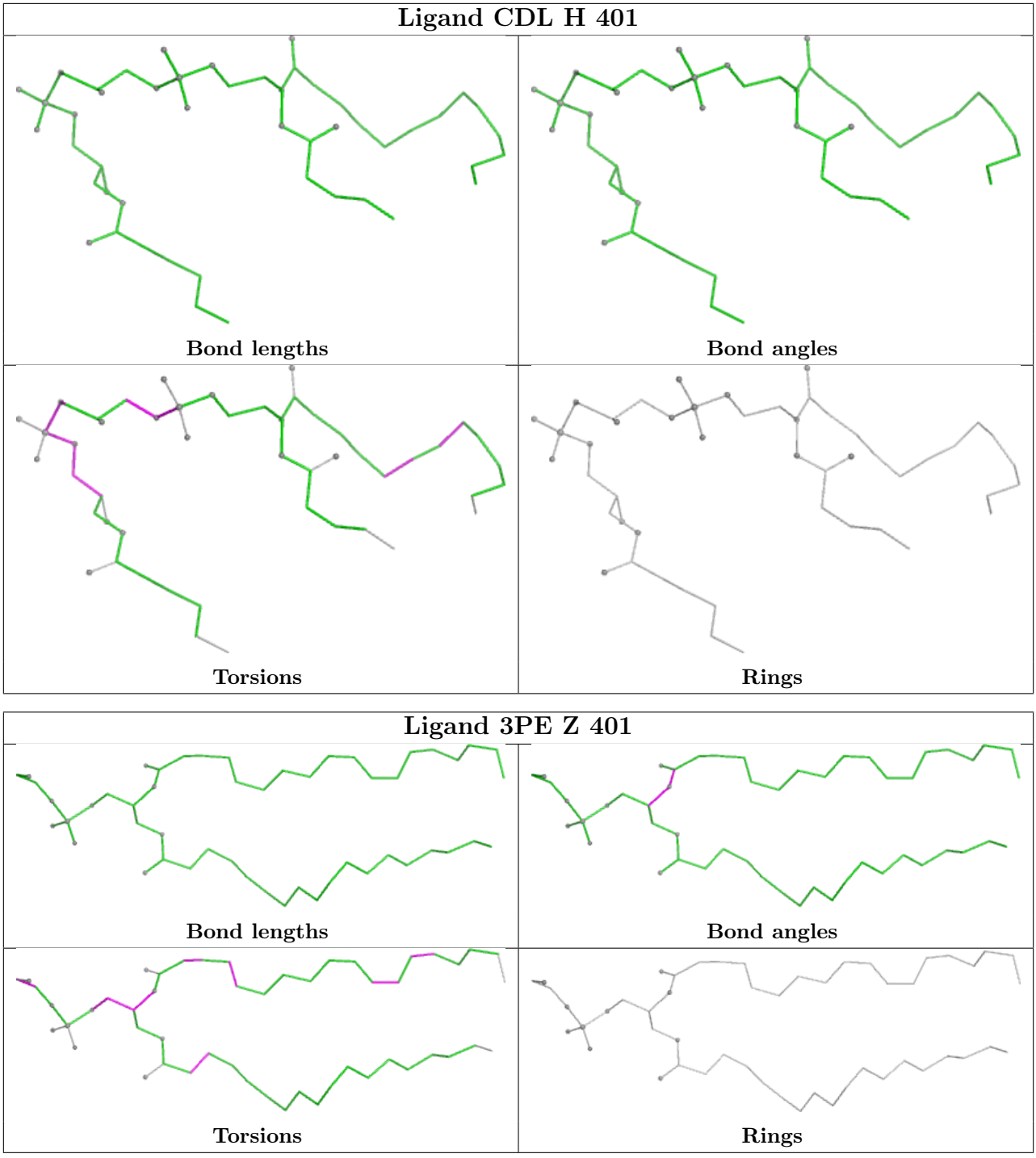
Bond angles



Torsions



Rings



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.

