Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 01:19 pm GMT

PDB ID	:	9R15 / pdb_00009r15
EMDB ID	:	EMD-53498
Title	:	Bovine complex I at pH 9.2 in the deactive state (consensus)
Authors	:	Fisher, W.; Grba, D.N.; Hirst, J.
Deposited on	:	2025-04-25
Resolution	:	2.31 Å(reported)
Based on initial model	:	7QSN

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:

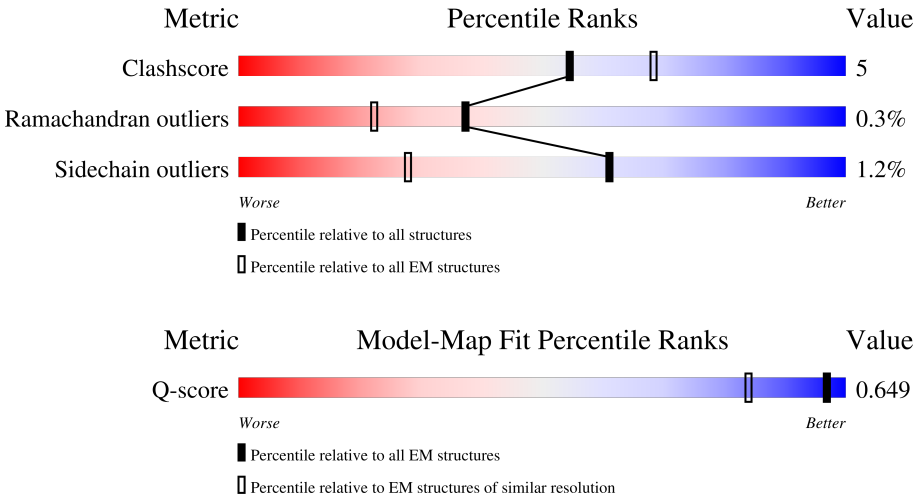
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 2.31 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.



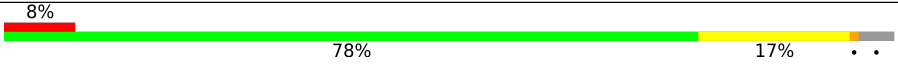
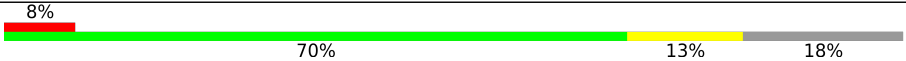
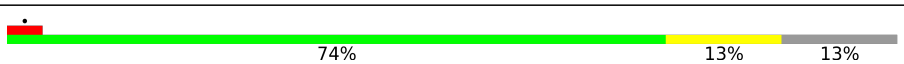
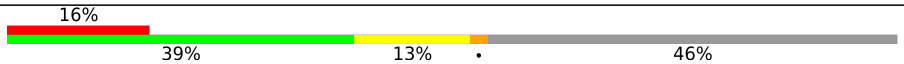
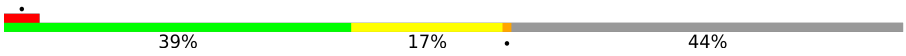
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4306 (1.81 - 2.81)

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	A	115	7%, 69%, 23%, 8%
2	B	216	62%, 9%, 28%
3	C	266	71%, 6%, 22%
4	D	463	82%, 10%, 8%

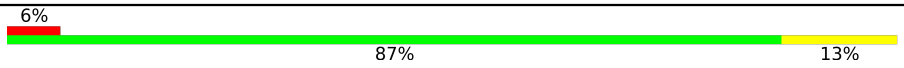
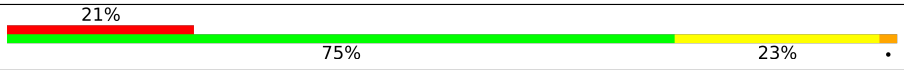
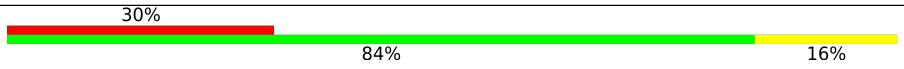
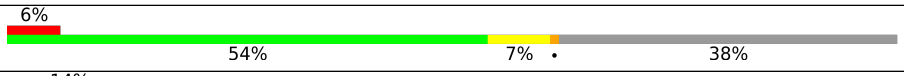
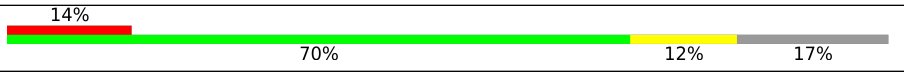
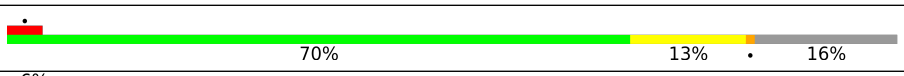
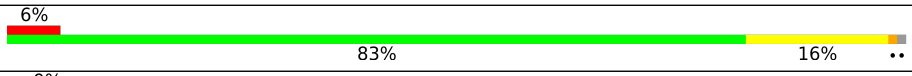
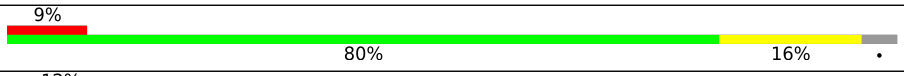
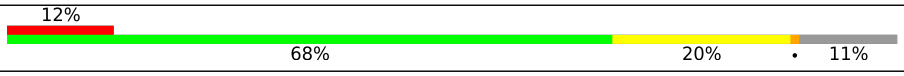
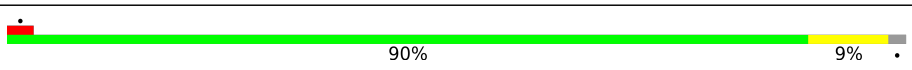
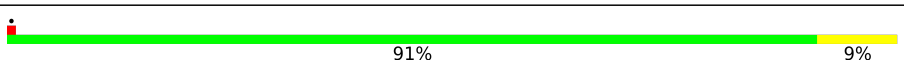
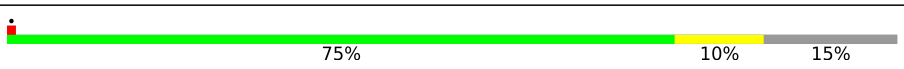
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 70327 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	106	852	578	124	145	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1248	795	225	214	14	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	426	3429	2190	592	622	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	1	0
			3336	2102	597	617	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	1	0
			2519	1687	388	421	23		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	168	Total	C	N	O	S	0	0
			1278	859	182	225	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	603	Total	C	N	O	S	0	0
			4775	3178	733	821	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	5	0
			3694	2461	578	616	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	1	0
			2739	1822	417	457	43		

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	313	Total	C	N	O	S	0	0
			2492	1604	445	438	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	141	Total	C	N	O	S	0	0
			1030	657	176	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	ACE	-	acetylation	UNP Q8HXG6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	121	Total	C	N	O	S	0	0
			999	650	172	172	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	ACE	-	acetylation	UNP Q02827

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	128	Total	C	N	O	S	0	0
			1097	722	191	183	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	0	ACE	-	acetylation	UNP Q02367

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	128	Total	C	N	O	0	0
			1067	684	188	195		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	1	0
			1498	958	276	257	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1450	909	268	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

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

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

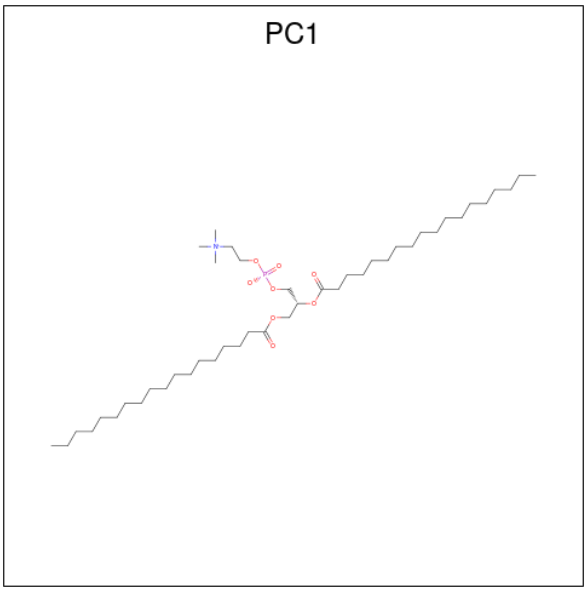
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	0	ACE	-	acetylation	UNP Q05752

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

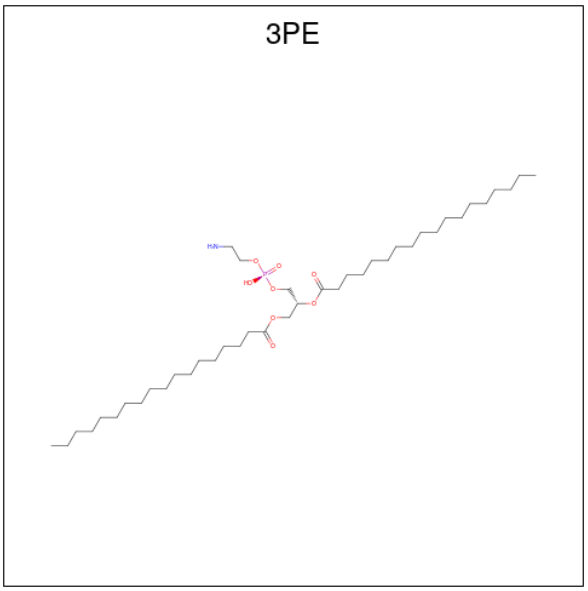
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

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



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

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



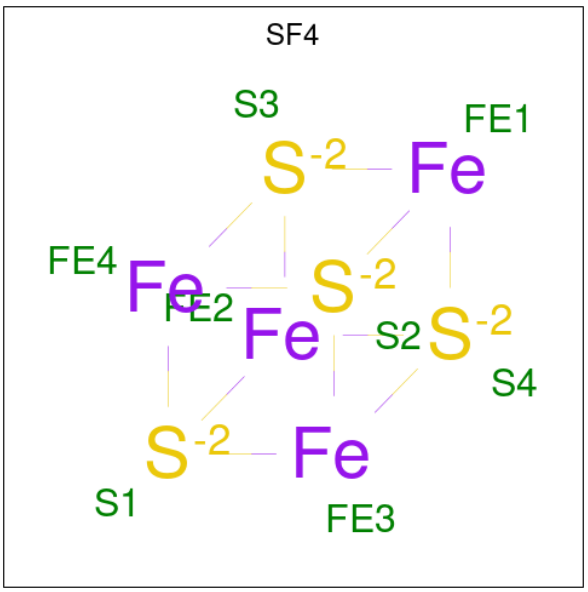
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	L	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	M	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	O	1	Total	C	N	O	P	0
			36	26	1	8	1	

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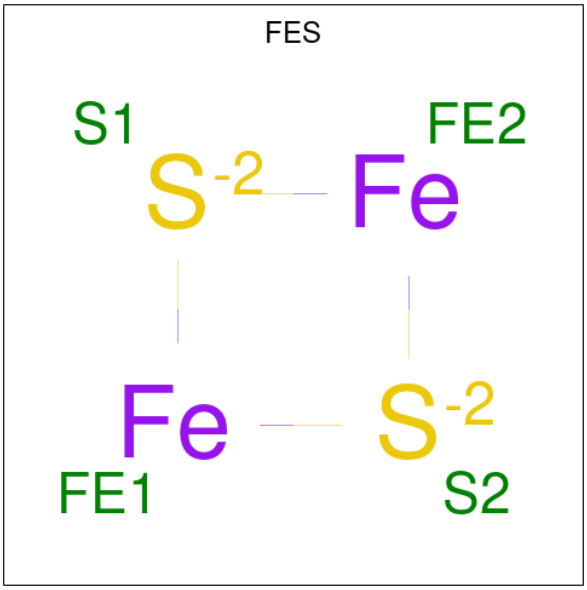
Mol	Chain	Residues	Atoms					AltConf
46	O	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	Y	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	b	1	Total	C	N	O	P	0
			51	41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

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



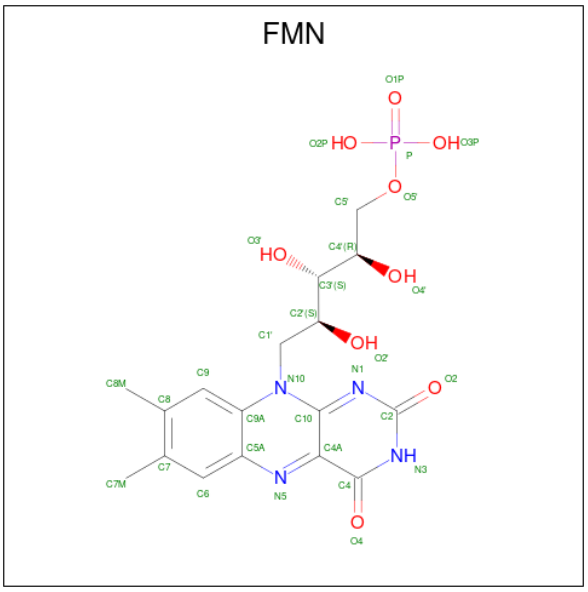
Mol	Chain	Residues	Atoms	AltConf
47	B	1	Total Fe S 8 4 4	0
47	F	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	G	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0
47	I	1	Total Fe S 8 4 4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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

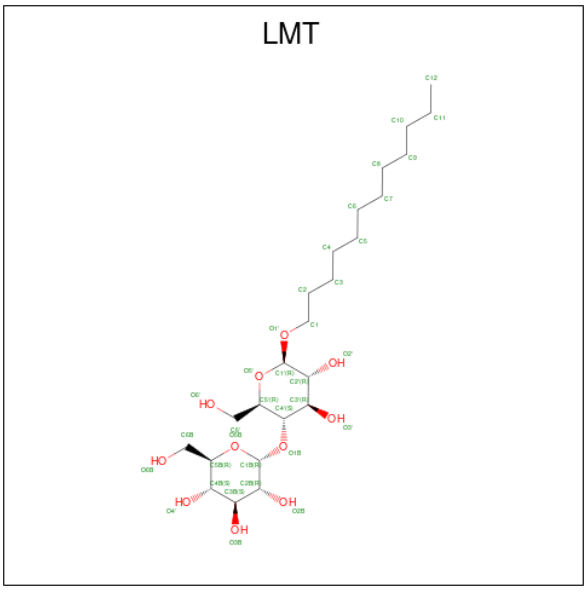


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

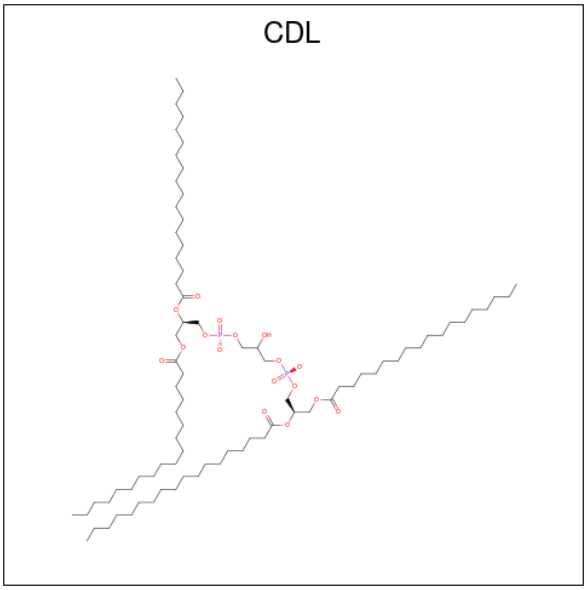
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
51	H	1	Total C O 35 24 11	0
51	L	1	Total C O 35 24 11	0
51	M	1	Total C O 35 24 11	0
51	Y	1	Total C O 35 24 11	0
51	Y	1	Total C O 35 24 11	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

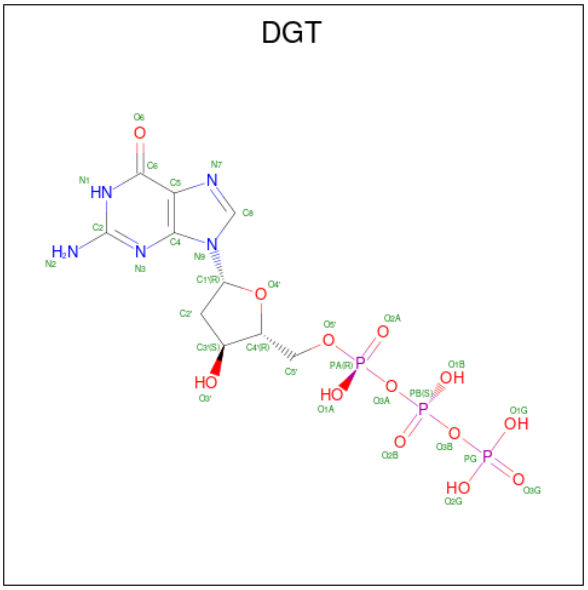


Mol	Chain	Residues	Atoms	AltConf
52	L	1	Total C O P 79 60 17 2	0
52	N	1	Total C O P 85 66 17 2	0
52	X	1	Total C O P 86 67 17 2	0
52	d	1	Total C O P 65 46 17 2	0
52	h	1	Total C O P 68 49 17 2	0
52	q	1	Total C O P 64 45 17 2	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

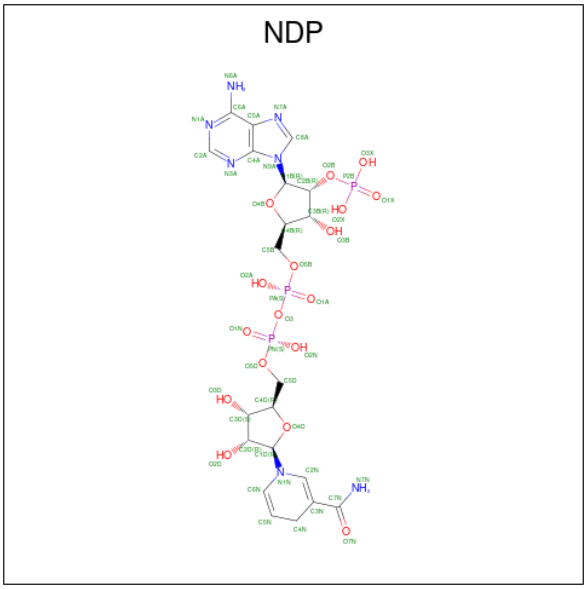
Mol	Chain	Residues	Atoms		AltConf
53	O	1	Total	Mg	0
			1	1	

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



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

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

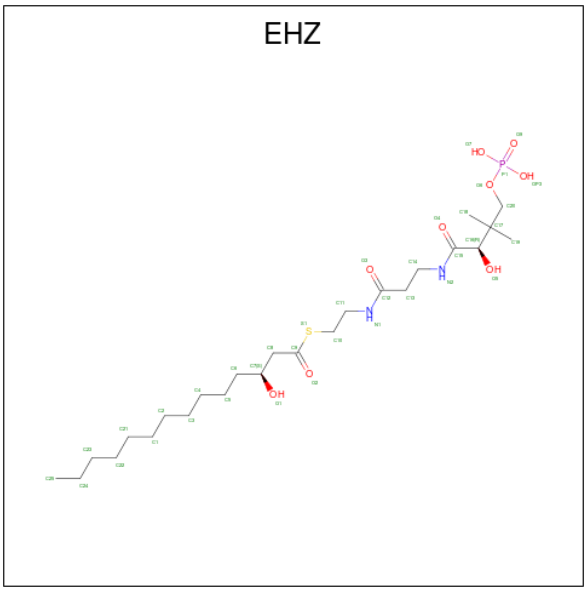


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

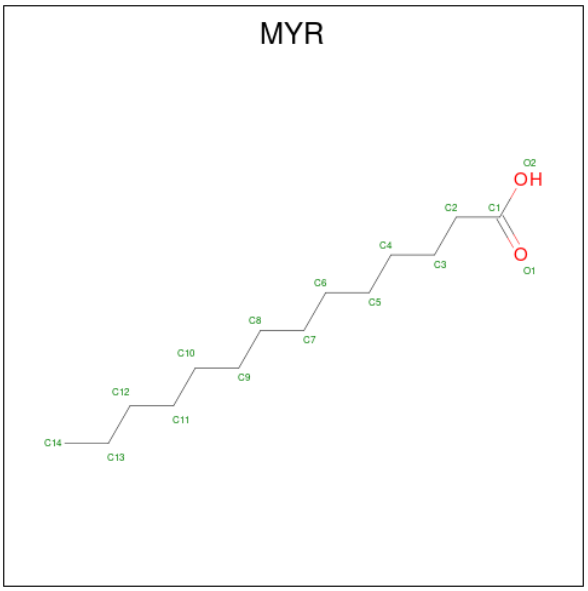
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

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



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

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	A	11	Total O 11 11	0
59	B	47	Total O 47 47	0
59	C	81	Total O 81 81	0
59	D	158	Total O 158 158	0
59	E	24	Total O 24 24	0
59	F	83	Total O 83 83	0
59	G	230	Total O 230 230	0
59	H	83	Total O 83 83	0
59	I	85	Total O 85 85	0
59	J	23	Total O 23 23	0
59	K	16	Total O 16 16	0

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Mol	Chain	Residues	Atoms	AltConf
59	L	133	Total O 133 133	0
59	M	125	Total O 125 125	0
59	N	81	Total O 81 81	0
59	O	38	Total O 38 38	0
59	P	55	Total O 55 55	0
59	Q	76	Total O 76 76	0
59	R	24	Total O 24 24	0
59	S	6	Total O 6 6	0
59	T	3	Total O 3 3	0
59	U	21	Total O 21 21	0
59	V	17	Total O 17 17	0
59	W	10	Total O 10 10	0
59	X	38	Total O 38 38	0
59	Y	6	Total O 6 6	0
59	Z	33	Total O 33 33	0
59	a	16	Total O 16 16	0
59	b	16	Total O 16 16	0
59	c	1	Total O 1 1	0
59	d	36	Total O 36 36	0
59	e	26	Total O 26 26	0
59	f	6	Total O 6 6	0

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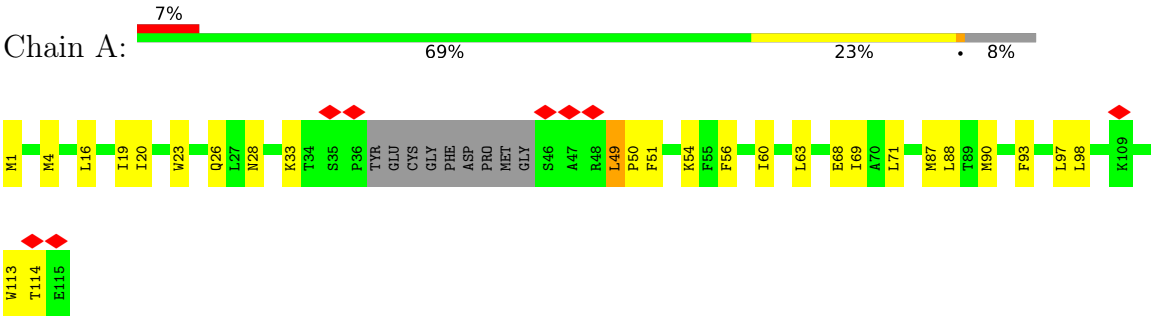
Mol	Chain	Residues	Atoms	AltConf
59	g	30	Total O 30 30	0
59	h	38	Total O 38 38	0
59	i	10	Total O 10 10	0
59	j	4	Total O 4 4	0
59	k	6	Total O 6 6	0
59	l	33	Total O 33 33	0
59	m	18	Total O 18 18	0
59	n	52	Total O 52 52	0
59	o	19	Total O 19 19	0
59	p	45	Total O 45 45	0
59	q	27	Total O 27 27	0
59	r	18	Total O 18 18	0
59	s	8	Total O 8 8	0

3 Residue-property plots (i)

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

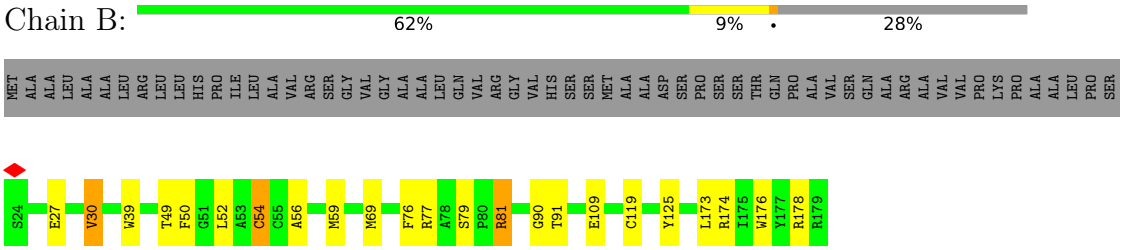
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



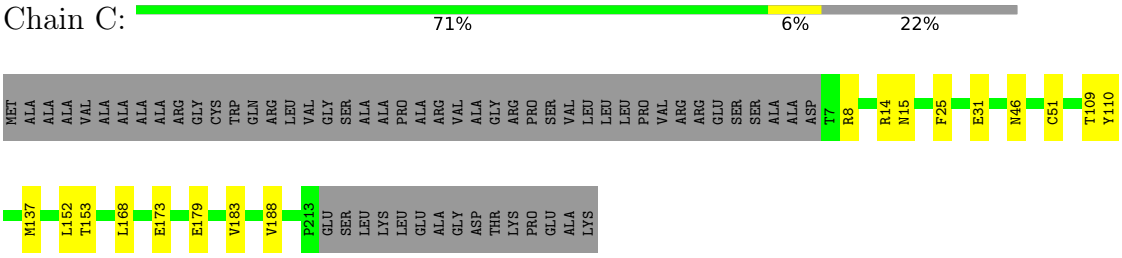
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



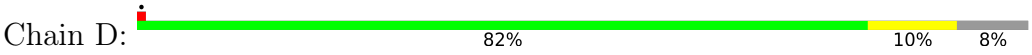
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

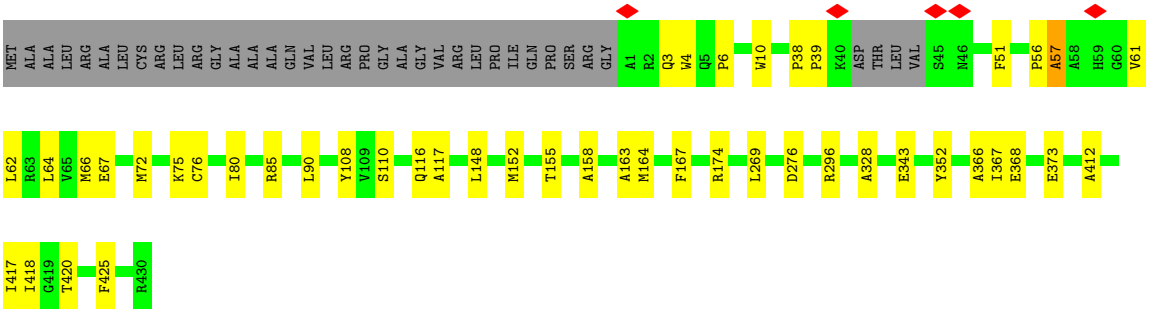
Chain C:



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

Chain D:

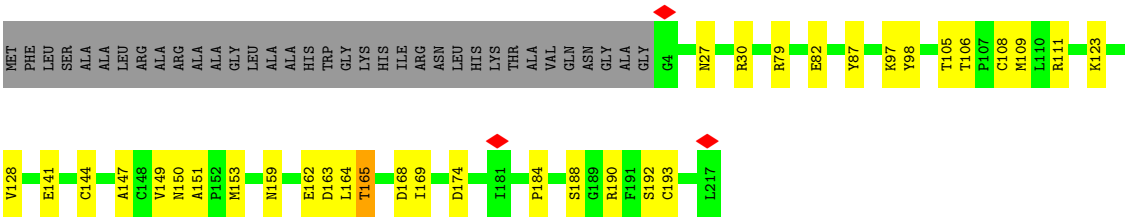




• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

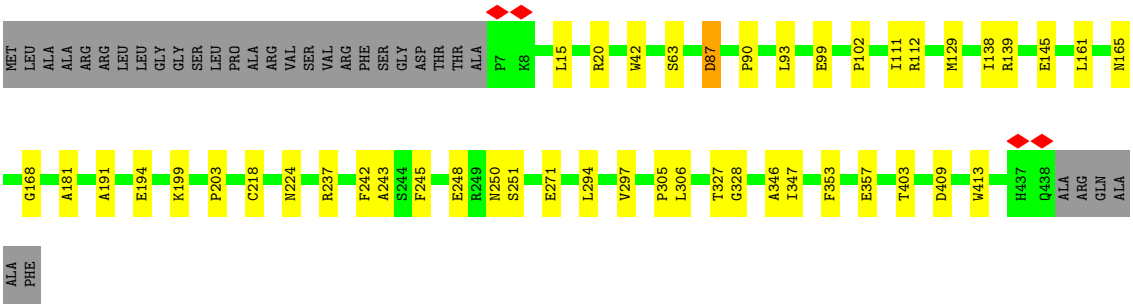




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

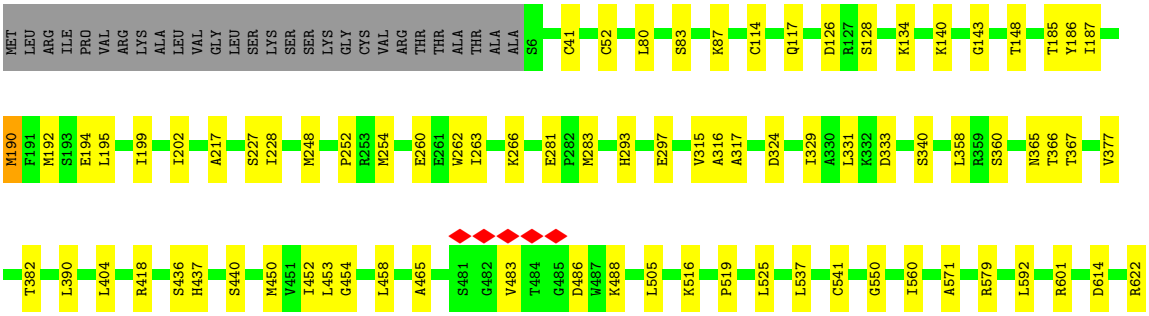


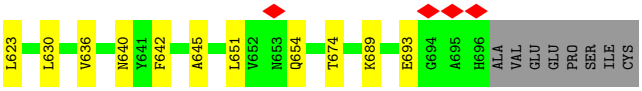


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

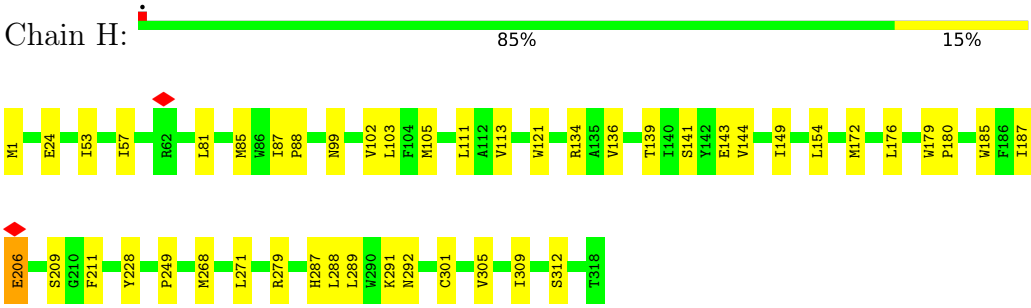
Chain G:



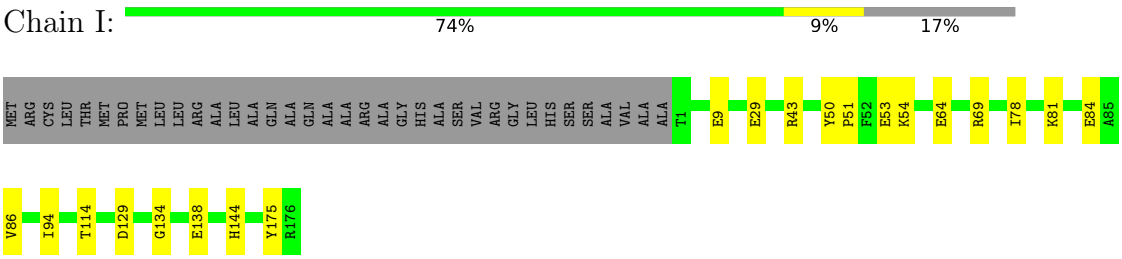




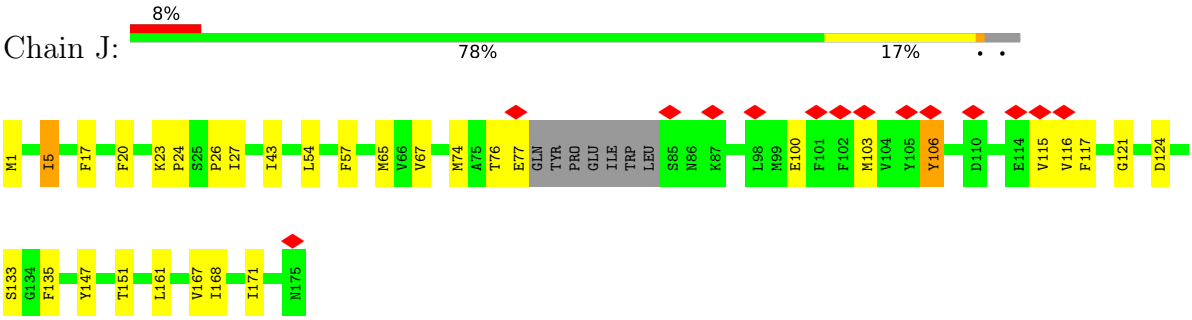
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



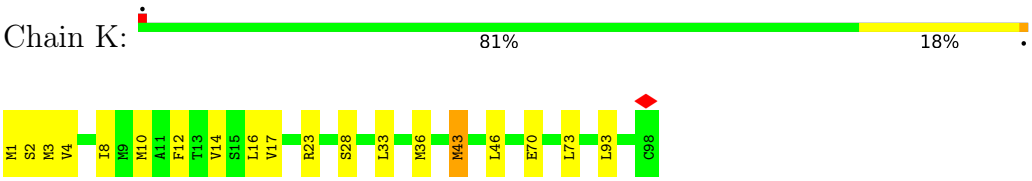
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



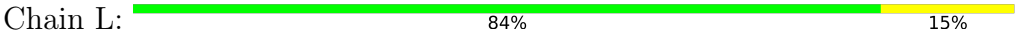
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

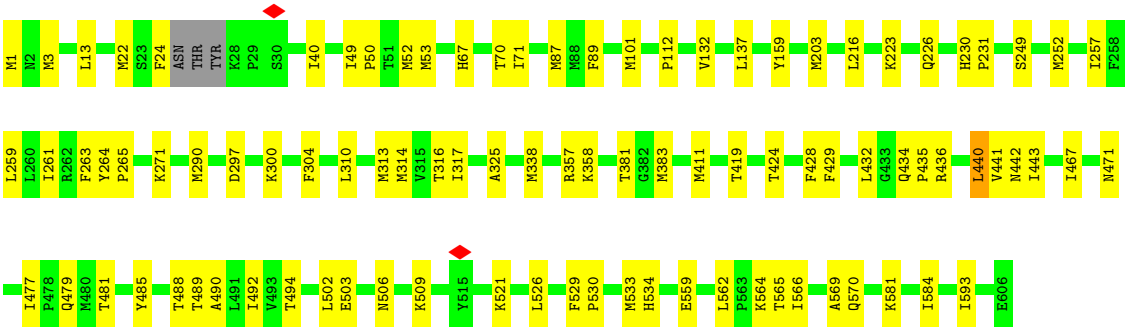


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



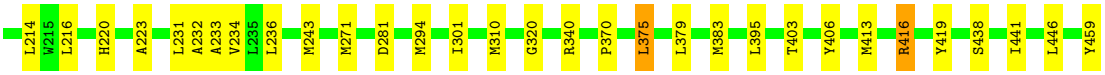


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



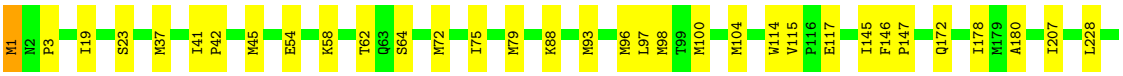




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:



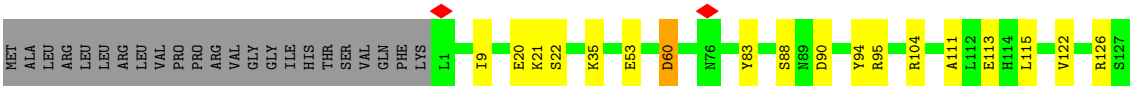


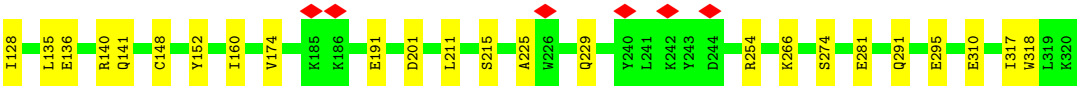


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:





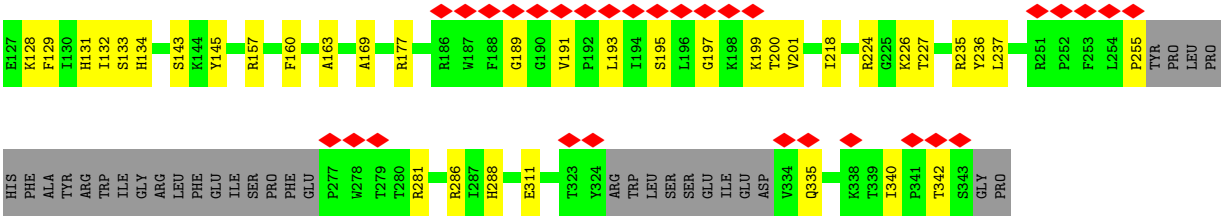


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



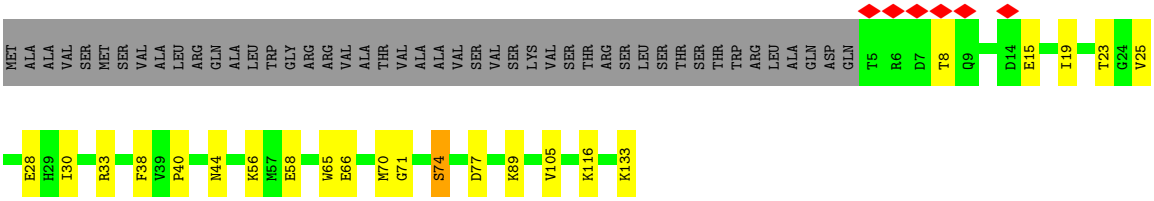




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:

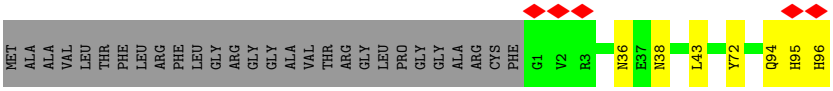




• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:

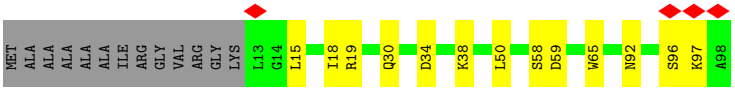




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

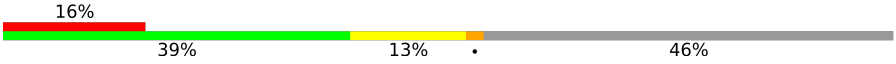
Chain S:

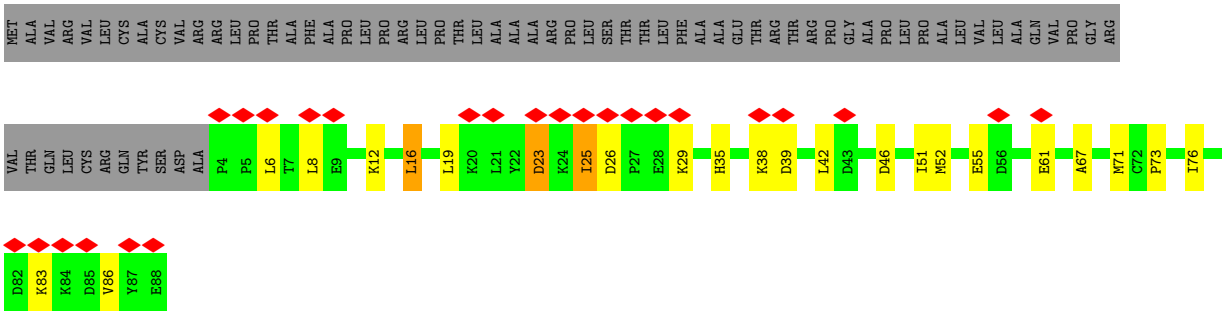




• Molecule 20: Acyl carrier protein, mitochondrial

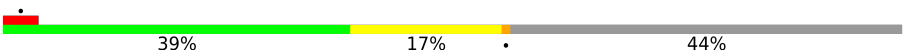
Chain T:

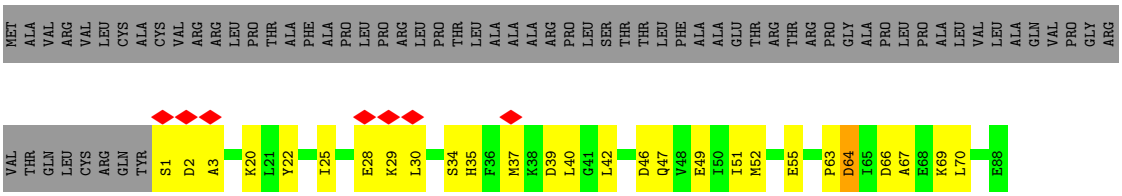




• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:

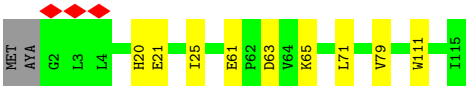




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:

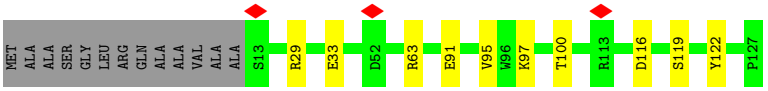




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

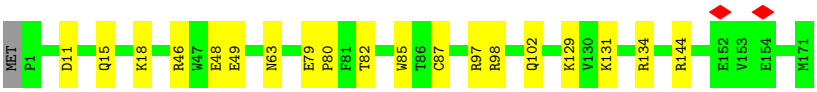




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

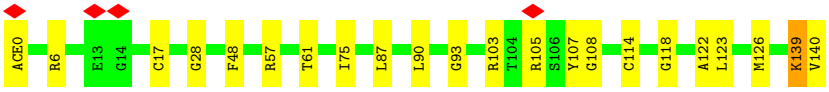




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:

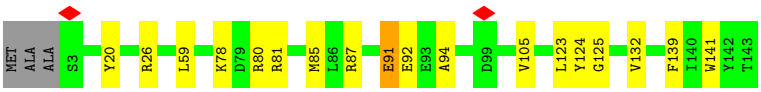




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

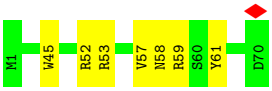




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:

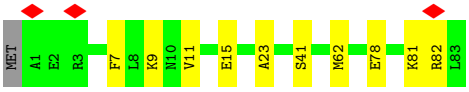




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:

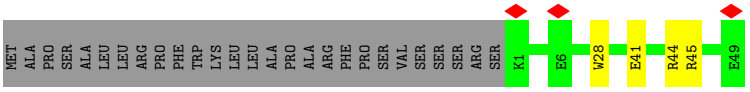




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:

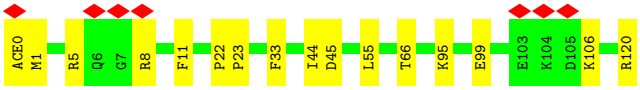




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:

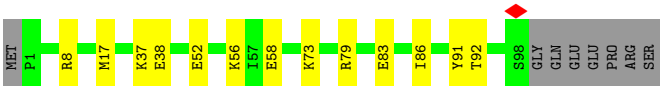




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:

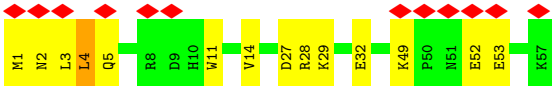




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:

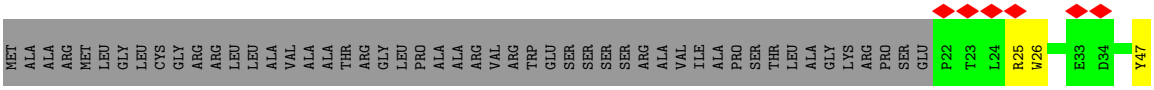


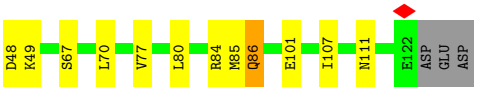


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:







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

Chain h:



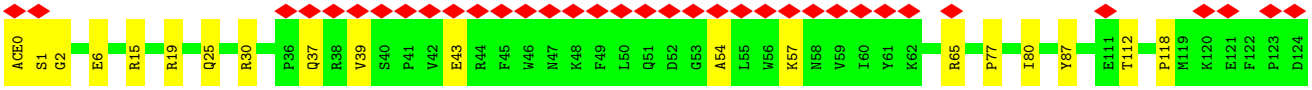




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



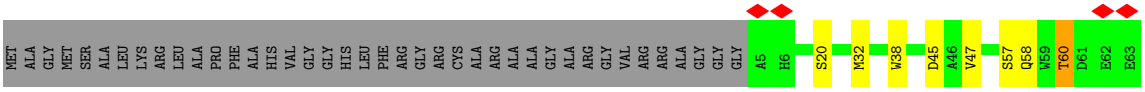


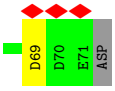


• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



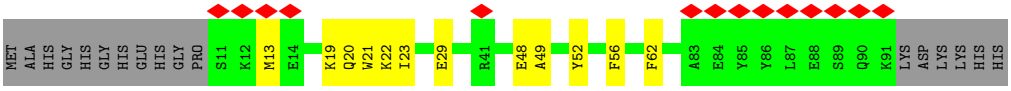




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:

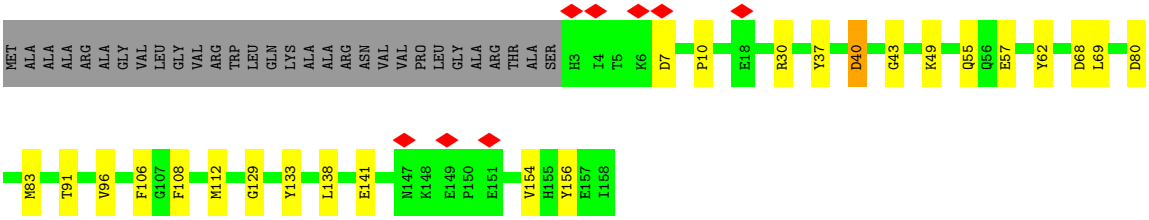




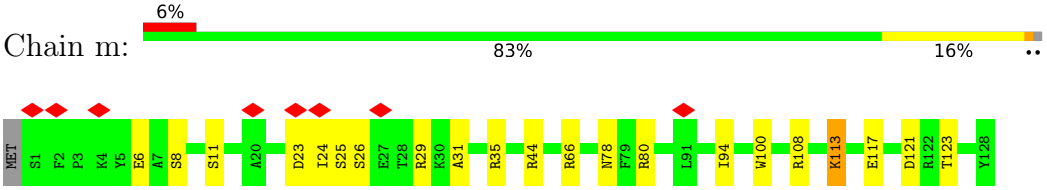
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:

