Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 11:14 am BST

PDB ID	:	9SMF / pdb_00009smf
EMDB ID	:	EMD-55030
Title	:	Reduced bovine complex I in lipid nanodisc, NADH-active-Q10
Authors	:	Chung, I.; Hirst, J.
Deposited on	:	2025-09-08
Resolution	:	2.51 Å(reported)
Based on initial model	:	7QSK

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

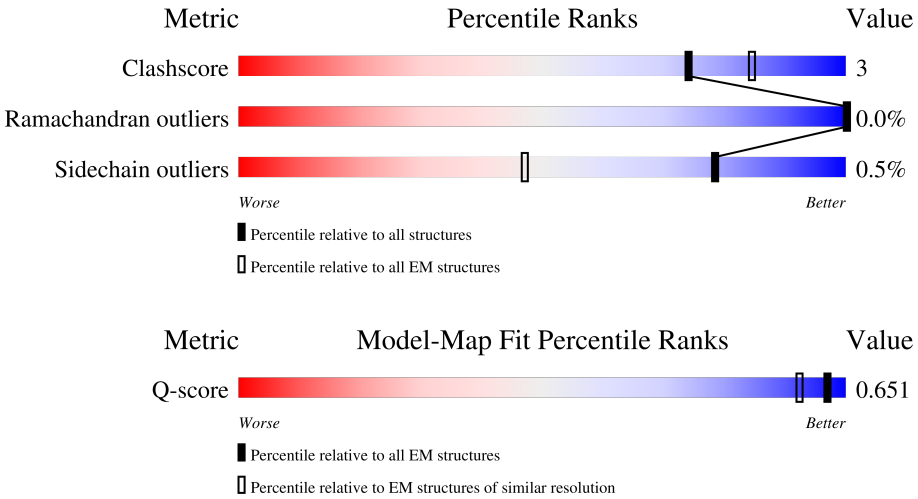
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.51 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.



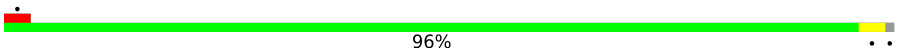
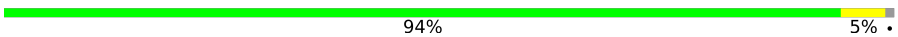
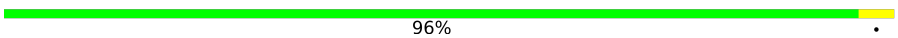
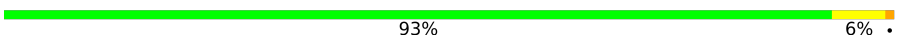
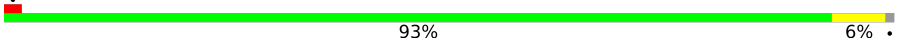
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7159 (2.01 - 3.01)

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	85% 15%
2	B	216	68% 6% 27%
3	C	266	73% 5% 21%
4	D	463	86% 7% 7%

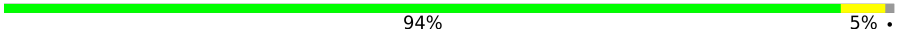
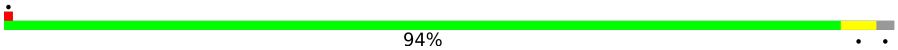
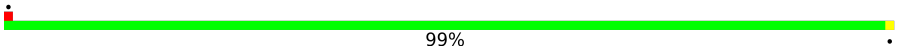
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 70931 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	115	921	622	133	159	7	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	158	1261	803	227	217	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	209	1738	1120	298	317	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	430	3459	2209	596	629	25	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1668	1064	280	314	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	433	Total	C	N	O	S	0	0
			3331	2099	595	617	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	690	Total	C	N	O	S	0	0
			5288	3312	922	1015	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	ACE	-	acetylation	UNP Q8HXG6

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	ACE	-	acetylation	UNP Q02827

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	100	Total	C	N	O	S	0	0
			838	528	160	144	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			854	548	141	161	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	143	Total	C	N	O	S	0	0
			1186	776	203	205	2		

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	1	ACE	-	acetylation	UNP Q02367

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1453	910	268	267	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	97	Total	C	N	O	S	0	0
			785	496	146	140	3		

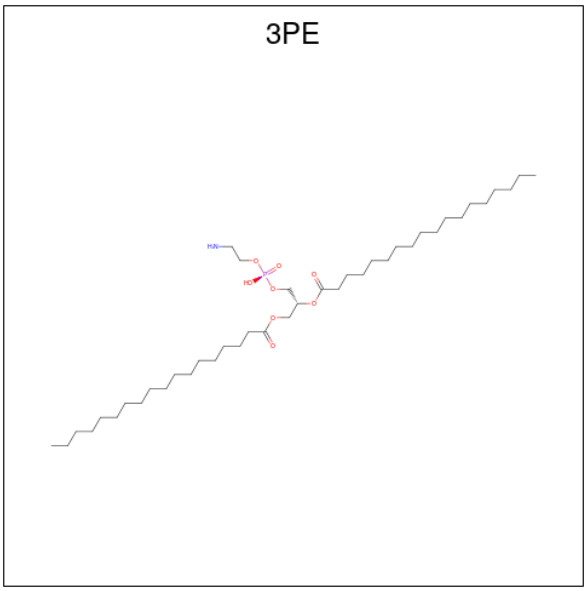
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	1	ACE	-	acetylation	UNP Q05752

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

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

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



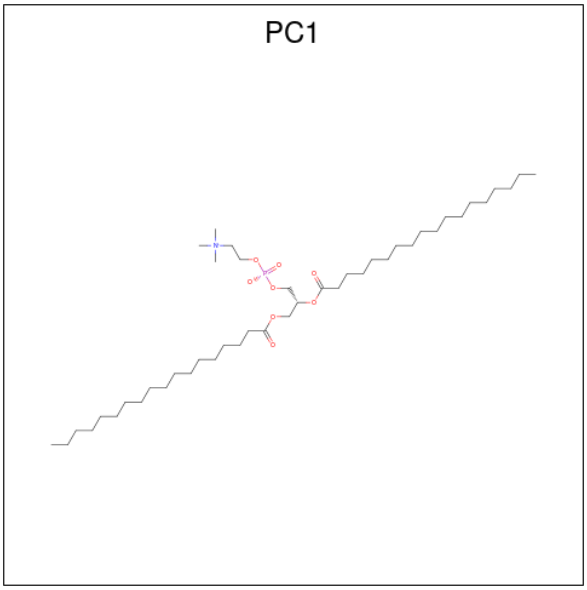
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	I	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	K	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	N	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	Y	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	Y	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	Y	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	b	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



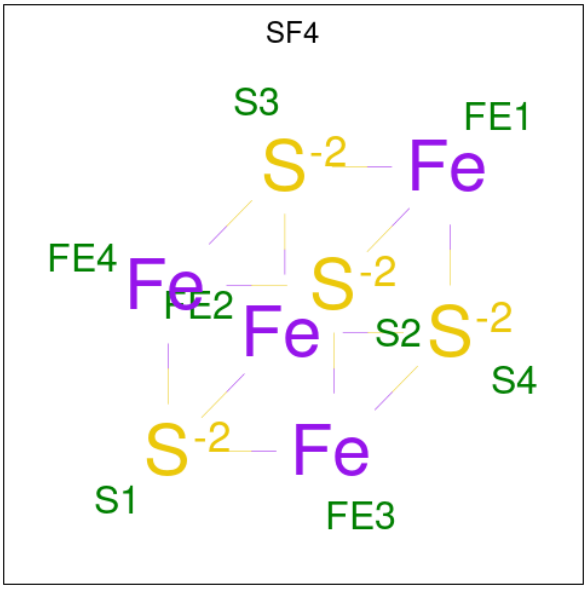
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	I	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	P	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	P	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	h	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



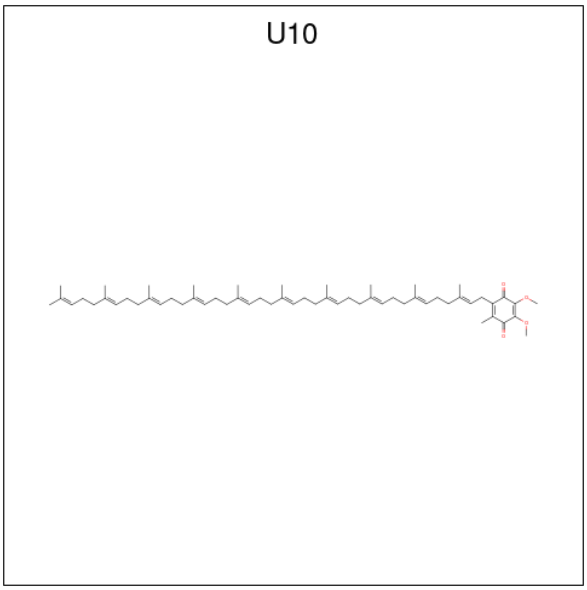
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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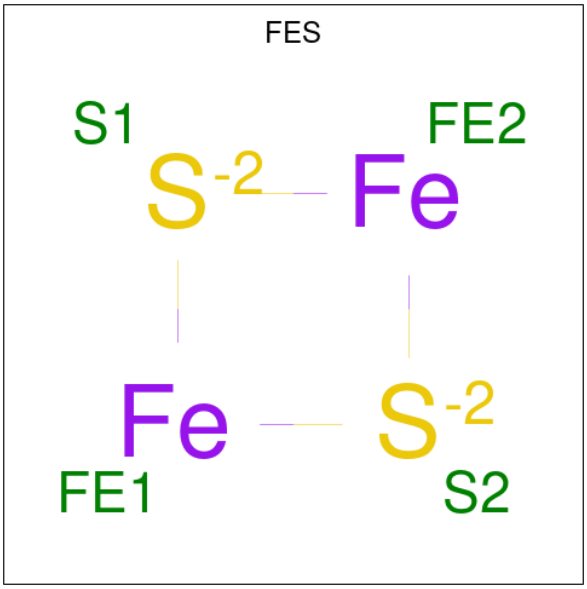
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	I	1	8	4	4	0

- Molecule 48 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



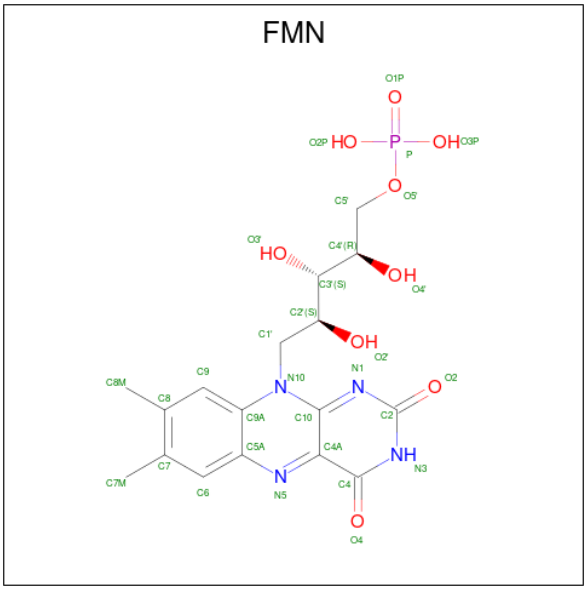
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	D	1	63	59	4	0

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



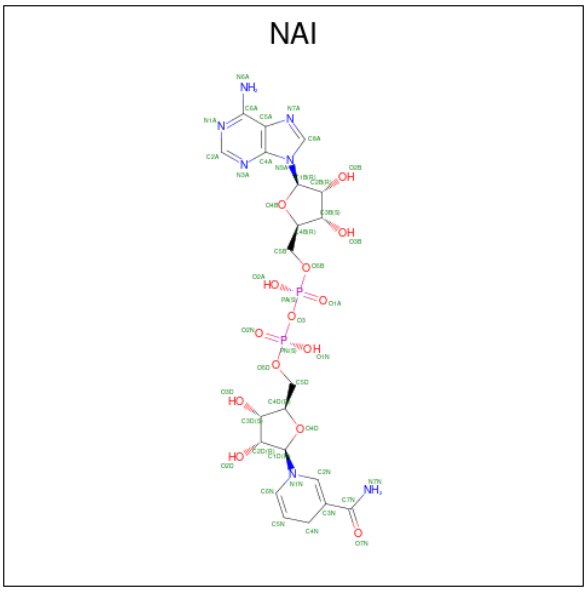
Mol	Chain	Residues	Atoms	AltConf
49	E	1	Total Fe S 4 2 2	0
49	G	1	Total Fe S 4 2 2	0

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



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

- Molecule 51 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

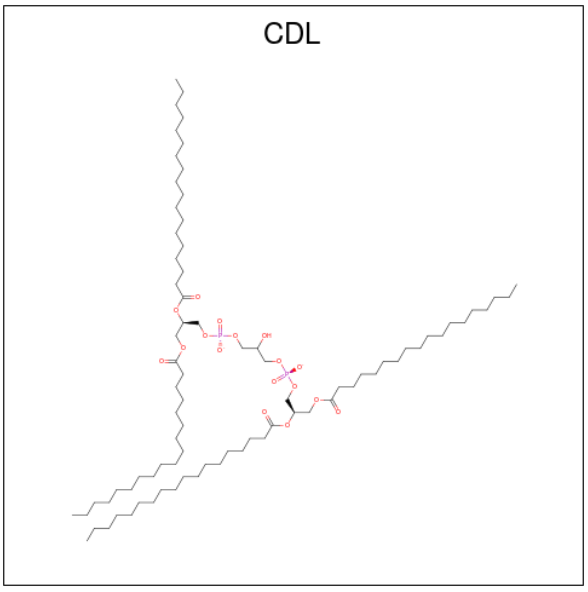


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

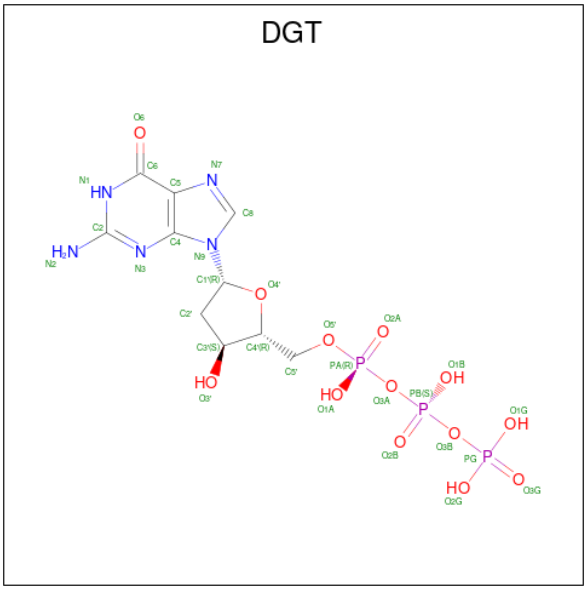
Mol	Chain	Residues	Atoms		AltConf
52	G	1	Total	K	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
53	H	1	Total	C	O	P	0
			69	50	17	2	
53	L	1	Total	C	O	P	0
			78	59	17	2	
53	N	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			62	43	17	2	
53	N	1	Total	C	O	P	0
			65	46	17	2	
53	X	1	Total	C	O	P	0
			86	67	17	2	
53	h	1	Total	C	O	P	0
			78	59	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

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

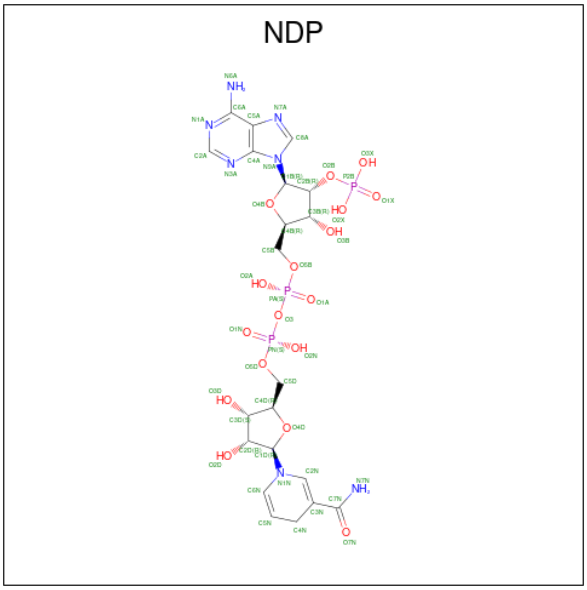


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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

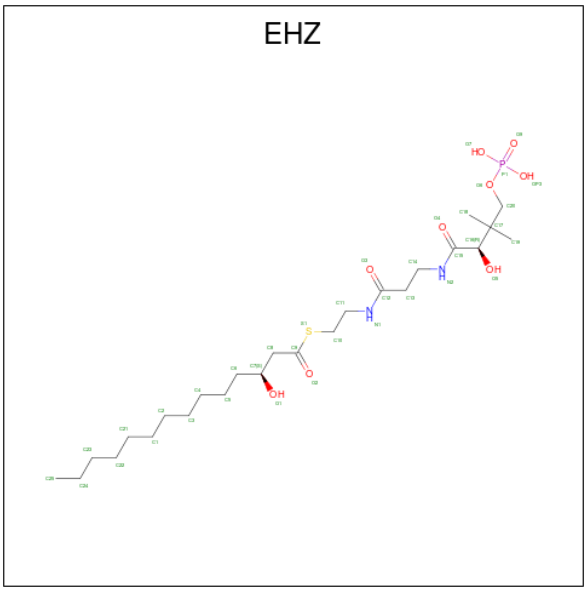


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

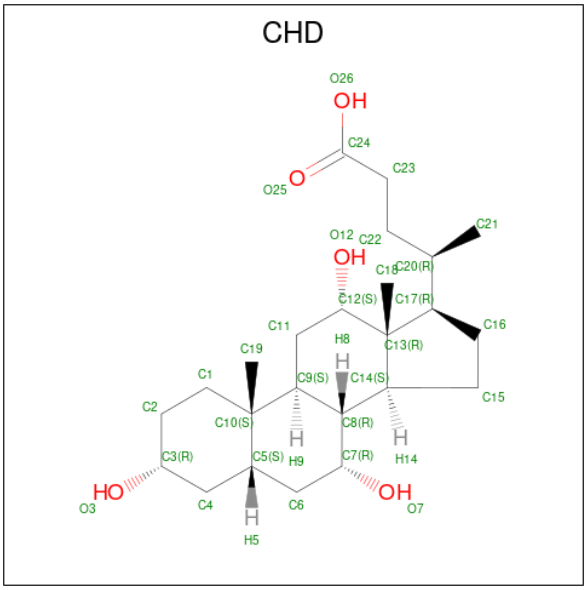
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

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



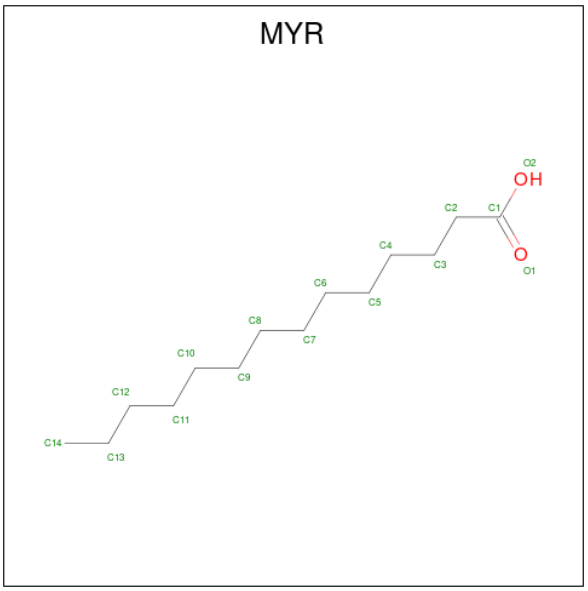
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	A	40	Total O 40 40	0
61	B	80	Total O 80 80	0
61	C	108	Total O 108 108	0
61	D	203	Total O 203 203	0
61	E	30	Total O 30 30	0
61	F	73	Total O 73 73	0
61	G	207	Total O 207 207	0
61	H	110	Total O 110 110	0
61	I	101	Total O 101 101	0
61	J	47	Total O 47 47	0
61	K	31	Total O 31 31	0

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Mol	Chain	Residues	Atoms	AltConf
61	L	78	Total O 78 78	0
61	M	132	Total O 132 132	0
61	N	92	Total O 92 92	0
61	O	22	Total O 22 22	0
61	P	90	Total O 90 90	0
61	Q	108	Total O 108 108	0
61	R	26	Total O 26 26	0
61	V	14	Total O 14 14	0
61	W	15	Total O 15 15	0
61	X	28	Total O 28 28	0
61	Y	2	Total O 2 2	0
61	Z	59	Total O 59 59	0
61	a	27	Total O 27 27	0
61	b	5	Total O 5 5	0
61	c	1	Total O 1 1	0
61	d	28	Total O 28 28	0
61	e	30	Total O 30 30	0
61	f	4	Total O 4 4	0
61	g	13	Total O 13 13	0
61	h	30	Total O 30 30	0
61	i	5	Total O 5 5	0

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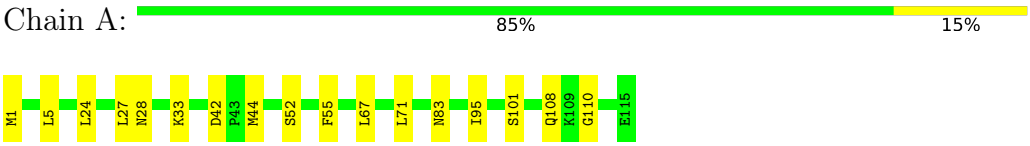
Mol	Chain	Residues	Atoms	AltConf
61	l	16	Total O 16 16	0
61	m	20	Total O 20 20	0
61	n	21	Total O 21 21	0
61	o	1	Total O 1 1	0
61	p	40	Total O 40 40	0
61	q	32	Total O 32 32	0
61	r	24	Total O 24 24	0
61	s	4	Total O 4 4	0

3 Residue-property plots (i)

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

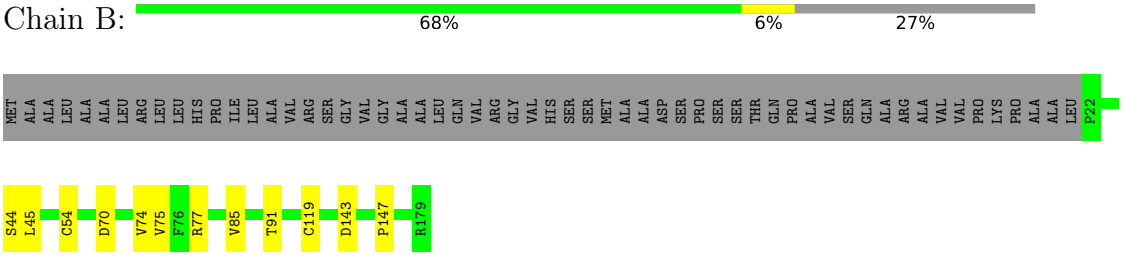
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



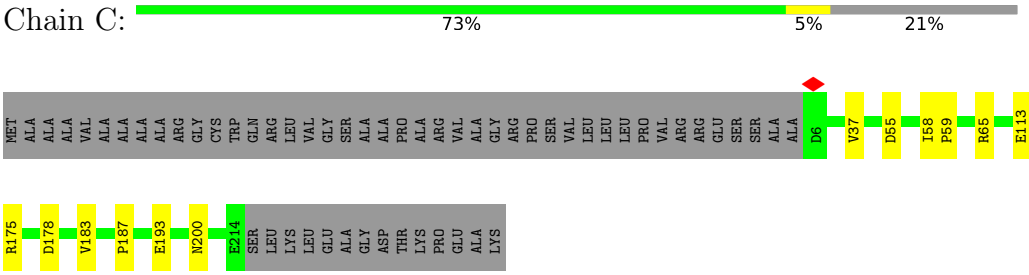
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



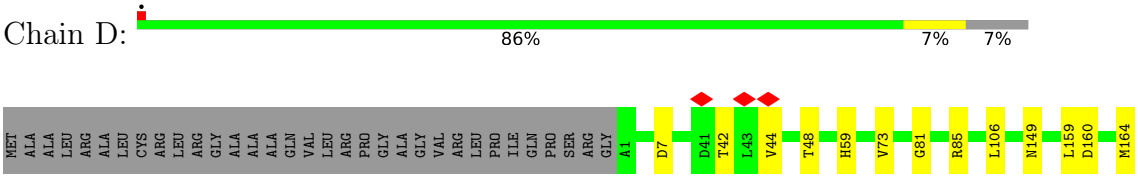
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

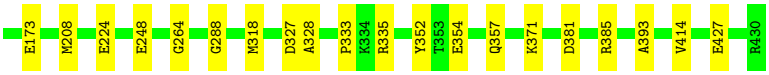
Chain C:



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

Chain D:





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

Chain E:

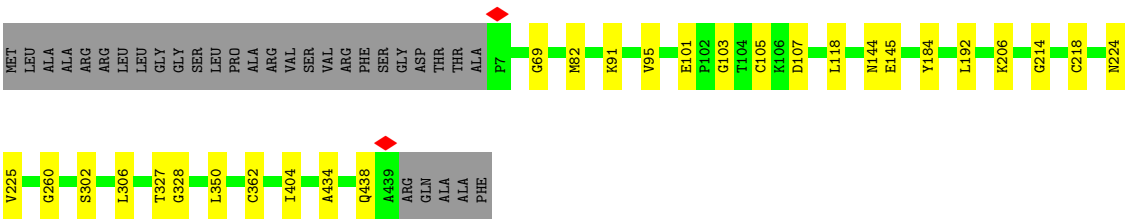




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

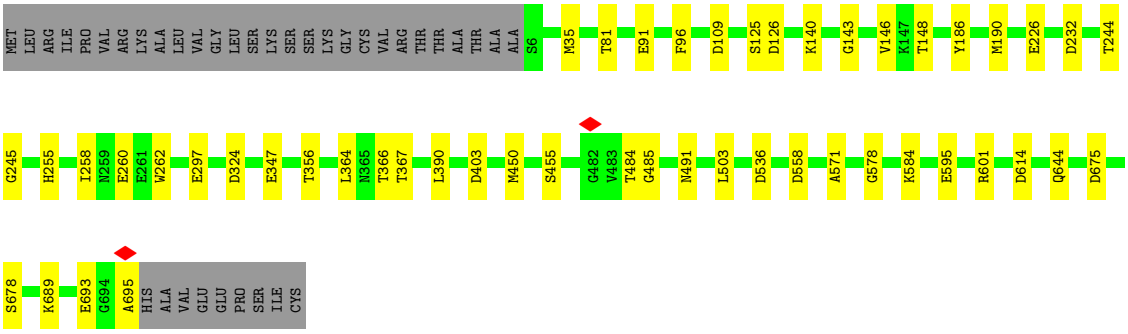




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

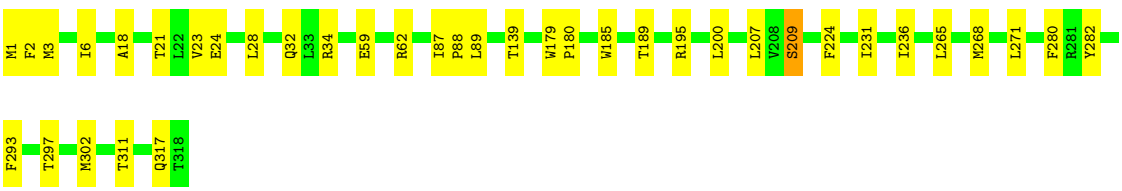




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

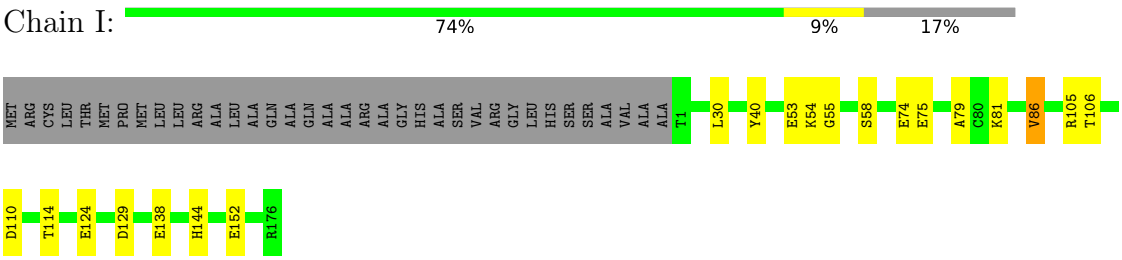
Chain H:





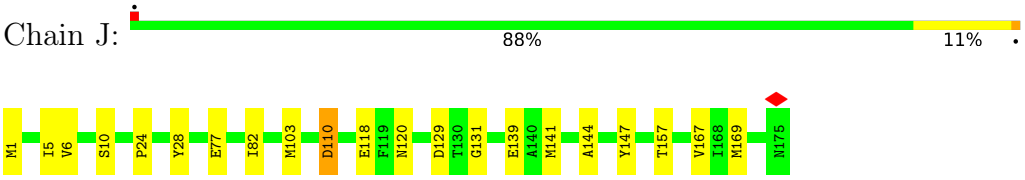
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



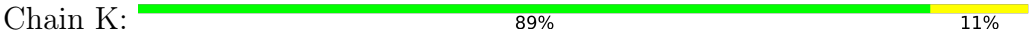
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

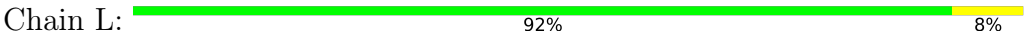
Chain K:

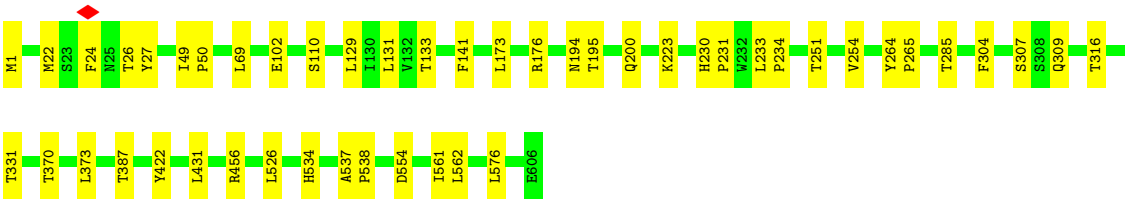




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

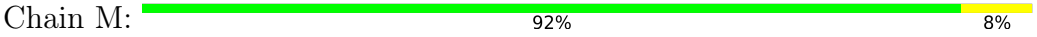
Chain L:

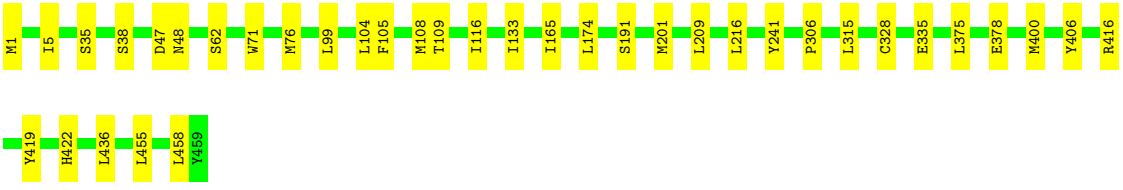




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

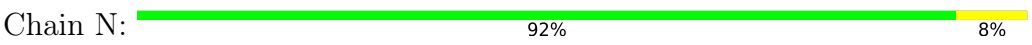
Chain M:





• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

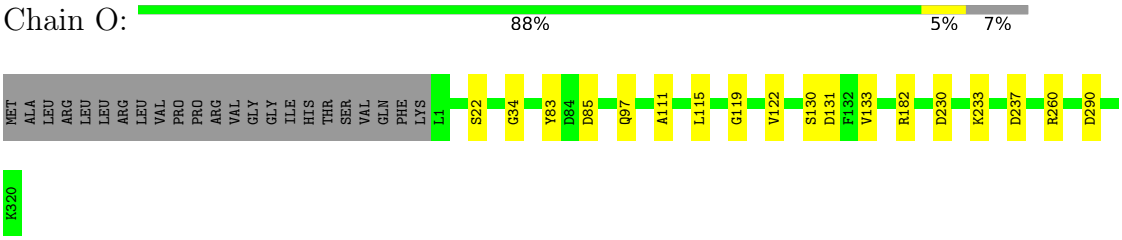
Chain N:





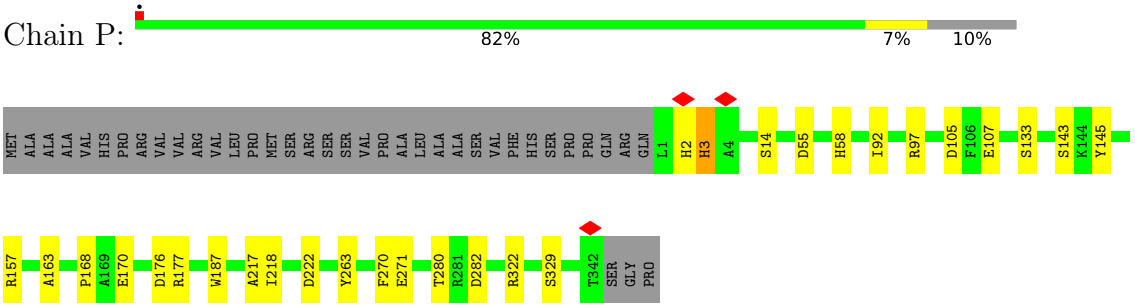
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:



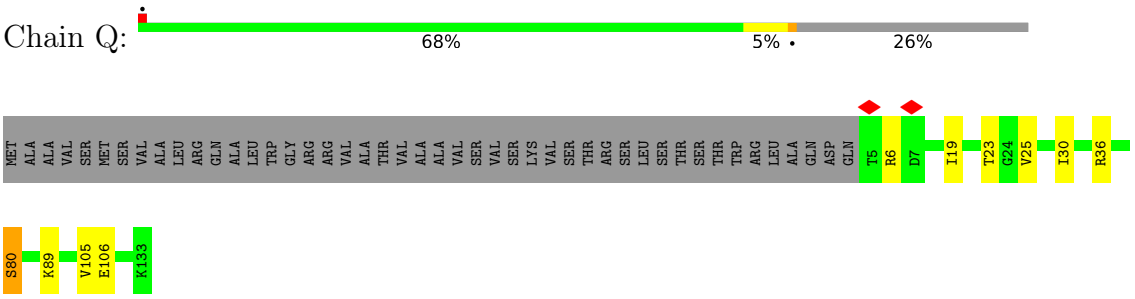
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



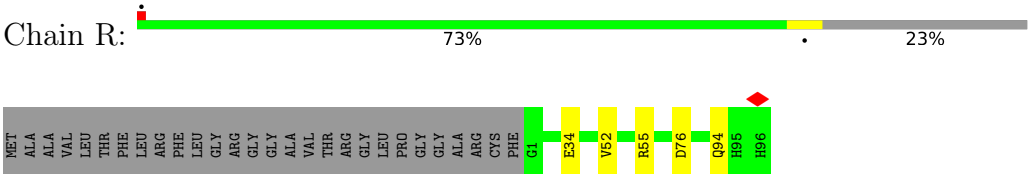
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



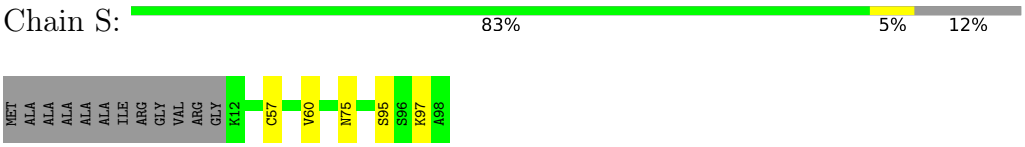
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



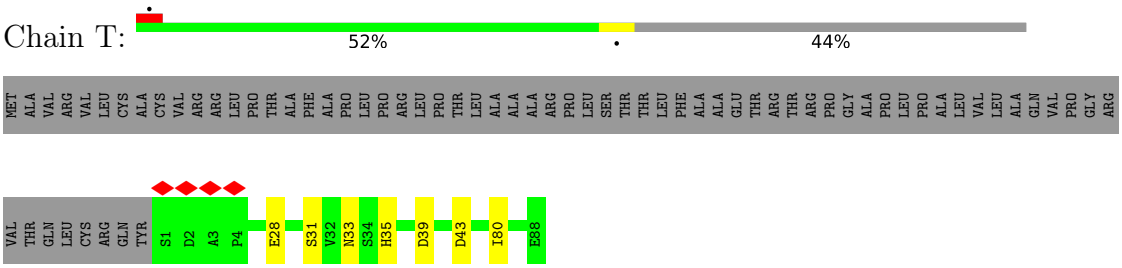
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



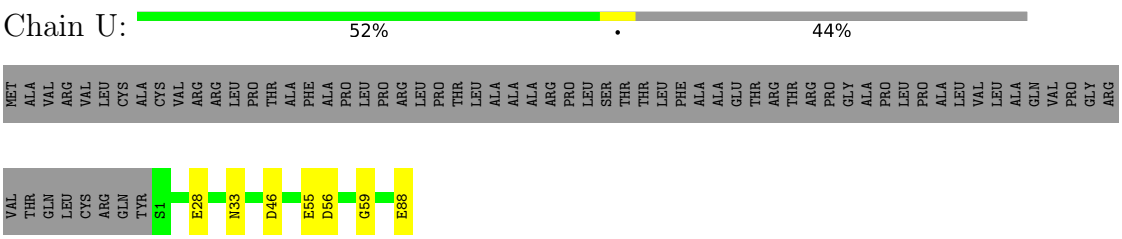
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



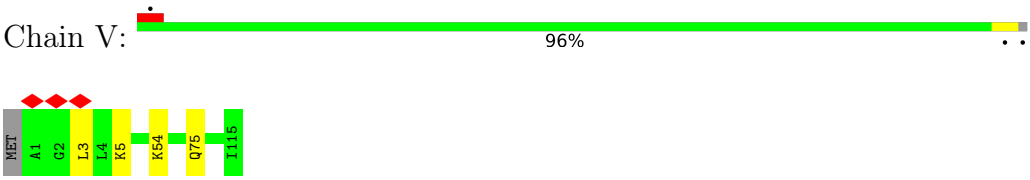
• Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



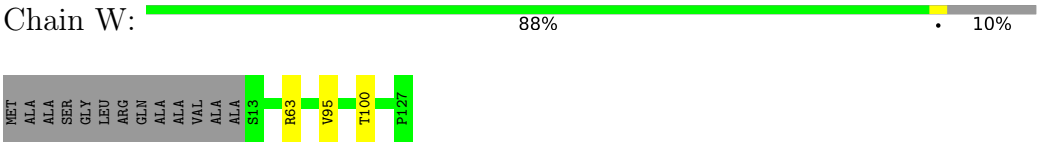
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



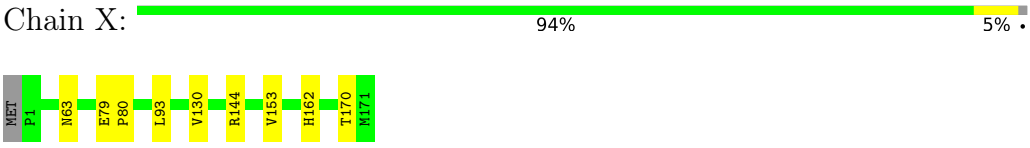
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



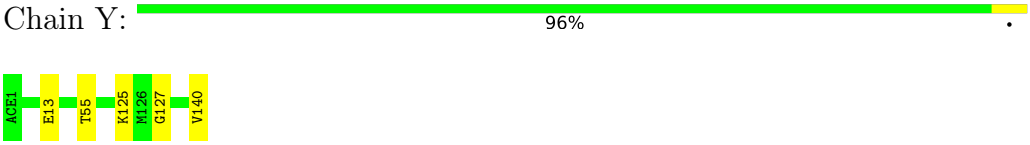
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



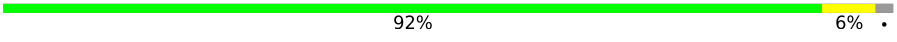
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



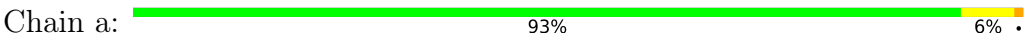
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

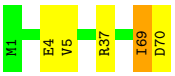
Chain Z:



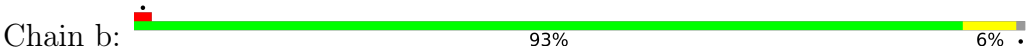


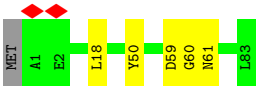
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1





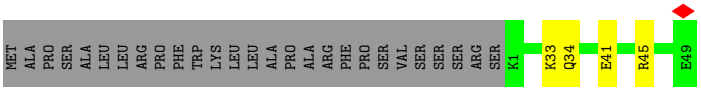
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



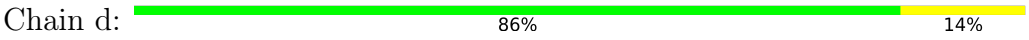


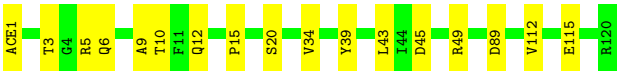
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



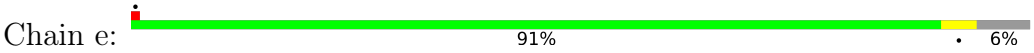


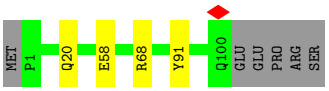
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



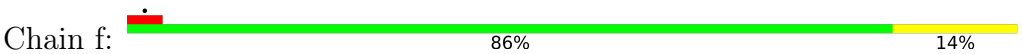


• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5





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

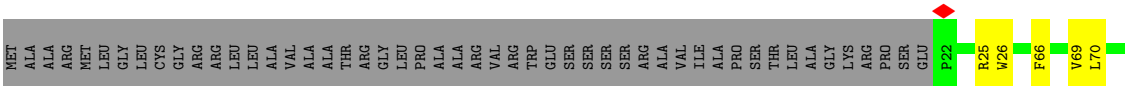


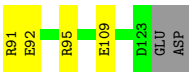


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



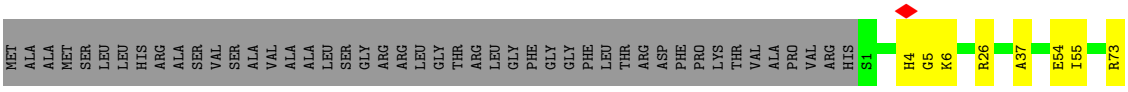


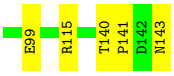


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:

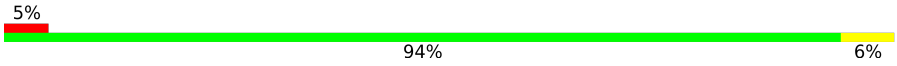






• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:

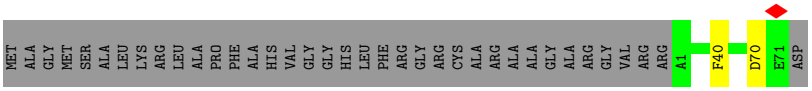




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:

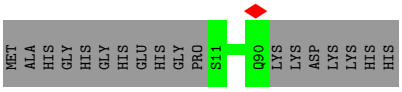




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:

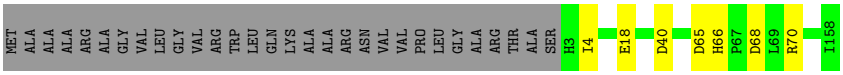




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

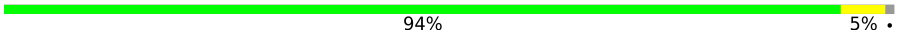
Chain l:

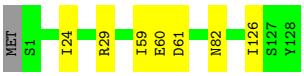




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:

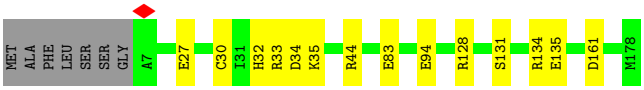




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

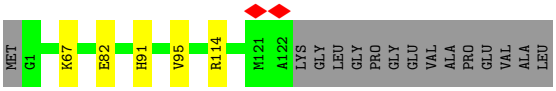




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

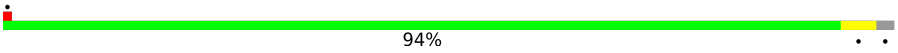
Chain o:





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

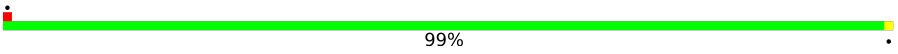
Chain p:

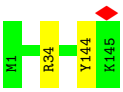




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:





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

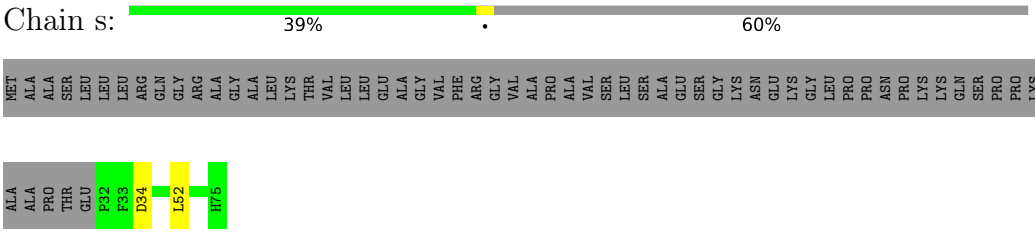
Chain r:





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

Chain s:


39%
60%
MET ALA ALA SER LEU LEU LEU ARG GLN GLY ARG ALA GLY ALA LEU LYS THR VAL LEU LEU GLU ALA GLY VAL PHE ARG GLY VAL ALA PRO ALA VAL SER LEU SER ALA GLU SER GLY LYS ASN GLU LYS GLY LEU PRO PRO ASN PRO LYS LYS GLN SER PRO PRO LYS LYS PRO VAL SER
ALA ALA PRO THR GLU P32 F33 D34 L52 H75

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.29	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	38.059	Depositor
Minimum map value	-14.540	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.938	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75375, 0.75375, 0.75375	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, DGT, NDP, ZN, SF4, ACE, 3PE, CDL, FES, MYR, U10, 2MR, FME, WYK, CHD, MG, FMN, EHZ, NAI, K

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	0.23	1/936 (0.1%)	0.29	0/1281
2	B	0.11	0/1280	0.29	0/1730
3	C	0.10	0/1789	0.30	0/2436
4	D	0.10	0/3537	0.25	0/4794
5	E	0.11	0/1708	0.31	0/2324
6	F	0.09	0/3406	0.28	0/4602
7	G	0.10	0/5376	0.29	0/7286
8	H	0.09	0/2571	0.28	0/3513
9	I	0.11	0/1445	0.27	0/1956
10	J	0.08	0/1370	0.22	0/1859
11	K	0.09	0/745	0.26	0/1008
12	L	0.10	0/4920	0.29	0/6694
13	M	0.08	0/3738	0.25	0/5097
14	N	0.10	0/2792	0.26	0/3800
15	O	0.12	0/2651	0.27	0/3587
16	P	0.11	0/2831	0.26	0/3841
17	Q	0.09	0/1072	0.25	0/1449
18	R	0.13	0/753	0.25	0/1014
19	S	0.10	0/711	0.31	0/956
20	T	0.14	0/719	0.39	0/971
20	U	0.12	0/719	0.32	0/971
21	V	0.10	0/948	0.24	0/1284
22	W	0.12	0/1000	0.31	0/1344
23	X	0.10	0/1439	0.27	0/1942
24	Y	0.19	0/1048	0.29	0/1423
25	Z	0.10	0/1181	0.26	0/1592
26	a	0.12	0/584	0.27	0/786
27	b	0.13	0/672	0.32	0/923
28	c	0.12	0/427	0.22	0/579
29	d	0.19	1/1027 (0.1%)	0.27	0/1387
30	e	0.09	0/859	0.25	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.12	0/505	0.36	0/681
32	g	0.11	0/881	0.31	0/1197
33	h	0.10	0/1221	0.27	0/1651
34	i	0.19	1/1134 (0.1%)	0.32	0/1544
35	j	0.13	0/624	0.31	0/855
36	k	0.10	0/663	0.29	0/895
37	l	0.11	0/1369	0.29	0/1873
38	m	0.10	0/1094	0.25	0/1480
39	n	0.10	0/1545	0.29	0/2092
40	o	0.10	0/1073	0.28	0/1437
41	p	0.09	0/1486	0.26	0/2004
42	q	0.12	0/1250	0.26	0/1698
43	r	0.22	1/804 (0.1%)	0.29	0/1088
44	s	0.09	0/383	0.24	0/518
All	All	0.11	4/68286 (0.0%)	0.28	0/92590

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
15	O	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	PHE	C-N	-6.36	1.25	1.33
29	d	1	ACE	C-N	5.02	1.45	1.34
43	r	1	ACE	C-N	5.00	1.45	1.34
34	i	1	ACE	C-N	5.00	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	182	ARG	Sidechain

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	921	0	952	14	0
2	B	1261	0	1256	10	0
3	C	1738	0	1685	12	0
4	D	3459	0	3404	30	0
5	E	1668	0	1672	13	0
6	F	3331	0	3287	21	0
7	G	5288	0	5309	34	0
8	H	2509	0	2621	26	0
9	I	1414	0	1370	15	0
10	J	1345	0	1352	21	0
11	K	745	0	785	10	0
12	L	4802	0	4960	28	0
13	M	3654	0	3852	27	0
14	N	2733	0	2912	24	0
15	O	2589	0	2565	13	0
16	P	2754	0	2773	23	0
17	Q	1049	0	1045	8	0
18	R	740	0	714	3	0
19	S	700	0	719	3	0
20	T	707	0	700	4	0
20	U	707	0	700	6	0
21	V	928	0	972	3	0
22	W	976	0	991	2	0
23	X	1402	0	1379	7	0
24	Y	1030	0	1039	4	0
25	Z	1152	0	1151	7	0
26	a	569	0	568	4	0
27	b	651	0	662	3	0
28	c	414	0	415	2	0
29	d	999	0	988	10	0
30	e	838	0	837	4	0
31	f	492	0	501	5	0
32	g	854	0	802	7	0
33	h	1186	0	1193	11	0
34	i	1097	0	1108	5	0
35	j	597	0	536	1	0
36	k	644	0	626	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l	1314	0	1210	6	0
38	m	1067	0	1067	7	0
39	n	1492	0	1438	9	0
40	o	1048	0	1016	4	0
41	p	1453	0	1425	6	0
42	q	1209	0	1182	2	0
43	r	785	0	795	4	0
44	s	371	0	344	2	0
45	A	47	0	71	1	0
45	H	34	0	42	2	0
45	I	45	0	67	1	0
45	K	42	0	58	0	0
45	L	153	0	208	4	0
45	M	50	0	77	0	0
45	N	49	0	75	0	0
45	P	35	0	44	3	0
45	Y	224	0	298	7	0
45	b	39	0	52	0	0
45	d	49	0	75	1	0
45	m	41	0	59	0	0
46	A	70	0	88	3	0
46	B	44	0	62	0	0
46	H	44	0	62	0	0
46	I	40	0	54	1	0
46	M	42	0	61	0	0
46	N	39	0	52	2	0
46	P	79	0	106	5	0
46	h	44	0	62	1	0
46	q	49	0	75	0	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	1	0
48	D	63	0	90	8	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	1	0
51	F	44	0	25	3	0
52	G	1	0	0	0	0
53	H	69	0	85	2	0
53	L	78	0	103	2	0
53	N	227	0	301	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	X	86	0	125	4	0
53	h	78	0	100	3	0
53	q	61	0	66	3	0
54	O	31	0	12	3	0
55	O	1	0	0	0	0
56	P	48	0	26	1	0
57	R	1	0	0	0	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	i	29	0	38	3	0
60	o	15	0	27	0	0
61	A	40	0	0	2	0
61	B	80	0	0	4	0
61	C	108	0	0	6	0
61	D	203	0	0	15	0
61	E	30	0	0	2	0
61	F	73	0	0	6	0
61	G	207	0	0	13	0
61	H	110	0	0	6	0
61	I	101	0	0	5	0
61	J	47	0	0	8	0
61	K	31	0	0	1	0
61	L	78	0	0	4	0
61	M	132	0	0	6	0
61	N	92	0	0	5	0
61	O	22	0	0	2	0
61	P	90	0	0	8	0
61	Q	108	0	0	1	0
61	R	26	0	0	1	0
61	V	14	0	0	1	0
61	W	15	0	0	0	0
61	X	28	0	0	1	0
61	Y	2	0	0	0	0
61	Z	59	0	0	3	0
61	a	27	0	0	2	0
61	b	5	0	0	0	0
61	c	1	0	0	0	0
61	d	28	0	0	1	0
61	e	30	0	0	1	0
61	f	4	0	0	1	0
61	g	13	0	0	1	0
61	h	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	i	5	0	0	0	0
61	l	16	0	0	1	0
61	m	20	0	0	2	0
61	n	21	0	0	3	0
61	o	1	0	0	0	0
61	p	40	0	0	2	0
61	q	32	0	0	0	0
61	r	24	0	0	1	0
61	s	4	0	0	0	0
All	All	70931	0	69643	437	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 (437) 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)
15:O:83:TYR:HH	54:O:401:DGT:HO3'	1.18	0.84
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.62	0.82
16:P:143:SER:OG	16:P:282:ASP:OD1	1.98	0.81
25:Z:92:GLU:OE1	30:e:91:TYR:OH	1.99	0.80
33:h:143:ASN:OD1	61:h:301:HOH:O	2.02	0.77
7:G:675:ASP:OD1	7:G:678:SER:OG	2.02	0.77
18:R:34:GLU:OE2	61:R:301:HOH:O	2.03	0.77
10:J:139:GLU:OE1	61:J:201:HOH:O	2.04	0.76
10:J:77:GLU:OE2	61:J:202:HOH:O	2.04	0.76
12:L:194:ASN:O	61:L:801:HOH:O	2.05	0.75
16:P:58:HIS:O	61:P:502:HOH:O	2.04	0.75
4:D:173:GLU:OE2	61:D:801:HOH:O	2.03	0.75
4:D:288:GLY:O	61:D:805:HOH:O	2.05	0.74
9:I:124:GLU:OE2	61:I:301:HOH:O	2.03	0.74
4:D:159:LEU:O	61:D:802:HOH:O	2.04	0.74
4:D:81:GLY:O	61:D:806:HOH:O	2.06	0.74
4:D:381:ASP:O	61:D:803:HOH:O	2.05	0.74
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.20	0.74
4:D:333:PRO:O	61:D:804:HOH:O	2.05	0.73
7:G:366:THR:O	7:G:367:THR:OG1	2.06	0.73
10:J:131:GLY:O	61:J:203:HOH:O	2.06	0.73
5:E:158:ASP:O	61:E:401:HOH:O	2.05	0.73
14:N:255:PRO:O	61:N:1001:HOH:O	2.06	0.73
10:J:144:ALA:O	61:J:204:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:22:SER:OG	15:O:119:GLY:O	2.03	0.73
13:M:419:TYR:O	61:M:601:HOH:O	2.06	0.73
11:K:57:SER:OG	61:K:201:HOH:O	2.07	0.73
33:h:140:THR:O	33:h:143:ASN:ND2	2.21	0.73
41:p:90:GLN:OE1	61:p:201:HOH:O	2.07	0.73
4:D:393:ALA:O	61:D:807:HOH:O	2.07	0.72
16:P:322:ARG:O	61:P:503:HOH:O	2.07	0.72
2:B:147:PRO:O	61:B:303:HOH:O	2.07	0.72
14:N:317:PHE:O	61:N:1002:HOH:O	2.07	0.72
2:B:143:ASP:OD2	61:B:301:HOH:O	2.06	0.72
4:D:248:GLU:OE2	61:D:808:HOH:O	2.08	0.72
30:e:20:GLN:O	61:e:201:HOH:O	2.08	0.72
31:f:31:ASP:OD2	61:f:101:HOH:O	2.07	0.72
7:G:91:GLU:OE2	61:G:903:HOH:O	2.07	0.72
7:G:584:LYS:NZ	61:G:915:HOH:O	2.22	0.72
1:A:42:ASP:OD1	61:A:301:HOH:O	2.08	0.71
2:B:44:SER:O	61:B:302:HOH:O	2.07	0.71
4:D:160:ASP:OD2	61:D:809:HOH:O	2.08	0.71
9:I:74:GLU:OE1	61:I:302:HOH:O	2.08	0.71
7:G:186:TYR:OH	61:G:902:HOH:O	2.07	0.71
10:J:24:PRO:O	61:J:205:HOH:O	2.08	0.71
37:l:65:ASP:OD2	61:l:201:HOH:O	2.08	0.71
7:G:260:GLU:OE1	61:G:905:HOH:O	2.08	0.71
39:n:94:GLU:O	61:n:201:HOH:O	2.09	0.71
53:L:702:CDL:H462	53:h:201:CDL:H762	1.73	0.70
15:O:290:ASP:OD1	61:O:501:HOH:O	2.08	0.70
5:E:134:ASP:N	5:E:134:ASP:OD1	2.24	0.70
21:V:54:LYS:NZ	61:V:201:HOH:O	2.24	0.70
25:Z:122:GLU:OE2	61:Z:201:HOH:O	2.09	0.70
7:G:96:PHE:O	61:G:904:HOH:O	2.08	0.70
10:J:103:MET:HE2	11:K:10:MET:HE2	1.74	0.70
5:E:45:ALA:O	61:E:402:HOH:O	2.10	0.69
7:G:146:VAL:O	61:G:906:HOH:O	2.09	0.69
14:N:269:GLU:OE1	61:N:1003:HOH:O	2.09	0.69
16:P:170:GLU:OE2	61:P:504:HOH:O	2.09	0.69
8:H:59:GLU:OE2	61:H:701:HOH:O	2.10	0.69
10:J:129:ASP:OD1	61:J:206:HOH:O	2.10	0.69
4:D:248:GLU:O	61:D:811:HOH:O	2.10	0.69
2:B:70:ASP:OD2	61:B:304:HOH:O	2.11	0.69
4:D:264:GLY:O	61:D:812:HOH:O	2.11	0.69
23:X:93:LEU:O	61:X:301:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:117:THR:O	61:Z:202:HOH:O	2.11	0.68
29:d:115:GLU:O	61:d:301:HOH:O	2.10	0.68
1:A:42:ASP:OD2	61:A:302:HOH:O	2.10	0.68
46:P:402:PC1:O12	61:P:505:HOH:O	2.10	0.68
10:J:141:MET:O	61:J:207:HOH:O	2.12	0.67
16:P:14:SER:OG	61:P:501:HOH:O	2.03	0.67
3:C:200:ASN:O	61:C:301:HOH:O	2.13	0.67
4:D:327:ASP:OD2	61:D:813:HOH:O	2.13	0.67
8:H:18:ALA:O	8:H:21:THR:OG1	2.12	0.67
13:M:241:TYR:OH	61:M:602:HOH:O	2.12	0.67
38:m:61:ASP:OD2	61:m:301:HOH:O	2.13	0.67
13:M:201:MET:HG3	45:Y:201:3PE:H2F2	1.75	0.67
33:h:141:PRO:O	61:h:303:HOH:O	2.14	0.66
53:H:602:CDL:OB3	61:H:702:HOH:O	2.12	0.66
3:C:159:GLY:O	61:C:302:HOH:O	2.14	0.66
12:L:309:GLN:NE2	61:L:805:HOH:O	2.28	0.66
6:F:101:GLU:O	61:F:601:HOH:O	2.13	0.66
9:I:152:GLU:OE1	61:I:303:HOH:O	2.12	0.66
45:L:701:3PE:N	61:L:806:HOH:O	2.28	0.66
14:N:336:MET:HE1	53:N:905:CDL:H461	1.78	0.66
38:m:126:ILE:O	61:m:302:HOH:O	2.14	0.66
16:P:217:ALA:O	61:P:506:HOH:O	2.14	0.65
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.30	0.65
7:G:232:ASP:O	61:G:907:HOH:O	2.12	0.65
9:I:110:ASP:OD1	61:I:304:HOH:O	2.14	0.65
7:G:109:ASP:OD2	61:G:909:HOH:O	2.15	0.65
39:n:128:ARG:O	61:n:202:HOH:O	2.13	0.65
51:F:503:NAI:O2A	61:F:602:HOH:O	2.14	0.65
7:G:595:GLU:OE2	61:G:908:HOH:O	2.15	0.65
59:i:201:CHD:H212	59:i:201:CHD:H12	1.78	0.65
7:G:244:THR:O	61:G:910:HOH:O	2.15	0.64
12:L:251:THR:O	12:L:254:VAL:HG22	1.97	0.64
13:M:48:ASN:OD1	61:M:603:HOH:O	2.15	0.64
4:D:224:GLU:OE1	9:I:40:TYR:OH	2.11	0.63
14:N:263:LYS:NZ	61:N:1007:HOH:O	2.23	0.63
16:P:177:ARG:NH2	61:P:510:HOH:O	2.29	0.63
7:G:644:GLN:N	7:G:644:GLN:OE1	2.31	0.63
34:i:105:PRO:O	40:o:67:LYS:NZ	2.31	0.63
4:D:381:ASP:OD2	61:D:814:HOH:O	2.16	0.63
4:D:385:ARG:NH2	61:D:819:HOH:O	2.32	0.62
6:F:144:ASN:ND2	61:F:606:HOH:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:LEU:HD22	2:B:85:VAL:CG2	2.30	0.62
8:H:282:TYR:OH	61:H:704:HOH:O	2.13	0.61
15:O:260:ARG:NH1	61:O:503:HOH:O	2.31	0.61
35:j:70:ASP:OD2	40:o:114:ARG:NH2	2.33	0.61
5:E:105:THR:HG22	5:E:106:THR:H	1.64	0.61
53:N:902:CDL:OB3	61:N:1004:HOH:O	2.16	0.61
3:C:113:GLU:OE1	61:C:303:HOH:O	2.16	0.61
14:N:215:MET:HE2	14:N:218:MET:CE	2.31	0.61
13:M:35:SER:O	13:M:38:SER:OG	2.18	0.60
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.83	0.60
39:n:83:GLU:OE1	61:n:203:HOH:O	2.16	0.60
12:L:26:THR:HG22	12:L:27:TYR:H	1.67	0.60
29:d:9:ALA:HB1	29:d:12:GLN:NE2	2.17	0.60
37:l:18:GLU:N	37:l:18:GLU:OE1	2.33	0.60
12:L:22:MET:SD	12:L:27:TYR:OH	2.53	0.60
12:L:173:LEU:HD23	45:L:701:3PE:H322	1.85	0.59
14:N:215:MET:HE2	14:N:218:MET:HE1	1.84	0.59
24:Y:127:GLY:HA3	45:Y:204:3PE:H241	1.83	0.59
10:J:10:SER:OG	11:K:7:ASN:ND2	2.35	0.59
26:a:37:ARG:NE	61:a:106:HOH:O	2.36	0.59
16:P:270:PHE:CD1	46:P:401:PC1:H351	2.38	0.59
7:G:689:LYS:NZ	7:G:693:GLU:OE2	2.28	0.58
9:I:55:GLY:O	61:I:305:HOH:O	2.17	0.58
48:D:701:U10:C13	48:D:701:U10:H101	2.33	0.58
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.36	0.58
7:G:140:LYS:O	7:G:148:THR:OG1	2.17	0.58
38:m:24:ILE:HD13	38:m:29:ARG:NE	2.19	0.58
29:d:5:ARG:NH1	29:d:89:ASP:OD1	2.37	0.57
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.36	0.57
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.33	0.57
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.87	0.57
33:h:54:GLU:OE2	33:h:55:ILE:N	2.38	0.57
15:O:230:ASP:OD1	15:O:233:LYS:N	2.37	0.56
7:G:578:GLY:O	61:G:911:HOH:O	2.17	0.56
14:N:261:MET:HE1	45:d:201:3PE:H2I1	1.85	0.56
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.39	0.56
10:J:157:THR:HG22	11:K:66:PHE:HE2	1.71	0.56
10:J:110:ASP:OD1	10:J:110:ASP:N	2.38	0.56
46:P:401:PC1:O22	46:P:401:PC1:H32	2.04	0.56
20:U:88:GLU:OE2	33:h:6:LYS:NZ	2.39	0.56
8:H:32:GLN:OE1	8:H:34:ARG:NH2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.41	0.55
14:N:336:MET:HE1	53:N:905:CDL:C46	2.36	0.55
43:r:69:MET:SD	43:r:70:SER:N	2.80	0.55
13:M:105:PHE:O	13:M:109:THR:OG1	2.15	0.55
17:Q:106:GLU:OE2	61:Q:201:HOH:O	2.18	0.55
8:H:311:THR:OG1	25:Z:50:MET:SD	2.65	0.54
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.39	0.54
48:D:701:U10:H402	8:H:224:PHE:CD2	2.42	0.54
13:M:416:ARG:O	61:M:604:HOH:O	2.18	0.54
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.54
3:C:175:ARG:NH1	61:C:311:HOH:O	2.39	0.54
6:F:82:MET:O	6:F:91:LYS:NZ	2.31	0.54
7:G:226:GLU:OE1	17:Q:36:ARG:NH2	2.40	0.54
53:N:905:CDL:C14	53:N:905:CDL:H711	2.37	0.53
1:A:83:ASN:ND2	46:A:203:PC1:O14	2.41	0.53
26:a:4:GLU:OE2	61:a:101:HOH:O	2.18	0.53
39:n:131:SER:OG	39:n:135:GLU:OE2	2.26	0.53
3:C:187:PRO:O	61:C:304:HOH:O	2.19	0.53
1:A:5:LEU:HD21	8:H:3:MET:SD	2.49	0.52
6:F:69:GLY:O	51:F:503:NAI:H2N	2.09	0.52
6:F:306:LEU:O	61:F:603:HOH:O	2.19	0.52
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.74	0.52
20:T:28:GLU:N	20:T:28:GLU:OE1	2.42	0.52
53:X:201:CDL:OB4	31:f:29:LYS:NZ	2.38	0.52
14:N:21:MET:HE1	46:N:904:PC1:H3B1	1.90	0.52
37:l:68:ASP:OD1	37:l:68:ASP:N	2.43	0.52
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.44	0.52
20:T:35:HIS:N	20:T:39:ASP:OD2	2.42	0.52
8:H:185:TRP:O	8:H:189:THR:HG23	2.09	0.52
9:I:79:ALA:HB2	9:I:106:THR:HG23	1.91	0.52
12:L:176:ARG:NH1	13:M:400:MET:O	2.43	0.52
15:O:85:ASP:OD1	15:O:85:ASP:N	2.42	0.52
16:P:55:ASP:OD2	61:P:507:HOH:O	2.18	0.52
10:J:120:ASN:O	61:J:208:HOH:O	2.19	0.51
4:D:42:THR:O	4:D:42:THR:HG23	2.09	0.51
7:G:356:THR:HG21	7:G:503:LEU:HD22	1.92	0.51
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.93	0.51
18:R:52:VAL:O	18:R:94:GLN:N	2.44	0.51
6:F:184:TYR:OH	51:F:503:NAI:H5N	2.11	0.51
16:P:187:TRP:CD1	45:P:404:3PE:H242	2.45	0.51
19:S:95:SER:O	19:S:97:LYS:NZ	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:265:LEU:CD1	45:H:601:3PE:H271	2.41	0.51
8:H:200:LEU:HD21	8:H:280:PHE:O	2.11	0.51
16:P:271:GLU:HG2	16:P:280:THR:HG22	1.93	0.51
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.45	0.50
15:O:83:TYR:OH	54:O:401:DGT:O3'	1.98	0.50
29:d:9:ALA:HB3	29:d:15:PRO:HG3	1.93	0.50
39:n:134:ARG:NH1	39:n:161:ASP:OD1	2.44	0.50
34:i:124:ASP:OD1	34:i:125:GLN:N	2.45	0.50
37:l:40:ASP:O	38:m:82:ASN:ND2	2.44	0.50
48:D:701:U10:H312	48:D:701:U10:H251	1.93	0.50
3:C:193:GLU:OE2	17:Q:80:SER:OG	2.21	0.50
5:E:55:GLN:NE2	5:E:91:ASN:OD1	2.44	0.50
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.93	0.50
13:M:335:GLU:OE2	61:M:606:HOH:O	2.19	0.50
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.93	0.50
46:I:204:PC1:O13	46:I:204:PC1:H152	2.12	0.50
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.50
45:Y:202:3PE:H231	45:Y:202:3PE:C3	2.42	0.49
1:A:44:MET:CE	4:D:48:THR:HG22	2.42	0.49
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.45	0.49
23:X:170:THR:OG1	53:X:201:CDL:OA3	2.13	0.49
46:A:202:PC1:O13	46:A:202:PC1:H133	2.13	0.49
5:E:111:ARG:NH1	6:F:260:GLY:O	2.45	0.49
5:E:79:ARG:NH1	5:E:82:GLU:OE2	2.44	0.49
7:G:484:THR:HG22	7:G:485:GLY:H	1.76	0.49
39:n:34:ASP:OD1	39:n:35:LYS:N	2.45	0.49
1:A:27:LEU:HD12	46:A:202:PC1:H131	1.94	0.49
5:E:55:GLN:O	5:E:59:GLY:N	2.38	0.49
18:R:55:ARG:NH2	18:R:76:ASP:OD2	2.46	0.49
48:D:701:U10:H202	48:D:701:U10:H161	1.94	0.49
6:F:206:LYS:NZ	61:F:608:HOH:O	2.43	0.49
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.39	0.49
40:o:91:HIS:O	40:o:95:VAL:HG23	2.13	0.49
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.46	0.48
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.94	0.48
32:g:91:ARG:NH2	61:g:202:HOH:O	2.46	0.48
7:G:190:MET:HE3	7:G:695:ALA:HB2	1.93	0.48
21:V:3:LEU:HD23	21:V:3:LEU:H	1.78	0.48
37:l:4:ILE:HD11	38:m:60:GLU:OE2	2.13	0.48
20:U:28:GLU:N	20:U:28:GLU:OE1	2.44	0.48
32:g:109:GLU:O	41:p:141:ARG:NE	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Z:202:HOH:O	30:e:68:ARG:NH2	2.45	0.48
32:g:25:ARG:O	32:g:26:TRP:CG	2.66	0.48
4:D:7:ASP:OD1	4:D:7:ASP:N	2.45	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
16:P:105:ASP:OD1	16:P:107:GLU:N	2.47	0.48
45:Y:203:3PE:H2B1	45:Y:204:3PE:H382	1.95	0.48
25:Z:67:ARG:NH2	27:b:50:TYR:O	2.47	0.48
1:A:28:ASN:O	1:A:33:LYS:NZ	2.46	0.48
6:F:145:GLU:OE1	6:F:145:GLU:N	2.41	0.48
9:I:30:LEU:HD13	45:I:201:3PE:H251	1.95	0.48
45:Y:203:3PE:H2I3	45:Y:204:3PE:H342	1.96	0.48
29:d:9:ALA:HB1	29:d:12:GLN:CD	2.38	0.48
6:F:118:LEU:HD13	6:F:225:VAL:HG13	1.96	0.47
53:h:201:CDL:H771	53:h:201:CDL:H732	1.96	0.47
16:P:2:HIS:O	16:P:3:HIS:HB3	2.15	0.47
23:X:144:ARG:NH2	30:e:58:GLU:OE1	2.47	0.47
7:G:245:GLY:O	61:G:912:HOH:O	2.20	0.47
8:H:23:VAL:HG11	8:H:268:MET:HE1	1.97	0.47
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.96	0.47
34:i:85:LEU:HD23	34:i:89:VAL:HG21	1.97	0.47
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.97	0.47
29:d:112:VAL:O	41:p:159:LYS:NZ	2.48	0.47
8:H:139:THR:OG1	61:H:703:HOH:O	2.12	0.47
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.46
13:M:47:ASP:OD1	13:M:48:ASN:N	2.48	0.46
34:i:65:ARG:HB3	59:i:201:CHD:H213	1.97	0.46
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.96	0.46
5:E:192:SER:OG	5:E:194:GLU:OE1	2.27	0.46
7:G:297:GLU:OE1	7:G:297:GLU:N	2.43	0.46
8:H:89:LEU:HD13	8:H:236:ILE:HG21	1.96	0.46
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.97	0.46
1:A:24:LEU:HD21	46:P:402:PC1:H3C2	1.97	0.46
1:A:110:GLY:HA3	10:J:169:MET:HE3	1.98	0.46
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.46
53:L:702:CDL:OB7	53:L:702:CDL:HB62	2.15	0.46
33:h:37:ALA:HA	53:h:201:CDL:H751	1.97	0.46
41:p:110:LYS:NZ	61:p:203:HOH:O	2.34	0.46
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.97	0.46
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.97	0.46
16:P:133:SER:O	16:P:168:PRO:HD2	2.15	0.46
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:P:401:PC1:H142	46:P:401:PC1:O13	2.15	0.46
2:B:91:THR:HA	2:B:119:CYS:HB3	1.97	0.46
9:I:54:LYS:NZ	9:I:138:GLU:OE2	2.49	0.46
43:r:2:SER:OG	61:r:201:HOH:O	2.19	0.46
10:J:157:THR:HG22	11:K:66:PHE:CE2	2.51	0.46
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.98	0.46
59:i:201:CHD:H212	59:i:201:CHD:C12	2.45	0.46
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.99	0.45
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.33	0.45
20:U:56:ASP:OD1	20:U:56:ASP:N	2.50	0.45
34:i:121:GLU:N	34:i:121:GLU:OE1	2.49	0.45
24:Y:55:THR:HG21	45:Y:205:3PE:H272	1.98	0.45
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.97	0.45
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.98	0.45
7:G:347:GLU:OE2	7:G:455:SER:OG	2.34	0.45
19:S:57:CYS:O	19:S:60:VAL:HG22	2.16	0.45
14:N:206:ILE:HD11	46:N:904:PC1:H382	1.98	0.45
45:Y:202:3PE:H231	45:Y:202:3PE:H31	1.99	0.45
12:L:69:LEU:HD21	13:M:455:LEU:HD11	1.98	0.45
40:o:82:GLU:N	40:o:82:GLU:OE1	2.50	0.45
53:q:202:CDL:H541	53:q:202:CDL:C73	2.46	0.45
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.45
7:G:558:ASP:OD1	42:q:144:TYR:OH	2.19	0.45
38:m:24:ILE:HD13	38:m:29:ARG:CZ	2.46	0.45
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.49	0.45
53:q:202:CDL:H541	53:q:202:CDL:H731	1.99	0.45
13:M:406:TYR:CD1	13:M:406:TYR:C	2.95	0.44
2:B:45:LEU:O	2:B:74:VAL:HA	2.18	0.44
7:G:143:GLY:HA2	7:G:190:MET:HE2	1.98	0.44
8:H:62:ARG:O	61:H:705:HOH:O	2.21	0.44
13:M:5:ILE:HG21	53:X:201:CDL:H612	1.97	0.44
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.00	0.44
14:N:237:THR:HG21	14:N:319:LEU:HD11	1.98	0.44
31:f:7:VAL:HG12	31:f:7:VAL:O	2.17	0.44
1:A:44:MET:HE3	4:D:48:THR:HG22	1.99	0.44
3:C:37:VAL:HG12	43:r:69:MET:CE	2.46	0.44
4:D:106:LEU:O	4:D:427:GLU:N	2.50	0.44
15:O:111:ALA:HB1	15:O:122:VAL:HG21	2.00	0.44
45:P:404:3PE:H231	45:P:404:3PE:H262	1.72	0.44
3:C:183:VAL:O	22:W:100:THR:OG1	2.31	0.44
6:F:192:LEU:C	6:F:192:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:33:ASN:OD1	20:U:33:ASN:N	2.51	0.44
16:P:176:ASP:OD1	16:P:177:ARG:N	2.50	0.44
12:L:534:HIS:ND1	45:L:701:3PE:O14	2.43	0.44
16:P:97:ARG:NH1	56:P:403:NDP:O2X	2.51	0.44
3:C:65:ARG:NH1	3:C:123:VAL:O	2.48	0.44
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.99	0.44
12:L:131:LEU:HD23	12:L:131:LEU:C	2.43	0.44
43:r:72:GLN:O	43:r:73:LYS:HB2	2.18	0.44
5:E:105:THR:HG22	5:E:106:THR:N	2.31	0.44
13:M:422:HIS:HB2	38:m:59:ILE:HD12	2.00	0.44
6:F:306:LEU:C	6:F:306:LEU:HD12	2.43	0.44
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.00	0.44
1:A:71:LEU:O	10:J:147:TYR:OH	2.32	0.43
4:D:328:ALA:HB3	7:G:126:ASP:HB2	2.00	0.43
16:P:222:ASP:OD1	16:P:222:ASP:N	2.42	0.43
11:K:66:PHE:CZ	14:N:31:ILE:HG23	2.52	0.43
16:P:157:ARG:NH1	16:P:163:ALA:O	2.51	0.43
3:C:178:ASP:OD1	61:C:305:HOH:O	2.21	0.43
6:F:214:GLY:N	6:F:218:CYS:O	2.51	0.43
12:L:24:PHE:O	33:h:26:ARG:HD3	2.18	0.43
2:B:45:LEU:HD22	2:B:85:VAL:HG21	2.00	0.43
10:J:28:TYR:CE2	10:J:82:ILE:HG22	2.54	0.43
37:l:66:HIS:O	37:l:70:ARG:N	2.51	0.43
20:U:46:ASP:OD1	39:n:44:ARG:NH2	2.46	0.43
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.99	0.43
53:q:202:CDL:H541	53:q:202:CDL:H742	2.00	0.43
48:D:701:U10:H101	48:D:701:U10:H13	1.99	0.43
19:S:75:ASN:OD1	19:S:75:ASN:N	2.50	0.43
29:d:45:ASP:OD1	29:d:49:ARG:NH1	2.46	0.43
5:E:34:ILE:HD11	44:s:52:LEU:HD22	2.00	0.43
13:M:108:MET:HE1	53:X:201:CDL:H242	2.00	0.43
16:P:176:ASP:O	16:P:177:ARG:HB2	2.18	0.43
4:D:44:VAL:O	4:D:44:VAL:HG13	2.19	0.43
48:D:701:U10:H201	48:D:701:U10:C23	2.49	0.43
13:M:165:ILE:HG21	14:N:268:GLN:HA	2.01	0.43
14:N:72:MET:HE3	14:N:76:ILE:HD11	2.00	0.43
14:N:215:MET:CE	14:N:247:THR:HB	2.49	0.43
9:I:75:GLU:O	9:I:105:ARG:NH1	2.52	0.43
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.01	0.43
12:L:223:LYS:NZ	61:L:811:HOH:O	2.44	0.43
12:L:264:TYR:N	12:L:265:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.52	0.43
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	2.01	0.43
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.00	0.43
41:p:127:GLU:OE1	41:p:127:GLU:N	2.48	0.43
10:J:118:GLU:N	10:J:118:GLU:OE1	2.52	0.43
15:O:237:ASP:N	15:O:237:ASP:OD1	2.52	0.43
26:a:69:ILE:O	26:a:70:ASP:C	2.62	0.43
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.49	0.42
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.48	0.42
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.59	0.42
14:N:207:ILE:HD13	14:N:262:PRO:HD3	2.01	0.42
20:U:55:GLU:O	20:U:59:GLY:N	2.52	0.42
7:G:366:THR:HB	7:G:450:MET:HE3	2.01	0.42
13:M:5:ILE:HG23	13:M:104:LEU:HD11	2.01	0.42
13:M:306:PRO:HA	13:M:458:LEU:HD22	2.02	0.42
6:F:434:ALA:O	6:F:438:GLN:HG2	2.20	0.42
15:O:130:SER:O	15:O:133:VAL:HG22	2.20	0.42
24:Y:13:GLU:OE2	24:Y:125:LYS:NZ	2.44	0.42
32:g:66:PHE:HD1	32:g:70:LEU:HD12	1.84	0.42
5:E:148:CYS:SG	6:F:103:GLY:N	2.85	0.42
21:V:5:LYS:NZ	21:V:75:GLN:OE1	2.47	0.42
33:h:73:ARG:NH2	46:h:202:PC1:O12	2.43	0.42
8:H:293:PHE:O	8:H:297:THR:OG1	2.35	0.42
20:T:43:ASP:OD1	22:W:63:ARG:NH2	2.53	0.42
6:F:107:ASP:OD2	61:F:604:HOH:O	2.22	0.42
53:N:905:CDL:H473	29:d:34:VAL:HG22	2.00	0.42
16:P:2:HIS:O	16:P:3:HIS:CB	2.67	0.42
13:M:315:LEU:HD21	13:M:378:GLU:N	2.35	0.42
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.85	0.42
12:L:422:TYR:CD1	12:L:422:TYR:C	2.98	0.42
45:A:201:3PE:H262	27:b:18:LEU:HD22	2.02	0.41
7:G:364:LEU:HD12	7:G:491:ASN:HB3	2.01	0.41
8:H:265:LEU:HD12	45:H:601:3PE:H271	2.00	0.41
11:K:43:MET:SD	14:N:72:MET:HE1	2.59	0.41
32:g:26:TRP:CD1	32:g:26:TRP:C	2.97	0.41
8:H:317:GLN:NE2	61:H:716:HOH:O	2.43	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.34	0.41
11:K:37:MET:SD	14:N:68:MET:HE1	2.60	0.41
13:M:104:LEU:HG	13:M:108:MET:HE2	2.01	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.41
14:N:215:MET:HE1	14:N:244:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:MET:HE3	8:H:28:LEU:HD11	2.03	0.41
12:L:331:THR:HB	12:L:387:THR:HG22	2.02	0.41
13:M:133:ILE:HD13	61:M:685:HOH:O	2.20	0.41
13:M:216:LEU:HD23	13:M:216:LEU:C	2.45	0.41
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.54	0.41
7:G:324:ASP:OD2	61:G:913:HOH:O	2.22	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.35	0.41
20:T:33:ASN:OD1	20:T:33:ASN:N	2.53	0.41
27:b:59:ASP:OD1	27:b:60:GLY:N	2.53	0.41
4:D:73:VAL:HG21	4:D:414:VAL:HG21	2.02	0.41
48:D:701:U10:H521	48:D:701:U10:H501	1.86	0.41
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.56	0.41
58:T:101:EHZ:O3	58:T:101:EHZ:N2	2.50	0.41
7:G:35:MET:HE2	7:G:81:THR:HB	2.02	0.41
8:H:207:LEU:O	8:H:209:SER:N	2.53	0.41
13:M:116:ILE:HG12	13:M:174:LEU:HD13	2.03	0.41
15:O:34:GLY:N	54:O:401:DGT:O1G	2.53	0.41
3:C:55:ASP:OD2	17:Q:6:ARG:NE	2.51	0.41
23:X:153:VAL:HG23	29:d:6:GLN:HB2	2.02	0.41
41:p:116:GLU:OE1	41:p:123:ASN:ND2	2.46	0.41
2:B:45:LEU:HD22	2:B:85:VAL:HG23	2.03	0.41
28:c:33:LYS:HG3	28:c:34:GLN:N	2.35	0.41
33:h:4:HIS:HB3	33:h:5:GLY:H	1.53	0.41
6:F:224:ASN:ND2	50:F:501:FMN:O2	2.49	0.41
45:L:701:3PE:H2G1	45:L:701:3PE:H2C1	2.02	0.41
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.21	0.41
31:f:11:TRP:O	31:f:14:VAL:HG22	2.21	0.41
39:n:30:CYS:O	39:n:32:HIS:N	2.53	0.41
44:s:34:ASP:OD1	44:s:34:ASP:N	2.54	0.41
32:g:92:GLU:OE2	32:g:95:ARG:NH2	2.50	0.41
4:D:208:MET:HE1	4:D:318:MET:CB	2.51	0.40
12:L:129:LEU:O	12:L:133:THR:OG1	2.31	0.40
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.03	0.40
13:M:76:MET:HE3	13:M:99:LEU:HD22	2.02	0.40
26:a:5:VAL:O	26:a:5:VAL:HG12	2.21	0.40
31:f:2:ASN:HA	31:f:6:VAL:HG21	2.03	0.40
53:H:602:CDL:OB3	53:H:602:CDL:O1	2.36	0.40
16:P:145:TYR:CD1	16:P:145:TYR:C	2.99	0.40
2:B:75:VAL:HG13	48:D:701:U10:C25	2.52	0.40
4:D:59:HIS:NE2	61:D:815:HOH:O	2.25	0.40
9:I:81:LYS:N	47:I:203:SF4:S1	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.50	0.40
12:L:561:ILE:HG13	12:L:562:LEU:N	2.37	0.40
16:P:187:TRP:CG	45:P:404:3PE:H242	2.57	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	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
2	B	155/216 (72%)	149 (96%)	6 (4%)	0	100	100
3	C	207/266 (78%)	204 (99%)	3 (1%)	0	100	100
4	D	427/463 (92%)	419 (98%)	8 (2%)	0	100	100
5	E	214/249 (86%)	208 (97%)	6 (3%)	0	100	100
6	F	431/464 (93%)	424 (98%)	7 (2%)	0	100	100
7	G	688/727 (95%)	673 (98%)	15 (2%)	0	100	100
8	H	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
9	I	174/212 (82%)	172 (99%)	2 (1%)	0	100	100
10	J	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
11	K	96/98 (98%)	96 (100%)	0	0	100	100
12	L	604/606 (100%)	585 (97%)	19 (3%)	0	100	100
13	M	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	340/380 (90%)	336 (99%)	3 (1%)	1 (0%)	36	55
17	Q	127/175 (73%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
19	S	85/99 (86%)	82 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
20	U	86/156 (55%)	86 (100%)	0	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	109 (96%)	3 (3%)	1 (1%)	14	27
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
30	e	98/106 (92%)	98 (100%)	0	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	100/154 (65%)	93 (93%)	7 (7%)	0	100	100
33	h	141/189 (75%)	136 (96%)	5 (4%)	0	100	100
34	i	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	78/98 (80%)	76 (97%)	2 (3%)	0	100	100
37	l	154/186 (83%)	151 (98%)	3 (2%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
39	n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	o	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
41	p	171/176 (97%)	171 (100%)	0	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	93/113 (82%)	91 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8210/9214 (89%)	8049 (98%)	159 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	3	HIS
22	W	95	VAL

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	100/100 (100%)	98 (98%)	2 (2%)	48 75
2	B	133/174 (76%)	132 (99%)	1 (1%)	73 88
3	C	190/228 (83%)	190 (100%)	0	100 100
4	D	370/392 (94%)	370 (100%)	0	100 100
5	E	183/205 (89%)	182 (100%)	1 (0%)	81 92
6	F	346/368 (94%)	345 (100%)	1 (0%)	86 94
7	G	578/608 (95%)	575 (100%)	3 (0%)	81 92
8	H	274/274 (100%)	273 (100%)	1 (0%)	84 93
9	I	151/175 (86%)	149 (99%)	2 (1%)	61 82
10	J	141/141 (100%)	140 (99%)	1 (1%)	76 89
11	K	85/85 (100%)	83 (98%)	2 (2%)	43 70
12	L	533/533 (100%)	527 (99%)	6 (1%)	65 84
13	M	412/412 (100%)	409 (99%)	3 (1%)	76 89
14	N	315/315 (100%)	315 (100%)	0	100 100
15	O	283/303 (93%)	283 (100%)	0	100 100
16	P	296/327 (90%)	294 (99%)	2 (1%)	76 89
17	Q	116/153 (76%)	115 (99%)	1 (1%)	70 87
18	R	79/97 (81%)	79 (100%)	0	100 100
19	S	77/82 (94%)	77 (100%)	0	100 100
20	T	81/135 (60%)	79 (98%)	2 (2%)	42 69
20	U	81/135 (60%)	81 (100%)	0	100 100
21	V	101/102 (99%)	101 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	W	107/114 (94%)	107 (100%)	0	100 100
23	X	154/155 (99%)	153 (99%)	1 (1%)	78 91
24	Y	101/101 (100%)	101 (100%)	0	100 100
25	Z	120/121 (99%)	120 (100%)	0	100 100
26	a	59/59 (100%)	58 (98%)	1 (2%)	53 78
27	b	71/72 (99%)	70 (99%)	1 (1%)	59 81
28	c	45/68 (66%)	45 (100%)	0	100 100
29	d	106/106 (100%)	103 (97%)	3 (3%)	38 66
30	e	90/96 (94%)	90 (100%)	0	100 100
31	f	54/54 (100%)	53 (98%)	1 (2%)	50 76
32	g	93/131 (71%)	93 (100%)	0	100 100
33	h	124/158 (78%)	124 (100%)	0	100 100
34	i	121/121 (100%)	121 (100%)	0	100 100
35	j	61/84 (73%)	60 (98%)	1 (2%)	55 79
36	k	62/76 (82%)	62 (100%)	0	100 100
37	l	140/159 (88%)	140 (100%)	0	100 100
38	m	114/115 (99%)	114 (100%)	0	100 100
39	n	156/161 (97%)	156 (100%)	0	100 100
40	o	110/120 (92%)	110 (100%)	0	100 100
41	p	155/157 (99%)	155 (100%)	0	100 100
42	q	131/131 (100%)	131 (100%)	0	100 100
43	r	86/96 (90%)	86 (100%)	0	100 100
44	s	43/92 (47%)	43 (100%)	0	100 100
All	All	7228/7891 (92%)	7192 (100%)	36 (0%)	78 92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	101	SER
2	B	54	CYS
5	E	134	ASP
6	F	105	CYS
7	G	125	SER

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Mol	Chain	Res	Type
7	G	403	ASP
7	G	536	ASP
8	H	209	SER
9	I	58	SER
9	I	86	VAL
10	J	110	ASP
11	K	2	SER
11	K	82	SER
12	L	110	SER
12	L	285	THR
12	L	307	SER
12	L	316	THR
12	L	554	ASP
12	L	576	LEU
13	M	62	SER
13	M	191	SER
13	M	209	LEU
16	P	263	TYR
16	P	329	SER
17	Q	80	SER
20	T	31	SER
20	T	80	ILE
23	X	130	VAL
26	a	69	ILE
27	b	61	ASN
29	d	3	THR
29	d	10	THR
29	d	20	SER
31	f	30	ASN
35	j	40	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	GLN
5	E	42	HIS
5	E	214	GLN
6	F	116	HIS
6	F	200	GLN
6	F	421	HIS
7	G	141	ASN
7	G	237	ASN

