Full wwPDB EM Validation Report ⓘ

Apr 1, 2023 – 10:22 am BST

PDB ID	:	8B6F
EMDB ID	:	EMD-15865
Title	:	Cryo-EM structure of NADH:ubiquinone oxidoreductase (complex-I) from respiratory supercomplex of Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on	:	2022-09-27
Resolution	:	2.80 Å(reported)

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

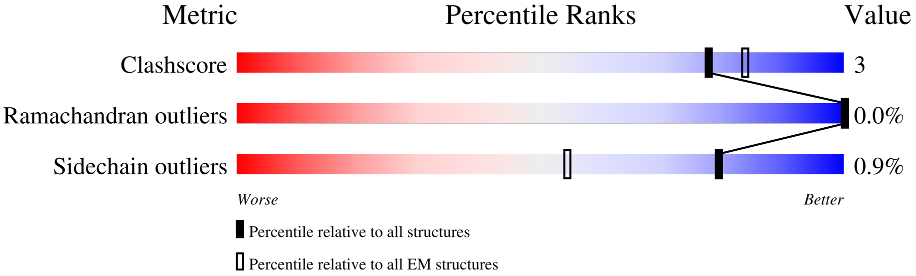
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance ⓘ

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

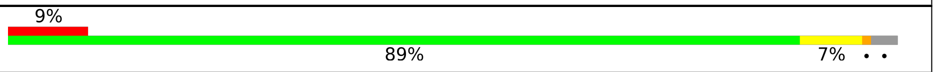
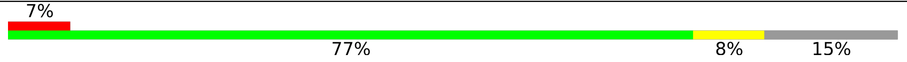
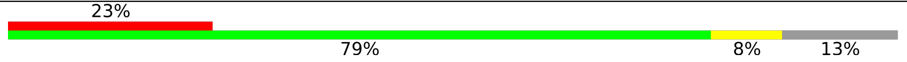
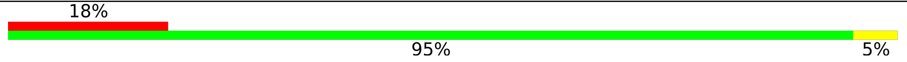
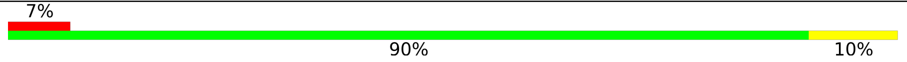
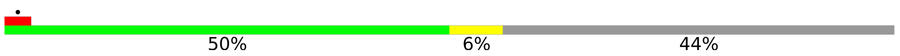
The reported resolution of this entry is 2.80 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A0	516	
2	A1	362	
3	A2	317	
4	A3	333	
5	A4	311	
6	A5	282	
7	A6	251	
8	A7	238	

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Mol	Chain	Length	Quality of chain
9	A8	217	7% 93% 7%
10	A9	231	6% 95% 5%
11	AA	750	10% 84% 11% 5%
12	AB	718	6% 85% 10% •
13	AC	505	• 90% 10%
14	AD	474	17% 82% 10% 7%
15	AE	442	• 87% 12%
16	AF	360	• 89% 11%
17	AG	346	• 96% •
18	AH	284	• 89% 11%
19	AI	274	16% 77% 7% 16%
20	AJ	255	• 93% 7%
21	AK	257	• 82% 8% 11%
22	AL	236	• 78% 14% 8%
23	AM	233	• 89% 9% ••
24	AN	206	• 70% 6% 24%
25	AO	198	• 87% 13%
26	AP	194	• 89% 9% •
27	AQ	189	• 94% 5% •
28	AR	185	6% 94% • •
29	AS	172	• 92% 7% •
30	AT	162	• 81% 17% ••
31	AU	150	13% 94% 5% •
32	AV	138	• 78% • 19%
33	AW	133	• 68% 5% 26%

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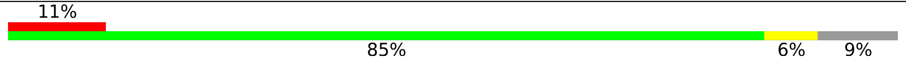
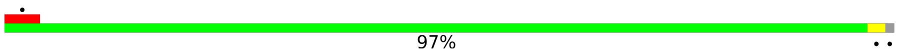
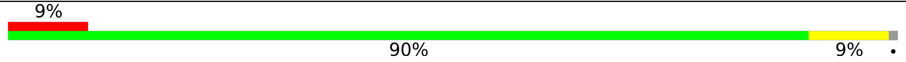
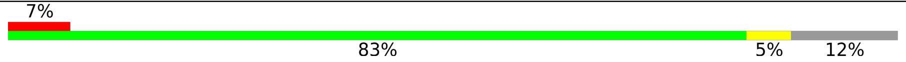
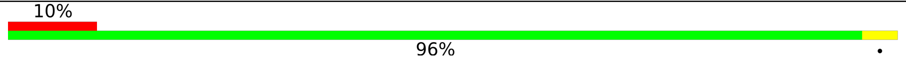
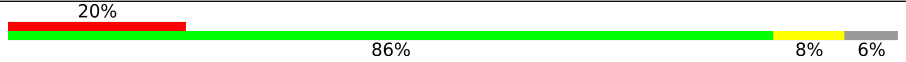
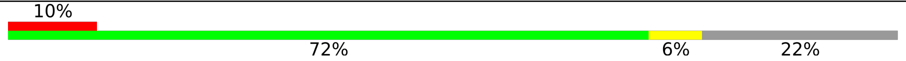
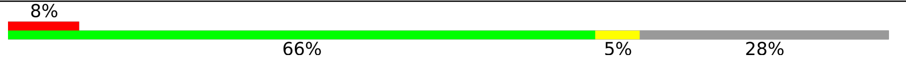
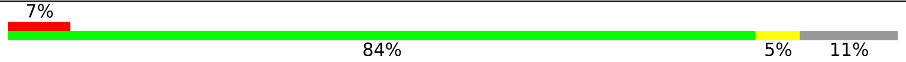
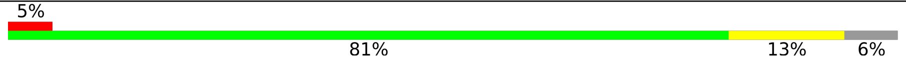
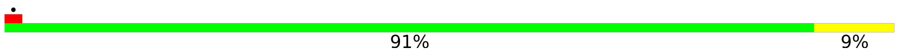
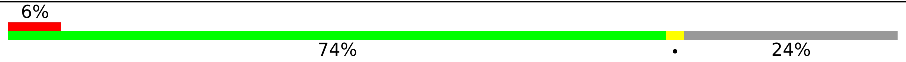
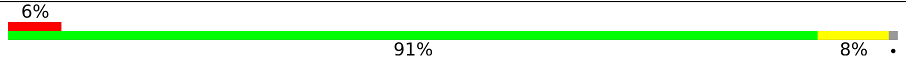
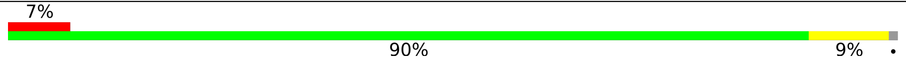
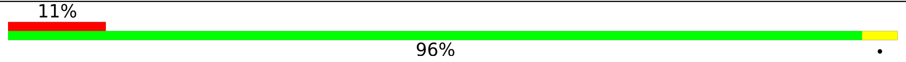
Mol	Chain	Length	Quality of chain
34	AX	121	
35	AY	116	
36	AZ	103	
37	B0	94	
38	B1	93	
39	B2	94	
40	B3	83	
41	B4	73	
42	B5	71	
43	B6	59	
44	BA	212	
45	BB	214	
46	BC	207	
47	BD	205	
48	BE	189	
49	BF	188	
50	BG	175	
51	BH	178	
52	BI	172	
53	BJ	166	
54	BK	144	
55	BL	143	
56	BM	135	
57	BN	135	
58	BO	136	

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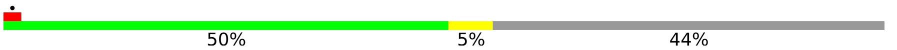
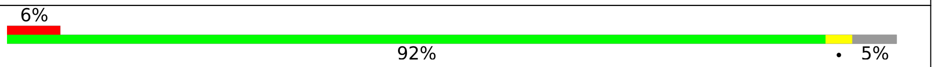
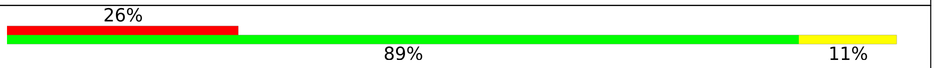
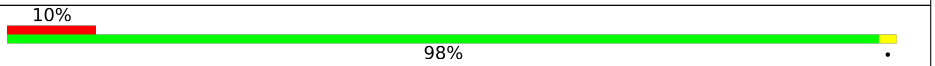
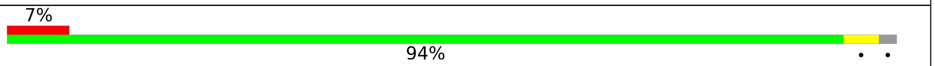
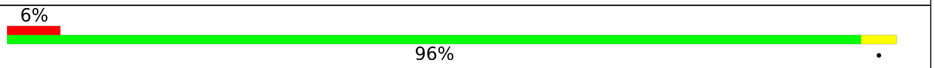
Mol	Chain	Length	Quality of chain
59	BP	129	
60	BQ	127	
61	BR	132	
62	BS	126	
63	BT	125	
64	BU	134	
65	BV	125	
66	BW	120	
67	BX	113	
68	BY	100	
69	BZ	102	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
78	FES	AI	301	-	-	X	-
79	SF4	AB	803	-	-	X	-
79	SF4	AL	302	-	-	X	-

2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 234355 atoms, of which 117595 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 Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A0	503	8090	2609	4019	699	750	13	0	0

- Molecule 2 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A1	338	5368	1737	2650	475	494	12	0	0

- Molecule 3 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	A2	269	4362	1392	2163	408	396	3	0	0

- Molecule 4 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A3	291	4523	1438	2260	390	434	1	0	0

- Molecule 5 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A4	311	4985	1583	2491	434	469	8	0	0

- Molecule 6 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	A5	282	4596	1478	2249	413	453	3	0	0

- Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	A6	230	3770	1241	1862	322	340	5	0	0

- Molecule 8 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	A7	133	2124	682	1040	182	209	11	0	0

- Molecule 9 is a protein called NDUTT15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	A8	217	3597	1153	1803	305	328	8	0	0

- Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	A9	231	3697	1219	1818	317	336	7	0	0

- Molecule 11 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AA	713	11919	4066	5978	855	1004	16	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AB	688	10762	3410	5359	935	1030	28	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AC	505	8393	2859	4223	601	692	18	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AD	441	6744	2140	3345	596	639	24	0	0

- Molecule 15 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	AE	441	7126	2285	3539	620	658	24	0	0

- Molecule 16 is a protein called Ymf65.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	AF	359	6216	2132	3148	435	494	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	208	VAL	GLY	conflict	UNP Q951A3

- Molecule 17 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	AG	346	5531	1766	2727	481	549	8	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	AH	283	4656	1581	2350	334	379	12	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AI	231	3710	1173	1848	321	358	10	0	0

- Molecule 20 is a protein called Ymf62.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AJ	254	4316	1478	2156	305	373	4	0	0

- Molecule 21 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AK	230	3519	1117	1740	306	351	5	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AL	218	3501	1155	1689	299	347	11	0	0

- Molecule 23 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AM	231	3558	1112	1788	316	335	7	0	0

- Molecule 24 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AN	157	2651	846	1329	221	249	6	0	0

- Molecule 25 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AO	198	3363	1097	1680	268	312	6	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AP	191	3104	1013	1505	301	280	5	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	AQ	187	3084	1027	1496	254	303	4	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	AR	181	2937	948	1445	267	269	8	0	0

- Molecule 29 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	AS	172	2802	903	1382	253	256	8	0	0

- Molecule 30 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	AT	161	2549	822	1272	220	225	10	0	0

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
31	AU	149	2436	800	1209	213	214	0	0

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
32	AV	112	1829	586	904	158	181	0	0

- Molecule 33 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	AW	98	1584	512	781	133	157	1	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	AX	121	2047	710	1020	143	170	4	0	0

- Molecule 35 is a protein called Ymf58.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AY	116	1944	648	987	142	163	4	0	0

- Molecule 36 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	AZ	94	1552	491	775	140	144	2	0	0

- Molecule 37 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
37	B0	93	1607	531	802	139	135	0	0

- Molecule 38 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	B1	92	1536	497	746	146	146	1	0	0

- Molecule 39 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	B2	93	1485	480	728	129	142	6	0	0

- Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	B3	73	1251	414	618	113	105	1	0	0

- Molecule 41 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	B4	73	1247	408	623	111	104	1	0	0

- Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	B5	54	917	305	464	71	75	2	0	0

- Molecule 43 is a protein called ND1b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	B6	59	1043	362	528	78	72	3	0	0

- Molecule 44 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	BA	199	3289	1071	1638	285	292	3	0	0

- Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	BB	167	2626	848	1280	228	265	5	0	0

- Molecule 46 is a protein called NDUB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	BC	173	2848	928	1406	244	264	6	0	0

- Molecule 47 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	BD	148	2414	764	1223	211	214	2	0	0

- Molecule 48 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	BE	168	2807	930	1385	227	260	5	0	0

- Molecule 49 is a protein called NDUB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	BF	177	2961	934	1486	267	270	4	0	0

- Molecule 50 is a protein called NDUA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	BG	160	2725	858	1376	256	227	8	0	0

- Molecule 51 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	BH	178	3036	1015	1554	215	247	5	0	0

- Molecule 52 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	BI	149	2318	731	1139	211	227	10	0	0

- Molecule 53 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	BJ	144	2361	767	1156	205	226	7	0	0

- Molecule 54 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	BK	109	1757	562	854	161	174	6	0	0

- Molecule 55 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	BL	142	Total	C	H	N	O	S	0	0
			2325	770	1138	202	209	6		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	BM	128	Total	C	H	N	O	S	0	0
			2074	695	1002	194	180	3		

- Molecule 57 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BN	133	Total	C	H	N	O	0	0
			2229	716	1126	196	191		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	BO	136	Total	C	H	N	O	S	0	0
			2156	690	1058	190	208	10		

- Molecule 59 is a protein called NDUB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	BP	72	Total	C	H	N	O	S	0	0
			1194	404	590	100	96	4		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	BQ	101	Total	C	H	N	O	S	0	0
			1674	547	829	140	153	5		

- Molecule 61 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	BR	91	Total	C	H	N	O	S	0	0
			1449	460	719	129	137	4		

- Molecule 62 is a protein called NDUB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	BS	120	Total 1907	C 621	H 941	N 167	O 175	S 3	0	0

- Molecule 63 is a protein called NDUB15.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	BT	125	Total 2016	C 696	H 953	N 172	O 190	S 5	0	0

- Molecule 64 is a protein called NDUTT16.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	BU	134	Total 2176	C 683	H 1094	N 194	O 204	S 1	0	0

- Molecule 65 is a protein called NDUTT17.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	BV	125	Total 2001	C 632	H 1014	N 177	O 177	S 1	0	0

- Molecule 66 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	BW	118	Total 1848	C 603	H 893	N 167	O 179	S 6	0	0

- Molecule 67 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BX	96	Total 1552	C 512	H 755	N 139	O 146	0	0

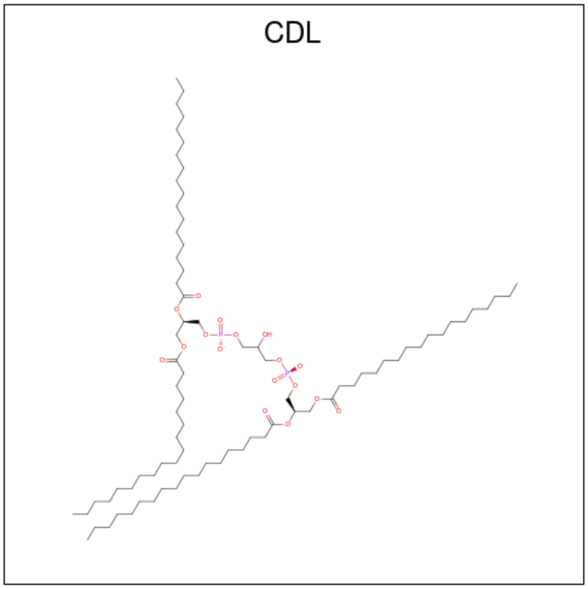
- Molecule 68 is a protein called Ymf57.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	BY	100	Total 1806	C 620	H 917	N 128	O 138	S 3	0	0

- Molecule 69 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	BZ	102	1690	553	840	139	150	8	0	0

- Molecule 70 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
70	A0	1	256	81	156	17	2	0
70	A0	1	256	81	156	17	2	0
70	A1	1	256	81	156	17	2	0
70	AA	1	256	81	156	17	2	0
70	AA	1	256	81	156	17	2	0
70	AC	1	256	81	156	17	2	0
70	AC	1	256	81	156	17	2	0
70	AF	1	256	81	156	17	2	0
70	AF	1	256	81	156	17	2	0
70	AM	1	256	81	156	17	2	0

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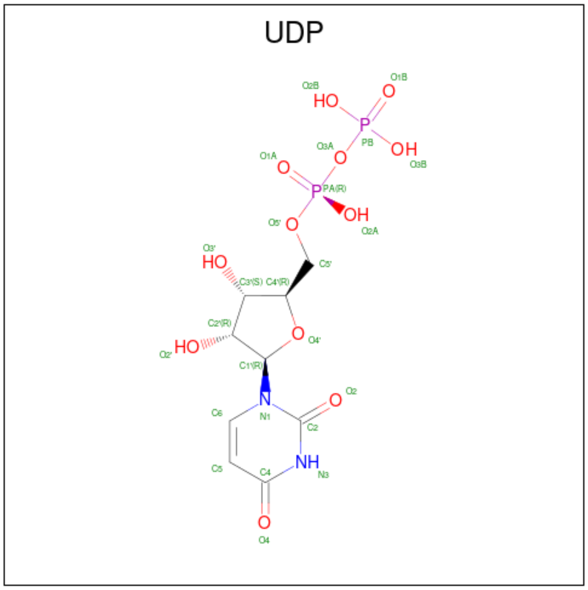
Mol	Chain	Residues	Atoms	AltConf
70	AP	1	Total C H O P 256 81 156 17 2	0
70	B0	1	Total C H O P 256 81 156 17 2	0
70	B0	1	Total C H O P 256 81 156 17 2	0
70	B1	1	Total C H O P 256 81 156 17 2	0
70	BC	1	Total C H O P 256 81 156 17 2	0
70	BC	1	Total C H O P 256 81 156 17 2	0
70	BE	1	Total C H O P 256 81 156 17 2	0
70	BG	1	Total C H O P 256 81 156 17 2	0
70	BL	1	Total C H O P 256 81 156 17 2	0
70	BT	1	Total C H O P 256 81 156 17 2	0
70	BV	1	Total C H O P 256 81 156 17 2	0
70	BY	1	Total C H O P 256 81 156 17 2	0

- Molecule 71 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

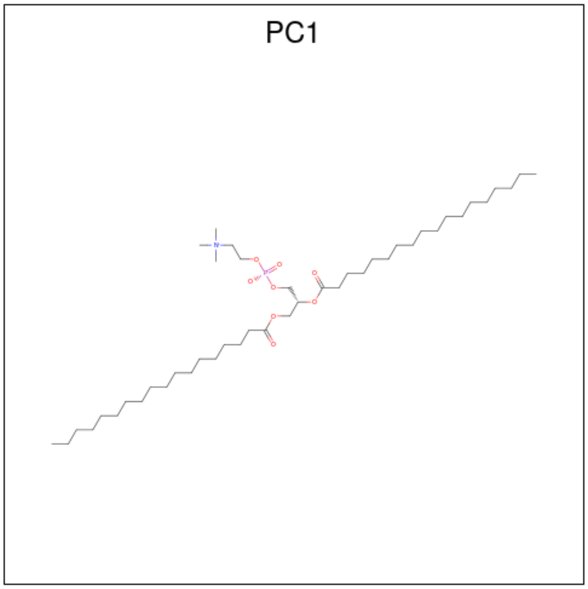


Mol	Chain	Residues	Atoms	AltConf
71	A0	1	Total C H N O P 36 9 11 2 12 2	0

- Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
72	A0	1	Total Mg 1 1	0
72	A8	1	Total Mg 1 1	0

- Molecule 73 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
73	A0	1	Total C H N O P 142 44 88 1 8 1	0
73	A1	1	Total C H N O P 142 44 88 1 8 1	0
73	A1	1	Total C H N O P 142 44 88 1 8 1	0
73	A2	1	Total C H N O P 142 44 88 1 8 1	0
73	A6	1	Total C H N O P 142 44 88 1 8 1	0
73	A6	1	Total C H N O P 142 44 88 1 8 1	0

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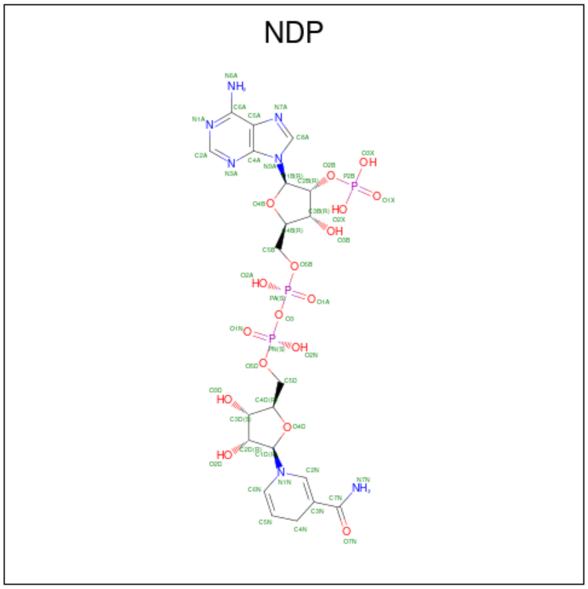
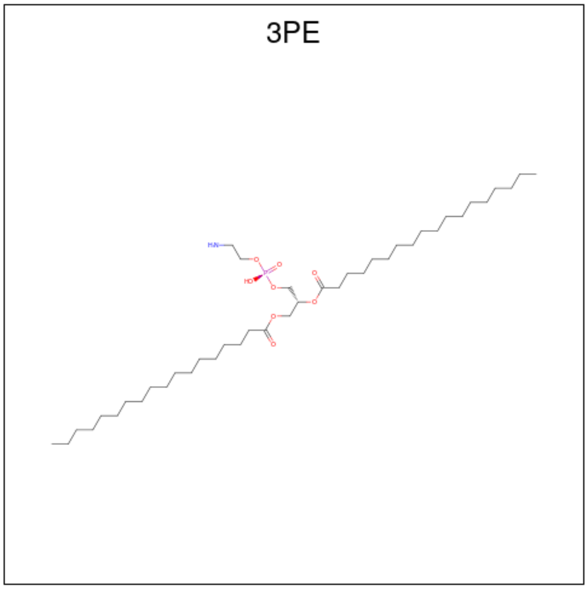
Mol	Chain	Residues	Atoms	AltConf
73	A9	1	Total C H N O P 142 44 88 1 8 1	0
73	A9	1	Total C H N O P 142 44 88 1 8 1	0
73	AA	1	Total C H N O P 142 44 88 1 8 1	0
73	AA	1	Total C H N O P 142 44 88 1 8 1	0
73	AA	1	Total C H N O P 142 44 88 1 8 1	0
73	AA	1	Total C H N O P 142 44 88 1 8 1	0
73	AA	1	Total C H N O P 142 44 88 1 8 1	0
73	AH	1	Total C H N O P 142 44 88 1 8 1	0
73	AJ	1	Total C H N O P 142 44 88 1 8 1	0
73	AL	1	Total C H N O P 142 44 88 1 8 1	0
73	AM	1	Total C H N O P 142 44 88 1 8 1	0
73	AQ	1	Total C H N O P 142 44 88 1 8 1	0
73	AU	1	Total C H N O P 142 44 88 1 8 1	0
73	AU	1	Total C H N O P 142 44 88 1 8 1	0
73	B1	1	Total C H N O P 142 44 88 1 8 1	0
73	B1	1	Total C H N O P 142 44 88 1 8 1	0
73	BQ	1	Total C H N O P 142 44 88 1 8 1	0
73	BS	1	Total C H N O P 142 44 88 1 8 1	0
73	BS	1	Total C H N O P 142 44 88 1 8 1	0
73	BT	1	Total C H N O P 142 44 88 1 8 1	0
73	BY	1	Total C H N O P 142 44 88 1 8 1	0

- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



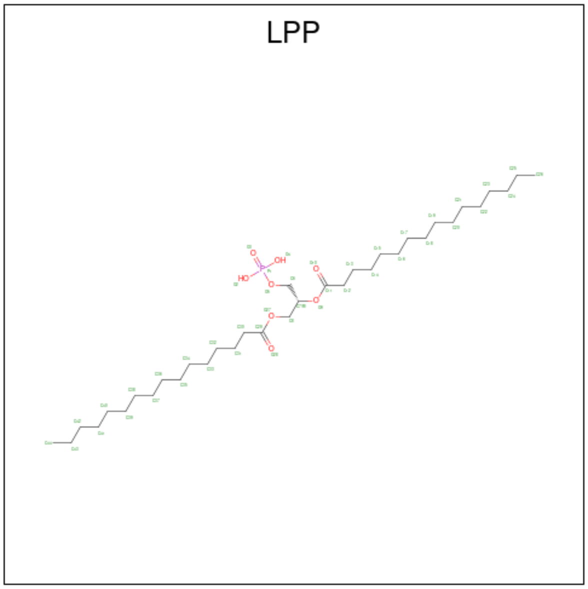
Mol	Chain	Residues	Atoms						AltConf
74	A1	1	Total 74	C 21	H 26	N 7	O 17	P 3	0

- Molecule 75 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



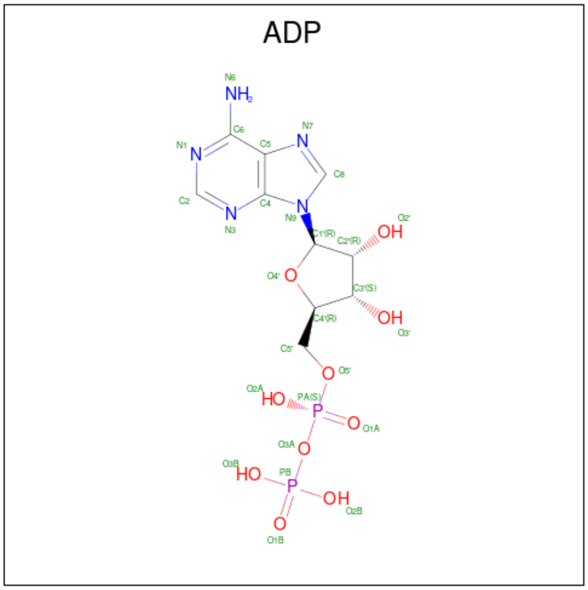
Mol	Chain	Residues	Atoms						AltConf
75	A2	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
75	A9	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
75	A9	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
75	AJ	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
75	BA	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
75	BP	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

- Molecule 76 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



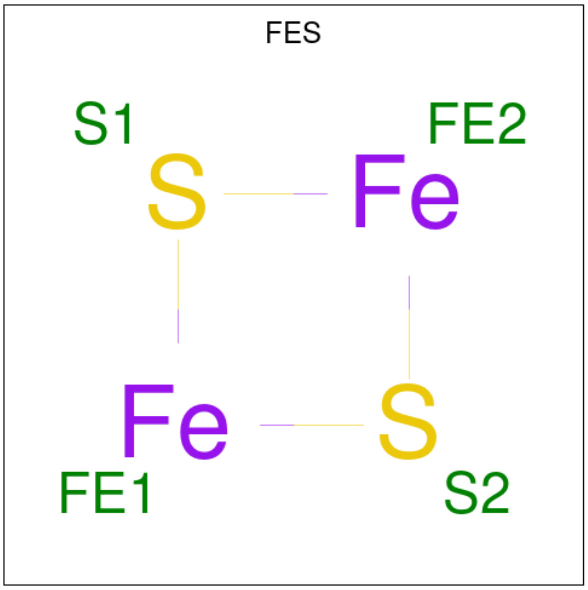
Mol	Chain	Residues	Atoms					AltConf
76	A6	1	Total 111	C 35	H 67	O 8	P 1	0
76	AA	1	Total 111	C 35	H 67	O 8	P 1	0
76	AL	1	Total 111	C 35	H 67	O 8	P 1	0
76	BN	1	Total 111	C 35	H 67	O 8	P 1	0

- Molecule 77 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
77	A8	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
77	AQ	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 78 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
78	AB	1	Total 4	Fe 2	S 2	0

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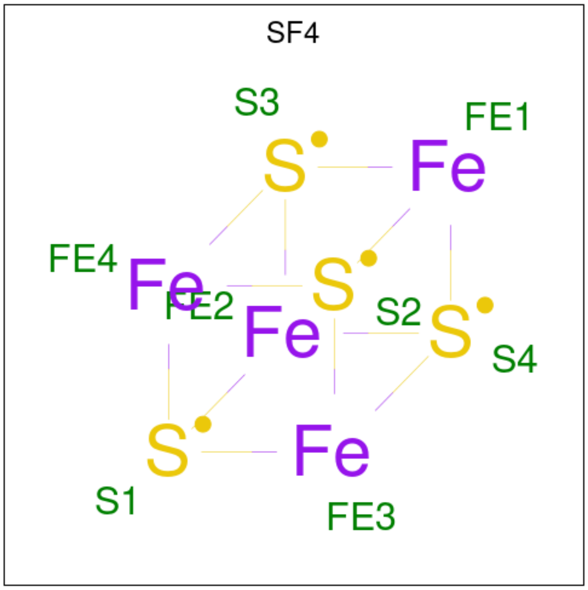
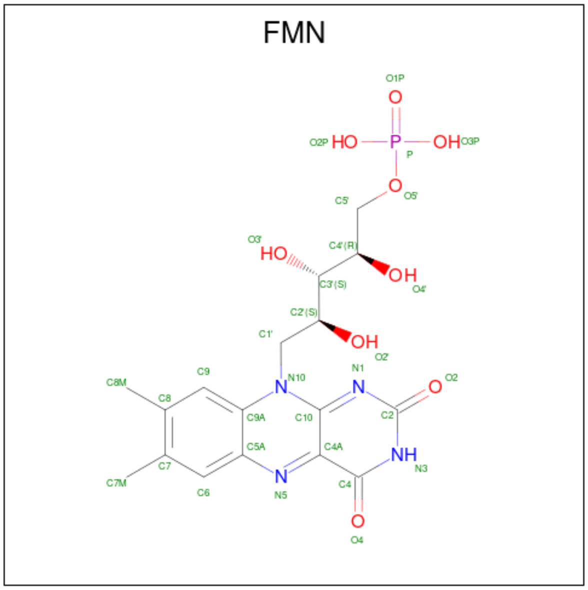
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
78	AI	1	4	2	2	0
			Total	Fe	S	
78	BI	1	4	2	2	0

- Molecule 79 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



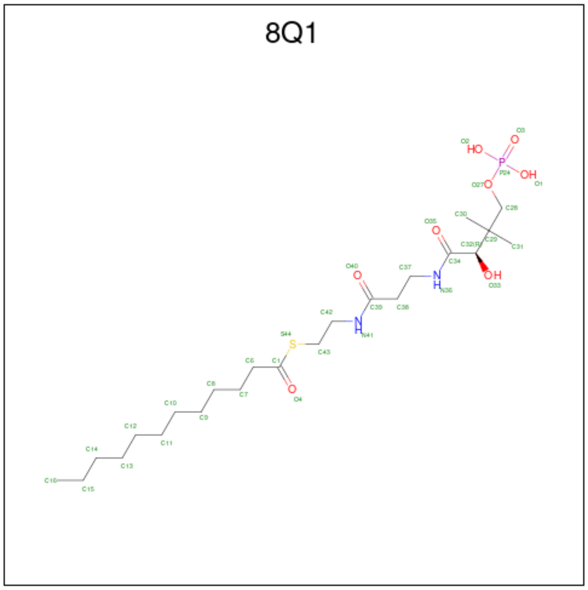
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
79	AB	1	8	4	4	0
			Total	Fe	S	
79	AB	1	8	4	4	0
			Total	Fe	S	
79	AD	1	8	4	4	0
			Total	Fe	S	
79	AL	1	8	4	4	0
			Total	Fe	S	
79	AL	1	8	4	4	0
			Total	Fe	S	
79	AT	1	8	4	4	0

- Molecule 80 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
80	AD	1	49	17	18	4	9	1	0

- Molecule 81 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
81	AS	1	77	23	43	2	7	1	1	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

Interest" by depositor).

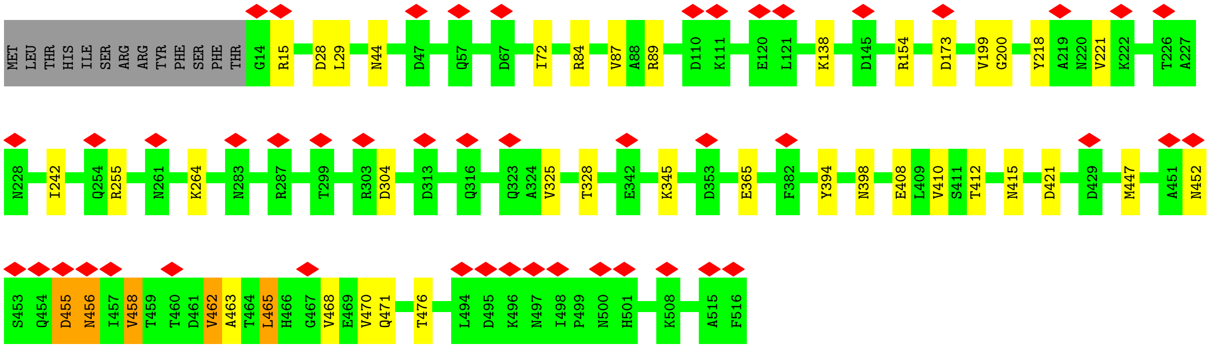
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	BR	1	1	1	0

3 Residue-property plots ⓘ

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.

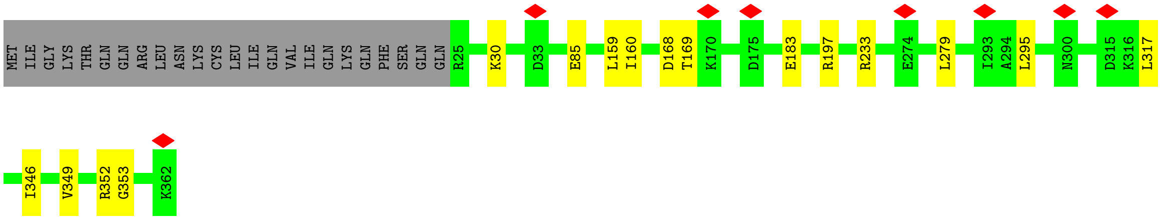
- Molecule 1: Lipid-A-disaccharide synthase

Chain A0:



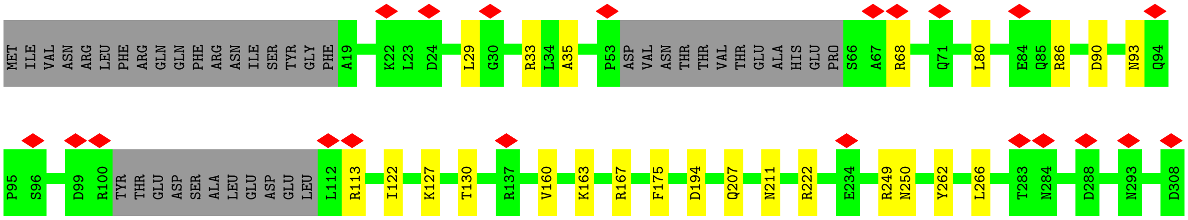
- Molecule 2: NAD-dependent epimerase/dehydratase family protein

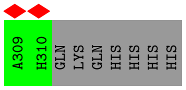
Chain A1:



- Molecule 3: DnaJ domain protein

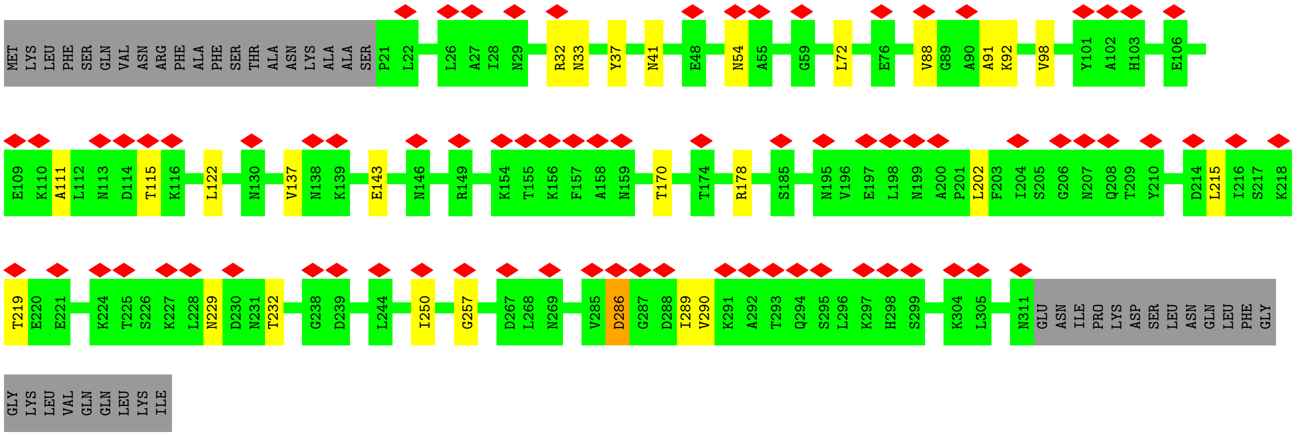
Chain A2:





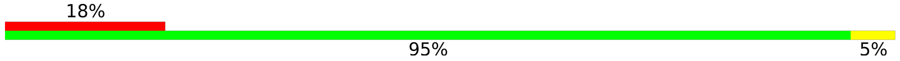
- Molecule 4: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

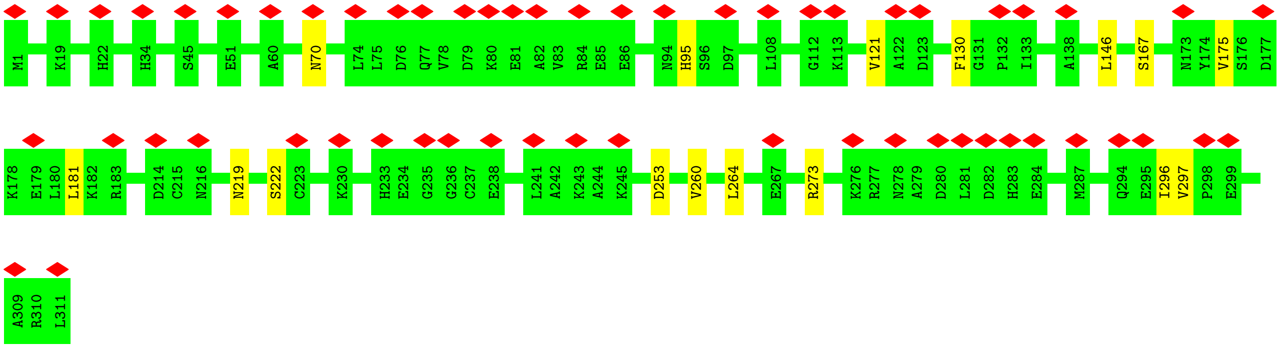
Chain A3:



- Molecule 5: RNase III domain-containing protein

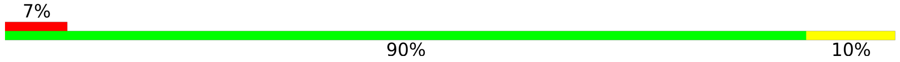
Chain A4:

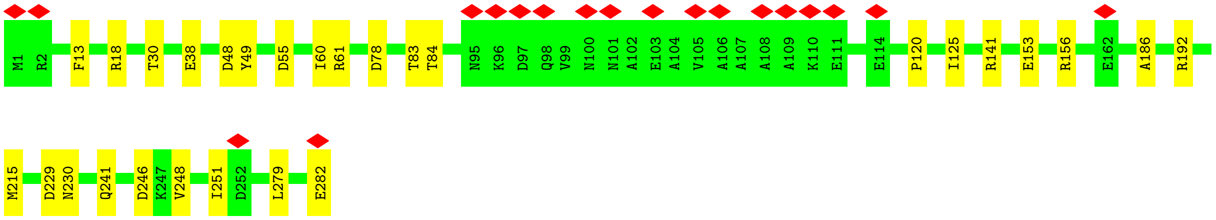




- Molecule 6: 37S ribosomal protein S25, mitochondrial

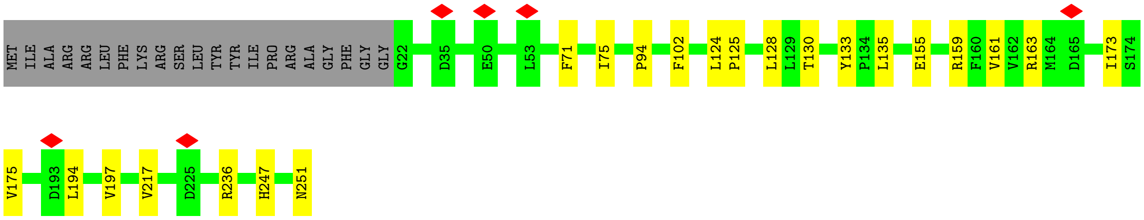
Chain A5:





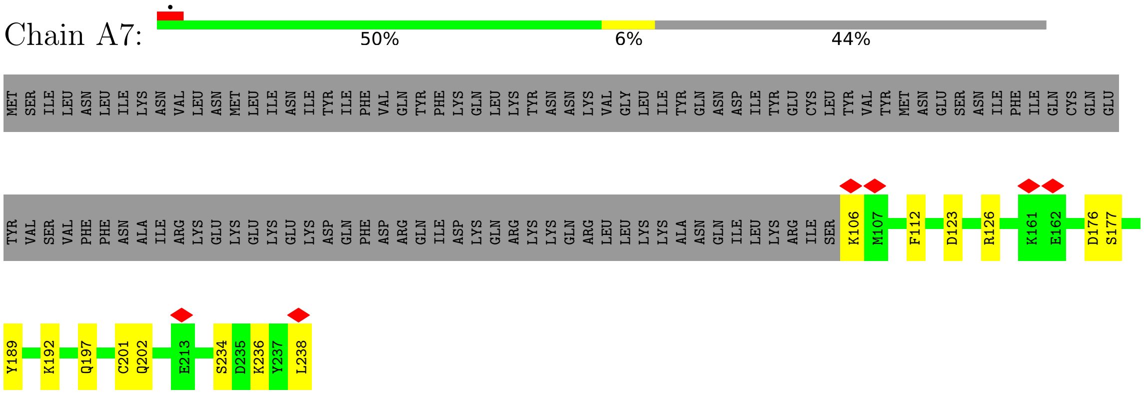
- Molecule 7: Transmembrane protein, putative

Chain A6:



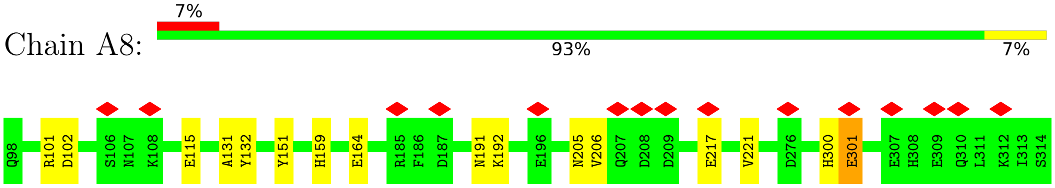
- Molecule 8: CX9C domain-containing protein

Chain A7:



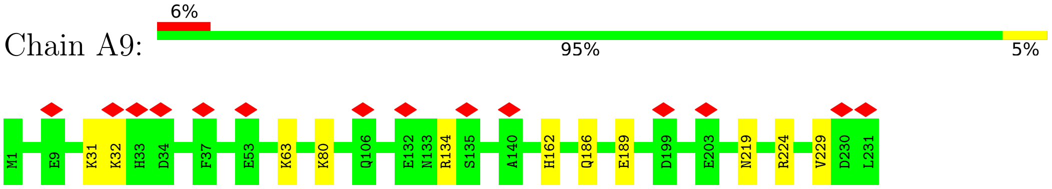
- Molecule 9: NDUTT15

Chain A8:



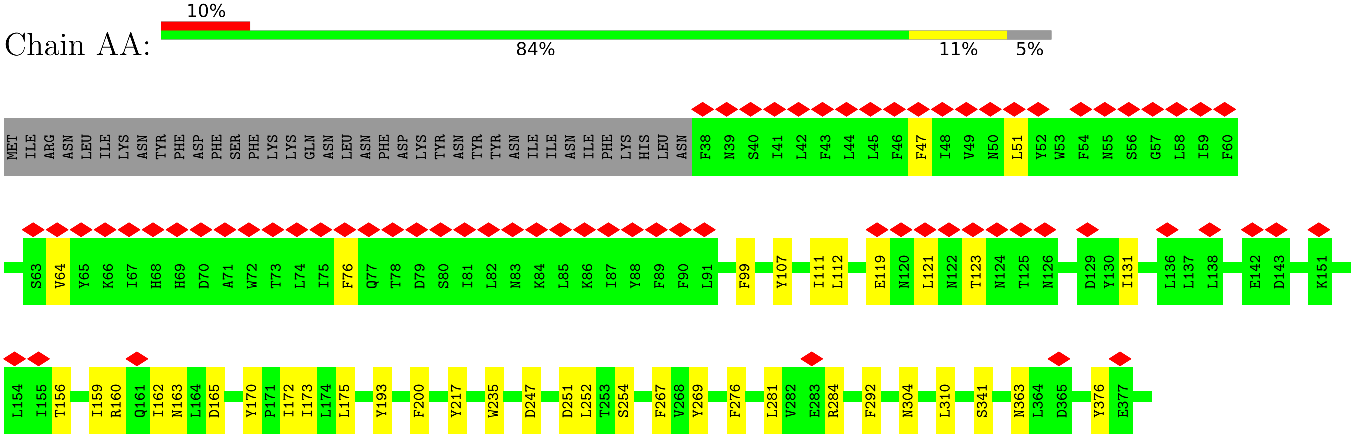
- Molecule 10: Transmembrane protein, putative

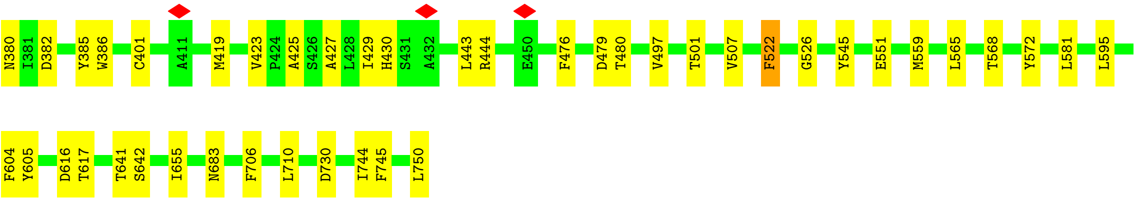
Chain A9:



- Molecule 11: NADH dehydrogenase subunit 5

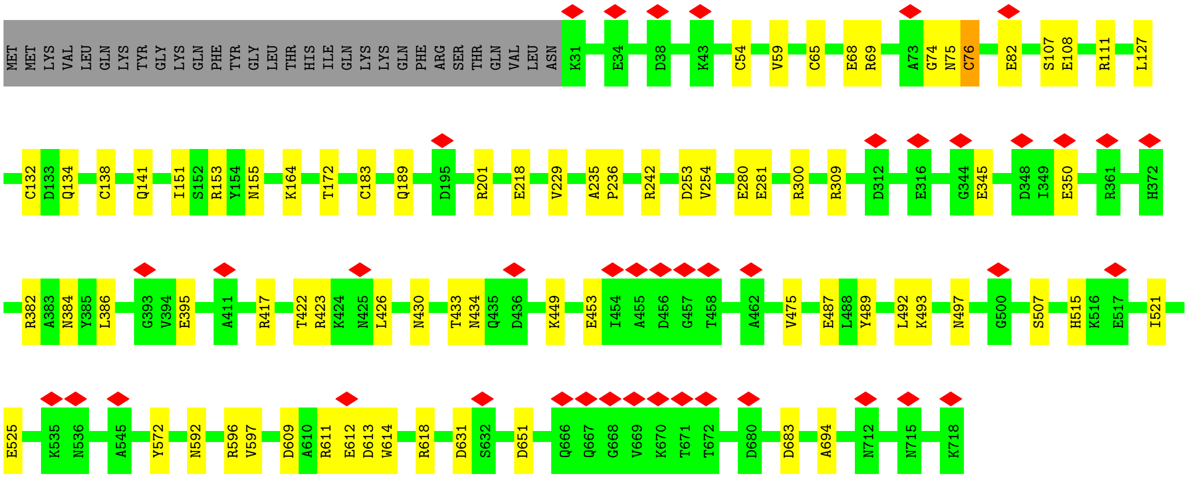
Chain AA:





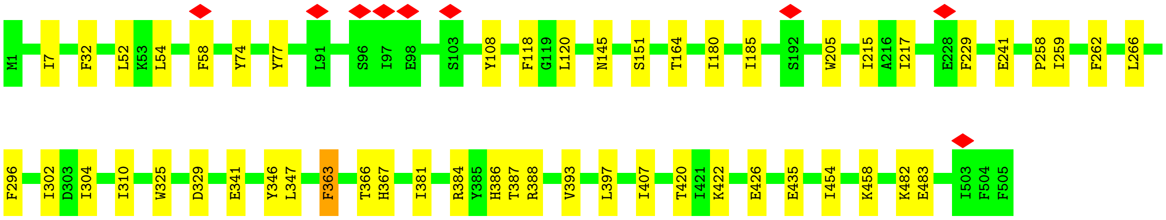
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain AB:



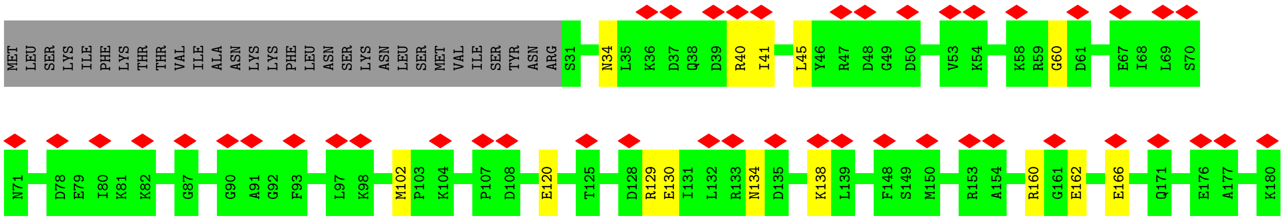
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

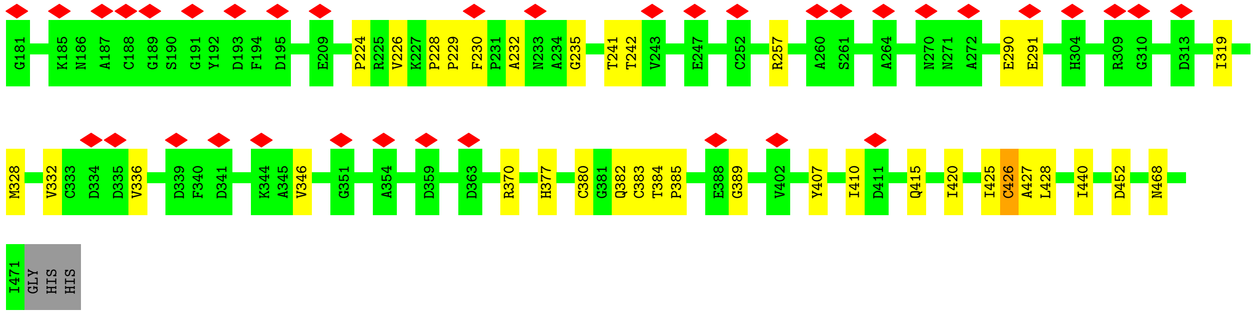
Chain AC:



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

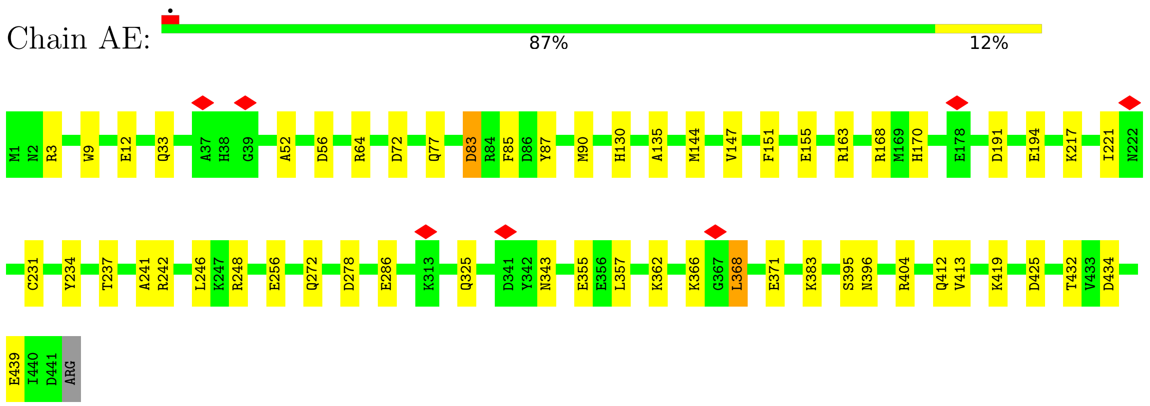
Chain AD:





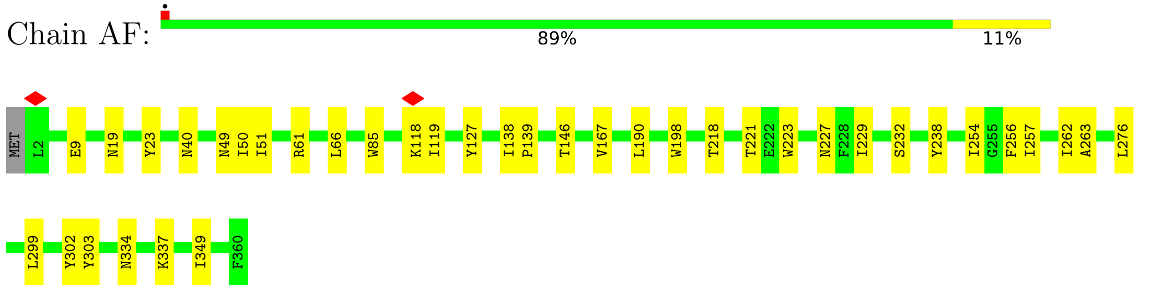
- Molecule 15: NADH dehydrogenase subunit 7

Chain AE:



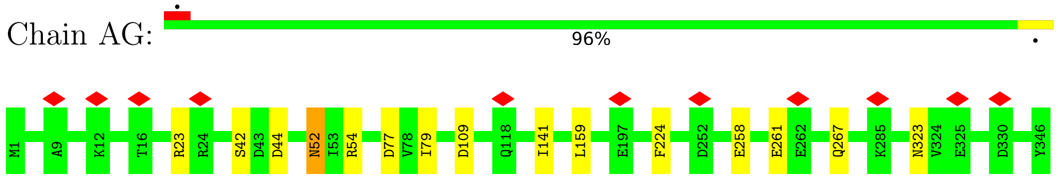
- Molecule 16: Ymf65

Chain AF:



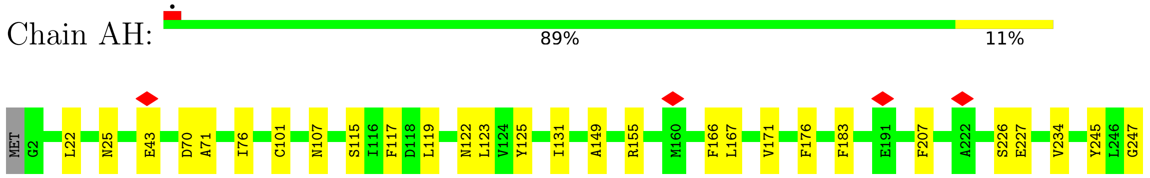
- Molecule 17: Transcription factor apfi protein, putative

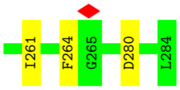
Chain AG:



- Molecule 18: NADH-ubiquinone oxidoreductase chain 1

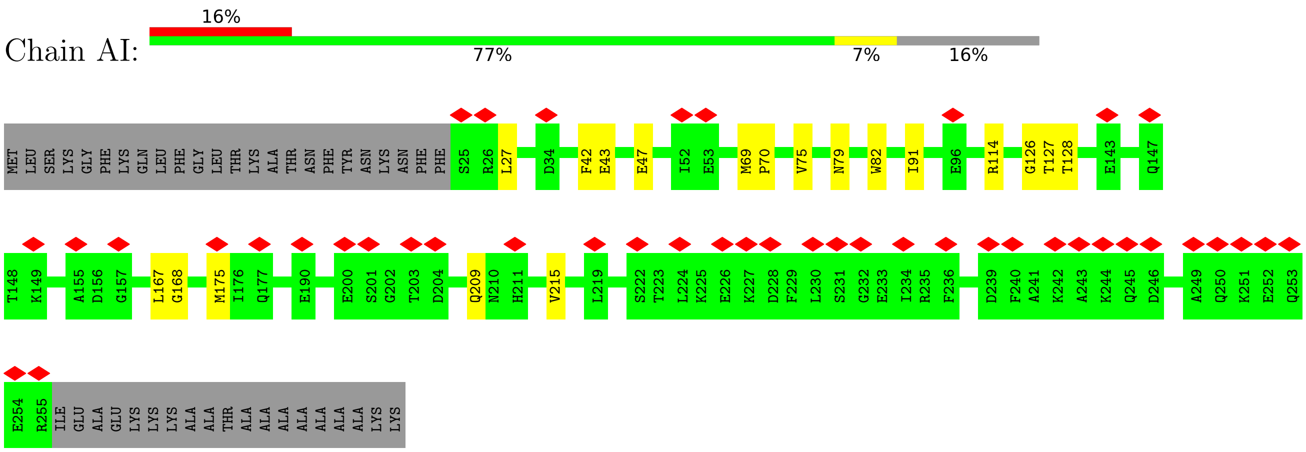
Chain AH:





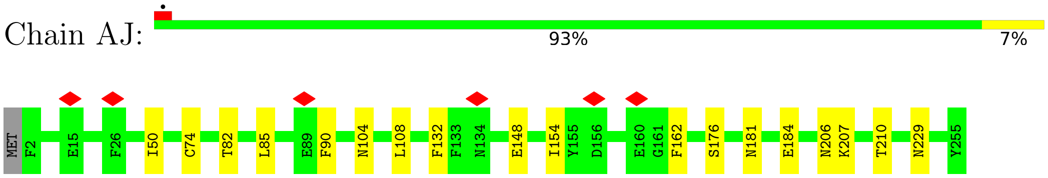
- Molecule 19: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain AI:



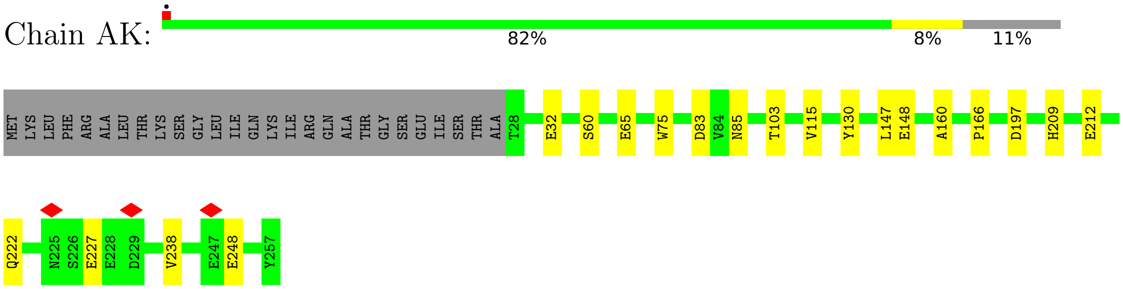
- Molecule 20: Ymf62

Chain AJ:



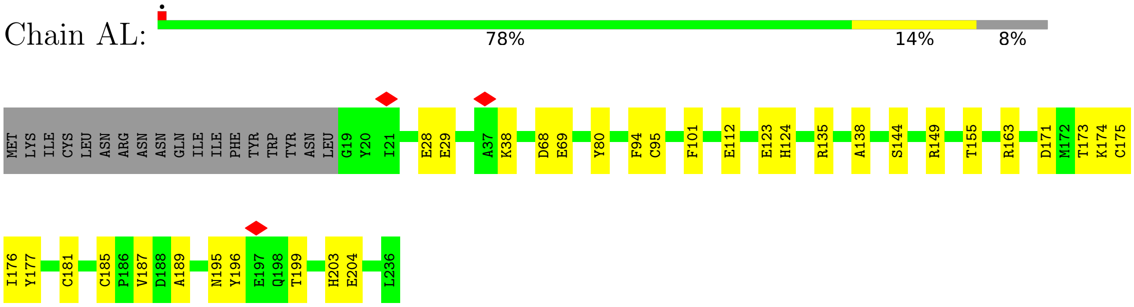
- Molecule 21: Gamma-carbonic anhydrase

Chain AK:



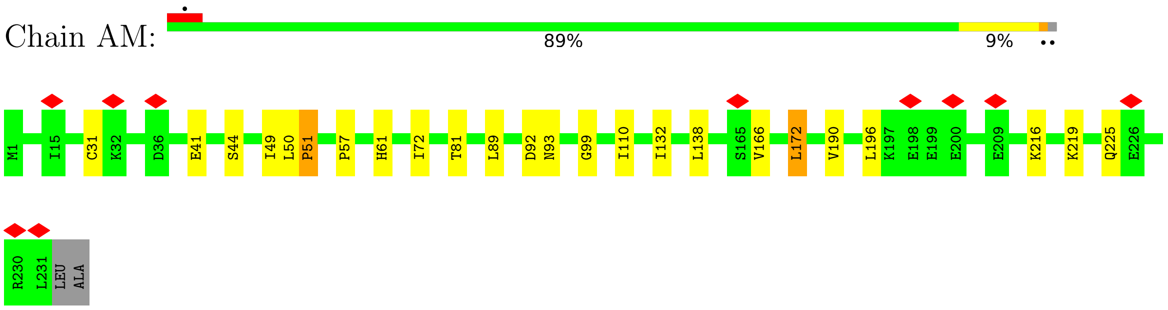
- Molecule 22: NADH-ubiquinone oxidoreductase 1, chain, putative

Chain AL:



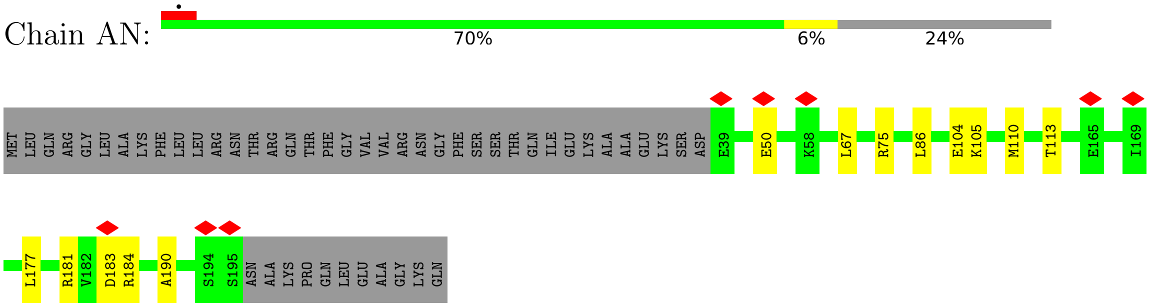
- Molecule 23: Gamma-carbonic anhydrase

Chain AM:



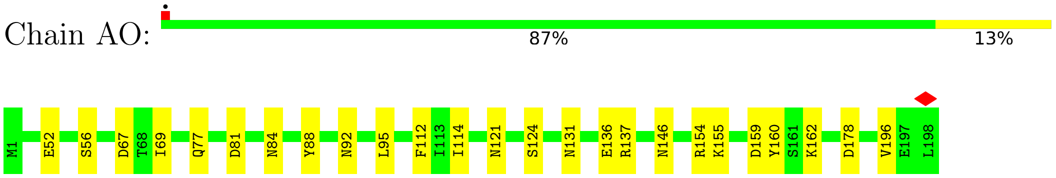
- Molecule 24: ETC complex I subunit motif protein

Chain AN:



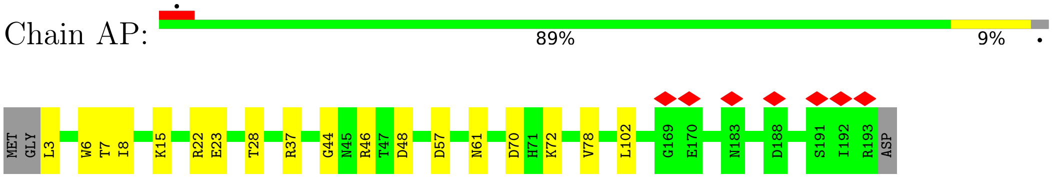
- Molecule 25: NADH dehydrogenase subunit 9

Chain AO:



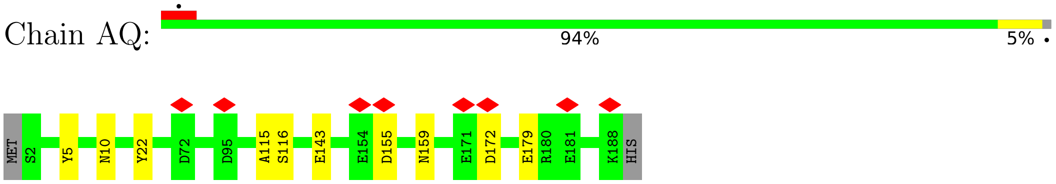
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AP:



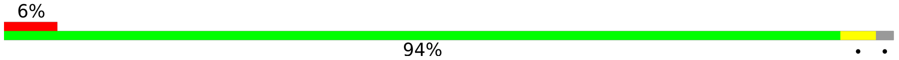
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

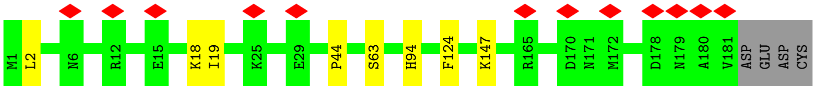
Chain AQ:



- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

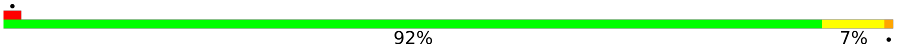
Chain AR:

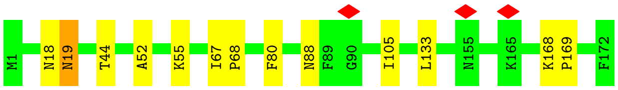




- Molecule 29: NADH dehydrogenase, putative

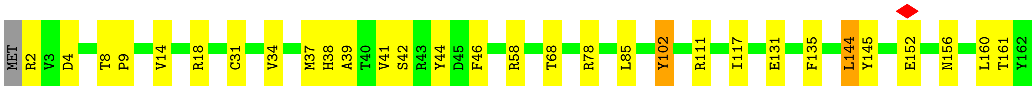
Chain AS:





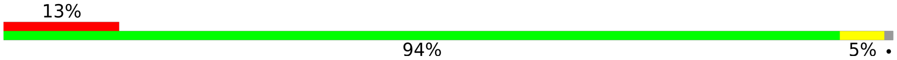
- Molecule 30: NADH dehydrogenase subunit 10

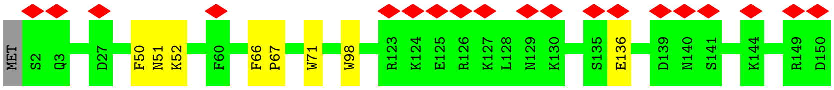
Chain AT:



- Molecule 31: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

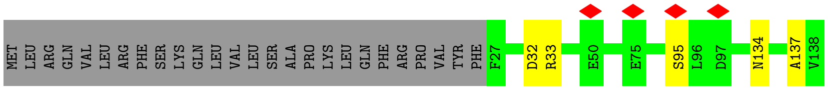
Chain AU:





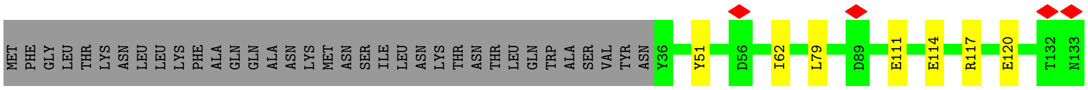
- Molecule 32: Acyl carrier protein

Chain AV:



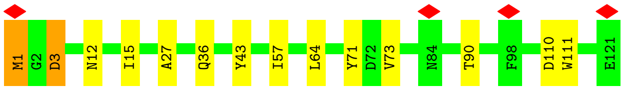
- Molecule 33: Acyl carrier protein

Chain AW:

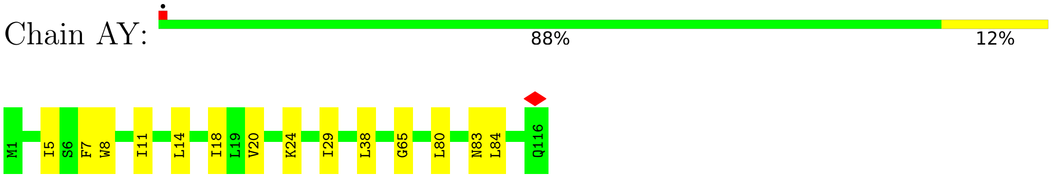


- Molecule 34: NADH-ubiquinone oxidoreductase chain 3

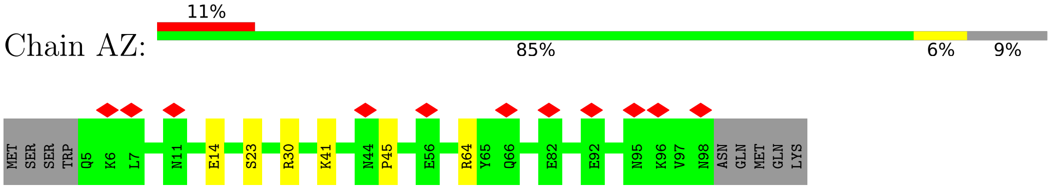
Chain AX:



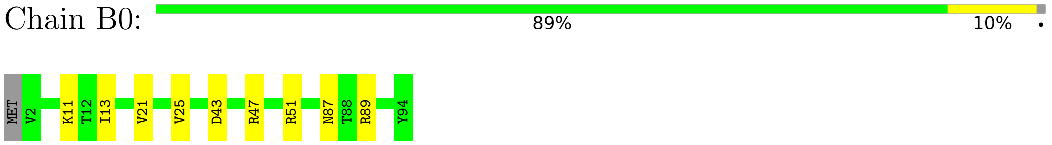
- Molecule 35: Ymf58



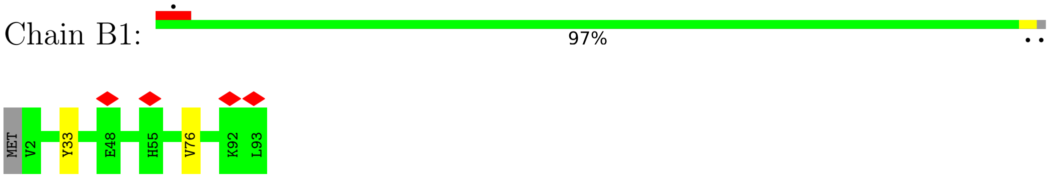
- Molecule 36: Ribosomal protein L51/S25/CI-B8 domain protein



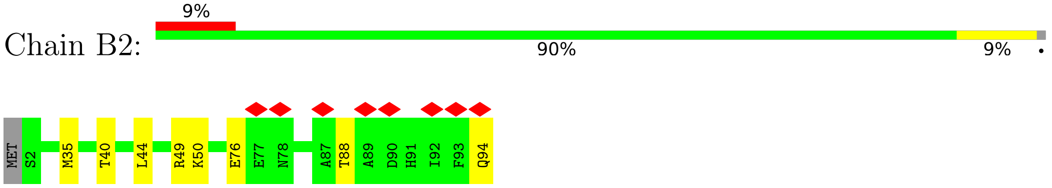
- Molecule 37: Transmembrane protein, putative



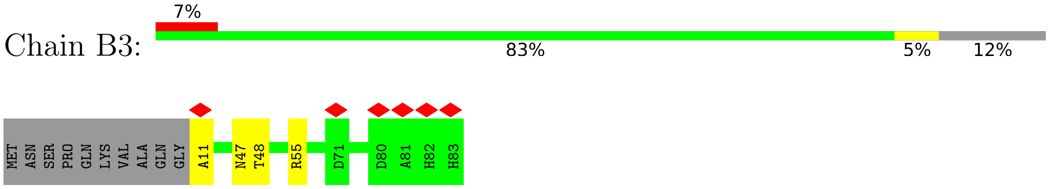
- Molecule 38: ATP synthase subunit e, mitochondrial



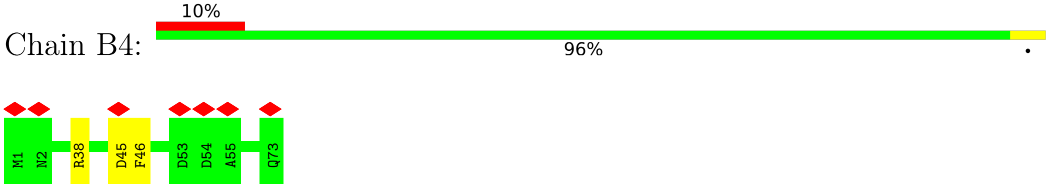
- Molecule 39: GRAM domain protein



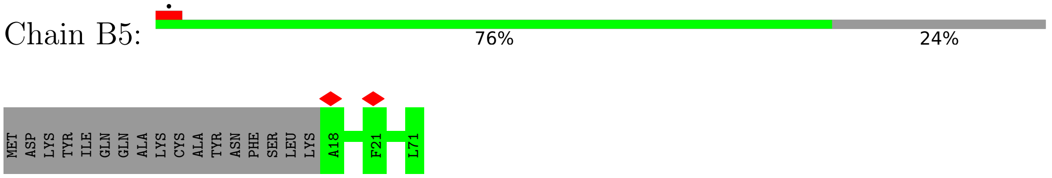
- Molecule 40: Transmembrane protein, putative



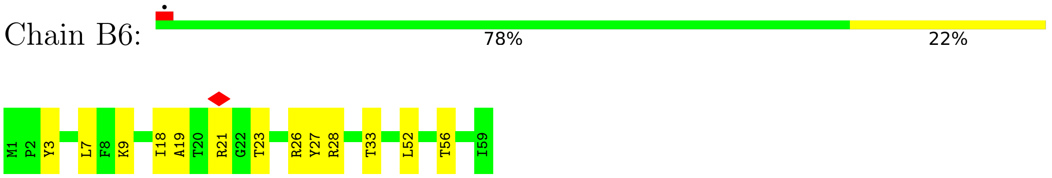
- Molecule 41: Transmembrane protein, putative



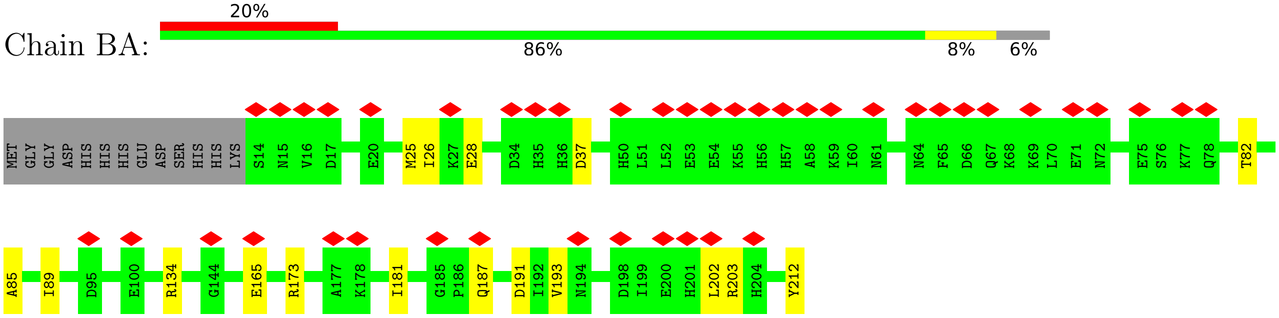
- Molecule 42: Transmembrane protein, putative



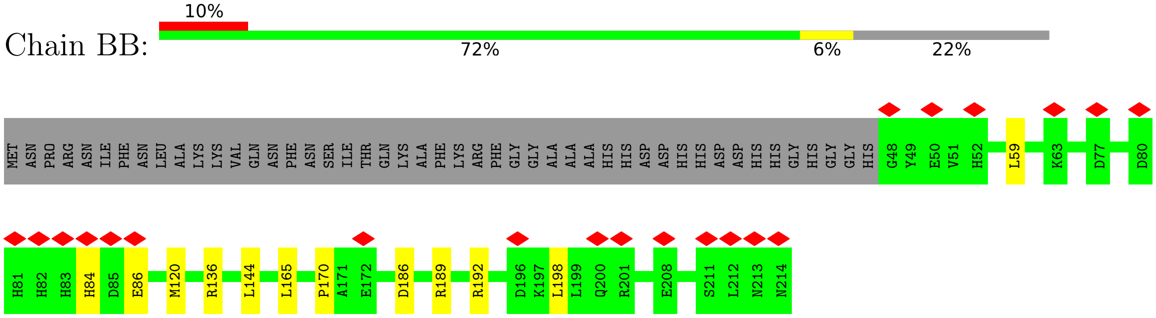
- Molecule 43: ND1b



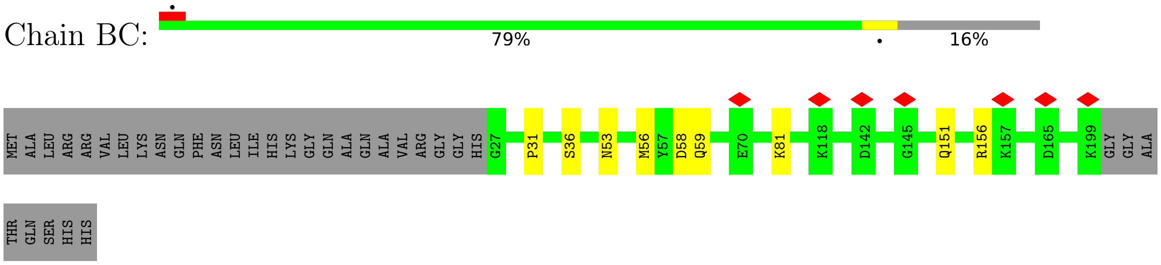
- Molecule 44: Transmembrane protein



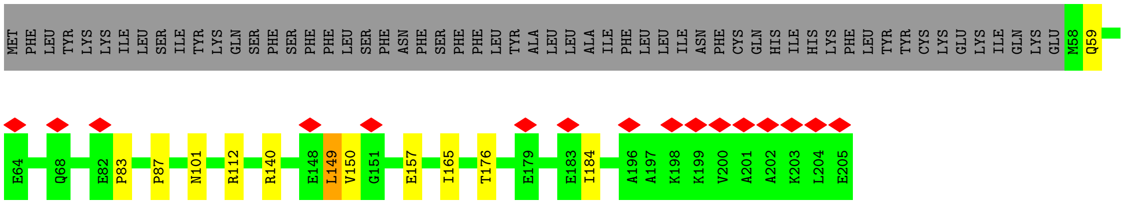
- Molecule 45: Transmembrane protein, putative



- Molecule 46: NDUB8

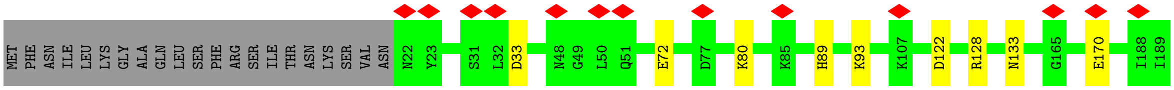


- Molecule 47: Transmembrane protein, putative



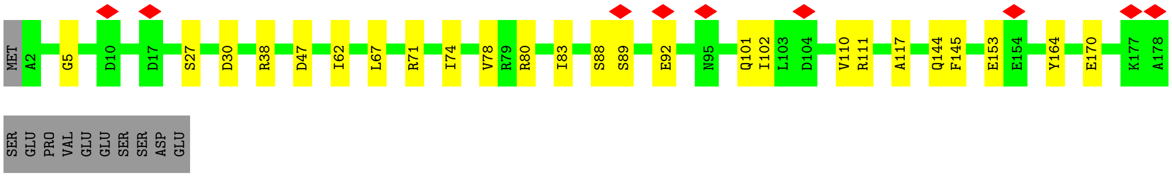
- Molecule 48: NDUPH2

Chain BE:



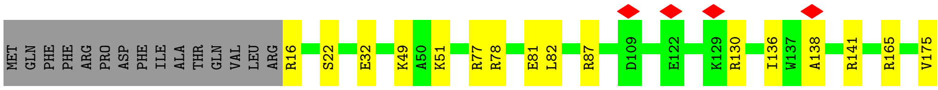
- Molecule 49: NDUB10

Chain BF:



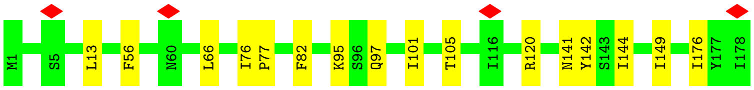
- Molecule 50: NDUA13

Chain BG:



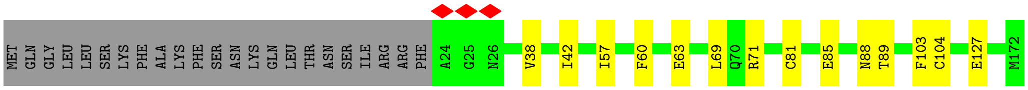
- Molecule 51: NADH dehydrogenase subunit 2

Chain BH:



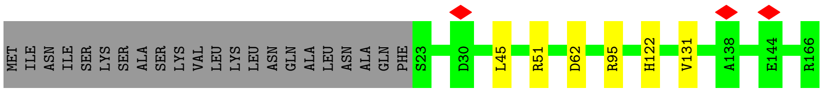
- Molecule 52: 2 iron, 2 sulfur cluster-binding protein

Chain BI:



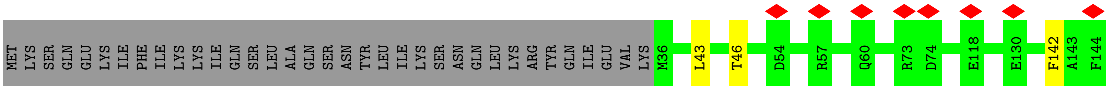
- Molecule 53: Thioredoxin

Chain BJ:



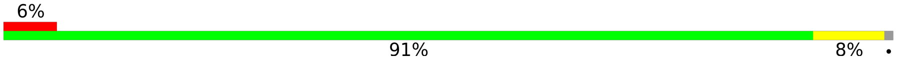
- Molecule 54: COX assembly mitochondrial protein

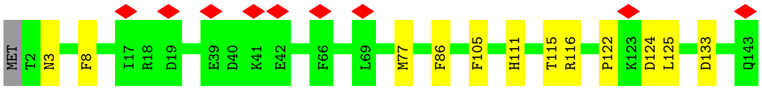
Chain BK:



- Molecule 55: Transmembrane protein, putative

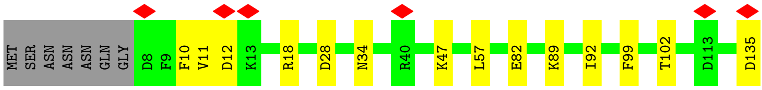
Chain BL:





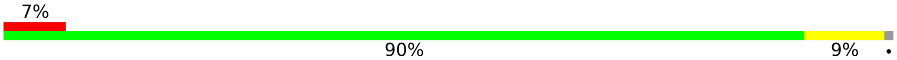
- Molecule 56: Transmembrane protein, putative

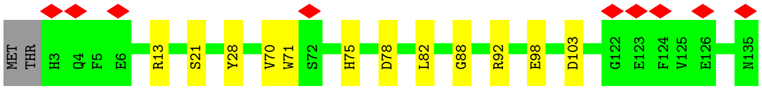
Chain BM:



- Molecule 57: PH domain-containing protein

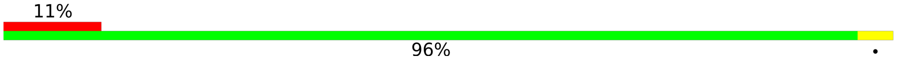
Chain BN:

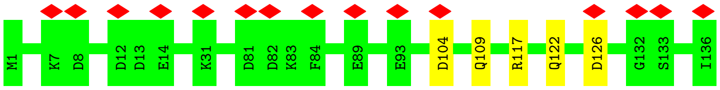




- Molecule 58: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

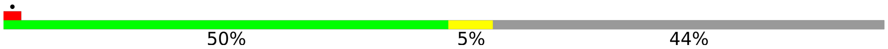
Chain BO:

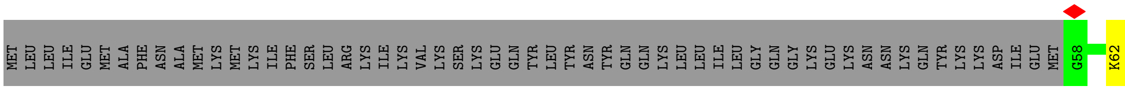


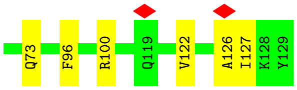


- Molecule 59: NDUB6

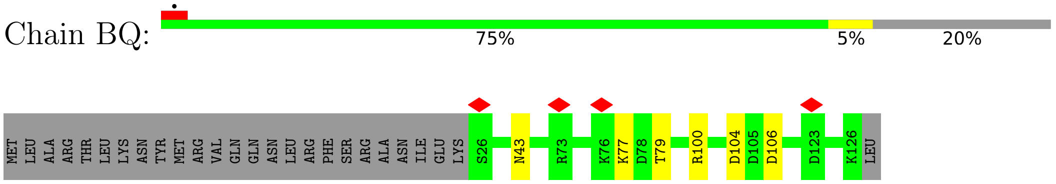
Chain BP:



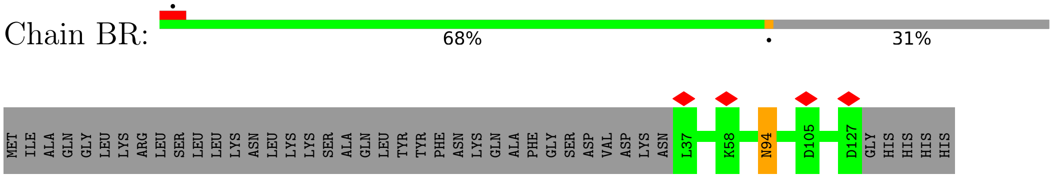




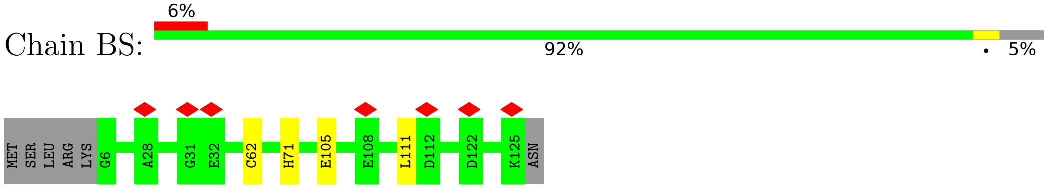
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



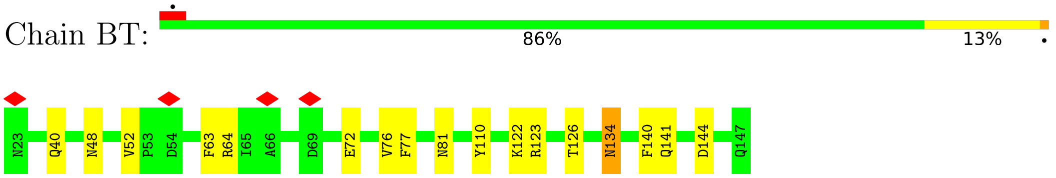
- Molecule 61: Zinc-finger protein



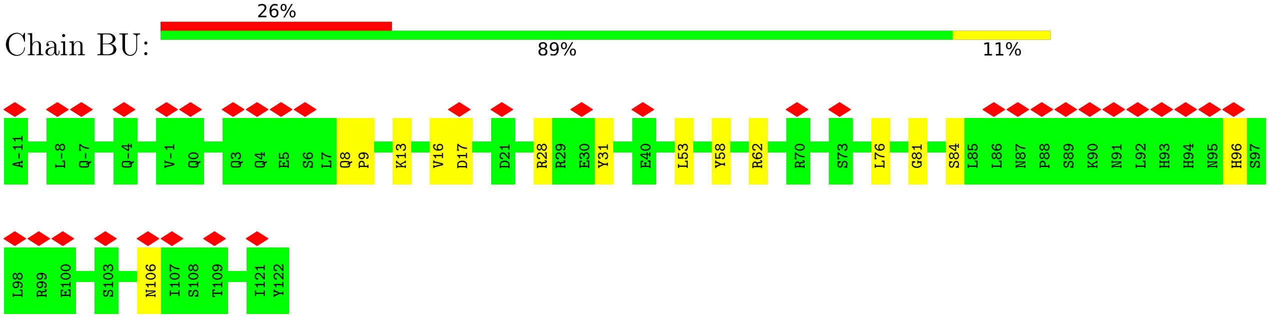
- Molecule 62: NDUB4



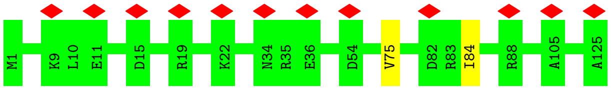
- Molecule 63: NDUB15



- Molecule 64: NDUTT16

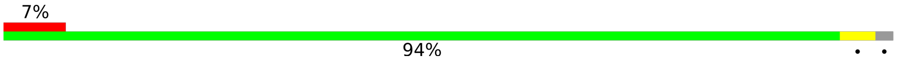


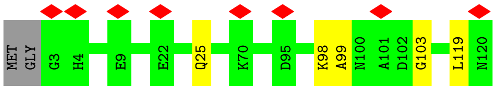
- Molecule 65: NDUTT17



- Molecule 66: CHCH domain-containing protein

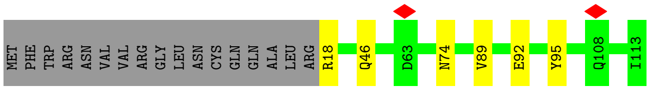
Chain BW:





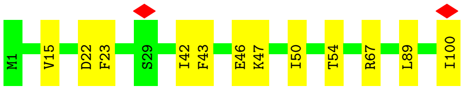
- Molecule 67: Transmembrane protein, putative

Chain BX:



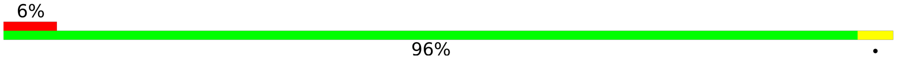
- Molecule 68: Ymf57

Chain BY:



- Molecule 69: Complex I-MNLL

Chain BZ:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	5.836	Depositor
Minimum map value	-2.721	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 8Q1, SF4, 3PE, PC1, LPP, UDP, NDP, MG, ZN, FMN, ADP, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A0	0.26	0/4166	0.44	0/5634
2	A1	0.26	0/2789	0.47	0/3777
3	A2	0.25	0/2248	0.48	0/3027
4	A3	0.25	0/2308	0.45	0/3134
5	A4	0.25	0/2542	0.43	0/3441
6	A5	0.24	0/2408	0.46	0/3269
7	A6	0.26	0/1963	0.47	0/2658
8	A7	0.26	0/1108	0.41	0/1488
9	A8	0.24	0/1833	0.44	0/2479
10	A9	0.26	0/1935	0.44	0/2616
11	AA	0.27	0/6132	0.40	0/8343
12	AB	0.26	0/5511	0.50	0/7465
13	AC	0.27	0/4303	0.40	0/5844
14	AD	0.26	0/3474	0.49	0/4699
15	AE	0.27	0/3669	0.48	0/4955
16	AF	0.27	0/3168	0.38	0/4307
17	AG	0.25	0/2865	0.47	0/3877
18	AH	0.27	0/2377	0.41	0/3234
19	AI	0.26	0/1899	0.46	0/2563
20	AJ	0.27	0/2224	0.39	0/3025
21	AK	0.26	0/1816	0.47	0/2475
22	AL	0.29	0/1867	0.55	0/2538
23	AM	0.26	0/1801	0.50	0/2449
24	AN	0.25	0/1351	0.44	0/1817
25	AO	0.25	0/1720	0.45	0/2322
26	AP	0.25	0/1654	0.49	0/2240
27	AQ	0.27	0/1636	0.43	0/2214
28	AR	0.26	0/1535	0.48	0/2077
29	AS	0.25	0/1458	0.47	0/1965
30	AT	0.28	0/1310	0.54	0/1779
31	AU	0.26	0/1261	0.47	0/1698
32	AV	0.25	0/941	0.43	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	AW	0.25	0/819	0.47	0/1110
34	AX	0.26	0/1061	0.39	0/1441
35	AY	0.25	0/982	0.40	0/1335
36	AZ	0.25	0/790	0.47	0/1066
37	B0	0.27	0/833	0.50	0/1132
38	B1	0.25	0/812	0.44	0/1093
39	B2	0.26	0/776	0.44	0/1048
40	B3	0.25	0/654	0.45	0/884
41	B4	0.26	0/642	0.47	0/865
42	B5	0.27	0/466	0.41	0/630
43	B6	0.28	0/535	0.43	0/727
44	BA	0.25	0/1696	0.41	0/2292
45	BB	0.25	0/1376	0.42	0/1862
46	BC	0.26	0/1479	0.47	0/1996
47	BD	0.25	0/1216	0.44	0/1643
48	BE	0.26	0/1462	0.43	0/1981
49	BF	0.25	0/1503	0.49	0/2018
50	BG	0.25	0/1379	0.49	0/1841
51	BH	0.27	0/1519	0.39	0/2058
52	BI	0.25	0/1203	0.48	0/1630
53	BJ	0.26	0/1234	0.44	0/1662
54	BK	0.26	0/923	0.43	0/1239
55	BL	0.26	0/1223	0.45	0/1648
56	BM	0.26	0/1110	0.46	0/1502
57	BN	0.25	0/1132	0.44	0/1534
58	BO	0.26	0/1120	0.46	0/1500
59	BP	0.30	0/631	0.42	0/860
60	BQ	0.26	0/868	0.43	0/1170
61	BR	0.25	0/747	0.45	0/1011
62	BS	0.26	0/991	0.42	0/1333
63	BT	0.28	0/1106	0.41	0/1504
64	BU	0.24	0/1102	0.45	0/1486
65	BV	0.25	0/1003	0.46	0/1353
66	BW	0.26	0/983	0.40	0/1327
67	BX	0.27	0/821	0.46	0/1111
68	BY	0.28	0/916	0.41	0/1224
69	BZ	0.26	0/873	0.43	0/1175
All	All	0.26	0/115258	0.45	0/155972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	4071	4019	4018	28	0
2	A1	2718	2650	2649	9	0
3	A2	2199	2163	2160	13	0
4	A3	2263	2260	2260	15	0
5	A4	2494	2491	2491	10	0
6	A5	2347	2249	2249	22	0
7	A6	1908	1862	1861	14	0
8	A7	1084	1040	1039	12	0
9	A8	1794	1803	1800	11	0
10	A9	1879	1818	1818	6	0
11	AA	5941	5978	5977	47	0
12	AB	5403	5359	5358	49	0
13	AC	4170	4223	4223	33	0
14	AD	3399	3345	3345	33	0
15	AE	3587	3539	3539	37	0
16	AF	3068	3148	3147	31	0
17	AG	2804	2727	2727	13	0
18	AH	2306	2350	2349	21	0
19	AI	1862	1848	1847	14	0
20	AJ	2160	2156	2155	13	0
21	AK	1779	1740	1739	15	0
22	AL	1812	1689	1688	27	0
23	AM	1770	1788	1788	15	0
24	AN	1322	1329	1328	10	0
25	AO	1683	1680	1680	17	0
26	AP	1599	1505	1504	13	0
27	AQ	1588	1496	1495	6	0
28	AR	1492	1445	1445	5	0
29	AS	1420	1382	1382	6	0
30	AT	1277	1272	1271	19	0
31	AU	1227	1209	1208	5	0
32	AV	925	904	903	4	0
33	AW	803	781	780	5	0
34	AX	1027	1020	1020	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	AY	957	987	987	13	0
36	AZ	777	775	774	3	0
37	B0	805	802	801	6	0
38	B1	790	746	745	1	0
39	B2	757	728	727	7	0
40	B3	633	618	617	4	0
41	B4	624	623	623	3	0
42	B5	453	464	463	0	0
43	B6	515	528	528	11	0
44	BA	1651	1638	1637	12	0
45	BB	1346	1280	1279	10	0
46	BC	1442	1406	1405	7	0
47	BD	1191	1223	1222	12	0
48	BE	1422	1385	1384	5	0
49	BF	1475	1486	1485	20	0
50	BG	1349	1376	1375	13	0
51	BH	1482	1554	1554	15	0
52	BI	1179	1139	1134	10	0
53	BJ	1205	1156	1155	3	0
54	BK	903	854	853	2	0
55	BL	1187	1138	1137	9	0
56	BM	1072	1002	1001	10	0
57	BN	1103	1126	1125	10	0
58	BO	1098	1058	1058	3	0
59	BP	604	590	589	7	0
60	BQ	845	829	828	7	0
61	BR	730	719	718	1	0
62	BS	966	941	940	5	0
63	BT	1063	953	950	9	0
64	BU	1082	1094	1094	9	0
65	BV	987	1014	1014	1	0
66	BW	955	893	892	4	0
67	BX	797	755	754	6	0
68	BY	889	917	917	10	0
69	BZ	850	840	840	4	0
70	A0	200	312	312	1	0
70	A1	100	156	156	0	0
70	AA	200	312	312	3	0
70	AC	200	312	312	0	0
70	AF	200	312	312	0	0
70	AM	100	156	156	0	0
70	AP	100	156	156	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	B0	200	312	312	1	0
70	B1	100	156	156	0	0
70	BC	200	312	312	1	0
70	BE	100	156	156	1	0
70	BG	100	156	156	0	0
70	BL	100	156	156	1	0
70	BT	100	156	156	0	0
70	BV	100	156	156	0	0
70	BY	100	156	156	0	0
71	A0	25	11	11	2	0
72	A0	1	0	0	0	0
72	A8	1	0	0	0	0
73	A0	54	88	88	0	0
73	A1	108	176	176	0	0
73	A2	54	88	88	0	0
73	A6	108	176	176	2	0
73	A9	108	176	176	0	0
73	AA	270	440	440	0	0
73	AH	54	88	88	0	0
73	AJ	54	88	88	0	0
73	AL	54	88	88	2	0
73	AM	54	88	88	0	0
73	AQ	54	88	88	0	0
73	AU	108	176	176	0	0
73	B1	108	176	176	0	0
73	BQ	54	88	88	0	0
73	BS	108	176	176	1	0
73	BT	54	88	88	1	0
73	BY	54	88	88	0	0
74	A1	48	26	25	0	0
75	A2	51	82	82	0	0
75	A9	102	164	164	1	0
75	AJ	51	82	82	0	0
75	BA	51	82	82	1	0
75	BP	51	82	82	0	0
76	A6	44	67	67	0	0
76	AA	44	67	67	1	0
76	AL	44	67	67	2	0
76	BN	44	67	67	0	0
77	A8	27	12	12	0	0
77	AQ	27	12	12	0	0
78	AB	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	AI	4	0	0	2	0
78	BI	4	0	0	1	0
79	AB	16	0	0	3	0
79	AD	8	0	0	1	0
79	AL	16	0	0	6	0
79	AT	8	0	0	0	0
80	AD	31	18	19	0	0
81	AS	34	43	0	2	0
82	BR	1	0	0	0	0
All	All	116760	117595	117495	670	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 (670) 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)
26:AP:3:LEU:N	70:AP:301:CDL:OA3	1.70	1.23
17:AG:54:ARG:O	23:AM:225:GLN:NE2	2.11	0.82
24:AN:105:LYS:NZ	25:AO:52:GLU:OE2	2.14	0.80
14:AD:40:ARG:NH1	14:AD:290:GLU:O	2.16	0.79
70:AP:301:CDL:OA4	70:AP:301:CDL:O1	2.00	0.79
15:AE:155:GLU:OE1	15:AE:168:ARG:NH2	2.16	0.78
12:AB:201:ARG:NH1	14:AD:377:HIS:O	2.18	0.77
12:AB:155:ASN:O	14:AD:468:ASN:ND2	2.18	0.77
25:AO:124:SER:OG	25:AO:136:GLU:OE1	2.01	0.77
10:A9:63:LYS:NZ	68:BY:100:ILE:OXT	2.18	0.77
1:A0:200:GLY:O	1:A0:476:THR:OG1	2.02	0.77
3:A2:167:ARG:NH1	21:AK:83:ASP:O	2.19	0.76
50:BG:77:ARG:NH1	60:BQ:104:ASP:OD1	2.19	0.76
16:AF:49:ASN:ND2	16:AF:51:ILE:O	2.19	0.75
12:AB:281:GLU:OE1	12:AB:596:ARG:NH2	2.19	0.75
2:A1:233:ARG:NH2	2:A1:317:LEU:O	2.19	0.75
17:AG:23:ARG:NH2	56:BM:18:ARG:O	2.19	0.75
11:AA:730:ASP:OD1	44:BA:134:ARG:NH2	2.20	0.74
11:AA:380:ASN:OD1	46:BC:156:ARG:NH1	2.20	0.74
13:AC:341:GLU:OE1	13:AC:367:HIS:ND1	2.21	0.74
16:AF:40:ASN:ND2	22:AL:68:ASP:OD1	2.20	0.74
24:AN:75:ARG:NH1	24:AN:113:THR:O	2.21	0.74
70:AA:901:CDL:OA3	48:BE:128:ARG:NH1	2.20	0.73
44:BA:203:ARG:NH2	62:BS:105:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AI:27:LEU:O	19:AI:114:ARG:NH2	2.22	0.73
25:AO:88:TYR:O	25:AO:92:ASN:ND2	2.21	0.73
14:AD:102:MET:SD	14:AD:242:THR:OG1	2.47	0.73
18:AH:155:ARG:NH1	18:AH:227:GLU:OE1	2.21	0.73
7:A6:251:ASN:O	40:B3:11:ALA:N	2.22	0.73
44:BA:187:GLN:NE2	44:BA:191:ASP:OD1	2.22	0.73
12:AB:384:ASN:O	12:AB:489:TYR:OH	2.05	0.73
18:AH:43:GLU:OE2	43:B6:21:ARG:NH2	2.23	0.72
4:A3:54:ASN:OD1	4:A3:92:LYS:NZ	2.21	0.72
3:A2:249:ARG:NH1	3:A2:250:ASN:OD1	2.23	0.72
52:BI:63:GLU:OE2	52:BI:71:ARG:NH2	2.22	0.72
53:BJ:51:ARG:NH1	53:BJ:62:ASP:OD2	2.22	0.72
22:AL:123:GLU:OE1	22:AL:195:ASN:ND2	2.22	0.72
21:AK:60:SER:OG	21:AK:75:TRP:O	2.09	0.71
26:AP:70:ASP:OD2	37:B0:11:LYS:NZ	2.20	0.71
4:A3:33:ASN:ND2	19:AI:43:GLU:OE1	2.23	0.70
44:BA:165:GLU:OE1	44:BA:173:ARG:NH2	2.23	0.70
14:AD:370:ARG:NE	19:AI:126:GLY:O	2.26	0.69
12:AB:487:GLU:N	12:AB:487:GLU:OE1	2.26	0.69
22:AL:69:GLU:OE2	56:BM:47:LYS:NZ	2.25	0.69
48:BE:72:GLU:OE1	48:BE:80:LYS:NZ	2.25	0.69
11:AA:247:ASP:OD1	11:AA:304:ASN:ND2	2.26	0.68
59:BP:73:GLN:N	59:BP:73:GLN:OE1	2.26	0.68
3:A2:167:ARG:NH2	21:AK:65:GLU:OE1	2.27	0.68
55:BL:116:ARG:NE	60:BQ:106:ASP:OD1	2.27	0.68
22:AL:181:CYS:HB3	79:AL:302:SF4:S3	2.34	0.67
2:A1:30:LYS:NZ	12:AB:609:ASP:OD2	2.28	0.67
6:A5:153:GLU:OE1	6:A5:156:ARG:NH2	2.27	0.67
13:AC:74:TYR:OH	63:BT:140:PHE:O	2.13	0.67
18:AH:70:ASP:OD1	18:AH:71:ALA:N	2.28	0.67
11:AA:254:SER:OG	11:AA:444:ARG:NH2	2.29	0.66
15:AE:383:LYS:NZ	15:AE:434:ASP:OD1	2.29	0.66
22:AL:196:TYR:OH	30:AT:131:GLU:OE1	2.11	0.66
36:AZ:41:LYS:NZ	36:AZ:45:PRO:O	2.29	0.66
8:A7:176:ASP:OD1	8:A7:177:SER:N	2.28	0.66
7:A6:155:GLU:OE2	7:A6:159:ARG:NE	2.28	0.66
66:BW:25:GLN:OE1	66:BW:25:GLN:N	2.29	0.65
1:A0:264:LYS:NZ	1:A0:304:ASP:O	2.26	0.65
18:AH:125:TYR:OH	34:AX:1:MET:O	2.09	0.65
29:AS:18:ASN:O	29:AS:19:ASN:ND2	2.28	0.65
6:A5:38:GLU:OE2	15:AE:163:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:162:GLU:N	14:AD:162:GLU:OE1	2.29	0.65
39:B2:49:ARG:NH1	50:BG:141:ARG:O	2.28	0.65
12:AB:395:GLU:OE2	12:AB:417:ARG:NH1	2.28	0.65
15:AE:64:ARG:HD3	30:AT:68:THR:HG21	1.79	0.65
17:AG:23:ARG:NH1	23:AM:31:CYS:SG	2.69	0.64
13:AC:215:ILE:HD11	51:BH:105:THR:HG21	1.78	0.64
31:AU:51:ASN:OD1	31:AU:52:LYS:N	2.30	0.64
13:AC:422:LYS:NZ	13:AC:426:GLU:OE2	2.31	0.64
14:AD:130:GLU:O	14:AD:134:ASN:ND2	2.31	0.64
1:A0:456:ASN:HB2	1:A0:471:GLN:HB3	1.80	0.64
12:AB:609:ASP:OD1	12:AB:611:ARG:NH1	2.30	0.63
51:BH:120:ARG:NH2	52:BI:88:ASN:OD1	2.31	0.63
3:A2:33:ARG:NH2	3:A2:93:ASN:O	2.31	0.63
70:AP:301:CDL:H1O1	70:AP:301:CDL:PA1	2.20	0.63
19:AI:168:GLY:N	78:AI:301:FES:S1	2.72	0.63
34:AX:90:THR:OG1	56:BM:92:ILE:O	2.16	0.63
11:AA:616:ASP:OD1	11:AA:617:THR:N	2.31	0.63
1:A0:218:TYR:CG	1:A0:463:ALA:HB1	2.34	0.63
81:AS:200:8Q1:P24	32:AV:95:SER:OG	2.57	0.63
2:A1:183:GLU:OE2	2:A1:197:ARG:NH2	2.32	0.62
6:A5:241:GLN:NE2	6:A5:246:ASP:OD2	2.32	0.62
13:AC:458:LYS:NZ	46:BC:56:MET:SD	2.72	0.62
36:AZ:14:GLU:OE1	36:AZ:64:ARG:NH2	2.31	0.62
11:AA:200:PHE:O	11:AA:269:TYR:OH	2.17	0.62
14:AD:120:GLU:O	14:AD:160:ARG:NH1	2.31	0.62
25:AO:121:ASN:OD1	25:AO:146:ASN:ND2	2.31	0.62
13:AC:108:TYR:HH	13:AC:164:THR:HG1	1.47	0.62
16:AF:190:LEU:HB2	35:AY:84:LEU:HD13	1.82	0.62
48:BE:170:GLU:N	48:BE:170:GLU:OE1	2.32	0.62
27:AQ:143:GLU:OE1	27:AQ:155:ASP:N	2.33	0.62
49:BF:5:GLY:N	49:BF:30:ASP:OD2	2.33	0.62
63:BT:110:TYR:OH	73:BT:202:PC1:O14	2.18	0.62
14:AD:60:GLY:O	14:AD:257:ARG:NH1	2.32	0.62
19:AI:167:LEU:N	78:AI:301:FES:S1	2.73	0.62
56:BM:11:VAL:HG12	56:BM:12:ASP:H	1.64	0.62
6:A5:229:ASP:OD1	6:A5:230:ASN:N	2.33	0.61
27:AQ:179:GLU:OE2	57:BN:28:TYR:OH	2.16	0.61
14:AD:383:CYS:HB3	14:AD:425:ILE:HD12	1.82	0.61
44:BA:134:ARG:NE	75:BA:301:3PE:O12	2.33	0.61
12:AB:507:SER:OG	24:AN:190:ALA:O	2.15	0.61
20:AJ:148:GLU:N	20:AJ:148:GLU:OE1	2.33	0.61