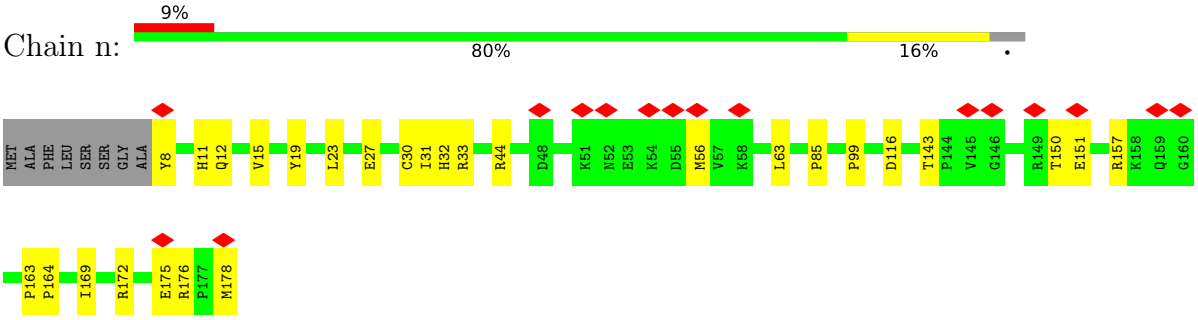




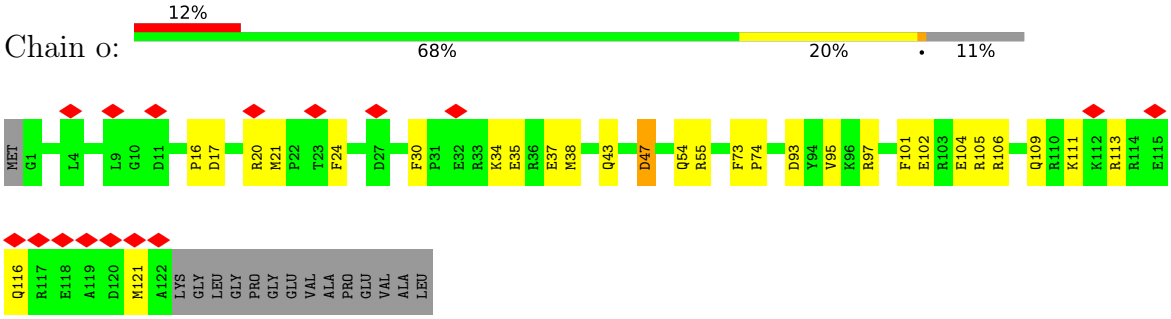
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



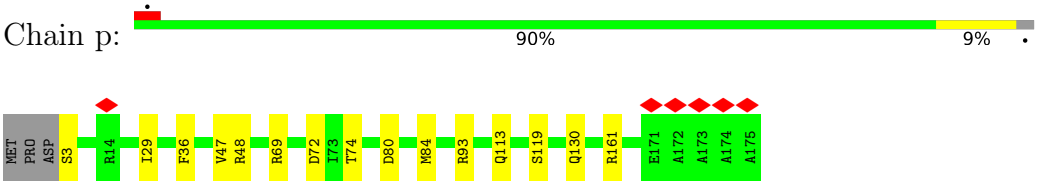
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



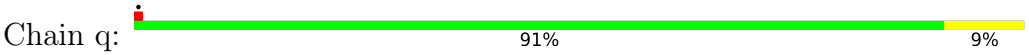
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

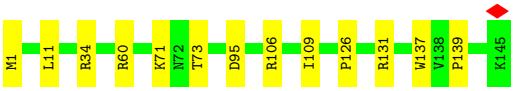


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



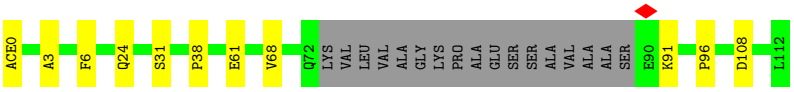
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





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

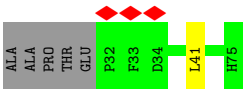




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	262659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Global and local CTF parameters were refined both in cycles in RELION then during refinement cycles in the final homogeneous refinement in cryoSPARC.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.608	Depositor
Minimum map value	-0.556	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.12	0/863	0.30	0/1181
2	B	0.14	0/1266	0.31	0/1711
3	C	0.12	0/1772	0.29	0/2413
4	D	0.12	0/3506	0.27	0/4749
5	E	0.09	0/1699	0.26	0/2312
6	F	0.10	0/3412	0.27	0/4610
7	G	0.11	0/5387	0.27	0/7301
8	H	0.12	0/2582	0.31	0/3528
9	I	0.12	0/1445	0.28	0/1956
10	J	0.10	0/1298	0.26	0/1757
11	K	0.10	0/745	0.24	0/1008
12	L	0.10	0/4891	0.28	0/6652
13	M	0.11	0/3779	0.27	0/5152
14	N	0.12	0/2801	0.27	0/3811
15	O	0.09	0/2651	0.23	0/3587
16	P	0.11	0/2554	0.27	0/3458
17	Q	0.10	0/1072	0.26	0/1449
18	R	0.11	0/753	0.25	0/1014
19	S	0.10	0/702	0.31	0/945
20	T	0.12	0/700	0.36	0/944
20	U	0.12	0/719	0.29	0/971
21	V	0.10	0/943	0.25	0/1277
22	W	0.09	0/1001	0.26	0/1345
23	X	0.10	0/1439	0.25	0/1942
24	Y	0.21	1/1048 (0.1%)	0.22	0/1423
25	Z	0.10	0/1181	0.22	0/1592
26	a	0.11	0/584	0.26	0/786
27	b	0.10	0/672	0.28	0/923
28	c	0.09	0/427	0.23	0/579
29	d	0.23	1/1027 (0.1%)	0.30	0/1387
30	e	0.13	0/846	0.31	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	f	0.13	0/505	0.31	0/681
32	g	0.10	0/873	0.27	0/1186
33	h	0.10	0/1188	0.22	0/1607
34	i	0.22	1/1134 (0.1%)	0.29	0/1544
35	j	0.09	0/607	0.25	0/833
36	k	0.12	0/672	0.28	0/906
37	l	0.11	0/1369	0.29	0/1873
38	m	0.10	0/1094	0.28	0/1480
39	n	0.09	0/1551	0.26	0/2099
40	o	0.12	0/1073	0.32	0/1437
41	p	0.10	0/1483	0.27	0/2000
42	q	0.11	0/1250	0.28	0/1698
43	r	0.25	1/795 (0.1%)	0.28	0/1077
44	s	0.09	0/383	0.25	0/518
All	All	0.12	4/67742 (0.0%)	0.27	0/91833

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	0	ACE	C-N	6.22	1.45	1.33
29	d	0	ACE	C-N	6.13	1.45	1.33
24	Y	0	ACE	C-N	6.12	1.45	1.33
43	r	0	ACE	C-N	6.03	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	852	0	896	24	0
2	B	1248	0	1243	13	0
3	C	1721	0	1675	13	0
4	D	3429	0	3372	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1659	0	1664	19	0
6	F	3336	0	3288	27	0
7	G	5298	0	5316	52	0
8	H	2519	0	2627	33	0
9	I	1414	0	1370	14	0
10	J	1278	0	1289	28	0
11	K	745	0	785	18	0
12	L	4775	0	4937	63	0
13	M	3694	0	3891	46	0
14	N	2739	0	2925	36	0
15	O	2589	0	2566	26	0
16	P	2492	0	2528	28	0
17	Q	1049	0	1045	12	0
18	R	740	0	714	5	0
19	S	691	0	706	7	0
20	T	688	0	684	16	0
20	U	707	0	700	18	0
21	V	923	0	964	5	0
22	W	977	0	994	6	0
23	X	1402	0	1383	14	0
24	Y	1030	0	1041	16	0
25	Z	1152	0	1151	14	0
26	a	569	0	568	5	0
27	b	651	0	662	7	0
28	c	414	0	415	4	0
29	d	999	0	988	13	0
30	e	825	0	826	9	0
31	f	492	0	501	9	0
32	g	846	0	798	12	0
33	h	1154	0	1168	12	0
34	i	1097	0	1108	13	0
35	j	580	0	519	4	0
36	k	653	0	639	7	0
37	l	1314	0	1210	20	0
38	m	1067	0	1067	18	0
39	n	1498	0	1445	20	0
40	o	1048	0	1018	22	0
41	p	1450	0	1426	14	0
42	q	1209	0	1182	9	0
43	r	776	0	782	8	0
44	s	371	0	344	0	0
45	A	50	0	77	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	51	0	79	3	0
45	H	46	0	69	3	0
45	M	46	0	69	4	0
45	N	40	0	54	2	0
45	O	30	0	34	1	0
46	A	84	0	119	3	0
46	H	36	0	49	1	0
46	I	102	0	164	4	0
46	K	43	0	60	2	0
46	L	127	0	182	7	0
46	M	125	0	178	3	0
46	N	51	0	82	6	0
46	O	77	0	102	4	0
46	Y	166	0	240	5	0
46	Z	43	0	63	3	0
46	b	51	0	82	2	0
46	d	49	0	75	3	0
46	h	36	0	46	1	0
46	j	39	0	55	1	0
46	m	40	0	57	1	0
46	p	39	0	52	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	H	35	0	46	1	0
51	L	35	0	46	0	0
51	M	35	0	46	1	0
51	Y	70	0	92	3	0
52	L	79	0	108	4	0
52	N	85	0	117	3	0
52	X	86	0	125	6	0
52	d	65	0	77	1	0
52	h	68	0	80	3	0
52	q	64	0	72	2	0
53	O	1	0	0	0	0
54	O	31	0	12	4	0
55	P	48	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	R	1	0	0	0	0
57	T	37	0	0	1	0
57	U	37	0	0	2	0
58	o	15	0	27	0	0
59	A	11	0	0	0	0
59	B	47	0	0	0	0
59	C	81	0	0	0	0
59	D	158	0	0	0	0
59	E	24	0	0	0	0
59	F	83	0	0	2	0
59	G	230	0	0	1	0
59	H	83	0	0	0	0
59	I	85	0	0	1	0
59	J	23	0	0	0	0
59	K	16	0	0	1	0
59	L	133	0	0	3	0
59	M	125	0	0	0	0
59	N	81	0	0	3	0
59	O	38	0	0	0	0
59	P	55	0	0	2	0
59	Q	76	0	0	1	0
59	R	24	0	0	1	0
59	S	6	0	0	0	0
59	T	3	0	0	0	0
59	U	21	0	0	0	0
59	V	17	0	0	0	0
59	W	10	0	0	0	0
59	X	38	0	0	1	0
59	Y	6	0	0	0	0
59	Z	33	0	0	1	0
59	a	16	0	0	1	0
59	b	16	0	0	0	0
59	c	1	0	0	0	0
59	d	36	0	0	0	0
59	e	26	0	0	0	0
59	f	6	0	0	1	0
59	g	30	0	0	1	0
59	h	38	0	0	2	0
59	i	10	0	0	2	0
59	j	4	0	0	0	0
59	k	6	0	0	0	0
59	l	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	m	18	0	0	0	0
59	n	52	0	0	0	0
59	o	19	0	0	1	0
59	p	45	0	0	1	0
59	q	27	0	0	1	0
59	r	18	0	0	0	0
59	s	8	0	0	0	0
All	All	70327	0	69301	696	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 (696) 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)
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.50	0.91
37:l:156:TYR:HA	40:o:35:GLU:HA	1.65	0.77
20:T:29:LYS:O	20:T:29:LYS:NZ	2.15	0.77
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.69	0.75
1:A:54:LYS:HD2	1:A:113:TRP:HA	1.68	0.75
13:M:57:PHE:HB3	13:M:113:MET:HE2	1.70	0.74
9:I:9:GLU:N	9:I:9:GLU:OE2	2.22	0.73
16:P:133:SER:OG	16:P:134:HIS:N	2.19	0.72
24:Y:57:ARG:HE	46:Y:204:3PE:H111	1.53	0.72
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.24	0.71
8:H:204:GLU:OE1	8:H:279:ARG:NH1	2.25	0.70
5:E:192:SER:OG	5:E:193:CYS:N	2.24	0.70
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.72	0.69
1:A:114:THR:HA	4:D:72:MET:HE3	1.74	0.69
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.11	0.68
7:G:217:ALA:HB2	7:G:248:MET:HE2	1.76	0.68
8:H:141:SER:HB3	8:H:289:LEU:HD22	1.76	0.68
40:o:34:LYS:HE2	40:o:34:LYS:HA	1.74	0.68
2:B:30:VAL:HG22	2:B:173:LEU:HB3	1.74	0.68
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.75	0.68
20:U:28:GLU:OE2	20:U:28:GLU:N	2.26	0.68
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.76	0.68
12:L:569:ALA:HB2	46:L:705:3PE:H261	1.74	0.68
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.74	0.68
31:f:53:GLU:OE2	31:f:53:GLU:N	2.27	0.67
29:d:120:ARG:O	38:m:108:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:X:201:CDL:H351	52:X:201:CDL:H531	1.76	0.66
35:j:38:TRP:NE1	46:j:101:3PE:O14	2.28	0.66
32:g:85:MET:HE1	41:p:93:ARG:HG2	1.78	0.66
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.29	0.66
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.29	0.65
39:n:56:MET:HA	39:n:56:MET:HE2	1.79	0.65
7:G:252:PRO:HG3	7:G:263:ILE:HG12	1.79	0.65
9:I:81:LYS:NZ	59:I:302:HOH:O	2.30	0.64
37:l:55:GLN:NE2	37:l:69:LEU:O	2.31	0.64
12:L:533:MET:HE3	12:L:533:MET:HA	1.78	0.64
12:L:297:ASP:HB3	12:L:300:LYS:HB2	1.79	0.64
12:L:159:TYR:HB2	13:M:416:ARG:HG2	1.80	0.64
19:S:92:ASN:O	19:S:96:SER:OG	2.15	0.63
20:U:25:ILE:HD11	20:U:42:LEU:HD11	1.80	0.63
1:A:28:ASN:HA	45:A:301:PC1:H32	1.78	0.63
37:l:30:ARG:HD3	38:m:35:ARG:HG2	1.80	0.63
15:O:291:GLN:NE2	15:O:295:GLU:OE2	2.31	0.63
38:m:8:SER:OG	38:m:11:SER:OG	2.17	0.63
12:L:565:THR:HG21	46:L:705:3PE:H321	1.80	0.62
13:M:88:ASN:HD21	13:M:91:ARG:HG3	1.63	0.62
34:i:43:GLU:N	34:i:43:GLU:OE2	2.32	0.62
37:l:40:ASP:O	38:m:80:ARG:NH1	2.32	0.62
12:L:24:PHE:HB3	33:h:26:ARG:HD3	1.80	0.62
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.31	0.62
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.79	0.62
20:U:22:TYR:OH	20:U:46:ASP:OD1	2.16	0.62
20:T:6:LEU:HB2	20:T:86:VAL:HG21	1.81	0.62
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.83	0.61
16:P:224:ARG:NH1	59:P:603:HOH:O	2.33	0.61
37:l:10:PRO:HD3	38:m:66:ARG:HG2	1.82	0.61
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.33	0.61
14:N:263[B]:LYS:NZ	59:N:505:HOH:O	2.34	0.61
4:D:412:ALA:HB2	8:H:205:SER:HB3	1.82	0.60
34:i:6:GLU:OE2	39:n:157:ARG:NH1	2.33	0.60
41:p:130:GLN:NE2	59:p:307:HOH:O	2.35	0.60
52:N:402:CDL:H712	45:O:401:PC1:H221	1.84	0.60
16:P:157:ARG:NH2	16:P:227:THR:OG1	2.34	0.60
20:U:20:LYS:HG3	20:U:30:LEU:HD23	1.84	0.60
10:J:171:ILE:HG23	14:N:45:MET:HE2	1.84	0.60
38:m:6:GLU:OE2	38:m:6:GLU:N	2.24	0.60
4:D:67:GLU:HB2	4:D:75:LYS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:15:LEU:H	19:S:97:LYS:HE3	1.66	0.59
8:H:249:PRO:HG2	23:X:98:ARG:HD2	1.83	0.59
45:N:403:PC1:H242	46:d:201:3PE:H221	1.83	0.59
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.16	0.59
4:D:3:GLN:NE2	13:M:137:GLY:O	2.36	0.59
26:a:53:ARG:NH2	59:a:101:HOH:O	2.35	0.59
2:B:49:THR:HG21	2:B:59:MET:HE2	1.83	0.59
19:S:18:ILE:HD12	19:S:50:LEU:HD21	1.83	0.59
19:S:30:GLN:NE2	19:S:34:ASP:OD1	2.35	0.59
25:Z:78:LYS:NZ	59:Z:305:HOH:O	2.36	0.59
20:T:23:ASP:N	20:T:23:ASP:OD1	2.35	0.58
32:g:47:TYR:OH	59:g:201:HOH:O	2.14	0.58
12:L:52:MET:HB3	41:p:29:ILE:HD11	1.85	0.58
24:Y:6:ARG:HH22	51:Y:206:LMT:H2'	1.68	0.58
20:T:51:ILE:HG13	20:T:67:ALA:HB1	1.85	0.58
13:M:133:ILE:HG12	13:M:223:ALA:HB2	1.85	0.58
15:O:83:TYR:HH	54:O:404:DGT:HO3'	1.51	0.58
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.86	0.57
6:F:112:ARG:HB3	6:F:145:GLU:HG3	1.85	0.57
6:F:15:LEU:O	6:F:20:ARG:NH1	2.32	0.57
52:L:702:CDL:H473	52:h:202:CDL:H751	1.85	0.57
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.86	0.57
15:O:95:ARG:NH1	15:O:281:GLU:O	2.37	0.57
16:P:128:LYS:NZ	16:P:218:ILE:O	2.33	0.57
29:d:99:GLU:OE1	29:d:99:GLU:N	2.22	0.57
32:g:48:ASP:OD1	32:g:49:LYS:N	2.37	0.57
12:L:87:MET:HA	12:L:87:MET:HE2	1.85	0.57
16:P:193:LEU:HD23	16:P:197:GLY:HA3	1.87	0.57
24:Y:61:THR:HG23	24:Y:103:ARG:HG3	1.87	0.57
17:Q:89:LYS:HD3	17:Q:105:VAL:HG11	1.86	0.57
29:d:1:MET:HG2	33:h:122:TRP:HB3	1.86	0.57
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.38	0.57
6:F:199:LYS:NZ	59:F:621:HOH:O	2.37	0.57
6:F:243:ALA:HA	6:F:251:SER:HB3	1.87	0.57
7:G:315:VAL:O	7:G:340:SER:OG	2.22	0.57
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.87	0.57
7:G:281:GLU:HG2	7:G:592:LEU:HD12	1.86	0.57
22:W:116:ASP:OD1	22:W:119:SER:OG	2.23	0.57
25:Z:125:GLY:O	30:e:79:ARG:NH1	2.37	0.57
37:l:133:TYR:HB3	37:l:138:LEU:HD23	1.87	0.57
9:I:43:ARG:HH11	43:r:24:GLN:HE22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:19:ARG:HB2	19:S:65:TRP:HB2	1.86	0.56
34:i:15:ARG:NH2	59:i:202:HOH:O	2.39	0.56
38:m:24:ILE:HD11	38:m:29:ARG:HG2	1.88	0.56
41:p:72:ASP:OD2	41:p:74:THR:OG1	2.21	0.56
7:G:114:CYS:HB3	7:G:117:GLN:HB2	1.88	0.56
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.37	0.56
5:E:159:ASN:HB3	5:E:184:PRO:HB3	1.87	0.56
20:T:73:PRO:HA	20:T:76:ILE:HD12	1.87	0.56
29:d:5:ARG:HB3	29:d:8:ARG:HB2	1.87	0.56
7:G:640:ASN:ND2	59:G:928:HOH:O	2.39	0.55
13:M:281:ASP:OD2	13:M:340:ARG:HB3	2.05	0.55
15:O:60:ASP:OD1	15:O:60:ASP:N	2.39	0.55
5:E:163:ASP:HB3	5:E:188:SER:HB3	1.87	0.55
12:L:358:LYS:NZ	59:L:833:HOH:O	2.40	0.55
2:B:69:MET:HE2	2:B:76:PHE:HA	1.88	0.55
13:M:73:LEU:HA	13:M:76:MET:HE3	1.89	0.55
14:N:274:ASN:ND2	59:N:509:HOH:O	2.35	0.55
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.89	0.55
20:U:1:SER:O	20:U:3:ALA:N	2.39	0.55
7:G:465:ALA:HB2	7:G:654:GLN:HB2	1.87	0.55
4:D:51:PHE:HB3	4:D:64:LEU:HB2	1.89	0.55
12:L:593:ILE:HD11	46:Y:205:3PE:H282	1.88	0.55
6:F:245:PHE:HB3	6:F:271:GLU:HG3	1.88	0.55
7:G:283:MET:HB2	7:G:560:ILE:HB	1.88	0.55
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.89	0.55
37:l:108:PHE:O	37:l:112:MET:HG2	2.06	0.55
7:G:382:THR:HB	7:G:454:GLY:HA3	1.89	0.55
12:L:442:ASN:ND2	59:L:835:HOH:O	2.40	0.55
12:L:467:ILE:O	12:L:471:ASN:ND2	2.30	0.55
57:U:101:EHZ:O3	39:n:11:HIS:NE2	2.33	0.55
29:d:11:PHE:O	30:e:8:ARG:NH1	2.39	0.54
32:g:67:SER:OG	33:h:28:TYR:O	2.22	0.54
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.39	0.54
20:U:35:HIS:CE1	20:U:37:MET:HB2	2.42	0.54
16:P:129:PHE:HE1	16:P:131:HIS:HB2	1.71	0.54
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.33	0.54
35:j:57:SER:OG	35:j:58:GLN:OE1	2.26	0.54
15:O:174:VAL:HG22	15:O:225:ALA:HB2	1.90	0.54
52:q:201:CDL:HB22	43:r:3:ALA:HA	1.90	0.54
40:o:116:GLN:N	40:o:116:GLN:OE1	2.41	0.54
14:N:146:PHE:CD1	14:N:147:PRO:HD3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:63:PRO:HG2	20:U:66:ASP:HB2	1.90	0.53
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.91	0.53
1:A:63:LEU:HB2	10:J:67:VAL:HG21	1.90	0.53
7:G:140:LYS:O	7:G:148:THR:OG1	2.18	0.53
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.90	0.53
16:P:10:LYS:NZ	17:Q:28:GLU:OE1	2.41	0.53
2:B:52:LEU:HB2	2:B:90:GLY:HA3	1.90	0.53
24:Y:87:LEU:HD12	24:Y:90:LEU:HD23	1.91	0.53
37:l:62:TYR:OH	39:n:151:GLU:OE2	2.27	0.53
16:P:52:GLU:HG3	16:P:54:TYR:H	1.72	0.53
57:U:101:EHZ:O2	57:U:101:EHZ:O1	2.23	0.53
40:o:16:PRO:HB3	40:o:104:GLU:HG2	1.90	0.53
4:D:269:LEU:HB2	4:D:368:GLU:HB2	1.90	0.53
20:U:47:GLN:NE2	20:U:70:LEU:O	2.41	0.53
23:X:87:CYS:SG	23:X:102:GLN:NE2	2.81	0.53
20:U:69:LYS:HA	34:i:2:GLY:HA2	1.91	0.53
39:n:15:VAL:HG22	39:n:63:LEU:HD13	1.91	0.53
5:E:149:VAL:O	5:E:190:ARG:NH2	2.39	0.53
42:q:1:MET:C	42:q:1:MET:HE3	2.33	0.53
8:H:176:LEU:HD13	46:Z:200:3PE:H3G2	1.91	0.52
3:C:179:GLU:OE1	16:P:37:HIS:NE2	2.37	0.52
4:D:158:ALA:HB1	4:D:163:ALA:HB3	1.91	0.52
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.39	0.52
13:M:370:PRO:HB3	13:M:375:LEU:HD22	1.90	0.52
37:l:129:GLY:N	40:o:97:ARG:O	2.39	0.52
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.91	0.52
15:O:113:GLU:OE1	15:O:266:LYS:NZ	2.42	0.52
1:A:23:TRP:HA	1:A:26:GLN:HG3	1.91	0.52
4:D:67:GLU:HA	4:D:67:GLU:OE1	2.09	0.52
4:D:148:LEU:HD23	4:D:174:ARG:HG2	1.92	0.52
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.73	0.52
12:L:506:ASN:OD1	12:L:509:LYS:NZ	2.42	0.52
23:X:48:GLU:OE1	23:X:134:ARG:NH2	2.35	0.52
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.42	0.52
12:L:559:GLU:HG2	13:M:214:LEU:HD13	1.92	0.52
13:M:74:PRO:O	13:M:78:MET:HG3	2.09	0.52
14:N:19:ILE:O	14:N:23:SER:OG	2.22	0.52
20:U:51:ILE:HG13	20:U:67:ALA:HB1	1.92	0.52
46:M:605:3PE:H231	29:d:55:LEU:HB2	1.92	0.52
2:B:91:THR:HA	2:B:119:CYS:HB3	1.91	0.52
4:D:117:ALA:HB2	4:D:367:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ASN:OD1	5:E:30:ARG:NH1	2.43	0.52
12:L:490:ALA:O	12:L:494:THR:OG1	2.25	0.52
13:M:271:MET:HE2	13:M:271:MET:HA	1.92	0.52
17:Q:116:LYS:NZ	59:Q:206:HOH:O	2.42	0.52
33:h:114:MET:HE2	33:h:121:PRO:HD2	1.93	0.52
13:M:76:MET:O	13:M:80:SER:OG	2.20	0.51
1:A:71:LEU:O	10:J:147:TYR:OH	2.20	0.51
15:O:88:SER:OG	15:O:90:ASP:OD1	2.25	0.51
37:l:68:ASP:N	37:l:68:ASP:OD1	2.42	0.51
7:G:333:ASP:OD2	7:G:622:ARG:NE	2.39	0.51
37:l:43:GLY:HA2	38:m:78:ASN:HB2	1.91	0.51
45:A:301:PC1:H11	2:B:176:TRP:HB2	1.93	0.51
1:A:88:LEU:HD23	46:A:303:3PE:H222	1.92	0.51
32:g:25:ARG:HG3	32:g:26:TRP:H	1.75	0.51
36:k:19:LYS:O	36:k:22:LYS:NZ	2.43	0.51
7:G:377:VAL:HG23	7:G:404:LEU:HD11	1.92	0.51
10:J:5:ILE:HG21	25:Z:141:TRP:HZ2	1.76	0.51
13:M:198:ALA:HB2	46:M:601:3PE:H292	1.91	0.51
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.93	0.51
33:h:12:LYS:NZ	59:h:307:HOH:O	2.43	0.51
34:i:37:GLN:HE22	34:i:39:VAL:HG13	1.76	0.51
8:H:87:ILE:HG12	8:H:88:PRO:HD3	1.93	0.51
10:J:115:VAL:O	10:J:117:PHE:N	2.44	0.51
12:L:485:TYR:O	12:L:489:THR:OG1	2.23	0.51
12:L:3:MET:HG3	41:p:36:PHE:CD1	2.46	0.50
1:A:49:LEU:H	1:A:50:PRO:HA	1.75	0.50
15:O:104:ARG:NH2	54:O:404:DGT:O6	2.43	0.50
1:A:51:PHE:CD1	10:J:74:MET:HE3	2.46	0.50
13:M:220[B]:HIS:CE1	13:M:232:ALA:HB2	2.46	0.50
14:N:242:VAL:HG11	46:N:401:3PE:H332	1.93	0.50
11:K:16:LEU:HB2	11:K:36:MET:HE3	1.92	0.50
13:M:403:THR:HA	13:M:406:TYR:CE2	2.47	0.50
13:M:216:LEU:HG	13:M:220[B]:HIS:HD2	1.76	0.50
13:M:459:TYR:O	32:g:84:ARG:NH1	2.44	0.50
14:N:1:FME:O1	15:O:254:ARG:NE	2.45	0.50
39:n:175:GLU:HG2	39:n:176:ARG:HG2	1.94	0.50
7:G:519:PRO:HD2	7:G:537:LEU:HD23	1.93	0.50
12:L:526:LEU:HD12	12:L:530:PRO:HG2	1.94	0.50
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.46	0.50
16:P:281:ARG:HA	16:P:281:ARG:NE	2.26	0.50
16:P:177:ARG:NH2	59:P:608:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:134:ARG:HE	8:H:206:GLU:CD	2.20	0.50
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.47	0.50
2:B:27:GLU:OE1	2:B:178:ARG:NH1	2.45	0.50
3:C:183:VAL:O	22:W:100:THR:OG1	2.19	0.50
7:G:365:ASN:HB3	7:G:488:LYS:HD3	1.94	0.50
3:C:14:ARG:HH11	3:C:14:ARG:HG2	1.77	0.49
7:G:297:GLU:HG3	22:W:122:TYR:CZ	2.47	0.49
35:j:60:THR:O	40:o:106:ARG:NH1	2.45	0.49
23:X:97:ARG:HD3	25:Z:59:LEU:HD13	1.94	0.49
23:X:98:ARG:NH1	59:X:306:HOH:O	2.44	0.49
3:C:173:GLU:HG2	3:C:188:VAL:HA	1.95	0.49
6:F:194:GLU:OE1	17:Q:133:LYS:NZ	2.44	0.49
46:M:601:3PE:H3C2	51:Y:201:LMT:H123	1.93	0.49
38:m:25:SER:OG	38:m:26:SER:N	2.44	0.49
6:F:248:GLU:O	6:F:250:ASN:ND2	2.46	0.49
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.93	0.49
34:i:30:ARG:NH2	39:n:116:ASP:OD1	2.37	0.49
40:o:113:ARG:NH2	59:o:304:HOH:O	2.39	0.49
52:q:201:CDL:H561	43:r:6:PHE:HE2	1.78	0.49
7:G:185:THR:O	7:G:187:ILE:N	2.45	0.49
12:L:13:LEU:HD23	34:i:77:PRO:HB3	1.93	0.49
40:o:16:PRO:HD3	40:o:105:ARG:HG2	1.95	0.49
38:m:121:ASP:OD1	38:m:123:THR:OG1	2.30	0.49
12:L:441:VAL:HG13	12:L:443:ILE:HD12	1.93	0.49
14:N:3:PRO:HB2	15:O:9:ILE:HD11	1.94	0.49
14:N:298:TYR:O	14:N:303:THR:OG1	2.24	0.49
46:A:302:3PE:H322	10:J:151:THR:HG21	1.95	0.49
3:C:51:CYS:HB3	21:V:111:TRP:CE2	2.48	0.49
7:G:190:MET:HB3	7:G:192:MET:HG2	1.95	0.49
9:I:54:LYS:NZ	9:I:138:GLU:OE2	2.46	0.49
8:H:111:LEU:HD11	10:J:57:PHE:CD1	2.48	0.48
12:L:223:LYS:NZ	59:L:844:HOH:O	2.46	0.48
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.93	0.48
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.37	0.48
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.12	0.48
16:P:237:LEU:HG	16:P:340:ILE:HD11	1.94	0.48
6:F:237:ARG:NH1	59:F:625:HOH:O	2.47	0.48
31:f:1:MET:HE2	31:f:4:LEU:HB2	1.95	0.48
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.48	0.48
33:h:111:ARG:NH1	59:h:309:HOH:O	2.45	0.48
38:m:113:LYS:HE3	38:m:113:LYS:HB3	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:199:ILE:HA	7:G:202:ILE:HG12	1.95	0.48
20:U:29:LYS:HB2	20:U:29:LYS:NZ	2.28	0.48
46:d:201:3PE:H382	46:d:201:3PE:H282	1.96	0.48
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.94	0.48
16:P:191:VAL:HG22	16:P:255:PRO:HA	1.95	0.48
8:H:205:SER:O	8:H:209:SER:OG	2.29	0.48
46:L:703:3PE:H362	45:M:602:PC1:H341	1.95	0.48
18:R:94:GLN:O	18:R:96:HIS:N	2.46	0.48
24:Y:90:LEU:HB2	24:Y:122:ALA:HB2	1.96	0.48
52:h:202:CDL:H561	41:p:47:VAL:HG21	1.96	0.48
1:A:4:MET:HE2	45:H:603:PC1:H251	1.96	0.48
6:F:63:SER:HB2	6:F:242:PHE:HB3	1.96	0.48
12:L:49:ILE:HB	12:L:50:PRO:HD3	1.96	0.48
45:M:602:PC1:H143	45:M:602:PC1:H112	1.70	0.48
15:O:310:GLU:HG3	15:O:317:ILE:HD12	1.96	0.48
20:U:51:ILE:O	20:U:55:GLU:HG3	2.14	0.48
23:X:144:ARG:NH1	30:e:58:GLU:OE2	2.46	0.48
31:f:2:ASN:O	31:f:4:LEU:N	2.47	0.48
33:h:19:LYS:HB3	33:h:19:LYS:HE3	1.55	0.48
36:k:23:ILE:HD12	36:k:29:GLU:HA	1.95	0.48
7:G:194:GLU:HG2	7:G:195:LEU:HG	1.96	0.47
11:K:14:VAL:HG22	46:K:101:3PE:H3C1	1.95	0.47
38:m:25:SER:O	38:m:29:ARG:HG3	2.14	0.47
14:N:238:PRO:O	14:N:241:THR:OG1	2.30	0.47
16:P:26:ALA:HA	16:P:31:GLY:HA3	1.97	0.47
6:F:191:ALA:HB2	6:F:203:PRO:HG3	1.97	0.47
6:F:294:LEU:HD11	6:F:297:VAL:HG23	1.96	0.47
7:G:358:LEU:HD12	7:G:645:ALA:HB2	1.95	0.47
12:L:521:LYS:HD3	37:l:96:VAL:HG22	1.97	0.47
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.96	0.47
31:f:29:LYS:NZ	31:f:32:GLU:OE1	2.47	0.47
23:X:129:LYS:NZ	27:b:62:MET:O	2.44	0.47
13:M:71:TRP:CD1	45:M:602:PC1:H2D2	2.49	0.47
21:V:20:HIS:NE2	21:V:61:GLU:O	2.44	0.47
27:b:78:GLU:OE1	27:b:82:ARG:NH1	2.42	0.47
38:m:44:ARG:HH12	39:n:143:THR:HG21	1.80	0.47
39:n:30:CYS:O	39:n:32:HIS:N	2.43	0.47
6:F:165:ASN:ND2	6:F:168:GLY:HA2	2.30	0.47
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.17	0.47
9:I:84:GLU:HB2	9:I:94:ILE:HD12	1.97	0.47
13:M:5:ILE:HG21	52:X:201:CDL:H611	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:94:LEU:HD23	16:P:132:ILE:HG13	1.96	0.47
8:H:287[A]:HIS:CD2	8:H:291:LYS:HD2	2.49	0.47
46:L:705:3PE:H11	24:Y:108:GLY:HA3	1.95	0.47
13:M:2:LEU:HB2	31:f:27:ASP:OD1	2.15	0.47
46:N:401:3PE:H342	46:O:405:3PE:H2A1	1.96	0.47
59:N:502:HOH:O	33:h:111:ARG:NH2	2.47	0.47
40:o:102:GLU:OE2	40:o:105:ARG:NH2	2.48	0.47
46:L:705:3PE:H262	46:L:705:3PE:H232	1.66	0.47
7:G:80:LEU:HB3	7:G:83:SER:HB3	1.97	0.47
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.97	0.47
11:K:70:GLU:OE2	59:K:201:HOH:O	2.20	0.47
20:T:26:ASP:OD2	20:T:29:LYS:HB3	2.15	0.47
37:l:7:ASP:OD1	37:l:7:ASP:N	2.36	0.47
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.96	0.46
8:H:53:ILE:O	8:H:57:ILE:HG12	2.15	0.46
9:I:175:TYR:CZ	43:r:38:PRO:HG3	2.50	0.46
16:P:157:ARG:NH2	16:P:226:LYS:O	2.38	0.46
34:i:54:ALA:HB3	34:i:57:LYS:HG2	1.96	0.46
7:G:41:CYS:HB3	7:G:52:CYS:HB3	1.98	0.46
7:G:283:MET:HE3	7:G:293:HIS:CE1	2.50	0.46
7:G:331:LEU:HD22	7:G:525:LEU:HD22	1.98	0.46
7:G:450:MET:HE2	7:G:452:ILE:HD11	1.98	0.46
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.48	0.46
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.32	0.46
27:b:81:LYS:HB2	27:b:81:LYS:HE3	1.61	0.46
5:E:87:TYR:HB3	6:F:181:ALA:O	2.15	0.46
8:H:113:VAL:HG22	8:H:136:VAL:HG22	1.97	0.46
11:K:17:VAL:HG12	46:K:101:3PE:H351	1.97	0.46
16:P:133:SER:O	55:P:501:NDP:H6N	2.15	0.46
26:a:57:VAL:HG23	26:a:59:ARG:HB2	1.98	0.46
3:C:8:ARG:NH2	43:r:61:GLU:OE2	2.38	0.46
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.97	0.46
12:L:564:LYS:NZ	51:M:604:LMT:O2B	2.43	0.46
21:V:63:ASP:OD2	21:V:65:LYS:N	2.47	0.46
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.45	0.46
11:K:93:LEU:HB3	14:N:54:GLU:HG3	1.97	0.46
20:T:29:LYS:HE3	20:T:39:ASP:HB3	1.97	0.46
25:Z:92:GLU:OE1	30:e:91:TYR:OH	2.23	0.46
38:m:113:LYS:O	38:m:117:GLU:HG3	2.15	0.46
40:o:73:PHE:CD1	40:o:74:PRO:HA	2.50	0.46
9:I:50:TYR:CD1	9:I:51:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:20:TYR:OH	43:r:108:ASP:OD2	2.23	0.46
42:q:131:ARG:NH2	59:q:303:HOH:O	2.48	0.46
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.80	0.46
16:P:79:ASP:OD2	16:P:82:ARG:NH2	2.49	0.46
34:i:126:HIS:O	34:i:127:HIS:ND1	2.49	0.46
3:C:137:MET:HE1	3:C:153:THR:HG23	1.98	0.46
7:G:227:SER:OG	7:G:228:ILE:N	2.48	0.46
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.46	0.46
7:G:418:ARG:HE	7:G:418:ARG:HB2	1.61	0.46
10:J:23:LYS:HE2	11:K:23:ARG:HG3	1.97	0.46
10:J:43:ILE:HG22	11:K:46:LEU:HD11	1.98	0.46
24:Y:122:ALA:O	24:Y:126:MET:HG3	2.16	0.46
1:A:54:LYS:HE3	1:A:54:LYS:HB2	1.51	0.46
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.98	0.46
13:M:379:LEU:O	13:M:383:MET:HG2	2.15	0.46
14:N:96:MET:O	14:N:100:MET:HG3	2.16	0.46
15:O:136:GLU:O	15:O:140:ARG:HG3	2.15	0.46
14:N:88:LYS:NZ	30:e:52:GLU:OE1	2.49	0.46
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.97	0.46
20:U:64:ASP:N	20:U:64:ASP:OD1	2.48	0.46
12:L:290:MET:HE3	12:L:290:MET:HB3	1.89	0.45
12:L:357:ARG:HG2	39:n:31:ILE:HG12	1.97	0.45
20:T:19:LEU:HD12	20:T:25:ILE:HD12	1.98	0.45
13:M:122:PHE:CE1	13:M:206:LYS:HD2	2.52	0.45
22:W:29:ARG:O	22:W:33:GLU:HG2	2.16	0.45
24:Y:28:GLY:HA2	46:Y:204:3PE:H2A1	1.97	0.45
20:T:35:HIS:CE1	20:T:71:MET:HG2	2.51	0.45
24:Y:139:LYS:HE2	24:Y:139:LYS:HB2	1.77	0.45
1:A:90:MET:SD	10:J:151:THR:HG23	2.57	0.45
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.51	0.45
15:O:20:GLU:HG2	15:O:21:LYS:HD2	1.99	0.45
5:E:97:LYS:NZ	5:E:98:TYR:OH	2.38	0.45
8:H:81:LEU:O	8:H:85:MET:HG2	2.16	0.45
8:H:103:LEU:HB3	10:J:54:LEU:HD13	1.98	0.45
30:e:56:LYS:NZ	30:e:56:LYS:HB3	2.32	0.45
38:m:24:ILE:HG12	39:n:8:TYR:CZ	2.52	0.45
7:G:486:ASP:OD1	7:G:486:ASP:N	2.36	0.45
12:L:89:PHE:CD2	12:L:132:VAL:HG21	2.51	0.45
52:L:702:CDL:H611	52:L:702:CDL:H642	1.63	0.45
52:N:402:CDL:H382	52:N:402:CDL:H351	1.87	0.45
7:G:537:LEU:HD22	7:G:541:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:288:LEU:O	8:H:292:ASN:HB2	2.16	0.45
11:K:12:PHE:CD2	14:N:72:MET:HE2	2.52	0.45
16:P:145:TYR:CD1	16:P:286:ARG:HD3	2.52	0.45
18:R:38:ASN:HB3	18:R:43:LEU:HD11	1.98	0.45
23:X:82:THR:HA	23:X:85:TRP:CD1	2.51	0.45
3:C:109:THR:OG1	3:C:110:TYR:N	2.49	0.45
4:D:56:PRO:HG3	8:H:211:PHE:CG	2.51	0.45
12:L:53:MET:HE2	12:L:53:MET:HB3	1.86	0.45
41:p:80:ASP:O	41:p:84:MET:HG3	2.17	0.45
14:N:314:LYS:NZ	15:O:274:SER:OG	2.47	0.45
15:O:225:ALA:O	15:O:229:GLN:NE2	2.50	0.45
33:h:73:ARG:H	33:h:73:ARG:HG2	1.61	0.45
39:n:169:ILE:O	39:n:172:ARG:NH1	2.50	0.45
5:E:128:VAL:HG11	5:E:141:GLU:HG3	1.99	0.45
6:F:99:GLU:O	6:F:139:ARG:NH1	2.50	0.45
12:L:434:GLN:HG3	36:k:52:TYR:CE2	2.52	0.45
37:l:57:GLU:OE2	37:l:91:THR:OG1	2.25	0.45
3:C:25:PHE:CE1	43:r:96:PRO:HD3	2.51	0.44
12:L:271:LYS:HB2	12:L:271:LYS:HE2	1.73	0.44
15:O:35:LYS:N	54:O:404:DGT:O2G	2.50	0.44
25:Z:26:ARG:HD2	25:Z:26:ARG:HA	1.72	0.44
27:b:23:ALA:HB2	46:b:101:3PE:H3B1	1.99	0.44
38:m:31:ALA:O	38:m:35:ARG:HG3	2.16	0.44
2:B:81:ARG:H	2:B:81:ARG:HG2	1.58	0.44
2:B:174:ARG:HB3	2:B:174:ARG:NH1	2.33	0.44
6:F:327:THR:OG1	6:F:328:GLY:N	2.42	0.44
46:H:601:3PE:H291	46:H:601:3PE:H2C2	1.72	0.44
12:L:226:GLN:HG3	12:L:314:MET:HE3	1.99	0.44
12:L:257:ILE:HG21	12:L:313:MET:HB3	1.98	0.44
4:D:64:LEU:HD11	4:D:418:ILE:HD11	2.00	0.44
7:G:579:ARG:HB2	7:G:636:VAL:HG22	1.99	0.44
17:Q:66:GLU:HG2	17:Q:71:GLY:HA2	1.99	0.44
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.51	0.44
46:Y:204:3PE:H381	46:Y:204:3PE:H352	1.61	0.44
27:b:15:GLU:HG3	46:b:101:3PE:H31	1.98	0.44
28:c:44:ARG:HG2	28:c:44:ARG:HH11	1.82	0.44
8:H:139:THR:O	8:H:143:GLU:HG3	2.17	0.44
25:Z:81:ARG:O	25:Z:85:MET:HG3	2.17	0.44
8:H:99:ASN:N	45:H:603:PC1:O12	2.50	0.44
8:H:179:TRP:HB2	46:I:204:3PE:H2B2	1.98	0.44
46:N:401:3PE:H2G2	46:N:401:3PE:H3B2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:305:PRO:HG3	6:F:413:TRP:HB3	2.00	0.44
25:Z:94:ALA:HB2	25:Z:105:VAL:HG11	1.99	0.44
29:d:45:ASP:OD1	52:d:202:CDL:O1	2.29	0.44
2:B:54:CYS:HB3	4:D:108:TYR:HB2	2.00	0.44
5:E:109:MET:HE1	6:F:346:ALA:HA	1.99	0.44
12:L:534:HIS:CD2	46:L:701:3PE:H232	2.53	0.44
12:L:566:ILE:O	12:L:570:GLN:HG2	2.18	0.44
14:N:346:LEU:HD21	46:d:201:3PE:H2D2	2.00	0.44
28:c:44:ARG:HG2	28:c:44:ARG:NH1	2.33	0.44
42:q:106:ARG:HB2	42:q:109:ILE:HG13	2.00	0.44
7:G:329:ILE:HD13	7:G:505:LEU:HD22	1.99	0.44
10:J:27:ILE:HD11	10:J:77:GLU:HB3	1.99	0.44
10:J:100:GLU:HA	10:J:103:MET:HE3	1.99	0.44
5:E:108:CYS:HA	5:E:151:ALA:HB1	1.99	0.44
7:G:366:THR:O	7:G:367:THR:OG1	2.34	0.44
14:N:250:SER:O	14:N:259:GLY:HA3	2.18	0.44
23:X:49:GLU:OE2	23:X:134:ARG:NH1	2.51	0.44
25:Z:87:ARG:O	25:Z:91:GLU:HG2	2.18	0.44
7:G:516:LYS:HA	7:G:516:LYS:HD3	1.85	0.43
13:M:90:THR:HG21	46:N:401:3PE:H12	2.00	0.43
14:N:75:ILE:O	14:N:79:MET:HG3	2.18	0.43
20:U:49:GLU:OE2	39:n:44:ARG:NH1	2.46	0.43
52:X:201:CDL:H332	29:d:33:PHE:HB2	1.99	0.43
40:o:24:PHE:HE1	40:o:111:LYS:HD3	1.83	0.43
1:A:87:MET:HG2	10:J:147:TYR:HB3	2.00	0.43
7:G:316:ALA:HB3	7:G:519:PRO:HG3	1.99	0.43
39:n:163:PRO:HA	39:n:164:PRO:HD3	1.94	0.43
1:A:87:MET:HE3	1:A:87:MET:HB3	1.85	0.43
45:B:202:PC1:H3A1	8:H:53:ILE:HD11	2.00	0.43
5:E:111:ARG:HD3	5:E:151:ALA:HB3	2.01	0.43
13:M:413:MET:HA	13:M:413:MET:HE2	1.99	0.43
16:P:201:VAL:HG11	16:P:235:ARG:HE	1.84	0.43
20:T:25:ILE:HD11	20:T:42:LEU:HD11	2.01	0.43
23:X:18:LYS:HB2	23:X:18:LYS:HE2	1.60	0.43
46:h:201:3PE:H282	46:h:201:3PE:H2B1	1.84	0.43
6:F:353:PHE:O	6:F:357:GLU:HG2	2.19	0.43
29:d:22:PRO:HA	29:d:23:PRO:HD3	1.90	0.43
4:D:56:PRO:HG3	8:H:211:PHE:CD1	2.53	0.43
12:L:203:MET:HB2	41:p:113:GLN:HG3	2.01	0.43
12:L:316:THR:HB	12:L:325:ALA:HB2	1.99	0.43
12:L:424:THR:HG23	36:k:62:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:MET:HE2	8:H:105:MET:HB3	1.83	0.43
14:N:100:MET:O	14:N:104:MET:HG3	2.17	0.43
37:l:129:GLY:O	40:o:97:ARG:NE	2.50	0.43
7:G:317:ALA:HB1	7:G:331:LEU:HD21	2.00	0.43
46:O:405:3PE:H252	46:O:405:3PE:H221	1.90	0.43
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.40	0.43
20:T:12:LYS:O	20:T:16:LEU:HB2	2.18	0.43
24:Y:93:GLY:HA3	24:Y:118:GLY:HA2	1.99	0.43
46:Z:200:3PE:H272	46:Z:200:3PE:H241	1.72	0.43
33:h:69:HIS:O	33:h:73:ARG:HG2	2.19	0.43
37:l:106:PHE:C	37:l:106:PHE:CD2	2.97	0.43
3:C:168:LEU:HD11	4:D:90:LEU:HD23	2.01	0.43
12:L:428:PHE:HA	12:L:432:LEU:HD12	2.01	0.43
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.19	0.43
34:i:15:ARG:O	34:i:19:ARG:HG3	2.19	0.43
45:A:301:PC1:H3F1	45:B:202:PC1:H3F1	2.01	0.43
7:G:689:LYS:NZ	7:G:693:GLU:OE1	2.48	0.43
9:I:9:GLU:H	9:I:9:GLU:CD	2.23	0.43
12:L:216:LEU:HD22	12:L:259:LEU:HD21	2.00	0.43
52:L:702:CDL:H382	52:L:702:CDL:H411	1.82	0.43
14:N:98:MET:HG2	14:N:145:ILE:HD13	2.00	0.43
46:N:401:3PE:H2F1	46:N:401:3PE:H2C1	1.79	0.43
52:N:402:CDL:H191	52:N:402:CDL:H391	2.01	0.43
15:O:83:TYR:OH	54:O:404:DGT:O3'	2.22	0.43
46:O:405:3PE:H351	29:d:44:ILE:HG13	2.00	0.43
20:U:34:SER:HB2	20:U:40:LEU:HD21	2.00	0.43
23:X:46:ARG:HA	23:X:46:ARG:HD2	1.88	0.43
52:X:201:CDL:H372	29:d:33:PHE:HA	1.99	0.43
29:d:95:LYS:HB3	29:d:95:LYS:HE2	1.54	0.43
30:e:73:LYS:NZ	30:e:73:LYS:HB3	2.34	0.43
52:h:202:CDL:H582	41:p:47:VAL:HG21	2.01	0.43
4:D:38:PRO:HA	4:D:39:PRO:HD3	1.91	0.43
12:L:435:PRO:HG3	36:k:56:PHE:CG	2.54	0.43
45:N:403:PC1:H111	45:N:403:PC1:H132	1.66	0.43
37:l:40:ASP:OD1	37:l:40:ASP:N	2.52	0.43
6:F:111:ILE:HD13	6:F:138:ILE:HD12	2.01	0.42
31:f:1:MET:HB3	31:f:5:GLN:HB2	2.01	0.42
40:o:37:GLU:OE2	40:o:38:MET:N	2.52	0.42
10:J:133:SER:O	10:J:133:SER:OG	2.34	0.42
12:L:261:ILE:HG13	12:L:317:ILE:HD11	2.02	0.42
13:M:42:MET:HE3	32:g:77:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:42:MET:HG2	32:g:80:LEU:HD11	2.02	0.42
16:P:160:PHE:HB3	16:P:163:ALA:HB2	2.00	0.42
46:m:201:3PE:H2I3	46:m:201:3PE:H2F1	1.77	0.42
39:n:19:TYR:CZ	39:n:23:LEU:HD11	2.53	0.42
1:A:69:ILE:HD11	8:H:144:VAL:HG13	2.00	0.42
4:D:155:THR:HB	4:D:167:PHE:HA	2.01	0.42
7:G:87:LYS:HB2	7:G:87:LYS:HE2	1.81	0.42
12:L:71:ILE:HG23	13:M:310:MET:HE1	2.00	0.42
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.32	0.42
52:X:201:CDL:H451	52:X:201:CDL:H422	1.84	0.42
42:q:60:ARG:HH22	42:q:95:ASP:HA	1.84	0.42
3:C:15:ASN:HB3	3:C:46:ASN:ND2	2.34	0.42
6:F:306:LEU:HD23	6:F:347:ILE:HD11	2.00	0.42
12:L:429:PHE:O	12:L:436:ARG:NH2	2.53	0.42
17:Q:40:PRO:HG3	17:Q:56:LYS:HG3	2.02	0.42
11:K:4:VAL:O	11:K:8:ILE:HG12	2.19	0.42
13:M:231:LEU:O	13:M:236:LEU:HG	2.20	0.42
1:A:19:ILE:HD12	1:A:19:ILE:C	2.45	0.42
5:E:105:THR:HG22	5:E:106:THR:H	1.84	0.42
6:F:90:PRO:O	6:F:218:CYS:HB3	2.19	0.42
8:H:172:MET:HB3	8:H:172:MET:HE2	1.69	0.42
14:N:93:MET:HE3	14:N:97:LEU:HG	2.01	0.42
14:N:172:GLN:HB2	14:N:178:ILE:HG13	2.02	0.42
15:O:94:TYR:CG	15:O:148:CYS:HB3	2.54	0.42
16:P:157:ARG:NH1	16:P:163:ALA:O	2.49	0.42
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.50	0.42
37:l:37:TYR:CE2	37:l:49:LYS:HD2	2.55	0.42
8:H:149:ILE:HG21	8:H:185:TRP:HB2	2.00	0.42
8:H:312:SER:HA	27:b:41:SER:OG	2.20	0.42
45:H:603:PC1:H352	45:H:603:PC1:H381	1.74	0.42
10:J:23:LYS:HD2	11:K:28:SER:HB3	2.01	0.42
10:J:65:MET:HE2	10:J:65:MET:HA	2.01	0.42
11:K:43:MET:HE1	14:N:72:MET:SD	2.59	0.42
12:L:477:ILE:HD11	40:o:54:GLN:HA	2.00	0.42
18:R:38:ASN:ND2	59:R:303:HOH:O	2.45	0.42
38:m:23:ASP:OD1	38:m:23:ASP:N	2.51	0.42
39:n:12:GLN:N	39:n:12:GLN:CD	2.78	0.42
2:B:109:GLU:OE1	16:P:54:TYR:OH	2.36	0.42
4:D:343:GLU:OE1	7:G:128:SER:HB2	2.20	0.42
15:O:22:SER:HB3	15:O:115:LEU:HD11	2.01	0.42
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:123:LEU:HB3	51:Y:206:LMT:H102	2.00	0.42
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.51	0.42
31:f:49:LYS:HB2	31:f:52:GLU:HB3	2.01	0.42
32:g:86:GLN:HE21	32:g:86:GLN:C	2.28	0.42
3:C:31:GLU:OE2	43:r:91:LYS:NZ	2.53	0.42
25:Z:123:LEU:HD23	25:Z:123:LEU:HA	1.86	0.42
35:j:69:ASP:OD1	40:o:113:ARG:NH2	2.52	0.42
36:k:21:TRP:HB3	36:k:49:ALA:HB3	2.02	0.42
40:o:21:MET:HE1	40:o:101:PHE:CD2	2.55	0.42
2:B:39:TRP:CZ2	45:B:202:PC1:H332	2.54	0.42
12:L:440:LEU:HD11	36:k:13:MET:HE1	2.01	0.42
13:M:141:GLU:H	13:M:141:GLU:CD	2.28	0.42
16:P:200:THR:HG21	16:P:288:HIS:HA	2.01	0.42
30:e:37:LYS:NZ	30:e:38:GLU:OE2	2.53	0.42
31:f:28:ARG:NH1	59:f:101:HOH:O	2.53	0.42
1:A:51:PHE:CG	10:J:74:MET:HE3	2.55	0.41
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.55	0.41
8:H:301:CYS:O	8:H:305:VAL:HG23	2.20	0.41
51:H:602:LMT:H91	51:H:602:LMT:H122	1.81	0.41
11:K:43:MET:HE3	11:K:43:MET:HB3	1.86	0.41
12:L:223:LYS:HD2	12:L:252:MET:HE3	2.02	0.41
13:M:220[B]:HIS:HE1	13:M:232:ALA:HB2	1.84	0.41
26:a:59:ARG:HG2	26:a:61:TYR:CZ	2.55	0.41
7:G:360:SER:HB2	7:G:642:PHE:CE2	2.55	0.41
10:J:106:TYR:HD1	10:J:106:TYR:HA	1.74	0.41
12:L:264:TYR:CD2	12:L:265:PRO:HD3	2.55	0.41
13:M:67:ILE:HG22	45:M:602:PC1:H2E2	2.01	0.41
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.45	0.41
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.47	0.41
7:G:623:LEU:HD22	7:G:630:LEU:HD13	2.01	0.41
12:L:40:ILE:HG13	12:L:101:MET:SD	2.60	0.41
13:M:233:ALA:HA	13:M:320:GLY:HA2	2.01	0.41
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.55	0.41
20:T:38:LYS:H	20:T:38:LYS:HG2	1.68	0.41
20:T:83:LYS:HE2	20:T:83:LYS:HB2	1.81	0.41
20:U:39:ASP:OD1	20:U:39:ASP:N	2.53	0.41
24:Y:17:CYS:SG	24:Y:75:ILE:HD13	2.60	0.41
40:o:17:ASP:OD2	40:o:20:ARG:HG3	2.20	0.41
1:A:19:ILE:HD12	1:A:20:ILE:N	2.34	0.41
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.55	0.41
11:K:10:MET:HE2	11:K:10:MET:HB2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:294:MET:HE2	13:M:294:MET:HA	2.02	0.41
20:T:55:GLU:HG2	20:T:61:GLU:HA	2.02	0.41
21:V:21:GLU:O	21:V:25:ILE:HD13	2.20	0.41
37:l:80:ASP:HB3	37:l:83:MET:HE3	2.02	0.41
42:q:71:LYS:HD3	42:q:73:THR:HG22	2.02	0.41
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.80	0.41
1:A:93:PHE:HD1	46:A:303:3PE:H2C2	1.85	0.41
5:E:147:ALA:HB3	5:E:153:MET:HE3	2.02	0.41
12:L:479:GLN:NE2	12:L:481:THR:O	2.54	0.41
14:N:207:ILE:HD13	14:N:262:PRO:HD3	2.03	0.41
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.03	0.41
24:Y:48:PHE:HA	46:Y:205:3PE:H32	2.03	0.41
6:F:42:TRP:CD2	6:F:161:LEU:HD13	2.55	0.41
12:L:488:THR:O	12:L:492:ILE:HG12	2.20	0.41
15:O:128:ILE:HD12	15:O:160:ILE:HG13	2.02	0.41
4:D:366:ALA:HB1	4:D:373:GLU:HG3	2.02	0.41
4:D:417:ILE:O	4:D:420:THR:HG22	2.20	0.41
7:G:437:HIS:O	7:G:440:SER:OG	2.26	0.41
17:Q:65:TRP:CE2	17:Q:74:SER:HB2	2.56	0.41
27:b:7:PHE:O	27:b:11:VAL:HG22	2.21	0.41
34:i:25:GLN:NE2	59:i:203:HOH:O	2.40	0.41
8:H:187:ILE:HD11	46:I:201:3PE:H281	2.02	0.41
9:I:64:GLU:O	9:I:134:GLY:N	2.46	0.41
11:K:70:GLU:HG3	14:N:37:MET:HE1	2.03	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.36	0.41
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.55	0.41
37:l:138:LEU:HD12	37:l:141:GLU:HB2	2.03	0.41
2:B:56:ALA:HB1	4:D:57:ALA:O	2.21	0.41
3:C:137:MET:HE3	3:C:152:LEU:HB2	2.02	0.41
7:G:134:LYS:HB2	18:R:72:TYR:CD1	2.55	0.41
7:G:453:LEU:HD21	7:G:458:LEU:HD21	2.01	0.41
7:G:550:GLY:HA3	42:q:137:TRP:CG	2.56	0.41
9:I:129:ASP:OD1	9:I:129:ASP:N	2.53	0.41
12:L:502:LEU:HD12	12:L:502:LEU:HA	1.83	0.41
12:L:584:ILE:HG12	14:N:58:LYS:HG2	2.03	0.41
13:M:419:TYR:CZ	39:n:99:PRO:HD3	2.56	0.41
15:O:318:TRP:H	15:O:318:TRP:CD1	2.38	0.41
46:O:403:3PE:H321	46:O:403:3PE:H352	1.84	0.41
16:P:157:ARG:HH21	16:P:227:THR:HG1	1.64	0.41
20:T:52:MET:HA	20:T:55:GLU:HB2	2.02	0.41
22:W:91:GLU:HB3	22:W:97:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:15:GLN:HE21	23:X:15:GLN:HB2	1.68	0.41
25:Z:139:PHE:HB2	26:a:45:TRP:CD1	2.55	0.41
34:i:87:TYR:CE1	41:p:48:ARG:HG2	2.56	0.41
41:p:72:ASP:OD2	41:p:72:ASP:C	2.64	0.41
4:D:152:MET:HE2	4:D:152:MET:HB2	1.96	0.41
5:E:164:LEU:HD13	5:E:169:ILE:HD13	2.03	0.41
12:L:338:MET:HE2	12:L:338:MET:HB3	1.89	0.41
46:L:703:3PE:H292	34:i:80:ILE:HG23	2.03	0.41
13:M:438:SER:HA	13:M:441:ILE:HG22	2.02	0.41
14:N:228:LEU:HD23	14:N:228:LEU:HA	1.85	0.41
40:o:24:PHE:CE1	40:o:111:LYS:HD3	2.56	0.41
40:o:93:ASP:N	40:o:93:ASP:OD2	2.53	0.41
5:E:123:LYS:NZ	5:E:174:ASP:OD1	2.34	0.40
7:G:143:GLY:HA2	7:G:190:MET:HG2	2.03	0.40
10:J:26:PRO:HG2	10:J:76:THR:HG21	2.03	0.40
12:L:383:MET:HE2	12:L:383:MET:HB2	1.91	0.40
52:X:201:CDL:H511	52:X:201:CDL:HB4	1.76	0.40
40:o:55:ARG:HH22	41:p:119:SER:HB3	1.86	0.40
4:D:4:TRP:CH2	13:M:140:THR:HG23	2.57	0.40
4:D:6:PRO:HB3	4:D:10:TRP:CD1	2.55	0.40
4:D:62:LEU:HD13	4:D:425:PHE:CZ	2.57	0.40
6:F:409:ASP:OD1	6:F:409:ASP:N	2.52	0.40
46:I:204:3PE:H2B1	46:Z:200:3PE:H3C1	2.02	0.40
46:I:204:3PE:H2C2	46:I:204:3PE:H291	1.63	0.40
10:J:121:GLY:HA2	11:K:3:MET:HE3	2.02	0.40
12:L:381:THR:HG22	12:L:419:THR:HG22	2.04	0.40
13:M:203:PHE:O	13:M:207:MET:HG2	2.21	0.40
17:Q:70:MET:SD	42:q:126:PRO:HB2	2.61	0.40
24:Y:105:ARG:HD2	24:Y:105:ARG:HA	1.89	0.40
32:g:70:LEU:HD23	32:g:70:LEU:HA	1.87	0.40
5:E:144:CYS:SG	6:F:102:PRO:HA	2.61	0.40
12:L:112:PRO:HG3	39:n:178:MET:HB3	2.03	0.40
12:L:310:LEU:HA	12:L:313:MET:HE3	2.04	0.40
19:S:59:ASP:N	19:S:59:ASP:OD1	2.55	0.40
20:U:52:MET:HE3	20:U:52:MET:HB3	1.77	0.40
41:p:69:ARG:HA	41:p:69:ARG:HD2	1.83	0.40
6:F:403:THR:HB	47:F:502:SF4:S4	2.61	0.40
7:G:254:MET:HA	7:G:260:GLU:O	2.21	0.40
7:G:266:LYS:NZ	7:G:674:THR:OG1	2.49	0.40
12:L:22:MET:HB3	12:L:22:MET:HE3	1.74	0.40
52:L:702:CDL:H402	13:M:446:LEU:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:242:VAL:HG21	46:N:401:3PE:H31	2.04	0.40
15:O:211:LEU:O	15:O:215:SER:OG	2.29	0.40
19:S:34:ASP:O	19:S:38:LYS:HG2	2.21	0.40
24:Y:105:ARG:HH22	24:Y:107:TYR:HE1	1.69	0.40
30:e:83:GLU:C	30:e:83:GLU:OE1	2.65	0.40
40:o:121:MET:HE2	40:o:121:MET:HB3	1.93	0.40
45:A:301:PC1:H143	45:A:301:PC1:H111	1.87	0.40
4:D:66:MET:HE3	4:D:76:CYS:SG	2.61	0.40
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.87	0.40
11:K:33:LEU:HD21	14:N:64:SER:HB3	2.03	0.40
13:M:173:SER:HB2	33:h:101:ALA:HB2	2.03	0.40
17:Q:38:PHE:HE1	17:Q:58:GLU:HG2	1.85	0.40
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	2.03	0.40
31:f:11:TRP:O	31:f:14:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	102/115 (89%)	95 (93%)	6 (6%)	1 (1%)	12 14
2	B	153/216 (71%)	144 (94%)	9 (6%)	0	100 100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100 100
4	D	421/463 (91%)	399 (95%)	19 (4%)	3 (1%)	18 22
5	E	212/249 (85%)	206 (97%)	6 (3%)	0	100 100
6	F	431/464 (93%)	413 (96%)	17 (4%)	1 (0%)	43 53
7	G	689/727 (95%)	670 (97%)	17 (2%)	2 (0%)	36 45
8	H	317/318 (100%)	306 (96%)	10 (3%)	1 (0%)	36 45
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	164/175 (94%)	152 (93%)	10 (6%)	2 (1%)	10 11
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100 100
12	L	599/606 (99%)	570 (95%)	27 (4%)	2 (0%)	36 45
13	M	462/459 (101%)	452 (98%)	10 (2%)	0	100 100
14	N	346/347 (100%)	338 (98%)	8 (2%)	0	100 100
15	O	318/343 (93%)	309 (97%)	9 (3%)	0	100 100
16	P	307/380 (81%)	289 (94%)	13 (4%)	5 (2%)	7 7
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100 100
18	R	94/124 (76%)	90 (96%)	3 (3%)	1 (1%)	11 12
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100 100
20	T	83/156 (53%)	76 (92%)	7 (8%)	0	100 100
20	U	86/156 (55%)	83 (96%)	2 (2%)	1 (1%)	10 11
21	V	112/116 (97%)	109 (97%)	3 (3%)	0	100 100
22	W	113/128 (88%)	109 (96%)	4 (4%)	0	100 100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
24	Y	139/141 (99%)	136 (98%)	3 (2%)	0	100 100
25	Z	139/144 (96%)	135 (97%)	4 (3%)	0	100 100
26	a	68/70 (97%)	68 (100%)	0	0	100 100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100 100
28	c	47/76 (62%)	44 (94%)	3 (6%)	0	100 100
29	d	119/121 (98%)	117 (98%)	2 (2%)	0	100 100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100 100
31	f	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	6 5
32	g	99/154 (64%)	94 (95%)	5 (5%)	0	100 100
33	h	136/189 (72%)	136 (100%)	0	0	100 100
34	i	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	16 19
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100 100
36	k	79/98 (81%)	75 (95%)	4 (5%)	0	100 100
37	l	154/186 (83%)	145 (94%)	8 (5%)	1 (1%)	21 25
38	m	126/129 (98%)	117 (93%)	9 (7%)	0	100 100
39	n	170/179 (95%)	163 (96%)	6 (4%)	1 (1%)	21 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	p	171/176 (97%)	169 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	92/113 (81%)	87 (95%)	5 (5%)	0	100	100
44	s	42/109 (38%)	37 (88%)	5 (12%)	0	100	100
All	All	8131/9214 (88%)	7824 (96%)	284 (4%)	23 (0%)	37	45

