Full wwPDB EM Validation Report (i)

Sep 11, 2026 – 03:21 am BST

PDB ID	:	7R4D / pdb_00007r4d
EMDB ID	:	EMD-14297
Title	:	Bovine complex I in the presence of IM1761092, deactive class vi (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

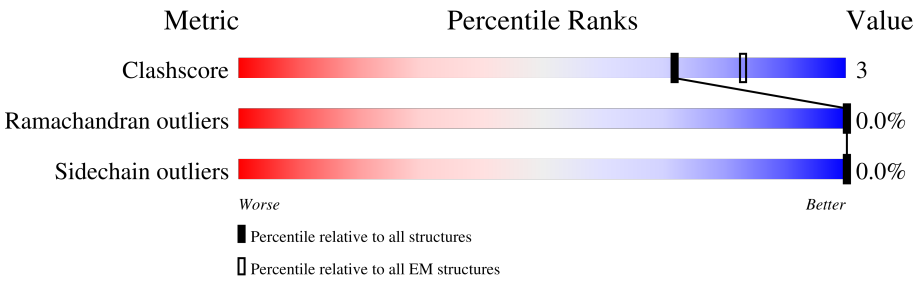
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

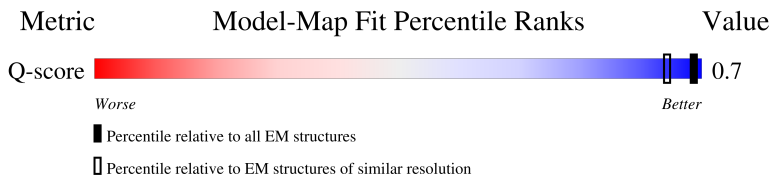
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	68% 18% 14%
2	B	216	63% 8% 29%
3	C	266	75% • 23%
4	D	463	84% 5% 10%

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Mol	Chain	Length	Quality of chain
5	E	249	81% 14%
6	F	464	85% 8% 8%
7	G	727	89% 6% 5%
8	H	318	83% 14%
9	I	212	78% 5% 17%
10	J	175	18% 87% 13%
11	K	98	81% 17%
12	L	606	89% 9%
13	M	459	88% 12%
14	N	347	90% 10%
15	O	343	85% 8% 7%
16	P	380	73% 24%
17	Q	175	68% 29%
18	R	124	71% 5% 24%
19	S	99	79% 5% 16%
20	T	156	8% 43% 5% 51%
20	U	156	47% 6% 46%
21	V	116	93%
22	W	128	82% 7% 11%
23	X	172	96%
24	Y	141	56% 87% 12%
25	Z	144	7% 92% 6%
26	a	70	89% 10%
27	b	84	5% 96%
28	c	76	55% 8% 37%

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Mol	Chain	Length	Quality of chain
29	d	120	89% 7%
30	e	106	76% 13% 10%
31	f	57	9% 84% 5% 11%
32	g	154	58% 5% 37%
33	h	189	69% 27%
34	i	127	74% 7% 19%
35	j	108	61% 38%
36	k	98	80% 19%
37	l	186	75% 9% 17%
38	m	129	78% 5% 16%
39	n	179	92%
40	o	137	84% 12%
41	p	176	94%
42	q	145	94% 5%
43	r	113	77% 6% 17%
44	s	109	38% 61%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 68004 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	99	799	547	116	131	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	154	1230	786	220	210	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	206	1714	1107	295	309	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	416	3362	2149	578	610	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
			Total	C	N	O	S		
5	E	213	1655	1057	277	311	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	429	3301	2080	589	612	20	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	309	2440	1636	375	406	23	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	174	1337	902	189	234	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	96	730	478	109	128	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	592	4695	3124	722	806	43	0	0

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

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

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

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

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

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

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
			Total	C	N	O	S		
16	P	290	2305	1474	416	410	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	83	669	419	125	123	2	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	114	971	622	180	165	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	69	561	361	103	92	5	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	48	405	268	69	68	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	51	444	291	78	74	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	97	813	523	133	153	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	103	884	584	149	150	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	79	638	418	107	111	2	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	121	1043	650	200	184	9	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	144	1201	773	215	209	4	0	0

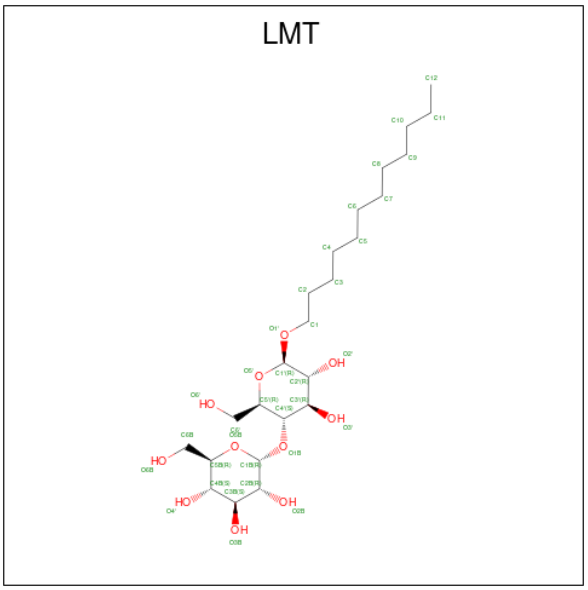
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	35	24	11	0
45	H	1	35	24	11	0
45	J	1	35	24	11	0
45	L	1	35	24	11	0
45	L	1	35	24	11	0
45	M	1	35	24	11	0
45	N	1	35	24	11	0

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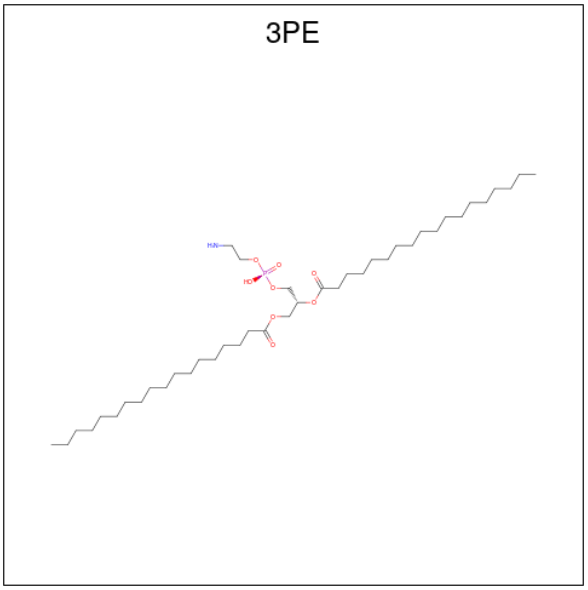
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	Y	1	35	24	11	0
			Total	C	O	
45	f	1	35	24	11	0
			Total	C	O	
45	h	1	35	24	11	0
			Total	C	O	
45	h	1	35	24	11	0
			Total	C	O	
45	j	1	35	24	11	0
			Total	C	O	
45	l	1	35	24	11	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	42	32	1	8	1	0
			Total	C	N	O	P	
46	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
46	H	1	34	24	1	8	1	0
			Total	C	N	O	P	
46	L	1	49	39	1	8	1	0
			Total	C	N	O	P	
46	L	1	45	35	1	8	1	0

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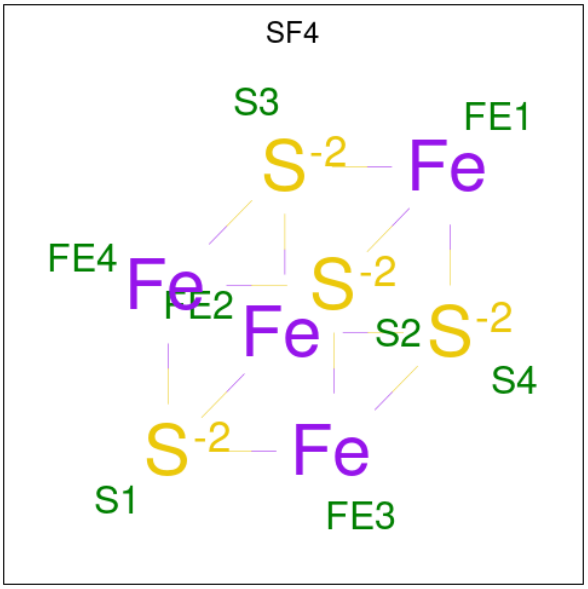
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	M	1	51	41	1	8	1	0
46	N	1	41	31	1	8	1	0
46	O	1	47	37	1	8	1	0
46	Y	1	40	30	1	8	1	0
46	Y	1	35	25	1	8	1	0
46	Y	1	29	19	1	8	1	0

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



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

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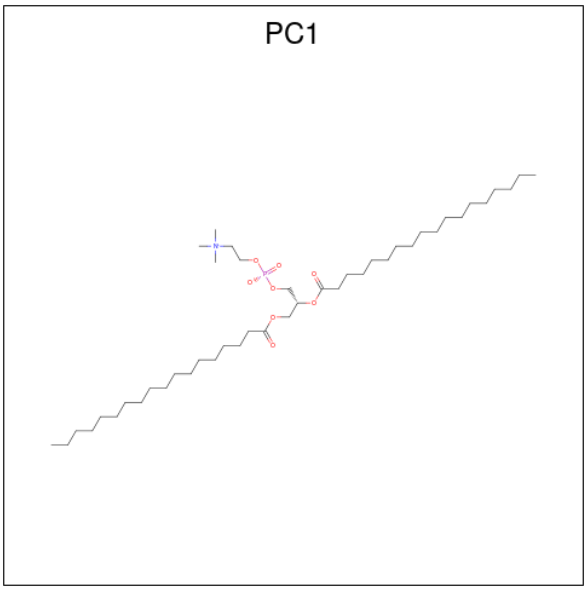
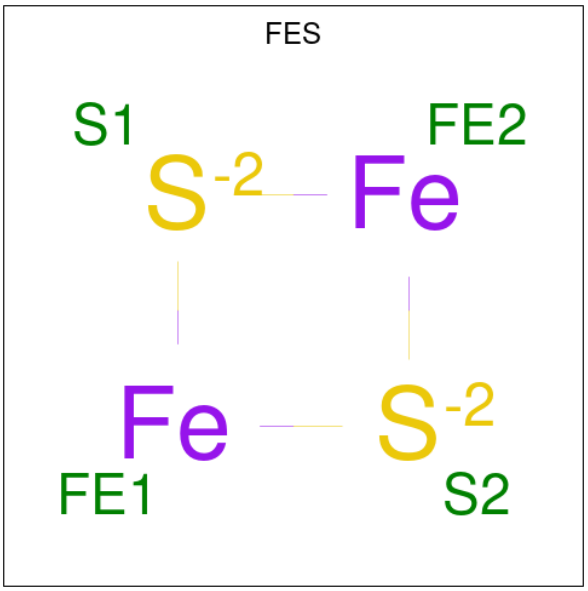
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	I	1	8	4	4	0

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



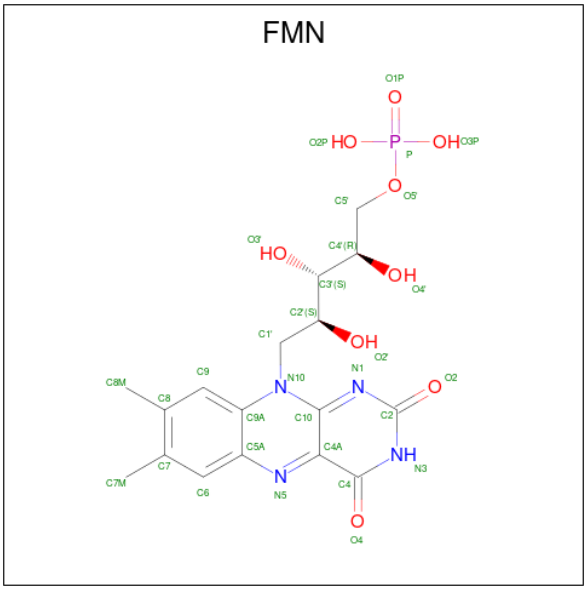
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	35	25	1	8	1	0
			Total	C	N	O	P	
48	M	1	49	39	1	8	1	0

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



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

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

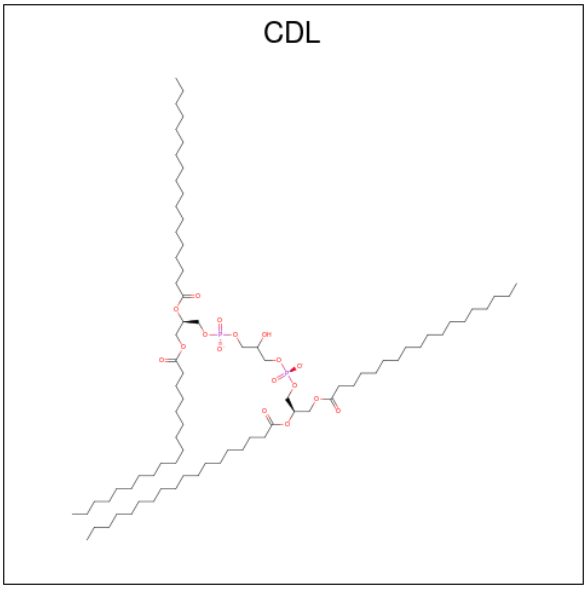


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	F	1	31	17	4	9	1	0

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

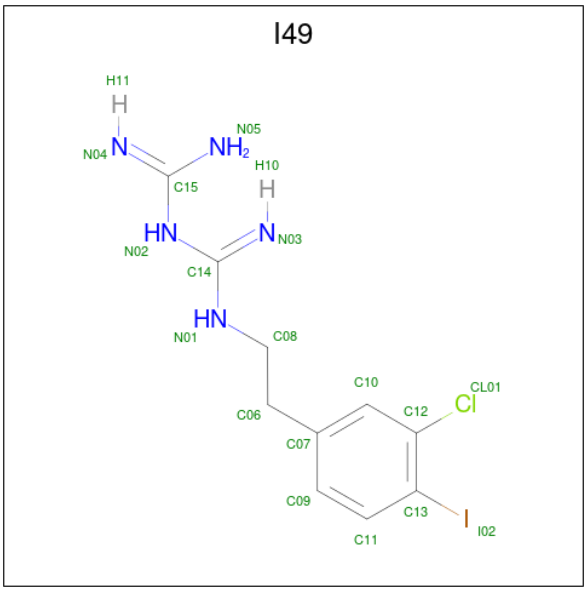
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	G	1	1	1	0

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



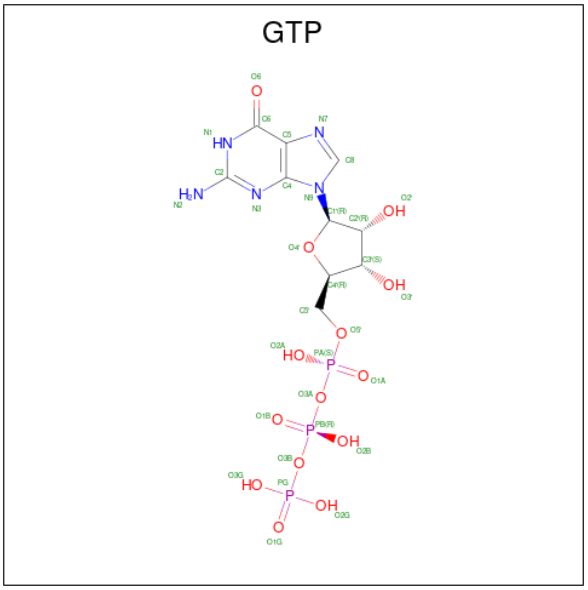
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	L	1	69	50	17	2	0
			Total	C	O	P	
52	X	1	68	49	17	2	0
			Total	C	O	P	
52	d	1	65	46	17	2	0
			Total	C	O	P	
52	h	1	67	48	17	2	0
			Total	C	O	P	
52	r	1	76	57	17	2	0

- Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (CCD ID: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



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

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

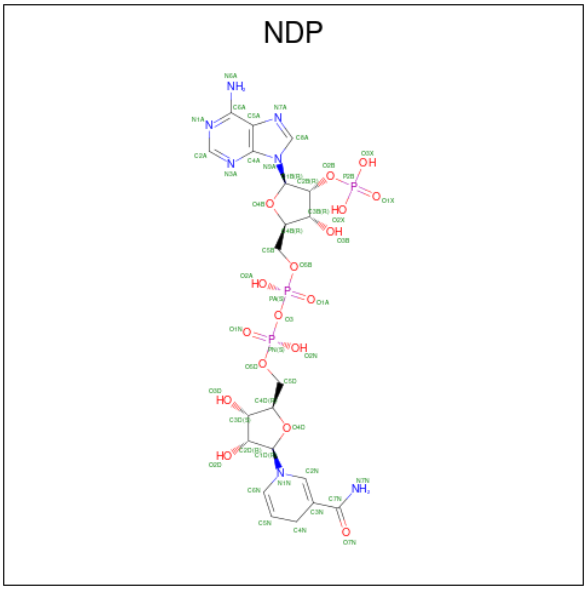


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	O	1	32	10	5	14	3	0

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

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

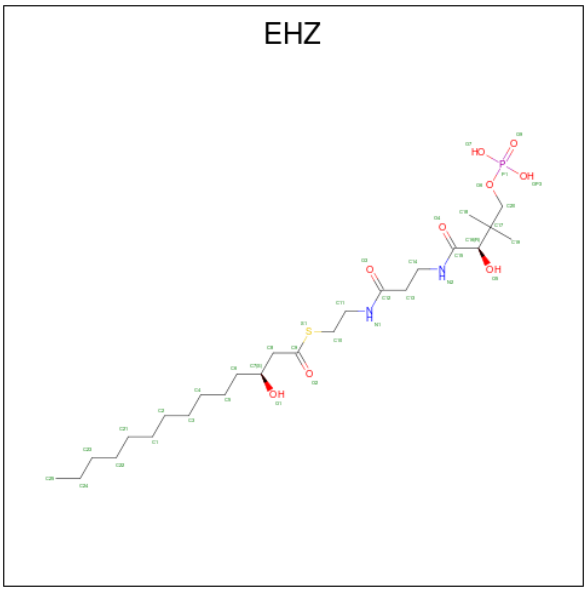


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	P	1	48	21	7	17	3	0

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

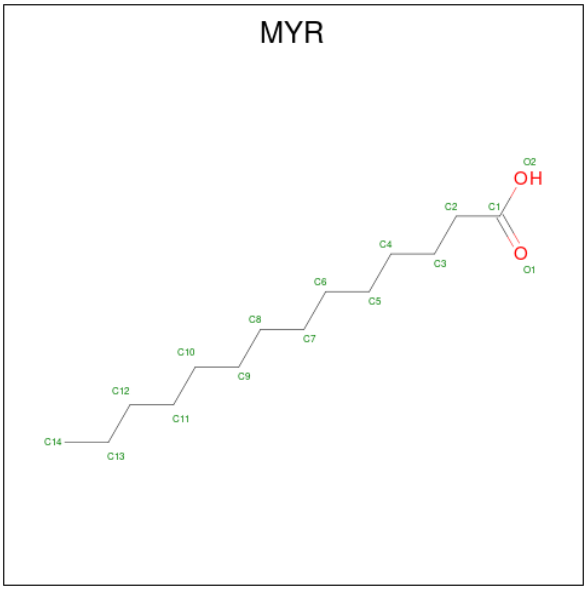
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	R	1	1	1	0

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



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

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	A	8	8	8	0
60	B	58	58	58	0
60	C	102	102	102	0
60	D	157	157	157	0
60	E	29	29	29	0
60	F	70	70	70	0
60	G	227	227	227	0
60	H	46	46	46	0
60	I	104	104	104	0
60	J	10	10	10	0
60	K	4	4	4	0
60	L	65	65	65	0
60	M	71	71	71	0
60	N	46	46	46	0
60	O	11	11	11	0
60	P	47	47	47	0
60	Q	74	74	74	0
60	R	47	47	47	0
60	S	2	2	2	0
60	T	1	1	1	0
60	U	23	23	23	0
60	V	13	13	13	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	W	18	18	18	0
			Total	O	
60	X	28	28	28	0
			Total	O	
60	Y	1	1	1	0
			Total	O	
60	Z	21	21	21	0
			Total	O	
60	a	19	19	19	0
			Total	O	
60	b	7	7	7	0
			Total	O	
60	c	1	1	1	0
			Total	O	
60	d	8	8	8	0
			Total	O	
60	e	15	15	15	0
			Total	O	
60	f	7	7	7	0
			Total	O	
60	g	9	9	9	0
			Total	O	
60	h	29	29	29	0
			Total	O	
60	i	7	7	7	0
			Total	O	
60	j	4	4	4	0
			Total	O	
60	k	7	7	7	0
			Total	O	
60	l	30	30	30	0
			Total	O	
60	m	18	18	18	0
			Total	O	
60	n	31	31	31	0
			Total	O	
60	o	22	22	22	0
			Total	O	
60	p	37	37	37	0
			Total	O	
60	q	40	40	40	0

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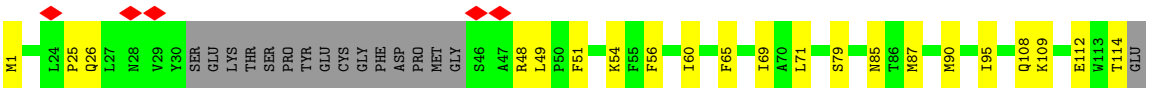
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	r	27	27	27	0
			Total	O	
60	s	6	6	6	0

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.

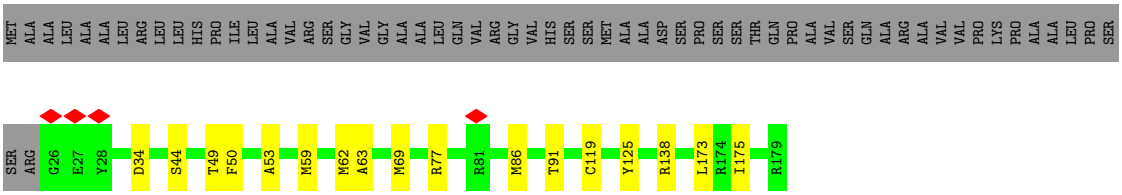
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 68% 18% 14%



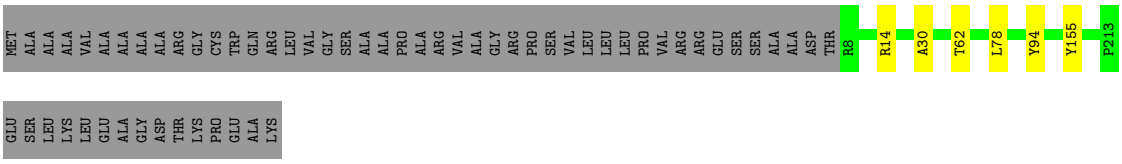
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 63% 8% 29%



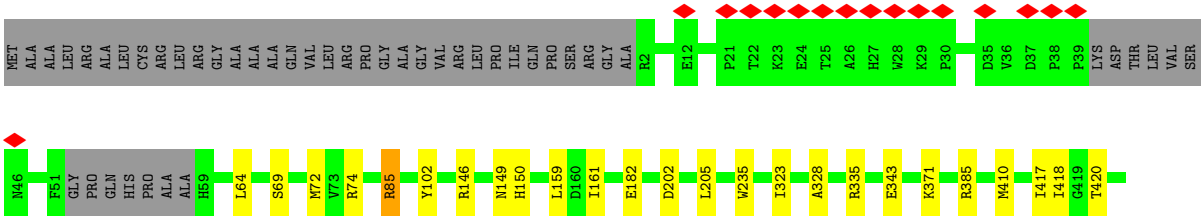
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 75% 23%



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

Chain D: 84% 5% 10%



R430

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

Chain E: 81% • 14%

MET PHE LEU SER ALA ALA LEU ARG ALA ARG ALA ALA GLY LEU ALA ALA HIS TRP GLY LYS HIS ILE ARG ASN LEU HIS LYS THR ALA VAL GLN ASN GLY ALA GLY GLY A5 Y38 M66 Y81 T105 T106 T132 P133 D134 N150 E162 I181 Q214 L217

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

Chain F: 85% 8% 8%

MET LEU ALA ALA ARG ARG LEU LEU GLY GLY SER LEU PRO ALA ARG VAL SER VAL ARG PHE SER GLY ASP THR THR ALA PRO LYS K9 R28 L93 V94 V95 D98 E99 T104 L118 C122 A134 L192 I193 E194 K199 R204 G214 V215 C218

E226 C235 F242 G252 V268 E269 L306 P364 V380 T403 R423 P424 R429 M430 Q431 Q432 Q435 Q436 H437 GLN ALA ARG GLN ALA ALA PHE

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

Chain G: 89% 6% 5%

MET LEU ARG ILE PRO VAL ARG LYS ALA LEU VAL GLY LEU SER LYS SER SER LYS GLY CYS VAL ARG THR THR ALA THR ALA ALA S6 M35 R39 E44 R45 L46 T81 I107 D126 K140 T148 Y186 C203 W262 D265 R276 E287

E297 M306 F310 D324 L364 V377 E387 L390 R396 L404 L415 T416 I452 L453 L458 A465 Q475 S480 S481 G482 V483 T484 N491 K569 S570 A571 G578 V585 D596 D635 L651 Q654 A680 S681 Q682 T683

M684 E693 GLY ALA HIS ALA VAL GLU GLU PRO SER ILE CYS

• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

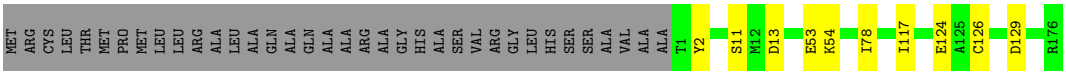
Chain H: 83% 14% •

M1 F2 I6 E24 D51 R62 P63 A64 T65 S66 S67 M70 M77 L81 I87 P88 V102 L103 V113 W118 W121 V136 Y142 I148 L154 F160 M172 L176 L200 E206 L207 VAL SER GLY PHE ASN VAL GLU TYR

ALA A217 L222 M225 Y228 M233 M234 N235 I236 F259 L271 R274 L285 L288 L289 N292 F293 L294 P295 C301 M302 V305 I309 T318

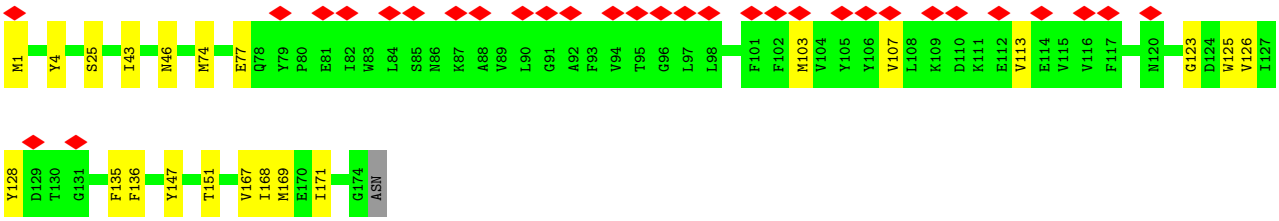
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I: 78% 5% 17%



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

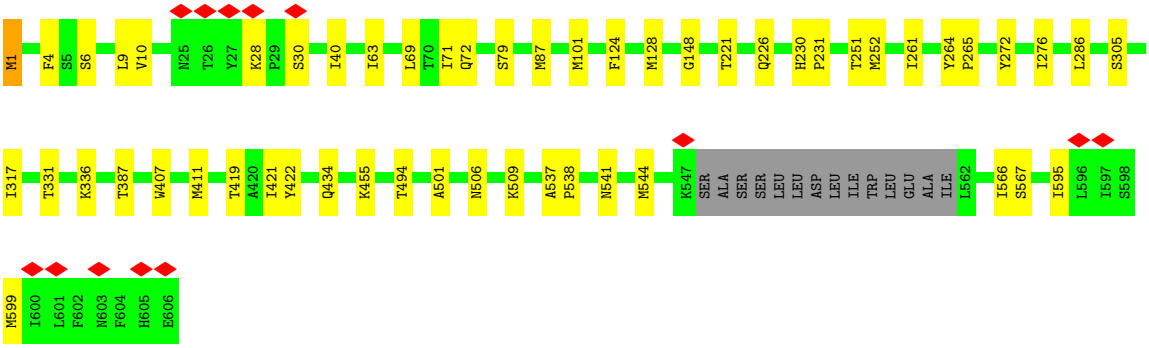


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

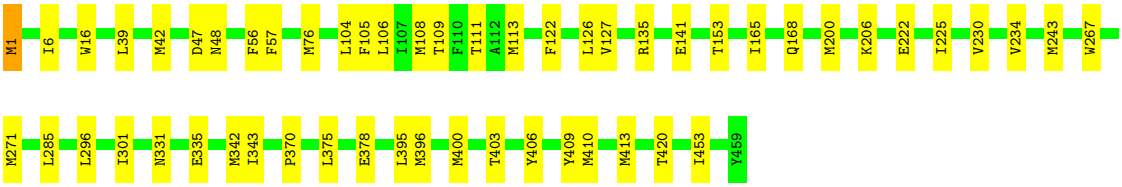
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

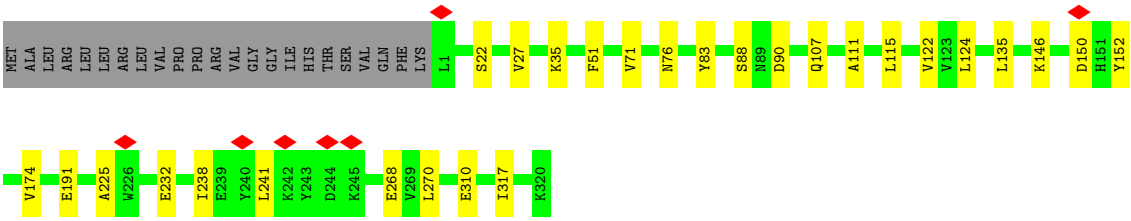


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:

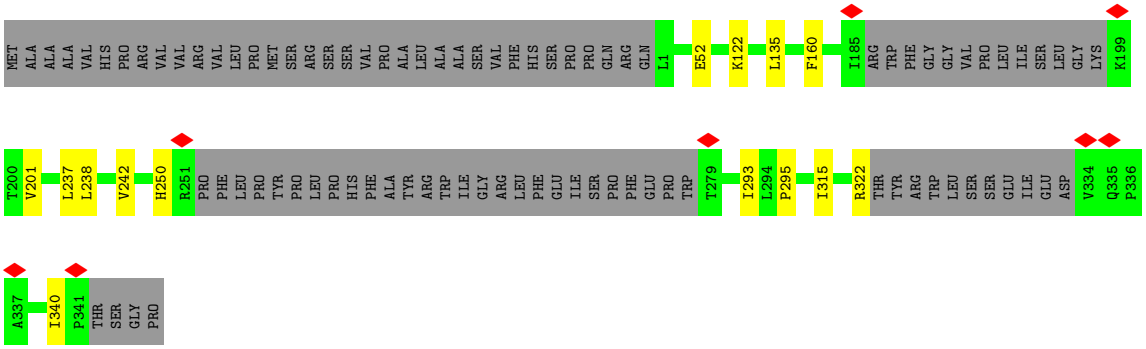
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



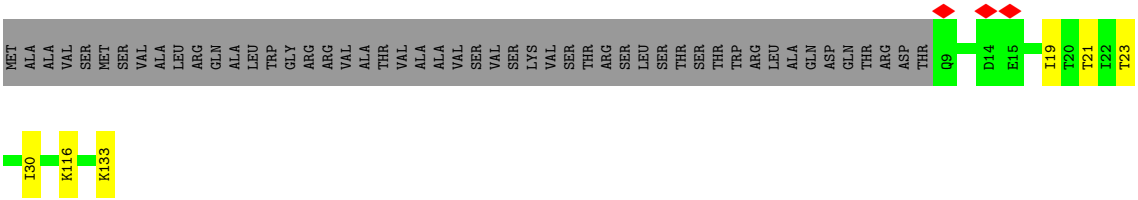
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



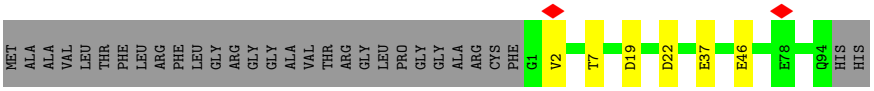
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



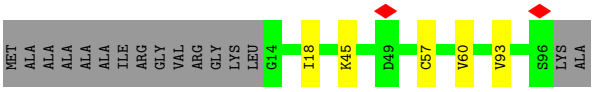
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



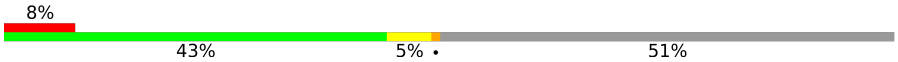
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

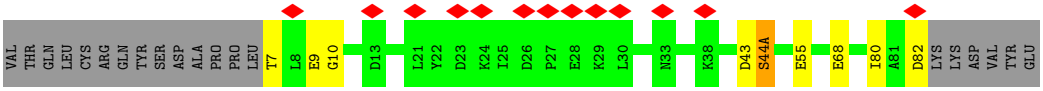
Chain S:



• Molecule 20: Acyl carrier protein, mitochondrial

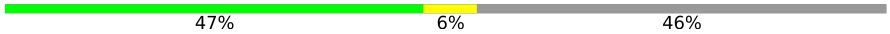
Chain T:

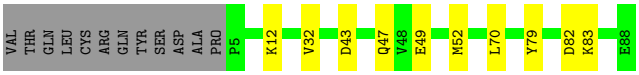




• Molecule 20: Acyl carrier protein, mitochondrial

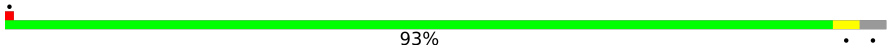
Chain U:

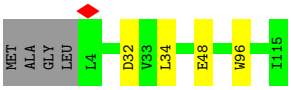




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



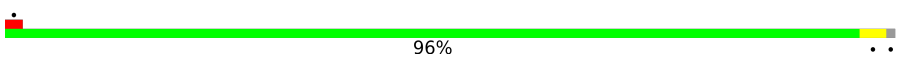


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

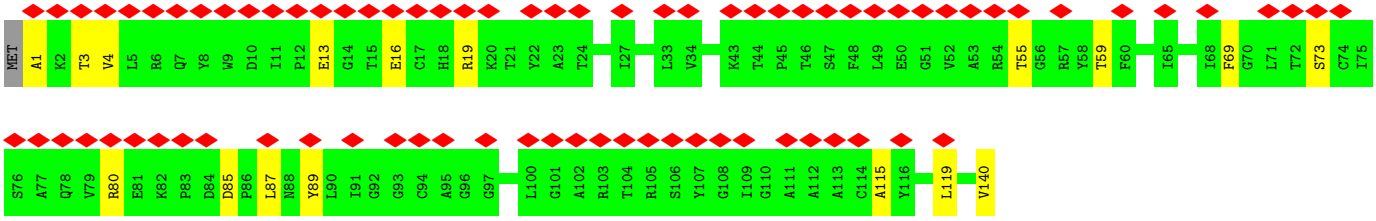
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



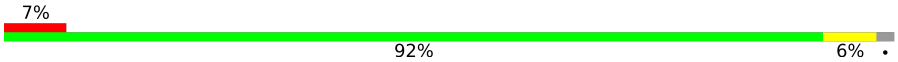
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

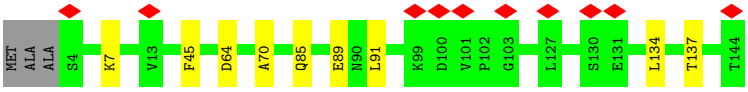
Chain Y:



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

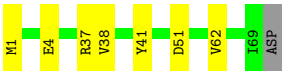
Chain Z:





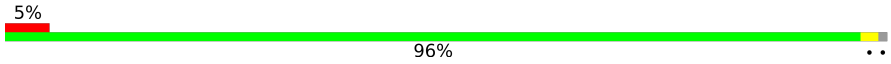
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

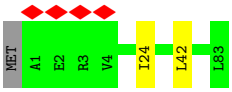
Chain a:



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

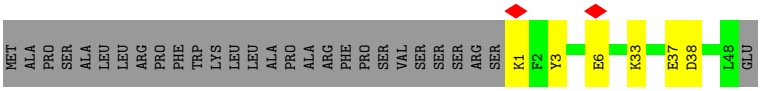
Chain b:





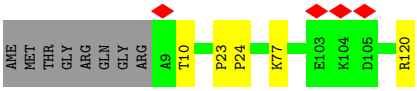
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



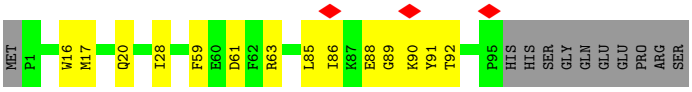
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



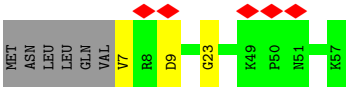
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



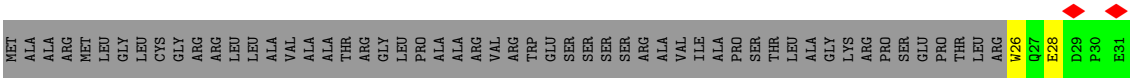
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



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

Chain g:

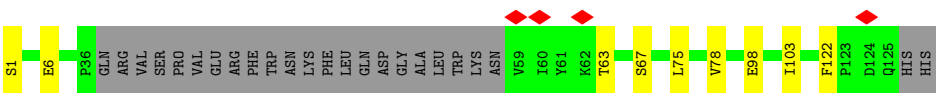


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

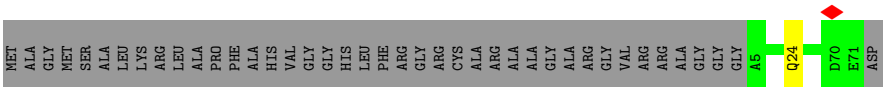
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



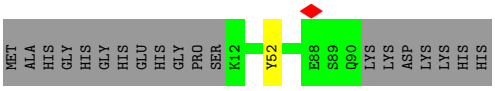
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



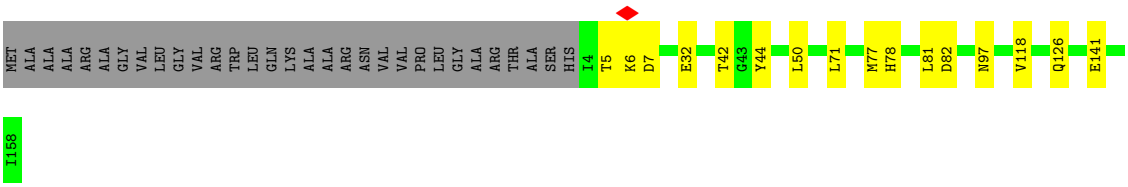
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



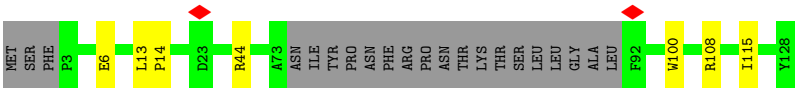
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



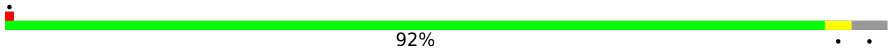
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

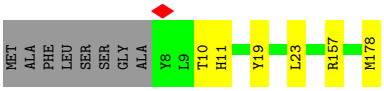
Chain m:



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

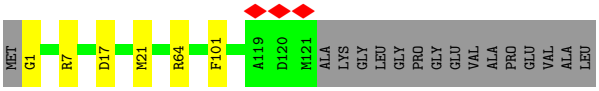
Chain n:





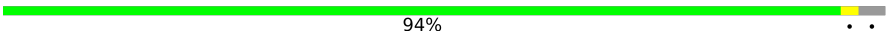
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



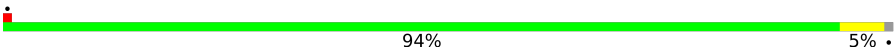
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

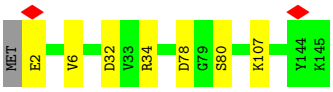
Chain p:



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

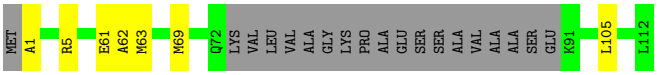
Chain q:





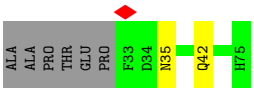
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122019	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	47.399	Depositor
Minimum map value	-18.669	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.090	Depositor
Recommended contour level	6	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.24	0/809	0.36	0/1108
2	B	0.27	0/1261	0.43	0/1706
3	C	0.24	0/1765	0.35	0/2403
4	D	0.23	0/3435	0.34	0/4650
5	E	0.22	0/1695	0.34	0/2307
6	F	0.23	0/3375	0.34	0/4561
7	G	0.23	0/5367	0.35	0/7274
8	H	0.25	0/2499	0.37	0/3413
9	I	0.25	0/1445	0.39	0/1956
10	J	0.22	0/1362	0.32	0/1848
11	K	0.29	0/730	0.39	0/988
12	L	0.27	0/4810	0.34	0/6541
13	M	0.26	0/3738	0.36	0/5097
14	N	0.25	0/2792	0.33	0/3800
15	O	0.26	0/2651	0.32	0/3587
16	P	0.22	0/2355	0.35	0/3182
17	Q	0.22	0/1039	0.33	0/1404
18	R	0.23	0/731	0.33	0/984
19	S	0.26	0/680	0.35	0/916
20	T	0.24	0/621	0.33	0/837
20	U	0.30	0/692	0.33	0/932
21	V	0.22	0/931	0.30	0/1261
22	W	0.23	0/995	0.33	0/1337
23	X	0.25	0/1439	0.35	0/1942
24	Y	0.16	0/1042	0.26	0/1414
25	Z	0.25	0/1181	0.33	0/1592
26	a	0.27	0/576	0.34	0/775
27	b	0.24	0/672	0.32	0/923
28	c	0.26	0/418	0.29	0/567
29	d	0.26	0/964	0.33	0/1305
30	e	0.26	0/818	0.37	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.25	0/457	0.35	0/616
32	g	0.28	0/839	0.38	0/1140
33	h	0.26	0/1188	0.33	0/1607
34	i	0.31	0/904	0.36	0/1230
35	j	0.29	0/607	0.31	0/833
36	k	0.27	0/657	0.29	0/887
37	l	0.29	0/1358	0.33	0/1858
38	m	0.28	0/929	0.34	0/1252
39	n	0.28	0/1540	0.37	0/2085
40	o	0.36	1/1068 (0.1%)	0.38	0/1430
41	p	0.30	0/1468	0.33	0/1979
42	q	0.21	0/1242	0.32	0/1688
43	r	0.21	0/780	0.34	0/1056
44	s	0.22	0/375	0.30	0/507
All	All	0.25	1/66300 (0.0%)	0.34	0/89871

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	o	1	GLY	CA-C	5.08	1.61	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

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	799	0	847	18	0
2	B	1230	0	1238	18	0
3	C	1714	0	1668	6	0
4	D	3362	0	3303	19	0
5	E	1655	0	1661	8	0
6	F	3301	0	3253	23	0
7	G	5279	0	5301	34	0
8	H	2440	0	2559	35	0
9	I	1414	0	1370	11	0
10	J	1337	0	1346	26	0
11	K	730	0	772	29	0
12	L	4695	0	4848	36	0
13	M	3654	0	3852	45	0
14	N	2733	0	2912	38	0
15	O	2589	0	2566	21	0
16	P	2305	0	2339	9	0
17	Q	1016	0	1014	5	0
18	R	720	0	700	4	0
19	S	669	0	677	4	0
20	T	612	0	604	6	0
20	U	681	0	677	7	0
21	V	911	0	950	3	0
22	W	971	0	989	7	0
23	X	1402	0	1383	5	0
24	Y	1030	0	1041	9	0
25	Z	1152	0	1151	10	0
26	a	561	0	564	6	0
27	b	651	0	662	2	0
28	c	405	0	409	4	0
29	d	934	0	919	5	0
30	e	799	0	807	14	0
31	f	444	0	444	2	0
32	g	813	0	759	5	0
33	h	1154	0	1168	7	0
34	i	884	0	905	6	0
35	j	580	0	519	1	0
36	k	638	0	621	1	0
37	l	1304	0	1203	12	0
38	m	908	0	903	6	0
39	n	1487	0	1433	6	0
40	o	1043	0	1011	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	p	1435	0	1411	3	0
42	q	1201	0	1170	6	0
43	r	767	0	776	5	0
44	s	364	0	336	2	0
45	A	35	0	46	3	0
45	H	35	0	46	0	0
45	J	35	0	46	0	0
45	L	70	0	92	1	0
45	M	35	0	46	2	0
45	N	35	0	46	3	0
45	Y	35	0	46	2	0
45	f	35	0	46	0	0
45	h	70	0	92	3	0
45	j	35	0	46	2	0
45	l	35	0	46	0	0
46	A	42	0	58	1	0
46	H	85	0	129	1	0
46	L	94	0	142	0	0
46	M	51	0	82	5	0
46	N	41	0	56	0	0
46	O	47	0	71	1	0
46	Y	104	0	133	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	1	0
47	I	16	0	0	1	0
48	B	35	0	44	0	0
48	M	49	0	75	1	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	L	69	0	82	1	0
52	X	68	0	80	0	0
52	d	65	0	77	0	0
52	h	67	0	81	2	0
52	r	76	0	96	0	0
53	N	17	0	0	1	0
54	O	32	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	0	0
57	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	T	37	0	0	0	0
58	U	37	0	0	0	0
59	o	15	0	27	2	0
60	A	8	0	0	0	0
60	B	58	0	0	1	0
60	C	102	0	0	1	0
60	D	157	0	0	2	0
60	E	29	0	0	1	0
60	F	70	0	0	1	0
60	G	227	0	0	6	0
60	H	46	0	0	0	0
60	I	104	0	0	2	0
60	J	10	0	0	0	0
60	K	4	0	0	0	0
60	L	65	0	0	1	0
60	M	71	0	0	2	0
60	N	46	0	0	2	0
60	O	11	0	0	1	0
60	P	47	0	0	1	0
60	Q	74	0	0	2	0
60	R	47	0	0	0	0
60	S	2	0	0	0	0
60	T	1	0	0	0	0
60	U	23	0	0	1	0
60	V	13	0	0	0	0
60	W	18	0	0	0	0
60	X	28	0	0	0	0
60	Y	1	0	0	0	0
60	Z	21	0	0	2	0
60	a	19	0	0	4	0
60	b	7	0	0	0	0
60	c	1	0	0	0	0
60	d	8	0	0	0	0
60	e	15	0	0	1	0
60	f	7	0	0	0	0
60	g	9	0	0	0	0
60	h	29	0	0	3	0
60	i	7	0	0	1	0
60	j	4	0	0	0	0
60	k	7	0	0	0	0
60	l	30	0	0	0	0
60	m	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	n	31	0	0	0	0
60	o	22	0	0	0	0
60	p	37	0	0	0	0
60	q	40	0	0	1	0
60	r	27	0	0	0	0
60	s	6	0	0	0	0
All	All	68004	0	66929	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (451) 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)
16:P:237:LEU:HD22	16:P:340:ILE:HD11	1.43	0.98
7:G:276:ARG:NH2	7:G:680:ALA:O	1.97	0.97
10:J:25:SER:OG	10:J:77:GLU:OE1	1.86	0.92
42:q:78:ASP:OD1	42:q:80:SER:OG	1.89	0.90
15:O:83:TYR:OH	54:O:1202:GTP:O2'	1.89	0.89
13:M:335:GLU:OE1	60:M:1401:HOH:O	1.92	0.88
1:A:85:ASN:OD1	45:A:301:LMT:O3'	1.92	0.87
37:l:97:ASN:ND2	38:m:6:GLU:OE1	2.08	0.86
14:N:214:THR:HG22	14:N:218:MET:HE2	1.58	0.85
37:l:5:THR:OG1	37:l:7:ASP:OD1	1.94	0.85
8:H:70:MET:HE1	8:H:121:TRP:HE3	1.43	0.83
42:q:32:ASP:OD2	60:q:201:HOH:O	1.94	0.83
14:N:196:TYR:O	53:N:503:I49:N05	2.11	0.83
6:F:432:GLN:O	6:F:436:GLN:NE2	2.12	0.82
1:A:54:LYS:NZ	1:A:112:GLU:O	2.12	0.80
33:h:141:PRO:O	60:h:1101:HOH:O	1.99	0.80
11:K:43:MET:HE1	14:N:72:MET:HE1	1.61	0.80
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.46	0.80
33:h:80:PHE:O	60:h:1102:HOH:O	2.00	0.80
9:I:11:SER:OG	9:I:13:ASP:OD2	2.00	0.79
45:h:1003:LMT:O6B	41:p:58:ASN:OD1	2.01	0.79
5:E:38:TYR:O	60:E:401:HOH:O	2.00	0.78
14:N:174:GLN:OE1	60:N:601:HOH:O	2.02	0.77
6:F:226:GLU:OE1	60:F:601:HOH:O	2.02	0.76
26:a:51:ASP:OD2	60:a:101:HOH:O	2.03	0.75
15:O:146:LYS:NZ	15:O:150:ASP:OD2	2.19	0.74
45:Y:602:LMT:O5B	45:Y:602:LMT:O6'	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:L:703:CDL:OA9	33:h:26:ARG:NH2	2.20	0.74
13:M:126:LEU:HD11	13:M:153:THR:HG21	1.69	0.74
12:L:286:LEU:HD13	12:L:411:MET:SD	2.28	0.74
22:W:42:GLU:OE2	22:W:46:THR:OG1	2.05	0.74
7:G:265:ASP:OD2	60:G:901:HOH:O	2.06	0.73
20:T:68:GLU:OE2	22:W:33:ARG:NE	2.22	0.73
12:L:72:GLN:OE1	60:L:801:HOH:O	2.07	0.72
8:H:70:MET:HE1	8:H:121:TRP:CE3	2.25	0.72
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.71	0.72
13:M:153:THR:HG23	13:M:206:LYS:NZ	2.03	0.72
6:F:431:GLN:O	6:F:435:GLN:NE2	2.22	0.72
9:I:54:LYS:O	60:I:301:HOH:O	2.08	0.72
17:Q:30:ILE:O	60:Q:201:HOH:O	2.08	0.71
13:M:42:MET:HE1	13:M:453:ILE:HD12	1.72	0.71
7:G:387:GLU:OE1	60:G:902:HOH:O	2.08	0.71
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.74	0.70
13:M:285:LEU:HD22	13:M:410:MET:CE	2.21	0.70
2:B:44:SER:OG	8:H:51:ASP:OD1	2.02	0.70
20:T:55:GLU:OE1	22:W:37:ARG:NH2	2.25	0.70
26:a:1:MET:N	26:a:4:GLU:OE2	2.23	0.69
33:h:47:ILE:O	60:h:1103:HOH:O	2.08	0.69
20:U:49:GLU:OE1	39:n:19:TYR:OH	2.09	0.69
15:O:107:GLN:OE1	60:O:1301:HOH:O	2.10	0.69
45:j:101:LMT:O3'	45:j:101:LMT:O2B	2.11	0.68
7:G:635:ASP:O	60:G:903:HOH:O	2.11	0.67
4:D:69:SER:OG	4:D:74:ARG:NH1	2.28	0.67
11:K:53:PHE:CE1	30:e:20:GLN:HA	2.30	0.67
25:Z:64:ASP:OD2	60:Z:201:HOH:O	2.11	0.67
20:T:7:THR:O	20:T:10:GLY:N	2.29	0.66
2:B:50:PHE:HE2	2:B:86:MET:HE2	1.60	0.66
17:Q:21:THR:HG21	22:W:73:ILE:HD11	1.77	0.66
12:L:494:THR:HG21	45:L:705:LMT:H121	1.77	0.66
7:G:578:GLY:O	60:G:905:HOH:O	2.14	0.66
25:Z:85:GLN:NE2	25:Z:89:GLU:OE1	2.26	0.66
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.31	0.65
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.31	0.65
11:K:53:PHE:CE2	11:K:56:ALA:HB2	2.31	0.65
7:G:684:MET:HA	7:G:684:MET:HE2	1.79	0.65
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.09	0.65
4:D:182:GLU:OE1	60:D:501:HOH:O	2.15	0.65
7:G:569:LYS:NZ	7:G:596:ASP:OD2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:176:LEU:HD21	25:Z:45:PHE:HD2	1.61	0.65
12:L:28:LYS:NZ	12:L:30:SER:OG	2.21	0.65
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.78	0.65
46:M:1301:3PE:H3D2	46:M:1301:3PE:H2I3	1.78	0.65
7:G:44:GLU:OE2	60:G:904:HOH:O	2.14	0.64
34:i:63:THR:O	34:i:67:SER:N	2.29	0.64
40:o:21:MET:HE1	40:o:101:PHE:HA	1.80	0.64
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.33	0.64
8:H:222:LEU:HD23	8:H:225:MET:HE2	1.80	0.64
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.32	0.63
20:U:12:LYS:HD2	20:U:32:VAL:HG11	1.81	0.63
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.81	0.63
2:B:62:MET:CE	2:B:69:MET:HE2	2.28	0.63
23:X:25:LYS:NZ	23:X:94:GLN:O	2.31	0.62
37:l:126:GLN:NE2	59:o:201:MYR:O1	2.30	0.62
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.33	0.62
8:H:24:GLU:OE1	8:H:274:ARG:NH1	2.33	0.61
46:H:402:3PE:H3C1	27:b:24:ILE:HD11	1.81	0.61
14:N:17:THR:HG22	14:N:21:MET:HE2	1.82	0.61
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.35	0.61
12:L:544:MET:HE1	13:M:271:MET:HE1	1.81	0.60
11:K:59:MET:HE2	14:N:84:TRP:HH2	1.66	0.60
11:K:70:GLU:OE2	14:N:64:SER:OG	2.13	0.60
15:O:191:GLU:OE2	54:O:1202:GTP:O3'	2.14	0.60
1:A:79:SER:HA	1:A:87:MET:HE2	1.83	0.60
11:K:43:MET:CE	14:N:72:MET:HE1	2.31	0.60
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.37	0.60
26:a:37:ARG:NE	60:a:104:HOH:O	2.27	0.60
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.84	0.59
34:i:103:ILE:O	60:i:201:HOH:O	2.16	0.59
15:O:174:VAL:HG22	15:O:225:ALA:HB2	1.84	0.59
30:e:61:ASP:OD2	60:e:201:HOH:O	2.16	0.59
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.33	0.59
20:U:79:TYR:OH	20:U:83:LYS:NZ	2.36	0.59
10:J:103:MET:O	10:J:107:VAL:HG23	2.03	0.58
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.84	0.58
4:D:205:LEU:HD13	25:Z:7:LYS:HZ2	1.68	0.58
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.86	0.58
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.33	0.58
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.85	0.58
13:M:153:THR:HG23	13:M:206:LYS:HZ2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:88:GLU:OE2	41:p:92:ARG:NH1	2.37	0.58
4:D:205:LEU:HD13	25:Z:7:LYS:NZ	2.19	0.57
23:X:44:LEU:HD22	23:X:130:VAL:CG2	2.35	0.57
7:G:415:LEU:O	7:G:416:THR:OG1	2.21	0.57
45:N:501:LMT:O6'	45:N:501:LMT:O1B	2.23	0.57
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.87	0.56
29:d:120:ARG:HD3	38:m:115:ILE:HD13	1.86	0.56
10:J:4:TYR:HE2	11:K:3:MET:HE1	1.71	0.56
24:Y:80:ARG:HH12	24:Y:87:LEU:HD23	1.70	0.56
12:L:506:ASN:OD1	12:L:509:LYS:NZ	2.30	0.55
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.89	0.55
8:H:318:THR:HG23	26:a:41:TYR:HE2	1.71	0.55
10:J:107:VAL:HG22	10:J:113:VAL:CG1	2.36	0.55
8:H:172:MET:SD	8:H:176:LEU:HD23	2.47	0.55
2:B:62:MET:HE2	2:B:69:MET:HE2	1.88	0.55
12:L:124:PHE:CE1	12:L:251:THR:HG21	2.42	0.55
14:N:179:MET:HE1	14:N:251:MET:HE1	1.89	0.55
26:a:38:VAL:O	60:a:102:HOH:O	2.18	0.55
15:O:238:ILE:HA	15:O:241:LEU:HD23	1.88	0.54
37:l:6:LYS:O	37:l:6:LYS:NZ	2.29	0.54
6:F:194:GLU:OE2	6:F:204:ARG:NE	2.25	0.54
13:M:57:PHE:CD1	13:M:113:MET:HG2	2.43	0.54
7:G:396:ARG:NH1	7:G:416:THR:O	2.40	0.54
7:G:465:ALA:HB2	7:G:654:GLN:OE1	2.07	0.53
14:N:321:LYS:NZ	15:O:268:GLU:OE2	2.41	0.53
11:K:37:MET:HE2	11:K:67:ALA:HB3	1.90	0.53
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.42	0.53
20:U:82:ASP:OD1	60:U:201:HOH:O	2.18	0.53
24:Y:16:GLU:OE1	24:Y:19:ARG:NE	2.40	0.53
13:M:285:LEU:HD22	13:M:410:MET:HE3	1.89	0.53
37:l:50:LEU:HD12	37:l:78:HIS:HA	1.89	0.53
12:L:69:LEU:HD21	12:L:71:ILE:HD11	1.89	0.53
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.90	0.53
12:L:40:ILE:HG13	12:L:101:MET:SD	2.49	0.53
8:H:222:LEU:HD23	8:H:225:MET:CE	2.39	0.52
12:L:87:MET:HA	12:L:87:MET:HE2	1.90	0.52
12:L:128:MET:HB2	12:L:251:THR:HG23	1.91	0.52
13:M:39:LEU:HB2	45:h:1002:LMT:H121	1.90	0.52
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.91	0.52
6:F:99:GLU:OE2	6:F:104:THR:HG22	2.10	0.52
10:J:43:ILE:HG22	11:K:46:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:33:LYS:O	28:c:37:GLU:OE1	2.27	0.52
13:M:1:FME:HE3	13:M:111:THR:HG21	1.92	0.52
30:e:17:MET:O	30:e:17:MET:HG2	2.10	0.52
13:M:153:THR:HG23	13:M:206:LYS:HZ1	1.72	0.52
5:E:214:GLN:NE2	6:F:235:CYS:O	2.42	0.52
45:j:101:LMT:H2O1	45:j:101:LMT:C3'	2.22	0.52
39:n:10:THR:HG22	39:n:11:HIS:N	2.24	0.52
10:J:46:ASN:O	10:J:128:TYR:OH	2.23	0.52
12:L:331:THR:HB	12:L:387:THR:HG22	1.92	0.52
46:M:1301:3PE:C33	14:N:242:VAL:HG11	2.40	0.52
45:M:1303:LMT:C1'	45:M:1303:LMT:H6'	2.21	0.52
13:M:370:PRO:HB3	13:M:375:LEU:HD22	1.92	0.51
30:e:85:LEU:O	30:e:89:GLY:N	2.43	0.51
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.40	0.51
16:P:135:LEU:O	60:P:601:HOH:O	2.18	0.51
5:E:66:MET:HE2	5:E:81:TYR:CD1	2.45	0.51
10:J:1:FME:HE1	25:Z:134:LEU:HD11	1.92	0.51
12:L:148:GLY:HA2	12:L:252:MET:HE3	1.93	0.51
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.92	0.51
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.45	0.51
13:M:42:MET:HE1	13:M:453:ILE:CD1	2.41	0.51
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.92	0.51
45:A:301:LMT:O3'	45:A:301:LMT:O5B	2.28	0.51
24:Y:13:GLU:OE2	24:Y:89:TYR:OH	2.25	0.51
1:A:114:THR:HA	4:D:72:MET:HE3	1.93	0.51
11:K:44:ALA:HB1	11:K:59:MET:HE1	1.92	0.51
2:B:91:THR:HA	2:B:119:CYS:HB3	1.93	0.50
8:H:200:LEU:HD22	8:H:285:LEU:HD21	1.92	0.50
10:J:4:TYR:CE2	11:K:3:MET:HE1	2.46	0.50
2:B:125:TYR:HB2	9:I:117:ILE:HG21	1.93	0.50
3:C:14:ARG:NH2	43:r:61:GLU:O	2.45	0.50
10:J:125:TRP:HB2	25:Z:137:THR:HG21	1.94	0.50
42:q:2:GLU:OE2	43:r:5:ARG:NH1	2.44	0.50
28:c:38:ASP:HB3	29:d:23:PRO:HG3	1.94	0.50
7:G:651:LEU:HD11	19:S:45:LYS:HE2	1.94	0.50
23:X:44:LEU:HD22	23:X:130:VAL:HG22	1.94	0.50
32:g:100:ARG:NH1	32:g:107:ILE:O	2.44	0.50
33:h:87:TYR:OH	41:p:86:GLU:HG2	2.12	0.50
43:r:62:ALA:O	43:r:63:MET:HE2	2.11	0.50
2:B:62:MET:HE3	2:B:69:MET:HE2	1.92	0.50
2:B:63:ALA:HA	2:B:69:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:TYR:CZ	43:r:105:LEU:HD23	2.46	0.49
11:K:53:PHE:HE1	30:e:20:GLN:HA	1.75	0.49
12:L:261:ILE:HG13	12:L:317:ILE:HD11	1.94	0.49
37:l:118:VAL:HG12	59:o:201:MYR:H141	1.93	0.49
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.94	0.49
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.94	0.49
24:Y:55:THR:O	24:Y:59:THR:OG1	2.23	0.49
21:V:34:LEU:HD13	21:V:48:GLU:HG3	1.95	0.49
3:C:78:LEU:HD13	3:C:94:TYR:CD2	2.48	0.49
5:E:181:ILE:HG23	5:E:181:ILE:O	2.10	0.49
15:O:232:GLU:OE1	15:O:232:GLU:N	2.46	0.49
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.95	0.49
37:l:71:LEU:HD11	37:l:81:LEU:HD21	1.94	0.49
5:E:132:THR:OG1	5:E:134:ASP:OD2	2.29	0.49
13:M:343:ILE:HG13	13:M:413:MET:HE2	1.94	0.49
12:L:251:THR:HG22	12:L:252:MET:N	2.28	0.48
15:O:27:VAL:HG12	15:O:35:LYS:HB2	1.95	0.48
8:H:233:MET:HE1	8:H:234:MET:CE	2.44	0.48
11:K:44:ALA:HB1	11:K:59:MET:CE	2.43	0.48
42:q:2:GLU:O	42:q:6:VAL:HG23	2.13	0.48
12:L:305:SER:OG	12:L:336:LYS:NZ	2.46	0.48
32:g:76:PHE:CG	45:h:1002:LMT:H123	2.49	0.48
1:A:49:LEU:O	1:A:51:PHE:N	2.47	0.48
2:B:59:MET:HE3	2:B:69:MET:HE1	1.95	0.48
45:M:1303:LMT:O1'	45:M:1303:LMT:O6'	2.27	0.48
14:N:314:LYS:NZ	15:O:270:LEU:O	2.47	0.48
6:F:28:ARG:NH1	44:s:35:ASN:O	2.46	0.48
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.96	0.48
13:M:403:THR:HA	13:M:406:TYR:CE1	2.48	0.48
13:M:126:LEU:HD11	13:M:153:THR:CG2	2.41	0.48
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.94	0.48
11:K:37:MET:HG3	11:K:67:ALA:CB	2.44	0.48
19:S:57:CYS:O	19:S:60:VAL:HG22	2.14	0.48
14:N:313:MET:HG2	15:O:270:LEU:HD13	1.96	0.48
18:R:46:GLU:OE1	42:q:107:LYS:NZ	2.47	0.48
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.54	0.47
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.95	0.47
13:M:127:VAL:HG11	46:M:1301:3PE:H2I2	1.95	0.47
14:N:298:TYR:O	14:N:303:THR:OG1	2.25	0.47
1:A:69:ILE:HD12	8:H:148:ILE:HG12	1.95	0.47
9:I:124:GLU:OE2	60:I:302:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:7:ARG:NH2	40:o:17:ASP:OD2	2.47	0.47
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.49	0.47
12:L:541:ASN:O	12:L:544:MET:HG3	2.15	0.47
13:M:267:TRP:CE2	13:M:271:MET:HE3	2.49	0.47
30:e:59:PHE:CE2	30:e:63:ARG:HD2	2.49	0.47
38:m:44:ARG:NH2	60:m:204:HOH:O	2.46	0.47
7:G:140:LYS:O	7:G:148:THR:OG1	2.30	0.47
8:H:87:ILE:N	8:H:88:PRO:CD	2.77	0.47
45:A:301:LMT:H6'1	27:b:42:LEU:HD22	1.97	0.47
2:B:49:THR:OG1	2:B:59:MET:HE2	2.15	0.47
16:P:122:LYS:HE3	16:P:160:PHE:CD1	2.49	0.47
16:P:250:HIS:CE1	16:P:322:ARG:NH1	2.82	0.47
30:e:88:GLU:OE1	30:e:90:LYS:NZ	2.43	0.47
4:D:146:ARG:HG2	4:D:150:HIS:CD2	2.50	0.47
10:J:171:ILE:HG23	14:N:45:MET:HE2	1.97	0.47
12:L:1:FME:HCN	12:L:4:PHE:H	1.79	0.47
13:M:56:PHE:HA	13:M:111:THR:O	2.15	0.47
31:f:7:VAL:HG12	31:f:9:ASP:H	1.79	0.47
37:l:32:GLU:N	37:l:32:GLU:OE1	2.45	0.47
4:D:64:LEU:HD11	4:D:418:ILE:HD11	1.96	0.46
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.48	0.46
37:l:77:MET:HE3	37:l:81:LEU:CD2	2.45	0.46
14:N:321:LYS:CE	15:O:268:GLU:OE2	2.63	0.46
15:O:310:GLU:HG3	15:O:317:ILE:HD12	1.96	0.46
34:i:6:GLU:OE2	39:n:157:ARG:NH1	2.35	0.46
5:E:105:THR:HG22	5:E:106:THR:H	1.80	0.46
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.97	0.46
7:G:377:VAL:HG13	7:G:452:ILE:CD1	2.45	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.98	0.46
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.98	0.46
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.16	0.46
17:Q:133:LYS:NZ	60:Q:204:HOH:O	2.39	0.46
4:D:385:ARG:NH1	60:D:507:HOH:O	2.38	0.46
13:M:342:MET:HE1	13:M:409:TYR:CE2	2.51	0.46
20:T:80:ILE:O	20:T:82:ASP:N	2.47	0.46
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.46	0.46
32:g:57:ASN:O	32:g:57:ASN:ND2	2.46	0.46
5:E:66:MET:HE1	7:G:186:TYR:CE2	2.51	0.46
1:A:108:GLN:HB2	10:J:169:MET:CE	2.46	0.46
4:D:72:MET:HE1	4:D:410:MET:HE2	1.97	0.46
14:N:323:MET:O	60:N:602:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:2:VAL:HG21	18:R:37:GLU:OE1	2.16	0.46
19:S:18:ILE:CD1	19:S:93:VAL:HG11	2.46	0.46
20:T:43:ASP:OD1	20:T:44(A):SER:N	2.41	0.46
24:Y:115:ALA:O	24:Y:119:LEU:HD23	2.15	0.46
8:H:113:VAL:HG21	8:H:136:VAL:HG13	1.97	0.45
13:M:141:GLU:HG2	13:M:222:GLU:CD	2.41	0.45
1:A:71:LEU:O	10:J:147:TYR:OH	2.30	0.45
2:B:50:PHE:CE2	2:B:86:MET:HE2	2.47	0.45
4:D:417:ILE:O	4:D:420:THR:HG22	2.16	0.45
11:K:40:LEU:HD21	14:N:72:MET:HE2	1.97	0.45
13:M:285:LEU:HD23	13:M:285:LEU:C	2.41	0.45
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.98	0.45
22:W:96:VAL:HG12	22:W:96:VAL:O	2.17	0.45
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.50	0.45
6:F:93:LEU:O	6:F:134:ALA:HA	2.17	0.45
12:L:455:LYS:NZ	35:j:24:GLN:OE1	2.35	0.45
8:H:103:LEU:HD21	8:H:160:PHE:CE1	2.52	0.45
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.46	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.45
24:Y:69:PHE:O	24:Y:73:SER:OG	2.28	0.45
10:J:135:PHE:CD2	10:J:135:PHE:O	2.70	0.45
13:M:135:ARG:NH1	14:N:301:THR:O	2.50	0.45
2:B:175:ILE:HD12	16:P:52:GLU:HG2	1.99	0.45
13:M:168:GLN:NE2	23:X:167:PHE:CE1	2.84	0.45
13:M:285:LEU:HD23	13:M:285:LEU:O	2.16	0.45
37:l:141:GLU:OE2	37:l:141:GLU:N	2.45	0.45
44:s:42:GLN:OE1	44:s:42:GLN:N	2.48	0.45
25:Z:70:ALA:O	60:Z:202:HOH:O	2.21	0.44
12:L:419:THR:HA	12:L:422:TYR:CE1	2.52	0.44
7:G:276:ARG:NH2	7:G:682:GLN:HG3	2.32	0.44
29:d:10:THR:O	29:d:10:THR:HG23	2.18	0.44
6:F:364:PRO:HB2	6:F:403:THR:HG22	1.99	0.44
7:G:46:LEU:O	17:Q:116:LYS:NZ	2.47	0.44
7:G:306:MET:HE3	7:G:310:PHE:HE2	1.81	0.44
46:M:1301:3PE:H332	14:N:242:VAL:HG11	2.00	0.44
3:C:155:TYR:O	60:C:301:HOH:O	2.21	0.44
8:H:233:MET:HE1	8:H:234:MET:HE3	2.00	0.44
10:J:123:GLY:O	10:J:126:VAL:HG22	2.18	0.44
10:J:136:PHE:CE2	30:e:28:ILE:HD11	2.52	0.44
13:M:106:LEU:HD13	13:M:234:VAL:HG11	2.00	0.44
30:e:86:ILE:HD11	30:e:91:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.99	0.44
13:M:105:PHE:O	13:M:109:THR:OG1	2.29	0.44
8:H:66:SER:OG	8:H:121:TRP:O	2.35	0.44
11:K:53:PHE:CD2	11:K:56:ALA:HB2	2.52	0.44
11:K:55:LEU:O	30:e:17:MET:HE2	2.18	0.44
13:M:296:LEU:HD21	13:M:396:MET:SD	2.58	0.44
11:K:53:PHE:CD1	30:e:20:GLN:HA	2.53	0.44
12:L:434:GLN:HG3	36:k:52:TYR:CE2	2.53	0.44
46:M:1301:3PE:H331	14:N:242:VAL:HG11	1.98	0.44
15:O:88:SER:OG	15:O:90:ASP:OD1	2.25	0.44
30:e:16:TRP:CH2	30:e:17:MET:HE3	2.53	0.44
10:J:135:PHE:O	10:J:135:PHE:CG	2.71	0.43
13:M:378:GLU:OE2	13:M:400:MET:HE2	2.18	0.43
37:l:82:ASP:OD1	37:l:82:ASP:N	2.51	0.43
34:i:122:PHE:HE2	40:o:64:ARG:HE	1.66	0.43
7:G:35:MET:SD	7:G:81:THR:CB	3.07	0.43
7:G:377:VAL:HG23	7:G:404:LEU:HD11	1.99	0.43
11:K:59:MET:HB3	11:K:60:PRO:HD3	2.00	0.43
28:c:1:LYS:NZ	28:c:3:TYR:O	2.50	0.43
32:g:101:GLU:HG2	32:g:107:ILE:HD11	2.00	0.43
13:M:6:ILE:HD12	31:f:23:GLY:HA2	2.00	0.43
3:C:62:THR:HG21	21:V:96:TRP:HH2	1.83	0.43
4:D:328:ALA:HB3	7:G:126:ASP:HB2	2.01	0.43
11:K:40:LEU:CD2	14:N:72:MET:HE2	2.48	0.43
12:L:272:TYR:CZ	12:L:276:ILE:HD11	2.54	0.43
12:L:595:ILE:HG21	45:N:501:LMT:C12	2.49	0.43
11:K:73:LEU:HD21	14:N:41:ILE:HG13	2.00	0.43
18:R:7:THR:O	18:R:7:THR:HG22	2.18	0.43
2:B:138:ARG:NH1	60:B:306:HOH:O	2.46	0.43
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.54	0.43
23:X:6:LEU:HD12	25:Z:91:LEU:HD22	2.00	0.43
24:Y:85:ASP:OD1	24:Y:87:LEU:HB3	2.19	0.43
34:i:75:LEU:O	34:i:78:VAL:HG12	2.19	0.43
6:F:380:VAL:O	6:F:429:ARG:NH2	2.46	0.43
8:H:288:LEU:O	8:H:292:ASN:HB2	2.18	0.43
11:K:53:PHE:CD2	11:K:56:ALA:CB	3.01	0.43
26:a:62:VAL:O	60:a:103:HOH:O	2.22	0.43
39:n:19:TYR:CZ	39:n:23:LEU:HD11	2.54	0.43
13:M:104:LEU:HG	13:M:108:MET:HE2	2.01	0.42
8:H:77:MET:HE3	8:H:81:LEU:HD11	2.01	0.42
11:K:53:PHE:CD1	30:e:20:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:54:ILE:HD13	22:W:107:PHE:CZ	2.54	0.42
3:C:78:LEU:HD13	3:C:94:TYR:CE2	2.55	0.42
4:D:335:ARG:NH2	9:I:129:ASP:OD2	2.46	0.42
8:H:70:MET:HE3	8:H:118:TRP:CD1	2.55	0.42
11:K:70:GLU:OE2	14:N:64:SER:CB	2.67	0.42
14:N:214:THR:HG22	14:N:218:MET:CE	2.41	0.42
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.00	0.42
15:O:111:ALA:HB1	15:O:122:VAL:HG21	2.02	0.42
12:L:9:LEU:HD22	52:h:1001:CDL:C22	2.49	0.42
48:M:1302:PC1:H142	52:h:1001:CDL:OA3	2.18	0.42
45:Y:602:LMT:H6'	45:Y:602:LMT:C1B	2.29	0.42
1:A:65:PHE:O	1:A:69:ILE:HG12	2.20	0.42
2:B:34:ASP:OD1	2:B:173:LEU:HB2	2.20	0.42
13:M:225:ILE:HD13	13:M:331:ASN:CB	2.49	0.42
28:c:6:GLU:OE2	28:c:6:GLU:HA	2.19	0.42
2:B:125:TYR:CE2	4:D:102:TYR:CD1	3.08	0.42
6:F:98:ASP:O	6:F:99:GLU:C	2.62	0.42
8:H:233:MET:SD	8:H:234:MET:HE2	2.60	0.42
16:P:293:ILE:HG22	16:P:295:PRO:HD3	2.01	0.42
1:A:90:MET:SD	10:J:151:THR:HG23	2.60	0.42
1:A:109:LYS:HE2	1:A:109:LYS:HA	2.02	0.42
7:G:306:MET:HE3	7:G:310:PHE:CE2	2.55	0.42
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.01	0.42
19:S:18:ILE:HD11	19:S:93:VAL:HG11	2.01	0.42
37:l:42:THR:HG21	37:l:44:TYR:CE2	2.55	0.42
6:F:268:VAL:HG22	6:F:269:GLU:N	2.35	0.42
6:F:423:ARG:N	6:F:424:PRO:HD2	2.35	0.42
8:H:24:GLU:HA	8:H:271:LEU:HD13	2.02	0.42
12:L:6:SER:O	12:L:10:VAL:HG23	2.19	0.42
10:J:167:VAL:O	10:J:171:ILE:HG12	2.19	0.42
13:M:200:MET:HE1	13:M:243:MET:HG2	2.02	0.42
20:T:7:THR:O	20:T:9:GLU:N	2.53	0.42
4:D:202:ASP:CA	4:D:323:ILE:HD13	2.49	0.41
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.55	0.41
13:M:122:PHE:CZ	13:M:206:LYS:HE2	2.55	0.41
11:K:44:ALA:CB	11:K:59:MET:HE1	2.50	0.41
1:A:25:PRO:O	1:A:26:GLN:CB	2.69	0.41
10:J:171:ILE:HD11	14:N:41:ILE:HG22	2.03	0.41
11:K:33:LEU:HD21	14:N:64:SER:HB3	2.02	0.41
13:M:370:PRO:HB3	13:M:375:LEU:CD2	2.49	0.41
24:Y:3:THR:HG23	24:Y:4:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:92:THR:HG23	30:e:92:THR:O	2.20	0.41
32:g:26:TRP:CD1	32:g:28:GLU:HB2	2.55	0.41
1:A:48:ARG:NH1	1:A:51:PHE:O	2.47	0.41
2:B:49:THR:HG21	2:B:59:MET:HG2	2.02	0.41
7:G:39:ARG:NH2	60:G:930:HOH:O	2.44	0.41
7:G:453:LEU:HD21	7:G:458:LEU:HD21	2.03	0.41
16:P:238:LEU:O	16:P:242:VAL:HG23	2.20	0.41
20:U:43:ASP:C	20:U:43:ASP:OD1	2.64	0.41
14:N:76:ILE:HD11	45:N:501:LMT:H62	2.02	0.41
6:F:403:THR:HB	47:F:502:SF4:S4	2.61	0.41
6:F:194:GLU:OE1	6:F:199:LYS:NZ	2.51	0.41
12:L:264:TYR:N	12:L:265:PRO:CD	2.84	0.41
3:C:30:ALA:HB1	43:r:69:MET:SD	2.61	0.41
8:H:113:VAL:CG2	8:H:136:VAL:HG22	2.51	0.41
10:J:167:VAL:HG13	14:N:42:PRO:HD3	2.02	0.41
13:M:16:TRP:CE2	46:O:1201:3PE:H271	2.56	0.41
15:O:88:SER:HG	15:O:90:ASP:CG	2.26	0.41
16:P:201:VAL:HG13	16:P:340:ILE:HD12	2.01	0.41
6:F:306:LEU:HD12	6:F:306:LEU:C	2.46	0.41
7:G:203:CYS:HA	47:G:802:SF4:S2	2.61	0.41
8:H:207:LEU:HD12	8:H:207:LEU:C	2.46	0.41
12:L:566:ILE:HG23	12:L:567:SER:N	2.35	0.41
13:M:420:THR:O	60:M:1402:HOH:O	2.22	0.41
14:N:250:SER:O	14:N:259:GLY:HA3	2.20	0.41
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.56	0.41
21:V:32:ASP:C	21:V:32:ASP:OD1	2.63	0.41
38:m:13:LEU:HD12	38:m:14:PRO:HD2	2.02	0.41
40:o:21:MET:CE	40:o:101:PHE:HA	2.49	0.41
6:F:214:GLY:N	6:F:218:CYS:O	2.48	0.41
12:L:1:FME:HG2	34:i:98:GLU:OE2	2.21	0.41
16:P:315:ILE:CD1	16:P:322:ARG:HH21	2.33	0.41
46:A:302:3PE:C2B	46:A:302:3PE:C2F	2.98	0.40
9:I:126:CYS:HA	47:I:202:SF4:S2	2.61	0.40
11:K:96:LEU:HD13	14:N:117:GLU:O	2.21	0.40
12:L:63:ILE:O	12:L:79:SER:HA	2.21	0.40
2:B:77:ARG:NH2	4:D:159:LEU:HD21	2.36	0.40
13:M:47:ASP:OD1	13:M:48:ASN:N	2.53	0.40
13:M:76:MET:SD	13:M:230:VAL:HB	2.62	0.40
33:h:10:ILE:HG23	39:n:178:MET:HG2	2.04	0.40
4:D:343:GLU:OE2	4:D:343:GLU:N	2.49	0.40
8:H:301:CYS:O	8:H:305:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:125:TRP:CB	25:Z:137:THR:HG21	2.51	0.40
11:K:4:VAL:HG11	11:K:46:LEU:CD2	2.51	0.40
12:L:407:TRP:CH2	12:L:411:MET:HE3	2.56	0.40
14:N:313:MET:HE3	14:N:313:MET:HB2	2.00	0.40
18:R:19:ASP:OD2	18:R:22:ASP:HB2	2.21	0.40
29:d:24:PRO:CD	29:d:77:LYS:HG2	2.51	0.40
29:d:120:ARG:O	38:m:108:ARG:NH2	2.54	0.40
6:F:192:LEU:HD23	6:F:192:LEU:C	2.47	0.40
7:G:569:LYS:HA	7:G:585:VAL:HG22	2.04	0.40
10:J:123:GLY:N	11:K:3:MET:HE3	2.35	0.40
12:L:599:MET:HE3	14:N:96:MET:HE1	2.02	0.40
20:U:47:GLN:NE2	20:U:70:LEU:O	2.50	0.40
8:H:142:TYR:CD1	8:H:289:LEU:HD12	2.57	0.40
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.04	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	95/115 (83%)	92 (97%)	3 (3%)	0	100	100
2	B	152/216 (70%)	144 (95%)	7 (5%)	1 (1%)	18	23
3	C	204/266 (77%)	199 (98%)	5 (2%)	0	100	100
4	D	409/463 (88%)	402 (98%)	7 (2%)	0	100	100
5	E	211/249 (85%)	208 (99%)	3 (1%)	0	100	100
6	F	427/464 (92%)	418 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	670 (98%)	16 (2%)	0	100	100
8	H	305/318 (96%)	296 (97%)	9 (3%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	172/175 (98%)	162 (94%)	10 (6%)	0	100	100
11	K	94/98 (96%)	91 (97%)	3 (3%)	0	100	100
12	L	588/606 (97%)	569 (97%)	19 (3%)	0	100	100
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	282/380 (74%)	278 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	92/124 (74%)	89 (97%)	3 (3%)	0	100	100
19	S	81/99 (82%)	80 (99%)	1 (1%)	0	100	100
20	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	95/154 (62%)	91 (96%)	4 (4%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	99/127 (78%)	96 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
38	m	104/129 (81%)	101 (97%)	3 (3%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
41	p	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	40 (98%)	1 (2%)	0	100	100
All	All	7943/9212 (86%)	7776 (98%)	166 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	53	ALA