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
20:AJ:184:GLU:N	20:AJ:184:GLU:OE1	2.34	0.61
9:A8:132:TYR:OH	22:AL:29:GLU:O	2.19	0.61
13:AC:325:TRP:O	46:BC:53:ASN:ND2	2.33	0.60
46:BC:151:GLN:N	46:BC:151:GLN:OE1	2.34	0.60
15:AE:425:ASP:OD1	43:B6:28:ARG:NH1	2.34	0.60
1:A0:15:ARG:NH1	1:A0:44:ASN:OD1	2.35	0.60
22:AL:199:THR:HG1	30:AT:135:PHE:HD2	1.48	0.60
25:AO:155:LYS:NZ	25:AO:162:LYS:O	2.34	0.60
11:AA:382:ASP:OD2	63:BT:123:ARG:NE	2.35	0.60
11:AA:572:TYR:HH	62:BS:62:CYS:HG	1.50	0.60
12:AB:350:GLU:OE1	12:AB:350:GLU:N	2.35	0.60
17:AG:258:GLU:OE1	60:BQ:43:ASN:ND2	2.35	0.59
37:B0:43:ASP:OD1	41:B4:38:ARG:NH1	2.35	0.59
16:AF:263:ALA:HB2	16:AF:349:ILE:HD11	1.83	0.59
12:AB:253:ASP:OD1	12:AB:254:VAL:N	2.35	0.59
11:AA:501:THR:O	11:AA:683:ASN:ND2	2.35	0.59
76:AL:304:LPP:O4	60:BQ:79:THR:OG1	2.21	0.59
5:A4:175:VAL:HG23	5:A4:181:LEU:HD22	1.84	0.59
64:BU:13:LYS:NZ	64:BU:17:ASP:OD1	2.36	0.59
45:BB:192:ARG:NH2	49:BF:170:GLU:OE1	2.35	0.59
60:BQ:100:ARG:NH1	60:BQ:104:ASP:OD2	2.36	0.59
58:BO:104:ASP:OD2	58:BO:109:GLN:NE2	2.36	0.59
68:BY:50:ILE:O	68:BY:54:THR:OG1	2.18	0.59
6:A5:215:MET:SD	15:AE:325:GLN:NE2	2.75	0.58
49:BF:101:GLN:NE2	59:BP:127:ILE:O	2.36	0.58
32:AV:33:ARG:NH1	52:BI:127:GLU:OE1	2.35	0.58
1:A0:365:GLU:OE2	71:A0:603:UDP:O2’	2.20	0.58
25:AO:95:LEU:HD11	25:AO:112:PHE:HB3	1.85	0.58
7:A6:217:VAL:O	7:A6:236:ARG:NH1	2.36	0.58
18:AH:264:PHE:O	43:B6:9:LYS:NZ	2.32	0.58
10:A9:186:GLN:N	10:A9:186:GLN:OE1	2.37	0.58
16:AF:61:ARG:NH1	31:AU:71:TRP:O	2.36	0.58
34:AX:3:ASP:OD1	34:AX:3:ASP:N	2.36	0.58
29:AS:88:ASN:ND2	29:AS:133:LEU:O	2.37	0.58
9:A8:101:ARG:NH2	9:A8:115:GLU:O	2.37	0.58
15:AE:155:GLU:OE2	30:AT:38:HIS:ND1	2.37	0.58
26:AP:6:TRP:NE1	26:AP:28:THR:O	2.36	0.58
9:A8:205:ASN:ND2	9:A8:205:ASN:O	2.37	0.58
47:BD:83:PRO:HD3	59:BP:122:VAL:HG21	1.85	0.57
14:AD:226:VAL:HG12	14:AD:228:PRO:HD3	1.86	0.57
29:AS:44:THR:O	29:AS:55:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AL:204:GLU:N	22:AL:204:GLU:OE1	2.35	0.57
13:AC:145:ASN:OD1	13:AC:145:ASN:N	2.35	0.57
22:AL:124:HIS:NE2	79:AL:302:SF4:S1	2.78	0.57
27:AQ:115:ALA:O	27:AQ:116:SER:OG	2.12	0.57
3:A2:113:ARG:NH1	3:A2:122:ILE:O	2.37	0.57
30:AT:4:ASP:OD2	30:AT:161:THR:OG1	2.18	0.57
55:BL:124:ASP:OD1	55:BL:125:LEU:N	2.38	0.57
17:AG:323:ASN:OD1	28:AR:63:SER:OG	2.17	0.56
24:AN:50:GLU:N	24:AN:50:GLU:OE1	2.37	0.56
10:A9:162:HIS:NE2	75:A9:602:3PE:O14	2.32	0.56
33:AW:114:GLU:O	33:AW:117:ARG:NH1	2.39	0.56
5:A4:253:ASP:OD2	5:A4:273:ARG:NE	2.34	0.56
11:AA:247:ASP:OD1	11:AA:247:ASP:N	2.39	0.56
35:AY:80:LEU:HG	35:AY:84:LEU:HD12	1.88	0.56
67:BX:46:GLN:N	67:BX:46:GLN:OE1	2.39	0.56
37:B0:47:ARG:NH1	37:B0:51:ARG:O	2.39	0.56
12:AB:68:GLU:OE1	12:AB:68:GLU:N	2.38	0.56
15:AE:33:GLN:OE1	34:AX:43:TYR:OH	2.18	0.56
19:AI:167:LEU:HB2	19:AI:175:MET:CE	2.36	0.56
4:A3:178:ARG:NE	12:AB:434:ASN:O	2.38	0.55
11:AA:551:GLU:N	11:AA:551:GLU:OE1	2.38	0.55
14:AD:426:CYS:O	14:AD:427:ALA:HB3	2.06	0.55
19:AI:79:ASN:OD1	19:AI:82:TRP:NE1	2.39	0.55
33:AW:62:ILE:HD12	45:BB:59:LEU:HD12	1.87	0.55
49:BF:88:SER:O	49:BF:89:SER:OG	2.19	0.55
1:A0:345:LYS:NZ	71:A0:603:UDP:O2'	2.39	0.55
3:A2:127:LYS:O	3:A2:130:THR:OG1	2.15	0.55
34:AX:64:LEU:HD13	43:B6:33:THR:HG21	1.87	0.55
64:BU:106:ASN:O	64:BU:106:ASN:ND2	2.40	0.55
14:AD:426:CYS:SG	14:AD:428:LEU:HB2	2.46	0.55
56:BM:28:ASP:O	56:BM:34:ASN:ND2	2.40	0.55
47:BD:149:LEU:O	49:BF:80:ARG:NH2	2.39	0.55
55:BL:77:MET:O	60:BQ:77:LYS:NZ	2.32	0.55
19:AI:75:VAL:HG21	19:AI:91:ILE:HD11	1.89	0.55
43:B6:19:ALA:O	43:B6:23:THR:HG23	2.06	0.55
56:BM:82:GLU:O	56:BM:89:LYS:NZ	2.40	0.55
63:BT:77:PHE:O	63:BT:81:ASN:ND2	2.38	0.55
5:A4:175:VAL:HG21	5:A4:296:ILE:HG21	1.88	0.54
8:A7:123:ASP:OD1	8:A7:126:ARG:NH2	2.39	0.54
30:AT:152:GLU:OE1	30:AT:152:GLU:N	2.40	0.54
50:BG:16:ARG:N	50:BG:22:SER:HG	2.03	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BN:75:HIS:HB3	57:BN:82:LEU:HD11	1.88	0.54
7:A6:71:PHE:CE2	7:A6:75:ILE:HD11	2.42	0.54
12:AB:475:VAL:HG21	12:AB:492:LEU:HD13	1.90	0.54
12:AB:597:VAL:O	12:AB:651:ASP:N	2.37	0.54
1:A0:255:ARG:NH2	1:A0:264:LYS:O	2.41	0.54
16:AF:276:LEU:O	16:AF:337:LYS:NZ	2.40	0.54
49:BF:92:GLU:OE1	49:BF:92:GLU:N	2.39	0.54
1:A0:412:THR:O	1:A0:415:ASN:ND2	2.38	0.54
22:AL:138:ALA:O	22:AL:163:ARG:NH2	2.39	0.54
54:BK:142:PHE:O	58:BO:117:ARG:NH1	2.36	0.54
22:AL:173:THR:HG21	22:AL:203:HIS:CD2	2.43	0.54
49:BF:153:GLU:OE1	49:BF:153:GLU:N	2.40	0.54
61:BR:94:ASN:ND2	61:BR:94:ASN:O	2.40	0.54
4:A3:215:LEU:O	4:A3:219:THR:HG23	2.07	0.54
6:A5:13:PHE:O	6:A5:18:ARG:NH2	2.40	0.53
10:A9:219:ASN:O	10:A9:224:ARG:NH2	2.41	0.53
27:AQ:10:ASN:O	27:AQ:10:ASN:ND2	2.41	0.53
4:A3:229:ASN:ND2	4:A3:232:THR:OG1	2.42	0.53
1:A0:465:LEU:HD12	1:A0:468:VAL:HG11	1.90	0.53
34:AX:71:TYR:OH	34:AX:110:ASP:OD2	2.26	0.53
39:B2:88:THR:O	39:B2:94:GLN:NE2	2.42	0.53
7:A6:130:THR:HG21	11:AA:744:ILE:HD13	1.91	0.53
15:AE:72:ASP:OD2	22:AL:149:ARG:NH2	2.41	0.53
16:AF:223:TRP:O	16:AF:227:ASN:ND2	2.41	0.53
6:A5:55:ASP:OD1	9:A8:151:TYR:OH	2.22	0.53
6:A5:141:ARG:NH1	24:AN:104:GLU:OE2	2.42	0.53
19:AI:209:GLN:OE1	19:AI:209:GLN:N	2.42	0.53
49:BF:144:GLN:OE1	49:BF:144:GLN:N	2.39	0.53
64:BU:58:TYR:OH	64:BU:62:ARG:NH1	2.38	0.53
6:A5:186:ALA:O	6:A5:192:ARG:NH1	2.41	0.53
9:A8:191:ASN:OD1	9:A8:192:LYS:N	2.42	0.53
14:AD:230:PHE:O	14:AD:232:ALA:N	2.43	0.52
4:A3:143:GLU:OE1	4:A3:143:GLU:N	2.40	0.52
11:AA:159:ILE:O	11:AA:162:ILE:HG22	2.10	0.52
12:AB:309:ARG:NH1	12:AB:572:TYR:O	2.43	0.52
28:AR:18:LYS:O	28:AR:147:LYS:NZ	2.39	0.52
44:BA:26:ILE:HG13	62:BS:111:LEU:HD13	1.92	0.52
6:A5:78:ASP:OD1	6:A5:125:ILE:HD11	2.10	0.52
5:A4:219:ASN:ND2	5:A4:222:SER:O	2.43	0.52
11:AA:251:ASP:OD1	11:AA:252:LEU:N	2.40	0.52
23:AM:92:ASP:OD1	23:AM:93:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A4:181:LEU:HD23	5:A4:297:VAL:HG21	1.92	0.52
11:AA:341:SER:HA	13:AC:454:ILE:HD11	1.92	0.52
12:AB:493:LYS:O	12:AB:497:ASN:ND2	2.40	0.52
17:AG:141:ILE:HG23	17:AG:159:LEU:HD11	1.91	0.52
57:BN:70:VAL:N	69:BZ:1:MET:O	2.41	0.52
25:AO:159:ASP:OD1	25:AO:160:TYR:N	2.41	0.51
12:AB:153:ARG:NH1	14:AD:415:GLN:OE1	2.44	0.51
47:BD:150:VAL:HG21	49:BF:83:ILE:HD12	1.92	0.51
51:BH:149:ILE:HD12	69:BZ:19:ALA:HA	1.92	0.51
4:A3:72:LEU:HD23	4:A3:98:VAL:HB	1.93	0.51
9:A8:300:HIS:ND1	9:A8:301:GLU:OE1	2.43	0.51
16:AF:232:SER:CB	39:B2:40:THR:HG21	2.40	0.51
12:AB:618:ARG:NH2	12:AB:631:ASP:OD1	2.40	0.51
13:AC:217:ILE:HD11	13:AC:296:PHE:CZ	2.46	0.51
51:BH:101:ILE:O	51:BH:105:THR:HG23	2.10	0.51
64:BU:9:PRO:O	64:BU:31:TYR:OH	2.25	0.51
5:A4:260:VAL:O	5:A4:264:LEU:N	2.38	0.51
30:AT:39:ALA:O	30:AT:44:TYR:O	2.28	0.51
45:BB:84:HIS:NE2	45:BB:86:GLU:OE2	2.44	0.51
1:A0:242:ILE:HD13	1:A0:462:VAL:HG11	1.93	0.51
12:AB:127:LEU:HB3	15:AE:357:LEU:HD22	1.93	0.51
1:A0:410:VAL:HG23	1:A0:410:VAL:O	2.09	0.51
8:A7:192:LYS:NZ	50:BG:81:GLU:OE1	2.43	0.51
11:AA:501:THR:HG22	11:AA:581:LEU:HA	1.93	0.50
12:AB:218:GLU:N	12:AB:218:GLU:OE1	2.43	0.50
23:AM:81:THR:OG1	23:AM:99:GLY:O	2.29	0.50
11:AA:427:ALA:HB2	11:AA:522:PHE:HB3	1.94	0.50
12:AB:74:GLY:O	14:AD:425:ILE:HD11	2.10	0.50
14:AD:228:PRO:N	14:AD:229:PRO:CD	2.74	0.50
18:AH:183:PHE:HB3	18:AH:261:ILE:HG21	1.93	0.50
46:BC:81:LYS:NZ	70:BC:302:CDL:OA4	2.35	0.50
1:A0:394:TYR:CZ	1:A0:410:VAL:HG21	2.46	0.50
22:AL:177:TYR:HA	79:AL:302:SF4:S1	2.51	0.50
51:BH:95:LYS:O	51:BH:97:GLN:NE2	2.44	0.50
2:A1:349:VAL:HG23	2:A1:349:VAL:O	2.12	0.50
11:AA:193:TYR:OH	70:AA:908:CDL:OB3	2.26	0.50
11:AA:376:TYR:OH	49:BF:71:ARG:NH2	2.44	0.50
22:AL:171:ASP:OD2	22:AL:174:LYS:NZ	2.38	0.50
11:AA:497:VAL:O	11:AA:501:THR:HG23	2.12	0.50
22:AL:95:CYS:SG	43:B6:23:THR:HG22	2.51	0.50
1:A0:199:VAL:HG23	1:A0:199:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:398:ASN:ND2	1:A0:408:GLU:OE2	2.43	0.50
1:A0:28:ASP:OD1	1:A0:29:LEU:N	2.45	0.50
8:A7:197:GLN:NE2	55:BL:133:ASP:OD2	2.45	0.50
57:BN:92:ARG:NH2	57:BN:103:ASP:OD2	2.44	0.50
1:A0:218:TYR:CD1	1:A0:463:ALA:HB1	2.47	0.49
12:AB:612:GLU:OE1	12:AB:614:TRP:NE1	2.40	0.49
21:AK:227:GLU:OE1	21:AK:227:GLU:N	2.37	0.49
15:AE:77:GLN:O	30:AT:102:TYR:OH	2.29	0.49
17:AG:267:GLN:HG2	24:AN:67:LEU:HD13	1.94	0.49
21:AK:32:GLU:N	21:AK:32:GLU:OE1	2.45	0.49
34:AX:111:TRP:CE2	56:BM:57:LEU:HD21	2.47	0.49
2:A1:279:LEU:HB3	2:A1:346:ILE:HD11	1.95	0.49
30:AT:78:ARG:HA	30:AT:117:ILE:HD11	1.93	0.49
50:BG:130:ARG:NH2	50:BG:138:ALA:O	2.45	0.49
11:AA:112:LEU:HD22	67:BX:89:VAL:HG21	1.94	0.49
66:BW:99:ALA:O	66:BW:103:GLY:HA2	2.13	0.49
4:A3:32:ARG:NH1	4:A3:257:GLY:O	2.45	0.49
11:AA:745:PHE:O	11:AA:750:LEU:N	2.44	0.49
57:BN:98:GLU:OE1	57:BN:98:GLU:N	2.39	0.49
20:AJ:132:PHE:CE1	68:BY:100:ILE:HD11	2.48	0.49
48:BE:33:ASP:OD1	48:BE:89:HIS:ND1	2.37	0.49
8:A7:192:LYS:NZ	55:BL:8:PHE:O	2.30	0.49
34:AX:73:VAL:HG11	35:AY:65:GLY:HA2	1.94	0.49
41:B4:45:ASP:OD1	41:B4:46:PHE:N	2.42	0.49
3:A2:29:LEU:HD12	3:A2:80:LEU:HD12	1.93	0.49
6:A5:251:ILE:HG22	6:A5:251:ILE:O	2.13	0.49
14:AD:332:VAL:O	14:AD:336:VAL:HG23	2.13	0.49
13:AC:151:SER:HB2	13:AC:185:ILE:HD11	1.94	0.48
14:AD:224:PRO:HG2	14:AD:426:CYS:CB	2.43	0.48
22:AL:124:HIS:CE1	79:AL:302:SF4:S1	3.07	0.48
2:A1:85:GLU:OE2	34:AX:36:GLN:NE2	2.46	0.48
12:AB:430:ASN:ND2	12:AB:433:THR:O	2.43	0.48
18:AH:43:GLU:HA	43:B6:18:ILE:HD13	1.94	0.48
6:A5:48:ASP:OD1	6:A5:49:TYR:N	2.46	0.48
21:AK:103:THR:HG22	21:AK:115:VAL:HG23	1.94	0.48
37:B0:87:ASN:O	37:B0:89:ARG:NH1	2.46	0.48
13:AC:77:TYR:OH	63:BT:144:ASP:OD2	2.24	0.48
15:AE:395:SER:OG	15:AE:396:ASN:N	2.46	0.48
4:A3:122:LEU:HD22	4:A3:137:VAL:HG21	1.95	0.48
14:AD:235:GLY:HA3	14:AD:241:THR:HG22	1.96	0.48
22:AL:176:ILE:O	79:AL:302:SF4:S4	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AL:185:CYS:HA	79:AL:301:SF4:S3	2.54	0.48
23:AM:89:LEU:HD22	23:AM:110:ILE:HD12	1.95	0.48
11:AA:162:ILE:HD13	76:AA:902:LPP:O27	2.14	0.48
12:AB:151:ILE:N	15:AE:355:GLU:OE1	2.47	0.48
13:AC:363:PHE:HA	13:AC:366:THR:HG22	1.95	0.48
21:AK:209:HIS:CE1	23:AM:72:ILE:HG21	2.48	0.48
25:AO:81:ASP:OD1	25:AO:84:ASN:ND2	2.46	0.48
25:AO:95:LEU:HD13	25:AO:114:ILE:HD13	1.95	0.48
54:BK:43:LEU:O	54:BK:46:THR:OG1	2.26	0.48
1:A0:154:ARG:NH2	1:A0:173:ASP:O	2.45	0.48
1:A0:221:VAL:HG21	1:A0:463:ALA:HB2	1.96	0.48
12:AB:108:GLU:OE2	12:AB:111:ARG:NH1	2.47	0.48
20:AJ:74:CYS:SG	20:AJ:82:THR:HG21	2.54	0.48
21:AK:197:ASP:OD2	67:BX:18:ARG:N	2.47	0.48
44:BA:89:ILE:HG12	44:BA:202:LEU:HD11	1.96	0.48
12:AB:141:GLN:NE2	79:AB:803:SF4:S4	2.87	0.48
16:AF:334:ASN:ND2	52:BI:103:PHE:O	2.47	0.48
51:BH:76:ILE:HG22	51:BH:77:PRO:HD2	1.95	0.48
68:BY:22:ASP:OD1	68:BY:23:PHE:N	2.47	0.48
8:A7:234:SER:O	50:BG:78:ARG:NH2	2.47	0.47
11:AA:292:PHE:CE2	11:AA:429:ILE:HG22	2.49	0.47
45:BB:120:MET:SD	59:BP:62:LYS:NZ	2.85	0.47
7:A6:247:HIS:O	7:A6:251:ASN:ND2	2.42	0.47
11:AA:479:ASP:OD1	11:AA:480:THR:N	2.46	0.47
14:AD:336:VAL:HG22	14:AD:346:VAL:HG21	1.95	0.47
45:BB:186:ASP:OD1	45:BB:189:ARG:NH1	2.47	0.47
3:A2:222:ARG:O	53:BJ:95:ARG:NH2	2.48	0.47
15:AE:272:GLN:N	15:AE:272:GLN:OE1	2.46	0.47
11:AA:545:TYR:CZ	40:B3:48:THR:HG22	2.50	0.47
35:AY:20:VAL:O	35:AY:24:LYS:NZ	2.33	0.47
51:BH:56:PHE:CB	51:BH:66:LEU:HD22	2.45	0.47
4:A3:286:ASP:O	4:A3:290:VAL:HG23	2.15	0.47
44:BA:25:MET:HB3	62:BS:111:LEU:HD11	1.96	0.47
47:BD:101:ASN:OD1	59:BP:100:ARG:NH2	2.42	0.47
55:BL:122:PRO:HD2	55:BL:125:LEU:HD12	1.97	0.47
8:A7:126:ARG:NH2	56:BM:135:ASP:OD2	2.42	0.47
76:AL:304:LPP:O4	50:BG:51:LYS:NZ	2.48	0.47
6:A5:60:ILE:HD12	6:A5:61:ARG:N	2.29	0.47
7:A6:161:VAL:HG13	7:A6:175:VAL:HG13	1.96	0.47
16:AF:146:THR:HB	16:AF:221:THR:HG23	1.95	0.47
13:AC:180:ILE:HD11	51:BH:76:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AD:45:LEU:O	14:AD:134:ASN:ND2	2.48	0.46
18:AH:76:ILE:HA	34:AX:27:ALA:HB1	1.97	0.46
31:AU:66:PHE:HB3	31:AU:67:PRO:HD3	1.96	0.46
47:BD:157:GLU:OE1	47:BD:157:GLU:N	2.44	0.46
51:BH:120:ARG:NH1	52:BI:85:GLU:OE1	2.48	0.46
3:A2:33:ARG:NE	3:A2:90:ASP:OD2	2.45	0.46
12:AB:395:GLU:OE1	24:AN:184:ARG:NH2	2.47	0.46
63:BT:134:ASN:OD1	63:BT:134:ASN:N	2.47	0.46
15:AE:12:GLU:OE1	20:AJ:229:ASN:ND2	2.47	0.46
15:AE:151:PHE:O	15:AE:155:GLU:HG2	2.15	0.46
16:AF:198:TRP:CH2	35:AY:29:ILE:HG22	2.51	0.46
30:AT:156:ASN:ND2	30:AT:160:LEU:O	2.43	0.46
12:AB:345:GLU:OE1	12:AB:345:GLU:N	2.47	0.46
13:AC:329:ASP:OD2	13:AC:388:ARG:NH1	2.49	0.46
17:AG:224:PHE:CE1	23:AM:41:GLU:HA	2.50	0.46
22:AL:101:PHE:CE1	37:B0:13:ILE:HD11	2.50	0.46
25:AO:178:ASP:OD1	30:AT:111:ARG:NH1	2.48	0.46
44:BA:28:GLU:O	66:BW:98:LYS:NZ	2.43	0.46
53:BJ:45:LEU:HD21	53:BJ:131:VAL:HG21	1.98	0.46
56:BM:99:PHE:HA	56:BM:102:THR:HG22	1.98	0.46
14:AD:41:ILE:O	14:AD:138:LYS:NZ	2.48	0.46
16:AF:138:ILE:N	16:AF:139:PRO:HD2	2.31	0.46
16:AF:218:THR:HG22	16:AF:229:ILE:HG21	1.98	0.46
51:BH:13:LEU:N	57:BN:88:GLY:O	2.43	0.46
14:AD:228:PRO:N	14:AD:229:PRO:HD2	2.30	0.46
15:AE:85:PHE:O	15:AE:439:GLU:N	2.49	0.46
18:AH:117:PHE:HB2	18:AH:119:LEU:HD13	1.97	0.46
18:AH:280:ASP:OD1	55:BL:3:ASN:ND2	2.49	0.46
25:AO:77:GLN:OE1	25:AO:77:GLN:N	2.46	0.46
6:A5:83:THR:HG22	6:A5:84:THR:H	1.81	0.46
17:AG:44:ASP:O	21:AK:222:GLN:NE2	2.43	0.46
18:AH:25:ASN:OD1	34:AX:12:ASN:ND2	2.49	0.46
2:A1:352:ARG:NH1	2:A1:353:GLY:O	2.49	0.46
12:AB:82:GLU:OE1	12:AB:107:SER:OG	2.32	0.46
15:AE:368:LEU:HD12	15:AE:368:LEU:O	2.16	0.46
18:AH:115:SER:O	50:BG:165:ARG:NH2	2.46	0.46
7:A6:94:PRO:O	7:A6:163:ARG:NH2	2.44	0.46
9:A8:206:VAL:O	9:A8:206:VAL:HG23	2.15	0.46
11:AA:443:LEU:HD11	11:AA:507:VAL:HG11	1.98	0.46
47:BD:176:THR:HG21	49:BF:164:TYR:OH	2.15	0.46
48:BE:89:HIS:O	48:BE:93:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:72:ILE:H	1:A0:72:ILE:HD12	1.80	0.45
3:A2:207:GLN:OE1	3:A2:211:ASN:ND2	2.49	0.45
16:AF:23:TYR:CE1	16:AF:66:LEU:HD12	2.51	0.45
57:BN:13:ARG:NH1	57:BN:21:SER:OG	2.47	0.45
1:A0:325:VAL:O	1:A0:328:THR:OG1	2.32	0.45
11:AA:170:TYR:OH	47:BD:87:PRO:HD3	2.16	0.45
81:AS:200:8Q1:O40	81:AS:200:8Q1:N36	2.47	0.45
70:B0:102:CDL:OA3	41:B4:38:ARG:NH2	2.49	0.45
6:A5:282:GLU:OXT	26:AP:22:ARG:NH1	2.48	0.45
12:AB:229:VAL:O	79:AB:803:SF4:S3	2.75	0.45
52:BI:104:CYS:O	78:BI:201:FES:S1	2.75	0.45
63:BT:72:GLU:O	63:BT:76:VAL:HG23	2.16	0.45
1:A0:458:VAL:HG13	1:A0:470:VAL:HG23	1.99	0.45
13:AC:7:ILE:HG23	13:AC:77:TYR:CZ	2.51	0.45
16:AF:19:ASN:OD1	31:AU:98:TRP:NE1	2.47	0.45
47:BD:140:ARG:NH1	67:BX:92:GLU:OE2	2.49	0.45
18:AH:149:ALA:HB2	18:AH:234:VAL:HG12	1.98	0.45
11:AA:107:TYR:CE2	11:AA:111:ILE:HD11	2.52	0.45
16:AF:257:ILE:HD13	16:AF:262:ILE:HD12	1.99	0.45
19:AI:47:GLU:OE1	19:AI:47:GLU:N	2.44	0.45
22:AL:135:ARG:O	22:AL:187:VAL:HG21	2.17	0.45
7:A6:197:VAL:HG13	7:A6:197:VAL:O	2.17	0.45
15:AE:83:ASP:N	15:AE:83:ASP:OD1	2.46	0.45
43:B6:3:TYR:O	43:B6:7:LEU:HD23	2.16	0.45
46:BC:58:ASP:OD1	46:BC:59:GLN:N	2.50	0.45
4:A3:111:ALA:O	4:A3:115:THR:HG22	2.17	0.45
10:A9:189:GLU:OE1	49:BF:27:SER:OG	2.34	0.45
11:AA:99:PHE:CE2	11:AA:131:ILE:HD11	2.52	0.45
13:AC:302:ILE:HG22	13:AC:304:ILE:HG22	1.97	0.45
18:AH:107:ASN:OD1	18:AH:122:ASN:ND2	2.47	0.45
22:AL:28:GLU:N	22:AL:28:GLU:OE1	2.50	0.45
1:A0:465:LEU:HD23	1:A0:465:LEU:N	2.32	0.45
9:A8:217:GLU:O	9:A8:221:VAL:HG12	2.17	0.45
11:AA:419:MET:SD	11:AA:430:HIS:NE2	2.90	0.45
11:AA:604:PHE:HZ	11:AA:710:LEU:HD22	1.81	0.45
13:AC:258:PRO:HG3	13:AC:266:LEU:HD22	1.98	0.45
5:A4:175:VAL:O	5:A4:175:VAL:HG22	2.17	0.44
12:AB:235:ALA:HB3	12:AB:236:PRO:HD3	1.99	0.44
17:AG:261:GLU:OE2	60:BQ:43:ASN:ND2	2.47	0.44
34:AX:73:VAL:HG11	35:AY:65:GLY:CA	2.47	0.44
40:B3:55:ARG:NH2	70:BE:201:CDL:OB4	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:BZ:16:ARG:NH2	69:BZ:29:THR:O	2.50	0.44
6:A5:55:ASP:O	15:AE:343:ASN:ND2	2.47	0.44
15:AE:412:GLN:NE2	25:AO:131:ASN:O	2.44	0.44
16:AF:302:TYR:CG	51:BH:176:ILE:HD11	2.53	0.44
30:AT:37:MET:O	30:AT:41:VAL:HG13	2.17	0.44
68:BY:43:PHE:O	68:BY:47:LYS:HB2	2.18	0.44
7:A6:173:ILE:HD12	7:A6:194:LEU:HD11	1.99	0.44
10:A9:229:VAL:N	57:BN:98:GLU:OE2	2.48	0.44
18:AH:101:CYS:HB2	18:AH:247:GLY:HA2	1.99	0.44
13:AC:482:LYS:HA	45:BB:144:LEU:HD12	1.99	0.44
21:AK:238:VAL:HG23	21:AK:238:VAL:O	2.18	0.44
52:BI:85:GLU:O	52:BI:89:THR:HG22	2.17	0.44
9:A8:101:ARG:NH1	9:A8:102:ASP:O	2.51	0.44
15:AE:52:ALA:O	15:AE:419:LYS:O	2.36	0.44
17:AG:52:ASN:O	17:AG:52:ASN:ND2	2.47	0.44
20:AJ:50:ILE:CG1	35:AY:18:ILE:HD12	2.48	0.44
20:AJ:206:ASN:O	35:AY:83:ASN:ND2	2.51	0.44
8:A7:106:LYS:N	39:B2:76:GLU:OE2	2.51	0.44
15:AE:77:GLN:NE2	22:AL:144:SER:O	2.51	0.44
23:AM:166:VAL:HG23	23:AM:196:LEU:HD11	1.98	0.44
26:AP:15:LYS:NZ	26:AP:44:GLY:O	2.50	0.44
12:AB:69:ARG:NH2	12:AB:280:GLU:OE1	2.50	0.44
12:AB:189:GLN:O	12:AB:423:ARG:NH2	2.47	0.44
18:AH:131:ILE:HG21	20:AJ:90:PHE:HB3	2.00	0.44
23:AM:172:LEU:O	23:AM:190:VAL:HG13	2.18	0.44
33:AW:51:TYR:CE2	46:BC:31:PRO:HG2	2.53	0.44
51:BH:77:PRO:HA	51:BH:82:PHE:CG	2.53	0.44
64:BU:81:GLY:O	64:BU:84:SER:OG	2.28	0.44
7:A6:124:LEU:HB3	7:A6:125:PRO:HD3	2.00	0.44
11:AA:476:PHE:CD1	68:BY:15:VAL:HG11	2.53	0.44
13:AC:387:THR:HG23	13:AC:393:VAL:CG2	2.47	0.44
14:AD:319:ILE:HG23	14:AD:319:ILE:O	2.18	0.44
16:AF:118:LYS:NZ	21:AK:248:GLU:OE2	2.47	0.44
33:AW:79:LEU:O	33:AW:120:GLU:N	2.50	0.44
51:BH:142:TYR:OH	69:BZ:16:ARG:NH1	2.51	0.44
15:AE:231:CYS:HB3	15:AE:246:LEU:HD11	2.00	0.43
7:A6:133:TYR:OH	44:BA:37:ASP:OD2	2.36	0.43
16:AF:227:ASN:ND2	16:AF:303:TYR:O	2.39	0.43
20:AJ:176:SER:O	20:AJ:181:ASN:N	2.48	0.43
26:AP:78:VAL:CG2	26:AP:102:LEU:HD11	2.48	0.43
8:A7:201:CYS:SG	8:A7:202:GLN:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:559:MET:HB2	70:AA:901:CDL:H273	2.00	0.43
13:AC:32:PHE:CD1	13:AC:52:LEU:HD11	2.53	0.43
29:AS:168:LYS:NZ	29:AS:169:PRO:O	2.39	0.43
31:AU:136:GLU:OE1	31:AU:136:GLU:N	2.43	0.43
44:BA:82:THR:HG21	44:BA:181:ILE:HG13	2.00	0.43
58:BO:122:GLN:NE2	58:BO:126:ASP:OD1	2.51	0.43
13:AC:420:THR:HG22	13:AC:422:LYS:H	1.82	0.43
15:AE:217:LYS:HB3	15:AE:221:ILE:HD12	2.01	0.43
15:AE:237:THR:HA	15:AE:241:ALA:HB2	2.00	0.43
17:AG:42:SER:HB3	23:AM:51:PRO:HD3	2.00	0.43
21:AK:160:ALA:HB3	23:AM:172:LEU:CD1	2.48	0.43
49:BF:67:LEU:HB3	49:BF:110:VAL:HG12	2.00	0.43
55:BL:111:HIS:O	55:BL:115:THR:OG1	2.26	0.43
13:AC:74:TYR:CD2	13:AC:120:LEU:HD12	2.54	0.43
16:AF:254:ILE:HD11	68:BY:89:LEU:HD22	2.01	0.43
64:BU:53:LEU:HD11	64:BU:76:LEU:HD11	2.01	0.43
11:AA:235:TRP:CH2	11:AA:310:LEU:HD22	2.54	0.43
22:AL:80:TYR:OH	73:AL:303:PC1:O12	2.29	0.43
24:AN:177:LEU:CD2	28:AR:2:LEU:HD11	2.49	0.43
49:BF:47:ASP:OD1	49:BF:47:ASP:N	2.51	0.43
14:AD:34:ASN:N	14:AD:291:GLU:OE2	2.51	0.43
17:AG:77:ASP:OD1	17:AG:79:ILE:HD11	2.19	0.43
18:AH:176:PHE:CE1	43:B6:52:LEU:HD23	2.53	0.43
21:AK:147:LEU:HD12	21:AK:166:PRO:HD3	1.99	0.43
23:AM:61:HIS:O	23:AM:219:LYS:NZ	2.52	0.43
23:AM:132:ILE:HD13	23:AM:138:LEU:HD11	2.00	0.43
32:AV:134:ASN:OD1	32:AV:137:ALA:N	2.50	0.43
3:A2:262:TYR:CE2	3:A2:266:LEU:HD11	2.54	0.43
5:A4:121:VAL:HG13	5:A4:146:LEU:HB3	2.01	0.43
12:AB:164:LYS:O	12:AB:172:THR:OG1	2.29	0.43
12:AB:132:CYS:O	12:AB:242:ARG:NH1	2.47	0.43
12:AB:382:ARG:NH2	12:AB:525:GLU:OE2	2.52	0.43
28:AR:19:ILE:HD11	28:AR:44:PRO:O	2.19	0.43
8:A7:112:PHE:HD2	50:BG:175:VAL:HG23	1.84	0.43
11:AA:641:THR:OG1	11:AA:642:SER:N	2.52	0.43
16:AF:119:ILE:CD1	51:BH:144:ILE:HD12	2.49	0.43
19:AI:127:THR:HG22	19:AI:128:THR:H	1.83	0.43
11:AA:565:LEU:O	11:AA:568:THR:OG1	2.32	0.42
26:AP:48:ASP:OD1	26:AP:48:ASP:N	2.51	0.42
43:B6:56:THR:CG2	56:BM:92:ILE:HD11	2.49	0.42
52:BI:38:VAL:O	52:BI:42:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BV:75:VAL:HG11	65:BV:84:ILE:HD13	2.00	0.42
1:A0:455:ASP:CG	1:A0:456:ASN:N	2.73	0.42
12:AB:183:CYS:HB3	79:AB:802:SF4:S2	2.58	0.42
14:AD:389:GLY:HA3	14:AD:420:ILE:HD11	2.00	0.42
26:AP:23:GLU:OE1	26:AP:23:GLU:N	2.51	0.42
30:AT:8:THR:HB	30:AT:9:PRO:HD3	2.01	0.42
30:AT:144:LEU:HD23	30:AT:145:TYR:N	2.34	0.42
49:BF:71:ARG:O	49:BF:74:ILE:HG22	2.19	0.42
4:A3:88:VAL:HG23	4:A3:250:ILE:HD12	2.02	0.42
9:A8:164:GLU:OE1	22:AL:38:LYS:NZ	2.49	0.42
16:AF:9:GLU:OE1	16:AF:85:TRP:N	2.41	0.42
1:A0:138:LYS:NZ	70:A0:602:CDL:OB4	2.45	0.42
2:A1:159:LEU:HD23	2:A1:160:ILE:N	2.34	0.42
15:AE:242:ARG:NH2	15:AE:286:GLU:OE2	2.50	0.42
19:AI:42:PHE:CZ	19:AI:75:VAL:HG22	2.54	0.42
22:AL:112:GLU:OE2	26:AP:37:ARG:NE	2.48	0.42
25:AO:52:GLU:O	25:AO:56:SER:N	2.53	0.42
26:AP:7:THR:HG22	26:AP:8:ILE:N	2.35	0.42
27:AQ:159:ASN:O	45:BB:136:ARG:NH2	2.48	0.42
3:A2:35:ALA:O	3:A2:86:ARG:NH2	2.49	0.42
13:AC:54:LEU:HD12	13:AC:58:PHE:CD2	2.54	0.42
14:AD:410:ILE:HG23	14:AD:440:ILE:HD12	2.02	0.42
16:AF:119:ILE:HD11	51:BH:141:ASN:CB	2.49	0.42
30:AT:34:VAL:HG12	30:AT:38:HIS:NE2	2.34	0.42
11:AA:281:LEU:HD13	11:AA:284:ARG:CZ	2.49	0.42
13:AC:381:ILE:HD11	13:AC:407:ILE:HD11	2.01	0.42
13:AC:384:ARG:NH2	13:AC:483:GLU:OE1	2.53	0.42
73:AL:303:PC1:O11	50:BG:49:LYS:NZ	2.53	0.42
33:AW:111:GLU:OE1	33:AW:111:GLU:N	2.46	0.42
44:BA:85:ALA:HB2	44:BA:193:VAL:HG23	2.02	0.42
50:BG:136:ILE:N	50:BG:136:ILE:HD12	2.34	0.42
11:AA:64:VAL:HG11	11:AA:76:PHE:HE1	1.85	0.42
13:AC:241:GLU:OE2	49:BF:38:ARG:NH2	2.53	0.42
16:AF:138:ILE:N	16:AF:139:PRO:CD	2.82	0.42
19:AI:167:LEU:HB2	19:AI:175:MET:HE1	2.01	0.42
27:AQ:172:ASP:OD1	64:BU:62:ARG:NH2	2.53	0.42
30:AT:18:ARG:HG3	30:AT:144:LEU:HD21	2.01	0.42
35:AY:7:PHE:O	35:AY:11:ILE:HG23	2.18	0.42
68:BY:42:ILE:O	68:BY:46:GLU:HB3	2.20	0.42
6:A5:84:THR:HG23	6:A5:120:PRO:HB2	2.02	0.42
11:AA:267:PHE:CZ	11:AA:655:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:422:THR:HA	12:AB:426:LEU:HB3	2.02	0.42
12:AB:449:LYS:NZ	12:AB:453:GLU:OE2	2.34	0.42
12:AB:592:ASN:OD1	12:AB:596:ARG:N	2.52	0.42
30:AT:58:ARG:O	30:AT:85:LEU:HD12	2.20	0.42
49:BF:78:VAL:CG2	49:BF:102:ILE:HD11	2.50	0.42
7:A6:128:LEU:HD22	73:A6:303:PC1:C3B	2.50	0.42
12:AB:515:HIS:HB2	12:AB:521:ILE:HD11	2.02	0.42
15:AE:3:ARG:NH2	16:AF:50:ILE:O	2.53	0.42
16:AF:254:ILE:HD11	68:BY:89:LEU:CD2	2.50	0.42
11:AA:423:VAL:HG11	11:AA:526:GLY:HA3	2.02	0.42
16:AF:256:PHE:CZ	16:AF:299:LEU:HD11	2.55	0.42
6:A5:30:THR:HG22	15:AE:194:GLU:OE1	2.20	0.41
8:A7:189:TYR:HB2	50:BG:82:LEU:HD13	2.02	0.41
11:AA:47:PHE:CE2	11:AA:51:LEU:HD11	2.55	0.41
12:AB:613:ASP:N	12:AB:613:ASP:OD1	2.53	0.41
15:AE:56:ASP:OD1	25:AO:154:ARG:NH2	2.51	0.41
15:AE:144:MET:O	15:AE:147:VAL:HG12	2.19	0.41
16:AF:229:ILE:HG23	39:B2:44:LEU:HD21	2.02	0.41
35:AY:5:ILE:HD12	35:AY:5:ILE:H	1.85	0.41
47:BD:165:ILE:HD12	49:BF:145:PHE:HB2	2.01	0.41
12:AB:75:ASN:OD1	12:AB:76:CYS:N	2.54	0.41
13:AC:435:GLU:OE1	63:BT:126:THR:OG1	2.32	0.41
15:AE:90:MET:SD	15:AE:170:HIS:N	2.84	0.41
16:AF:127:TYR:HA	16:AF:167:VAL:HG21	2.03	0.41
18:AH:226:SER:OG	43:B6:26:ARG:NH2	2.53	0.41
29:AS:67:ILE:N	29:AS:68:PRO:HD2	2.35	0.41
1:A0:84:ARG:HA	1:A0:87:VAL:HG22	2.02	0.41
5:A4:175:VAL:CG2	5:A4:181:LEU:HD22	2.50	0.41
6:A5:83:THR:HG22	6:A5:84:THR:N	2.35	0.41
12:AB:300:ARG:NE	12:AB:694:ALA:O	2.41	0.41
13:AC:386:HIS:NE2	63:BT:64:ARG:O	2.52	0.41
14:AD:328:MET:HE1	14:AD:336:VAL:HG11	2.02	0.41
25:AO:196:VAL:HG22	28:AR:124:PHE:CZ	2.55	0.41
32:AV:32:ASP:O	68:BY:67:ARG:NH2	2.48	0.41
35:AY:8:TRP:CE3	35:AY:11:ILE:HD11	2.55	0.41
15:AE:248:ARG:NH2	15:AE:256:GLU:OE1	2.49	0.41
22:AL:124:HIS:CD2	22:AL:181:CYS:SG	3.13	0.41
4:A3:170:THR:HG22	12:AB:683:ASP:OD2	2.20	0.41
14:AD:129:ARG:NH2	14:AD:166:GLU:OE2	2.54	0.41
25:AO:67:ASP:OD1	25:AO:69:ILE:HG22	2.21	0.41
25:AO:137:ARG:NE	25:AO:154:ARG:O	2.52	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
36:AZ:23:SER:O	36:AZ:30:ARG:NH2	2.54	0.41
4:A3:91:ALA:HA	4:A3:202:LEU:HD13	2.01	0.41
11:AA:121:LEU:O	11:AA:123:THR:N	2.54	0.41
14:AD:407:TYR:OH	14:AD:452:ASP:OD2	2.37	0.41
18:AH:76:ILE:HD13	30:AT:14:VAL:HG13	2.03	0.41
23:AM:49:ILE:HG23	23:AM:57:PRO:HG2	2.03	0.41
37:B0:21:VAL:O	37:B0:25:VAL:HG23	2.19	0.41
38:B1:76:VAL:HG11	39:B2:35:MET:CE	2.51	0.41
13:AC:151:SER:CB	13:AC:185:ILE:HD11	2.50	0.41
15:AE:234:TYR:CG	15:AE:413:VAL:HG12	2.55	0.41
20:AJ:85:LEU:CD1	35:AY:38:LEU:HD22	2.51	0.41
50:BG:32:GLU:OE1	50:BG:32:GLU:N	2.49	0.41
57:BN:78:ASP:OD1	57:BN:78:ASP:N	2.54	0.41
1:A0:89:ARG:HA	1:A0:89:ARG:NE	2.36	0.41
11:AA:173:ILE:HG12	11:AA:217:TYR:CD2	2.56	0.41
11:AA:175:LEU:HD13	59:BP:96:PHE:HA	2.02	0.41
13:AC:259:ILE:O	13:AC:262:PHE:N	2.53	0.41
19:AI:69:MET:HB2	19:AI:70:PRO:HD3	2.01	0.41
29:AS:52:ALA:HB1	29:AS:105:ILE:HG21	2.02	0.41
40:B3:47:ASN:OD1	40:B3:48:THR:N	2.54	0.41
62:BS:71:HIS:NE2	73:BS:1301:PC1:O14	2.39	0.41
2:A1:168:ASP:OD1	2:A1:169:THR:N	2.53	0.41
12:AB:134:GLN:O	12:AB:138:CYS:HB2	2.20	0.41
13:AC:310:ILE:HG23	13:AC:347:LEU:HD11	2.03	0.41
20:AJ:104:ASN:ND2	20:AJ:108:LEU:O	2.51	0.41
20:AJ:207:LYS:O	20:AJ:210:THR:HG22	2.20	0.41
21:AK:148:GLU:OE1	21:AK:148:GLU:N	2.45	0.41
22:AL:185:CYS:SG	22:AL:189:ALA:N	2.87	0.41
24:AN:181:ARG:NE	24:AN:183:ASP:OD1	2.52	0.41
26:AP:57:ASP:OD1	26:AP:61:ASN:N	2.54	0.41
64:BU:16:VAL:HG13	64:BU:28:ARG:HG3	2.02	0.41
73:A6:303:PC1:H133	73:A6:303:PC1:O13	2.21	0.41
15:AE:371:GLU:OE1	15:AE:371:GLU:N	2.51	0.41
16:AF:138:ILE:HG22	16:AF:139:PRO:HD3	2.03	0.41
45:BB:198:LEU:HB3	47:BD:184:ILE:HG21	2.03	0.41
47:BD:112:ARG:NH2	67:BX:74:ASN:OD1	2.51	0.41
52:BI:57:ILE:CD1	52:BI:69:LEU:HD23	2.51	0.41
64:BU:8:GLN:N	64:BU:9:PRO:HD2	2.36	0.41
6:A5:279:LEU:HD11	26:AP:46:ARG:HE	1.86	0.40
13:AC:397:LEU:HD23	13:AC:397:LEU:O	2.21	0.40
14:AD:384:THR:CG2	14:AD:385:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AE:135:ALA:HB1	15:AE:147:VAL:HA	2.03	0.40
21:AK:212:GLU:HB3	23:AM:50:LEU:HD11	2.04	0.40
35:AY:14:LEU:O	35:AY:18:ILE:HG12	2.22	0.40
52:BI:42:ILE:HG22	52:BI:60:PHE:CZ	2.56	0.40
18:AH:123:LEU:HD13	18:AH:171:VAL:HG13	2.03	0.40
6:A5:248:VAL:HG22	6:A5:248:VAL:O	2.21	0.40
8:A7:236:LYS:HE2	8:A7:238:LEU:HD22	2.04	0.40
11:AA:425:ALA:O	11:AA:429:ILE:HG23	2.22	0.40
11:AA:497:VAL:HG21	11:AA:595:LEU:HD21	2.03	0.40
14:AD:382:GLN:N	79:AD:501:SF4:S4	2.94	0.40
16:AF:238:TYR:O	39:B2:50:LYS:NZ	2.41	0.40
20:AJ:154:ILE:N	20:AJ:154:ILE:HD12	2.37	0.40
45:BB:165:LEU:HD21	67:BX:95:TYR:HA	2.04	0.40
57:BN:70:VAL:HG13	57:BN:71:TRP:N	2.36	0.40
1:A0:242:ILE:HD11	1:A0:462:VAL:HG21	2.03	0.40
3:A2:160:VAL:HG11	3:A2:163:LYS:HD2	2.04	0.40
4:A3:37:TYR:O	4:A3:41:ASN:N	2.55	0.40
5:A4:130:PHE:HE2	5:A4:167:SER:HG	1.67	0.40
12:AB:54:CYS:HB3	12:AB:59:VAL:HG13	2.03	0.40
12:AB:74:GLY:HA2	78:AB:801:FES:S2	2.62	0.40
15:AE:362:LYS:O	15:AE:366:LYS:O	2.39	0.40
18:AH:22:LEU:HD21	34:AX:15:ILE:HG21	2.04	0.40
24:AN:86:LEU:HD11	24:AN:110:MET:HE1	2.03	0.40
47:BD:59:GLN:O	59:BP:126:ALA:N	2.54	0.40
49:BF:111:ARG:HB2	49:BF:117:ALA:HB2	2.04	0.40
6:A5:30:THR:HG21	26:AP:72:LYS:CD	2.52	0.40
7:A6:135:LEU:HD12	66:BW:119:LEU:HB3	2.03	0.40
9:A8:131:ALA:O	9:A8:159:HIS:NE2	2.51	0.40
30:AT:2:ARG:NH1	30:AT:161:THR:O	2.50	0.40
45:BB:170:PRO:HB2	49:BF:62:ILE:HD12	2.03	0.40
55:BL:86:PHE:N	70:BL:301:CDL:OA4	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A0	501/516 (97%)	486 (97%)	15 (3%)	0	100	100
2	A1	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
3	A2	263/317 (83%)	260 (99%)	3 (1%)	0	100	100
4	A3	289/333 (87%)	285 (99%)	4 (1%)	0	100	100
5	A4	309/311 (99%)	302 (98%)	7 (2%)	0	100	100
6	A5	280/282 (99%)	279 (100%)	1 (0%)	0	100	100
7	A6	228/251 (91%)	224 (98%)	4 (2%)	0	100	100
8	A7	131/238 (55%)	129 (98%)	2 (2%)	0	100	100
9	A8	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
10	A9	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
11	AA	711/750 (95%)	691 (97%)	19 (3%)	1 (0%)	51	81
12	AB	686/718 (96%)	671 (98%)	15 (2%)	0	100	100
13	AC	503/505 (100%)	490 (97%)	13 (3%)	0	100	100
14	AD	439/474 (93%)	425 (97%)	14 (3%)	0	100	100
15	AE	439/442 (99%)	430 (98%)	9 (2%)	0	100	100
16	AF	357/360 (99%)	348 (98%)	9 (2%)	0	100	100
17	AG	344/346 (99%)	339 (98%)	5 (2%)	0	100	100
18	AH	281/284 (99%)	273 (97%)	8 (3%)	0	100	100
19	AI	229/274 (84%)	228 (100%)	1 (0%)	0	100	100
20	AJ	252/255 (99%)	246 (98%)	6 (2%)	0	100	100
21	AK	228/257 (89%)	220 (96%)	8 (4%)	0	100	100
22	AL	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
23	AM	229/233 (98%)	220 (96%)	8 (4%)	1 (0%)	34	66
24	AN	155/206 (75%)	155 (100%)	0	0	100	100
25	AO	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
26	AP	189/194 (97%)	183 (97%)	6 (3%)	0	100	100
27	AQ	185/189 (98%)	182 (98%)	3 (2%)	0	100	100
28	AR	179/185 (97%)	177 (99%)	2 (1%)	0	100	100
29	AS	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
30	AT	159/162 (98%)	152 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
32	AV	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
33	AW	96/133 (72%)	94 (98%)	2 (2%)	0	100	100
34	AX	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
35	AY	114/116 (98%)	114 (100%)	0	0	100	100
36	AZ	92/103 (89%)	89 (97%)	3 (3%)	0	100	100
37	B0	91/94 (97%)	91 (100%)	0	0	100	100
38	B1	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
39	B2	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
40	B3	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
41	B4	71/73 (97%)	71 (100%)	0	0	100	100
42	B5	52/71 (73%)	52 (100%)	0	0	100	100
43	B6	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
44	BA	197/212 (93%)	194 (98%)	3 (2%)	0	100	100
45	BB	165/214 (77%)	164 (99%)	1 (1%)	0	100	100
46	BC	171/207 (83%)	170 (99%)	1 (1%)	0	100	100
47	BD	146/205 (71%)	145 (99%)	1 (1%)	0	100	100
48	BE	166/189 (88%)	160 (96%)	6 (4%)	0	100	100
49	BF	175/188 (93%)	167 (95%)	8 (5%)	0	100	100
50	BG	158/175 (90%)	154 (98%)	4 (2%)	0	100	100
51	BH	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
52	BI	147/172 (86%)	145 (99%)	2 (1%)	0	100	100
53	BJ	142/166 (86%)	142 (100%)	0	0	100	100
54	BK	107/144 (74%)	106 (99%)	1 (1%)	0	100	100
55	BL	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
56	BM	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
57	BN	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
58	BO	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
59	BP	70/129 (54%)	69 (99%)	1 (1%)	0	100	100
60	BQ	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
61	BR	89/132 (67%)	88 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	BS	118/126 (94%)	115 (98%)	3 (2%)	0	100	100
63	BT	123/125 (98%)	123 (100%)	0	0	100	100
64	BU	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
65	BV	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
66	BW	116/120 (97%)	111 (96%)	5 (4%)	0	100	100
67	BX	94/113 (83%)	93 (99%)	1 (1%)	0	100	100
68	BY	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
69	BZ	100/102 (98%)	100 (100%)	0	0	100	100
All	All	13572/14758 (92%)	13286 (98%)	284 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	AA	119	GLU
23	AM	51	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	441/454 (97%)	433 (98%)	8 (2%)	59	86
2	A1	288/311 (93%)	287 (100%)	1 (0%)	92	98
3	A2	225/270 (83%)	222 (99%)	3 (1%)	69	91
4	A3	244/280 (87%)	242 (99%)	2 (1%)	81	94
5	A4	275/275 (100%)	273 (99%)	2 (1%)	84	95
6	A5	257/257 (100%)	257 (100%)	0	100	100
7	A6	207/223 (93%)	206 (100%)	1 (0%)	88	96
8	A7	122/224 (54%)	122 (100%)	0	100	100
9	A8	195/195 (100%)	194 (100%)	1 (0%)	88	96
10	A9	199/199 (100%)	195 (98%)	4 (2%)	55	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AA	657/694 (95%)	644 (98%)	13 (2%)	55	84
12	AB	589/617 (96%)	586 (100%)	3 (0%)	88	96
13	AC	463/463 (100%)	458 (99%)	5 (1%)	73	92
14	AD	361/392 (92%)	359 (99%)	2 (1%)	86	96
15	AE	398/399 (100%)	389 (98%)	9 (2%)	50	82
16	AF	346/347 (100%)	346 (100%)	0	100	100
17	AG	309/309 (100%)	307 (99%)	2 (1%)	86	96
18	AH	249/250 (100%)	245 (98%)	4 (2%)	62	88
19	AI	206/236 (87%)	205 (100%)	1 (0%)	88	96
20	AJ	243/244 (100%)	242 (100%)	1 (0%)	91	97
21	AK	196/218 (90%)	194 (99%)	2 (1%)	76	93
22	AL	197/215 (92%)	194 (98%)	3 (2%)	65	89
23	AM	196/197 (100%)	193 (98%)	3 (2%)	65	89
24	AN	146/186 (78%)	146 (100%)	0	100	100
25	AO	191/191 (100%)	191 (100%)	0	100	100
26	AP	168/170 (99%)	168 (100%)	0	100	100
27	AQ	170/172 (99%)	168 (99%)	2 (1%)	71	92
28	AR	159/163 (98%)	158 (99%)	1 (1%)	86	96
29	AS	154/154 (100%)	152 (99%)	2 (1%)	69	91
30	AT	136/137 (99%)	131 (96%)	5 (4%)	34	68
31	AU	132/133 (99%)	131 (99%)	1 (1%)	81	94
32	AV	104/129 (81%)	104 (100%)	0	100	100
33	AW	87/119 (73%)	87 (100%)	0	100	100
34	AX	112/112 (100%)	109 (97%)	3 (3%)	44	78
35	AY	108/108 (100%)	108 (100%)	0	100	100
36	AZ	84/93 (90%)	84 (100%)	0	100	100
37	B0	88/89 (99%)	88 (100%)	0	100	100
38	B1	83/84 (99%)	82 (99%)	1 (1%)	71	92
39	B2	82/83 (99%)	82 (100%)	0	100	100
40	B3	66/74 (89%)	66 (100%)	0	100	100
41	B4	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	B5	48/63 (76%)	48 (100%)	0	100	100
43	B6	55/55 (100%)	54 (98%)	1 (2%)	59	86
44	BA	179/190 (94%)	178 (99%)	1 (1%)	86	96
45	BB	145/182 (80%)	145 (100%)	0	100	100
46	BC	155/180 (86%)	154 (99%)	1 (1%)	86	96
47	BD	124/179 (69%)	123 (99%)	1 (1%)	81	94
48	BE	159/178 (89%)	157 (99%)	2 (1%)	69	91
49	BF	161/172 (94%)	161 (100%)	0	100	100
50	BG	142/156 (91%)	141 (99%)	1 (1%)	84	95
51	BH	170/170 (100%)	170 (100%)	0	100	100
52	BI	131/152 (86%)	130 (99%)	1 (1%)	81	94
53	BJ	128/147 (87%)	127 (99%)	1 (1%)	81	94
54	BK	97/131 (74%)	97 (100%)	0	100	100
55	BL	124/125 (99%)	123 (99%)	1 (1%)	81	94
56	BM	108/114 (95%)	107 (99%)	1 (1%)	78	94
57	BN	120/122 (98%)	120 (100%)	0	100	100
58	BO	122/122 (100%)	122 (100%)	0	100	100
59	BP	64/117 (55%)	64 (100%)	0	100	100
60	BQ	93/117 (80%)	93 (100%)	0	100	100
61	BR	81/116 (70%)	80 (99%)	1 (1%)	71	92
62	BS	103/109 (94%)	103 (100%)	0	100	100
63	BT	110/110 (100%)	103 (94%)	7 (6%)	17	45
64	BU	121/121 (100%)	120 (99%)	1 (1%)	81	94
65	BV	102/102 (100%)	102 (100%)	0	100	100
66	BW	98/99 (99%)	98 (100%)	0	100	100
67	BX	81/97 (84%)	81 (100%)	0	100	100
68	BY	98/98 (100%)	98 (100%)	0	100	100
69	BZ	89/89 (100%)	89 (100%)	0	100	100
All	All	12206/13144 (93%)	12101 (99%)	105 (1%)	79	94

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	421	ASP
1	A0	447	MET
1	A0	452	ASN
1	A0	455	ASP
1	A0	456	ASN
1	A0	458	VAL
1	A0	462	VAL
1	A0	465	LEU
2	A1	295	LEU
3	A2	68	ARG
3	A2	175	PHE
3	A2	194	ASP
4	A3	286	ASP
4	A3	289	ILE
5	A4	70	ASN
5	A4	95	HIS
7	A6	102	PHE
9	A8	301	GLU
10	A9	31	LYS
10	A9	32	LYS
10	A9	80	LYS
10	A9	134	ARG
11	AA	156	THR
11	AA	160	ARG
11	AA	163	ASN
11	AA	165	ASP
11	AA	172	ILE
11	AA	276	PHE
11	AA	363	ASN
11	AA	385	TYR
11	AA	386	TRP
11	AA	401	CYS
11	AA	522	PHE
11	AA	605	TYR
11	AA	706	PHE
12	AB	65	CYS
12	AB	76	CYS
12	AB	386	LEU
13	AC	118	PHE
13	AC	205	TRP
13	AC	229	PHE
13	AC	346	TYR
13	AC	363	PHE

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Mol	Chain	Res	Type
14	AD	380	CYS
14	AD	426	CYS
15	AE	9	TRP
15	AE	83	ASP
15	AE	87	TYR
15	AE	130	HIS
15	AE	191	ASP
15	AE	278	ASP
15	AE	368	LEU
15	AE	404	ARG
15	AE	432	THR
17	AG	52	ASN
17	AG	109	ASP
18	AH	166	PHE
18	AH	167	LEU
18	AH	207	PHE
18	AH	245	TYR
19	AI	215	VAL
20	AJ	162	PHE
21	AK	85	ASN
21	AK	130	TYR
22	AL	94	PHE
22	AL	155	THR
22	AL	175	CYS
23	AM	44	SER
23	AM	172	LEU
23	AM	216	LYS
27	AQ	5	TYR
27	AQ	22	TYR
28	AR	94	HIS
29	AS	19	ASN
29	AS	80	PHE
30	AT	31	CYS
30	AT	42	SER
30	AT	46	PHE
30	AT	102	TYR
30	AT	144	LEU
31	AU	50	PHE
34	AX	1	MET
34	AX	3	ASP
34	AX	57	ILE
38	B1	33	TYR

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Mol	Chain	Res	Type
43	B6	27	TYR
44	BA	212	TYR
46	BC	36	SER
47	BD	149	LEU
48	BE	122	ASP
48	BE	133	ASN
50	BG	87	ARG
52	BI	81	CYS
53	BJ	122	HIS
55	BL	105	PHE
56	BM	10	PHE
61	BR	94	ASN
63	BT	40	GLN
63	BT	48	ASN
63	BT	52	VAL
63	BT	63	PHE
63	BT	122	LYS
63	BT	134	ASN
63	BT	141	GLN
64	BU	96	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	450	GLN
1	A0	452	ASN
5	A4	283	HIS
11	AA	168	ASN
27	AQ	63	ASN
61	BR	109	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 77 ligands modelled in this entry, 3 are monoatomic - leaving 74 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	$\#\|Z\| > 2$
70	CDL	A1	402	-	99,99,99	1.20	7 (7%)	105,111,111	0.68	2 (1%)
70	CDL	AF	401	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	1 (0%)
73	PC1	A6	303	-	53,53,53	1.07	3 (5%)	59,61,61	0.60	1 (1%)
73	PC1	AQ	202	-	53,53,53	1.09	3 (5%)	59,61,61	0.63	1 (1%)
75	3PE	BA	301	-	50,50,50	1.06	5 (10%)	53,55,55	0.58	0
70	CDL	AC	802	-	99,99,99	1.18	7 (7%)	105,111,111	0.67	0
70	CDL	BC	302	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	1 (0%)
70	CDL	BY	201	-	99,99,99	1.20	8 (8%)	105,111,111	0.73	2 (1%)
71	UDP	A0	603	72	24,26,26	3.62	14 (58%)	37,40,40	1.49	5 (13%)
73	PC1	A9	604	-	53,53,53	1.05	3 (5%)	59,61,61	0.63	0
74	NDP	A1	401	-	45,52,52	4.23	20 (44%)	53,80,80	1.66	5 (9%)
70	CDL	BC	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.74	1 (0%)
70	CDL	AM	301	-	99,99,99	1.21	9 (9%)	105,111,111	0.69	2 (1%)
70	CDL	B0	101	-	99,99,99	1.19	7 (7%)	105,111,111	0.72	2 (1%)
70	CDL	BT	201	-	99,99,99	1.21	8 (8%)	105,111,111	0.67	2 (1%)
73	PC1	A0	605	-	53,53,53	1.07	3 (5%)	59,61,61	0.59	0
76	LPP	AA	902	-	43,43,43	0.91	3 (6%)	47,48,48	0.71	1 (2%)
73	PC1	AU	201	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	BY	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.61	1 (1%)
75	3PE	A2	401	-	50,50,50	1.07	5 (10%)	53,55,55	0.65	1 (1%)
81	8Q1	AS	200	-	27,33,34	1.59	4 (14%)	32,40,43	1.53	6 (18%)
76	LPP	A6	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.93	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
73	PC1	BS	1301	-	53,53,53	1.04	3 (5%)	59,61,61	0.66	2 (3%)
75	3PE	A9	603	-	50,50,50	1.07	5 (10%)	53,55,55	0.66	1 (1%)
73	PC1	AA	904	-	53,53,53	1.04	3 (5%)	59,61,61	0.72	1 (1%)
73	PC1	B1	403	-	53,53,53	1.07	3 (5%)	59,61,61	0.54	0
70	CDL	BV	201	-	99,99,99	1.17	7 (7%)	105,111,111	0.66	0
77	ADP	A8	401	72	24,29,29	3.56	10 (41%)	29,45,45	3.39	6 (20%)
79	SF4	AL	301	22	0,12,12	-	-	-		
70	CDL	B0	102	-	99,99,99	1.19	7 (7%)	105,111,111	0.68	2 (1%)
70	CDL	BL	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.72	2 (1%)
70	CDL	AC	801	-	99,99,99	1.15	7 (7%)	105,111,111	0.74	2 (1%)
73	PC1	A2	402	-	53,53,53	1.05	3 (5%)	59,61,61	0.62	0
73	PC1	BT	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.71	2 (3%)
73	PC1	AA	905	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	AM	302	-	53,53,53	1.06	3 (5%)	59,61,61	0.62	1 (1%)
78	FES	BI	201	52	0,4,4	-	-	-		
76	LPP	BN	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.73	1 (2%)
79	SF4	AD	501	14	0,12,12	-	-	-		
70	CDL	AF	402	-	99,99,99	1.19	7 (7%)	105,111,111	0.70	2 (1%)
73	PC1	BS	1302	-	53,53,53	1.06	3 (5%)	59,61,61	0.60	1 (1%)
79	SF4	AB	802	12	0,12,12	-	-	-		
73	PC1	AU	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.62	0
70	CDL	AP	301	-	99,99,99	1.17	6 (6%)	105,111,111	0.75	0
70	CDL	BG	201	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	3 (2%)
79	SF4	AT	201	30	0,12,12	-	-	-		
73	PC1	A1	404	-	53,53,53	1.06	3 (5%)	59,61,61	0.75	2 (3%)
77	ADP	AQ	201	-	24,29,29	3.55	9 (37%)	29,45,45	3.43	7 (24%)
80	FMN	AD	502	-	33,33,33	0.72	0	48,50,50	0.78	0
78	FES	AB	801	12	0,4,4	-	-	-		
73	PC1	A9	601	-	53,53,53	1.07	3 (5%)	59,61,61	0.58	1 (1%)
73	PC1	BQ	401	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	AA	903	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
70	CDL	AA	908	-	99,99,99	1.16	6 (6%)	105,111,111	0.68	1 (0%)
76	LPP	AL	304	-	43,43,43	0.90	3 (6%)	47,48,48	0.68	1 (2%)
73	PC1	A1	403	-	53,53,53	1.09	3 (5%)	59,61,61	0.62	1 (1%)
79	SF4	AL	302	22	0,12,12	-	-	-		
73	PC1	AH	301	-	53,53,53	1.07	3 (5%)	59,61,61	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
78	FES	AI	301	19	0,4,4	-	-	-		
70	CDL	BE	201	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	2 (1%)
73	PC1	AA	907	-	53,53,53	1.07	3 (5%)	59,61,61	0.56	1 (1%)
73	PC1	AJ	501	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
73	PC1	AL	303	-	53,53,53	1.06	3 (5%)	59,61,61	0.72	1 (1%)
70	CDL	A0	601	-	99,99,99	1.17	7 (7%)	105,111,111	0.77	1 (0%)
70	CDL	AA	901	-	99,99,99	1.19	7 (7%)	105,111,111	0.74	2 (1%)
73	PC1	B1	401	-	53,53,53	1.07	3 (5%)	59,61,61	0.68	1 (1%)
70	CDL	B1	402	-	99,99,99	1.19	7 (7%)	105,111,111	0.64	1 (0%)
73	PC1	A6	302	-	53,53,53	1.08	3 (5%)	59,61,61	0.66	1 (1%)
79	SF4	AB	803	12	0,12,12	-	-	-		
73	PC1	AA	906	-	53,53,53	1.06	3 (5%)	59,61,61	0.68	1 (1%)
70	CDL	A0	602	-	99,99,99	1.19	8 (8%)	105,111,111	0.75	2 (1%)
75	3PE	AJ	502	-	50,50,50	1.05	5 (10%)	53,55,55	0.71	1 (1%)
75	3PE	A9	602	-	50,50,50	1.09	5 (10%)	53,55,55	1.01	5 (9%)
75	3PE	BP	201	-	50,50,50	1.07	5 (10%)	53,55,55	0.71	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	A1	402	-	-	33/110/110/110	-
70	CDL	AF	401	-	-	20/110/110/110	-
73	PC1	A6	303	-	-	9/57/57/57	-
73	PC1	AQ	202	-	-	18/57/57/57	-
75	3PE	BA	301	-	-	19/54/54/54	-
70	CDL	AC	802	-	-	26/110/110/110	-
70	CDL	BC	302	-	-	23/110/110/110	-
70	CDL	BY	201	-	-	21/110/110/110	-
71	UDP	A0	603	72	-	7/16/32/32	0/2/2/2
73	PC1	A9	604	-	-	20/57/57/57	-
74	NDP	A1	401	-	-	7/30/77/77	0/5/5/5
70	CDL	BC	301	-	-	19/110/110/110	-
70	CDL	AM	301	-	-	26/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	B0	101	-	-	30/110/110/110	-
70	CDL	BT	201	-	-	21/110/110/110	-
73	PC1	A0	605	-	-	14/57/57/57	-
76	LPP	AA	902	-	-	10/45/45/45	-
73	PC1	AU	201	-	-	12/57/57/57	-
73	PC1	BY	202	-	-	12/57/57/57	-
75	3PE	A2	401	-	-	8/54/54/54	-
81	8Q1	AS	200	-	-	10/38/40/41	-
76	LPP	A6	301	-	-	9/45/45/45	-
73	PC1	BS	1301	-	-	16/57/57/57	-
75	3PE	A9	603	-	-	7/54/54/54	-
73	PC1	AA	904	-	-	15/57/57/57	-
73	PC1	B1	403	-	-	15/57/57/57	-
70	CDL	BV	201	-	-	18/110/110/110	-
77	ADP	A8	401	72	-	0/12/32/32	0/3/3/3
79	SF4	AL	301	22	-	-	0/6/5/5
70	CDL	B0	102	-	-	21/110/110/110	-
70	CDL	BL	301	-	-	17/110/110/110	-
70	CDL	AC	801	-	-	25/110/110/110	-
73	PC1	A2	402	-	-	8/57/57/57	-
73	PC1	BT	202	-	-	13/57/57/57	-
73	PC1	AA	905	-	-	17/57/57/57	-
73	PC1	AM	302	-	-	17/57/57/57	-
78	FES	BI	201	52	-	-	0/1/1/1
76	LPP	BN	301	-	-	7/45/45/45	-
79	SF4	AD	501	14	-	-	0/6/5/5
70	CDL	AF	402	-	-	27/110/110/110	-
73	PC1	BS	1302	-	-	10/57/57/57	-
79	SF4	AB	802	12	-	-	0/6/5/5
73	PC1	AU	202	-	-	13/57/57/57	-
70	CDL	AP	301	-	-	24/110/110/110	-
70	CDL	BG	201	-	-	36/110/110/110	-
79	SF4	AT	201	30	-	-	0/6/5/5
73	PC1	A1	404	-	-	13/57/57/57	-
77	ADP	AQ	201	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	FMN	AD	502	-	-	7/18/18/18	0/3/3/3
78	FES	AB	801	12	-	-	0/1/1/1
73	PC1	A9	601	-	-	15/57/57/57	-
73	PC1	BQ	401	-	-	21/57/57/57	-
73	PC1	AA	903	-	-	14/57/57/57	-
70	CDL	AA	908	-	-	31/110/110/110	-
76	LPP	AL	304	-	-	4/45/45/45	-
73	PC1	A1	403	-	-	6/57/57/57	-
79	SF4	AL	302	22	-	-	0/6/5/5
73	PC1	AH	301	-	-	8/57/57/57	-
78	FES	AI	301	19	-	-	0/1/1/1
70	CDL	BE	201	-	-	31/110/110/110	-
73	PC1	AA	907	-	-	21/57/57/57	-
73	PC1	AJ	501	-	-	17/57/57/57	-
73	PC1	AL	303	-	-	9/57/57/57	-
70	CDL	A0	601	-	-	21/110/110/110	-
70	CDL	AA	901	-	-	23/110/110/110	-
73	PC1	B1	401	-	-	18/57/57/57	-
70	CDL	B1	402	-	-	26/110/110/110	-
73	PC1	A6	302	-	-	11/57/57/57	-
79	SF4	AB	803	12	-	-	0/6/5/5
73	PC1	AA	906	-	-	20/57/57/57	-
70	CDL	A0	602	-	-	25/110/110/110	-
75	3PE	AJ	502	-	-	12/54/54/54	-
75	3PE	A9	602	-	-	16/54/54/54	-
75	3PE	BP	201	-	-	13/54/54/54	-