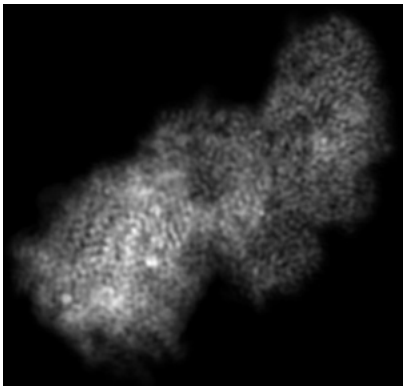
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19147. These allow visual inspection of the internal detail of the map and identification of artifacts.

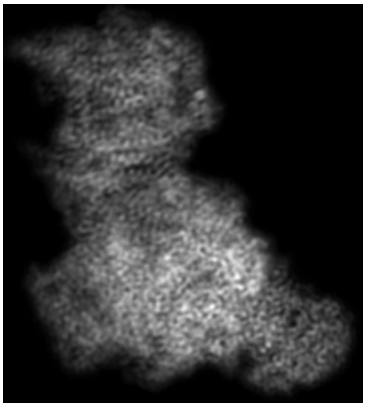
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

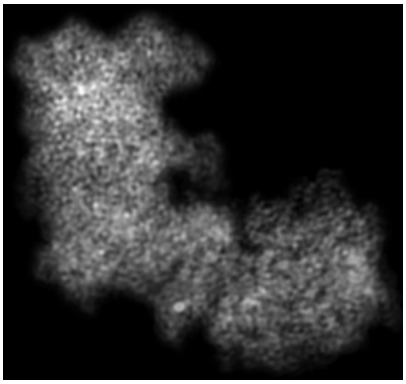
6.1.1 Primary map



X



Y

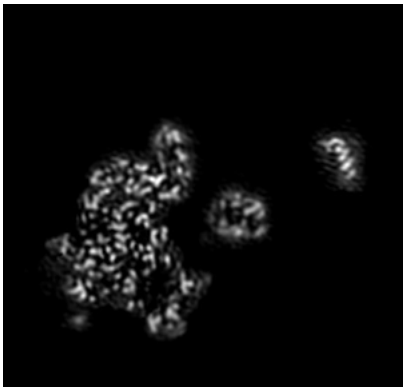


Z

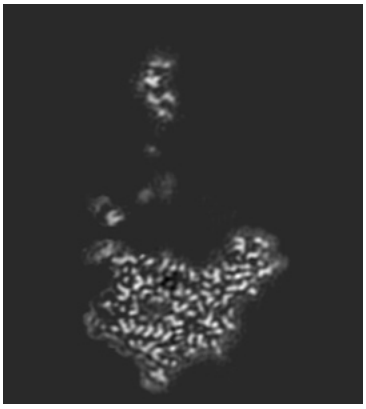
The images above show the map projected in three orthogonal directions.

6.2 Central slices

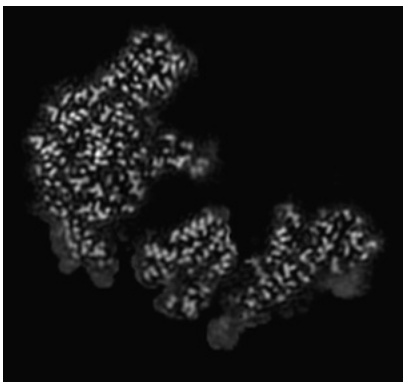
6.2.1 Primary map



X Index: 107



Y Index: 100

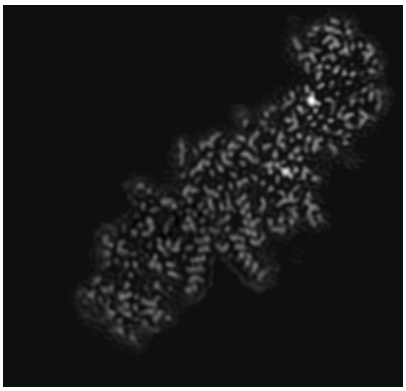


Z Index: 96

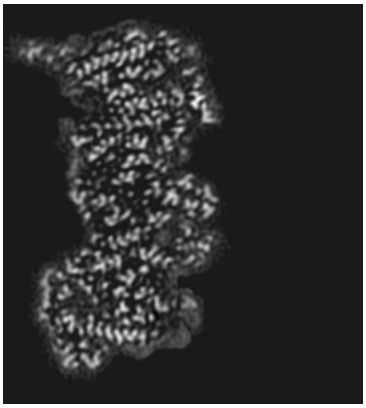
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