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Mol	Chain	Res	Type
7	G	401	HIS
7	G	581	GLN
11	K	50	ASN
12	L	25	ASN
12	L	59	GLN
12	L	518	ASN
12	L	603	ASN
13	M	48	ASN
13	M	139	GLN
13	M	168	GLN
13	M	187	HIS
13	M	293	HIS
13	M	366	ASN
13	M	399	ASN
14	N	134	GLN
15	O	190	HIS
15	O	251	GLN
15	O	287	HIS
16	P	93	ASN
16	P	131	HIS
16	P	260	HIS
17	Q	29	HIS
22	W	69	ASN
26	a	27	HIS
29	d	12	GLN
29	d	79	GLN
29	d	117	HIS
33	h	124	HIS
33	h	143	ASN
35	j	6	HIS
36	k	47	ASN
37	l	104	HIS
39	n	77	GLN
40	o	49	GLN
40	o	116	GLN
41	p	54	GLN
41	p	90	GLN
41	p	133	GLN
42	q	5	GLN
42	q	13	GLN
43	r	51	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FME	H	1	8	8,9,10	1.51	1 (12%)	7,9,11	1.70	2 (28%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	7,9,11	1.64	2 (28%)
13	FME	M	1	13	8,9,10	1.50	1 (12%)	7,9,11	1.67	1 (14%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.74	3 (42%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	7,9,11	1.66	2 (28%)
4	2MR	D	85	4	10,12,13	2.44	2 (20%)	5,13,15	1.21	0
12	FME	L	1	12	8,9,10	1.51	1 (12%)	7,9,11	1.60	1 (14%)
2	WYK	B	77	2	9,11,12	2.53	2 (22%)	7,13,15	0.60	0
11	FME	K	1	11	8,9,10	1.51	1 (12%)	7,9,11	1.65	2 (28%)

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
8	FME	H	1	8	-	2/7/9/11	-
10	FME	J	1	10	-	5/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
14	FME	N	1	14	-	1/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WYK	B	77	2	-	1/10/11/13	-
11	FME	K	1	11	-	2/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	WYK	CZ-NE	6.70	1.46	1.33
4	D	85	2MR	CZ-NH2	5.37	1.45	1.33
4	D	85	2MR	CZ-NE	5.21	1.45	1.34
10	J	1	FME	CN-N	3.70	1.45	1.33
12	L	1	FME	CN-N	3.67	1.45	1.33
11	K	1	FME	CN-N	3.67	1.45	1.33
8	H	1	FME	CN-N	3.66	1.45	1.33
13	M	1	FME	CN-N	3.66	1.45	1.33
14	N	1	FME	CN-N	3.65	1.45	1.33
1	A	1	FME	CN-N	3.64	1.45	1.33
2	B	77	WYK	CZ-NH2	-2.18	1.25	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	FME	CE-SD-CG	2.84	110.16	100.40
13	M	1	FME	CE-SD-CG	2.72	109.74	100.40
1	A	1	FME	CE-SD-CG	2.69	109.62	100.40
14	N	1	FME	CE-SD-CG	2.67	109.57	100.40
11	K	1	FME	CE-SD-CG	2.62	109.42	100.40
10	J	1	FME	CE-SD-CG	2.52	109.07	100.40
12	L	1	FME	CE-SD-CG	2.51	109.03	100.40
1	A	1	FME	O1-CN-N	-2.10	119.74	125.27
1	A	1	FME	CA-N-CN	-2.08	119.62	122.82
8	H	1	FME	O1-CN-N	-2.02	119.95	125.27
10	J	1	FME	O1-CN-N	-2.02	119.96	125.27
14	N	1	FME	O1-CN-N	-2.01	119.97	125.27
11	K	1	FME	O1-CN-N	-2.01	119.99	125.27

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	C-CA-CB-CG

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 3 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	3PE	N	901	-	48,48,50	0.88	4 (8%)	51,53,55	1.01	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	CDL	N	905	-	64,64,99	1.09	7 (10%)	70,76,111	1.14	4 (5%)
60	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.86	0
53	CDL	N	902	-	99,99,99	0.91	7 (7%)	105,111,111	1.07	5 (4%)
46	PC1	P	401	-	32,32,53	1.55	6 (18%)	38,40,61	1.01	2 (5%)
53	CDL	q	202	-	60,60,99	1.13	7 (11%)	66,72,111	1.12	5 (7%)
45	3PE	L	704	-	30,30,50	1.09	4 (13%)	33,35,55	1.17	2 (6%)
45	3PE	Y	206	-	48,48,50	0.89	4 (8%)	51,53,55	1.04	2 (3%)
46	PC1	A	203	-	34,34,53	1.52	6 (17%)	40,42,61	1.07	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-		
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.47	4 (11%)
45	3PE	Y	203	-	39,39,50	0.97	4 (10%)	42,44,55	1.10	2 (4%)
56	NDP	P	403	-	49,52,52	3.98	25 (51%)	66,80,80	2.02	14 (21%)
45	3PE	P	404	-	34,34,50	1.03	4 (11%)	37,39,55	1.18	3 (8%)
47	SF4	I	202	9	0,12,12	-	-	-		
49	FES	G	803	7	0,4,4	-	-	-		
49	FES	E	301	5	0,4,4	-	-	-		
50	FMN	F	501	-	33,33,33	2.79	10 (30%)	48,50,50	1.74	14 (29%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	N	904	-	38,38,53	1.46	6 (15%)	44,46,61	1.13	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-		
53	CDL	N	903	-	61,61,99	1.13	6 (9%)	67,73,111	1.27	5 (7%)
58	EHZ	T	101	20	29,36,37	1.70	5 (17%)	35,44,47	1.46	3 (8%)
46	PC1	B	202	-	43,43,53	1.40	6 (13%)	49,51,61	0.98	2 (4%)
46	PC1	q	201	-	48,48,53	1.36	6 (12%)	54,56,61	1.00	2 (3%)
45	3PE	L	701	-	45,45,50	0.92	4 (8%)	48,50,55	1.01	2 (4%)
45	3PE	Y	205	-	26,26,50	1.15	4 (15%)	29,31,55	1.17	2 (6%)
47	SF4	G	801	7	0,12,12	-	-	-		
59	CHD	i	201	-	32,32,32	3.24	10 (31%)	51,51,51	1.88	14 (27%)
45	3PE	Y	201	-	42,42,50	0.93	4 (9%)	45,47,55	1.13	2 (4%)
45	3PE	H	601	-	33,33,50	1.04	4 (12%)	36,38,55	1.16	2 (5%)
46	PC1	A	202	-	34,34,53	1.53	6 (17%)	40,42,61	1.02	2 (5%)
48	U10	D	701	-	63,63,63	2.13	16 (25%)	76,79,79	1.63	19 (25%)
45	3PE	Y	202	-	30,30,50	1.08	4 (13%)	33,35,55	1.11	2 (6%)
53	CDL	X	201	-	85,85,99	0.97	7 (8%)	91,97,111	1.07	4 (4%)
54	DGT	O	401	55	29,33,33	3.19	14 (48%)	44,52,52	2.10	12 (27%)
45	3PE	L	705	-	30,30,50	1.10	4 (13%)	33,35,55	1.07	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	0.97	2 (3%)
45	3PE	L	703	-	44,44,50	0.92	4 (9%)	47,49,55	1.04	2 (4%)
46	PC1	H	603	-	43,43,53	1.42	6 (13%)	49,51,61	0.91	2 (4%)
45	3PE	m	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.09	2 (4%)
45	3PE	K	101	-	41,41,50	0.94	4 (9%)	44,46,55	1.07	2 (4%)
53	CDL	L	702	-	77,77,99	1.02	7 (9%)	83,89,111	1.01	4 (4%)
45	3PE	M	502	-	49,49,50	0.87	4 (8%)	52,54,55	1.08	2 (3%)
46	PC1	I	204	-	39,39,53	1.46	6 (15%)	45,47,61	1.01	2 (4%)
45	3PE	Y	204	-	33,33,50	1.05	4 (12%)	36,38,55	1.13	2 (5%)
53	CDL	h	201	-	77,77,99	1.02	7 (9%)	83,89,111	1.06	4 (4%)
45	3PE	A	201	-	46,46,50	0.91	4 (8%)	49,51,55	0.99	2 (4%)
46	PC1	h	202	-	43,43,53	1.39	6 (13%)	49,51,61	1.03	2 (4%)
46	PC1	P	402	-	45,45,53	1.37	6 (13%)	51,53,61	0.95	2 (3%)
45	3PE	I	201	-	44,44,50	0.91	4 (9%)	47,49,55	1.09	2 (4%)
53	CDL	H	602	-	68,68,99	1.08	7 (10%)	74,80,111	1.09	4 (5%)
46	PC1	M	501	-	41,41,53	1.40	6 (14%)	47,49,61	1.10	2 (4%)
45	3PE	b	101	-	38,38,50	0.98	4 (10%)	41,43,55	1.09	2 (4%)
51	NAI	F	503	-	45,48,48	3.73	20 (44%)	60,73,73	1.79	14 (23%)
47	SF4	I	203	9	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	N	901	-	-	20/52/52/54	-
53	CDL	N	905	-	-	37/75/75/110	-
60	MYR	o	201	40	-	1/11/12/13	-
53	CDL	N	902	-	-	40/110/110/110	-
46	PC1	P	401	-	-	8/36/36/57	-
53	CDL	q	202	-	-	32/71/71/110	-
45	3PE	L	704	-	-	15/34/34/54	-
45	3PE	Y	206	-	-	20/52/52/54	-
46	PC1	A	203	-	-	15/38/38/57	-
47	SF4	G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	U	101	20	-	10/42/44/45	-
45	3PE	Y	203	-	-	12/43/43/54	-
56	NDP	P	403	-	-	4/34/77/77	0/5/5/5
45	3PE	P	404	-	-	20/38/38/54	-
47	SF4	I	202	9	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1
49	FES	E	301	5	-	-	0/1/1/1
50	FMN	F	501	-	-	5/18/18/18	0/3/3/3
47	SF4	B	201	2	-	-	0/6/5/5
46	PC1	N	904	-	-	13/42/42/57	-
47	SF4	F	502	6	-	-	0/6/5/5
53	CDL	N	903	-	-	34/71/71/110	-
58	EHZ	T	101	20	-	19/42/44/45	-
46	PC1	B	202	-	-	14/47/47/57	-
46	PC1	q	201	-	-	25/52/52/57	-
45	3PE	L	701	-	-	22/49/49/54	-
45	3PE	Y	205	-	-	14/30/30/54	-
59	CHD	i	201	-	-	2/9/74/74	0/4/4/4
47	SF4	G	801	7	-	-	0/6/5/5
45	3PE	Y	201	-	-	19/46/46/54	-
45	3PE	H	601	-	-	16/37/37/54	-
46	PC1	A	202	-	-	14/38/38/57	-
48	U10	D	701	-	-	17/63/87/87	0/1/1/1
45	3PE	Y	202	-	-	12/34/34/54	-
53	CDL	X	201	-	-	40/96/96/110	-
54	DGT	O	401	55	-	4/22/34/34	0/3/3/3
45	3PE	L	705	-	-	11/34/34/54	-
45	3PE	d	201	-	-	26/52/52/54	-
45	3PE	L	703	-	-	24/48/48/54	-
46	PC1	H	603	-	-	21/47/47/57	-
45	3PE	m	201	-	-	25/44/44/54	-
45	3PE	K	101	-	-	24/45/45/54	-
53	CDL	L	702	-	-	30/88/88/110	-
45	3PE	M	502	-	-	23/53/53/54	-
46	PC1	I	204	-	-	21/43/43/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Y	204	-	-	17/37/37/54	-
53	CDL	h	201	-	-	34/88/88/110	-
45	3PE	A	201	-	-	28/50/50/54	-
46	PC1	h	202	-	-	18/47/47/57	-
46	PC1	P	402	-	-	11/49/49/57	-
45	3PE	I	201	-	-	18/48/48/54	-
53	CDL	H	602	-	-	42/79/79/110	-
46	PC1	M	501	-	-	11/45/45/57	-
45	3PE	b	101	-	-	12/42/42/54	-
51	NAI	F	503	-	-	7/29/72/72	0/5/5/5
47	SF4	I	203	9	-	-	0/6/5/5

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	403	NDP	C6N-C5N	12.16	1.55	1.33
51	F	503	NAI	C6N-C5N	11.12	1.53	1.33
48	D	701	U10	C6-C1	9.59	1.52	1.35
59	i	201	CHD	C11-C12	8.74	1.68	1.53
51	F	503	NAI	O4B-C1B	8.65	1.62	1.42
56	P	403	NDP	C2B-C1B	-8.53	1.31	1.53
56	P	403	NDP	O4B-C1B	8.50	1.62	1.42
51	F	503	NAI	O4D-C1D	8.31	1.61	1.42
56	P	403	NDP	C7N-N7N	8.27	1.55	1.33
56	P	403	NDP	O4D-C1D	8.20	1.61	1.42
54	O	401	DGT	C2'-C3'	-7.64	1.32	1.52
50	F	501	FMN	C4A-N5	7.22	1.44	1.30
56	P	403	NDP	C2D-C1D	-7.18	1.30	1.53
59	i	201	CHD	C16-C15	7.14	1.73	1.54
51	F	503	NAI	C2B-C1B	-7.03	1.31	1.53
51	F	503	NAI	C2D-C1D	-6.78	1.31	1.53
50	F	501	FMN	C10-N1	6.59	1.46	1.33
51	F	503	NAI	O4D-C4D	-6.53	1.30	1.45
54	O	401	DGT	C4-N3	6.49	1.49	1.34
56	P	403	NDP	O4D-C4D	-6.37	1.30	1.45
51	F	503	NAI	C2N-C3N	6.30	1.52	1.34
51	F	503	NAI	O4B-C4B	-6.23	1.31	1.45
59	i	201	CHD	C13-C17	6.01	1.65	1.55
56	P	403	NDP	C6A-N6A	5.60	1.48	1.34
59	i	201	CHD	C8-C9	5.56	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	O	401	DGT	C2-N3	5.52	1.46	1.33
58	U	101	EHZ	C15-N2	5.42	1.45	1.33
56	P	403	NDP	P2B-O2B	5.42	1.69	1.59
54	O	401	DGT	O4'-C4'	5.37	1.57	1.45
58	T	101	EHZ	C12-N1	5.36	1.45	1.33
58	T	101	EHZ	C15-N2	5.33	1.45	1.33
58	U	101	EHZ	C12-N1	5.29	1.45	1.33
59	i	201	CHD	C20-C17	-5.28	1.45	1.54
50	F	501	FMN	C5A-N5	5.27	1.49	1.39
54	O	401	DGT	O4'-C1'	-5.20	1.30	1.42
59	i	201	CHD	O12-C12	-5.12	1.35	1.43
50	F	501	FMN	C9A-N10	5.10	1.50	1.41
56	P	403	NDP	O4B-C4B	-5.07	1.33	1.45
59	i	201	CHD	C6-C5	4.83	1.61	1.53
50	F	501	FMN	C2-N1	4.78	1.48	1.36
54	O	401	DGT	C2-N2	4.73	1.45	1.34
56	P	403	NDP	C2N-C3N	4.71	1.48	1.34
51	F	503	NAI	C6A-N6A	4.61	1.45	1.34
51	F	503	NAI	C7N-N7N	4.57	1.45	1.33
48	D	701	U10	C4-C3	4.31	1.53	1.36
50	F	501	FMN	C2-N3	4.27	1.49	1.39
59	i	201	CHD	C15-C14	4.15	1.63	1.54
59	i	201	CHD	C6-C7	4.04	1.59	1.52
56	P	403	NDP	O7N-C7N	-4.04	1.14	1.24
56	P	403	NDP	O2D-C2D	4.01	1.52	1.43
50	F	501	FMN	C4-N3	3.94	1.46	1.38
56	P	403	NDP	C5A-C4A	-3.89	1.31	1.39
54	O	401	DGT	C2'-C1'	3.88	1.63	1.52
46	q	201	PC1	O31-C31	3.87	1.44	1.33
46	N	904	PC1	O31-C31	3.85	1.44	1.33
46	H	603	PC1	O31-C31	3.85	1.44	1.33
46	A	203	PC1	O31-C31	3.85	1.44	1.33
54	O	401	DGT	C5'-C4'	-3.85	1.39	1.51
46	I	204	PC1	O31-C31	3.82	1.44	1.33
46	P	401	PC1	O31-C31	3.79	1.44	1.33
46	B	202	PC1	O31-C31	3.79	1.44	1.33
46	M	501	PC1	O31-C31	3.79	1.44	1.33
50	F	501	FMN	C10-N10	3.78	1.45	1.37
46	A	202	PC1	O31-C31	3.77	1.44	1.33
46	P	402	PC1	O31-C31	3.77	1.44	1.33
46	h	202	PC1	O31-C31	3.76	1.44	1.33
46	P	401	PC1	O21-C21	3.71	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	202	PC1	O21-C21	3.69	1.44	1.34
46	q	201	PC1	O21-C21	3.65	1.44	1.34
46	h	202	PC1	O21-C21	3.64	1.44	1.34
46	I	204	PC1	O21-C21	3.60	1.44	1.34
46	N	904	PC1	O21-C21	3.60	1.44	1.34
46	B	202	PC1	O21-C21	3.59	1.44	1.34
46	A	203	PC1	O21-C21	3.58	1.44	1.34
46	H	603	PC1	O21-C21	3.56	1.44	1.34
46	M	501	PC1	O21-C21	3.49	1.44	1.34
56	P	403	NDP	C8A-N9A	-3.48	1.31	1.37
46	P	402	PC1	O21-C21	3.44	1.44	1.34
56	P	403	NDP	C4N-C3N	3.31	1.56	1.49
51	F	503	NAI	C6N-N1N	3.21	1.45	1.37
54	O	401	DGT	C5-N7	-3.10	1.33	1.39
50	F	501	FMN	O2-C2	-2.96	1.18	1.24
51	F	503	NAI	O3B-C3B	-2.96	1.36	1.43
51	F	503	NAI	O3D-C3D	-2.92	1.36	1.43
51	F	503	NAI	O2B-C2B	2.91	1.49	1.43
53	N	903	CDL	OB6-CB5	2.91	1.41	1.35
51	F	503	NAI	O2D-C2D	2.91	1.49	1.43
56	P	403	NDP	C4N-C5N	2.83	1.56	1.48
48	D	701	U10	C7-C6	2.77	1.56	1.51
53	N	902	CDL	OB8-CB7	2.74	1.41	1.33
53	H	602	CDL	OB8-CB7	2.72	1.41	1.33
50	F	501	FMN	O4-C4	-2.69	1.18	1.23
53	q	202	CDL	OB8-CB7	2.69	1.41	1.33
53	X	201	CDL	OB8-CB7	2.69	1.41	1.33
48	D	701	U10	C7-C8	2.69	1.54	1.50
53	N	905	CDL	OB8-CB7	2.68	1.41	1.33
53	q	202	CDL	OA6-CA4	-2.68	1.39	1.46
51	F	503	NAI	C5A-C4A	-2.67	1.34	1.39
54	O	401	DGT	C2-N1	2.67	1.44	1.37
54	O	401	DGT	O3'-C3'	2.66	1.49	1.43
48	D	701	U10	C16-C14	2.66	1.56	1.51
53	N	903	CDL	OB8-CB7	2.65	1.41	1.33
53	h	201	CDL	OB8-CB7	2.64	1.41	1.33
53	L	702	CDL	OB8-CB7	2.64	1.41	1.33
53	h	201	CDL	OA6-CA4	-2.63	1.40	1.46
46	P	402	PC1	O21-C2	-2.63	1.40	1.46
53	X	201	CDL	OA6-CA4	-2.62	1.40	1.46
53	N	905	CDL	OA6-CA4	-2.59	1.40	1.46
53	N	902	CDL	OA6-CA4	-2.58	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	K	101	3PE	O21-C2	-2.58	1.40	1.46
45	Y	206	3PE	O21-C2	-2.58	1.40	1.46
53	N	903	CDL	OA8-CA7	2.57	1.40	1.33
45	L	701	3PE	O21-C2	-2.56	1.40	1.46
54	O	401	DGT	C5-C6	2.54	1.53	1.44
46	H	603	PC1	O21-C2	-2.54	1.40	1.46
53	X	201	CDL	OB6-CB5	2.53	1.41	1.34
53	H	602	CDL	OB6-CB4	-2.53	1.40	1.46
46	B	202	PC1	O21-C2	-2.53	1.40	1.46
53	L	702	CDL	OB6-CB5	2.53	1.41	1.34
53	X	201	CDL	OA8-CA7	2.52	1.40	1.33
53	q	202	CDL	OB6-CB5	2.52	1.41	1.34
45	A	201	3PE	O21-C2	-2.52	1.40	1.46
45	L	703	3PE	O31-C31	2.52	1.40	1.33
53	N	902	CDL	OB6-CB5	2.52	1.41	1.34
45	Y	204	3PE	O21-C2	-2.51	1.40	1.46
53	N	905	CDL	OB6-CB5	2.51	1.41	1.34
56	P	403	NDP	C6N-N1N	2.51	1.43	1.37
46	I	204	PC1	O21-C2	-2.51	1.40	1.46
45	b	101	3PE	O21-C2	-2.51	1.40	1.46
53	L	702	CDL	OA6-CA4	-2.51	1.40	1.46
46	A	203	PC1	O21-C2	-2.51	1.40	1.46
45	H	601	3PE	O21-C2	-2.50	1.40	1.46
45	L	703	3PE	O21-C2	-2.50	1.40	1.46
56	P	403	NDP	O3D-C3D	-2.49	1.37	1.43
58	T	101	EHZ	C9-S1	2.49	1.82	1.76
46	N	904	PC1	O21-C2	-2.49	1.40	1.46
46	M	501	PC1	O21-C2	-2.49	1.40	1.46
46	h	202	PC1	O21-C2	-2.49	1.40	1.46
53	h	201	CDL	OB6-CB5	2.49	1.41	1.34
45	Y	204	3PE	O31-C31	2.49	1.40	1.33
53	H	602	CDL	OA8-CA7	2.49	1.40	1.33
45	Y	203	3PE	O31-C31	2.48	1.40	1.33
45	Y	201	3PE	O21-C2	-2.48	1.40	1.46
56	P	403	NDP	O3B-C3B	-2.48	1.37	1.43
53	N	903	CDL	OA6-CA4	-2.48	1.40	1.46
45	L	705	3PE	O21-C2	-2.47	1.40	1.46
53	L	702	CDL	OA8-CA7	2.47	1.40	1.33
45	m	201	3PE	O21-C2	-2.47	1.40	1.46
45	d	201	3PE	O21-C2	-2.46	1.40	1.46
45	Y	203	3PE	O21-C2	-2.46	1.40	1.46
45	I	201	3PE	O21-C2	-2.45	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	b	101	3PE	O31-C31	2.45	1.40	1.33
54	O	401	DGT	O6-C6	-2.45	1.18	1.23
45	Y	206	3PE	O31-C31	2.44	1.40	1.33
45	H	601	3PE	O31-C31	2.44	1.40	1.33
51	F	503	NAI	C5A-N7A	-2.44	1.34	1.39
48	D	701	U10	C6-C5	2.44	1.53	1.46
54	O	401	DGT	C6-N1	2.44	1.43	1.38
45	M	502	3PE	O31-C31	2.44	1.40	1.33
45	d	201	3PE	O31-C31	2.43	1.40	1.33
45	Y	201	3PE	O31-C31	2.43	1.40	1.33
53	h	201	CDL	OA8-CA7	2.42	1.40	1.33
45	L	704	3PE	O31-C31	2.42	1.40	1.33
45	N	901	3PE	O31-C31	2.42	1.40	1.33
45	L	705	3PE	O31-C31	2.41	1.40	1.33
56	P	403	NDP	C7N-C3N	2.41	1.53	1.48
59	i	201	CHD	C13-C12	-2.41	1.50	1.54
53	L	702	CDL	OB6-CB4	-2.41	1.40	1.46
45	A	201	3PE	O31-C31	2.41	1.40	1.33
53	N	902	CDL	OB6-CB4	-2.41	1.40	1.46
53	h	201	CDL	OB6-CB4	-2.40	1.40	1.46
46	A	202	PC1	O21-C2	-2.40	1.40	1.46
46	q	201	PC1	C22-C21	2.40	1.57	1.50
51	F	503	NAI	O7N-C7N	-2.40	1.18	1.24
48	D	701	U10	C26-C24	2.39	1.56	1.51
45	m	201	3PE	O31-C31	2.39	1.40	1.33
46	H	603	PC1	P-O11	2.38	1.68	1.59
48	D	701	U10	C41-C39	2.38	1.56	1.51
53	N	905	CDL	OB6-CB4	-2.38	1.40	1.46
53	N	902	CDL	OA8-CA7	2.38	1.40	1.33
53	H	602	CDL	OB6-CB5	2.38	1.41	1.34
45	I	201	3PE	O31-C31	2.37	1.40	1.33
53	q	202	CDL	OA8-CA7	2.37	1.40	1.33
45	P	404	3PE	O31-C31	2.37	1.40	1.33
45	Y	205	3PE	O31-C31	2.37	1.40	1.33
58	U	101	EHZ	C9-S1	2.37	1.81	1.76
56	P	403	NDP	C5A-N7A	-2.36	1.34	1.39
46	P	401	PC1	P-O11	2.35	1.68	1.59
48	D	701	U10	O2-C2	-2.35	1.18	1.23
45	K	101	3PE	O31-C31	2.35	1.40	1.33
46	h	202	PC1	P-O11	2.34	1.68	1.59
46	A	203	PC1	P-O11	2.34	1.68	1.59
58	T	101	EHZ	O4-C15	-2.34	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	D	701	U10	O5-C5	-2.34	1.18	1.23
46	A	202	PC1	P-O11	2.34	1.68	1.59
46	I	204	PC1	P-O11	2.34	1.68	1.59
46	q	201	PC1	P-O11	2.33	1.68	1.59
53	N	905	CDL	OA8-CA7	2.33	1.40	1.33
46	I	204	PC1	C22-C21	2.33	1.57	1.50
46	A	202	PC1	C22-C21	2.32	1.57	1.50
53	N	903	CDL	OB6-CB4	-2.32	1.40	1.46
45	Y	205	3PE	O21-C2	-2.31	1.40	1.46
46	N	904	PC1	P-O11	2.31	1.68	1.59
46	P	401	PC1	O21-C2	-2.31	1.40	1.46
46	M	501	PC1	P-O11	2.31	1.68	1.59
53	H	602	CDL	OA6-CA4	-2.30	1.40	1.46
53	X	201	CDL	OB6-CB4	-2.30	1.40	1.46
53	q	202	CDL	OB6-CB4	-2.30	1.40	1.46
48	D	701	U10	C11-C9	2.29	1.56	1.51
46	q	201	PC1	O21-C2	-2.29	1.40	1.46
46	B	202	PC1	C22-C21	2.29	1.57	1.50
46	M	501	PC1	C22-C21	2.29	1.57	1.50
45	L	701	3PE	O31-C31	2.29	1.40	1.33
56	P	403	NDP	PA-O5B	2.29	1.68	1.59
46	P	401	PC1	C22-C21	2.28	1.57	1.50
48	D	701	U10	C31-C29	2.28	1.56	1.51
45	P	404	3PE	O21-C2	-2.28	1.40	1.46
46	B	202	PC1	P-O11	2.27	1.68	1.59
58	T	101	EHZ	O3-C12	-2.27	1.18	1.23
45	Y	202	3PE	O31-C31	2.27	1.40	1.33
45	N	901	3PE	O21-C2	-2.27	1.40	1.46
58	U	101	EHZ	O4-C15	-2.26	1.18	1.23
46	N	904	PC1	C22-C21	2.26	1.57	1.50
46	A	203	PC1	C22-C21	2.26	1.57	1.50
46	P	402	PC1	P-O11	2.26	1.68	1.59
46	H	603	PC1	C22-C21	2.25	1.57	1.50
45	P	404	3PE	O21-C21	2.24	1.40	1.34
46	h	202	PC1	C22-C21	2.24	1.57	1.50
56	P	403	NDP	P2B-O1X	2.23	1.57	1.50
45	Y	202	3PE	O21-C21	2.23	1.40	1.34
45	L	701	3PE	O21-C21	2.22	1.40	1.34
45	N	901	3PE	O21-C21	2.22	1.40	1.34
58	U	101	EHZ	O3-C12	-2.22	1.18	1.23
45	L	701	3PE	O31-C3	-2.22	1.40	1.45
53	L	702	CDL	OA6-CA5	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	704	3PE	O21-C2	-2.22	1.41	1.46
45	M	502	3PE	O21-C21	2.21	1.40	1.34
53	H	602	CDL	OA8-CA6	-2.21	1.40	1.45
53	H	602	CDL	OA6-CA5	2.21	1.40	1.34
45	A	201	3PE	O21-C21	2.20	1.40	1.34
45	Y	202	3PE	O21-C2	-2.20	1.41	1.46
45	Y	202	3PE	O31-C3	-2.20	1.40	1.45
45	L	704	3PE	O21-C21	2.18	1.40	1.34
45	Y	205	3PE	O21-C21	2.18	1.40	1.34
45	d	201	3PE	O31-C3	-2.17	1.40	1.45
45	L	705	3PE	O21-C21	2.17	1.40	1.34
51	F	503	NAI	C7N-C3N	2.17	1.53	1.48
53	N	905	CDL	OA6-CA5	2.16	1.40	1.34
45	Y	201	3PE	O21-C21	2.16	1.40	1.34
45	d	201	3PE	O21-C21	2.15	1.40	1.34
45	Y	206	3PE	O21-C21	2.15	1.40	1.34
53	N	905	CDL	OA8-CA6	-2.15	1.40	1.45
45	P	404	3PE	O31-C3	-2.15	1.40	1.45
53	X	201	CDL	OA6-CA5	2.15	1.40	1.34
45	I	201	3PE	O21-C21	2.14	1.40	1.34
46	P	402	PC1	C22-C21	2.14	1.57	1.50
45	Y	204	3PE	O21-C21	2.14	1.40	1.34
45	L	703	3PE	O21-C21	2.14	1.40	1.34
45	A	201	3PE	O31-C3	-2.14	1.40	1.45
45	K	101	3PE	O21-C21	2.13	1.40	1.34
45	Y	203	3PE	O21-C21	2.13	1.40	1.34
53	N	902	CDL	OA8-CA6	-2.13	1.40	1.45
45	H	601	3PE	O21-C21	2.13	1.40	1.34
45	N	901	3PE	O31-C3	-2.13	1.40	1.45
45	M	502	3PE	O21-C2	-2.13	1.41	1.46
53	h	201	CDL	OA6-CA5	2.12	1.40	1.34
46	A	203	PC1	P-O13	2.11	1.67	1.59
45	L	705	3PE	O31-C3	-2.11	1.40	1.45
45	m	201	3PE	O31-C3	-2.11	1.40	1.45
45	I	201	3PE	O31-C3	-2.11	1.40	1.45
48	D	701	U10	O3-C3M	-2.11	1.40	1.45
45	L	704	3PE	O31-C3	-2.11	1.40	1.45
45	H	601	3PE	O31-C3	-2.11	1.40	1.45
53	q	202	CDL	OA8-CA6	-2.11	1.40	1.45
46	h	202	PC1	P-O13	2.10	1.67	1.59
53	N	903	CDL	OA6-CA5	2.10	1.40	1.34
46	H	603	PC1	P-O13	2.10	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	403	NDP	C5B-C4B	2.10	1.58	1.51
53	h	201	CDL	OA8-CA6	-2.10	1.40	1.45
45	K	101	3PE	O31-C3	-2.10	1.40	1.45
46	I	204	PC1	P-O13	2.10	1.67	1.59
46	q	201	PC1	P-O13	2.09	1.67	1.59
45	M	502	3PE	O31-C3	-2.09	1.40	1.45
45	Y	204	3PE	O31-C3	-2.09	1.40	1.45
53	N	902	CDL	OA6-CA5	2.09	1.40	1.34
46	A	202	PC1	P-O13	2.08	1.67	1.59
45	m	201	3PE	O21-C21	2.08	1.40	1.34
45	Y	206	3PE	O31-C3	-2.08	1.40	1.45
46	B	202	PC1	P-O13	2.07	1.67	1.59
45	Y	205	3PE	O31-C3	-2.07	1.40	1.45
46	M	501	PC1	P-O13	2.07	1.67	1.59
51	F	503	NAI	C8A-N9A	-2.07	1.33	1.37
46	P	401	PC1	P-O13	2.06	1.67	1.59
45	Y	203	3PE	O31-C3	-2.06	1.40	1.45
46	P	402	PC1	P-O13	2.06	1.67	1.59
45	b	101	3PE	O21-C21	2.05	1.40	1.34
45	Y	201	3PE	O31-C3	-2.05	1.40	1.45
48	D	701	U10	C21-C19	2.05	1.55	1.51
53	L	702	CDL	OA8-CA6	-2.04	1.40	1.45
45	b	101	3PE	O31-C3	-2.04	1.40	1.45
46	N	904	PC1	P-O13	2.04	1.67	1.59
45	L	703	3PE	O31-C3	-2.03	1.40	1.45
48	D	701	U10	C18-C19	2.03	1.37	1.33
53	q	202	CDL	OA6-CA5	2.01	1.40	1.34
53	X	201	CDL	OA8-CA6	-2.01	1.40	1.45
48	D	701	U10	C51-C49	2.00	1.55	1.51

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	N	903	CDL	OB6-CB5-C51	6.05	122.23	111.09
56	P	403	NDP	N6A-C6A-N1A	-5.81	105.63	118.35
54	O	401	DGT	C5-C4-N3	-5.50	119.53	128.46
56	P	403	NDP	C4A-N9A-C1B	-5.40	113.73	126.59
56	P	403	NDP	N3A-C2A-N1A	-5.38	120.19	128.60
51	F	503	NAI	N3A-C2A-N1A	-5.35	120.23	128.60
54	O	401	DGT	C1'-N9-C8	5.33	139.79	127.85
56	P	403	NDP	C5A-C4A-N3A	-5.33	119.80	126.75
51	F	503	NAI	C5A-C4A-N3A	-5.18	119.99	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	U	101	EHZ	C8-C9-S1	5.17	120.03	113.63
59	i	201	CHD	C17-C13-C12	5.09	122.31	117.67
56	P	403	NDP	C1B-N9A-C8A	4.87	138.12	127.14
54	O	401	DGT	C1'-N9-C4	-4.83	112.08	125.48
58	T	101	EHZ	C8-C9-S1	4.79	119.55	113.63
56	P	403	NDP	C5A-C6A-N6A	4.76	133.78	123.43
50	F	501	FMN	C9-C8-C7	4.61	126.28	119.67
59	i	201	CHD	C18-C13-C12	-4.60	104.38	109.07
54	O	401	DGT	C2-N3-C4	4.59	120.48	112.30
45	P	404	3PE	O21-C21-C22	4.58	121.37	111.50
50	F	501	FMN	C7M-C7-C6	4.41	127.64	119.49
46	N	904	PC1	O21-C21-C22	4.39	120.95	111.50
53	N	902	CDL	OA6-CA5-C11	4.30	120.76	111.50
46	M	501	PC1	O21-C21-C22	4.28	120.72	111.50
53	X	201	CDL	OB6-CB5-C51	4.26	120.69	111.50
45	I	201	3PE	O21-C21-C22	4.23	120.62	111.50
56	P	403	NDP	N9A-C8A-N7A	-4.21	108.16	113.91
45	M	502	3PE	O21-C21-C22	4.19	120.53	111.50
59	i	201	CHD	C14-C13-C12	4.18	111.30	107.40
45	Y	203	3PE	O21-C21-C22	4.15	120.45	111.50
51	F	503	NAI	N9A-C8A-N7A	-4.15	108.24	113.91
45	m	201	3PE	O21-C21-C22	4.10	120.34	111.50
59	i	201	CHD	C13-C17-C20	-4.09	114.61	119.50
53	h	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
53	N	905	CDL	OA6-CA5-C11	4.08	120.28	111.50
51	F	503	NAI	N6A-C6A-N1A	-4.07	109.44	118.35
45	Y	202	3PE	O21-C21-C22	4.06	120.25	111.50
53	H	602	CDL	OA6-CA5-C11	4.05	120.24	111.50
46	h	202	PC1	O21-C21-C22	4.03	120.19	111.50
45	L	703	3PE	O21-C21-C22	4.00	120.12	111.50
45	Y	201	3PE	O21-C21-C22	3.95	120.02	111.50
46	A	203	PC1	O21-C21-C22	3.95	120.01	111.50
45	K	101	3PE	O21-C21-C22	3.94	119.99	111.50
46	B	202	PC1	O21-C21-C22	3.93	119.98	111.50
46	A	202	PC1	O21-C21-C22	3.92	119.95	111.50
46	q	201	PC1	O21-C21-C22	3.92	119.95	111.50
45	L	704	3PE	O21-C21-C22	3.92	119.94	111.50
46	P	401	PC1	O21-C21-C22	3.89	119.89	111.50
45	Y	204	3PE	O21-C21-C22	3.85	119.80	111.50
45	Y	205	3PE	O21-C21-C22	3.83	119.76	111.50
53	q	202	CDL	OA6-CA5-C11	3.82	119.73	111.50
45	N	901	3PE	O21-C21-C22	3.82	119.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	N	903	CDL	OA6-CA5-C11	3.79	119.67	111.50
59	i	201	CHD	C17-C13-C14	3.78	103.90	100.09
46	P	402	PC1	O21-C21-C22	3.77	119.63	111.50
45	L	701	3PE	O21-C21-C22	3.76	119.61	111.50
45	L	705	3PE	O21-C21-C22	3.76	119.59	111.50
45	b	101	3PE	O21-C21-C22	3.75	119.59	111.50
53	X	201	CDL	OA6-CA5-C11	3.75	119.58	111.50
46	I	204	PC1	O21-C21-C22	3.74	119.56	111.50
45	H	601	3PE	O21-C21-C22	3.74	119.56	111.50
53	q	202	CDL	OB6-CB5-C51	3.73	119.54	111.50
56	P	403	NDP	C2A-N3A-C4A	3.65	120.37	111.75
45	A	201	3PE	O21-C21-C22	3.60	119.25	111.50
45	d	201	3PE	O21-C21-C22	3.58	119.23	111.50
48	D	701	U10	C50-C49-C51	3.58	121.29	115.27
45	Y	206	3PE	O21-C21-C22	3.53	119.11	111.50
53	H	602	CDL	OB6-CB5-C51	3.53	119.10	111.50
53	N	902	CDL	OB6-CB5-C51	3.51	119.06	111.50
48	D	701	U10	C30-C29-C31	3.49	121.14	115.27
51	F	503	NAI	C2A-N3A-C4A	3.47	119.96	111.75
53	h	201	CDL	OA6-CA5-C11	3.47	118.98	111.50
48	D	701	U10	C40-C39-C41	3.45	121.07	115.27
54	O	401	DGT	N9-C4-N3	3.43	132.83	125.94
53	L	702	CDL	OB6-CB5-C51	3.43	118.89	111.50
53	L	702	CDL	OA6-CA5-C11	3.43	118.89	111.50
46	H	603	PC1	O21-C21-C22	3.40	118.83	111.50
53	N	905	CDL	OB6-CB5-C51	3.35	120.15	110.80
50	F	501	FMN	C8M-C8-C7	-3.34	113.89	120.74
50	F	501	FMN	C4-N3-C2	-3.30	119.54	125.64
51	F	503	NAI	C5A-C6A-N6A	3.25	130.50	123.43
48	D	701	U10	C15-C14-C16	3.22	120.69	115.27
45	H	601	3PE	O31-C31-C32	3.22	119.82	111.38
56	P	403	NDP	N3A-C4A-N9A	3.21	132.38	127.08
53	N	903	CDL	OA8-CA7-C31	3.20	121.96	111.91
58	T	101	EHZ	C10-S1-C9	3.17	111.75	101.87
54	O	401	DGT	C2-N1-C6	-3.08	119.48	125.10
51	F	503	NAI	C5A-N7A-C8A	3.06	107.86	103.51
51	F	503	NAI	N3A-C4A-N9A	3.02	132.06	127.08
56	P	403	NDP	C5A-N7A-C8A	3.01	107.79	103.51
48	D	701	U10	C45-C44-C46	3.00	120.32	115.27
59	i	201	CHD	C18-C13-C17	-2.95	106.59	111.21
54	O	401	DGT	N9-C8-N7	-2.90	107.94	113.39
45	Y	204	3PE	O31-C31-C32	2.85	120.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	Y	201	3PE	O31-C31-C32	2.83	120.78	111.91
45	N	901	3PE	O31-C31-C32	2.81	120.74	111.91
48	D	701	U10	C20-C19-C21	2.81	120.00	115.27
54	O	401	DGT	PA-O3A-PB	-2.78	123.28	132.83
45	L	704	3PE	O31-C31-C32	2.77	120.59	111.91
48	D	701	U10	C37-C38-C39	-2.76	121.02	127.66
51	F	503	NAI	C4D-O4D-C1D	-2.75	103.39	109.47
45	m	201	3PE	O31-C31-C32	2.75	120.55	111.91
56	P	403	NDP	PN-O3-PA	-2.75	123.38	132.83
53	q	202	CDL	OA8-CA7-C31	2.74	120.50	111.91
46	I	204	PC1	O31-C31-C32	2.74	120.50	111.91
54	O	401	DGT	PB-O3B-PG	-2.74	123.44	132.83
48	D	701	U10	C47-C48-C49	-2.73	121.09	127.66
50	F	501	FMN	C6-C7-C8	-2.71	115.79	119.67
45	Y	206	3PE	O31-C31-C32	2.70	120.38	111.91
54	O	401	DGT	C5-C6-N1	2.70	120.04	113.19
50	F	501	FMN	C4A-C10-N10	2.68	120.40	116.48
46	q	201	PC1	O31-C31-C32	2.67	120.30	111.91
59	i	201	CHD	C11-C12-C13	2.67	113.98	111.24
53	h	201	CDL	OA8-CA7-C31	2.65	120.23	111.91
45	I	201	3PE	O31-C31-C32	2.65	120.21	111.91
53	N	905	CDL	OB8-CB7-C71	2.64	120.21	111.91
45	P	404	3PE	O31-C31-C32	2.64	120.20	111.91
53	N	902	CDL	OB8-CB7-C71	2.64	120.20	111.91
51	F	503	NAI	PN-O3-PA	-2.64	123.77	132.83
48	D	701	U10	C42-C43-C44	-2.63	121.33	127.66
45	b	101	3PE	O31-C31-C32	2.60	120.08	111.91
53	L	702	CDL	OA8-CA7-C31	2.60	120.08	111.91
45	M	502	3PE	O31-C31-C32	2.60	120.06	111.91
46	M	501	PC1	O31-C31-C32	2.59	120.05	111.91
50	F	501	FMN	C4A-C4-N3	2.58	119.75	113.19
45	L	705	3PE	O31-C31-C32	2.57	119.99	111.91
46	H	603	PC1	O31-C31-C32	2.57	119.98	111.91
53	X	201	CDL	OB8-CB7-C71	2.57	119.97	111.91
53	L	702	CDL	OB8-CB7-C71	2.57	119.97	111.91
46	A	202	PC1	O31-C31-C32	2.56	119.95	111.91
46	A	203	PC1	O31-C31-C32	2.56	119.95	111.91
46	P	401	PC1	O31-C31-C32	2.56	119.94	111.91
46	N	904	PC1	O31-C31-C32	2.55	119.92	111.91
53	X	201	CDL	OA8-CA7-C31	2.54	119.89	111.91
53	q	202	CDL	OB8-CB7-C71	2.53	119.84	111.91
53	N	905	CDL	OA8-CA7-C31	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	D	701	U10	C1M-C1-C6	-2.50	120.32	124.40
50	F	501	FMN	O4-C4-C4A	-2.50	119.98	126.60
54	O	401	DGT	O6-C6-C5	-2.50	119.98	126.60
45	L	703	3PE	O31-C31-C32	2.49	119.74	111.91
45	K	101	3PE	O31-C31-C32	2.49	119.72	111.91
53	N	902	CDL	OA8-CA7-C31	2.49	119.72	111.91
45	Y	205	3PE	O31-C31-C32	2.48	119.69	111.91
53	h	201	CDL	OB8-CB7-C71	2.48	119.68	111.91
53	N	903	CDL	OB8-CB7-C71	2.46	119.63	111.91
45	Y	203	3PE	O31-C31-C32	2.45	119.59	111.91
50	F	501	FMN	C9A-C5A-N5	-2.44	119.78	122.43
45	L	701	3PE	O31-C31-C32	2.43	119.53	111.91
48	D	701	U10	C25-C24-C23	-2.43	117.45	123.68
45	d	201	3PE	O31-C31-C32	2.43	119.53	111.91
48	D	701	U10	C25-C24-C26	2.41	119.32	115.27
53	H	602	CDL	OA8-CA7-C31	2.39	119.42	111.91
50	F	501	FMN	C10-C4A-N5	-2.38	119.80	124.86
45	A	201	3PE	O31-C31-C32	2.37	119.34	111.91
59	i	201	CHD	C14-C8-C9	2.37	112.96	109.71
59	i	201	CHD	C6-C5-C4	-2.36	108.48	111.19
59	i	201	CHD	C23-C22-C20	-2.34	110.24	114.52
53	H	602	CDL	OB8-CB7-C71	2.33	119.21	111.91
46	P	402	PC1	O31-C31-C32	2.31	119.14	111.91
46	B	202	PC1	O31-C31-C32	2.30	119.14	111.91
59	i	201	CHD	C18-C13-C14	-2.30	107.61	111.21
48	D	701	U10	C35-C34-C33	-2.30	117.78	123.68
50	F	501	FMN	C6-C5A-C9A	2.27	122.15	118.94
48	D	701	U10	C10-C9-C8	-2.24	117.93	123.68
54	O	401	DGT	C8-N7-C5	2.24	108.29	104.24
56	P	403	NDP	C4A-N9A-C8A	2.23	108.15	105.73
45	Y	202	3PE	O31-C31-C32	2.23	118.90	111.91
46	h	202	PC1	O31-C31-C32	2.22	118.88	111.91
58	T	101	EHZ	C13-C12-N1	2.21	120.14	116.42
58	U	101	EHZ	C13-C12-N1	2.21	120.14	116.42
48	D	701	U10	C30-C29-C28	-2.17	118.10	123.68
48	D	701	U10	C35-C34-C36	2.17	118.93	115.27
56	P	403	NDP	C2B-C1B-N9A	-2.17	109.88	113.53
58	U	101	EHZ	C10-S1-C9	2.16	108.61	101.87
51	F	503	NAI	C4A-C5A-N7A	-2.14	108.01	110.62
48	D	701	U10	C12-C13-C14	-2.14	122.51	127.66
53	N	902	CDL	CA4-OA6-CA5	-2.13	112.55	117.79
59	i	201	CHD	C21-C20-C17	-2.13	109.67	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	F	503	NAI	C3D-C2D-C1D	2.12	105.46	101.43
58	U	101	EHZ	C7-C8-C9	-2.12	109.05	113.89
50	F	501	FMN	C4A-C10-N1	-2.09	119.88	124.73
48	D	701	U10	C56-C54-C55	2.09	119.21	114.60
56	P	403	NDP	C4A-C5A-N7A	-2.08	108.09	110.62
50	F	501	FMN	C4-C4A-C10	2.07	120.27	116.79
53	N	903	CDL	OB6-CB5-OB7	-2.06	118.88	122.96
45	P	404	3PE	O21-C21-O22	-2.05	118.74	123.70
59	i	201	CHD	C21-C20-C22	-2.05	107.15	110.36
53	q	202	CDL	CA4-OA6-CA5	-2.05	112.74	117.79
48	D	701	U10	C22-C23-C24	-2.05	122.73	127.66
51	F	503	NAI	C4A-N9A-C8A	2.05	107.94	105.73
59	i	201	CHD	C15-C14-C8	2.03	121.17	118.33
50	F	501	FMN	C7M-C7-C8	-2.03	116.57	120.74
51	F	503	NAI	C3N-C2N-N1N	-2.01	120.23	123.10

There are no chirality outliers.