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	199	LYS
34	i	118	PRO
6	F	87	ASP
18	R	95	HIS
31	f	3	LEU
4	D	57	ALA
7	G	186	TYR
7	G	651	LEU
10	J	24	PRO
12	L	562	LEU
16	P	169	ALA
16	P	195	SER
20	U	2	ASP
4	D	61	VAL
8	H	206	GLU
12	L	249	SER
16	P	335	GLN
37	l	40	ASP
10	J	116	VAL
16	P	189	GLY
1	A	49	LEU
39	n	85	PRO
4	D	80	ILE

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	A	93/100 (93%)	90 (97%)	3 (3%)	34	50
2	B	131/174 (75%)	125 (95%)	6 (5%)	24	35
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	366/392 (93%)	364 (100%)	2 (0%)	81	89
5	E	183/205 (89%)	182 (100%)	1 (0%)	81	89
6	F	347/368 (94%)	346 (100%)	1 (0%)	86	92
7	G	579/608 (95%)	576 (100%)	3 (0%)	81	89
8	H	275/274 (100%)	272 (99%)	3 (1%)	65	80
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	76
10	J	134/141 (95%)	131 (98%)	3 (2%)	45	63
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	60
12	L	530/533 (99%)	526 (99%)	4 (1%)	73	85
13	M	416/412 (101%)	412 (99%)	4 (1%)	68	81
14	N	316/315 (100%)	316 (100%)	0	100	100
15	O	283/303 (93%)	281 (99%)	2 (1%)	76	86
16	P	269/327 (82%)	267 (99%)	2 (1%)	76	86
17	Q	116/153 (76%)	112 (97%)	4 (3%)	32	47
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	76/82 (93%)	75 (99%)	1 (1%)	61	76
20	T	79/135 (58%)	75 (95%)	4 (5%)	21	31
20	U	81/135 (60%)	80 (99%)	1 (1%)	63	78
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	83
23	X	154/155 (99%)	152 (99%)	2 (1%)	61	76
24	Y	101/101 (100%)	99 (98%)	2 (2%)	48	66
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	85
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	70 (99%)	1 (1%)	59	75
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	106/106 (100%)	105 (99%)	1 (1%)	70	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	e	89/96 (93%)	86 (97%)	3 (3%)	32 47
31	f	54/54 (100%)	53 (98%)	1 (2%)	50 67
32	g	92/131 (70%)	91 (99%)	1 (1%)	65 80
33	h	121/158 (77%)	121 (100%)	0	100 100
34	i	121/121 (100%)	118 (98%)	3 (2%)	42 59
35	j	61/84 (73%)	56 (92%)	5 (8%)	10 14
36	k	63/76 (83%)	61 (97%)	2 (3%)	34 50
37	l	140/159 (88%)	139 (99%)	1 (1%)	76 86
38	m	114/115 (99%)	112 (98%)	2 (2%)	51 69
39	n	157/161 (98%)	156 (99%)	1 (1%)	78 88
40	o	110/120 (92%)	106 (96%)	4 (4%)	31 45
41	p	154/157 (98%)	153 (99%)	1 (1%)	78 88
42	q	131/131 (100%)	130 (99%)	1 (1%)	73 85
43	r	85/96 (88%)	83 (98%)	2 (2%)	43 60
44	s	43/92 (47%)	42 (98%)	1 (2%)	44 62
All	All	7177/7891 (91%)	7093 (99%)	84 (1%)	61 78

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	97	LEU
1	A	98	LEU
2	B	30	VAL
2	B	50	PHE
2	B	54	CYS
2	B	79	SER
2	B	81	ARG
2	B	125	TYR
4	D	110	SER
4	D	164	MET
5	E	165	THR
6	F	87	ASP
7	G	190	MET
7	G	436	SER
7	G	483	VAL
8	H	121	TRP

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Mol	Chain	Res	Type
8	H	194	ASN
8	H	268	MET
9	I	29	GLU
9	I	78	ILE
10	J	5	ILE
10	J	106	TYR
10	J	135	PHE
11	K	2	SER
11	K	43	MET
12	L	411	MET
12	L	440	LEU
12	L	503	GLU
12	L	581	LYS
13	M	114	GLU
13	M	116	ILE
13	M	375	LEU
13	M	416	ARG
15	O	60	ASP
15	O	191	GLU
16	P	143	SER
16	P	342	THR
17	Q	8	THR
17	Q	15	GLU
17	Q	44	ASN
17	Q	74	SER
19	S	58	SER
20	T	8	LEU
20	T	16	LEU
20	T	23	ASP
20	T	25	ILE
20	U	64	ASP
22	W	95	VAL
23	X	11	ASP
23	X	131	LYS
24	Y	114	CYS
24	Y	139	LYS
25	Z	91	GLU
27	b	9	LYS
29	d	106	LYS
30	e	17	MET
30	e	86	ILE
30	e	92	THR

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Mol	Chain	Res	Type
31	f	4	LEU
32	g	86	GLN
34	i	1	SER
34	i	65	ARG
34	i	112	THR
35	j	20	SER
35	j	32	MET
35	j	45	ASP
35	j	47	VAL
35	j	60	THR
36	k	20	GLN
36	k	48	GLU
37	l	154	VAL
38	m	94	ILE
38	m	113	LYS
39	n	150	THR
40	o	30	PHE
40	o	47	ASP
40	o	95	VAL
40	o	109	GLN
41	p	3	SER
42	q	11	LEU
43	r	31	SER
43	r	68	VAL
44	s	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
2	B	106	GLN
3	C	160	HIS
3	C	192	GLN
3	C	211	GLN
4	D	13	GLN
4	D	127	ASN
5	E	42	HIS
5	E	74	GLN
5	E	99	HIS
6	F	200	GLN
6	F	373	ASN
6	F	421	HIS

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Mol	Chain	Res	Type
7	G	237	ASN
7	G	293	HIS
7	G	311	GLN
7	G	392	ASN
7	G	475	GLN
7	G	517	ASN
7	G	644	GLN
8	H	5	ASN
8	H	47	GLN
8	H	99	ASN
8	H	304	HIS
9	I	23	GLN
11	K	7	ASN
12	L	56	HIS
12	L	135	ASN
12	L	199	GLN
12	L	514	HIS
12	L	541	ASN
12	L	603	ASN
13	M	82	HIS
13	M	88	ASN
13	M	175	ASN
13	M	180	GLN
13	M	188	ASN
13	M	399	ASN
13	M	415	GLN
14	N	48	HIS
14	N	186	HIS
14	N	289	ASN
15	O	57	HIS
15	O	271	ASN
15	O	291	GLN
15	O	294	GLN
17	Q	50	ASN
19	S	80	ASN
22	W	44	ASN
22	W	98	GLN
23	X	15	GLN
23	X	29	HIS
24	Y	7	GLN
25	Z	60	GLN
25	Z	84	GLN

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Mol	Chain	Res	Type
27	b	51	ASN
27	b	73	GLN
29	d	79	GLN
29	d	117	HIS
31	f	30	ASN
33	h	143	ASN
34	i	37	GLN
34	i	47	ASN
34	i	82	HIS
37	l	155	HIS
38	m	32	GLN
39	n	140	GLN
40	o	46	ASN
41	p	58	ASN
41	p	123	ASN
41	p	133	GLN
42	q	72	ASN
43	r	24	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	2MR	D	85	4	10,12,13	2.40	2 (20%)	5,13,15	1.78	1 (20%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	7,9,11	1.69	2 (28%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.64	1 (14%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.69	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	L	1	12	8,9,10	1.52	1 (12%)	7,9,11	1.61	1 (14%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.63	2 (28%)
13	FME	M	1	13	8,9,10	1.49	1 (12%)	7,9,11	1.74	3 (42%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	7,9,11	1.60	2 (28%)
2	WYK	B	77	2	9,11,12	2.49	2 (22%)	7,13,15	0.27	0

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	WYK	CZ-NE	6.56	1.46	1.33
4	D	85	2MR	CZ-NH2	5.29	1.45	1.33
4	D	85	2MR	CZ-NE	5.04	1.45	1.34
8	H	1	FME	CN-N	3.69	1.45	1.33
12	L	1	FME	CN-N	3.68	1.45	1.33
1	A	1	FME	CN-N	3.67	1.45	1.33
11	K	1	FME	CN-N	3.66	1.45	1.33
10	J	1	FME	CN-N	3.66	1.45	1.33
14	N	1	FME	CN-N	3.64	1.45	1.33
13	M	1	FME	CN-N	3.61	1.45	1.33
2	B	77	WYK	CZ-NH2	-2.21	1.25	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	85	2MR	CD-NE-CZ	-3.20	117.42	123.41
14	N	1	FME	CE-SD-CG	2.71	109.70	100.40
13	M	1	FME	CE-SD-CG	2.69	109.64	100.40
1	A	1	FME	CE-SD-CG	2.66	109.53	100.40
8	H	1	FME	CE-SD-CG	2.64	109.46	100.40
10	J	1	FME	CE-SD-CG	2.63	109.44	100.40
12	L	1	FME	CE-SD-CG	2.63	109.42	100.40
11	K	1	FME	CE-SD-CG	2.57	109.22	100.40
13	M	1	FME	CA-N-CN	-2.17	119.49	122.82
10	J	1	FME	O1-CN-N	-2.09	119.76	125.27
14	N	1	FME	O1-CN-N	-2.06	119.85	125.27
8	H	1	FME	O1-CN-N	-2.05	119.86	125.27
13	M	1	FME	O1-CN-N	-2.03	119.92	125.27
11	K	1	FME	O1-CN-N	-2.02	119.94	125.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	PC1	M	602	-	45,45,53	1.38	6 (13%)	51,53,61	1.05	2 (3%)
46	3PE	I	204	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	M	601	-	42,42,50	0.92	4 (9%)	45,47,55	1.18	2 (4%)
46	3PE	Y	205	-	31,31,50	1.07	4 (12%)	34,36,55	1.16	2 (5%)
47	SF4	I	203	9	0,12,12	-	-	-		
48	FES	E	301	5	0,4,4	-	-	-		
52	CDL	N	402	-	84,84,99	0.98	7 (8%)	90,96,111	1.13	4 (4%)
51	LMT	Y	201	-	36,36,36	1.16	2 (5%)	47,47,47	1.05	3 (6%)
46	3PE	d	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.09	2 (3%)
46	3PE	A	303	-	36,36,50	1.01	4 (11%)	39,41,55	1.11	2 (5%)
51	LMT	M	604	-	36,36,36	1.18	2 (5%)	47,47,47	1.01	1 (2%)
46	3PE	b	101	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
52	CDL	X	201	-	85,85,99	0.97	7 (8%)	91,97,111	1.10	4 (4%)
47	SF4	G	802	7	0,12,12	-	-	-		
46	3PE	m	201	-	39,39,50	0.97	4 (10%)	42,44,55	1.13	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
46	3PE	M	603	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-		
52	CDL	d	202	-	64,64,99	1.09	7 (10%)	70,76,111	1.14	4 (5%)
46	3PE	H	601	-	35,35,50	1.01	4 (11%)	38,40,55	1.17	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	CDL	h	202	-	67,67,99	1.09	7 (10%)	73,79,111	1.16	4 (5%)
46	3PE	j	101	-	38,38,50	0.98	4 (10%)	41,43,55	1.13	2 (4%)
45	PC1	B	202	-	50,50,53	1.33	6 (12%)	56,58,61	1.04	2 (3%)
51	LMT	L	704	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
45	PC1	O	401	-	29,29,53	1.51	6 (20%)	35,37,61	1.06	1 (2%)
46	3PE	A	302	-	46,46,50	0.90	4 (8%)	49,51,55	1.08	2 (4%)
45	PC1	N	403	-	39,39,53	1.45	5 (12%)	45,47,61	1.06	2 (4%)
46	3PE	L	705	-	44,44,50	0.91	4 (9%)	47,49,55	1.11	2 (4%)
46	3PE	Z	200	-	42,42,50	0.94	4 (9%)	45,47,55	1.08	2 (4%)
49	FMN	F	501	-	33,33,33	2.78	10 (30%)	48,50,50	1.86	16 (33%)
58	MYR	o	201	40	14,14,15	0.44	0	13,13,15	0.92	0
46	3PE	p	201	-	38,38,50	0.98	4 (10%)	41,43,55	1.11	2 (4%)
51	LMT	H	602	-	36,36,36	1.15	2 (5%)	47,47,47	0.99	1 (2%)
55	NDP	P	501	-	49,52,52	4.00	25 (51%)	66,80,80	2.05	14 (21%)
47	SF4	I	202	9	0,12,12	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
45	PC1	A	301	-	49,49,53	1.35	6 (12%)	55,57,61	1.03	2 (3%)
57	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.57	5 (14%)
57	EHZ	T	101	20	29,36,37	1.73	5 (17%)	35,44,47	1.43	5 (14%)
45	PC1	H	603	-	45,45,53	1.37	6 (13%)	51,53,61	1.04	2 (3%)
54	DGT	O	404	53	29,33,33	3.18	14 (48%)	44,52,52	2.12	12 (27%)
46	3PE	Y	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.07	2 (3%)
46	3PE	Y	202	-	38,38,50	0.98	4 (10%)	41,43,55	1.15	2 (4%)
46	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
46	3PE	K	101	-	42,42,50	0.93	4 (9%)	45,47,55	1.10	2 (4%)
52	CDL	L	702	-	78,78,99	1.01	7 (8%)	84,90,111	1.11	4 (4%)
52	CDL	q	201	-	63,63,99	1.12	7 (11%)	69,75,111	1.14	4 (5%)
46	3PE	h	201	-	35,35,50	1.02	4 (11%)	38,40,55	1.15	2 (5%)
46	3PE	O	403	-	35,35,50	1.02	4 (11%)	38,40,55	1.16	2 (5%)
51	LMT	Y	206	-	36,36,36	1.15	2 (5%)	47,47,47	1.00	1 (2%)
46	3PE	Y	204	-	43,43,50	0.92	4 (9%)	46,48,55	1.11	2 (4%)
46	3PE	M	605	-	30,30,50	1.10	4 (13%)	33,35,55	1.16	2 (6%)
46	3PE	O	405	-	40,40,50	0.96	4 (10%)	43,45,55	1.13	2 (4%)
46	3PE	L	701	-	38,38,50	0.98	4 (10%)	41,43,55	1.10	2 (4%)
46	3PE	L	703	-	42,42,50	0.93	4 (9%)	45,47,55	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	N	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PC1	M	602	-	-	22/49/49/57	-
46	3PE	I	204	-	-	24/54/54/54	-
46	3PE	M	601	-	-	23/46/46/54	-
46	3PE	Y	205	-	-	18/35/35/54	-
47	SF4	I	203	9	-	-	0/6/5/5
48	FES	E	301	5	-	-	0/1/1/1
52	CDL	N	402	-	-	49/95/95/110	-
51	LMT	Y	201	-	-	11/21/61/61	0/2/2/2
46	3PE	d	201	-	-	22/52/52/54	-
46	3PE	A	303	-	-	10/40/40/54	-
51	LMT	M	604	-	-	10/21/61/61	0/2/2/2
46	3PE	b	101	-	-	25/54/54/54	-
52	CDL	X	201	-	-	46/96/96/110	-
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	m	201	-	-	17/43/43/54	-
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	M	603	-	-	24/54/54/54	-
48	FES	G	803	7	-	-	0/1/1/1
52	CDL	d	202	-	-	36/75/75/110	-
46	3PE	H	601	-	-	16/39/39/54	-
52	CDL	h	202	-	-	32/78/78/110	-
46	3PE	j	101	-	-	16/42/42/54	-
45	PC1	B	202	-	-	24/54/54/57	-
51	LMT	L	704	-	-	9/21/61/61	0/2/2/2
45	PC1	O	401	-	-	11/32/32/57	-
46	3PE	A	302	-	-	25/50/50/54	-
45	PC1	N	403	-	-	24/43/43/57	-
46	3PE	L	705	-	-	20/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	Z	200	-	-	18/46/46/54	-
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
58	MYR	o	201	40	-	6/11/12/13	-
46	3PE	p	201	-	-	25/42/42/54	-
51	LMT	H	602	-	-	8/21/61/61	0/2/2/2
55	NDP	P	501	-	-	8/34/77/77	0/5/5/5
57	EHZ	U	101	20	-	18/42/44/45	-
47	SF4	B	201	2	-	-	0/6/5/5
45	PC1	A	301	-	-	19/53/53/57	-
47	SF4	I	202	9	-	-	0/6/5/5
57	EHZ	T	101	20	-	11/42/44/45	-
45	PC1	H	603	-	-	20/49/49/57	-
54	DGT	O	404	53	-	6/22/34/34	0/3/3/3
46	3PE	Y	203	-	-	28/54/54/54	-
46	3PE	Y	202	-	-	16/42/42/54	-
46	3PE	I	201	-	-	19/54/54/54	-
46	3PE	K	101	-	-	21/46/46/54	-
52	CDL	L	702	-	-	46/89/89/110	-
52	CDL	q	201	-	-	28/74/74/110	-
46	3PE	h	201	-	-	16/39/39/54	-
46	3PE	O	403	-	-	20/39/39/54	-
51	LMT	Y	206	-	-	9/21/61/61	0/2/2/2
46	3PE	Y	204	-	-	23/47/47/54	-
46	3PE	M	605	-	-	16/34/34/54	-
46	3PE	O	405	-	-	18/44/44/54	-
46	3PE	L	701	-	-	14/42/42/54	-
46	3PE	L	703	-	-	21/46/46/54	-
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	N	401	-	-	23/54/54/54	-

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	C6N-C5N	12.16	1.55	1.33
55	P	501	NDP	C2B-C1B	-8.70	1.30	1.53
55	P	501	NDP	C7N-N7N	8.35	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	501	NDP	O4B-C1B	8.25	1.61	1.42
55	P	501	NDP	O4D-C1D	8.11	1.61	1.42
54	O	404	DGT	C2'-C3'	-7.59	1.32	1.52
49	F	501	FMN	C4A-N5	7.33	1.45	1.30
55	P	501	NDP	C2D-C1D	-7.32	1.30	1.53
49	F	501	FMN	C10-N1	6.65	1.46	1.33
55	P	501	NDP	O4D-C4D	-6.49	1.30	1.45
54	O	404	DGT	C4-N3	6.36	1.49	1.34
57	T	101	EHZ	C15-N2	5.64	1.45	1.33
55	P	501	NDP	C6A-N6A	5.60	1.48	1.34
55	P	501	NDP	P2B-O2B	5.56	1.69	1.59
54	O	404	DGT	C2-N3	5.45	1.46	1.33
57	U	101	EHZ	C15-N2	5.40	1.45	1.33
54	O	404	DGT	O4'-C4'	5.36	1.57	1.45
57	T	101	EHZ	C12-N1	5.36	1.45	1.33
57	U	101	EHZ	C12-N1	5.35	1.45	1.33
49	F	501	FMN	C5A-N5	5.24	1.49	1.39
55	P	501	NDP	O4B-C4B	-5.23	1.33	1.45
54	O	404	DGT	O4'-C1'	-5.15	1.30	1.42
49	F	501	FMN	C2-N1	4.91	1.48	1.36
55	P	501	NDP	C2N-C3N	4.77	1.48	1.34
54	O	404	DGT	C2-N2	4.75	1.45	1.34
49	F	501	FMN	C9A-N10	4.62	1.49	1.41
49	F	501	FMN	C2-N3	4.33	1.49	1.39
55	P	501	NDP	C5A-C4A	-4.04	1.31	1.39
55	P	501	NDP	O7N-C7N	-4.03	1.14	1.24
55	P	501	NDP	O2D-C2D	3.97	1.52	1.43
54	O	404	DGT	C2'-C1'	3.91	1.63	1.52
49	F	501	FMN	C4-N3	3.89	1.46	1.38
54	O	404	DGT	C5'-C4'	-3.81	1.39	1.51
45	B	202	PC1	O31-C31	3.81	1.44	1.33
45	M	602	PC1	O31-C31	3.79	1.44	1.33
45	N	403	PC1	O31-C31	3.78	1.44	1.33
45	A	301	PC1	O31-C31	3.77	1.44	1.33
49	F	501	FMN	C10-N10	3.77	1.45	1.37
45	H	603	PC1	O31-C31	3.70	1.44	1.33
51	M	604	LMT	O5'-C1'	3.65	1.51	1.41
45	A	301	PC1	O21-C21	3.63	1.44	1.34
45	N	403	PC1	O21-C21	3.62	1.44	1.34
45	B	202	PC1	O21-C21	3.59	1.44	1.34
45	O	401	PC1	O21-C21	3.58	1.44	1.34
55	P	501	NDP	C8A-N9A	-3.56	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	602	PC1	O21-C21	3.52	1.44	1.34
45	H	603	PC1	O21-C21	3.49	1.44	1.34
51	Y	201	LMT	O5B-C1B	3.48	1.50	1.41
51	Y	206	LMT	O5'-C1'	3.48	1.50	1.41
55	P	501	NDP	C4N-C3N	3.39	1.56	1.49
51	H	602	LMT	O5B-C1B	3.33	1.50	1.41
51	Y	201	LMT	O5'-C1'	3.32	1.50	1.41
51	Y	206	LMT	O5B-C1B	3.30	1.50	1.41
51	L	704	LMT	O5'-C1'	3.26	1.50	1.41
51	M	604	LMT	O5B-C1B	3.26	1.50	1.41
51	H	602	LMT	O5'-C1'	3.24	1.50	1.41
51	L	704	LMT	O5B-C1B	3.16	1.49	1.41
49	F	501	FMN	O2-C2	-3.00	1.18	1.24
54	O	404	DGT	C5-N7	-2.95	1.33	1.39
55	P	501	NDP	C4N-C5N	2.80	1.56	1.48
54	O	404	DGT	C2-N1	2.77	1.44	1.37
52	q	201	CDL	OB8-CB7	2.76	1.41	1.33
52	L	702	CDL	OB8-CB7	2.74	1.41	1.33
52	d	202	CDL	OB8-CB7	2.70	1.41	1.33
54	O	404	DGT	O3'-C3'	2.69	1.49	1.43
52	X	201	CDL	OB8-CB7	2.69	1.41	1.33
52	h	202	CDL	OA6-CA4	-2.67	1.39	1.46
49	F	501	FMN	O4-C4	-2.66	1.18	1.23
52	X	201	CDL	OA6-CA4	-2.65	1.40	1.46
52	h	202	CDL	OB8-CB7	2.64	1.41	1.33
52	N	402	CDL	OB8-CB7	2.63	1.41	1.33
52	L	702	CDL	OA6-CA4	-2.59	1.40	1.46
45	H	603	PC1	O21-C2	-2.58	1.40	1.46
45	M	602	PC1	O21-C2	-2.58	1.40	1.46
52	q	201	CDL	OA6-CA4	-2.58	1.40	1.46
52	N	402	CDL	OA6-CA4	-2.58	1.40	1.46
46	b	101	3PE	O21-C2	-2.58	1.40	1.46
45	A	301	PC1	O21-C2	-2.57	1.40	1.46
46	A	303	3PE	O21-C2	-2.56	1.40	1.46
46	L	701	3PE	O21-C2	-2.56	1.40	1.46
46	N	401	3PE	O21-C2	-2.56	1.40	1.46
46	O	405	3PE	O21-C2	-2.54	1.40	1.46
46	Y	202	3PE	O21-C2	-2.54	1.40	1.46
52	d	202	CDL	OA6-CA4	-2.54	1.40	1.46
55	P	501	NDP	O3B-C3B	-2.53	1.37	1.43
52	N	402	CDL	OB6-CB5	2.53	1.41	1.34
46	m	201	3PE	O21-C2	-2.53	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	601	3PE	O21-C2	-2.52	1.40	1.46
46	L	705	3PE	O21-C2	-2.52	1.40	1.46
46	I	204	3PE	O21-C2	-2.52	1.40	1.46
54	O	404	DGT	C5-C6	2.52	1.53	1.44
46	Z	200	3PE	O21-C2	-2.51	1.40	1.46
55	P	501	NDP	O3D-C3D	-2.51	1.37	1.43
46	I	201	3PE	O21-C2	-2.51	1.40	1.46
46	A	302	3PE	O21-C2	-2.50	1.40	1.46
46	Y	204	3PE	O21-C2	-2.50	1.40	1.46
46	j	101	3PE	O21-C2	-2.50	1.40	1.46
46	M	605	3PE	O21-C2	-2.50	1.40	1.46
54	O	404	DGT	C6-N1	2.50	1.43	1.38
46	Y	203	3PE	O21-C2	-2.49	1.40	1.46
45	B	202	PC1	O21-C2	-2.49	1.40	1.46
52	d	202	CDL	OB6-CB5	2.49	1.41	1.34
46	K	101	3PE	O21-C2	-2.48	1.40	1.46
46	h	201	3PE	O21-C2	-2.48	1.40	1.46
52	h	202	CDL	OB6-CB4	-2.48	1.40	1.46
52	q	201	CDL	OB6-CB4	-2.48	1.40	1.46
46	Y	205	3PE	O21-C2	-2.48	1.40	1.46
52	L	702	CDL	OB6-CB4	-2.48	1.40	1.46
52	X	201	CDL	OB6-CB5	2.48	1.41	1.34
55	P	501	NDP	C6N-N1N	2.48	1.43	1.37
46	O	405	3PE	O31-C31	2.47	1.40	1.33
55	P	501	NDP	C5A-N7A	-2.47	1.34	1.39
52	h	202	CDL	OA8-CA7	2.47	1.40	1.33
46	H	601	3PE	O21-C2	-2.47	1.40	1.46
46	L	703	3PE	O21-C2	-2.47	1.40	1.46
46	A	303	3PE	O31-C31	2.47	1.40	1.33
55	P	501	NDP	C7N-C3N	2.47	1.54	1.48
45	N	403	PC1	O21-C2	-2.47	1.40	1.46
46	p	201	3PE	O21-C2	-2.47	1.40	1.46
45	O	401	PC1	O21-C2	-2.46	1.40	1.46
46	p	201	3PE	O31-C31	2.46	1.40	1.33
52	X	201	CDL	OA8-CA7	2.46	1.40	1.33
52	X	201	CDL	OB6-CB4	-2.45	1.40	1.46
52	q	201	CDL	OB6-CB5	2.45	1.41	1.34
54	O	404	DGT	O6-C6	-2.45	1.18	1.23
52	q	201	CDL	OA8-CA7	2.45	1.40	1.33
52	L	702	CDL	OA8-CA7	2.45	1.40	1.33
52	h	202	CDL	OB6-CB5	2.44	1.41	1.34
46	A	302	3PE	O31-C31	2.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	U	101	EHZ	C9-S1	2.44	1.82	1.76
46	O	403	3PE	O21-C2	-2.44	1.40	1.46
46	O	403	3PE	O31-C31	2.44	1.40	1.33
46	d	201	3PE	O21-C2	-2.43	1.40	1.46
46	M	603	3PE	O21-C2	-2.43	1.40	1.46
46	L	705	3PE	O31-C31	2.43	1.40	1.33
46	j	101	3PE	O31-C31	2.43	1.40	1.33
46	h	201	3PE	O31-C31	2.42	1.40	1.33
46	I	201	3PE	O31-C31	2.42	1.40	1.33
46	L	701	3PE	O31-C31	2.41	1.40	1.33
46	L	703	3PE	O31-C31	2.41	1.40	1.33
52	N	402	CDL	OA8-CA7	2.41	1.40	1.33
46	Y	204	3PE	O31-C31	2.41	1.40	1.33
57	T	101	EHZ	C9-S1	2.41	1.82	1.76
52	d	202	CDL	OB6-CB4	-2.41	1.40	1.46
46	M	605	3PE	O31-C31	2.40	1.40	1.33
46	d	201	3PE	O31-C31	2.40	1.40	1.33
46	Y	205	3PE	O31-C31	2.40	1.40	1.33
52	N	402	CDL	OB6-CB4	-2.40	1.40	1.46
46	H	601	3PE	O31-C31	2.39	1.40	1.33
46	Y	202	3PE	O31-C31	2.39	1.40	1.33
46	I	204	3PE	O31-C31	2.39	1.40	1.33
52	L	702	CDL	OB6-CB5	2.38	1.41	1.34
45	O	401	PC1	P-O11	2.38	1.68	1.59
46	Y	203	3PE	O31-C31	2.38	1.40	1.33
46	K	101	3PE	O31-C31	2.38	1.40	1.33
46	m	201	3PE	O31-C31	2.37	1.40	1.33
45	M	602	PC1	P-O11	2.37	1.68	1.59
46	Z	200	3PE	O31-C31	2.36	1.40	1.33
46	M	601	3PE	O31-C31	2.36	1.40	1.33
45	N	403	PC1	C22-C21	2.36	1.57	1.50
46	M	603	3PE	O31-C31	2.36	1.40	1.33
46	N	401	3PE	O31-C31	2.35	1.40	1.33
52	d	202	CDL	OA8-CA7	2.35	1.40	1.33
46	b	101	3PE	O31-C31	2.33	1.40	1.33
45	N	403	PC1	P-O11	2.33	1.68	1.59
55	P	501	NDP	PA-O5B	2.32	1.68	1.59
45	B	202	PC1	P-O11	2.32	1.68	1.59
55	P	501	NDP	P2B-O1X	2.32	1.58	1.50
45	O	401	PC1	C22-C21	2.31	1.57	1.50
45	A	301	PC1	P-O11	2.30	1.68	1.59
45	A	301	PC1	C22-C21	2.30	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	603	3PE	O21-C21	2.28	1.40	1.34
45	H	603	PC1	C22-C21	2.28	1.57	1.50
57	T	101	EHZ	O4-C15	-2.28	1.18	1.23
45	B	202	PC1	C22-C21	2.28	1.57	1.50
45	M	602	PC1	C22-C21	2.27	1.57	1.50
45	O	401	PC1	O31-C31	2.26	1.44	1.33
45	H	603	PC1	P-O11	2.25	1.68	1.59
57	T	101	EHZ	O3-C12	-2.24	1.18	1.23
46	O	403	3PE	O21-C21	2.21	1.40	1.34
46	N	401	3PE	O31-C3	-2.21	1.40	1.45
52	d	202	CDL	OA8-CA6	-2.19	1.40	1.45
46	I	201	3PE	O31-C3	-2.19	1.40	1.45
46	Z	200	3PE	O21-C21	2.19	1.40	1.34
46	d	201	3PE	O21-C21	2.18	1.40	1.34
46	L	703	3PE	O21-C21	2.18	1.40	1.34
46	Y	203	3PE	O31-C3	-2.18	1.40	1.45
46	h	201	3PE	O21-C21	2.18	1.40	1.34
57	U	101	EHZ	O3-C12	-2.18	1.18	1.23
46	Z	200	3PE	O31-C3	-2.17	1.40	1.45
52	d	202	CDL	OA6-CA5	2.17	1.40	1.34
46	M	605	3PE	O21-C21	2.17	1.40	1.34
57	U	101	EHZ	O4-C15	-2.17	1.19	1.23
46	K	101	3PE	O21-C21	2.17	1.40	1.34
46	Y	202	3PE	O31-C3	-2.16	1.40	1.45
46	M	603	3PE	O31-C3	-2.16	1.40	1.45
46	I	201	3PE	O21-C21	2.16	1.40	1.34
46	m	201	3PE	O21-C21	2.15	1.40	1.34
52	q	201	CDL	OA8-CA6	-2.15	1.40	1.45
46	O	405	3PE	O21-C21	2.15	1.40	1.34
46	A	302	3PE	O21-C21	2.14	1.40	1.34
46	L	701	3PE	O21-C21	2.14	1.40	1.34
46	p	201	3PE	O21-C21	2.14	1.40	1.34
55	P	501	NDP	C5B-C4B	2.14	1.58	1.51
52	q	201	CDL	OA6-CA5	2.14	1.40	1.34
46	Y	205	3PE	O21-C21	2.14	1.40	1.34
46	Y	202	3PE	O21-C21	2.14	1.40	1.34
46	Y	203	3PE	O21-C21	2.14	1.40	1.34
46	H	601	3PE	O21-C21	2.13	1.40	1.34
46	M	605	3PE	O31-C3	-2.13	1.40	1.45
46	I	204	3PE	O21-C21	2.13	1.40	1.34
46	L	701	3PE	O31-C3	-2.13	1.40	1.45
52	h	202	CDL	OA8-CA6	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	703	3PE	O31-C3	-2.13	1.40	1.45
46	O	403	3PE	O31-C3	-2.12	1.40	1.45
46	b	101	3PE	O31-C3	-2.12	1.40	1.45
46	j	101	3PE	O21-C21	2.12	1.40	1.34
46	H	601	3PE	O31-C3	-2.12	1.40	1.45
46	d	201	3PE	O31-C3	-2.12	1.40	1.45
52	N	402	CDL	OA6-CA5	2.12	1.40	1.34
46	L	705	3PE	O21-C21	2.11	1.40	1.34
46	N	401	3PE	O21-C21	2.11	1.40	1.34
46	I	204	3PE	O31-C3	-2.11	1.40	1.45
45	O	401	PC1	P-O13	2.11	1.67	1.59
46	L	705	3PE	O31-C3	-2.11	1.40	1.45
45	M	602	PC1	P-O13	2.11	1.67	1.59
52	L	702	CDL	OA6-CA5	2.11	1.40	1.34
46	m	201	3PE	O31-C3	-2.11	1.40	1.45
46	h	201	3PE	O31-C3	-2.10	1.40	1.45
52	X	201	CDL	OA8-CA6	-2.10	1.40	1.45
46	j	101	3PE	O31-C3	-2.10	1.40	1.45
46	K	101	3PE	O31-C3	-2.10	1.40	1.45
52	L	702	CDL	OA8-CA6	-2.09	1.40	1.45
46	M	601	3PE	O31-C3	-2.09	1.40	1.45
46	Y	204	3PE	O21-C21	2.09	1.40	1.34
52	X	201	CDL	OA6-CA5	2.09	1.40	1.34
46	M	601	3PE	O21-C21	2.08	1.40	1.34
45	A	301	PC1	P-O13	2.08	1.67	1.59
46	b	101	3PE	O21-C21	2.08	1.40	1.34
46	p	201	3PE	O31-C3	-2.07	1.40	1.45
46	A	303	3PE	O21-C21	2.07	1.40	1.34
46	A	302	3PE	O31-C3	-2.07	1.40	1.45
46	Y	204	3PE	O31-C3	-2.07	1.40	1.45
52	N	402	CDL	OA8-CA6	-2.07	1.40	1.45
46	A	303	3PE	O31-C3	-2.07	1.40	1.45
46	O	405	3PE	O31-C3	-2.06	1.40	1.45
46	Y	205	3PE	O31-C3	-2.06	1.40	1.45
45	B	202	PC1	P-O13	2.05	1.67	1.59
52	h	202	CDL	OA6-CA5	2.04	1.40	1.34
45	H	603	PC1	P-O13	2.03	1.67	1.59