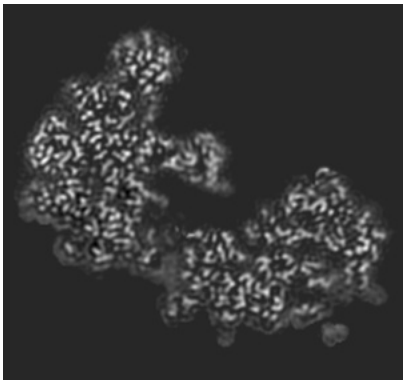
6.3.1 Primary map



X Index: 41



Y Index: 63

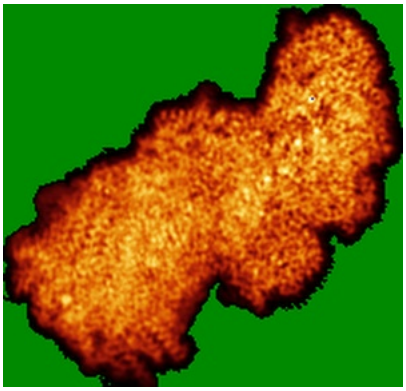


Z Index: 87

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

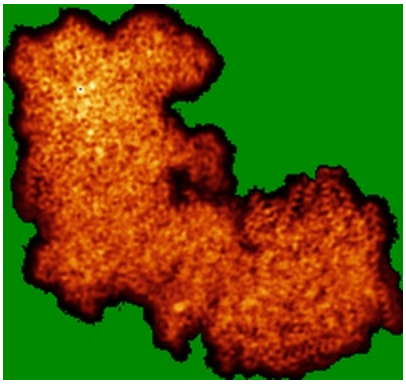
6.4.1 Primary map



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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

