Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 08:27 PM JST

PDB ID	:	7DGR
EMDB ID	:	EMD-30674
Title	:	Activity optimized supercomplex state2
Authors	:	Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on	:	2020-11-12
Resolution	:	4.60 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

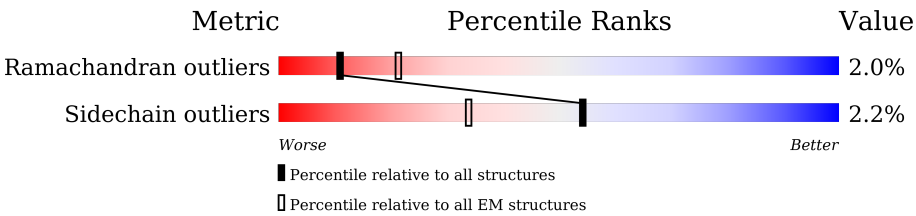
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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)
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	9	217	89% 5% • 5%
2	4	459	95% •
3	2	347	95% • ••
4	7	175	5% 92% 5% • •
5	6	606	98% •
6	5	98	93% • ••
7	3	115	9% 94% • •
8	1	318	89% 11% •
9	8	444	93% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	A	704	92% 6%
11	B	430	6% 94% 6%
12	C	228	89% 9%
13	D	179	77% 7% 15%
14	E	176	91% 7%
15	F	75	36% 63%
16	G	133	91% 8%
17	H	105	87% 5% 9%
18	I	96	69% 26%
19	J	70	96%
20	K	98	84% 14%
21	L	83	5% 95%
22	N	115	96%
23	O	127	87% 10%
24	P	112	9% 77% 20%
25	Q	171	95%
26	R	345	5% 88% 8%
27	S	320	95% 5%
28	T	140	5% 70% 26%
29	U	145	18% 88% 9%
30	V	143	92%
31	M	88	83% 8% 9%
31	W	88	92% 6%
32	X	57	82% 14%
33	Y	72	78% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Z	98	72% 24%
35	a	128	9% 88% 11%
36	b	143	94%
37	c	128	70% 30%
38	d	117	88% 9%
39	f	178	91% 6%
40	h	125	64% 33%
41	i	49	78% 22%
42	j	120	12% 91% 6%
43	g	176	96%
44	e	158	77% 10% 11%
45	k	480	92% 7%
45	w	480	90% 9%
46	l	453	91% 8%
46	x	453	91% 8%
47	m	379	14% 99%
47	y	379	18% 99%
48	o	241	95% 5%
48	z	241	5% 95% 5%
49	A0	196	11% 78% 18%
49	p	196	68% 6% 23%
50	A1	111	9% 89% 5%
50	q	111	95% 5%
51	A2	82	20% 99%
51	r	82	17% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	B3	91	12% 73% 24%
52	s	91	7% 70% 26%
53	A3	56	25% 59% 7% 30%
53	t	56	14% 55% 41%
54	B2	64	30% 97%
54	u	64	8% 97%
55	B1	78	19% 8% 72%
55	v	78	19% 77%
56	A9	514	37% 92% 8%
57	C4	227	17% 90% 10%
58	C2	261	51% 90% 10%
59	A7	169	58% 80% 5% 15%
60	C0	152	61% 68% 28%
61	A6	129	47% 70% 5% 24%
62	A4	97	74% 64% 22% 13%
63	A5	86	31% 76% 12% 13%
64	B4	74	55% 92% 7%
65	C3	80	59% 61% 6% 30%
66	B0	80	38% 59% 39%
67	C1	63	49% 71% 25%
68	A8	70	47% 57% 39%

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
79	HEA	A9	601	X	-	-	-
79	HEA	A9	602	X	-	-	-

2 Entry composition (i)

There are 81 unique types of molecules in this entry. The entry contains 107305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9	207	1578	1006	269	293	10	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	458	3577	2382	561	599	35	1	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	344	2681	1779	413	449	40	0	0

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	172	1239	838	182	211	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	606	4766	3172	732	820	42	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	96	712	464	110	125	13	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	3	112	879	593	128	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1	318	2503	1678	385	417	23	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	427	3065	1927	563	559	16	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	688	5218	3273	920	988	37	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	430	3422	2185	588	624	25	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	208	1726	1114	297	312	3	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	152	1206	772	212	208	14	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	176	1401	880	243	267	11	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	28	186	118	32	35	1	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	123	985	622	178	182	3	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	H	96	780	494	147	134	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	I	71	533	332	99	99	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	69	530	344	96	88	2	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	K	84	656	412	126	118	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	L	80	602	398	97	105	2	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	111	862	559	149	152	2	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	114	925	595	170	156	4	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	90	702	445	129	126	2	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	168	1345	851	242	243	9	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	319	2407	1548	431	425	3	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	N	O	S		
27	S	319	2299	1457	395	438	9	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	138	923	586	163	168	6	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	132	1019	659	179	178	3	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	138	1087	699	186	193	9	0	0

- Molecule 31 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	86	616	400	98	114	4	0	0
31	M	80	642	413	96	128	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	X	49	372	243	64	65	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	57	409	277	65	66	1	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	74	493	320	89	82	2	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	a	114	857	550	159	148	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b	139	1032	672	190	168	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	c	90	617	391	119	107	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	d	107	713	448	134	127	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	f	167	1156	739	205	208	4	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	84	658	423	115	118	2	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	i	38	277	185	46	46	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	113	883	580	149	151	3	0	0

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	g	173	1351	849	246	248	8	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	e	141	864	539	161	160	4	0	0

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	446	3454	2159	608	667	20	0	0
45	w	436	3385	2117	599	649	20	0	0

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	l	419	3135	1969	553	606	7	0	0
46	x	419	3141	1972	556	606	7	0	0

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	m	379	3011	2018	472	502	19	0	0
47	y	379	3011	2018	472	502	19	0	0

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	o	241	1919	1225	330	349	15	0	0
48	z	241	1906	1216	329	347	14	0	0

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	p	151	938	572	170	194	2	0	0
49	A0	188	1117	679	207	229	2	0	0

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	q	106	916	579	167	168	2	0	0
50	A1	106	916	579	167	168	2	0	0

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	r	81	682	441	128	112	1	0	0
51	A2	81	676	438	125	112	1	0	0

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s	67	548	332	99	112	5	0	0
52	B3	69	566	342	101	118	5	0	0

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	t	33	262	174	46	42	0	0
53	A3	39	318	212	56	50	0	0

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	u	62	511	335	89	87	0	0
54	B2	62	511	335	89	87	0	0

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	v	18	114	70	22	22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	B1	22	148	91	30	27	0	0

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	A9	514	4025	2690	623	677	35	0	0

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	C4	227	1822	1184	281	339	18	0	0

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	C2	261	2124	1420	338	353	13	0	0

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	A7	144	1195	777	196	218	4	0	0

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	C0	109	878	558	150	168	2	0	0

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	A6	98	748	464	134	145	5	0	0

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	A4	84	671	431	129	110	1	0	0

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	A5	75	628	395	114	114	5	0	0

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	B4	73	598	388	107	99	4	0	0

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	C3	56	441	285	73	80	3	0	0

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	B0	49	384	250	65	67	2	0	0

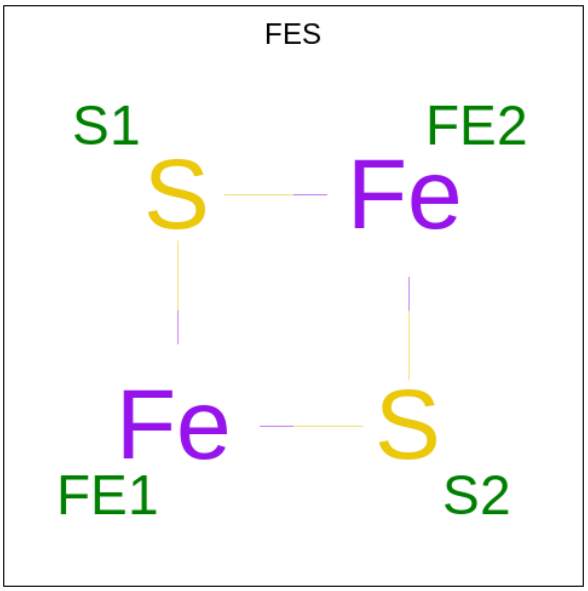
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	C1	47	386	257	65	62	2	0	0

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

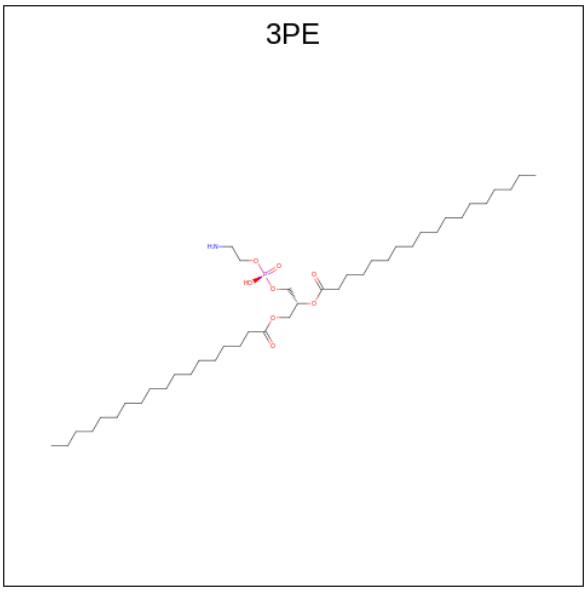
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	A8	43	335	223	53	59	0	0

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



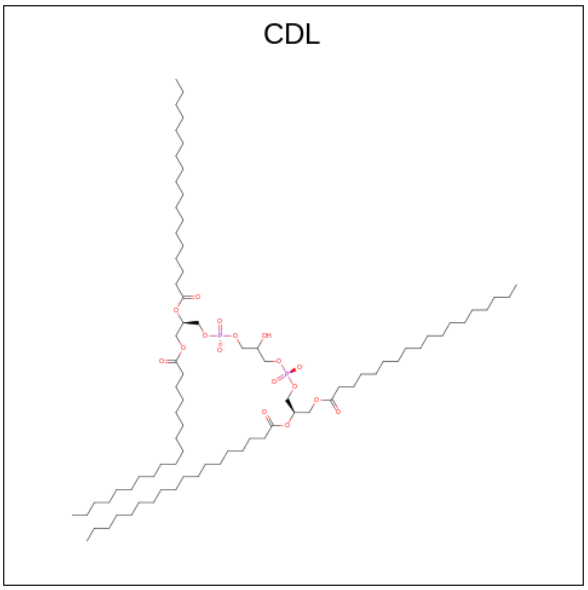
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
69	9	1	4	2	2	0
69	A	1	4	2	2	0
69	m	1	4	2	2	0

- Molecule 70 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



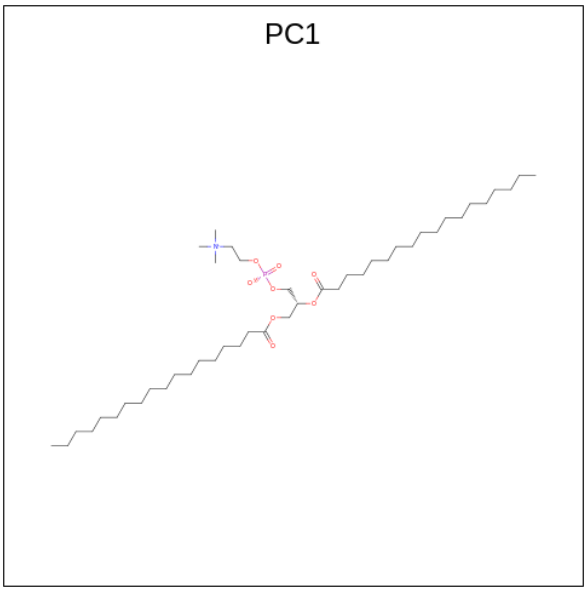
Mol	Chain	Residues	Atoms					AltConf
70	4	1	Total 82	C 62	N 2	O 16	P 2	0
70	4	1	Total 82	C 62	N 2	O 16	P 2	0
70	2	1	Total 46	C 36	N 1	O 8	P 1	0
70	B	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 71 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



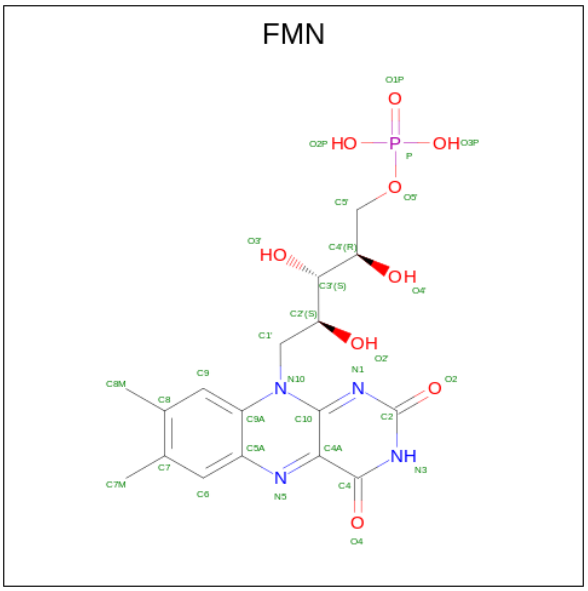
Mol	Chain	Residues	Atoms				AltConf
71	4	1	Total 82	C 63	O 17	P 2	0
71	6	1	Total 64	C 45	O 17	P 2	0
71	J	1	Total 58	C 39	O 17	P 2	0

- Molecule 72 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



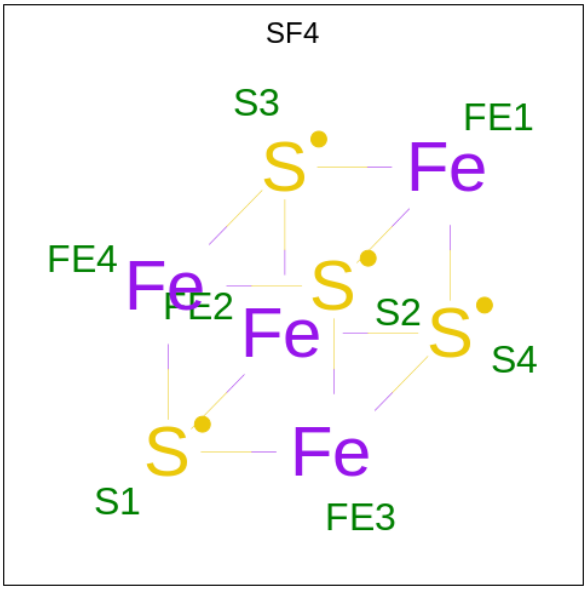
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
72	4	1	46	36	1	8	1	0
			Total	C	N	O	P	
72	2	1	46	36	1	8	1	0
			Total	C	N	O	P	
72	L	1	47	37	1	8	1	0
			Total	C	N	O	P	
72	S	1	47	37	1	8	1	0
			Total	C	N	O	P	
72	j	1	39	29	1	8	1	0

- Molecule 73 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	N	O	P	
73	8	1	31	17	4	9	1	0

- Molecule 74 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
74	8	1	8	4	4	0
			Total	Fe	S	
74	A	1	16	8	8	0
			Total	Fe	S	
74	A	1	16	8	8	0

Continued on next page...

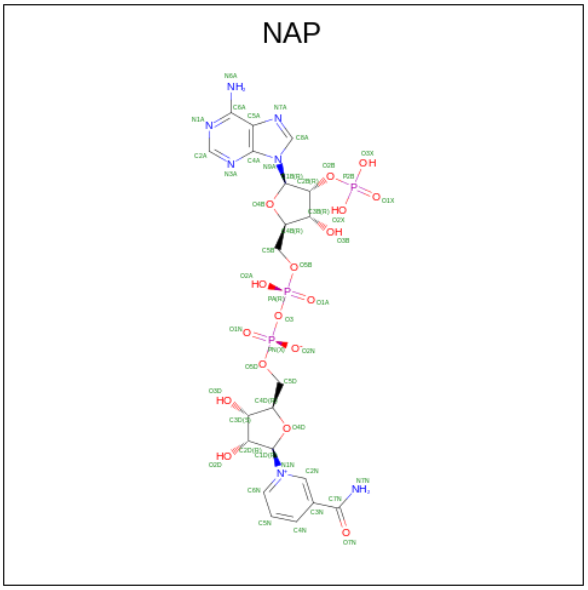
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
74	D	1	8	4	4	0
			Total	Fe	S	
74	E	1	16	8	8	0
			Total	Fe	S	
74	E	1	16	8	8	0

- Molecule 75 is ZINC ION (three-letter code: ZN) (formula: Zn).