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	A1	401	NDP	O4B-C1B	14.77	1.61	1.41
74	A1	401	NDP	C6N-C5N	12.07	1.54	1.33
77	AQ	201	ADP	C2’-C3’	-11.05	1.23	1.53
77	A8	401	ADP	C2’-C3’	-10.99	1.23	1.53
74	A1	401	NDP	C2D-C3D	-10.66	1.24	1.53
71	A0	603	UDP	C3’-C2’	-8.28	1.30	1.53
71	A0	603	UDP	C2-N1	6.54	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	A0	603	UDP	C2-N3	6.51	1.49	1.38
74	A1	401	NDP	C2N-C3N	6.50	1.53	1.34
77	A8	401	ADP	O4'-C1'	6.45	1.50	1.41
77	AQ	201	ADP	O4'-C1'	6.27	1.49	1.41
74	A1	401	NDP	O4D-C4D	-6.20	1.31	1.45
77	AQ	201	ADP	O4'-C4'	-6.11	1.31	1.45
74	A1	401	NDP	O4B-C4B	-6.09	1.31	1.45
77	A8	401	ADP	O4'-C4'	-6.02	1.31	1.45
71	A0	603	UDP	C6-C5	5.84	1.48	1.35
77	A8	401	ADP	C3'-C4'	5.41	1.66	1.53
74	A1	401	NDP	C7N-N7N	5.38	1.47	1.33
77	AQ	201	ADP	C3'-C4'	5.35	1.66	1.53
74	A1	401	NDP	C3D-C4D	5.09	1.66	1.53
81	AS	200	8Q1	C34-N36	4.97	1.44	1.33
77	A8	401	ADP	C2'-C1'	4.82	1.61	1.53
71	A0	603	UDP	O4'-C1'	-4.77	1.30	1.42
77	AQ	201	ADP	C2'-C1'	4.76	1.61	1.53
74	A1	401	NDP	C6N-N1N	4.52	1.48	1.37
71	A0	603	UDP	O4'-C4'	4.50	1.55	1.45
81	AS	200	8Q1	C39-N41	4.47	1.43	1.33
71	A0	603	UDP	C4-N3	4.22	1.46	1.38
74	A1	401	NDP	C1D-N1N	-3.97	1.35	1.46
77	A8	401	ADP	O2'-C2'	3.80	1.51	1.43
70	BC	301	CDL	OA8-CA7	3.70	1.44	1.33
74	A1	401	NDP	O2D-C2D	3.70	1.51	1.43
73	A1	403	PC1	O31-C31	3.69	1.44	1.33
70	AF	401	CDL	OA8-CA7	3.68	1.44	1.33
77	AQ	201	ADP	O2'-C2'	3.66	1.51	1.43
74	A1	401	NDP	P2B-O2B	3.63	1.66	1.59
70	AF	402	CDL	OA8-CA7	3.62	1.43	1.33
70	B0	101	CDL	OA8-CA7	3.62	1.43	1.33
73	A1	404	PC1	O31-C31	3.60	1.43	1.33
70	AA	901	CDL	OA8-CA7	3.60	1.43	1.33
70	AC	801	CDL	OA8-CA7	3.59	1.43	1.33
70	B1	402	CDL	OA8-CA7	3.59	1.43	1.33
70	BY	201	CDL	OA8-CA7	3.58	1.43	1.33
70	AF	401	CDL	OB8-CB7	3.57	1.43	1.33
70	AM	301	CDL	OA8-CA7	3.56	1.43	1.33
70	BT	201	CDL	OA8-CA7	3.55	1.43	1.33
73	A9	604	PC1	O31-C31	3.53	1.43	1.33
73	BT	202	PC1	O31-C31	3.53	1.43	1.33
70	B0	102	CDL	OA8-CA7	3.53	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	BV	201	CDL	OA8-CA7	3.51	1.43	1.33
73	AA	906	PC1	O31-C31	3.50	1.43	1.33
70	BL	301	CDL	OA8-CA7	3.49	1.43	1.33
73	AM	302	PC1	O31-C31	3.49	1.43	1.33
73	AA	904	PC1	O31-C31	3.49	1.43	1.33
70	A0	602	CDL	OA8-CA7	3.48	1.43	1.33
70	AC	802	CDL	OA8-CA7	3.48	1.43	1.33
70	A1	402	CDL	OA8-CA7	3.47	1.43	1.33
73	AQ	202	PC1	O31-C31	3.47	1.43	1.33
70	AA	908	CDL	OA8-CA7	3.45	1.43	1.33
70	BG	201	CDL	OA8-CA7	3.45	1.43	1.33
73	BS	1302	PC1	O31-C31	3.45	1.43	1.33
73	AL	303	PC1	O31-C31	3.45	1.43	1.33
73	A9	601	PC1	O31-C31	3.44	1.43	1.33
75	A9	602	3PE	O31-C31	3.44	1.43	1.33
73	A2	402	PC1	O31-C31	3.44	1.43	1.33
70	BC	302	CDL	OA8-CA7	3.43	1.43	1.33
73	AA	903	PC1	O31-C31	3.43	1.43	1.33
70	AP	301	CDL	OB8-CB7	3.43	1.43	1.33
70	A0	601	CDL	OA8-CA7	3.42	1.43	1.33
73	A6	303	PC1	O31-C31	3.41	1.43	1.33
73	A6	302	PC1	O31-C31	3.41	1.43	1.33
70	BE	201	CDL	OA8-CA7	3.40	1.43	1.33
77	A8	401	ADP	O3'-C3'	3.40	1.51	1.43
74	A1	401	NDP	O4D-C1D	3.38	1.50	1.42
75	BP	201	3PE	O31-C31	3.38	1.43	1.33
70	AA	901	CDL	OB8-CB7	3.38	1.43	1.33
70	AM	301	CDL	OB6-CB5	3.37	1.43	1.34
73	B1	403	PC1	O31-C31	3.37	1.43	1.33
73	AU	202	PC1	O31-C31	3.37	1.43	1.33
70	A0	602	CDL	OB8-CB7	3.37	1.43	1.33
73	AU	201	PC1	O31-C31	3.37	1.43	1.33
73	BS	1301	PC1	O31-C31	3.35	1.43	1.33
70	BT	201	CDL	OB6-CB5	3.35	1.43	1.34
73	B1	401	PC1	O31-C31	3.35	1.43	1.33
77	AQ	201	ADP	O3'-C3'	3.35	1.50	1.43
73	BQ	401	PC1	O31-C31	3.34	1.43	1.33
73	A0	605	PC1	O31-C31	3.34	1.43	1.33
73	AJ	501	PC1	O31-C31	3.34	1.43	1.33
70	BE	201	CDL	OB8-CB7	3.34	1.43	1.33
70	BC	302	CDL	OB8-CB7	3.33	1.43	1.33
73	AA	905	PC1	O31-C31	3.31	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	AH	301	PC1	O31-C31	3.31	1.43	1.33
73	BY	202	PC1	O31-C31	3.29	1.43	1.33
70	AA	908	CDL	OB8-CB7	3.29	1.43	1.33
73	AA	907	PC1	O31-C31	3.29	1.42	1.33
70	AM	301	CDL	OA6-CA5	3.28	1.43	1.34
70	BT	201	CDL	OB8-CB7	3.28	1.42	1.33
75	BA	301	3PE	O21-C2	-3.27	1.38	1.46
75	A9	603	3PE	O31-C31	3.27	1.42	1.33
70	BG	201	CDL	OB8-CB7	3.26	1.42	1.33
70	BC	301	CDL	OB8-CB7	3.26	1.42	1.33
71	A0	603	UDP	C5'-C4'	-3.26	1.41	1.51
70	B0	101	CDL	OB8-CB7	3.25	1.42	1.33
75	A2	401	3PE	O31-C31	3.24	1.42	1.33
70	BC	302	CDL	OB6-CB5	3.24	1.43	1.34
70	BY	201	CDL	OB6-CB5	3.24	1.43	1.34
70	A0	601	CDL	OB8-CB7	3.24	1.42	1.33
70	AP	301	CDL	OB6-CB5	3.23	1.43	1.34
70	BY	201	CDL	OB8-CB7	3.23	1.42	1.33
70	BC	301	CDL	OB6-CB5	3.23	1.43	1.34
70	AM	301	CDL	OB8-CB7	3.22	1.42	1.33
70	AP	301	CDL	OA8-CA7	3.21	1.42	1.33
70	BE	201	CDL	OA6-CA5	3.21	1.43	1.34
70	BV	201	CDL	OB6-CB5	3.21	1.43	1.34
70	AA	901	CDL	OA6-CA5	3.21	1.43	1.34
70	BL	301	CDL	OB6-CB5	3.20	1.43	1.34
70	BG	201	CDL	OB6-CB5	3.19	1.43	1.34
70	AF	402	CDL	OB8-CB7	3.17	1.42	1.33
70	AC	802	CDL	OA6-CA5	3.17	1.43	1.34
70	AF	401	CDL	OB6-CB5	3.17	1.43	1.34
70	AC	801	CDL	OB8-CB7	3.16	1.42	1.33
70	BE	201	CDL	OB6-CB5	3.16	1.43	1.34
70	AC	802	CDL	OB8-CB7	3.16	1.42	1.33
70	A0	601	CDL	OA6-CA5	3.15	1.43	1.34
70	B0	101	CDL	OB6-CB5	3.15	1.43	1.34
70	BY	201	CDL	OA6-CA5	3.14	1.43	1.34
70	BL	301	CDL	OA6-CA5	3.13	1.43	1.34
70	A1	402	CDL	OA6-CA5	3.13	1.43	1.34
70	A1	402	CDL	OB8-CB7	3.13	1.42	1.33
70	B0	102	CDL	OB8-CB7	3.12	1.42	1.33
70	B1	402	CDL	OB8-CB7	3.11	1.42	1.33
70	AF	402	CDL	OA6-CA5	3.11	1.43	1.34
75	AJ	502	3PE	O21-C2	-3.11	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	A2	401	3PE	O21-C2	-3.10	1.38	1.46
70	A0	602	CDL	OA6-CA5	3.10	1.43	1.34
70	B1	402	CDL	OB6-CB5	3.10	1.43	1.34
70	A1	402	CDL	OB6-CB5	3.09	1.43	1.34
70	BL	301	CDL	OB8-CB7	3.09	1.42	1.33
70	A0	602	CDL	OB6-CB5	3.09	1.43	1.34
70	AC	802	CDL	OB6-CB5	3.09	1.43	1.34
75	BA	301	3PE	O31-C31	3.09	1.42	1.33
75	A9	603	3PE	O21-C2	-3.08	1.38	1.46
70	B1	402	CDL	OA6-CA5	3.07	1.43	1.34
74	A1	401	NDP	O3B-C3B	-3.07	1.35	1.43
70	BC	302	CDL	OA6-CA5	3.06	1.42	1.34
70	BV	201	CDL	OB8-CB7	3.04	1.42	1.33
70	AF	402	CDL	OB6-CB5	3.04	1.42	1.34
70	B0	101	CDL	OA6-CA5	3.04	1.42	1.34
70	BC	301	CDL	OA6-CA5	3.04	1.42	1.34
70	AA	908	CDL	OB6-CB5	3.03	1.42	1.34
75	AJ	502	3PE	O31-C31	3.03	1.42	1.33
70	BG	201	CDL	OA6-CA5	3.03	1.42	1.34
70	BV	201	CDL	OA6-CA5	3.03	1.42	1.34
70	B0	102	CDL	OB6-CB5	3.01	1.42	1.34
70	AC	801	CDL	OA6-CA5	3.01	1.42	1.34
70	B0	102	CDL	OA6-CA5	3.01	1.42	1.34
70	A0	601	CDL	OB6-CB5	3.00	1.42	1.34
70	BT	201	CDL	OA6-CA5	3.00	1.42	1.34
70	AA	908	CDL	OA6-CA5	2.99	1.42	1.34
70	AA	901	CDL	OB6-CB5	2.97	1.42	1.34
70	AC	801	CDL	OB6-CB5	2.97	1.42	1.34
70	AP	301	CDL	OA6-CA5	2.97	1.42	1.34
74	A1	401	NDP	C5A-C4A	-2.95	1.33	1.40
71	A0	603	UDP	C2'-C1'	2.94	1.62	1.53
70	AF	401	CDL	OA6-CA5	2.92	1.42	1.34
71	A0	603	UDP	O3'-C3'	2.91	1.49	1.43
71	A0	603	UDP	O4-C4	-2.89	1.18	1.24
74	A1	401	NDP	C7N-C3N	2.84	1.54	1.48
71	A0	603	UDP	C6-N1	2.84	1.44	1.38
74	A1	401	NDP	O3D-C3D	2.81	1.49	1.43
73	AQ	202	PC1	O21-C21	2.74	1.42	1.34
76	AL	304	LPP	O9-C7	-2.72	1.39	1.46
73	AU	201	PC1	O21-C2	-2.66	1.39	1.46
73	B1	403	PC1	O21-C2	-2.66	1.39	1.46
75	A9	602	3PE	O21-C21	2.65	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	AU	202	PC1	O21-C2	-2.65	1.40	1.46
73	A9	601	PC1	O21-C2	-2.64	1.40	1.46
75	BP	201	3PE	O21-C21	2.63	1.41	1.34
74	A1	401	NDP	O7N-C7N	-2.62	1.18	1.24
71	A0	603	UDP	C5-C4	2.60	1.49	1.43
70	AC	802	CDL	OB6-CB4	-2.60	1.40	1.46
73	BY	202	PC1	O21-C2	-2.59	1.40	1.46
70	AF	402	CDL	OB6-CB4	-2.59	1.40	1.46
73	AA	906	PC1	O21-C21	2.59	1.41	1.34
76	BN	301	LPP	O9-C7	-2.57	1.40	1.46
73	AA	907	PC1	O21-C21	2.57	1.41	1.34
70	A0	601	CDL	OB6-CB4	-2.57	1.40	1.46
77	AQ	201	ADP	C5-C4	-2.57	1.34	1.40
76	AA	902	LPP	O9-C7	-2.57	1.40	1.46
73	AA	905	PC1	O21-C2	-2.55	1.40	1.46
73	BQ	401	PC1	O21-C2	-2.55	1.40	1.46
81	AS	200	8Q1	O40-C39	-2.54	1.18	1.23
70	B0	102	CDL	OB6-CB4	-2.54	1.40	1.46
73	AH	301	PC1	O21-C2	-2.54	1.40	1.46
76	A6	301	LPP	O9-C11	2.54	1.41	1.34
73	AH	301	PC1	O21-C21	2.53	1.41	1.34
73	A6	303	PC1	O21-C21	2.53	1.41	1.34
73	B1	401	PC1	O21-C2	-2.53	1.40	1.46
70	AC	801	CDL	OA6-CA4	-2.52	1.40	1.46
70	AC	801	CDL	OB6-CB4	-2.50	1.40	1.46
77	A8	401	ADP	C5-C4	-2.50	1.34	1.40
73	A6	302	PC1	O21-C2	-2.50	1.40	1.46
73	A0	605	PC1	O21-C2	-2.50	1.40	1.46
73	A9	604	PC1	O21-C21	2.50	1.41	1.34
75	BP	201	3PE	O21-C2	-2.49	1.40	1.46
70	B0	102	CDL	OA6-CA4	-2.49	1.40	1.46
77	A8	401	ADP	C6-N6	2.49	1.43	1.34
73	AA	903	PC1	O21-C2	-2.49	1.40	1.46
73	BT	202	PC1	O21-C2	-2.48	1.40	1.46
73	AA	907	PC1	O21-C2	-2.48	1.40	1.46
73	A0	605	PC1	O21-C21	2.48	1.41	1.34
70	BC	301	CDL	OB6-CB4	-2.48	1.40	1.46
70	BG	201	CDL	OB6-CB4	-2.48	1.40	1.46
73	BS	1302	PC1	O21-C21	2.47	1.41	1.34
73	BS	1302	PC1	O21-C2	-2.47	1.40	1.46
73	AM	302	PC1	O21-C21	2.47	1.41	1.34
70	B1	402	CDL	OB6-CB4	-2.47	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	A2	401	3PE	O21-C21	2.47	1.41	1.34
70	BV	201	CDL	OA6-CA4	-2.47	1.40	1.46
73	A1	403	PC1	O21-C2	-2.46	1.40	1.46
73	AM	302	PC1	O21-C2	-2.46	1.40	1.46
70	BL	301	CDL	OB6-CB4	-2.46	1.40	1.46
73	AJ	501	PC1	O21-C2	-2.46	1.40	1.46
70	AA	901	CDL	OB6-CB4	-2.46	1.40	1.46
73	AA	905	PC1	O21-C21	2.46	1.41	1.34
73	A6	302	PC1	O21-C21	2.45	1.41	1.34
73	B1	401	PC1	O21-C21	2.45	1.41	1.34
73	AA	904	PC1	O21-C2	-2.44	1.40	1.46
73	AL	303	PC1	O21-C2	-2.43	1.40	1.46
71	A0	603	UDP	O2-C2	-2.42	1.18	1.23
77	AQ	201	ADP	C6-N6	2.42	1.42	1.34
73	AA	903	PC1	O21-C21	2.42	1.41	1.34
73	AA	904	PC1	O21-C21	2.42	1.41	1.34
75	A9	602	3PE	P-O11	2.41	1.69	1.59
75	A9	603	3PE	O21-C21	2.41	1.41	1.34
70	A1	402	CDL	OA6-CA4	-2.41	1.40	1.46
70	AF	401	CDL	OA6-CA4	-2.40	1.40	1.46
70	AA	908	CDL	OA6-CA4	-2.40	1.40	1.46
73	BS	1301	PC1	O21-C2	-2.40	1.40	1.46
73	BS	1301	PC1	O21-C21	2.39	1.41	1.34
76	AA	902	LPP	O27-C29	2.39	1.40	1.33
73	A2	402	PC1	O21-C2	-2.39	1.40	1.46
73	AL	303	PC1	O21-C21	2.38	1.41	1.34
74	A1	401	NDP	C6A-N6A	2.38	1.42	1.34
73	A6	303	PC1	O21-C2	-2.38	1.40	1.46
76	BN	301	LPP	O27-C8	-2.38	1.39	1.45
70	BV	201	CDL	OB6-CB4	-2.38	1.40	1.46
73	AJ	501	PC1	O21-C21	2.37	1.41	1.34
81	AS	200	8Q1	O35-C34	-2.37	1.18	1.23
73	BQ	401	PC1	O21-C21	2.37	1.41	1.34
73	AU	202	PC1	O21-C21	2.37	1.41	1.34
76	AL	304	LPP	O27-C8	-2.36	1.39	1.45
70	BT	201	CDL	OB6-CB4	-2.36	1.40	1.46
73	A1	403	PC1	O21-C21	2.36	1.41	1.34
76	AL	304	LPP	O27-C29	2.36	1.40	1.33
75	BA	301	3PE	O21-C21	2.36	1.41	1.34
70	A0	602	CDL	OB6-CB4	-2.35	1.40	1.46
73	A2	402	PC1	O21-C21	2.35	1.40	1.34
70	B0	101	CDL	OA6-CA4	-2.35	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	A9	604	PC1	O21-C2	-2.35	1.40	1.46
70	B1	402	CDL	OA6-CA4	-2.35	1.40	1.46
75	BP	201	3PE	P-O11	2.35	1.68	1.59
73	BY	202	PC1	O21-C21	2.34	1.40	1.34
70	BL	301	CDL	OA6-CA4	-2.34	1.40	1.46
73	A1	404	PC1	O21-C21	2.34	1.40	1.34
76	A6	301	LPP	O27-C8	-2.34	1.39	1.45
73	A9	601	PC1	O21-C21	2.34	1.40	1.34
75	AJ	502	3PE	O21-C21	2.33	1.40	1.34
75	A9	602	3PE	O21-C2	-2.32	1.40	1.46
70	AF	402	CDL	OA6-CA4	-2.32	1.40	1.46
74	A1	401	NDP	C2D-C1D	2.32	1.60	1.53
73	AU	201	PC1	O21-C21	2.30	1.40	1.34
70	BC	301	CDL	OA6-CA4	-2.30	1.40	1.46
75	BA	301	3PE	P-O11	2.30	1.68	1.59
70	BT	201	CDL	OA6-CA4	-2.29	1.40	1.46
73	BT	202	PC1	O21-C21	2.29	1.40	1.34
70	BC	302	CDL	OA6-CA4	-2.29	1.40	1.46
70	BC	302	CDL	OB6-CB4	-2.29	1.40	1.46
75	A2	401	3PE	P-O11	2.28	1.68	1.59
76	AA	902	LPP	O27-C8	-2.26	1.40	1.45
70	A1	402	CDL	OB6-CB4	-2.25	1.41	1.46
70	AA	901	CDL	OA6-CA4	-2.25	1.41	1.46
70	AA	908	CDL	OB6-CB4	-2.25	1.41	1.46
70	BE	201	CDL	OB6-CB4	-2.24	1.41	1.46
73	A1	404	PC1	O21-C2	-2.24	1.41	1.46
76	BN	301	LPP	O27-C29	2.24	1.39	1.33
73	AA	906	PC1	O21-C2	-2.23	1.41	1.46
73	B1	403	PC1	O21-C21	2.23	1.40	1.34
70	BG	201	CDL	OA6-CA4	-2.23	1.41	1.46
70	BY	201	CDL	PA1-OA5	2.22	1.68	1.59
70	A1	402	CDL	PA1-OA5	2.20	1.68	1.59
75	A9	603	3PE	P-O11	2.19	1.68	1.59
70	AA	901	CDL	PA1-OA5	2.19	1.68	1.59
75	AJ	502	3PE	P-O11	2.18	1.68	1.59
76	A6	301	LPP	O27-C29	2.18	1.39	1.33
70	A0	601	CDL	OA6-CA4	-2.17	1.41	1.46
70	B0	101	CDL	OB6-CB4	-2.16	1.41	1.46
70	AC	802	CDL	PA1-OA5	2.15	1.68	1.59
70	A0	602	CDL	OA6-CA4	-2.15	1.41	1.46
70	A0	601	CDL	PA1-OA5	2.14	1.68	1.59
70	BG	201	CDL	PA1-OA5	2.14	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	BY	201	CDL	OA6-CA4	-2.14	1.41	1.46
70	AM	301	CDL	PA1-OA5	2.14	1.67	1.59
70	AF	401	CDL	PA1-OA5	2.12	1.67	1.59
70	BT	201	CDL	PA1-OA5	2.12	1.67	1.59
70	B0	102	CDL	PA1-OA5	2.12	1.67	1.59
70	BE	201	CDL	PA1-OA5	2.11	1.67	1.59
75	BP	201	3PE	P-O13	2.11	1.67	1.59
70	BL	301	CDL	PA1-OA5	2.10	1.67	1.59
77	A8	401	ADP	C2-N3	2.09	1.35	1.32
70	AF	401	CDL	C71-CB7	2.09	1.56	1.50
70	AC	802	CDL	OA6-CA4	-2.09	1.41	1.46
75	BA	301	3PE	P-O13	2.08	1.67	1.59
70	BV	201	CDL	PA1-OA5	2.08	1.67	1.59
70	AM	301	CDL	PA1-OA2	2.08	1.67	1.59
73	AQ	202	PC1	O21-C2	-2.08	1.41	1.46
75	A9	602	3PE	P-O13	2.07	1.67	1.59
70	AF	402	CDL	PA1-OA5	2.07	1.67	1.59
70	AP	301	CDL	OB6-CB4	-2.07	1.41	1.46
75	A9	603	3PE	P-O13	2.07	1.67	1.59
70	AP	301	CDL	OA6-CA4	-2.06	1.41	1.46
70	AF	401	CDL	OB6-CB4	-2.06	1.41	1.46
70	BY	201	CDL	C51-CB5	2.06	1.56	1.50
70	B1	402	CDL	PA1-OA5	2.05	1.67	1.59
70	BE	201	CDL	OA6-CA4	-2.05	1.41	1.46
70	BC	302	CDL	PA1-OA5	2.05	1.67	1.59
75	AJ	502	3PE	P-O13	2.05	1.67	1.59
70	AM	301	CDL	OB6-CB4	-2.05	1.41	1.46
70	A0	602	CDL	C71-CB7	2.04	1.56	1.50
75	A2	401	3PE	P-O13	2.03	1.67	1.59
70	B0	101	CDL	PA1-OA5	2.03	1.67	1.59
70	A0	602	CDL	PA1-OA5	2.02	1.67	1.59
70	AM	301	CDL	C51-CB5	2.01	1.56	1.50
70	BT	201	CDL	C71-CB7	2.01	1.56	1.50
70	AM	301	CDL	OA6-CA4	-2.01	1.41	1.46
70	BC	301	CDL	PA1-OA5	2.01	1.67	1.59
70	AC	801	CDL	PA1-OA5	2.00	1.67	1.59
70	BY	201	CDL	OB6-CB4	-2.00	1.41	1.46
70	BE	201	CDL	C71-CB7	2.00	1.56	1.50

All (96) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	AQ	201	ADP	C1'-N9-C4	10.73	145.50	126.64
77	A8	401	ADP	C1'-N9-C4	10.72	145.48	126.64
77	A8	401	ADP	C5-C6-N6	10.44	136.21	120.35
77	AQ	201	ADP	C5-C6-N6	10.28	135.98	120.35
74	A1	401	NDP	C5A-C6A-N6A	7.25	131.37	120.35
77	A8	401	ADP	N6-C6-N1	-7.10	103.83	118.57
77	AQ	201	ADP	N6-C6-N1	-6.99	104.06	118.57
77	A8	401	ADP	N3-C2-N1	-5.71	119.76	128.68
77	AQ	201	ADP	N3-C2-N1	-5.63	119.88	128.68
74	A1	401	NDP	N3A-C2A-N1A	-5.36	120.31	128.68
74	A1	401	NDP	N6A-C6A-N1A	-5.01	108.17	118.57
71	A0	603	UDP	C4-N3-C2	-4.95	120.05	126.58
76	A6	301	LPP	O9-C11-C12	4.59	121.40	111.50
75	A9	602	3PE	C2-O21-C21	4.09	127.86	117.79
81	AS	200	8Q1	C37-C38-C39	-4.05	105.61	112.36
71	A0	603	UDP	N3-C2-N1	3.93	120.11	114.89
81	AS	200	8Q1	C38-C37-N36	-3.71	104.41	111.90
81	AS	200	8Q1	C6-C1-S44	3.35	117.35	113.46
81	AS	200	8Q1	C43-S44-C1	3.18	111.78	101.87
70	A0	602	CDL	OB6-CB5-C51	3.12	118.23	111.50
77	AQ	201	ADP	O4'-C1'-C2'	-3.12	102.37	106.93
73	B1	401	PC1	O21-C21-C22	3.03	118.04	111.50
75	A9	602	3PE	O31-C31-C32	3.02	121.38	111.91
71	A0	603	UDP	C5-C4-N3	2.99	119.31	114.84
70	BY	201	CDL	OB6-CB5-C51	2.95	117.86	111.50
70	A0	601	CDL	OA6-CA5-C11	2.90	117.74	111.50
70	BE	201	CDL	OB6-CB5-C51	2.89	117.72	111.50
70	BC	302	CDL	OB6-CB5-C51	2.86	117.67	111.50
73	A1	404	PC1	O21-C21-C22	2.86	117.67	111.50
70	BY	201	CDL	OA6-CA5-C11	2.85	117.64	111.50
73	BT	202	PC1	O21-C21-C22	2.84	117.62	111.50
76	BN	301	LPP	O9-C11-C12	2.84	117.62	111.50
81	AS	200	8Q1	C7-C6-C1	-2.82	106.08	112.33
73	A6	302	PC1	O21-C21-C22	2.80	117.54	111.50
74	A1	401	NDP	PN-O3-PA	-2.76	123.34	132.83
75	BP	201	3PE	O21-C21-C22	2.75	117.43	111.50
73	AJ	501	PC1	O21-C21-C22	2.74	117.42	111.50
70	AF	401	CDL	OB6-CB5-C51	2.72	117.36	111.50
71	A0	603	UDP	PA-O3A-PB	-2.72	123.50	132.83
75	AJ	502	3PE	O21-C21-C22	2.71	117.33	111.50
71	A0	603	UDP	O4-C4-C5	-2.68	120.45	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	AL	303	PC1	O21-C21-C22	2.68	117.27	111.50
75	A9	602	3PE	O21-C21-C22	2.67	117.27	111.50
73	AQ	202	PC1	O21-C21-C22	2.67	117.25	111.50
70	A0	602	CDL	OA6-CA5-C11	2.66	117.23	111.50
70	BG	201	CDL	CA4-OA6-CA5	-2.59	111.42	117.79
70	AA	901	CDL	OB6-CB5-C51	2.58	117.06	111.50
70	BE	201	CDL	OA6-CA5-C11	2.54	116.98	111.50
76	AL	304	LPP	O9-C11-C12	2.53	116.95	111.50
73	A6	303	PC1	O21-C21-C22	2.51	116.91	111.50
76	AA	902	LPP	O9-C11-C12	2.48	116.84	111.50
70	BL	301	CDL	OA6-CA5-C11	2.48	116.84	111.50
77	A8	401	ADP	O4'-C1'-C2'	-2.47	103.32	106.93
70	AA	901	CDL	OA6-CA5-C11	2.46	116.81	111.50
70	AM	301	CDL	OB6-CB5-C51	2.45	116.77	111.50
70	A1	402	CDL	OB6-CB5-C51	2.44	116.75	111.50
70	AM	301	CDL	OA6-CA5-C11	2.43	116.74	111.50
70	BG	201	CDL	OA6-CA5-C11	2.42	116.72	111.50
73	AA	903	PC1	O21-C21-C22	2.40	116.68	111.50
73	AA	906	PC1	O21-C21-C22	2.35	116.56	111.50
73	BS	1301	PC1	O21-C21-C22	2.35	116.56	111.50
73	AM	302	PC1	O21-C21-C22	2.34	116.55	111.50
70	AC	801	CDL	OB6-CB5-C51	2.33	116.53	111.50
77	AQ	201	ADP	PA-O3A-PB	-2.32	124.85	132.83
70	B0	101	CDL	OA6-CA5-C11	2.32	116.50	111.50
81	AS	200	8Q1	O4-C1-C6	-2.32	121.25	123.99
73	BY	202	PC1	O21-C21-C22	2.32	116.50	111.50
74	A1	401	NDP	C3D-C2D-C1D	2.30	105.80	101.43
75	A9	602	3PE	O21-C2-C1	2.29	116.68	108.40
70	BC	301	CDL	OA6-CA5-C11	2.26	116.38	111.50
73	BT	202	PC1	C2-O21-C21	-2.25	112.25	117.79
70	BG	201	CDL	OB6-CB5-C51	2.25	116.34	111.50
70	B0	101	CDL	OB6-CB5-C51	2.25	116.34	111.50
73	AA	904	PC1	O21-C21-C22	2.21	116.26	111.50
70	AF	402	CDL	OA6-CA5-C11	2.20	116.24	111.50
73	A1	403	PC1	O21-C21-C22	2.18	116.20	111.50
70	B1	402	CDL	OB6-CB5-C51	2.17	116.18	111.50
70	AF	402	CDL	OB6-CB5-C51	2.16	116.17	111.50
70	B0	102	CDL	OB6-CB5-C51	2.16	116.16	111.50
70	BL	301	CDL	OB6-CB5-C51	2.13	116.09	111.50
73	A9	601	PC1	O21-C21-C22	2.12	116.07	111.50
75	A2	401	3PE	O21-C21-C22	2.11	116.06	111.50
73	BS	1302	PC1	O21-C21-C22	2.11	116.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	BS	1301	PC1	C2-O21-C21	-2.10	112.63	117.79
70	BT	201	CDL	OA6-CA5-C11	2.09	116.00	111.50
70	BT	201	CDL	OB6-CB5-C51	2.08	115.98	111.50
75	A9	603	3PE	O21-C21-C22	2.07	115.95	111.50
77	AQ	201	ADP	C3'-C2'-C1'	2.06	104.08	100.98
70	AA	908	CDL	OB6-CB5-C51	2.06	115.94	111.50
70	A1	402	CDL	OA6-CA5-C11	2.05	115.92	111.50
70	B0	102	CDL	OA6-CA5-C11	2.05	115.91	111.50
70	AC	801	CDL	OA6-CA5-C11	2.05	115.91	111.50
75	A9	602	3PE	O31-C31-O32	-2.04	118.44	123.59
73	A1	404	PC1	O31-C31-C32	2.03	118.29	111.91
73	AA	907	PC1	O21-C21-C22	2.02	115.86	111.50
77	A8	401	ADP	PA-O3A-PB	-2.01	125.93	132.83

There are no chirality outliers.

All (1063) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A0	601	CDL	C11-CA5-OA6-CA4
70	A0	601	CDL	CB3-OB5-PB2-OB4
70	A0	601	CDL	C51-CB5-OB6-CB4
70	A0	602	CDL	C1-CB2-OB2-PB2
70	A0	602	CDL	OB5-CB3-CB4-OB6
70	A1	402	CDL	CB2-C1-CA2-OA2
70	A1	402	CDL	CA3-OA5-PA1-OA2
70	A1	402	CDL	CA3-OA5-PA1-OA3
70	A1	402	CDL	CA3-OA5-PA1-OA4
70	A1	402	CDL	CB2-OB2-PB2-OB3
70	A1	402	CDL	CB2-OB2-PB2-OB5
70	A1	402	CDL	CB3-OB5-PB2-OB3
70	AA	901	CDL	C51-CB5-OB6-CB4
70	AA	908	CDL	CA2-C1-CB2-OB2
70	AA	908	CDL	OA5-CA3-CA4-OA6
70	AA	908	CDL	C11-CA5-OA6-CA4
70	AA	908	CDL	CB3-OB5-PB2-OB4
70	AA	908	CDL	C51-CB5-OB6-CB4
70	AC	801	CDL	CB3-OB5-PB2-OB4
70	AC	802	CDL	CB2-OB2-PB2-OB4
70	AC	802	CDL	CB3-OB5-PB2-OB2
70	AC	802	CDL	CB3-OB5-PB2-OB3
70	AC	802	CDL	CB3-OB5-PB2-OB4
70	AF	401	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
70	AF	401	CDL	OB7-CB5-OB6-CB4
70	AF	402	CDL	CB3-OB5-PB2-OB4
70	AF	402	CDL	OB6-CB4-CB6-OB8
70	AM	301	CDL	O1-C1-CA2-OA2
70	AM	301	CDL	OA5-CA3-CA4-OA6
70	AM	301	CDL	C11-CA5-OA6-CA4
70	AM	301	CDL	CB2-OB2-PB2-OB3
70	AM	301	CDL	OB6-CB4-CB6-OB8
70	AP	301	CDL	CA3-OA5-PA1-OA2
70	AP	301	CDL	CA3-OA5-PA1-OA3
70	AP	301	CDL	CA3-OA5-PA1-OA4
70	AP	301	CDL	C11-CA5-OA6-CA4
70	AP	301	CDL	CB2-OB2-PB2-OB3
70	AP	301	CDL	CB2-OB2-PB2-OB5
70	AP	301	CDL	OB7-CB5-OB6-CB4
70	B0	101	CDL	OB7-CB5-OB6-CB4
70	B0	101	CDL	C51-CB5-OB6-CB4
70	B0	102	CDL	CA2-C1-CB2-OB2
70	B0	102	CDL	OA6-CA4-CA6-OA8
70	B1	402	CDL	CA3-OA5-PA1-OA3
70	B1	402	CDL	CB2-OB2-PB2-OB3
70	B1	402	CDL	CB2-OB2-PB2-OB4
70	B1	402	CDL	OB9-CB7-OB8-CB6
70	BC	302	CDL	CB3-OB5-PB2-OB4
70	BE	201	CDL	CA2-C1-CB2-OB2
70	BE	201	CDL	CA3-OA5-PA1-OA3
70	BE	201	CDL	C11-CA5-OA6-CA4
70	BE	201	CDL	CB2-OB2-PB2-OB3
70	BE	201	CDL	OB7-CB5-OB6-CB4
70	BG	201	CDL	CA2-OA2-PA1-OA3
70	BG	201	CDL	CA3-OA5-PA1-OA3
70	BG	201	CDL	C11-CA5-OA6-CA4
70	BG	201	CDL	CB2-OB2-PB2-OB3
70	BG	201	CDL	CB3-OB5-PB2-OB3
70	BL	301	CDL	CB3-OB5-PB2-OB3
70	BL	301	CDL	OB5-CB3-CB4-OB6
70	BT	201	CDL	CA2-OA2-PA1-OA3
70	BT	201	CDL	C11-CA5-OA6-CA4
70	BT	201	CDL	CB2-OB2-PB2-OB3
70	BT	201	CDL	OB7-CB5-OB6-CB4
70	BT	201	CDL	C51-CB5-OB6-CB4
70	BY	201	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
70	BY	201	CDL	C51-CB5-OB6-CB4
71	A0	603	UDP	C5'-O5'-PA-O1A
73	A0	605	PC1	C1-O11-P-O12
73	A0	605	PC1	C1-O11-P-O14
73	A0	605	PC1	C1-O11-P-O13
73	A1	404	PC1	O11-C1-C2-O21
73	A1	404	PC1	O22-C21-O21-C2
73	A2	402	PC1	C22-C21-O21-C2
73	A6	303	PC1	C11-O13-P-O14
73	A9	601	PC1	O13-C11-C12-N
73	A9	604	PC1	C11-O13-P-O14
73	A9	604	PC1	C1-O11-P-O12
73	A9	604	PC1	O22-C21-O21-C2
73	A9	604	PC1	C22-C21-O21-C2
73	AA	904	PC1	C22-C21-O21-C2
73	AA	905	PC1	C1-O11-P-O14
73	AA	905	PC1	C1-O11-P-O13
73	AA	905	PC1	O13-C11-C12-N
73	AA	906	PC1	C11-O13-P-O14
73	AA	907	PC1	C1-O11-P-O12
73	AA	907	PC1	C1-O11-P-O14
73	AA	907	PC1	C1-O11-P-O13
73	AA	907	PC1	O13-C11-C12-N
73	AA	907	PC1	C2-C1-O11-P
73	AH	301	PC1	C11-O13-P-O14
73	AJ	501	PC1	C1-O11-P-O12
73	AJ	501	PC1	C1-O11-P-O14
73	AJ	501	PC1	C1-O11-P-O13
73	AJ	501	PC1	O13-C11-C12-N
73	AL	303	PC1	O13-C11-C12-N
73	AL	303	PC1	O22-C21-O21-C2
73	AM	302	PC1	C11-O13-P-O12
73	AM	302	PC1	C1-O11-P-O12
73	AM	302	PC1	C1-O11-P-O14
73	AM	302	PC1	C1-O11-P-O13
73	AM	302	PC1	C22-C21-O21-C2
73	AQ	202	PC1	C11-O13-P-O14
73	AQ	202	PC1	C1-O11-P-O14
73	AU	201	PC1	C11-O13-P-O12
73	AU	201	PC1	C11-O13-P-O11
73	AU	202	PC1	O21-C2-C3-O31
73	B1	401	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
73	B1	401	PC1	C1-O11-P-O12
73	B1	401	PC1	C1-O11-P-O14
73	B1	401	PC1	C2-C1-O11-P
73	B1	401	PC1	O21-C2-C3-O31
73	B1	403	PC1	C11-O13-P-O14
73	B1	403	PC1	C11-O13-P-O11
73	BQ	401	PC1	C11-O13-P-O12
73	BQ	401	PC1	C12-C11-O13-P
73	BQ	401	PC1	O13-C11-C12-N
73	BS	1301	PC1	C11-O13-P-O12
73	BS	1301	PC1	C11-O13-P-O14
73	BS	1301	PC1	C11-O13-P-O11
73	BS	1301	PC1	C1-O11-P-O14
73	BS	1301	PC1	O22-C21-O21-C2
73	BS	1301	PC1	C22-C21-O21-C2
73	BS	1302	PC1	C11-O13-P-O12
73	BS	1302	PC1	C1-O11-P-O12
73	BS	1302	PC1	C1-O11-P-O13
73	BT	202	PC1	C11-O13-P-O14
73	BT	202	PC1	C1-O11-P-O12
73	BT	202	PC1	C1-O11-P-O14
73	BT	202	PC1	O22-C21-O21-C2
73	BT	202	PC1	C22-C21-O21-C2
73	BY	202	PC1	C11-O13-P-O14
73	BY	202	PC1	C11-O13-P-O11
75	A2	401	3PE	O11-C1-C2-O21
75	A9	602	3PE	O21-C2-C3-O31
75	A9	602	3PE	C22-C21-O21-C2
75	A9	603	3PE	C1-O11-P-O12
75	AJ	502	3PE	C11-O13-P-O14
75	AJ	502	3PE	O13-C11-C12-N
75	BA	301	3PE	C11-O13-P-O11
75	BA	301	3PE	C11-O13-P-O12
75	BA	301	3PE	C11-O13-P-O14
75	BP	201	3PE	C1-O11-P-O14
76	A6	301	LPP	C6-O5-P1-O2
76	A6	301	LPP	C6-O5-P1-O3
76	A6	301	LPP	C6-O5-P1-O4
76	A6	301	LPP	O10-C11-O9-C7
76	A6	301	LPP	C12-C11-O9-C7
76	AA	902	LPP	C6-O5-P1-O2
76	AA	902	LPP	C6-O5-P1-O4