All (907) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O14
45	H	601	3PE	C1-O11-P-O12
45	H	601	3PE	C1-O11-P-O13
45	H	601	3PE	C1-O11-P-O14
45	I	201	3PE	C1-O11-P-O12
45	I	201	3PE	C1-O11-P-O13
45	I	201	3PE	C1-O11-P-O14
45	I	201	3PE	C22-C21-O21-C2
45	K	101	3PE	C1-O11-P-O14
45	K	101	3PE	O11-C1-C2-O21
45	K	101	3PE	C22-C21-O21-C2
45	L	701	3PE	C1-O11-P-O14
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	O13-C11-C12-N
45	L	704	3PE	C1-O11-P-O12
45	L	704	3PE	C1-O11-P-O14
45	L	704	3PE	O13-C11-C12-N
45	L	704	3PE	C3-C2-O21-C21
45	L	704	3PE	C22-C21-O21-C2
45	L	705	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	M	502	3PE	C1-O11-P-O12
45	M	502	3PE	C12-C11-O13-P
45	M	502	3PE	C22-C21-O21-C2
45	N	901	3PE	C1-O11-P-O12
45	N	901	3PE	C1-O11-P-O14
45	N	901	3PE	C22-C21-O21-C2
45	P	404	3PE	O22-C21-O21-C2
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	O13-C11-C12-N
45	Y	201	3PE	O11-C1-C2-O21
45	Y	202	3PE	C2-C1-O11-P
45	Y	202	3PE	C22-C21-O21-C2
45	Y	204	3PE	C1-O11-P-O12
45	Y	205	3PE	C11-O13-P-O12
45	Y	205	3PE	C22-C21-O21-C2
45	Y	206	3PE	C1-O11-P-O14
45	Y	206	3PE	O13-C11-C12-N
45	b	101	3PE	C11-O13-P-O14
45	b	101	3PE	O13-C11-C12-N
45	d	201	3PE	C1-O11-P-O12
45	d	201	3PE	C1-O11-P-O13
45	d	201	3PE	C1-O11-P-O14
45	d	201	3PE	C11-O13-P-O11
45	d	201	3PE	C11-O13-P-O14
45	d	201	3PE	C12-C11-O13-P
45	d	201	3PE	O11-C1-C2-O21
45	m	201	3PE	C12-C11-O13-P
45	m	201	3PE	C22-C21-O21-C2
46	A	202	PC1	O13-C11-C12-N
46	A	203	PC1	C22-C21-O21-C2
46	B	202	PC1	C22-C21-O21-C2
46	H	603	PC1	C1-O11-P-O12
46	H	603	PC1	C1-O11-P-O14
46	H	603	PC1	O13-C11-C12-N
46	I	204	PC1	C1-O11-P-O12
46	M	501	PC1	C11-O13-P-O11
46	P	401	PC1	C2-C1-O11-P
46	h	202	PC1	C11-O13-P-O14
46	h	202	PC1	C11-O13-P-O11
46	h	202	PC1	C2-C1-O11-P
46	q	201	PC1	C22-C21-O21-C2
48	D	701	U10	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
51	F	503	NAI	C5B-O5B-PA-O1A
51	F	503	NAI	C5B-O5B-PA-O3
53	H	602	CDL	CA2-OA2-PA1-OA4
53	H	602	CDL	CA3-OA5-PA1-OA3
53	H	602	CDL	C11-CA5-OA6-CA4
53	H	602	CDL	C1-CB2-OB2-PB2
53	H	602	CDL	CB2-OB2-PB2-OB3
53	H	602	CDL	CB2-OB2-PB2-OB4
53	H	602	CDL	CB2-OB2-PB2-OB5
53	H	602	CDL	CB3-OB5-PB2-OB2
53	H	602	CDL	CB3-OB5-PB2-OB4
53	L	702	CDL	O1-C1-CB2-OB2
53	L	702	CDL	CB2-OB2-PB2-OB3
53	L	702	CDL	CB2-OB2-PB2-OB4
53	L	702	CDL	CB2-OB2-PB2-OB5
53	L	702	CDL	CB3-OB5-PB2-OB2
53	L	702	CDL	CB3-OB5-PB2-OB4
53	N	902	CDL	CA2-OA2-PA1-OA3
53	N	902	CDL	CA2-OA2-PA1-OA4
53	N	902	CDL	CA2-OA2-PA1-OA5
53	N	902	CDL	CB2-OB2-PB2-OB3
53	N	902	CDL	CB2-OB2-PB2-OB4
53	N	902	CDL	CB2-OB2-PB2-OB5
53	N	902	CDL	OB9-CB7-OB8-CB6
53	N	902	CDL	C71-CB7-OB8-CB6
53	N	903	CDL	CA2-OA2-PA1-OA4
53	N	903	CDL	CA4-CA3-OA5-PA1
53	N	903	CDL	C11-CA5-OA6-CA4
53	N	903	CDL	CB2-OB2-PB2-OB3
53	N	903	CDL	CB2-OB2-PB2-OB4
53	N	905	CDL	CA3-OA5-PA1-OA4
53	N	905	CDL	CB2-OB2-PB2-OB3
53	N	905	CDL	CB2-OB2-PB2-OB4
53	X	201	CDL	CA3-OA5-PA1-OA4
53	X	201	CDL	CA4-CA3-OA5-PA1
53	X	201	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CB2-OB2-PB2-OB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	OB7-CB5-OB6-CB4
53	q	202	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
53	q	202	CDL	CA2-OA2-PA1-OA4
53	q	202	CDL	OA7-CA5-OA6-CA4
53	q	202	CDL	CB2-OB2-PB2-OB4
54	O	401	DGT	C5'-O5'-PA-O3A
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	S1-C10-C11-N1
58	T	101	EHZ	C15-C16-C17-C20
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
45	L	701	3PE	O32-C31-O31-C3
45	Y	206	3PE	O32-C31-O31-C3
46	q	201	PC1	O32-C31-O31-C3
45	K	101	3PE	C32-C31-O31-C3
46	h	202	PC1	C32-C31-O31-C3
45	K	101	3PE	O32-C31-O31-C3
45	N	901	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
46	N	904	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
53	L	702	CDL	OB9-CB7-OB8-CB6
53	N	903	CDL	OA9-CA7-OA8-CA6
45	H	601	3PE	O22-C21-O21-C2
45	I	201	3PE	O22-C21-O21-C2
45	K	101	3PE	O22-C21-O21-C2
45	L	704	3PE	O22-C21-O21-C2
45	M	502	3PE	O22-C21-O21-C2
45	N	901	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	m	201	3PE	O22-C21-O21-C2
46	A	203	PC1	O22-C21-O21-C2
46	B	202	PC1	O22-C21-O21-C2
46	q	201	PC1	O22-C21-O21-C2
53	H	602	CDL	OB7-CB5-OB6-CB4
53	N	903	CDL	OA7-CA5-OA6-CA4
53	X	201	CDL	OB7-CB5-OB6-CB4
45	L	701	3PE	C32-C31-O31-C3
45	L	705	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
46	N	904	PC1	C32-C31-O31-C3
46	q	201	PC1	C32-C31-O31-C3
45	H	601	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	P	404	3PE	C22-C21-O21-C2
53	N	902	CDL	C11-CA5-OA6-CA4
53	h	201	CDL	C51-CB5-OB6-CB4
53	q	202	CDL	C11-CA5-OA6-CA4
53	N	903	CDL	C51-CB5-OB6-CB4
53	H	602	CDL	OA9-CA7-OA8-CA6
53	N	903	CDL	OB7-CB5-OB6-CB4
48	D	701	U10	C13-C14-C16-C17
45	L	704	3PE	C32-C31-O31-C3
45	M	502	3PE	C32-C31-O31-C3
45	N	901	3PE	C32-C31-O31-C3
45	P	404	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
45	Y	205	3PE	C32-C31-O31-C3
45	b	101	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
46	P	401	PC1	C32-C31-O31-C3
53	H	602	CDL	C31-CA7-OA8-CA6
53	L	702	CDL	C71-CB7-OB8-CB6
53	N	903	CDL	C31-CA7-OA8-CA6
45	Y	205	3PE	O22-C21-O21-C2
53	H	602	CDL	OA7-CA5-OA6-CA4
53	N	902	CDL	OA7-CA5-OA6-CA4
45	L	705	3PE	O32-C31-O31-C3
46	P	401	PC1	O32-C31-O31-C3
53	N	902	CDL	O1-C1-CB2-OB2
53	N	903	CDL	O1-C1-CA2-OA2
53	N	905	CDL	O1-C1-CB2-OB2
53	h	201	CDL	C71-CB7-OB8-CB6
45	b	101	3PE	O32-C31-O31-C3
45	L	701	3PE	C22-C21-O21-C2
45	Y	201	3PE	C22-C21-O21-C2
53	H	602	CDL	C51-CB5-OB6-CB4
53	L	702	CDL	CA5-C11-C12-C13
46	M	501	PC1	C32-C31-O31-C3
45	M	502	3PE	O32-C31-O31-C3
45	P	404	3PE	O32-C31-O31-C3
53	N	902	CDL	C16-C17-C18-C19
48	D	701	U10	C30-C29-C31-C32
48	D	701	U10	C40-C39-C41-C42
48	D	701	U10	C50-C49-C51-C52

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Mol	Chain	Res	Type	Atoms
48	D	701	U10	C28-C29-C31-C32
48	D	701	U10	C38-C39-C41-C42
48	D	701	U10	C48-C49-C51-C52
45	L	704	3PE	O32-C31-O31-C3
45	Y	205	3PE	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
48	D	701	U10	C24-C26-C27-C28
45	Y	202	3PE	C32-C31-O31-C3
46	M	501	PC1	O32-C31-O31-C3
53	h	201	CDL	OB9-CB7-OB8-CB6
53	X	201	CDL	CA2-C1-CB2-OB2
45	L	701	3PE	O22-C21-O21-C2
45	Y	201	3PE	O22-C21-O21-C2
45	Y	202	3PE	O32-C31-O31-C3
45	d	201	3PE	C32-C31-O31-C3
46	H	603	PC1	C32-C31-O31-C3
46	I	204	PC1	C32-C31-O31-C3
53	h	201	CDL	O1-C1-CB2-OB2
53	h	201	CDL	C57-C58-C59-C60
46	N	904	PC1	C21-C22-C23-C24
53	H	602	CDL	CA5-C11-C12-C13
53	N	903	CDL	CA5-C11-C12-C13
46	H	603	PC1	O32-C31-O31-C3
53	N	905	CDL	C31-CA7-OA8-CA6
46	A	203	PC1	C31-C32-C33-C34
53	N	902	CDL	CA5-C11-C12-C13
53	N	905	CDL	CA5-C11-C12-C13
45	Y	204	3PE	C22-C23-C24-C25
53	L	702	CDL	CB4-CB3-OB5-PB2
53	X	201	CDL	C17-C18-C19-C20
46	I	204	PC1	O32-C31-O31-C3
53	N	902	CDL	C58-C59-C60-C61
45	Y	204	3PE	C31-C32-C33-C34
45	m	201	3PE	C31-C32-C33-C34
53	X	201	CDL	O1-C1-CB2-OB2
45	d	201	3PE	O32-C31-O31-C3
53	N	905	CDL	OA9-CA7-OA8-CA6
46	H	603	PC1	C36-C37-C38-C39
45	A	201	3PE	C1-O11-P-O13
45	K	101	3PE	C1-O11-P-O13
45	L	703	3PE	C11-O13-P-O11
45	L	704	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	L	705	3PE	C1-O11-P-O13
45	M	502	3PE	C1-O11-P-O13
45	N	901	3PE	C1-O11-P-O13
45	P	404	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O13
45	Y	204	3PE	C1-O11-P-O13
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C11-O13-P-O11
45	Y	206	3PE	C1-O11-P-O13
45	m	201	3PE	C1-O11-P-O13
46	H	603	PC1	C1-O11-P-O13
46	h	202	PC1	C1-O11-P-O13
46	q	201	PC1	C11-O13-P-O11
46	q	201	PC1	C1-O11-P-O13
53	H	602	CDL	CA2-OA2-PA1-OA5
53	H	602	CDL	CA3-OA5-PA1-OA2
53	N	903	CDL	CA2-OA2-PA1-OA5
53	N	903	CDL	CB2-OB2-PB2-OB5
53	N	905	CDL	CA2-OA2-PA1-OA5
53	N	905	CDL	CA3-OA5-PA1-OA2
53	N	905	CDL	CB2-OB2-PB2-OB5
53	X	201	CDL	CA3-OA5-PA1-OA2
53	X	201	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	CA2-OA2-PA1-OA5
53	q	202	CDL	CA2-OA2-PA1-OA5
53	q	202	CDL	CB2-OB2-PB2-OB5
53	N	903	CDL	C12-C13-C14-C15
53	L	702	CDL	CA2-C1-CB2-OB2
53	N	903	CDL	CB2-C1-CA2-OA2
46	A	203	PC1	C32-C31-O31-C3
53	L	702	CDL	CB5-C51-C52-C53
53	H	602	CDL	CB5-C51-C52-C53
45	b	101	3PE	C22-C21-O21-C2
53	N	905	CDL	C11-CA5-OA6-CA4
53	N	905	CDL	C51-CB5-OB6-CB4
45	K	101	3PE	C27-C28-C29-C2A
45	Y	201	3PE	C23-C24-C25-C26
53	L	702	CDL	C32-C33-C34-C35
53	N	902	CDL	C60-C61-C62-C63
53	N	903	CDL	C17-C18-C19-C20
53	X	201	CDL	C63-C64-C65-C66
45	L	701	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C39-C3A-C3B-C3C
45	L	703	3PE	C3A-C3B-C3C-C3D
45	M	502	3PE	C3-C2-O21-C21
45	Y	205	3PE	C3-C2-O21-C21
45	Y	206	3PE	O22-C21-O21-C2
53	N	905	CDL	OA7-CA5-OA6-CA4
53	N	905	CDL	OB7-CB5-OB6-CB4
45	Y	204	3PE	C34-C35-C36-C37
46	q	201	PC1	C32-C33-C34-C35
53	N	902	CDL	C19-C20-C21-C22
53	N	905	CDL	CB4-CB3-OB5-PB2
45	Y	201	3PE	C26-C27-C28-C29
45	m	201	3PE	C24-C25-C26-C27
53	H	602	CDL	C58-C59-C60-C61
46	h	202	PC1	C22-C23-C24-C25
53	X	201	CDL	C14-C15-C16-C17
58	U	101	EHZ	C1-C21-C22-C23
45	N	901	3PE	C22-C23-C24-C25
46	H	603	PC1	C38-C39-C3A-C3B
53	N	902	CDL	C75-C76-C77-C78
45	A	201	3PE	C26-C27-C28-C29
45	M	502	3PE	C38-C39-C3A-C3B
53	L	702	CDL	C12-C13-C14-C15
46	q	201	PC1	C2-C3-O31-C31
46	A	203	PC1	C35-C36-C37-C38
46	N	904	PC1	C35-C36-C37-C38
46	h	202	PC1	C33-C34-C35-C36
45	Y	206	3PE	C37-C38-C39-C3A
46	A	202	PC1	C26-C27-C28-C29
45	b	101	3PE	O22-C21-O21-C2
45	Y	206	3PE	C22-C21-O21-C2
53	H	602	CDL	C63-C64-C65-C66
45	m	201	3PE	C21-C22-C23-C24
53	h	201	CDL	CA5-C11-C12-C13
45	M	502	3PE	C34-C35-C36-C37
45	Y	203	3PE	C28-C29-C2A-C2B
45	d	201	3PE	C35-C36-C37-C38
46	B	202	PC1	C35-C36-C37-C38
46	M	501	PC1	C29-C2A-C2B-C2C
53	X	201	CDL	C20-C21-C22-C23
53	h	201	CDL	C73-C74-C75-C76
45	L	703	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
53	N	905	CDL	C76-C77-C78-C79
46	A	203	PC1	C22-C23-C24-C25
46	N	904	PC1	C32-C33-C34-C35
45	N	901	3PE	C31-C32-C33-C34
45	Y	201	3PE	C2C-C2D-C2E-C2F
45	Y	206	3PE	C22-C23-C24-C25
45	d	201	3PE	C32-C33-C34-C35
46	I	204	PC1	C33-C34-C35-C36
45	L	701	3PE	C26-C27-C28-C29
46	M	501	PC1	C32-C33-C34-C35
53	h	201	CDL	C39-C40-C41-C42
45	I	201	3PE	C2C-C2D-C2E-C2F
46	M	501	PC1	C2B-C2C-C2D-C2E
46	q	201	PC1	C34-C35-C36-C37
53	N	903	CDL	C33-C34-C35-C36
53	q	202	CDL	CA3-CA4-CA6-OA8
53	H	602	CDL	C51-C52-C53-C54
45	K	101	3PE	C29-C2A-C2B-C2C
45	d	201	3PE	C22-C23-C24-C25
58	T	101	EHZ	C1-C21-C22-C23
53	X	201	CDL	CA7-C31-C32-C33
53	N	902	CDL	C37-C38-C39-C40
53	q	202	CDL	C17-C18-C19-C20
46	A	203	PC1	O32-C31-O31-C3
58	U	101	EHZ	C3-C4-C5-C6
45	L	703	3PE	C33-C34-C35-C36
53	X	201	CDL	C51-C52-C53-C54
53	X	201	CDL	C59-C60-C61-C62
46	h	202	PC1	C26-C27-C28-C29
53	X	201	CDL	C58-C59-C60-C61
45	m	201	3PE	C2D-C2E-C2F-C2G
45	M	502	3PE	C3A-C3B-C3C-C3D
46	q	201	PC1	C2A-C2B-C2C-C2D
53	X	201	CDL	C24-C25-C26-C27
45	P	404	3PE	C36-C37-C38-C39
45	Y	204	3PE	C36-C37-C38-C39
53	N	902	CDL	C71-C72-C73-C74
53	N	902	CDL	CB5-C51-C52-C53
45	d	201	3PE	C34-C35-C36-C37
53	N	905	CDL	C71-C72-C73-C74
58	T	101	EHZ	C12-C13-C14-N2
45	L	703	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C22-C21-O21-C2
46	H	603	PC1	O11-C1-C2-O21
45	M	502	3PE	C27-C28-C29-C2A
45	d	201	3PE	C38-C39-C3A-C3B
45	d	201	3PE	C25-C26-C27-C28
45	L	703	3PE	O22-C21-O21-C2
46	q	201	PC1	C21-C22-C23-C24
45	d	201	3PE	C27-C28-C29-C2A
46	I	204	PC1	O21-C2-C3-O31
45	L	701	3PE	C39-C3A-C3B-C3C
45	N	901	3PE	C2B-C2C-C2D-C2E
45	Y	202	3PE	C32-C33-C34-C35
45	d	201	3PE	C24-C25-C26-C27
45	N	901	3PE	C36-C37-C38-C39
45	Y	201	3PE	C2A-C2B-C2C-C2D
46	h	202	PC1	C2A-C2B-C2C-C2D
53	L	702	CDL	C41-C42-C43-C44
45	Y	204	3PE	C22-C21-O21-C2
45	d	201	3PE	C29-C2A-C2B-C2C
53	L	702	CDL	C71-C72-C73-C74
58	U	101	EHZ	C21-C1-C2-C3
45	A	201	3PE	C11-O13-P-O11
46	I	204	PC1	C11-O13-P-O11
46	I	204	PC1	C1-O11-P-O13
56	P	403	NDP	O4D-C1D-N1N-C6N
58	U	101	EHZ	C2-C1-C21-C22
53	N	903	CDL	C1-CA2-OA2-PA1
45	N	901	3PE	C33-C34-C35-C36
53	N	905	CDL	C77-C78-C79-C80
45	L	704	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
45	d	201	3PE	O11-C1-C2-C3
53	q	202	CDL	C12-C13-C14-C15
45	A	201	3PE	C28-C29-C2A-C2B
45	M	502	3PE	C37-C38-C39-C3A
53	N	902	CDL	CA2-C1-CB2-OB2
53	N	905	CDL	CA2-C1-CB2-OB2
45	I	201	3PE	C28-C29-C2A-C2B
45	Y	205	3PE	C22-C23-C24-C25
53	N	905	CDL	C34-C35-C36-C37
45	A	201	3PE	C1-C2-C3-O31
45	H	601	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	b	101	3PE	C23-C24-C25-C26
46	A	203	PC1	C1-C2-C3-O31
45	m	201	3PE	C35-C36-C37-C38
46	N	904	PC1	C2-C3-O31-C31
45	A	201	3PE	C2B-C2C-C2D-C2E
46	H	603	PC1	C2B-C2C-C2D-C2E
45	L	703	3PE	C38-C39-C3A-C3B
45	A	201	3PE	C38-C39-C3A-C3B
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
46	N	904	PC1	C23-C24-C25-C26
53	L	702	CDL	CB6-CB4-OB6-CB5
45	Y	206	3PE	C28-C29-C2A-C2B
53	H	602	CDL	C53-C54-C55-C56
53	N	903	CDL	C13-C14-C15-C16
45	Y	206	3PE	O21-C21-C22-C23
46	B	202	PC1	C33-C34-C35-C36
53	H	602	CDL	C12-C13-C14-C15
53	N	903	CDL	O1-C1-CB2-OB2
45	P	404	3PE	C23-C24-C25-C26
45	m	201	3PE	C2A-C2B-C2C-C2D
53	N	903	CDL	C39-C40-C41-C42
45	P	404	3PE	O31-C31-C32-C33
45	L	701	3PE	C2C-C2D-C2E-C2F
58	T	101	EHZ	O5-C16-C17-C18
58	T	101	EHZ	O5-C16-C17-C19
45	L	703	3PE	C36-C37-C38-C39
53	N	902	CDL	C33-C34-C35-C36
53	X	201	CDL	C52-C51-CB5-OB6
46	A	202	PC1	C22-C23-C24-C25
51	F	503	NAI	PN-O3-PA-O1A
45	K	101	3PE	C38-C39-C3A-C3B
53	N	903	CDL	C21-C22-C23-C24
53	N	903	CDL	CA2-C1-CB2-OB2
45	m	201	3PE	C33-C34-C35-C36
53	q	202	CDL	C18-C19-C20-C21
45	A	201	3PE	C32-C31-O31-C3
45	Y	201	3PE	C24-C25-C26-C27
53	N	902	CDL	C51-C52-C53-C54
53	h	201	CDL	C76-C77-C78-C79
53	q	202	CDL	C52-C53-C54-C55
46	I	204	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
53	N	902	CDL	C40-C41-C42-C43
51	F	503	NAI	C3D-C4D-C5D-O5D
45	Y	201	3PE	O11-C1-C2-C3
45	m	201	3PE	O11-C1-C2-C3
46	H	603	PC1	O11-C1-C2-C3
46	I	204	PC1	O11-C1-C2-C3
53	N	902	CDL	OA5-CA3-CA4-CA6
48	D	701	U10	C39-C41-C42-C43
45	H	601	3PE	C26-C27-C28-C29
46	H	603	PC1	C22-C23-C24-C25
46	A	202	PC1	C32-C31-O31-C3
45	Y	204	3PE	O22-C21-O21-C2
53	X	201	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	C71-CB7-OB8-CB6
53	N	903	CDL	C34-C35-C36-C37
45	L	701	3PE	C2F-C2G-C2H-C2I
53	L	702	CDL	C62-C63-C64-C65
53	h	201	CDL	C35-C36-C37-C38
45	d	201	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
46	I	204	PC1	C1-C2-C3-O31
53	N	905	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	CA3-CA4-CA6-OA8
45	H	601	3PE	C23-C24-C25-C26
45	P	404	3PE	C38-C39-C3A-C3B
46	M	501	PC1	C25-C26-C27-C28
46	P	402	PC1	C25-C26-C27-C28
58	T	101	EHZ	C22-C23-C24-C25
45	Y	201	3PE	C1-O11-P-O13
45	b	101	3PE	C1-O11-P-O13
46	A	202	PC1	C11-O13-P-O11
46	N	904	PC1	C31-C32-C33-C34
53	L	702	CDL	C35-C36-C37-C38
45	Y	204	3PE	O11-C1-C2-O21
46	I	204	PC1	O11-C1-C2-O21
46	M	501	PC1	O11-C1-C2-O21
53	N	905	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	OA5-CA3-CA4-OA6
53	q	202	CDL	OB5-CB3-CB4-OB6
46	P	402	PC1	C32-C31-O31-C3
45	M	502	3PE	C35-C36-C37-C38
45	K	101	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	O31-C31-C32-C33
53	h	201	CDL	C36-C37-C38-C39
46	I	204	PC1	C24-C25-C26-C27
45	A	201	3PE	O21-C2-C3-O31
45	L	701	3PE	O21-C2-C3-O31
53	H	602	CDL	OB6-CB4-CB6-OB8
53	N	905	CDL	OB6-CB4-CB6-OB8
45	N	901	3PE	C27-C28-C29-C2A
53	h	201	CDL	C34-C35-C36-C37
58	T	101	EHZ	C2-C3-C4-C5
53	N	902	CDL	C73-C74-C75-C76
53	q	202	CDL	C71-C72-C73-C74
45	M	502	3PE	C2-C1-O11-P
50	F	501	FMN	C4'-C5'-O5'-P
53	N	902	CDL	C35-C36-C37-C38
46	I	204	PC1	C39-C3A-C3B-C3C
53	L	702	CDL	C15-C16-C17-C18
53	X	201	CDL	C57-C58-C59-C60
58	T	101	EHZ	O2-C9-S1-C10
45	A	201	3PE	O32-C31-O31-C3
45	M	502	3PE	C3F-C3G-C3H-C3I
45	A	201	3PE	O11-C1-C2-C3
45	K	101	3PE	O11-C1-C2-C3
53	H	602	CDL	OB5-CB3-CB4-CB6
53	h	201	CDL	OB5-CB3-CB4-CB6
45	Y	202	3PE	O21-C21-C22-C23
45	Y	204	3PE	O31-C31-C32-C33
45	d	201	3PE	C2A-C2B-C2C-C2D
46	H	603	PC1	C23-C24-C25-C26
53	N	902	CDL	C52-C53-C54-C55
45	M	502	3PE	C2A-C2B-C2C-C2D
53	q	202	CDL	C51-CB5-OB6-CB4
58	U	101	EHZ	C5-C6-C7-C8
46	A	202	PC1	O32-C31-O31-C3
45	Y	205	3PE	O31-C31-C32-C33
45	Y	203	3PE	C32-C33-C34-C35
58	T	101	EHZ	C8-C9-S1-C10
45	Y	201	3PE	C27-C28-C29-C2A
46	N	904	PC1	C37-C38-C39-C3A
45	N	901	3PE	C2-C1-O11-P
45	b	101	3PE	C2-C1-O11-P
46	N	904	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	N	902	CDL	OA5-CA3-CA4-OA6
53	X	201	CDL	OB5-CB3-CB4-OB6
53	q	202	CDL	CA7-C31-C32-C33
53	h	201	CDL	C17-C18-C19-C20
53	q	202	CDL	OB7-CB5-OB6-CB4
58	T	101	EHZ	C15-C16-C17-C19
58	U	101	EHZ	O1-C7-C8-C9
53	X	201	CDL	OA9-CA7-OA8-CA6
53	X	201	CDL	OB9-CB7-OB8-CB6
46	A	202	PC1	O21-C2-C3-O31
46	A	203	PC1	O21-C2-C3-O31
46	N	904	PC1	O21-C2-C3-O31
51	F	503	NAI	C5D-O5D-PN-O3
45	A	201	3PE	C23-C24-C25-C26
46	P	402	PC1	O32-C31-O31-C3
53	N	902	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C36-C37-C38-C39
53	h	201	CDL	C37-C38-C39-C40
46	P	402	PC1	C35-C36-C37-C38
45	H	601	3PE	C22-C23-C24-C25
46	H	603	PC1	C29-C2A-C2B-C2C
46	I	204	PC1	C35-C36-C37-C38
45	M	502	3PE	C11-O13-P-O11
45	Y	204	3PE	C11-O13-P-O11
53	N	903	CDL	C19-C20-C21-C22
53	q	202	CDL	O1-C1-CB2-OB2
53	H	602	CDL	C14-C15-C16-C17
53	N	905	CDL	C43-C44-C45-C46
53	N	905	CDL	CA4-CA3-OA5-PA1
45	K	101	3PE	C1-O11-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	705	3PE	C1-O11-P-O12
45	M	502	3PE	C1-O11-P-O14
45	P	404	3PE	C1-O11-P-O12
45	P	404	3PE	C1-O11-P-O14
45	P	404	3PE	C11-O13-P-O12
45	Y	203	3PE	C1-O11-P-O12
45	Y	205	3PE	C1-O11-P-O12
45	Y	205	3PE	C1-O11-P-O14
45	m	201	3PE	C1-O11-P-O12
45	m	201	3PE	C1-O11-P-O14
46	I	204	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
46	I	204	PC1	C1-O11-P-O14
46	M	501	PC1	C11-O13-P-O12
46	h	202	PC1	C1-O11-P-O12
46	h	202	PC1	C1-O11-P-O14
46	q	201	PC1	C11-O13-P-O12
46	q	201	PC1	C1-O11-P-O12
48	D	701	U10	C6-C7-C8-C9
53	H	602	CDL	CA2-OA2-PA1-OA3
53	H	602	CDL	CA3-OA5-PA1-OA4
53	H	602	CDL	CB3-OB5-PB2-OB3
53	L	702	CDL	CB3-OB5-PB2-OB3
53	N	903	CDL	CA2-OA2-PA1-OA3
53	N	905	CDL	CA2-OA2-PA1-OA3
53	N	905	CDL	CA3-OA5-PA1-OA3
53	X	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
54	O	401	DGT	C5'-O5'-PA-O1A
46	P	401	PC1	C21-C22-C23-C24
53	H	602	CDL	C71-CB7-OB8-CB6
53	X	201	CDL	OB5-CB3-CB4-CB6
45	L	703	3PE	C29-C2A-C2B-C2C
45	K	101	3PE	O13-C11-C12-N
46	A	202	PC1	C32-C33-C34-C35
45	L	703	3PE	C34-C35-C36-C37
46	q	201	PC1	C2C-C2D-C2E-C2F
45	Y	204	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	L	705	3PE	C21-C22-C23-C24
53	H	602	CDL	CA7-C31-C32-C33
45	I	201	3PE	C23-C24-C25-C26
45	P	404	3PE	C33-C34-C35-C36
53	L	702	CDL	OB7-CB5-OB6-CB4
45	A	201	3PE	O11-C1-C2-O21
45	L	701	3PE	O11-C1-C2-O21
45	L	704	3PE	O11-C1-C2-O21
45	L	705	3PE	O11-C1-C2-O21
45	m	201	3PE	O11-C1-C2-O21
53	H	602	CDL	OB5-CB3-CB4-OB6
53	L	702	CDL	OB5-CB3-CB4-OB6
56	P	403	NDP	O4D-C4D-C5D-O5D
53	h	201	CDL	C13-C14-C15-C16
45	H	601	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
53	N	902	CDL	C51-CB5-OB6-CB4
53	H	602	CDL	OB9-CB7-OB8-CB6
46	P	402	PC1	C27-C28-C29-C2A
45	L	705	3PE	C35-C36-C37-C38
46	h	202	PC1	C2D-C2E-C2F-C2G
58	T	101	EHZ	O5-C16-C17-C20
45	H	601	3PE	O21-C2-C3-O31
46	q	201	PC1	O21-C2-C3-O31
53	h	201	CDL	OA6-CA4-CA6-OA8
53	q	202	CDL	OA6-CA4-CA6-OA8
53	q	202	CDL	C51-C52-C53-C54
53	N	905	CDL	C44-C45-C46-C47
45	m	201	3PE	C2-C1-O11-P
45	L	701	3PE	C31-C32-C33-C34
53	h	201	CDL	C55-C56-C57-C58
45	d	201	3PE	O31-C31-C32-C33
45	L	701	3PE	C27-C28-C29-C2A
53	N	902	CDL	C53-C54-C55-C56
45	Y	203	3PE	O21-C21-C22-C23
46	P	401	PC1	O21-C21-C22-C23
53	N	905	CDL	C31-C32-C33-C34
45	L	701	3PE	C36-C37-C38-C39
45	Y	201	3PE	O21-C21-C22-C23
45	H	601	3PE	C1-C2-O21-C21
45	I	201	3PE	C1-C2-O21-C21
45	N	901	3PE	C3-C2-O21-C21
45	P	404	3PE	C3-C2-O21-C21
45	Y	202	3PE	C1-C2-O21-C21
46	P	401	PC1	C3-C2-O21-C21
46	q	201	PC1	C3-C2-O21-C21
53	H	602	CDL	CA6-CA4-OA6-CA5
45	L	701	3PE	O11-C1-C2-C3
46	M	501	PC1	O11-C1-C2-C3
53	X	201	CDL	C12-C11-CA5-OA6
53	h	201	CDL	C75-C76-C77-C78
45	L	703	3PE	C27-C28-C29-C2A
45	M	502	3PE	C3E-C3F-C3G-C3H
45	Y	202	3PE	C22-C23-C24-C25
46	q	201	PC1	C2E-C2F-C2G-C2H
45	A	201	3PE	O21-C21-C22-C23
48	D	701	U10	C34-C36-C37-C38
45	d	201	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	I	201	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O11
45	Y	202	3PE	C1-O11-P-O13
45	Y	203	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O11
46	A	203	PC1	C11-O13-P-O11
46	B	202	PC1	C11-O13-P-O11
53	N	902	CDL	CB3-OB5-PB2-OB2
46	P	402	PC1	C3A-C3B-C3C-C3D
53	L	702	CDL	C56-C57-C58-C59
51	F	503	NAI	O4D-C1D-N1N-C2N
53	h	201	CDL	OA7-CA5-OA6-CA4
45	Y	201	3PE	C32-C33-C34-C35
48	D	701	U10	C5-C4-O4-C4M
46	H	603	PC1	C27-C28-C29-C2A
50	F	501	FMN	C2'-C3'-C4'-O4'
45	I	201	3PE	C2-C1-O11-P
45	L	705	3PE	C2-C1-O11-P
53	X	201	CDL	C1-CB2-OB2-PB2
45	K	101	3PE	C34-C35-C36-C37
46	P	402	PC1	O21-C21-C22-C23
45	A	201	3PE	C34-C35-C36-C37
53	N	902	CDL	C11-C12-C13-C14
53	h	201	CDL	CA2-C1-CB2-OB2
45	A	201	3PE	C25-C26-C27-C28
53	X	201	CDL	CB7-C71-C72-C73
45	Y	201	3PE	C28-C29-C2A-C2B
46	P	402	PC1	C34-C35-C36-C37
59	i	201	CHD	C22-C23-C24-O26
45	Y	206	3PE	O22-C21-C22-C23
45	Y	203	3PE	O22-C21-O21-C2
45	M	502	3PE	O11-C1-C2-C3
45	H	601	3PE	O13-C11-C12-N
45	Y	204	3PE	O13-C11-C12-N
45	A	201	3PE	C29-C2A-C2B-C2C
53	N	903	CDL	OA5-CA3-CA4-OA6
45	L	703	3PE	C23-C24-C25-C26
45	P	404	3PE	C32-C33-C34-C35
46	A	203	PC1	C32-C33-C34-C35
45	I	201	3PE	C33-C34-C35-C36
45	H	601	3PE	O32-C31-C32-C33
45	Y	201	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C2-C1-O11-P
45	L	704	3PE	C2-C1-O11-P
45	P	404	3PE	C2-C1-O11-P
58	U	101	EHZ	S1-C10-C11-N1
45	L	701	3PE	C34-C35-C36-C37
45	Y	206	3PE	C2B-C2C-C2D-C2E
59	i	201	CHD	C22-C23-C24-O25
50	F	501	FMN	O3'-C3'-C4'-C5'
45	m	201	3PE	C26-C27-C28-C29
53	H	602	CDL	C55-C56-C57-C58
56	P	403	NDP	O4B-C4B-C5B-O5B
45	Y	206	3PE	C23-C24-C25-C26
46	I	204	PC1	C37-C38-C39-C3A
46	P	402	PC1	C1-C2-C3-O31
53	X	201	CDL	CB3-CB4-CB6-OB8
45	K	101	3PE	C24-C25-C26-C27
48	D	701	U10	C19-C21-C22-C23
45	I	201	3PE	C3-C2-O21-C21
53	X	201	CDL	CB6-CB4-OB6-CB5
46	q	201	PC1	C36-C37-C38-C39
46	I	204	PC1	O22-C21-O21-C2
53	N	905	CDL	C73-C74-C75-C76
45	m	201	3PE	C2B-C2C-C2D-C2E
45	L	705	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
53	N	905	CDL	OB5-CB3-CB4-CB6
45	N	901	3PE	C37-C38-C39-C3A
45	Y	201	3PE	C25-C26-C27-C28
45	Y	203	3PE	C22-C21-O21-C2
53	L	702	CDL	C51-CB5-OB6-CB4
45	d	201	3PE	C21-C22-C23-C24
46	q	201	PC1	C2B-C2C-C2D-C2E
58	T	101	EHZ	C11-C10-S1-C9
45	I	201	3PE	O21-C2-C3-O31
53	N	903	CDL	OA6-CA4-CA6-OA8
53	X	201	CDL	C11-C12-C13-C14
53	H	602	CDL	C56-C57-C58-C59
46	H	603	PC1	C32-C33-C34-C35
53	X	201	CDL	C53-C54-C55-C56
48	D	701	U10	C9-C11-C12-C13
48	D	701	U10	C49-C51-C52-C53
53	H	602	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
45	P	404	3PE	C35-C36-C37-C38
45	Y	201	3PE	C2E-C2F-C2G-C2H
46	H	603	PC1	C35-C36-C37-C38
53	X	201	CDL	C41-C42-C43-C44
46	q	201	PC1	O31-C31-C32-C33
54	O	401	DGT	PB-O3A-PA-O1A
48	D	701	U10	C16-C17-C18-C19
53	h	201	CDL	C11-C12-C13-C14
45	P	404	3PE	O32-C31-C32-C33
46	B	202	PC1	C27-C28-C29-C2A
45	d	201	3PE	C37-C38-C39-C3A
46	q	201	PC1	C1-C2-C3-O31
58	U	101	EHZ	C1-C2-C3-C4
45	K	101	3PE	C33-C34-C35-C36
45	L	703	3PE	C26-C27-C28-C29
45	d	201	3PE	C2C-C2D-C2E-C2F
46	P	401	PC1	C25-C26-C27-C28
53	X	201	CDL	C52-C51-CB5-OB7
46	I	204	PC1	C38-C39-C3A-C3B
58	T	101	EHZ	C21-C1-C2-C3
53	L	702	CDL	OB5-CB3-CB4-CB6
53	h	201	CDL	OA5-CA3-CA4-CA6
53	q	202	CDL	OB5-CB3-CB4-CB6
53	N	902	CDL	C42-C43-C44-C45
45	L	705	3PE	O13-C11-C12-N
45	N	901	3PE	C29-C2A-C2B-C2C
50	F	501	FMN	C2'-C3'-C4'-C5'
45	Y	206	3PE	C2-C1-O11-P
53	L	702	CDL	CB2-C1-CA2-OA2
46	A	203	PC1	C33-C34-C35-C36
46	h	202	PC1	O21-C2-C3-O31
53	N	902	CDL	OB6-CB4-CB6-OB8
53	h	201	CDL	C11-CA5-OA6-CA4
45	L	701	3PE	C1-O11-P-O13
46	H	603	PC1	O21-C21-C22-C23
45	m	201	3PE	O31-C31-C32-C33
45	m	201	3PE	O21-C21-C22-C23
46	h	202	PC1	O31-C31-C32-C33
53	q	202	CDL	C52-C51-CB5-OB6
45	H	601	3PE	C3-C2-O21-C21
53	N	902	CDL	C63-C64-C65-C66
45	I	201	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
53	L	702	CDL	C12-C11-CA5-OA6
45	A	201	3PE	C36-C37-C38-C39
45	A	201	3PE	O31-C31-C32-C33
45	N	901	3PE	O31-C31-C32-C33
53	H	602	CDL	C52-C51-CB5-OB6
53	q	202	CDL	C32-C31-CA7-OA8
53	H	602	CDL	CB3-CB4-CB6-OB8
45	I	201	3PE	C32-C33-C34-C35
45	L	703	3PE	O31-C31-C32-C33
45	M	502	3PE	O21-C21-C22-C23
53	X	201	CDL	C12-C13-C14-C15
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	C15-C16-C17-C18
53	N	903	CDL	OA5-CA3-CA4-CA6
45	L	703	3PE	O21-C21-C22-C23
45	K	101	3PE	O21-C2-C3-O31
53	N	903	CDL	OB6-CB4-CB6-OB8
46	M	501	PC1	C2F-C2G-C2H-C2I
53	N	902	CDL	C39-C40-C41-C42
46	A	203	PC1	O32-C31-C32-C33
56	P	403	NDP	C2B-O2B-P2B-O3X
46	I	204	PC1	C22-C21-O21-C2
45	K	101	3PE	O21-C21-C22-C23
45	P	404	3PE	O21-C21-C22-C23
53	N	905	CDL	C12-C11-CA5-OA6
45	K	101	3PE	C32-C33-C34-C35
53	N	903	CDL	C37-C38-C39-C40
46	N	904	PC1	O21-C21-C22-C23
46	q	201	PC1	C26-C27-C28-C29
53	L	702	CDL	C39-C40-C41-C42
60	o	201	MYR	C3-C4-C5-C6
53	N	902	CDL	C84-C85-C86-C87
46	B	202	PC1	O21-C21-C22-C23
53	q	202	CDL	C72-C73-C74-C75
53	q	202	CDL	C73-C74-C75-C76
45	m	201	3PE	O32-C31-C32-C33
53	q	202	CDL	C32-C31-CA7-OA9
45	L	703	3PE	O32-C31-C32-C33
53	q	202	CDL	C19-C20-C21-C22
45	I	201	3PE	O22-C21-C22-C23
53	L	702	CDL	C12-C11-CA5-OA7
53	H	602	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
45	N	901	3PE	O32-C31-C32-C33
53	q	202	CDL	C52-C51-CB5-OB7
45	L	701	3PE	C1-C2-C3-O31
50	F	501	FMN	O3'-C3'-C4'-O4'
46	H	603	PC1	O22-C21-C22-C23
45	M	502	3PE	C39-C3A-C3B-C3C
46	P	402	PC1	O31-C31-C32-C33
53	q	202	CDL	C1-CB2-OB2-PB2
46	h	202	PC1	O32-C31-C32-C33
46	q	201	PC1	C2D-C2E-C2F-C2G
45	A	201	3PE	C33-C34-C35-C36
45	H	601	3PE	C11-O13-P-O12
45	L	703	3PE	C1-O11-P-O14
45	L	704	3PE	C11-O13-P-O14
45	Y	202	3PE	C1-O11-P-O14
45	Y	203	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O14
45	Y	206	3PE	C11-O13-P-O14
45	m	201	3PE	C11-O13-P-O14
46	A	202	PC1	C11-O13-P-O12
46	A	202	PC1	C1-O11-P-O14
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C1-O11-P-O14
46	H	603	PC1	C11-O13-P-O14
46	I	204	PC1	C11-O13-P-O14
46	q	201	PC1	C11-O13-P-O14
51	F	503	NAI	C5B-O5B-PA-O2A
53	N	905	CDL	CA2-OA2-PA1-OA4
53	N	905	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	CB3-OB5-PB2-OB3
53	q	202	CDL	CB3-OB5-PB2-OB3
54	O	401	DGT	C5'-O5'-PA-O2A
45	A	201	3PE	O32-C31-C32-C33
46	N	904	PC1	O22-C21-C22-C23
53	X	201	CDL	OA5-CA3-CA4-CA6
45	A	201	3PE	O13-C11-C12-N
45	I	201	3PE	O13-C11-C12-N
45	L	701	3PE	O13-C11-C12-N
45	Y	205	3PE	O13-C11-C12-N
45	L	703	3PE	O22-C21-C22-C23
45	K	101	3PE	C35-C36-C37-C38
53	N	905	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C32-C33-C34-C35
45	Y	206	3PE	O31-C31-C32-C33
45	P	404	3PE	O22-C21-C22-C23
45	Y	204	3PE	O32-C31-C32-C33
45	A	201	3PE	C12-C11-O13-P
45	N	901	3PE	C12-C11-O13-P
45	Y	203	3PE	C12-C11-O13-P
45	b	101	3PE	C12-C11-O13-P
46	A	203	PC1	C12-C11-O13-P
46	P	401	PC1	C12-C11-O13-P
53	N	903	CDL	CA3-CA4-OA6-CA5
46	B	202	PC1	O22-C21-C22-C23
53	N	905	CDL	C12-C11-CA5-OA7
53	N	903	CDL	C15-C16-C17-C18
46	A	202	PC1	O21-C21-C22-C23
53	N	902	CDL	C52-C51-CB5-OB6
45	Y	202	3PE	O22-C21-C22-C23
45	Y	205	3PE	O32-C31-C32-C33
53	H	602	CDL	C12-C11-CA5-OA6
53	h	201	CDL	C71-C72-C73-C74
45	Y	204	3PE	O21-C21-C22-C23
45	L	701	3PE	C22-C23-C24-C25
45	K	101	3PE	O32-C31-C32-C33
45	A	201	3PE	C35-C36-C37-C38
45	b	101	3PE	C22-C23-C24-C25
46	A	202	PC1	O22-C21-C22-C23
46	P	402	PC1	O32-C31-C32-C33
46	H	603	PC1	C28-C29-C2A-C2B
53	h	201	CDL	C74-C75-C76-C77
53	q	202	CDL	C53-C54-C55-C56
45	K	101	3PE	O31-C31-C32-C33
45	L	704	3PE	O31-C31-C32-C33
46	h	202	PC1	O21-C21-C22-C23
45	Y	206	3PE	O32-C31-C32-C33
46	q	201	PC1	C23-C24-C25-C26
53	H	602	CDL	C12-C11-CA5-OA7
46	A	202	PC1	C24-C25-C26-C27
53	N	905	CDL	C39-C40-C41-C42
46	B	202	PC1	O31-C31-C32-C33
45	L	701	3PE	C21-C22-C23-C24
45	K	101	3PE	O22-C21-C22-C23
46	h	202	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C3A-C3B-C3C-C3D
53	X	201	CDL	C15-C16-C17-C18
53	q	202	CDL	C54-C55-C56-C57