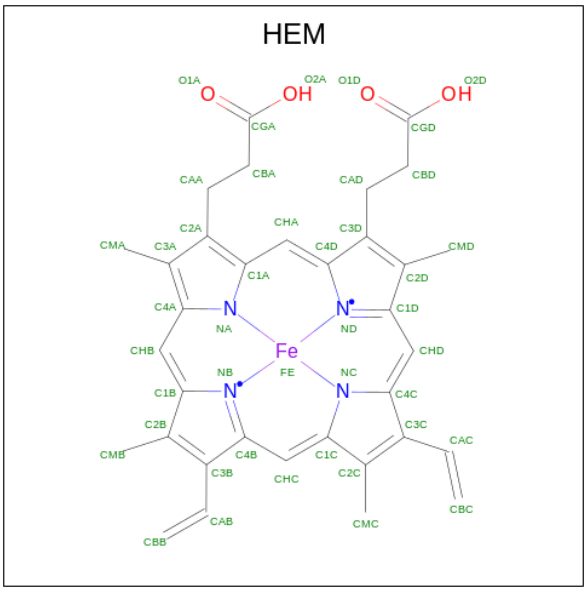
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
75	I	1	1	1	0
			Total	Zn	
75	A6	1	1	1	0

- Molecule 76 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



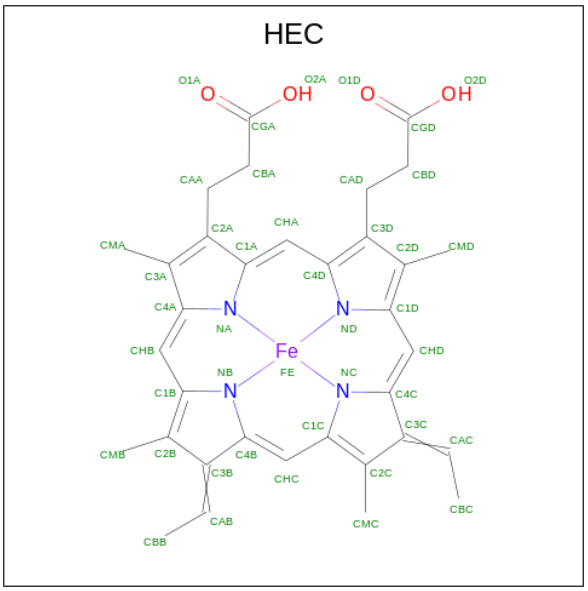
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	R	1	48	21	7	17	3	0

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



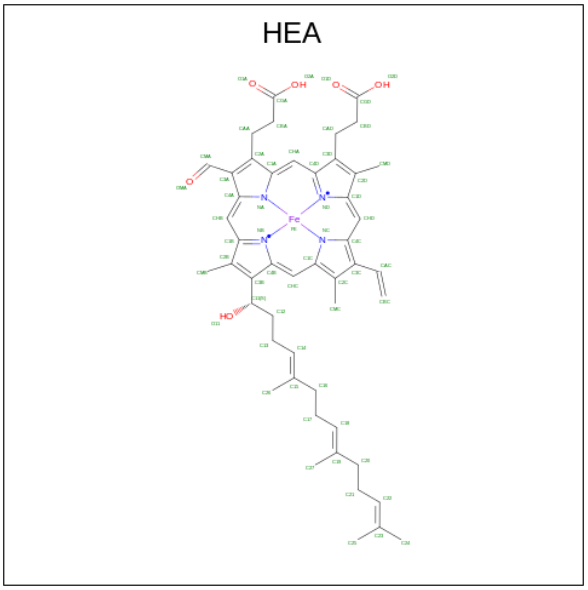
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
77	m	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
77	m	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
77	y	1	86	68	2	8	8	0
			Total	C	Fe	N	O	
77	y	1	86	68	2	8	8	0

- Molecule 78 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
78	o	1	Total 43	C 34	Fe 1	N 4	O 4	0
78	z	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
79	A9	1	Total 120	C 98	Fe 2	N 8	O 12	0
79	A9	1	Total 120	C 98	Fe 2	N 8	O 12	0

- Molecule 80 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	A9	1	Total 1	Cu 1	0
80	C4	2	Total 2	Cu 2	0

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

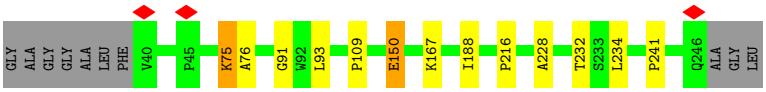
Mol	Chain	Residues	Atoms		AltConf
81	A9	1	Total 1	Mg 1	0

3 Residue-property plots (i)

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

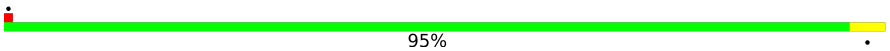
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

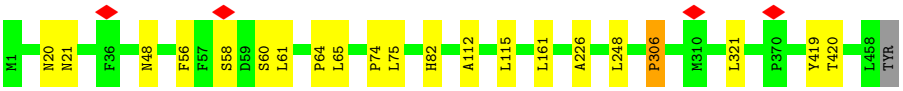
Chain 9:



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

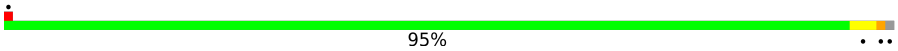
Chain 4:

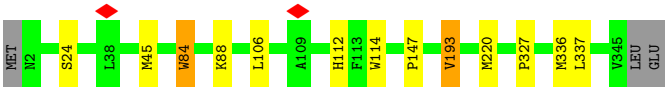




- Molecule 3: NADH-ubiquinone oxidoreductase chain 2

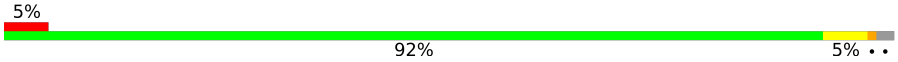
Chain 2:

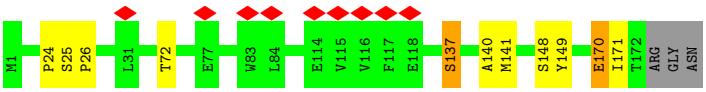




- Molecule 4: NADH-ubiquinone oxidoreductase chain 6

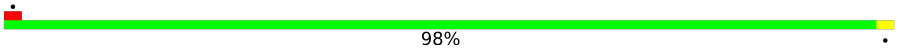
Chain 7:

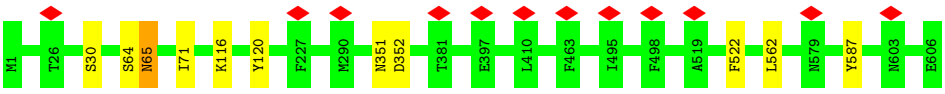




- Molecule 5: NADH-ubiquinone oxidoreductase chain 5

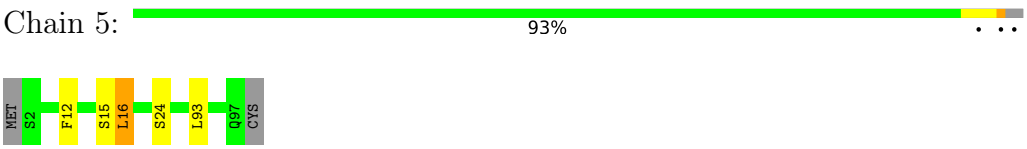
Chain 6:





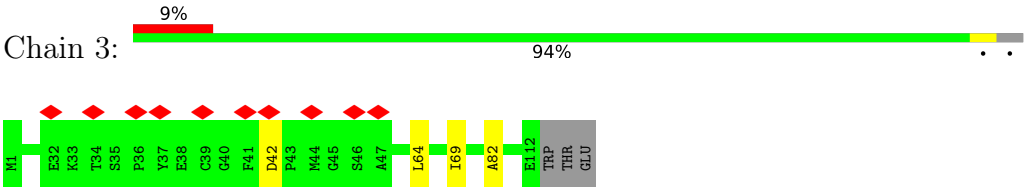
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5:



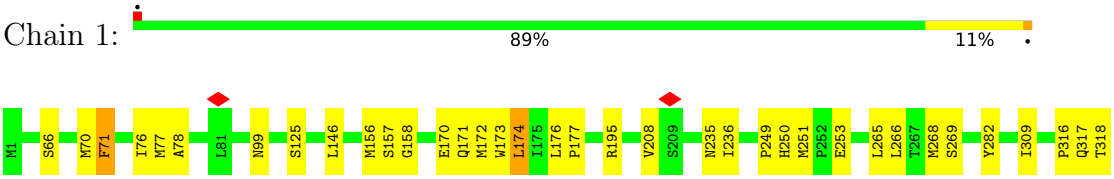
• Molecule 7: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



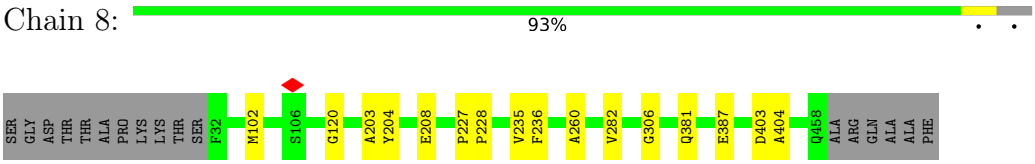
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1:



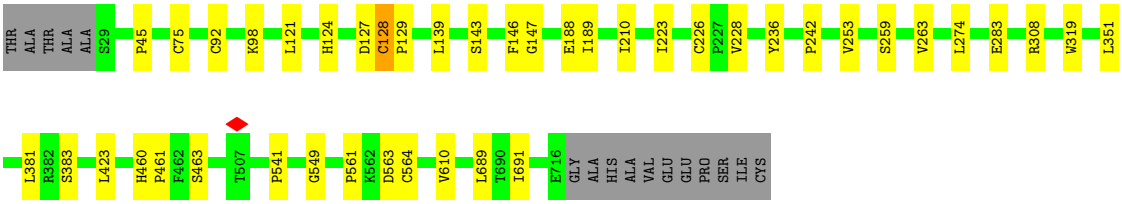
• Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 8:



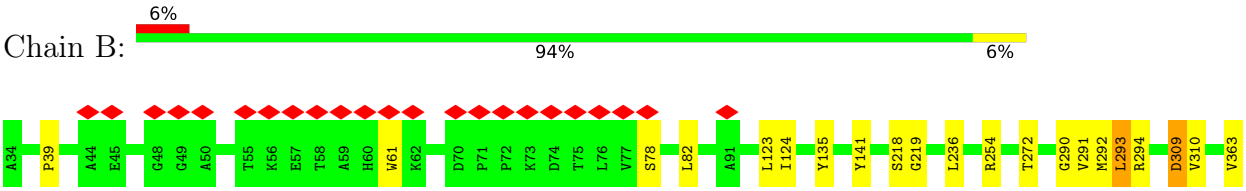
• Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

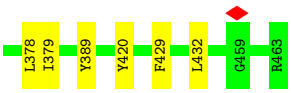
Chain A:



• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

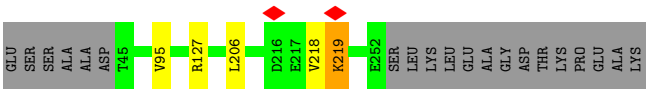
Chain B:





• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



• Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

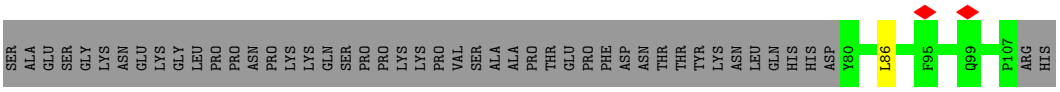
Chain D:

• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E:

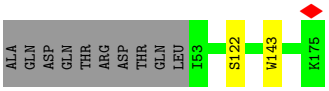
• Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:



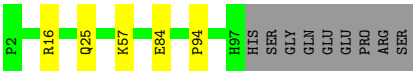
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G:



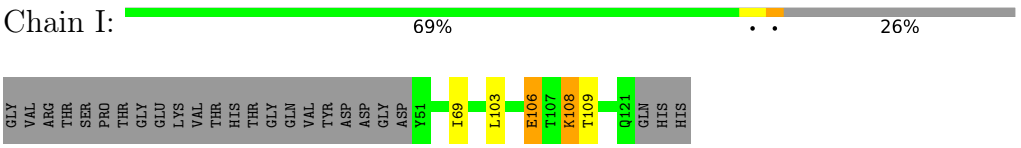
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain H:



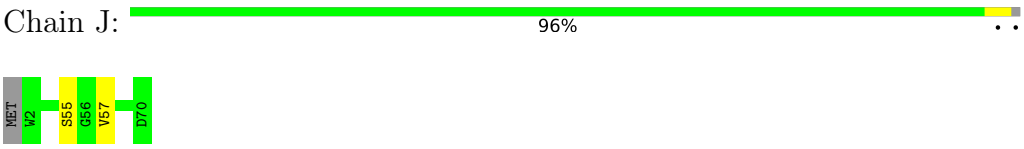
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain I:



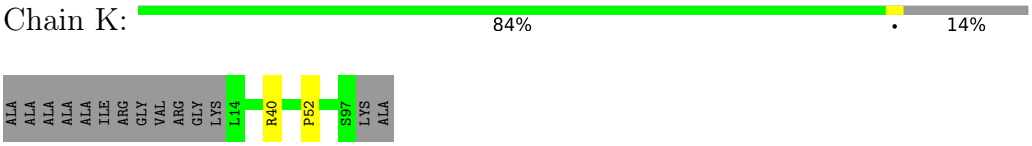
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain J:



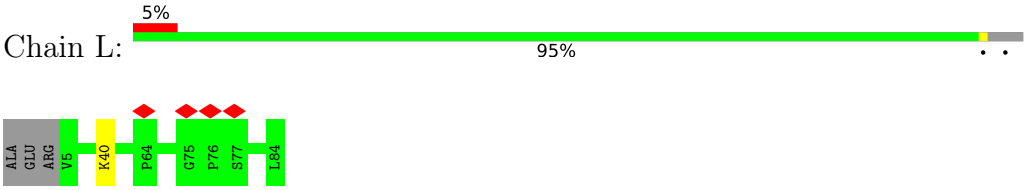
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain K:



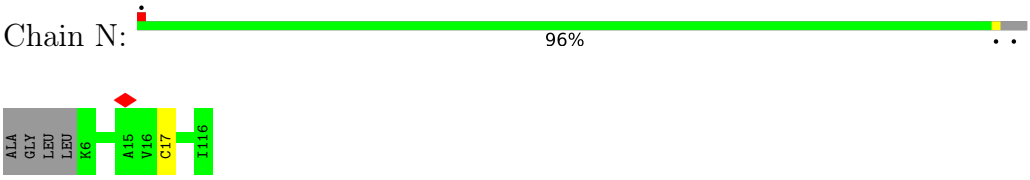
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain L:



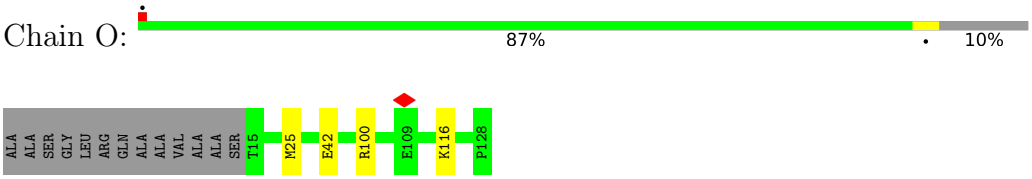
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N:



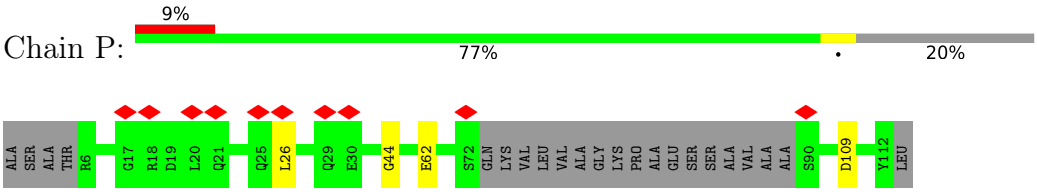
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O:



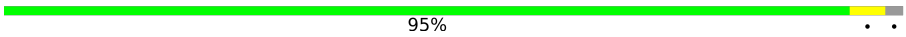
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

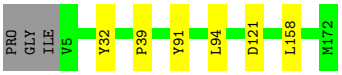
Chain P:



• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

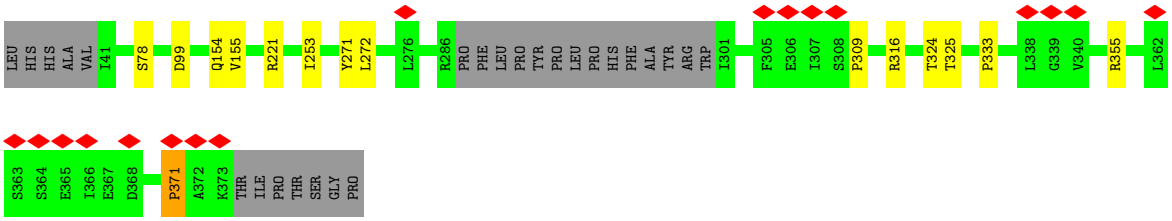
Chain Q:





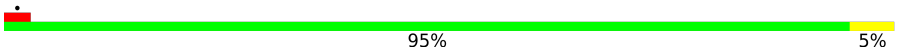
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

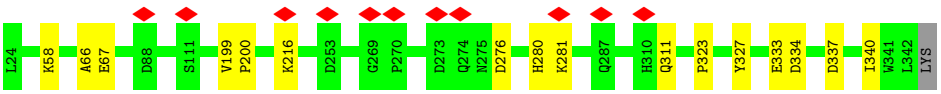
Chain R:



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

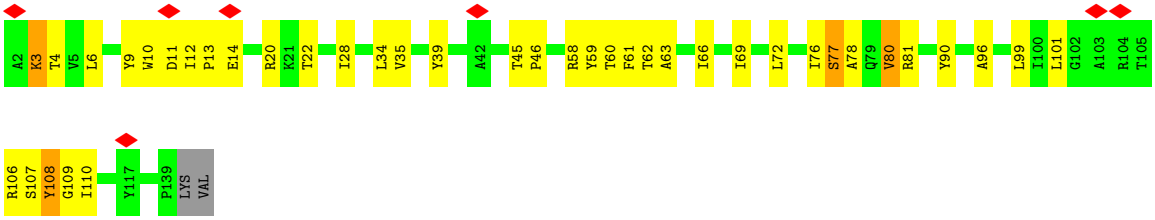
Chain S:





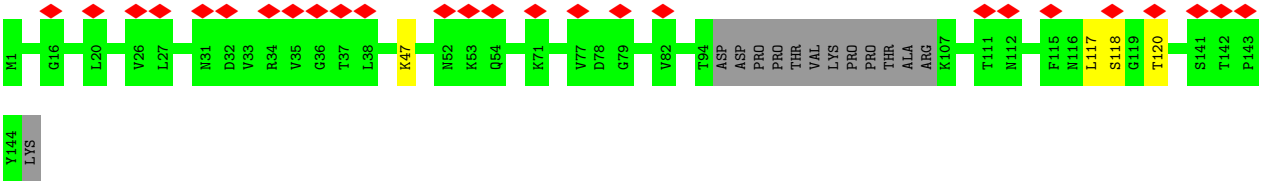
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T:



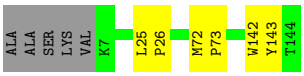
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain U:



• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain V: 92%

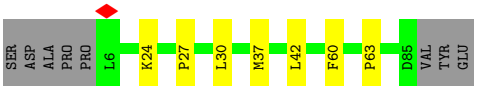


• Molecule 31: Acyl carrier protein, mitochondrial

Chain W: 92% 6%

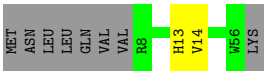
• Molecule 31: Acyl carrier protein, mitochondrial

Chain M: 83% 8% 9%



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

Chain X: 82% 14%

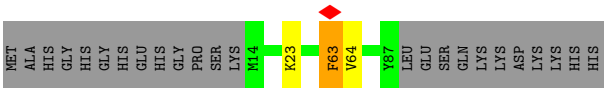


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 78% 21%

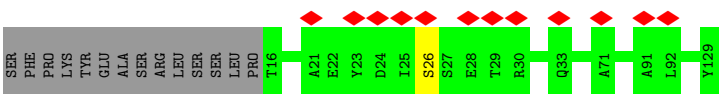
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 72% 24%



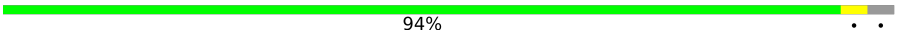
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

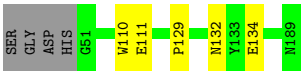
Chain a: 9% 88% 11%



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

Chain b:





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

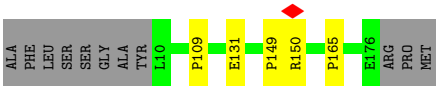
Chain c:

• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain d:

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

Chain f:

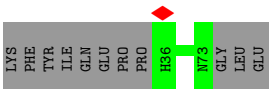


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain h:

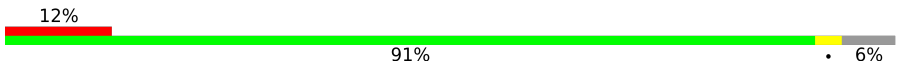
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

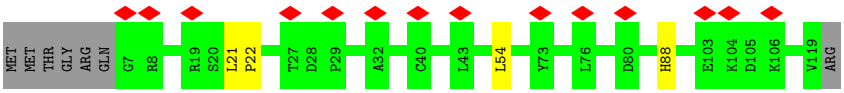
Chain i:



• Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C2

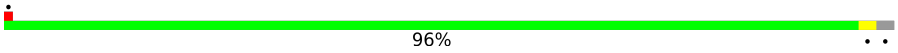
Chain j:

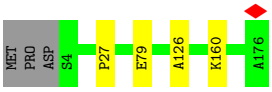




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

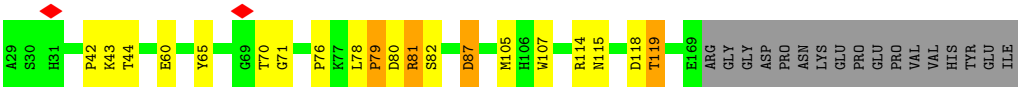
Chain g:





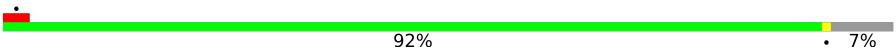
• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

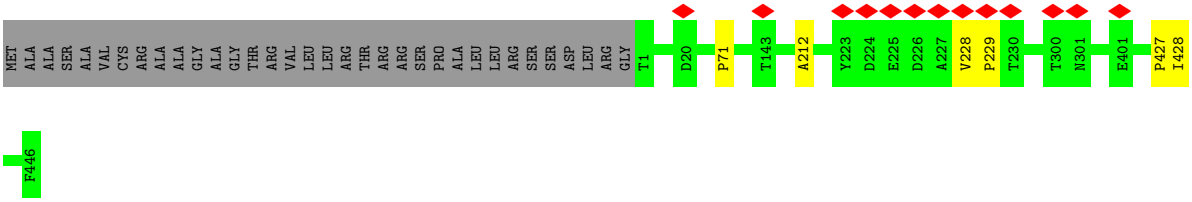
Chain e:



• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

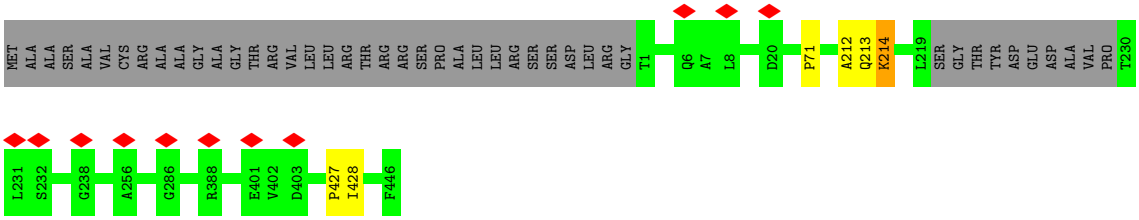
Chain k:





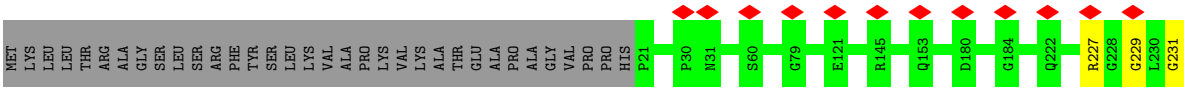
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

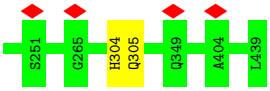
Chain w:



• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

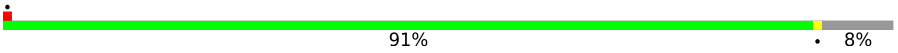
Chain l:

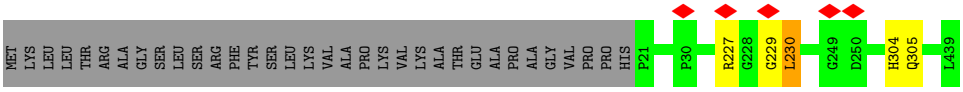




• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

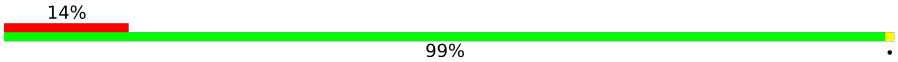
Chain x:

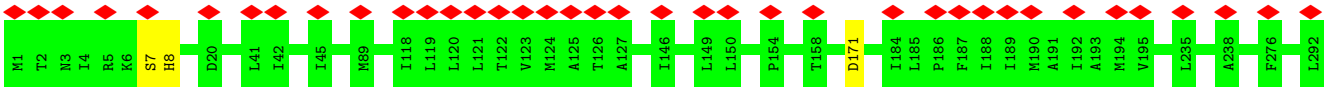


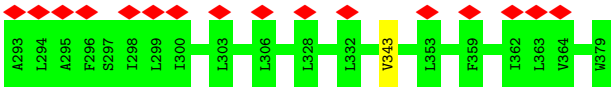


• Molecule 47: Cytochrome b

Chain m:

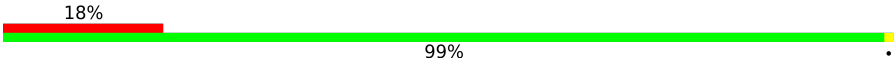


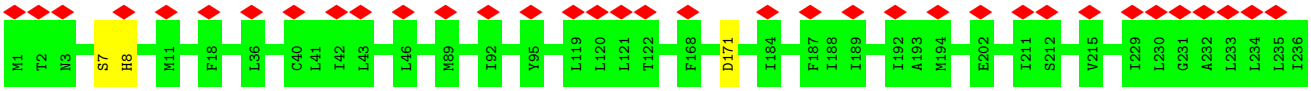


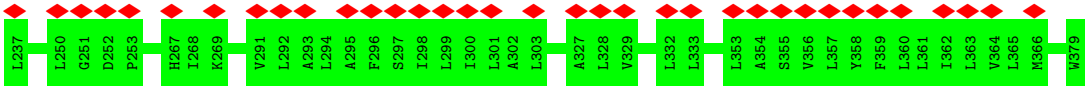


• Molecule 47: Cytochrome b

Chain y:

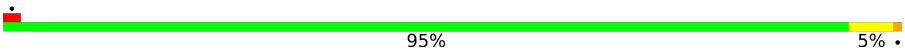


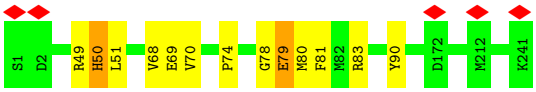




• Molecule 48: Cytochrome c1, heme protein, mitochondrial

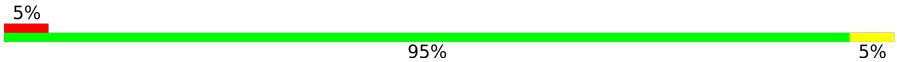
Chain o:

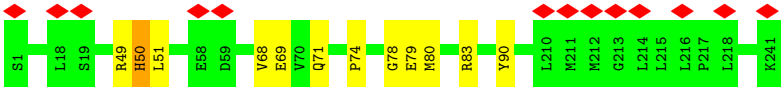




• Molecule 48: Cytochrome c1, heme protein, mitochondrial

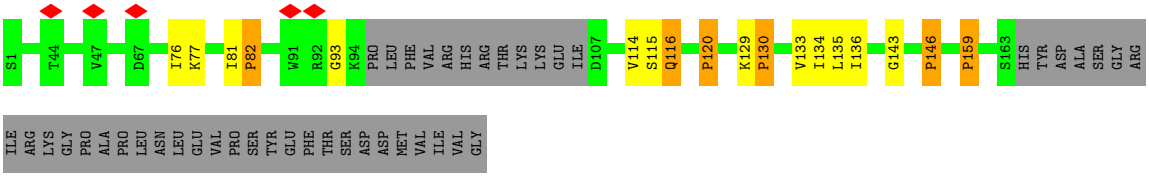
Chain z:





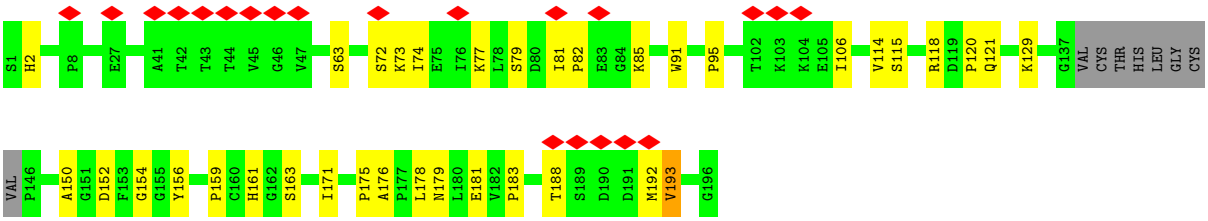
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain p:



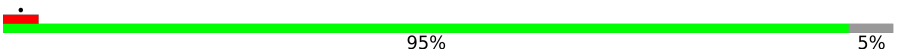
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

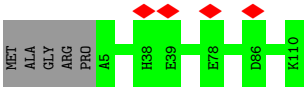
Chain A0:



- Molecule 50: Cytochrome b-c1 complex subunit 7

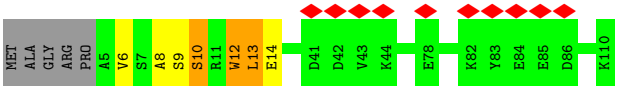
Chain q:





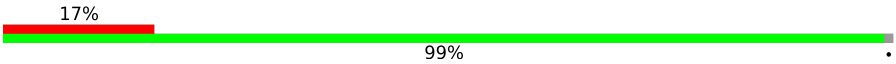
- Molecule 50: Cytochrome b-c1 complex subunit 7

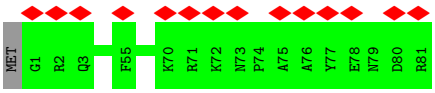
Chain A1:



- Molecule 51: Cytochrome b-c1 complex subunit 8

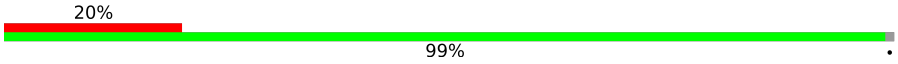
Chain r:

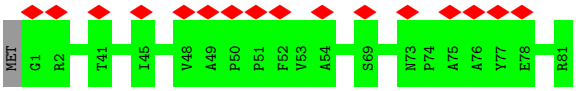




- Molecule 51: Cytochrome b-c1 complex subunit 8

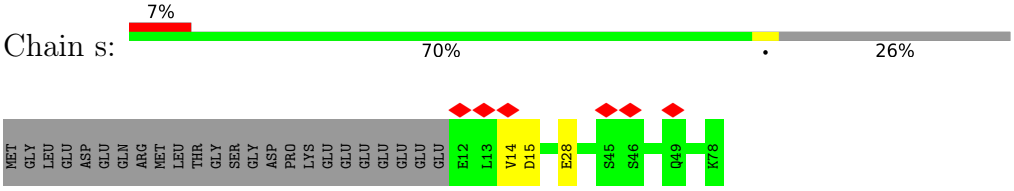
Chain A2:





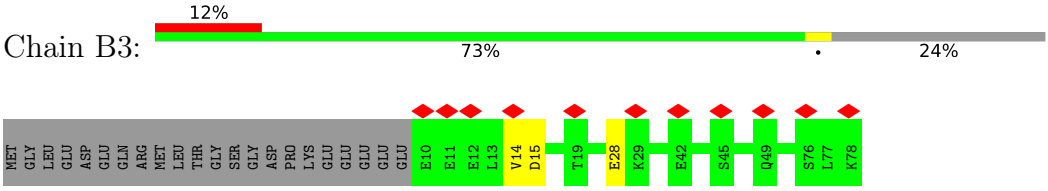
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain s:



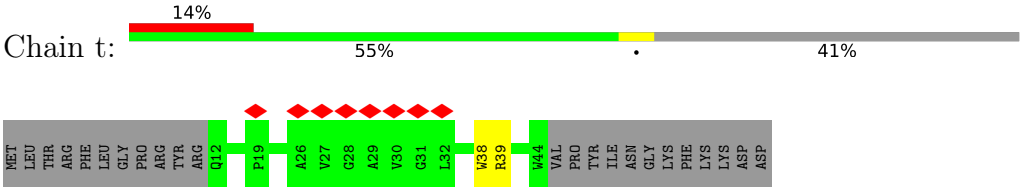
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain B3:



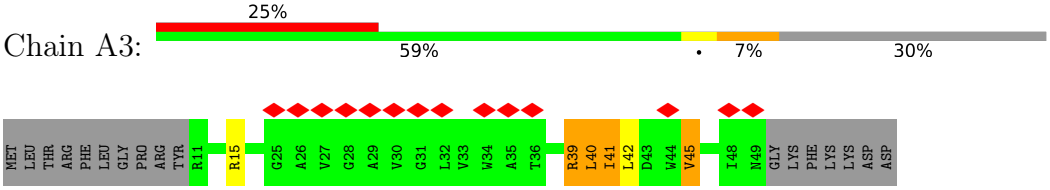
• Molecule 53: Cytochrome b-c1 complex subunit 10