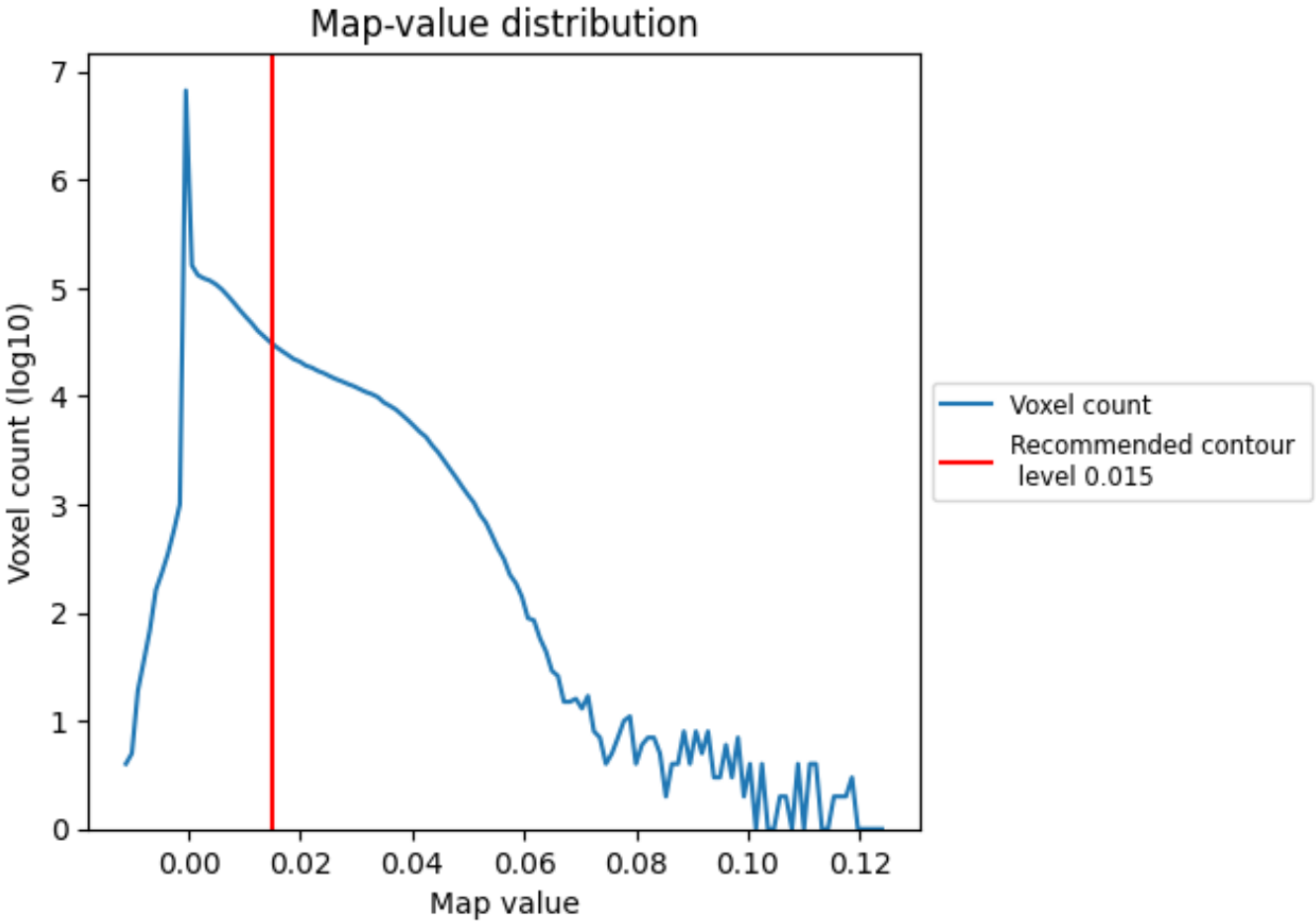
6.6 Mask visualisation (i)

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

7 Map analysis