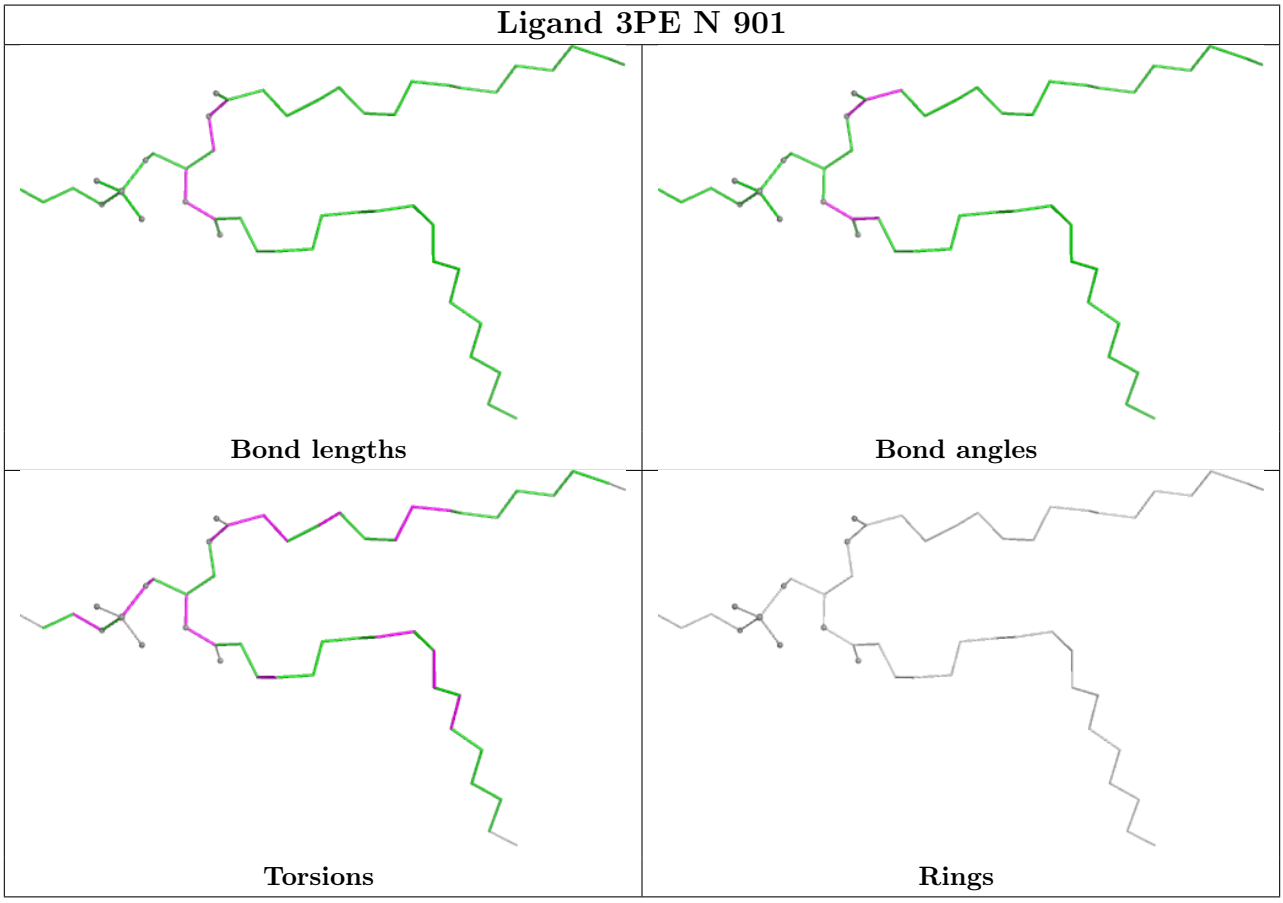
There are no ring outliers.

34 monomers are involved in 71 short contacts:

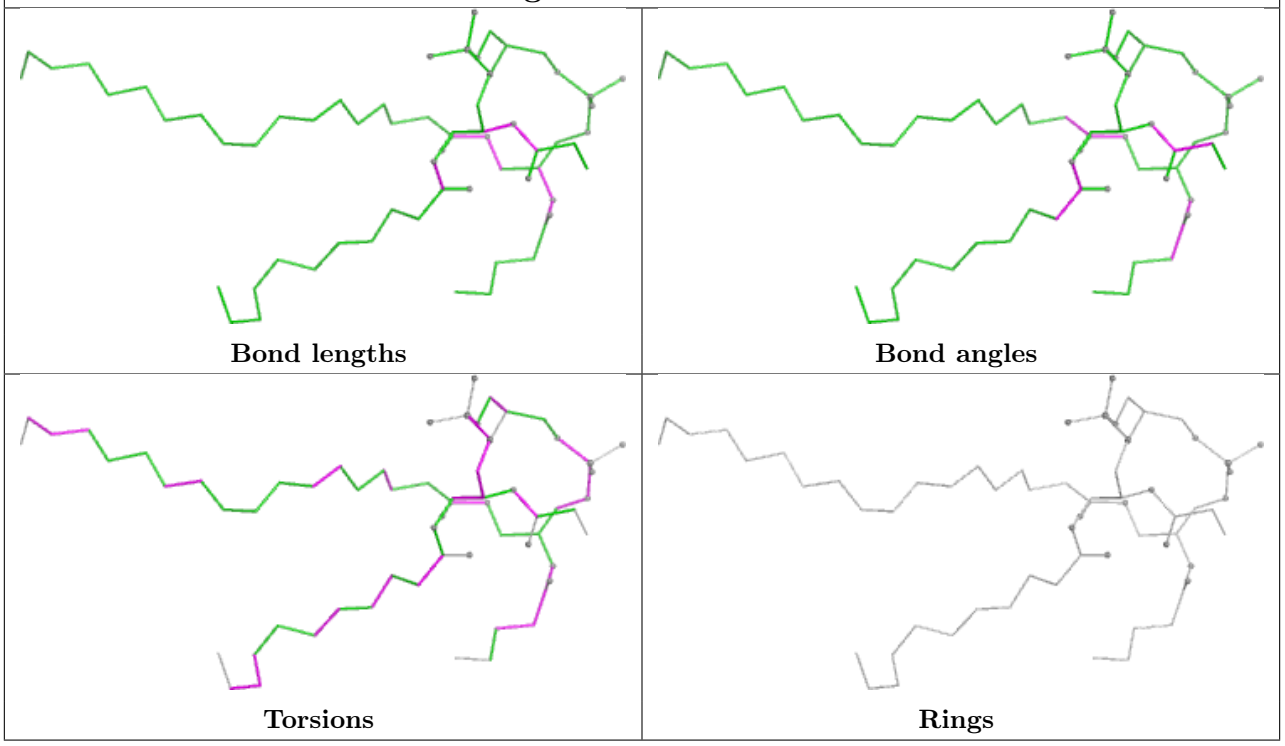
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	N	905	CDL	4	0
53	N	902	CDL	1	0
46	P	401	PC1	3	0
53	q	202	CDL	3	0
46	A	203	PC1	1	0
58	U	101	EHZ	1	0
45	Y	203	3PE	2	0
56	P	403	NDP	1	0
45	P	404	3PE	3	0
50	F	501	FMN	1	0
46	N	904	PC1	2	0
58	T	101	EHZ	1	0
45	L	701	3PE	4	0
45	Y	205	3PE	1	0
59	i	201	CHD	3	0
45	Y	201	3PE	1	0
45	H	601	3PE	2	0
46	A	202	PC1	2	0
48	D	701	U10	8	0
45	Y	202	3PE	2	0
53	X	201	CDL	4	0
54	O	401	DGT	3	0
45	d	201	3PE	1	0
53	L	702	CDL	2	0
46	I	204	PC1	1	0
45	Y	204	3PE	3	0
53	h	201	CDL	3	0
45	A	201	3PE	1	0
46	h	202	PC1	1	0
46	P	402	PC1	2	0
45	I	201	3PE	1	0
53	H	602	CDL	2	0
51	F	503	NAI	3	0
47	I	203	SF4	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.