Chain t:



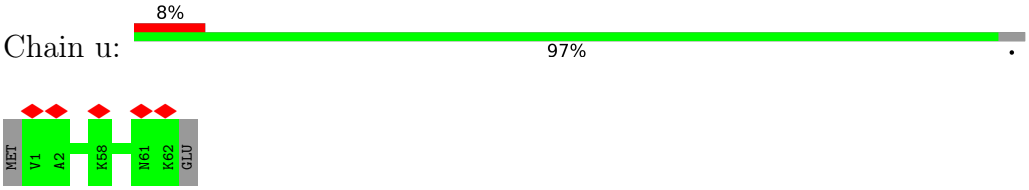
• Molecule 53: Cytochrome b-c1 complex subunit 10

Chain A3:



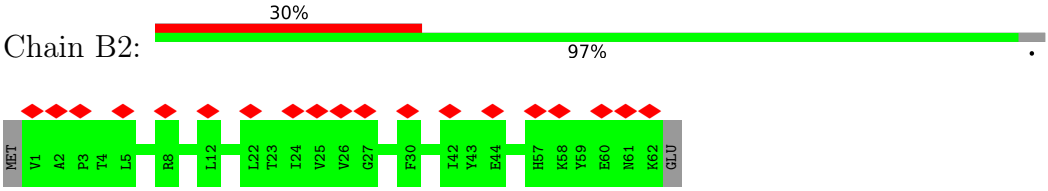
• Molecule 54: Cytochrome b-c1 complex subunit 9

Chain u:



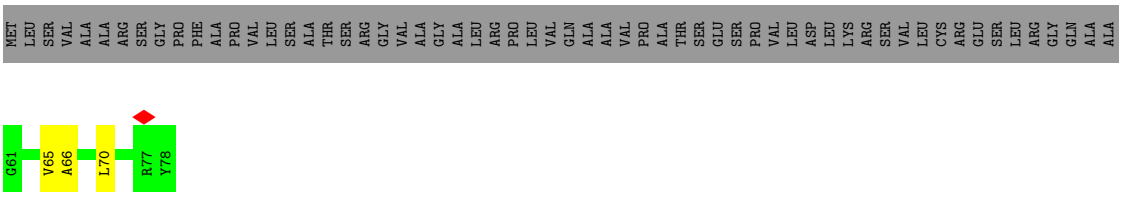
• Molecule 54: Cytochrome b-c1 complex subunit 9

Chain B2:



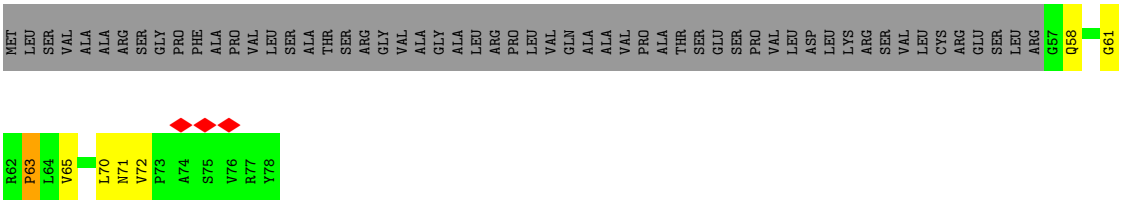
• Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain v:



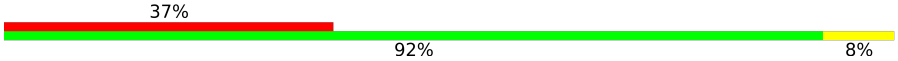
• Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

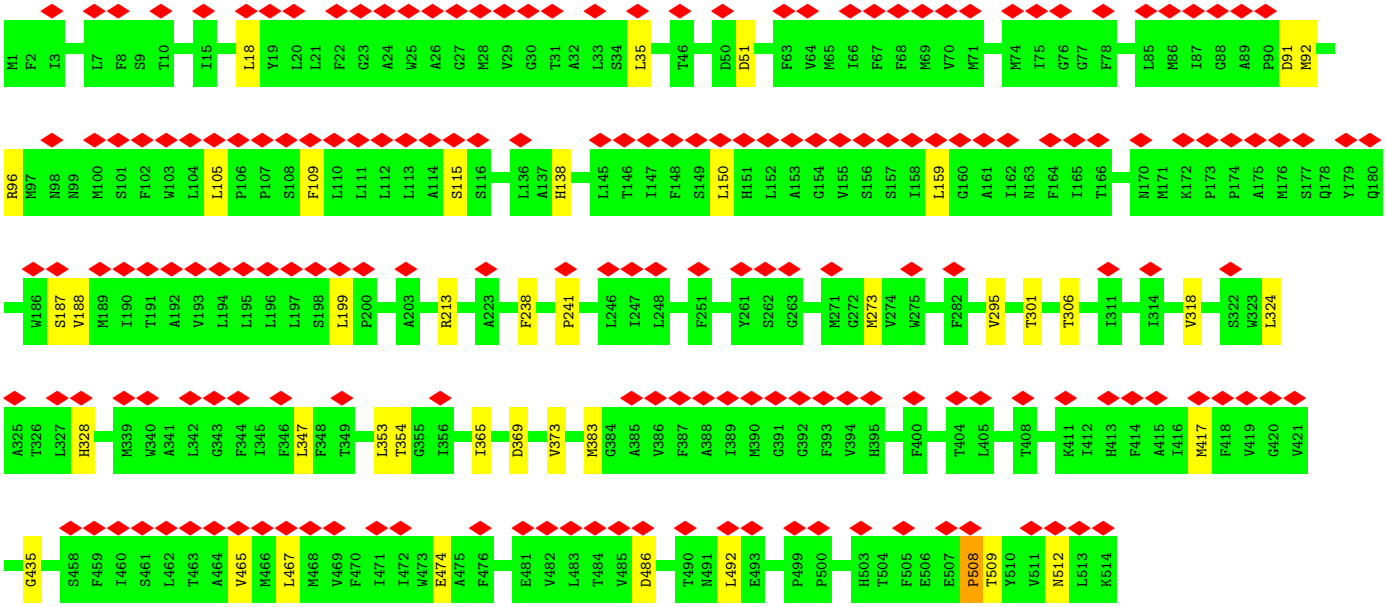
Chain B1:



• Molecule 56: Cytochrome c oxidase subunit 1

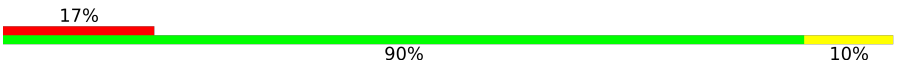
Chain A9:

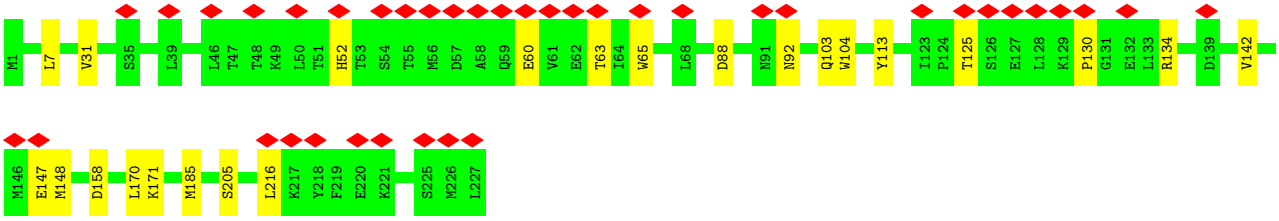




• Molecule 57: Cytochrome c oxidase subunit 2

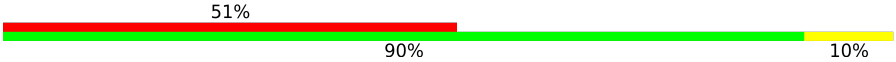
Chain C4:

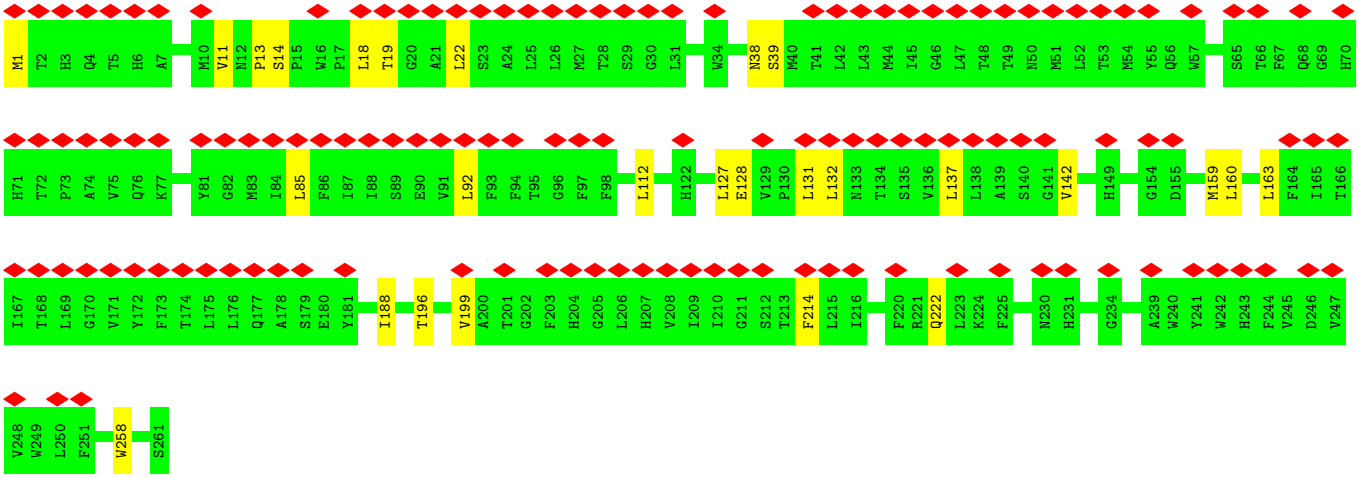




- Molecule 58: Cytochrome c oxidase subunit 3

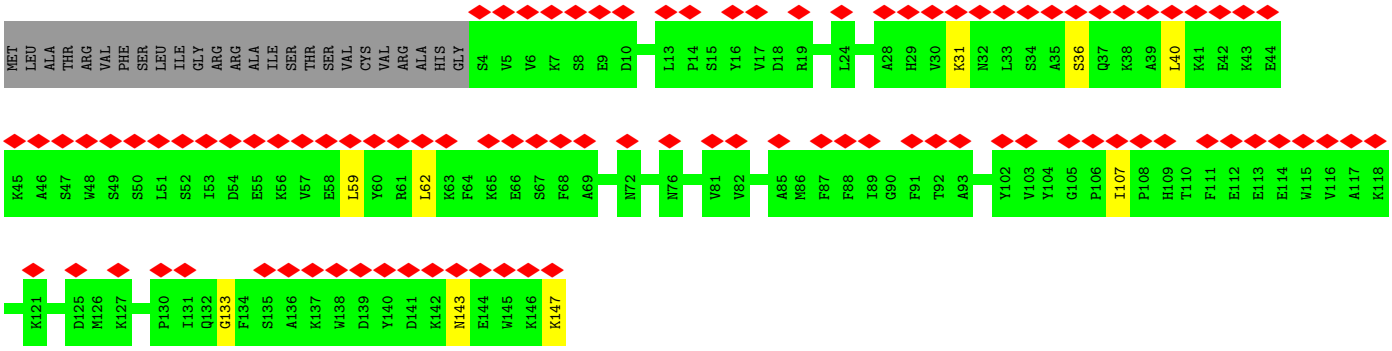
Chain C2:





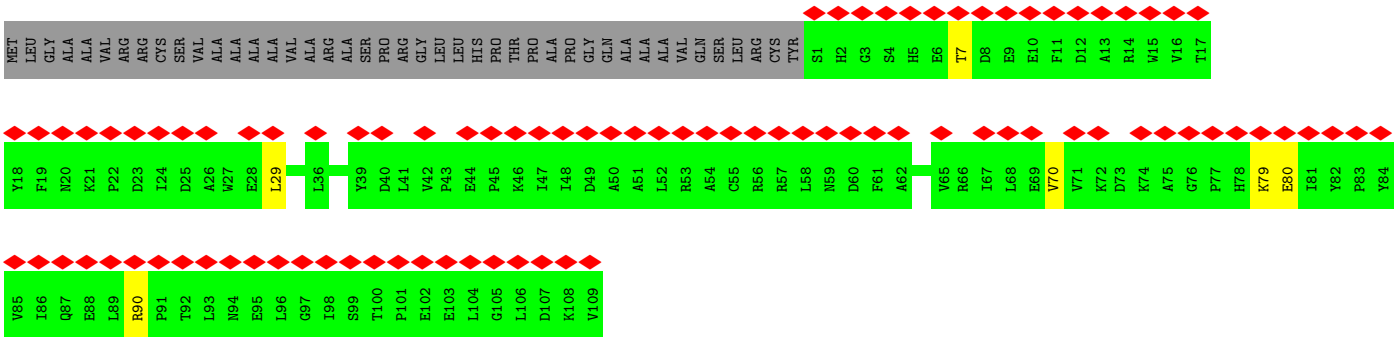
- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain A7:



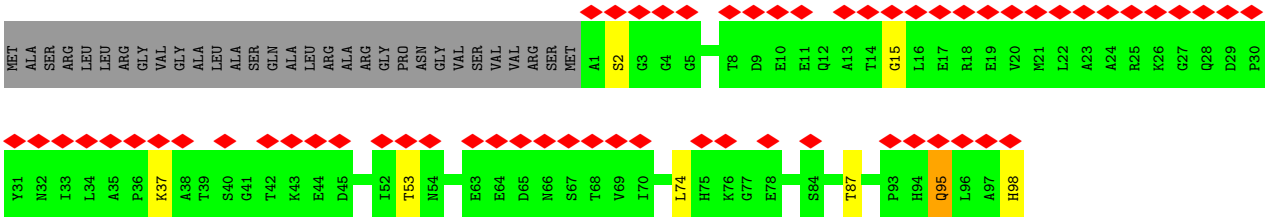
- Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

Chain C0:



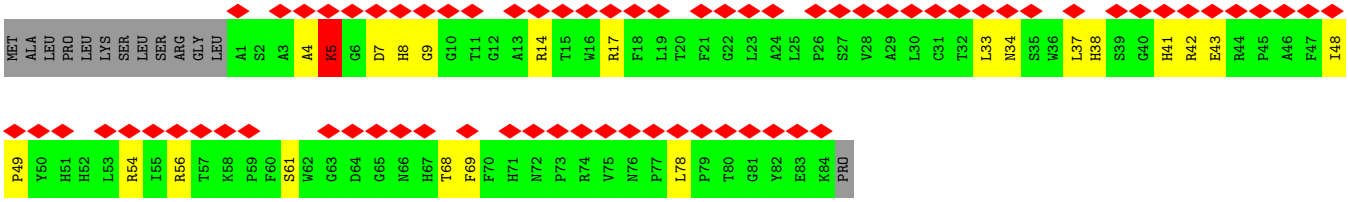
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial

Chain A6:



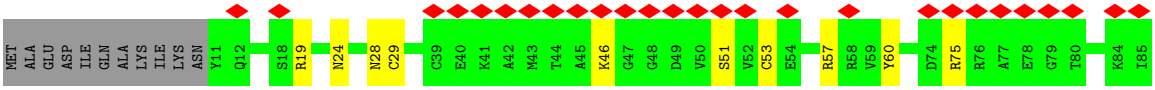
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain A4:



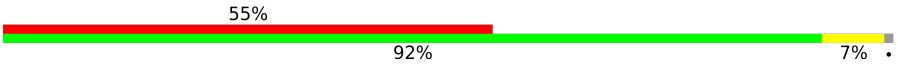
- Molecule 63: Cytochrome c oxidase subunit 6B1

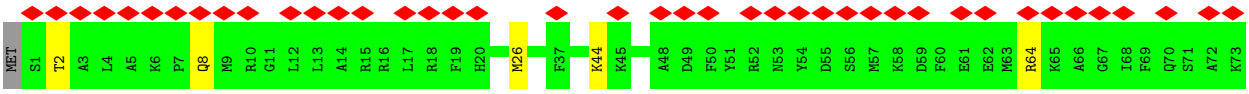
Chain A5:



- Molecule 64: Cytochrome c oxidase subunit 6C

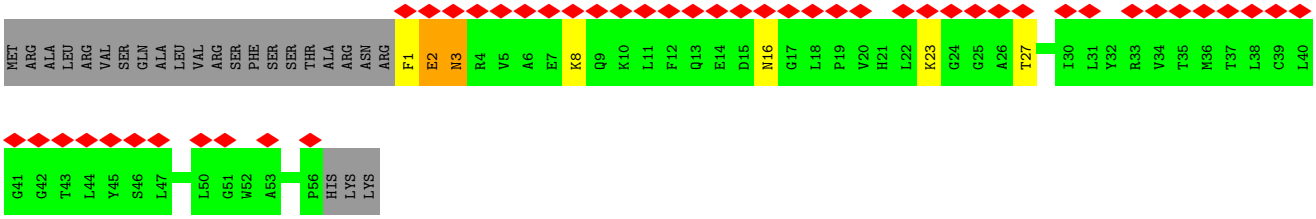
Chain B4:





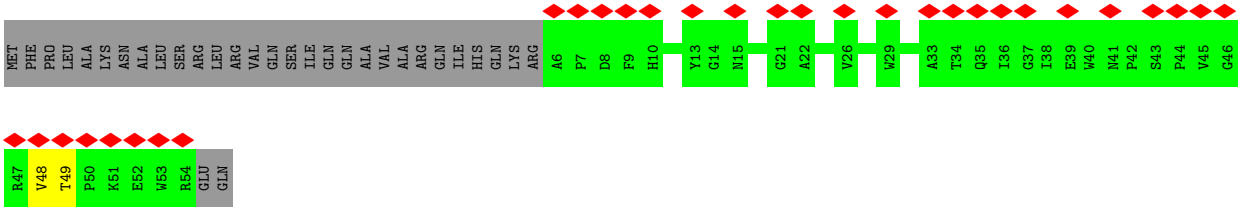
- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain C3:



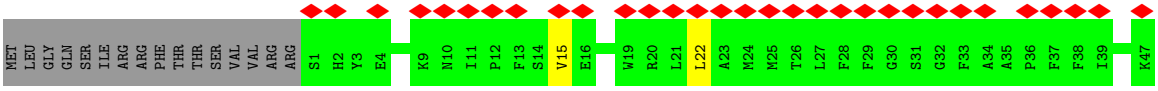
- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial

Chain B0:



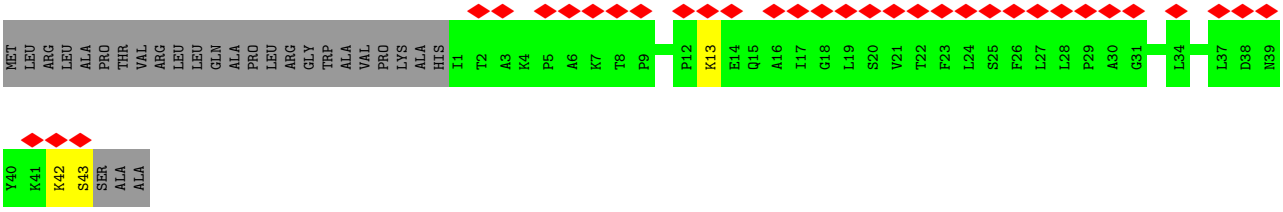
- Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial

Chain C1:



- Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial

Chain A8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.509	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 3PE, HEC, ZN, NAP, SF4, CU, FMN, FES, CDL, HEA, MG, PC1

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	9	0.50	0/1617	0.62	0/2206
2	4	0.61	1/3674 (0.0%)	0.80	4/5020 (0.1%)
3	2	0.72	1/2749 (0.0%)	0.85	0/3744
4	7	0.61	0/1271	0.74	0/1735
5	6	0.46	0/4893	0.65	1/6661 (0.0%)
6	5	0.63	0/721	0.84	2/977 (0.2%)
7	3	0.53	0/902	0.76	1/1233 (0.1%)
8	1	0.64	0/2575	0.83	3/3518 (0.1%)
9	8	0.50	0/3136	0.64	1/4258 (0.0%)
10	A	0.69	4/5304 (0.1%)	0.82	7/7193 (0.1%)
11	B	0.92	1/3512 (0.0%)	0.92	12/4763 (0.3%)
12	C	0.84	0/1777	0.78	1/2420 (0.0%)
13	D	0.95	2/1237 (0.2%)	0.87	2/1676 (0.1%)
14	E	0.96	4/1431 (0.3%)	0.98	8/1938 (0.4%)
15	F	0.33	0/191	0.82	0/262
16	G	0.78	0/1008	0.80	0/1363
17	H	0.55	0/800	0.73	0/1076
18	I	0.56	0/541	0.85	0/726
19	J	0.60	0/545	0.61	0/740
20	K	0.44	0/667	0.58	0/900
21	L	0.47	0/623	0.60	0/862
22	N	0.50	0/882	0.66	0/1203
23	O	0.54	0/948	0.67	0/1279
24	P	0.51	0/723	0.73	1/985 (0.1%)
25	Q	0.48	0/1381	0.66	0/1869
26	R	0.50	0/2465	0.69	0/3349
27	S	0.38	0/2348	0.71	1/3198 (0.0%)
28	T	0.42	0/938	0.65	0/1278
29	U	0.48	0/1053	0.72	1/1439 (0.1%)
30	V	0.53	0/1115	0.67	0/1508
31	M	0.46	0/651	0.69	1/876 (0.1%)
31	W	0.39	0/624	0.59	0/847

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	X	0.37	0/383	0.56	0/523
33	Y	0.40	0/428	0.59	0/592
34	Z	0.38	0/506	0.57	0/688
35	a	0.50	0/878	0.60	0/1195
36	b	0.52	0/1058	0.68	0/1434
37	c	0.36	0/632	0.74	2/871 (0.2%)
38	d	0.36	0/729	0.56	1/996 (0.1%)
39	f	0.38	0/1191	0.55	0/1639
40	h	0.50	0/679	0.65	0/926
41	i	0.38	0/286	0.52	0/392
42	j	0.55	0/912	0.67	1/1240 (0.1%)
43	g	0.48	0/1380	0.59	1/1872 (0.1%)
44	e	0.38	0/888	0.73	1/1234 (0.1%)
45	k	0.50	0/3527	0.60	0/4787
45	w	0.50	0/3455	0.59	0/4685
46	l	0.45	0/3192	0.55	0/4329
46	x	0.45	0/3198	0.56	2/4336 (0.0%)
47	m	0.60	0/3108	0.60	0/4252
47	y	0.60	0/3108	0.60	0/4252
48	o	0.52	0/1978	0.63	3/2684 (0.1%)
48	z	0.53	0/1965	0.62	1/2669 (0.0%)
49	A0	0.39	0/1124	0.62	0/1538
49	p	0.46	0/945	0.88	5/1288 (0.4%)
50	A1	0.53	0/935	0.53	0/1253
50	q	0.51	0/935	0.55	0/1253
51	A2	0.49	0/698	0.53	0/944
51	r	0.49	0/704	0.53	0/951
52	B3	0.36	0/571	0.59	1/765 (0.1%)
52	s	0.37	0/553	0.58	1/741 (0.1%)
53	A3	0.47	0/330	0.70	1/457 (0.2%)
53	t	0.36	0/272	0.50	0/377
54	B2	0.42	0/524	0.48	0/707
54	u	0.42	0/524	0.48	0/707
55	B1	0.50	0/149	0.95	0/203
55	v	0.44	0/114	0.94	1/156 (0.6%)
56	A9	0.60	0/4164	0.76	1/5688 (0.0%)
57	C4	0.57	0/1868	0.79	0/2544
58	C2	0.56	0/2211	0.68	0/3023
59	A7	0.57	0/1229	0.65	1/1658 (0.1%)
60	C0	0.50	0/898	0.66	0/1218
61	A6	0.56	0/765	0.81	0/1038
62	A4	0.54	0/698	0.73	1/950 (0.1%)
63	A5	0.55	0/648	0.73	0/877

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
64	B4	0.60	0/611	0.64	0/810
65	C3	0.61	0/451	0.72	0/610
66	B0	0.57	0/398	0.66	0/546
67	C1	0.63	0/399	0.62	0/534
68	A8	0.51	0/345	0.65	0/470
All	All	0.57	13/108846 (0.0%)	0.70	70/148004 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9	0	6
2	4	0	9
3	2	0	10
4	7	0	6
5	6	0	5
6	5	0	4
7	3	0	2
8	1	0	3
9	8	0	8
10	A	0	16
11	B	0	4
13	D	0	6
14	E	0	5
17	H	0	2
18	I	0	1
20	K	0	1
21	L	0	1
22	N	0	1
23	O	0	1
24	P	0	3
25	Q	0	2
26	R	0	9
27	S	0	4
29	U	0	3
30	V	0	2
31	M	0	3
31	W	0	2
34	Z	0	2
35	a	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
36	b	0	4
38	d	0	1
39	f	0	3
40	h	0	3
42	j	0	2
43	g	0	1
44	e	0	7
45	k	0	3
45	w	0	4
46	l	0	5
46	x	0	3
47	m	0	4
47	y	0	3
48	o	0	7
48	z	0	7
49	A0	0	3
49	p	0	6
53	A3	0	1
55	B1	0	5
All	All	0	194

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	135	TYR	CE1-CZ	-7.40	1.28	1.38
14	E	123	CYS	CB-SG	-6.99	1.70	1.82
14	E	116	CYS	CB-SG	-6.28	1.71	1.82
10	A	92	CYS	CB-SG	-5.91	1.72	1.81
3	2	193	VAL	CB-CG2	-5.57	1.41	1.52
13	D	163	TYR	CE2-CZ	-5.50	1.31	1.38
2	4	161	LEU	CA-C	-5.44	1.38	1.52
13	D	163	TYR	CD2-CE2	-5.41	1.31	1.39
10	A	75	CYS	CB-SG	-5.30	1.73	1.81
14	E	122	VAL	CB-CG1	-5.28	1.41	1.52
10	A	226	CYS	CB-SG	-5.28	1.73	1.81
14	E	120	GLU	CG-CD	-5.18	1.44	1.51
10	A	228	VAL	CB-CG1	-5.08	1.42	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	199	VAL	C-N-CD	-15.74	85.97	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	E	140	ARG	CG-CD-NE	8.45	129.55	111.80
10	A	139	LEU	CA-CB-CG	-8.02	96.85	115.30
14	E	118	LEU	CB-CG-CD2	-7.90	97.57	111.00
37	c	36	PRO	C-N-CD	-7.73	103.60	120.60
10	A	121	LEU	CA-CB-CG	-7.67	97.66	115.30
10	A	610	VAL	C-N-CA	-7.33	103.37	121.70
49	p	146	PRO	N-CA-CB	7.22	111.97	103.30
14	E	170	GLY	C-N-CD	-7.14	104.89	120.60
11	B	363	VAL	C-N-CA	-6.68	105.00	121.70
11	B	123	LEU	CB-CG-CD1	-6.56	99.85	111.00
59	A7	133	GLY	N-CA-C	6.43	129.19	113.10
14	E	70	LEU	CA-CB-CG	-6.25	100.93	115.30
11	B	379	ILE	CG1-CB-CG2	-6.25	97.66	111.40
49	p	82	PRO	N-CA-CB	6.17	110.71	103.30
11	B	420	TYR	N-CA-C	-6.16	94.36	111.00
11	B	309	ASP	N-CA-C	-6.13	94.44	111.00
48	o	80	MET	CA-CB-CG	6.11	123.69	113.30
11	B	82	LEU	CA-CB-CG	6.11	129.35	115.30
12	C	206	LEU	CB-CG-CD2	-6.11	100.62	111.00
11	B	218	SER	C-N-CA	-6.05	109.59	122.30
2	4	75	LEU	CB-CG-CD2	-6.04	100.72	111.00
11	B	293	LEU	N-CA-C	-6.04	94.70	111.00
31	M	42	LEU	CA-CB-CG	6.02	129.14	115.30
2	4	115	LEU	CA-CB-CG	-6.00	101.51	115.30
53	A3	15	ARG	NE-CZ-NH2	-5.99	117.30	120.30
14	E	140	ARG	CA-CB-CG	5.97	126.54	113.40
7	3	64	LEU	CA-CB-CG	-5.96	101.59	115.30
49	p	130	PRO	N-CA-CB	5.93	110.42	103.30
11	B	123	LEU	CA-CB-CG	5.89	128.86	115.30
14	E	140	ARG	CB-CG-CD	-5.89	96.29	111.60
11	B	292	MET	C-N-CA	5.89	136.42	121.70
10	A	351	LEU	CA-CB-CG	-5.86	101.81	115.30
29	U	120	THR	C-N-CD	-5.85	107.72	120.60
46	x	230	LEU	N-CA-C	5.85	126.80	111.00
49	p	120	PRO	N-CA-CB	5.71	110.15	103.30
37	c	36	PRO	C-N-CA	5.71	145.97	122.00
48	o	79	GLU	N-CA-C	5.67	126.32	111.00
8	1	146	LEU	CB-CG-CD1	-5.66	101.38	111.00
11	B	378	LEU	CA-CB-CG	-5.62	102.38	115.30
14	E	122	VAL	CB-CA-C	-5.58	100.80	111.40
5	6	562	LEU	CA-CB-CG	-5.56	102.51	115.30
6	5	16	LEU	CA-CB-CG	-5.45	102.76	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	159	PRO	N-CA-CB	5.45	109.83	103.30
10	A	381	LEU	CB-CG-CD2	-5.42	101.78	111.00
55	v	70	LEU	CA-CB-CG	5.40	127.72	115.30
10	A	381	LEU	CA-CB-CG	5.35	127.60	115.30
48	o	90	TYR	C-N-CA	-5.34	108.35	121.70
44	e	119	THR	N-CA-C	5.34	125.41	111.00
48	z	90	TYR	C-N-CA	-5.32	108.39	121.70
2	4	248	LEU	CB-CG-CD1	-5.32	101.97	111.00
13	D	172	GLY	N-CA-C	5.28	126.31	113.10
62	A4	5	LYS	N-CA-C	5.22	125.09	111.00
8	1	158	GLY	N-CA-C	5.21	126.11	113.10
42	j	22	PRO	C-N-CD	-5.20	109.15	120.60
24	P	26	LEU	CA-CB-CG	5.20	127.27	115.30
11	B	124	ILE	CG1-CB-CG2	-5.19	99.98	111.40
38	d	18	ASP	CB-CG-OD2	5.19	122.97	118.30
10	A	423	LEU	CA-CB-CG	5.18	127.21	115.30
56	A9	435	GLY	N-CA-C	5.15	125.97	113.10
6	5	12	PHE	C-N-CA	-5.12	108.91	121.70
52	s	15	ASP	CB-CG-OD1	5.10	122.89	118.30
2	4	321	LEU	CA-CB-CG	-5.09	103.59	115.30
8	1	253	GLU	C-N-CA	-5.09	108.97	121.70
13	D	193	LEU	CA-CB-CG	-5.09	103.60	115.30
43	g	27	PRO	C-N-CA	-5.06	109.04	121.70
52	B3	15	ASP	CB-CG-OD1	5.05	122.85	118.30
46	x	304	HIS	C-N-CA	5.02	134.26	121.70
14	E	86	TYR	CA-CB-CG	-5.01	103.88	113.40
9	8	120	GLY	C-N-CA	-5.01	109.18	121.70

There are no chirality outliers.