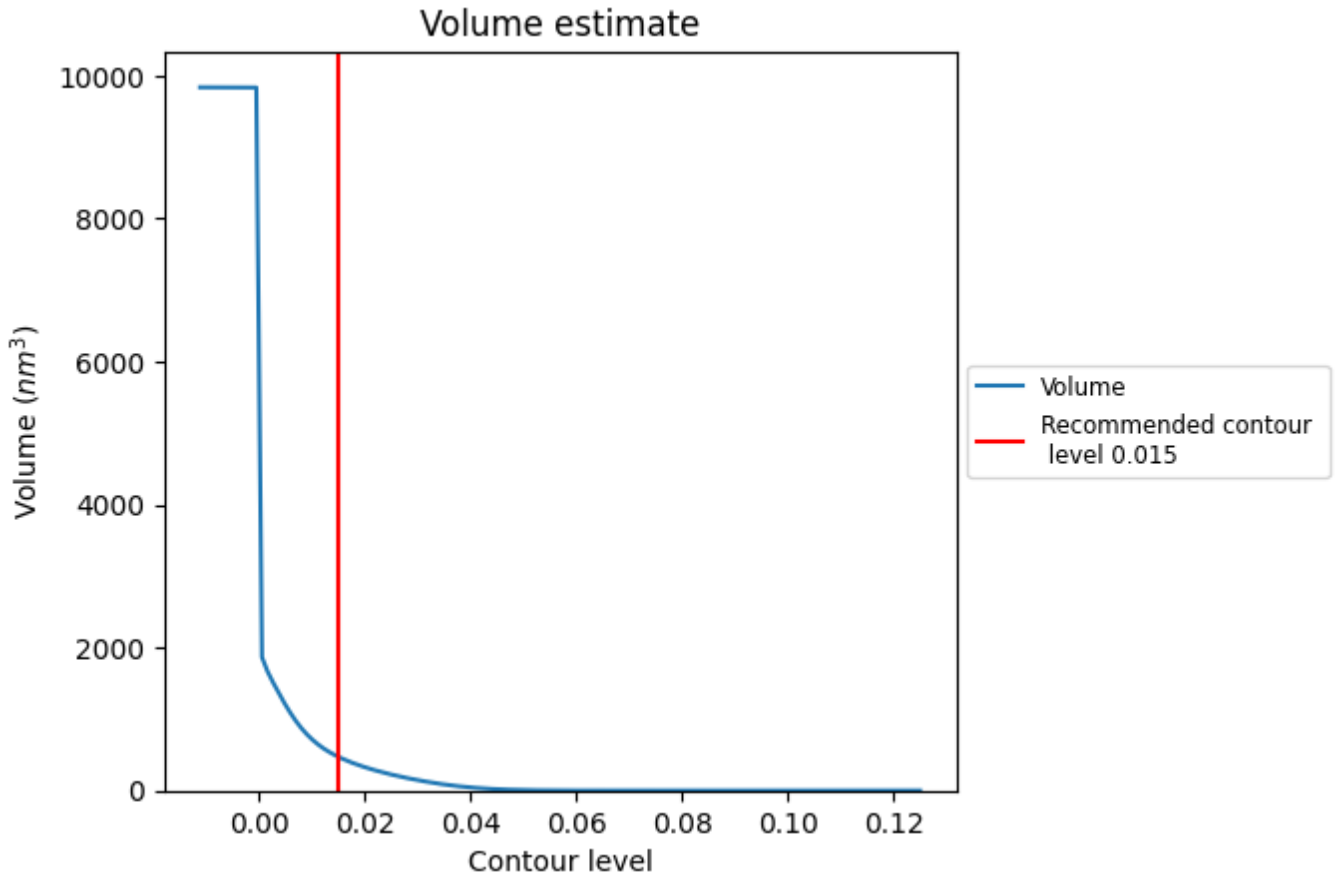
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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