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	404	DGT	C1'-N9-C8	6.13	141.59	127.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	404	DGT	C1'-N9-C4	-5.56	110.07	125.48
55	P	501	NDP	C4A-N9A-C1B	-5.54	113.39	126.59
55	P	501	NDP	N6A-C6A-N1A	-5.54	106.22	118.35
55	P	501	NDP	N3A-C2A-N1A	-5.45	120.08	128.60
55	P	501	NDP	C5A-C4A-N3A	-5.39	119.71	126.75
57	U	101	EHZ	C8-C9-S1	5.30	120.19	113.63
49	F	501	FMN	C9-C8-C7	5.07	126.93	119.67
54	O	404	DGT	C5-C4-N3	-4.98	120.38	128.46
49	F	501	FMN	C7M-C7-C6	4.91	128.57	119.49
55	P	501	NDP	C1B-N9A-C8A	4.86	138.11	127.14
57	T	101	EHZ	C8-C9-S1	4.57	119.28	113.63
55	P	501	NDP	C5A-C6A-N6A	4.47	133.16	123.43
55	P	501	NDP	N9A-C8A-N7A	-4.46	107.81	113.91
52	N	402	CDL	OB6-CB5-C51	4.35	120.87	111.50
49	F	501	FMN	C8M-C8-C7	-4.34	111.84	120.74
54	O	404	DGT	C2-N3-C4	4.33	120.02	112.30
46	O	403	3PE	O21-C21-C22	4.24	120.64	111.50
46	Y	202	3PE	O21-C21-C22	4.14	120.43	111.50
46	M	603	3PE	O21-C21-C22	4.14	120.42	111.50
46	M	601	3PE	O21-C21-C22	4.12	120.38	111.50
45	N	403	PC1	O21-C21-C22	4.05	120.22	111.50
46	I	201	3PE	O21-C21-C22	4.04	120.20	111.50
52	d	202	CDL	OA6-CA5-C11	4.03	120.18	111.50
46	h	201	3PE	O21-C21-C22	4.01	120.15	111.50
46	j	101	3PE	O21-C21-C22	4.01	120.14	111.50
46	M	605	3PE	O21-C21-C22	4.01	120.14	111.50
45	O	401	PC1	O21-C21-C22	4.00	120.12	111.50
46	d	201	3PE	O21-C21-C22	4.00	120.12	111.50
46	b	101	3PE	O21-C21-C22	4.00	120.12	111.50
52	L	702	CDL	OB6-CB5-C51	3.99	120.10	111.50
46	Y	205	3PE	O21-C21-C22	3.99	120.10	111.50
46	m	201	3PE	O21-C21-C22	3.99	120.09	111.50
46	L	705	3PE	O21-C21-C22	3.98	120.07	111.50
52	X	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
52	h	202	CDL	OA6-CA5-C11	3.97	120.06	111.50
52	N	402	CDL	OA6-CA5-C11	3.96	120.04	111.50
46	Y	204	3PE	O21-C21-C22	3.95	120.02	111.50
46	H	601	3PE	O21-C21-C22	3.94	120.00	111.50
52	h	202	CDL	OB6-CB5-C51	3.93	119.97	111.50
45	B	202	PC1	O21-C21-C22	3.92	119.96	111.50
52	q	201	CDL	OA6-CA5-C11	3.92	119.94	111.50
46	L	703	3PE	O21-C21-C22	3.92	119.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	O	405	3PE	O21-C21-C22	3.91	119.93	111.50
46	K	101	3PE	O21-C21-C22	3.91	119.92	111.50
45	H	603	PC1	O21-C21-C22	3.91	119.92	111.50
46	Y	203	3PE	O21-C21-C22	3.88	119.87	111.50
52	L	702	CDL	OA6-CA5-C11	3.87	119.85	111.50
46	p	201	3PE	O21-C21-C22	3.87	119.83	111.50
46	A	303	3PE	O21-C21-C22	3.87	119.83	111.50
52	q	201	CDL	OB6-CB5-C51	3.86	119.82	111.50
46	N	401	3PE	O21-C21-C22	3.86	119.82	111.50
46	I	204	3PE	O21-C21-C22	3.84	119.77	111.50
46	A	302	3PE	O21-C21-C22	3.80	119.70	111.50
45	M	602	PC1	O21-C21-C22	3.80	119.68	111.50
46	Z	200	3PE	O21-C21-C22	3.80	119.68	111.50
46	L	701	3PE	O21-C21-C22	3.78	119.64	111.50
52	X	201	CDL	OA6-CA5-C11	3.70	119.48	111.50
55	P	501	NDP	C2A-N3A-C4A	3.67	120.43	111.75
45	A	301	PC1	O21-C21-C22	3.64	119.35	111.50
55	P	501	NDP	N3A-C4A-N9A	3.40	132.68	127.08
46	H	601	3PE	O31-C31-C32	3.35	120.16	111.38
49	F	501	FMN	C4-N3-C2	-3.34	119.47	125.64
52	d	202	CDL	OB6-CB5-C51	3.30	120.00	110.80
51	Y	206	LMT	C1B-O1B-C4'	-3.23	109.96	117.96
55	P	501	NDP	C5A-N7A-C8A	3.09	107.90	103.51
54	O	404	DGT	N9-C8-N7	-2.99	107.75	113.39
51	L	704	LMT	C1B-O1B-C4'	-2.98	110.58	117.96
51	H	602	LMT	C1B-O1B-C4'	-2.98	110.59	117.96
54	O	404	DGT	C2-N1-C6	-2.95	119.72	125.10
54	O	404	DGT	N9-C4-N3	2.89	131.73	125.94
49	F	501	FMN	C7M-C7-C8	-2.88	114.84	120.74
52	h	202	CDL	OA8-CA7-C31	2.81	120.73	111.91
46	M	601	3PE	O31-C31-C32	2.75	120.55	111.91
46	A	302	3PE	O31-C31-C32	2.74	120.50	111.91
46	O	405	3PE	O31-C31-C32	2.73	120.48	111.91
45	B	202	PC1	O31-C31-C32	2.73	120.47	111.91
52	N	402	CDL	OA8-CA7-C31	2.72	120.46	111.91
46	p	201	3PE	O31-C31-C32	2.71	120.41	111.91
52	L	702	CDL	OB8-CB7-C71	2.70	120.39	111.91
52	q	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
46	d	201	3PE	O31-C31-C32	2.66	120.27	111.91
46	Y	205	3PE	O31-C31-C32	2.64	120.20	111.91
54	O	404	DGT	C5-C6-N1	2.63	119.87	113.19
55	P	501	NDP	PN-O3-PA	-2.63	123.81	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	Y	201	LMT	C1B-C2B-C3B	2.63	115.47	110.00
55	P	501	NDP	C2B-C1B-N9A	-2.62	109.11	113.53
46	O	403	3PE	O31-C31-C32	2.62	120.13	111.91
49	F	501	FMN	O4-C4-C4A	-2.62	119.66	126.60
52	d	202	CDL	OB8-CB7-C71	2.61	120.11	111.91
52	q	201	CDL	OA8-CA7-C31	2.61	120.10	111.91
49	F	501	FMN	C4A-C4-N3	2.60	119.80	113.19
52	N	402	CDL	OB8-CB7-C71	2.60	120.08	111.91
46	L	701	3PE	O31-C31-C32	2.60	120.06	111.91
46	j	101	3PE	O31-C31-C32	2.59	120.04	111.91
46	A	303	3PE	O31-C31-C32	2.59	120.03	111.91
46	m	201	3PE	O31-C31-C32	2.58	120.02	111.91
46	M	603	3PE	O31-C31-C32	2.58	120.01	111.91
52	X	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
46	K	101	3PE	O31-C31-C32	2.58	120.00	111.91
57	T	101	EHZ	C10-S1-C9	2.58	109.90	101.87
46	Y	202	3PE	O31-C31-C32	2.58	119.99	111.91
46	Y	204	3PE	O31-C31-C32	2.57	119.97	111.91
52	L	702	CDL	OA8-CA7-C31	2.57	119.97	111.91
45	A	301	PC1	O31-C31-C32	2.57	119.97	111.91
46	N	401	3PE	O31-C31-C32	2.57	119.96	111.91
52	X	201	CDL	OA8-CA7-C31	2.56	119.96	111.91
55	P	501	NDP	C4A-N9A-C8A	2.56	108.50	105.73
46	L	703	3PE	O31-C31-C32	2.56	119.94	111.91
45	M	602	PC1	O31-C31-C32	2.56	119.93	111.91
57	U	101	EHZ	C10-S1-C9	2.54	109.78	101.87
46	h	201	3PE	O31-C31-C32	2.53	119.85	111.91
45	N	403	PC1	O31-C31-C32	2.53	119.83	111.91
46	L	705	3PE	O31-C31-C32	2.52	119.82	111.91
46	Z	200	3PE	O31-C31-C32	2.52	119.81	111.91
46	I	201	3PE	O31-C31-C32	2.51	119.80	111.91
54	O	404	DGT	PA-O3A-PB	-2.51	124.22	132.83
54	O	404	DGT	PB-O3B-PG	-2.50	124.25	132.83
45	H	603	PC1	O31-C31-C32	2.49	119.73	111.91
46	b	101	3PE	O31-C31-C32	2.49	119.71	111.91
46	M	605	3PE	O31-C31-C32	2.48	119.69	111.91
52	d	202	CDL	OA8-CA7-C31	2.47	119.67	111.91
52	h	202	CDL	OB8-CB7-C71	2.46	119.64	111.91
46	I	204	3PE	O31-C31-C32	2.45	119.60	111.91
54	O	404	DGT	O6-C6-C5	-2.45	120.10	126.60
51	Y	201	LMT	C1B-O1B-C4'	-2.42	111.97	117.96
46	Y	203	3PE	O31-C31-C32	2.40	119.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	F	501	FMN	C4A-C10-N10	2.37	119.95	116.48
49	F	501	FMN	C9A-C5A-N5	-2.35	119.88	122.43
57	U	101	EHZ	C14-C13-C12	-2.27	108.58	112.36
57	U	101	EHZ	C13-C12-N1	2.19	120.11	116.42
49	F	501	FMN	C6-C5A-C9A	2.17	122.00	118.94
54	O	404	DGT	C8-N7-C5	2.16	108.14	104.24
49	F	501	FMN	C6-C7-C8	-2.15	116.58	119.67
49	F	501	FMN	C10-C4A-N5	-2.14	120.31	124.86
51	Y	201	LMT	O5B-C1B-C2B	2.12	114.84	110.35
49	F	501	FMN	C4-C4A-C10	2.11	120.34	116.79
57	T	101	EHZ	C16-C15-N2	2.11	120.78	116.58
57	T	101	EHZ	O2-C9-S1	-2.11	119.88	122.61
49	F	501	FMN	C9A-C9-C8	-2.08	115.11	119.30
49	F	501	FMN	C5A-C9A-N10	2.08	120.10	117.95
57	T	101	EHZ	C13-C12-N1	2.06	119.89	116.42
49	F	501	FMN	C4A-C10-N1	-2.06	119.95	124.73
57	U	101	EHZ	O2-C9-S1	-2.05	119.95	122.61
51	M	604	LMT	C1B-O1B-C4'	-2.03	112.93	117.96
55	P	501	NDP	C4A-C5A-N7A	-2.00	108.18	110.62

There are no chirality outliers.

All (974) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C11-O13-P-O12
45	B	202	PC1	C11-O13-P-O14
45	B	202	PC1	C22-C21-O21-C2
45	H	603	PC1	O11-C1-C2-O21
45	M	602	PC1	C11-O13-P-O14
45	N	403	PC1	C11-O13-P-O12
45	N	403	PC1	C1-O11-P-O12
45	N	403	PC1	C1-O11-P-O14
45	O	401	PC1	C1-O11-P-O13
46	A	302	3PE	O22-C21-O21-C2
46	A	303	3PE	O11-C1-C2-O21
46	A	303	3PE	O22-C21-O21-C2
46	H	601	3PE	C1-O11-P-O12
46	H	601	3PE	C1-O11-P-O14
46	I	201	3PE	C1-O11-P-O12
46	I	201	3PE	C1-O11-P-O14
46	I	204	3PE	C1-O11-P-O12
46	I	204	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
46	K	101	3PE	C1-O11-P-O12
46	K	101	3PE	C1-O11-P-O13
46	K	101	3PE	C1-O11-P-O14
46	K	101	3PE	O13-C11-C12-N
46	K	101	3PE	O21-C2-C3-O31
46	K	101	3PE	C22-C21-O21-C2
46	L	701	3PE	C1-O11-P-O12
46	L	701	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O14
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	L	705	3PE	C1-O11-P-O12
46	L	705	3PE	C1-O11-P-O13
46	L	705	3PE	C1-O11-P-O14
46	L	705	3PE	O22-C21-O21-C2
46	L	705	3PE	C22-C21-O21-C2
46	M	601	3PE	C11-O13-P-O12
46	M	601	3PE	C11-O13-P-O14
46	M	601	3PE	O11-C1-C2-O21
46	M	603	3PE	C1-O11-P-O12
46	M	603	3PE	C1-O11-P-O14
46	M	603	3PE	O22-C21-O21-C2
46	M	603	3PE	C22-C21-O21-C2
46	M	605	3PE	C1-O11-P-O12
46	M	605	3PE	C1-O11-P-O13
46	M	605	3PE	O11-C1-C2-O21
46	M	605	3PE	O22-C21-O21-C2
46	N	401	3PE	C1-O11-P-O14
46	O	403	3PE	C1-O11-P-O12
46	O	403	3PE	C1-O11-P-O13
46	O	403	3PE	C1-O11-P-O14
46	O	403	3PE	O22-C21-O21-C2
46	O	405	3PE	C1-O11-P-O12
46	O	405	3PE	C1-O11-P-O13
46	O	405	3PE	C1-O11-P-O14
46	O	405	3PE	O22-C21-O21-C2
46	Y	202	3PE	O13-C11-C12-N
46	Y	202	3PE	O21-C2-C3-O31
46	Y	202	3PE	O22-C21-O21-C2
46	Y	202	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C1-O11-P-O14
46	Y	203	3PE	O22-C21-O21-C2
46	Y	204	3PE	C1-O11-P-O12
46	Y	204	3PE	C1-O11-P-O13
46	Y	204	3PE	C1-O11-P-O14
46	Y	204	3PE	C11-O13-P-O12
46	Y	204	3PE	C11-O13-P-O14
46	Y	204	3PE	O13-C11-C12-N
46	Y	205	3PE	C1-O11-P-O12
46	Y	205	3PE	C1-O11-P-O14
46	Y	205	3PE	O11-C1-C2-O21
46	Z	200	3PE	C1-O11-P-O12
46	b	101	3PE	C1-O11-P-O12
46	b	101	3PE	C1-O11-P-O14
46	b	101	3PE	O13-C11-C12-N
46	d	201	3PE	O11-C1-C2-O21
46	h	201	3PE	C1-O11-P-O12
46	h	201	3PE	C1-O11-P-O13
46	h	201	3PE	C1-O11-P-O14
46	m	201	3PE	C1-O11-P-O12
46	m	201	3PE	C1-O11-P-O13
46	m	201	3PE	C1-O11-P-O14
46	m	201	3PE	C22-C21-O21-C2
46	p	201	3PE	C1-O11-P-O12
46	p	201	3PE	C1-O11-P-O14
46	p	201	3PE	C11-O13-P-O14
51	Y	206	LMT	C2'-C1'-O1'-C1
51	Y	206	LMT	O5'-C1'-O1'-C1
51	Y	206	LMT	C2-C1-O1'-C1'
52	L	702	CDL	CA2-OA2-PA1-OA4
52	N	402	CDL	C1-CA2-OA2-PA1
52	N	402	CDL	CA2-OA2-PA1-OA4
52	N	402	CDL	CB2-OB2-PB2-OB3
52	N	402	CDL	CB2-OB2-PB2-OB4
52	N	402	CDL	OB7-CB5-OB6-CB4
52	N	402	CDL	C51-CB5-OB6-CB4
52	X	201	CDL	CA2-C1-CB2-OB2
52	X	201	CDL	CA2-OA2-PA1-OA3
52	X	201	CDL	OB7-CB5-OB6-CB4
52	X	201	CDL	C51-CB5-OB6-CB4
52	d	202	CDL	CB2-C1-CA2-OA2
52	d	202	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	d	202	CDL	CA2-OA2-PA1-OA4
52	d	202	CDL	CB2-OB2-PB2-OB3
52	d	202	CDL	CB2-OB2-PB2-OB4
52	d	202	CDL	CB2-OB2-PB2-OB5
52	h	202	CDL	CA3-OA5-PA1-OA2
52	h	202	CDL	CA3-OA5-PA1-OA3
52	q	201	CDL	CB2-OB2-PB2-OB4
54	O	404	DGT	C5'-O5'-PA-O3A
54	O	404	DGT	C5'-O5'-PA-O1A
54	O	404	DGT	C5'-O5'-PA-O2A
55	P	501	NDP	C5B-O5B-PA-O1A
55	P	501	NDP	C5B-O5B-PA-O3
55	P	501	NDP	C2B-O2B-P2B-O3X
57	T	101	EHZ	C6-C7-C8-C9
57	T	101	EHZ	C11-C10-S1-C9
57	T	101	EHZ	C16-C17-C20-O6
57	T	101	EHZ	C18-C17-C20-O6
57	T	101	EHZ	C19-C17-C20-O6
57	U	101	EHZ	O1-C7-C8-C9
57	U	101	EHZ	C6-C7-C8-C9
57	U	101	EHZ	S1-C10-C11-N1
57	U	101	EHZ	C15-C16-C17-C18
57	U	101	EHZ	C15-C16-C17-C19
57	U	101	EHZ	C15-C16-C17-C20
57	U	101	EHZ	O5-C16-C17-C18
57	U	101	EHZ	O5-C16-C17-C19
57	U	101	EHZ	O5-C16-C17-C20
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
46	O	403	3PE	O32-C31-O31-C3
46	O	405	3PE	O32-C31-O31-C3
46	Y	204	3PE	O32-C31-O31-C3
46	d	201	3PE	O32-C31-O31-C3
46	p	201	3PE	O32-C31-O31-C3
45	N	403	PC1	C32-C31-O31-C3
46	O	403	3PE	C32-C31-O31-C3
46	O	405	3PE	C32-C31-O31-C3
46	d	201	3PE	C32-C31-O31-C3
45	N	403	PC1	O32-C31-O31-C3
46	A	302	3PE	O32-C31-O31-C3
46	A	303	3PE	O32-C31-O31-C3
46	M	605	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	j	101	3PE	O32-C31-O31-C3
52	L	702	CDL	OB9-CB7-OB8-CB6
52	X	201	CDL	OB9-CB7-OB8-CB6
52	h	202	CDL	OA9-CA7-OA8-CA6
52	q	201	CDL	OA9-CA7-OA8-CA6
45	B	202	PC1	O22-C21-O21-C2
46	K	101	3PE	O22-C21-O21-C2
46	m	201	3PE	O22-C21-O21-C2
45	A	301	PC1	C32-C31-O31-C3
46	A	302	3PE	C32-C31-O31-C3
46	A	303	3PE	C32-C31-O31-C3
46	M	605	3PE	C32-C31-O31-C3
46	N	401	3PE	C32-C31-O31-C3
46	Y	204	3PE	C32-C31-O31-C3
46	j	101	3PE	C32-C31-O31-C3
46	p	201	3PE	C32-C31-O31-C3
52	L	702	CDL	C71-CB7-OB8-CB6
46	A	302	3PE	C22-C21-O21-C2
46	A	303	3PE	C22-C21-O21-C2
46	M	605	3PE	C22-C21-O21-C2
46	O	403	3PE	C22-C21-O21-C2
46	O	405	3PE	C22-C21-O21-C2
46	Y	203	3PE	C22-C21-O21-C2
51	M	604	LMT	O5'-C5'-C6'-O6'
51	Y	206	LMT	O5B-C5B-C6B-O6B
52	X	201	CDL	C71-CB7-OB8-CB6
52	h	202	CDL	C31-CA7-OA8-CA6
52	q	201	CDL	C31-CA7-OA8-CA6
51	Y	201	LMT	O5B-C5B-C6B-O6B
46	N	401	3PE	O32-C31-O31-C3
52	d	202	CDL	O1-C1-CA2-OA2
45	A	301	PC1	O32-C31-O31-C3
51	Y	201	LMT	C4B-C5B-C6B-O6B
52	d	202	CDL	C51-CB5-OB6-CB4
52	h	202	CDL	C51-CB5-OB6-CB4
52	L	702	CDL	CA5-C11-C12-C13
51	Y	201	LMT	O5'-C5'-C6'-O6'
51	Y	206	LMT	C4B-C5B-C6B-O6B
55	P	501	NDP	O4B-C4B-C5B-O5B
51	L	704	LMT	O5B-C5B-C6B-O6B
52	h	202	CDL	OB7-CB5-OB6-CB4
45	M	602	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
51	M	604	LMT	C4'-C5'-C6'-O6'
46	h	201	3PE	C32-C31-O31-C3
52	L	702	CDL	CB2-C1-CA2-OA2
46	h	201	3PE	O32-C31-O31-C3
52	q	201	CDL	CB5-C51-C52-C53
51	M	604	LMT	C3'-C4'-O1B-C1B
51	Y	201	LMT	C4'-C5'-C6'-O6'
51	H	602	LMT	C2-C3-C4-C5
46	N	401	3PE	O11-C1-C2-O21
52	N	402	CDL	O1-C1-CB2-OB2
52	X	201	CDL	O1-C1-CB2-OB2
46	M	603	3PE	C34-C35-C36-C37
51	H	602	LMT	C4'-C5'-C6'-O6'
52	d	202	CDL	OB7-CB5-OB6-CB4
46	I	201	3PE	C21-C22-C23-C24
45	H	603	PC1	C21-C22-C23-C24
46	K	101	3PE	C31-C32-C33-C34
51	L	704	LMT	C4B-C5B-C6B-O6B
45	O	401	PC1	C21-C22-C23-C24
46	O	405	3PE	C21-C22-C23-C24
46	b	101	3PE	C31-C32-C33-C34
52	X	201	CDL	CA5-C11-C12-C13
52	X	201	CDL	CB5-C51-C52-C53
52	d	202	CDL	CA5-C11-C12-C13
52	h	202	CDL	CB5-C51-C52-C53
52	q	201	CDL	CB7-C71-C72-C73
46	O	405	3PE	C31-C32-C33-C34
46	Y	205	3PE	C31-C32-C33-C34
46	Z	200	3PE	C21-C22-C23-C24
52	d	202	CDL	CA7-C31-C32-C33
46	O	403	3PE	C32-C33-C34-C35
52	N	402	CDL	C19-C20-C21-C22
45	H	603	PC1	C31-C32-C33-C34
46	I	204	3PE	C29-C2A-C2B-C2C
45	B	202	PC1	C11-O13-P-O11
45	M	602	PC1	C11-O13-P-O11
45	N	403	PC1	C11-O13-P-O11
45	N	403	PC1	C1-O11-P-O13
45	O	401	PC1	C11-O13-P-O11
46	H	601	3PE	C1-O11-P-O13
46	I	201	3PE	C1-O11-P-O13
46	I	204	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	C11-O13-P-O11
46	M	601	3PE	C1-O11-P-O13
46	M	603	3PE	C1-O11-P-O13
46	N	401	3PE	C1-O11-P-O13
46	Y	203	3PE	C1-O11-P-O13
46	Y	204	3PE	C11-O13-P-O11
46	Y	205	3PE	C1-O11-P-O13
46	Z	200	3PE	C1-O11-P-O13
46	b	101	3PE	C1-O11-P-O13
46	d	201	3PE	C1-O11-P-O13
46	j	101	3PE	C1-O11-P-O13
46	p	201	3PE	C1-O11-P-O13
52	L	702	CDL	CA2-OA2-PA1-OA5
52	N	402	CDL	CA2-OA2-PA1-OA5
52	N	402	CDL	CB2-OB2-PB2-OB5
52	X	201	CDL	CA2-OA2-PA1-OA5
52	X	201	CDL	CB2-OB2-PB2-OB5
52	d	202	CDL	CA2-OA2-PA1-OA5
52	d	202	CDL	CA3-OA5-PA1-OA2
52	q	201	CDL	CB2-OB2-PB2-OB5
46	A	302	3PE	C31-C32-C33-C34
46	M	603	3PE	C32-C31-O31-C3
45	M	602	PC1	C25-C26-C27-C28
46	M	601	3PE	C22-C21-O21-C2
45	B	202	PC1	C3C-C3D-C3E-C3F
45	N	403	PC1	C3C-C3D-C3E-C3F
46	Y	203	3PE	C34-C35-C36-C37
46	m	201	3PE	C22-C23-C24-C25
52	X	201	CDL	C34-C35-C36-C37
52	X	201	CDL	C51-C52-C53-C54
52	d	202	CDL	C33-C34-C35-C36
52	q	201	CDL	C71-C72-C73-C74
45	N	403	PC1	C3B-C3C-C3D-C3E
46	L	703	3PE	C36-C37-C38-C39
46	M	603	3PE	C26-C27-C28-C29
52	X	201	CDL	C23-C24-C25-C26
52	q	201	CDL	C17-C18-C19-C20
46	M	601	3PE	O22-C21-O21-C2
46	M	601	3PE	C34-C35-C36-C37
52	X	201	CDL	C35-C36-C37-C38
45	N	403	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
46	Y	204	3PE	C25-C26-C27-C28
52	N	402	CDL	C14-C15-C16-C17
52	X	201	CDL	C55-C56-C57-C58
46	I	204	3PE	C3B-C3C-C3D-C3E
46	K	101	3PE	C29-C2A-C2B-C2C
46	N	401	3PE	C32-C33-C34-C35
46	Z	200	3PE	C3C-C3D-C3E-C3F
46	b	101	3PE	C24-C25-C26-C27
52	L	702	CDL	C36-C37-C38-C39
51	Y	201	LMT	C2'-C1'-O1'-C1
45	A	301	PC1	C28-C29-C2A-C2B
46	L	705	3PE	C36-C37-C38-C39
46	p	201	3PE	C27-C28-C29-C2A
52	N	402	CDL	C61-C62-C63-C64
52	X	201	CDL	C19-C20-C21-C22
52	X	201	CDL	C33-C34-C35-C36
52	d	202	CDL	C76-C77-C78-C79
52	h	202	CDL	C51-C52-C53-C54
58	o	201	MYR	C3-C4-C5-C6
45	A	301	PC1	C3E-C3F-C3G-C3H
46	h	201	3PE	C25-C26-C27-C28
46	p	201	3PE	C34-C35-C36-C37
52	X	201	CDL	C22-C23-C24-C25
52	X	201	CDL	C63-C64-C65-C66
52	d	202	CDL	C31-C32-C33-C34
52	L	702	CDL	CB4-CB6-OB8-CB7
45	B	202	PC1	C2A-C2B-C2C-C2D
45	B	202	PC1	C33-C34-C35-C36
45	M	602	PC1	C23-C24-C25-C26
45	M	602	PC1	C27-C28-C29-C2A
46	M	603	3PE	C27-C28-C29-C2A
52	N	402	CDL	C12-C13-C14-C15
52	h	202	CDL	C53-C54-C55-C56
52	q	201	CDL	C51-C52-C53-C54
45	B	202	PC1	C38-C39-C3A-C3B
45	M	602	PC1	C2C-C2D-C2E-C2F
46	A	302	3PE	C3A-C3B-C3C-C3D
46	H	601	3PE	C24-C25-C26-C27
46	H	601	3PE	C2C-C2D-C2E-C2F
46	m	201	3PE	C2C-C2D-C2E-C2F
46	p	201	3PE	C33-C34-C35-C36
46	I	204	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C32-C33-C34-C35
46	Y	202	3PE	C26-C27-C28-C29
46	j	101	3PE	C23-C24-C25-C26
51	L	704	LMT	C4-C5-C6-C7
46	M	605	3PE	C21-C22-C23-C24
52	h	202	CDL	CA5-C11-C12-C13
52	q	201	CDL	CA7-C31-C32-C33
45	A	301	PC1	C2A-C2B-C2C-C2D
46	I	204	3PE	C36-C37-C38-C39
46	Y	204	3PE	C33-C34-C35-C36
46	p	201	3PE	C23-C24-C25-C26
46	p	201	3PE	C2A-C2B-C2C-C2D
51	M	604	LMT	O1'-C1-C2-C3
52	L	702	CDL	C31-C32-C33-C34
52	N	402	CDL	C15-C16-C17-C18
52	X	201	CDL	C31-C32-C33-C34
58	o	201	MYR	C10-C11-C12-C13
51	Y	201	LMT	O5'-C1'-O1'-C1
52	N	402	CDL	C31-C32-C33-C34
46	I	204	3PE	C2A-C2B-C2C-C2D
46	I	204	3PE	C2D-C2E-C2F-C2G
46	K	101	3PE	C35-C36-C37-C38
46	M	601	3PE	C33-C34-C35-C36
51	M	604	LMT	C11-C10-C9-C8
52	L	702	CDL	C52-C53-C54-C55
52	X	201	CDL	C21-C22-C23-C24
52	d	202	CDL	C71-C72-C73-C74
52	q	201	CDL	C31-C32-C33-C34
46	L	705	3PE	C21-C22-C23-C24
46	I	201	3PE	C34-C35-C36-C37
46	d	201	3PE	C34-C35-C36-C37
45	H	603	PC1	C32-C31-O31-C3
46	M	603	3PE	C22-C23-C24-C25
52	L	702	CDL	C33-C34-C35-C36
51	Y	201	LMT	C2-C1-O1'-C1'
46	H	601	3PE	C25-C26-C27-C28
46	Y	205	3PE	C34-C35-C36-C37
46	b	101	3PE	C32-C33-C34-C35
46	m	201	3PE	C29-C2A-C2B-C2C
46	L	703	3PE	C31-C32-C33-C34
46	p	201	3PE	C31-C32-C33-C34
46	A	302	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
46	A	302	3PE	C36-C37-C38-C39
46	M	603	3PE	C3C-C3D-C3E-C3F
46	Y	205	3PE	C23-C24-C25-C26
51	M	604	LMT	C2-C3-C4-C5
52	N	402	CDL	C56-C57-C58-C59
52	h	202	CDL	C55-C56-C57-C58
52	h	202	CDL	C73-C74-C75-C76
46	Y	203	3PE	C31-C32-C33-C34
52	N	402	CDL	CB5-C51-C52-C53
46	K	101	3PE	C28-C29-C2A-C2B
57	U	101	EHZ	C1-C21-C22-C23
46	L	703	3PE	C32-C31-O31-C3
52	X	201	CDL	C11-CA5-OA6-CA4
52	h	202	CDL	C11-CA5-OA6-CA4
46	Y	203	3PE	C3B-C3C-C3D-C3E
46	Y	203	3PE	C22-C23-C24-C25
52	N	402	CDL	C60-C61-C62-C63
52	X	201	CDL	C52-C53-C54-C55
51	H	602	LMT	O5'-C5'-C6'-O6'
45	M	602	PC1	C26-C27-C28-C29
46	p	201	3PE	C2C-C2D-C2E-C2F
52	L	702	CDL	O1-C1-CA2-OA2
46	M	605	3PE	C33-C34-C35-C36
51	M	604	LMT	C6-C7-C8-C9
46	M	603	3PE	O32-C31-O31-C3
45	M	602	PC1	C31-C32-C33-C34
46	b	101	3PE	C25-C26-C27-C28
46	m	201	3PE	C2D-C2E-C2F-C2G
52	X	201	CDL	OA7-CA5-OA6-CA4
52	h	202	CDL	OA7-CA5-OA6-CA4
46	K	101	3PE	C34-C35-C36-C37
51	M	604	LMT	C3-C4-C5-C6
52	L	702	CDL	C57-C58-C59-C60
52	h	202	CDL	C75-C76-C77-C78
45	H	603	PC1	C25-C26-C27-C28
46	H	601	3PE	C2B-C2C-C2D-C2E
46	Y	203	3PE	C2E-C2F-C2G-C2H
51	H	602	LMT	C7-C8-C9-C10
58	o	201	MYR	C2-C3-C4-C5
52	q	201	CDL	C11-CA5-OA6-CA4
45	H	603	PC1	C28-C29-C2A-C2B
45	M	602	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	Z	200	3PE	C34-C35-C36-C37
46	h	201	3PE	C33-C34-C35-C36
52	N	402	CDL	C34-C35-C36-C37
45	H	603	PC1	O32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
45	H	603	PC1	C2E-C2F-C2G-C2H
58	o	201	MYR	C4-C5-C6-C7
46	I	204	3PE	O22-C21-O21-C2
46	O	403	3PE	C21-C22-C23-C24
45	A	301	PC1	C22-C23-C24-C25
46	A	302	3PE	C35-C36-C37-C38
52	L	702	CDL	C34-C35-C36-C37
52	X	201	CDL	C41-C42-C43-C44
46	L	705	3PE	C28-C29-C2A-C2B
52	N	402	CDL	CA5-C11-C12-C13
46	A	302	3PE	C37-C38-C39-C3A
46	M	601	3PE	C23-C24-C25-C26
46	Y	204	3PE	C23-C24-C25-C26
46	b	101	3PE	C3B-C3C-C3D-C3E
46	j	101	3PE	C22-C23-C24-C25
52	L	702	CDL	C51-C52-C53-C54
52	X	201	CDL	C36-C37-C38-C39
52	d	202	CDL	C40-C41-C42-C43
58	o	201	MYR	C6-C7-C8-C9
46	L	703	3PE	C3E-C3F-C3G-C3H
46	M	603	3PE	C37-C38-C39-C3A
57	T	101	EHZ	C12-C13-C14-N2
45	H	603	PC1	C33-C34-C35-C36
45	M	602	PC1	C34-C35-C36-C37
45	N	403	PC1	C32-C33-C34-C35
46	I	201	3PE	C2B-C2C-C2D-C2E
46	Y	203	3PE	C3E-C3F-C3G-C3H
46	Y	204	3PE	C2C-C2D-C2E-C2F
57	T	101	EHZ	C21-C22-C23-C24
46	N	401	3PE	C22-C21-O21-C2
46	Y	204	3PE	C22-C21-O21-C2
46	Y	205	3PE	C22-C21-O21-C2
52	L	702	CDL	C51-CB5-OB6-CB4
52	d	202	CDL	C11-CA5-OA6-CA4
45	O	401	PC1	O11-C1-C2-O21
46	K	101	3PE	C32-C33-C34-C35
52	N	402	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
52	d	202	CDL	OA7-CA5-OA6-CA4
52	q	201	CDL	OA7-CA5-OA6-CA4
52	q	201	CDL	CA5-C11-C12-C13
52	N	402	CDL	C17-C18-C19-C20
46	L	705	3PE	C22-C23-C24-C25
52	L	702	CDL	C62-C63-C64-C65
46	L	703	3PE	C24-C25-C26-C27
52	L	702	CDL	C37-C38-C39-C40
52	N	402	CDL	C71-C72-C73-C74
45	A	301	PC1	C36-C37-C38-C39
46	Y	204	3PE	O22-C21-O21-C2
46	Y	205	3PE	C24-C25-C26-C27
46	M	601	3PE	C11-O13-P-O11
51	H	602	LMT	O5B-C5B-C6B-O6B
52	X	201	CDL	C12-C13-C14-C15
45	A	301	PC1	O11-C1-C2-C3
45	H	603	PC1	O11-C1-C2-C3
46	A	302	3PE	O11-C1-C2-C3
46	A	303	3PE	O11-C1-C2-C3
46	L	703	3PE	O11-C1-C2-C3
46	N	401	3PE	O11-C1-C2-C3
46	O	403	3PE	O11-C1-C2-C3
46	d	201	3PE	O11-C1-C2-C3
45	H	603	PC1	C23-C24-C25-C26
46	d	201	3PE	C39-C3A-C3B-C3C
46	O	403	3PE	C34-C35-C36-C37
46	d	201	3PE	C26-C27-C28-C29
52	L	702	CDL	C61-C62-C63-C64
52	N	402	CDL	C75-C76-C77-C78
46	N	401	3PE	O22-C21-O21-C2
46	Y	205	3PE	O22-C21-O21-C2
52	h	202	CDL	C31-C32-C33-C34
58	o	201	MYR	C7-C8-C9-C10
46	N	401	3PE	C26-C27-C28-C29
45	B	202	PC1	C1-C2-C3-O31
46	H	601	3PE	C1-C2-C3-O31
46	I	201	3PE	C22-C23-C24-C25
46	I	204	3PE	C22-C23-C24-C25
46	Y	202	3PE	C1-C2-C3-O31
46	p	201	3PE	C1-C2-C3-O31
52	N	402	CDL	CA3-CA4-CA6-OA8
52	N	402	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
52	d	202	CDL	CA3-CA4-CA6-OA8
52	d	202	CDL	C74-C75-C76-C77
52	h	202	CDL	CB3-CB4-CB6-OB8
52	q	201	CDL	CA3-CA4-CA6-OA8
46	Y	203	3PE	C32-C31-O31-C3
46	d	201	3PE	C32-C33-C34-C35
46	p	201	3PE	C32-C33-C34-C35
52	N	402	CDL	C55-C56-C57-C58
46	b	101	3PE	C3D-C3E-C3F-C3G
52	L	702	CDL	C71-C72-C73-C74
46	A	302	3PE	C21-C22-C23-C24
45	M	602	PC1	C35-C36-C37-C38
46	L	703	3PE	C34-C35-C36-C37
52	N	402	CDL	C76-C77-C78-C79
57	U	101	EHZ	O4-C15-C16-O5
46	Z	200	3PE	C39-C3A-C3B-C3C
45	N	403	PC1	C22-C21-O21-C2
46	L	701	3PE	C22-C21-O21-C2
46	p	201	3PE	C35-C36-C37-C38
57	U	101	EHZ	C5-C6-C7-O1
46	L	701	3PE	C27-C28-C29-C2A
51	M	604	LMT	C5'-C4'-O1B-C1B
52	d	202	CDL	C77-C78-C79-C80
46	N	401	3PE	C22-C23-C24-C25
46	I	201	3PE	C32-C31-O31-C3
46	Y	203	3PE	O11-C1-C2-O21
52	L	702	CDL	OB5-CB3-CB4-OB6
52	L	702	CDL	C59-C60-C61-C62
52	h	202	CDL	C76-C77-C78-C79
45	A	301	PC1	O21-C2-C3-O31
45	M	602	PC1	O21-C2-C3-O31
46	M	603	3PE	O21-C2-C3-O31
46	I	204	3PE	C32-C33-C34-C35
46	Y	203	3PE	C2F-C2G-C2H-C2I
46	H	601	3PE	C22-C23-C24-C25
46	N	401	3PE	C38-C39-C3A-C3B
52	q	201	CDL	C14-C15-C16-C17
52	d	202	CDL	C73-C74-C75-C76
45	O	401	PC1	C26-C27-C28-C29
46	M	603	3PE	C3F-C3G-C3H-C3I
52	N	402	CDL	C73-C74-C75-C76
46	L	703	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	N	401	3PE	C3D-C3E-C3F-C3G
46	j	101	3PE	C22-C21-O21-C2
46	I	204	3PE	O11-C1-C2-C3
46	M	601	3PE	O11-C1-C2-C3
52	L	702	CDL	OB5-CB3-CB4-CB6
45	O	401	PC1	C23-C24-C25-C26
46	d	201	3PE	C35-C36-C37-C38
45	N	403	PC1	C39-C3A-C3B-C3C
52	h	202	CDL	O1-C1-CA2-OA2
52	L	702	CDL	OB7-CB5-OB6-CB4
46	Y	203	3PE	O32-C31-O31-C3
46	I	204	3PE	C25-C26-C27-C28
46	L	705	3PE	C23-C24-C25-C26
46	N	401	3PE	C34-C35-C36-C37
52	h	202	CDL	C71-CB7-OB8-CB6
46	b	101	3PE	O21-C21-C22-C23
51	H	602	LMT	C2-C1-O1'-C1'
45	A	301	PC1	C3F-C3G-C3H-C3I
46	M	605	3PE	C23-C24-C25-C26
46	Z	200	3PE	C32-C31-O31-C3
46	K	101	3PE	C3A-C3B-C3C-C3D
45	H	603	PC1	C1-C2-C3-O31
46	I	204	3PE	C1-C2-C3-O31
46	K	101	3PE	C1-C2-C3-O31
46	M	605	3PE	C1-C2-C3-O31
46	Y	204	3PE	C1-C2-C3-O31
46	Y	205	3PE	C1-C2-C3-O31
46	b	101	3PE	C1-C2-C3-O31
46	j	101	3PE	C1-C2-C3-O31
52	N	402	CDL	CB3-CB4-CB6-OB8
52	q	201	CDL	CB3-CB4-CB6-OB8
46	O	405	3PE	C28-C29-C2A-C2B
51	Y	206	LMT	C2-C3-C4-C5
46	H	601	3PE	C21-C22-C23-C24
46	d	201	3PE	C21-C22-C23-C24
45	H	603	PC1	C37-C38-C39-C3A
46	A	302	3PE	C38-C39-C3A-C3B
46	L	705	3PE	C33-C34-C35-C36
46	N	401	3PE	C2D-C2E-C2F-C2G
51	Y	201	LMT	C7-C8-C9-C10
46	O	405	3PE	C32-C33-C34-C35
46	O	405	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
52	N	402	CDL	C54-C55-C56-C57
52	d	202	CDL	C75-C76-C77-C78
46	Y	202	3PE	C33-C34-C35-C36
45	H	603	PC1	C29-C2A-C2B-C2C
46	A	302	3PE	O11-C1-C2-O21
46	m	201	3PE	O11-C1-C2-O21
46	L	701	3PE	O22-C21-O21-C2
46	I	201	3PE	O32-C31-O31-C3
46	A	302	3PE	C27-C28-C29-C2A
52	q	201	CDL	C19-C20-C21-C22
46	K	101	3PE	C3C-C3D-C3E-C3F
46	I	204	3PE	O21-C2-C3-O31
46	Y	205	3PE	O21-C2-C3-O31
46	b	101	3PE	O21-C2-C3-O31
46	j	101	3PE	O21-C2-C3-O31
46	p	201	3PE	O21-C2-C3-O31
52	N	402	CDL	OA6-CA4-CA6-OA8
52	N	402	CDL	OB6-CB4-CB6-OB8
52	d	202	CDL	OA6-CA4-CA6-OA8
52	h	202	CDL	OB6-CB4-CB6-OB8
52	X	201	CDL	C62-C63-C64-C65
52	L	702	CDL	CA2-C1-CB2-OB2
52	d	202	CDL	CA2-C1-CB2-OB2
45	N	403	PC1	O22-C21-O21-C2
46	j	101	3PE	C33-C34-C35-C36
51	Y	201	LMT	C2-C3-C4-C5
46	M	603	3PE	C2-C1-O11-P
45	B	202	PC1	C24-C25-C26-C27
46	O	405	3PE	C33-C34-C35-C36
52	h	202	CDL	C60-C61-C62-C63
52	L	702	CDL	C52-C51-CB5-OB6
52	N	402	CDL	C53-C54-C55-C56
45	M	602	PC1	C24-C25-C26-C27
45	N	403	PC1	C31-C32-C33-C34
46	j	101	3PE	O22-C21-O21-C2
52	N	402	CDL	C11-CA5-OA6-CA4
52	X	201	CDL	C58-C59-C60-C61
52	X	201	CDL	C64-C65-C66-C67
51	L	704	LMT	C9-C10-C11-C12
51	Y	206	LMT	O1'-C1-C2-C3
51	L	704	LMT	C4'-C5'-C6'-O6'
46	Y	202	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	b	101	3PE	C23-C24-C25-C26
46	L	701	3PE	O11-C1-C2-C3
46	L	705	3PE	O11-C1-C2-C3
46	M	605	3PE	O11-C1-C2-C3
46	Y	203	3PE	O11-C1-C2-C3
46	Y	205	3PE	O11-C1-C2-C3
46	m	201	3PE	O11-C1-C2-C3
46	p	201	3PE	O11-C1-C2-C3
46	M	603	3PE	C3B-C3C-C3D-C3E
46	Z	200	3PE	C22-C23-C24-C25
46	M	601	3PE	C28-C29-C2A-C2B
52	N	402	CDL	C21-C22-C23-C24
57	U	101	EHZ	N2-C15-C16-O5
46	Y	203	3PE	C2D-C2E-C2F-C2G
52	N	402	CDL	CA7-C31-C32-C33
52	L	702	CDL	C12-C13-C14-C15
52	L	702	CDL	C54-C55-C56-C57
46	L	703	3PE	C32-C33-C34-C35
45	B	202	PC1	C34-C35-C36-C37
52	L	702	CDL	CB3-CB4-CB6-OB8
52	d	202	CDL	CA4-CA3-OA5-PA1
45	B	202	PC1	C35-C36-C37-C38
46	H	601	3PE	O11-C1-C2-O21
46	I	204	3PE	C2F-C2G-C2H-C2I
52	X	201	CDL	C32-C33-C34-C35
46	Y	204	3PE	C36-C37-C38-C39
45	A	301	PC1	C37-C38-C39-C3A
52	N	402	CDL	OA7-CA5-OA6-CA4
46	Z	200	3PE	O32-C31-O31-C3
46	M	601	3PE	C32-C33-C34-C35
46	Y	202	3PE	C23-C24-C25-C26
46	j	101	3PE	C29-C2A-C2B-C2C
45	B	202	PC1	O21-C2-C3-O31
46	H	601	3PE	O21-C2-C3-O31
46	h	201	3PE	O21-C2-C3-O31
52	h	202	CDL	OB9-CB7-OB8-CB6
52	L	702	CDL	C15-C16-C17-C18
46	M	603	3PE	C33-C34-C35-C36
46	N	401	3PE	C35-C36-C37-C38
45	M	602	PC1	C2B-C2C-C2D-C2E
45	B	202	PC1	C2B-C2C-C2D-C2E
57	U	101	EHZ	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
54	O	404	DGT	PB-O3A-PA-O1A
45	A	301	PC1	C29-C2A-C2B-C2C
57	U	101	EHZ	C21-C22-C23-C24
52	h	202	CDL	CA2-OA2-PA1-OA5
45	B	202	PC1	C2-C1-O11-P
46	L	705	3PE	C2-C1-O11-P
49	F	501	FMN	C4'-C5'-O5'-P
46	Z	200	3PE	C3E-C3F-C3G-C3H
45	M	602	PC1	C11-O13-P-O12
45	N	403	PC1	C11-O13-P-O14
45	O	401	PC1	C11-O13-P-O12
45	O	401	PC1	C1-O11-P-O12
46	I	204	3PE	C1-O11-P-O14
46	L	703	3PE	C1-O11-P-O14
46	M	601	3PE	C1-O11-P-O12
46	M	605	3PE	C1-O11-P-O14
46	Y	202	3PE	C1-O11-P-O14
46	d	201	3PE	C1-O11-P-O12
46	d	201	3PE	C1-O11-P-O14
46	j	101	3PE	C1-O11-P-O14
52	L	702	CDL	CA2-OA2-PA1-OA3
52	X	201	CDL	CA2-OA2-PA1-OA4
52	X	201	CDL	CB2-OB2-PB2-OB3
52	X	201	CDL	CB2-OB2-PB2-OB4
52	d	202	CDL	CA3-OA5-PA1-OA3
52	h	202	CDL	CA2-OA2-PA1-OA4
52	h	202	CDL	CB2-OB2-PB2-OB3
52	q	201	CDL	CA2-OA2-PA1-OA3
45	M	602	PC1	C21-C22-C23-C24
46	L	705	3PE	C31-C32-C33-C34
46	m	201	3PE	C21-C22-C23-C24
46	H	601	3PE	O11-C1-C2-C3
52	X	201	CDL	OA5-CA3-CA4-CA6
46	I	204	3PE	C3E-C3F-C3G-C3H
46	I	204	3PE	C38-C39-C3A-C3B
51	M	604	LMT	C1-C2-C3-C4
51	Y	206	LMT	C1-C2-C3-C4
52	L	702	CDL	C56-C57-C58-C59
52	q	201	CDL	C18-C19-C20-C21
46	M	605	3PE	C12-C11-O13-P
46	Y	202	3PE	C12-C11-O13-P
46	h	201	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
52	h	202	CDL	CA7-C31-C32-C33
45	A	301	PC1	C35-C36-C37-C38
45	H	603	PC1	C2B-C2C-C2D-C2E
46	M	601	3PE	O21-C21-C22-C23
45	A	301	PC1	O11-C1-C2-O21
46	L	701	3PE	O11-C1-C2-O21
46	L	703	3PE	O11-C1-C2-O21
46	L	705	3PE	O11-C1-C2-O21
46	h	201	3PE	O11-C1-C2-O21
46	p	201	3PE	O11-C1-C2-O21
52	X	201	CDL	OA5-CA3-CA4-OA6
55	P	501	NDP	C3B-C4B-C5B-O5B
52	L	702	CDL	C14-C15-C16-C17
46	Y	203	3PE	C3F-C3G-C3H-C3I
46	d	201	3PE	C2E-C2F-C2G-C2H
46	Z	200	3PE	C38-C39-C3A-C3B
55	P	501	NDP	O4D-C1D-N1N-C6N
46	I	204	3PE	C31-C32-C33-C34
52	L	702	CDL	C42-C43-C44-C45
52	L	702	CDL	O1-C1-CB2-OB2
46	Z	200	3PE	C32-C33-C34-C35
46	p	201	3PE	C21-C22-C23-C24
52	N	402	CDL	CB7-C71-C72-C73
45	A	301	PC1	O13-C11-C12-N
45	A	301	PC1	C3C-C3D-C3E-C3F
45	M	602	PC1	C1-C2-C3-O31
45	M	602	PC1	C22-C23-C24-C25
46	d	201	3PE	C1-C2-C3-O31
45	H	603	PC1	O21-C2-C3-O31
46	M	605	3PE	O21-C2-C3-O31
46	Y	204	3PE	O21-C2-C3-O31
46	d	201	3PE	O21-C2-C3-O31
52	L	702	CDL	OB6-CB4-CB6-OB8
51	L	704	LMT	C6-C7-C8-C9
45	B	202	PC1	C22-C23-C24-C25
46	L	703	3PE	O21-C21-C22-C23
45	H	603	PC1	C35-C36-C37-C38
46	Y	203	3PE	C2-C1-O11-P
46	L	701	3PE	C35-C36-C37-C38
46	I	201	3PE	C36-C37-C38-C39
52	q	201	CDL	C53-C54-C55-C56
46	m	201	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
52	d	202	CDL	C72-C73-C74-C75
46	O	403	3PE	C22-C23-C24-C25
46	L	701	3PE	C29-C2A-C2B-C2C
52	N	402	CDL	C74-C75-C76-C77
51	L	704	LMT	C2-C3-C4-C5
52	L	702	CDL	C43-C44-C45-C46
46	Y	202	3PE	C25-C26-C27-C28
57	U	101	EHZ	C3-C4-C5-C6
46	I	204	3PE	C2B-C2C-C2D-C2E
46	N	401	3PE	C2F-C2G-C2H-C2I
52	X	201	CDL	C39-C40-C41-C42
46	M	603	3PE	C35-C36-C37-C38
46	K	101	3PE	C1-C2-O21-C21
46	O	403	3PE	C1-C2-O21-C21
45	O	401	PC1	O11-C1-C2-C3
46	M	603	3PE	C2D-C2E-C2F-C2G
51	H	602	LMT	C5-C6-C7-C8
46	Y	203	3PE	C33-C34-C35-C36
52	X	201	CDL	C56-C57-C58-C59
46	p	201	3PE	C2-C1-O11-P
49	F	501	FMN	C5'-O5'-P-O1P
46	O	403	3PE	O11-C1-C2-O21
46	I	201	3PE	C24-C25-C26-C27
46	Y	204	3PE	C2D-C2E-C2F-C2G
52	q	201	CDL	OA6-CA4-CA6-OA8
46	A	302	3PE	C11-O13-P-O11
46	A	303	3PE	C1-O11-P-O13
46	I	204	3PE	C11-O13-P-O11
46	L	705	3PE	C11-O13-P-O11
46	M	603	3PE	C11-O13-P-O11
46	Y	202	3PE	C11-O13-P-O11
46	Y	203	3PE	C11-O13-P-O11
46	Y	205	3PE	C11-O13-P-O11
46	d	201	3PE	C11-O13-P-O11
46	m	201	3PE	C11-O13-P-O11
52	d	202	CDL	CB3-OB5-PB2-OB2
52	h	202	CDL	CB2-OB2-PB2-OB5
46	Y	203	3PE	C36-C37-C38-C39
45	A	301	PC1	C1-C2-C3-O31
46	M	603	3PE	C1-C2-C3-O31
51	L	704	LMT	C5-C6-C7-C8
52	d	202	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
46	A	302	3PE	C39-C3A-C3B-C3C
51	Y	201	LMT	C1-C2-C3-C4
45	H	603	PC1	C2D-C2E-C2F-C2G
46	H	601	3PE	C2-C1-O11-P
52	N	402	CDL	CA4-CA3-OA5-PA1
52	N	402	CDL	CB4-CB3-OB5-PB2
46	d	201	3PE	C3A-C3B-C3C-C3D
52	N	402	CDL	CA2-C1-CB2-OB2
52	h	202	CDL	CB2-C1-CA2-OA2
52	N	402	CDL	C57-C58-C59-C60
46	Y	204	3PE	O21-C21-C22-C23
46	A	303	3PE	O13-C11-C12-N
52	L	702	CDL	C35-C36-C37-C38
46	b	101	3PE	C38-C39-C3A-C3B
46	b	101	3PE	C2E-C2F-C2G-C2H
46	O	405	3PE	C35-C36-C37-C38
46	Y	203	3PE	C35-C36-C37-C38
57	T	101	EHZ	C3-C4-C5-C6
46	Z	200	3PE	C25-C26-C27-C28
46	O	403	3PE	O21-C2-C3-O31
46	L	701	3PE	C25-C26-C27-C28
46	L	703	3PE	C25-C26-C27-C28
46	I	201	3PE	C33-C34-C35-C36
51	H	602	LMT	C11-C10-C9-C8
46	h	201	3PE	C1-C2-C3-O31
46	I	201	3PE	C2E-C2F-C2G-C2H
57	T	101	EHZ	C22-C23-C24-C25
46	M	601	3PE	C35-C36-C37-C38
45	B	202	PC1	C26-C27-C28-C29
46	O	403	3PE	C3-C2-O21-C21
46	I	201	3PE	C32-C33-C34-C35
46	b	101	3PE	C2F-C2G-C2H-C2I
46	d	201	3PE	C33-C34-C35-C36
46	Y	203	3PE	C3C-C3D-C3E-C3F
52	X	201	CDL	C24-C25-C26-C27
46	O	405	3PE	C2B-C2C-C2D-C2E
46	I	204	3PE	C27-C28-C29-C2A
46	M	601	3PE	C37-C38-C39-C3A
46	I	201	3PE	C3A-C3B-C3C-C3D
46	O	405	3PE	C34-C35-C36-C37
57	T	101	EHZ	C4-C5-C6-C7
46	M	601	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	Y	204	3PE	C35-C36-C37-C38
46	h	201	3PE	O11-C1-C2-C3
45	N	403	PC1	C3A-C3B-C3C-C3D
46	b	101	3PE	C28-C29-C2A-C2B
45	H	603	PC1	C24-C25-C26-C27
46	p	201	3PE	C22-C23-C24-C25
46	I	201	3PE	C25-C26-C27-C28
52	q	201	CDL	OB6-CB4-CB6-OB8
46	b	101	3PE	C2A-C2B-C2C-C2D
52	h	202	CDL	C11-C12-C13-C14
46	p	201	3PE	C28-C29-C2A-C2B
46	b	101	3PE	C39-C3A-C3B-C3C
46	I	201	3PE	C35-C36-C37-C38
46	M	601	3PE	C2C-C2D-C2E-C2F
46	Y	202	3PE	C2-C1-O11-P
54	O	404	DGT	PG-O3B-PB-O2B
55	P	501	NDP	PN-O3-PA-O1A
45	B	202	PC1	O32-C31-O31-C3
46	L	701	3PE	C28-C29-C2A-C2B
52	d	202	CDL	C52-C51-CB5-OB7
45	B	202	PC1	C32-C31-O31-C3
46	M	603	3PE	C23-C24-C25-C26
45	B	202	PC1	C27-C28-C29-C2A
45	N	403	PC1	C23-C24-C25-C26
46	M	601	3PE	C2-C1-O11-P
45	O	401	PC1	C24-C25-C26-C27
46	b	101	3PE	O22-C21-C22-C23
51	Y	206	LMT	C11-C10-C9-C8
55	P	501	NDP	O4D-C4D-C5D-O5D
46	Y	204	3PE	C31-C32-C33-C34
46	j	101	3PE	O21-C21-C22-C23
51	Y	201	LMT	O1'-C1-C2-C3
46	K	101	3PE	O31-C31-C32-C33
52	L	702	CDL	C12-C11-CA5-OA6
46	A	302	3PE	C3B-C3C-C3D-C3E
52	N	402	CDL	C72-C71-CB7-OB8
46	N	401	3PE	C39-C3A-C3B-C3C
52	L	702	CDL	C13-C14-C15-C16
45	N	403	PC1	O21-C21-C22-C23
46	b	101	3PE	O31-C31-C32-C33
46	A	303	3PE	C33-C34-C35-C36
46	Z	200	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
46	Z	200	3PE	O31-C31-C32-C33
45	N	403	PC1	C11-C12-N-C13
46	I	201	3PE	C29-C2A-C2B-C2C
46	j	101	3PE	C2E-C2F-C2G-C2H
45	A	301	PC1	O21-C21-C22-C23
46	A	302	3PE	O21-C21-C22-C23
51	L	704	LMT	O5'-C5'-C6'-O6'
46	j	101	3PE	C31-C32-C33-C34
57	T	101	EHZ	O1-C7-C8-C9
52	X	201	CDL	C52-C51-CB5-OB6
46	d	201	3PE	C2F-C2G-C2H-C2I
46	N	401	3PE	O21-C21-C22-C23
52	q	201	CDL	C52-C51-CB5-OB6
52	L	702	CDL	C55-C56-C57-C58
45	B	202	PC1	O21-C21-C22-C23
46	H	601	3PE	O21-C21-C22-C23
46	Y	205	3PE	O31-C31-C32-C33
46	d	201	3PE	O21-C21-C22-C23
46	L	703	3PE	C22-C23-C24-C25
52	d	202	CDL	C43-C44-C45-C46
46	L	705	3PE	C27-C28-C29-C2A
49	F	501	FMN	O2'-C2'-C3'-O3'
46	K	101	3PE	O21-C21-C22-C23
52	X	201	CDL	C15-C16-C17-C18
46	A	303	3PE	C25-C26-C27-C28
46	p	201	3PE	O21-C21-C22-C23
46	N	401	3PE	C2E-C2F-C2G-C2H
46	Y	203	3PE	C2A-C2B-C2C-C2D
52	d	202	CDL	O1-C1-CB2-OB2
54	O	404	DGT	O4'-C4'-C5'-O5'
46	Z	200	3PE	C37-C38-C39-C3A
52	q	201	CDL	C15-C16-C17-C18
46	O	405	3PE	C27-C28-C29-C2A
46	A	302	3PE	C22-C23-C24-C25
52	X	201	CDL	C53-C54-C55-C56
46	O	403	3PE	O21-C21-C22-C23
46	h	201	3PE	O31-C31-C32-C33
52	N	402	CDL	C35-C36-C37-C38
45	M	602	PC1	C32-C31-O31-C3
46	N	401	3PE	C37-C38-C39-C3A
45	M	602	PC1	O32-C31-O31-C3
46	L	705	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	N	401	3PE	C25-C26-C27-C28
45	N	403	PC1	O22-C21-C22-C23
46	K	101	3PE	O22-C21-C22-C23
46	j	101	3PE	O22-C21-C22-C23
46	b	101	3PE	C3E-C3F-C3G-C3H
46	Z	200	3PE	O32-C31-C32-C33
52	X	201	CDL	C52-C51-CB5-OB7
46	K	101	3PE	O32-C31-C32-C33
52	N	402	CDL	C72-C71-CB7-OB9
52	L	702	CDL	C58-C59-C60-C61
52	X	201	CDL	C12-C11-CA5-OA6
52	q	201	CDL	C1-CA2-OA2-PA1
46	Z	200	3PE	C33-C34-C35-C36
46	d	201	3PE	O22-C21-C22-C23
45	O	401	PC1	C11-O13-P-O14
46	A	302	3PE	C1-O11-P-O14
46	A	302	3PE	C11-O13-P-O14
46	L	705	3PE	C11-O13-P-O14
46	M	601	3PE	C1-O11-P-O14
46	Y	203	3PE	C11-O13-P-O14
46	h	201	3PE	C11-O13-P-O14
46	m	201	3PE	C11-O13-P-O14
52	L	702	CDL	CA3-OA5-PA1-OA4
52	L	702	CDL	CB2-OB2-PB2-OB4
52	h	202	CDL	CA2-OA2-PA1-OA3
52	h	202	CDL	CB3-OB5-PB2-OB3
45	A	301	PC1	O22-C21-C22-C23
46	H	601	3PE	O22-C21-C22-C23
46	Y	205	3PE	O32-C31-C32-C33
46	b	101	3PE	O32-C31-C32-C33
46	h	201	3PE	O32-C31-C32-C33
52	L	702	CDL	C12-C11-CA5-OA7
52	q	201	CDL	C52-C51-CB5-OB7
46	m	201	3PE	O21-C21-C22-C23
46	I	201	3PE	O13-C11-C12-N
46	Y	203	3PE	O13-C11-C12-N
46	A	302	3PE	O22-C21-C22-C23
46	N	401	3PE	O22-C21-C22-C23
46	O	403	3PE	O22-C21-C22-C23
46	L	703	3PE	C33-C34-C35-C36
46	Y	205	3PE	C32-C33-C34-C35
52	L	702	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C25-C26-C27-C28
46	L	701	3PE	C33-C34-C35-C36
46	O	405	3PE	C2A-C2B-C2C-C2D
46	M	603	3PE	C12-C11-O13-P
46	O	403	3PE	C12-C11-O13-P
46	Y	204	3PE	C12-C11-O13-P
46	Y	205	3PE	C12-C11-O13-P
46	m	201	3PE	C12-C11-O13-P
46	b	101	3PE	C34-C35-C36-C37
45	H	603	PC1	O21-C21-C22-C23
45	B	202	PC1	O22-C21-C22-C23
45	N	403	PC1	C11-C12-N-C14
52	d	202	CDL	C35-C36-C37-C38
46	M	605	3PE	C34-C35-C36-C37
46	M	601	3PE	C36-C37-C38-C39
46	h	201	3PE	C28-C29-C2A-C2B
46	O	403	3PE	O31-C31-C32-C33
46	Y	202	3PE	O21-C21-C22-C23
46	p	201	3PE	O22-C21-C22-C23
46	Y	203	3PE	C3D-C3E-C3F-C3G
52	X	201	CDL	C12-C11-CA5-OA7
46	Y	203	3PE	C32-C33-C34-C35
45	N	403	PC1	O31-C31-C32-C33
46	A	302	3PE	O31-C31-C32-C33
52	N	402	CDL	C52-C51-CB5-OB6
46	L	705	3PE	O32-C31-C32-C33
46	Y	202	3PE	O22-C21-C22-C23
45	M	602	PC1	O31-C31-C32-C33
46	A	302	3PE	O32-C31-C32-C33
52	N	402	CDL	C52-C51-CB5-OB7
45	N	403	PC1	C11-C12-N-C15
52	q	201	CDL	C52-C53-C54-C55