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	86/100 (86%)	86 (100%)	0	100	100
2	B	130/175 (74%)	130 (100%)	0	100	100
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	360/392 (92%)	360 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	343/368 (93%)	343 (100%)	0	100	100
7	G	578/608 (95%)	577 (100%)	1 (0%)	87	94
8	H	267/274 (97%)	267 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	83/85 (98%)	83 (100%)	0	100	100
12	L	521/533 (98%)	521 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	249/327 (76%)	249 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	74/82 (90%)	74 (100%)	0	100	100
20	T	70/135 (52%)	69 (99%)	1 (1%)	59	76
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	88/131 (67%)	88 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	98 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	96/115 (84%)	96 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	7028/7892 (89%)	7026 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
7	G	475	GLN
20	T	44(A)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	39	GLN
3	C	102	ASN
4	D	13	GLN
4	D	127	ASN
4	D	150	HIS
4	D	200	HIS
5	E	155	GLN
6	F	150	GLN
6	F	200	GLN
6	F	421	HIS
6	F	435	GLN
7	G	155	GLN
7	G	430	GLN
7	G	441	GLN
7	G	475	GLN
7	G	653	ASN
8	H	47	GLN
8	H	287	HIS
11	K	52	HIS
12	L	31	ASN
12	L	200	GLN
12	L	269	ASN
12	L	479	GLN
13	M	168	GLN
13	M	251	ASN
13	M	304	GLN
13	M	338	HIS
13	M	366	ASN
13	M	415	GLN

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Mol	Chain	Res	Type
14	N	63	GLN
14	N	120	GLN
14	N	174	GLN
14	N	268	GLN
15	O	89	ASN
15	O	180	GLN
15	O	184	GLN
15	O	188	ASN
15	O	190	HIS
15	O	271	ASN
15	O	288	GLN
16	P	8	HIS
16	P	93	ASN
16	P	250	HIS
16	P	288	HIS
17	Q	50	ASN
18	R	90	GLN
19	S	80	ASN
21	V	52	ASN
21	V	95	GLN
23	X	64	GLN
23	X	76	HIS
25	Z	112	HIS
28	c	5	GLN
29	d	117	HIS
33	h	63	HIS
33	h	124	HIS
34	i	125	GLN
35	j	58	GLN
39	n	61	GLN
39	n	72	HIS
39	n	159	GLN
40	o	42	GLN
41	p	120	HIS
42	q	17	HIS
42	q	31	ASN
42	q	69	ASN
42	q	112	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FME	M	1	13	8,9,10	0.93	0	7,9,11	0.97	1 (14%)
12	FME	L	1	12	8,9,10	0.97	1 (12%)	7,9,11	0.83	0
34	SAC	i	1	34	7,8,9	1.86	1 (14%)	8,9,11	1.95	1 (12%)
1	FME	A	1	1	8,9,10	0.99	1 (12%)	7,9,11	0.73	0
10	FME	J	1	10	8,9,10	0.97	0	7,9,11	0.73	0
8	FME	H	1	8	8,9,10	0.97	0	7,9,11	0.92	0
14	FME	N	1	14	8,9,10	0.95	0	7,9,11	1.20	1 (14%)
4	2MR	D	85	4	10,12,13	2.66	4 (40%)	5,13,15	1.16	1 (20%)
43	AYA	r	1	43	6,7,8	1.79	1 (16%)	5,8,10	1.19	1 (20%)
24	AYA	Y	1	24	6,7,8	1.82	2 (33%)	5,8,10	1.28	1 (20%)
11	FME	K	1	11	8,9,10	0.92	0	7,9,11	0.82	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
13	FME	M	1	13	-	0/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
34	SAC	i	1	34	-	4/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
24	AYA	Y	1	24	-	0/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	1/7/9/11	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.14	1.44	1.33
4	D	85	2MR	CZ-NE	4.69	1.44	1.34
34	i	1	SAC	O-C	4.25	1.36	1.19
4	D	85	2MR	O-C	3.89	1.35	1.19
43	r	1	AYA	CT-N	3.27	1.45	1.34
24	Y	1	AYA	CT-N	3.25	1.45	1.34
1	A	1	FME	CA-N	-2.07	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.07	1.42	1.46
12	L	1	FME	CA-N	-2.04	1.43	1.46
24	Y	1	AYA	OT-CT	-2.03	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.63	112.65	124.78
4	D	85	2MR	NE-CZ-NH2	-2.30	117.37	119.48
24	Y	1	AYA	CM-CT-N	2.20	119.83	116.10
14	N	1	FME	C-CA-N	2.16	113.63	109.73
43	r	1	AYA	CM-CT-N	2.12	119.69	116.10
13	M	1	FME	C-CA-N	2.06	113.46	109.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CA-N-CN
10	J	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
12	L	1	FME	2	0
10	J	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 3 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	3PE	H	402	-	50,50,50	0.86	4 (8%)	53,55,55	0.93	2 (3%)
46	3PE	O	1201	-	46,46,50	0.90	4 (8%)	49,51,55	1.09	2 (4%)
45	LMT	h	1002	-	36,36,36	1.19	3 (8%)	47,47,47	1.20	3 (6%)
45	LMT	L	702	-	36,36,36	1.16	3 (8%)	47,47,47	0.87	1 (2%)
52	CDL	X	1701	-	67,67,99	1.05	7 (10%)	73,79,111	1.20	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	LMT	L	705	-	36,36,36	1.20	3 (8%)	47,47,47	1.36	7 (14%)
45	LMT	M	1303	-	36,36,36	1.24	4 (11%)	47,47,47	0.98	4 (8%)
46	3PE	L	701	-	48,48,50	0.86	2 (4%)	51,53,55	1.05	2 (3%)
46	3PE	Y	601	-	39,39,50	0.94	4 (10%)	42,44,55	1.05	2 (4%)
54	GTP	O	1202	55	30,34,34	3.05	11 (36%)	46,54,54	2.03	17 (36%)
58	EHZ	U	101	20	29,36,37	1.66	5 (17%)	35,44,47	1.54	3 (8%)
45	LMT	f	1901	-	36,36,36	1.19	4 (11%)	47,47,47	1.02	2 (4%)
46	3PE	N	502	-	40,40,50	0.95	4 (10%)	43,45,55	1.15	2 (4%)
48	PC1	B	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.13	2 (5%)
46	3PE	L	704	-	44,44,50	0.91	3 (6%)	47,49,55	1.06	3 (6%)
46	3PE	Y	604	-	28,28,50	1.12	4 (14%)	31,33,55	1.21	2 (6%)
47	SF4	I	201	9	0,12,12	-	-	-		
45	LMT	J	201	-	36,36,36	1.24	4 (11%)	47,47,47	1.24	7 (14%)
59	MYR	o	201	40	14,14,15	0.96	0	13,13,15	0.72	0
45	LMT	j	101	-	36,36,36	1.20	3 (8%)	47,47,47	0.79	0
45	LMT	N	501	-	36,36,36	1.19	3 (8%)	47,47,47	0.96	1 (2%)
45	LMT	A	301	-	36,36,36	1.20	2 (5%)	47,47,47	1.00	3 (6%)
47	SF4	F	502	6	0,12,12	-	-	-		
52	CDL	L	703	-	68,68,99	1.03	6 (8%)	74,80,111	1.12	4 (5%)
49	FES	E	301	5	0,4,4	-	-	-		
46	3PE	Y	603	-	34,34,50	1.04	4 (11%)	37,39,55	1.16	2 (5%)
50	FMN	F	501	-	33,33,33	1.10	1 (3%)	48,50,50	1.31	8 (16%)
46	3PE	M	1301	-	50,50,50	0.86	3 (6%)	53,55,55	1.11	2 (3%)
47	SF4	G	801	7	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
45	LMT	Y	602	-	36,36,36	1.18	3 (8%)	47,47,47	0.98	3 (6%)
53	I49	N	503	-	15,17,17	1.56	2 (13%)	21,22,22	1.72	4 (19%)
52	CDL	d	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.18	4 (5%)
46	3PE	A	302	-	41,41,50	0.92	4 (9%)	44,46,55	1.09	2 (4%)
46	3PE	H	403	-	33,33,50	1.36	3 (9%)	34,37,55	1.23	2 (5%)
49	FES	G	803	7	0,4,4	-	-	-		
45	LMT	H	401	-	36,36,36	1.22	2 (5%)	47,47,47	0.94	0
56	NDP	P	501	-	49,52,52	2.19	5 (10%)	66,80,80	1.57	13 (19%)
48	PC1	M	1302	-	48,48,53	1.00	4 (8%)	54,56,61	0.98	2 (3%)
47	SF4	I	202	9	0,12,12	-	-	-		
52	CDL	r	201	-	75,75,99	1.00	8 (10%)	81,87,111	1.11	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	EHZ	T	101	20	29,36,37	1.67	5 (17%)	35,44,47	1.48	6 (17%)
45	LMT	l	201	-	36,36,36	1.19	3 (8%)	47,47,47	0.87	1 (2%)
47	SF4	B	201	2	0,12,12	-	-	-		
52	CDL	h	1001	-	66,66,99	1.06	6 (9%)	72,78,111	1.24	4 (5%)
45	LMT	h	1003	-	36,36,36	1.17	3 (8%)	47,47,47	1.09	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	H	402	-	-	16/54/54/54	-
46	3PE	O	1201	-	-	26/50/50/54	-
45	LMT	h	1002	-	-	10/21/61/61	0/2/2/2
45	LMT	L	702	-	-	3/21/61/61	0/2/2/2
52	CDL	X	1701	-	-	32/78/78/110	-
45	LMT	L	705	-	-	7/21/61/61	0/2/2/2
45	LMT	M	1303	-	-	8/21/61/61	0/2/2/2
46	3PE	L	701	-	-	20/52/52/54	-
46	3PE	Y	601	-	-	15/43/43/54	-
54	GTP	O	1202	55	-	7/22/38/38	0/3/3/3
58	EHZ	U	101	20	-	4/42/44/45	-
45	LMT	f	1901	-	-	9/21/61/61	0/2/2/2
46	3PE	N	502	-	-	22/44/44/54	-
48	PC1	B	202	-	-	13/38/38/57	-
46	3PE	L	704	-	-	21/48/48/54	-
46	3PE	Y	604	-	-	12/32/32/54	-
47	SF4	I	201	9	-	-	0/6/5/5
45	LMT	J	201	-	-	7/21/61/61	0/2/2/2
59	MYR	o	201	40	-	4/11/12/13	-
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
45	LMT	N	501	-	-	7/21/61/61	0/2/2/2
45	LMT	A	301	-	-	10/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5
52	CDL	L	703	-	-	33/79/79/110	-
49	FES	E	301	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	Y	603	-	-	20/38/38/54	-
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
46	3PE	M	1301	-	-	20/54/54/54	-
47	SF4	G	801	7	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
45	LMT	Y	602	-	-	10/21/61/61	0/2/2/2
53	I49	N	503	-	-	3/10/10/10	0/1/1/1
52	CDL	d	201	-	-	31/75/75/110	-
46	3PE	A	302	-	-	26/45/45/54	-
46	3PE	H	403	-	-	17/36/36/54	-
49	FES	G	803	7	-	-	0/1/1/1
45	LMT	H	401	-	-	9/21/61/61	0/2/2/2
56	NDP	P	501	-	-	7/34/77/77	0/5/5/5
48	PC1	M	1302	-	-	16/52/52/57	-
47	SF4	I	202	9	-	-	0/6/5/5
52	CDL	r	201	-	-	37/86/86/110	-
58	EHZ	T	101	20	-	13/42/44/45	-
45	LMT	l	201	-	-	4/21/61/61	0/2/2/2
47	SF4	B	201	2	-	-	0/6/5/5
52	CDL	h	1001	-	-	32/77/77/110	-
45	LMT	h	1003	-	-	4/21/61/61	0/2/2/2

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.42	1.82	1.59
54	O	1202	GTP	O6-C6	8.58	1.39	1.23
54	O	1202	GTP	C5-N7	6.92	1.52	1.39
46	H	403	3PE	O21-C2	-5.30	1.40	1.46
58	U	101	EHZ	C15-N2	5.23	1.45	1.33
58	T	101	EHZ	C12-N1	5.17	1.45	1.33
58	T	101	EHZ	C15-N2	5.16	1.44	1.33
58	U	101	EHZ	C12-N1	4.92	1.44	1.33
53	N	503	I49	C15-N02	-4.85	1.30	1.37
54	O	1202	GTP	C2-N2	4.79	1.45	1.34
54	O	1202	GTP	C2-N1	4.72	1.49	1.37
54	O	1202	GTP	C2-N3	4.47	1.43	1.33
54	O	1202	GTP	C8-N9	-4.44	1.27	1.37
45	L	705	LMT	O5B-C1B	3.92	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	PN-O5D	3.63	1.74	1.59
45	H	401	LMT	O5B-C1B	3.62	1.51	1.41
54	O	1202	GTP	C4-N9	-3.61	1.28	1.38
50	F	501	FMN	C4A-N5	3.54	1.37	1.30
45	l	201	LMT	O5B-C1B	3.46	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.46	1.50	1.41
45	N	501	LMT	O5B-C1B	3.46	1.50	1.41
45	f	1901	LMT	O5B-C1B	3.46	1.50	1.41
45	Y	602	LMT	O5B-C1B	3.43	1.50	1.41
45	M	1303	LMT	O5B-C1B	3.43	1.50	1.41
45	j	101	LMT	O5B-C1B	3.42	1.50	1.41
45	J	201	LMT	O5B-C1B	3.41	1.50	1.41
45	M	1303	LMT	O5'-C1'	3.38	1.50	1.41
45	A	301	LMT	O5B-C1B	3.35	1.50	1.41
45	L	702	LMT	O5B-C1B	3.34	1.50	1.41
45	J	201	LMT	O5'-C1'	3.28	1.50	1.41
45	j	101	LMT	O5'-C1'	3.18	1.49	1.41
45	h	1003	LMT	O5B-C1B	3.11	1.49	1.41
45	A	301	LMT	O5'-C1'	3.11	1.49	1.41
53	N	503	I49	C14-N03	3.09	1.38	1.29
45	N	501	LMT	O5'-C1'	3.09	1.49	1.41
45	h	1002	LMT	O5'-C1'	3.08	1.49	1.41
56	P	501	NDP	O2B-C2B	-3.05	1.33	1.44
45	l	201	LMT	O5'-C1'	3.02	1.49	1.41
45	H	401	LMT	O5'-C1'	3.01	1.49	1.41
45	h	1003	LMT	O5'-C1'	3.00	1.49	1.41
45	f	1901	LMT	O5'-C1'	2.97	1.49	1.41
46	H	403	3PE	O21-C21	2.96	1.40	1.33
52	r	201	CDL	OB6-CB4	-2.81	1.39	1.46
45	L	702	LMT	O5'-C1'	2.81	1.49	1.41
45	Y	602	LMT	O5'-C1'	2.80	1.49	1.41
46	L	701	3PE	O21-C2	-2.80	1.39	1.46
52	L	703	CDL	OB6-CB4	-2.80	1.39	1.46
45	L	705	LMT	O5'-C1'	2.77	1.48	1.41
46	L	704	3PE	O21-C2	-2.77	1.39	1.46
48	M	1302	PC1	O21-C2	-2.74	1.39	1.46
52	L	703	CDL	OA6-CA4	-2.73	1.39	1.46
54	O	1202	GTP	O4'-C1'	2.73	1.48	1.42
52	r	201	CDL	OA6-CA4	-2.73	1.39	1.46
46	M	1301	3PE	O21-C2	-2.72	1.39	1.46
52	h	1001	CDL	OB6-CB4	-2.72	1.39	1.46
46	L	701	3PE	O31-C3	-2.70	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	h	1001	CDL	OB8-CB6	-2.67	1.39	1.45
52	d	201	CDL	OB6-CB4	-2.66	1.39	1.46
46	H	402	3PE	O31-C3	-2.63	1.39	1.45
52	h	1001	CDL	OA6-CA4	-2.61	1.40	1.46
52	X	1701	CDL	OA6-CA4	-2.60	1.40	1.46
52	d	201	CDL	OA6-CA4	-2.60	1.40	1.46
46	O	1201	3PE	O21-C2	-2.57	1.40	1.46
58	U	101	EHZ	O3-C12	-2.56	1.18	1.23
46	Y	604	3PE	O21-C2	-2.54	1.40	1.46
46	Y	603	3PE	O21-C2	-2.53	1.40	1.46
58	T	101	EHZ	O4-C15	-2.53	1.18	1.23
52	X	1701	CDL	OB6-CB4	-2.52	1.40	1.46
46	N	502	3PE	O21-C2	-2.49	1.40	1.46
46	Y	601	3PE	O21-C2	-2.49	1.40	1.46
48	B	202	PC1	O21-C2	-2.48	1.40	1.46
45	L	705	LMT	O5B-C5B	2.48	1.50	1.44
46	A	302	3PE	O31-C31	2.47	1.40	1.33
52	L	703	CDL	OB8-CB7	2.44	1.40	1.33
46	M	1301	3PE	O31-C3	-2.43	1.39	1.45
52	r	201	CDL	OA8-CA6	-2.43	1.39	1.45
46	H	402	3PE	O21-C2	-2.42	1.40	1.46
46	O	1201	3PE	O31-C31	2.42	1.40	1.33
52	X	1701	CDL	OA8-CA7	2.42	1.40	1.33
48	M	1302	PC1	O31-C3	-2.41	1.39	1.45
58	U	101	EHZ	O4-C15	-2.39	1.18	1.23
54	O	1202	GTP	PG-O2G	-2.39	1.45	1.54
52	d	201	CDL	OA8-CA6	-2.38	1.39	1.45
52	X	1701	CDL	OB8-CB7	2.37	1.40	1.33
54	O	1202	GTP	C2'-C3'	-2.37	1.46	1.53
52	d	201	CDL	OB8-CB7	2.35	1.40	1.33
58	T	101	EHZ	O3-C12	-2.34	1.18	1.23
54	O	1202	GTP	PG-O3G	-2.34	1.45	1.54
52	r	201	CDL	OB8-CB7	2.33	1.40	1.33
46	L	704	3PE	O31-C3	-2.33	1.39	1.45
46	Y	603	3PE	O31-C31	2.33	1.40	1.33
46	H	403	3PE	O31-C31	2.32	1.40	1.33
45	J	201	LMT	O5'-C5'	2.32	1.50	1.44
48	B	202	PC1	O21-C21	2.29	1.40	1.34
52	L	703	CDL	OA8-CA7	2.28	1.40	1.33
52	h	1001	CDL	OA8-CA7	2.27	1.40	1.33
46	O	1201	3PE	O31-C3	-2.26	1.40	1.45
46	N	502	3PE	O31-C31	2.25	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	502	3PE	O31-C3	-2.25	1.40	1.45
46	Y	604	3PE	O31-C31	2.24	1.39	1.33
48	B	202	PC1	O31-C31	2.24	1.39	1.33
52	r	201	CDL	OB8-CB6	-2.24	1.40	1.45
52	X	1701	CDL	OA8-CA6	-2.24	1.40	1.45
45	L	702	LMT	O5B-C5B	2.23	1.49	1.44
46	Y	601	3PE	O31-C31	2.23	1.39	1.33
45	h	1002	LMT	O5B-C5B	2.23	1.49	1.44
52	d	201	CDL	OB8-CB6	-2.22	1.40	1.45
46	O	1201	3PE	O21-C21	2.22	1.40	1.34
46	L	704	3PE	O31-C31	2.21	1.39	1.33
48	M	1302	PC1	O31-C31	2.21	1.39	1.33
46	Y	604	3PE	O31-C3	-2.21	1.40	1.45
46	Y	603	3PE	O31-C3	-2.20	1.40	1.45
46	M	1301	3PE	O31-C31	2.19	1.39	1.33
45	h	1003	LMT	O5'-C5'	2.18	1.49	1.44
45	Y	602	LMT	O5B-C5B	2.18	1.49	1.44
52	X	1701	CDL	OA6-CA5	2.18	1.40	1.34
52	d	201	CDL	OA8-CA7	2.17	1.39	1.33
52	L	703	CDL	OA8-CA6	-2.17	1.40	1.45
45	f	1901	LMT	O5'-C5'	2.16	1.49	1.44
45	J	201	LMT	O5B-C5B	2.16	1.49	1.44
45	N	501	LMT	O5B-C5B	2.15	1.49	1.44
46	H	402	3PE	O21-C21	2.14	1.40	1.34
46	N	502	3PE	O21-C21	2.14	1.40	1.34
46	A	302	3PE	O21-C2	-2.14	1.41	1.46
48	B	202	PC1	O31-C3	-2.14	1.40	1.45
46	Y	601	3PE	O31-C3	-2.13	1.40	1.45
58	U	101	EHZ	C9-S1	2.12	1.81	1.76
52	X	1701	CDL	OB8-CB6	-2.12	1.40	1.45
52	h	1001	CDL	OB8-CB7	2.12	1.39	1.33
45	M	1303	LMT	O5'-C5'	2.11	1.49	1.44
45	l	201	LMT	O5B-C5B	2.11	1.49	1.44
52	r	201	CDL	OA8-CA7	2.11	1.39	1.33
46	A	302	3PE	O21-C21	2.09	1.40	1.34
45	f	1901	LMT	O5B-C5B	2.08	1.49	1.44
46	H	402	3PE	O31-C31	2.07	1.39	1.33
52	d	201	CDL	OA6-CA5	2.07	1.40	1.34
48	M	1302	PC1	O21-C21	2.06	1.40	1.34
46	A	302	3PE	O31-C3	-2.05	1.40	1.45
52	r	201	CDL	OA6-CA5	2.05	1.40	1.34
56	P	501	NDP	C2A-N1A	2.04	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	601	3PE	O21-C21	2.04	1.40	1.34
45	M	1303	LMT	O5B-C5B	2.04	1.49	1.44
46	Y	604	3PE	O21-C21	2.04	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.04	1.40	1.34
46	Y	603	3PE	O21-C21	2.03	1.40	1.34
52	L	703	CDL	OB8-CB6	-2.03	1.40	1.45
52	d	201	CDL	OB6-CB5	2.03	1.40	1.34
56	P	501	NDP	O3D-C3D	-2.02	1.38	1.43
58	T	101	EHZ	O6-C20	-2.02	1.39	1.44
52	r	201	CDL	OB6-CB5	2.01	1.40	1.34
45	j	101	LMT	O5B-C5B	2.01	1.49	1.44