The volume at the recommended contour level is 470 nm^3; this corresponds to an approximate mass of 425 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.

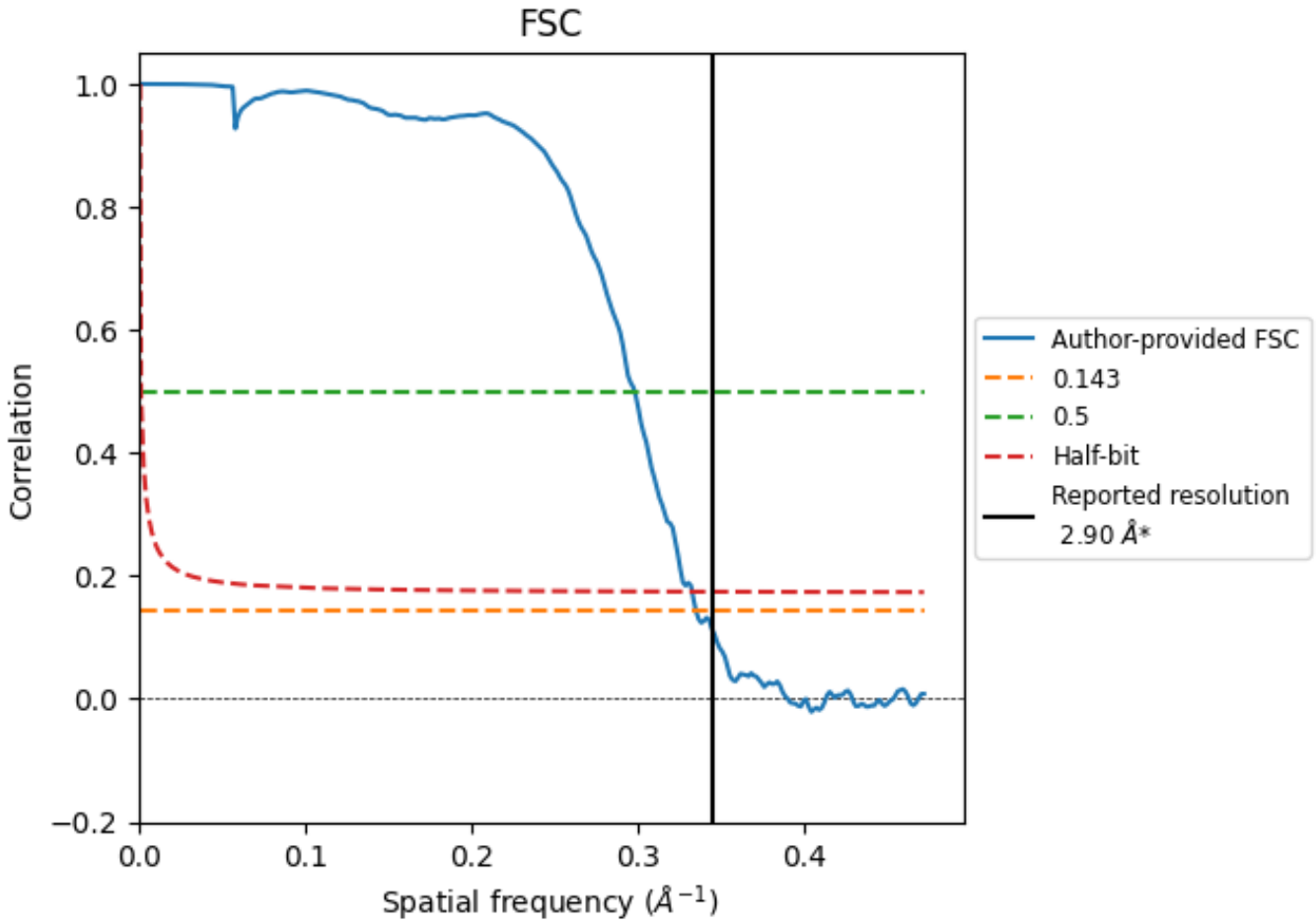
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