There are no ring outliers.

44 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	M	602	PC1	4	0
46	I	204	3PE	3	0
46	M	601	3PE	2	0
46	Y	205	3PE	2	0
52	N	402	CDL	3	0

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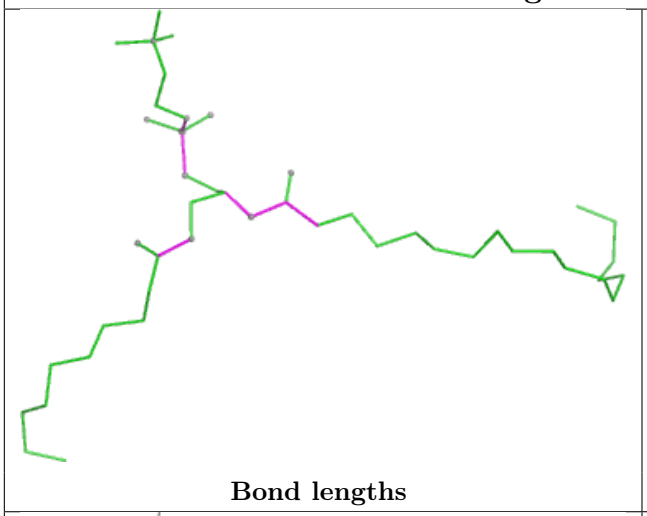
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	Y	201	LMT	1	0
46	d	201	3PE	3	0
46	A	303	3PE	2	0
51	M	604	LMT	1	0
46	b	101	3PE	2	0
52	X	201	CDL	6	0
46	m	201	3PE	1	0
47	F	502	SF4	1	0
52	d	202	CDL	1	0
46	H	601	3PE	1	0
52	h	202	CDL	3	0
46	j	101	3PE	1	0
45	B	202	PC1	3	0
45	O	401	PC1	1	0
46	A	302	3PE	1	0
45	N	403	PC1	2	0
46	L	705	3PE	4	0
46	Z	200	3PE	3	0
49	F	501	FMN	1	0
51	H	602	LMT	1	0
55	P	501	NDP	1	0
45	A	301	PC1	4	0
57	U	101	EHZ	2	0
57	T	101	EHZ	1	0
45	H	603	PC1	3	0
54	O	404	DGT	4	0
46	I	201	3PE	1	0
46	K	101	3PE	2	0
52	L	702	CDL	4	0
52	q	201	CDL	2	0
46	h	201	3PE	1	0
46	O	403	3PE	1	0
51	Y	206	LMT	2	0
46	Y	204	3PE	3	0
46	M	605	3PE	1	0
46	O	405	3PE	3	0
46	L	701	3PE	1	0
46	L	703	3PE	2	0
46	N	401	3PE	6	0

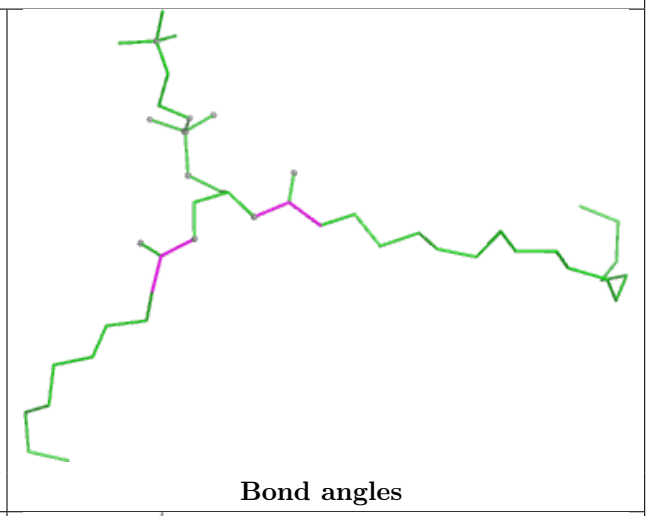
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

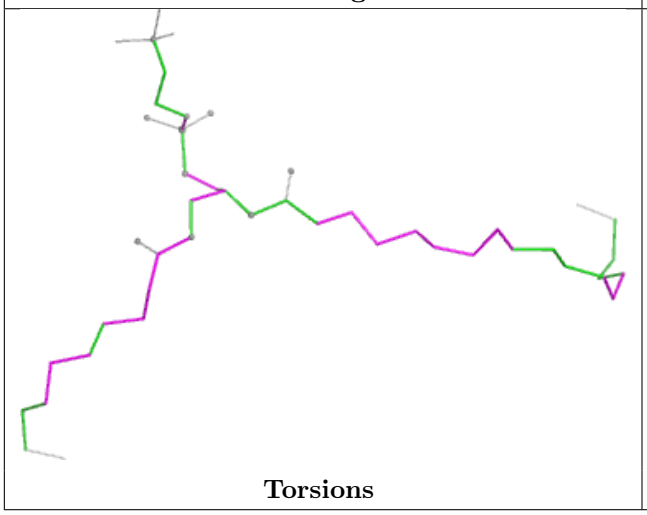
Ligand PC1 M 602



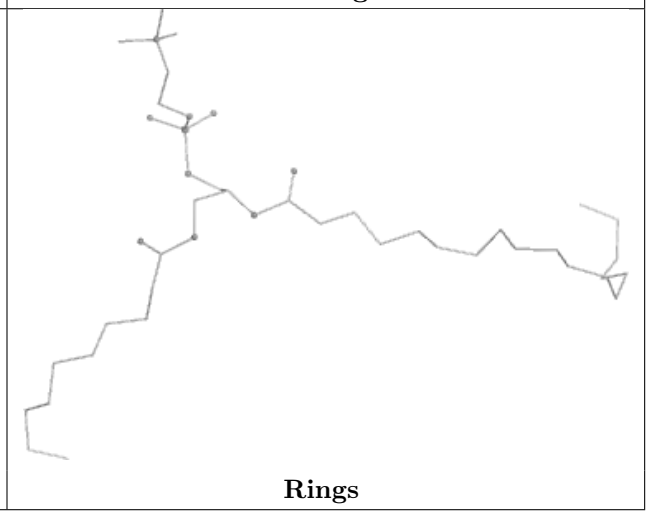
Bond lengths



Bond angles

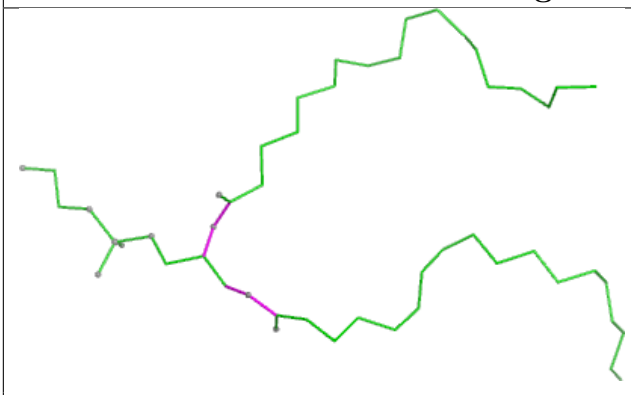


Torsions

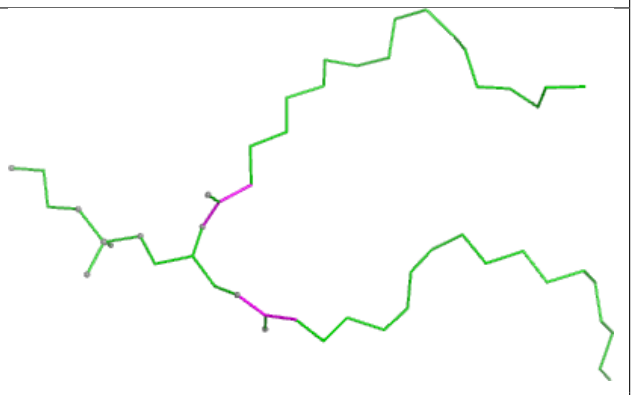


Rings

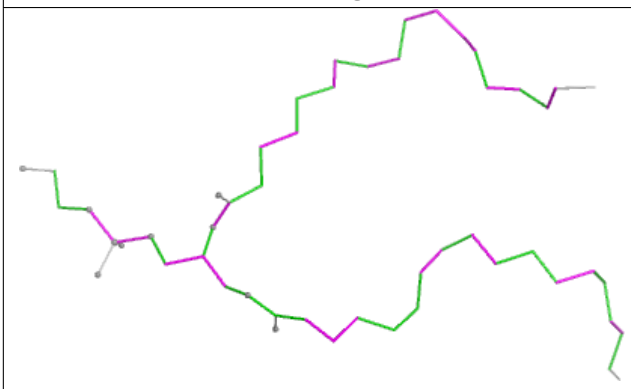
Ligand 3PE I 204



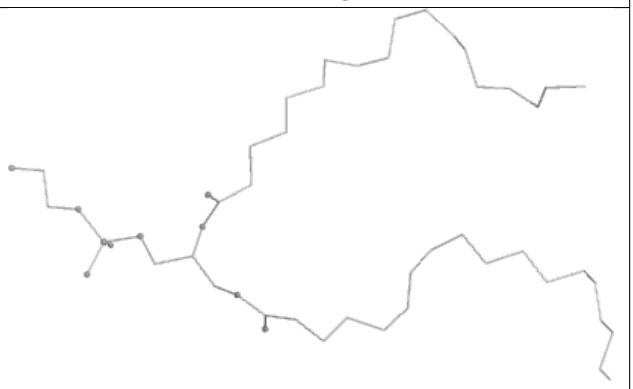
Bond lengths



Bond angles

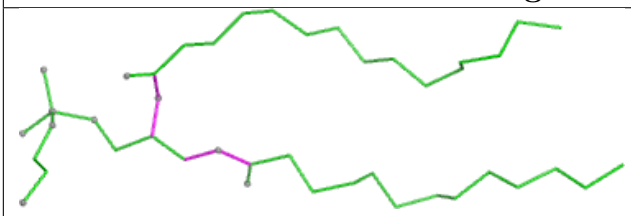


Torsions

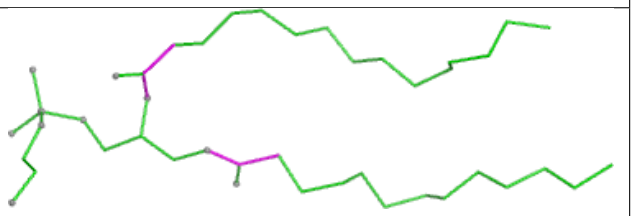


Rings

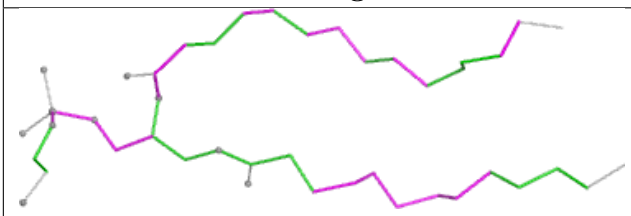
Ligand 3PE M 601



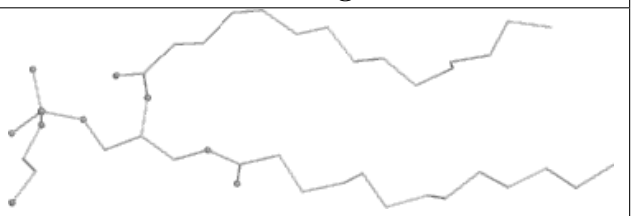
Bond lengths



Bond angles

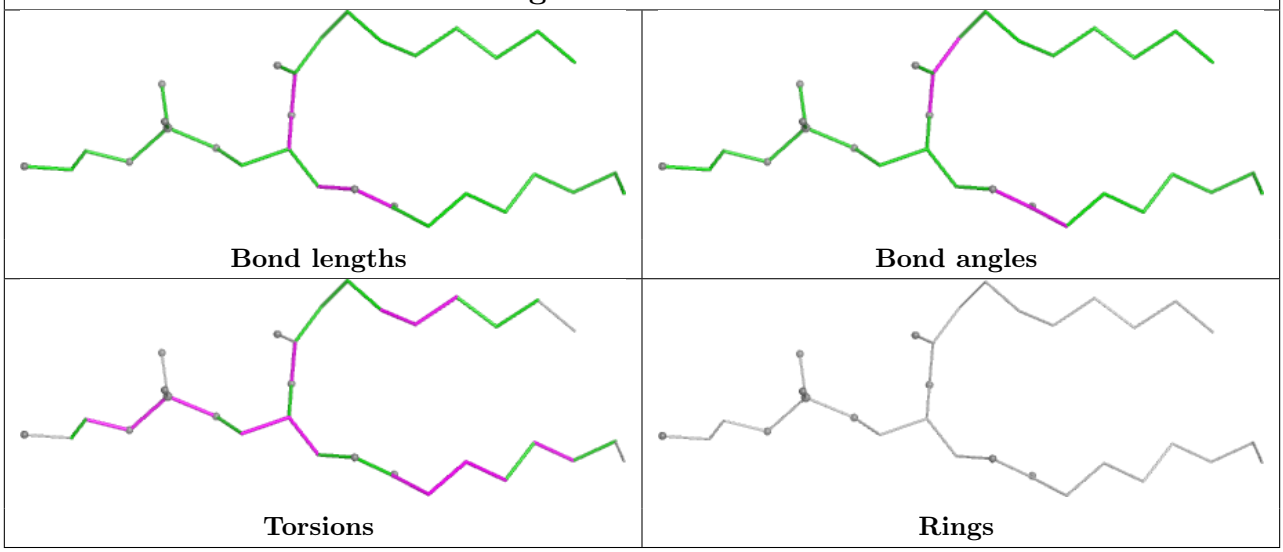


Torsions

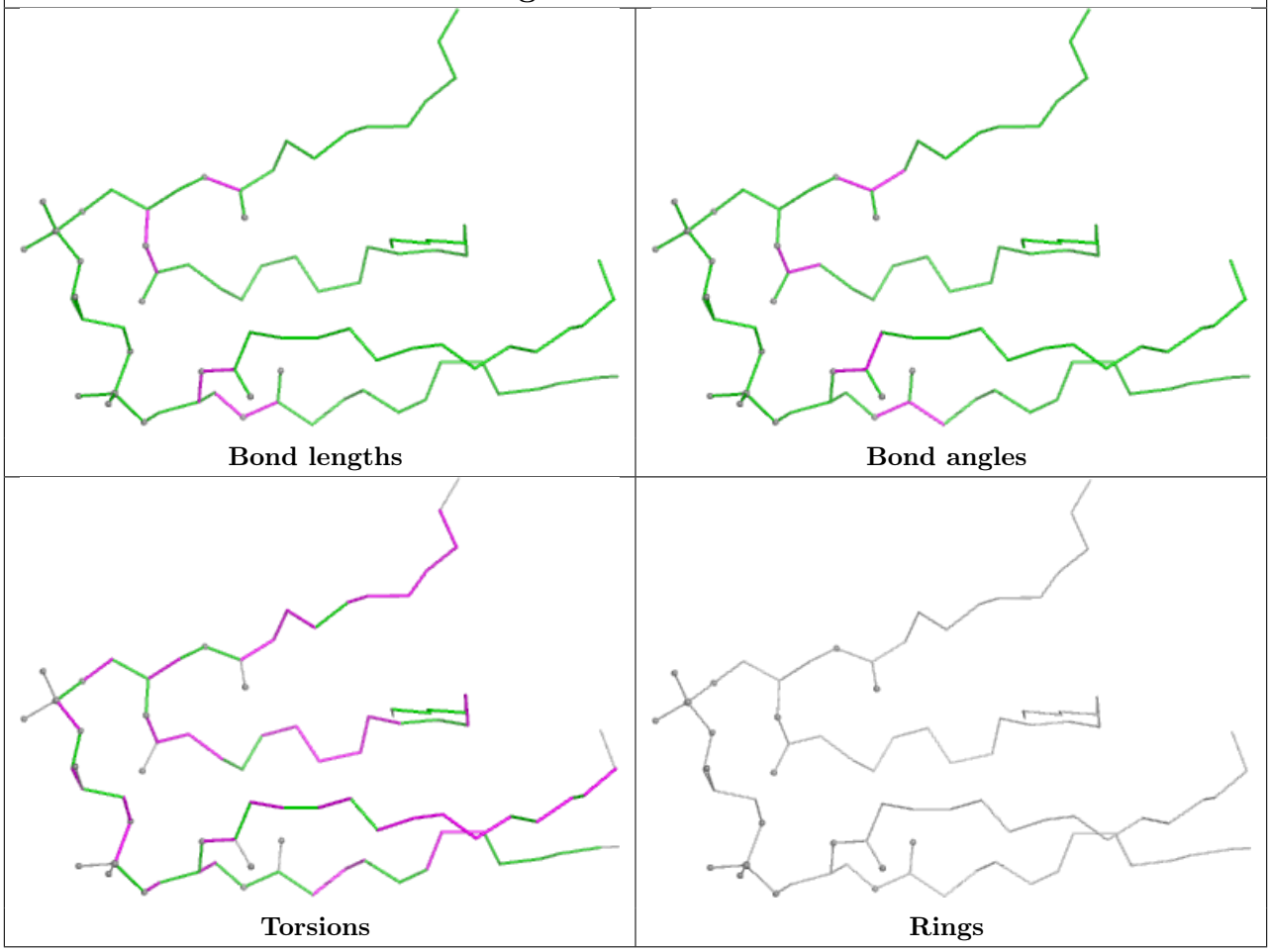


Rings

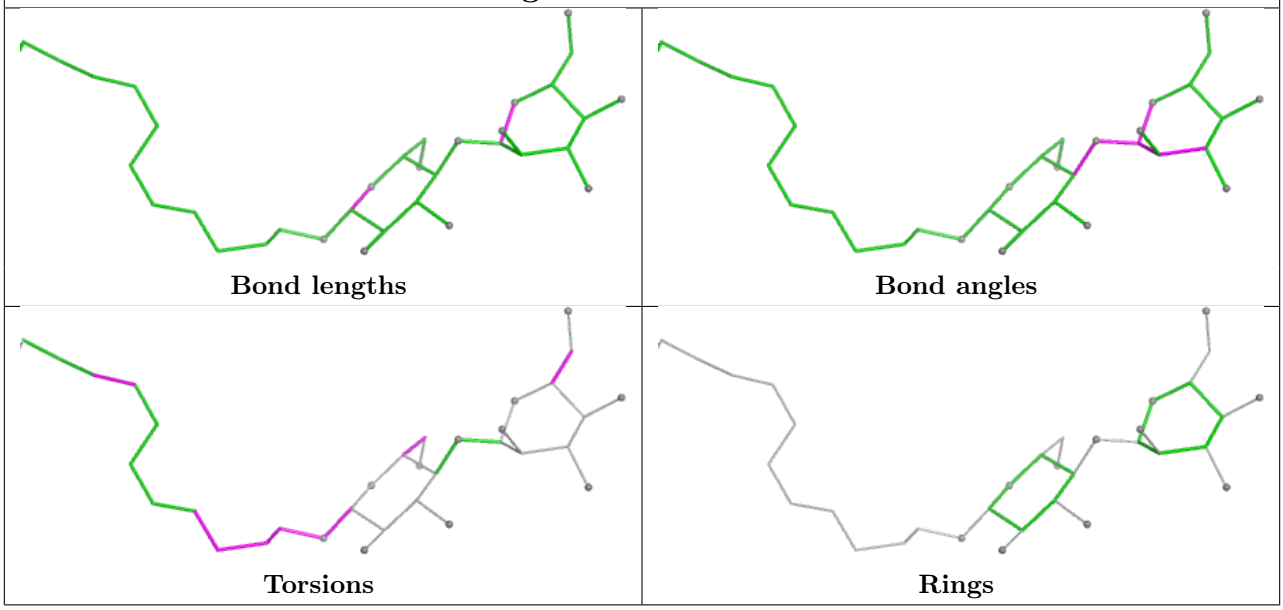
Ligand 3PE Y 205



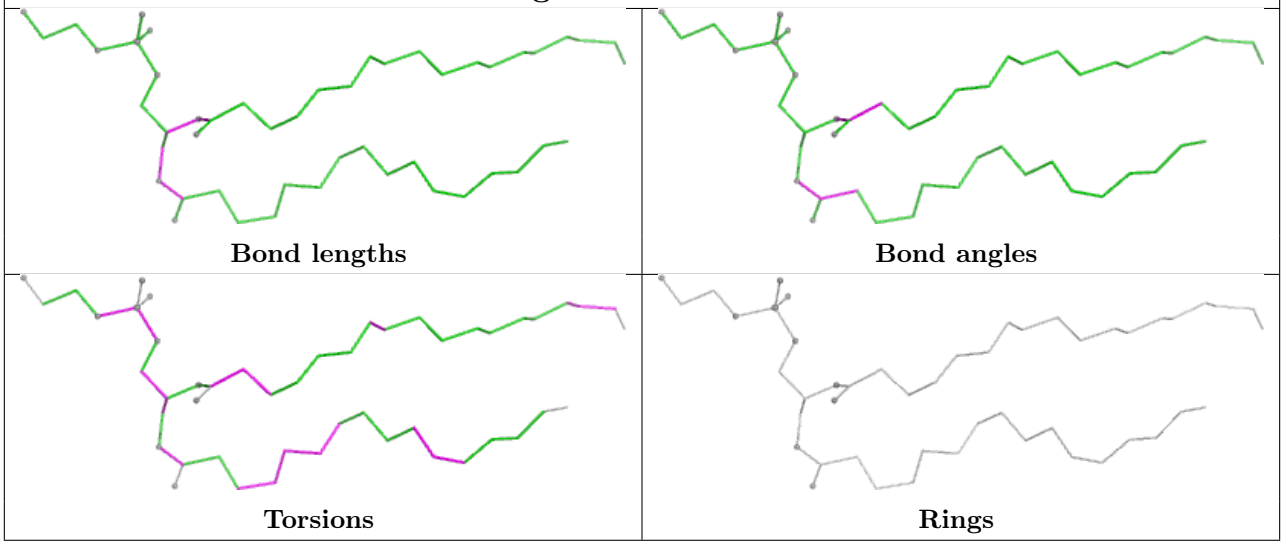
Ligand CDL N 402



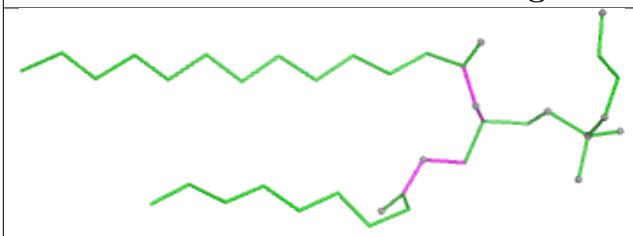
Ligand LMT Y 201



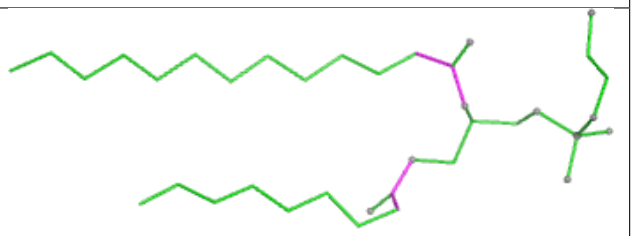
Ligand 3PE d 201



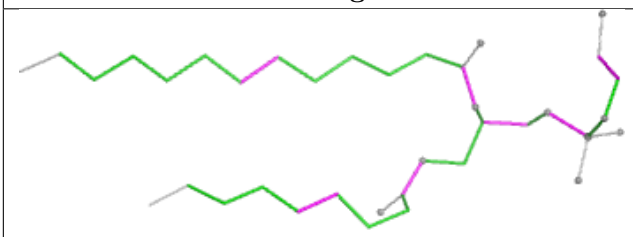
Ligand 3PE A 303



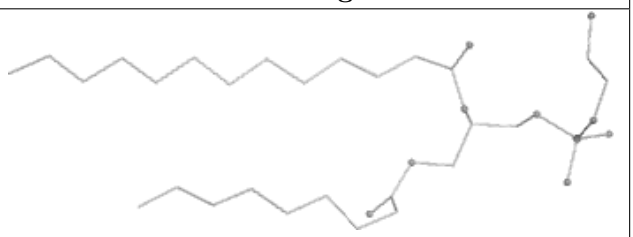
Bond lengths



Bond angles

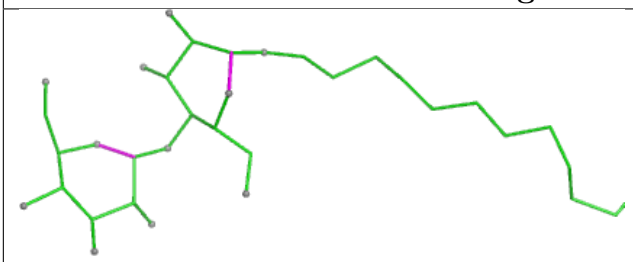


Torsions

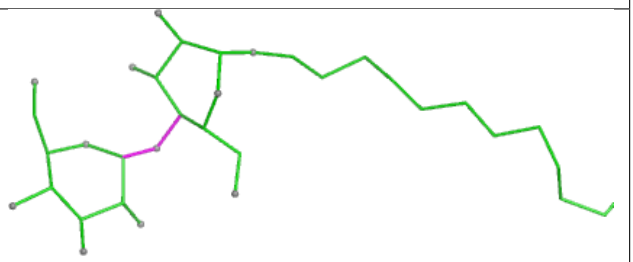


Rings

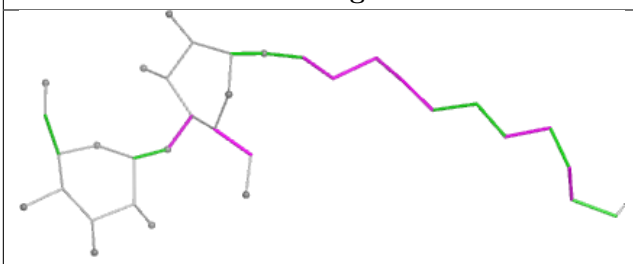
Ligand LMT M 604



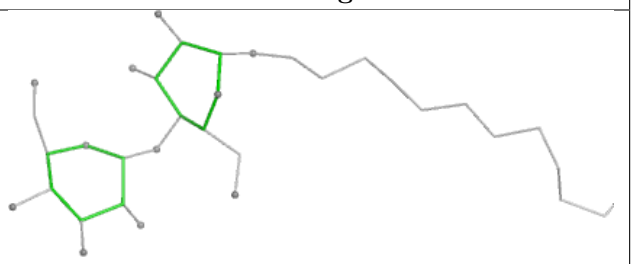
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Bond angles