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	1202	GTP	C8-N9-C4	7.38	120.11	106.05
56	P	501	NDP	PN-O3-PA	-6.62	110.12	132.83
58	U	101	EHZ	C8-C9-S1	6.36	121.50	113.63
58	T	101	EHZ	C8-C9-S1	5.63	120.59	113.63
46	H	403	3PE	O21-C21-O22	-4.92	119.31	125.57
52	X	1701	CDL	OB6-CB5-C51	4.62	121.45	111.50
52	h	1001	CDL	OB6-CB5-C51	4.58	121.38	111.50
53	N	503	I49	N01-C14-N03	4.49	128.67	120.26
52	d	201	CDL	OA6-CA5-C11	4.35	120.87	111.50
48	B	202	PC1	O21-C21-C22	4.27	120.70	111.50
46	Y	604	3PE	O21-C21-C22	4.25	120.66	111.50
45	J	201	LMT	O5'-C5'-C4'	4.23	118.67	109.75
52	X	1701	CDL	OA6-CA5-C11	4.20	120.56	111.50
46	Y	603	3PE	O21-C21-C22	4.11	120.35	111.50
46	N	502	3PE	O21-C21-C22	4.10	120.35	111.50
46	O	1201	3PE	O21-C21-C22	4.01	120.15	111.50
45	h	1003	LMT	O5'-C5'-C4'	3.96	118.10	109.75
46	A	302	3PE	O21-C21-C22	3.85	119.79	111.50
46	M	1301	3PE	O21-C21-C22	3.85	119.79	111.50
52	h	1001	CDL	OA6-CA5-C11	3.79	119.68	111.50
52	r	201	CDL	OB6-CB5-C51	3.77	119.62	111.50
45	L	705	LMT	O5B-C5B-C4B	3.66	116.33	109.69
48	M	1302	PC1	O21-C21-C22	3.64	119.34	111.50
52	L	703	CDL	OB6-CB5-C51	3.63	119.33	111.50
52	L	703	CDL	OA6-CA5-C11	3.63	119.32	111.50
46	Y	601	3PE	O21-C21-C22	3.60	119.26	111.50
56	P	501	NDP	O2B-P2B-O1X	-3.51	95.84	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	r	201	CDL	OA6-CA5-C11	3.49	119.03	111.50
45	f	1901	LMT	O5'-C5'-C4'	3.43	116.99	109.75
50	F	501	FMN	C4-N3-C2	-3.32	119.50	125.64
52	d	201	CDL	OB6-CB5-C51	3.32	120.05	110.80
46	L	701	3PE	O21-C21-C22	3.31	118.64	111.50
45	L	705	LMT	C1B-O5B-C5B	3.30	120.16	113.69
54	O	1202	GTP	C2-N1-C6	-3.22	119.22	125.10
46	L	704	3PE	O21-C21-C22	3.13	118.24	111.50
45	h	1002	LMT	C1'-C2'-C3'	3.09	116.44	110.00
52	h	1001	CDL	OA8-CA7-C31	3.09	121.59	111.91
46	H	402	3PE	O21-C21-C22	3.07	118.11	111.50
46	H	403	3PE	O31-C31-C32	3.03	121.42	111.91
52	d	201	CDL	OA8-CA7-C31	3.00	121.32	111.91
54	O	1202	GTP	O2G-PG-O3B	2.98	114.62	104.64
52	X	1701	CDL	OB8-CB7-C71	2.97	121.22	111.91
46	O	1201	3PE	O31-C31-C32	2.94	121.13	111.91
54	O	1202	GTP	O3G-PG-O3B	2.93	114.45	104.64
54	O	1202	GTP	C3'-C2'-C1'	2.91	106.95	101.43
50	F	501	FMN	C4A-C10-N10	2.88	120.69	116.48
52	L	703	CDL	OA8-CA7-C31	2.84	120.82	111.91
53	N	503	I49	N05-C15-N04	-2.81	111.60	120.26
52	h	1001	CDL	OB8-CB7-C71	2.80	120.70	111.91
45	A	301	LMT	C1B-O5B-C5B	-2.80	108.19	113.69
56	P	501	NDP	PA-O5B-C5B	-2.79	105.31	121.68
45	L	705	LMT	C1'-O5'-C5'	-2.79	108.22	113.69
52	X	1701	CDL	OA8-CA7-C31	2.79	120.65	111.91
46	Y	603	3PE	O31-C31-C32	2.78	120.64	111.91
45	L	705	LMT	C2'-C3'-C4'	2.78	116.03	109.68
46	N	502	3PE	O31-C31-C32	2.78	120.63	111.91
54	O	1202	GTP	PB-O3B-PG	-2.77	123.31	132.83
50	F	501	FMN	C4A-C4-N3	2.77	120.21	113.19
45	A	301	LMT	O1B-C4'-C3'	2.76	114.63	107.28
46	L	704	3PE	O31-C31-C32	2.76	120.56	111.91
52	r	201	CDL	OA8-CA7-C31	2.74	120.50	111.91
58	T	101	EHZ	O2-C9-S1	-2.71	119.09	122.61
48	B	202	PC1	O31-C31-C32	2.67	120.30	111.91
45	J	201	LMT	C1'-O5'-C5'	2.67	118.93	113.69
46	M	1301	3PE	O31-C31-C32	2.63	120.17	111.91
46	Y	604	3PE	O31-C31-C32	2.62	120.13	111.91
54	O	1202	GTP	PA-O3A-PB	-2.61	123.89	132.83
58	T	101	EHZ	C13-C12-N1	2.60	120.81	116.42
46	Y	601	3PE	O31-C31-C32	2.59	120.03	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	O	1202	GTP	C5-C6-N1	2.59	119.76	113.19
52	d	201	CDL	OB8-CB7-C71	2.58	120.02	111.91
50	F	501	FMN	O4-C4-C4A	-2.57	119.78	126.60
48	M	1302	PC1	O31-C31-C32	2.57	119.96	111.91
52	L	703	CDL	OB8-CB7-C71	2.56	119.93	111.91
54	O	1202	GTP	C2'-C3'-C4'	2.55	107.60	102.64
45	L	705	LMT	C1'-C2'-C3'	2.54	115.29	110.00
56	P	501	NDP	N3A-C4A-N9A	2.54	131.26	127.08
56	P	501	NDP	O3X-P2B-O2X	2.51	117.24	107.64
54	O	1202	GTP	O2A-PA-O1A	-2.51	99.84	112.24
54	O	1202	GTP	C1'-N9-C8	-2.49	119.60	126.70
54	O	1202	GTP	O6-C6-C5	-2.49	120.00	126.60
45	h	1002	LMT	C2'-C3'-C4'	2.48	115.35	109.68
52	r	201	CDL	OB8-CB7-C71	2.47	119.64	111.91
45	h	1002	LMT	C1-O1'-C1'	2.47	117.93	113.84
58	U	101	EHZ	O2-C9-S1	-2.45	119.43	122.61
45	L	705	LMT	O5B-C1B-C2B	2.45	115.53	110.35
45	f	1901	LMT	C3'-C4'-C5'	2.44	116.52	110.93
56	P	501	NDP	PN-O5D-C5D	-2.42	107.50	121.68
45	J	201	LMT	O5B-C5B-C4B	2.38	114.01	109.69
45	L	705	LMT	C6B-C5B-C4B	-2.38	107.43	113.00
56	P	501	NDP	C2A-N1A-C6A	-2.37	114.69	118.77
46	L	701	3PE	O31-C31-C32	2.36	119.30	111.91
58	U	101	EHZ	C13-C12-N1	2.35	120.37	116.42
46	A	302	3PE	O31-C31-C32	2.35	119.27	111.91
45	J	201	LMT	C3B-C4B-C5B	2.33	114.40	110.24
45	h	1003	LMT	C1B-O1B-C4'	-2.33	112.21	117.96
45	Y	602	LMT	C1'-C2'-C3'	2.31	114.80	110.00
50	F	501	FMN	C10-C4A-N5	-2.29	120.00	124.86
45	L	702	LMT	C1B-O1B-C4'	-2.28	112.32	117.96
45	A	301	LMT	C1'-O5'-C5'	-2.28	109.21	113.69
56	P	501	NDP	O5D-PN-O1N	-2.27	100.18	109.07
53	N	503	I49	C14-N02-C15	-2.26	121.44	125.21
56	P	501	NDP	O2N-PN-O1N	2.24	123.33	112.24
56	P	501	NDP	C5A-C4A-N3A	-2.24	123.83	126.75
54	O	1202	GTP	O2B-PB-O1B	-2.24	101.17	112.24
54	O	1202	GTP	N9-C8-N7	-2.22	109.22	113.39
45	J	201	LMT	C1-O1'-C1'	2.21	117.51	113.84
54	O	1202	GTP	C5-C4-N9	-2.20	101.64	105.63
46	H	402	3PE	O31-C31-C32	2.19	118.79	111.91
50	F	501	FMN	C4A-C10-N1	-2.17	119.68	124.73
58	T	101	EHZ	C13-C14-N2	-2.17	107.52	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	Y	602	LMT	C2'-C3'-C4'	2.13	114.55	109.68
56	P	501	NDP	O4B-C4B-C3B	2.13	109.32	105.11
45	M	1303	LMT	O5'-C5'-C4'	2.11	114.21	109.75
58	T	101	EHZ	C19-C17-C16	2.11	112.48	108.82
45	l	201	LMT	C1B-O1B-C4'	-2.10	112.76	117.96
45	J	201	LMT	C3'-C4'-C5'	2.10	115.74	110.93
58	T	101	EHZ	C16-C15-N2	2.09	120.74	116.58
54	O	1202	GTP	C1'-N9-C4	-2.09	120.29	126.50
56	P	501	NDP	O7N-C7N-N7N	-2.09	117.99	122.88
50	F	501	FMN	C5'-C4'-C3'	-2.07	108.21	112.20
45	M	1303	LMT	O5B-C5B-C4B	2.06	113.43	109.69
56	P	501	NDP	C2B-C1B-N9A	-2.06	110.07	113.53
45	M	1303	LMT	C1'-O5'-C5'	2.05	117.72	113.69
45	N	501	LMT	O1B-C4'-C3'	2.05	112.72	107.28
53	N	503	I49	C09-C07-C10	2.04	121.39	118.54
45	M	1303	LMT	C3B-C4B-C5B	2.03	113.86	110.24
54	O	1202	GTP	C6-C5-N7	2.03	134.02	130.25
50	F	501	FMN	C9A-C5A-N5	-2.01	120.25	122.43
45	J	201	LMT	C1B-O1B-C4'	-2.01	112.99	117.96
46	L	704	3PE	C23-C22-C21	-2.01	106.32	113.62
45	Y	602	LMT	C1-O1'-C1'	2.01	117.17	113.84

There are no chirality outliers.

All (546) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	J	201	LMT	C2-C1-O1'-C1'
45	h	1003	LMT	C2-C1-O1'-C1'
46	A	302	3PE	C1-O11-P-O12
46	A	302	3PE	C1-O11-P-O14
46	A	302	3PE	C11-O13-P-O14
46	A	302	3PE	O13-C11-C12-N
46	A	302	3PE	O21-C2-C3-O31
46	A	302	3PE	C1-C2-O21-C21
46	A	302	3PE	O22-C21-O21-C2
46	A	302	3PE	C22-C21-O21-C2
46	H	402	3PE	C11-O13-P-O14
46	H	403	3PE	C2-C1-O11-P
46	H	403	3PE	O13-C11-C12-N
46	H	403	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
46	H	403	3PE	O22-C21-O21-C2
46	L	704	3PE	C11-O13-P-O12
46	M	1301	3PE	O13-C11-C12-N
46	N	502	3PE	O13-C11-C12-N
46	O	1201	3PE	C22-C21-O21-C2
46	Y	601	3PE	O13-C11-C12-N
46	Y	603	3PE	C11-O13-P-O11
46	Y	603	3PE	C11-O13-P-O12
46	Y	603	3PE	C11-O13-P-O14
46	Y	603	3PE	C22-C21-O21-C2
46	Y	604	3PE	C1-O11-P-O13
46	Y	604	3PE	O22-C21-O21-C2
52	L	703	CDL	CA2-OA2-PA1-OA3
52	X	1701	CDL	OA7-CA5-OA6-CA4
52	X	1701	CDL	CB2-OB2-PB2-OB3
52	X	1701	CDL	OB6-CB4-CB6-OB8
52	d	201	CDL	CA3-OA5-PA1-OA2
52	d	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	CA3-OA5-PA1-OA4
52	d	201	CDL	C11-CA5-OA6-CA4
52	d	201	CDL	C51-CB5-OB6-CB4
52	h	1001	CDL	CA2-C1-CB2-OB2
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CA3-OA5-PA1-OA4
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB2-OB2-PB2-OB5
52	r	201	CDL	CB3-OB5-PB2-OB3
53	N	503	I49	C07-C06-C08-N01
53	N	503	I49	N01-C14-N02-C15
53	N	503	I49	N03-C14-N02-C15
54	O	1202	GTP	PB-O3B-PG-O2G
54	O	1202	GTP	C5'-O5'-PA-O3A
54	O	1202	GTP	C5'-O5'-PA-O2A
56	P	501	NDP	C2B-O2B-P2B-O1X
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-C17
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	O4-C15-C16-C17
58	U	101	EHZ	C5-C6-C7-C8
45	M	1303	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C3'-C4'-O1B-C1B
46	O	1201	3PE	O32-C31-O31-C3
52	X	1701	CDL	OB9-CB7-OB8-CB6
45	L	705	LMT	O5B-C1B-O1B-C4'
45	f	1901	LMT	O5B-C1B-O1B-C4'
46	O	1201	3PE	C32-C31-O31-C3
52	X	1701	CDL	C71-CB7-OB8-CB6
46	M	1301	3PE	O32-C31-O31-C3
46	Y	604	3PE	O32-C31-O31-C3
52	X	1701	CDL	OA9-CA7-OA8-CA6
52	d	201	CDL	OB9-CB7-OB8-CB6
45	M	1303	LMT	C2B-C1B-O1B-C4'
46	Y	603	3PE	O22-C21-O21-C2
52	d	201	CDL	OB7-CB5-OB6-CB4
46	Y	604	3PE	C32-C31-O31-C3
52	X	1701	CDL	C31-CA7-OA8-CA6
46	Y	604	3PE	C22-C21-O21-C2
52	X	1701	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C51-CB5-OB6-CB4
45	Y	602	LMT	O5B-C5B-C6B-O6B
45	J	201	LMT	C4B-C5B-C6B-O6B
45	N	501	LMT	C3'-C4'-O1B-C1B
46	M	1301	3PE	C32-C31-O31-C3
46	N	502	3PE	C32-C31-O31-C3
52	d	201	CDL	C71-CB7-OB8-CB6
46	O	1201	3PE	O22-C21-O21-C2
52	d	201	CDL	OA7-CA5-OA6-CA4
52	r	201	CDL	OA7-CA5-OA6-CA4
46	Y	603	3PE	O32-C31-O31-C3
52	h	1001	CDL	OB9-CB7-OB8-CB6
52	h	1001	CDL	O1-C1-CB2-OB2
46	Y	603	3PE	C32-C31-O31-C3
52	h	1001	CDL	C71-CB7-OB8-CB6
45	N	501	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	O5'-C5'-C6'-O6'
46	L	701	3PE	C22-C21-O21-C2
45	A	301	LMT	O5B-C5B-C6B-O6B
45	A	301	LMT	O5'-C5'-C6'-O6'
45	f	1901	LMT	O5'-C5'-C6'-O6'
45	Y	602	LMT	O5'-C5'-C6'-O6'
56	P	501	NDP	O4B-C4B-C5B-O5B
56	P	501	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
56	P	501	NDP	C3D-C4D-C5D-O5D
45	Y	602	LMT	C4B-C5B-C6B-O6B
48	M	1302	PC1	C2-C1-O11-P
45	h	1003	LMT	C2-C3-C4-C5
45	N	501	LMT	C4'-C5'-C6'-O6'
45	J	201	LMT	O5B-C5B-C6B-O6B
46	N	502	3PE	O32-C31-O31-C3
45	H	401	LMT	O5'-C1'-O1'-C1
45	J	201	LMT	O5'-C1'-O1'-C1
46	L	704	3PE	C32-C31-O31-C3
52	L	703	CDL	CB2-C1-CA2-OA2
46	L	701	3PE	O22-C21-O21-C2
46	L	704	3PE	O32-C31-O31-C3
45	H	401	LMT	C3'-C4'-O1B-C1B
48	B	202	PC1	C32-C31-O31-C3
48	M	1302	PC1	C32-C31-O31-C3
45	M	1303	LMT	C3'-C4'-O1B-C1B
52	L	703	CDL	O1-C1-CA2-OA2
45	f	1901	LMT	C2'-C1'-O1'-C1
48	B	202	PC1	O32-C31-O31-C3
48	M	1302	PC1	O32-C31-O31-C3
45	f	1901	LMT	C2B-C1B-O1B-C4'
46	L	701	3PE	C32-C31-O31-C3
52	X	1701	CDL	CA7-C31-C32-C33
48	B	202	PC1	C21-C22-C23-C24
45	N	501	LMT	O1'-C1-C2-C3
45	L	705	LMT	O5'-C5'-C6'-O6'
46	H	402	3PE	C21-C22-C23-C24
46	L	701	3PE	C31-C32-C33-C34
52	h	1001	CDL	CB5-C51-C52-C53
45	J	201	LMT	O5B-C1B-O1B-C4'
45	Y	602	LMT	C4'-C5'-C6'-O6'
46	H	402	3PE	C26-C27-C28-C29
45	J	201	LMT	C2B-C1B-O1B-C4'
45	A	301	LMT	C2-C3-C4-C5
52	X	1701	CDL	O1-C1-CB2-OB2
45	A	301	LMT	C4'-C5'-C6'-O6'
45	A	301	LMT	C4B-C5B-C6B-O6B
45	M	1303	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	O32-C31-O31-C3
46	A	302	3PE	C1-O11-P-O13
46	A	302	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	H	402	3PE	C11-O13-P-O11
46	L	704	3PE	C1-O11-P-O13
46	L	704	3PE	C11-O13-P-O11
52	L	703	CDL	CA2-OA2-PA1-OA5
52	d	201	CDL	CA2-OA2-PA1-OA5
46	L	701	3PE	C21-C22-C23-C24
45	h	1002	LMT	C4'-C5'-C6'-O6'
45	M	1303	LMT	C5'-C4'-O1B-C1B
52	X	1701	CDL	CA2-C1-CB2-OB2
45	j	101	LMT	O5'-C5'-C6'-O6'
52	r	201	CDL	C13-C14-C15-C16
52	L	703	CDL	C51-CB5-OB6-CB4
45	h	1002	LMT	C4-C5-C6-C7
45	j	101	LMT	C5-C6-C7-C8
46	L	704	3PE	C38-C39-C3A-C3B
46	O	1201	3PE	C34-C35-C36-C37
52	h	1001	CDL	C22-C23-C24-C25
52	r	201	CDL	C38-C39-C40-C41
45	L	702	LMT	C11-C10-C9-C8
48	B	202	PC1	C24-C25-C26-C27
52	L	703	CDL	OB7-CB5-OB6-CB4
46	O	1201	3PE	C21-C22-C23-C24
52	X	1701	CDL	CB5-C51-C52-C53
46	M	1301	3PE	C2D-C2E-C2F-C2G
48	M	1302	PC1	C2C-C2D-C2E-C2F
46	H	403	3PE	C3D-C3E-C3F-C3G
52	X	1701	CDL	C15-C16-C17-C18
52	r	201	CDL	C71-C72-C73-C74
46	M	1301	3PE	C35-C36-C37-C38
45	L	705	LMT	C2'-C1'-O1'-C1
46	A	302	3PE	C2A-C2B-C2C-C2D
52	L	703	CDL	C54-C55-C56-C57
52	X	1701	CDL	C57-C58-C59-C60
45	h	1003	LMT	C4-C5-C6-C7
46	H	403	3PE	C33-C34-C35-C36
52	X	1701	CDL	C51-C52-C53-C54
52	h	1001	CDL	C71-C72-C73-C74
58	T	101	EHZ	C3-C4-C5-C6
48	M	1302	PC1	C23-C24-C25-C26
52	X	1701	CDL	C55-C56-C57-C58
52	h	1001	CDL	C31-C32-C33-C34
52	r	201	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	C57-C58-C59-C60
46	A	302	3PE	C28-C29-C2A-C2B
46	H	402	3PE	C3A-C3B-C3C-C3D
48	M	1302	PC1	C26-C27-C28-C29
52	L	703	CDL	C35-C36-C37-C38
52	h	1001	CDL	C12-C13-C14-C15
46	A	302	3PE	C21-C22-C23-C24
52	X	1701	CDL	CA5-C11-C12-C13
45	N	501	LMT	C5-C6-C7-C8
46	H	403	3PE	C32-C33-C34-C35
46	H	403	3PE	C35-C36-C37-C38
46	O	1201	3PE	C33-C34-C35-C36
52	X	1701	CDL	C71-C72-C73-C74
52	X	1701	CDL	C73-C74-C75-C76
45	L	705	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
46	L	701	3PE	C2B-C2C-C2D-C2E
46	L	704	3PE	C3A-C3B-C3C-C3D
46	M	1301	3PE	C3D-C3E-C3F-C3G
46	Y	601	3PE	C23-C24-C25-C26
52	L	703	CDL	C12-C13-C14-C15
59	o	201	MYR	C11-C10-C9-C8
46	Y	604	3PE	O13-C11-C12-N
48	M	1302	PC1	C39-C3A-C3B-C3C
52	h	1001	CDL	C31-CA7-OA8-CA6
45	H	401	LMT	C7-C8-C9-C10
46	H	402	3PE	C33-C34-C35-C36
59	o	201	MYR	C2-C3-C4-C5
45	M	1303	LMT	C2-C1-O1'-C1'
46	M	1301	3PE	C27-C28-C29-C2A
52	X	1701	CDL	C11-C12-C13-C14
46	M	1301	3PE	C1-C2-C3-O31
52	r	201	CDL	CB3-CB4-CB6-OB8
48	M	1302	PC1	C2A-C2B-C2C-C2D
46	H	403	3PE	C32-C31-O31-C3
45	H	401	LMT	C3-C4-C5-C6
48	M	1302	PC1	C32-C33-C34-C35
46	A	302	3PE	C32-C33-C34-C35
46	L	701	3PE	C22-C23-C24-C25
48	M	1302	PC1	C2E-C2F-C2G-C2H
59	o	201	MYR	C4-C5-C6-C7
46	N	502	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
46	A	302	3PE	C26-C27-C28-C29
52	h	1001	CDL	C72-C73-C74-C75
58	T	101	EHZ	C21-C1-C2-C3
45	H	401	LMT	C4'-C5'-C6'-O6'
52	r	201	CDL	C37-C38-C39-C40
52	d	201	CDL	CA5-C11-C12-C13
45	j	101	LMT	C1-C2-C3-C4
46	Y	604	3PE	C32-C33-C34-C35
52	X	1701	CDL	C20-C21-C22-C23
46	Y	604	3PE	C21-C22-C23-C24
46	H	403	3PE	O32-C31-O31-C3
52	h	1001	CDL	OA9-CA7-OA8-CA6
46	N	502	3PE	C35-C36-C37-C38
46	N	502	3PE	O22-C21-O21-C2
46	L	701	3PE	C2A-C2B-C2C-C2D
46	N	502	3PE	C32-C33-C34-C35
45	M	1303	LMT	O5'-C5'-C6'-O6'
45	l	201	LMT	C4-C5-C6-C7
52	r	201	CDL	C59-C60-C61-C62
46	L	704	3PE	C22-C21-O21-C2
46	N	502	3PE	C22-C21-O21-C2
48	B	202	PC1	C22-C21-O21-C2
46	N	502	3PE	C29-C2A-C2B-C2C
48	M	1302	PC1	C36-C37-C38-C39
48	M	1302	PC1	O21-C2-C3-O31
46	A	302	3PE	C2C-C2D-C2E-C2F
52	h	1001	CDL	C15-C16-C17-C18
48	M	1302	PC1	C29-C2A-C2B-C2C
58	T	101	EHZ	C1-C2-C3-C4
46	L	704	3PE	O22-C21-O21-C2
46	M	1301	3PE	C33-C34-C35-C36
45	f	1901	LMT	C1-C2-C3-C4
46	N	502	3PE	C11-O13-P-O11
46	O	1201	3PE	C1-O11-P-O13
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	L	703	CDL	C52-C53-C54-C55
45	J	201	LMT	O5'-C5'-C6'-O6'
52	L	703	CDL	OB5-CB3-CB4-CB6
45	h	1002	LMT	C5'-C4'-O1B-C1B
46	Y	601	3PE	C2A-C2B-C2C-C2D
46	M	1301	3PE	C3C-C3D-C3E-C3F
46	L	701	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	C33-C34-C35-C36
46	M	1301	3PE	C23-C24-C25-C26
52	d	201	CDL	C38-C39-C40-C41
46	H	402	3PE	C35-C36-C37-C38
46	L	701	3PE	C1-C2-C3-O31
52	r	201	CDL	CA3-CA4-CA6-OA8
45	h	1002	LMT	O5B-C5B-C6B-O6B
58	U	101	EHZ	C1-C2-C3-C4
45	L	702	LMT	C4-C5-C6-C7
46	Y	603	3PE	C32-C33-C34-C35
45	f	1901	LMT	O5'-C1'-O1'-C1
58	T	101	EHZ	O4-C15-C16-O5
45	L	705	LMT	C2B-C1B-O1B-C4'
58	U	101	EHZ	C1-C21-C22-C23
46	L	704	3PE	C31-C32-C33-C34
46	L	701	3PE	C25-C26-C27-C28
46	A	302	3PE	C39-C3A-C3B-C3C
45	N	501	LMT	O5B-C5B-C6B-O6B
58	U	101	EHZ	C5-C6-C7-O1
46	O	1201	3PE	C3A-C3B-C3C-C3D
52	r	201	CDL	C35-C36-C37-C38
46	H	402	3PE	C32-C31-O31-C3
46	Y	601	3PE	C33-C34-C35-C36
45	h	1002	LMT	C3'-C4'-O1B-C1B
45	h	1002	LMT	O5B-C1B-O1B-C4'
46	H	402	3PE	C3B-C3C-C3D-C3E
52	L	703	CDL	C34-C35-C36-C37
52	d	201	CDL	C76-C77-C78-C79
52	r	201	CDL	C71-CB7-OB8-CB6
46	L	704	3PE	O11-C1-C2-O21
48	M	1302	PC1	C34-C35-C36-C37
52	L	703	CDL	C71-C72-C73-C74
46	Y	603	3PE	C34-C35-C36-C37
52	X	1701	CDL	C19-C20-C21-C22
46	O	1201	3PE	O21-C2-C3-O31
52	r	201	CDL	OB6-CB4-CB6-OB8
46	L	701	3PE	C33-C34-C35-C36
46	O	1201	3PE	C3C-C3D-C3E-C3F
46	Y	601	3PE	C26-C27-C28-C29
52	d	201	CDL	C74-C75-C76-C77
46	Y	601	3PE	C32-C33-C34-C35
52	r	201	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
46	H	402	3PE	C2A-C2B-C2C-C2D
46	H	403	3PE	C3C-C3D-C3E-C3F
46	L	704	3PE	C25-C26-C27-C28
48	B	202	PC1	C32-C33-C34-C35
56	P	501	NDP	PN-O3-PA-O1A
48	B	202	PC1	O22-C21-O21-C2
52	r	201	CDL	C15-C16-C17-C18
52	L	703	CDL	CB5-C51-C52-C53
46	L	704	3PE	O11-C1-C2-C3
46	N	502	3PE	O11-C1-C2-C3
52	h	1001	CDL	OA5-CA3-CA4-CA6
45	f	1901	LMT	O5B-C5B-C6B-O6B
52	r	201	CDL	CA5-C11-C12-C13
46	H	402	3PE	O32-C31-O31-C3
45	H	401	LMT	C5'-C4'-O1B-C1B
46	H	402	3PE	C23-C24-C25-C26
46	H	402	3PE	C32-C33-C34-C35
45	Y	602	LMT	C2-C1-O1'-C1'
52	X	1701	CDL	C17-C18-C19-C20
52	L	703	CDL	C31-CA7-OA8-CA6
48	B	202	PC1	C1-C2-C3-O31
48	M	1302	PC1	C1-C2-C3-O31
52	L	703	CDL	CB3-CB4-CB6-OB8
46	O	1201	3PE	C35-C36-C37-C38
46	M	1301	3PE	C3A-C3B-C3C-C3D
52	L	703	CDL	C32-C33-C34-C35
46	L	701	3PE	C39-C3A-C3B-C3C
52	X	1701	CDL	CB2-OB2-PB2-OB5
46	N	502	3PE	O11-C1-C2-O21
52	L	703	CDL	OB5-CB3-CB4-OB6
52	h	1001	CDL	OA5-CA3-CA4-OA6
52	r	201	CDL	OB9-CB7-OB8-CB6
52	L	703	CDL	C60-C61-C62-C63
52	d	201	CDL	C39-C40-C41-C42
46	L	701	3PE	O21-C2-C3-O31
48	B	202	PC1	O21-C2-C3-O31
46	M	1301	3PE	C29-C2A-C2B-C2C
46	O	1201	3PE	C28-C29-C2A-C2B
59	o	201	MYR	C9-C10-C11-C12
48	B	202	PC1	C2-C1-O11-P
46	M	1301	3PE	C25-C26-C27-C28
46	N	502	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C27-C28-C29-C2A
52	L	703	CDL	C55-C56-C57-C58
46	Y	603	3PE	O11-C1-C2-C3
56	P	501	NDP	O4D-C1D-N1N-C6N
52	r	201	CDL	C31-CA7-OA8-CA6
46	Y	604	3PE	C31-C32-C33-C34
45	l	201	LMT	O1'-C1-C2-C3
45	h	1003	LMT	C4'-C5'-C6'-O6'
46	N	502	3PE	C33-C34-C35-C36
58	T	101	EHZ	C12-C13-C14-N2
46	A	302	3PE	C1-C2-C3-O31
52	X	1701	CDL	CB3-CB4-CB6-OB8
52	r	201	CDL	C33-C34-C35-C36
52	X	1701	CDL	CB2-C1-CA2-OA2
52	X	1701	CDL	O1-C1-CA2-OA2
58	T	101	EHZ	O1-C7-C8-C9
52	L	703	CDL	OA9-CA7-OA8-CA6
46	L	704	3PE	C22-C23-C24-C25
46	H	403	3PE	C31-C32-C33-C34
45	M	1303	LMT	C9-C10-C11-C12
45	H	401	LMT	O5B-C5B-C6B-O6B
46	O	1201	3PE	C26-C27-C28-C29
45	A	301	LMT	O1'-C1-C2-C3
45	j	101	LMT	O1'-C1-C2-C3
46	H	402	3PE	C2C-C2D-C2E-C2F
46	Y	601	3PE	C1-O11-P-O13
52	d	201	CDL	C31-C32-C33-C34
46	N	502	3PE	C31-C32-C33-C34
52	r	201	CDL	OA9-CA7-OA8-CA6
46	H	403	3PE	C11-O13-P-O14
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C1-O11-P-O14
46	N	502	3PE	C11-O13-P-O12
46	O	1201	3PE	C1-O11-P-O14
46	Y	601	3PE	C1-O11-P-O12
46	Y	601	3PE	C1-O11-P-O14
52	d	201	CDL	CA2-OA2-PA1-OA3
52	d	201	CDL	CA2-OA2-PA1-OA4
52	h	1001	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CB2-OB2-PB2-OB4
54	O	1202	GTP	C5'-O5'-PA-O1A
52	d	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	OA5-CA3-CA4-CA6
58	T	101	EHZ	C4-C5-C6-C7
45	l	201	LMT	C1-C2-C3-C4
46	M	1301	3PE	C12-C11-O13-P
46	Y	603	3PE	C12-C11-O13-P
52	L	703	CDL	CA7-C31-C32-C33
46	Y	603	3PE	O11-C1-C2-O21
52	d	201	CDL	OA5-CA3-CA4-OA6
45	L	705	LMT	C4B-C5B-C6B-O6B
52	X	1701	CDL	C52-C51-CB5-OB6
45	N	501	LMT	C5'-C4'-O1B-C1B
52	r	201	CDL	C56-C57-C58-C59
45	f	1901	LMT	C4'-C5'-C6'-O6'
46	O	1201	3PE	C1-C2-C3-O31
46	Y	603	3PE	C1-C2-C3-O31
52	X	1701	CDL	CA3-CA4-CA6-OA8
46	M	1301	3PE	O21-C2-C3-O31
46	Y	603	3PE	O21-C2-C3-O31
52	L	703	CDL	OB6-CB4-CB6-OB8
52	h	1001	CDL	OA6-CA4-CA6-OA8
52	r	201	CDL	OA6-CA4-CA6-OA8
46	L	704	3PE	C34-C35-C36-C37
46	L	701	3PE	C2E-C2F-C2G-C2H
46	A	302	3PE	C27-C28-C29-C2A
45	Y	602	LMT	C1-C2-C3-C4
45	f	1901	LMT	C5-C6-C7-C8
52	h	1001	CDL	C33-C34-C35-C36
46	O	1201	3PE	C25-C26-C27-C28
46	H	403	3PE	O31-C31-C32-C33
45	H	401	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	C6-C7-C8-C9
46	O	1201	3PE	C39-C3A-C3B-C3C
46	N	502	3PE	C28-C29-C2A-C2B
45	l	201	LMT	C5-C6-C7-C8
52	h	1001	CDL	C16-C17-C18-C19
46	Y	601	3PE	C28-C29-C2A-C2B
52	X	1701	CDL	OA6-CA4-CA6-OA8
46	Y	603	3PE	C37-C38-C39-C3A
46	Y	603	3PE	C1-O11-P-O13
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	r	201	CDL	CA3-OA5-PA1-OA2
48	M	1302	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
52	X	1701	CDL	C74-C75-C76-C77
46	Y	604	3PE	C33-C34-C35-C36
46	H	403	3PE	C1-C2-C3-O31
46	A	302	3PE	C2B-C2C-C2D-C2E
46	H	402	3PE	C31-C32-C33-C34
46	Y	601	3PE	C2C-C2D-C2E-C2F
50	F	501	FMN	C4'-C5'-O5'-P
46	L	704	3PE	O21-C21-C22-C23
46	O	1201	3PE	O13-C11-C12-N
45	h	1002	LMT	C2B-C1B-O1B-C4'
45	Y	602	LMT	C2'-C1'-O1'-C1
46	A	302	3PE	C23-C24-C25-C26
52	L	703	CDL	CB4-CB3-OB5-PB2
54	O	1202	GTP	C4'-C5'-O5'-PA
52	L	703	CDL	OA7-CA5-OA6-CA4
46	Y	603	3PE	C3B-C3C-C3D-C3E
46	N	502	3PE	C26-C27-C28-C29
52	h	1001	CDL	CA3-CA4-CA6-OA8
45	Y	602	LMT	O5'-C1'-O1'-C1
52	h	1001	CDL	CA6-CA4-OA6-CA5
46	H	403	3PE	C11-O13-P-O11
46	Y	601	3PE	O21-C21-C22-C23
52	X	1701	CDL	CB4-CB3-OB5-PB2
45	j	101	LMT	O5B-C1B-O1B-C4'
46	L	701	3PE	C35-C36-C37-C38
45	Y	602	LMT	C3'-C4'-O1B-C1B
48	B	202	PC1	C33-C34-C35-C36
46	O	1201	3PE	C32-C33-C34-C35
45	j	101	LMT	O5'-C1'-O1'-C1
45	Y	602	LMT	C5'-C4'-O1B-C1B
54	O	1202	GTP	PG-O3B-PB-O1B
52	L	703	CDL	C38-C39-C40-C41
46	M	1301	3PE	C2F-C2G-C2H-C2I
45	j	101	LMT	C2B-C1B-O1B-C4'
52	r	201	CDL	C14-C15-C16-C17
45	L	705	LMT	C4'-C5'-C6'-O6'
46	M	1301	3PE	C22-C23-C24-C25
52	d	201	CDL	OB5-CB3-CB4-OB6
52	r	201	CDL	OB5-CB3-CB4-OB6
45	A	301	LMT	C1-C2-C3-C4
52	r	201	CDL	C52-C53-C54-C55
52	r	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	O13-C11-C12-N
46	Y	603	3PE	O13-C11-C12-N
46	O	1201	3PE	C2B-C2C-C2D-C2E
46	L	704	3PE	C29-C2A-C2B-C2C
46	L	704	3PE	C28-C29-C2A-C2B
46	Y	601	3PE	C2F-C2G-C2H-C2I
54	O	1202	GTP	PB-O3B-PG-O1G
46	O	1201	3PE	O21-C21-C22-C23
46	N	502	3PE	O21-C21-C22-C23
52	h	1001	CDL	CA3-CA4-OA6-CA5
46	H	402	3PE	C25-C26-C27-C28
52	d	201	CDL	C41-C42-C43-C44
52	r	201	CDL	C11-C12-C13-C14
46	N	502	3PE	O31-C31-C32-C33
48	B	202	PC1	O21-C21-C22-C23
46	A	302	3PE	O31-C31-C32-C33
52	d	201	CDL	C72-C71-CB7-OB8
45	j	101	LMT	C4-C5-C6-C7
52	d	201	CDL	OB5-CB3-CB4-CB6
52	r	201	CDL	C72-C71-CB7-OB8
46	A	302	3PE	O21-C21-C22-C23
52	d	201	CDL	C71-C72-C73-C74
52	r	201	CDL	C52-C51-CB5-OB6
46	A	302	3PE	C33-C34-C35-C36
46	Y	604	3PE	C22-C23-C24-C25
56	P	501	NDP	PN-O3-PA-O2A
52	L	703	CDL	C11-CA5-OA6-CA4
48	B	202	PC1	O22-C21-C22-C23
52	h	1001	CDL	C19-C20-C21-C22
46	H	403	3PE	C3A-C3B-C3C-C3D
52	d	201	CDL	C35-C36-C37-C38
46	L	704	3PE	C39-C3A-C3B-C3C
46	A	302	3PE	O32-C31-C32-C33
46	O	1201	3PE	O22-C21-C22-C23
52	d	201	CDL	CA3-CA4-CA6-OA8
52	L	703	CDL	CA4-CA3-OA5-PA1
46	A	302	3PE	O22-C21-C22-C23
46	Y	601	3PE	O32-C31-O31-C3
46	L	701	3PE	C1-O11-P-O14
46	M	1301	3PE	C1-O11-P-O14
46	N	502	3PE	C11-O13-P-O14
46	O	1201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
52	L	703	CDL	CA3-OA5-PA1-OA3
52	L	703	CDL	CB2-OB2-PB2-OB3
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	r	201	CDL	CA2-OA2-PA1-OA3
52	r	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	C72-C71-CB7-OB9
46	Y	604	3PE	O31-C31-C32-C33
46	N	502	3PE	O22-C21-C22-C23
46	O	1201	3PE	C38-C39-C3A-C3B
52	L	703	CDL	C32-C31-CA7-OA8
46	Y	603	3PE	C39-C3A-C3B-C3C
46	Y	603	3PE	C3A-C3B-C3C-C3D
46	Y	601	3PE	C12-C11-O13-P
52	d	201	CDL	C40-C41-C42-C43
52	r	201	CDL	C72-C71-CB7-OB9
50	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C5-C6-C7-O1
45	L	702	LMT	C2-C1-O1'-C1'
45	j	101	LMT	C2-C1-O1'-C1'
52	h	1001	CDL	C32-C31-CA7-OA8
46	O	1201	3PE	C2A-C2B-C2C-C2D
52	r	201	CDL	C52-C51-CB5-OB7
52	L	703	CDL	C32-C31-CA7-OA9
45	H	401	LMT	C5-C6-C7-C8
46	M	1301	3PE	C26-C27-C28-C29
52	L	703	CDL	C72-C71-CB7-OB8