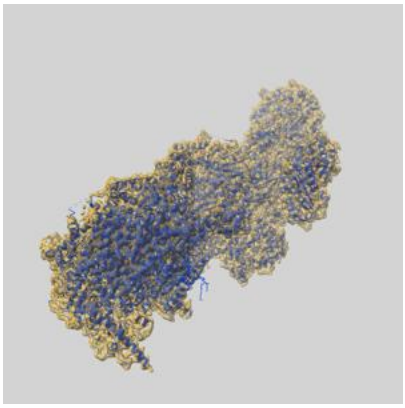
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.99	3.36	3.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

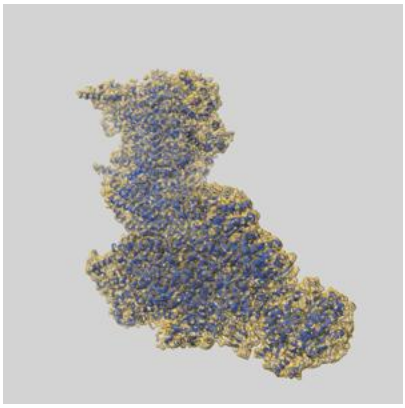
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19147 and PDB model 8RGR. Per-residue inclusion information can be found in section 3 on page 20.

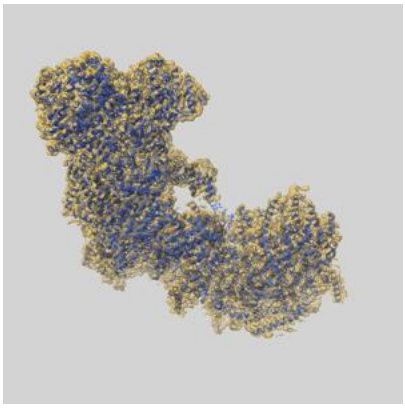
9.1 Map-model overlay



X



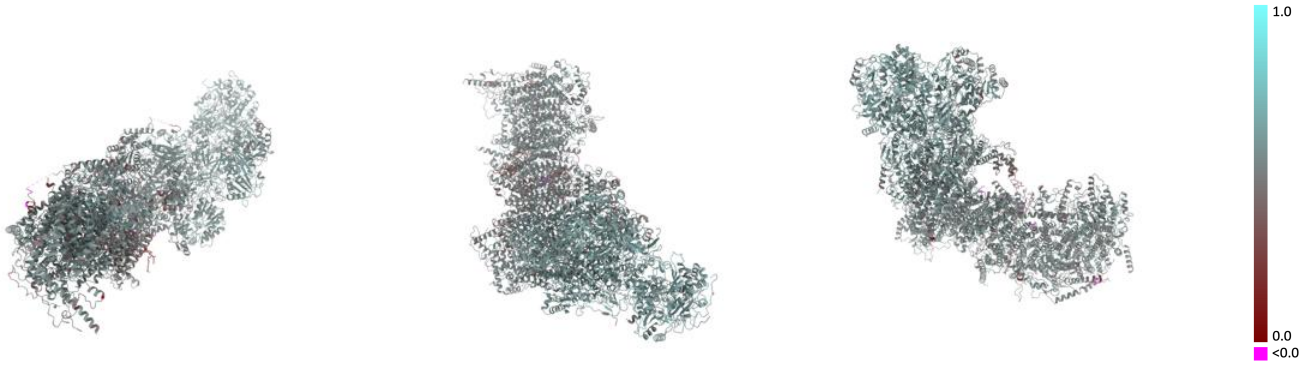
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

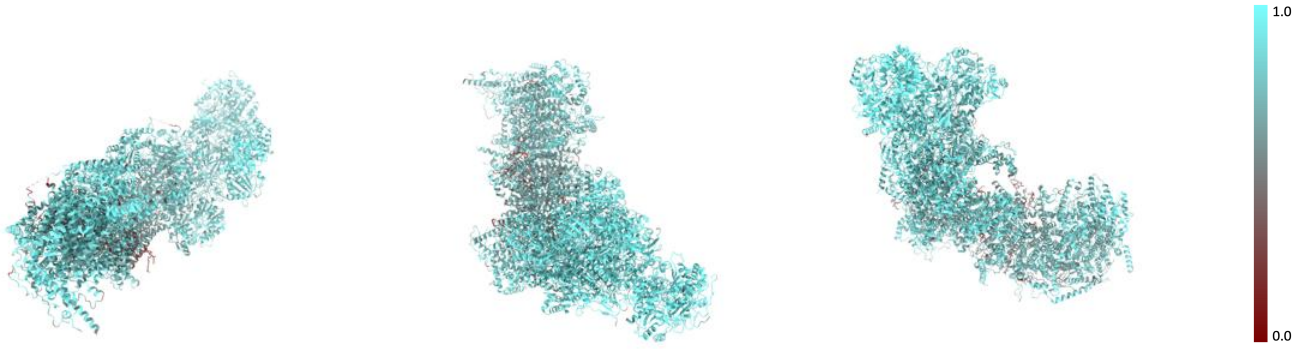
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