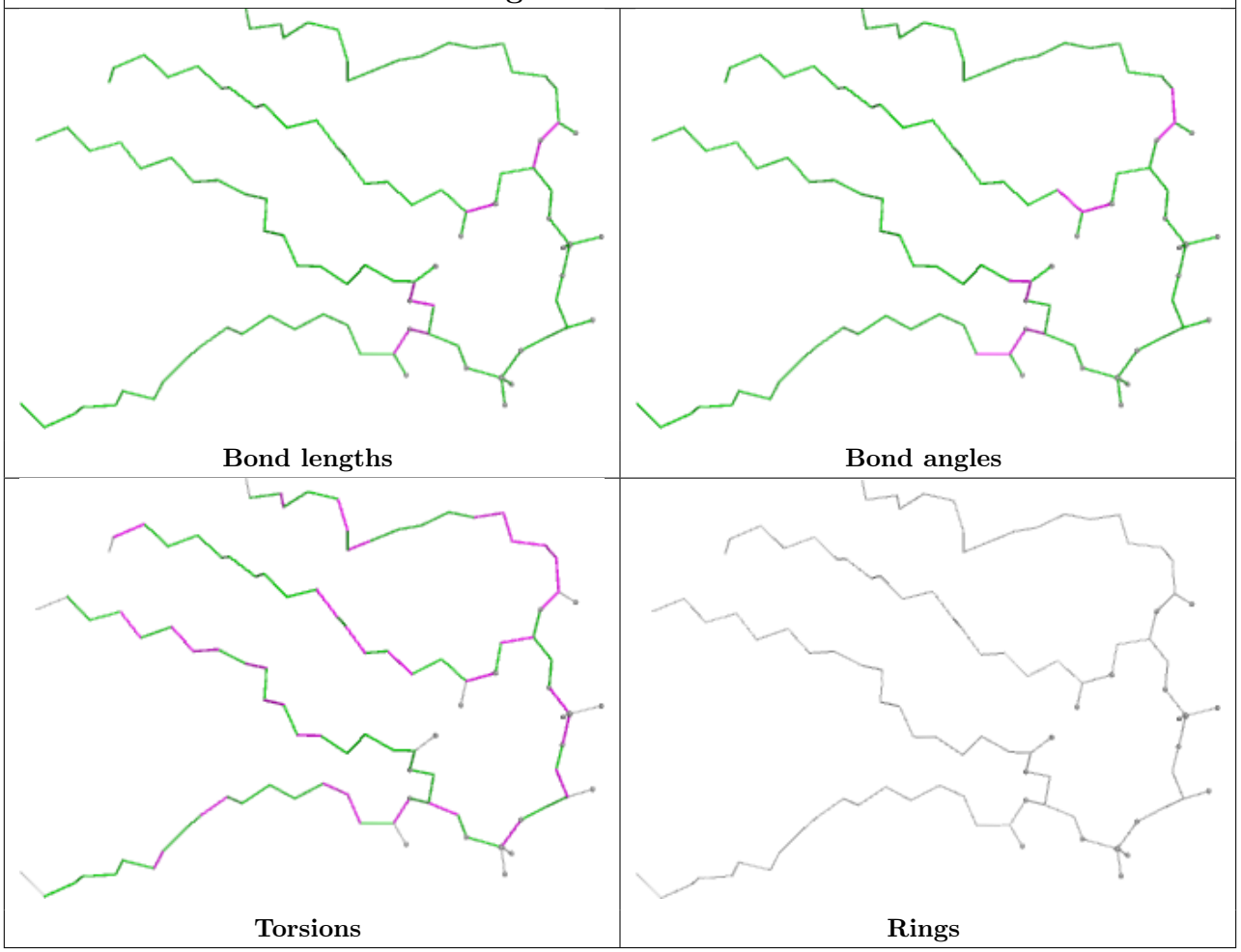
Ligand 3PE N 901



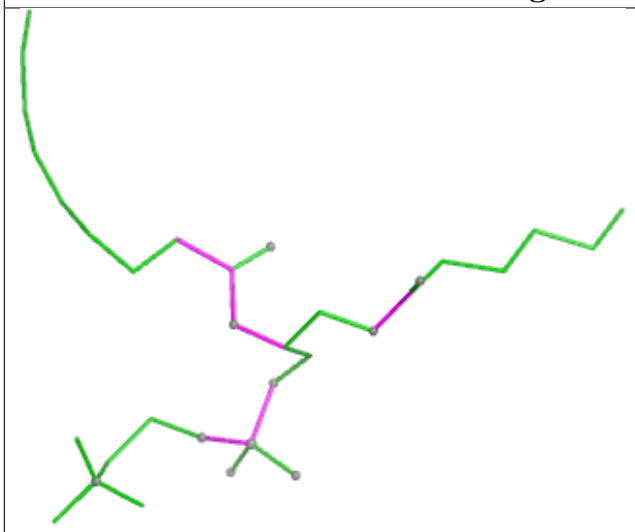
Ligand CDL N 905



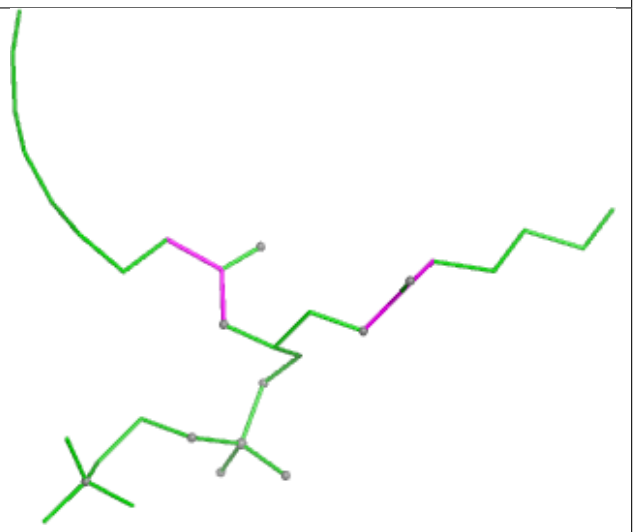
Ligand CDL N 902



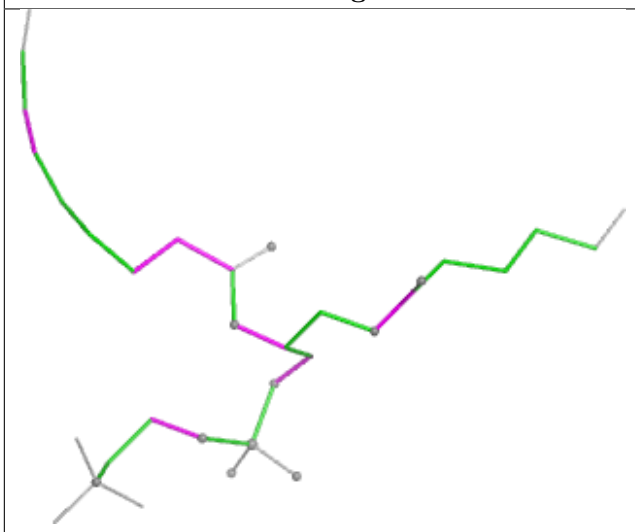
Ligand PC1 P 401



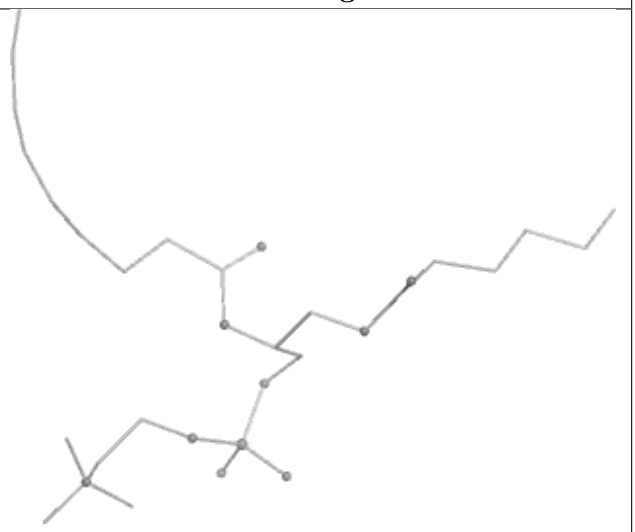
Bond lengths



Bond angles

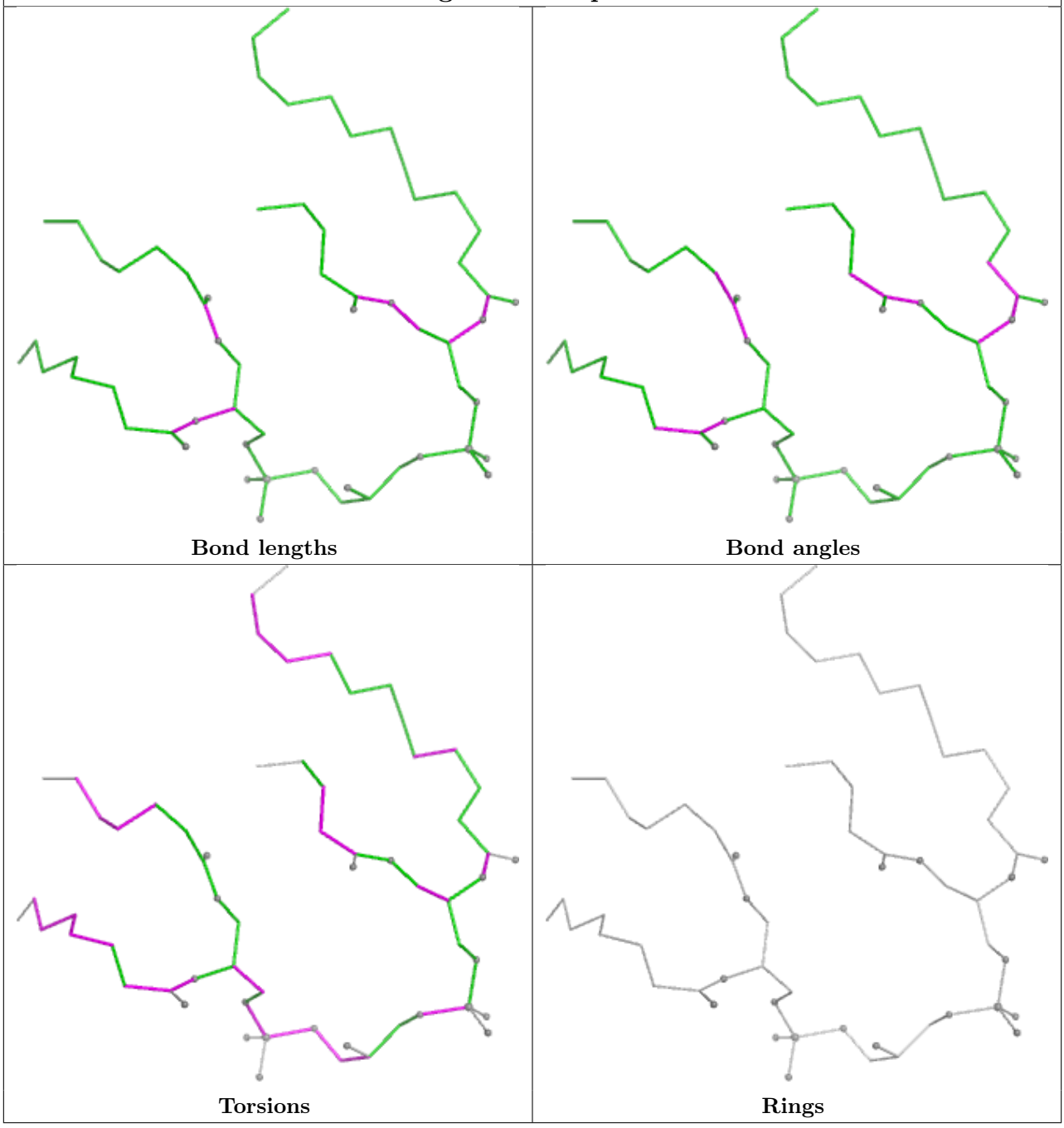


Torsions



Rings

Ligand CDL q 202



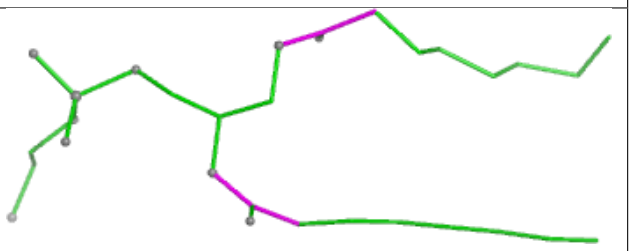
Bond lengths | Bond angles

Torsions | Rings

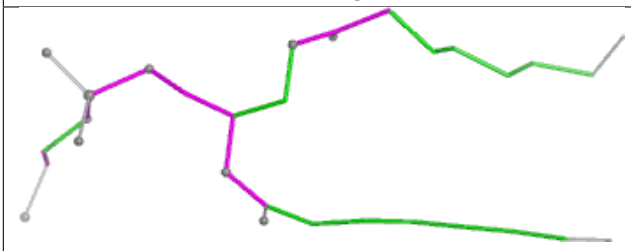
Ligand 3PE L 704



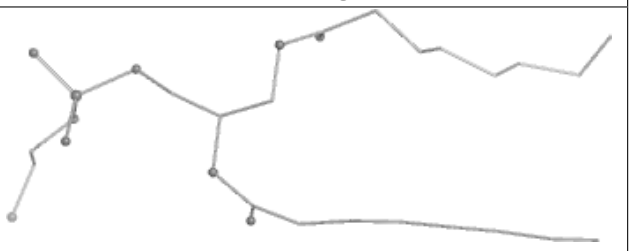
Bond lengths



Bond angles

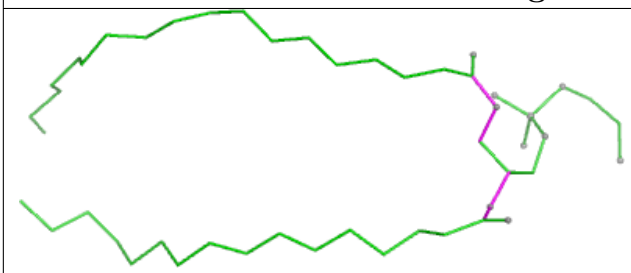


Torsions

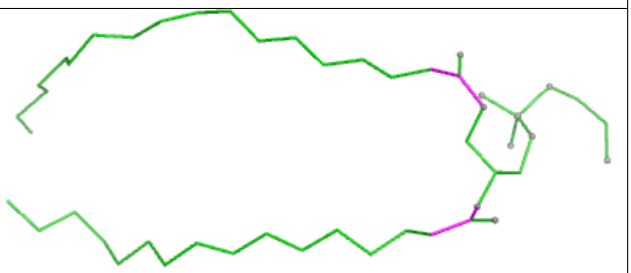


Rings

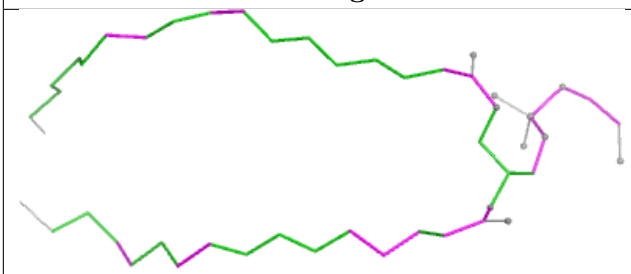
Ligand 3PE Y 206



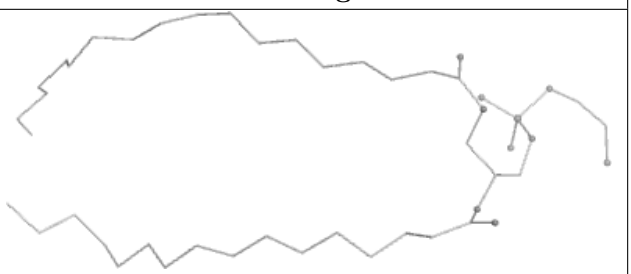
Bond lengths



Bond angles

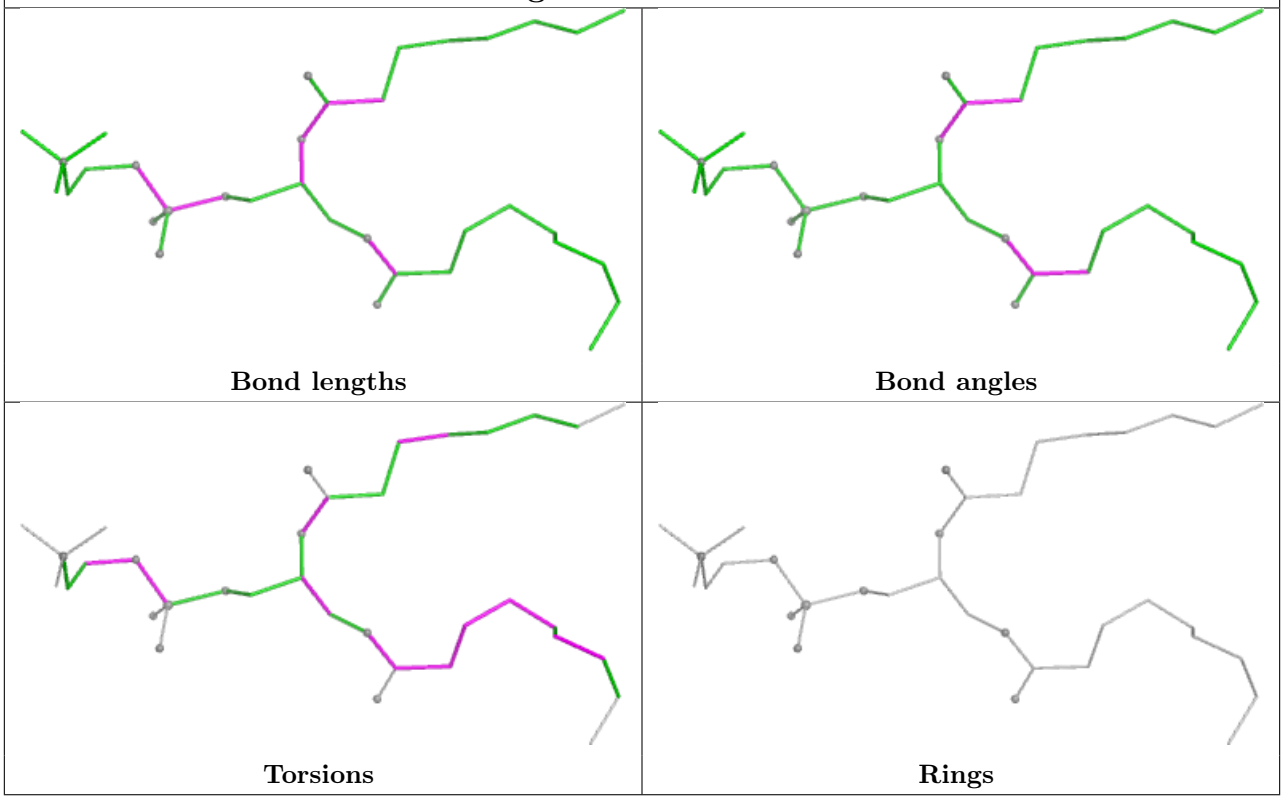


Torsions

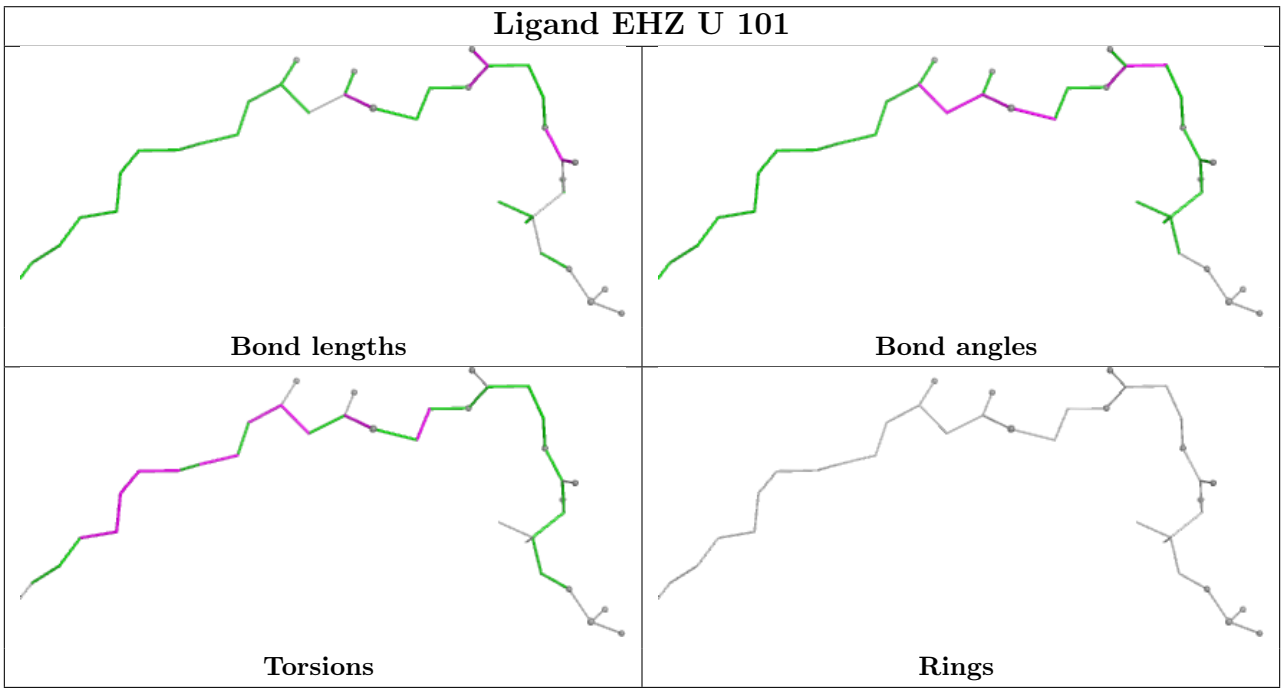


Rings

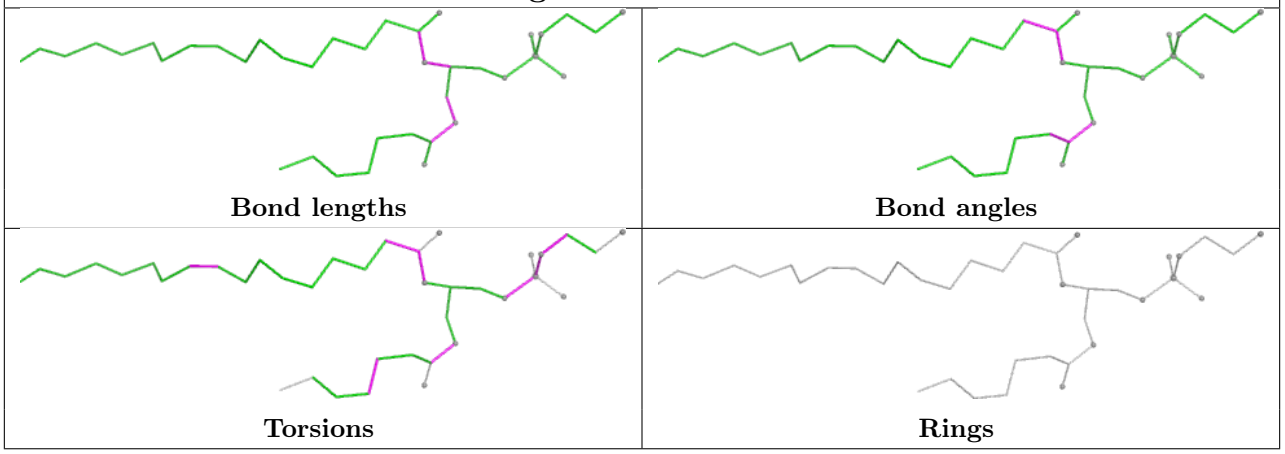
Ligand PC1 A 203



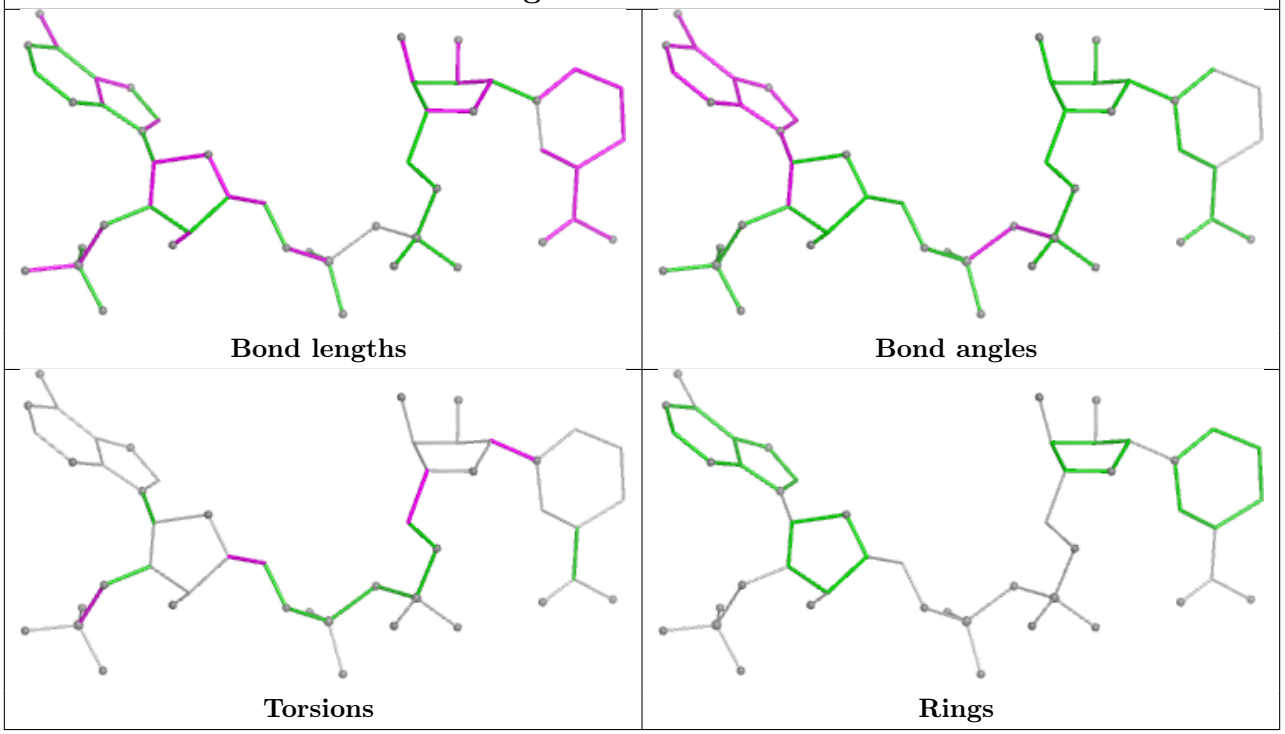
Ligand EHZ U 101



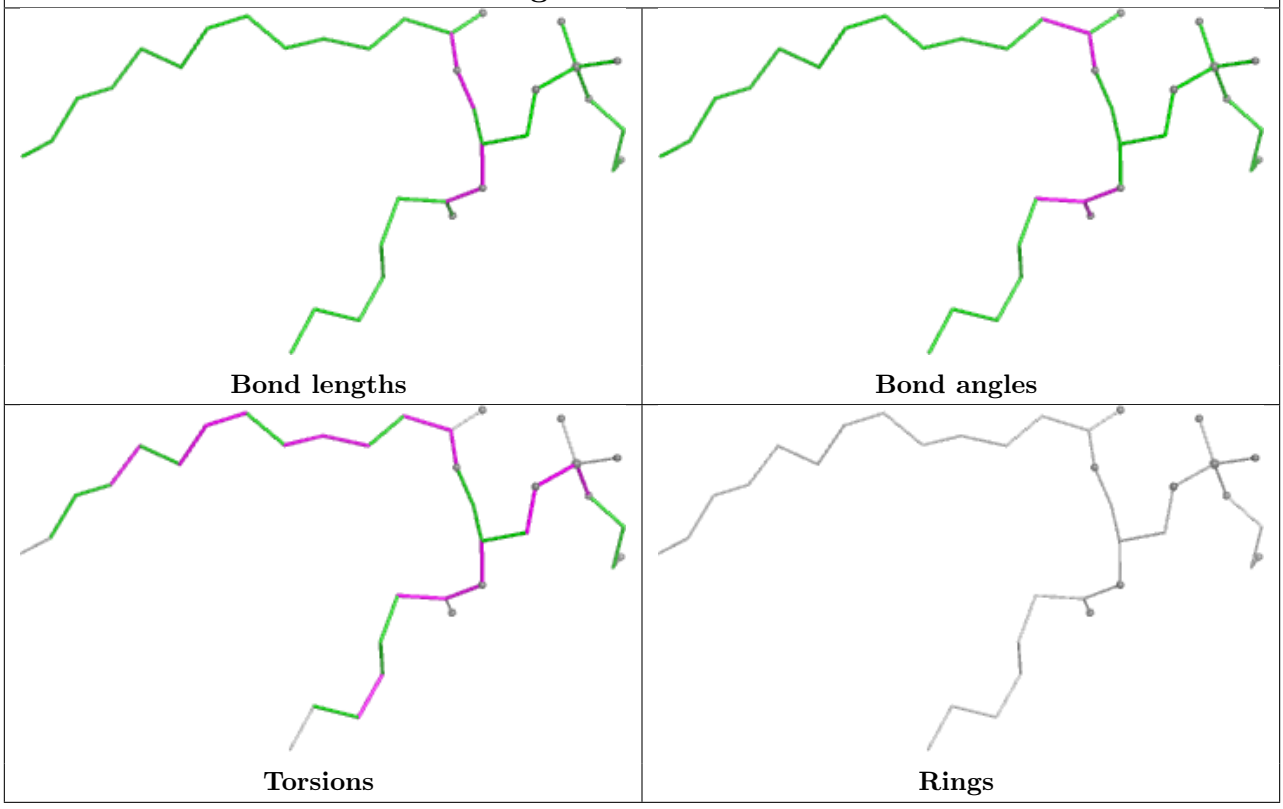
Ligand 3PE Y 203



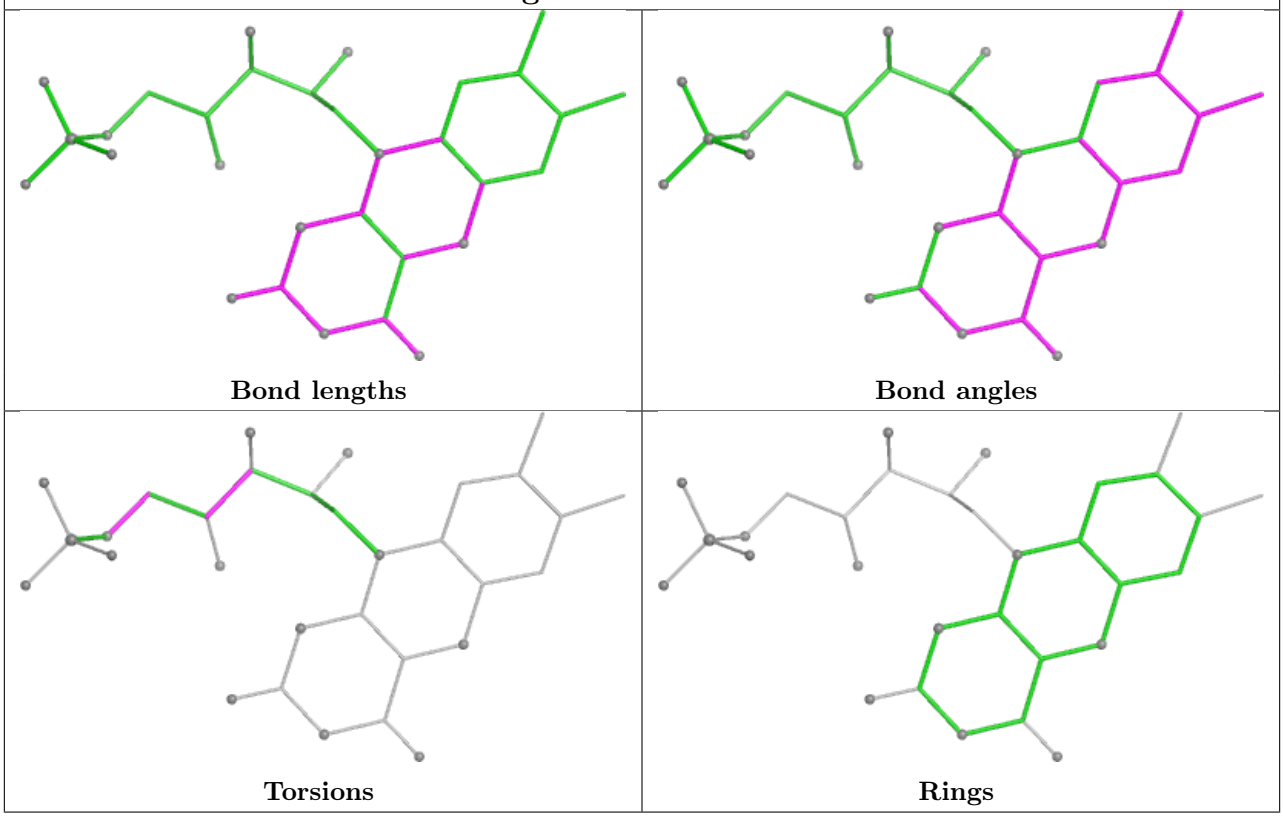
Ligand NDP P 403



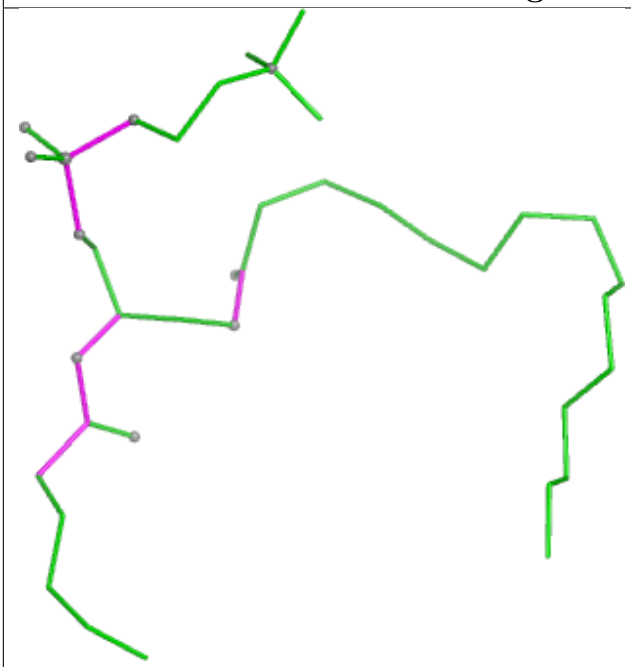
Ligand 3PE P 404



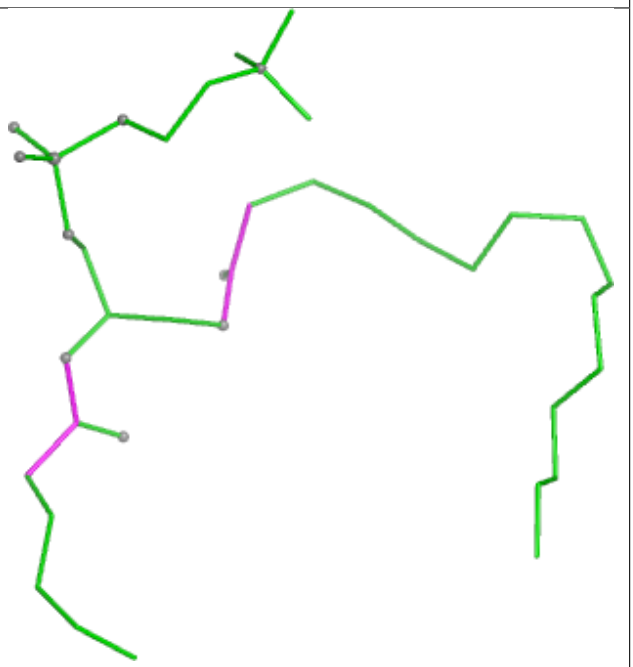
Ligand FMN F 501



Ligand PC1 N 904



Bond lengths



Bond angles

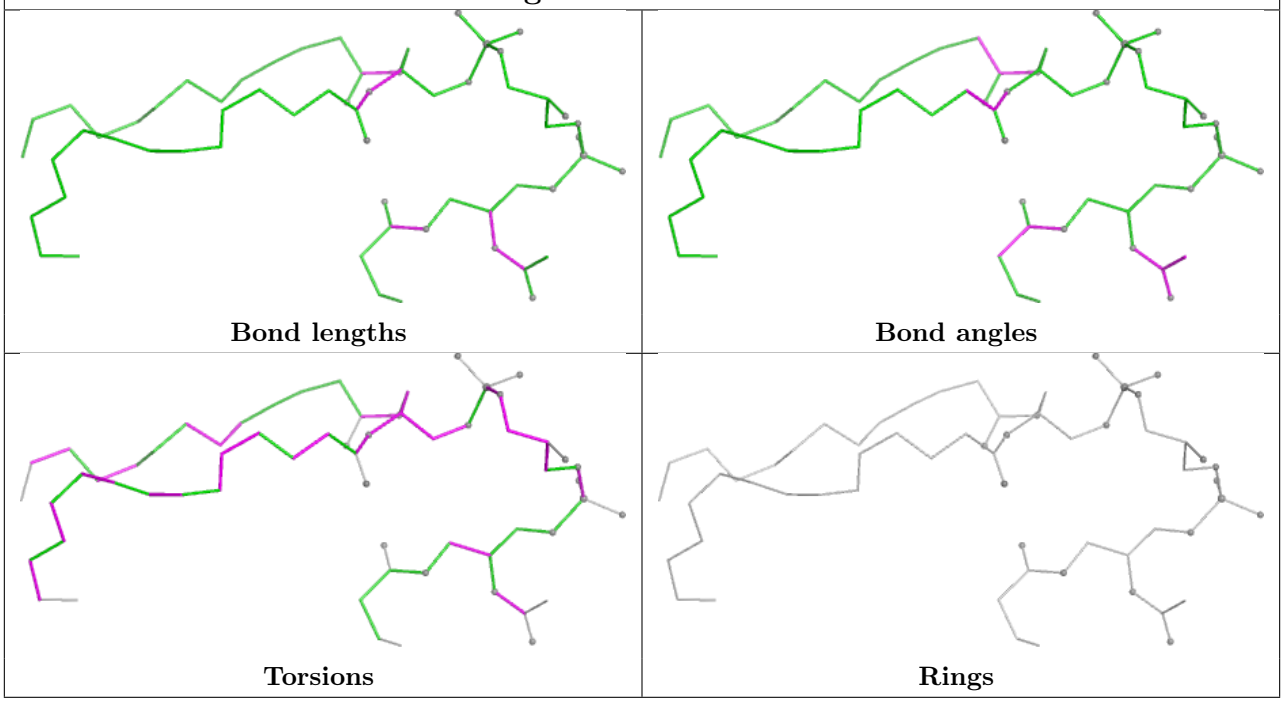


Torsions

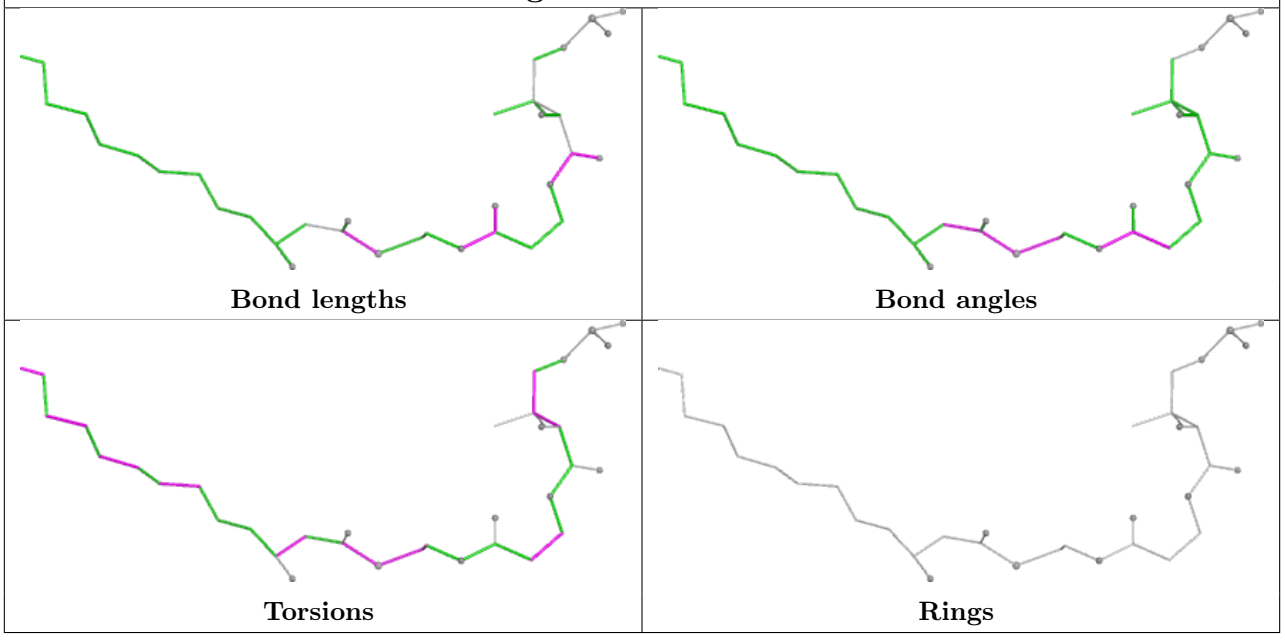


Rings

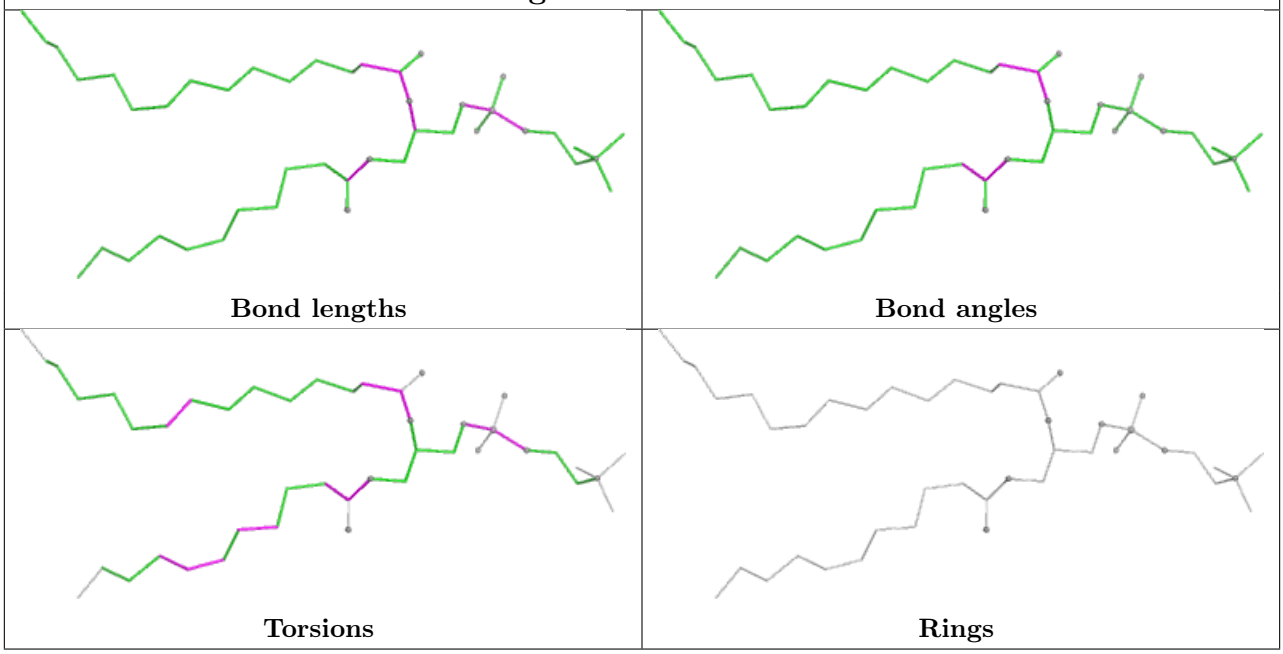
Ligand CDL N 903



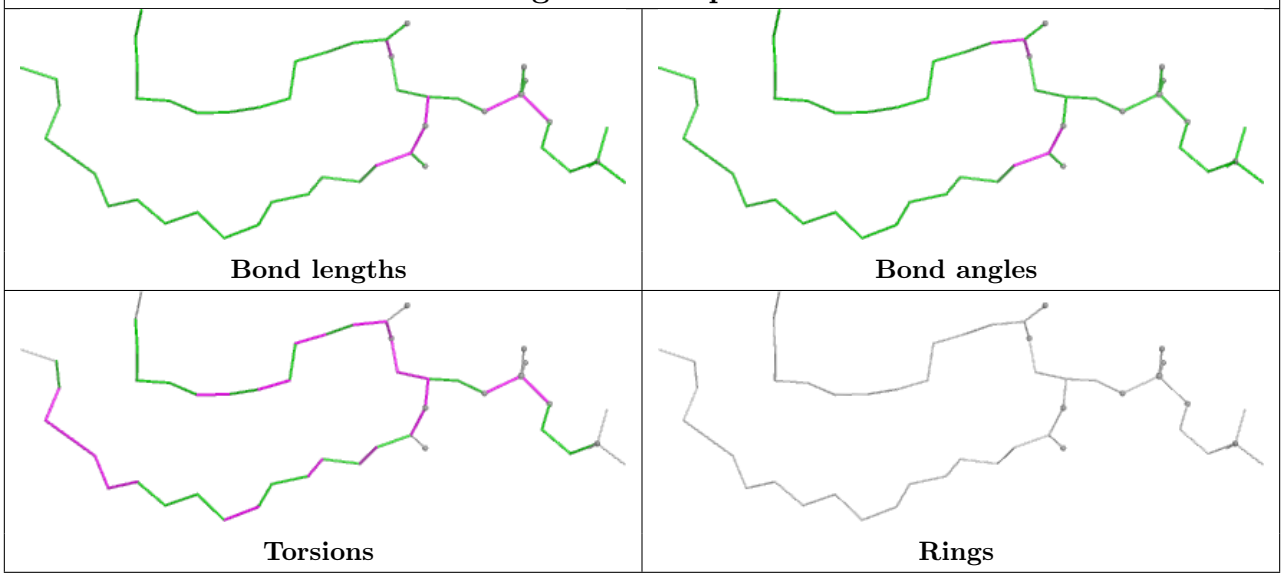
Ligand EHZ T 101



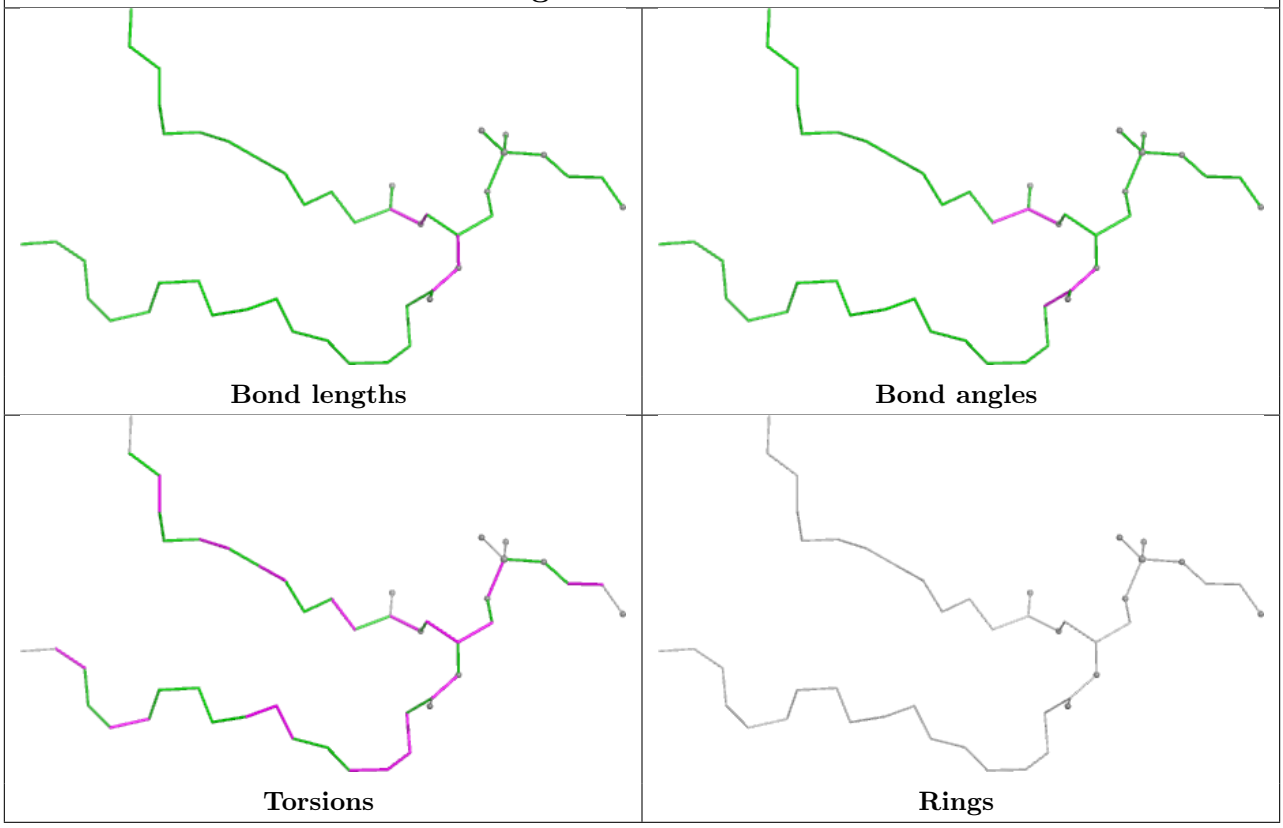
Ligand PC1 B 202



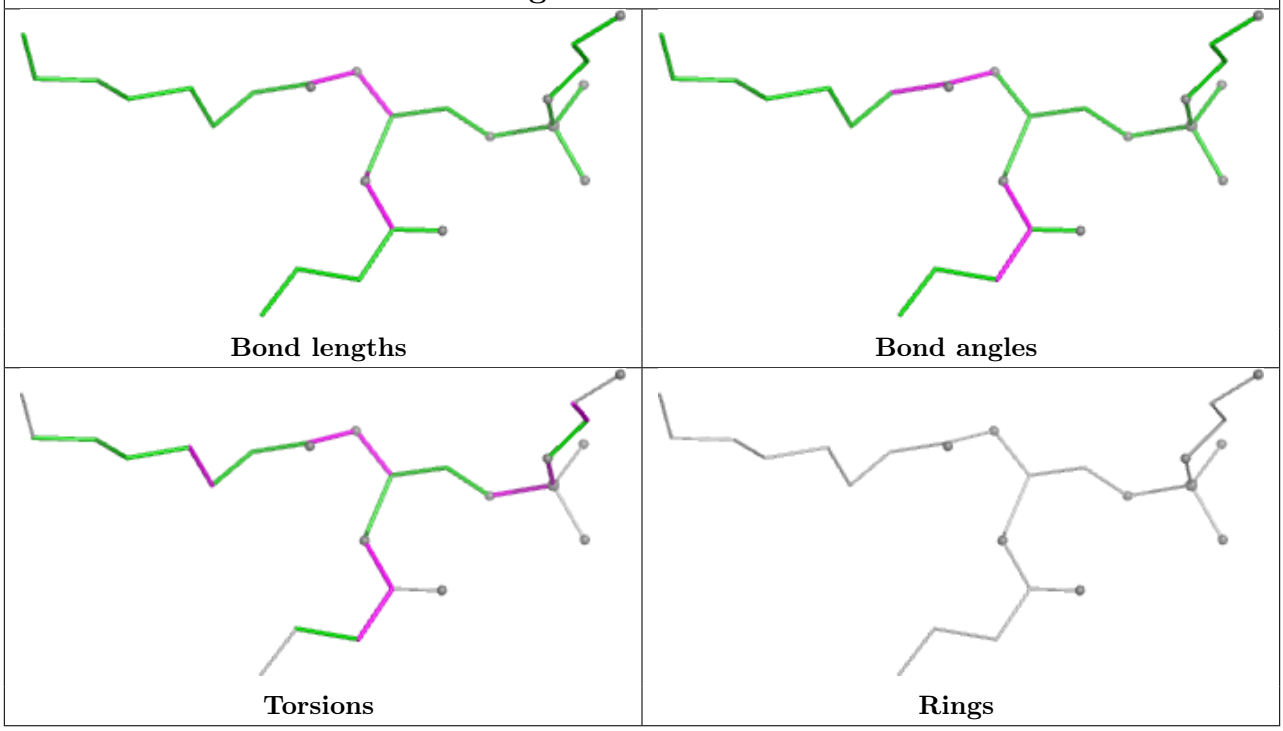
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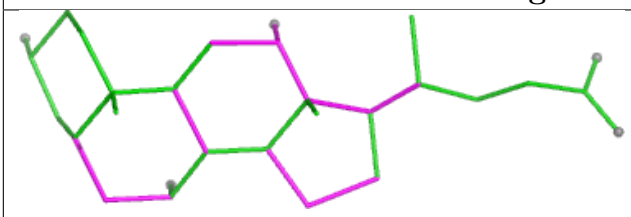
Ligand 3PE L 701



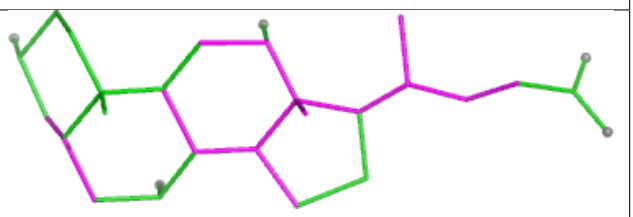
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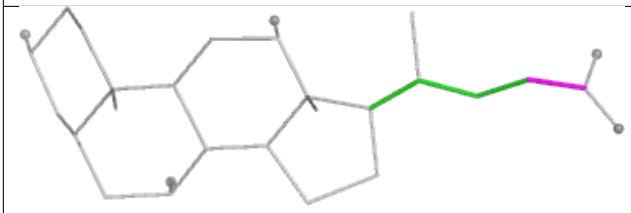
Ligand CHD i 201



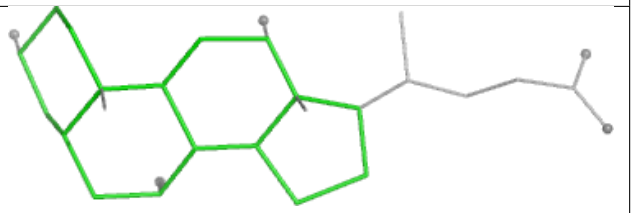
Bond lengths



Bond angles

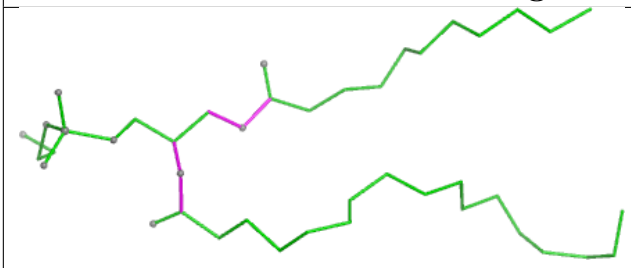


Torsions

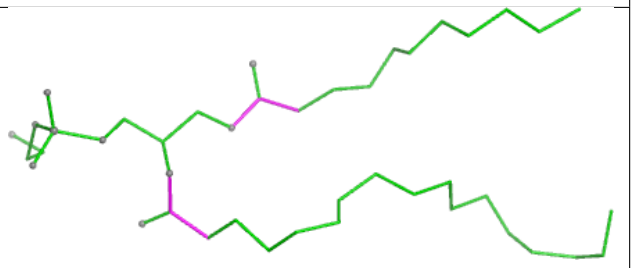


Rings

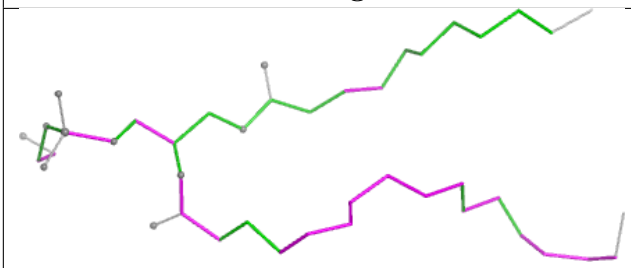
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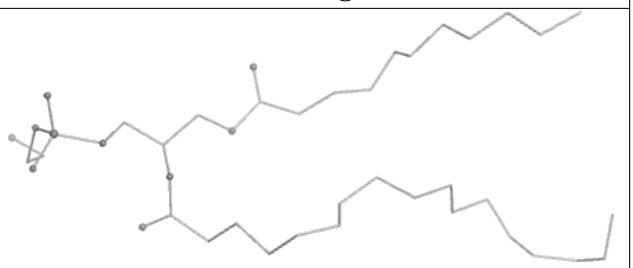
Bond lengths



Bond angles

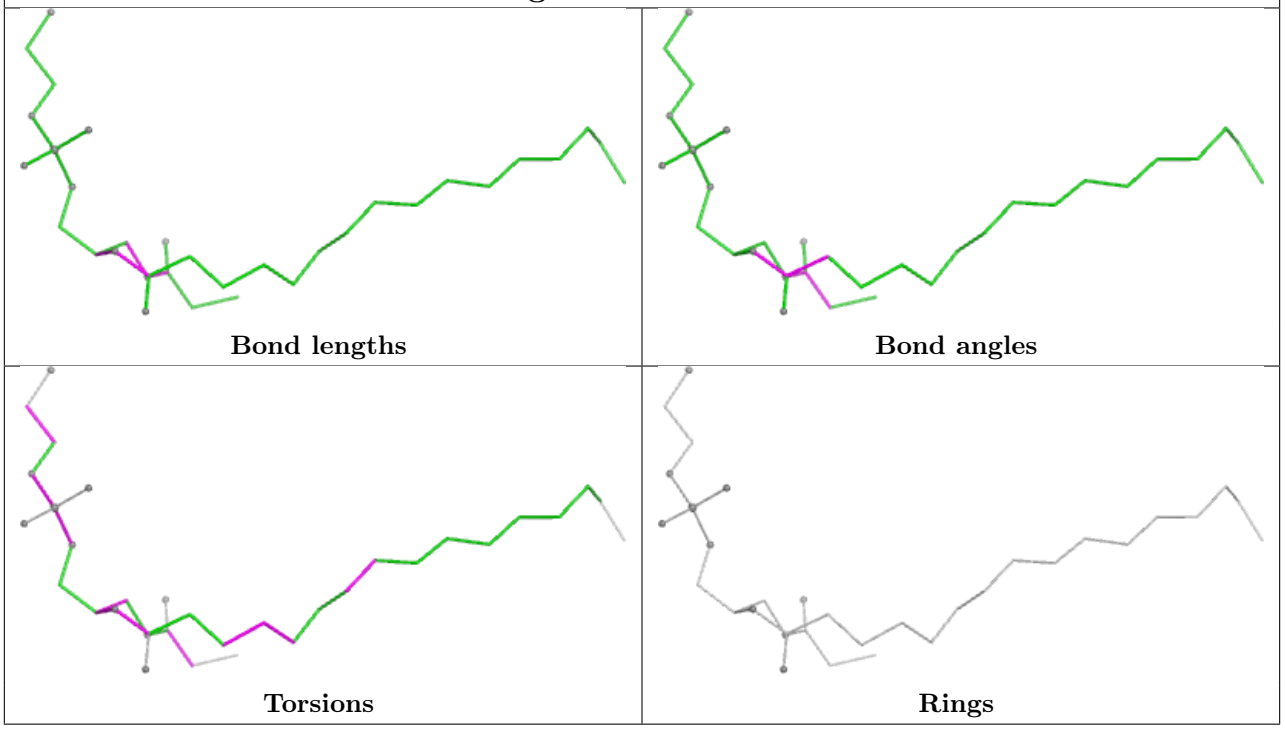


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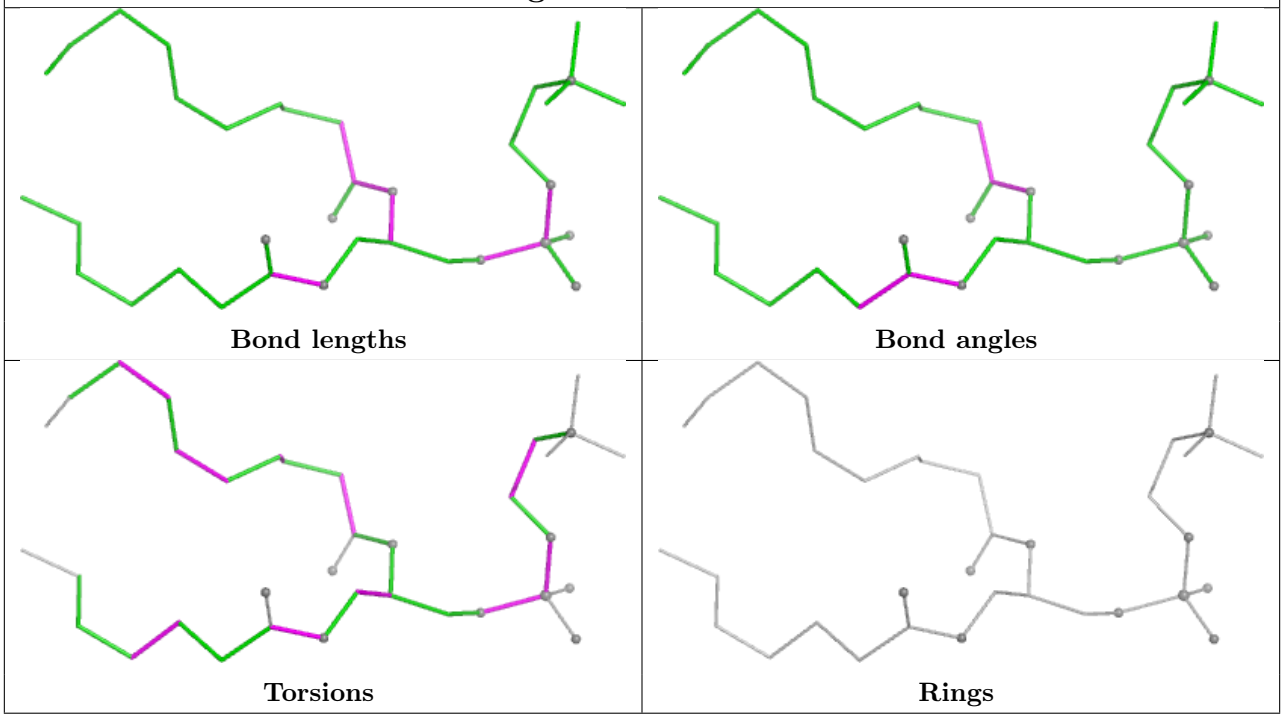


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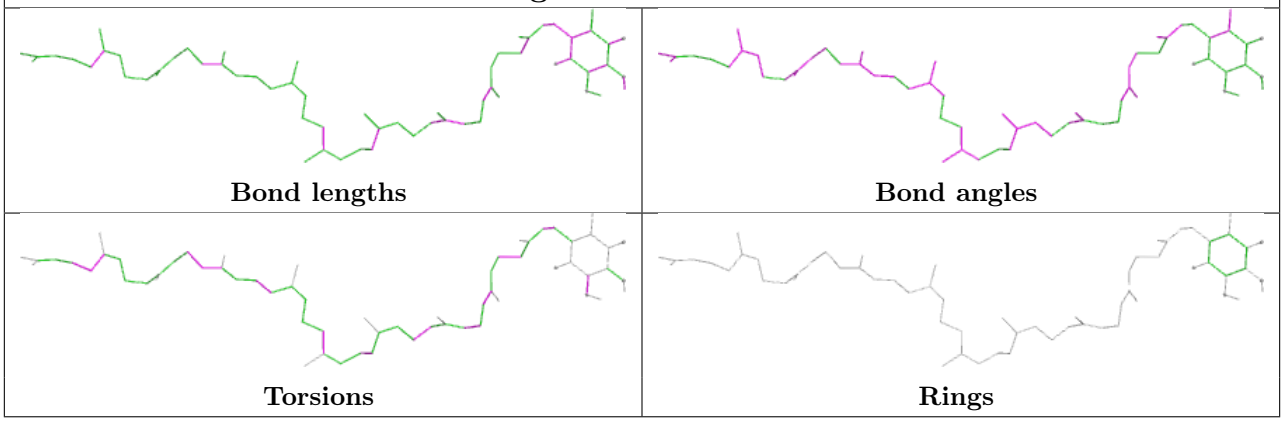
Ligand 3PE H 601



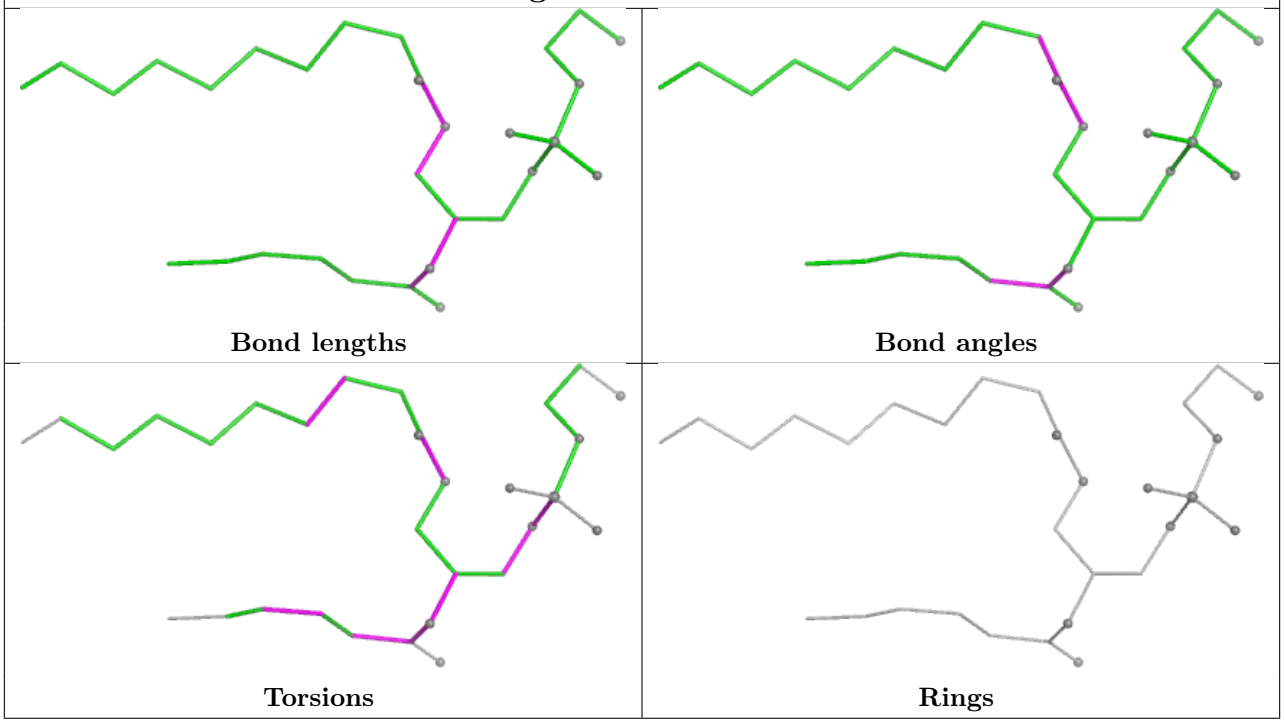
Ligand PC1 A 202



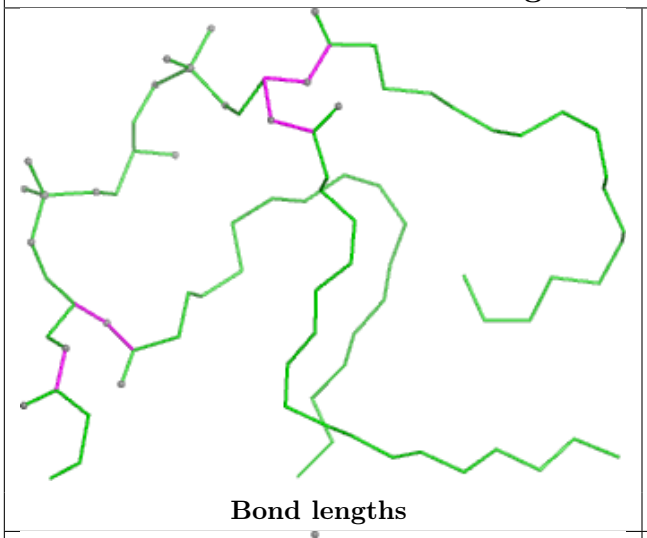
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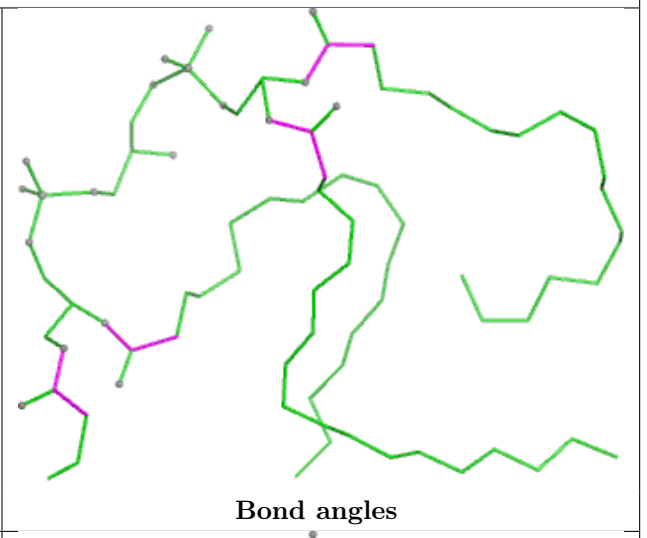
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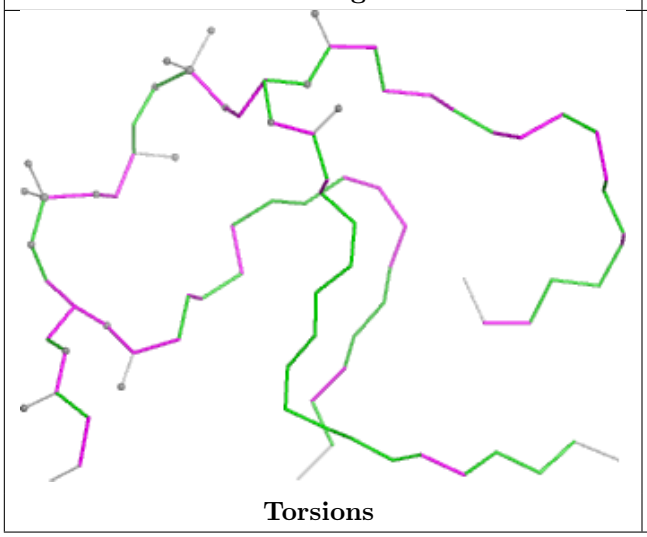
Ligand CDL X 201



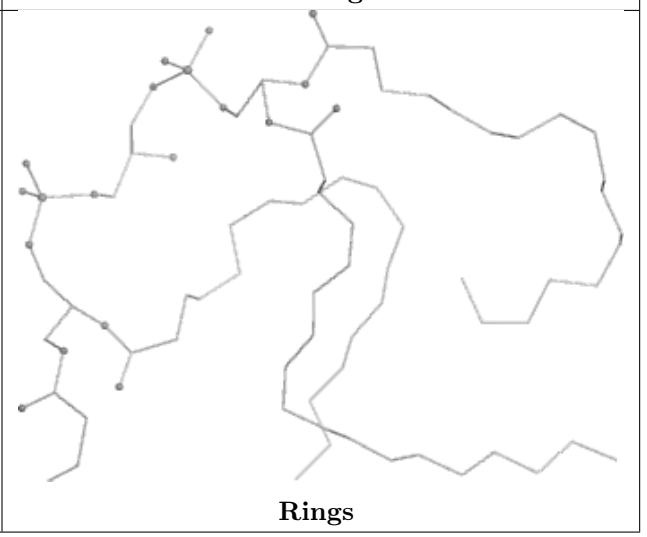
Bond lengths



Bond angles

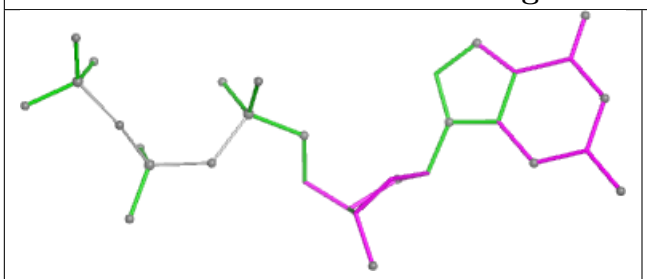


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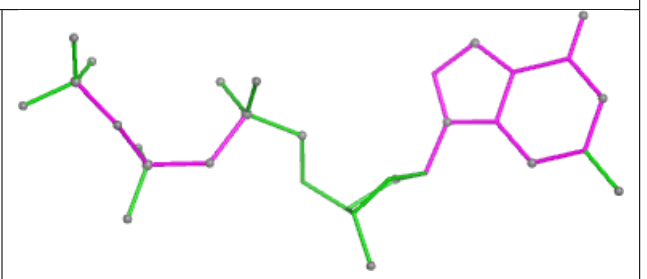


Rings

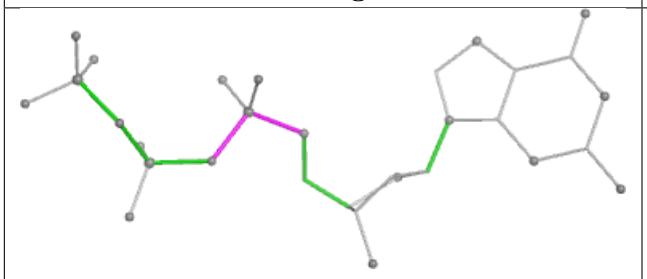
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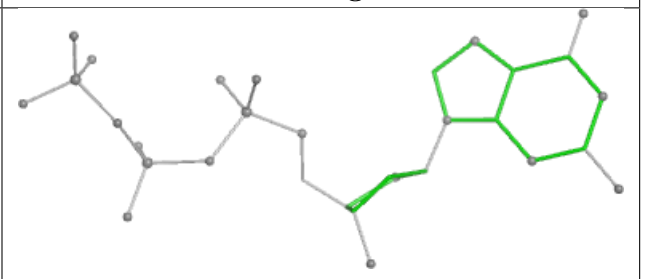
Bond lengths



Bond angles

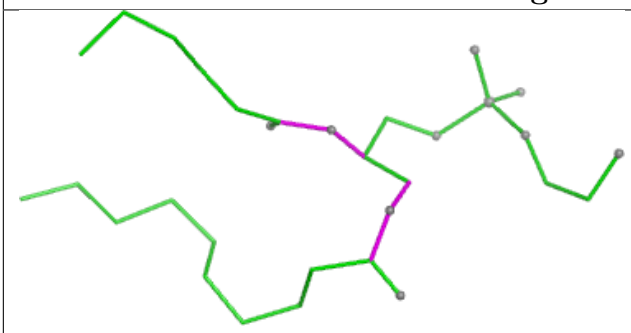


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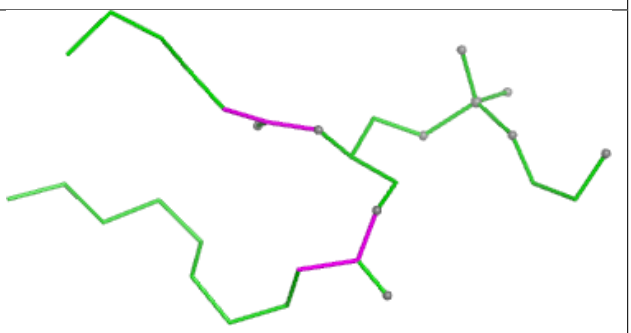


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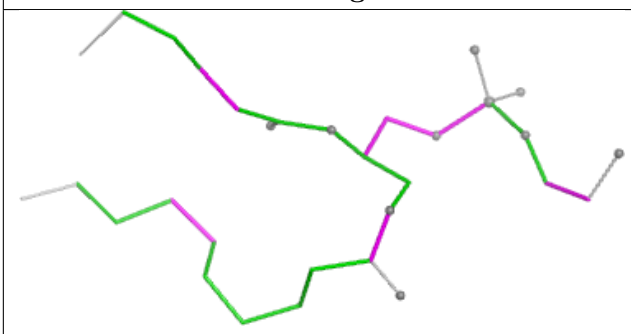
Ligand 3PE L 705