There are no ring outliers.

21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	H	402	3PE	1	0
46	O	1201	3PE	1	0
45	h	1002	LMT	2	0
45	L	705	LMT	1	0
45	M	1303	LMT	2	0
54	O	1202	GTP	2	0
59	o	201	MYR	2	0
45	j	101	LMT	2	0
45	N	501	LMT	3	0
45	A	301	LMT	3	0
47	F	502	SF4	1	0

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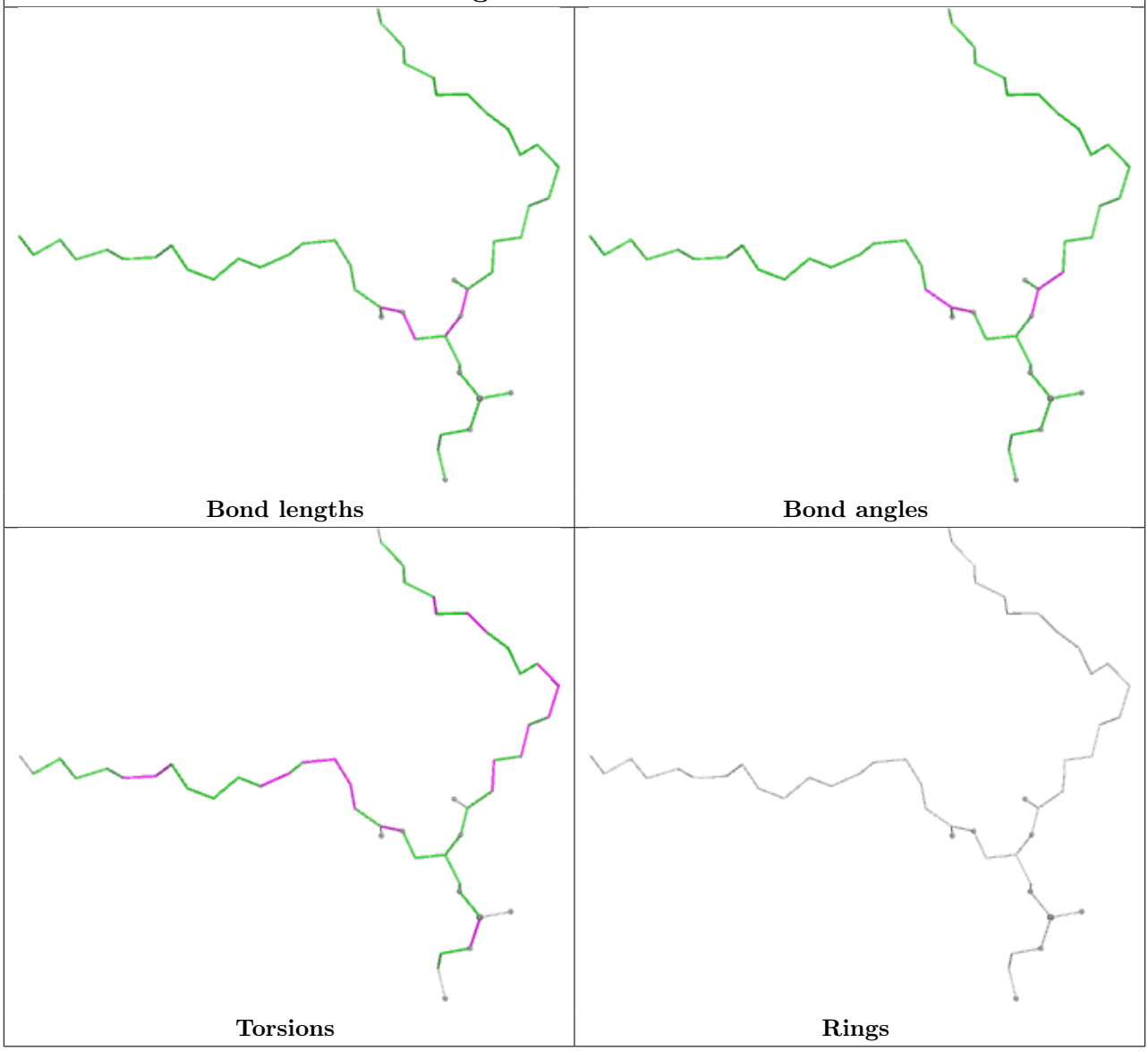
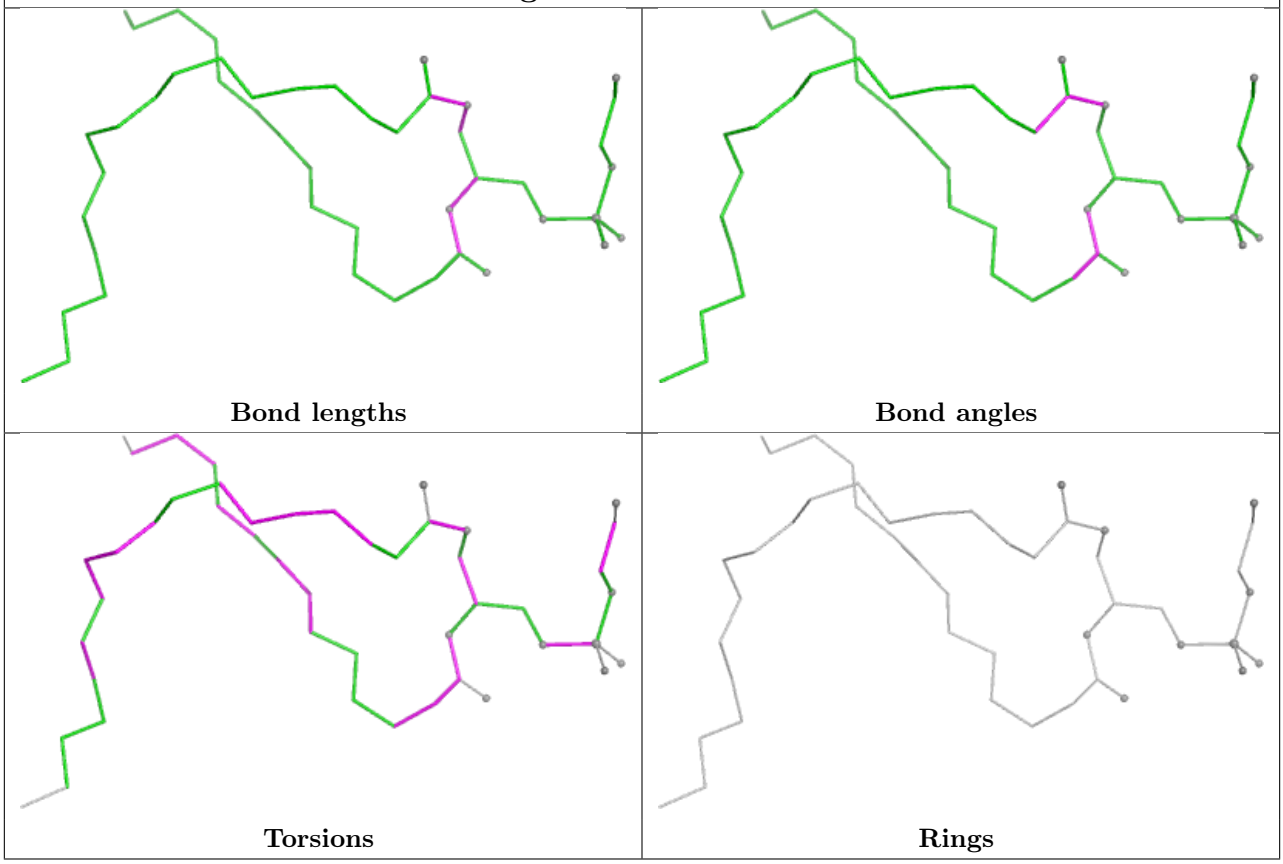
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	L	703	CDL	1	0
46	M	1301	3PE	5	0
47	G	802	SF4	1	0
45	Y	602	LMT	2	0
53	N	503	I49	1	0
46	A	302	3PE	1	0
48	M	1302	PC1	1	0
47	I	202	SF4	1	0
52	h	1001	CDL	2	0
45	h	1003	LMT	1	0

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

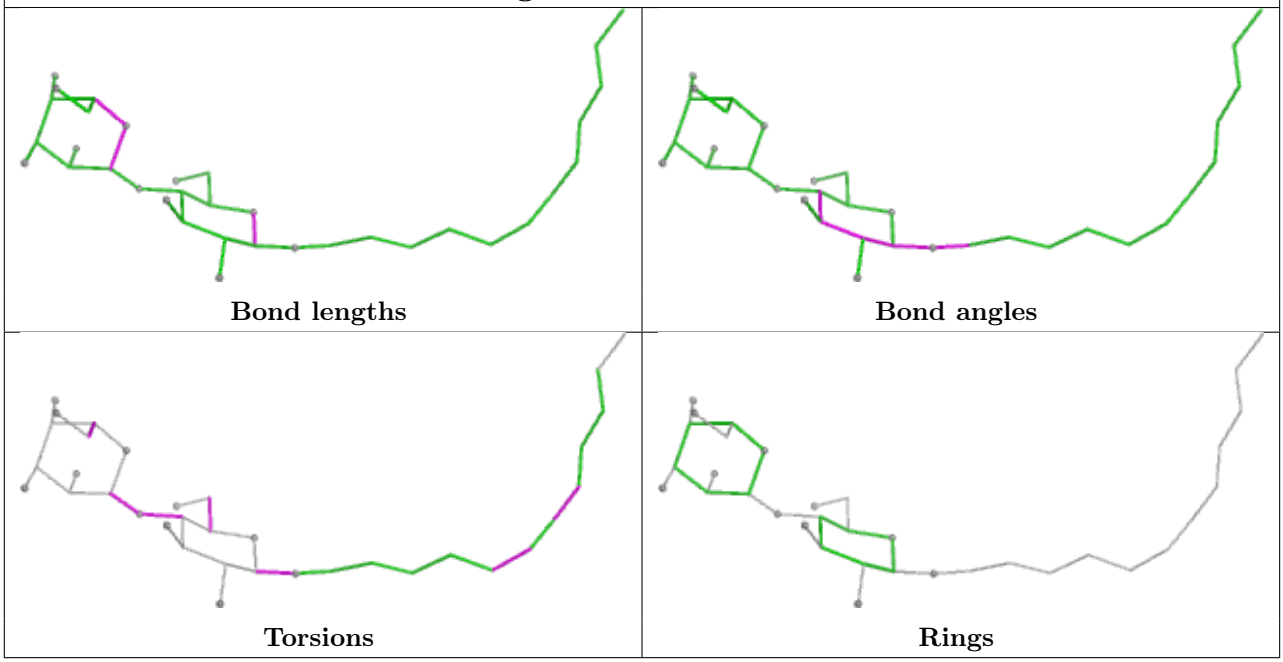
Ligand 3PE H 402



Ligand 3PE O 1201



Ligand LMT h 1002



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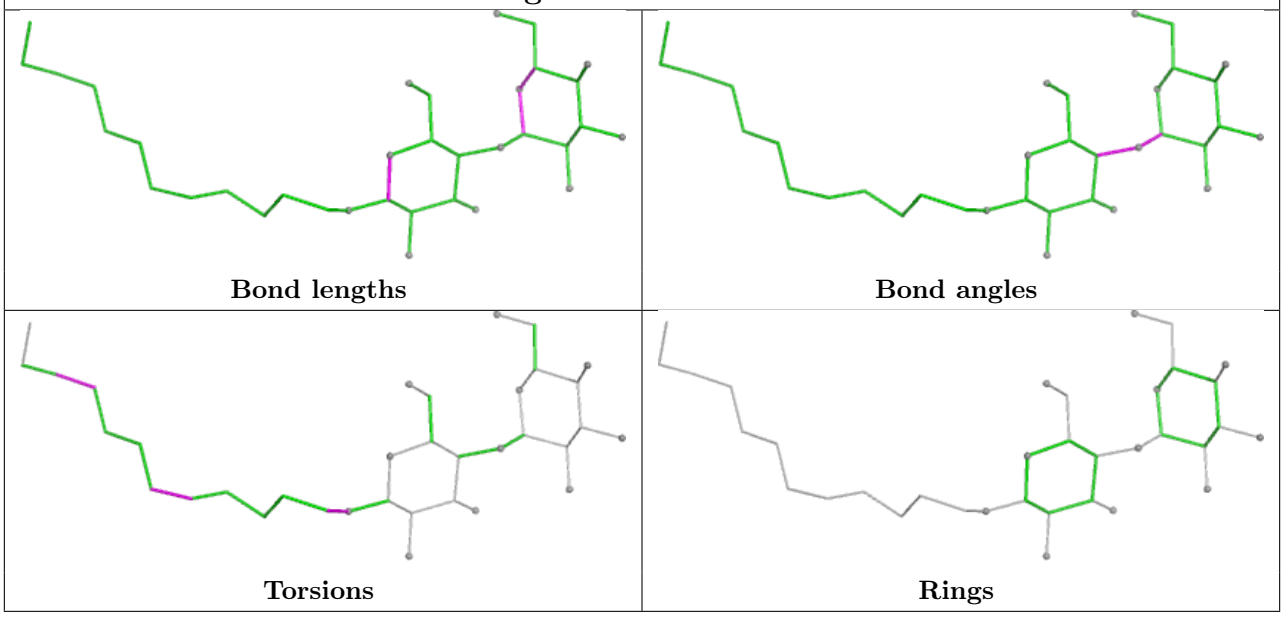
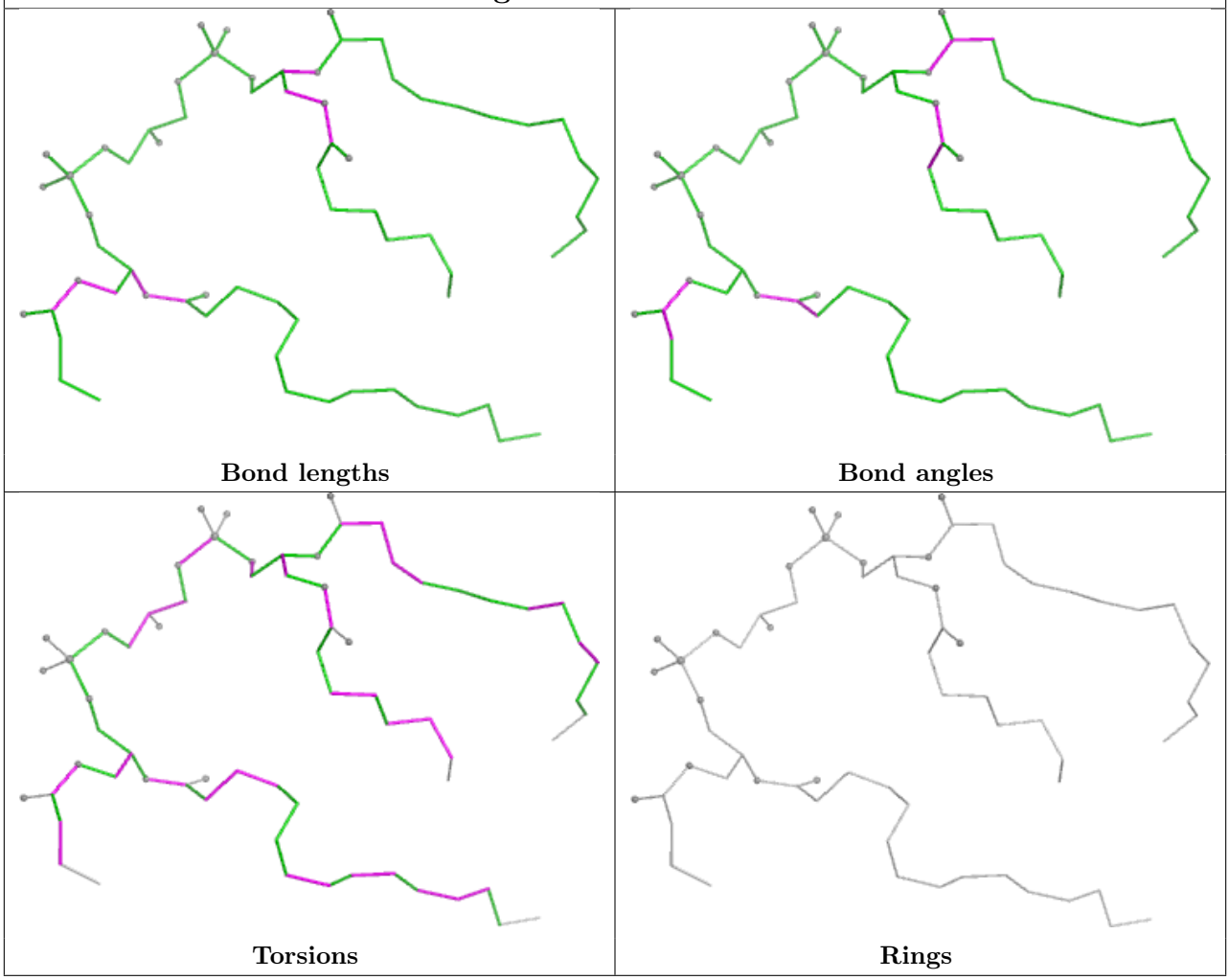


Ligand CDL X 1701



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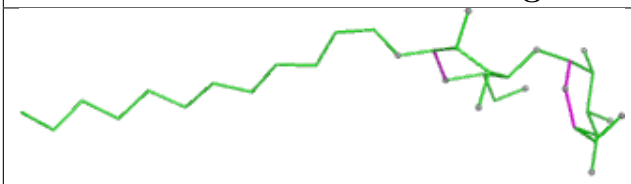
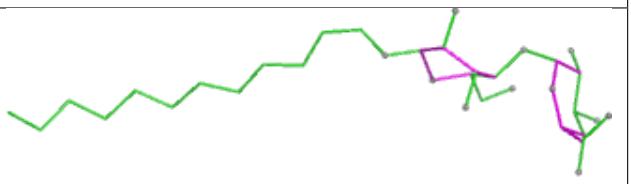
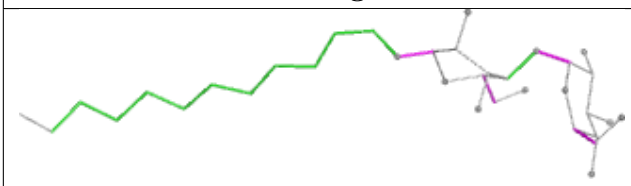
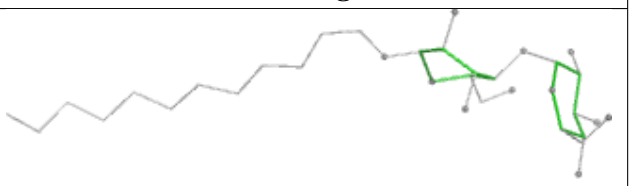
 Bond lengths	 Bond angles
 Torsions	 Rings

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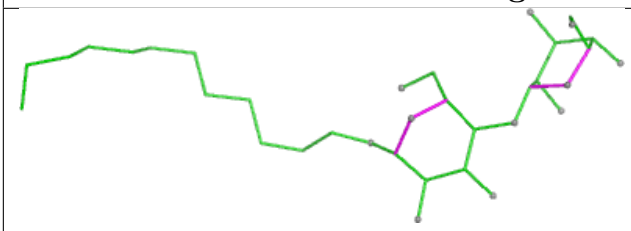
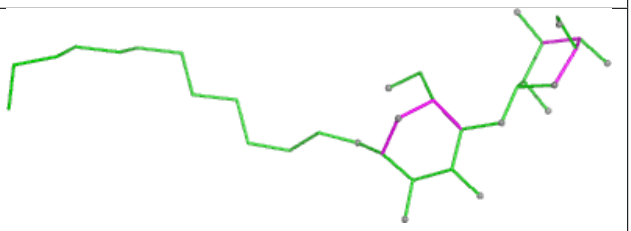
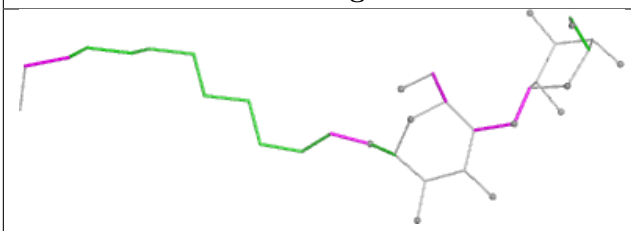
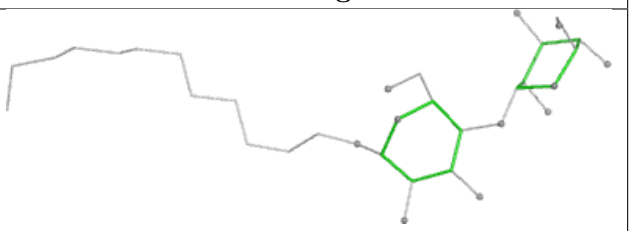
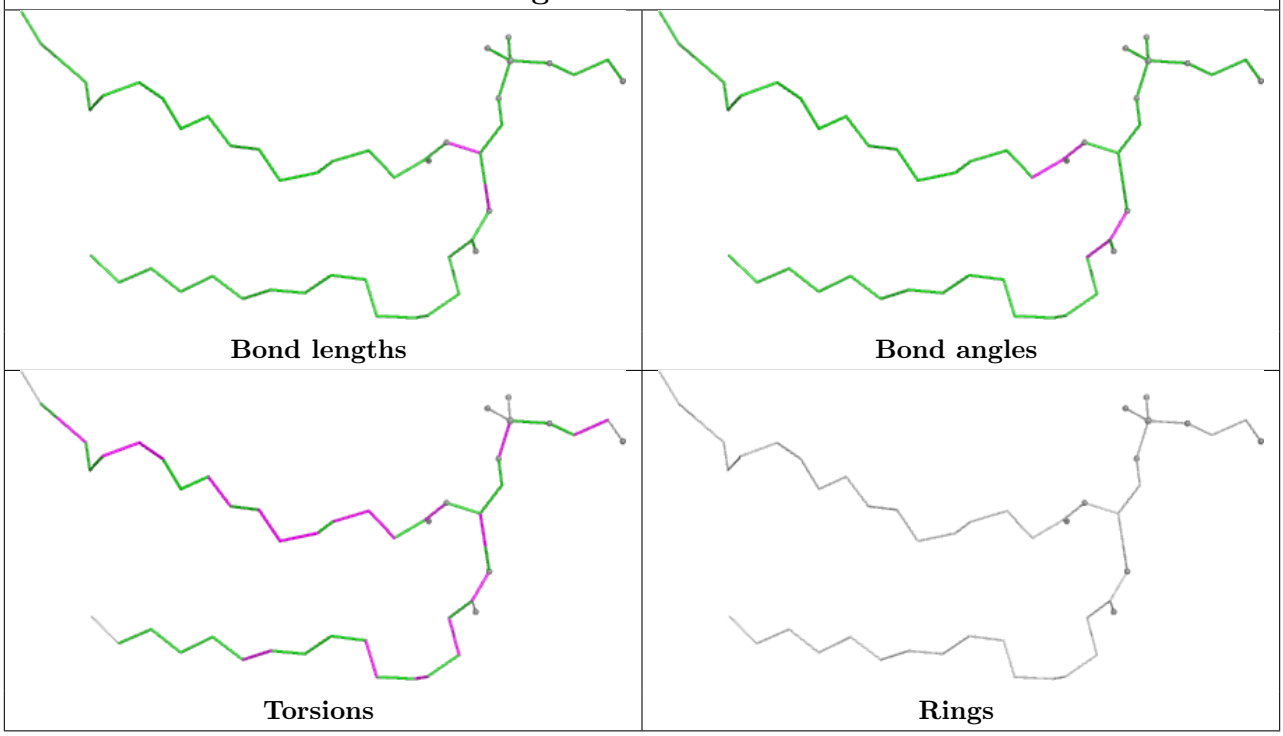
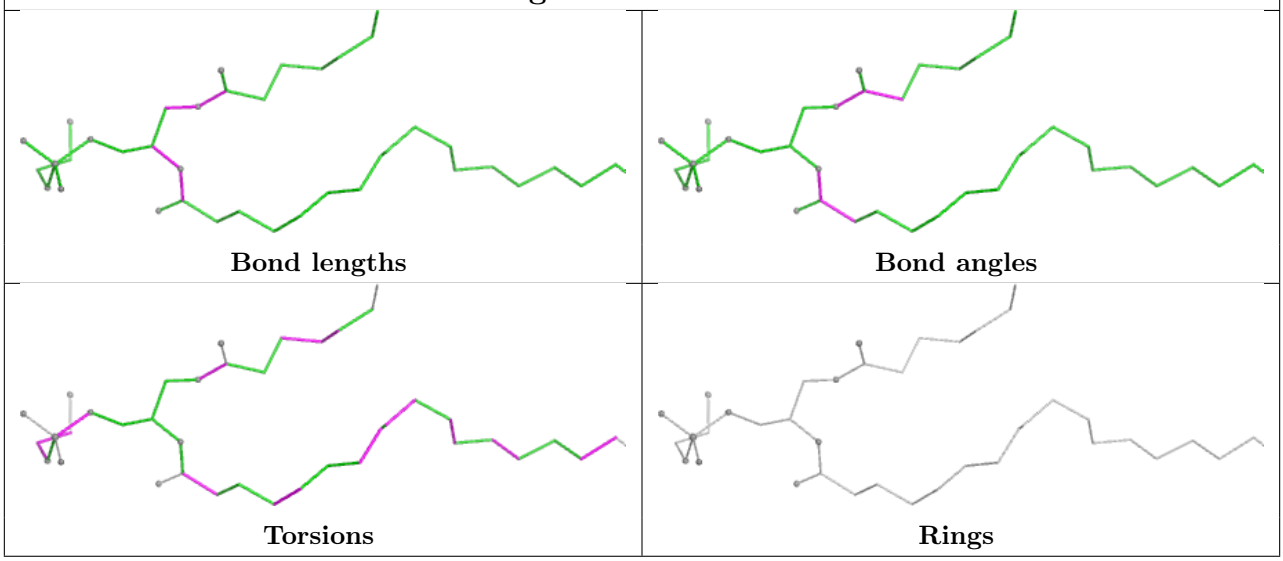
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE L 701