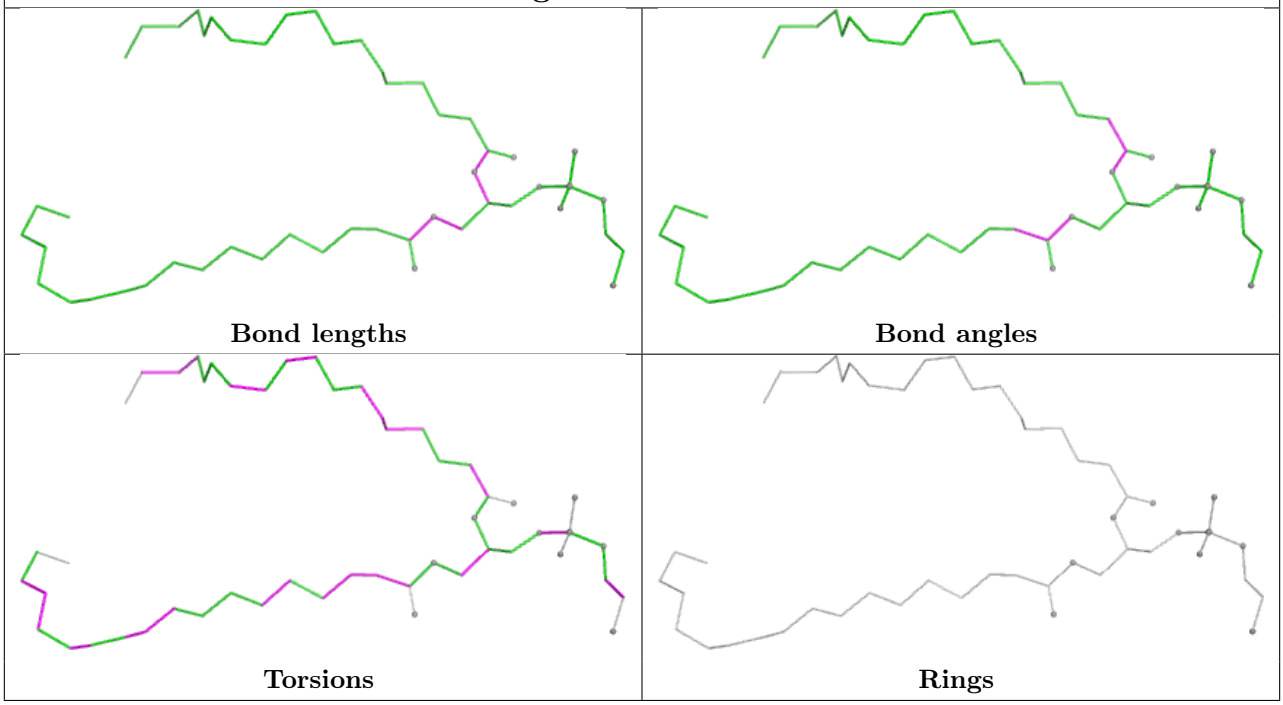


Torsions



Rings

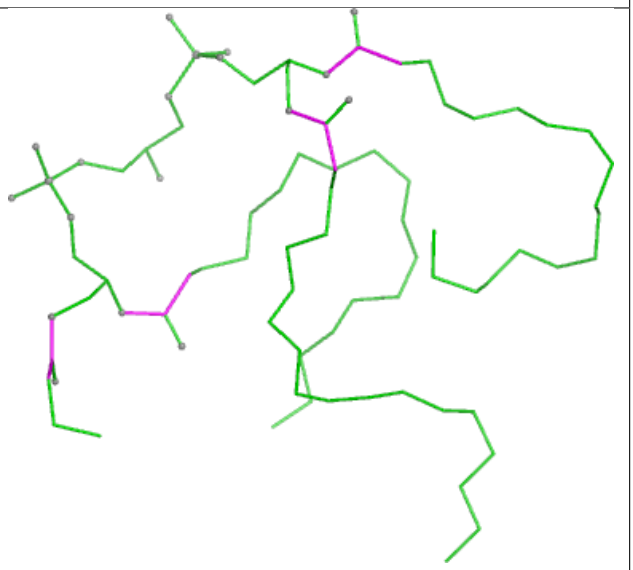
Ligand 3PE b 101



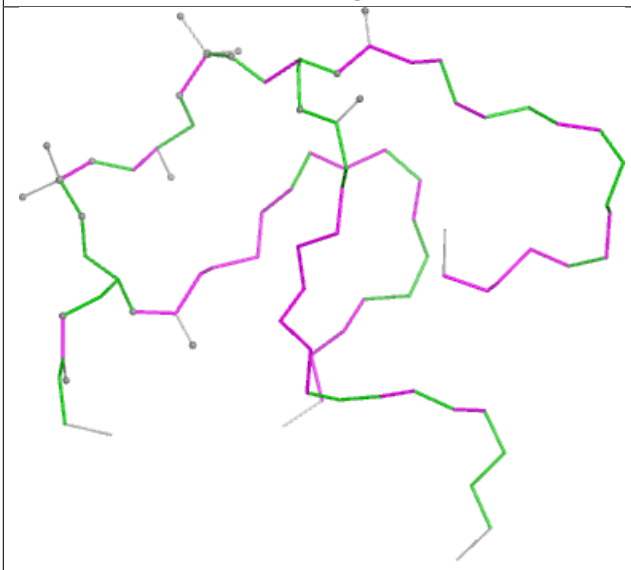
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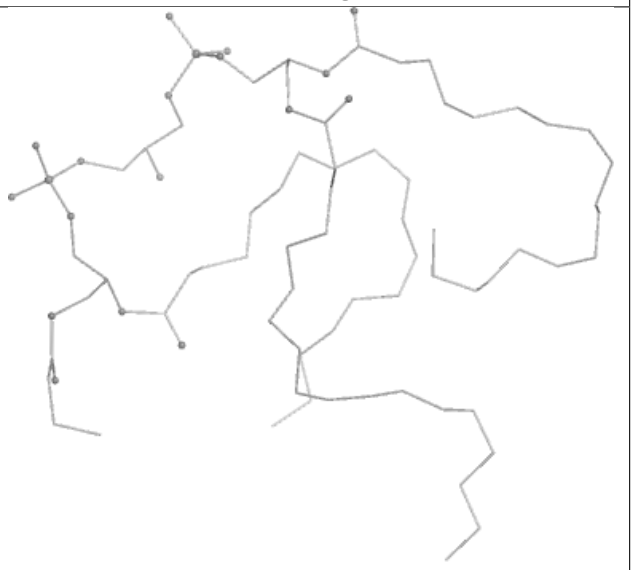
Bond lengths



Bond angles

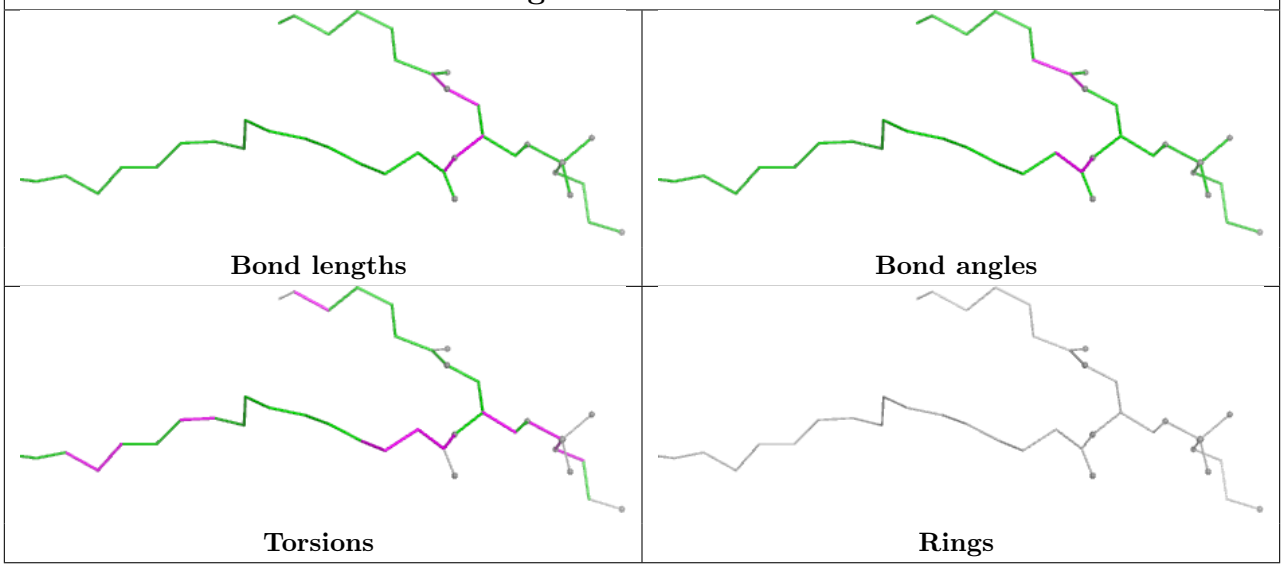


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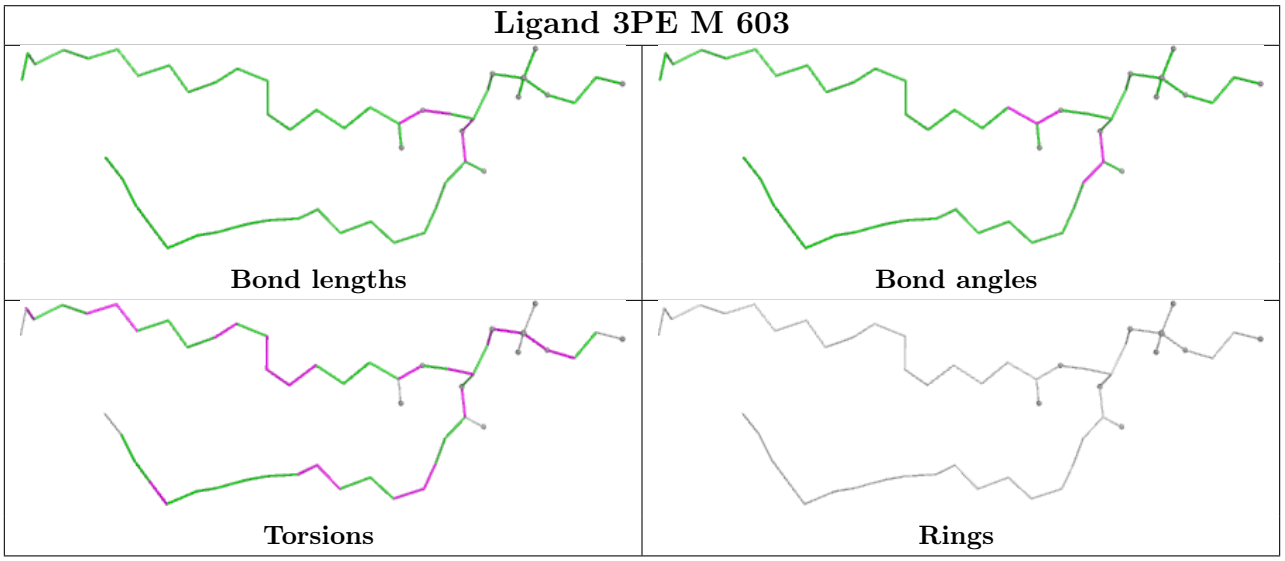


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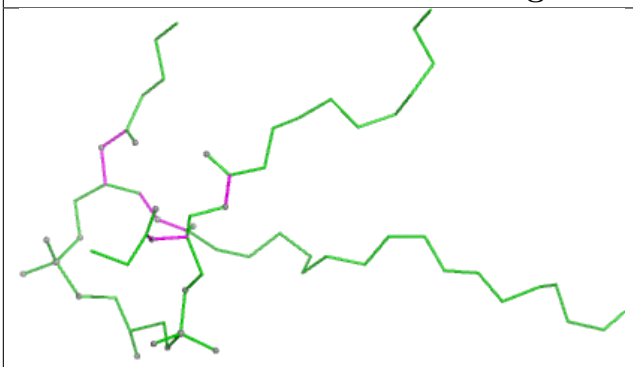
Ligand 3PE m 201



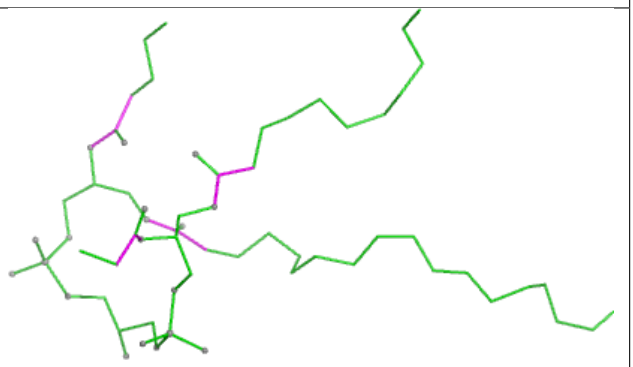
Ligand 3PE M 603



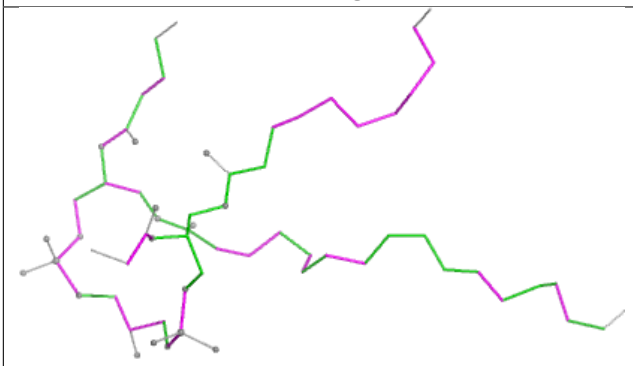
Ligand CDL d 202



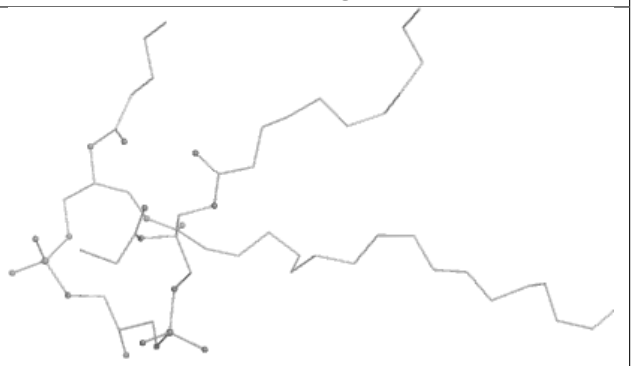
Bond lengths



Bond angles

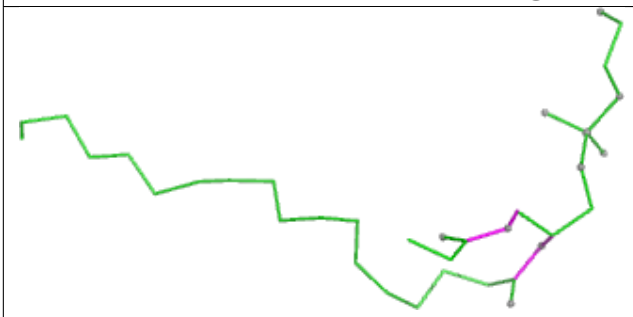


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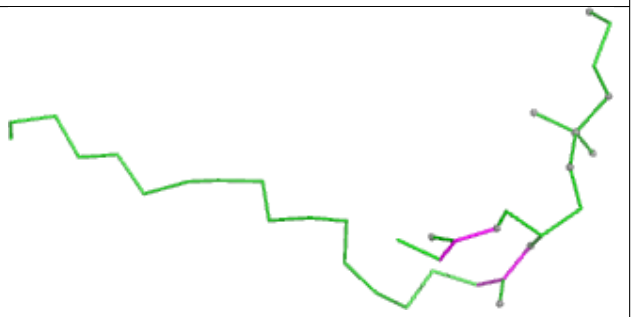


Rings

Ligand 3PE H 601



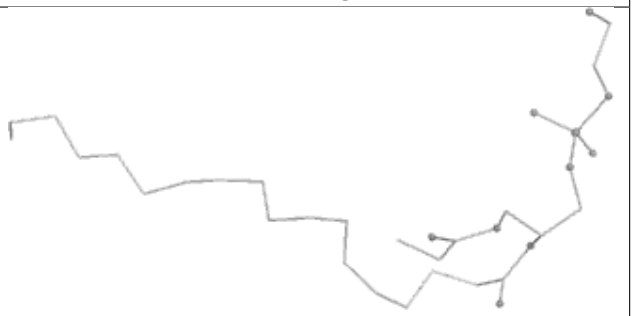
Bond lengths



Bond angles

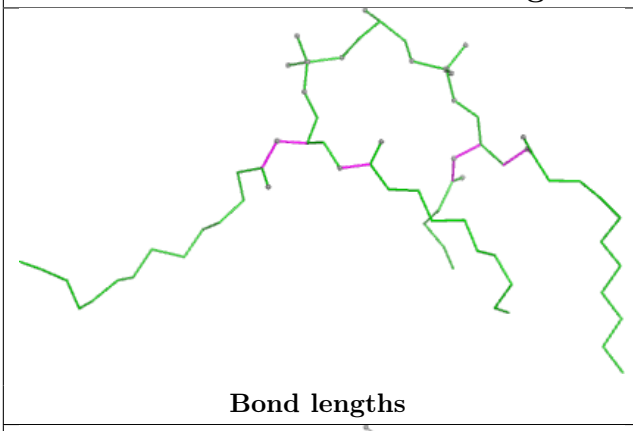


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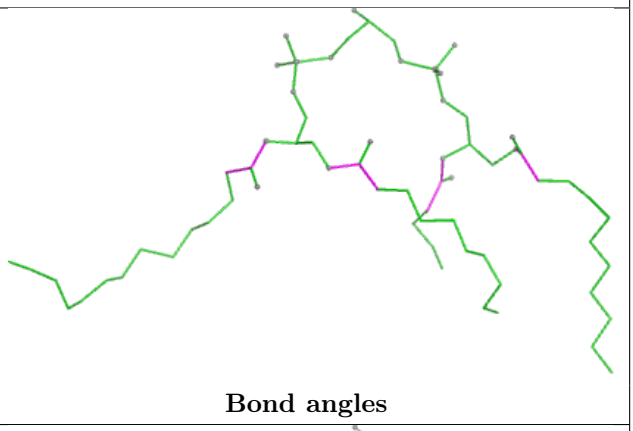


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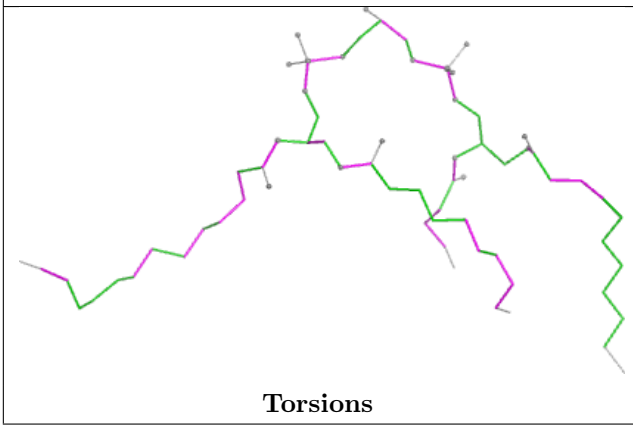
Ligand CDL h 202



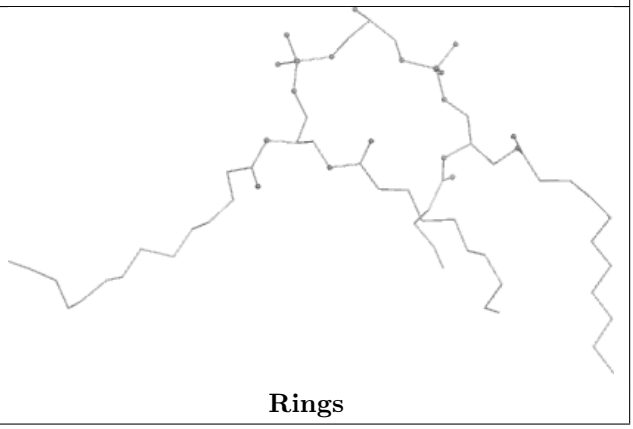
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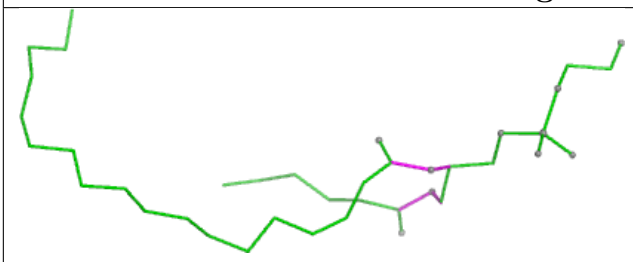


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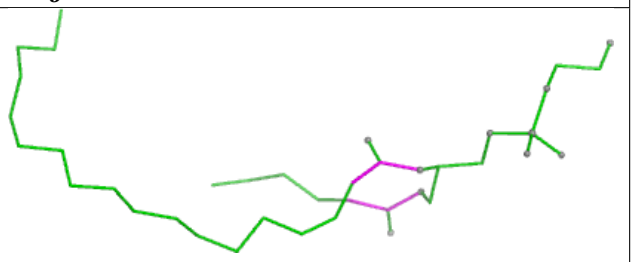


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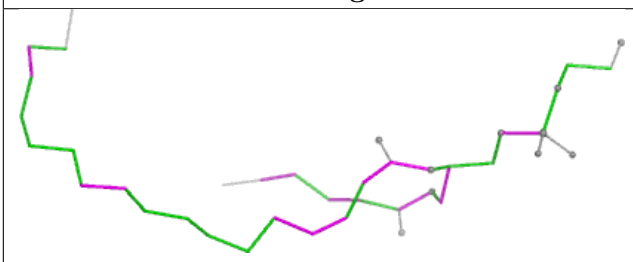
Ligand 3PE j 101



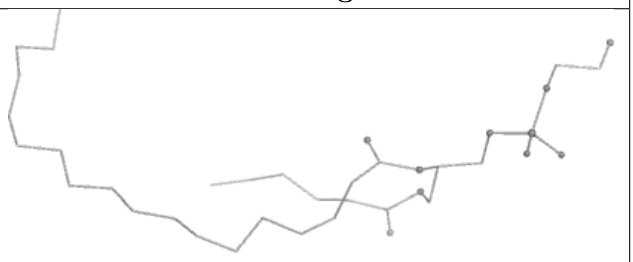
Bond lengths



Bond angles

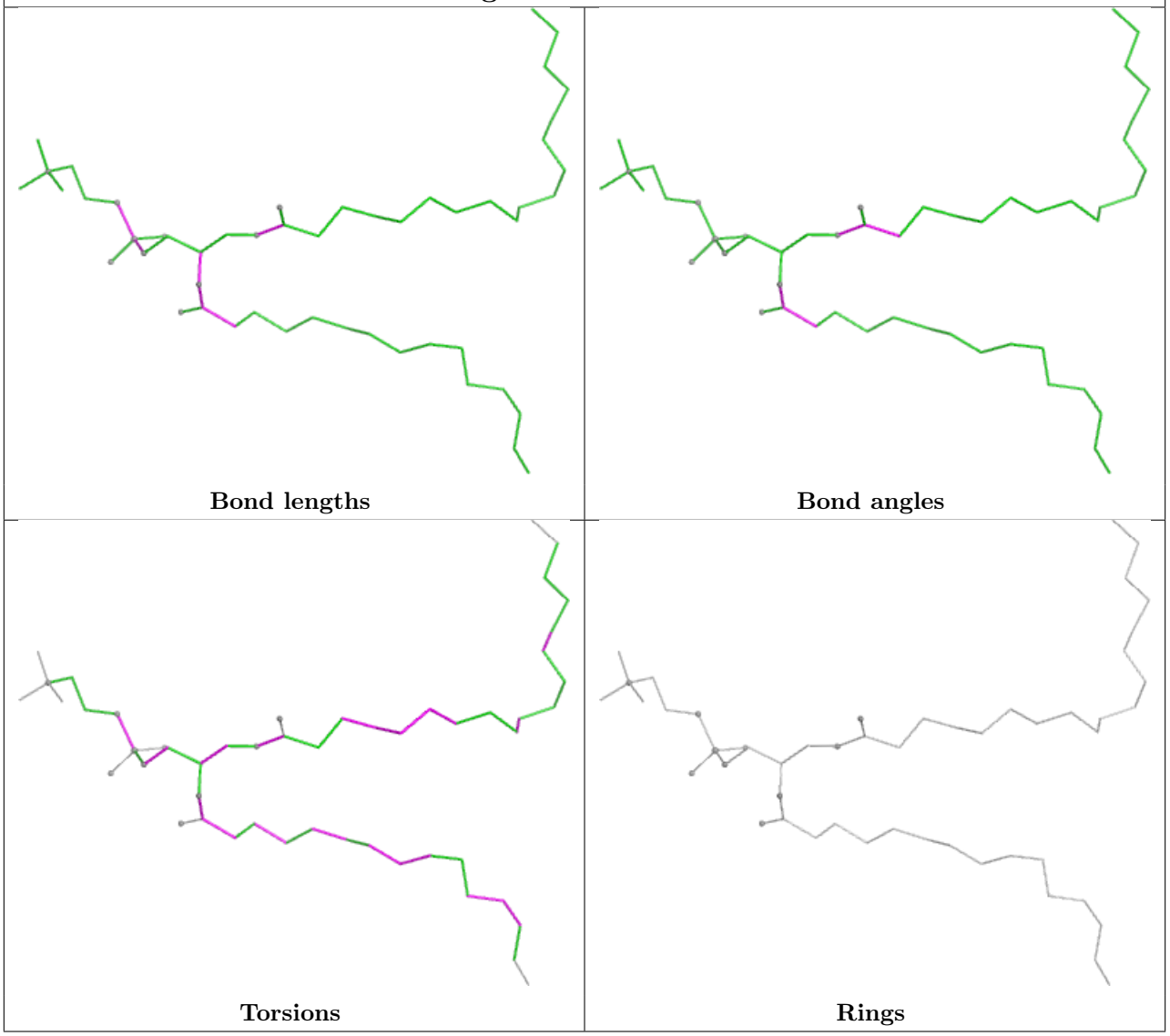


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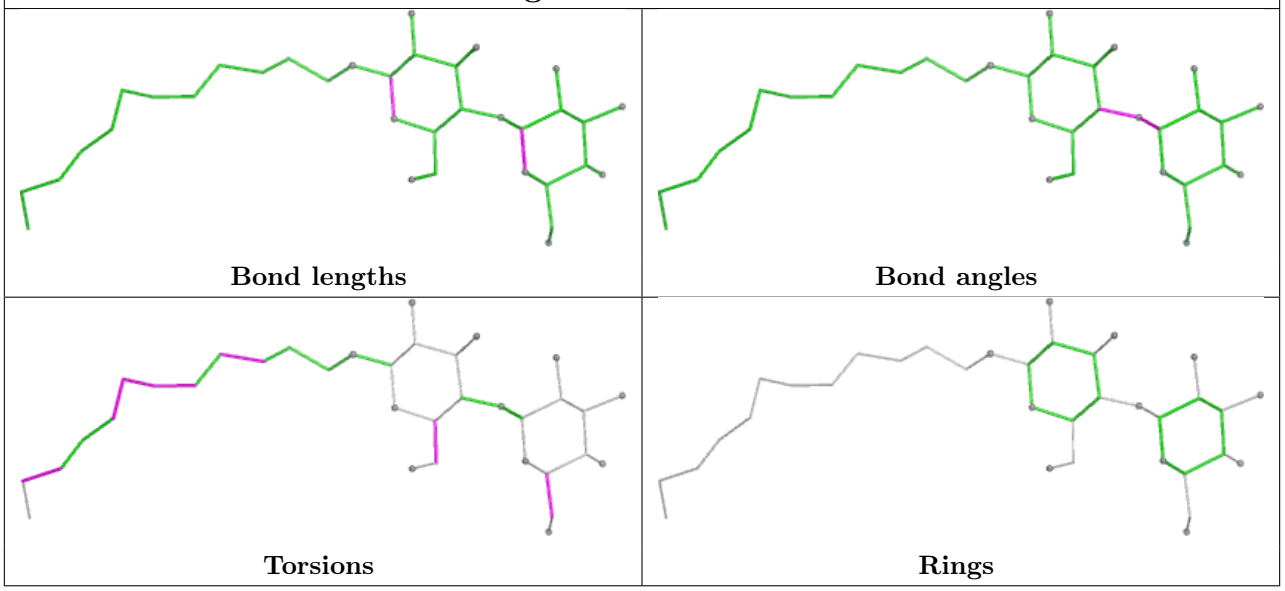


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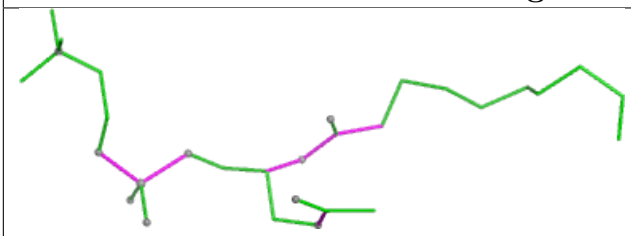
Ligand PC1 B 202



Ligand LMT L 704



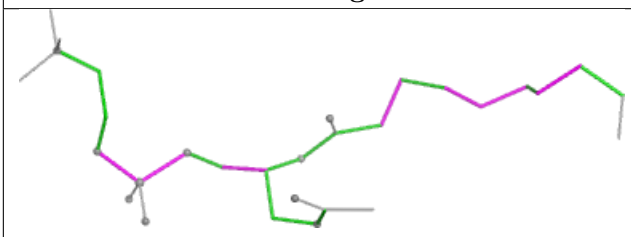
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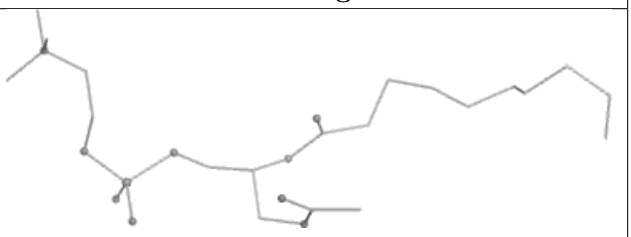
Bond lengths



Bond angles

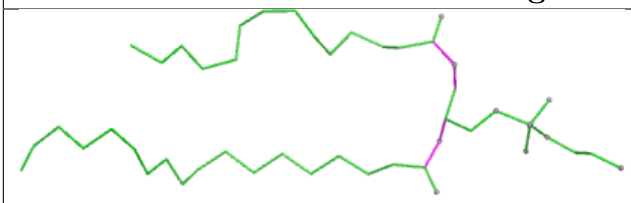


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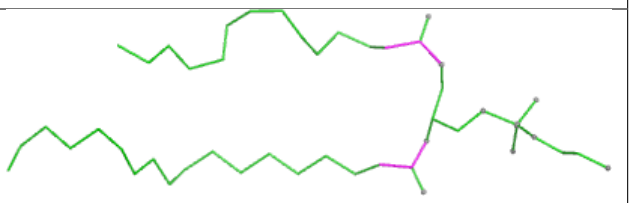


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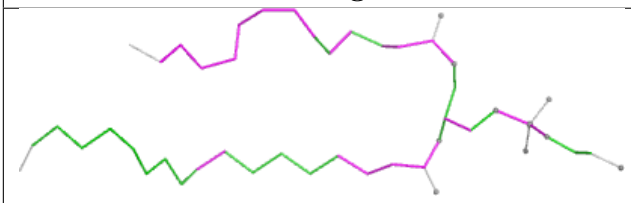
Ligand 3PE A 302



Bond lengths



Bond angles

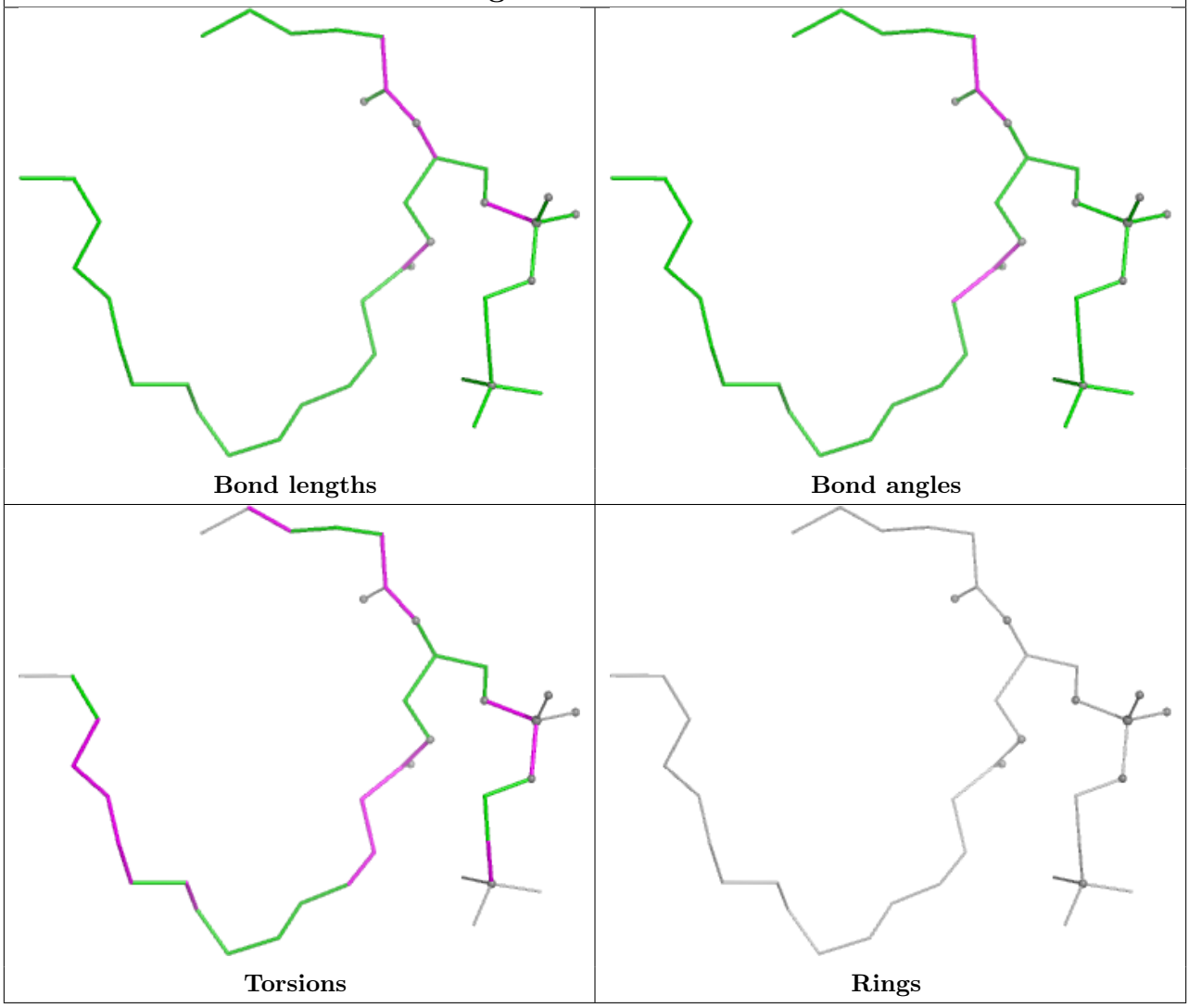


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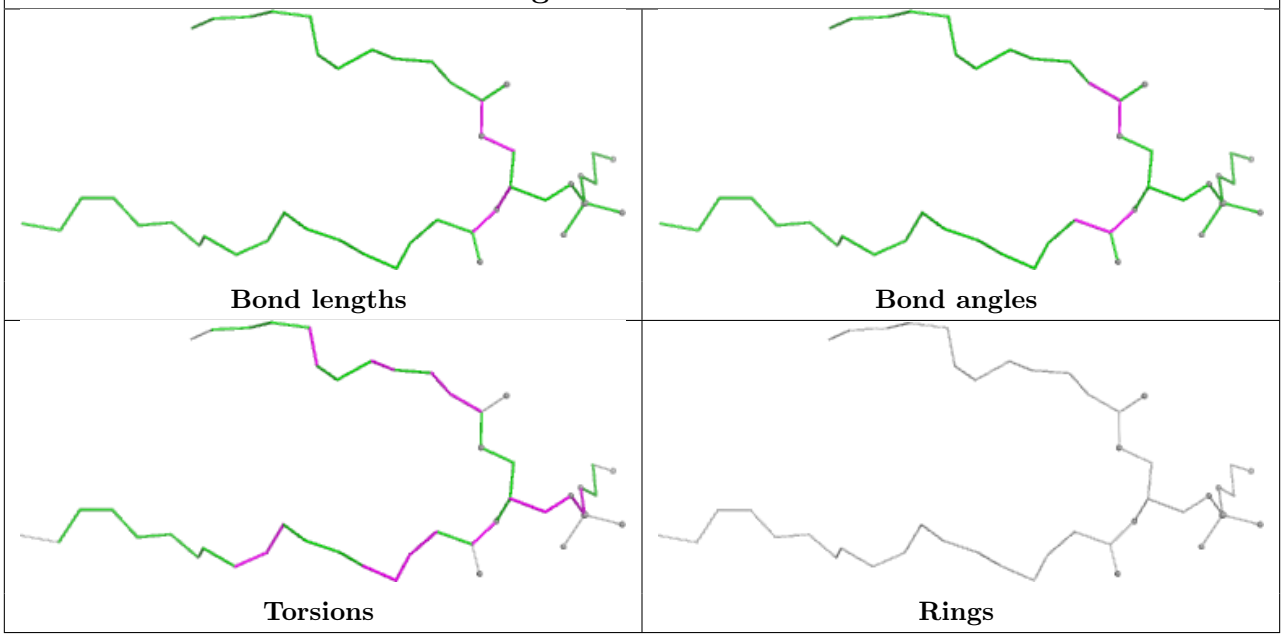


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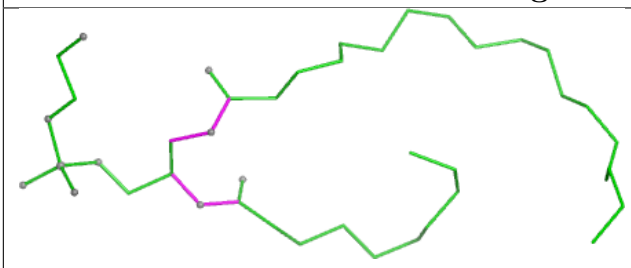
Ligand PC1 N 403



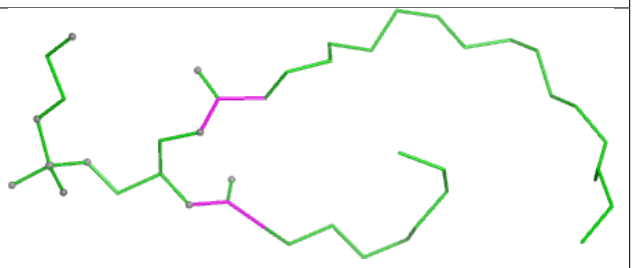
Ligand 3PE L 705



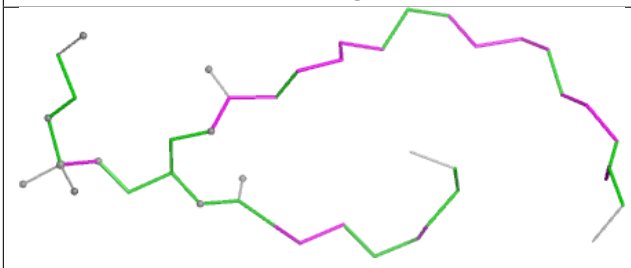
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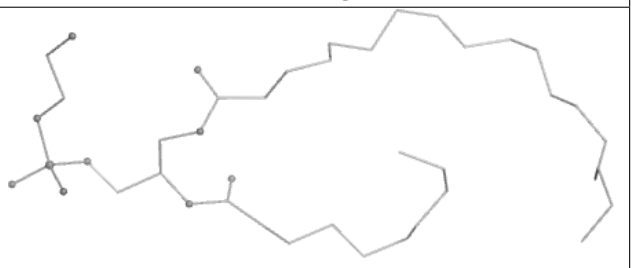
Bond lengths



Bond angles

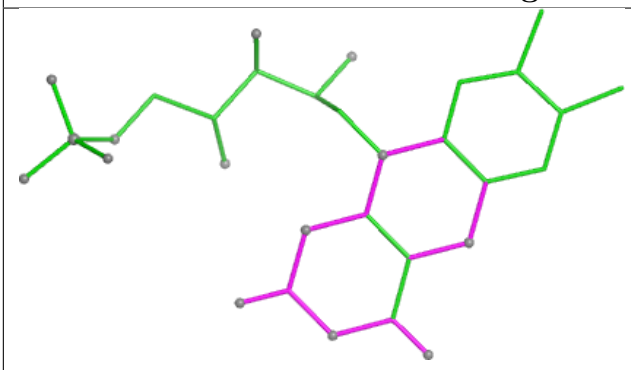


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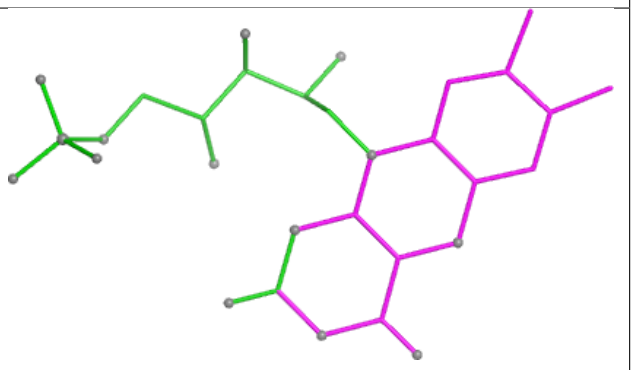


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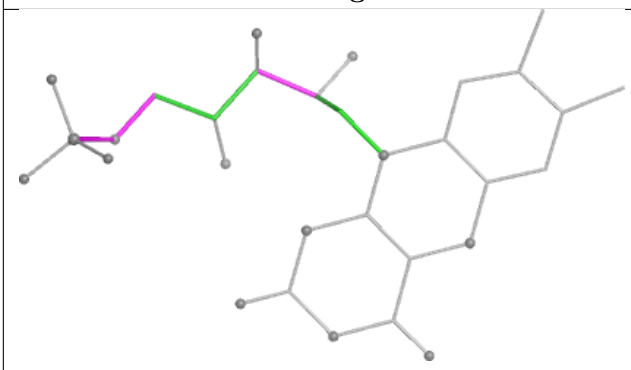
Ligand FMN F 501



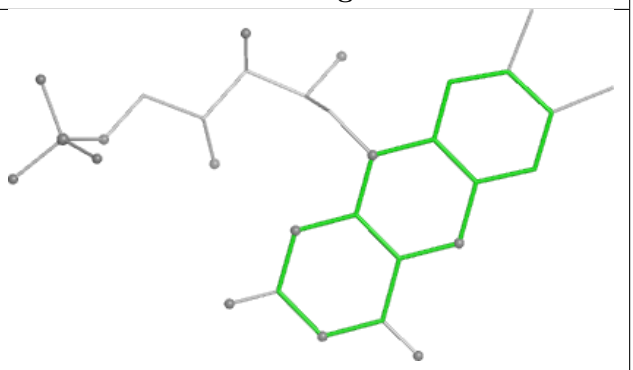
Bond lengths



Bond angles

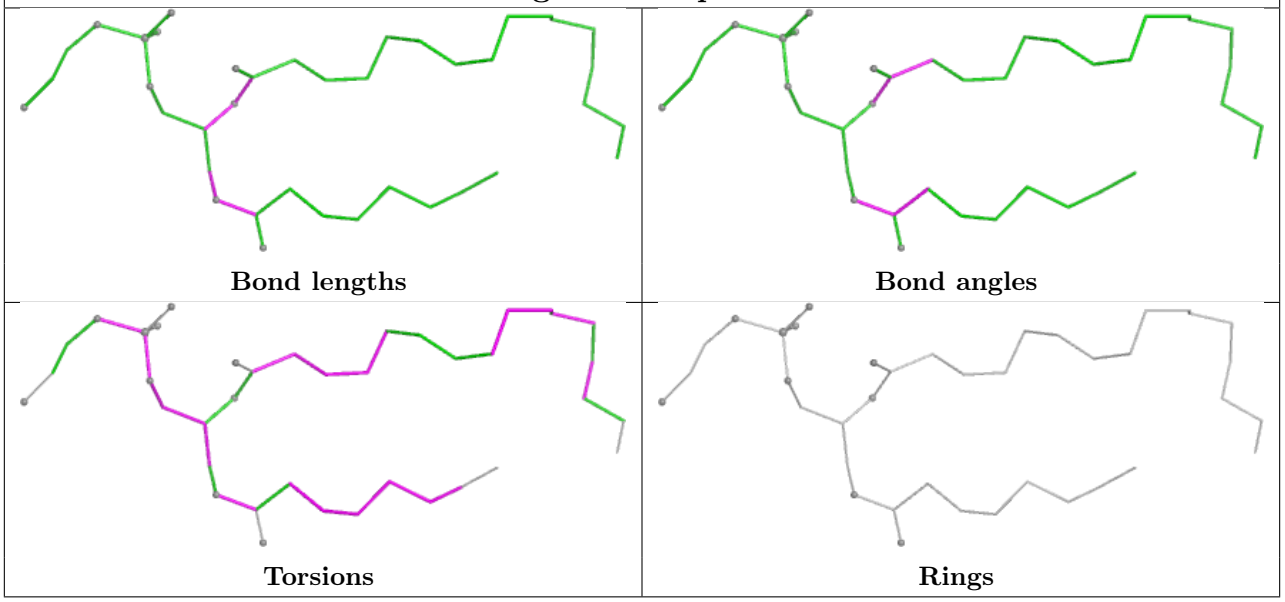


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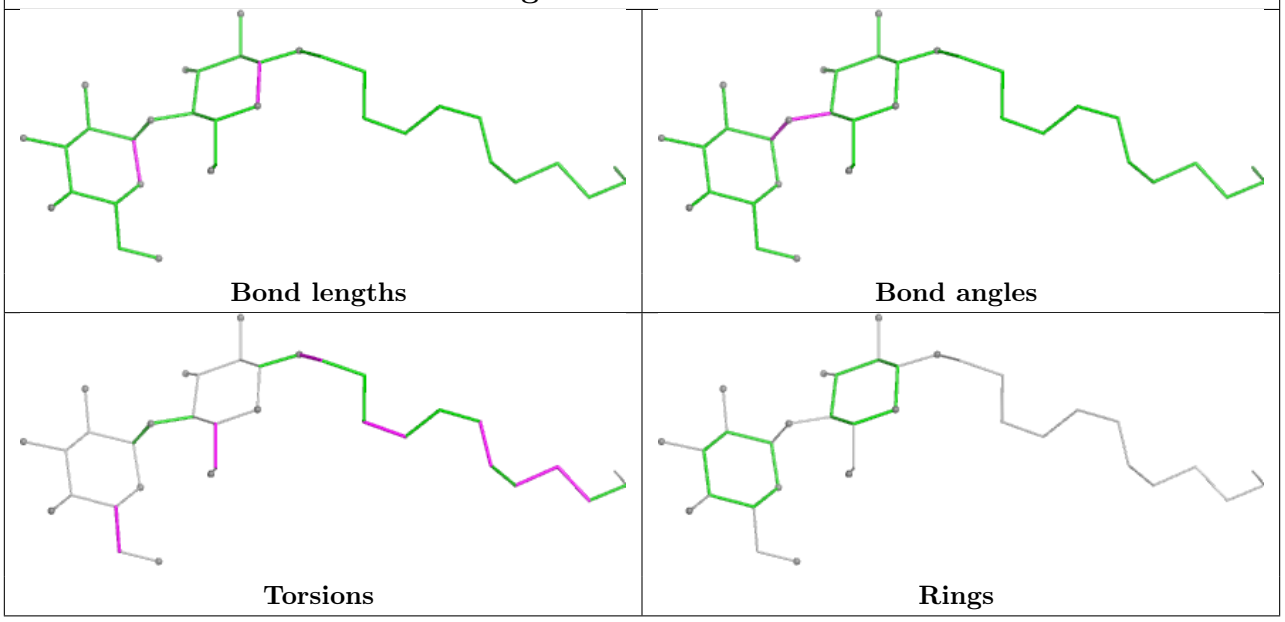


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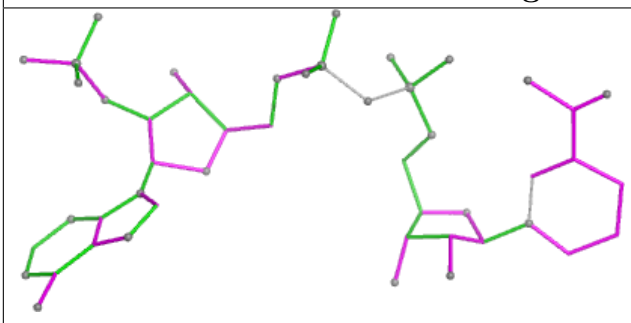
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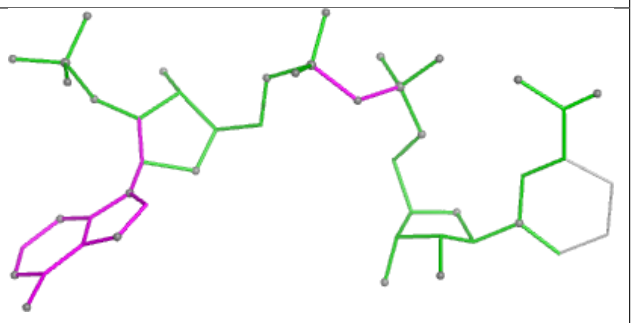
Ligand LMT H 602



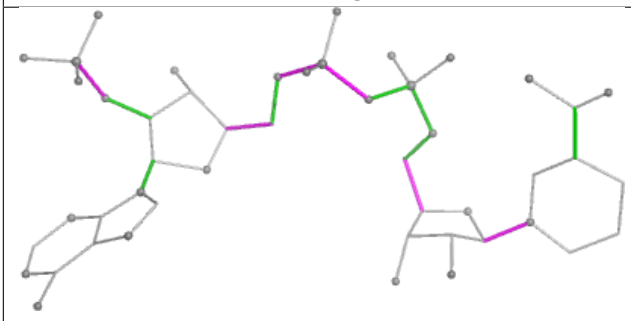
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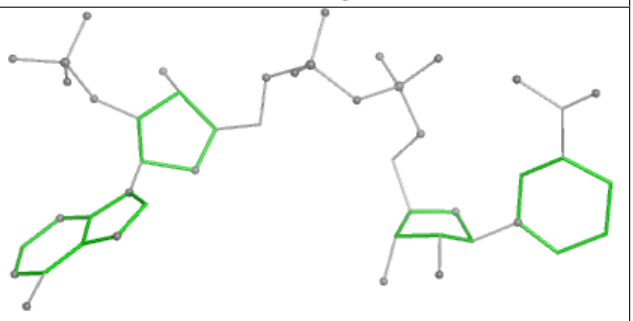
Bond lengths