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Mol	Chain	Res	Type	Atoms
81	AS	200	8Q1	C28-C29-C32-C34
81	AS	200	8Q1	C28-C29-C32-O33
81	AS	200	8Q1	C30-C29-C32-C34
81	AS	200	8Q1	C30-C29-C32-O33
81	AS	200	8Q1	C31-C29-C32-C34
81	AS	200	8Q1	C31-C29-C32-O33
81	AS	200	8Q1	O33-C32-C34-O35
81	AS	200	8Q1	C42-C43-S44-C1
70	A1	402	CDL	OB9-CB7-OB8-CB6
73	AA	906	PC1	O32-C31-O31-C3
70	A1	402	CDL	C71-CB7-OB8-CB6
75	BA	301	3PE	C32-C31-O31-C3
70	A0	602	CDL	OA9-CA7-OA8-CA6
70	AF	402	CDL	OB9-CB7-OB8-CB6
70	BG	201	CDL	OB9-CB7-OB8-CB6
73	AA	904	PC1	O32-C31-O31-C3
73	AA	907	PC1	O32-C31-O31-C3
73	B1	403	PC1	O32-C31-O31-C3
75	BA	301	3PE	O32-C31-O31-C3
70	A0	601	CDL	OA7-CA5-OA6-CA4
70	A0	601	CDL	OB7-CB5-OB6-CB4
70	A0	602	CDL	OB7-CB5-OB6-CB4
70	AA	901	CDL	OB7-CB5-OB6-CB4
70	AA	908	CDL	OA7-CA5-OA6-CA4
70	AM	301	CDL	OA7-CA5-OA6-CA4
70	B0	101	CDL	OA7-CA5-OA6-CA4
70	BG	201	CDL	OA7-CA5-OA6-CA4
70	BT	201	CDL	OA7-CA5-OA6-CA4
70	BY	201	CDL	OB7-CB5-OB6-CB4
73	A1	403	PC1	O22-C21-O21-C2
73	A2	402	PC1	O22-C21-O21-C2
73	AA	904	PC1	O22-C21-O21-C2
73	AM	302	PC1	O22-C21-O21-C2
75	A9	602	3PE	O22-C21-O21-C2
70	B0	102	CDL	OA9-CA7-OA8-CA6
70	A0	602	CDL	C31-CA7-OA8-CA6
70	AF	402	CDL	C71-CB7-OB8-CB6
70	B1	402	CDL	C71-CB7-OB8-CB6
73	AA	904	PC1	C32-C31-O31-C3
73	AA	906	PC1	C32-C31-O31-C3
73	B1	403	PC1	C32-C31-O31-C3
70	A0	602	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
70	AF	401	CDL	C51-CB5-OB6-CB4
70	AP	301	CDL	C51-CB5-OB6-CB4
70	B0	101	CDL	C11-CA5-OA6-CA4
70	BE	201	CDL	C51-CB5-OB6-CB4
73	A1	403	PC1	C22-C21-O21-C2
73	A1	404	PC1	C22-C21-O21-C2
73	AL	303	PC1	C22-C21-O21-C2
70	A0	601	CDL	OB9-CB7-OB8-CB6
70	A1	402	CDL	C31-CA7-OA8-CA6
70	B0	102	CDL	C31-CA7-OA8-CA6
70	BG	201	CDL	C71-CB7-OB8-CB6
73	A9	601	PC1	C32-C31-O31-C3
73	AA	907	PC1	C32-C31-O31-C3
70	AA	908	CDL	OB7-CB5-OB6-CB4
70	AP	301	CDL	OA7-CA5-OA6-CA4
70	BE	201	CDL	OA7-CA5-OA6-CA4
71	A0	603	UDP	O4'-C1'-N1-C2
70	A1	402	CDL	O1-C1-CA2-OA2
70	AA	908	CDL	O1-C1-CB2-OB2
70	B0	101	CDL	O1-C1-CB2-OB2
70	B0	102	CDL	O1-C1-CB2-OB2
70	BE	201	CDL	O1-C1-CB2-OB2
70	A0	601	CDL	C31-CA7-OA8-CA6
70	A0	601	CDL	C71-CB7-OB8-CB6
70	B0	102	CDL	C71-CB7-OB8-CB6
75	A9	602	3PE	C32-C31-O31-C3
73	A9	601	PC1	O32-C31-O31-C3
75	A9	602	3PE	O32-C31-O31-C3
70	A1	402	CDL	C11-CA5-OA6-CA4
70	BV	201	CDL	C51-CB5-OB6-CB4
75	A2	401	3PE	C22-C21-O21-C2
70	A0	601	CDL	OA9-CA7-OA8-CA6
70	A1	402	CDL	OA7-CA5-OA6-CA4
70	A1	402	CDL	OA9-CA7-OA8-CA6
70	B0	102	CDL	OB9-CB7-OB8-CB6
73	AA	905	PC1	C32-C31-O31-C3
70	AM	301	CDL	CB2-C1-CA2-OA2
70	BV	201	CDL	CB2-C1-CA2-OA2
70	B0	101	CDL	C71-CB7-OB8-CB6
70	B1	402	CDL	C31-CA7-OA8-CA6
70	BT	201	CDL	C71-CB7-OB8-CB6
73	AH	301	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
73	AQ	202	PC1	C32-C31-O31-C3
70	A1	402	CDL	O1-C1-CB2-OB2
70	BV	201	CDL	O1-C1-CA2-OA2
70	BC	302	CDL	OB6-CB4-CB6-OB8
70	BC	302	CDL	CB5-C51-C52-C53
70	BG	201	CDL	CA5-C11-C12-C13
70	BV	201	CDL	CA5-C11-C12-C13
70	B0	101	CDL	OB9-CB7-OB8-CB6
70	B1	402	CDL	OA9-CA7-OA8-CA6
73	AQ	202	PC1	O32-C31-O31-C3
70	AM	301	CDL	C31-CA7-OA8-CA6
70	B0	101	CDL	CA5-C11-C12-C13
70	BT	201	CDL	OB9-CB7-OB8-CB6
70	A0	602	CDL	CA5-C11-C12-C13
70	B0	102	CDL	CA5-C11-C12-C13
76	AA	902	LPP	C11-C12-C13-C14
71	A0	603	UDP	C3'-C4'-C5'-O5'
71	A0	603	UDP	O4'-C4'-C5'-O5'
75	A2	401	3PE	C32-C31-O31-C3
70	BV	201	CDL	OB7-CB5-OB6-CB4
73	A0	605	PC1	C2-C1-O11-P
73	AU	201	PC1	C2-C1-O11-P
70	AA	908	CDL	CA5-C11-C12-C13
70	AC	801	CDL	CA5-C11-C12-C13
70	AF	402	CDL	C11-CA5-OA6-CA4
73	B1	401	PC1	C22-C21-O21-C2
73	AH	301	PC1	O32-C31-O31-C3
70	BC	301	CDL	CA5-C11-C12-C13
75	A2	401	3PE	O22-C21-O21-C2
73	A9	604	PC1	C32-C31-O31-C3
70	AC	801	CDL	C14-C15-C16-C17
70	AM	301	CDL	OA9-CA7-OA8-CA6
73	AA	905	PC1	O32-C31-O31-C3
70	A0	602	CDL	C11-CA5-OA6-CA4
70	BC	301	CDL	C11-CA5-OA6-CA4
73	A0	605	PC1	C22-C21-O21-C2
75	BA	301	3PE	C24-C25-C26-C27
70	A0	601	CDL	CB3-OB5-PB2-OB2
70	A0	602	CDL	CB3-OB5-PB2-OB2
70	AA	901	CDL	CA3-OA5-PA1-OA2
70	AA	901	CDL	CB2-OB2-PB2-OB5
70	AC	801	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
70	AC	802	CDL	CB2-OB2-PB2-OB5
70	AM	301	CDL	CB3-OB5-PB2-OB2
70	B0	101	CDL	CB2-OB2-PB2-OB5
70	B1	402	CDL	CA3-OA5-PA1-OA2
70	B1	402	CDL	CB2-OB2-PB2-OB5
70	BC	301	CDL	CA2-OA2-PA1-OA5
70	BC	301	CDL	CA3-OA5-PA1-OA2
70	BC	302	CDL	CA3-OA5-PA1-OA2
70	BC	302	CDL	CB3-OB5-PB2-OB2
70	BE	201	CDL	CA3-OA5-PA1-OA2
70	BG	201	CDL	CA2-OA2-PA1-OA5
70	BG	201	CDL	CA3-OA5-PA1-OA2
73	A1	403	PC1	C1-O11-P-O13
73	A9	604	PC1	C11-O13-P-O11
73	A9	604	PC1	C1-O11-P-O13
73	AA	903	PC1	C1-O11-P-O13
73	AA	905	PC1	C11-O13-P-O11
73	AA	907	PC1	C11-O13-P-O11
73	AQ	202	PC1	C1-O11-P-O13
73	AU	201	PC1	C1-O11-P-O13
73	B1	401	PC1	C1-O11-P-O13
73	B1	403	PC1	C1-O11-P-O13
73	BQ	401	PC1	C11-O13-P-O11
73	BS	1301	PC1	C1-O11-P-O13
73	BS	1302	PC1	C11-O13-P-O11
73	BT	202	PC1	C1-O11-P-O13
75	A9	603	3PE	C1-O11-P-O13
75	AJ	502	3PE	C11-O13-P-O11
75	BP	201	3PE	C1-O11-P-O13
70	AF	401	CDL	CA5-C11-C12-C13
75	A2	401	3PE	O32-C31-O31-C3
70	A0	602	CDL	OA7-CA5-OA6-CA4
70	AF	402	CDL	OA7-CA5-OA6-CA4
70	BC	301	CDL	OA7-CA5-OA6-CA4
73	B1	401	PC1	O22-C21-O21-C2
73	A1	404	PC1	C32-C31-O31-C3
74	A1	401	NDP	O4D-C1D-N1N-C6N
70	AC	802	CDL	C11-CA5-OA6-CA4
70	BG	201	CDL	C51-CB5-OB6-CB4
70	BL	301	CDL	C11-CA5-OA6-CA4
70	AA	901	CDL	C17-C18-C19-C20
73	A6	302	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
70	AA	901	CDL	C23-C24-C25-C26
70	AC	802	CDL	OA7-CA5-OA6-CA4
70	BG	201	CDL	OB7-CB5-OB6-CB4
70	BL	301	CDL	OA7-CA5-OA6-CA4
73	A0	605	PC1	O22-C21-O21-C2
73	B1	403	PC1	C36-C37-C38-C39
75	BA	301	3PE	C2D-C2E-C2F-C2G
70	A0	601	CDL	O1-C1-CB2-OB2
70	A0	602	CDL	O1-C1-CB2-OB2
70	BE	201	CDL	O1-C1-CA2-OA2
70	B0	102	CDL	C13-C14-C15-C16
70	B1	402	CDL	C80-C81-C82-C83
70	BL	301	CDL	CA5-C11-C12-C13
73	BY	202	PC1	C21-C22-C23-C24
70	A0	601	CDL	C13-C14-C15-C16
73	A1	403	PC1	C3B-C3C-C3D-C3E
76	AA	902	LPP	C17-C18-C19-C20
73	A9	604	PC1	O32-C31-O31-C3
73	AJ	501	PC1	C3C-C3D-C3E-C3F
70	BY	201	CDL	CA5-C11-C12-C13
70	AC	802	CDL	C13-C14-C15-C16
70	BG	201	CDL	C34-C35-C36-C37
73	A9	601	PC1	O22-C21-O21-C2
73	A9	601	PC1	C22-C21-O21-C2
73	BQ	401	PC1	C22-C21-O21-C2
73	AA	904	PC1	C3D-C3E-C3F-C3G
70	BE	201	CDL	CA5-C11-C12-C13
70	BT	201	CDL	CA5-C11-C12-C13
70	AA	908	CDL	C41-C42-C43-C44
70	AA	908	CDL	C73-C74-C75-C76
73	AU	202	PC1	C3C-C3D-C3E-C3F
73	A1	404	PC1	O32-C31-O31-C3
70	B1	402	CDL	C56-C57-C58-C59
73	A9	601	PC1	C3B-C3C-C3D-C3E
70	BT	201	CDL	C73-C74-C75-C76
73	A9	604	PC1	C3C-C3D-C3E-C3F
75	BA	301	3PE	C34-C35-C36-C37
70	BY	201	CDL	C56-C57-C58-C59
70	AC	802	CDL	C80-C81-C82-C83
73	BS	1302	PC1	C36-C37-C38-C39
70	AC	802	CDL	C32-C33-C34-C35
73	AL	303	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
73	BY	202	PC1	C29-C2A-C2B-C2C
70	BL	301	CDL	CB3-CB4-CB6-OB8
71	A0	603	UDP	O4'-C1'-N1-C6
70	BC	302	CDL	C11-CA5-OA6-CA4
73	AA	905	PC1	C22-C21-O21-C2
75	AJ	502	3PE	C22-C21-O21-C2
70	A1	402	CDL	C40-C41-C42-C43
73	AQ	202	PC1	C26-C27-C28-C29
70	A0	602	CDL	C57-C58-C59-C60
70	AA	908	CDL	C53-C54-C55-C56
70	A0	601	CDL	CA2-C1-CB2-OB2
73	AA	903	PC1	C34-C35-C36-C37
73	AA	905	PC1	O22-C21-O21-C2
73	BQ	401	PC1	O22-C21-O21-C2
75	AJ	502	3PE	O22-C21-O21-C2
70	BT	201	CDL	C82-C83-C84-C85
70	BV	201	CDL	C37-C38-C39-C40
70	A0	602	CDL	C1-CA2-OA2-PA1
70	AC	802	CDL	C55-C56-C57-C58
70	AF	402	CDL	C71-C72-C73-C74
73	AQ	202	PC1	C2B-C2C-C2D-C2E
70	AA	908	CDL	C59-C60-C61-C62
73	BQ	401	PC1	C32-C31-O31-C3
70	AF	401	CDL	C11-CA5-OA6-CA4
73	AU	202	PC1	C22-C21-O21-C2
70	BY	201	CDL	C36-C37-C38-C39
70	AC	801	CDL	C55-C56-C57-C58
73	AQ	202	PC1	C3C-C3D-C3E-C3F
73	A0	605	PC1	C2C-C2D-C2E-C2F
73	BQ	401	PC1	C35-C36-C37-C38
73	BT	202	PC1	C33-C34-C35-C36
76	AL	304	LPP	C20-C21-C22-C23
70	BC	302	CDL	OA7-CA5-OA6-CA4
73	B1	403	PC1	C31-C32-C33-C34
73	A6	303	PC1	C32-C31-O31-C3
75	AJ	502	3PE	C3E-C3F-C3G-C3H
76	BN	301	LPP	C39-C40-C41-C42
70	AA	901	CDL	C36-C37-C38-C39
73	BS	1302	PC1	C32-C33-C34-C35
75	BA	301	3PE	C25-C26-C27-C28
70	AA	908	CDL	C60-C61-C62-C63
70	AC	802	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
70	AF	401	CDL	C61-C62-C63-C64
73	AA	904	PC1	C3F-C3G-C3H-C3I
70	BY	201	CDL	C71-CB7-OB8-CB6
70	AA	901	CDL	C11-C12-C13-C14
70	AC	801	CDL	C78-C79-C80-C81
70	AC	802	CDL	C42-C43-C44-C45
70	B0	102	CDL	C58-C59-C60-C61
70	A1	402	CDL	C51-CB5-OB6-CB4
70	AA	901	CDL	C11-CA5-OA6-CA4
70	AC	801	CDL	C51-CB5-OB6-CB4
70	A1	402	CDL	OA5-CA3-CA4-OA6
73	AA	905	PC1	O11-C1-C2-O21
70	AA	908	CDL	C12-C13-C14-C15
70	B0	101	CDL	C52-C53-C54-C55
70	BE	201	CDL	C11-C12-C13-C14
75	A9	602	3PE	C35-C36-C37-C38
70	B1	402	CDL	C76-C77-C78-C79
73	BS	1301	PC1	C2C-C2D-C2E-C2F
70	AC	801	CDL	OB7-CB5-OB6-CB4
73	A9	601	PC1	C23-C24-C25-C26
73	AA	907	PC1	O21-C2-C3-O31
76	BN	301	LPP	O9-C7-C8-O27
70	A0	602	CDL	C14-C15-C16-C17
70	BE	201	CDL	C19-C20-C21-C22
73	AA	903	PC1	C38-C39-C3A-C3B
70	B0	101	CDL	C40-C41-C42-C43
73	AU	201	PC1	C23-C24-C25-C26
73	AA	906	PC1	C21-C22-C23-C24
70	AC	802	CDL	C73-C74-C75-C76
70	AF	401	CDL	C63-C64-C65-C66
70	B0	101	CDL	C13-C14-C15-C16
73	BS	1301	PC1	C34-C35-C36-C37
76	AL	304	LPP	C40-C41-C42-C43
73	BQ	401	PC1	O32-C31-O31-C3
70	AF	401	CDL	OA7-CA5-OA6-CA4
73	AU	202	PC1	O22-C21-O21-C2
73	A6	303	PC1	C22-C21-O21-C2
75	A9	602	3PE	C3D-C3E-C3F-C3G
80	AD	502	FMN	C2'-C3'-C4'-O4'
70	AC	801	CDL	CB3-OB5-PB2-OB2
70	BY	201	CDL	CA3-OA5-PA1-OA2
73	AA	906	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
73	AM	302	PC1	C11-O13-P-O11
73	B1	401	PC1	C11-O13-P-O11
70	BG	201	CDL	C13-C14-C15-C16
70	BL	301	CDL	C21-C22-C23-C24
73	A9	601	PC1	C2D-C2E-C2F-C2G
73	B1	403	PC1	C2C-C2D-C2E-C2F
70	AC	802	CDL	CA4-CA3-OA5-PA1
70	AP	301	CDL	C1-CA2-OA2-PA1
73	A6	302	PC1	C28-C29-C2A-C2B
70	A0	602	CDL	OB5-CB3-CB4-CB6
70	AM	301	CDL	OA5-CA3-CA4-CA6
70	BC	301	CDL	OA5-CA3-CA4-CA6
70	BL	301	CDL	OB5-CB3-CB4-CB6
70	BY	201	CDL	OA5-CA3-CA4-CA6
73	A1	404	PC1	O11-C1-C2-C3
73	A9	601	PC1	O11-C1-C2-C3
76	BN	301	LPP	O5-C6-C7-C8
70	AM	301	CDL	C11-C12-C13-C14
73	B1	401	PC1	C3B-C3C-C3D-C3E
70	AF	402	CDL	C37-C38-C39-C40
73	B1	401	PC1	C2E-C2F-C2G-C2H
70	AC	801	CDL	C76-C77-C78-C79
70	BC	301	CDL	C35-C36-C37-C38
70	A1	402	CDL	CA2-C1-CB2-OB2
70	B0	101	CDL	CA2-C1-CB2-OB2
73	A6	303	PC1	O22-C21-O21-C2
70	AA	908	CDL	C61-C62-C63-C64
70	AM	301	CDL	C82-C83-C84-C85
70	AF	402	CDL	C39-C40-C41-C42
70	AF	402	CDL	CB3-CB4-CB6-OB8
70	AM	301	CDL	CB3-CB4-CB6-OB8
70	AP	301	CDL	CA3-CA4-CA6-OA8
70	B0	102	CDL	C43-C44-C45-C46
70	BV	201	CDL	CB3-CB4-CB6-OB8
73	A6	302	PC1	C1-C2-C3-O31
73	A6	303	PC1	C1-C2-C3-O31
73	BS	1301	PC1	C1-C2-C3-O31
73	BS	1301	PC1	C3E-C3F-C3G-C3H
75	A9	602	3PE	C1-C2-C3-O31
70	A0	602	CDL	C13-C14-C15-C16
73	A6	303	PC1	O32-C31-O31-C3
75	AJ	502	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
70	BY	201	CDL	C76-C77-C78-C79
70	B1	402	CDL	C34-C35-C36-C37
70	AF	401	CDL	C31-CA7-OA8-CA6
70	BY	201	CDL	C20-C21-C22-C23
70	AM	301	CDL	C51-CB5-OB6-CB4
73	AU	201	PC1	C32-C31-O31-C3
75	AJ	502	3PE	C32-C31-O31-C3
73	A6	302	PC1	C3C-C3D-C3E-C3F
70	AP	301	CDL	CA3-CA4-OA6-CA5
73	AA	906	PC1	C3-C2-O21-C21
70	BE	201	CDL	C71-CB7-OB8-CB6
70	BY	201	CDL	OB9-CB7-OB8-CB6
73	A9	601	PC1	O11-C1-C2-O21
73	A9	604	PC1	O11-C1-C2-O21
75	AJ	502	3PE	O11-C1-C2-O21
76	BN	301	LPP	O5-C6-C7-O9
70	AC	802	CDL	C60-C61-C62-C63
70	BG	201	CDL	C60-C61-C62-C63
73	A1	404	PC1	C31-C32-C33-C34
73	AJ	501	PC1	C21-C22-C23-C24
70	AP	301	CDL	C74-C75-C76-C77
70	BG	201	CDL	OA6-CA4-CA6-OA8
70	BV	201	CDL	OB6-CB4-CB6-OB8
73	A1	404	PC1	O21-C2-C3-O31
70	B0	102	CDL	C15-C16-C17-C18
70	A1	402	CDL	OB7-CB5-OB6-CB4
73	B1	403	PC1	C2D-C2E-C2F-C2G
73	AA	903	PC1	C32-C31-O31-C3
70	B0	101	CDL	C38-C39-C40-C41
70	AF	401	CDL	OA9-CA7-OA8-CA6
70	AA	908	CDL	C38-C39-C40-C41
70	AA	901	CDL	OA7-CA5-OA6-CA4
70	BG	201	CDL	C11-C12-C13-C14
73	A0	605	PC1	C32-C31-O31-C3
73	BS	1301	PC1	C32-C31-O31-C3
70	A1	402	CDL	C82-C83-C84-C85
70	AC	801	CDL	C62-C63-C64-C65
70	A1	402	CDL	OA5-CA3-CA4-CA6
70	AA	908	CDL	OA5-CA3-CA4-CA6
70	AC	801	CDL	OA5-CA3-CA4-CA6
70	AF	402	CDL	OB5-CB3-CB4-CB6
70	B1	402	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
70	BC	302	CDL	OA5-CA3-CA4-CA6
70	BC	302	CDL	OB5-CB3-CB4-CB6
73	A6	302	PC1	O11-C1-C2-C3
73	AA	905	PC1	O11-C1-C2-C3
73	AJ	501	PC1	O11-C1-C2-C3
73	AU	201	PC1	O11-C1-C2-C3
73	B1	403	PC1	O11-C1-C2-C3
73	BQ	401	PC1	C23-C24-C25-C26
70	AC	801	CDL	C54-C55-C56-C57
70	BC	302	CDL	C12-C13-C14-C15
70	BG	201	CDL	C31-CA7-OA8-CA6
70	BG	201	CDL	C53-C54-C55-C56
70	AC	801	CDL	C1-CB2-OB2-PB2
75	BA	301	3PE	C2-C1-O11-P
75	BP	201	3PE	C2-C1-O11-P
70	AP	301	CDL	CA5-C11-C12-C13
75	AJ	502	3PE	O32-C31-O31-C3
73	AH	301	PC1	C3C-C3D-C3E-C3F
70	A0	601	CDL	CA3-CA4-CA6-OA8
70	B0	102	CDL	CA3-CA4-CA6-OA8
70	BC	302	CDL	CB3-CB4-CB6-OB8
70	BE	201	CDL	CA3-CA4-CA6-OA8
70	BE	201	CDL	CB3-CB4-CB6-OB8
70	BG	201	CDL	CB3-CB4-CB6-OB8
73	AA	906	PC1	C1-C2-C3-O31
73	AA	907	PC1	C1-C2-C3-O31
73	B1	401	PC1	C1-C2-C3-O31
73	BT	202	PC1	C1-C2-C3-O31
73	BY	202	PC1	C1-C2-C3-O31
75	BA	301	3PE	C1-C2-C3-O31
76	BN	301	LPP	C6-C7-C8-O27
70	AP	301	CDL	C14-C15-C16-C17
75	A9	603	3PE	C2F-C2G-C2H-C2I
70	AA	901	CDL	CA5-C11-C12-C13
73	AU	201	PC1	O32-C31-O31-C3
81	AS	200	8Q1	C7-C8-C9-C10
70	AF	401	CDL	CA3-OA5-PA1-OA2
73	BQ	401	PC1	C1-O11-P-O13
70	BE	201	CDL	OB9-CB7-OB8-CB6
73	AQ	202	PC1	C28-C29-C2A-C2B
70	A1	402	CDL	OB5-CB3-CB4-OB6
70	B1	402	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
70	BC	302	CDL	OA5-CA3-CA4-OA6
70	BC	302	CDL	C32-C31-CA7-OA8
70	BL	301	CDL	O1-C1-CA2-OA2
70	A1	402	CDL	C84-C85-C86-C87
73	AA	903	PC1	O32-C31-O31-C3
70	A0	601	CDL	OA6-CA4-CA6-OA8
70	B0	101	CDL	OB6-CB4-CB6-OB8
70	B1	402	CDL	OA6-CA4-CA6-OA8
73	A6	302	PC1	O21-C2-C3-O31
73	BT	202	PC1	O21-C2-C3-O31
73	AA	905	PC1	C3D-C3E-C3F-C3G
70	AM	301	CDL	OB7-CB5-OB6-CB4
70	AP	301	CDL	CB4-CB3-OB5-PB2
70	BG	201	CDL	C1-CB2-OB2-PB2
73	BY	202	PC1	C2-C1-O11-P
70	A0	602	CDL	C40-C41-C42-C43
73	AA	904	PC1	C11-C12-N-C13
73	AA	905	PC1	C3B-C3C-C3D-C3E
73	BS	1301	PC1	O32-C31-O31-C3
70	AF	402	CDL	CA5-C11-C12-C13
73	A6	302	PC1	C36-C37-C38-C39
70	AA	901	CDL	OA5-CA3-CA4-CA6
73	AA	907	PC1	O11-C1-C2-C3
73	AL	303	PC1	O11-C1-C2-C3
73	BQ	401	PC1	O11-C1-C2-C3
75	A2	401	3PE	O11-C1-C2-C3
75	A9	602	3PE	O11-C1-C2-C3
75	BA	301	3PE	C22-C21-O21-C2
70	AA	908	CDL	C82-C83-C84-C85
73	B1	401	PC1	C32-C31-O31-C3
70	AA	901	CDL	C22-C23-C24-C25
70	A1	402	CDL	CB6-CB4-OB6-CB5
70	AC	802	CDL	CA6-CA4-OA6-CA5
70	AM	301	CDL	CB3-CB4-OB6-CB5
70	A0	602	CDL	C71-CB7-OB8-CB6
80	AD	502	FMN	O2'-C2'-C3'-C4'
73	A0	605	PC1	C3C-C3D-C3E-C3F
73	B1	401	PC1	C33-C34-C35-C36
70	AA	901	CDL	CA4-CA3-OA5-PA1
70	AF	401	CDL	CB4-CB3-OB5-PB2
70	AM	301	CDL	CB4-CB3-OB5-PB2
70	BG	201	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
70	BV	201	CDL	CA3-CA4-CA6-OA8
73	A2	402	PC1	C1-C2-C3-O31
73	AU	202	PC1	C1-C2-C3-O31
75	BP	201	3PE	C1-C2-C3-O31
76	A6	301	LPP	C7-C6-O5-P1
70	AC	801	CDL	OA5-CA3-CA4-OA6
70	AF	402	CDL	OA5-CA3-CA4-OA6
70	B1	402	CDL	OA5-CA3-CA4-OA6
70	BC	302	CDL	OB5-CB3-CB4-OB6
73	A6	302	PC1	O11-C1-C2-O21
73	AA	907	PC1	O11-C1-C2-O21
73	AJ	501	PC1	O11-C1-C2-O21
73	AL	303	PC1	O11-C1-C2-O21
73	AQ	202	PC1	O11-C1-C2-O21
73	BQ	401	PC1	O11-C1-C2-O21
73	AA	907	PC1	C37-C38-C39-C3A
75	BA	301	3PE	O22-C21-O21-C2
77	AQ	201	ADP	PA-O3A-PB-O2B
70	BG	201	CDL	OA9-CA7-OA8-CA6
73	A0	605	PC1	O32-C31-O31-C3
73	AA	906	PC1	C3E-C3F-C3G-C3H
70	BG	201	CDL	OB6-CB4-CB6-OB8
73	A6	303	PC1	O21-C2-C3-O31
73	AA	903	PC1	O21-C2-C3-O31
73	AA	906	PC1	O21-C2-C3-O31
73	BY	202	PC1	O21-C2-C3-O31
71	A0	603	UDP	C5'-O5'-PA-O3A
70	AA	901	CDL	C81-C82-C83-C84
73	B1	401	PC1	O32-C31-O31-C3
73	A9	604	PC1	C3D-C3E-C3F-C3G
73	AM	302	PC1	C3C-C3D-C3E-C3F
73	AA	907	PC1	C22-C23-C24-C25
70	AC	802	CDL	C61-C62-C63-C64
73	AL	303	PC1	C29-C2A-C2B-C2C
70	AA	908	CDL	CB3-OB5-PB2-OB2
70	AC	802	CDL	CA3-OA5-PA1-OA2
70	AM	301	CDL	CB2-OB2-PB2-OB5
70	B0	101	CDL	CA2-OA2-PA1-OA5
70	BG	201	CDL	CB3-OB5-PB2-OB2
70	BL	301	CDL	CB3-OB5-PB2-OB2
70	BY	201	CDL	CB2-OB2-PB2-OB5
73	AH	301	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
73	AU	202	PC1	C11-O13-P-O11
73	BT	202	PC1	C11-O13-P-O11
73	BT	202	PC1	C3B-C3C-C3D-C3E
70	A1	402	CDL	CB4-CB3-OB5-PB2
70	AA	908	CDL	CB4-CB3-OB5-PB2
70	AC	802	CDL	CB4-CB3-OB5-PB2
70	B0	102	CDL	CA4-CA3-OA5-PA1
80	AD	502	FMN	C4'-C5'-O5'-P
70	A0	601	CDL	CB3-OB5-PB2-OB3
70	A0	602	CDL	CB3-OB5-PB2-OB3
70	AA	901	CDL	CA3-OA5-PA1-OA3
70	AA	901	CDL	CA3-OA5-PA1-OA4
70	AA	901	CDL	CB2-OB2-PB2-OB3
70	AC	801	CDL	CA3-OA5-PA1-OA3
70	AC	801	CDL	CB3-OB5-PB2-OB3
70	AF	401	CDL	CA3-OA5-PA1-OA4
70	AM	301	CDL	CB3-OB5-PB2-OB3
70	B0	101	CDL	CB2-OB2-PB2-OB3
70	B1	402	CDL	CA3-OA5-PA1-OA4
70	BC	301	CDL	CA2-OA2-PA1-OA3
70	BC	301	CDL	CA3-OA5-PA1-OA3
70	BC	301	CDL	CA3-OA5-PA1-OA4
70	BC	302	CDL	CA3-OA5-PA1-OA3
70	BE	201	CDL	CA3-OA5-PA1-OA4
70	BG	201	CDL	CA2-OA2-PA1-OA4
70	BG	201	CDL	CB3-OB5-PB2-OB4
71	A0	603	UDP	C5'-O5'-PA-O2A
73	A1	403	PC1	C1-O11-P-O14
73	A9	604	PC1	C11-O13-P-O12
73	A9	604	PC1	C1-O11-P-O14
73	AA	903	PC1	C1-O11-P-O14
73	AA	904	PC1	C11-C12-N-C14
73	AA	905	PC1	C11-O13-P-O12
73	AA	905	PC1	C11-O13-P-O14
73	AA	907	PC1	C11-O13-P-O12
73	AA	907	PC1	C11-O13-P-O14
73	AM	302	PC1	C11-O13-P-O14
73	AQ	202	PC1	C1-O11-P-O12
73	AU	201	PC1	C11-O13-P-O14
73	AU	201	PC1	C1-O11-P-O14
73	B1	401	PC1	C11-O13-P-O12
73	B1	403	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
73	BS	1301	PC1	C1-O11-P-O12
73	BS	1302	PC1	C1-O11-P-O14
75	AJ	502	3PE	C11-O13-P-O12
75	BP	201	3PE	C1-O11-P-O12
70	AC	801	CDL	OB5-CB3-CB4-CB6
70	AF	402	CDL	OA5-CA3-CA4-CA6
70	B0	101	CDL	OA5-CA3-CA4-CA6
73	AA	903	PC1	O11-C1-C2-C3
73	AA	904	PC1	O11-C1-C2-C3
73	AQ	202	PC1	O11-C1-C2-C3
73	BS	1302	PC1	O11-C1-C2-C3
75	BP	201	3PE	O11-C1-C2-C3
73	A9	604	PC1	C12-C11-O13-P
73	AU	202	PC1	C12-C11-O13-P
75	A9	603	3PE	C12-C11-O13-P
75	BP	201	3PE	C12-C11-O13-P
70	A0	601	CDL	C11-C12-C13-C14
70	A0	602	CDL	C41-C42-C43-C44
73	A2	402	PC1	C3D-C3E-C3F-C3G
70	A0	602	CDL	OB9-CB7-OB8-CB6
70	BE	201	CDL	C31-CA7-OA8-CA6
76	AA	902	LPP	C34-C35-C36-C37
70	AA	901	CDL	OA5-CA3-CA4-OA6
70	AC	801	CDL	OB5-CB3-CB4-OB6
70	AF	402	CDL	OB5-CB3-CB4-OB6
70	AP	301	CDL	OB5-CB3-CB4-OB6
70	BE	201	CDL	OA5-CA3-CA4-OA6
70	BG	201	CDL	OB5-CB3-CB4-OB6
70	BT	201	CDL	OB5-CB3-CB4-OB6
70	BY	201	CDL	OA5-CA3-CA4-OA6
73	AA	903	PC1	O11-C1-C2-O21
73	AA	904	PC1	O11-C1-C2-O21
73	AU	201	PC1	O11-C1-C2-O21
73	B1	403	PC1	O11-C1-C2-O21
73	BS	1302	PC1	O11-C1-C2-O21
73	A9	604	PC1	C24-C25-C26-C27
70	BC	302	CDL	C34-C35-C36-C37
73	A2	402	PC1	C37-C38-C39-C3A
70	AF	401	CDL	CA3-CA4-CA6-OA8
73	A1	404	PC1	C1-C2-C3-O31
73	A2	402	PC1	O13-C11-C12-N
73	A9	604	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
73	AA	906	PC1	O13-C11-C12-N
73	AH	301	PC1	O13-C11-C12-N
73	AQ	202	PC1	O13-C11-C12-N
73	AU	201	PC1	O13-C11-C12-N
73	AU	202	PC1	O13-C11-C12-N
73	B1	403	PC1	O13-C11-C12-N
70	AA	908	CDL	OA6-CA4-CA6-OA8
70	AF	401	CDL	OA6-CA4-CA6-OA8
70	BE	201	CDL	OB6-CB4-CB6-OB8
70	BL	301	CDL	OB6-CB4-CB6-OB8
70	BV	201	CDL	OA6-CA4-CA6-OA8
73	A2	402	PC1	O21-C2-C3-O31
73	BS	1301	PC1	O21-C2-C3-O31
75	BA	301	3PE	O21-C2-C3-O31
73	AA	906	PC1	C3B-C3C-C3D-C3E
75	BA	301	3PE	C26-C27-C28-C29
75	AJ	502	3PE	O21-C21-C22-C23
70	AF	401	CDL	C1-CB2-OB2-PB2
70	BE	201	CDL	OA9-CA7-OA8-CA6
73	AA	906	PC1	C2C-C2D-C2E-C2F
73	AA	906	PC1	C3D-C3E-C3F-C3G
73	AJ	501	PC1	C2F-C2G-C2H-C2I
76	AL	304	LPP	C14-C15-C16-C17
70	A1	402	CDL	C71-C72-C73-C74
70	B0	101	CDL	C76-C77-C78-C79
70	BT	201	CDL	C15-C16-C17-C18
73	AA	903	PC1	C23-C24-C25-C26
73	A0	605	PC1	O31-C31-C32-C33
70	A1	402	CDL	CA6-CA4-OA6-CA5
70	AA	908	CDL	CB3-CB4-OB6-CB5
70	BY	201	CDL	CB6-CB4-OB6-CB5
73	AM	302	PC1	C3-C2-O21-C21
73	AQ	202	PC1	C1-C2-O21-C21
75	A9	602	3PE	C1-C2-O21-C21
75	BP	201	3PE	C3-C2-O21-C21
70	AP	301	CDL	OB5-CB3-CB4-CB6
73	A9	604	PC1	O11-C1-C2-C3
70	A1	402	CDL	CB7-C71-C72-C73
70	AC	802	CDL	C72-C71-CB7-OB8
75	A9	602	3PE	C29-C2A-C2B-C2C
70	AC	801	CDL	C1-CA2-OA2-PA1
70	BY	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
73	AJ	501	PC1	O32-C31-O31-C3
70	BC	301	CDL	OA5-CA3-CA4-OA6
73	AM	302	PC1	O11-C1-C2-O21
70	B1	402	CDL	C11-C12-C13-C14
70	BV	201	CDL	C17-C18-C19-C20
73	AA	904	PC1	C11-C12-N-C15
80	AD	502	FMN	C2'-C3'-C4'-C5'
73	AJ	501	PC1	C32-C31-O31-C3
70	BV	201	CDL	C72-C71-CB7-OB8
70	AA	908	CDL	C31-CA7-OA8-CA6
70	A0	601	CDL	CB2-OB2-PB2-OB5
70	AA	901	CDL	CA2-OA2-PA1-OA5
70	AC	801	CDL	CB2-OB2-PB2-OB5
70	AF	402	CDL	CA2-OA2-PA1-OA5
70	B0	102	CDL	CA2-OA2-PA1-OA5
70	B0	102	CDL	CB2-OB2-PB2-OB5
70	BC	301	CDL	CB2-OB2-PB2-OB5
70	BE	201	CDL	CA2-OA2-PA1-OA5
70	BE	201	CDL	CB2-OB2-PB2-OB5
70	BG	201	CDL	CB2-OB2-PB2-OB5
70	BT	201	CDL	CA2-OA2-PA1-OA5
70	BT	201	CDL	CB2-OB2-PB2-OB5
70	BY	201	CDL	CA2-OA2-PA1-OA5
73	A6	302	PC1	C11-O13-P-O11
73	A6	303	PC1	C11-O13-P-O11
73	A9	601	PC1	C1-O11-P-O13
73	AA	904	PC1	C1-O11-P-O13
73	AQ	202	PC1	C11-O13-P-O11
73	BY	202	PC1	C1-O11-P-O13
75	A9	602	3PE	C1-O11-P-O13
75	BP	201	3PE	C11-O13-P-O11
70	BC	302	CDL	CA5-C11-C12-C13
70	BE	201	CDL	C13-C14-C15-C16
70	AC	801	CDL	C19-C20-C21-C22
70	AA	908	CDL	CA3-CA4-CA6-OA8
70	B0	101	CDL	CB3-CB4-CB6-OB8
70	BG	201	CDL	CA3-CA4-CA6-OA8
70	B0	101	CDL	C75-C76-C77-C78
70	AA	901	CDL	C32-C31-CA7-OA8
70	AM	301	CDL	C37-C38-C39-C40
74	A1	401	NDP	PN-O3-PA-O1A
74	A1	401	NDP	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
73	AQ	202	PC1	C3B-C3C-C3D-C3E
70	B0	101	CDL	C18-C19-C20-C21
73	BY	202	PC1	C32-C31-O31-C3
70	A0	601	CDL	C1-CA2-OA2-PA1
70	A0	601	CDL	CA4-CA3-OA5-PA1
70	BL	301	CDL	CA4-CA3-OA5-PA1
70	BY	201	CDL	CA4-CA3-OA5-PA1
70	B0	101	CDL	C31-C32-C33-C34
70	BE	201	CDL	CB2-C1-CA2-OA2
70	AM	301	CDL	C71-CB7-OB8-CB6
70	BL	301	CDL	C71-CB7-OB8-CB6
70	BL	301	CDL	OB9-CB7-OB8-CB6
75	BP	201	3PE	C36-C37-C38-C39
70	AA	908	CDL	OA9-CA7-OA8-CA6
73	AM	302	PC1	C32-C31-O31-C3
73	BT	202	PC1	C32-C31-O31-C3
73	AH	301	PC1	O11-C1-C2-C3
73	BT	202	PC1	O32-C31-O31-C3
75	A9	603	3PE	O13-C11-C12-N
70	AM	301	CDL	OB9-CB7-OB8-CB6
70	BV	201	CDL	CB5-C51-C52-C53
70	AF	402	CDL	C79-C80-C81-C82
73	AU	202	PC1	C3E-C3F-C3G-C3H
73	AM	302	PC1	O32-C31-O31-C3
73	A9	601	PC1	C3D-C3E-C3F-C3G
73	AU	202	PC1	C3B-C3C-C3D-C3E
70	AC	802	CDL	C44-C45-C46-C47
75	BA	301	3PE	C2B-C2C-C2D-C2E
70	A1	402	CDL	OB6-CB4-CB6-OB8
73	AL	303	PC1	C2-C1-O11-P
70	AF	401	CDL	C64-C65-C66-C67
73	BQ	401	PC1	C34-C35-C36-C37
73	AA	907	PC1	C29-C2A-C2B-C2C
73	B1	403	PC1	C37-C38-C39-C3A
73	A2	402	PC1	C33-C34-C35-C36
73	A9	601	PC1	C1-C2-C3-O31
73	AA	905	PC1	C1-C2-C3-O31
76	AA	902	LPP	C31-C32-C33-C34
70	BG	201	CDL	C74-C75-C76-C77
73	BQ	401	PC1	C27-C28-C29-C2A
70	AF	402	CDL	CB3-CB4-OB6-CB5
70	AF	402	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
70	BC	302	CDL	CA3-CA4-OA6-CA5
70	BE	201	CDL	CA6-CA4-OA6-CA5
73	A1	403	PC1	C1-C2-O21-C21
73	A1	404	PC1	C1-O11-P-O13
70	A0	602	CDL	OA5-CA3-CA4-OA6
70	B0	101	CDL	OA5-CA3-CA4-OA6
70	A1	402	CDL	OB5-CB3-CB4-CB6
70	AC	802	CDL	C53-C54-C55-C56
73	AA	906	PC1	C2F-C2G-C2H-C2I
73	BY	202	PC1	O32-C31-O31-C3
80	AD	502	FMN	O3'-C3'-C4'-C5'
75	A9	602	3PE	C31-C32-C33-C34
70	B1	402	CDL	C77-C78-C79-C80
70	BE	201	CDL	OA6-CA4-CA6-OA8
70	AC	802	CDL	C74-C75-C76-C77
70	BG	201	CDL	C75-C76-C77-C78
70	B1	402	CDL	C1-CA2-OA2-PA1
80	AD	502	FMN	O2'-C2'-C3'-O3'
70	AC	801	CDL	C63-C64-C65-C66
73	AJ	501	PC1	O21-C21-C22-C23
70	AA	908	CDL	C42-C43-C44-C45
73	AL	303	PC1	C23-C24-C25-C26
70	BT	201	CDL	C16-C17-C18-C19
70	AM	301	CDL	C32-C33-C34-C35
75	BP	201	3PE	O22-C21-O21-C2
70	AF	402	CDL	C77-C78-C79-C80
70	AP	301	CDL	C79-C80-C81-C82
70	BE	201	CDL	OA5-CA3-CA4-CA6
70	BT	201	CDL	OA5-CA3-CA4-CA6
73	AA	904	PC1	C2B-C2C-C2D-C2E
80	AD	502	FMN	O3'-C3'-C4'-O4'
70	AA	908	CDL	C72-C73-C74-C75
73	AA	905	PC1	O21-C2-C3-O31
70	AA	908	CDL	C39-C40-C41-C42
73	BQ	401	PC1	O21-C21-C22-C23
75	A9	602	3PE	O21-C21-C22-C23
70	AA	908	CDL	C33-C34-C35-C36
73	AA	906	PC1	C22-C23-C24-C25
76	AL	304	LPP	C6-O5-P1-O4
81	AS	200	8Q1	O33-C32-C34-N36
70	B0	101	CDL	C32-C31-CA7-OA8
70	BC	301	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
70	BC	302	CDL	C72-C71-CB7-OB8
73	B1	401	PC1	O31-C31-C32-C33
73	B1	403	PC1	C22-C23-C24-C25
73	AU	202	PC1	O31-C31-C32-C33
75	BA	301	3PE	O21-C21-C22-C23
76	BN	301	LPP	O9-C11-C12-C13
73	A1	404	PC1	C3-C2-O21-C21
70	A0	602	CDL	C72-C71-CB7-OB8
70	B1	402	CDL	C72-C71-CB7-OB8
70	BL	301	CDL	C32-C31-CA7-OA8
73	AJ	501	PC1	O31-C31-C32-C33
73	BQ	401	PC1	O31-C31-C32-C33
70	AF	401	CDL	C32-C31-CA7-OA8
73	A0	605	PC1	O21-C21-C22-C23
73	AM	302	PC1	O31-C31-C32-C33
70	A1	402	CDL	C15-C16-C17-C18
70	A0	602	CDL	C12-C13-C14-C15
75	A2	401	3PE	C1-C2-C3-O31
76	AA	902	LPP	C7-C6-O5-P1
75	BP	201	3PE	C37-C38-C39-C3A
70	BC	302	CDL	OA9-CA7-OA8-CA6
70	AP	301	CDL	C12-C13-C14-C15
70	BC	302	CDL	C31-CA7-OA8-CA6
70	AM	301	CDL	C32-C31-CA7-OA8
70	AF	402	CDL	C78-C79-C80-C81
70	AP	301	CDL	C78-C79-C80-C81
73	A9	601	PC1	C2C-C2D-C2E-C2F
70	BV	201	CDL	C76-C77-C78-C79
70	BV	201	CDL	C36-C37-C38-C39
70	BG	201	CDL	OB5-CB3-CB4-CB6
70	B0	101	CDL	C15-C16-C17-C18
73	A9	601	PC1	O21-C2-C3-O31
75	A2	401	3PE	O21-C2-C3-O31
70	A0	601	CDL	CA5-C11-C12-C13
70	BV	201	CDL	C13-C14-C15-C16
73	AA	904	PC1	O21-C21-C22-C23
73	AA	906	PC1	O21-C21-C22-C23
75	A9	603	3PE	O21-C21-C22-C23
76	AA	902	LPP	O27-C29-C30-C31
73	A1	404	PC1	C2-C3-O31-C31
74	A1	401	NDP	C2B-O2B-P2B-O3X
70	BC	302	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
73	A6	302	PC1	O31-C31-C32-C33
70	B0	102	CDL	OB7-CB5-OB6-CB4
76	A6	301	LPP	O9-C11-C12-C13
70	BY	201	CDL	C17-C18-C19-C20
73	BY	202	PC1	C34-C35-C36-C37
73	AA	906	PC1	C2-C3-O31-C31
74	A1	401	NDP	O4B-C4B-C5B-O5B
70	BT	201	CDL	C32-C31-CA7-OA8
75	BP	201	3PE	C22-C21-O21-C2
73	AM	302	PC1	O32-C31-C32-C33
70	B0	101	CDL	C16-C17-C18-C19
73	BS	1302	PC1	C33-C34-C35-C36
73	AU	202	PC1	O32-C31-C32-C33
70	BC	302	CDL	C72-C71-CB7-OB9
70	BL	301	CDL	C32-C31-CA7-OA9
70	AC	801	CDL	C34-C35-C36-C37
70	BC	301	CDL	C12-C11-CA5-OA7
70	B0	102	CDL	C36-C37-C38-C39
75	BA	301	3PE	C38-C39-C3A-C3B
70	A0	602	CDL	C72-C71-CB7-OB9
70	B0	101	CDL	C32-C31-CA7-OA9
73	AJ	501	PC1	O32-C31-C32-C33
73	B1	401	PC1	O32-C31-C32-C33
73	BQ	401	PC1	O22-C21-C22-C23
75	A9	602	3PE	O22-C21-C22-C23
75	A9	603	3PE	O22-C21-C22-C23
73	AA	903	PC1	C1-C2-C3-O31
70	AF	402	CDL	C32-C31-CA7-OA8
70	B0	102	CDL	C32-C31-CA7-OA8
70	AF	402	CDL	CB3-OB5-PB2-OB2
73	BS	1301	PC1	C23-C24-C25-C26
70	BV	201	CDL	C51-C52-C53-C54
73	BQ	401	PC1	C3E-C3F-C3G-C3H
76	BN	301	LPP	O27-C29-C30-C31
70	B1	402	CDL	OB7-CB5-OB6-CB4
73	AA	903	PC1	O22-C21-O21-C2
70	B0	102	CDL	CB4-CB3-OB5-PB2
74	A1	401	NDP	C4D-C5D-O5D-PN
76	AA	902	LPP	C35-C36-C37-C38
70	AF	401	CDL	C32-C31-CA7-OA9
75	BA	301	3PE	O22-C21-C22-C23
73	AA	907	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
73	AA	907	PC1	C33-C34-C35-C36
70	AA	908	CDL	CB3-OB5-PB2-OB3
70	AC	801	CDL	CB2-OB2-PB2-OB3
70	AF	402	CDL	CA2-OA2-PA1-OA3
70	AF	402	CDL	CB3-OB5-PB2-OB3
70	B0	101	CDL	CB2-OB2-PB2-OB4
70	BC	301	CDL	CB2-OB2-PB2-OB3
70	BG	201	CDL	CA3-OA5-PA1-OA4
70	BY	201	CDL	CA2-OA2-PA1-OA3
70	BY	201	CDL	CA3-OA5-PA1-OA3
73	AA	903	PC1	C11-O13-P-O14
73	AQ	202	PC1	C11-O13-P-O12
73	AU	202	PC1	C1-O11-P-O14
73	BQ	401	PC1	C1-O11-P-O14
73	BY	202	PC1	C1-O11-P-O14
74	A1	401	NDP	C5D-O5D-PN-O1N
70	AC	802	CDL	OA6-CA4-CA6-OA8
73	AQ	202	PC1	C23-C24-C25-C26
70	AM	301	CDL	C32-C31-CA7-OA9
73	BQ	401	PC1	O32-C31-C32-C33
76	AA	902	LPP	O28-C29-C30-C31
70	BT	201	CDL	OB5-CB3-CB4-CB6
70	B1	402	CDL	C72-C71-CB7-OB9
70	BT	201	CDL	C32-C31-CA7-OA9
70	BL	301	CDL	C72-C71-CB7-OB8
70	BC	301	CDL	C32-C31-CA7-OA8
73	AA	903	PC1	C21-C22-C23-C24
73	A6	302	PC1	O32-C31-C32-C33
73	A1	404	PC1	C2A-C2B-C2C-C2D
73	A0	605	PC1	C12-C11-O13-P
73	AJ	501	PC1	C1-C2-O21-C21
73	AJ	501	PC1	C3-C2-O21-C21
75	A9	602	3PE	C12-C11-O13-P
73	A0	605	PC1	O22-C21-C22-C23
73	AA	906	PC1	O22-C21-C22-C23
70	BE	201	CDL	C32-C31-CA7-OA8
70	AP	301	CDL	C32-C31-CA7-OA8
70	BC	301	CDL	C72-C71-CB7-OB8
70	BG	201	CDL	C72-C71-CB7-OB8
70	AC	802	CDL	C78-C79-C80-C81
70	AP	301	CDL	C52-C51-CB5-OB6
70	B0	101	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
70	B1	402	CDL	C12-C11-CA5-OA6
73	A9	604	PC1	O21-C21-C22-C23
73	A9	604	PC1	O31-C31-C32-C33
73	AH	301	PC1	O21-C21-C22-C23
70	AA	901	CDL	CB2-C1-CA2-OA2
70	AF	401	CDL	C60-C61-C62-C63
70	BV	201	CDL	C75-C76-C77-C78
76	A6	301	LPP	O10-C11-C12-C13
70	BT	201	CDL	OA5-CA3-CA4-OA6
70	AF	402	CDL	C32-C31-CA7-OA9
73	AA	904	PC1	O22-C21-C22-C23
73	AM	302	PC1	O22-C21-C22-C23
73	AA	905	PC1	O21-C21-C22-C23
73	AA	906	PC1	O31-C31-C32-C33
73	AM	302	PC1	O21-C21-C22-C23
70	A1	402	CDL	C14-C15-C16-C17
70	BE	201	CDL	C32-C31-CA7-OA9
73	AA	907	PC1	O31-C31-C32-C33
70	AP	301	CDL	C32-C31-CA7-OA9
70	B0	102	CDL	C32-C31-CA7-OA9
70	BC	301	CDL	C72-C71-CB7-OB9
73	AJ	501	PC1	C38-C39-C3A-C3B
70	AF	402	CDL	C72-C71-CB7-OB8
73	AA	907	PC1	O21-C21-C22-C23
76	A6	301	LPP	O27-C29-C30-C31
70	B1	402	CDL	C55-C56-C57-C58
70	BC	301	CDL	C32-C31-CA7-OA9
73	AA	906	PC1	O32-C31-C32-C33
70	AA	901	CDL	C52-C53-C54-C55
73	A9	604	PC1	O32-C31-C32-C33
73	A6	303	PC1	C33-C34-C35-C36

There are no ring outliers.

26 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	A6	303	PC1	2	0
75	BA	301	3PE	1	0
70	BC	302	CDL	1	0
71	A0	603	UDP	2	0
76	AA	902	LPP	1	0
81	AS	200	8Q1	2	0

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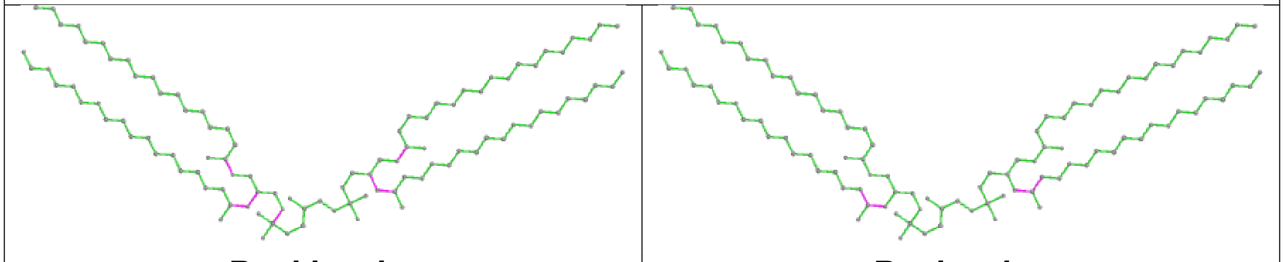
Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	BS	1301	PC1	1	0
79	AL	301	SF4	1	0
70	B0	102	CDL	1	0
70	BL	301	CDL	1	0
73	BT	202	PC1	1	0
78	BI	201	FES	1	0
79	AD	501	SF4	1	0
79	AB	802	SF4	1	0
70	AP	301	CDL	3	0
78	AB	801	FES	1	0
70	AA	908	CDL	1	0
76	AL	304	LPP	2	0
79	AL	302	SF4	5	0
78	AI	301	FES	2	0
70	BE	201	CDL	1	0
73	AL	303	PC1	2	0
70	AA	901	CDL	2	0
79	AB	803	SF4	2	0
70	A0	602	CDL	1	0
75	A9	602	3PE	1	0

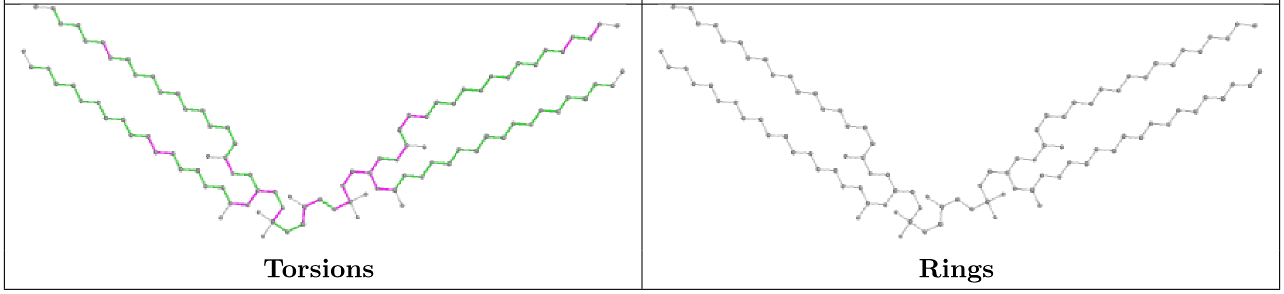
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 CDL A1 402



Bond lengths

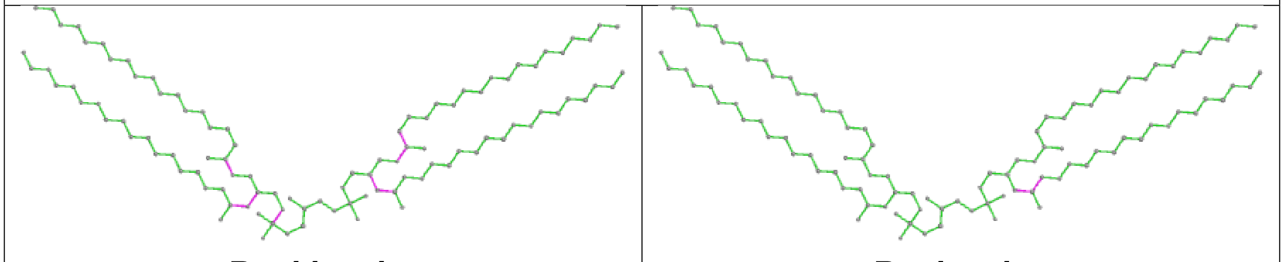
Bond angles



Torsions

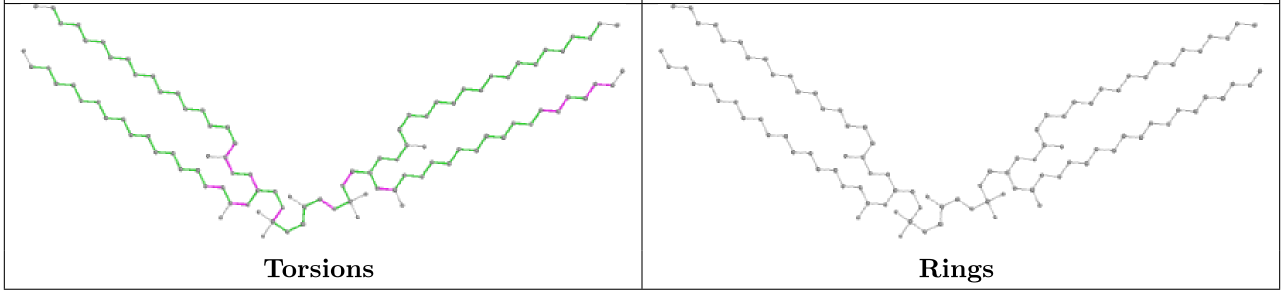
Rings

Ligand CDL AF 401



Bond lengths

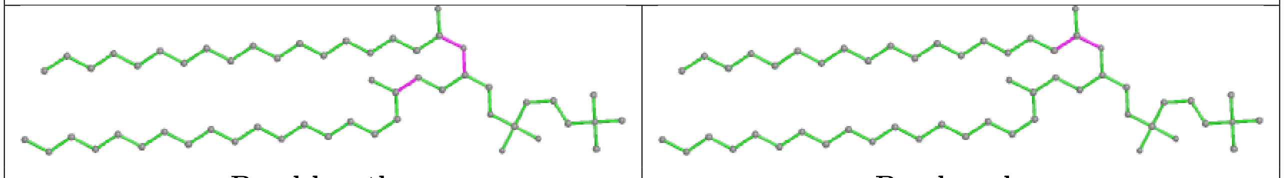
Bond angles



Torsions

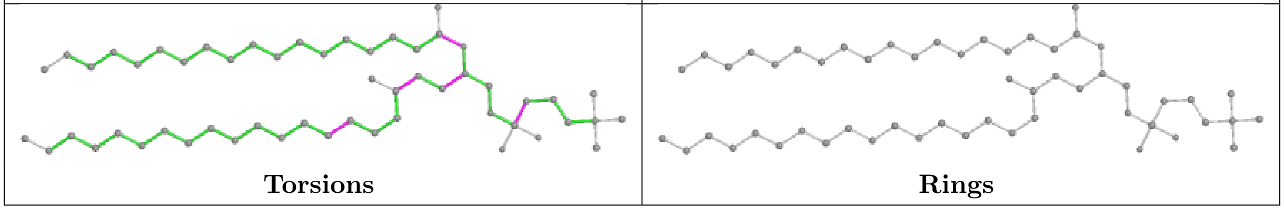
Rings

Ligand PC1 A6 303



Bond lengths

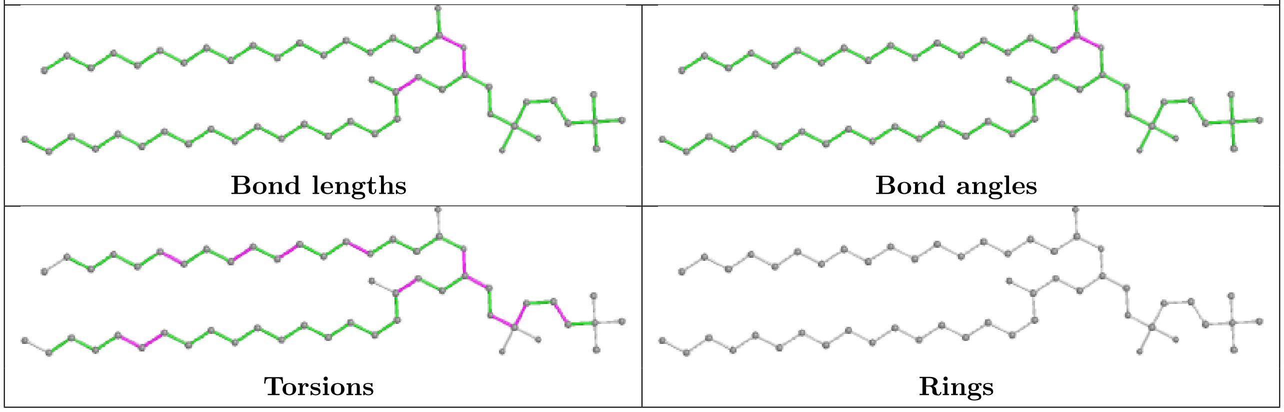
Bond angles



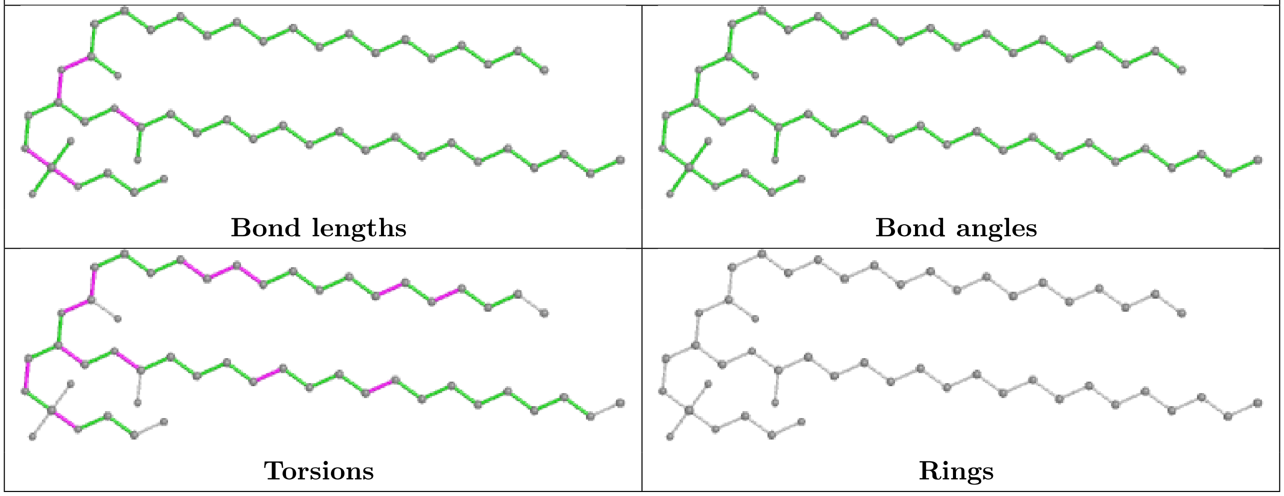
Torsions

Rings

Ligand PC1 AQ 202



Ligand 3PE BA 301



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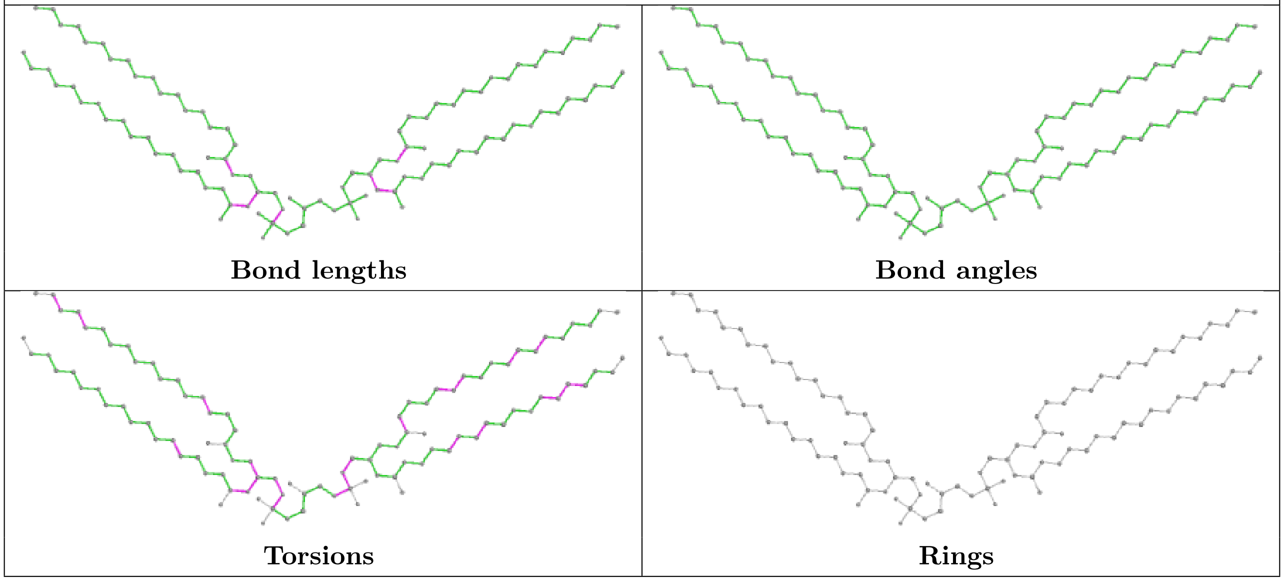

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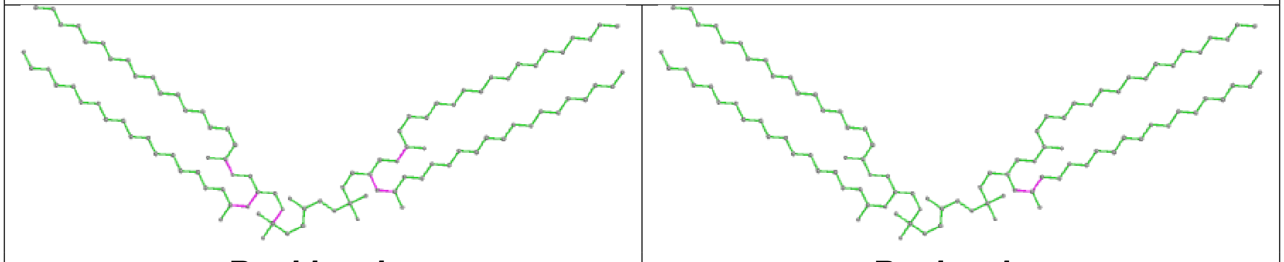
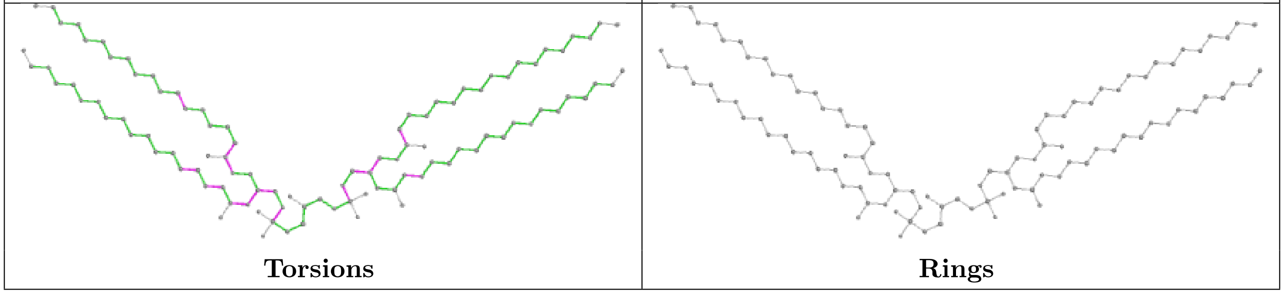


Bond lengths

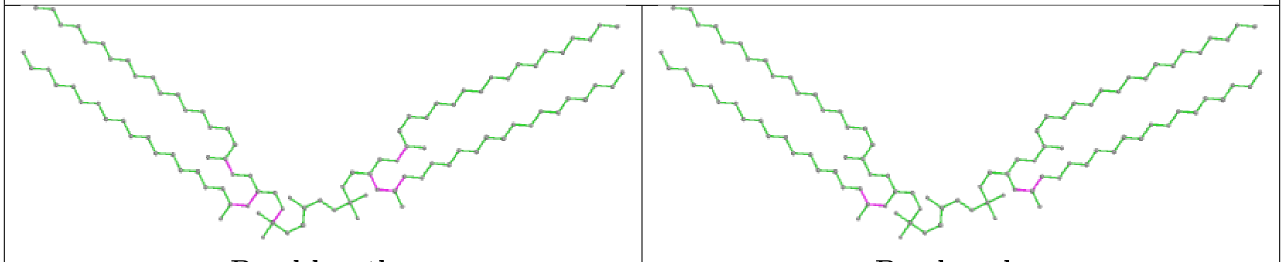
Bond angles



Torsions

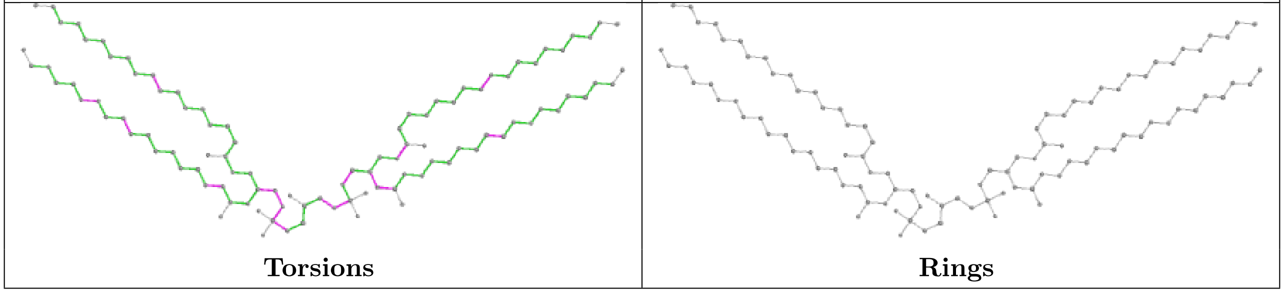
Rings

Ligand CDL BY 201



Bond lengths

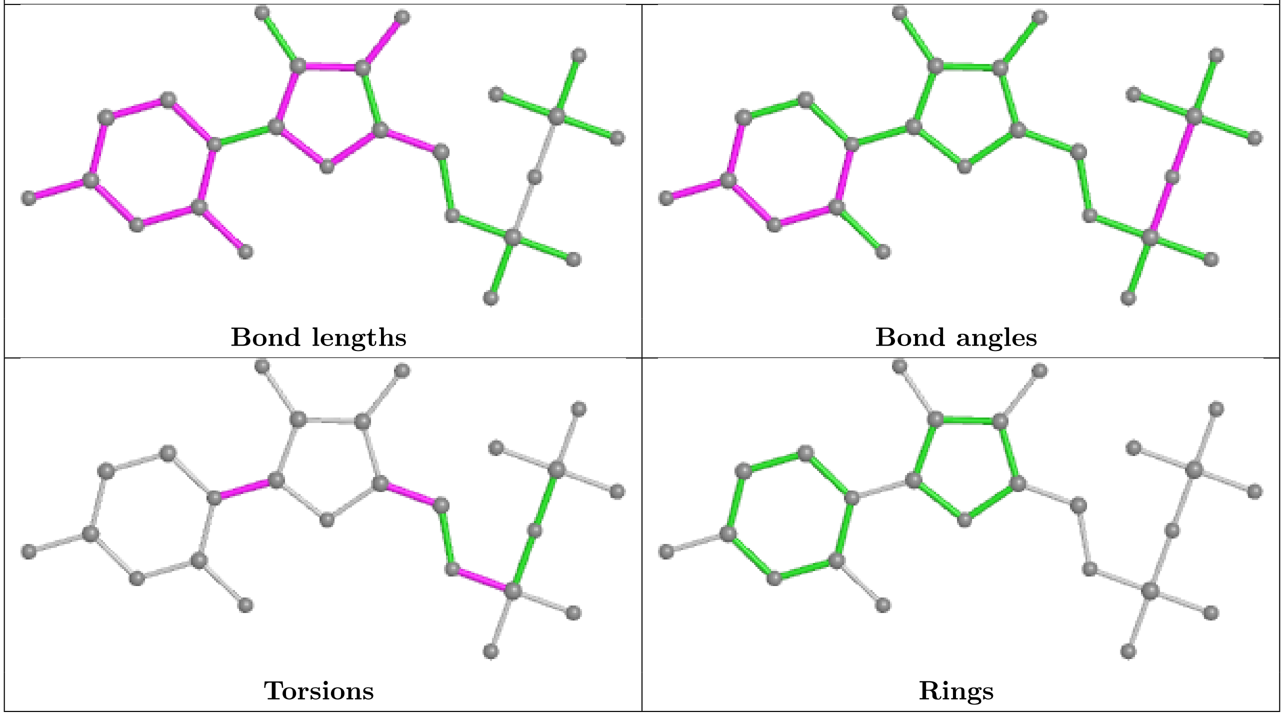
Bond angles



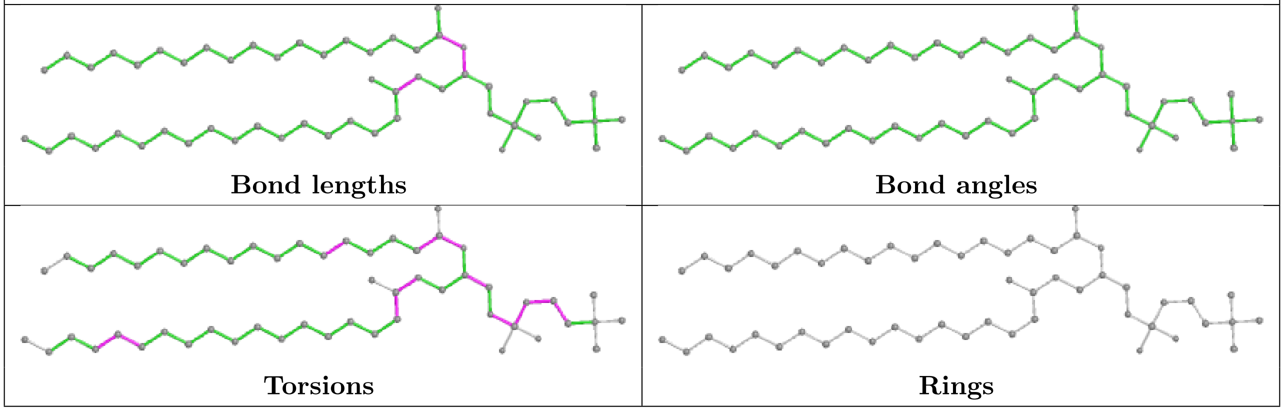
Torsions

Rings

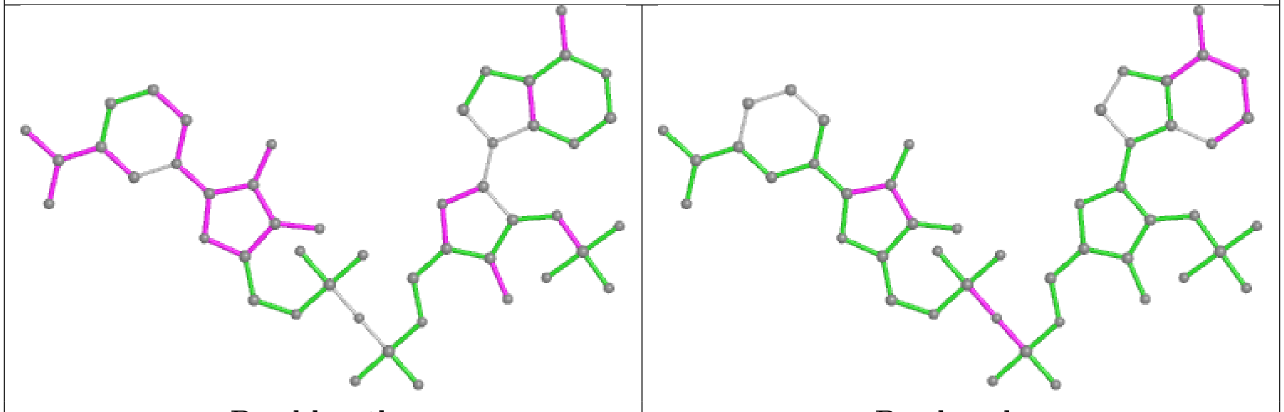
Ligand UDP A0 603



Ligand PC1 A9 604

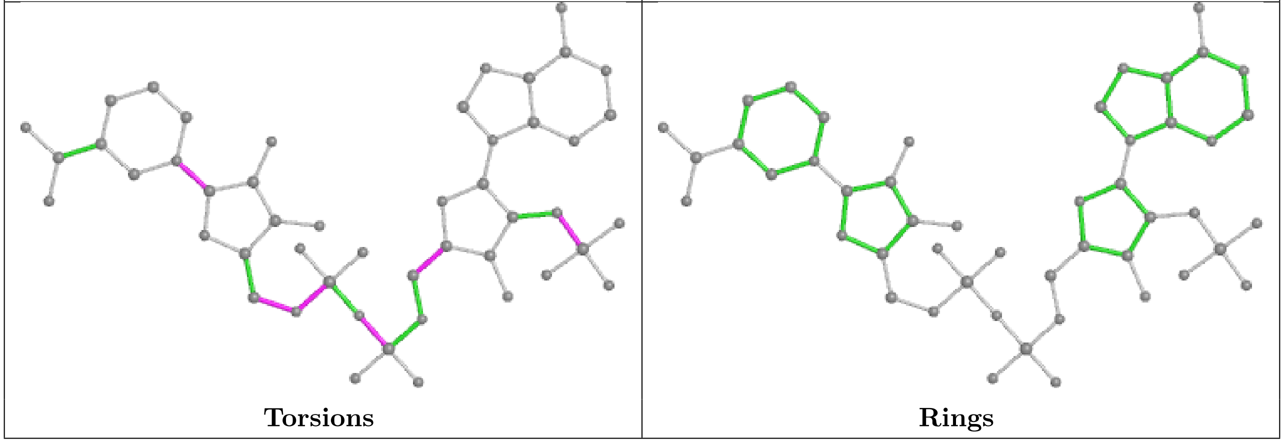


Ligand NDP A1 401



Bond lengths

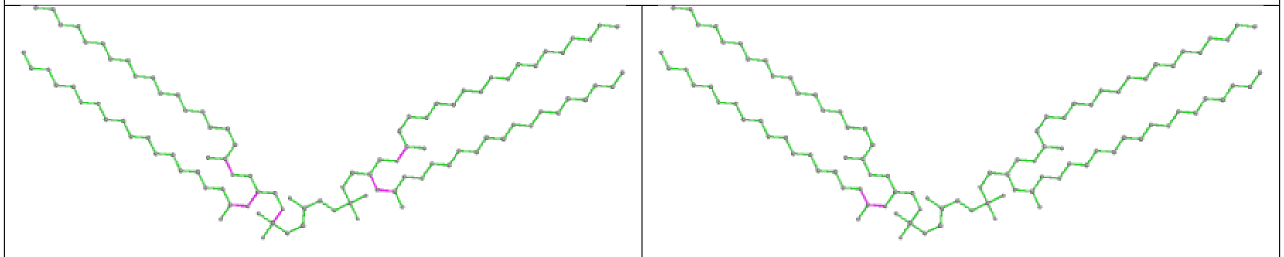
Bond angles



Torsions

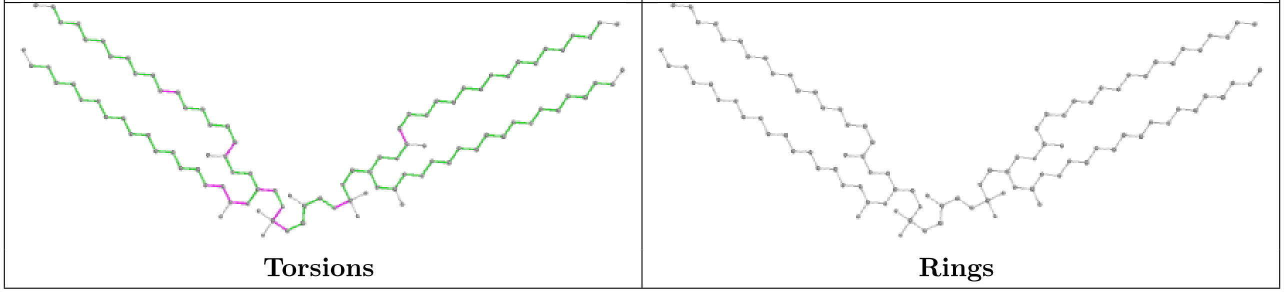
Rings

Ligand CDL BC 301



Bond lengths

Bond angles



Torsions

Rings

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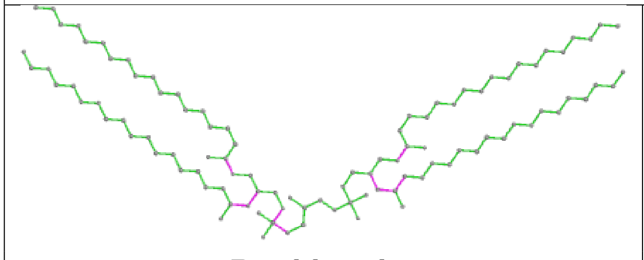
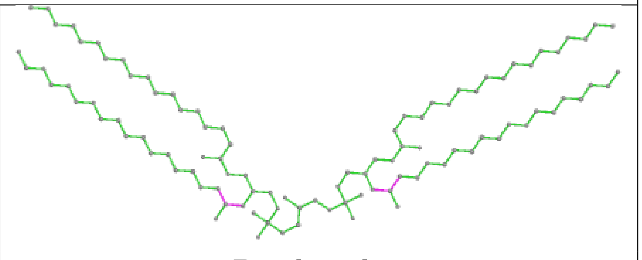
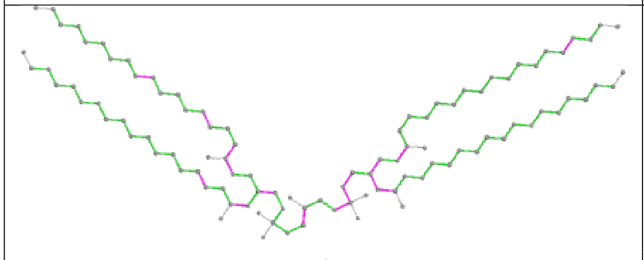