Ligand 3PE Y 601



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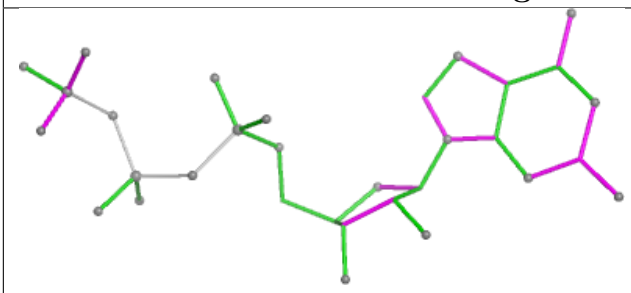
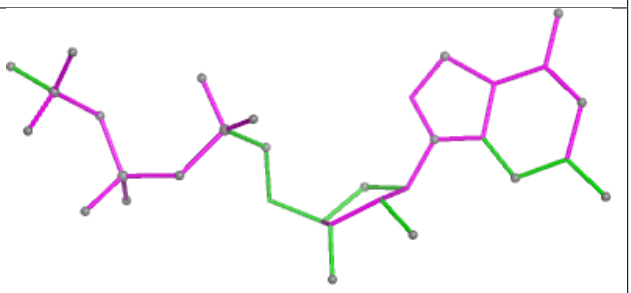
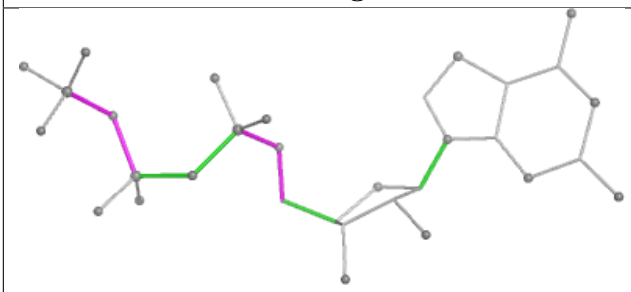
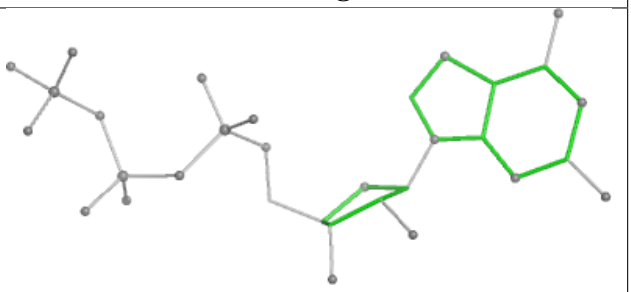
 Bond lengths	 Bond angles
 Torsions	 Rings

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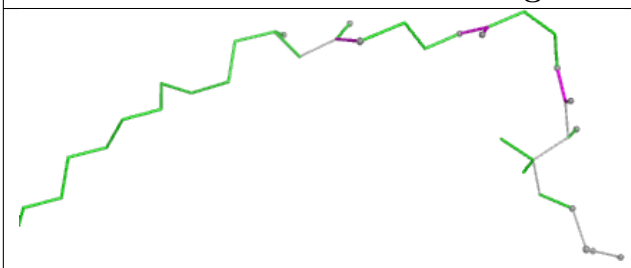
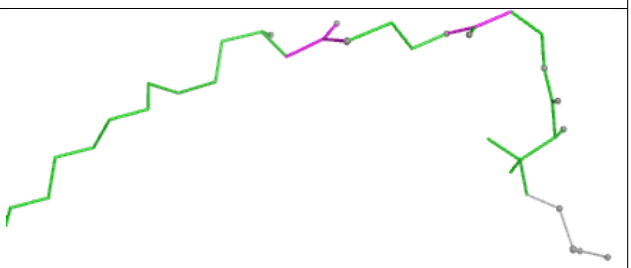
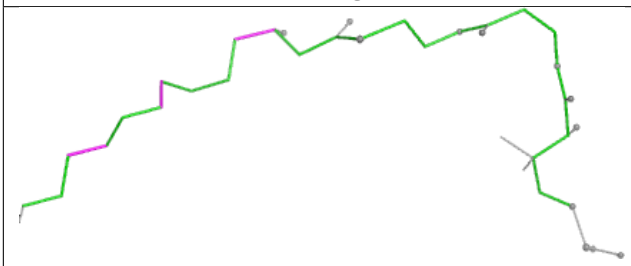
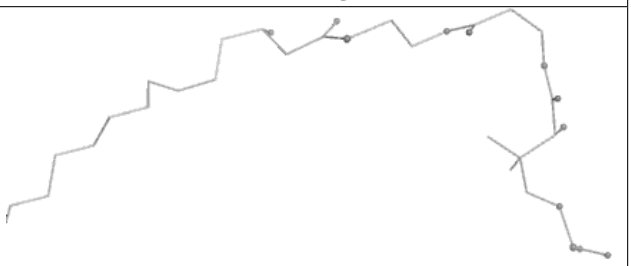
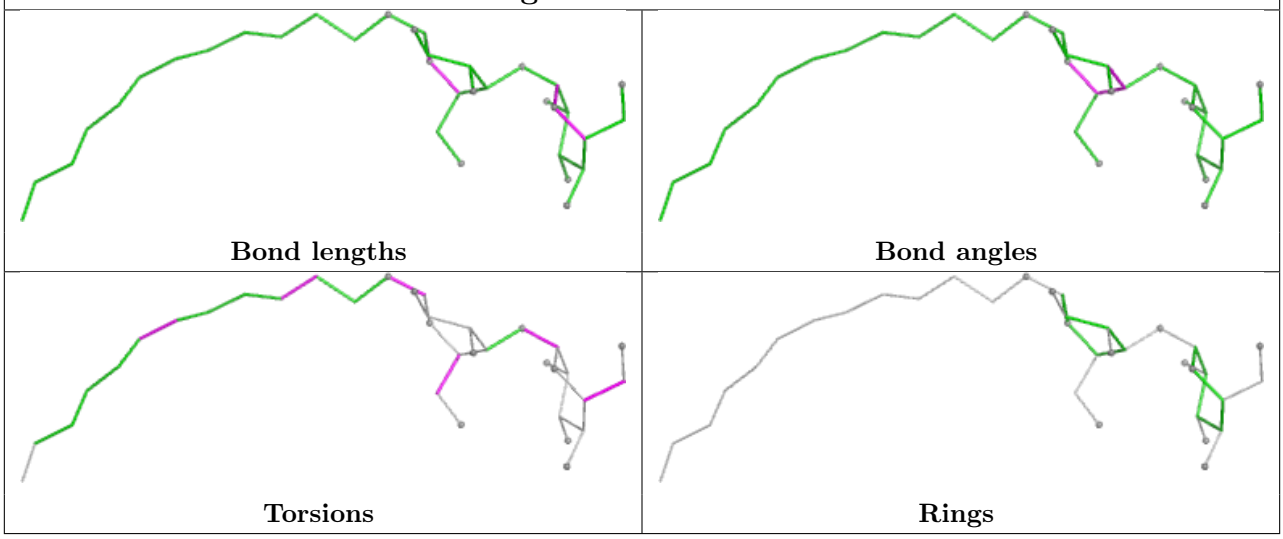
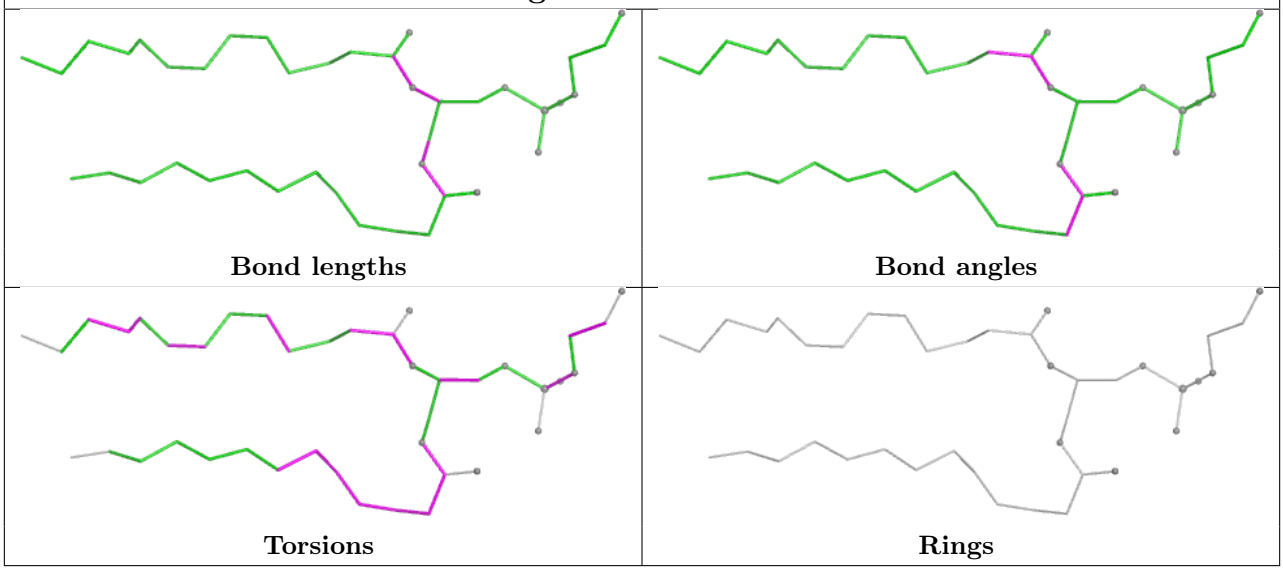
 Bond lengths	 Bond angles
 Torsions	 Rings

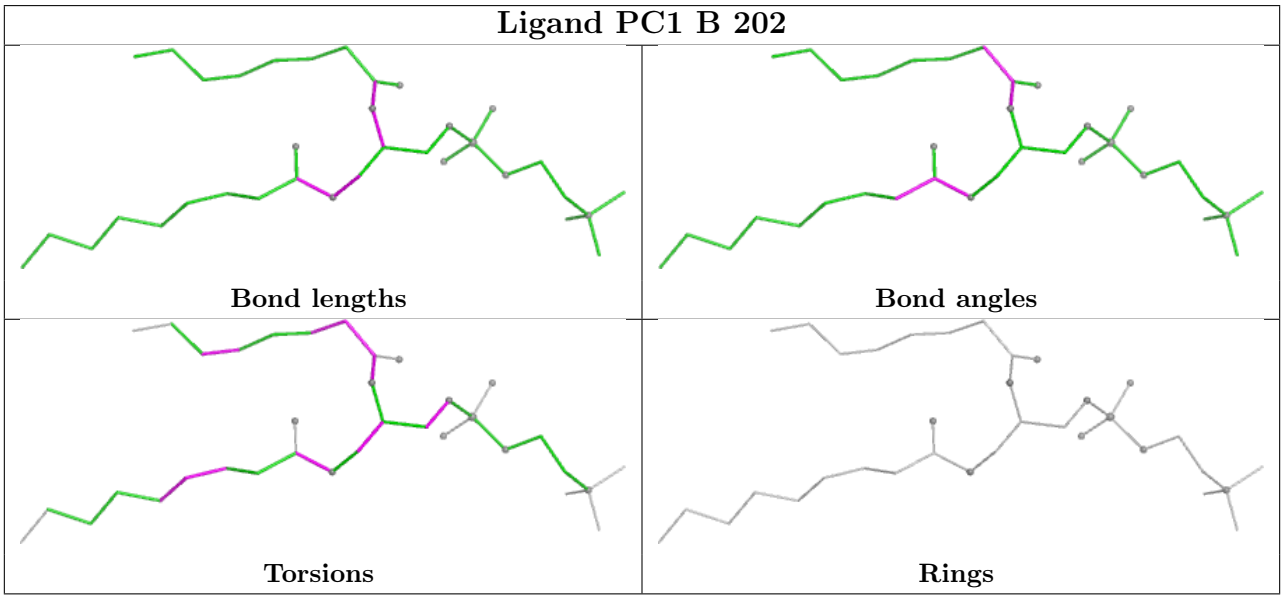
Ligand LMT f 1901



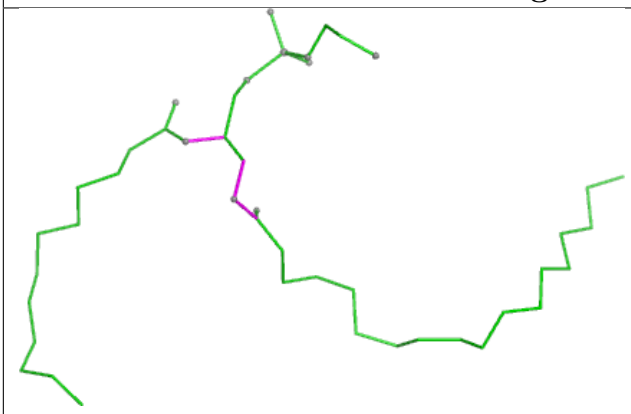
Ligand 3PE N 502



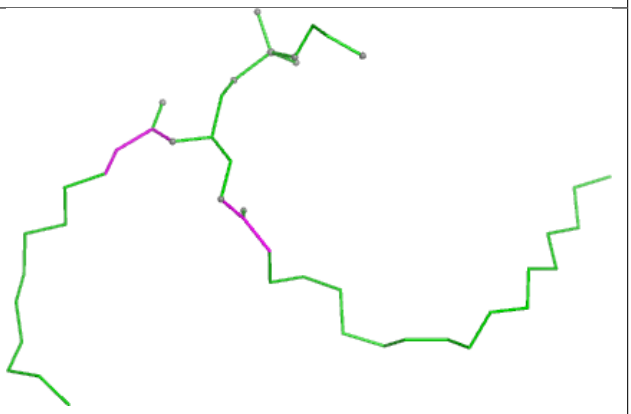
Ligand PC1 B 202



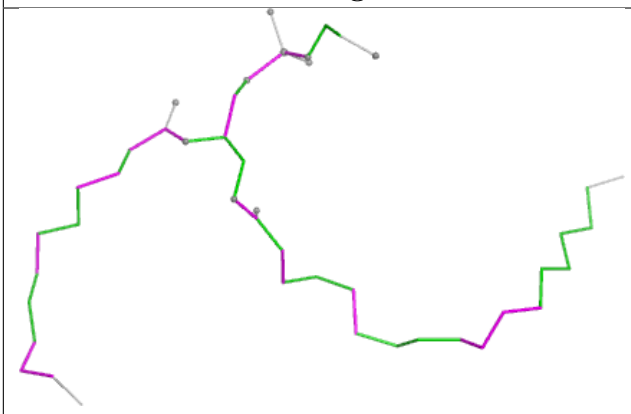
Ligand 3PE L 704



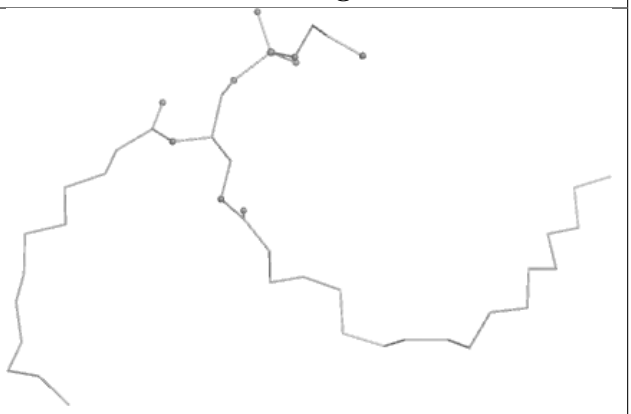
Bond lengths



Bond angles

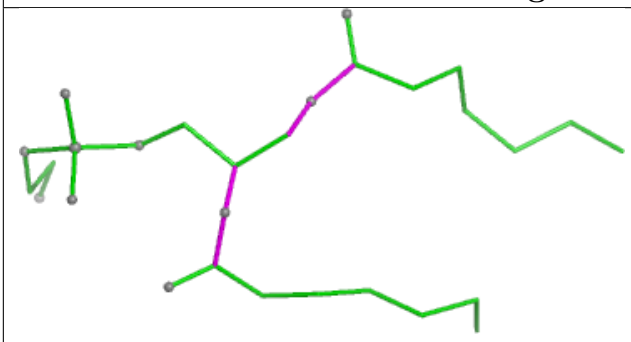


Torsions

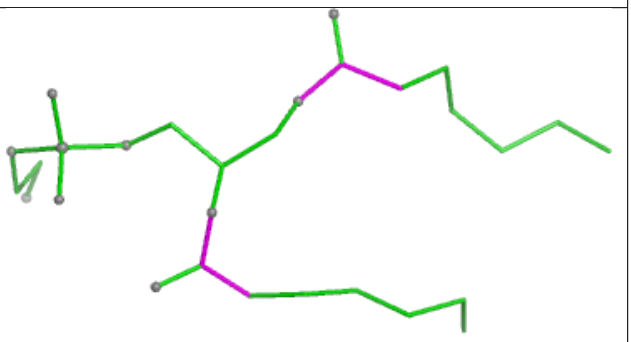


Rings

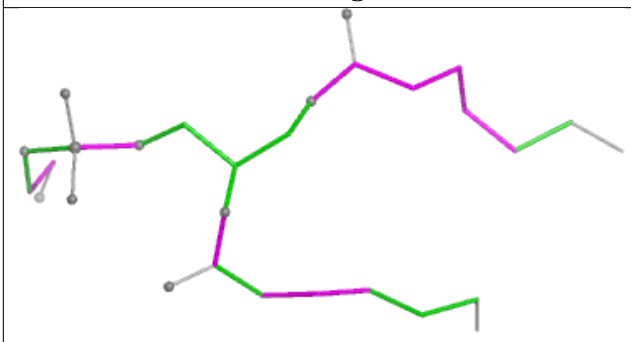
Ligand 3PE Y 604



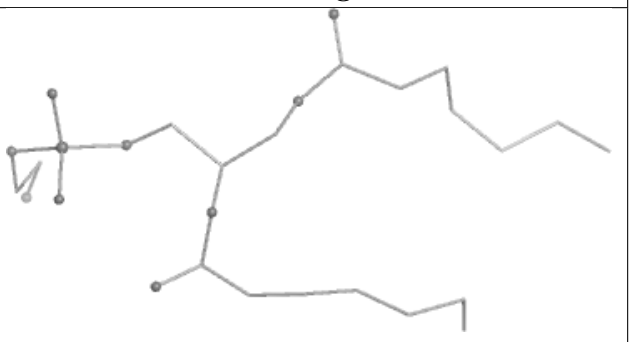
Bond lengths



Bond angles

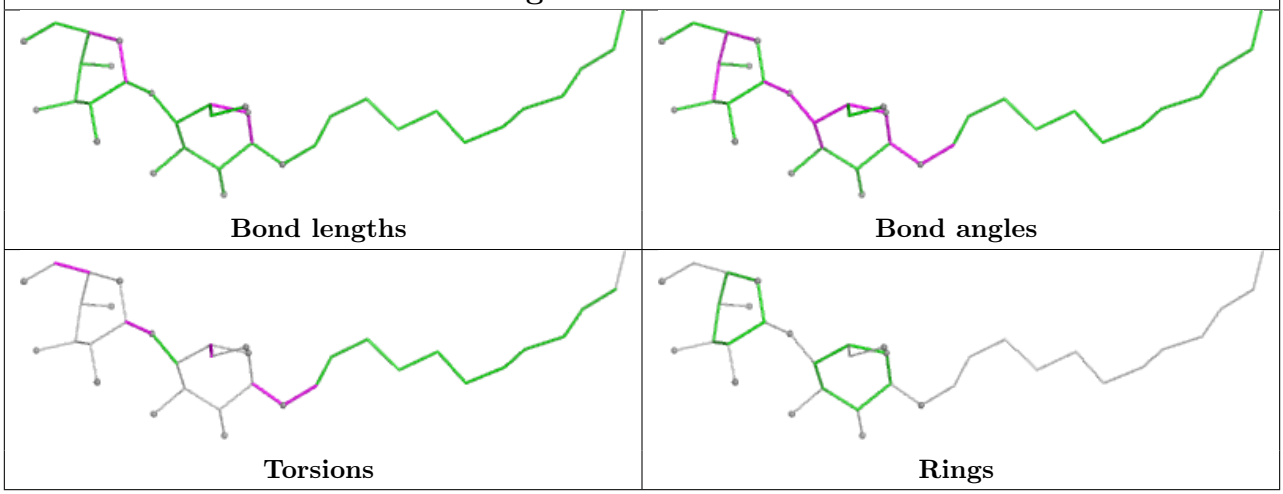


Torsions

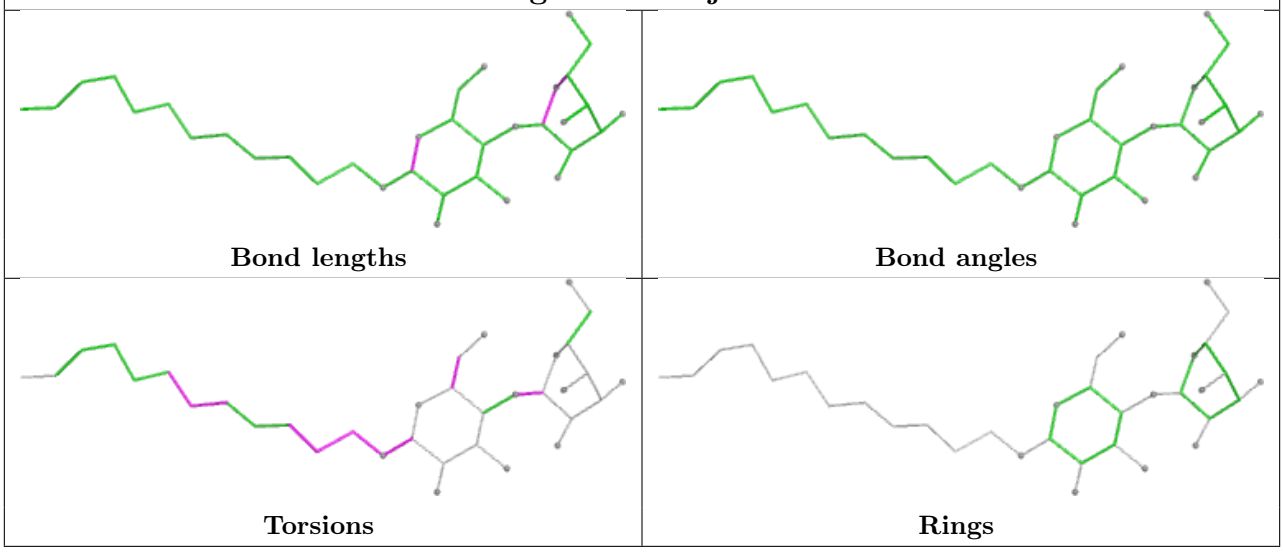


Rings

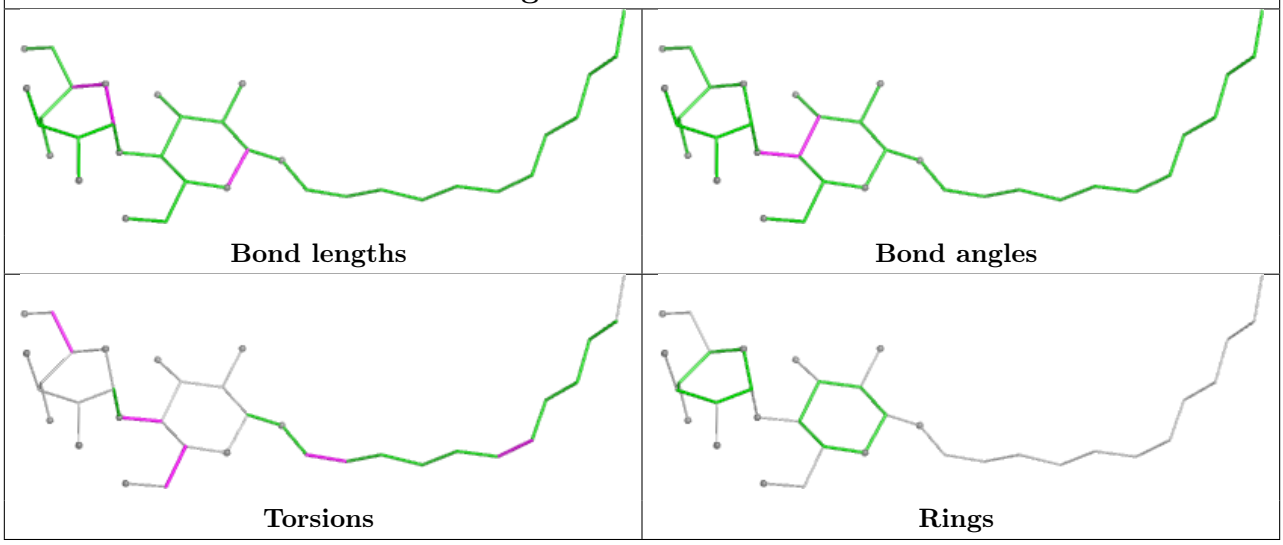
Ligand LMT J 201

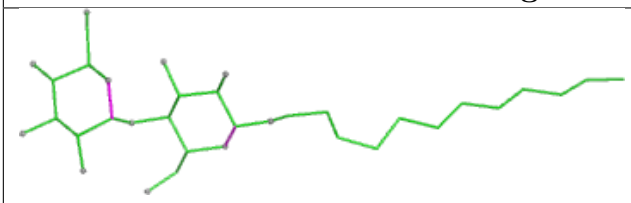
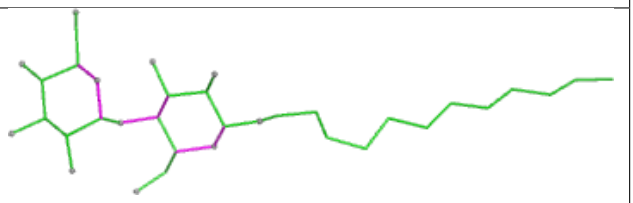
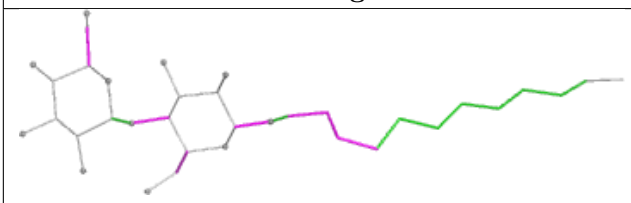
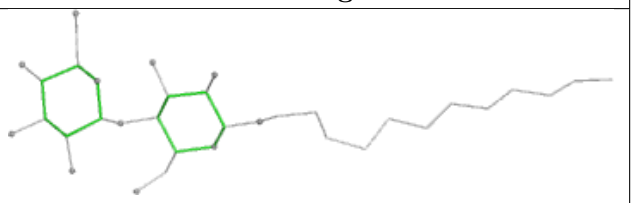


Ligand LMT j 101

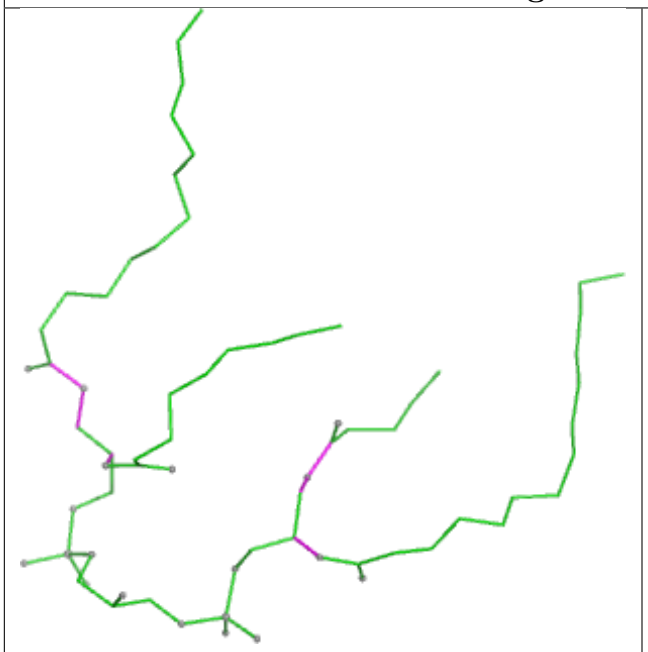


Ligand LMT N 501

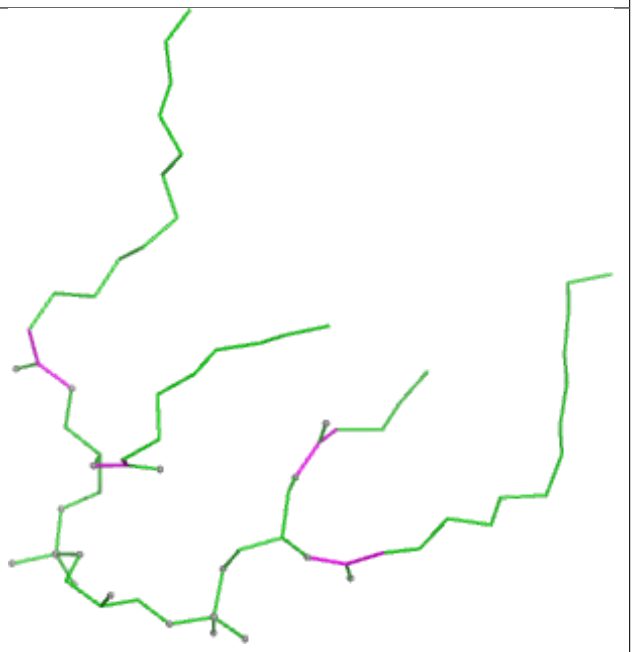


Ligand LMT A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

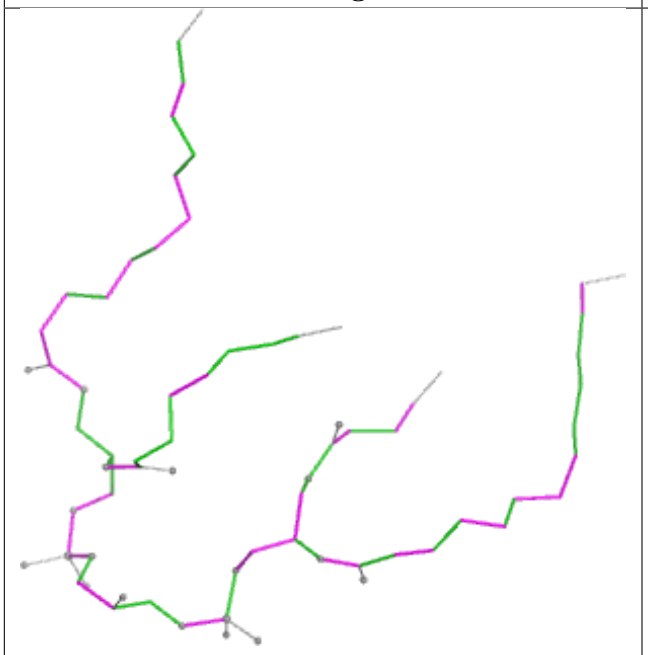
Ligand CDL L 703



Bond lengths

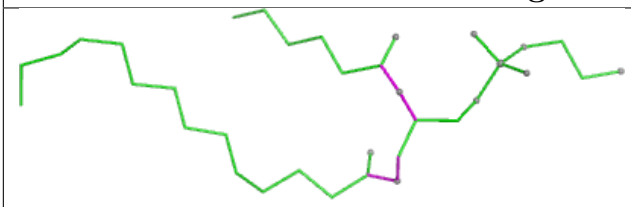
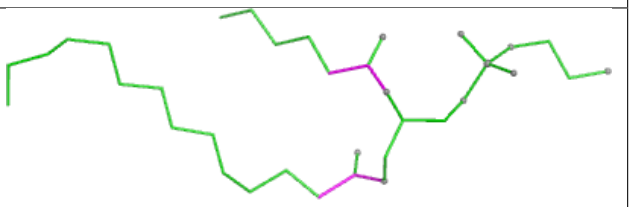
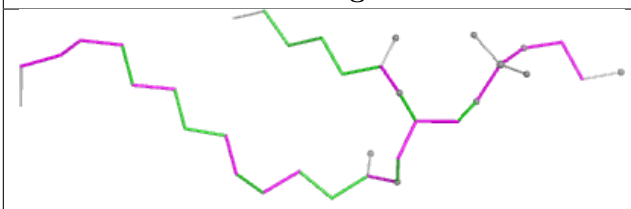
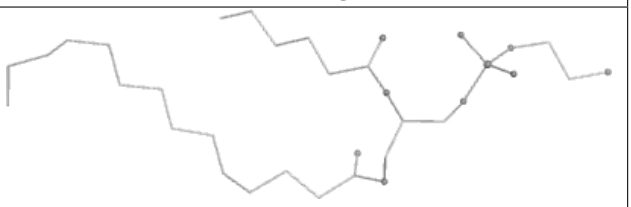