All (194) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	125	SER	Peptide
8	1	195	ARG	Peptide
8	1	66	SER	Mainchain
3	2	106	LEU	Peptide
3	2	112	HIS	Peptide
3	2	147	PRO	Peptide
3	2	193	VAL	Peptide
3	2	220	MET	Peptide
3	2	24	SER	Peptide
3	2	327	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	2	336	MET	Peptide
3	2	337	LEU	Peptide
3	2	45	MET	Peptide
7	3	42	ASP	Peptide
7	3	69	ILE	Peptide
2	4	20	ASN	Peptide
2	4	226	ALA	Peptide
2	4	306	PRO	Peptide
2	4	419	TYR	Peptide
2	4	48	ASN	Peptide
2	4	56	PHE	Peptide
2	4	60	SER	Peptide
2	4	64	PRO	Peptide
2	4	74	PRO	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
6	5	93	LEU	Peptide
5	6	30	SER	Peptide
5	6	351	ASN	Peptide
5	6	522	PHE	Peptide
5	6	64	SER	Peptide
5	6	65	ASN	Peptide
4	7	137	SER	Peptide
4	7	170	GLU	Peptide
4	7	24	PRO	Peptide
4	7	25	SER	Peptide
4	7	26	PRO	Peptide
4	7	72	THR	Peptide
9	8	102	MET	Peptide
9	8	203	ALA	Peptide
9	8	204	TYR	Peptide
9	8	208	GLU	Peptide
9	8	228	PRO	Peptide
9	8	260	ALA	Peptide
9	8	306	GLY	Peptide
9	8	404	ALA	Peptide
1	9	109	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	228	ALA	Peptide
1	9	75	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	9	91	GLY	Peptide
10	A	124	HIS	Peptide
10	A	127	ASP	Peptide
10	A	128	CYS	Peptide
10	A	143	SER	Peptide
10	A	147	GLY	Peptide
10	A	236	TYR	Peptide
10	A	253	VAL	Peptide
10	A	259	SER	Peptide
10	A	274	LEU	Peptide
10	A	308	ARG	Peptide
10	A	460	HIS	Peptide
10	A	549	GLY	Peptide
10	A	564	CYS	Peptide
10	A	689	LEU	Peptide
10	A	691	ILE	Peptide
10	A	98	LYS	Peptide
49	A0	161	HIS	Peptide
49	A0	192	MET	Peptide
49	A0	193	VAL	Peptide
53	A3	45	VAL	Peptide
11	B	219	GLY	Peptide
11	B	272	THR	Peptide
11	B	290	GLY	Peptide
11	B	309	ASP	Peptide
55	B1	58	GLN	Peptide
55	B1	61	GLY	Peptide
55	B1	63	PRO	Peptide
55	B1	70	LEU	Peptide
55	B1	71	ASN	Peptide
13	D	113	PHE	Peptide
13	D	126	ALA	Peptide
13	D	161	GLY	Peptide
13	D	184	PRO	Peptide
13	D	186	CYS	Peptide
13	D	188	PRO	Peptide
14	E	106	TYR	Peptide
14	E	107	PRO	Peptide
14	E	108	SER	Peptide
14	E	75	SER	Peptide
14	E	85	ASN	Peptide
17	H	84	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
17	H	94	PRO	Peptide
18	I	69	ILE	Peptide
20	K	40	ARG	Peptide
21	L	40	LYS	Peptide
31	M	24	LYS	Peptide
31	M	37	MET	Peptide
31	M	63	PRO	Peptide
22	N	17	CYS	Peptide
23	O	42	GLU	Peptide
24	P	109	ASP	Peptide
24	P	44	GLY	Peptide
24	P	62	GLU	Peptide
25	Q	39	PRO	Peptide
25	Q	91	TYR	Peptide
26	R	154	GLN	Peptide
26	R	221	ARG	Peptide
26	R	253	ILE	Peptide
26	R	271	TYR	Peptide
26	R	324	THR	Peptide
26	R	333	PRO	Peptide
26	R	355	ARG	Peptide
26	R	371	PRO	Peptide
26	R	78	SER	Peptide
27	S	311	GLN	Peptide
27	S	337	ASP	Peptide
27	S	66	ALA	Peptide
27	S	67	GLU	Peptide
29	U	117	LEU	Peptide
29	U	118	SER	Peptide
29	U	47	LYS	Peptide
30	V	142	TRP	Peptide
30	V	72	MET	Peptide
31	W	128	PHE	Peptide
31	W	154	VAL	Peptide
34	Z	23	LYS	Peptide
34	Z	63	PHE	Peptide
35	a	26	SER	Peptide
36	b	110	TRP	Peptide
36	b	129	PRO	Peptide
36	b	132	ASN	Peptide
36	b	134	GLU	Peptide
38	d	18	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
44	e	107	TRP	Peptide
44	e	60	GLU	Peptide
44	e	65	TYR	Peptide
44	e	79	PRO	Peptide
44	e	80	ASP	Peptide
44	e	81	ARG	Peptide
44	e	87	ASP	Peptide
39	f	109	PRO	Peptide
39	f	131	GLU	Peptide
39	f	150	ARG	Peptide
43	g	160	LYS	Peptide
40	h	133	GLY	Peptide
40	h	80	PRO	Peptide
40	h	81	ALA	Peptide
42	j	21	LEU	Peptide
42	j	54	LEU	Peptide
45	k	212	ALA	Peptide
45	k	228	VAL	Peptide
45	k	428	ILE	Peptide
46	l	227	ARG	Peptide
46	l	229	GLY	Mainchain,Peptide
46	l	231	GLY	Peptide
46	l	304	HIS	Peptide
47	m	171	ASP	Peptide
47	m	343	VAL	Mainchain
47	m	7	SER	Peptide
47	m	8	HIS	Peptide
48	o	50	HIS	Peptide
48	o	68	VAL	Peptide
48	o	69	GLU	Mainchain
48	o	78	GLY	Peptide
48	o	79	GLU	Peptide
48	o	81	PHE	Peptide
48	o	83	ARG	Peptide
49	p	116	GLN	Peptide
49	p	133	VAL	Peptide
49	p	135	LEU	Peptide
49	p	143	GLY	Peptide
49	p	76	ILE	Peptide
49	p	77	LYS	Peptide
45	w	212	ALA	Peptide
45	w	213	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
45	w	214	LYS	Mainchain
45	w	428	ILE	Peptide
46	x	227	ARG	Peptide
46	x	229	GLY	Mainchain
46	x	230	LEU	Peptide
47	y	171	ASP	Peptide
47	y	7	SER	Peptide
47	y	8	HIS	Peptide
48	z	50	HIS	Peptide
48	z	68	VAL	Peptide
48	z	69	GLU	Mainchain,Peptide
48	z	71	GLN	Peptide
48	z	78	GLY	Peptide
48	z	83	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	29
2	4	457/459 (100%)	393 (86%)	56 (12%)	8 (2%)	8	42
3	2	342/347 (99%)	283 (83%)	57 (17%)	2 (1%)	25	65
4	7	170/175 (97%)	138 (81%)	25 (15%)	7 (4%)	3	25
5	6	604/606 (100%)	517 (86%)	84 (14%)	3 (0%)	29	68
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	17	56
8	1	316/318 (99%)	255 (81%)	48 (15%)	13 (4%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	9	45
10	A	686/704 (97%)	559 (82%)	112 (16%)	15 (2%)	6	37
11	B	428/430 (100%)	343 (80%)	79 (18%)	6 (1%)	11	47
12	C	206/228 (90%)	173 (84%)	30 (15%)	3 (2%)	10	46
13	D	150/179 (84%)	121 (81%)	25 (17%)	4 (3%)	5	34
14	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	9	43
15	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	3	27
16	G	121/133 (91%)	101 (84%)	19 (16%)	1 (1%)	19	60
17	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	4	30
18	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	25
19	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	4	31
20	K	82/98 (84%)	65 (79%)	16 (20%)	1 (1%)	13	50
21	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
22	N	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
23	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	5	34
24	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
25	Q	166/171 (97%)	112 (68%)	51 (31%)	3 (2%)	8	42
26	R	315/345 (91%)	243 (77%)	65 (21%)	7 (2%)	6	37
27	S	317/320 (99%)	240 (76%)	67 (21%)	10 (3%)	4	30
28	T	136/140 (97%)	102 (75%)	15 (11%)	19 (14%)	0	4
29	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
30	V	136/143 (95%)	110 (81%)	22 (16%)	4 (3%)	4	32
31	M	78/88 (89%)	56 (72%)	19 (24%)	3 (4%)	3	27
31	W	84/88 (96%)	68 (81%)	15 (18%)	1 (1%)	13	50
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	25
33	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	8	42
34	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	5	33
35	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
36	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	22	62
37	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
38	d	105/117 (90%)	87 (83%)	15 (14%)	3 (3%)	4	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	f	165/178 (93%)	130 (79%)	33 (20%)	2 (1%)	13	50
40	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	3	27
41	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
42	j	111/120 (92%)	94 (85%)	17 (15%)	0	100	100
43	g	171/176 (97%)	141 (82%)	29 (17%)	1 (1%)	25	65
44	e	139/158 (88%)	81 (58%)	45 (32%)	13 (9%)	0	12
45	k	444/480 (92%)	407 (92%)	34 (8%)	3 (1%)	22	62
45	w	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	22	62
46	l	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	47	81
46	x	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	47	81
47	m	377/379 (100%)	348 (92%)	29 (8%)	0	100	100
47	y	377/379 (100%)	349 (93%)	28 (7%)	0	100	100
48	o	239/241 (99%)	213 (89%)	21 (9%)	5 (2%)	7	38
48	z	239/241 (99%)	213 (89%)	20 (8%)	6 (2%)	5	35
49	A0	184/196 (94%)	105 (57%)	48 (26%)	31 (17%)	0	3
49	p	147/196 (75%)	101 (69%)	33 (22%)	13 (9%)	1	12
50	A1	104/111 (94%)	91 (88%)	7 (7%)	6 (6%)	1	20
50	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
51	A2	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
51	r	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
52	B3	67/91 (74%)	59 (88%)	6 (9%)	2 (3%)	4	31
52	s	65/91 (71%)	58 (89%)	5 (8%)	2 (3%)	4	31
53	A3	37/56 (66%)	23 (62%)	10 (27%)	4 (11%)	0	8
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	4	30
54	B2	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
54	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
55	B1	20/78 (26%)	10 (50%)	7 (35%)	3 (15%)	0	4
55	v	16/78 (20%)	8 (50%)	6 (38%)	2 (12%)	0	5
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
57	C4	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
58	C2	259/261 (99%)	249 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	C0	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	A6	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	3	25
62	A4	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	19
63	A5	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	11	47
64	B4	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	C3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	3	27
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	C1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13638/14963 (91%)	11529 (84%)	1839 (14%)	270 (2%)	11	40

All (270) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	84	TRP
4	7	141	MET
4	7	171	ILE
8	1	170	GLU
8	1	174	LEU
8	1	268	MET
10	A	383	SER
10	A	461	PRO
10	A	463	SER
11	B	294	ARG
13	D	146	GLU
18	I	106	GLU
18	I	109	THR
27	S	200	PRO
27	S	276	ASP
28	T	4	THR
28	T	12	ILE
28	T	13	PRO
28	T	45	THR
28	T	46	PRO
28	T	61	PHE
28	T	63	ALA
28	T	80	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	T	96	ALA
28	T	110	ILE
30	V	143	TYR
34	Z	63	PHE
34	Z	64	VAL
40	h	81	ALA
40	h	82	VAL
44	e	42	PRO
44	e	81	ARG
44	e	82	SER
44	e	115	ASN
49	p	82	PRO
49	p	120	PRO
49	p	129	LYS
49	p	146	PRO
49	p	159	PRO
52	s	14	VAL
48	z	80	MET
49	A0	82	PRO
49	A0	95	PRO
49	A0	118	ARG
49	A0	120	PRO
49	A0	121	GLN
49	A0	150	ALA
49	A0	159	PRO
49	A0	163	SER
49	A0	175	PRO
49	A0	176	ALA
49	A0	183	PRO
50	A1	14	GLU
52	B3	14	VAL
53	A3	39	ARG
53	A3	40	LEU
56	A9	328	HIS
56	A9	508	PRO
61	A6	2	SER
61	A6	87	THR
61	A6	95	GLN
62	A4	4	ALA
62	A4	9	GLY
63	A5	46	LYS
65	C3	2	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9	75	LYS
1	9	76	ALA
2	4	21	ASN
2	4	420	THR
3	2	88	LYS
8	1	76	ILE
8	1	78	ALA
8	1	173	TRP
8	1	176	LEU
8	1	282	TYR
10	A	189	ILE
11	B	310	VAL
12	C	219	LYS
13	D	147	PRO
13	D	184	PRO
17	H	16	ARG
23	O	100	ARG
26	R	155	VAL
26	R	272	LEU
26	R	309	PRO
27	S	58	LYS
28	T	3	LYS
28	T	90	TYR
28	T	108	TYR
28	T	109	GLY
32	X	14	VAL
44	e	43	LYS
44	e	71	GLY
46	l	305	GLN
49	p	115	SER
49	p	130	PRO
55	v	65	VAL
48	z	79	GLU
49	A0	77	LYS
49	A0	81	ILE
49	A0	129	LYS
49	A0	156	TYR
49	A0	188	THR
50	A1	13	LEU
55	B1	65	VAL
62	A4	5	LYS
2	4	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	4	65	LEU
4	7	140	ALA
4	7	148	SER
4	7	170	GLU
5	6	352	ASP
7	3	82	ALA
8	1	177	PRO
9	8	235	VAL
9	8	403	ASP
10	A	129	PRO
10	A	283	GLU
10	A	541	PRO
11	B	291	VAL
11	B	293	LEU
20	K	52	PRO
25	Q	94	LEU
25	Q	121	ASP
26	R	99	ASP
27	S	280	HIS
27	S	333	GLU
28	T	78	ALA
31	W	129	GLU
43	g	126	ALA
44	e	70	THR
48	o	50	HIS
49	p	81	ILE
49	p	134	ILE
53	t	38	TRP
48	z	50	HIS
49	A0	91	TRP
49	A0	114	VAL
49	A0	154	GLY
49	A0	181	GLU
50	A1	6	VAL
53	A3	41	ILE
57	C4	104	TRP
62	A4	61	SER
8	1	71	PHE
12	C	127	ARG
13	D	103	ARG
14	E	106	TYR
14	E	107	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	G	122	SER
17	H	57	LYS
18	I	108	LYS
23	O	25	MET
26	R	325	THR
27	S	216	LYS
27	S	281	LYS
28	T	11	ASP
28	T	62	THR
30	V	26	PRO
38	d	19	PRO
38	d	39	MET
39	f	165	PRO
44	e	76	PRO
31	M	30	LEU
31	M	60	PHE
45	k	229	PRO
45	k	427	PRO
48	o	51	LEU
49	p	116	GLN
55	v	66	ALA
45	w	214	LYS
45	w	427	PRO
48	z	51	LEU
49	A0	79	SER
49	A0	85	LYS
49	A0	115	SER
49	A0	152	ASP
49	A0	178	LEU
49	A0	179	ASN
50	A1	10	SER
50	A1	12	TRP
53	A3	42	LEU
56	A9	51	ASP
1	9	150	GLU
1	9	232	THR
1	9	234	LEU
2	4	58	SER
2	4	112	ALA
8	1	316	PRO
9	8	236	PHE
9	8	282	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	8	381	GLN
10	A	563	ASP
11	B	78	SER
25	Q	32	TYR
26	R	316	ARG
27	S	334	ASP
28	T	35	VAL
28	T	77	SER
30	V	25	LEU
32	X	13	HIS
36	b	111	GLU
44	e	79	PRO
49	p	136	ILE
46	x	305	GLN
49	A0	2	HIS
49	A0	63	SER
49	A0	171	ILE
57	C4	103	GLN
65	C3	3	ASN
2	4	82	HIS
4	7	137	SER
4	7	149	TYR
5	6	65	ASN
9	8	227	PRO
9	8	387	GLU
10	A	128	CYS
10	A	188	GLU
10	A	242	PRO
15	F	86	LEU
19	J	55	SER
23	O	116	LYS
39	f	149	PRO
44	e	105	MET
48	o	49	ARG
52	s	28	GLU
48	z	49	ARG
50	A1	8	ALA
52	B3	28	GLU
56	A9	91	ASP
57	C4	158	ASP
62	A4	49	PRO
5	6	71	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	561	PRO
11	B	39	PRO
19	J	57	VAL
38	d	40	VAL
44	e	44	THR
49	A0	106	ILE
8	1	249	PRO
26	R	371	PRO
30	V	73	PRO
40	h	80	PRO
48	o	70	VAL
49	p	93	GLY
55	B1	63	PRO
55	B1	72	VAL
8	1	208	VAL
10	A	45	PRO
10	A	210	ILE
12	C	218	VAL
33	Y	90	PRO
45	k	71	PRO
45	w	71	PRO
61	A6	15	GLY
1	9	241	PRO
2	4	306	PRO
10	A	263	VAL
14	E	171	PRO
17	H	25	GLN
48	o	74	PRO
49	p	114	VAL
48	z	74	PRO
49	A0	193	VAL
1	9	216	PRO
27	S	340	ILE
44	e	78	LEU
44	e	87	ASP
31	M	27	PRO
27	S	323	PRO