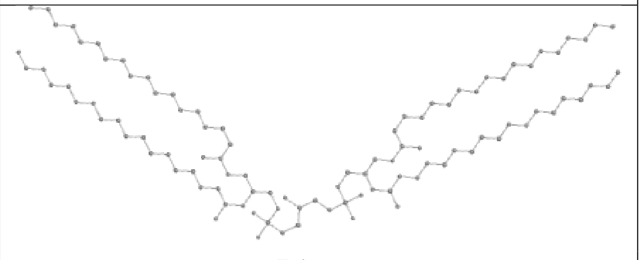
Bond lengths



Bond angles

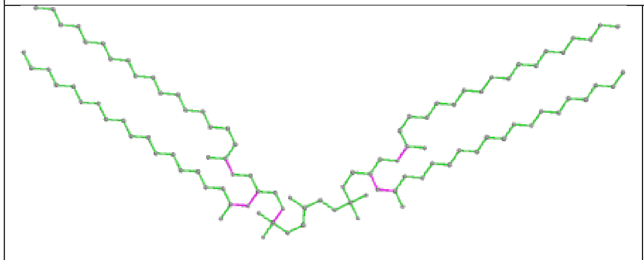


Torsions



Rings

Ligand CDL B0 101



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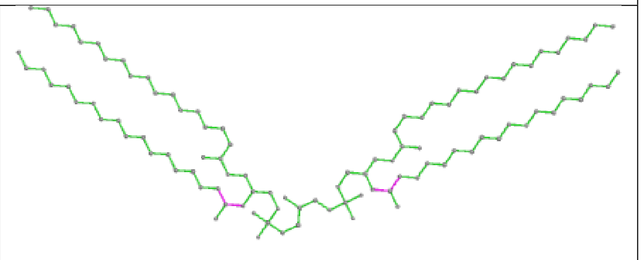

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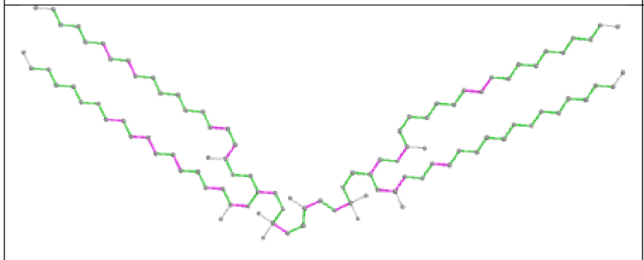

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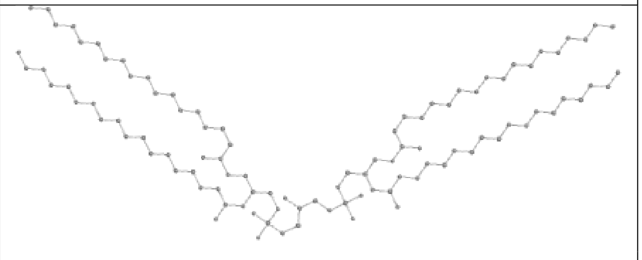
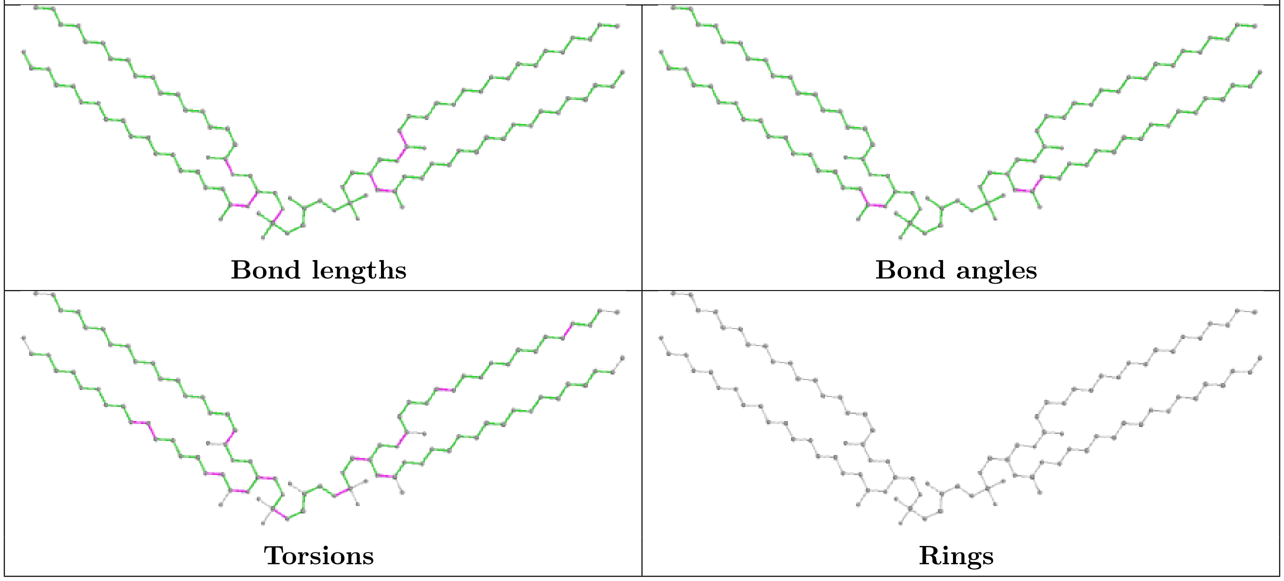


Rings

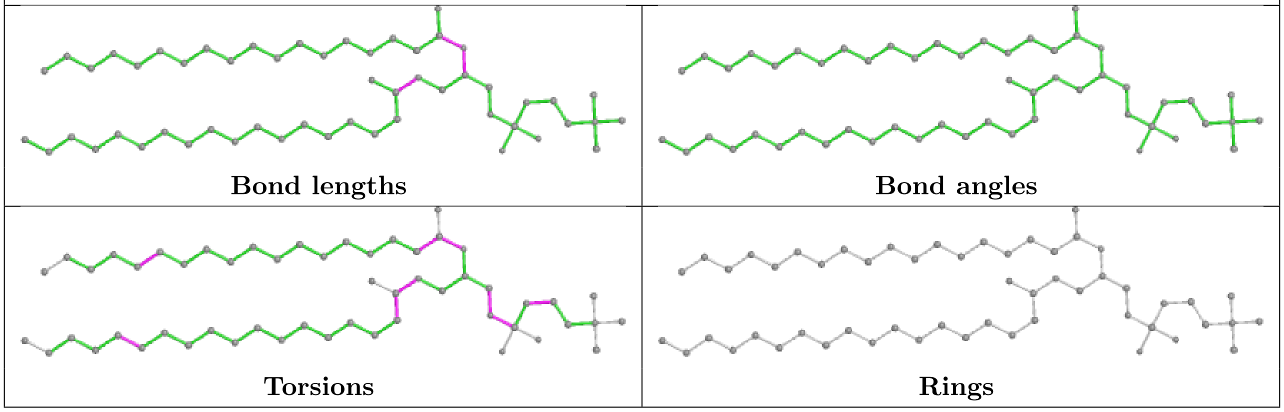
Ligand CDL BT 201



Bond lengths Bond angles

Torsions Rings

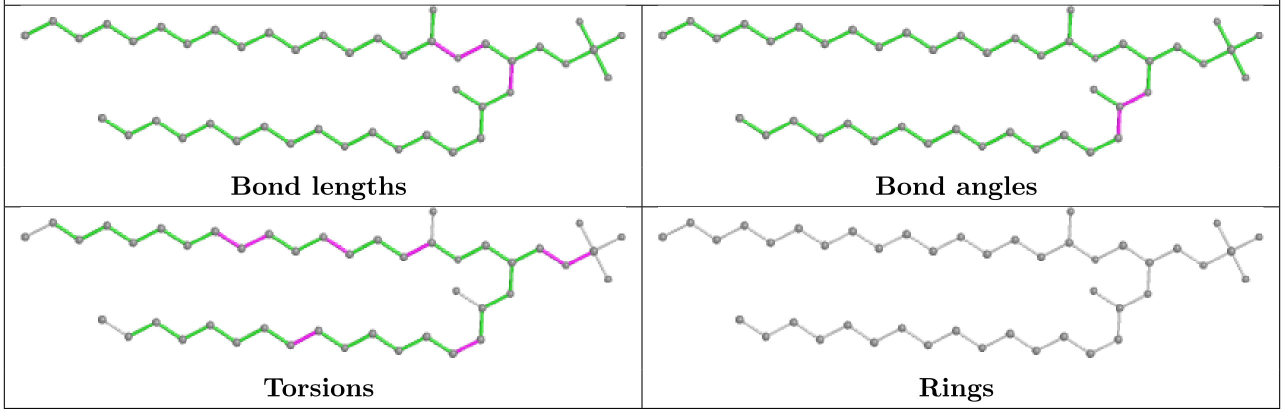
Ligand PC1 A0 605



Bond lengths Bond angles

Torsions Rings

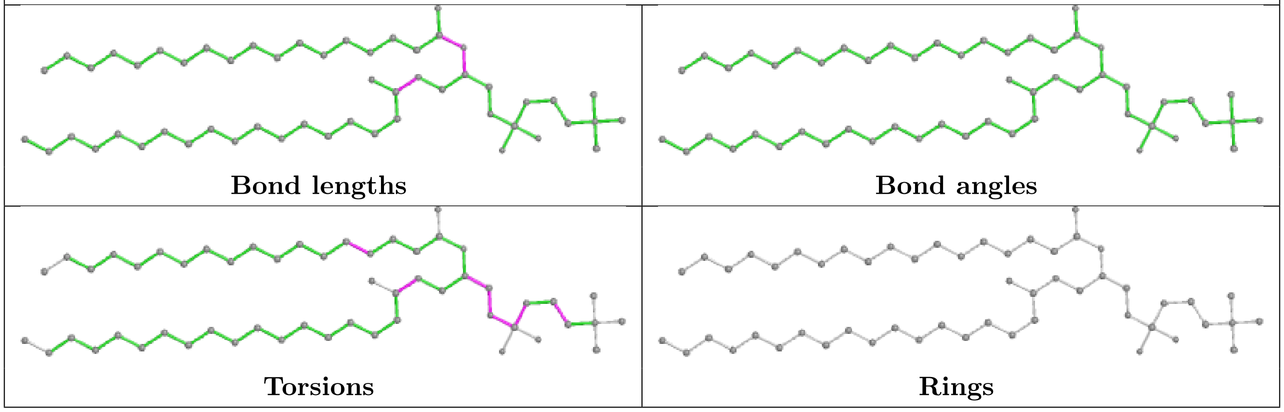
Ligand LPP AA 902



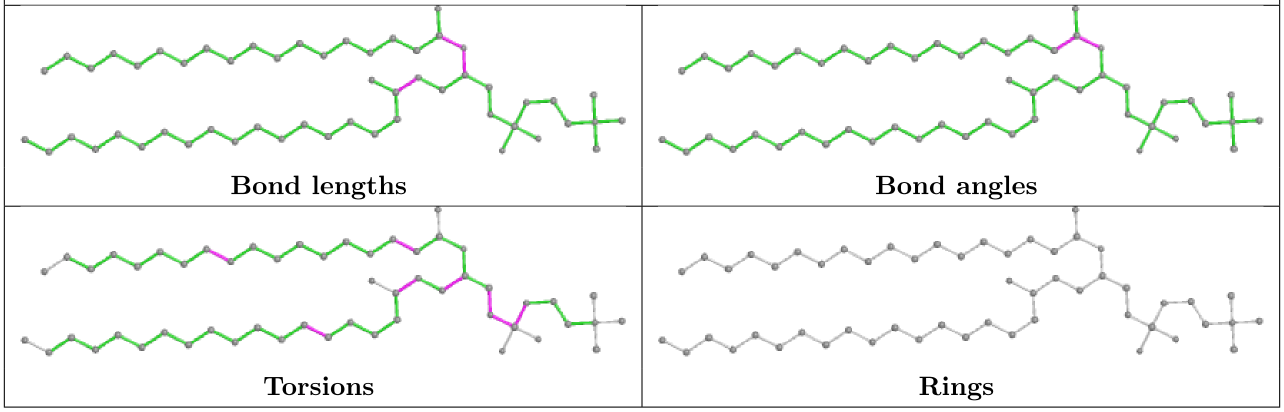
Bond lengths Bond angles

Torsions Rings

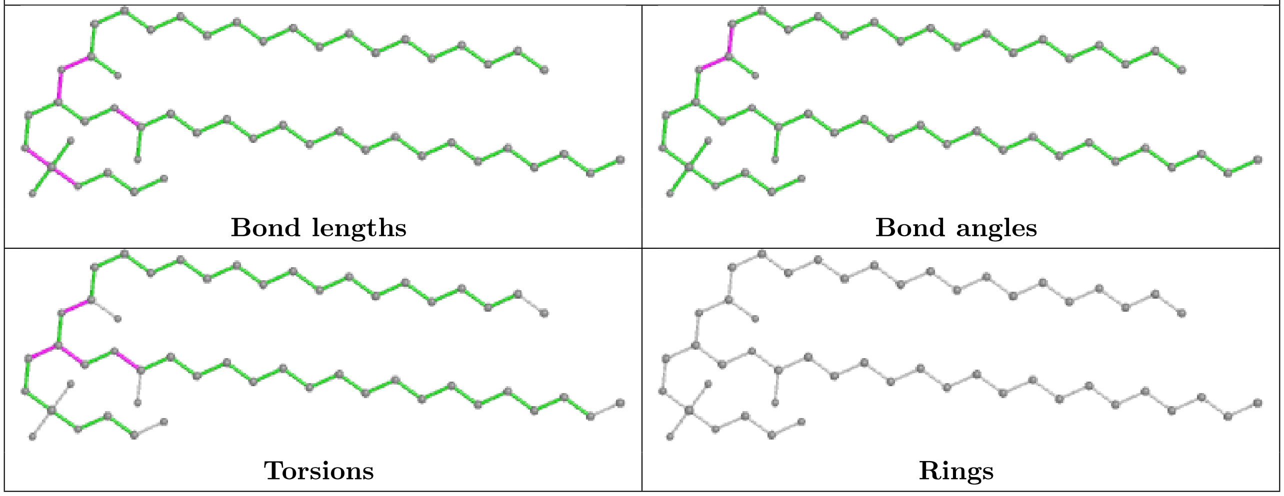
Ligand PC1 AU 201


Bond lengths
Bond angles
Torsions
Rings

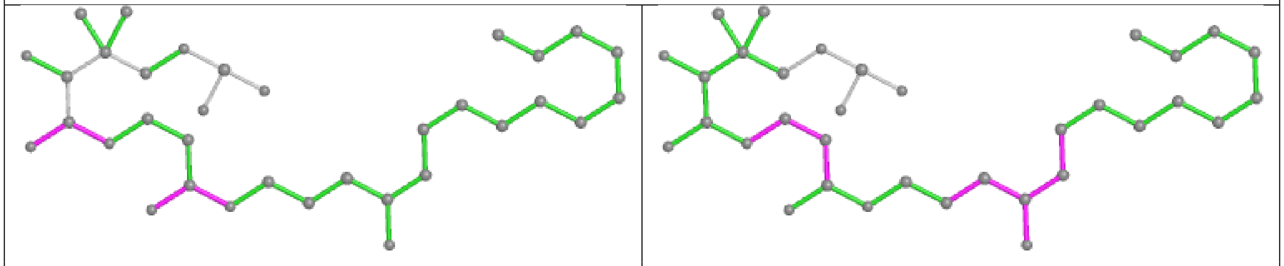
Ligand PC1 BY 202


Bond lengths
Bond angles
Torsions
Rings

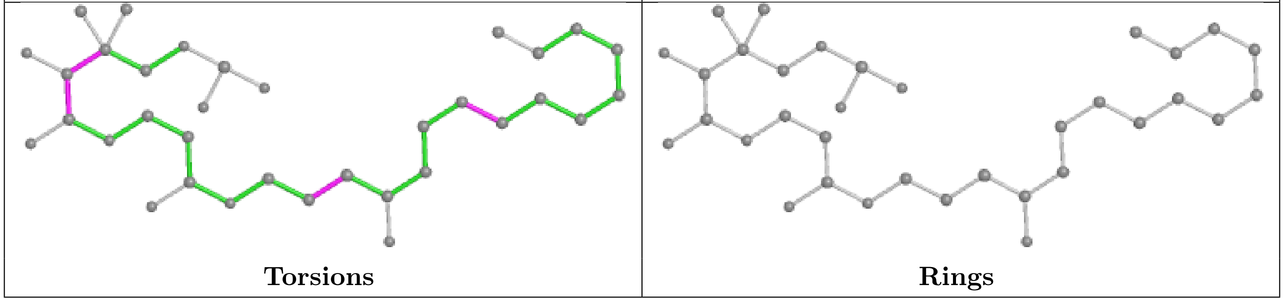
Ligand 3PE A2 401


Bond lengths
Bond angles
Torsions
Rings

Ligand 8Q1 AS 200

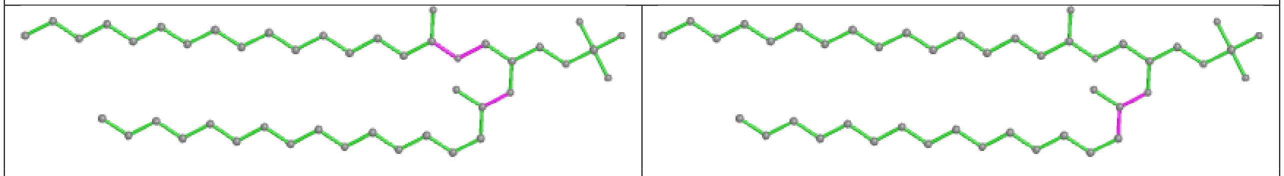


Bond lengths Bond angles

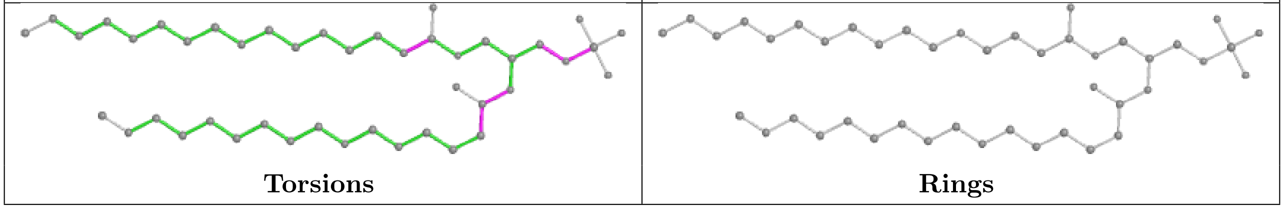


Torsions Rings

Ligand LPP A6 301

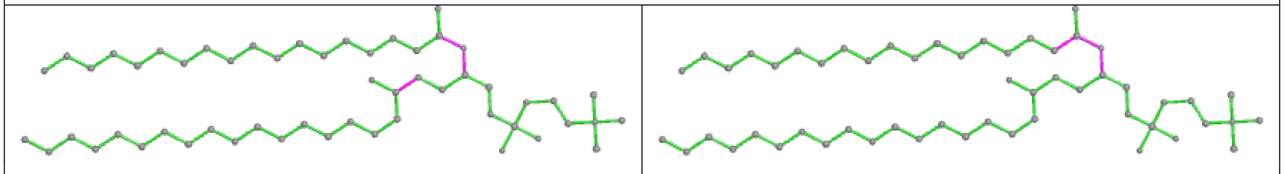


Bond lengths Bond angles

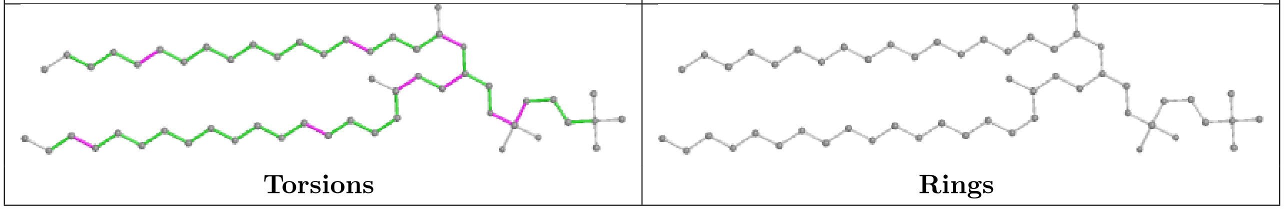


Torsions Rings

Ligand PC1 BS 1301

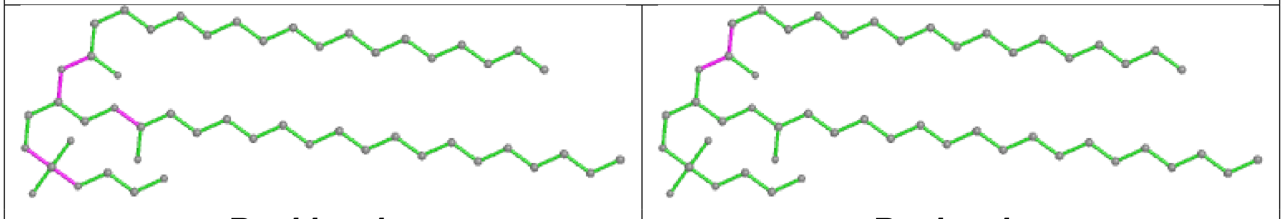


Bond lengths Bond angles



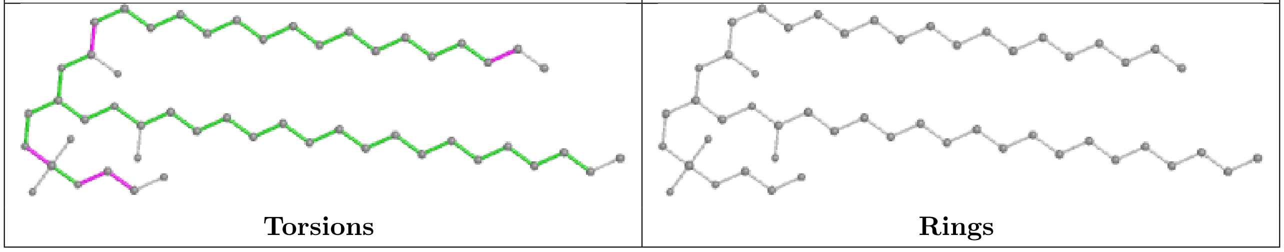
Torsions Rings

Ligand 3PE A9 603



Bond lengths

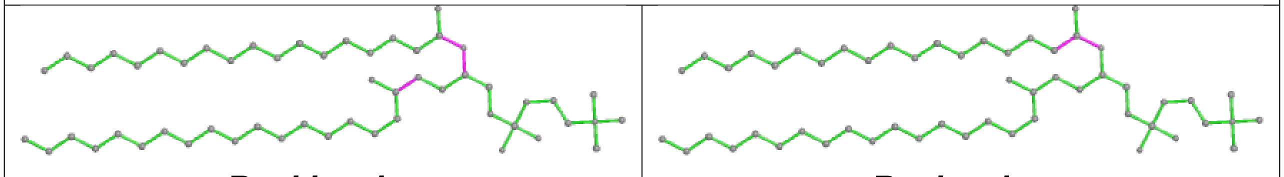
Bond angles



Torsions

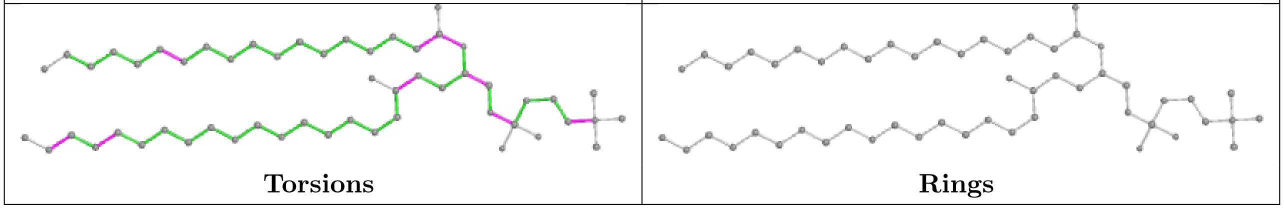
Rings

Ligand PC1 AA 904



Bond lengths

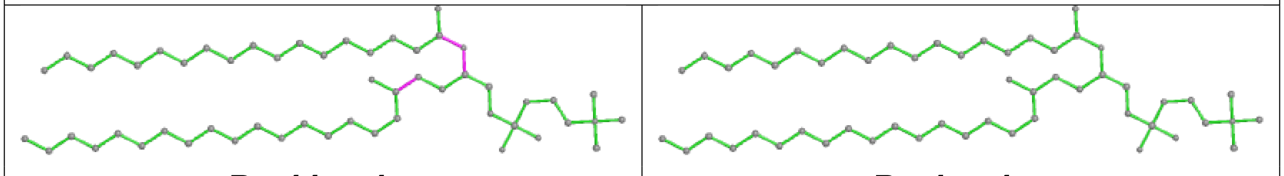
Bond angles



Torsions

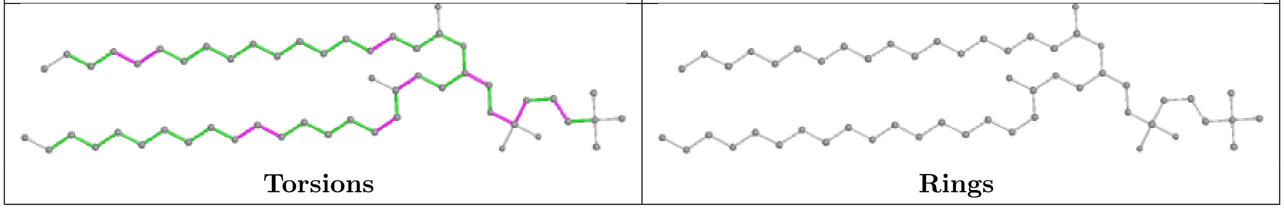
Rings

Ligand PC1 B1 403



Bond lengths

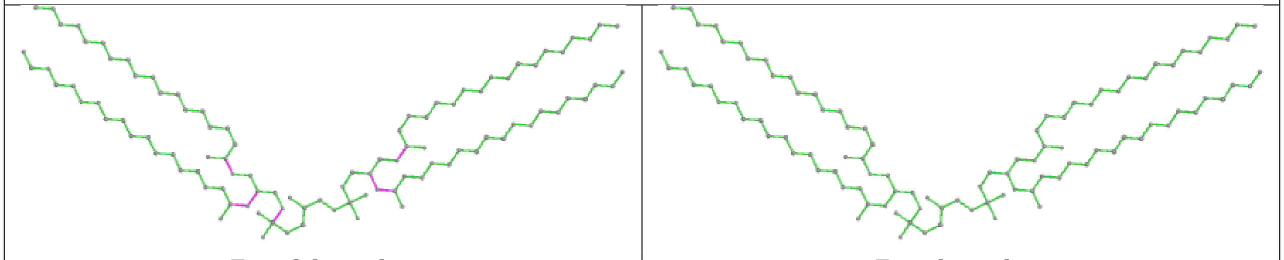
Bond angles



Torsions

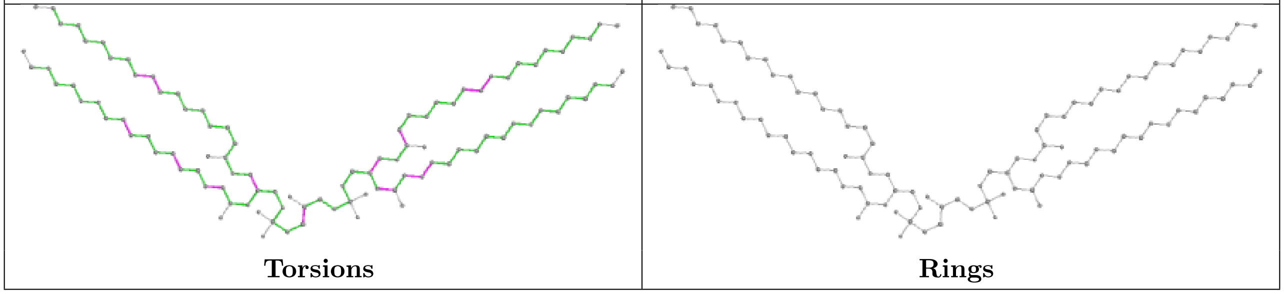
Rings

Ligand CDL BV 201



Bond lengths

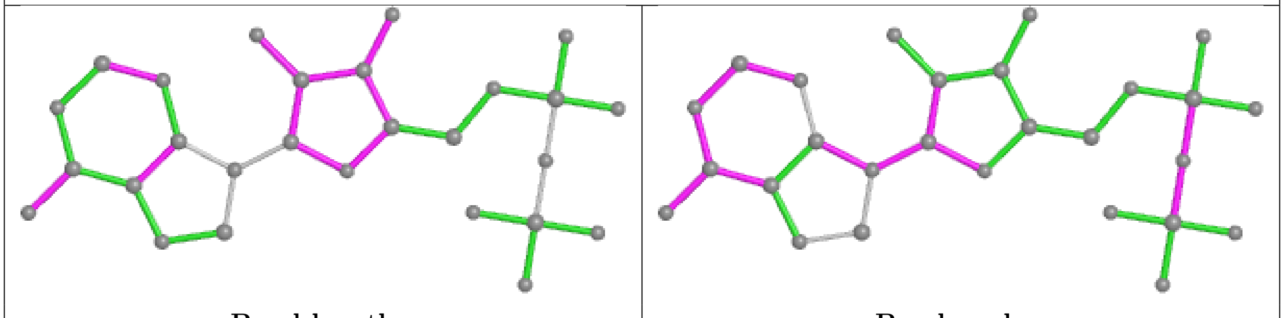
Bond angles



Torsions

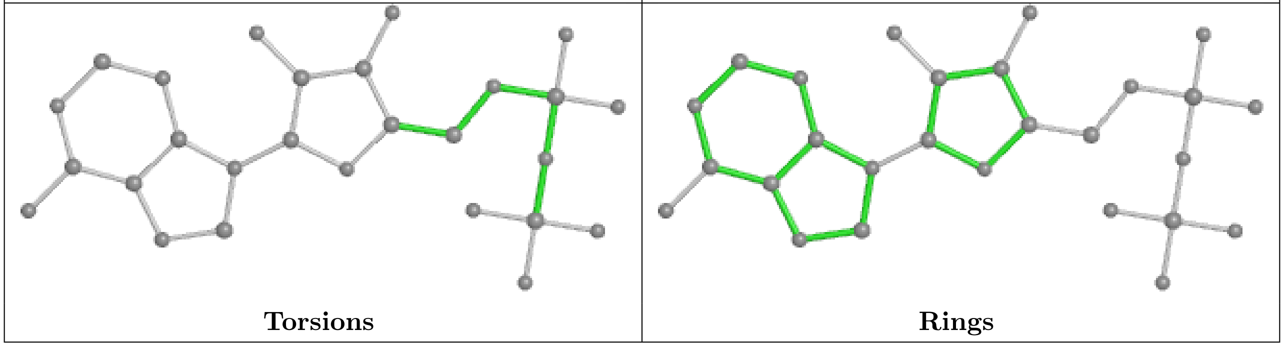
Rings

Ligand ADP A8 401



Bond lengths

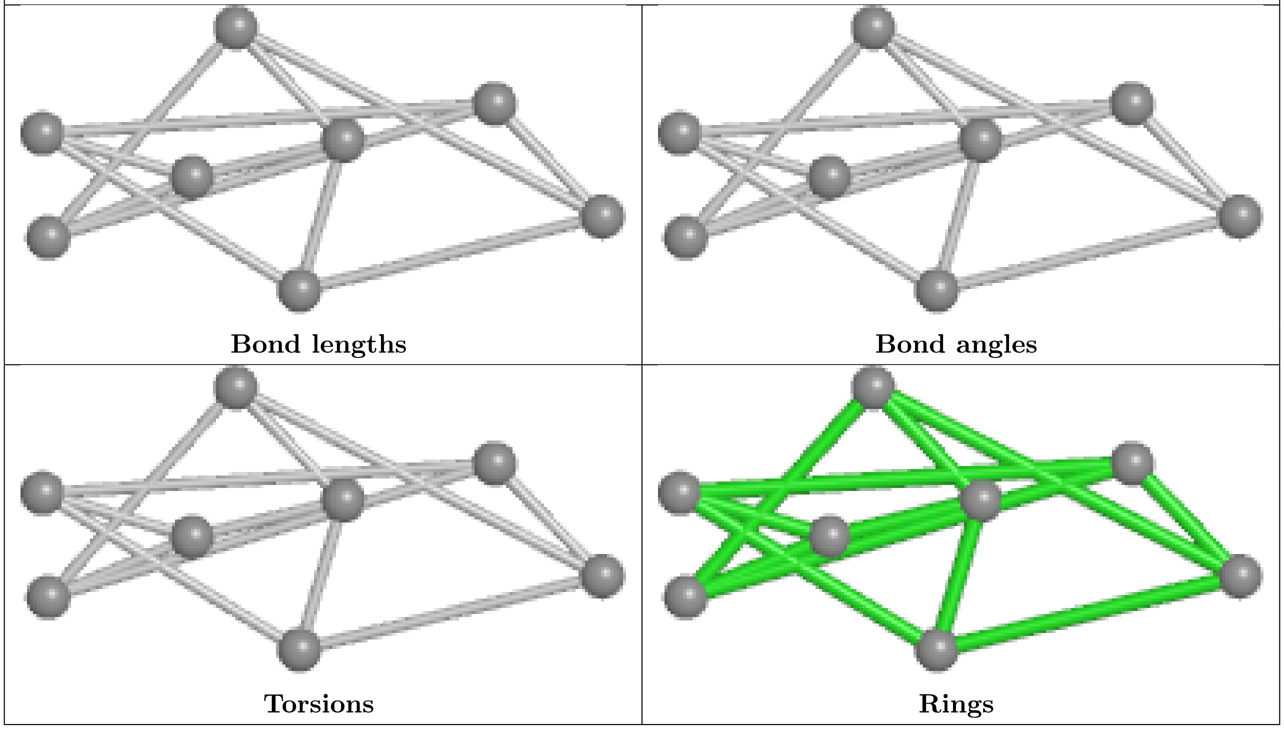
Bond angles



Torsions

Rings

Ligand SF4 AL 301



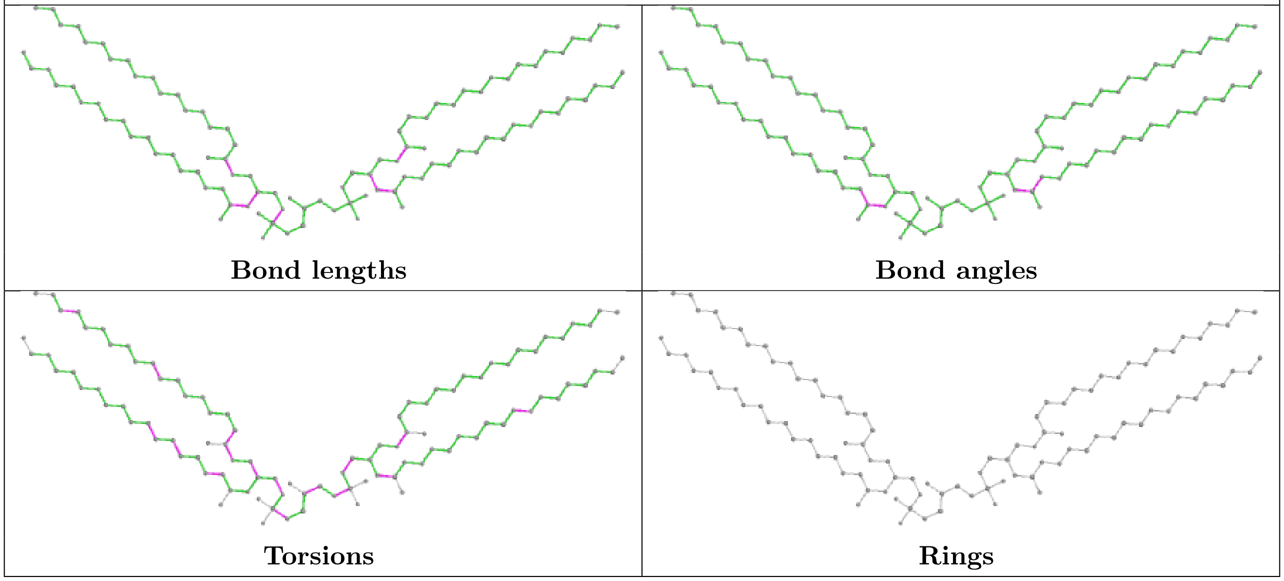
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL B0 102



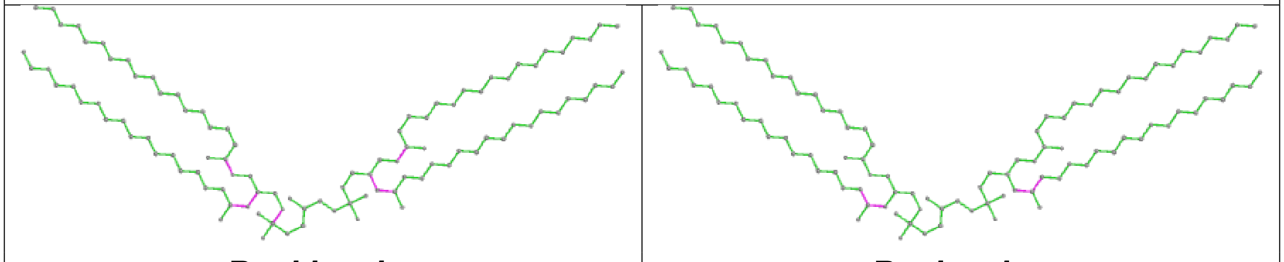
Bond lengths

Bond angles

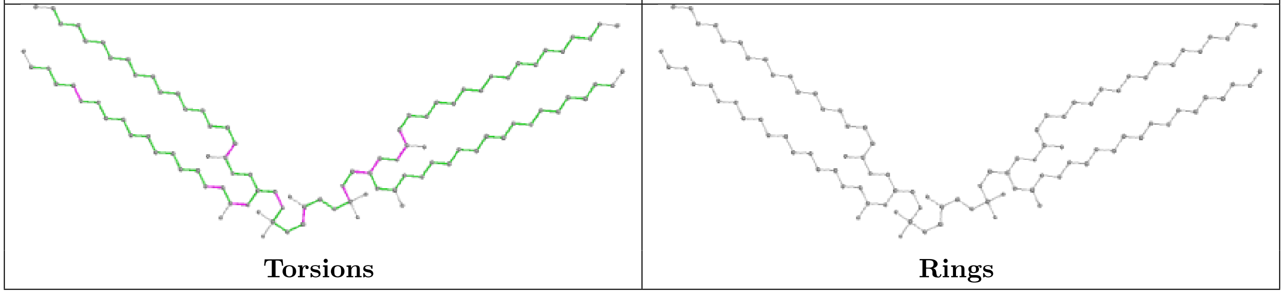
Torsions

Rings

Ligand CDL BL 301

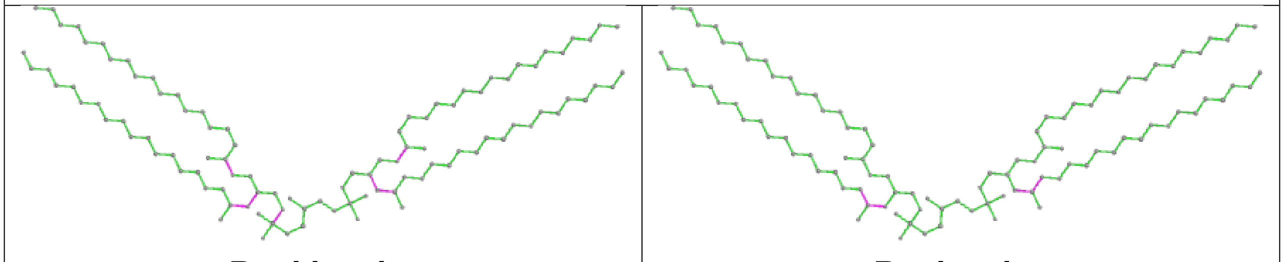


Bond lengths Bond angles

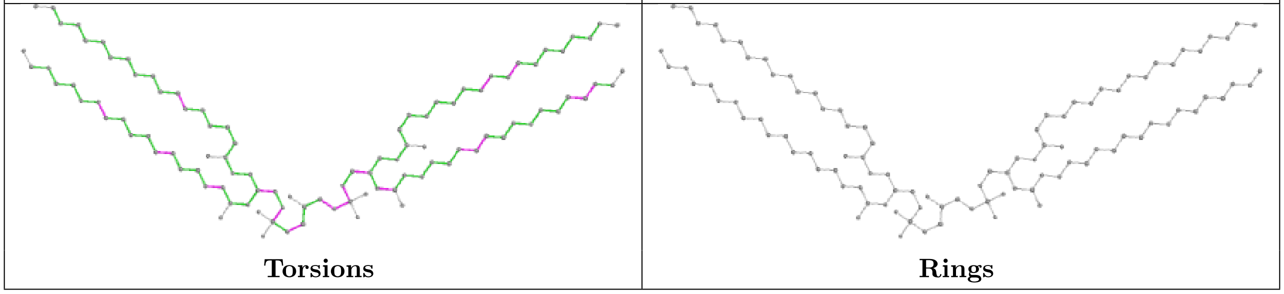


Torsions Rings

Ligand CDL AC 801

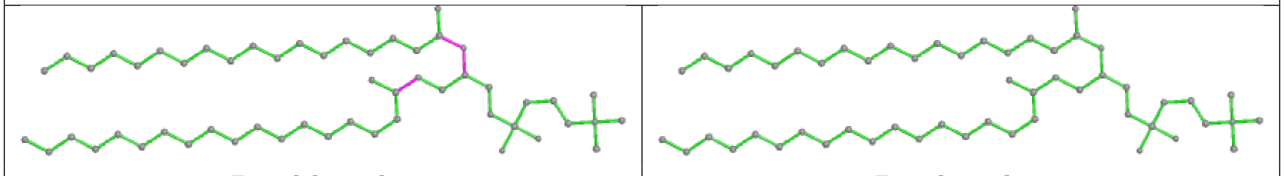


Bond lengths Bond angles

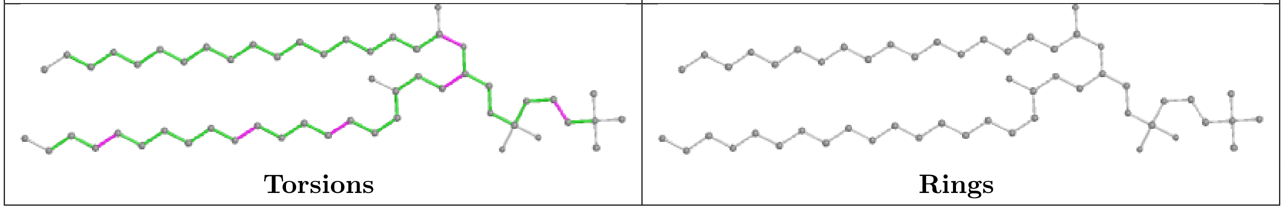


Torsions Rings

Ligand PC1 A2 402

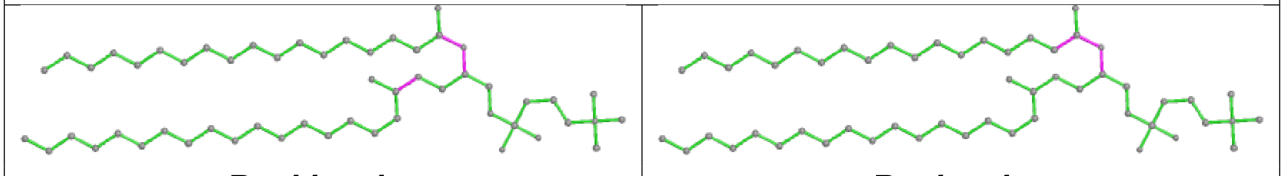


Bond lengths Bond angles



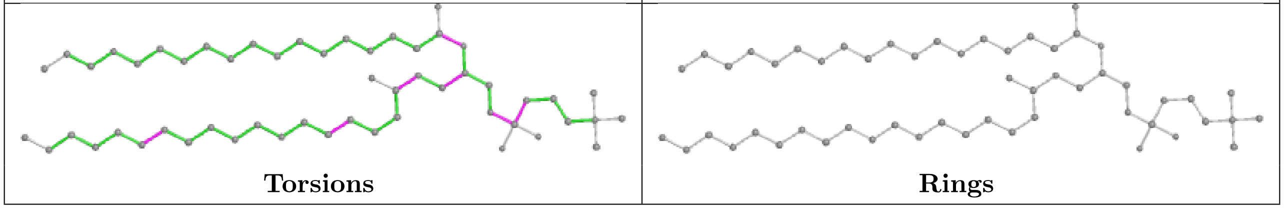
Torsions Rings

Ligand PC1 BT 202



Bond lengths

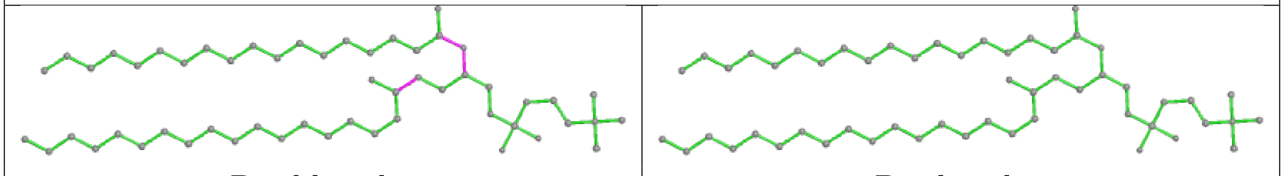
Bond angles



Torsions

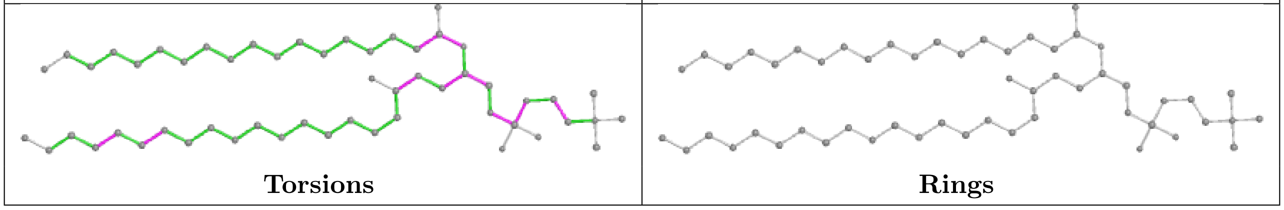
Rings

Ligand PC1 AA 905



Bond lengths

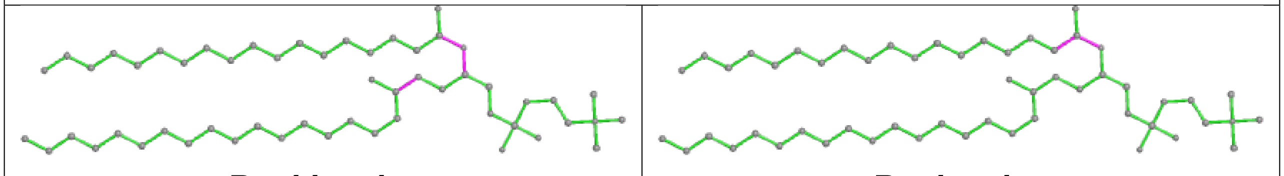
Bond angles



Torsions

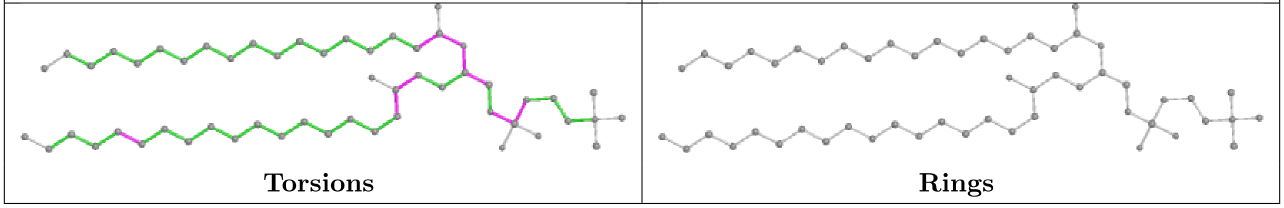
Rings

Ligand PC1 AM 302



Bond lengths

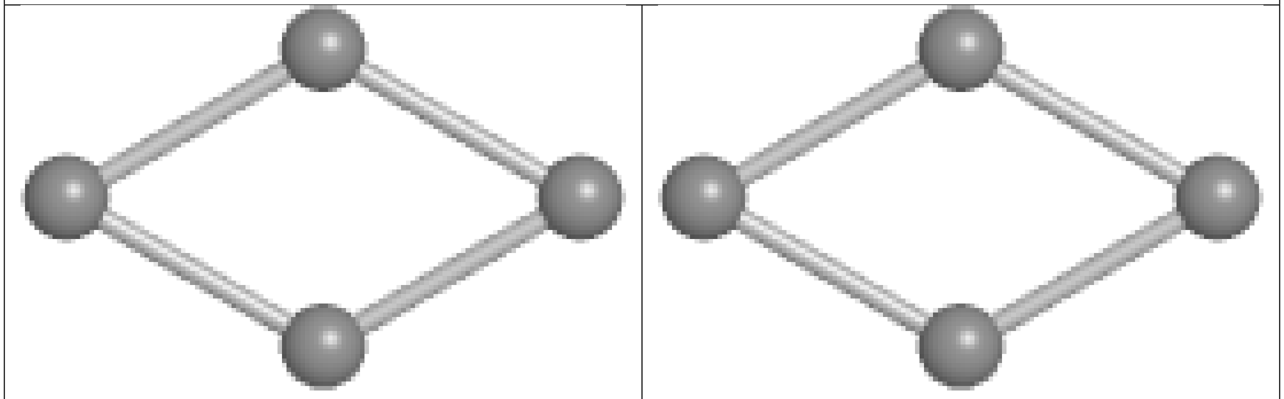
Bond angles



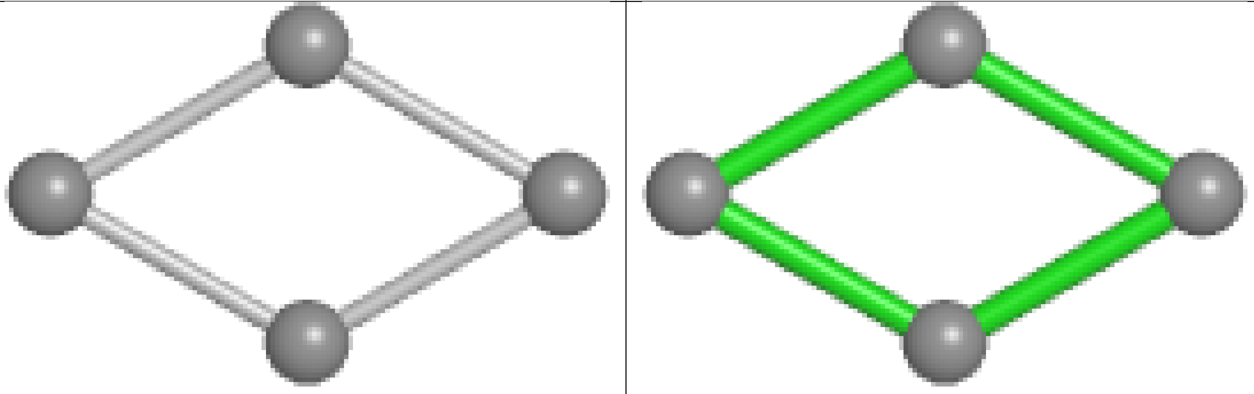
Torsions

Rings

Ligand FES BI 201

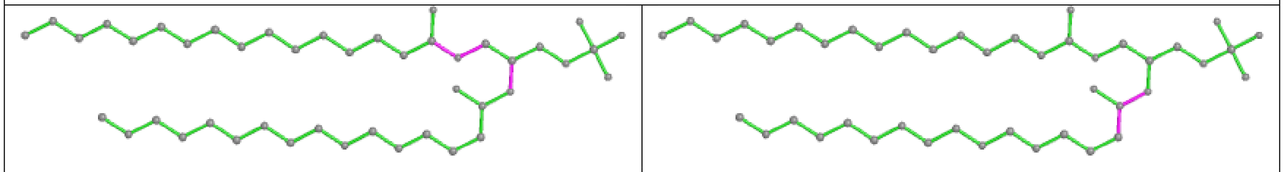


Bond lengths Bond angles

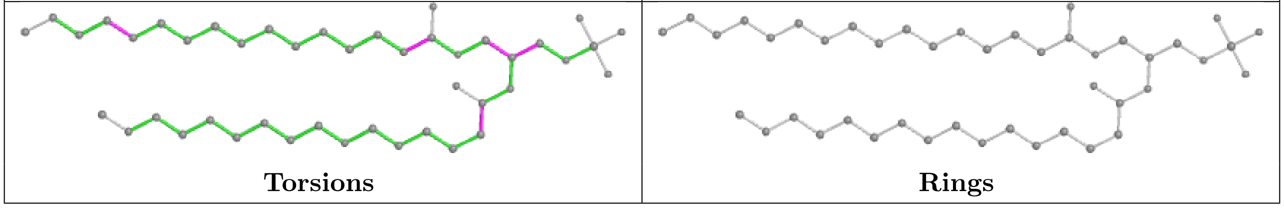


Torsions Rings

Ligand LPP BN 301

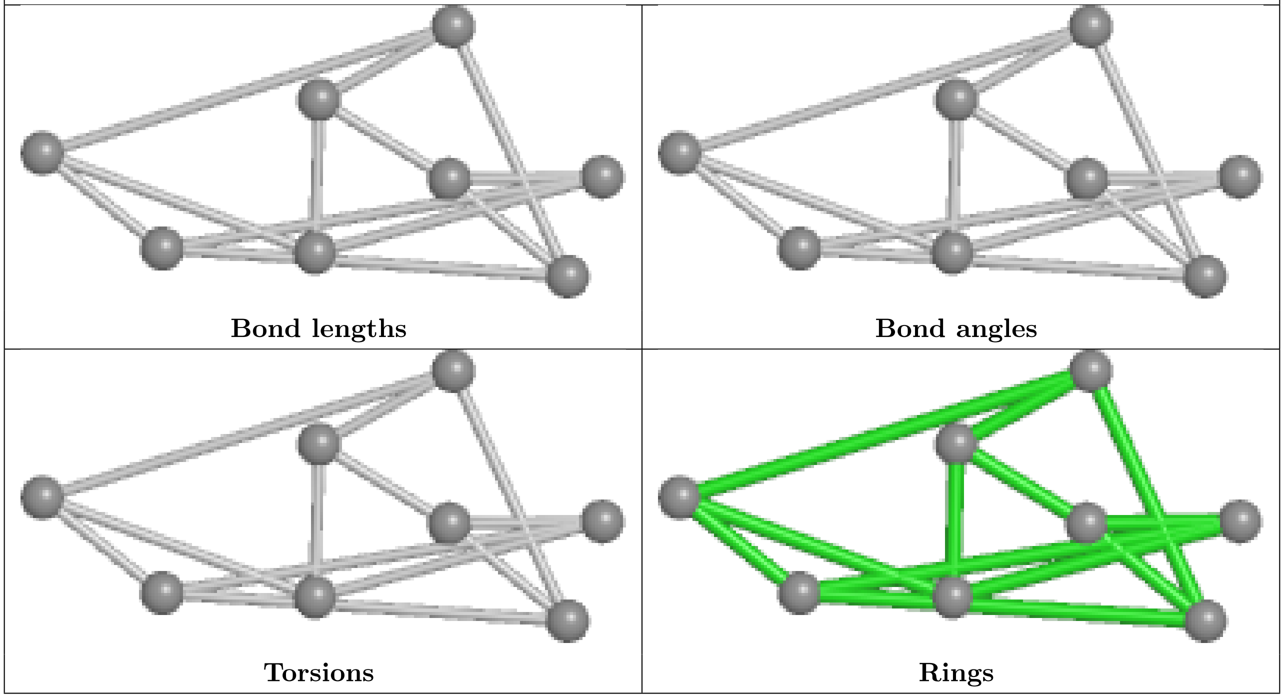


Bond lengths Bond angles



Torsions Rings

Ligand SF4 AD 501



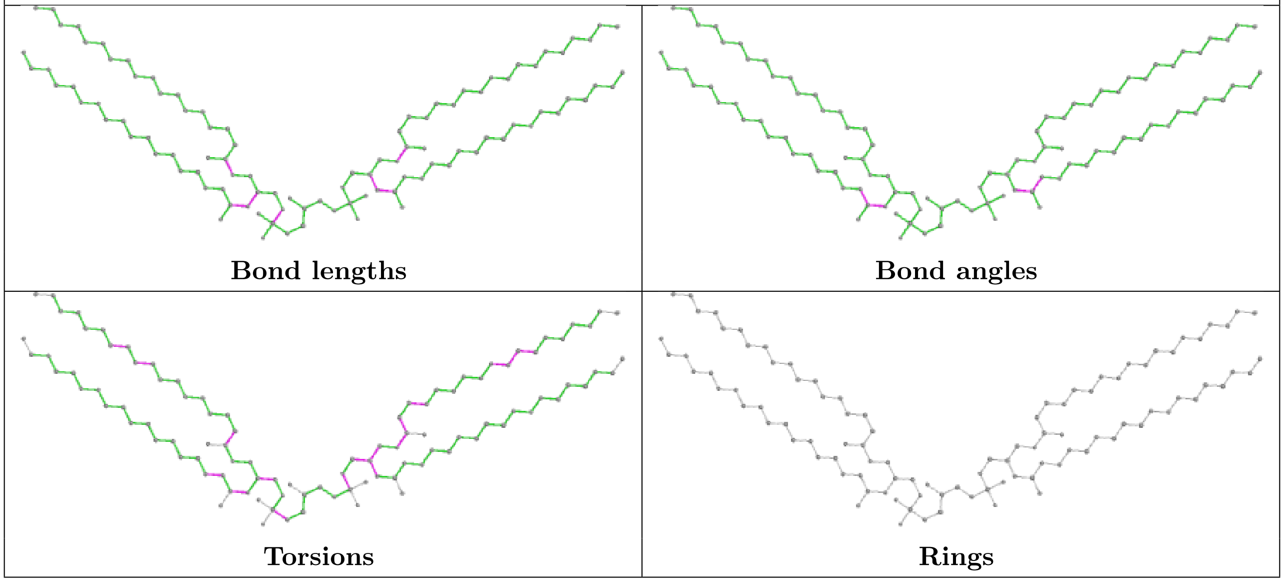
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL AF 402