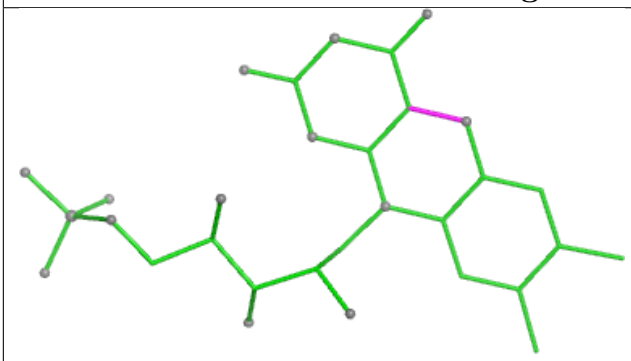
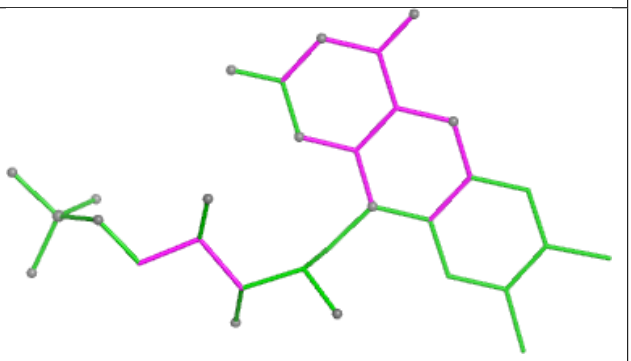
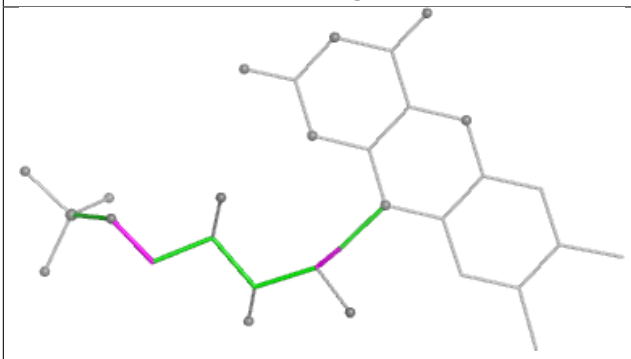
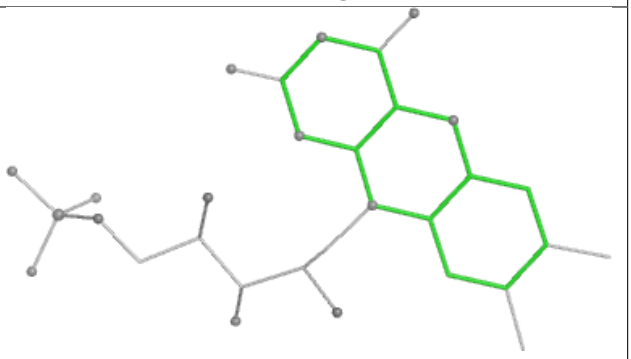
Bond angles



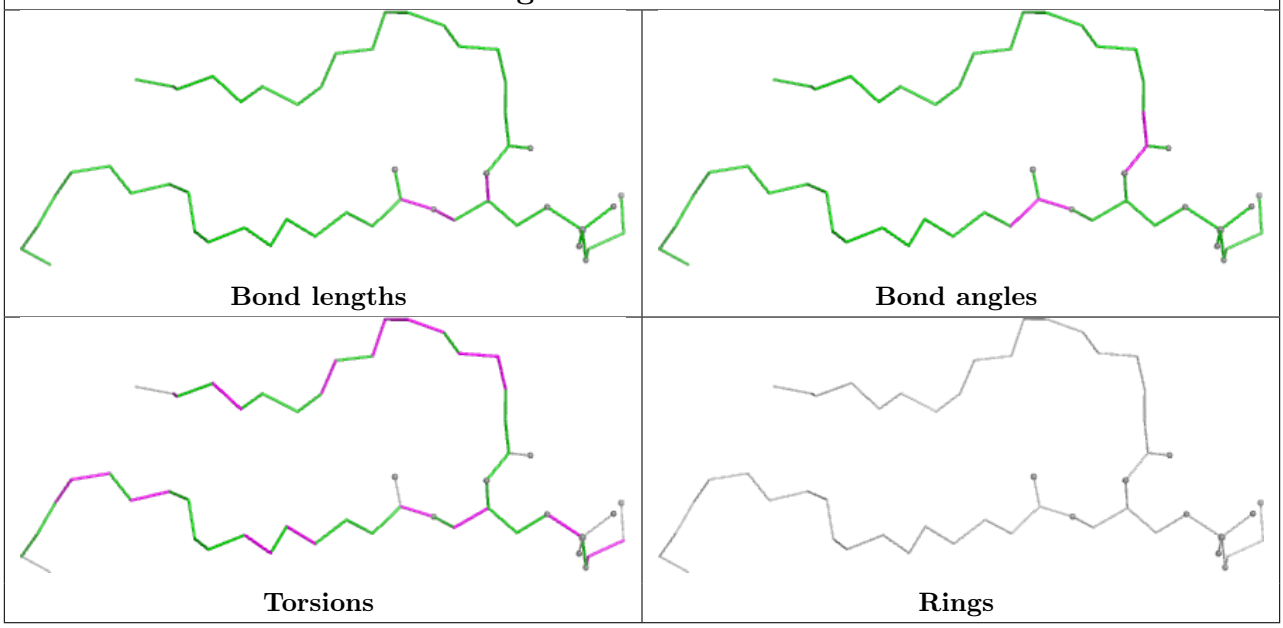
Torsions

Rings

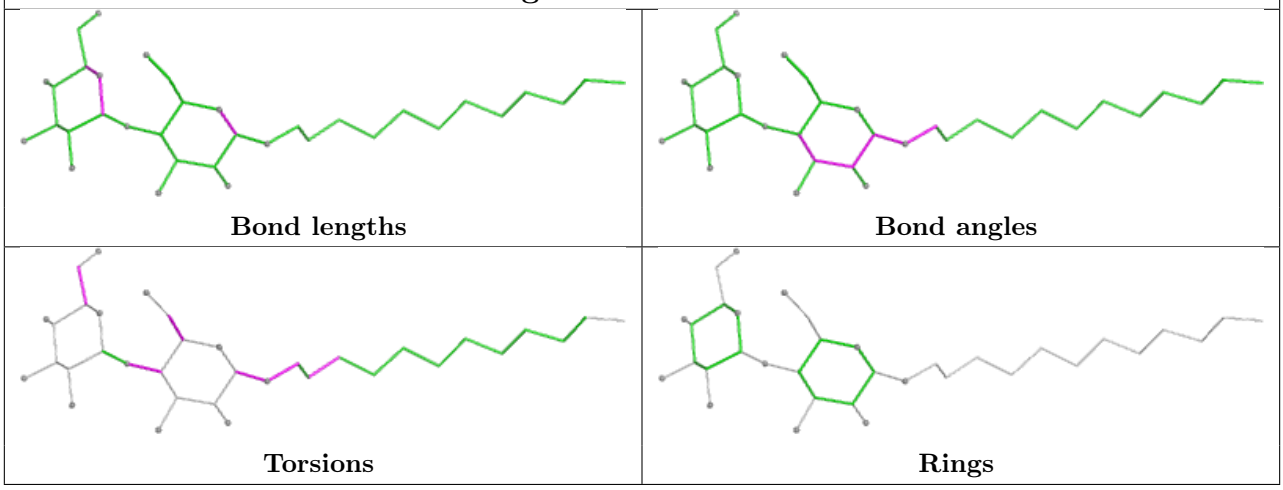
Ligand 3PE Y 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN F 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

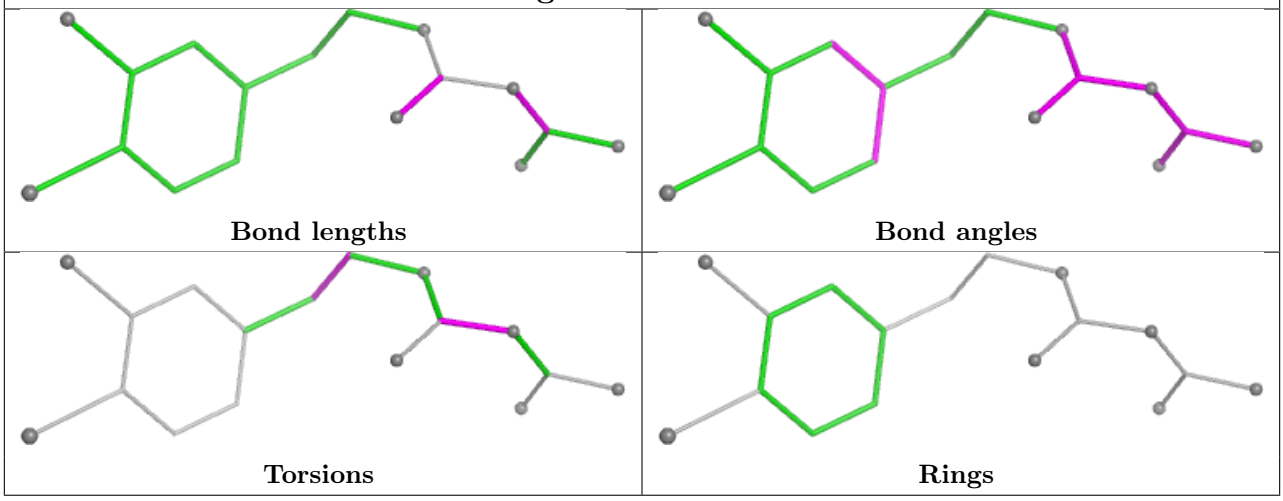
Ligand 3PE M 1301



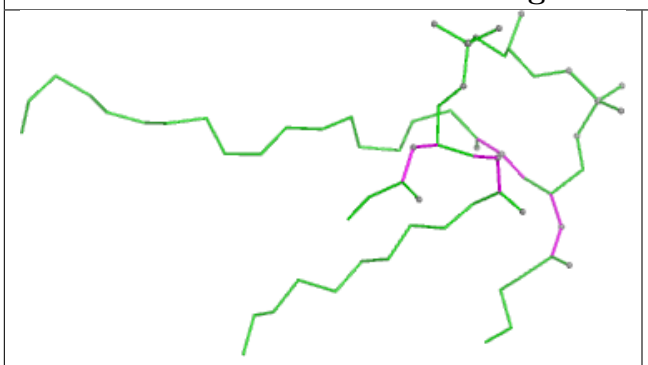
Ligand LMT Y 602



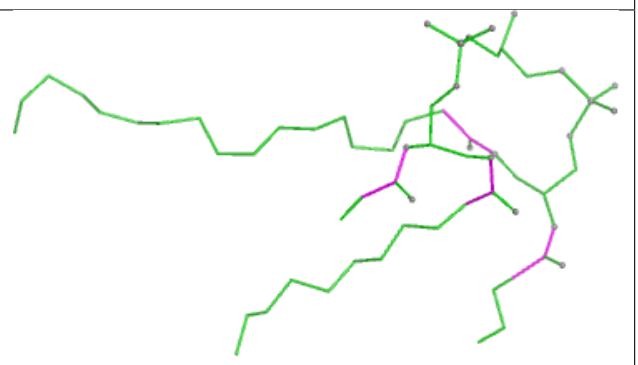
Ligand I49 N 503



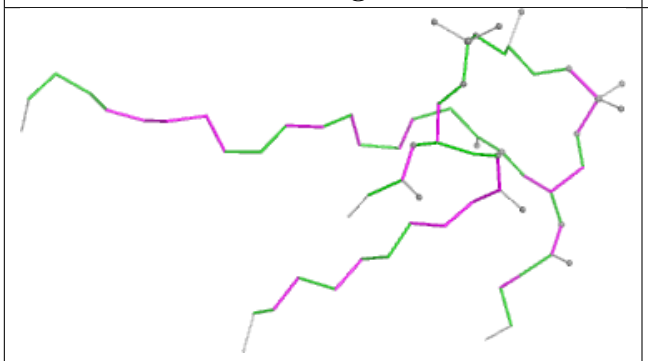
Ligand CDL d 201



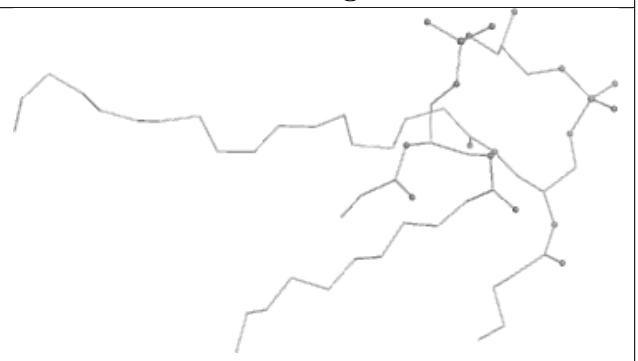
Bond lengths



Bond angles

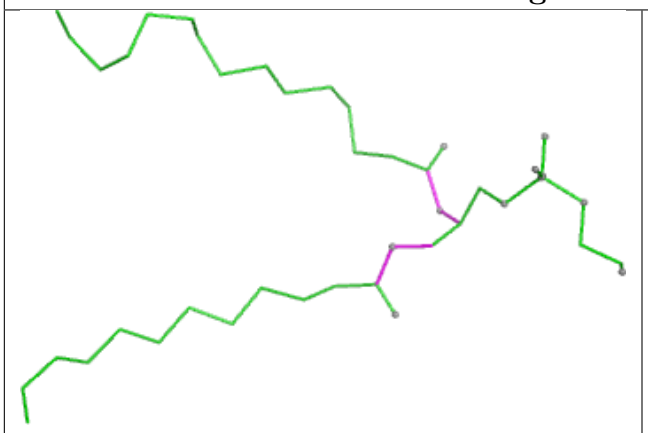


Torsions

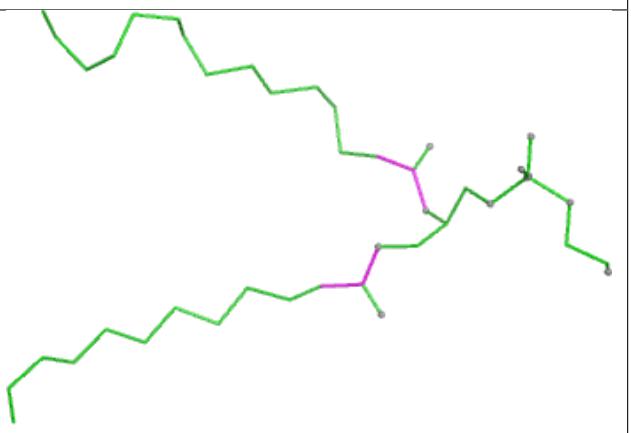


Rings

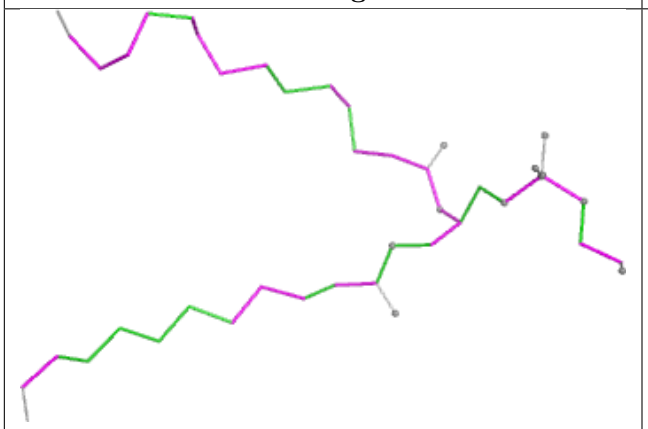
Ligand 3PE A 302



Bond lengths



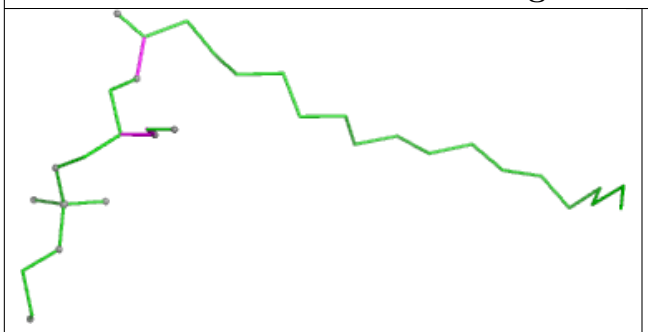
Bond angles



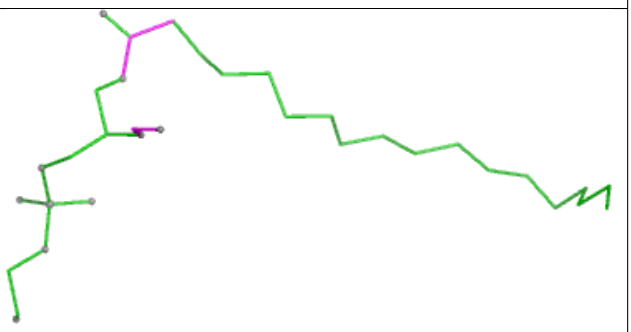
Torsions

Rings

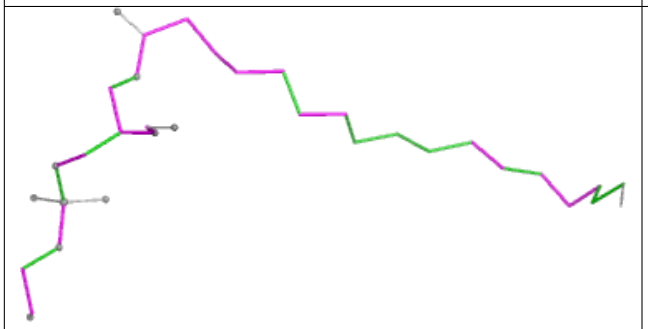
Ligand 3PE H 403



Bond lengths

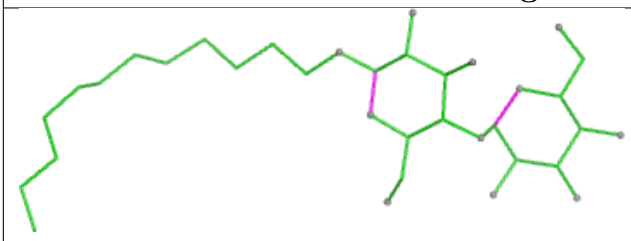
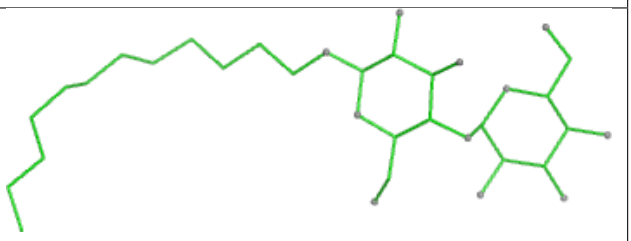
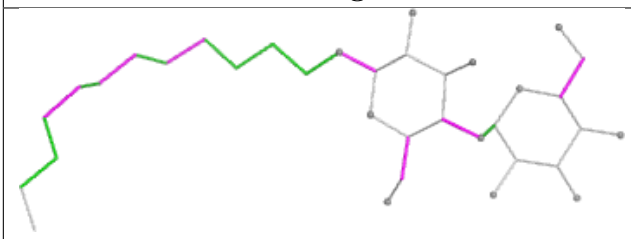
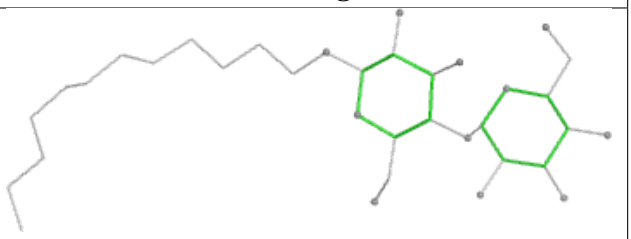


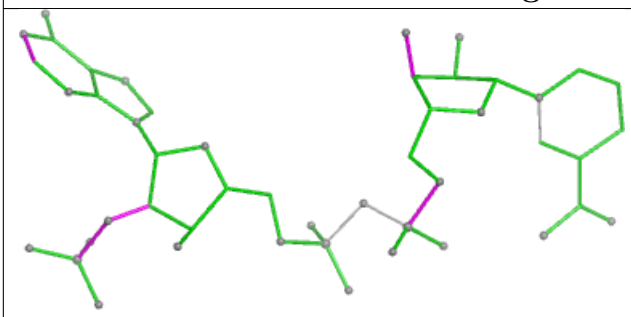
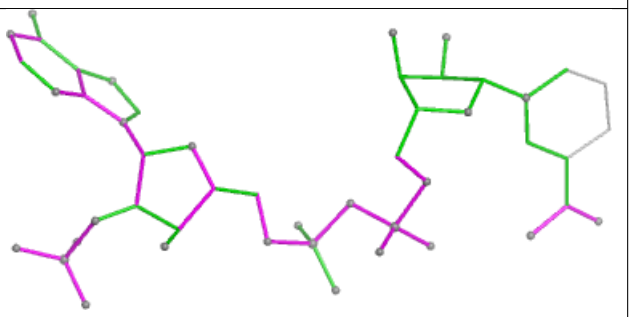
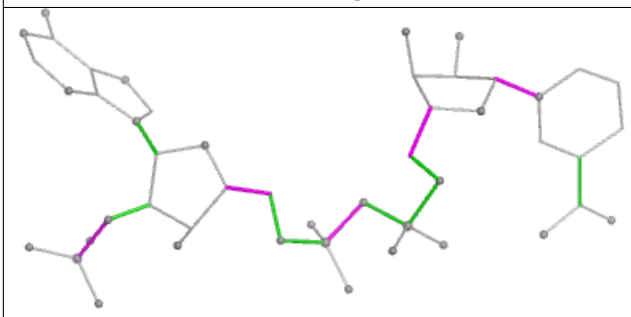
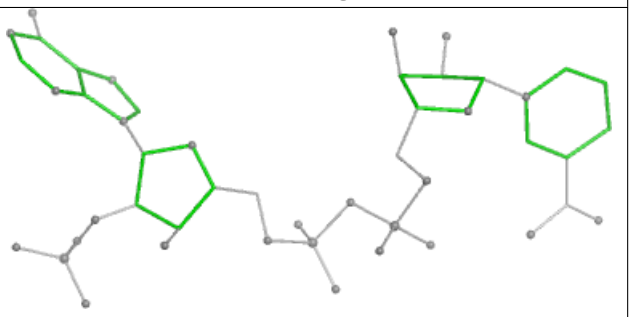
Bond angles



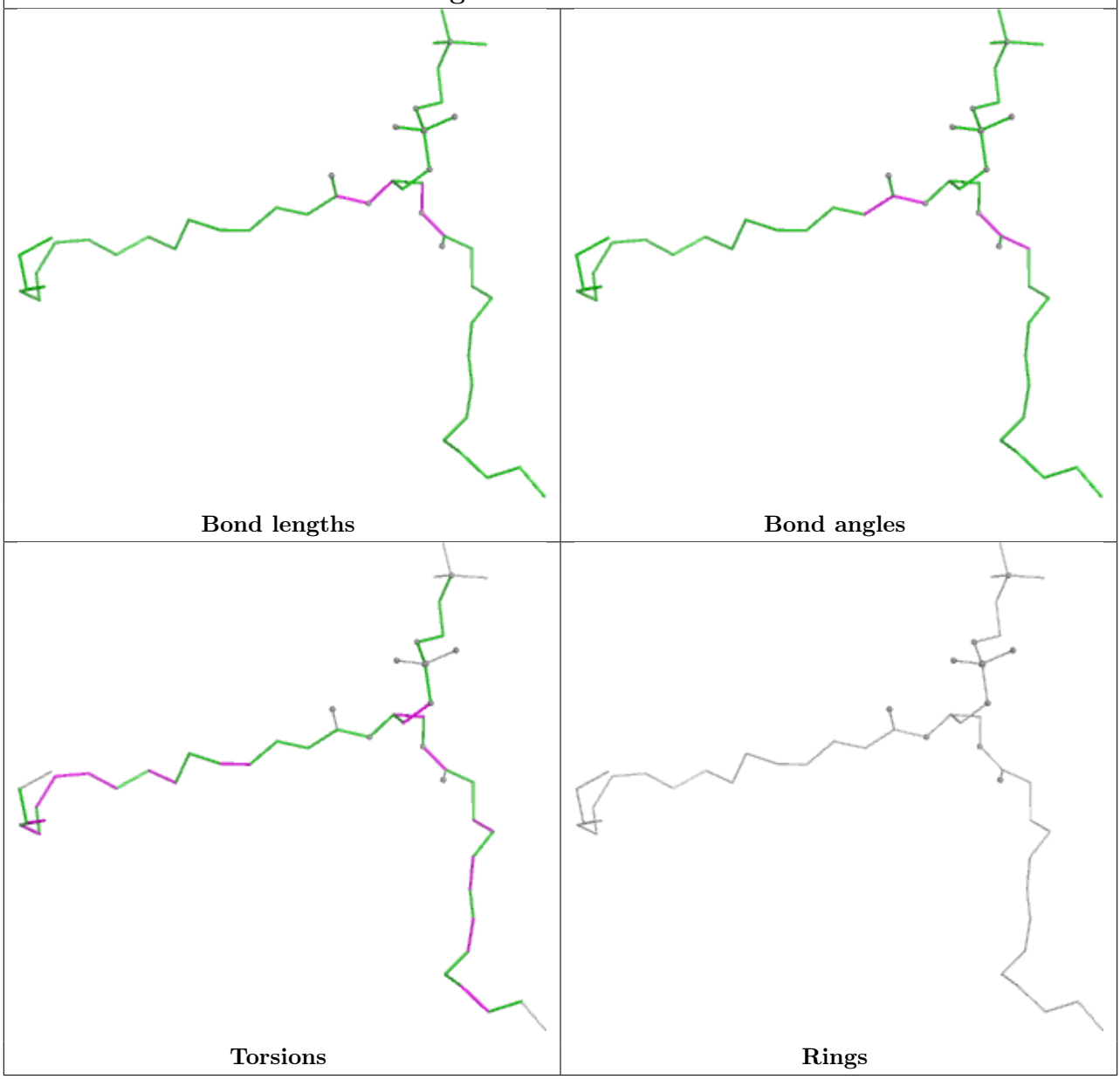
Torsions

Rings

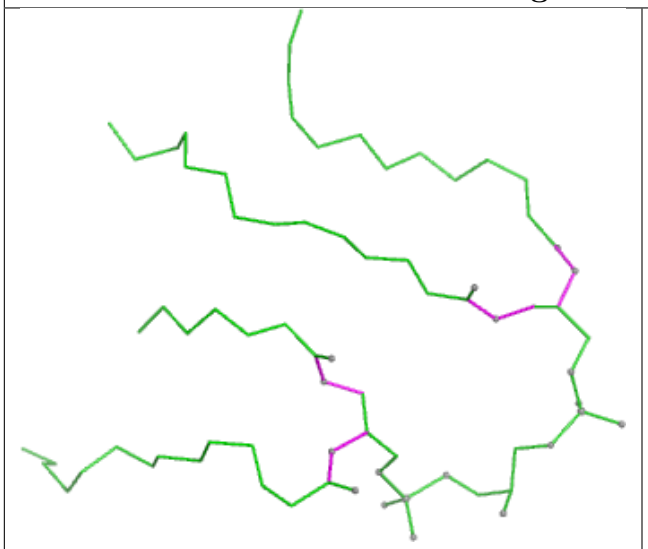
Ligand LMT H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NDP P 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