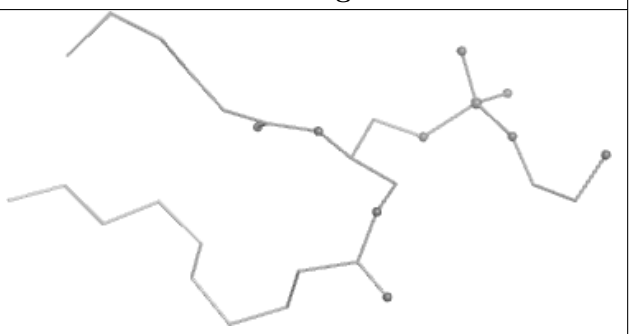
Bond lengths



Bond angles

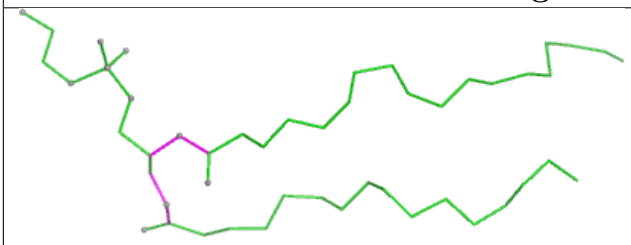


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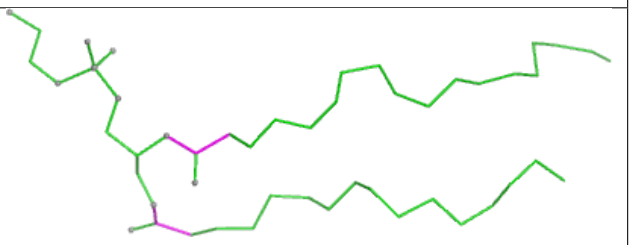


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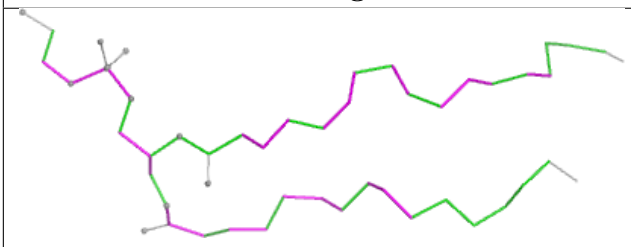
Ligand 3PE d 201



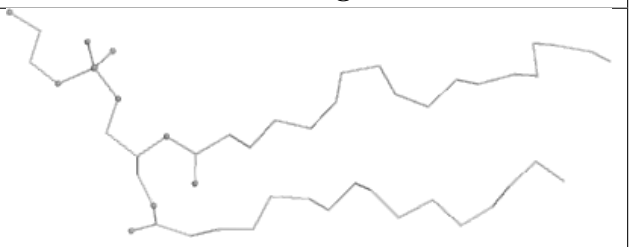
Bond lengths



Bond angles

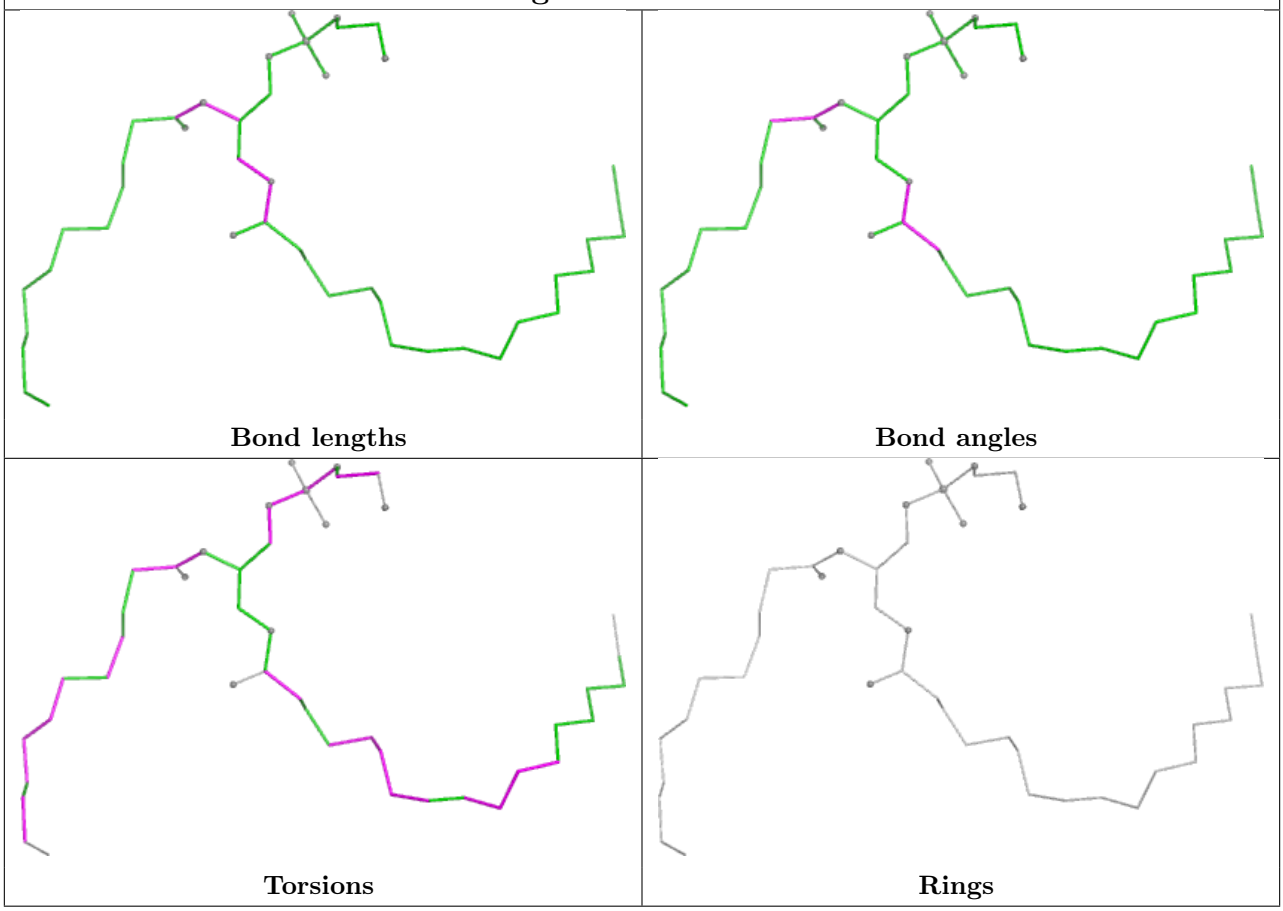


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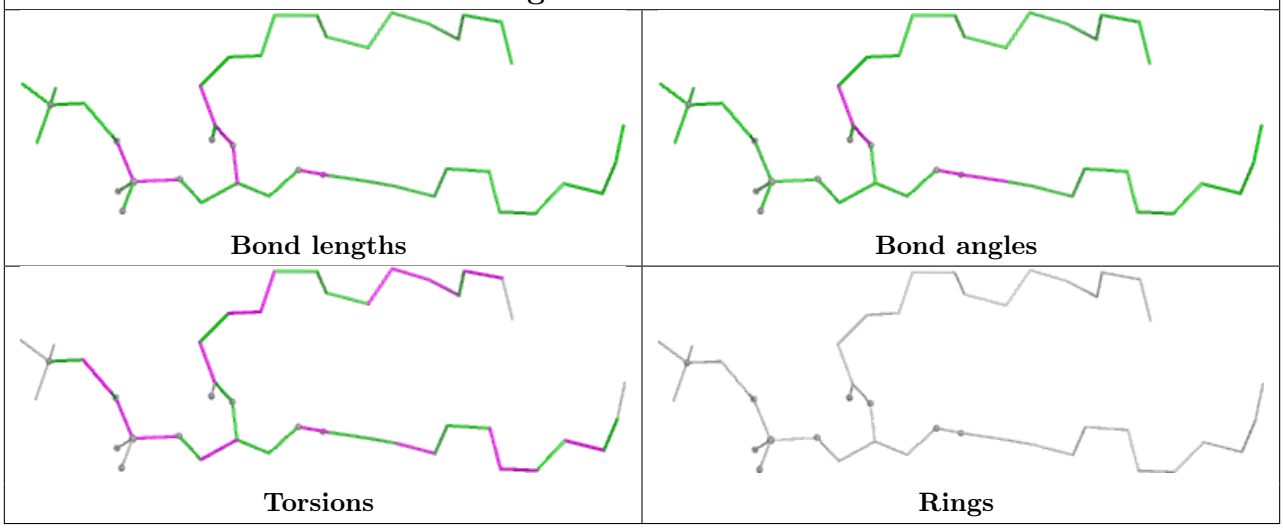


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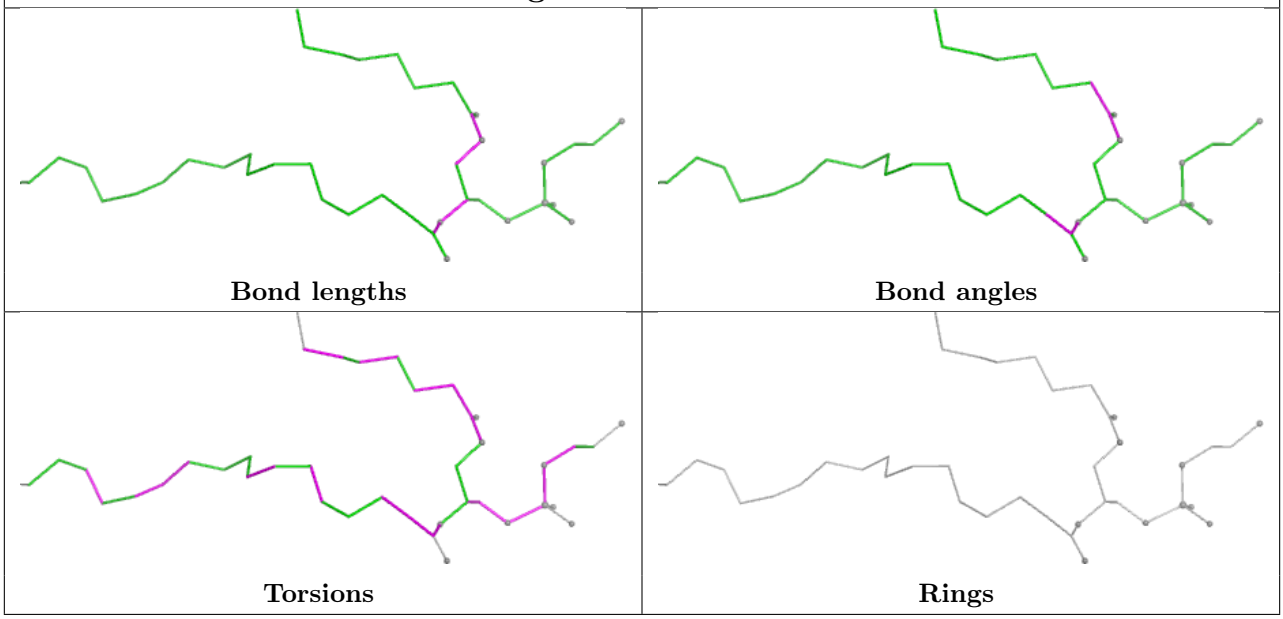
Ligand 3PE L 703



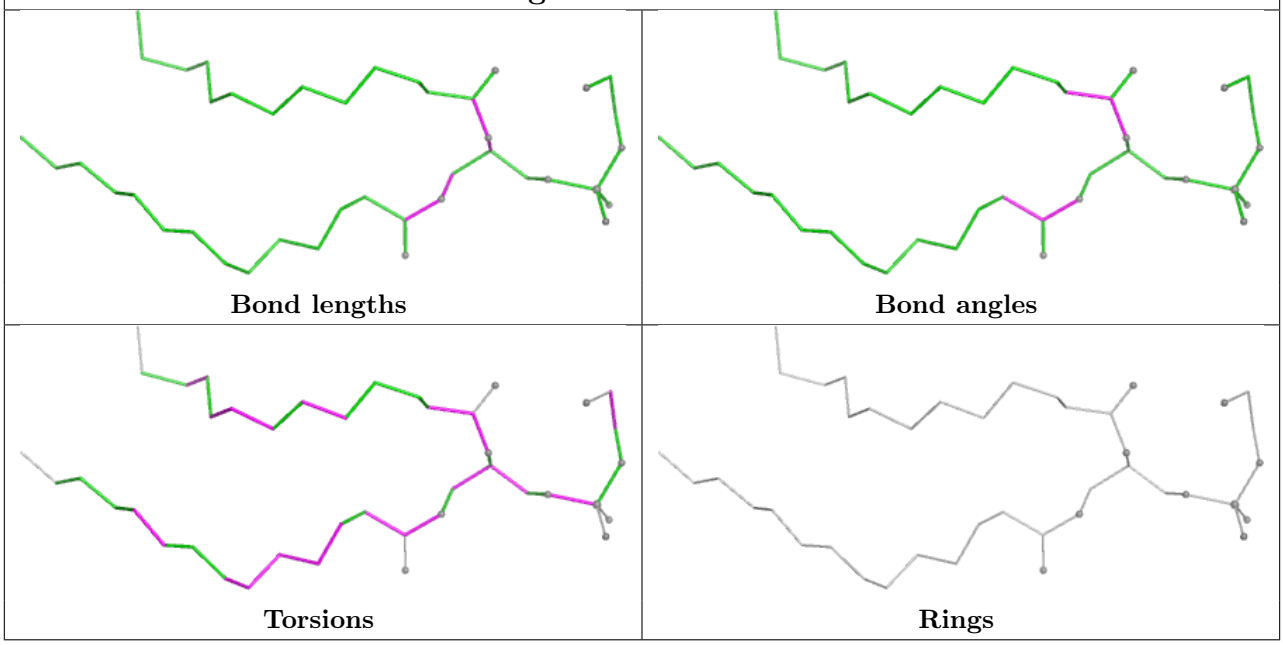
Ligand PC1 H 603



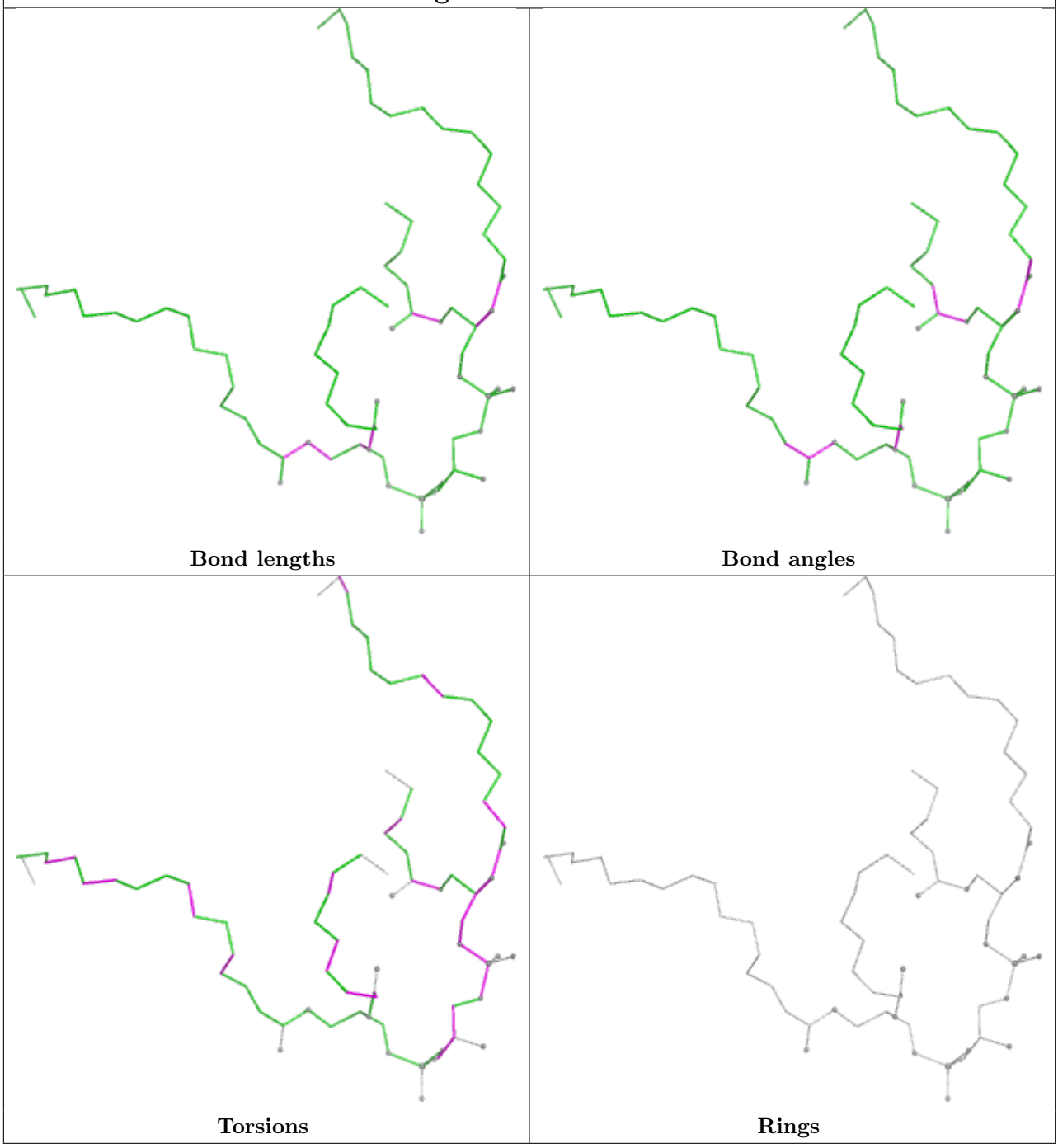
Ligand 3PE m 201



Ligand 3PE K 101



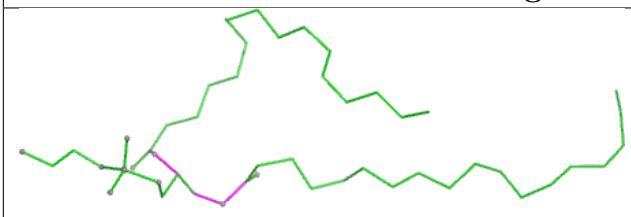
Ligand CDL L 702



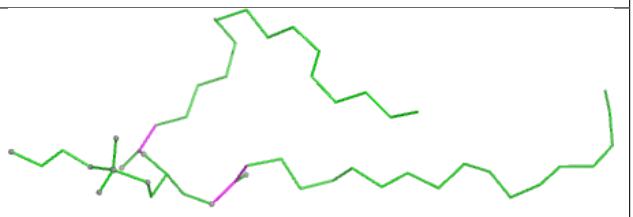
Bond lengths | Bond angles

Torsions | Rings

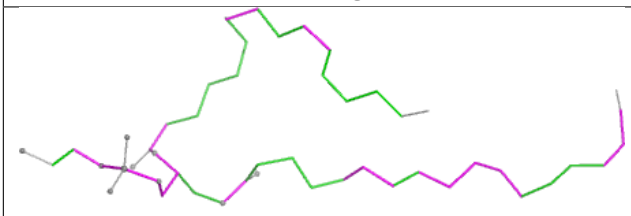
Ligand 3PE M 502



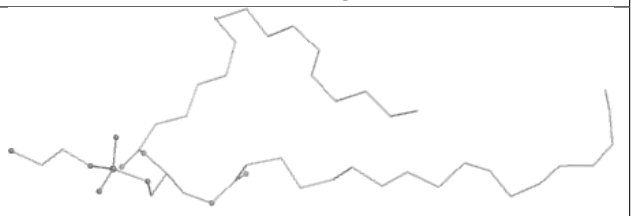
Bond lengths



Bond angles

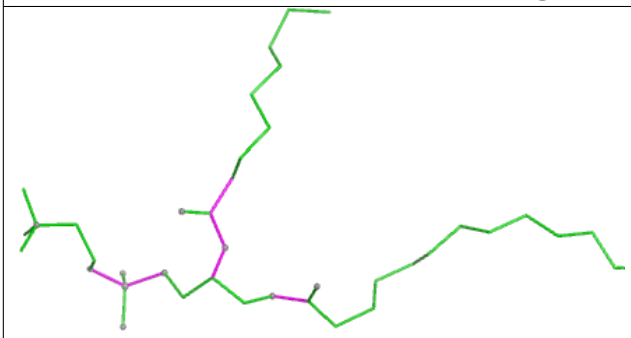


Torsions

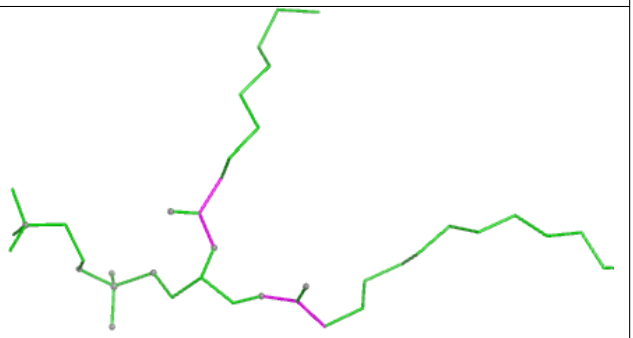


Rings

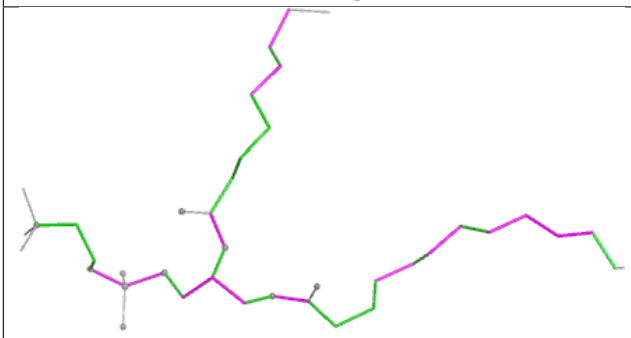
Ligand PC1 I 204



Bond lengths



Bond angles

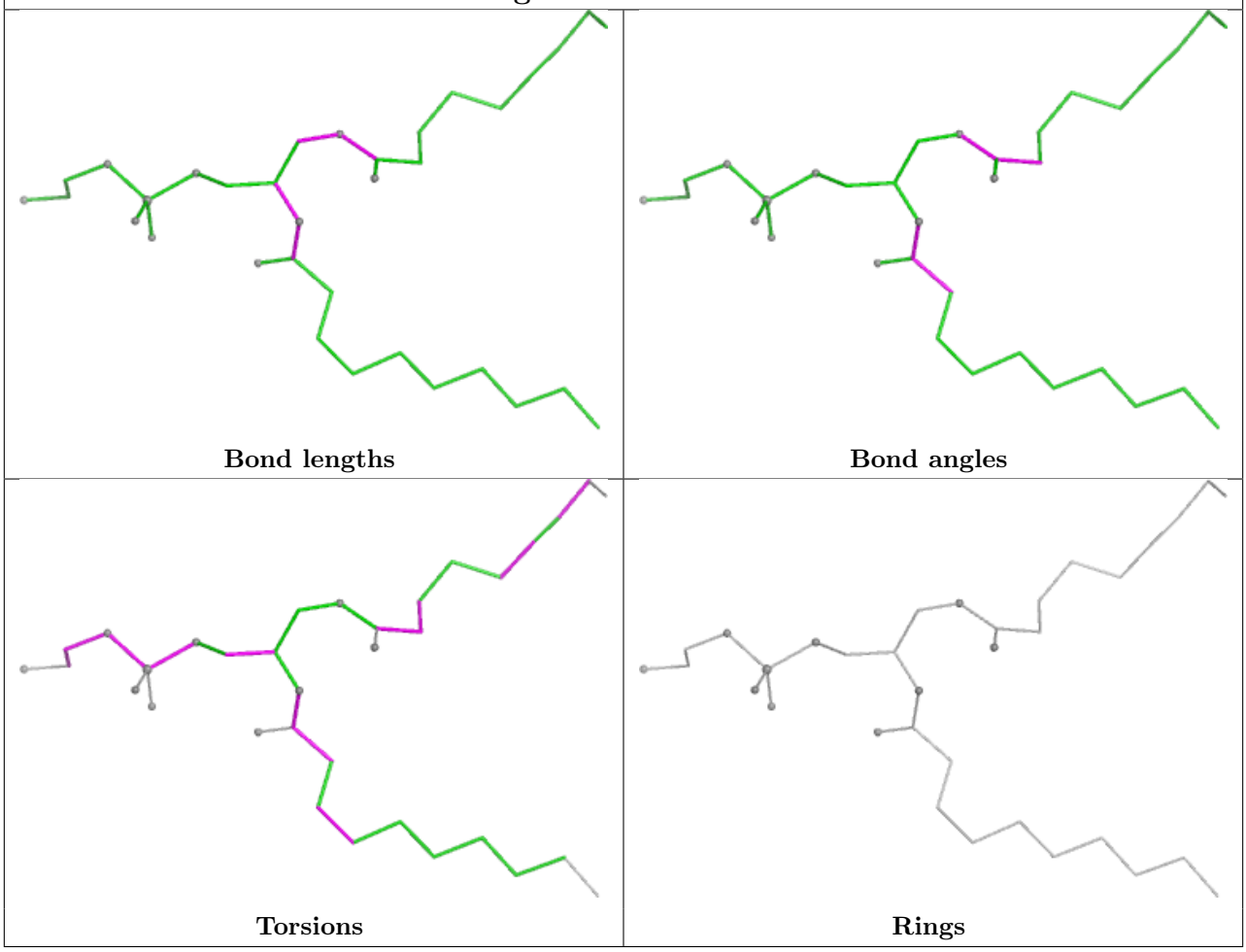


Torsions



Rings

Ligand 3PE Y 204



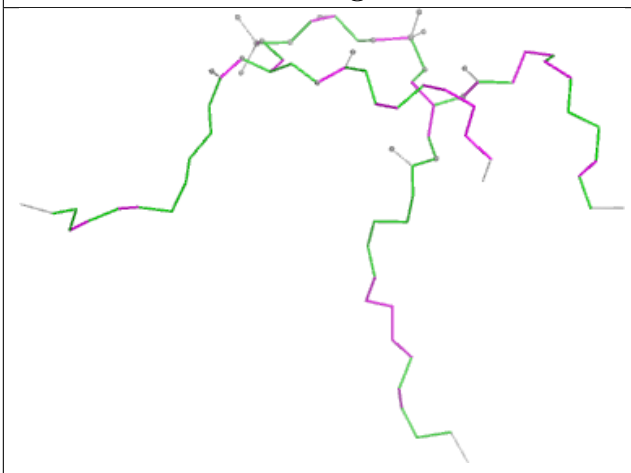
Ligand CDL h 201



Bond lengths



Bond angles

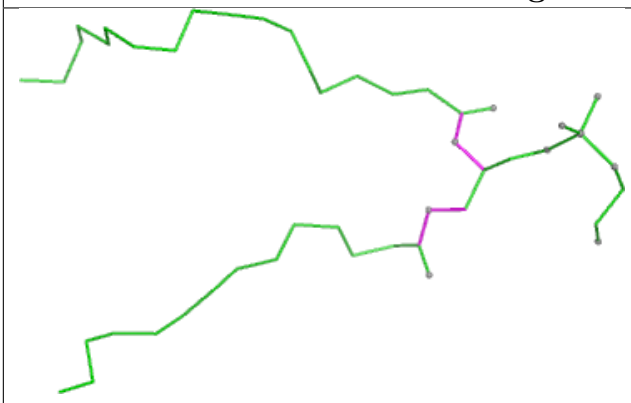


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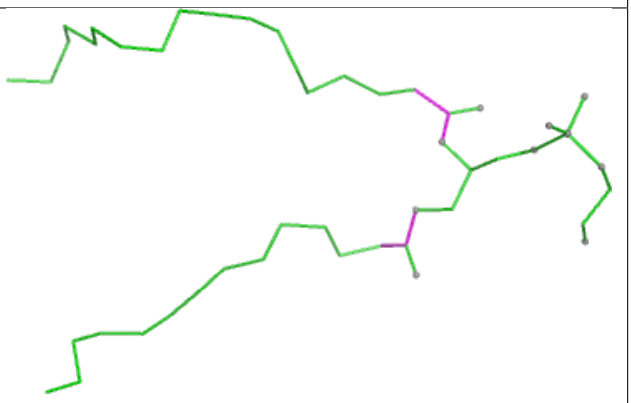


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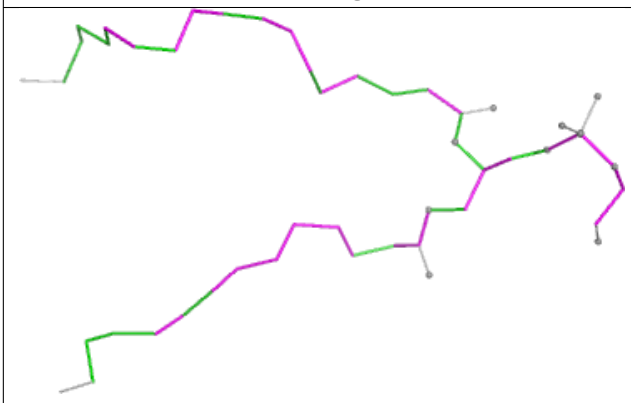
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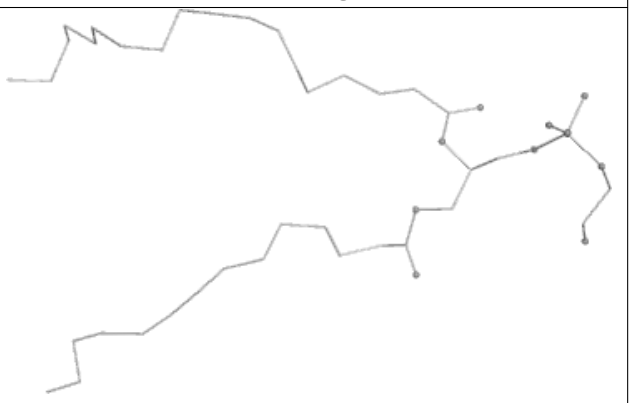
Bond lengths



Bond angles

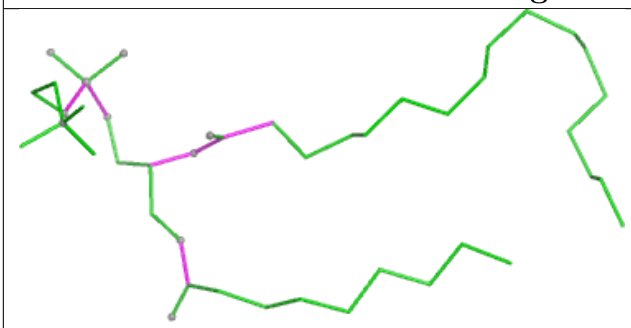


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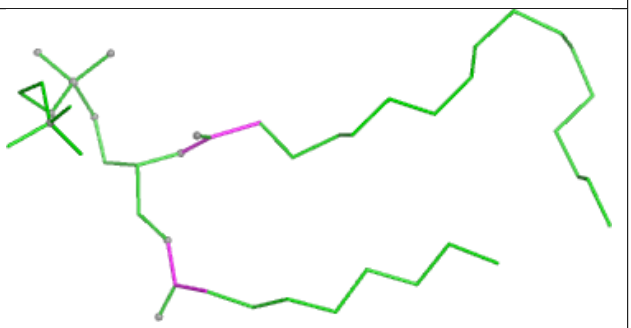


Rings

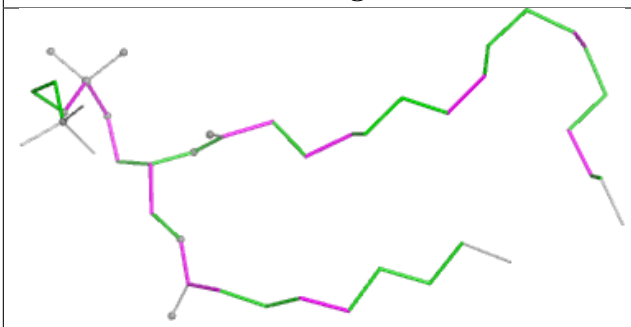
Ligand PC1 h 202



Bond lengths



Bond angles

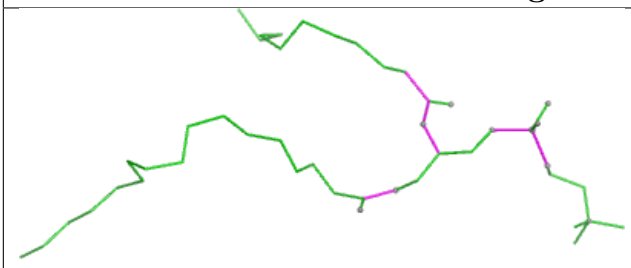


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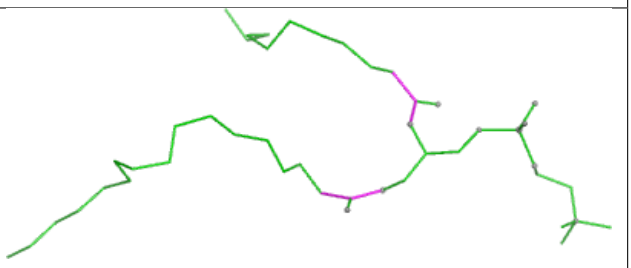


Rings

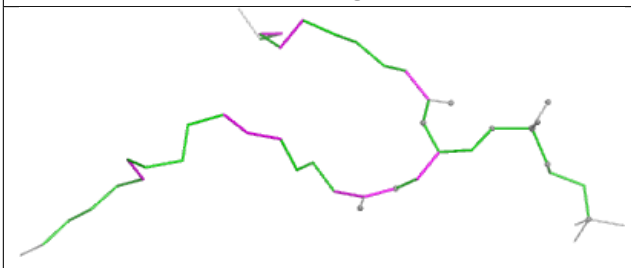
Ligand PC1 P 402



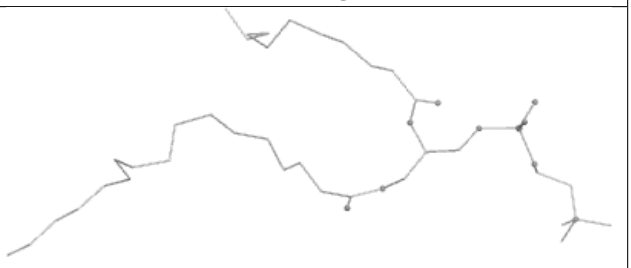
Bond lengths



Bond angles

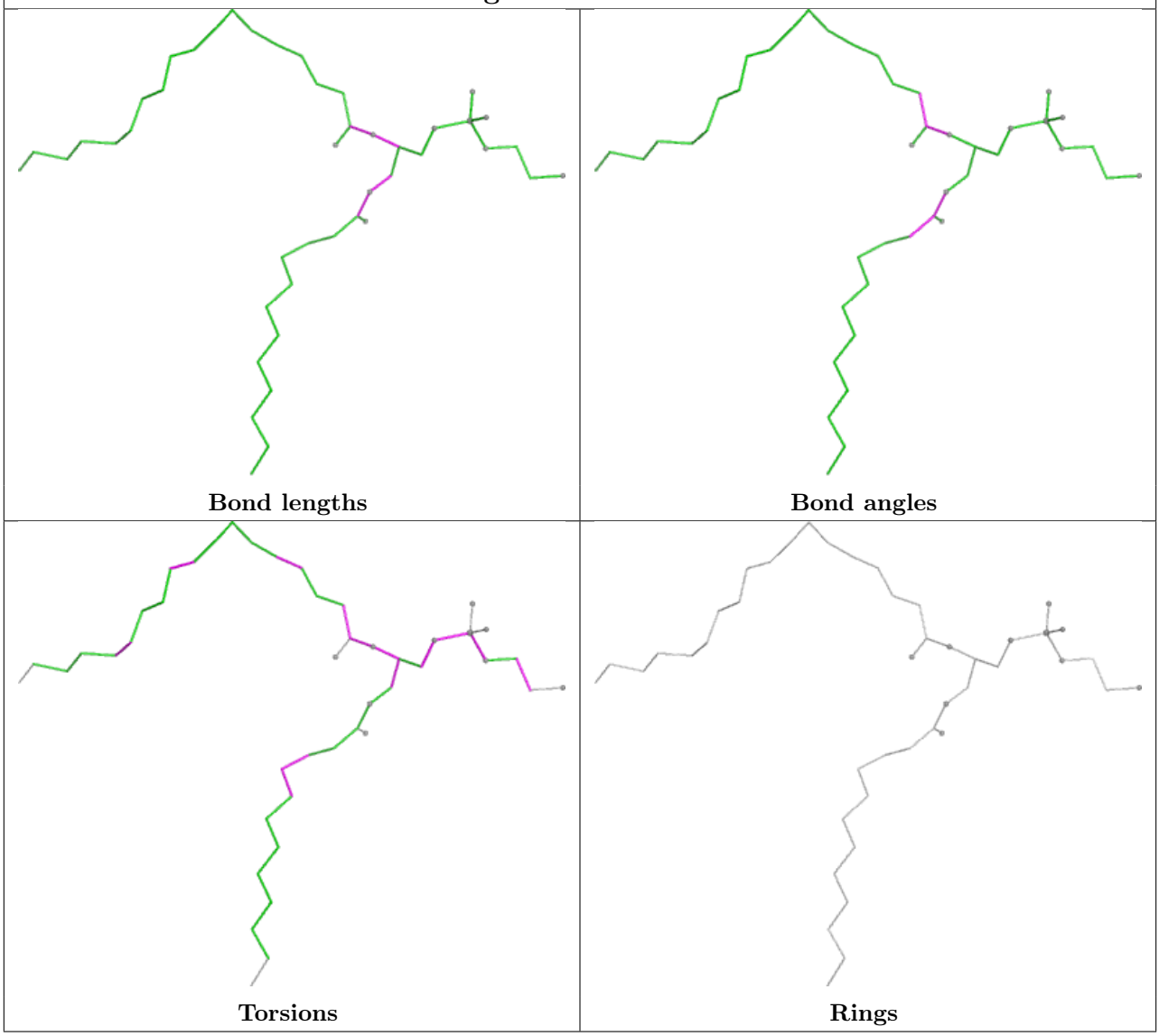


Torsions

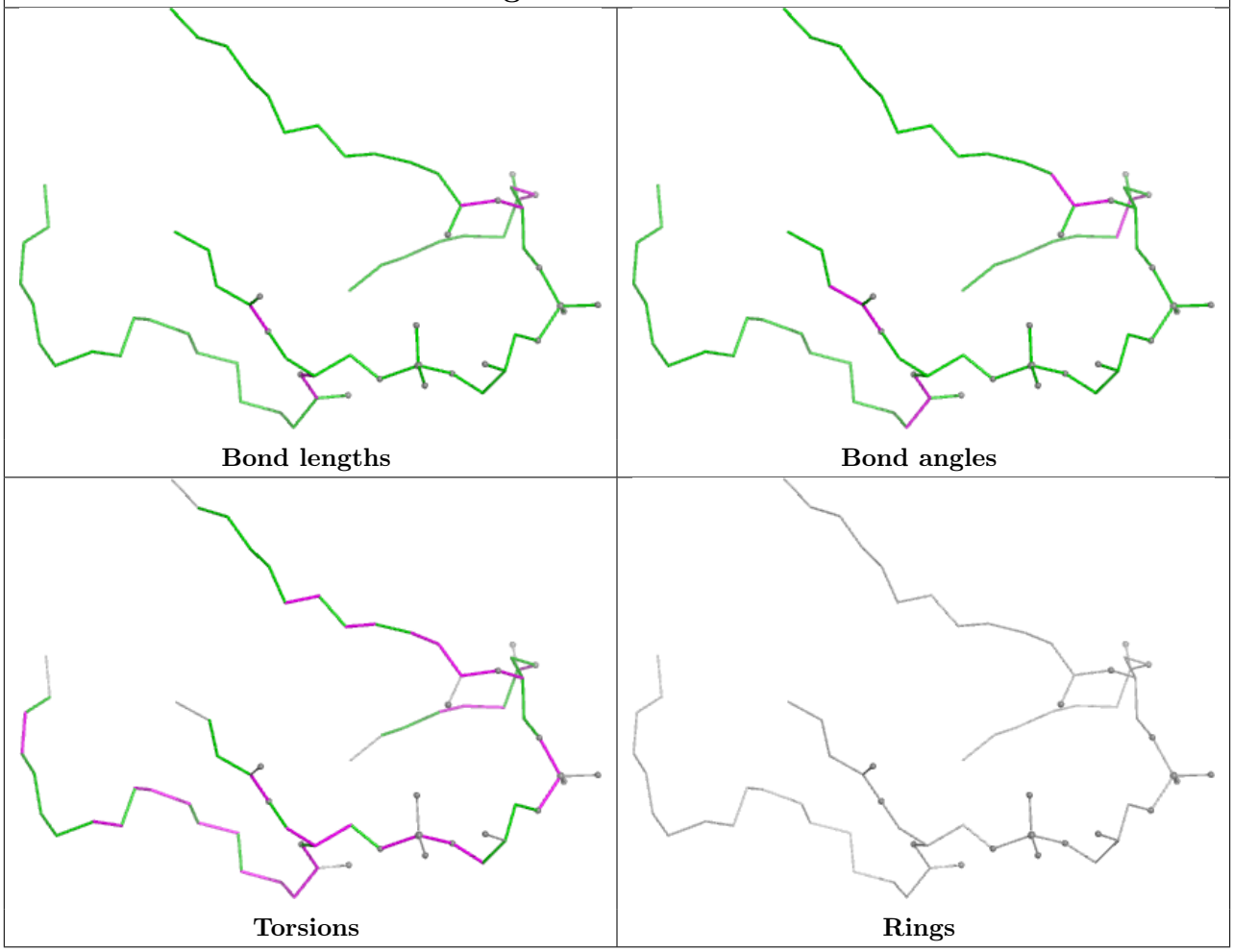


Rings

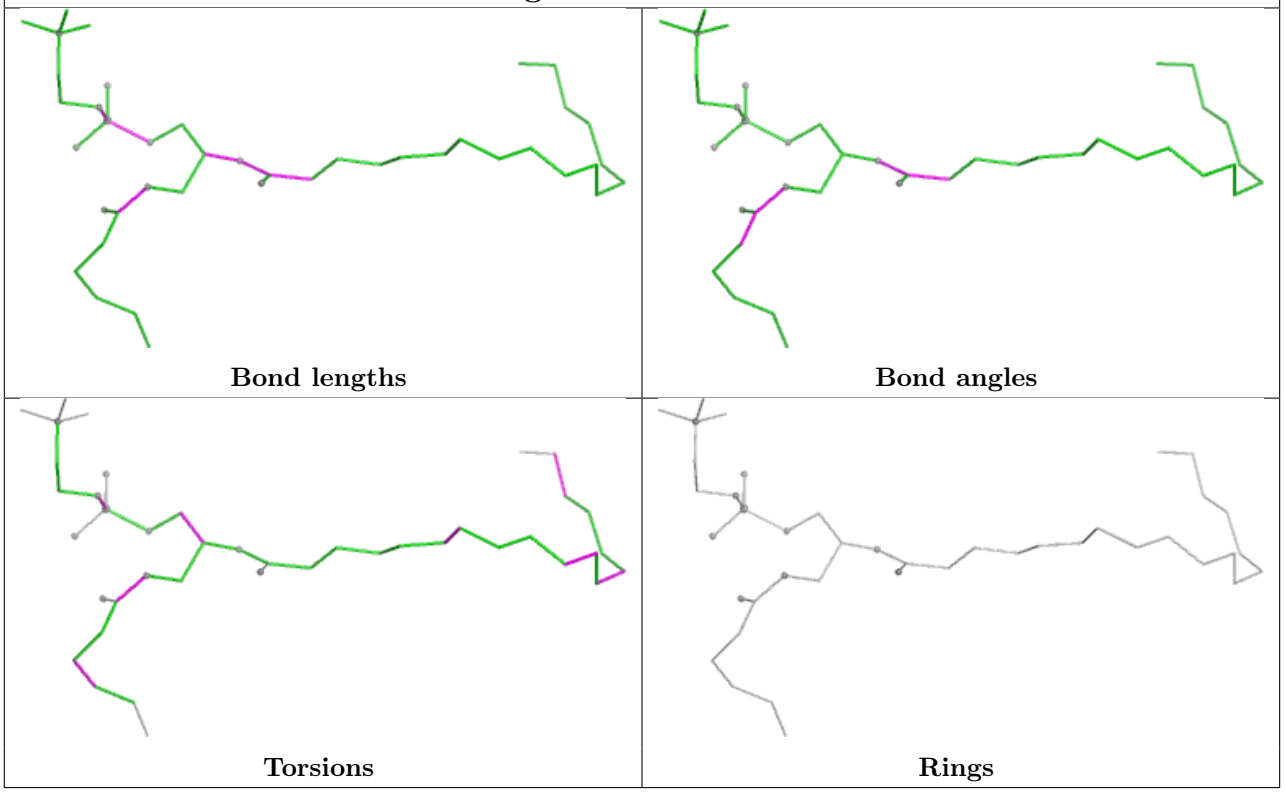
Ligand 3PE I 201



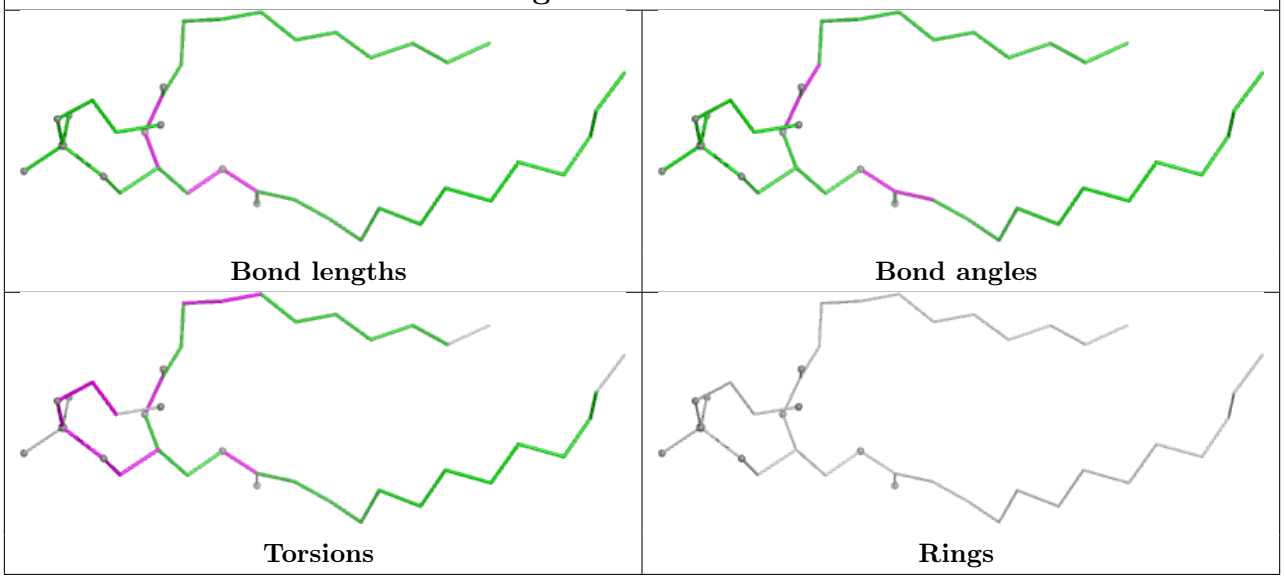
Ligand CDL H 602



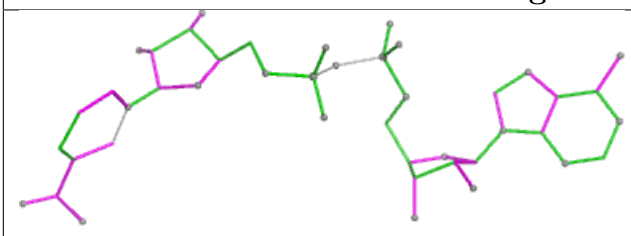
Ligand PC1 M 501



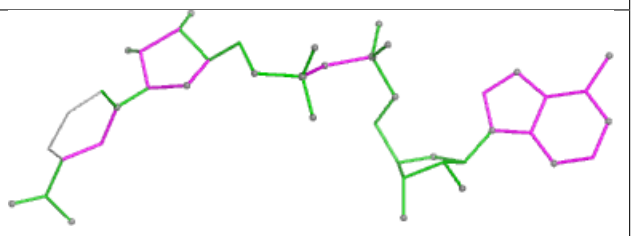
Ligand 3PE b 101



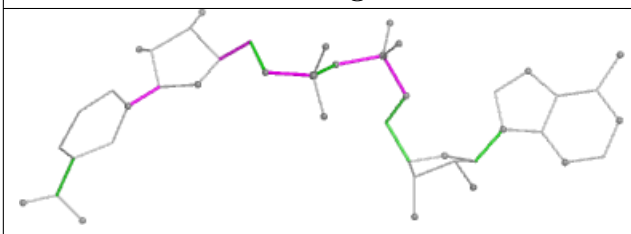
Ligand NAI F 503



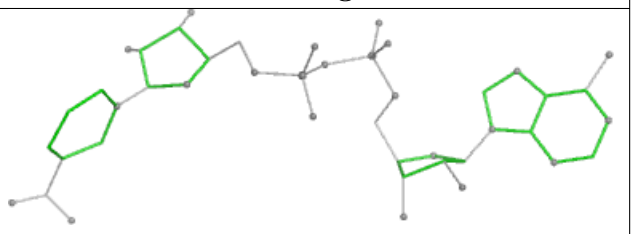
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

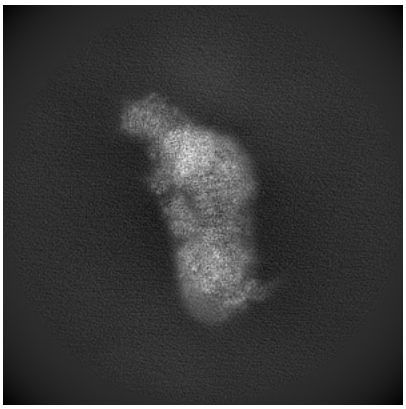
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55030. These allow visual inspection of the internal detail of the map and identification of artifacts.