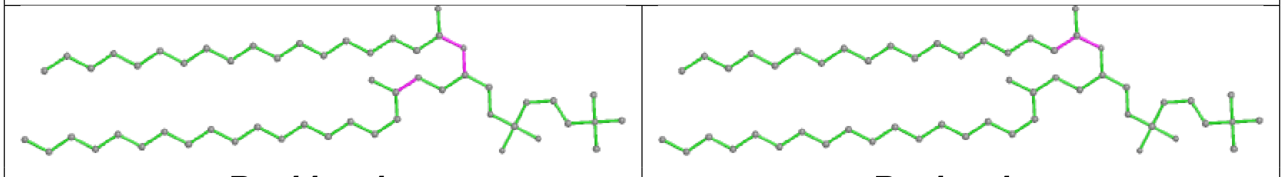
Bond lengths

Bond angles

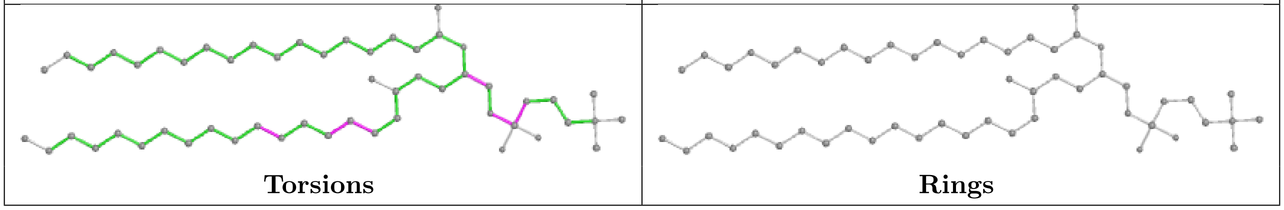
Torsions

Rings

Ligand PC1 BS 1302

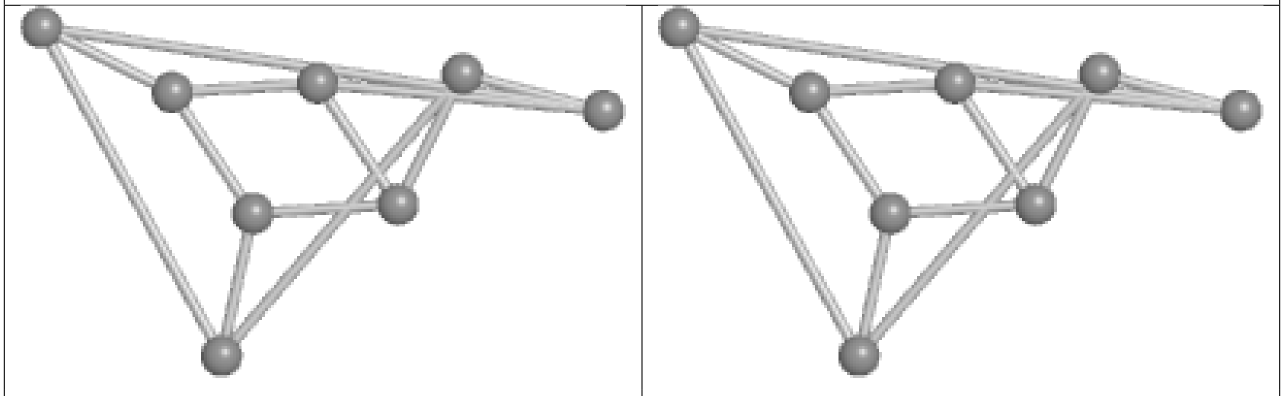


Bond lengths Bond angles

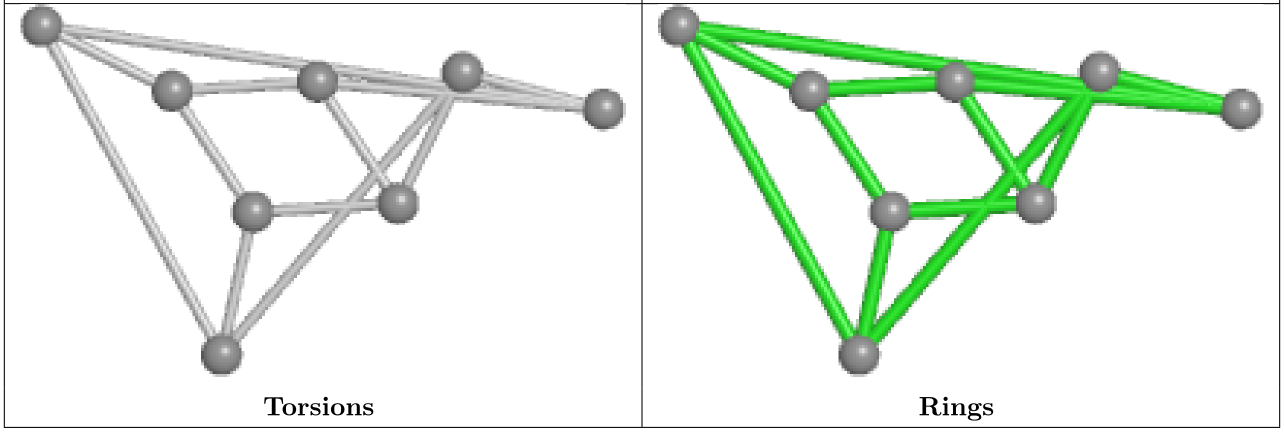


Torsions Rings

Ligand SF4 AB 802



Bond lengths Bond angles



Torsions Rings

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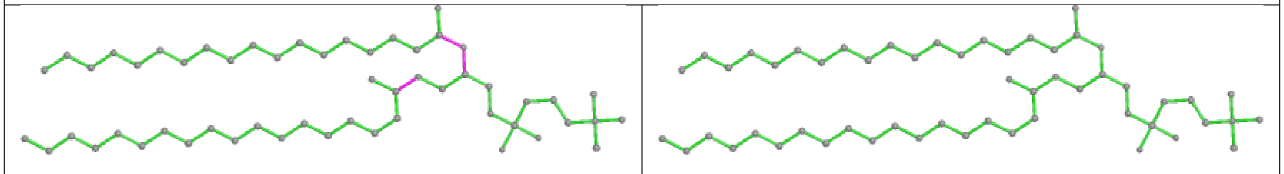
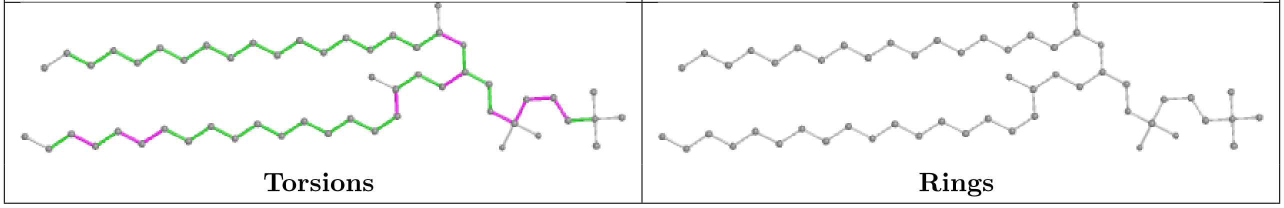
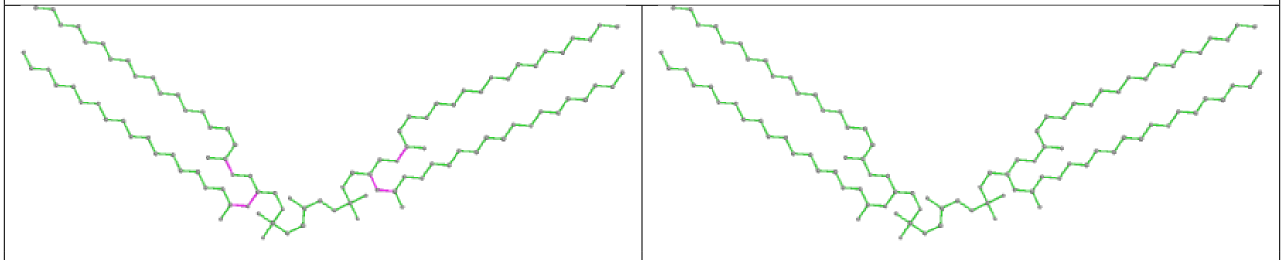


Bond lengths **Bond angles**

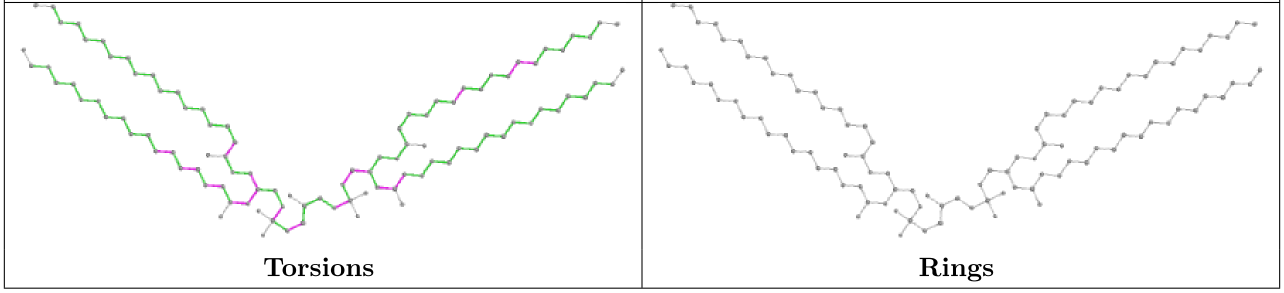


Torsions **Rings**

Ligand CDL AP 301

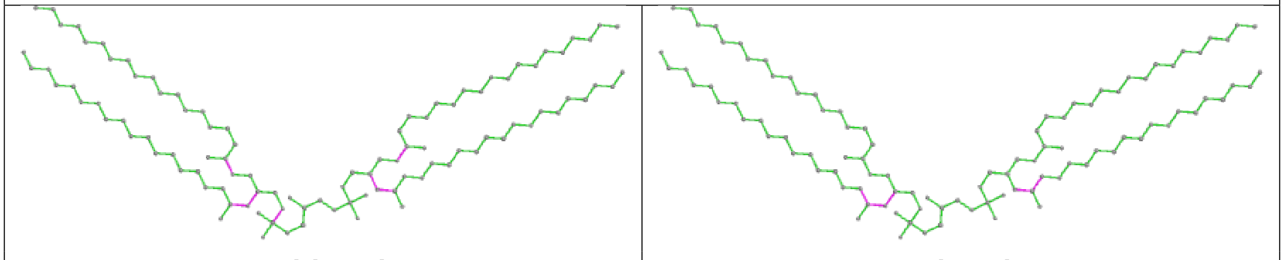


Bond lengths **Bond angles**

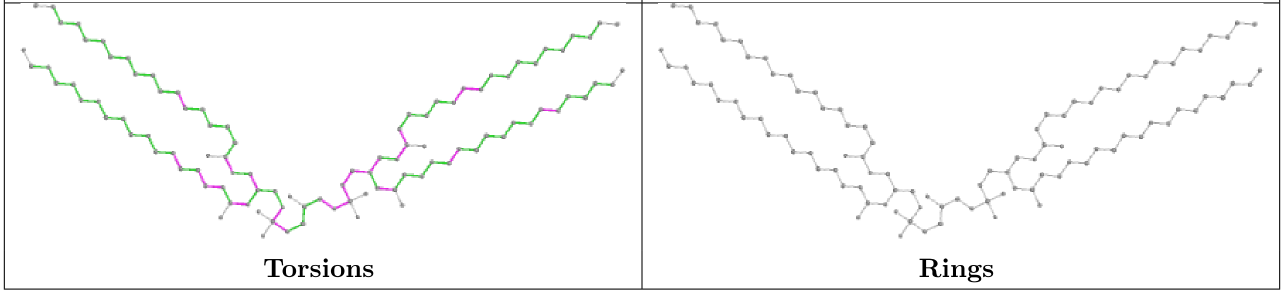


Torsions **Rings**

Ligand CDL BG 201

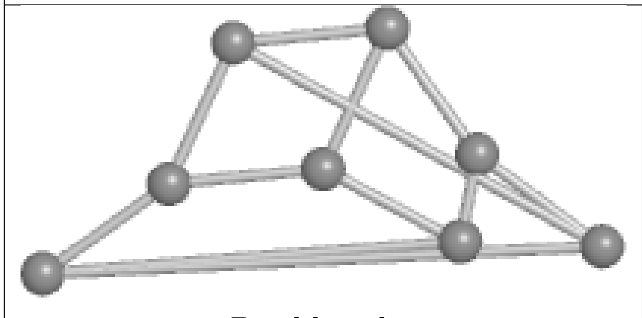


Bond lengths **Bond angles**

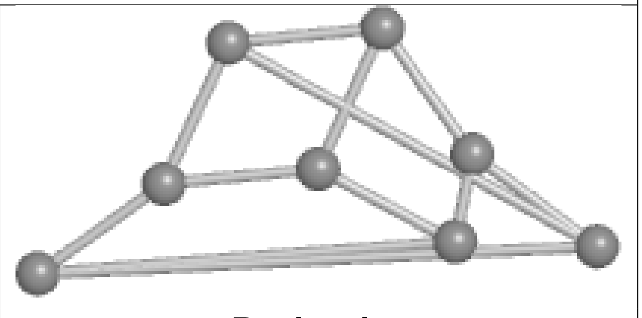


Torsions **Rings**

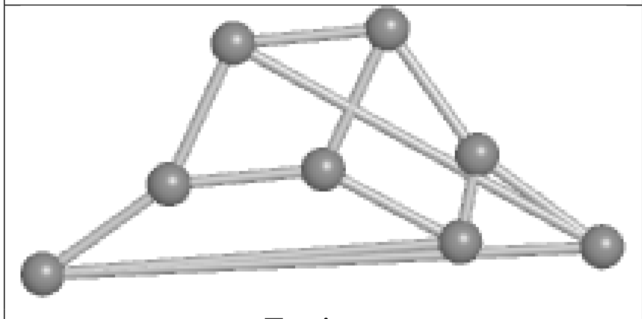
Ligand SF4 AT 201



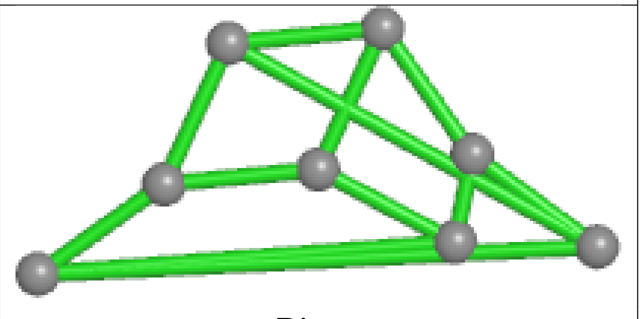
Bond lengths



Bond angles

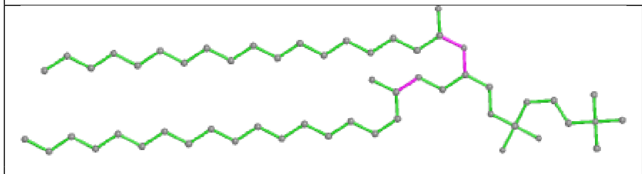


Torsions

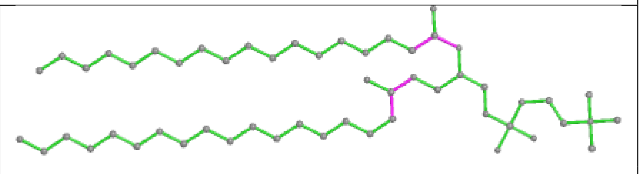


Rings

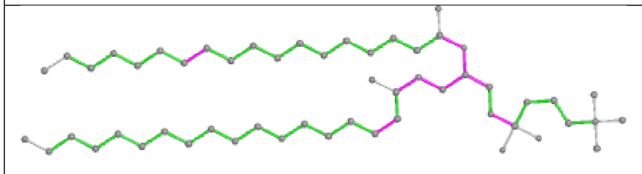
Ligand PC1 A1 404



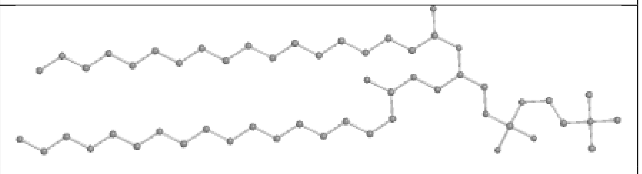
Bond lengths



Bond angles

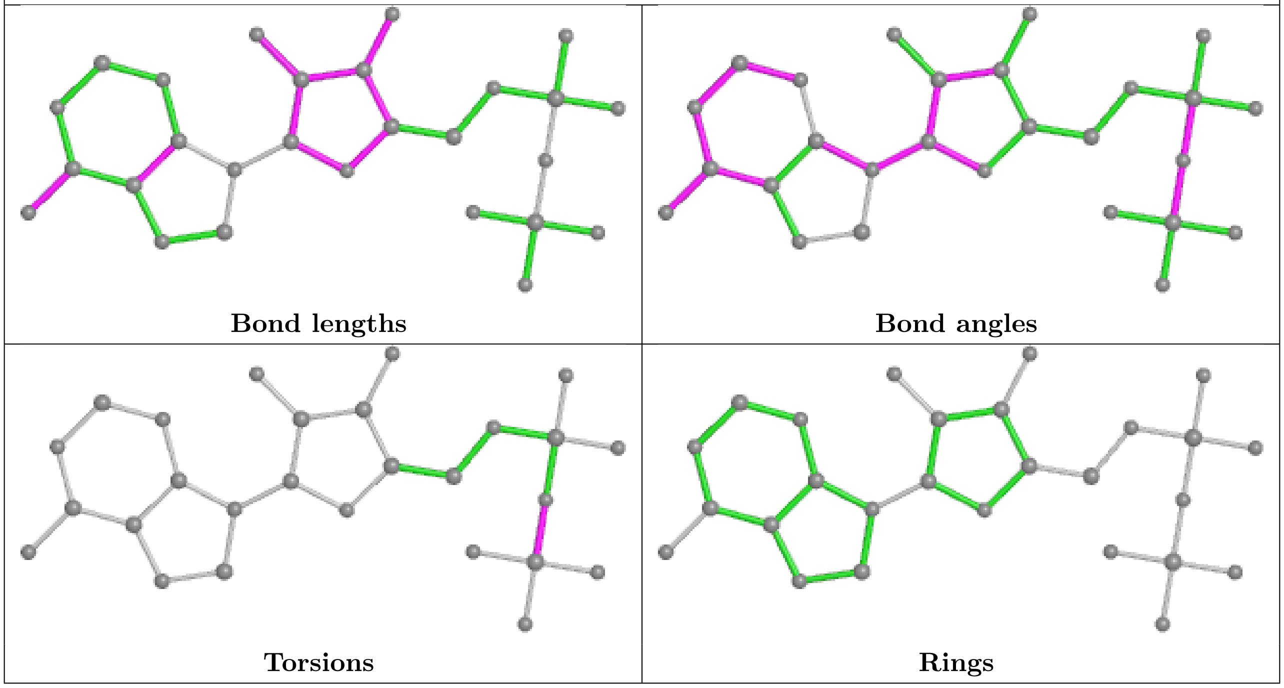


Torsions



Rings

Ligand ADP AQ 201



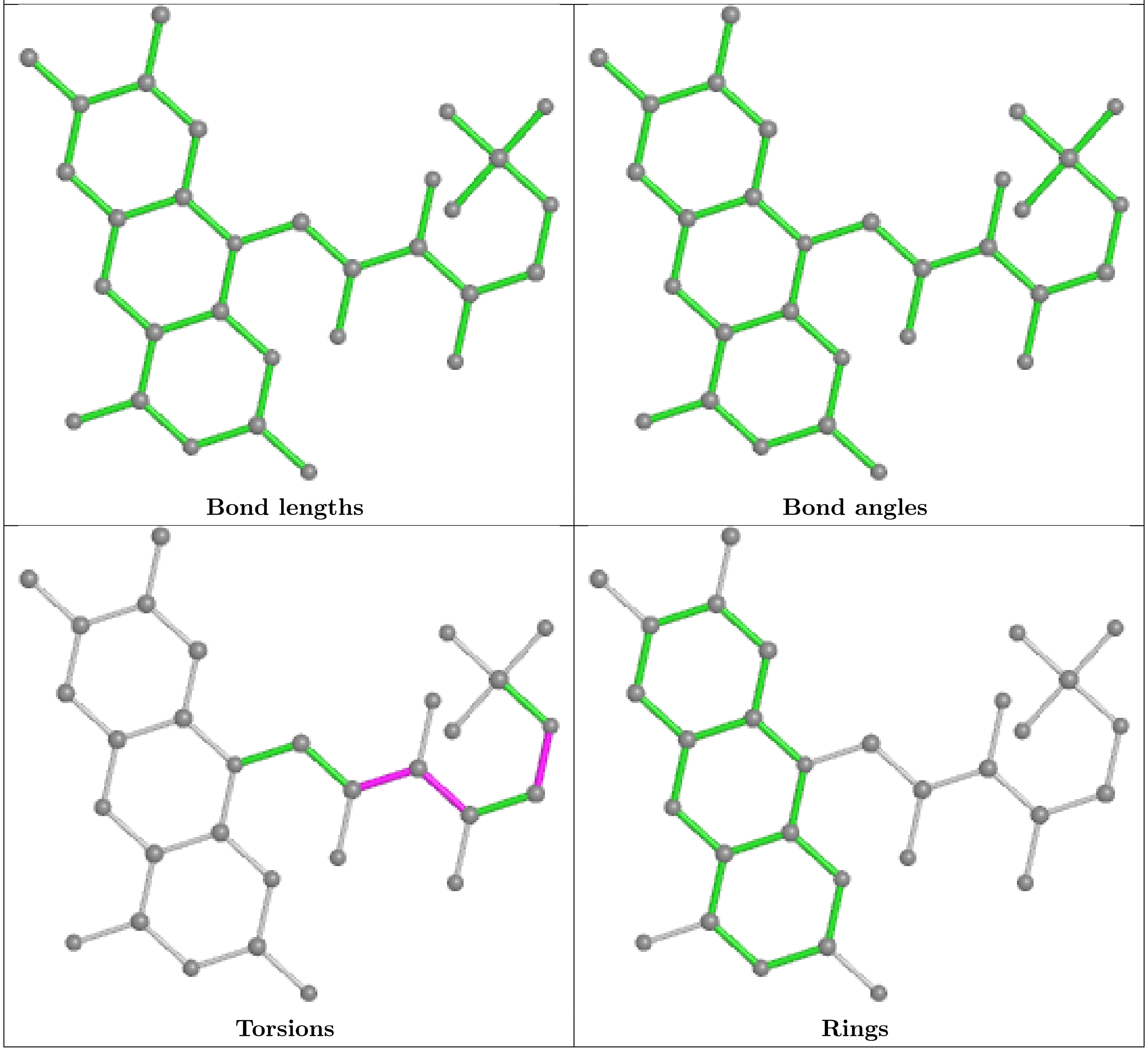
Bond lengths

Bond angles

Torsions

Rings

Ligand FMN AD 502



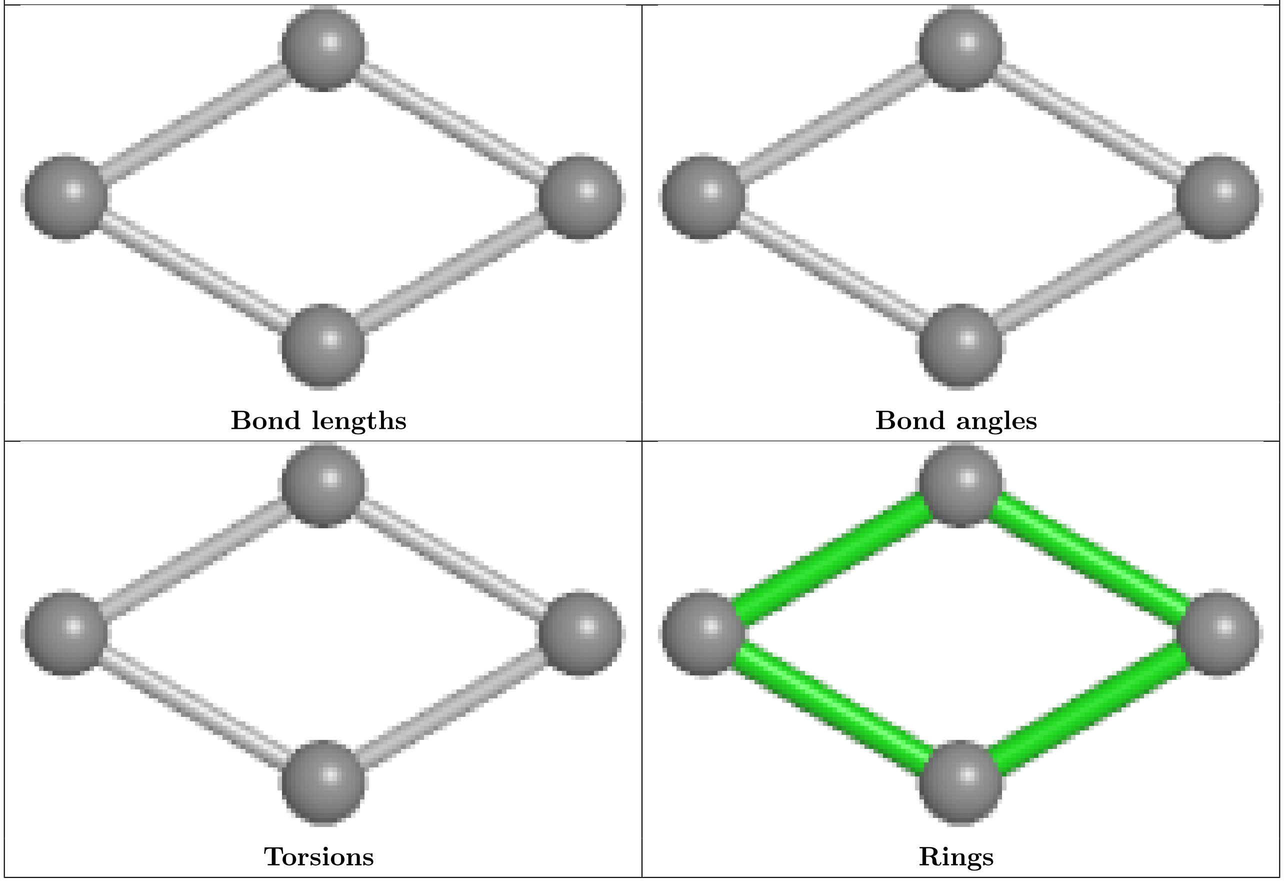
Bond lengths

Bond angles

Torsions

Rings

Ligand FES AB 801



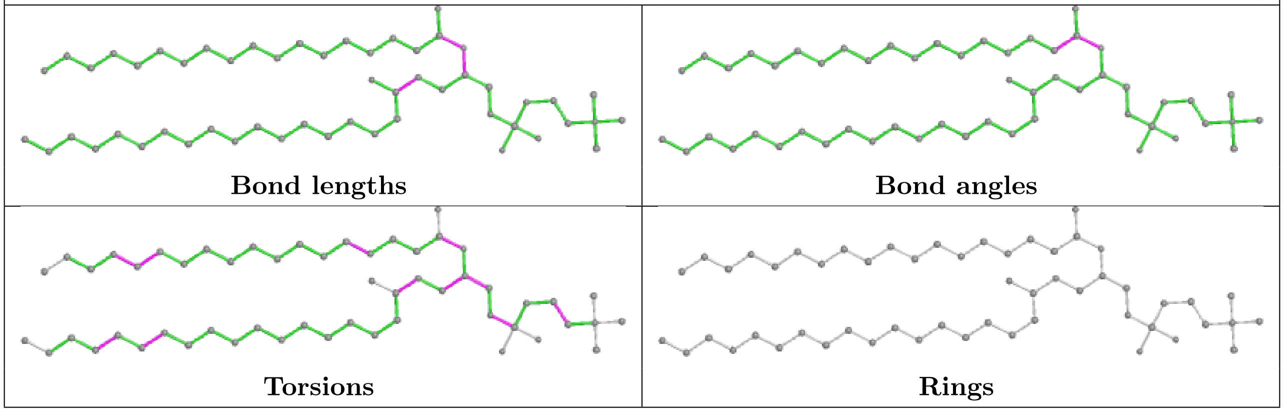
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A9 601



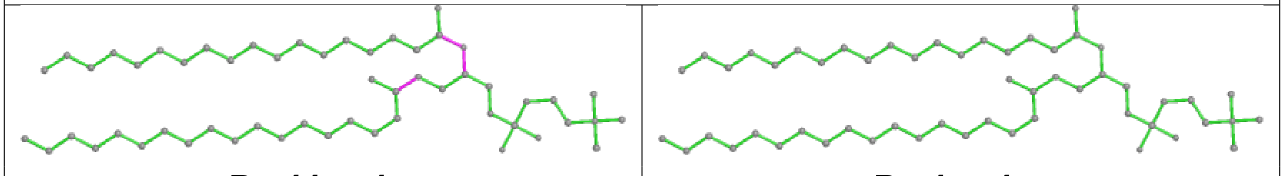
Bond lengths

Bond angles

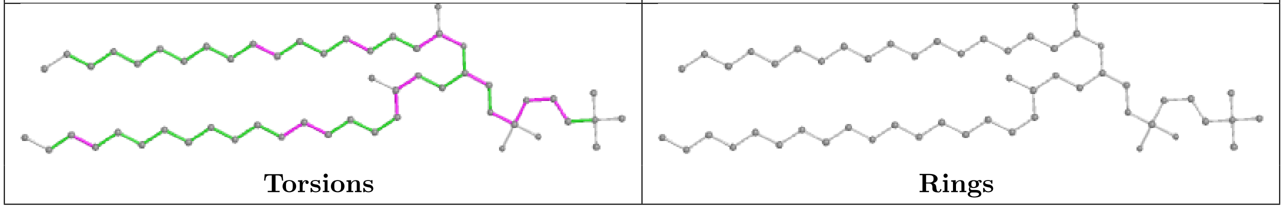
Torsions

Rings

Ligand PC1 BQ 401

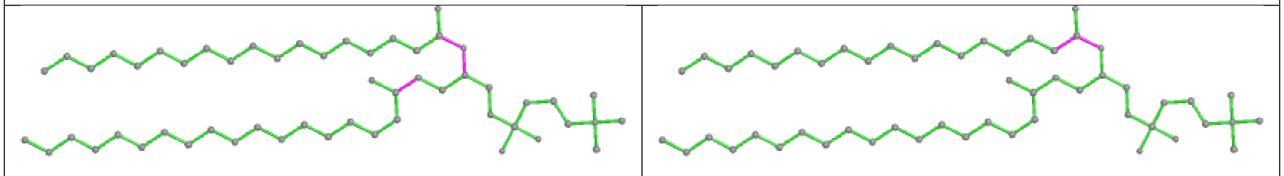


Bond lengths Bond angles

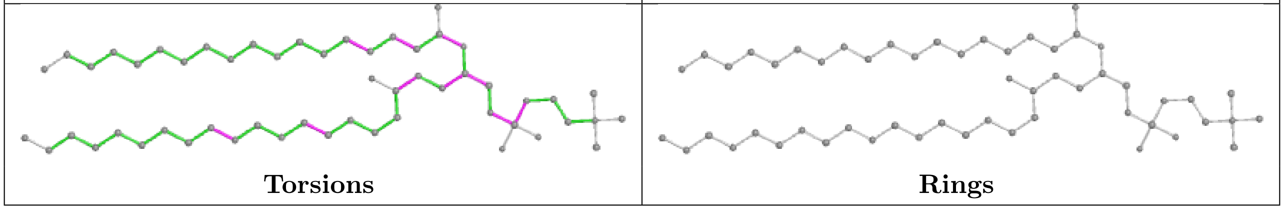


Torsions Rings

Ligand PC1 AA 903

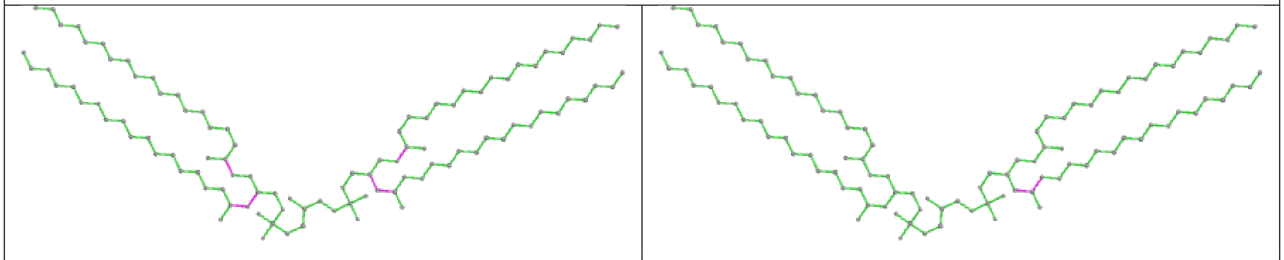


Bond lengths Bond angles

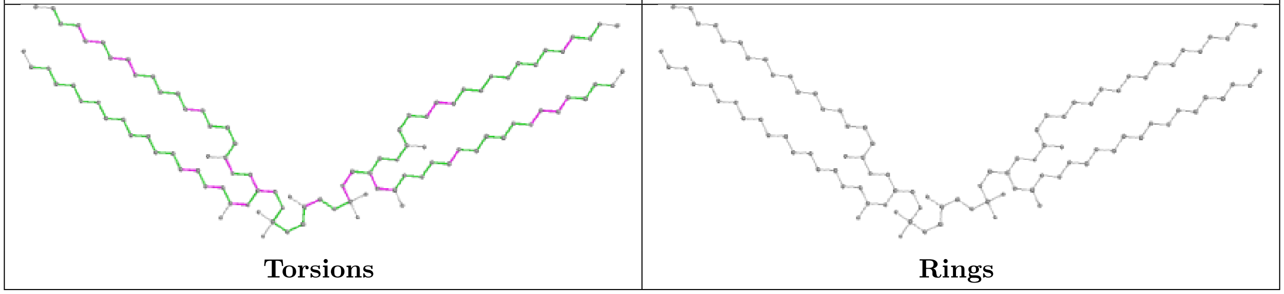


Torsions Rings

Ligand CDL AA 908

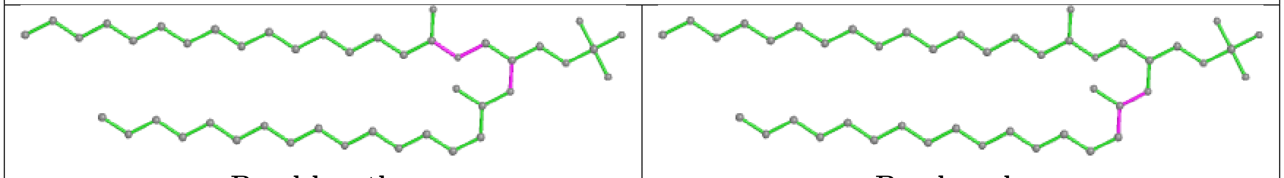


Bond lengths Bond angles



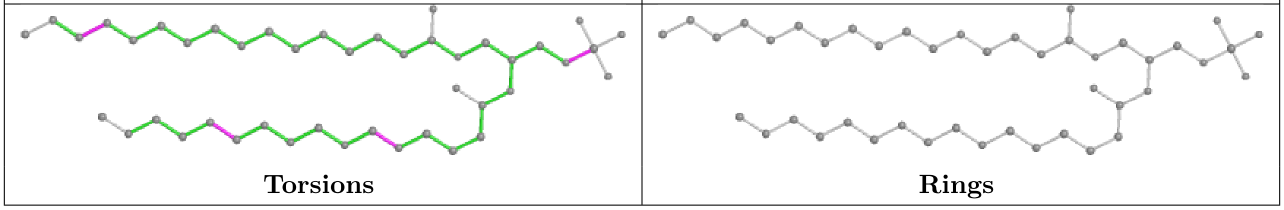
Torsions Rings

Ligand LPP AL 304



Bond lengths

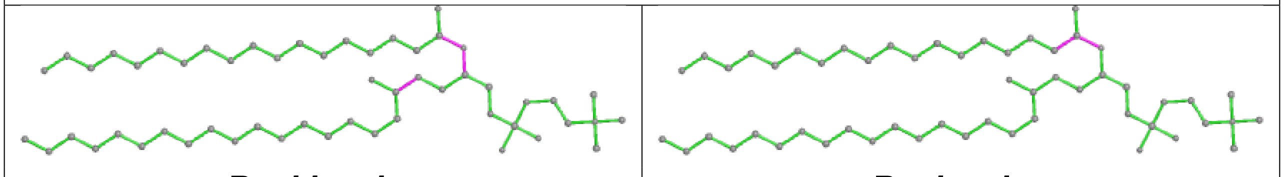
Bond angles



Torsions

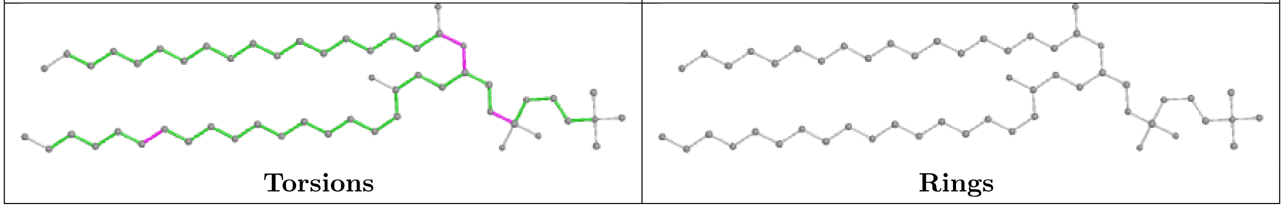
Rings

Ligand PC1 A1 403



Bond lengths

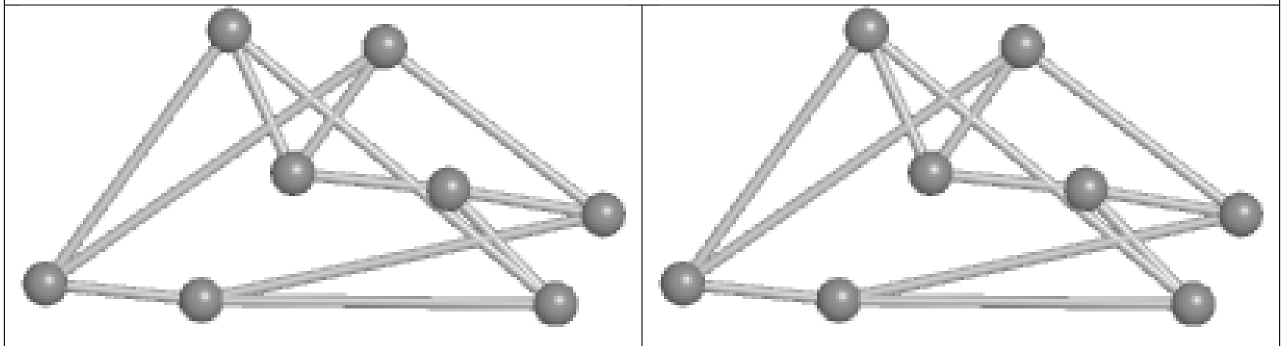
Bond angles



Torsions

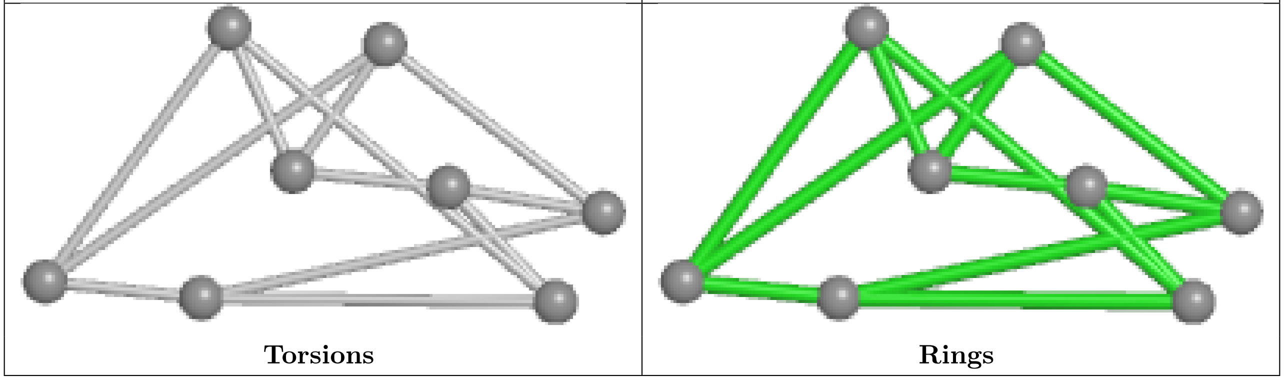
Rings

Ligand SF4 AL 302



Bond lengths

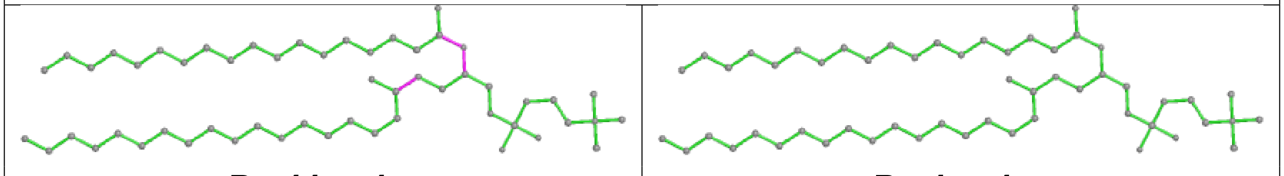
Bond angles



Torsions

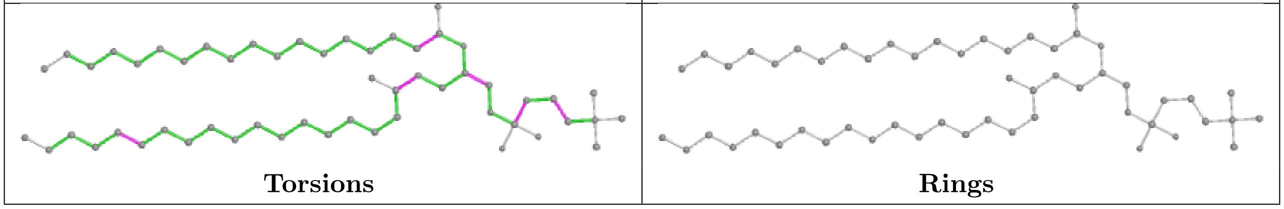
Rings

Ligand PC1 AH 301



Bond lengths

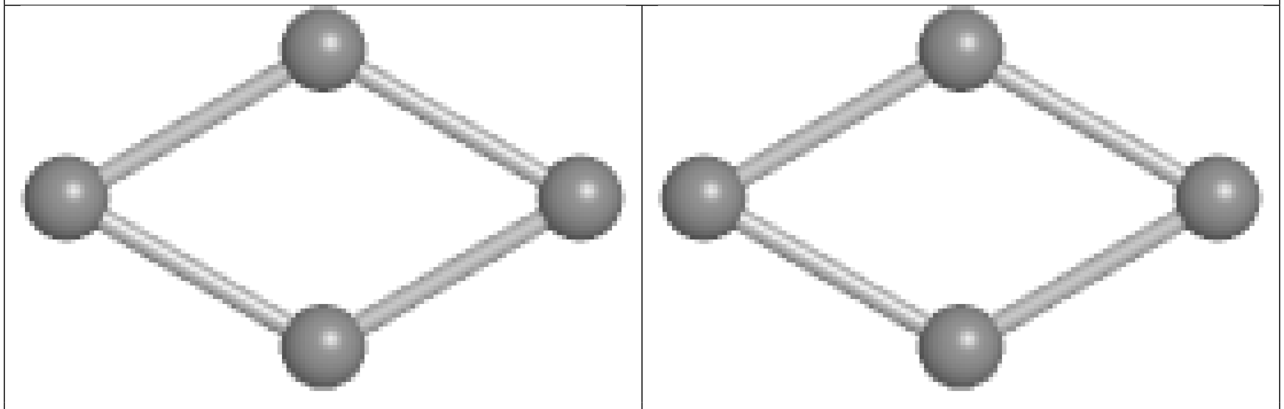
Bond angles



Torsions

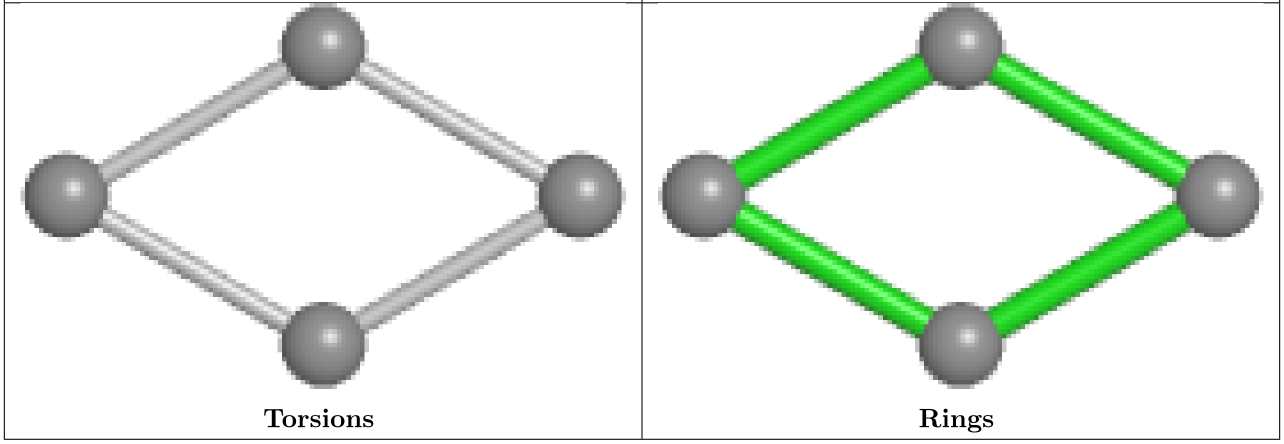
Rings

Ligand FES AI 301



Bond lengths

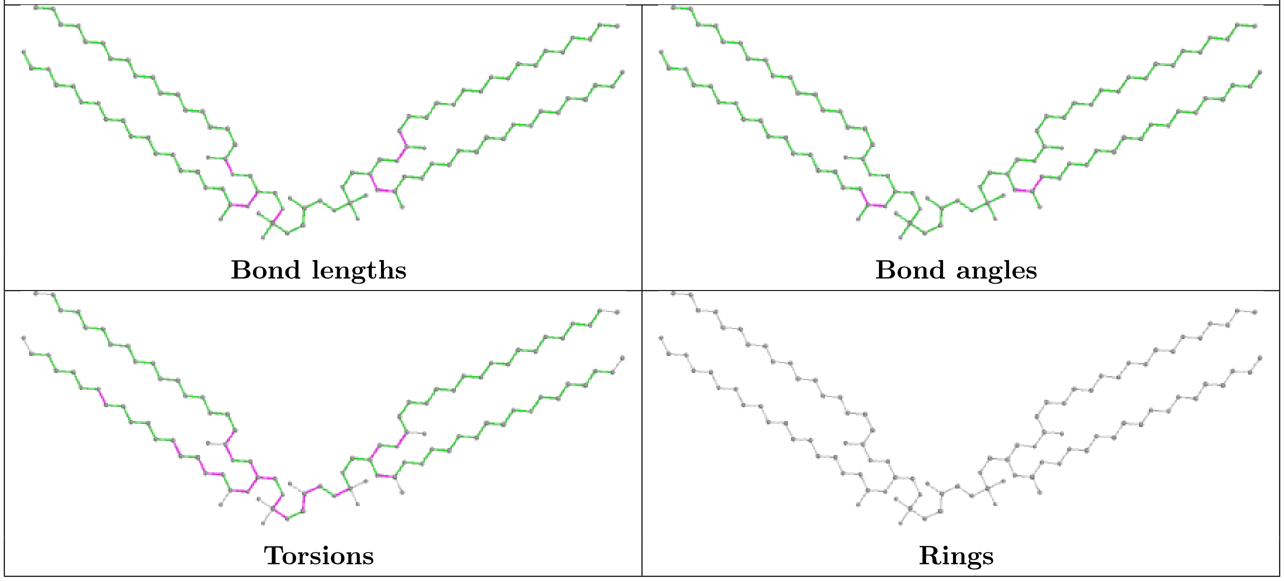
Bond angles



Torsions

Rings

Ligand CDL BE 201



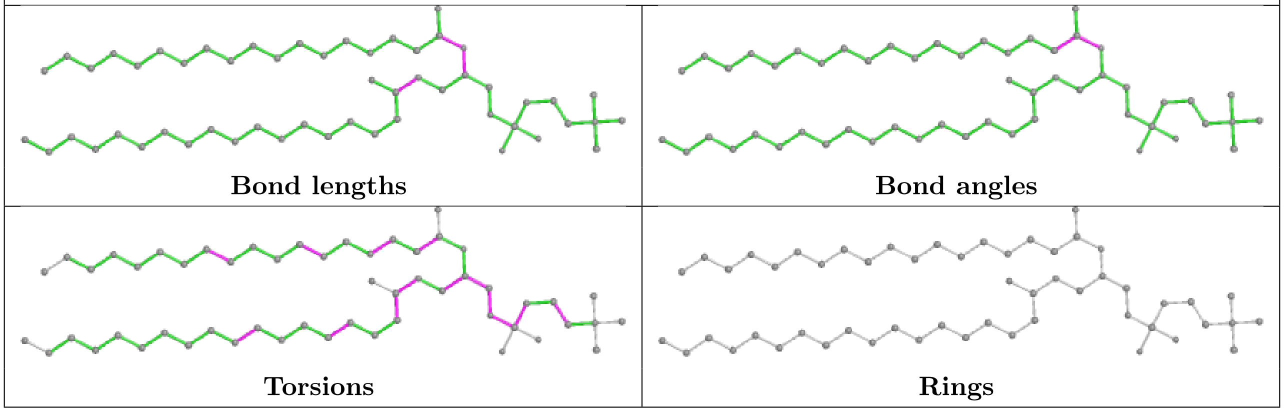
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 AA 907



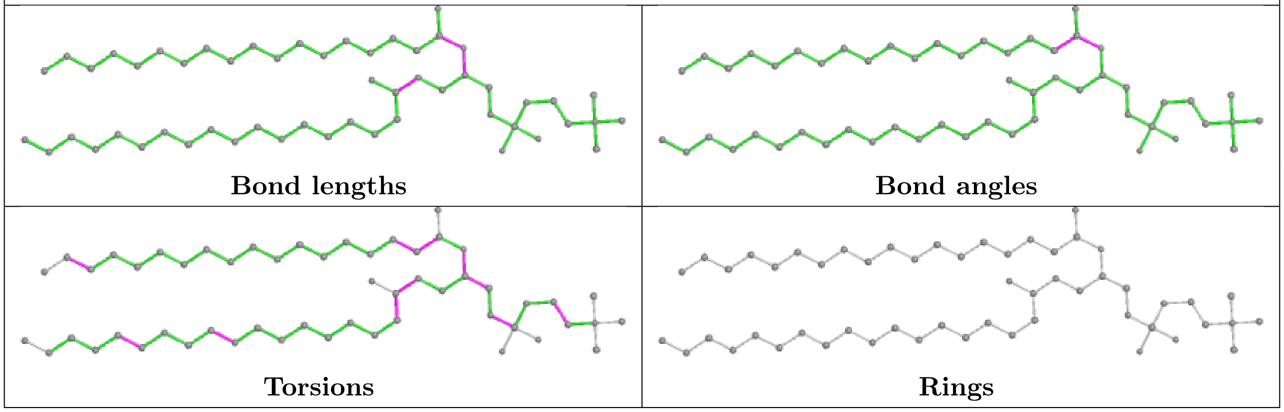
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 AJ 501