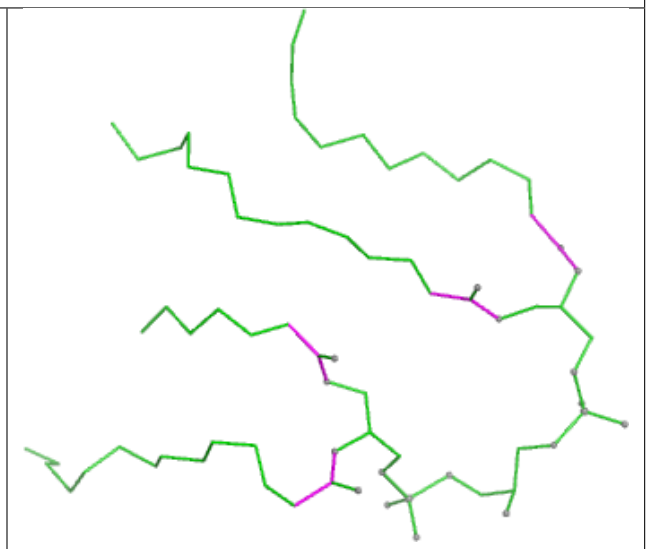
Ligand PC1 M 1302



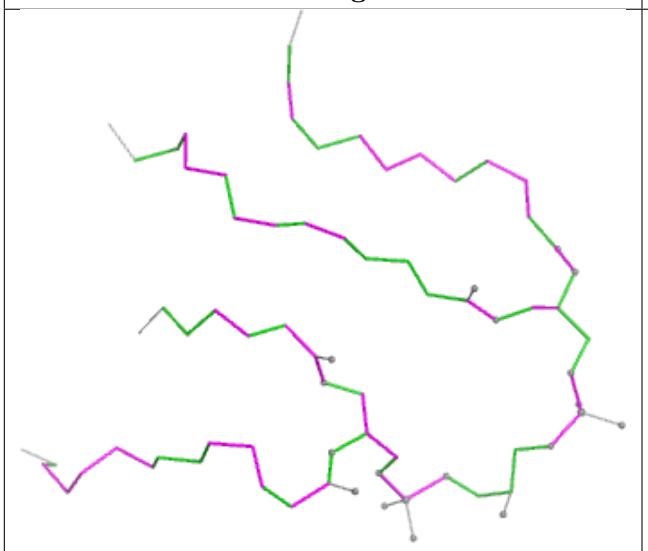
Ligand CDL r 201



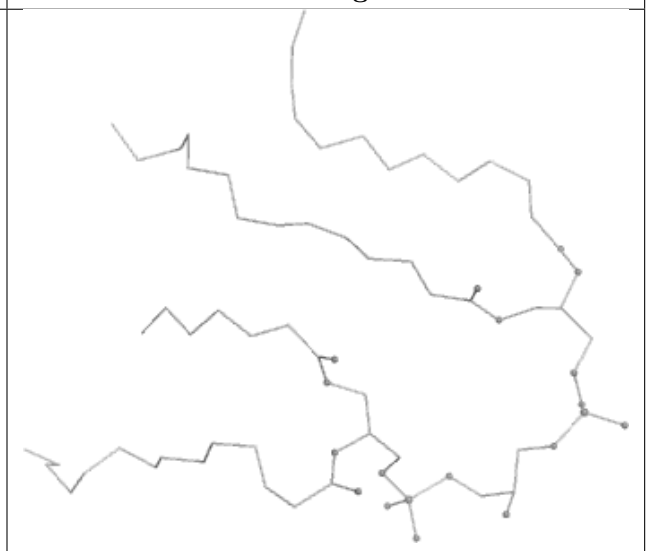
Bond lengths



Bond angles

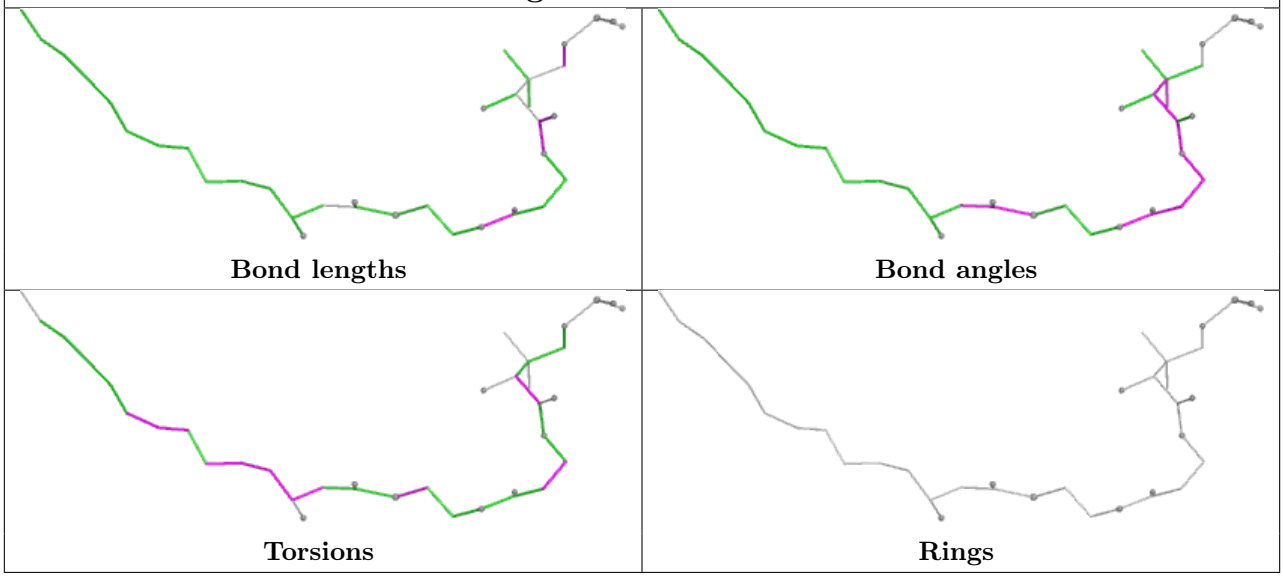


Torsions

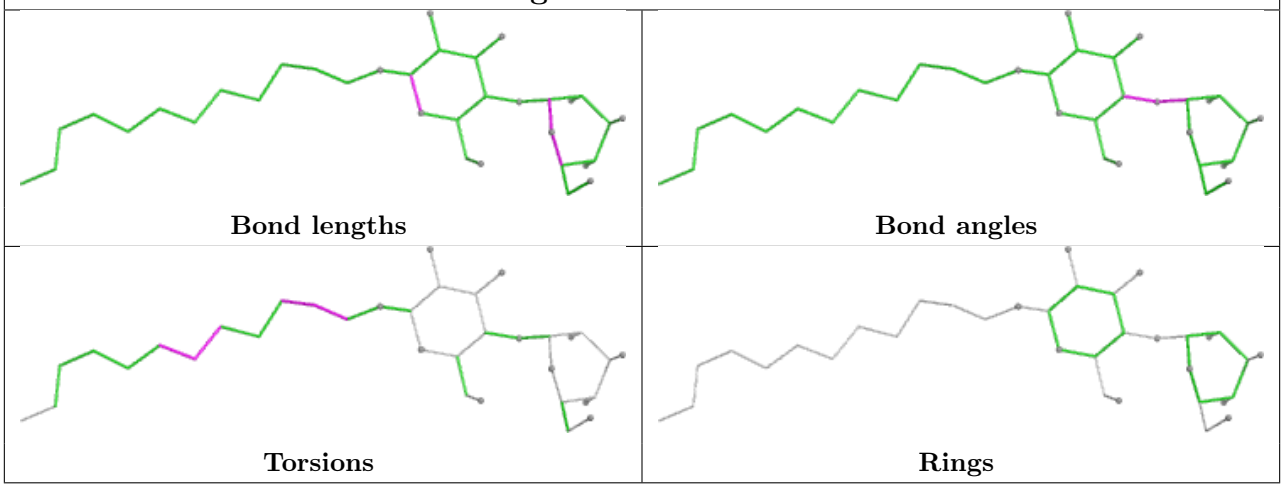


Rings

Ligand EHZ T 101

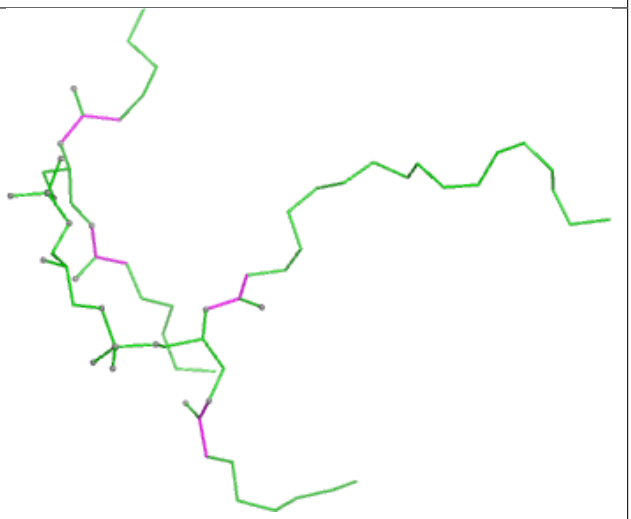


Ligand LMT l 201

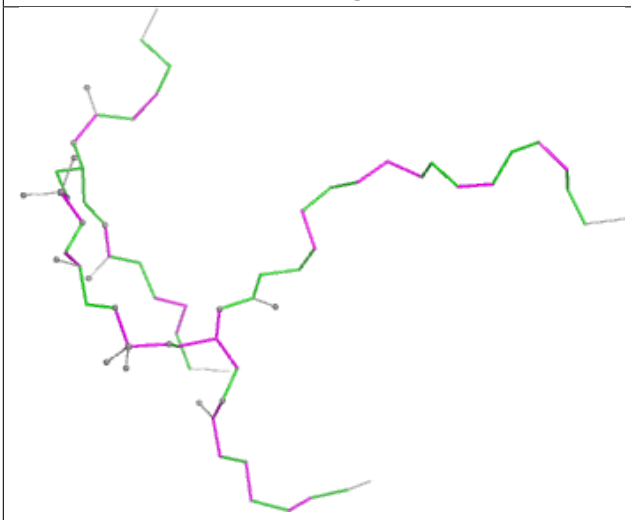


Ligand CDL h 1001

Bond lengths



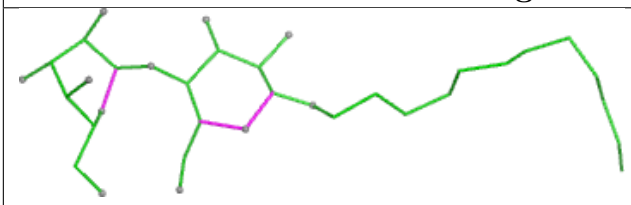
Bond angles



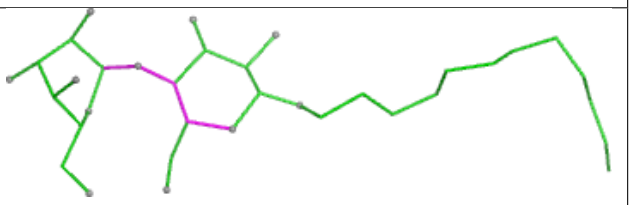
Torsions

Rings

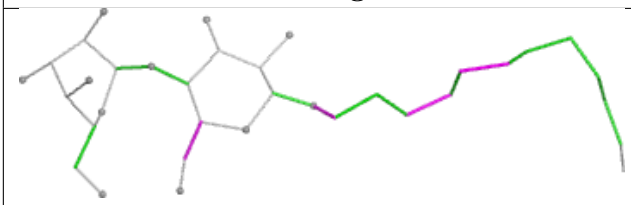
Ligand LMT h 1003



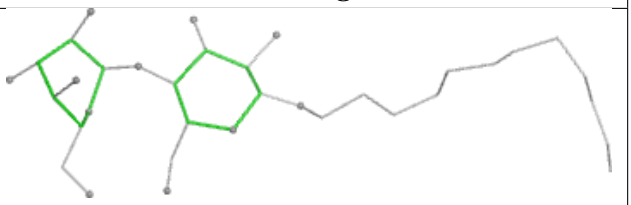
Bond lengths



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.

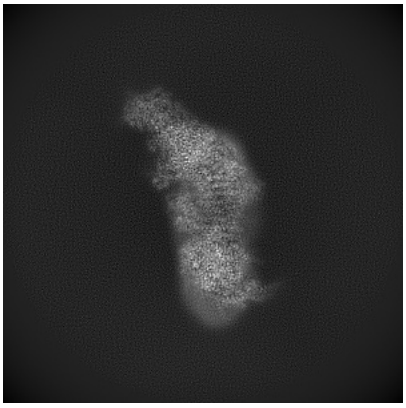
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14297. These allow visual inspection of the internal detail of the map and identification of artifacts.

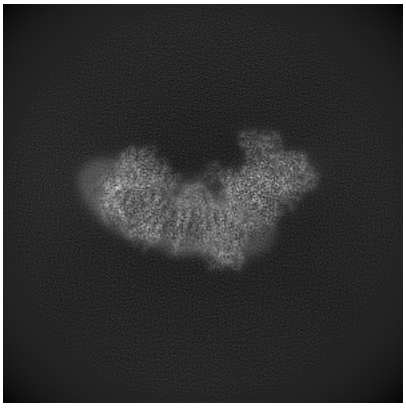
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

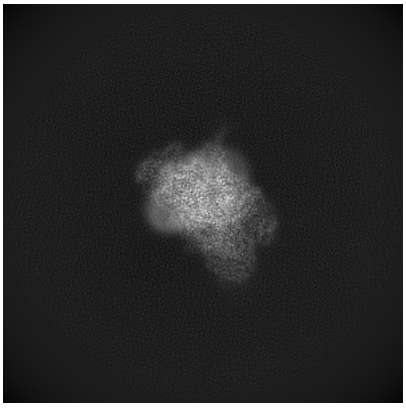
6.1.1 Primary map



X



Y

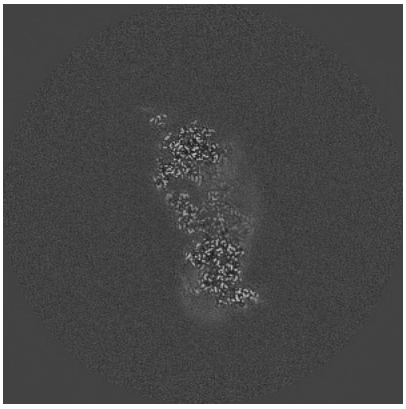


Z

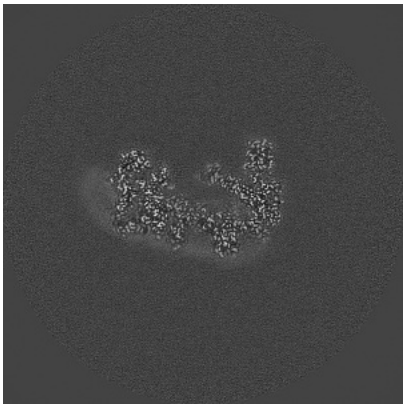
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 330



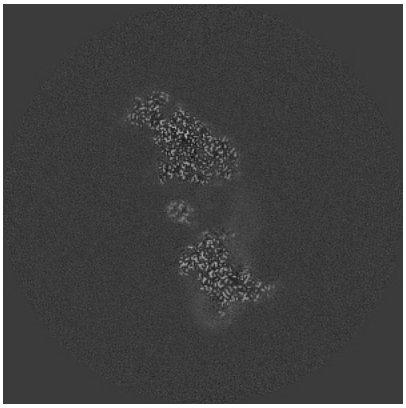
Y Index: 330

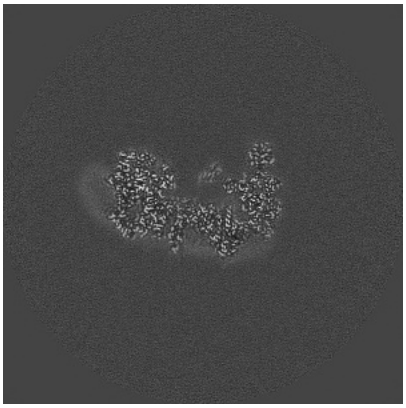
Z Index: 330

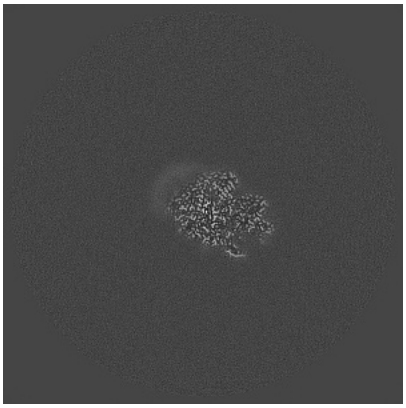
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 358

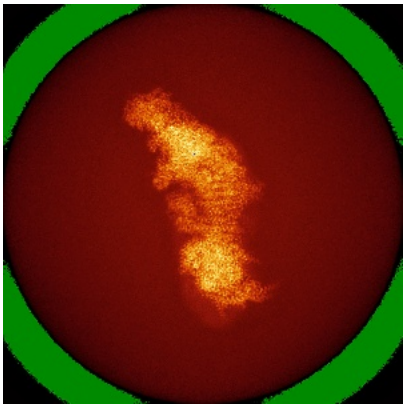

Y Index: 337

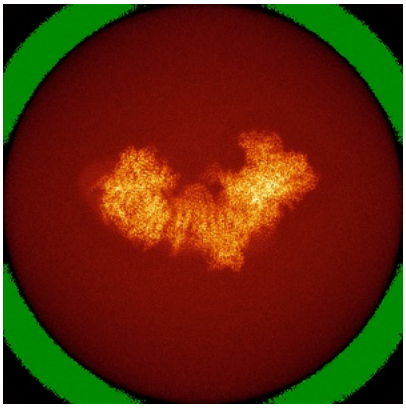

Z Index: 422

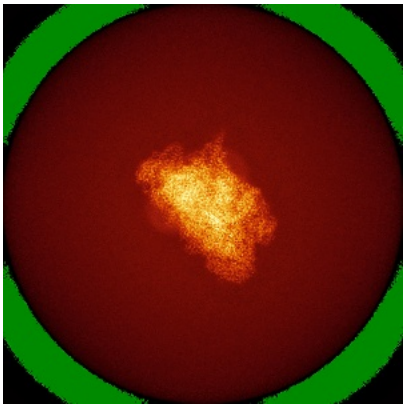
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

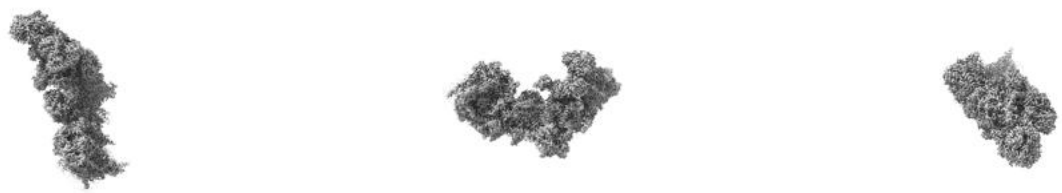

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

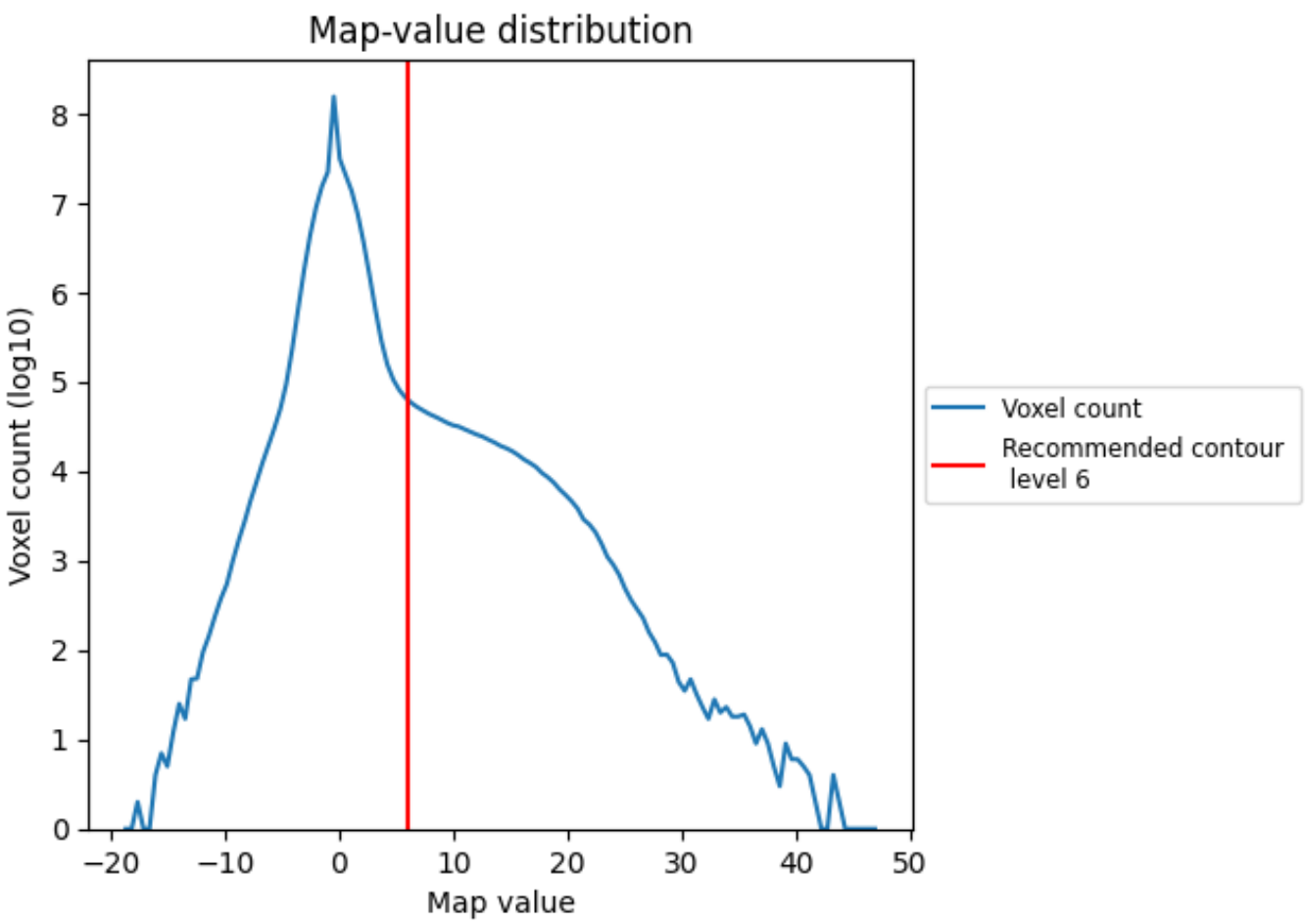
6.6 Mask visualisation (i)

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

7 Map analysis (i)

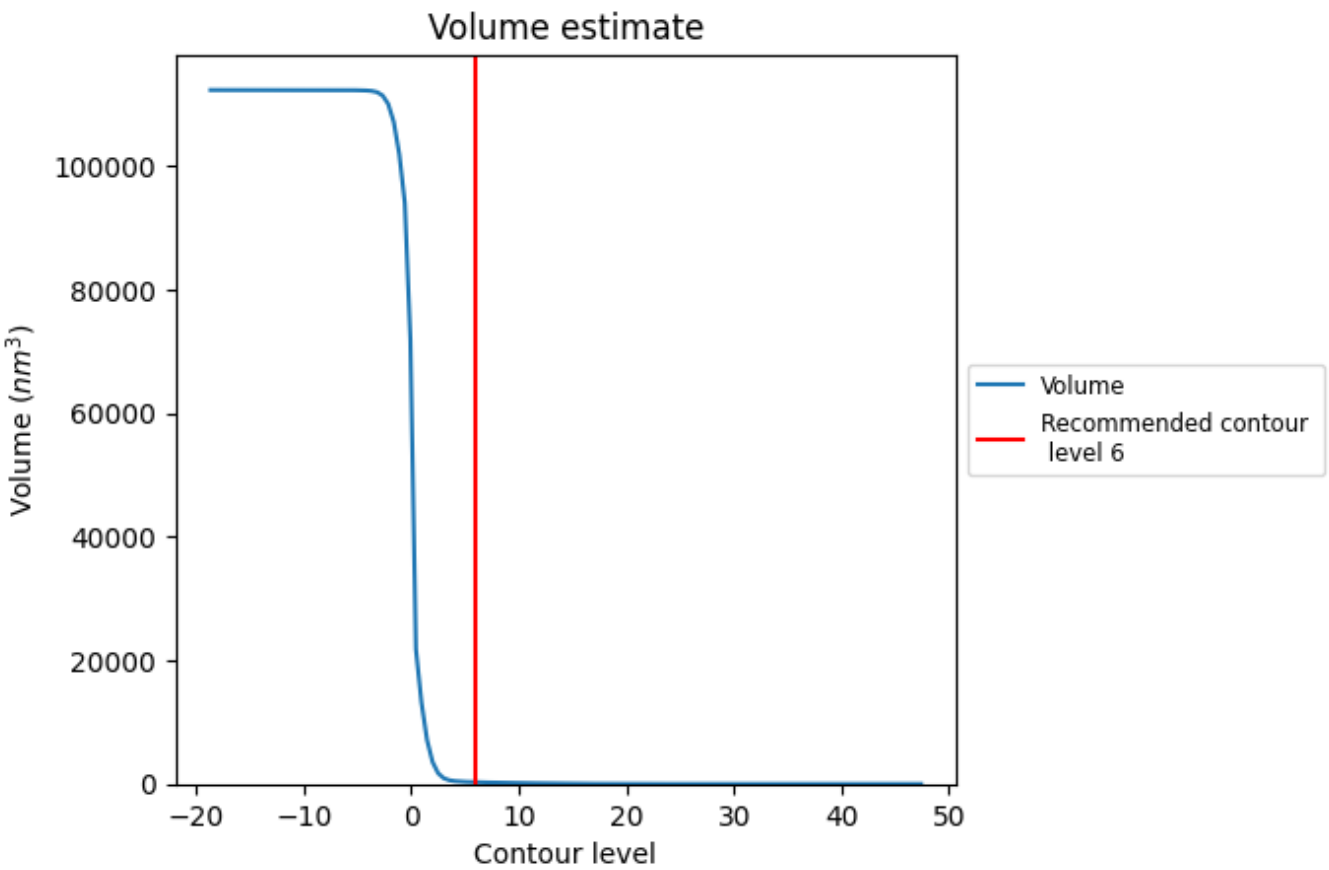
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

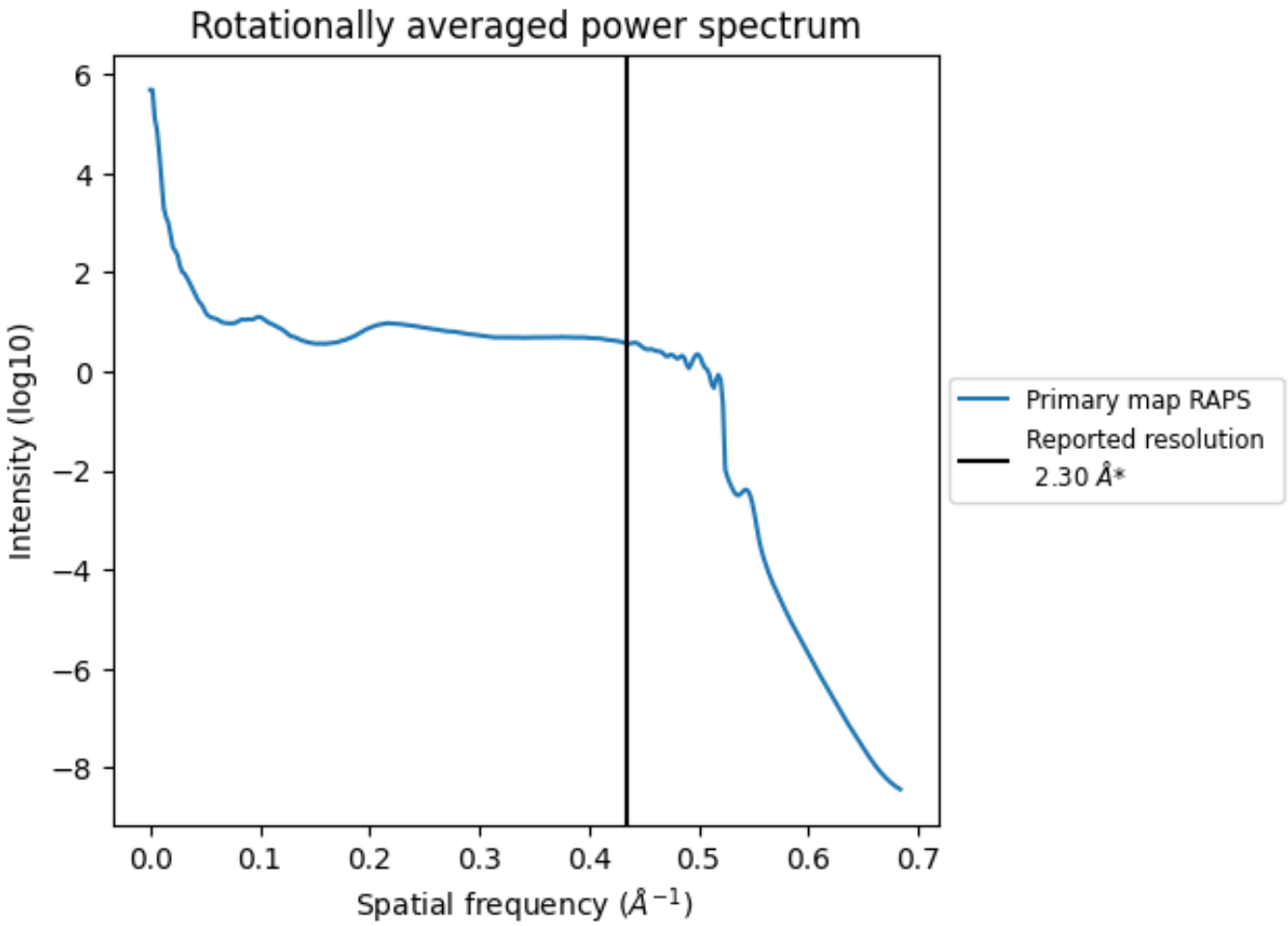
7.2 Volume estimate (i)



The volume at the recommended contour level is 287 nm^3; this corresponds to an approximate mass of 259 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 0.435 Å^{-1}

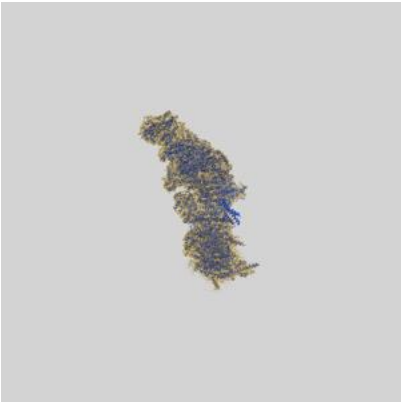
8 Fourier-Shell correlation (i)

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

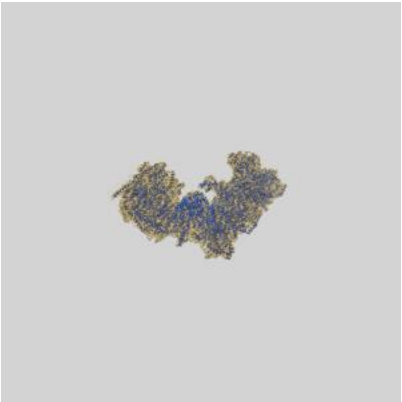
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14297 and PDB model 7R4D. Per-residue inclusion information can be found in section 3 on page 24.

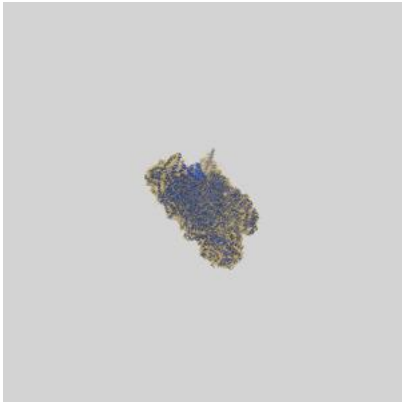
9.1 Map-model overlay (i)



X



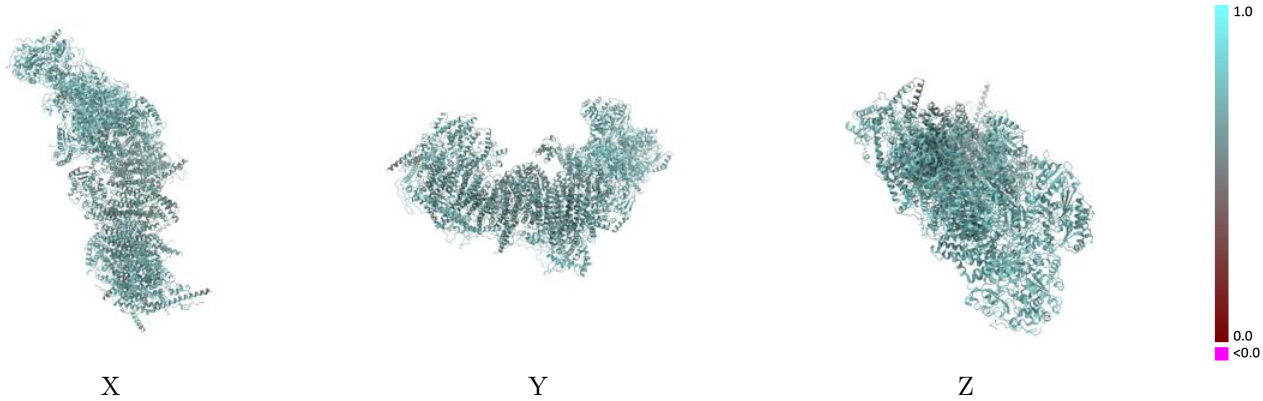
Y



Z

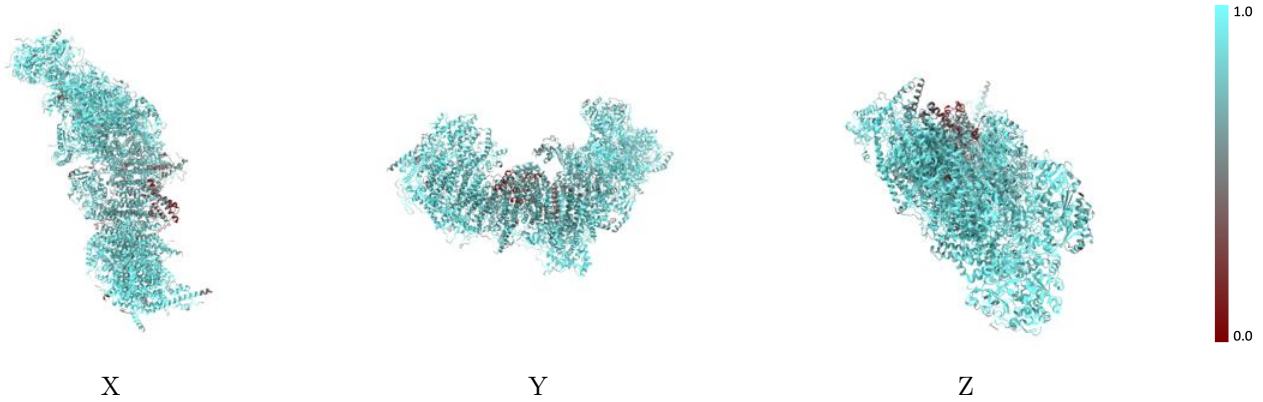
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



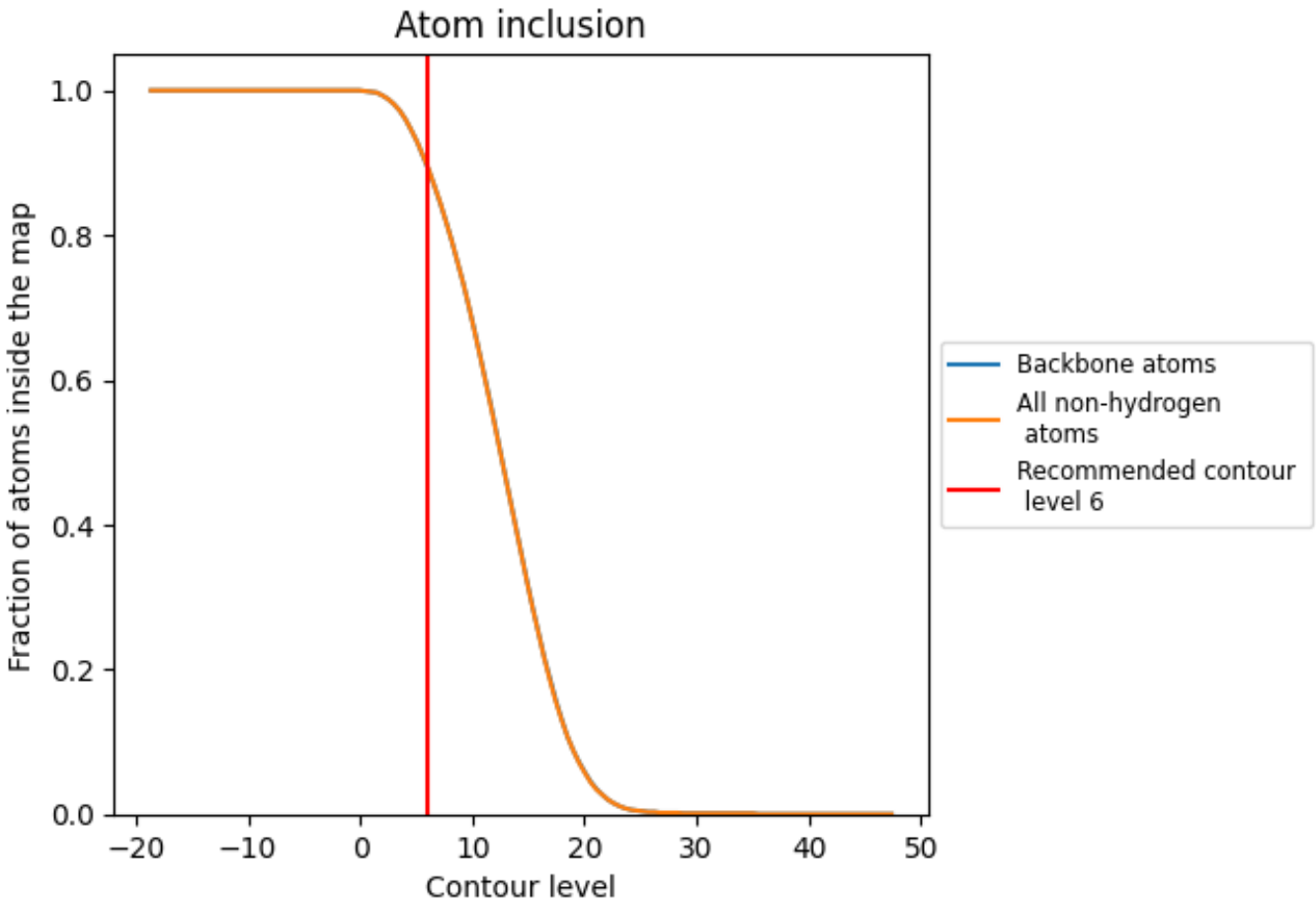
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.8950	0.7000
A	0.8180	0.6700
B	0.9280	0.7330
C	0.9680	0.7480
D	0.9180	0.7390
E	0.9120	0.7030
F	0.9440	0.7150
G	0.9290	0.7240
H	0.9300	0.7130
I	0.9730	0.7520
J	0.7540	0.6630
K	0.9350	0.7100
L	0.9280	0.6950
M	0.9560	0.7120
N	0.9500	0.7120
O	0.8370	0.6620
P	0.8820	0.7040
Q	0.9240	0.7350
R	0.9230	0.7220
S	0.8630	0.6860
T	0.6540	0.6010
U	0.9480	0.6930
V	0.8880	0.7100
W	0.8880	0.7110
X	0.8820	0.6820
Y	0.3840	0.6060
Z	0.8720	0.6890
a	0.9670	0.7080
b	0.8740	0.6750
c	0.7850	0.6440
d	0.8650	0.6850
e	0.8510	0.6650
f	0.8090	0.6580
g	0.8660	0.6800
h	0.9050	0.6920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8890	0.6650
j	0.8770	0.6520
k	0.8920	0.6420
l	0.9250	0.6850
m	0.8840	0.6740
n	0.9340	0.6900
o	0.9020	0.6550
p	0.9230	0.6890
q	0.9010	0.7210
r	0.8850	0.7170
s	0.8990	0.6980