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	169/183 (92%)	167 (99%)	2 (1%)	71	84
2	4	389/413 (94%)	389 (100%)	0	100	100
3	2	304/316 (96%)	302 (99%)	2 (1%)	84	90
4	7	116/142 (82%)	116 (100%)	0	100	100
5	6	524/534 (98%)	521 (99%)	3 (1%)	86	92
6	5	80/86 (93%)	80 (100%)	0	100	100
7	3	95/101 (94%)	95 (100%)	0	100	100
8	1	274/275 (100%)	255 (93%)	19 (7%)	15	42
9	8	270/353 (76%)	270 (100%)	0	100	100
10	A	560/588 (95%)	557 (100%)	3 (0%)	88	93
11	B	363/371 (98%)	356 (98%)	7 (2%)	57	75
12	C	188/204 (92%)	186 (99%)	2 (1%)	73	85
13	D	127/150 (85%)	124 (98%)	3 (2%)	49	69
14	E	148/151 (98%)	148 (100%)	0	100	100
15	F	14/69 (20%)	14 (100%)	0	100	100
16	G	106/119 (89%)	105 (99%)	1 (1%)	78	87
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	53/79 (67%)	50 (94%)	3 (6%)	20	47
19	J	50/59 (85%)	50 (100%)	0	100	100
20	K	67/81 (83%)	67 (100%)	0	100	100
21	L	63/71 (89%)	63 (100%)	0	100	100
22	N	88/101 (87%)	88 (100%)	0	100	100
23	O	95/113 (84%)	95 (100%)	0	100	100
24	P	73/96 (76%)	73 (100%)	0	100	100
25	Q	142/154 (92%)	141 (99%)	1 (1%)	84	90
26	R	232/298 (78%)	232 (100%)	0	100	100
27	S	205/283 (72%)	204 (100%)	1 (0%)	88	93
28	T	73/101 (72%)	48 (66%)	25 (34%)	0	1
29	U	95/131 (72%)	95 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	V	106/120 (88%)	106 (100%)	0	100	100
31	M	73/81 (90%)	73 (100%)	0	100	100
31	W	57/81 (70%)	55 (96%)	2 (4%)	36	60
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/76 (37%)	28 (100%)	0	100	100
35	a	70/114 (61%)	70 (100%)	0	100	100
36	b	85/124 (68%)	85 (100%)	0	100	100
37	c	45/122 (37%)	45 (100%)	0	100	100
38	d	44/107 (41%)	44 (100%)	0	100	100
39	f	80/160 (50%)	80 (100%)	0	100	100
40	h	63/112 (56%)	63 (100%)	0	100	100
41	i	23/45 (51%)	23 (100%)	0	100	100
42	j	86/106 (81%)	85 (99%)	1 (1%)	71	84
43	g	130/157 (83%)	129 (99%)	1 (1%)	81	89
44	e	44/141 (31%)	41 (93%)	3 (7%)	16	42
45	k	369/394 (94%)	369 (100%)	0	100	100
45	w	362/394 (92%)	362 (100%)	0	100	100
46	l	327/355 (92%)	327 (100%)	0	100	100
46	x	328/355 (92%)	328 (100%)	0	100	100
47	m	327/327 (100%)	327 (100%)	0	100	100
47	y	327/327 (100%)	327 (100%)	0	100	100
48	o	206/206 (100%)	206 (100%)	0	100	100
48	z	202/206 (98%)	202 (100%)	0	100	100
49	A0	64/168 (38%)	61 (95%)	3 (5%)	26	52
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	92 (96%)	4 (4%)	30	55
50	q	96/99 (97%)	96 (100%)	0	100	100
51	A2	70/72 (97%)	70 (100%)	0	100	100
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B3	66/85 (78%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	31/46 (67%)	27 (87%)	4 (13%)	4	20
53	t	24/46 (52%)	23 (96%)	1 (4%)	30	55
54	B2	52/54 (96%)	52 (100%)	0	100	100
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B1	15/60 (25%)	15 (100%)	0	100	100
55	v	11/60 (18%)	11 (100%)	0	100	100
56	A9	427/427 (100%)	389 (91%)	38 (9%)	9	33
57	C4	211/211 (100%)	191 (90%)	20 (10%)	8	29
58	C2	226/226 (100%)	199 (88%)	27 (12%)	5	22
59	A7	128/148 (86%)	120 (94%)	8 (6%)	18	44
60	C0	95/123 (77%)	89 (94%)	6 (6%)	18	44
61	A6	81/103 (79%)	76 (94%)	5 (6%)	18	45
62	A4	68/79 (86%)	50 (74%)	18 (26%)	0	4
63	A5	67/76 (88%)	58 (87%)	9 (13%)	4	20
64	B4	58/59 (98%)	53 (91%)	5 (9%)	10	35
65	C3	47/68 (69%)	40 (85%)	7 (15%)	3	16
66	B0	39/66 (59%)	37 (95%)	2 (5%)	24	50
67	C1	40/55 (73%)	38 (95%)	2 (5%)	24	51
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	37
All	All	10787/12809 (84%)	10546 (98%)	241 (2%)	54	71

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9	93	LEU
1	9	188	ILE
3	2	84	TRP
3	2	114	TRP
5	6	116	LYS
5	6	120	TYR
5	6	587	TYR
8	1	70	MET
8	1	71	PHE
8	1	77	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1	99	ASN
8	1	156	MET
8	1	157	SER
8	1	171	GLN
8	1	172	MET
8	1	174	LEU
8	1	235	ASN
8	1	236	ILE
8	1	250	HIS
8	1	251	MET
8	1	265	LEU
8	1	266	LEU
8	1	269	SER
8	1	309	ILE
8	1	317	GLN
8	1	318	THR
10	A	146	PHE
10	A	223	ILE
10	A	319	TRP
11	B	61	TRP
11	B	141	TYR
11	B	236	LEU
11	B	254	ARG
11	B	389	TYR
11	B	429	PHE
11	B	432	LEU
12	C	95	VAL
12	C	219	LYS
13	D	138	ARG
13	D	146	GLU
13	D	175	ARG
16	G	143	TRP
18	I	103	LEU
18	I	106	GLU
18	I	108	LYS
25	Q	158	LEU
27	S	327	TYR
28	T	3	LYS
28	T	6	LEU
28	T	9	TYR
28	T	10	TRP
28	T	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	T	20	ARG
28	T	22	THR
28	T	28	ILE
28	T	34	LEU
28	T	39	TYR
28	T	58	ARG
28	T	59	TYR
28	T	60	THR
28	T	66	ILE
28	T	69	ILE
28	T	72	LEU
28	T	76	ILE
28	T	77	SER
28	T	80	VAL
28	T	81	ARG
28	T	99	LEU
28	T	101	LEU
28	T	106	ARG
28	T	107	SER
28	T	108	TYR
31	W	106	LYS
31	W	108	LEU
42	j	88	HIS
43	g	79	GLU
44	e	114	ARG
44	e	118	ASP
44	e	119	THR
53	t	39	ARG
49	A0	72	SER
49	A0	73	LYS
49	A0	74	ILE
50	A1	9	SER
50	A1	10	SER
50	A1	12	TRP
50	A1	13	LEU
53	A3	39	ARG
53	A3	40	LEU
53	A3	41	ILE
53	A3	45	VAL
56	A9	18	LEU
56	A9	35	LEU
56	A9	92	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	A9	96	ARG
56	A9	105	LEU
56	A9	109	PHE
56	A9	115	SER
56	A9	138	HIS
56	A9	150	LEU
56	A9	159	LEU
56	A9	187	SER
56	A9	188	VAL
56	A9	199	LEU
56	A9	213	ARG
56	A9	238	PHE
56	A9	241	PRO
56	A9	273	MET
56	A9	295	VAL
56	A9	301	THR
56	A9	306	THR
56	A9	318	VAL
56	A9	324	LEU
56	A9	347	LEU
56	A9	353	LEU
56	A9	354	THR
56	A9	365	ILE
56	A9	369	ASP
56	A9	373	VAL
56	A9	383	MET
56	A9	417	MET
56	A9	465	VAL
56	A9	467	LEU
56	A9	474	GLU
56	A9	486	ASP
56	A9	492	LEU
56	A9	508	PRO
56	A9	509	THR
56	A9	512	ASN
57	C4	7	LEU
57	C4	31	VAL
57	C4	52	HIS
57	C4	60	GLU
57	C4	63	THR
57	C4	65	TRP
57	C4	88	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	C4	92	ASN
57	C4	113	TYR
57	C4	125	THR
57	C4	130	PRO
57	C4	134	ARG
57	C4	142	VAL
57	C4	147	GLU
57	C4	148	MET
57	C4	170	LEU
57	C4	171	LYS
57	C4	185	MET
57	C4	205	SER
57	C4	216	LEU
58	C2	1	MET
58	C2	11	VAL
58	C2	13	PRO
58	C2	14	SER
58	C2	18	LEU
58	C2	19	THR
58	C2	22	LEU
58	C2	38	ASN
58	C2	39	SER
58	C2	85	LEU
58	C2	92	LEU
58	C2	112	LEU
58	C2	127	LEU
58	C2	128	GLU
58	C2	131	LEU
58	C2	132	LEU
58	C2	137	LEU
58	C2	142	VAL
58	C2	159	MET
58	C2	160	LEU
58	C2	163	LEU
58	C2	188	ILE
58	C2	196	THR
58	C2	199	VAL
58	C2	214	PHE
58	C2	222	GLN
58	C2	258	TRP
59	A7	31	LYS
59	A7	36	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	A7	40	LEU
59	A7	59	LEU
59	A7	62	LEU
59	A7	107	ILE
59	A7	143	ASN
59	A7	147	LYS
60	C0	7	THR
60	C0	29	LEU
60	C0	70	VAL
60	C0	79	LYS
60	C0	80	GLU
60	C0	90	ARG
61	A6	37	LYS
61	A6	53	THR
61	A6	74	LEU
61	A6	95	GLN
61	A6	98	HIS
62	A4	5	LYS
62	A4	7	ASP
62	A4	8	HIS
62	A4	14	ARG
62	A4	17	ARG
62	A4	33	LEU
62	A4	34	ASN
62	A4	37	LEU
62	A4	38	HIS
62	A4	41	HIS
62	A4	42	ARG
62	A4	43	GLU
62	A4	48	ILE
62	A4	54	ARG
62	A4	56	ARG
62	A4	68	THR
62	A4	69	PHE
62	A4	78	LEU
63	A5	19	ARG
63	A5	24	ASN
63	A5	28	ASN
63	A5	29	CYS
63	A5	51	SER
63	A5	53	CYS
63	A5	57	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	A5	60	TYR
63	A5	75	ARG
64	B4	2	THR
64	B4	8	GLN
64	B4	26	MET
64	B4	44	LYS
64	B4	64	ARG
65	C3	1	PHE
65	C3	2	GLU
65	C3	3	ASN
65	C3	8	LYS
65	C3	16	ASN
65	C3	23	LYS
65	C3	27	THR
66	B0	48	VAL
66	B0	49	THR
67	C1	15	VAL
67	C1	22	LEU
68	A8	13	LYS
68	A8	42	LYS
68	A8	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	9	41	HIS
1	9	87	GLN
2	4	30	HIS
2	4	44	GLN
2	4	331	ASN
2	4	366	ASN
2	4	422	HIS
2	4	440	HIS
3	2	36	ASN
3	2	49	ASN
5	6	59	GLN
5	6	248	HIS
5	6	470	ASN
5	6	546	GLN
5	6	605	HIS
6	5	7	ASN
6	5	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1	5	ASN
8	1	169	GLN
8	1	171	GLN
8	1	230	ASN
8	1	287	HIS
8	1	317	GLN
9	8	103	ASN
9	8	168	ASN
9	8	281	HIS
9	8	393	ASN
9	8	422	HIS
10	A	282	ASN
10	A	359	ASN
10	A	460	HIS
10	A	571	HIS
10	A	572	HIS
11	B	79	ASN
11	B	160	ASN
11	B	182	ASN
11	B	183	HIS
11	B	234	GLN
11	B	349	ASN
11	B	381	HIS
12	C	230	GLN
14	E	85	ASN
14	E	204	ASN
16	G	88	GLN
16	G	92	ASN
17	H	21	GLN
17	H	82	GLN
19	J	40	HIS
21	L	71	GLN
23	O	102	HIS
24	P	52	ASN
25	Q	35	GLN
26	R	71	ASN
26	R	251	ASN
26	R	323	HIS
26	R	331	HIS
27	S	120	GLN
27	S	164	GLN
27	S	190	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	U	123	GLN
30	V	76	GLN
31	W	115	GLN
32	X	13	HIS
33	Y	86	HIS
35	a	79	ASN
37	c	83	HIS
38	d	61	HIS
38	d	92	HIS
40	h	70	ASN
40	h	74	HIS
40	h	115	GLN
41	i	62	HIS
43	g	144	HIS
31	M	35	HIS
31	M	74	GLN
45	k	61	HIS
45	k	119	ASN
45	k	207	GLN
45	k	252	HIS
45	k	323	HIS
45	k	363	ASN
46	l	31	ASN
46	l	125	ASN
46	l	254	HIS
46	l	290	ASN
46	l	354	ASN
47	m	3	ASN
47	m	8	HIS
47	m	16	ASN
47	m	32	ASN
47	m	201	HIS
47	m	374	ASN
48	o	23	HIS
49	p	53	ASN
45	w	61	HIS
45	w	207	GLN
45	w	252	HIS
45	w	323	HIS
45	w	363	ASN
46	x	31	ASN
46	x	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	x	254	HIS
46	x	290	ASN
46	x	304	HIS
46	x	354	ASN
47	y	3	ASN
47	y	8	HIS
47	y	16	ASN
47	y	32	ASN
47	y	201	HIS
47	y	374	ASN
48	z	75	ASN
49	A0	53	ASN
56	A9	11	ASN
56	A9	12	HIS
56	A9	43	GLN
56	A9	99	ASN
56	A9	170	ASN
56	A9	256	HIS
56	A9	360	ASN
56	A9	413	HIS
56	A9	512	ASN
57	C4	103	GLN
57	C4	203	ASN
58	C2	6	HIS
58	C2	12	ASN
58	C2	133	ASN
58	C2	148	HIS
58	C2	158	HIS
58	C2	207	HIS
58	C2	222	GLN
58	C2	232	HIS
59	A7	109	HIS
60	C0	34	ASN
61	A6	66	ASN
62	A4	52	HIS
63	A5	23	GLN
63	A5	24	ASN
63	A5	25	GLN
63	A5	28	ASN
63	A5	37	HIS
65	C3	3	ASN
65	C3	16	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	B0	10	HIS
66	B0	15	ASN
66	B0	41	ASN
67	C1	42	HIS
68	A8	39	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
78	HEC	z	301	48	32,50,50	2.50	5 (15%)	24,82,82	1.62	6 (25%)
71	CDL	6	701	-	63,63,99	1.08	7 (11%)	69,75,111	1.26	4 (5%)
74	SF4	A	801	10	0,12,12	-	-	-		
70	3PE	B	501	-	50,50,50	0.87	2 (4%)	53,55,55	1.34	4 (7%)
78	HEC	o	301	48	32,50,50	2.51	5 (15%)	24,82,82	1.61	6 (25%)
77	HEM	m	401	47	41,50,50	1.73	10 (24%)	45,82,82	1.45	5 (11%)
79	HEA	A9	602	56	57,67,67	1.48	6 (10%)	61,103,103	1.45	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	FES	m	403	-	0,4,4	-	-	-		
72	PC1	L	200	-	46,46,53	0.98	3 (6%)	52,54,61	1.08	2 (3%)
73	FMN	8	501	-	33,33,33	1.19	2 (6%)	48,50,50	1.62	12 (25%)
72	PC1	S	401	27	46,46,53	1.03	4 (8%)	52,54,61	1.07	2 (3%)
72	PC1	4	504	-	45,45,53	1.05	3 (6%)	51,53,61	1.13	2 (3%)
76	NAP	R	601	-	45,52,52	4.72	18 (40%)	56,80,80	1.90	7 (12%)
77	HEM	y	401	47	41,50,50	1.73	11 (26%)	45,82,82	1.45	5 (11%)
79	HEA	A9	601	56	57,67,67	1.24	6 (10%)	61,103,103	1.47	12 (19%)
72	PC1	j	201	-	38,38,53	1.15	6 (15%)	44,46,61	1.06	2 (4%)
70	3PE	4	503	-	40,40,50	0.90	3 (7%)	43,45,55	1.38	2 (4%)
74	SF4	D	301	13	0,12,12	-	-	-		
74	SF4	A	802	-	0,12,12	-	-	-		
77	HEM	m	402	47	41,50,50	1.75	12 (29%)	45,82,82	1.29	4 (8%)
77	HEM	y	402	47	41,50,50	1.74	12 (29%)	45,82,82	1.28	4 (8%)
71	CDL	J	101	-	57,57,99	1.16	7 (12%)	63,69,111	1.19	5 (7%)
69	FES	9	301	1	0,4,4	-	-	-		
72	PC1	2	402	-	45,45,53	1.02	2 (4%)	51,53,61	0.99	2 (3%)
74	SF4	E	302	14	0,12,12	-	-	-		
70	3PE	2	401	-	45,45,50	0.89	3 (6%)	48,50,55	1.08	2 (4%)
74	SF4	8	502	-	0,12,12	-	-	-		
70	3PE	4	501	-	40,40,50	1.03	2 (5%)	43,45,55	1.10	3 (6%)
69	FES	A	803	10	0,4,4	-	-	-		
71	CDL	4	502	-	81,81,99	0.98	6 (7%)	87,93,111	1.15	4 (4%)
74	SF4	E	301	14	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
78	HEC	z	301	48	-	5/10/54/54	-
71	CDL	6	701	-	-	34/74/74/110	-
74	SF4	A	801	10	-	-	0/6/5/5
70	3PE	B	501	-	-	28/54/54/54	-
78	HEC	o	301	48	-	5/10/54/54	-
77	HEM	m	401	47	-	4/12/54/54	-
79	HEA	A9	602	56	3/3/7/16	5/32/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	PC1	L	200	-	-	23/50/50/57	-
69	FES	m	403	-	-	-	0/1/1/1
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
72	PC1	S	401	27	-	30/50/50/57	-
72	PC1	4	504	-	-	23/49/49/57	-
76	NAP	R	601	-	-	14/31/67/67	0/5/5/5
77	HEM	y	401	47	-	4/12/54/54	-
79	HEA	A9	601	56	3/3/7/16	7/32/76/76	-
72	PC1	j	201	-	-	21/42/42/57	-
70	3PE	4	503	-	-	25/44/44/54	-
74	SF4	D	301	13	-	-	0/6/5/5
74	SF4	A	802	-	-	-	0/6/5/5
77	HEM	m	402	47	-	2/12/54/54	-
77	HEM	y	402	47	-	2/12/54/54	-
71	CDL	J	101	-	-	24/68/68/110	-
69	FES	9	301	1	-	-	0/1/1/1
72	PC1	2	402	-	-	30/49/49/57	-
74	SF4	E	302	14	-	-	0/6/5/5
70	3PE	2	401	-	-	20/49/49/54	-
74	SF4	8	502	-	-	-	0/6/5/5
70	3PE	4	501	-	-	29/44/44/54	-
69	FES	A	803	10	-	-	0/1/1/1
71	CDL	4	502	-	-	41/92/92/110	-
74	SF4	E	301	14	-	-	0/6/5/5