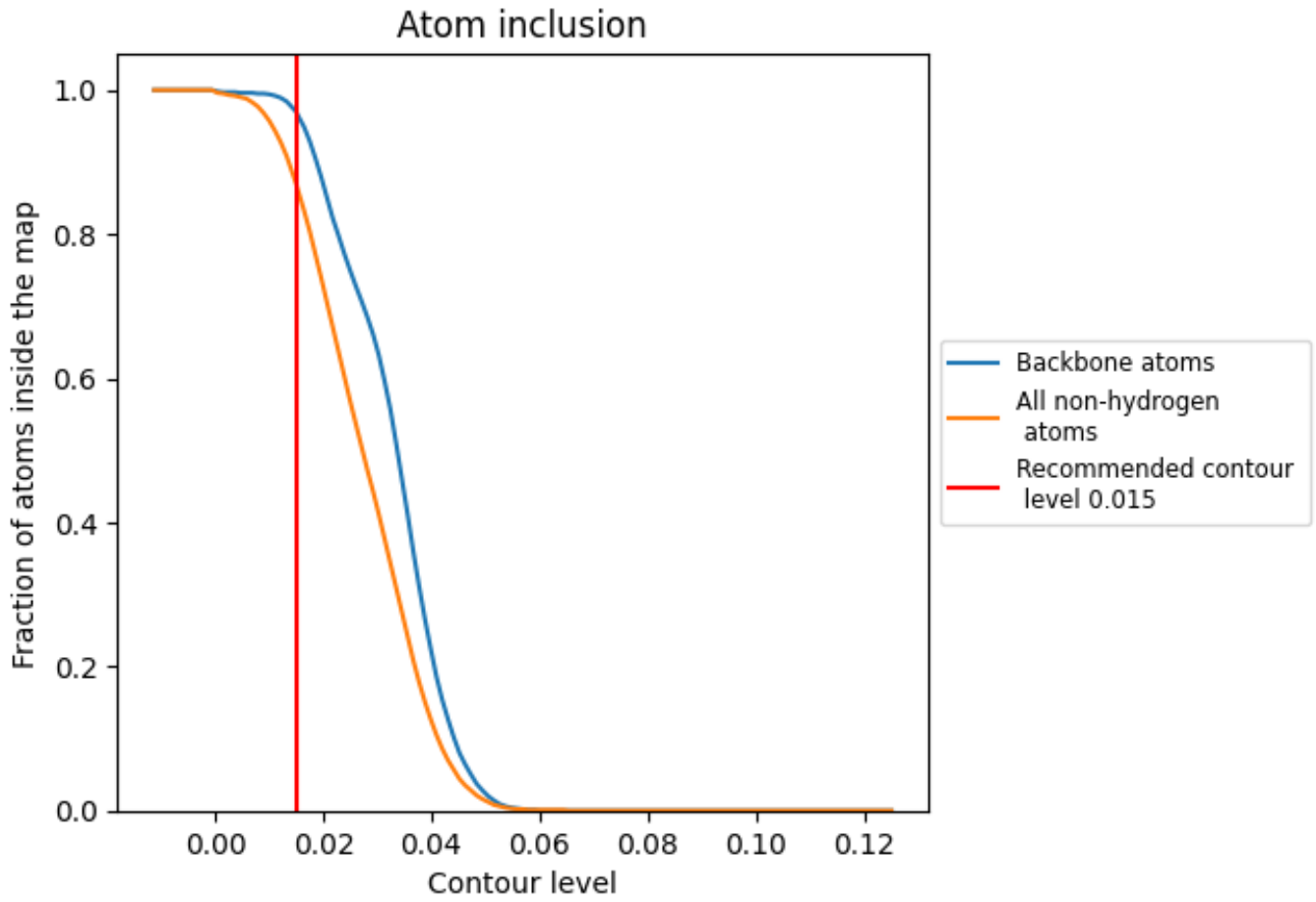
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.5450
1	0.9570	0.5860
2	0.9460	0.5790
3	0.9350	0.5810
6	0.9070	0.5730
7	0.9370	0.5870
9	0.9180	0.5830
A	0.8040	0.5400
C	0.9260	0.5820
D	0.8600	0.5450
H	0.8610	0.5450
J	0.7320	0.4960
K	0.7890	0.5290
L	0.8390	0.5340
M	0.8410	0.5460
N	0.8060	0.5360
O	0.8900	0.5340
P	0.9030	0.5650
Q	0.9040	0.5870
S	0.9320	0.5320
T	0.7780	0.4510
U	0.8690	0.5230
V	0.8990	0.5510
W	0.8940	0.5570
X	0.9030	0.5320
Y	0.6830	0.4630
Z	0.8700	0.5390
a	0.8860	0.5440
b	0.8640	0.5200
c	0.8220	0.5100
d	0.8070	0.5290
e	0.8520	0.5340
f	0.7970	0.5070
g	0.8320	0.5050
h	0.8770	0.5330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.7880	0.4800
j	0.8500	0.4990
k	0.8930	0.5230
l	0.8650	0.5430
m	0.7550	0.4960
n	0.8790	0.5320
o	0.8490	0.5000
p	0.8960	0.5300
q	0.9390	0.5790
r	0.8610	0.5560
s	0.9090	0.5610