Bond angles



Torsions



Rings

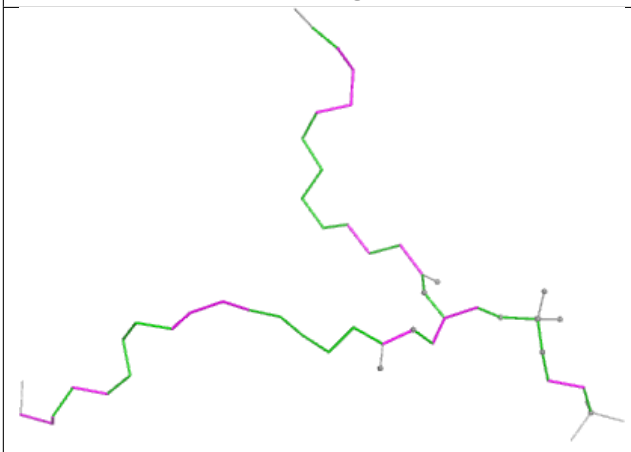
Ligand PC1 A 301



Bond lengths



Bond angles

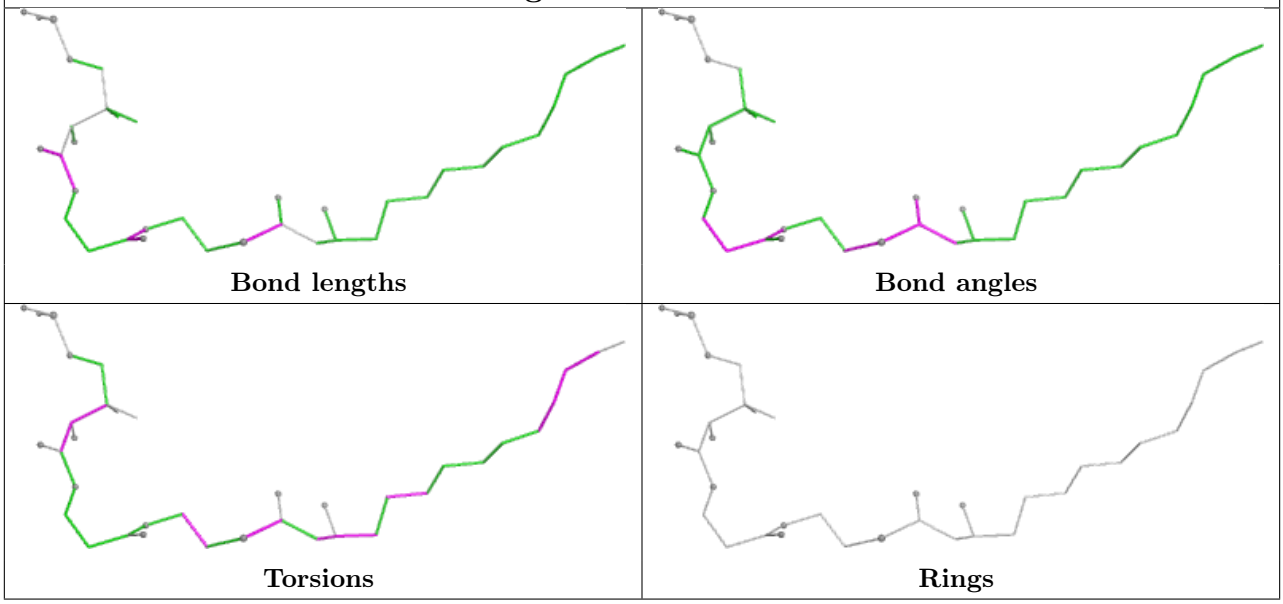


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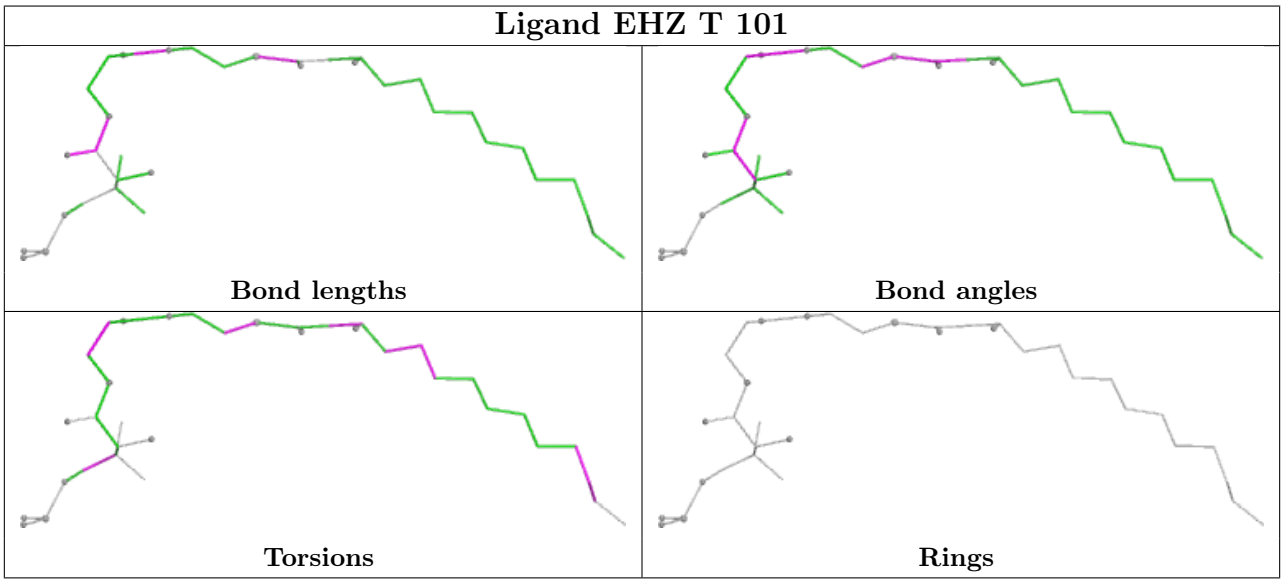


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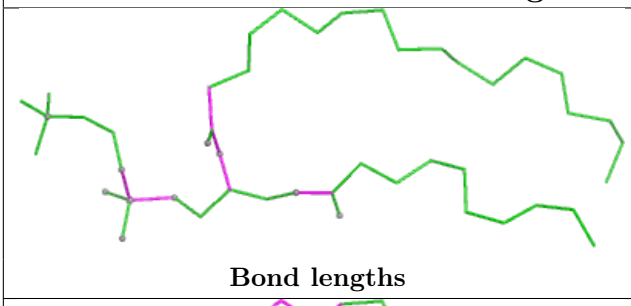
Ligand EHZ U 101



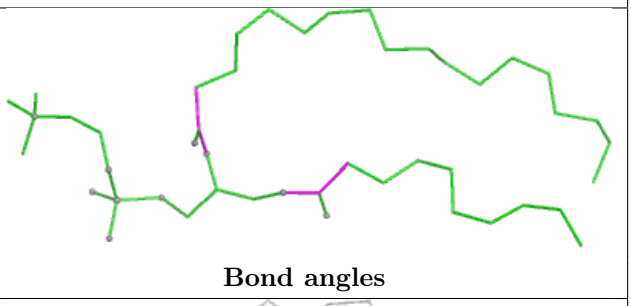
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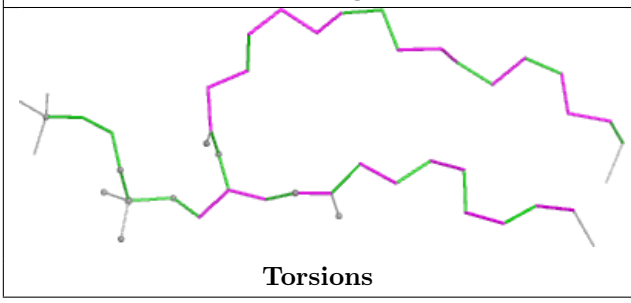
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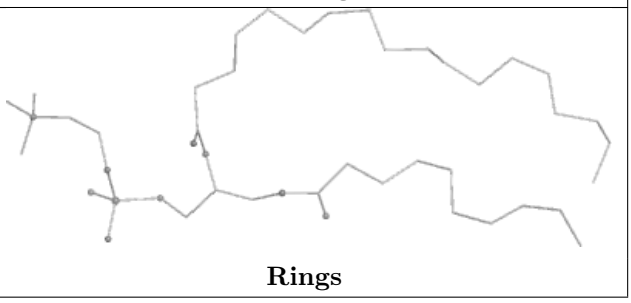
Bond lengths



Bond angles

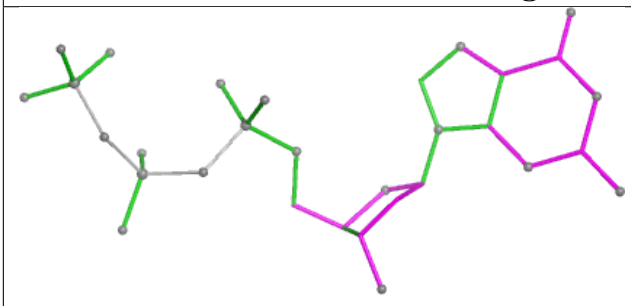


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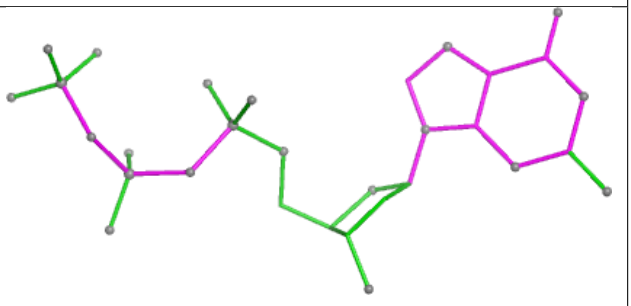


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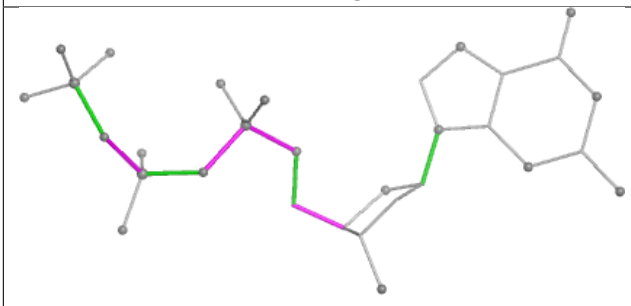
Ligand DGT O 404