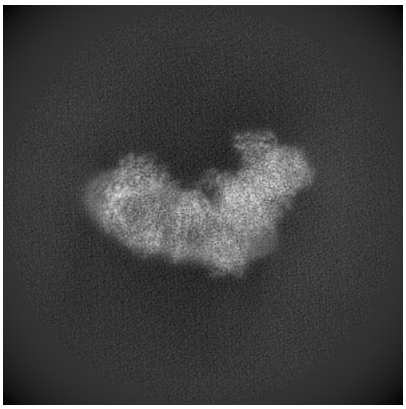
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

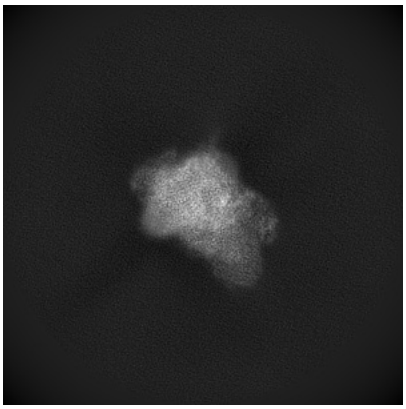
6.1.1 Primary map



X

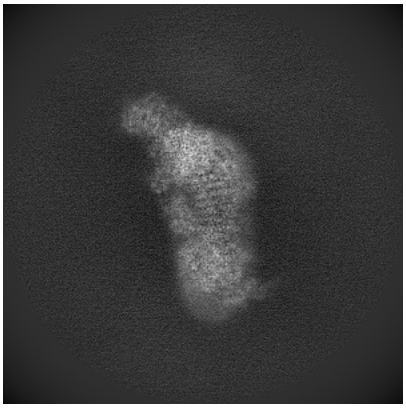


Y

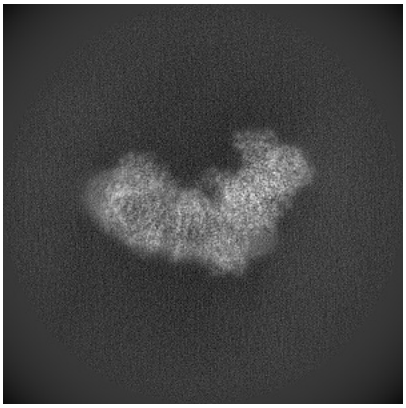


Z

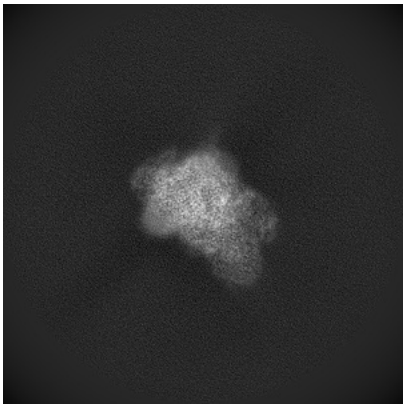
6.1.2 Raw map



X



Y

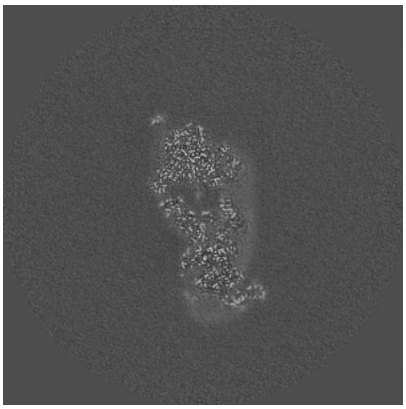


Z

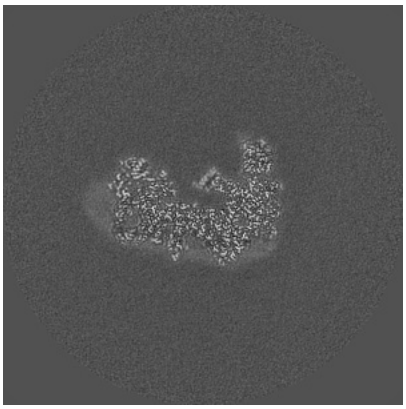
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

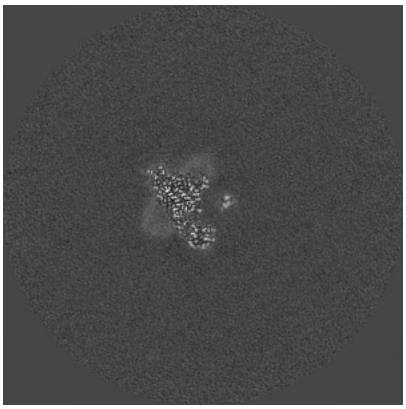
6.2.1 Primary map



X Index: 320

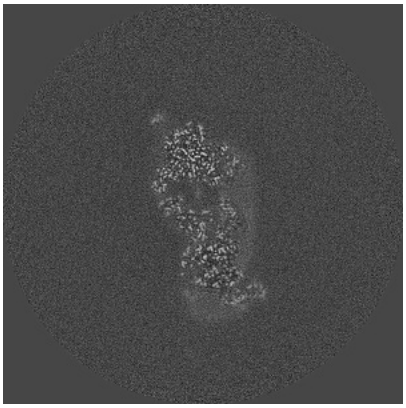


Y Index: 320

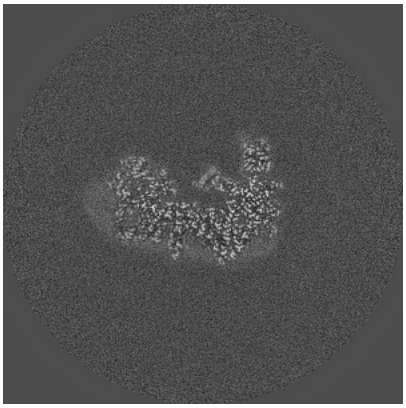


Z Index: 320

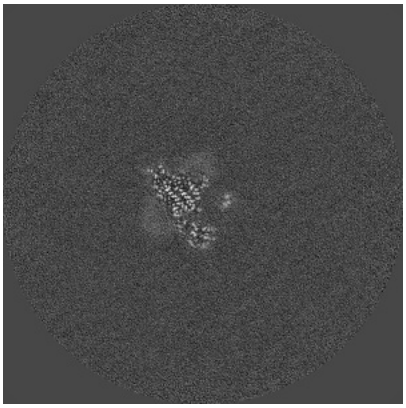
6.2.2 Raw map



X Index: 320



Y Index: 320



Z Index: 320

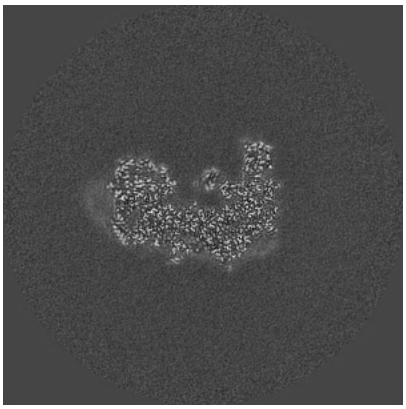
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

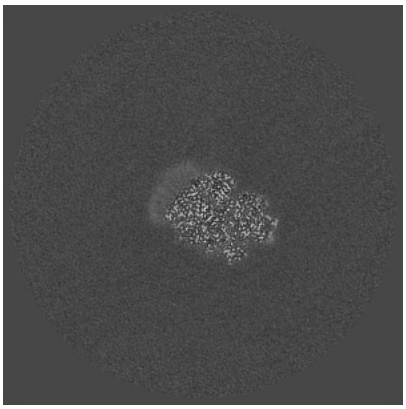
6.3.1 Primary map



X Index: 337

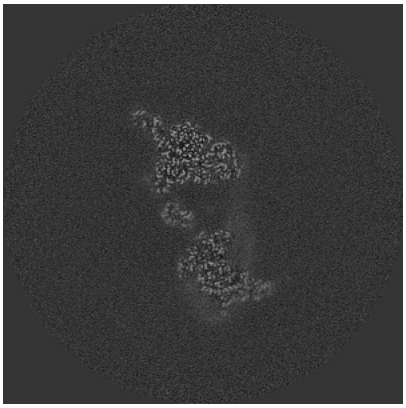


Y Index: 325

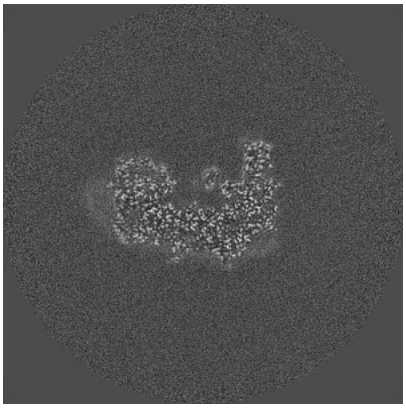


Z Index: 408

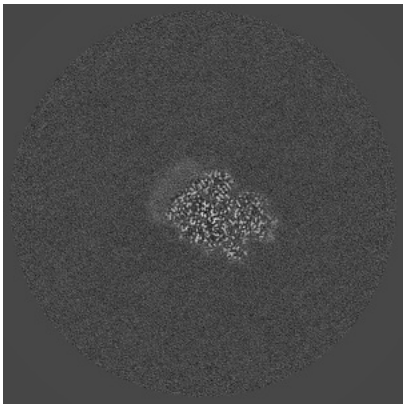
6.3.2 Raw map



X Index: 336



Y Index: 325

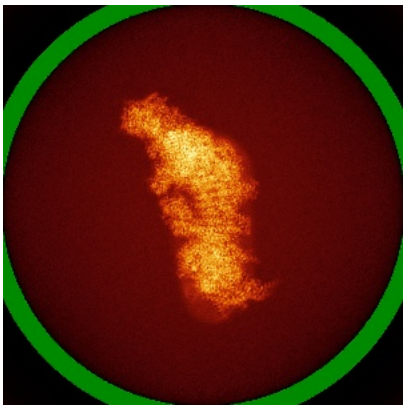


Z Index: 407

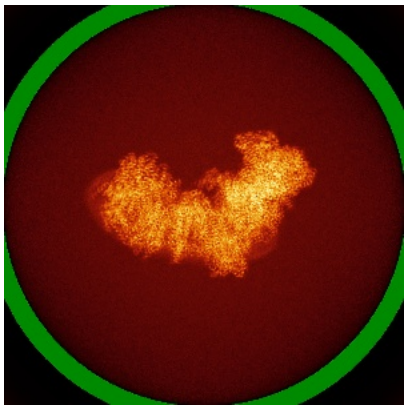
The images above show the largest variance slices of the map in three orthogonal directions.

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

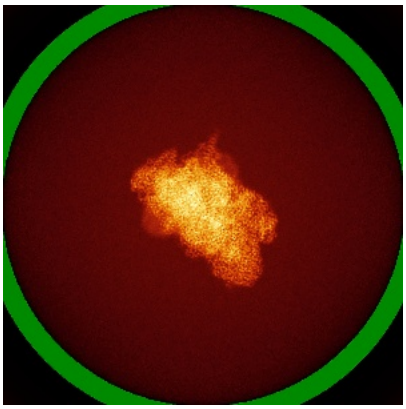
6.4.1 Primary map



X

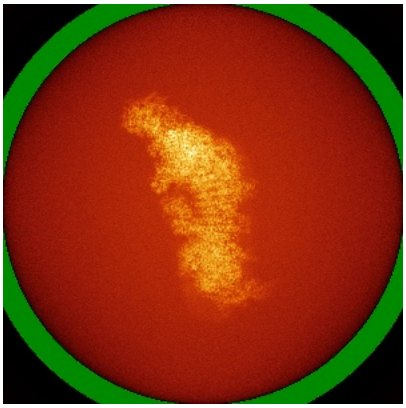


Y

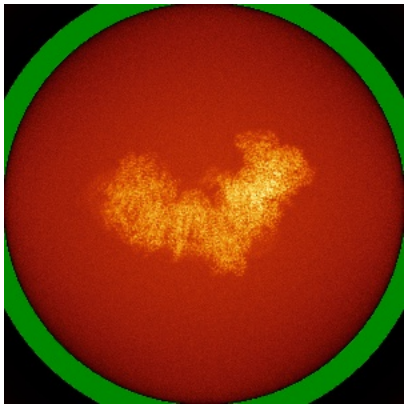


Z

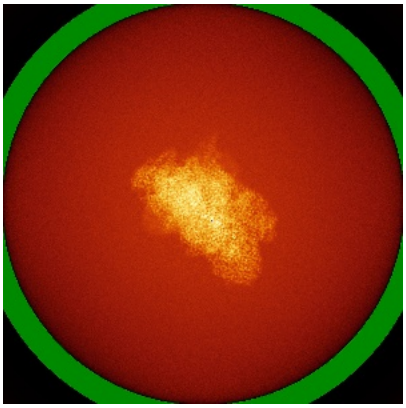
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

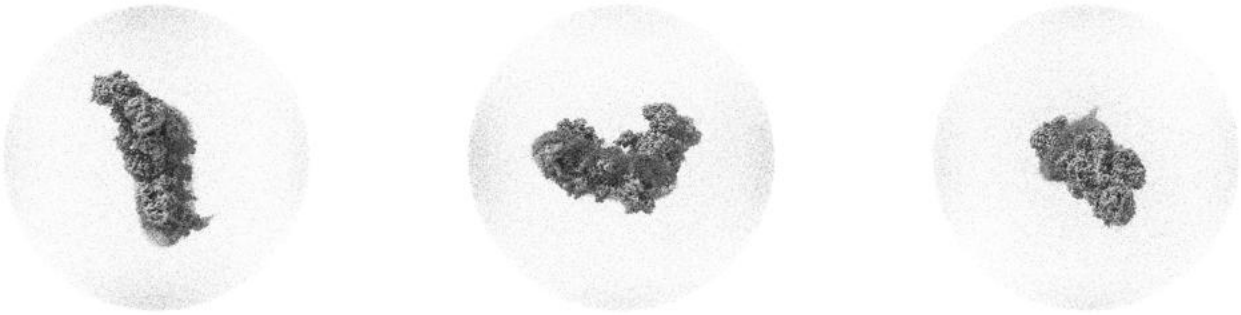
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

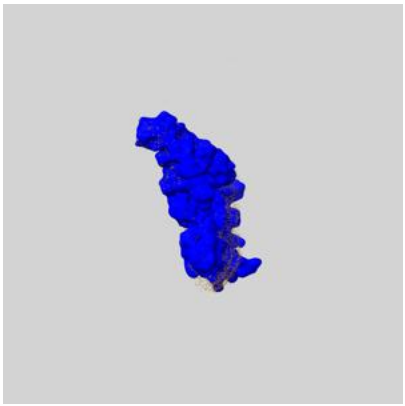
6.6 Mask visualisation

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

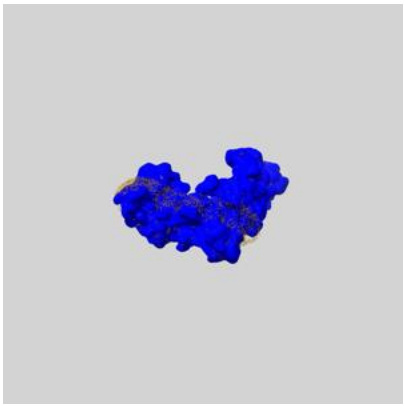
A mask typically either:

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

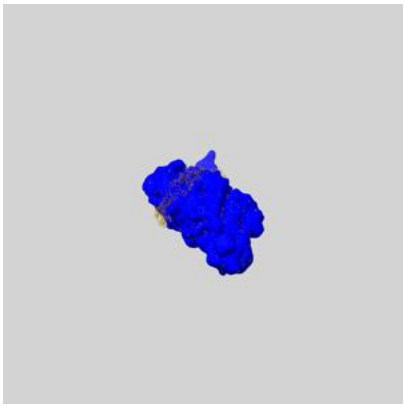
6.6.1 emd_55030_msk_1.map



X



Y

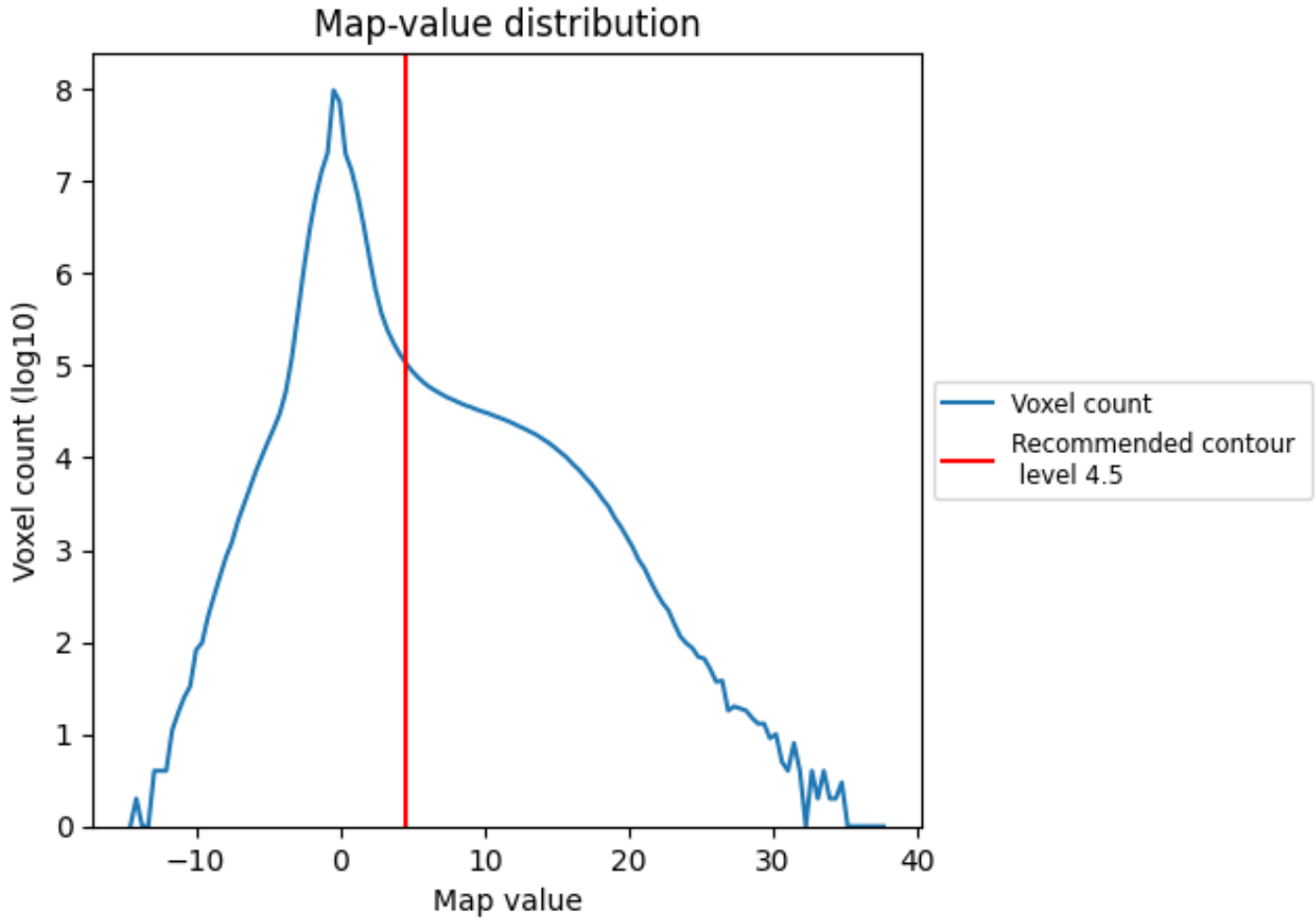


Z

7 Map analysis

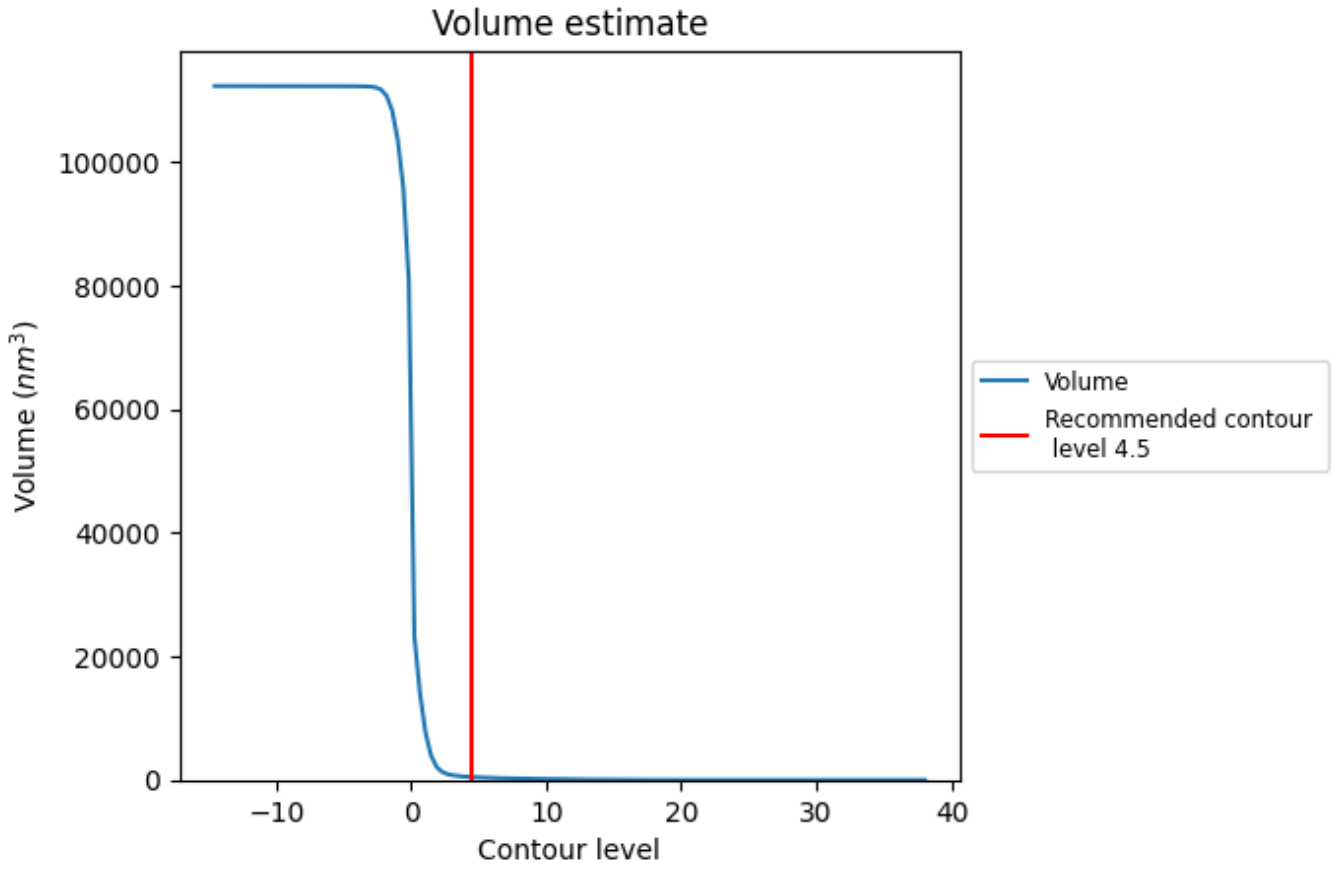
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

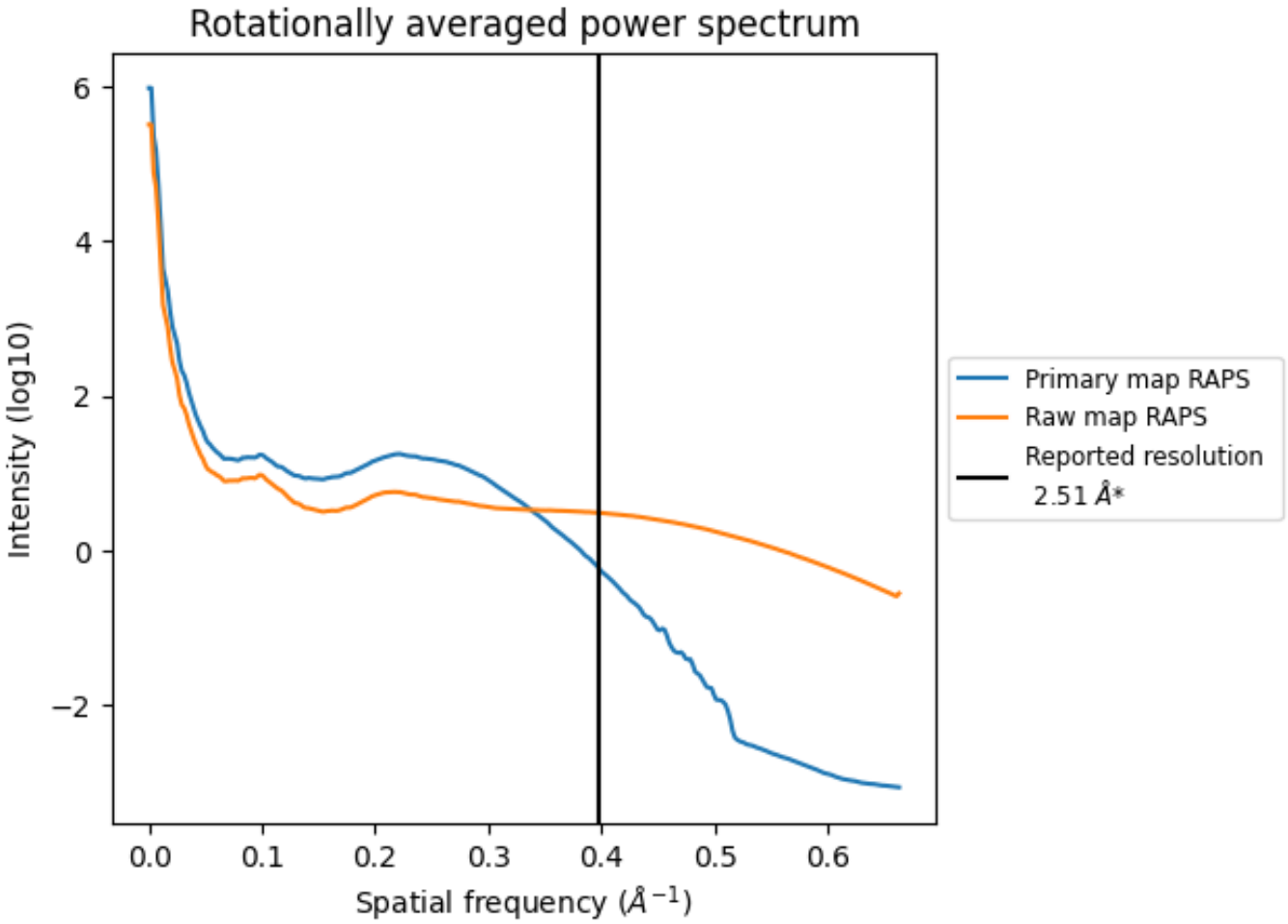
7.2 Volume estimate



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 424 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)

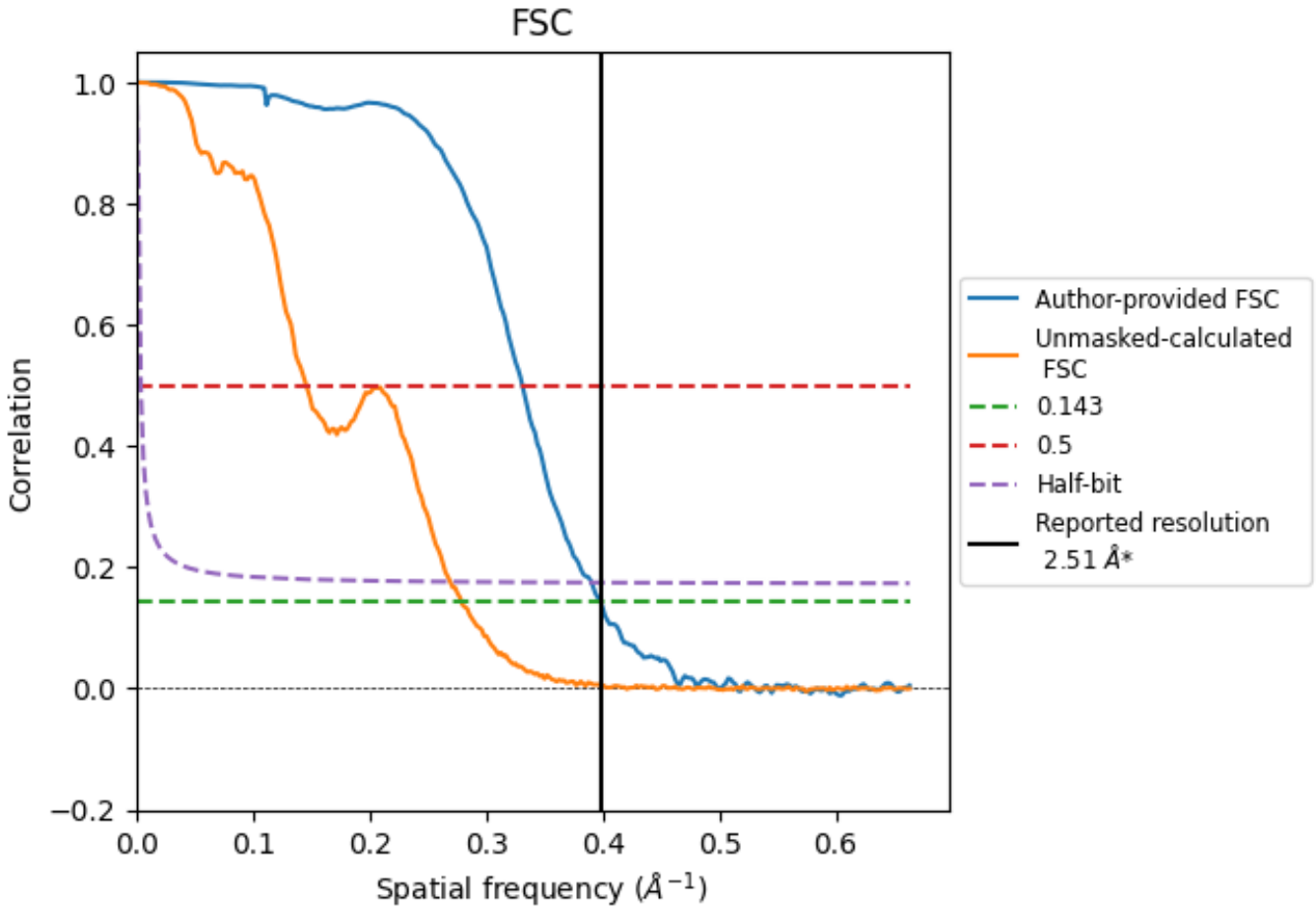


*Reported resolution corresponds to spatial frequency of 0.398 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.398 Å^{-1}

8.2 Resolution estimates (i)

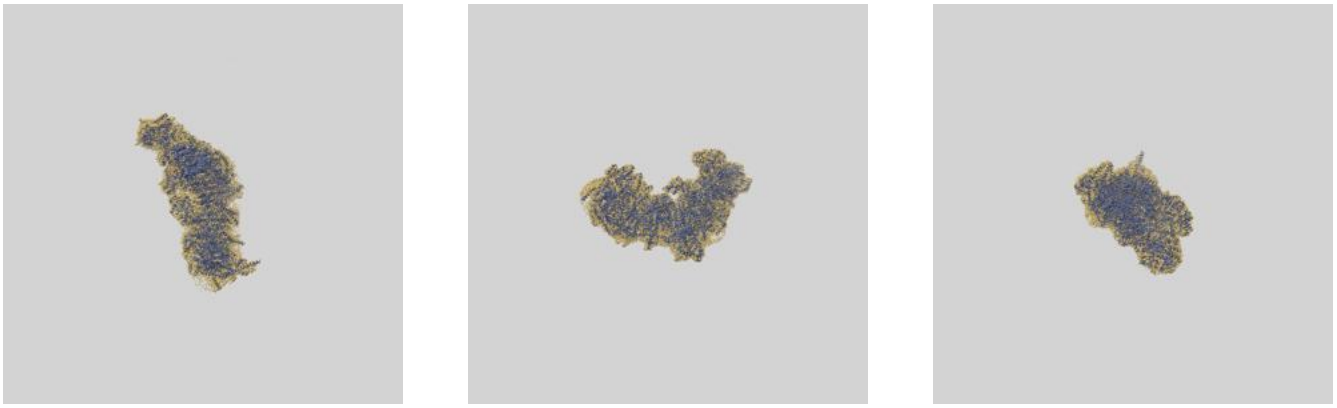
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.51	3.02	2.56
Unmasked-calculated*	3.58	6.85	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 2.51 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55030 and PDB model 9SMF. Per-residue inclusion information can be found in section 3 on page 25.

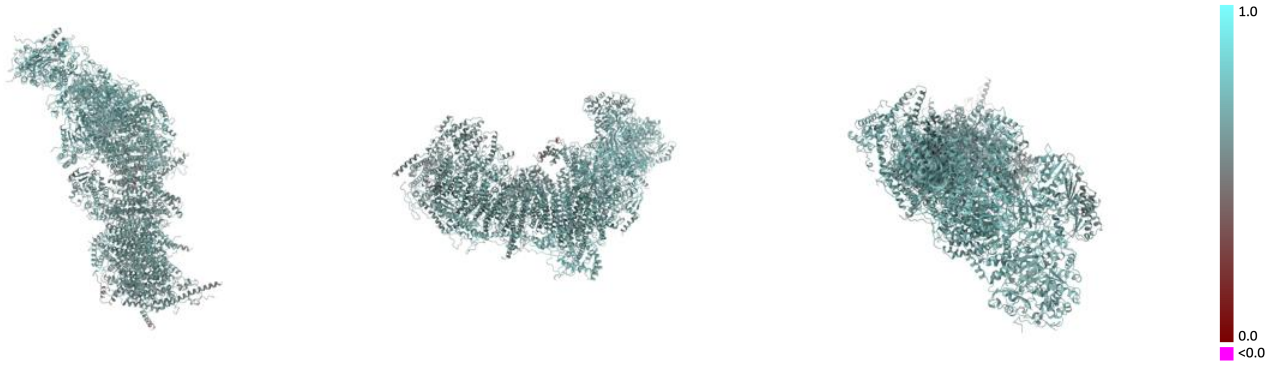
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

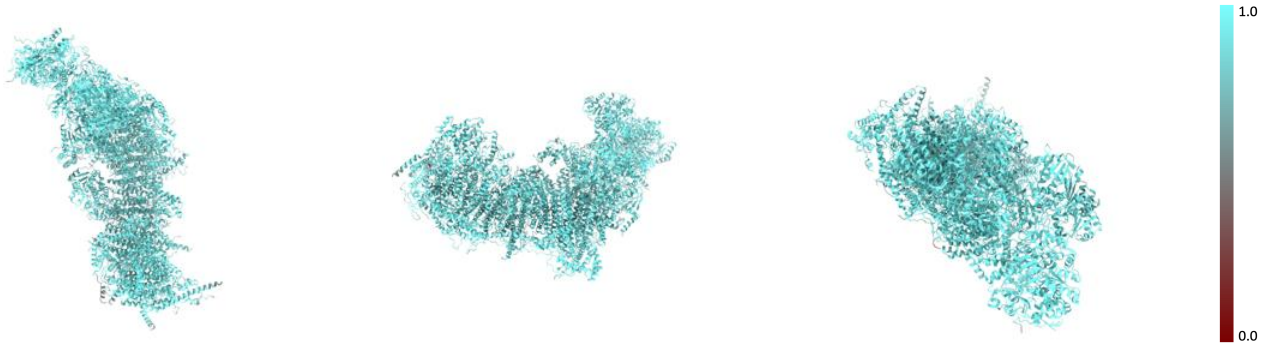
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

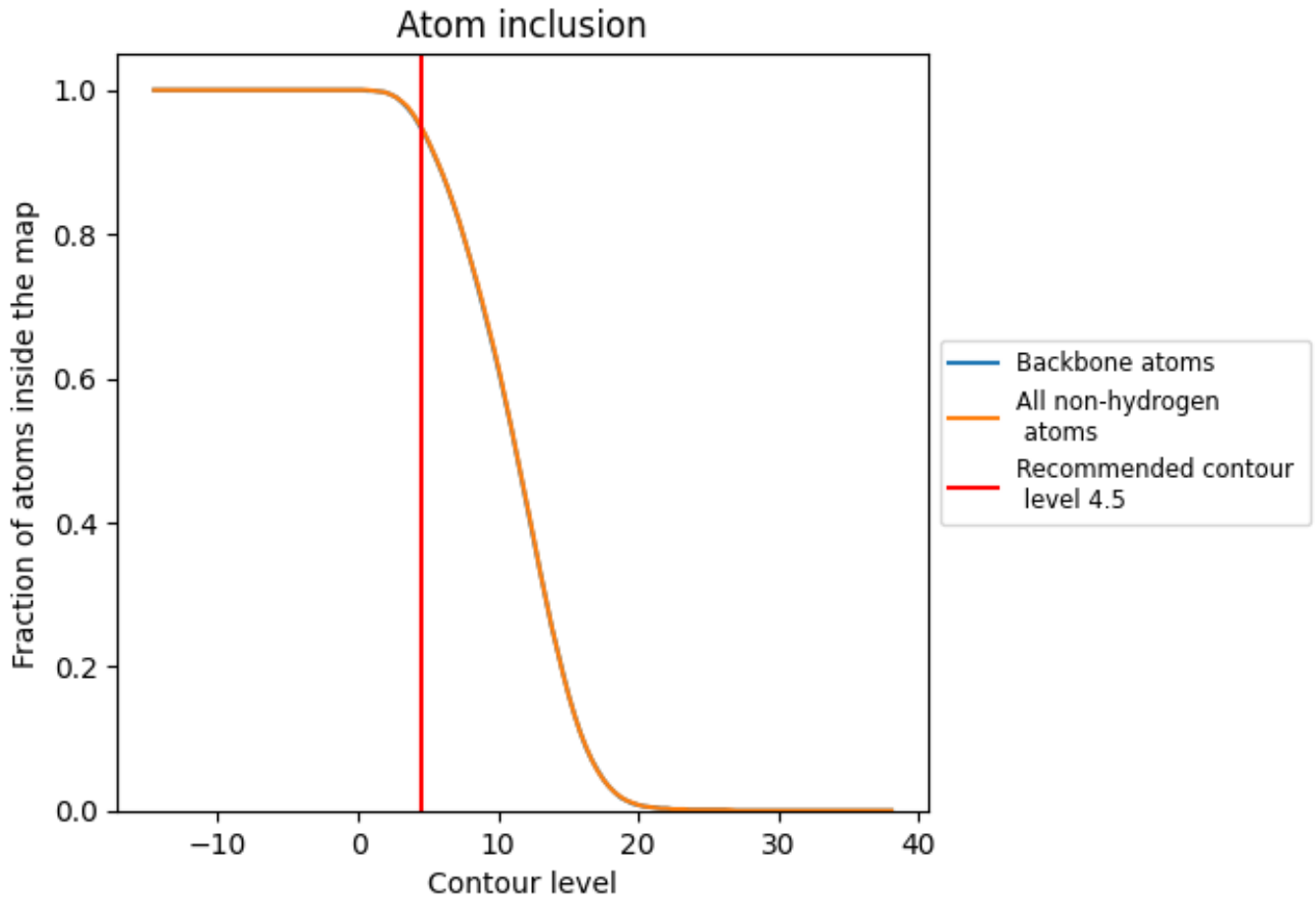
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.6510
A	0.9570	0.6780
B	0.9870	0.7010
C	0.9800	0.7000
D	0.9770	0.7020
E	0.9520	0.6370
F	0.9750	0.6590
G	0.9640	0.6660
H	0.9760	0.6910
I	0.9860	0.7020
J	0.9650	0.6690
K	0.9860	0.6900
L	0.9550	0.6360
M	0.9860	0.6850
N	0.9740	0.6830
O	0.9440	0.6260
P	0.9520	0.6580
Q	0.9580	0.6820
R	0.9490	0.6750
S	0.9020	0.5740
T	0.8050	0.5080
U	0.8900	0.5650
V	0.9350	0.6600
W	0.9410	0.6580
X	0.9350	0.6450
Y	0.9150	0.5970
Z	0.9530	0.6560
a	0.9800	0.6700
b	0.9190	0.6210
c	0.9010	0.6130
d	0.9460	0.6500
e	0.9340	0.6480
f	0.8620	0.5990
g	0.9150	0.6320
h	0.9500	0.6480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8290	0.5570
j	0.9020	0.5660
k	0.8760	0.5520
l	0.9430	0.6100
m	0.9340	0.6210
n	0.9300	0.6030
o	0.8880	0.5540
p	0.9350	0.6270
q	0.9280	0.6610
r	0.9510	0.6690
s	0.9500	0.6340