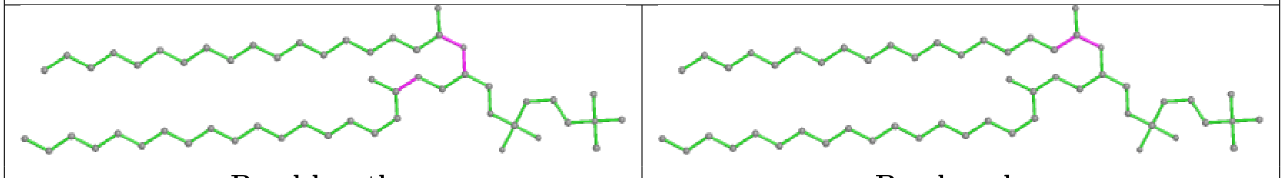
Bond lengths

Bond angles

Torsions

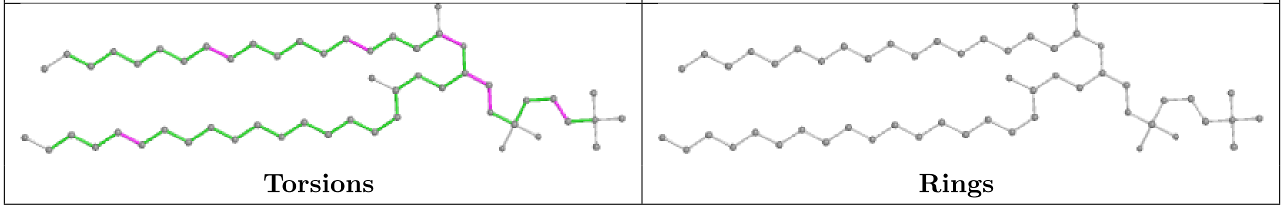
Rings

Ligand PC1 AL 303



Bond lengths

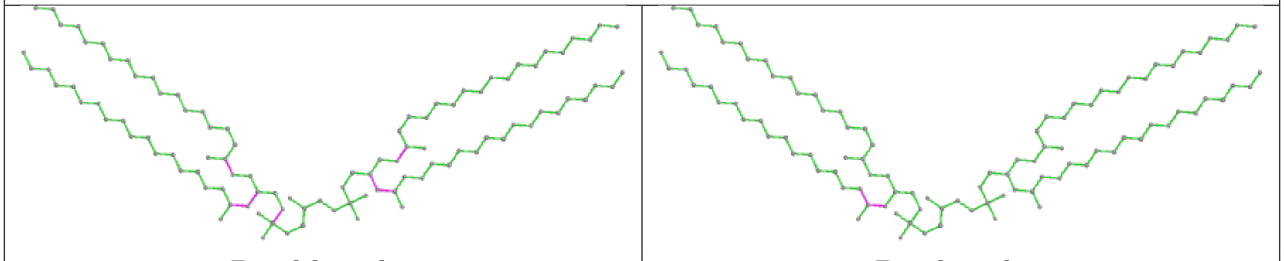
Bond angles



Torsions

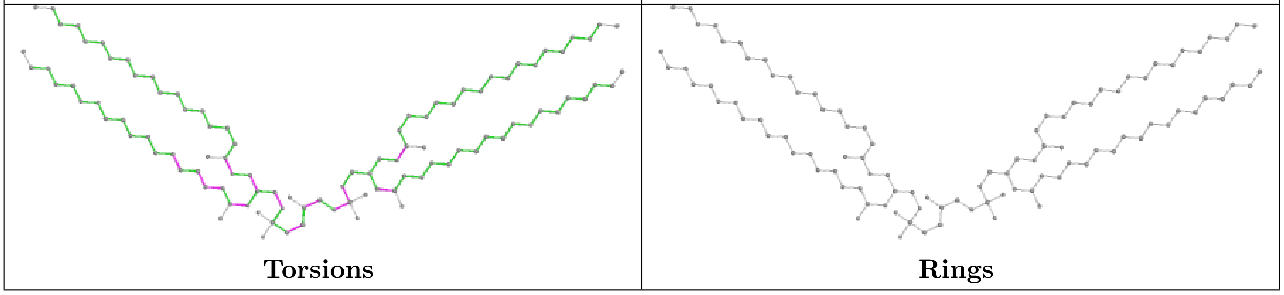
Rings

Ligand CDL A0 601



Bond lengths

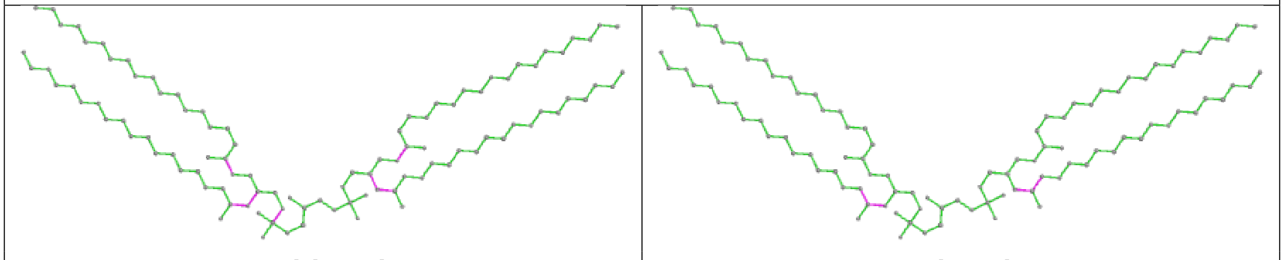
Bond angles



Torsions

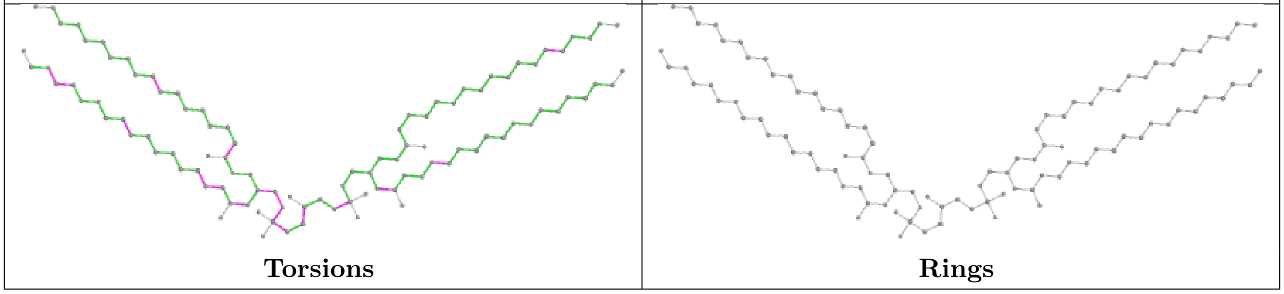
Rings

Ligand CDL AA 901



Bond lengths

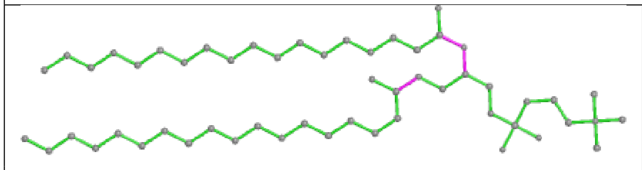
Bond angles

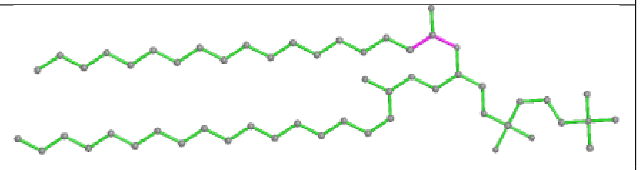


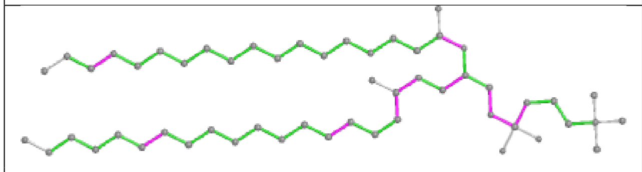
Torsions

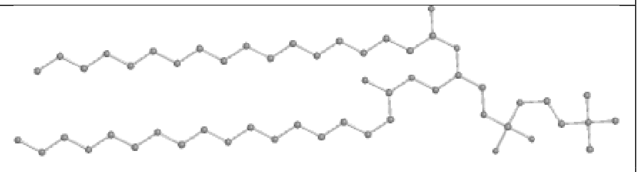
Rings

Ligand PC1 B1 401

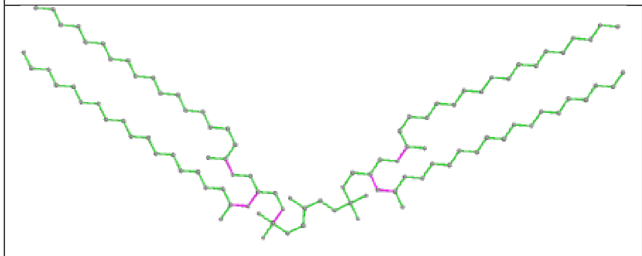

Bond lengths

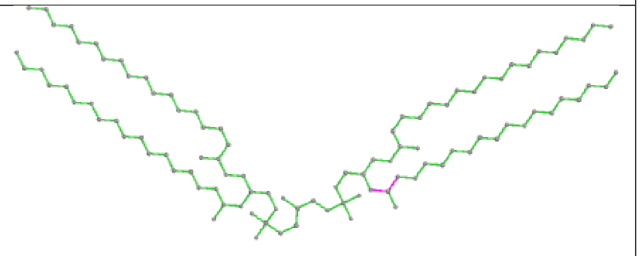

Bond angles

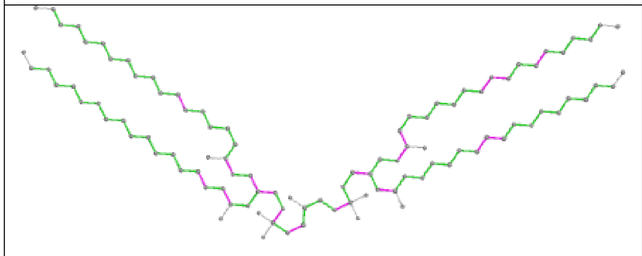

Torsions

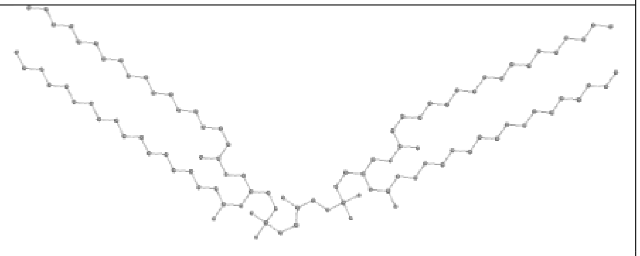

Rings

Ligand CDL B1 402

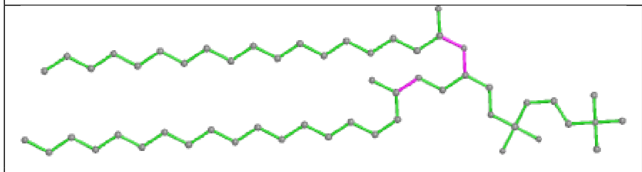

Bond lengths

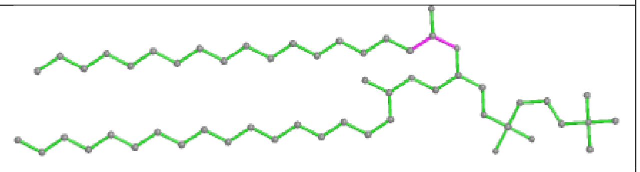

Bond angles

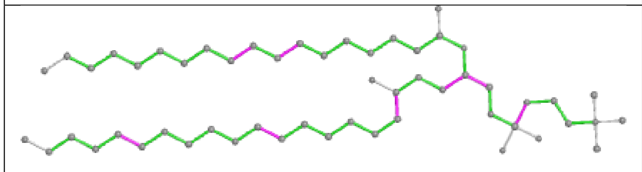

Torsions

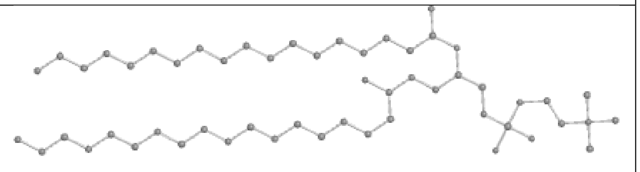

Rings

Ligand PC1 A6 302

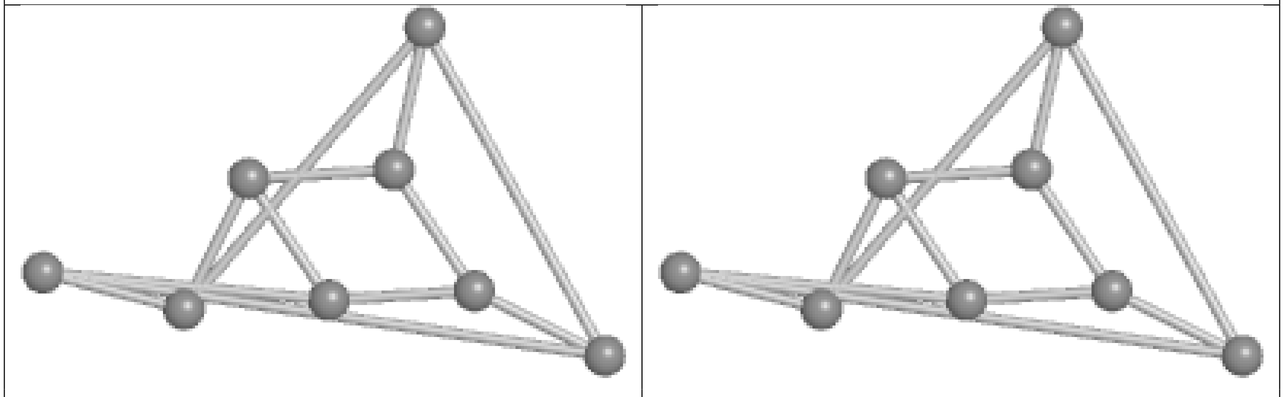

Bond lengths


Bond angles


Torsions

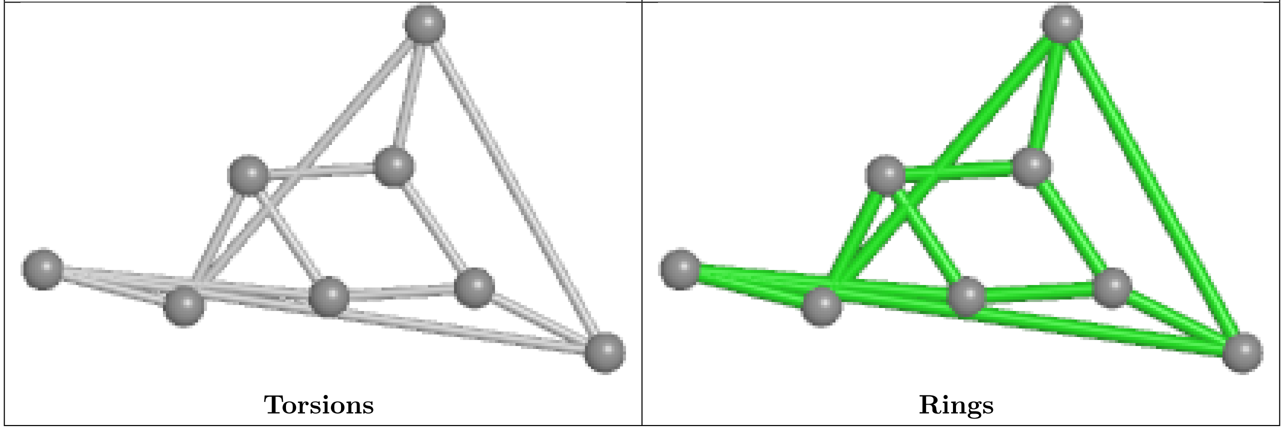

Rings

Ligand SF4 AB 803



Bond lengths

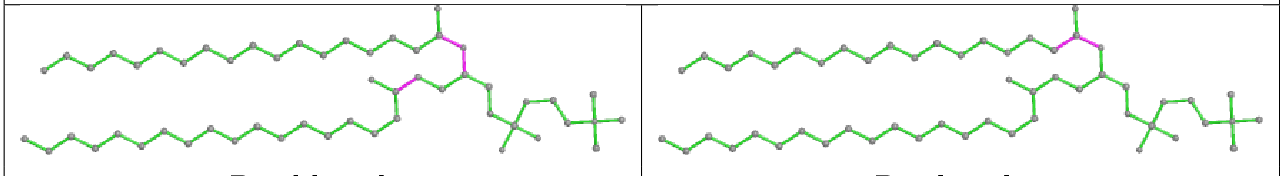
Bond angles



Torsions

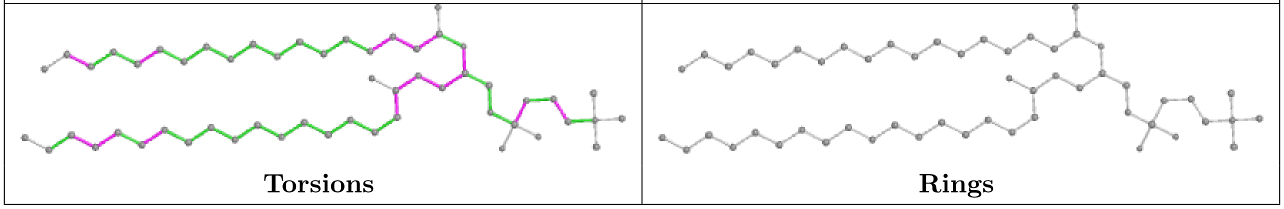
Rings

Ligand PC1 AA 906



Bond lengths

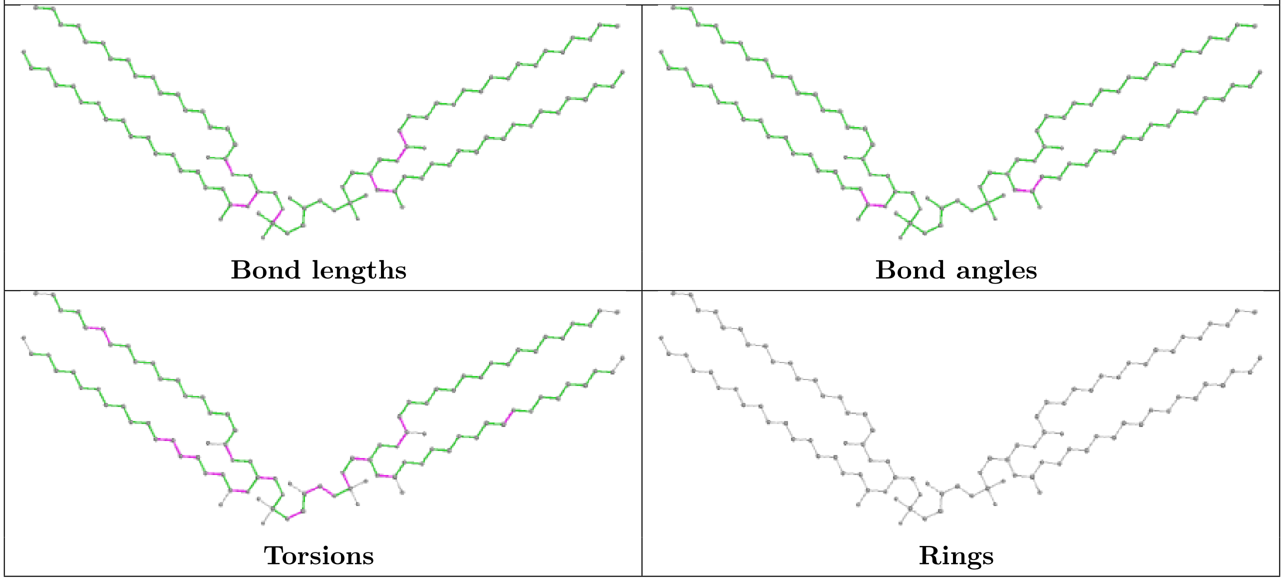
Bond angles



Torsions

Rings

Ligand CDL A0 602



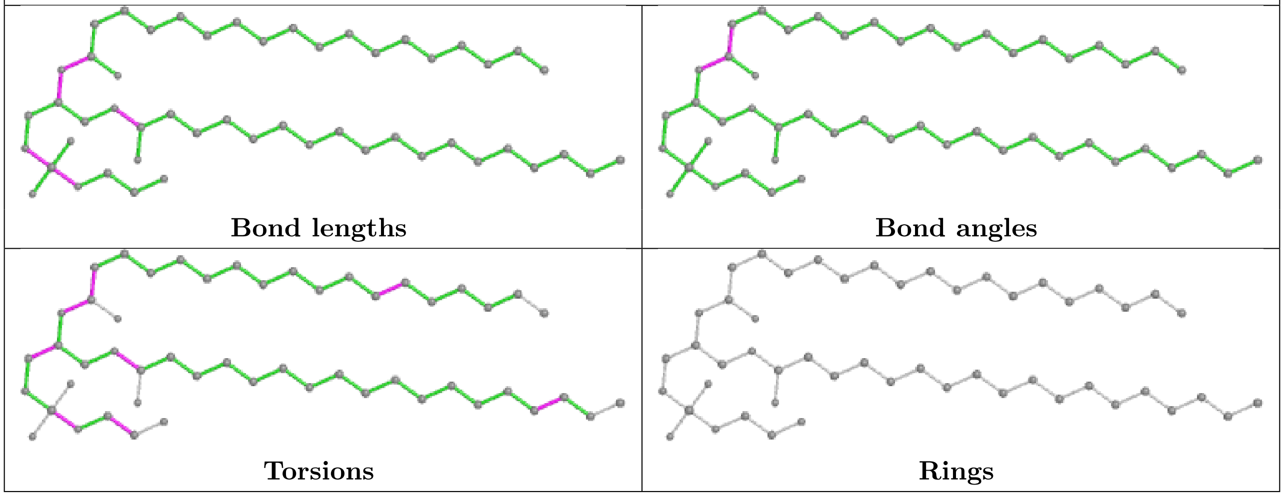
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE AJ 502



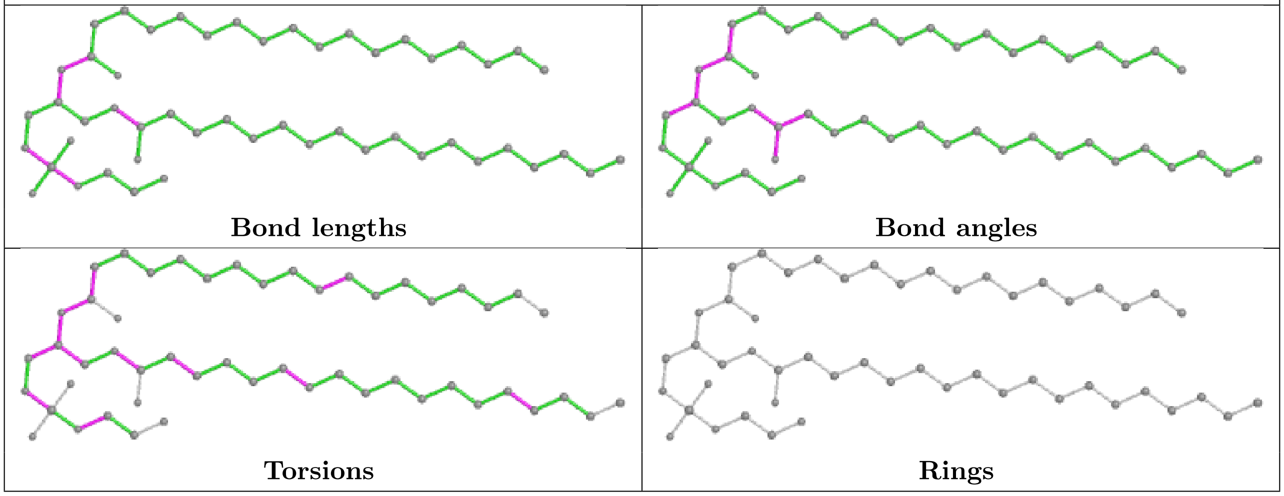
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE A9 602



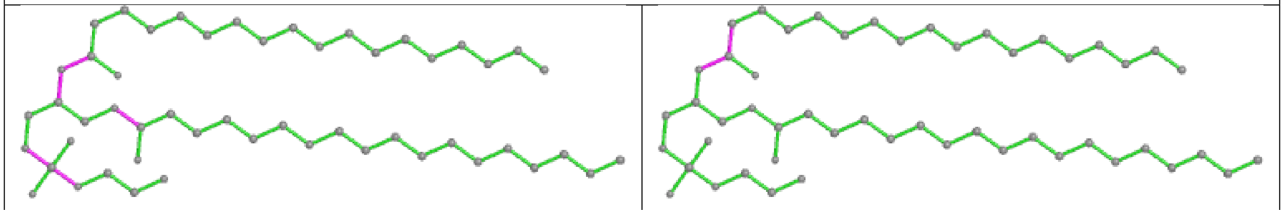
Bond lengths

Bond angles

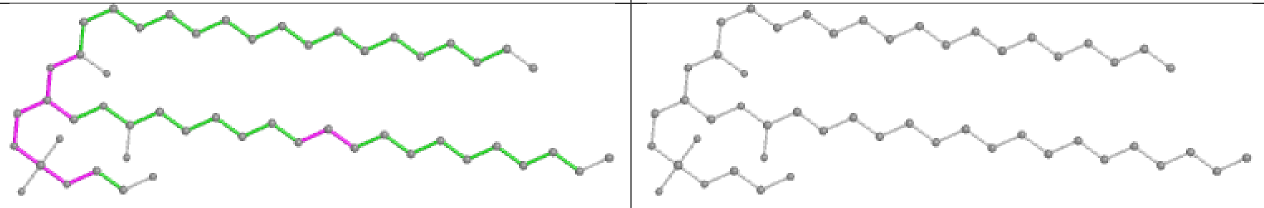
Torsions

Rings

Ligand 3PE BP 201



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.

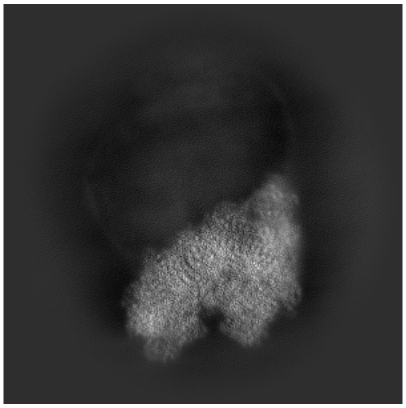
6 Map visualisation ⓘ

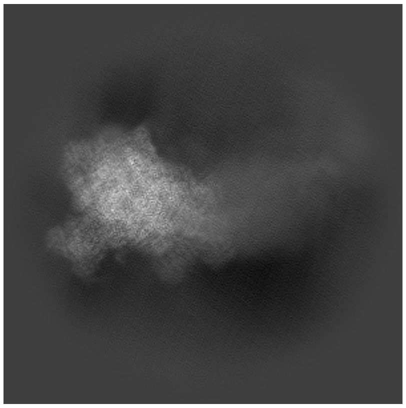
This section contains visualisations of the EMDB entry EMD-15865. These allow visual inspection of the internal detail of the map and identification of artifacts.

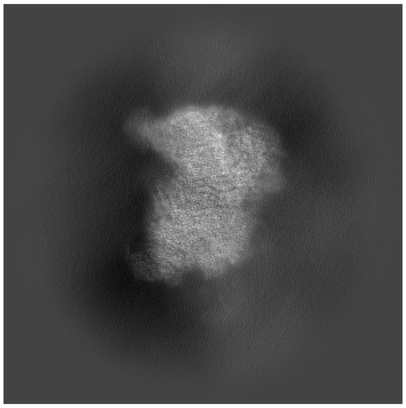
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

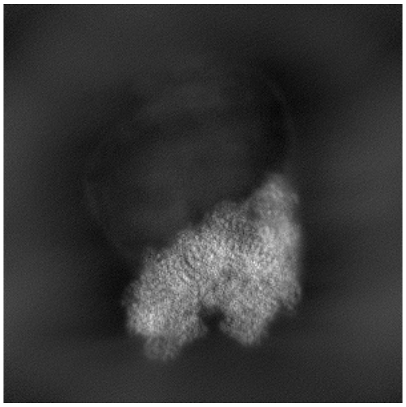
6.1.1 Primary map

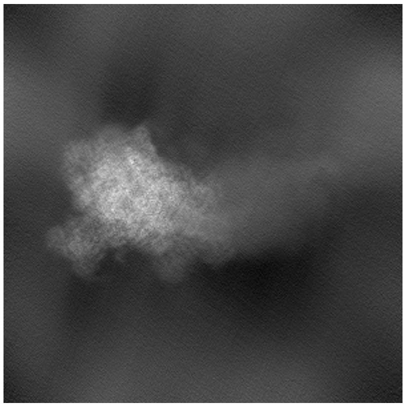

X

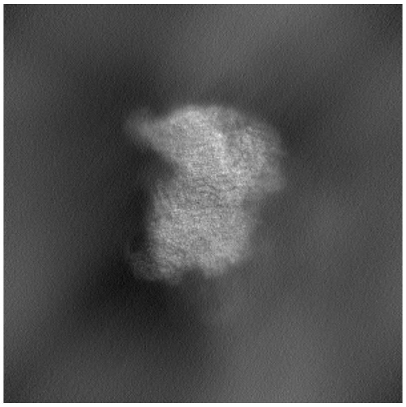

Y


Z

6.1.2 Raw map


X

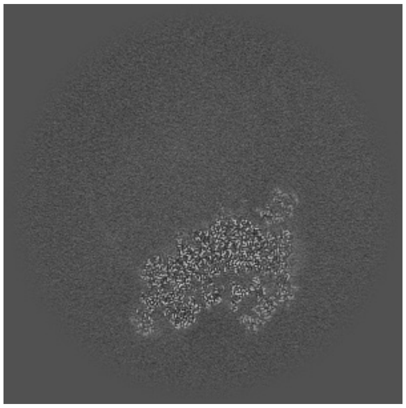

Y


Z

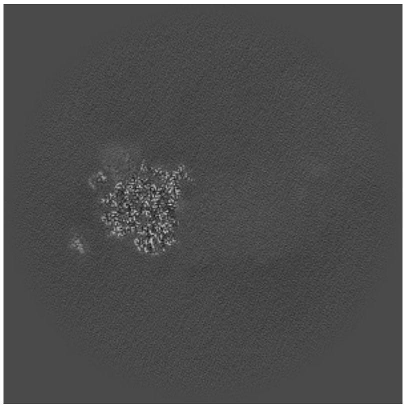
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

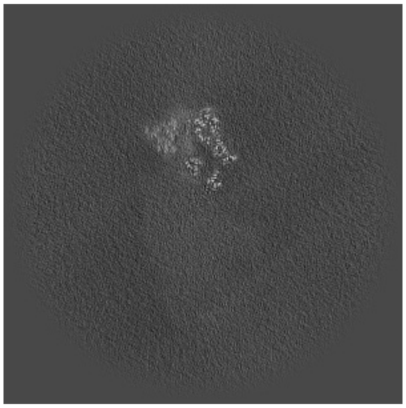
6.2.1 Primary map



X Index: 240

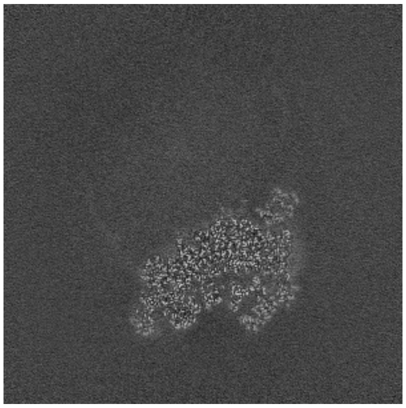


Y Index: 240

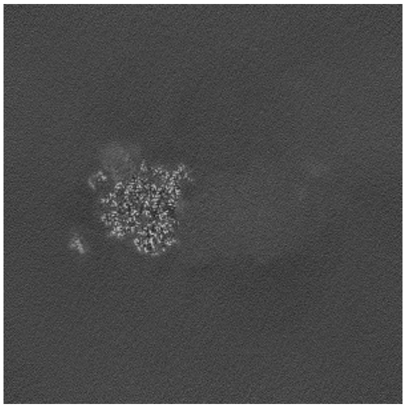


Z Index: 240

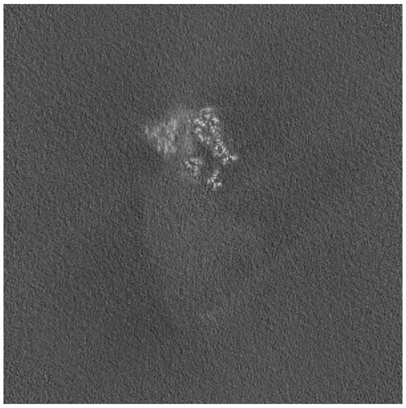
6.2.2 Raw map



X Index: 240



Y Index: 240

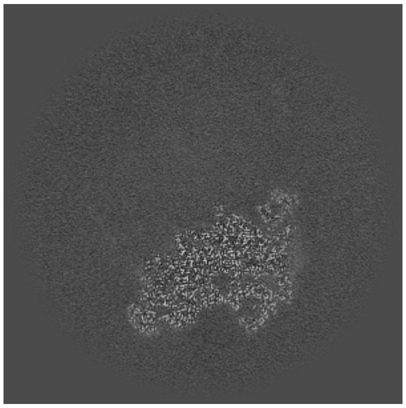


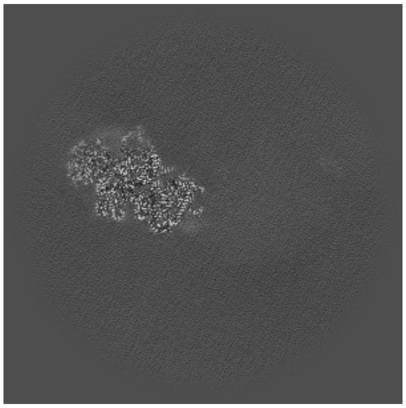
Z Index: 240

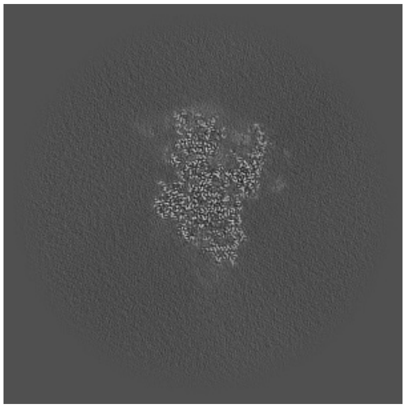
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

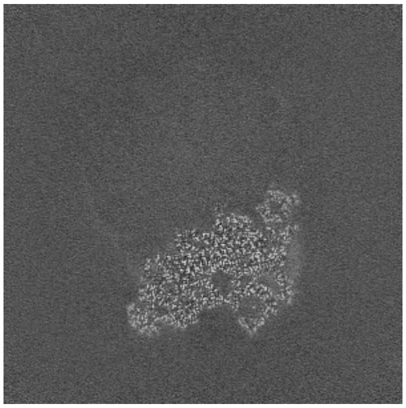
6.3.1 Primary map

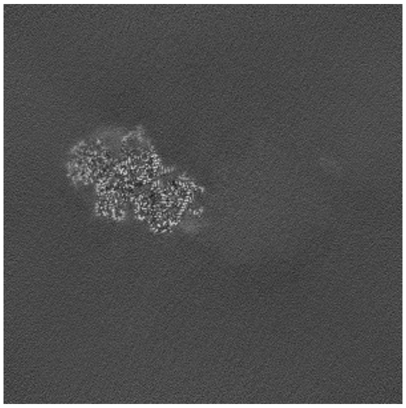

X Index: 243

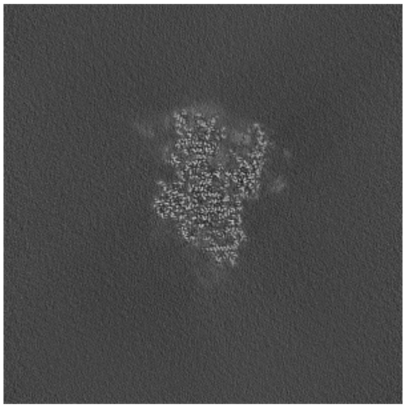

Y Index: 278


Z Index: 177

6.3.2 Raw map


X Index: 244

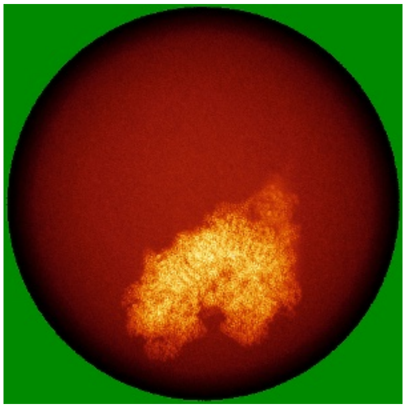

Y Index: 278

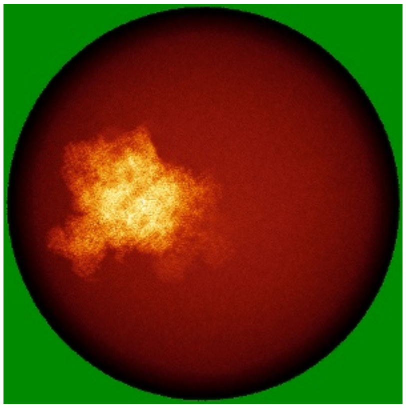

Z Index: 177

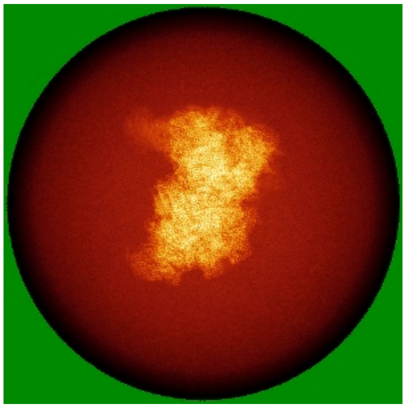
The images above show the largest variance slices of the map in three orthogonal directions.

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

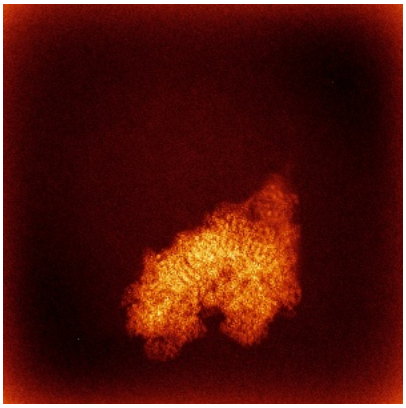
6.4.1 Primary map

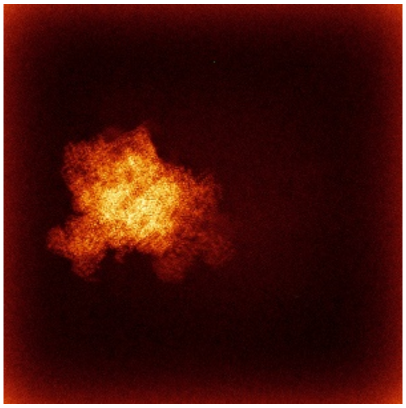

X

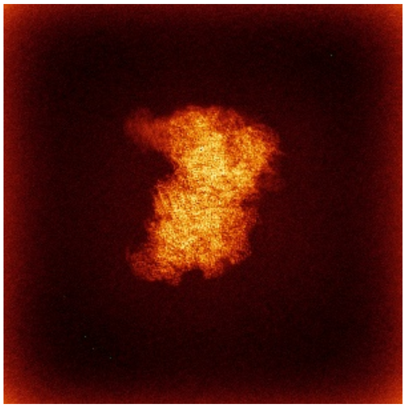

Y


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

6.5.1 Primary map

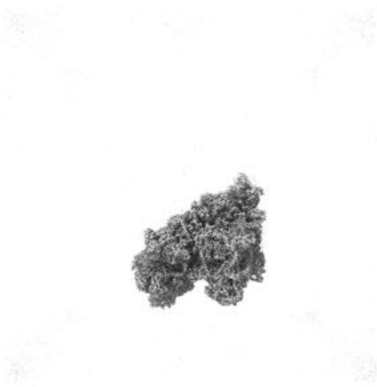
X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

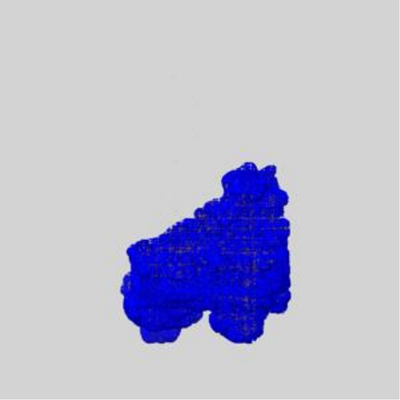
6.6 Mask visualisation (i)

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

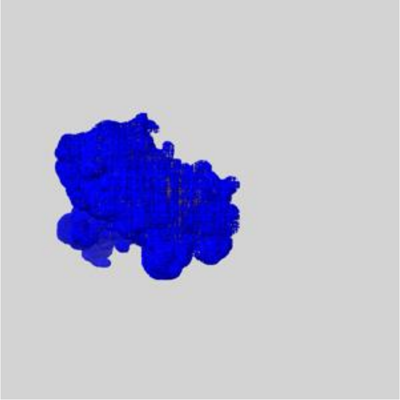
A mask typically either:

- 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_15865_msk_1.map (i)



X



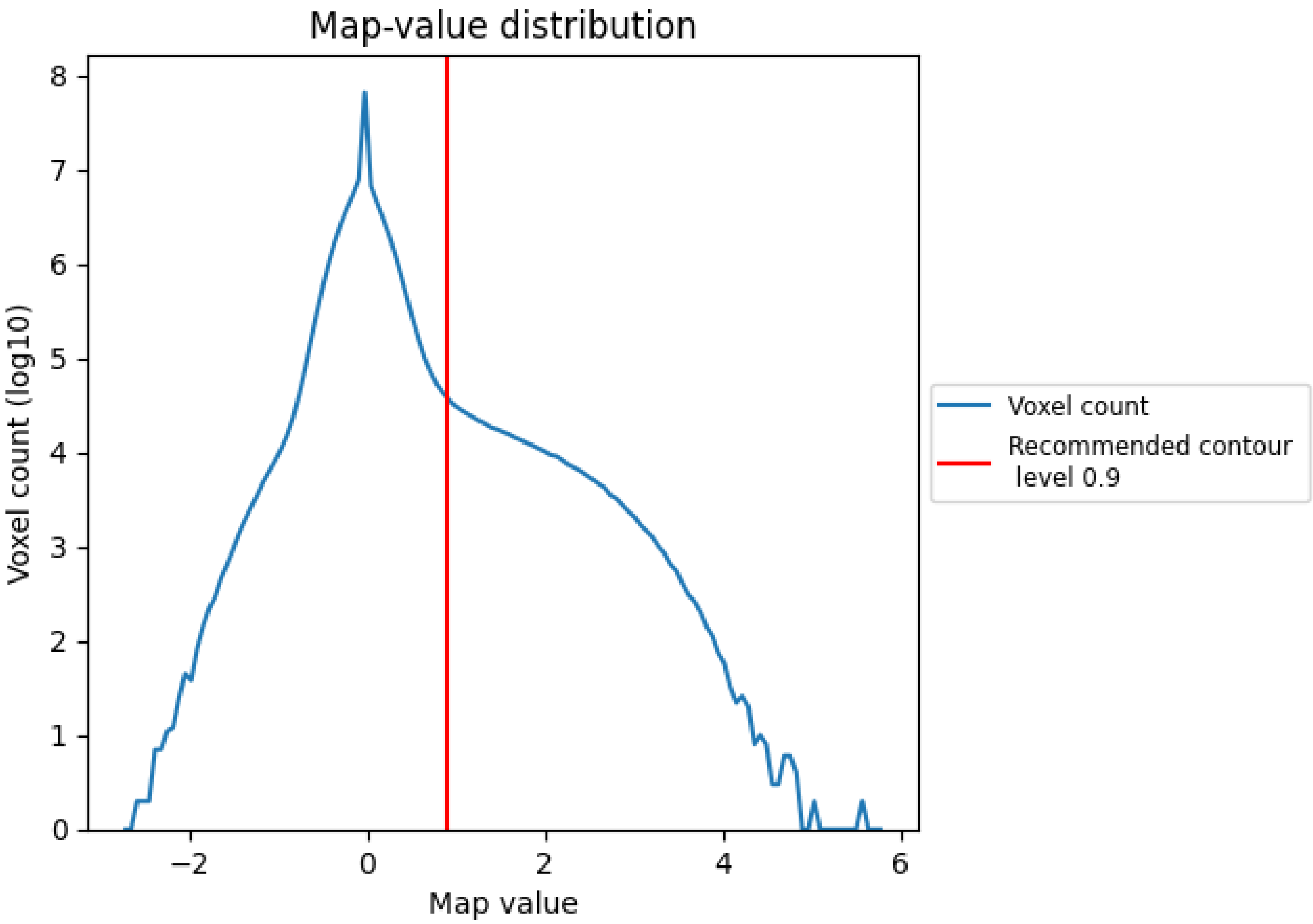
Y

Z

7 Map analysis ⓘ

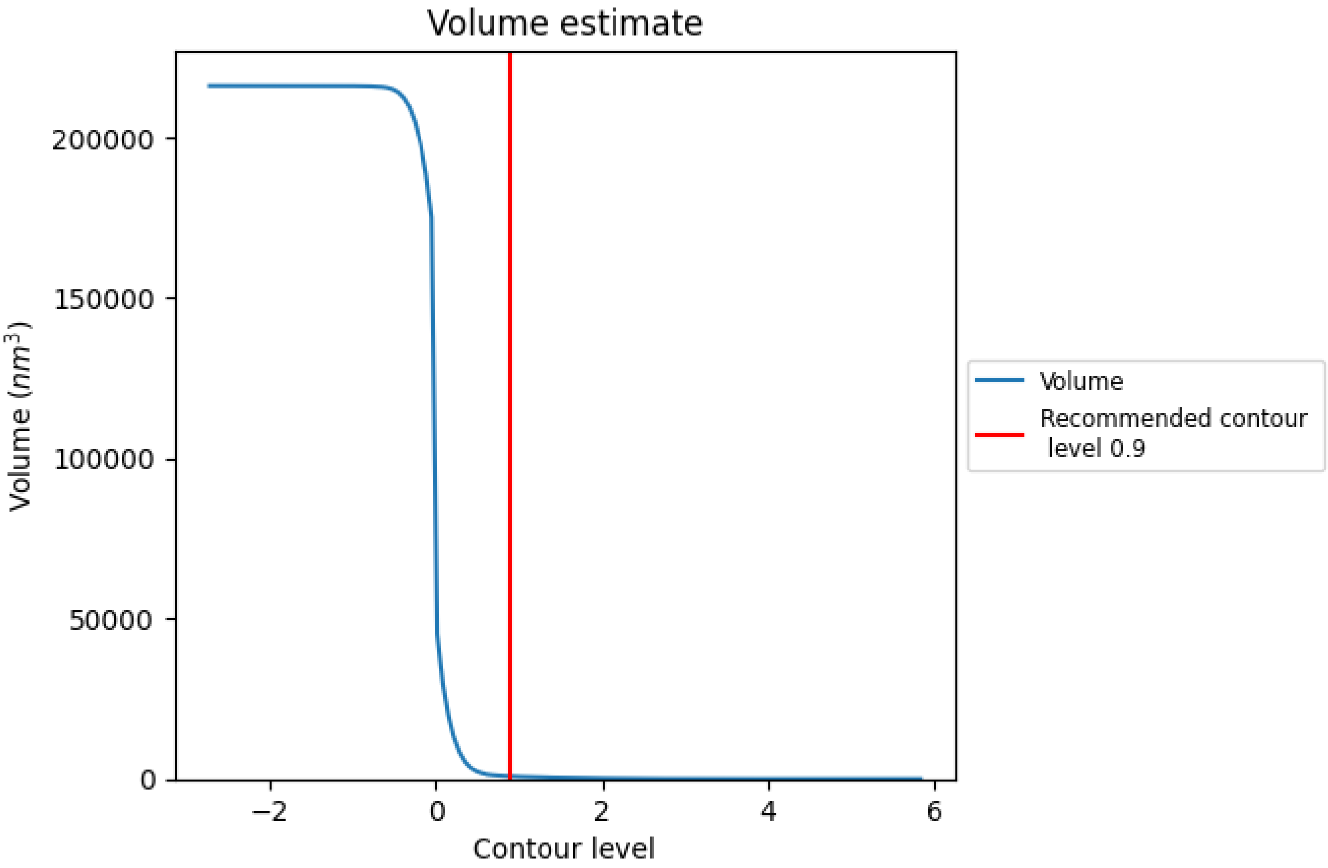
This section contains the results of statistical analysis of the map.

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.

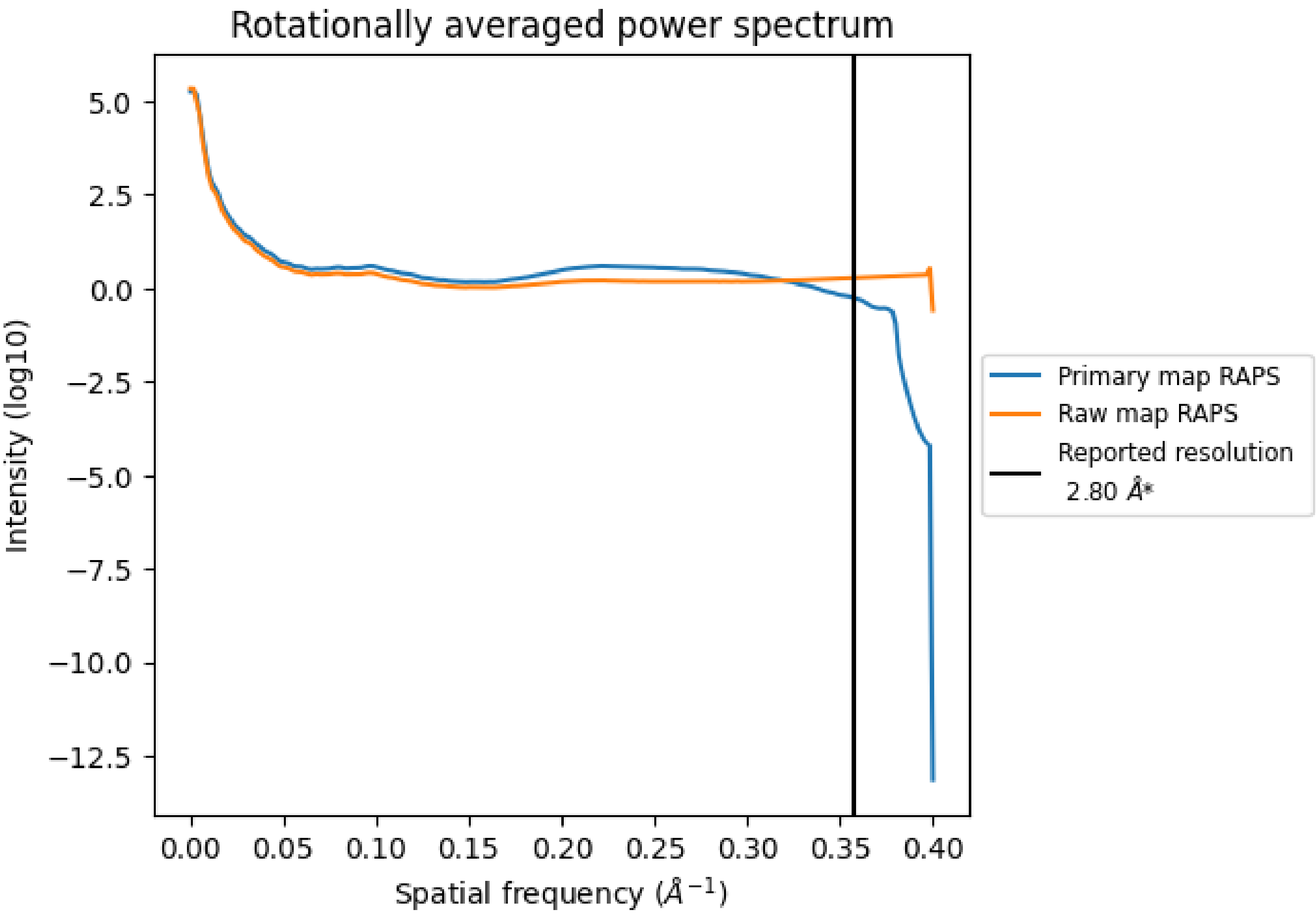
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 843 nm^3; this corresponds to an approximate mass of 762 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

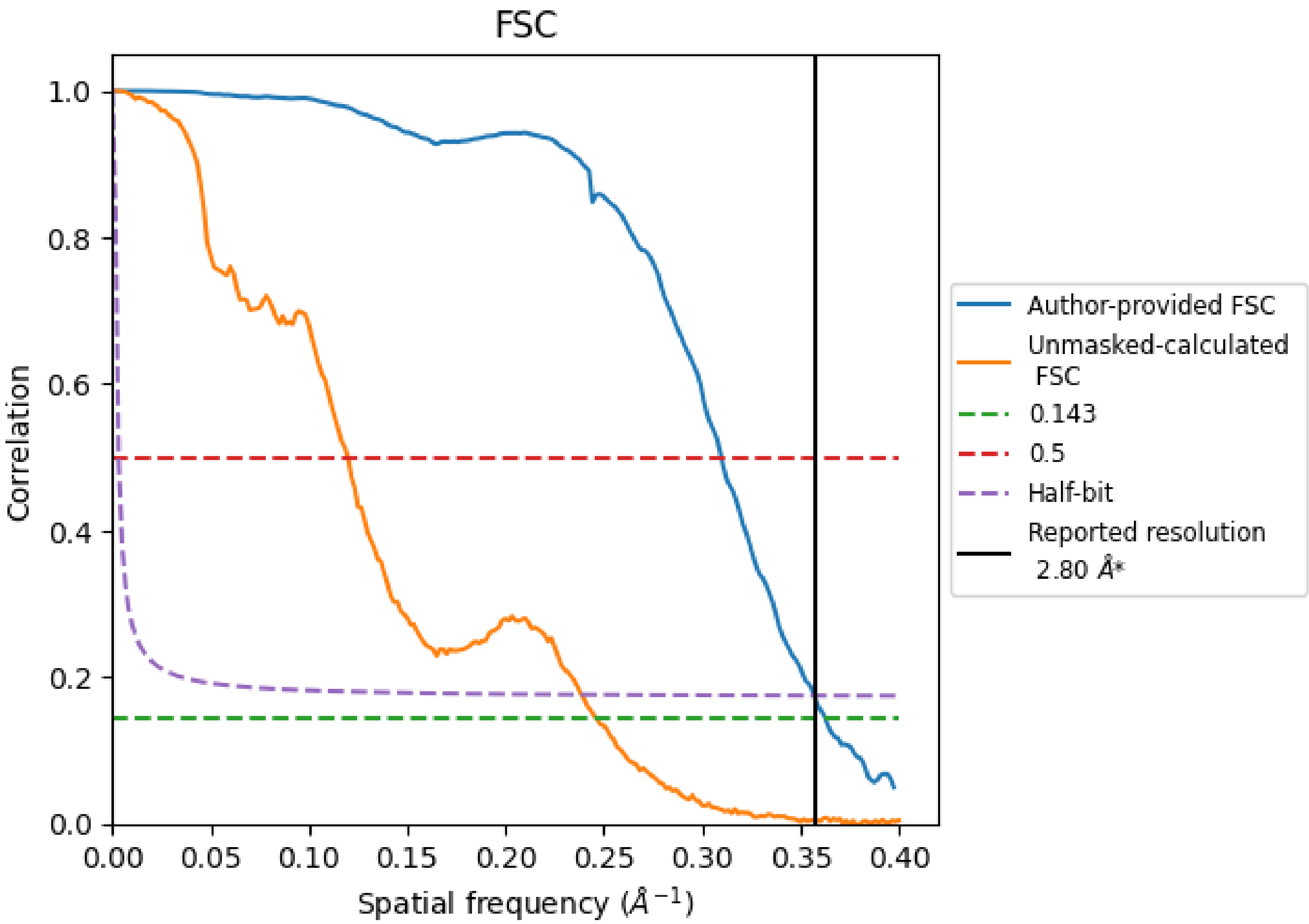


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 $Å^{-1}$

8.2 Resolution estimates

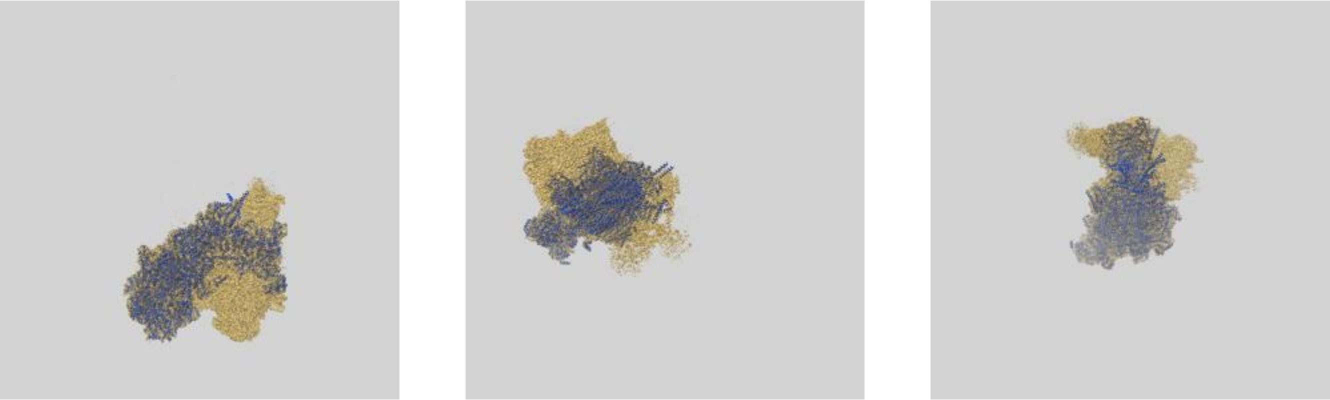
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.23	2.80
Unmasked-calculated*	4.06	8.35	4.19

*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 4.06 differs from the reported value 2.8 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-15865 and PDB model 8B6F. Per-residue inclusion information can be found in section 3 on page 26.

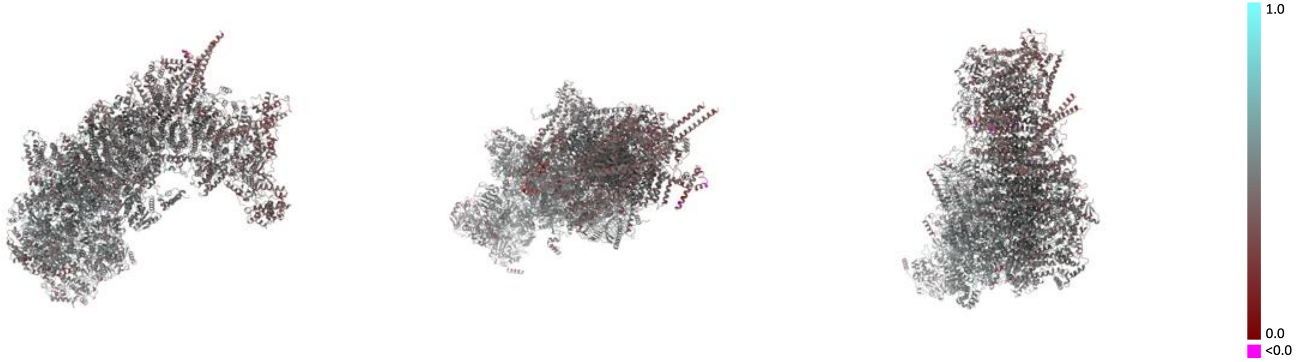
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

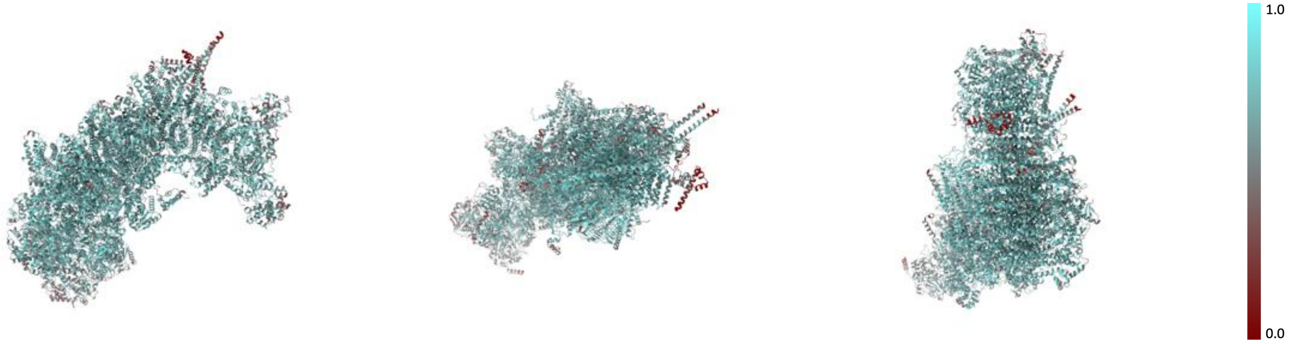
9.2 Q-score mapped to coordinate model ⓘ



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.

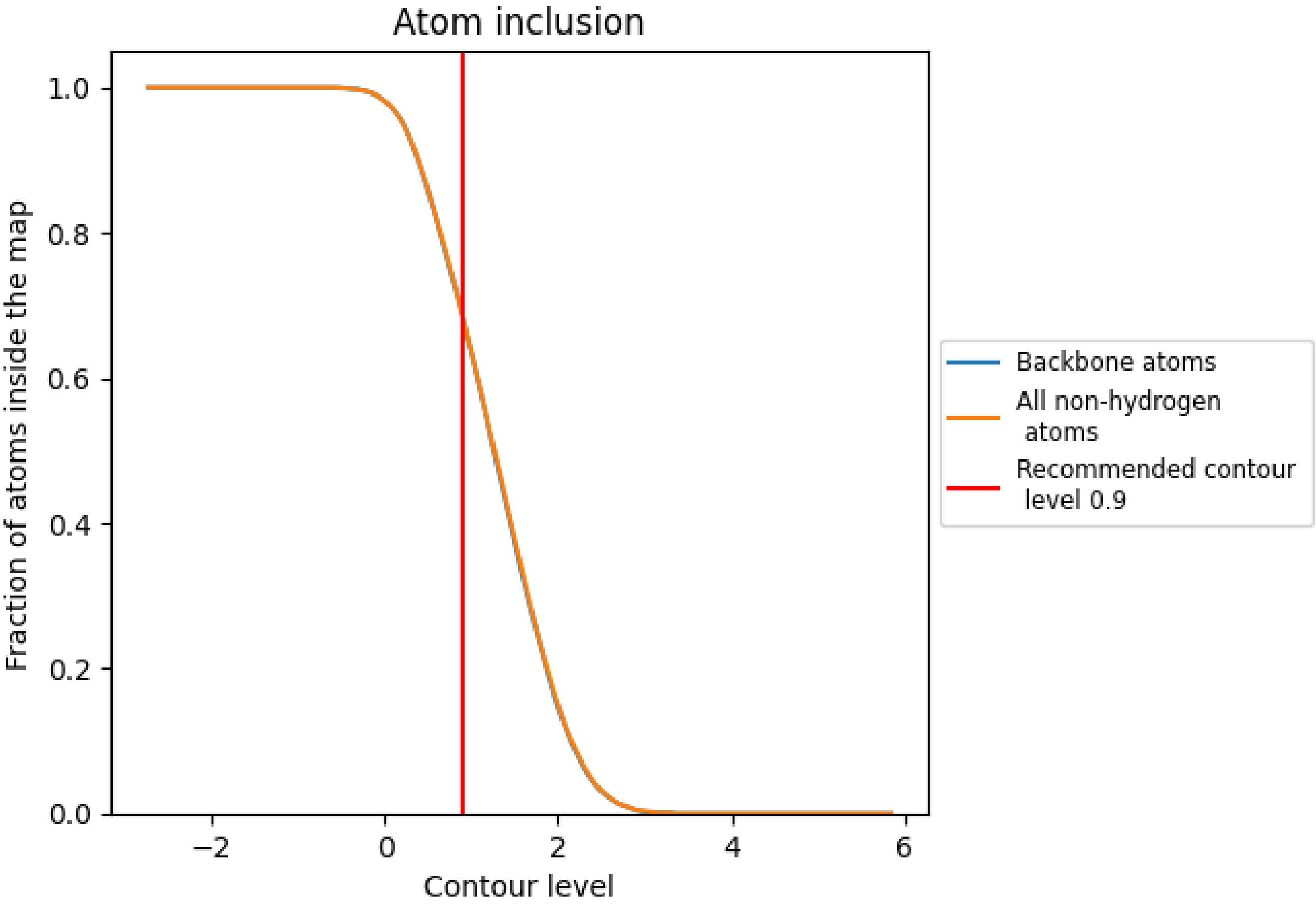
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6850	0.4630
A0	0.6510	0.4540
A1	0.7180	0.4840
A2	0.6830	0.4610
A3	0.5250	0.4510
A4	0.5720	0.3870
A5	0.7200	0.4890
A6	0.6880	0.4230
A7	0.7030	0.4540
A8	0.7050	0.5010
A9	0.6710	0.4470
AA	0.6540	0.4260
AB	0.6810	0.4860
AC	0.7300	0.4560
AD	0.6030	0.4830
AE	0.7770	0.5050
AF	0.7440	0.4730
AG	0.7320	0.4920
AH	0.7330	0.4880
AI	0.5940	0.4700
AJ	0.7320	0.4760
AK	0.7860	0.4980
AL	0.7750	0.5100
AM	0.7110	0.4730
AN	0.7220	0.5010
AO	0.7760	0.5070
AP	0.7300	0.4960
AQ	0.7220	0.4490
AR	0.7110	0.5000
AS	0.7760	0.4920
AT	0.7850	0.5010
AU	0.6610	0.4630
AV	0.7020	0.4770
AW	0.7040	0.4570
AX	0.7480	0.4870

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Chain	Atom inclusion	Q-score
AY	0.7590	0.4970
AZ	0.6130	0.4490
B0	0.6870	0.4590
B1	0.6490	0.4560
B2	0.6810	0.4490
B3	0.7020	0.4380
B4	0.6300	0.4390
B5	0.6950	0.4610
B6	0.7880	0.5130
BA	0.5750	0.3710
BB	0.6560	0.4170
BC	0.6560	0.4260
BD	0.6600	0.4210
BE	0.6510	0.4250
BF	0.7190	0.4340
BG	0.7080	0.4670
BH	0.7700	0.4720
BI	0.7840	0.4840
BJ	0.7350	0.4660
BK	0.6760	0.4410
BL	0.6770	0.4640
BM	0.7490	0.4790
BN	0.6820	0.4520
BO	0.6460	0.4250
BP	0.7360	0.4550
BQ	0.6620	0.4510
BR	0.7480	0.5090
BS	0.6650	0.4120
BT	0.6930	0.4480
BU	0.5560	0.4140
BV	0.6830	0.4420
BW	0.6900	0.4210
BX	0.7190	0.4580
BY	0.7080	0.4600
BZ	0.7220	0.4640