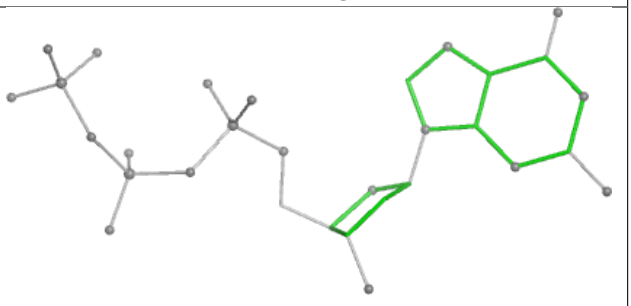
Bond lengths



Bond angles

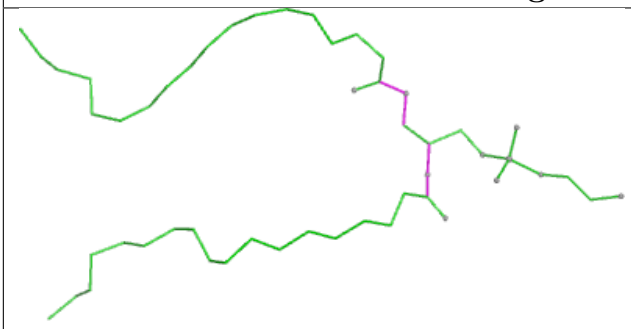


Torsions

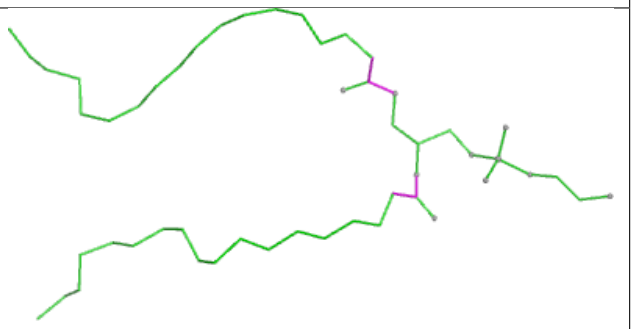


Rings

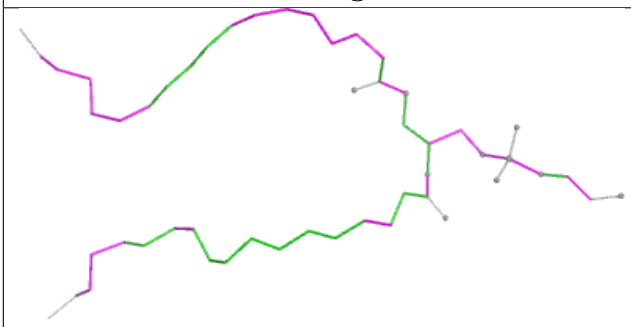
Ligand 3PE Y 203



Bond lengths



Bond angles

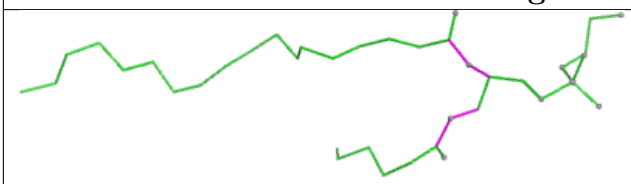


Torsions

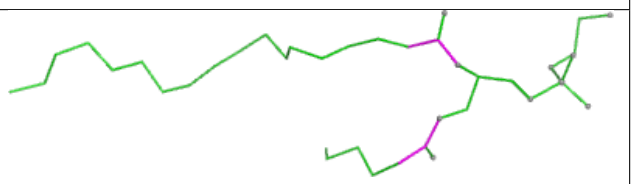


Rings

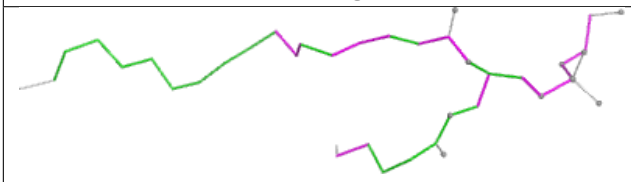
Ligand 3PE Y 202



Bond lengths



Bond angles

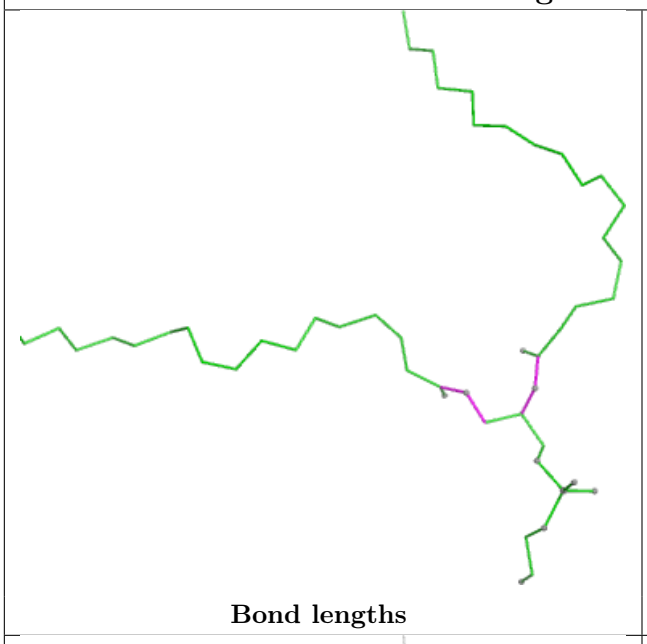


Torsions

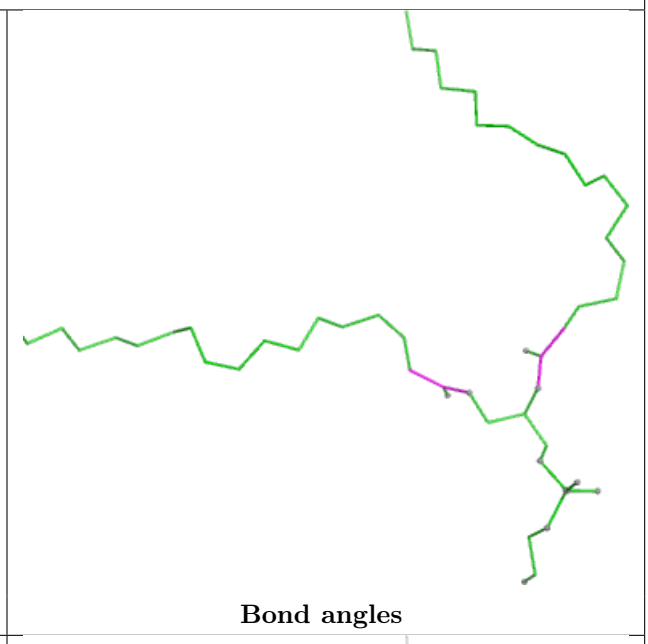


Rings

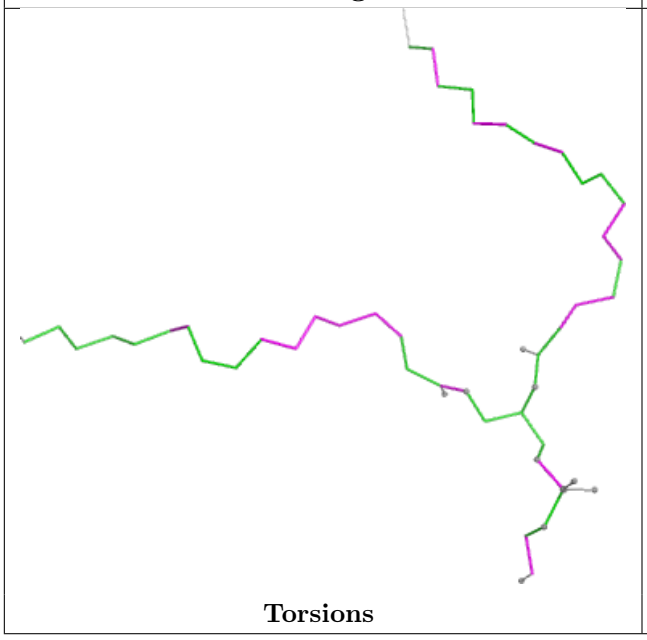
Ligand 3PE I 201



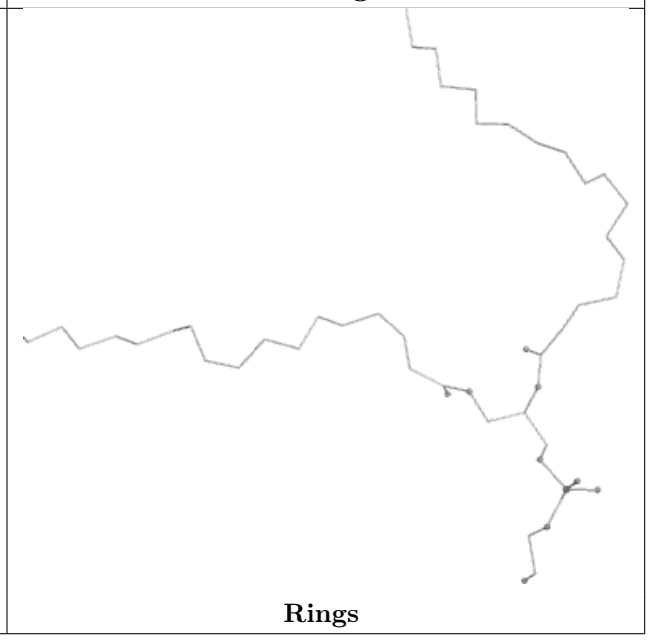
Bond lengths



Bond angles

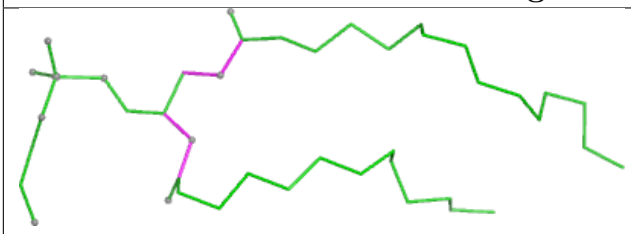


Torsions

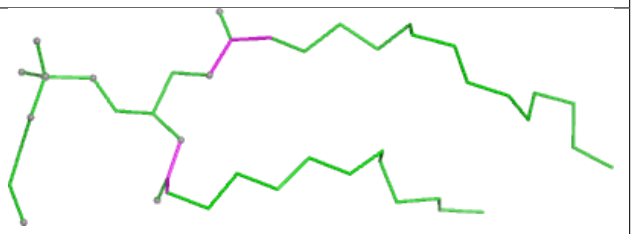


Rings

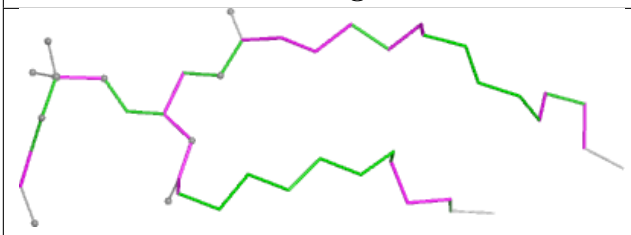
Ligand 3PE K 101



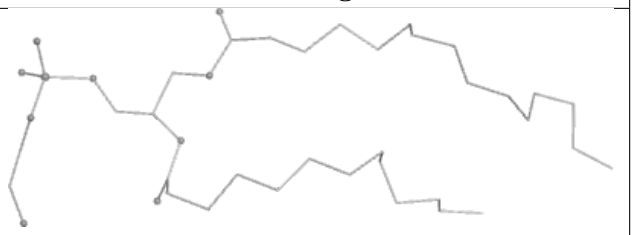
Bond lengths



Bond angles

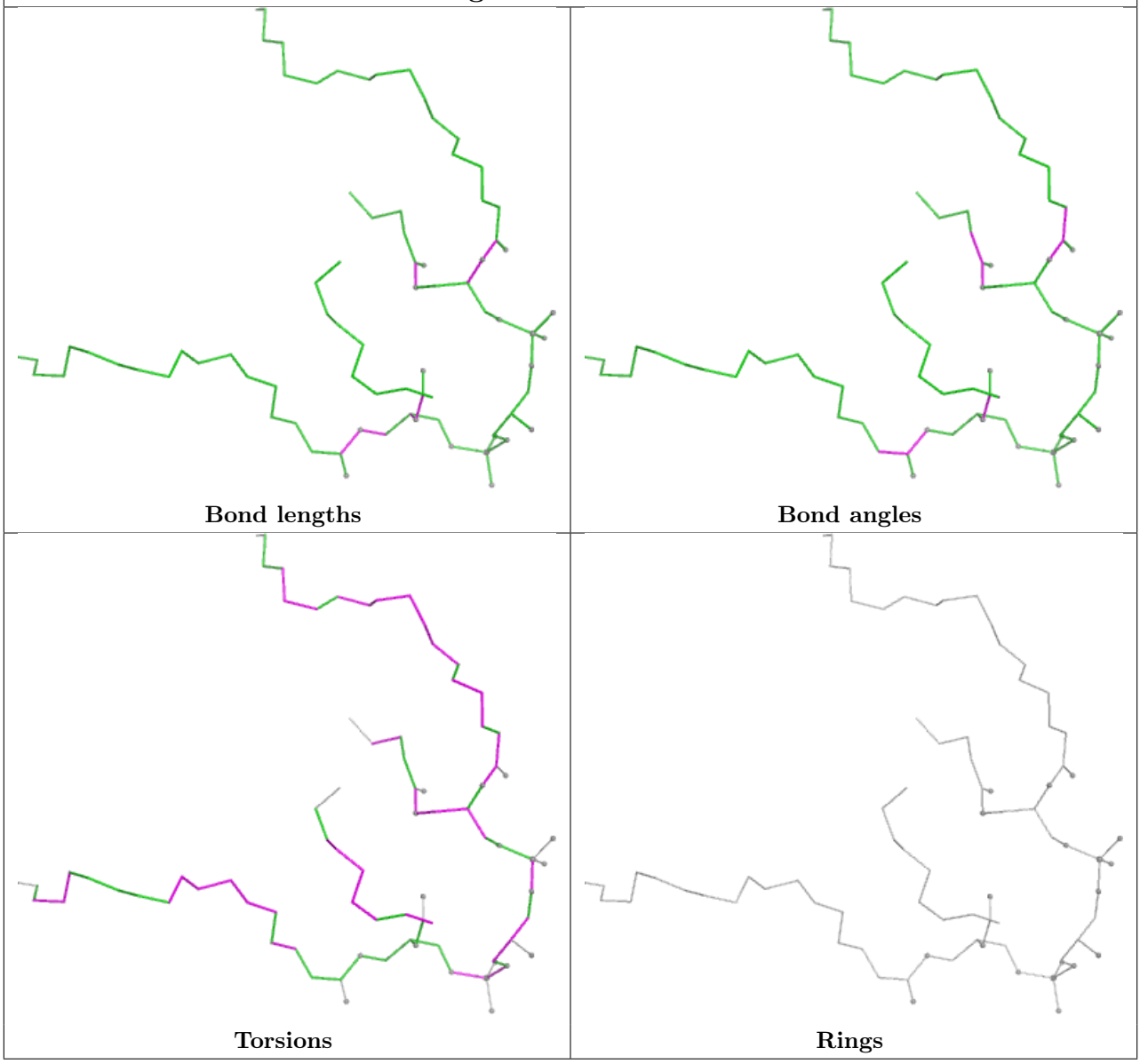


Torsions

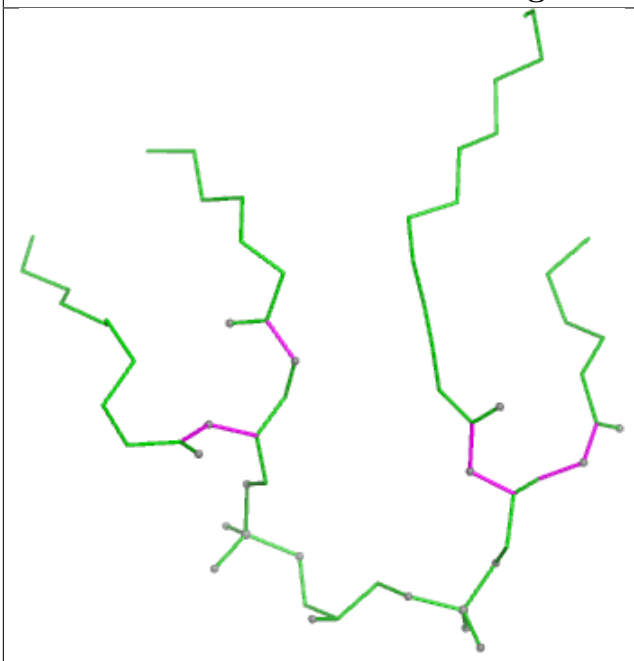


Rings

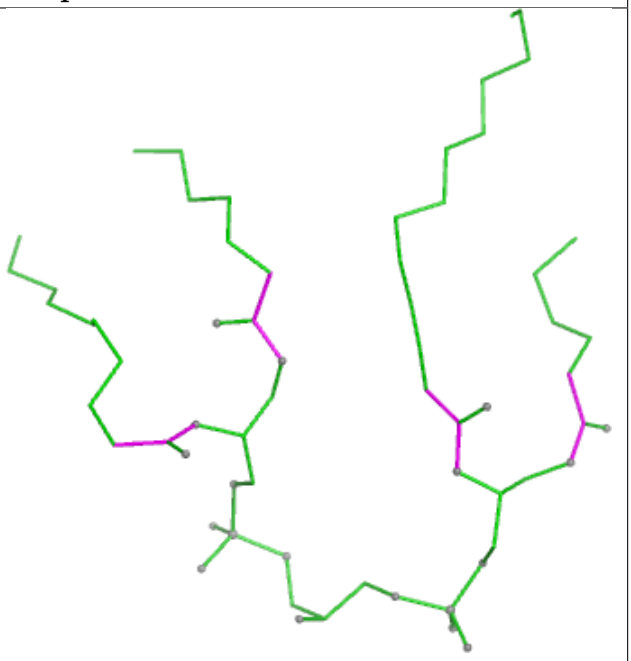
Ligand CDL L 702



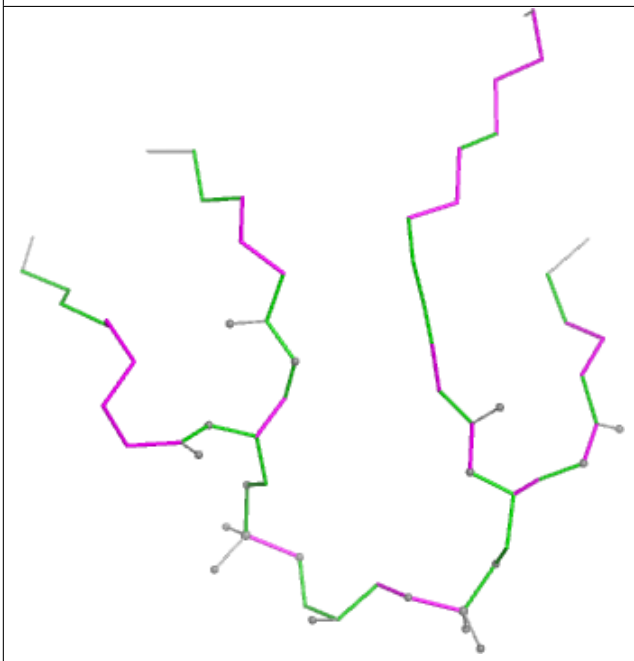
Ligand CDL q 201



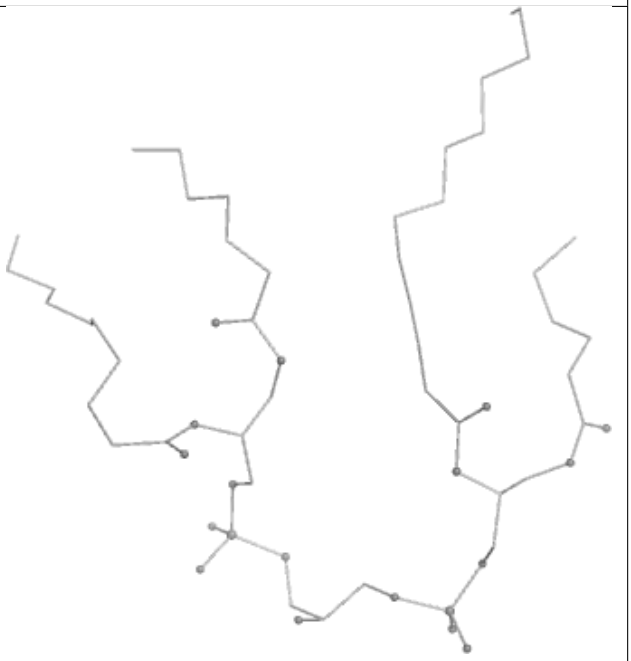
Bond lengths



Bond angles

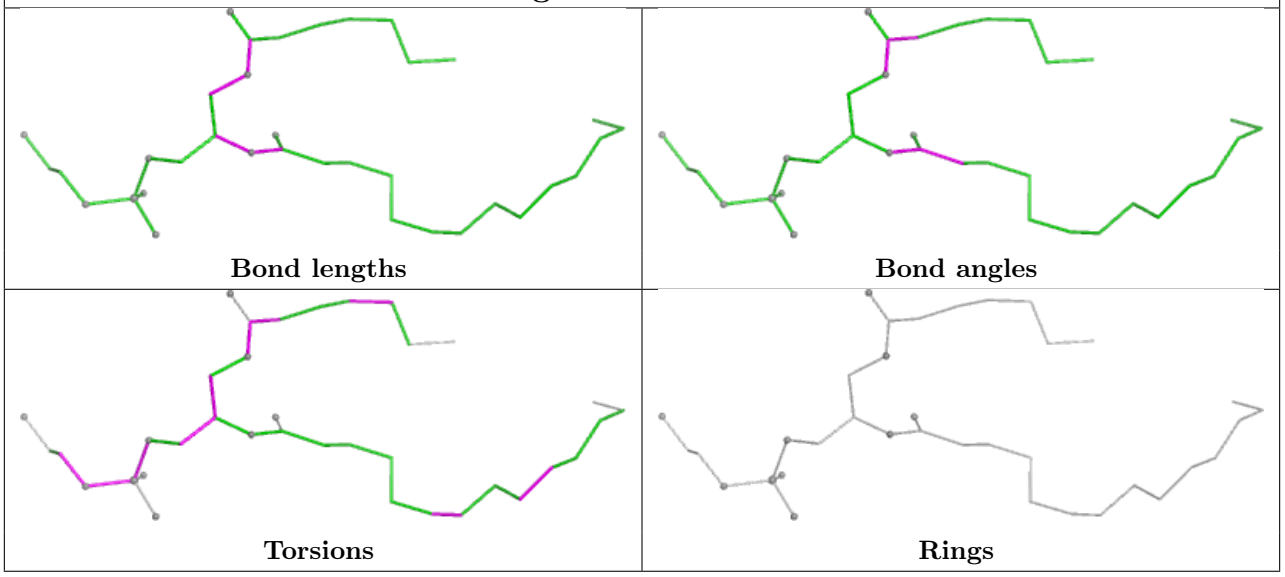


Torsions

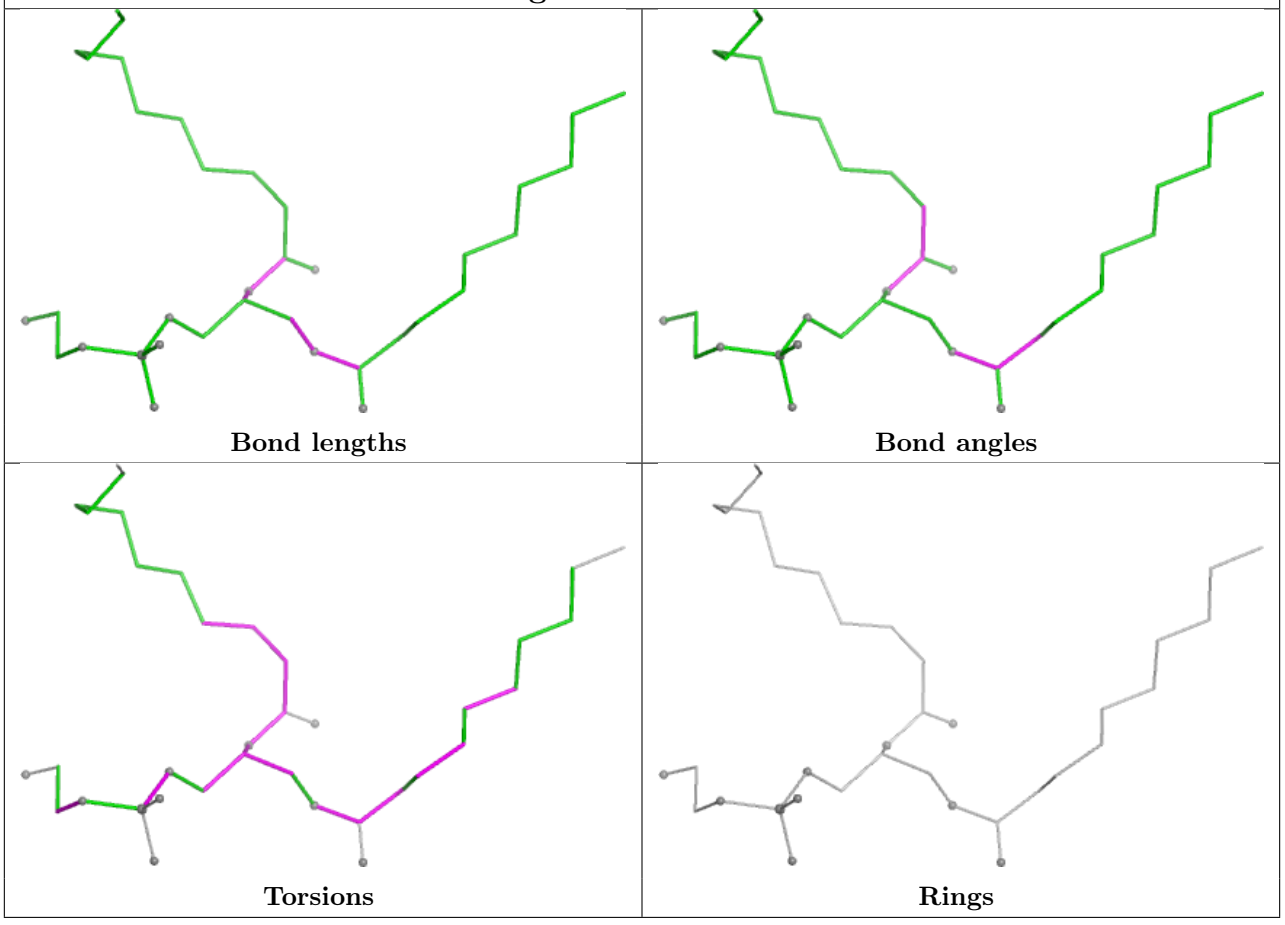


Rings

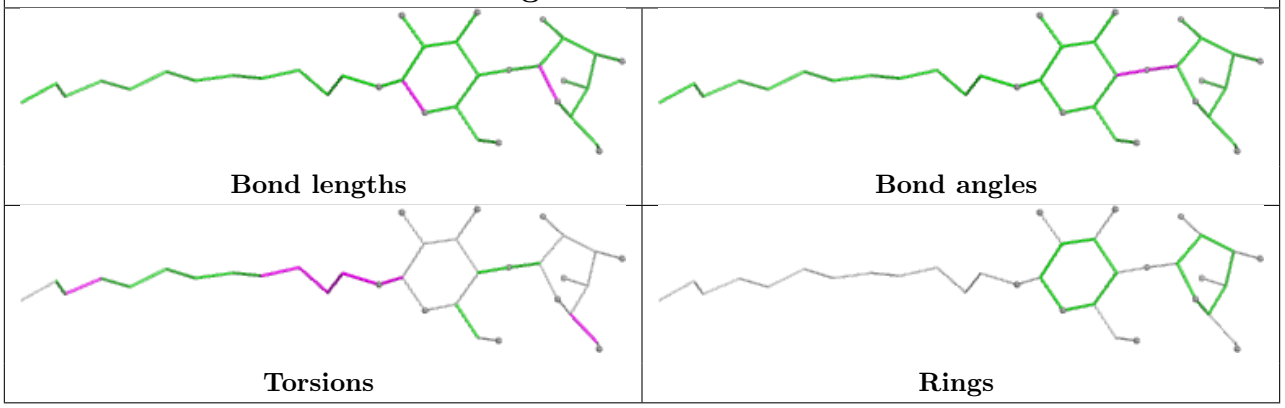
Ligand 3PE h 201



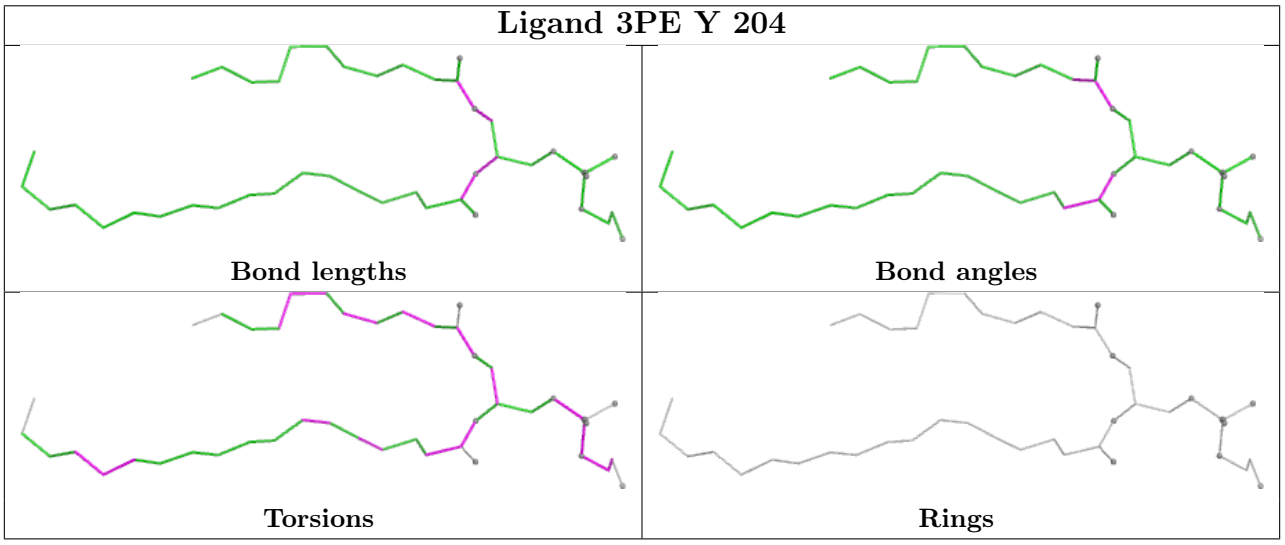
Ligand 3PE O 403



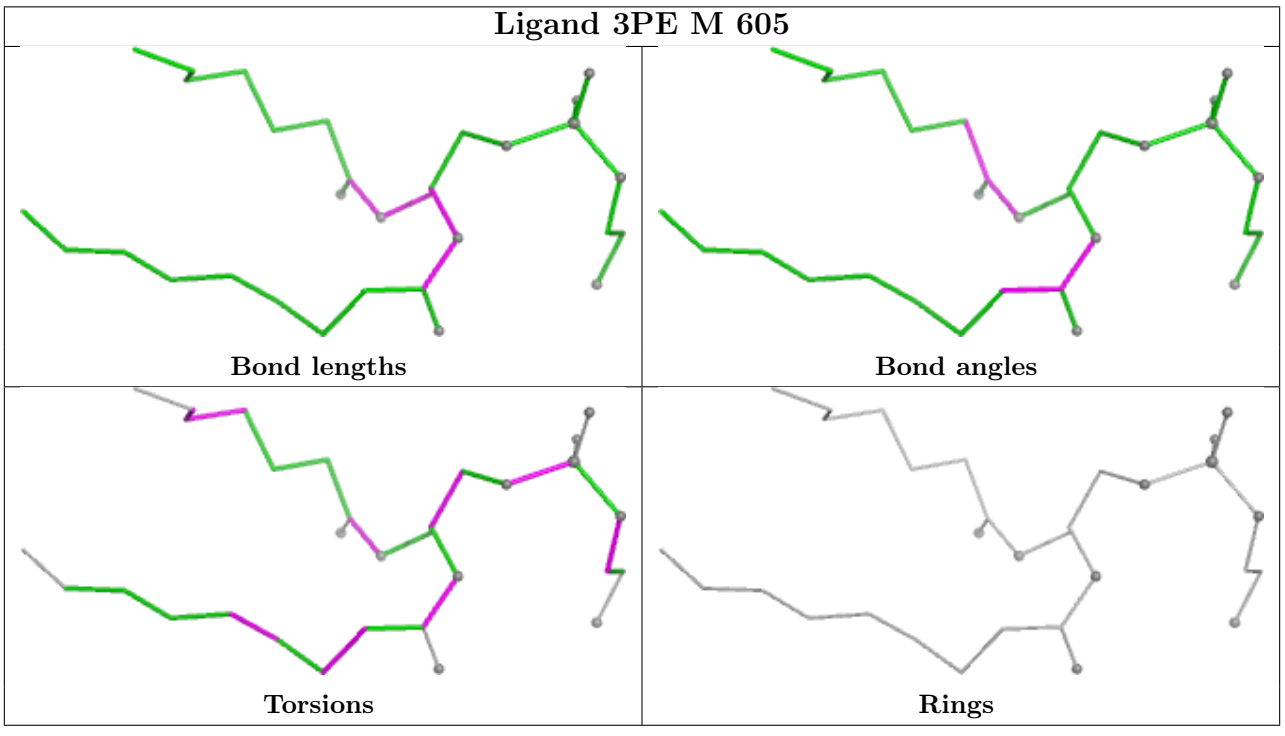
Ligand LMT Y 206



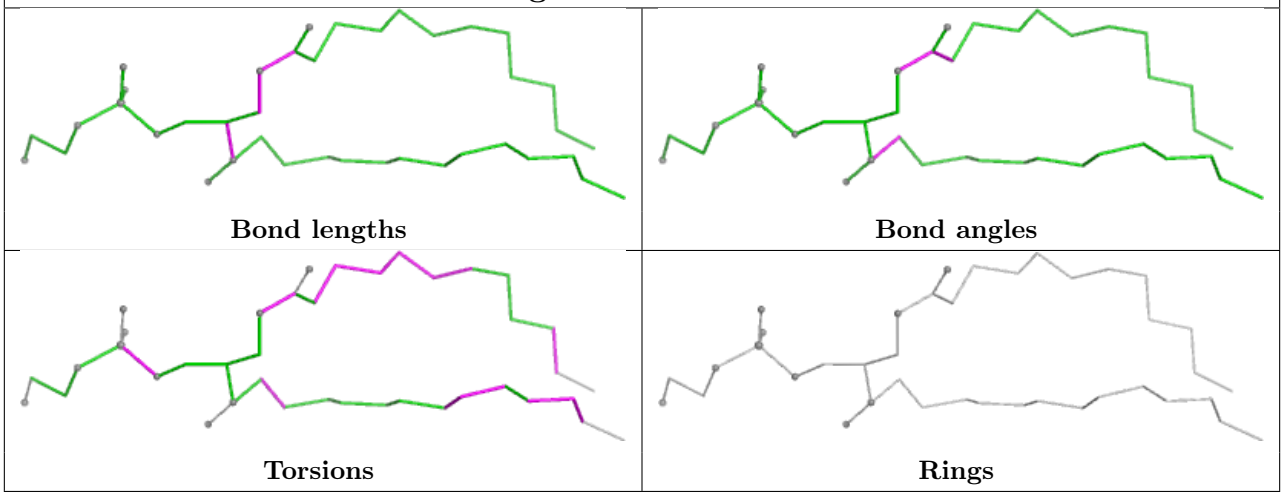
Ligand 3PE Y 204



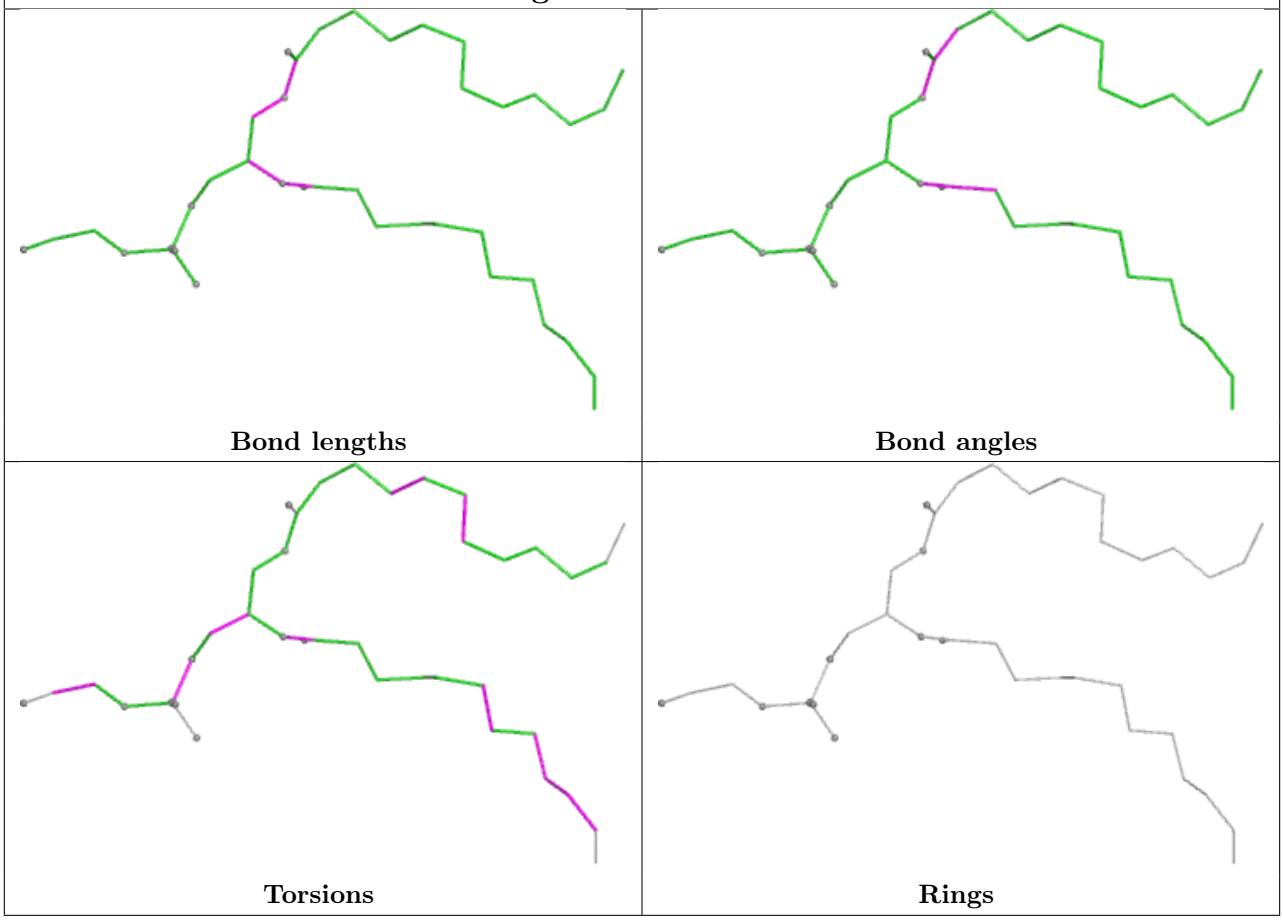
Ligand 3PE M 605



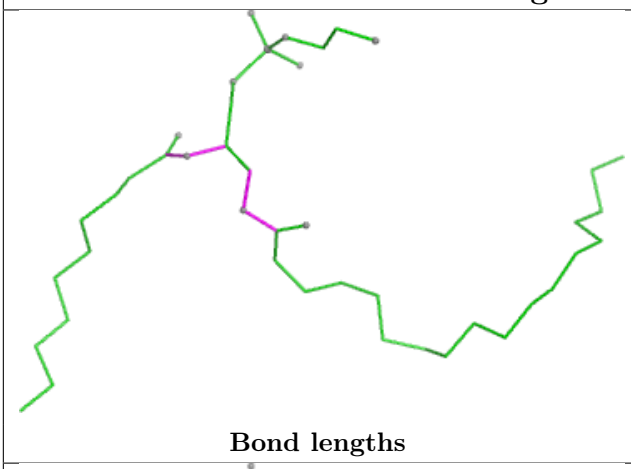
Ligand 3PE O 405



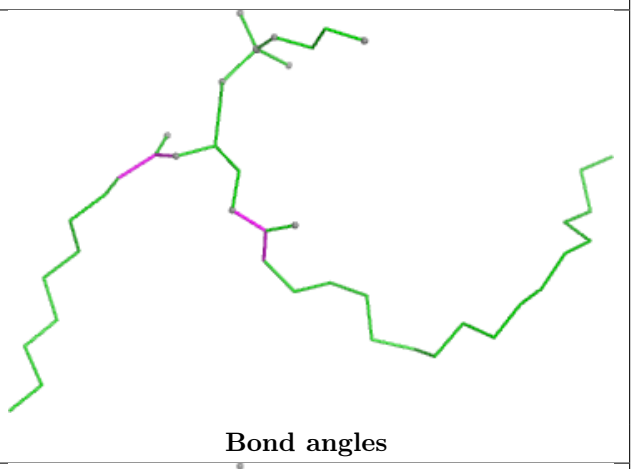
Ligand 3PE L 701



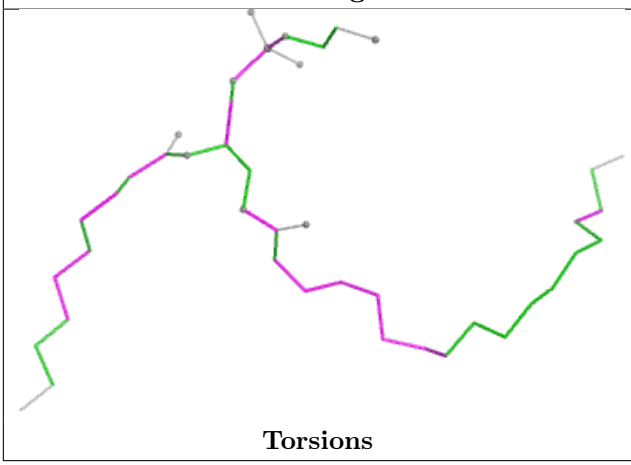
Ligand 3PE L 703



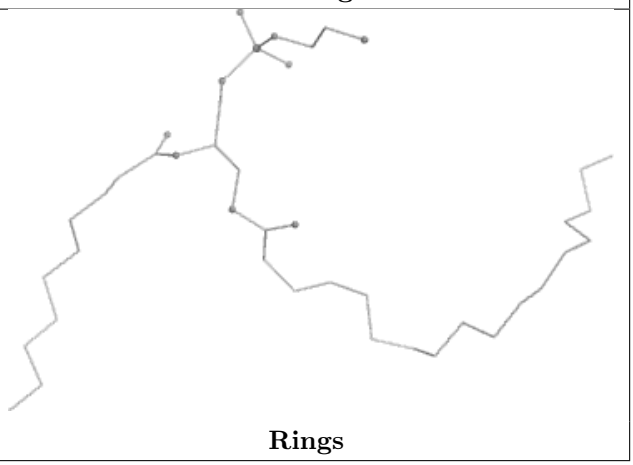
Bond lengths



Bond angles

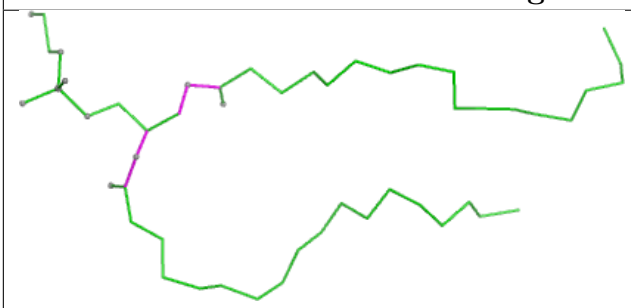


Torsions

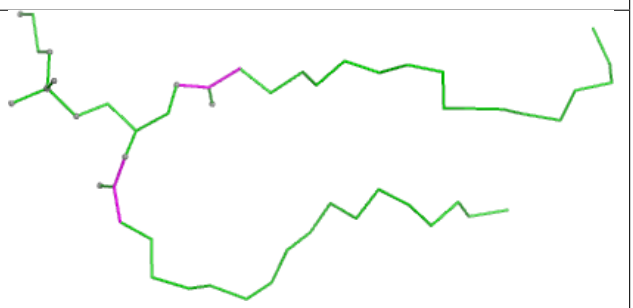


Rings

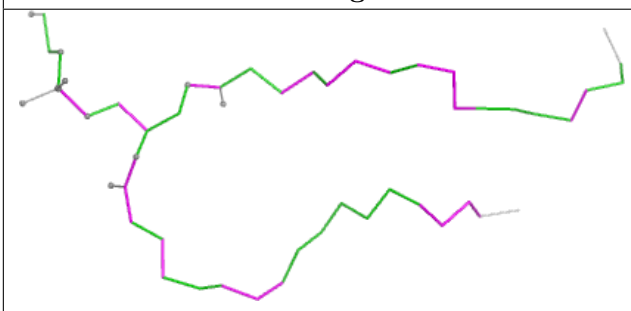
Ligand 3PE N 401



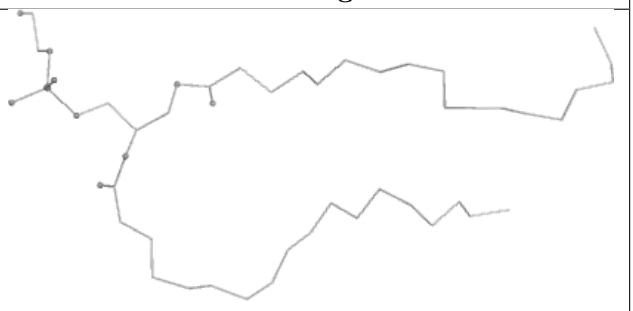
Bond lengths



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.

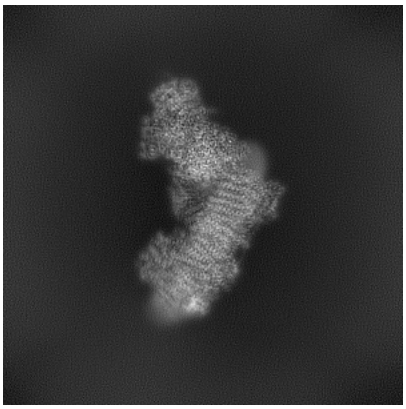
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53498. These allow visual inspection of the internal detail of the map and identification of artifacts.

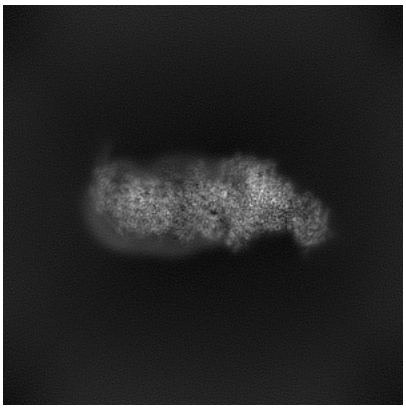
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

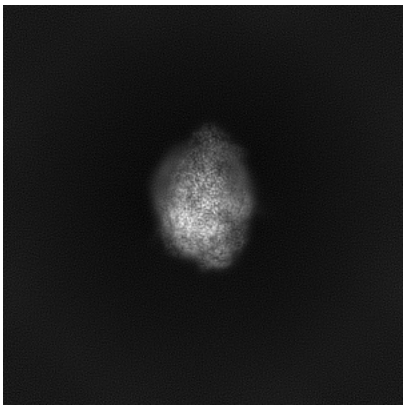
6.1.1 Primary map



X

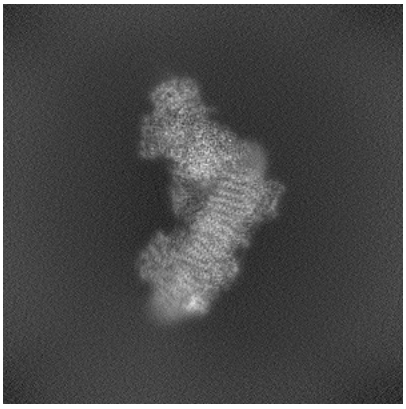


Y

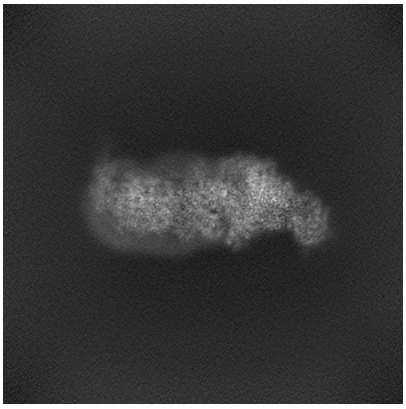


Z

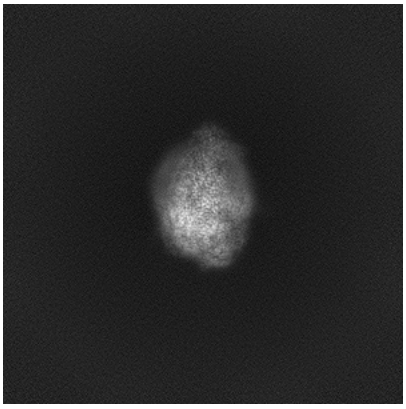
6.1.2 Raw map



X



Y

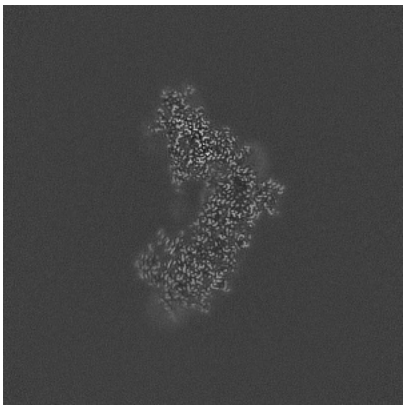


Z

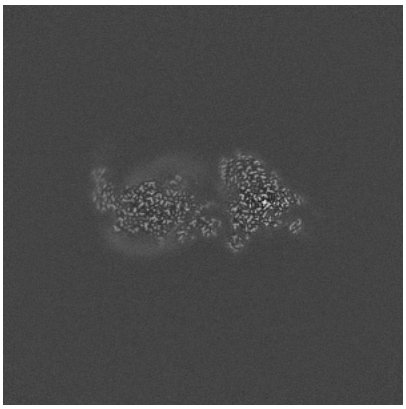
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

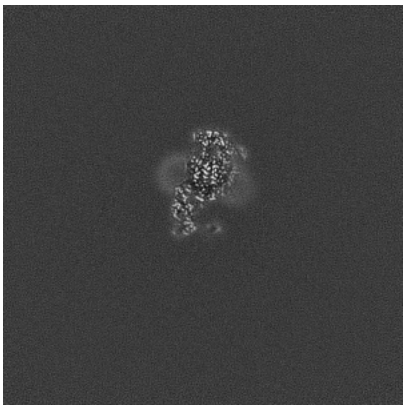
6.2.1 Primary map



X Index: 300

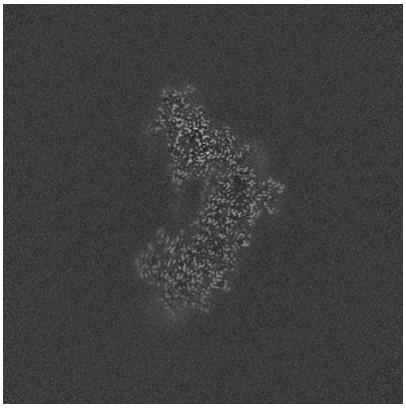


Y Index: 300

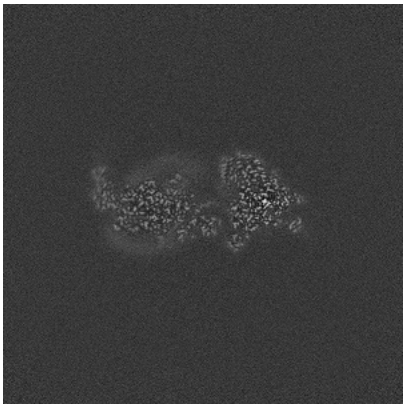


Z Index: 300

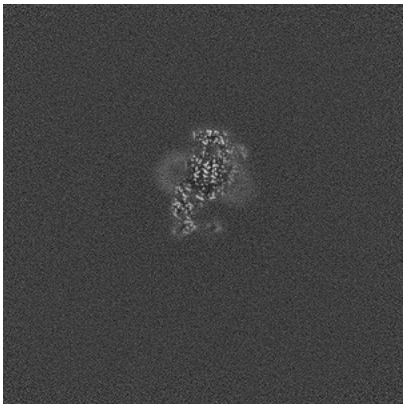
6.2.2 Raw map



X Index: 300



Y Index: 300

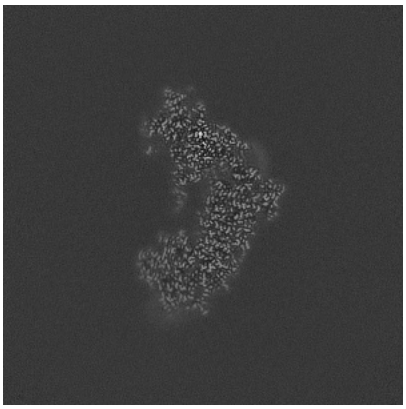


Z Index: 300

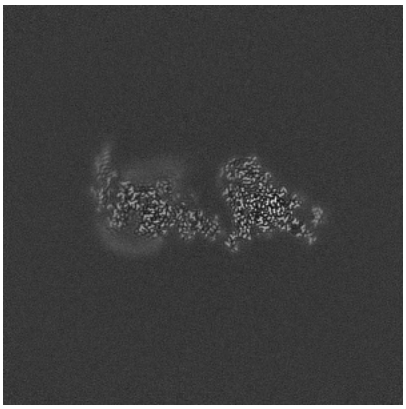
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

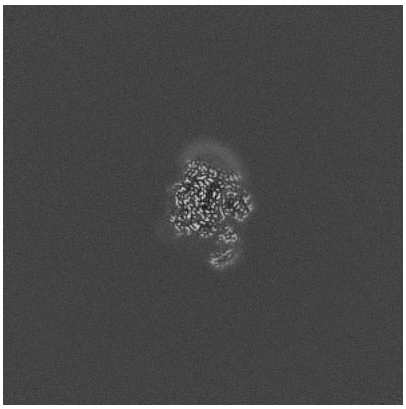
6.3.1 Primary map



X Index: 306

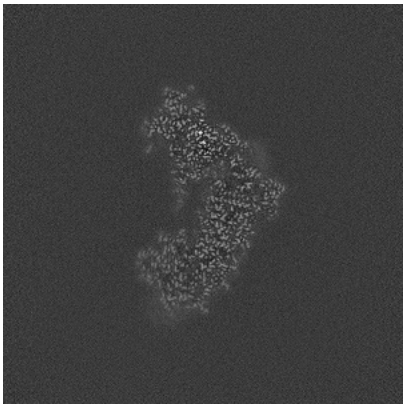


Y Index: 290

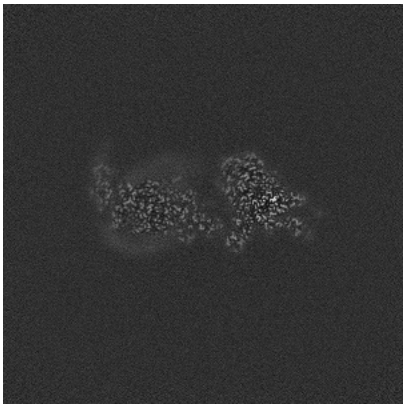


Z Index: 372

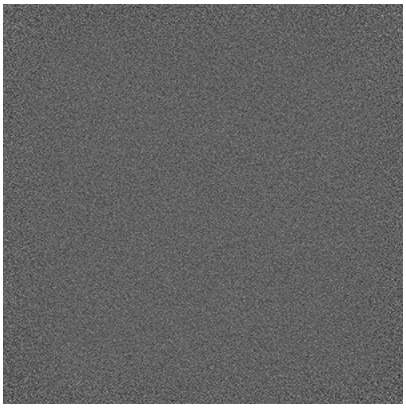
6.3.2 Raw map



X Index: 305



Y Index: 296

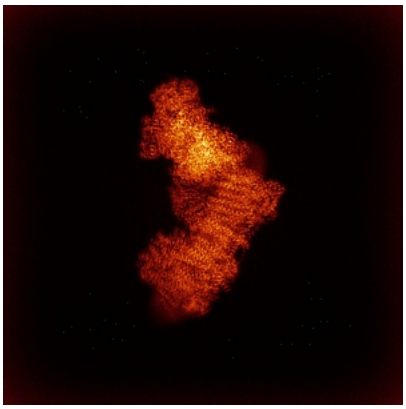


Z Index: 0

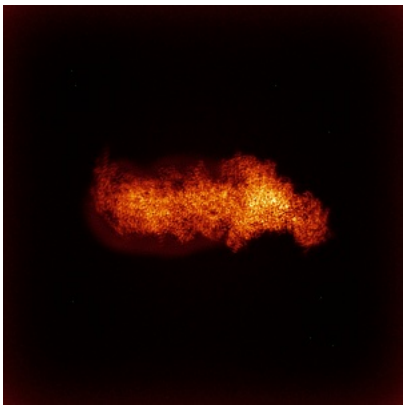
The images above show the largest variance slices of the map in three orthogonal directions.

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

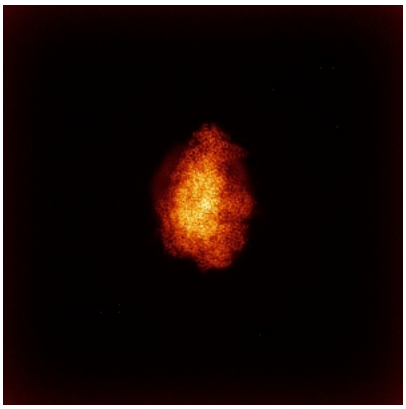
6.4.1 Primary map



X

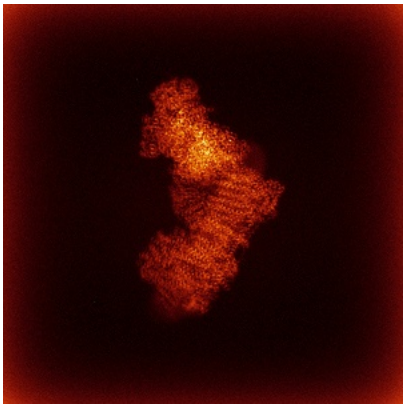


Y

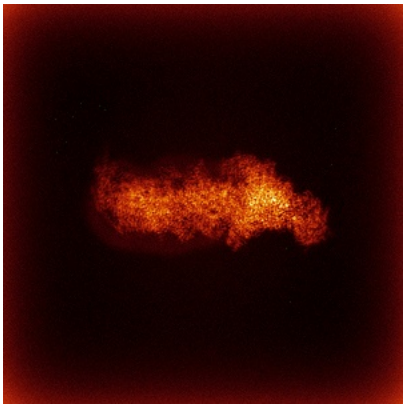


Z

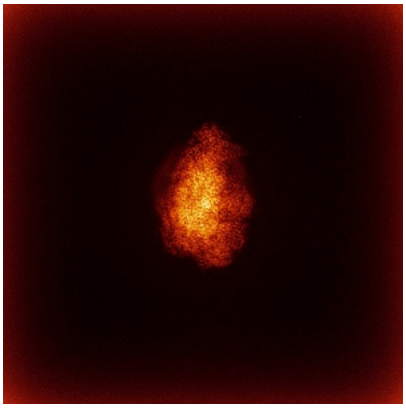
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

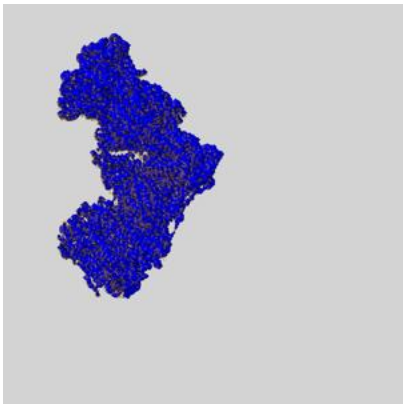
6.6 Mask visualisation

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

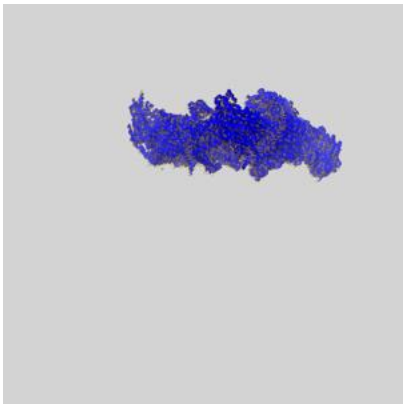
A mask typically either:

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

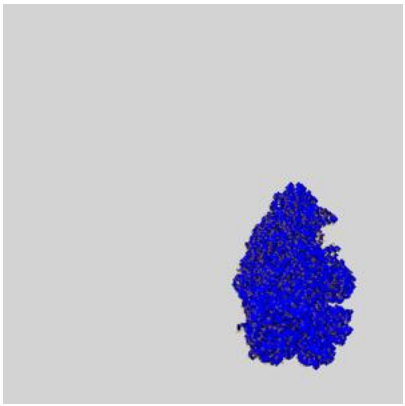
6.6.1 emd_53498_msk_1.map



X



Y

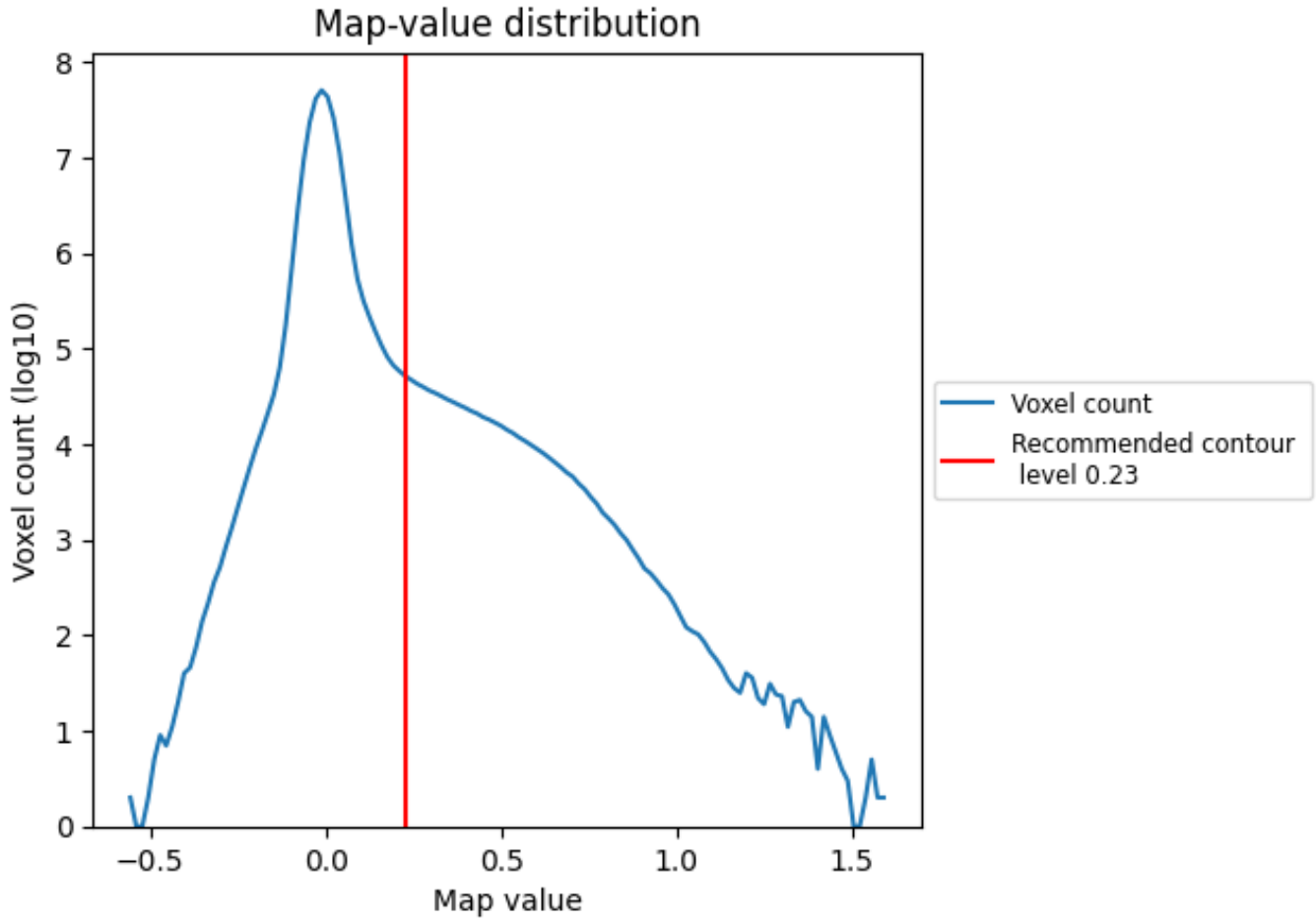


Z

7 Map analysis

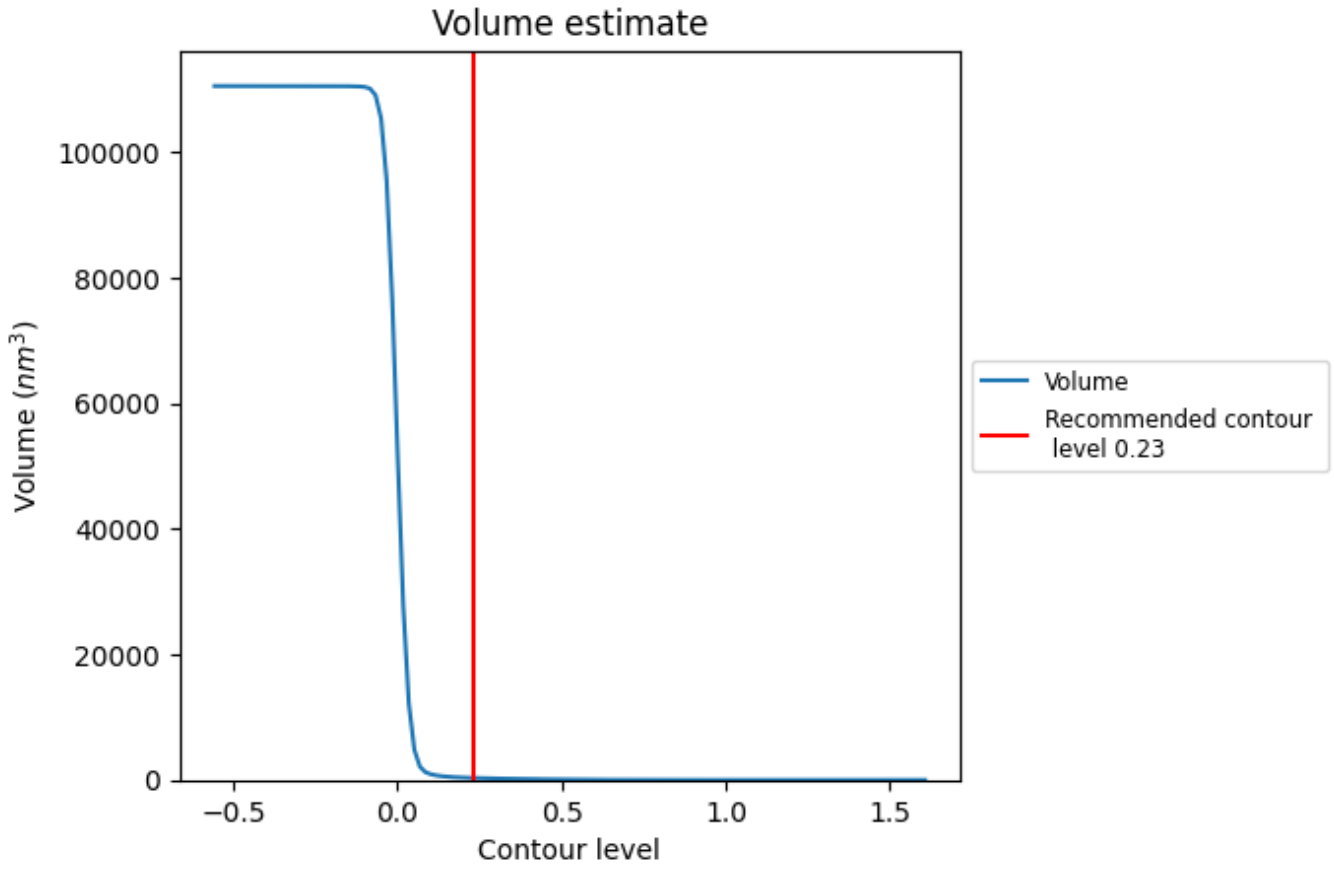
This section contains the results of statistical analysis of the map.

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.

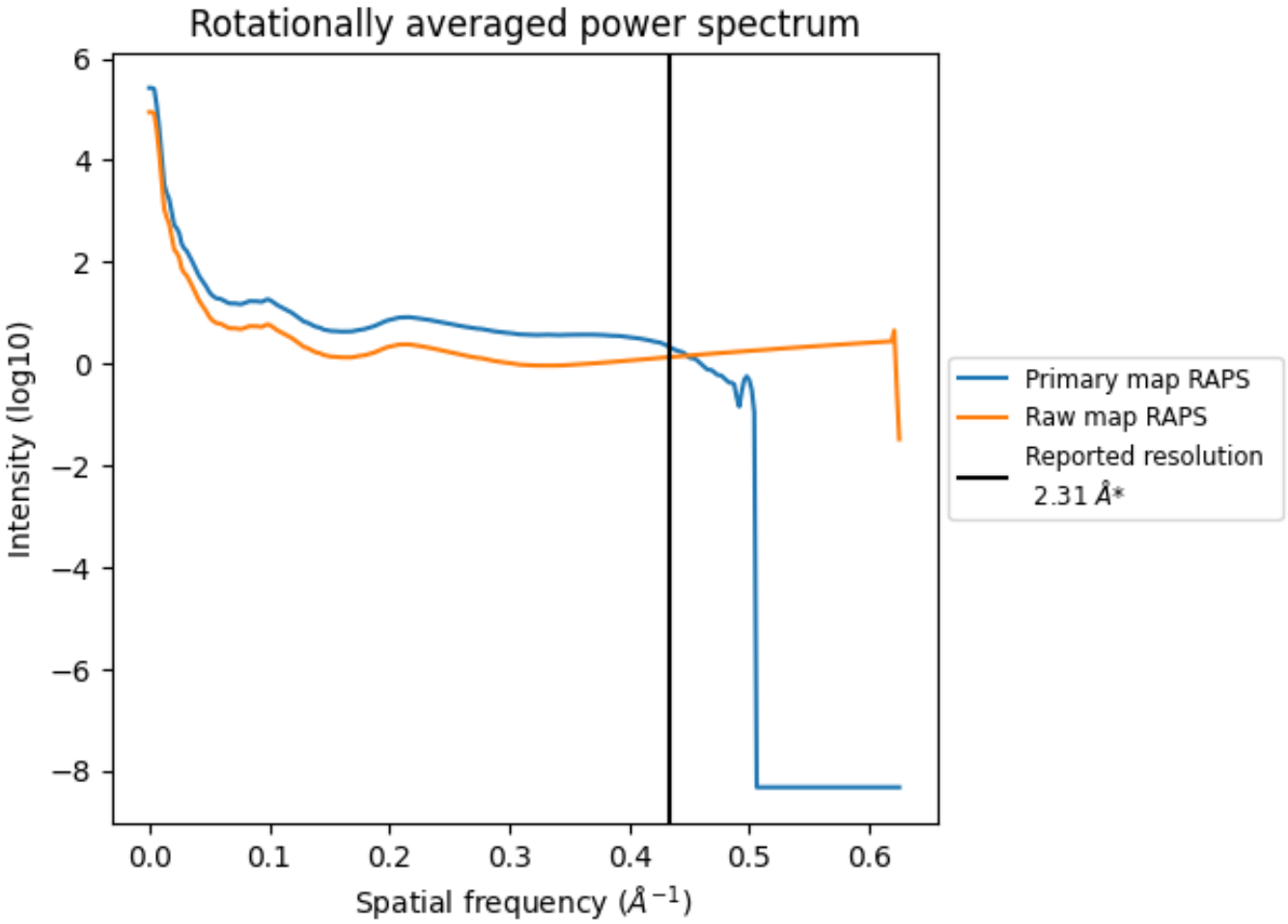
7.2 Volume estimate



The volume at the recommended contour level is 321 nm^3; this corresponds to an approximate mass of 290 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 (i)

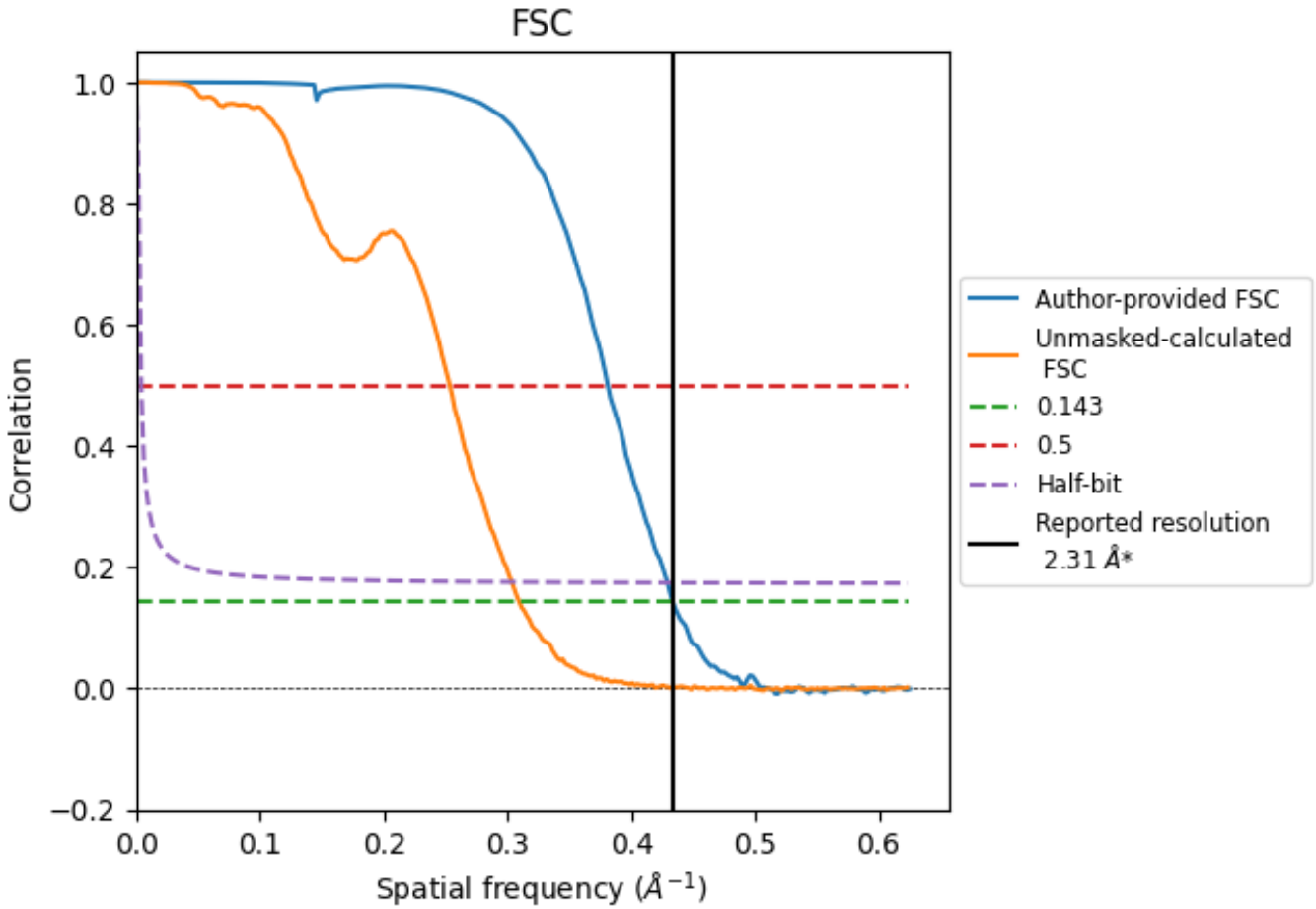


*Reported resolution corresponds to spatial frequency of 0.433 Å^{-1}

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 0.433 Å^{-1}

8.2 Resolution estimates (i)

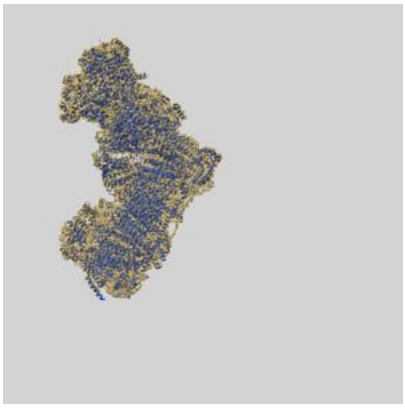
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.31	2.62	2.33
Unmasked-calculated*	3.23	3.95	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.31 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53498 and PDB model 9R15. Per-residue inclusion information can be found in section 3 on page 24.

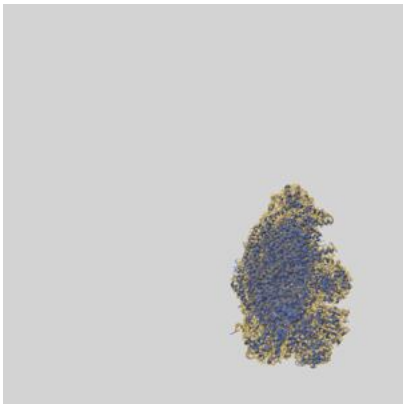
9.1 Map-model overlay



X



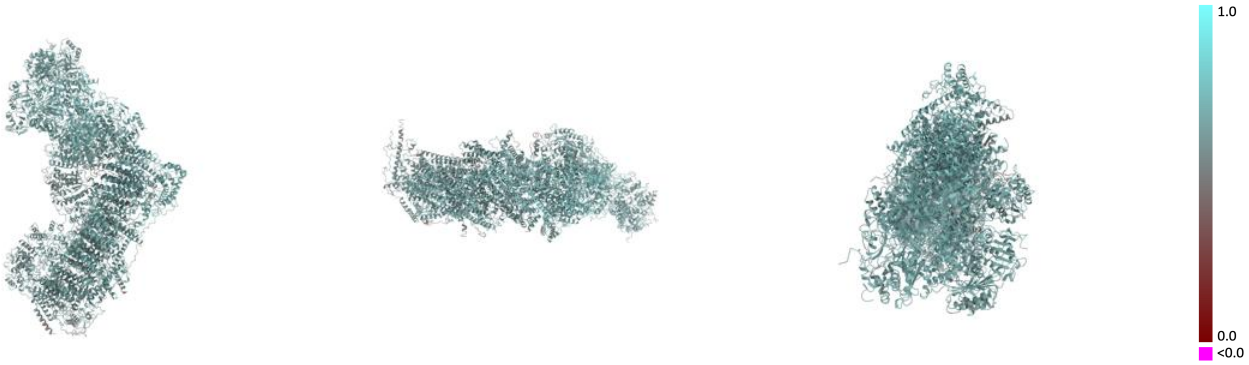
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23 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.

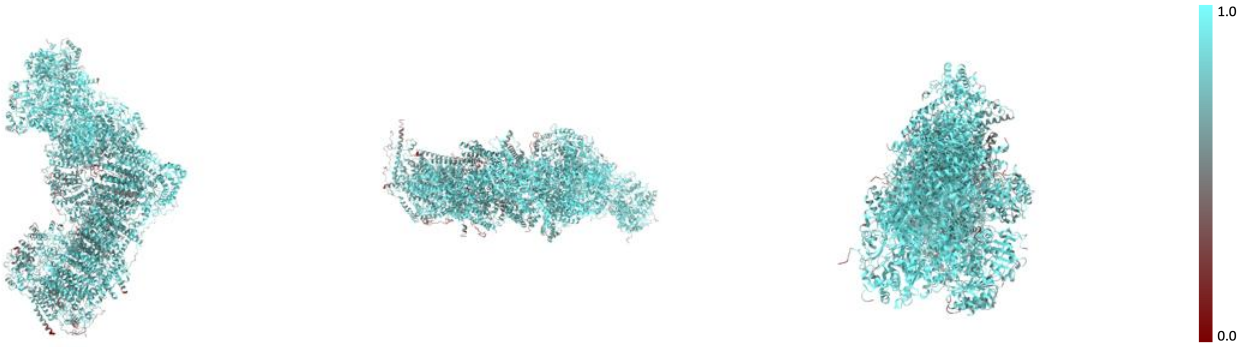
9.2 Q-score mapped to coordinate model (i)



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.

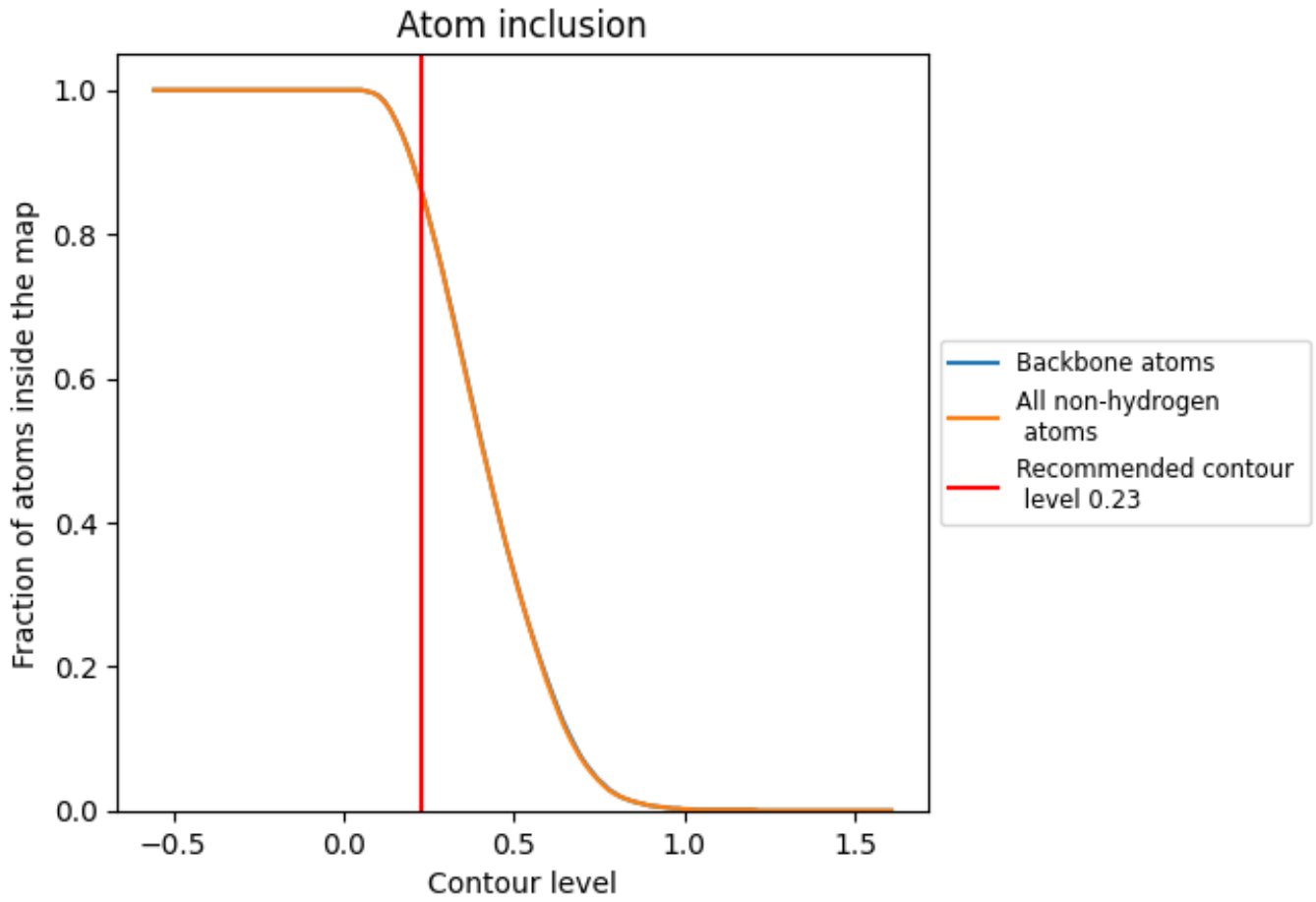
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.23).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.6490
A	0.7790	0.6400
B	0.9440	0.6870
C	0.9600	0.6940
D	0.9470	0.6950
E	0.8660	0.6270
F	0.9030	0.6450
G	0.9170	0.6660
H	0.9340	0.6830
I	0.9590	0.6980
J	0.8160	0.6450
K	0.9100	0.6790
L	0.8490	0.6360
M	0.9440	0.6750
N	0.9340	0.6840
O	0.8010	0.6310
P	0.7940	0.6170
Q	0.8940	0.6810
R	0.9020	0.6700
S	0.7990	0.6120
T	0.5480	0.5380
U	0.6920	0.5890
V	0.8590	0.6480
W	0.8690	0.6580
X	0.8680	0.6540
Y	0.6960	0.6230
Z	0.8840	0.6630
a	0.9470	0.6780
b	0.8630	0.6500
c	0.8020	0.6280
d	0.8660	0.6540
e	0.8830	0.6540
f	0.7390	0.6100
g	0.8370	0.6460
h	0.8710	0.6590



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Chain	Atom inclusion	Q-score
i	0.6140	0.5550
j	0.6630	0.5760
k	0.6230	0.5550
l	0.8080	0.6140
m	0.7530	0.6240
n	0.7790	0.6110
o	0.6820	0.5510
p	0.8360	0.6280
q	0.9220	0.6780
r	0.9230	0.6740
s	0.8430	0.6210