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	C2D-C1D	-15.67	1.30	1.53
76	R	601	NAP	O4D-C1D	15.38	1.62	1.41
76	R	601	NAP	O4B-C1B	15.02	1.62	1.41
78	z	301	HEC	C3C-C2C	-8.60	1.31	1.40
78	o	301	HEC	C3C-C2C	-8.54	1.31	1.40
78	o	301	HEC	C2B-C3B	-8.24	1.32	1.40
78	z	301	HEC	C2B-C3B	-8.14	1.32	1.40
76	R	601	NAP	O4D-C4D	-7.08	1.29	1.45
76	R	601	NAP	C7N-N7N	6.91	1.46	1.33
79	A9	602	HEA	C3A-C2A	-6.56	1.31	1.40
77	m	402	HEM	C3C-C2C	-6.50	1.31	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	402	HEM	C3C-C2C	-6.47	1.31	1.40
76	R	601	NAP	O4B-C4B	-6.15	1.31	1.45
77	y	401	HEM	C3C-C2C	-6.13	1.31	1.40
77	m	401	HEM	C3C-C2C	-6.12	1.31	1.40
76	R	601	NAP	C3N-C7N	4.72	1.57	1.50
78	o	301	HEC	C3D-C2D	4.68	1.51	1.37
78	z	301	HEC	C3D-C2D	4.67	1.51	1.37
76	R	601	NAP	O3D-C3D	-4.32	1.32	1.43
70	4	501	3PE	O31-C31	4.26	1.45	1.33
70	4	501	3PE	O21-C21	4.12	1.45	1.34
79	A9	602	HEA	C3A-CMA	-3.86	1.37	1.46
76	R	601	NAP	O7N-C7N	-3.67	1.17	1.24
76	R	601	NAP	O2D-C2D	3.57	1.51	1.43
79	A9	601	HEA	C3C-C2C	-3.25	1.35	1.40
77	y	401	HEM	C3D-C2D	-3.01	1.30	1.36
72	4	504	PC1	O21-C2	-2.98	1.39	1.46
76	R	601	NAP	C5A-C4A	-2.97	1.33	1.40
79	A9	601	HEA	C3A-CMA	-2.94	1.39	1.46
76	R	601	NAP	O3B-C3B	-2.94	1.36	1.43
70	B	501	3PE	O21-C2	-2.92	1.39	1.46
77	m	401	HEM	C3D-C2D	-2.91	1.30	1.36
71	6	701	CDL	OA6-CA4	-2.78	1.39	1.46
79	A9	601	HEA	C4C-NC	2.74	1.41	1.36
76	R	601	NAP	C6A-N6A	2.74	1.44	1.34
71	J	101	CDL	OB6-CB4	-2.73	1.39	1.46
71	4	502	CDL	OB8-CB7	2.73	1.41	1.33
73	8	501	FMN	C4A-N5	2.70	1.36	1.30
71	4	502	CDL	OA6-CA4	-2.69	1.39	1.46
77	y	401	HEM	C4A-CHB	-2.65	1.33	1.41
71	J	101	CDL	OA6-CA4	-2.65	1.40	1.46
70	2	401	3PE	O21-C2	-2.63	1.40	1.46
77	y	401	HEM	C3B-C2B	-2.62	1.32	1.37
79	A9	602	HEA	C3C-C2C	-2.62	1.36	1.40
77	m	401	HEM	C4A-CHB	-2.62	1.33	1.41
79	A9	602	HEA	C1D-C2D	2.62	1.49	1.44
79	A9	602	HEA	C1D-ND	-2.61	1.35	1.40
77	m	401	HEM	C3B-C2B	-2.60	1.32	1.37
77	y	402	HEM	C4A-CHB	-2.58	1.33	1.41
77	m	402	HEM	C4A-CHB	-2.58	1.33	1.41
76	R	601	NAP	C4N-C3N	-2.58	1.34	1.39
70	B	501	3PE	O31-C3	-2.57	1.39	1.45
71	J	101	CDL	OA8-CA7	2.56	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	m	401	HEM	C3C-CAC	2.55	1.53	1.47
71	4	502	CDL	OB6-CB5	2.54	1.41	1.34
70	4	503	3PE	O31-C3	-2.53	1.39	1.45
77	m	402	HEM	C3B-C2B	-2.52	1.32	1.37
77	y	401	HEM	C2A-C3A	-2.52	1.30	1.37
72	L	200	PC1	O21-C2	-2.51	1.40	1.46
72	2	402	PC1	O21-C21	2.51	1.41	1.34
77	y	402	HEM	C3C-CAC	2.51	1.52	1.47
77	m	402	HEM	C3C-CAC	2.50	1.52	1.47
77	y	402	HEM	CAB-C3B	2.50	1.54	1.47
76	R	601	NAP	PA-O5B	2.49	1.69	1.59
77	m	401	HEM	C2A-C3A	-2.49	1.30	1.37
71	4	502	CDL	OA8-CA7	2.49	1.40	1.33
77	y	402	HEM	C3B-C2B	-2.48	1.32	1.37
72	S	401	PC1	O21-C2	-2.48	1.40	1.46
72	4	504	PC1	O31-C3	-2.47	1.39	1.45
77	m	402	HEM	CAB-C3B	2.47	1.54	1.47
72	S	401	PC1	O31-C31	2.46	1.40	1.33
72	j	201	PC1	O31-C31	2.46	1.40	1.33
72	2	402	PC1	O31-C31	2.45	1.40	1.33
77	y	401	HEM	C3C-CAC	2.45	1.52	1.47
71	6	701	CDL	OA8-CA6	-2.44	1.39	1.45
77	m	401	HEM	C1A-CHA	-2.44	1.34	1.41
76	R	601	NAP	C5A-N7A	-2.44	1.30	1.39
71	6	701	CDL	OB6-CB5	2.43	1.41	1.34
77	m	402	HEM	C3D-C2D	-2.43	1.31	1.36
71	6	701	CDL	OB8-CB6	-2.42	1.39	1.45
77	y	401	HEM	C1A-CHA	-2.42	1.34	1.41
77	y	402	HEM	C3D-C2D	-2.41	1.31	1.36
77	m	401	HEM	C1B-NB	-2.40	1.36	1.40
77	m	401	HEM	CHD-C1D	-2.37	1.34	1.41
77	y	401	HEM	CHD-C1D	-2.36	1.34	1.41
79	A9	602	HEA	CMD-C2D	2.36	1.55	1.50
77	m	402	HEM	C2A-C3A	-2.34	1.30	1.37
77	y	402	HEM	C2A-C3A	-2.34	1.30	1.37
77	y	401	HEM	C1B-NB	-2.32	1.36	1.40
71	J	101	CDL	OB8-CB7	2.32	1.40	1.33
77	m	402	HEM	CHC-C4B	-2.31	1.34	1.41
72	j	201	PC1	O21-C21	2.31	1.40	1.34
72	L	200	PC1	O31-C3	-2.30	1.39	1.45
70	2	401	3PE	O31-C31	2.30	1.40	1.33
77	y	402	HEM	CHC-C4B	-2.28	1.34	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	j	201	PC1	O21-C2	-2.25	1.41	1.46
78	o	301	HEC	C4D-CHA	-2.24	1.34	1.41
77	m	402	HEM	C1B-NB	-2.22	1.36	1.40
77	y	402	HEM	C1B-NB	-2.21	1.36	1.40
71	J	101	CDL	OB8-CB6	-2.20	1.40	1.45
78	z	301	HEC	C4D-CHA	-2.20	1.34	1.41
70	4	503	3PE	O21-C21	2.19	1.40	1.34
71	6	701	CDL	OA8-CA7	2.18	1.39	1.33
71	J	101	CDL	OB6-CB5	2.17	1.40	1.34
71	J	101	CDL	OA6-CA5	2.17	1.40	1.34
72	S	401	PC1	O31-C3	-2.16	1.40	1.45
78	z	301	HEC	C2A-C3A	-2.16	1.31	1.37
78	o	301	HEC	C2A-C3A	-2.16	1.31	1.37
77	m	402	HEM	CHD-C1D	-2.15	1.34	1.41
77	m	402	HEM	C1A-CHA	-2.15	1.35	1.41
73	8	501	FMN	C4A-C10	-2.15	1.37	1.44
77	m	402	HEM	C4D-ND	-2.14	1.36	1.40
72	j	201	PC1	O31-C3	-2.14	1.40	1.45
77	m	401	HEM	CAB-C3B	2.14	1.53	1.47
77	y	402	HEM	CHD-C1D	-2.13	1.34	1.41
77	y	402	HEM	C1A-CHA	-2.12	1.35	1.41
72	S	401	PC1	O21-C21	2.12	1.40	1.34
77	y	401	HEM	CAB-C3B	2.12	1.53	1.47
72	4	504	PC1	O31-C31	2.12	1.39	1.33
79	A9	601	HEA	C3A-C2A	-2.11	1.37	1.40
79	A9	601	HEA	C1C-NC	2.11	1.40	1.36
76	R	601	NAP	P2B-O2B	2.11	1.63	1.59
70	2	401	3PE	O31-C3	-2.11	1.40	1.45
72	L	200	PC1	O21-C21	2.10	1.40	1.34
71	4	502	CDL	OA8-CA6	-2.09	1.40	1.45
71	4	502	CDL	OA6-CA5	2.09	1.40	1.34
72	j	201	PC1	C12-N	-2.07	1.44	1.51
76	R	601	NAP	C2A-N3A	2.07	1.35	1.32
79	A9	601	HEA	CHD-C1D	2.07	1.40	1.35
77	y	402	HEM	C4D-ND	-2.05	1.36	1.40
72	j	201	PC1	C13-N	-2.04	1.44	1.50
71	6	701	CDL	OB6-CB4	-2.03	1.41	1.46
71	6	701	CDL	OA6-CA5	2.02	1.40	1.34
70	4	503	3PE	O21-C2	-2.02	1.41	1.46
77	y	401	HEM	C4D-ND	-2.02	1.36	1.40

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	R	601	NAP	C5A-C6A-N6A	7.64	131.96	120.35
76	R	601	NAP	N3A-C2A-N1A	-6.43	118.62	128.68
76	R	601	NAP	N6A-C6A-N1A	-5.97	106.17	118.57
70	B	501	3PE	O21-C21-C22	5.41	123.16	111.50
70	4	503	3PE	O21-C21-C22	5.12	122.53	111.50
71	6	701	CDL	OB6-CB5-C51	4.63	121.49	111.50
77	y	401	HEM	CBA-CAA-C2A	-4.46	105.01	112.62
77	m	401	HEM	CBA-CAA-C2A	-4.44	105.04	112.62
71	J	101	CDL	OA6-CA5-C11	4.43	121.04	111.50
71	4	502	CDL	OA6-CA5-C11	4.15	120.44	111.50
72	S	401	PC1	O21-C21-C22	4.13	120.39	111.50
71	6	701	CDL	OA6-CA5-C11	4.10	120.33	111.50
77	y	402	HEM	CBA-CAA-C2A	-4.10	105.63	112.62
77	m	402	HEM	CBA-CAA-C2A	-4.07	105.67	112.62
72	4	504	PC1	O21-C21-C22	4.06	120.25	111.50
70	4	501	3PE	O21-C21-C22	4.02	120.16	111.50
73	8	501	FMN	C4-N3-C2	-3.98	118.29	125.64
79	A9	601	HEA	C17-C18-C19	-3.97	118.09	127.66
76	R	601	NAP	C1B-N9A-C4A	-3.93	119.74	126.64
77	m	401	HEM	CAD-CBD-CGD	-3.89	105.23	113.60
77	y	401	HEM	CAD-CBD-CGD	-3.85	105.31	113.60
71	4	502	CDL	OB6-CB5-C51	3.81	119.70	111.50
72	L	200	PC1	O21-C21-C22	3.75	119.59	111.50
70	2	401	3PE	O21-C21-C22	3.63	119.32	111.50
79	A9	602	HEA	C4A-CHB-C1B	3.59	127.29	122.56
78	z	301	HEC	CMC-C2C-C1C	-3.54	123.02	128.46
78	o	301	HEC	CMC-C2C-C1C	-3.53	123.03	128.46
72	2	402	PC1	O21-C21-C22	3.45	118.94	111.50
71	J	101	CDL	OB6-CB5-C51	3.44	118.92	111.50
72	j	201	PC1	O21-C21-C22	3.37	120.20	110.80
70	B	501	3PE	O31-C31-C32	3.28	122.21	111.91
79	A9	601	HEA	C13-C14-C15	-3.18	120.00	127.66
73	8	501	FMN	C4A-C10-N10	3.10	121.02	116.48
73	8	501	FMN	C4A-C10-N1	-3.09	117.55	124.73
73	8	501	FMN	C5A-C9A-N10	3.09	121.15	117.95
71	4	502	CDL	OB8-CB7-C71	3.05	121.49	111.91
77	y	401	HEM	CMC-C2C-C3C	3.04	130.36	124.68
73	8	501	FMN	O4-C4-C4A	-3.03	118.56	126.60
77	m	401	HEM	CBD-CAD-C3D	-3.03	104.21	112.63
77	m	401	HEM	CMC-C2C-C3C	3.03	130.35	124.68
77	m	402	HEM	CAA-CBA-CGA	-3.02	105.30	113.76
77	y	402	HEM	CAA-CBA-CGA	-3.01	105.32	113.76
77	y	401	HEM	CBD-CAD-C3D	-3.00	104.28	112.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	y	402	HEM	CMC-C2C-C3C	2.96	130.22	124.68
77	m	402	HEM	CMC-C2C-C3C	2.92	130.15	124.68
76	R	601	NAP	PN-O3-PA	-2.90	122.87	132.83
72	4	504	PC1	O31-C31-C32	2.88	120.94	111.91
71	4	502	CDL	OA8-CA7-C31	2.88	120.93	111.91
71	J	101	CDL	OA8-CA7-C31	2.87	120.92	111.91
79	A9	602	HEA	CBA-CAA-C2A	2.85	117.40	112.60
73	8	501	FMN	C4A-C4-N3	2.84	120.41	113.19
78	o	301	HEC	CBD-CAD-C3D	-2.81	107.82	112.62
79	A9	601	HEA	C1B-C2B-C3B	2.81	110.16	106.80
71	6	701	CDL	OA8-CA7-C31	2.81	120.72	111.91
78	z	301	HEC	CBD-CAD-C3D	-2.79	107.86	112.62
72	j	201	PC1	O31-C31-C32	2.78	120.65	111.91
78	z	301	HEC	C1D-C2D-C3D	-2.78	105.06	107.00
72	S	401	PC1	O31-C31-C32	2.72	120.44	111.91
78	o	301	HEC	C1D-C2D-C3D	-2.72	105.11	107.00
71	J	101	CDL	OB8-CB7-C71	2.71	120.41	111.91
71	6	701	CDL	OB8-CB7-C71	2.70	120.39	111.91
73	8	501	FMN	C4-C4A-C10	2.67	121.28	116.79
77	m	402	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
77	y	402	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
78	o	301	HEC	CBA-CAA-C2A	-2.64	108.16	112.60
70	4	501	3PE	O31-C31-C32	2.63	120.17	111.91
70	2	401	3PE	O31-C31-C32	2.61	120.10	111.91
72	2	402	PC1	O31-C31-C32	2.61	120.09	111.91
78	z	301	HEC	CBA-CAA-C2A	-2.61	108.21	112.60
79	A9	602	HEA	CMD-C2D-C1D	2.57	128.95	125.04
79	A9	602	HEA	C4D-CHA-C1A	2.53	125.89	122.56
70	4	501	3PE	C2-O21-C21	-2.45	111.76	117.79
79	A9	602	HEA	CMC-C2C-C3C	2.42	129.22	124.68
79	A9	602	HEA	C1D-C2D-C3D	-2.42	104.41	106.96
70	4	503	3PE	C23-C22-C21	-2.41	104.84	113.62
79	A9	601	HEA	C17-C16-C15	-2.41	105.06	112.98
79	A9	601	HEA	C20-C19-C18	2.35	125.88	121.12
79	A9	602	HEA	CMB-C2B-C3B	-2.35	125.86	130.34
79	A9	601	HEA	C16-C17-C18	-2.34	104.19	111.88
76	R	601	NAP	C2N-C3N-C4N	2.34	120.91	118.26
73	8	501	FMN	O2'-C2'-C3'	-2.32	103.45	109.10
73	8	501	FMN	C10-N1-C2	2.32	121.55	116.90
79	A9	602	HEA	C13-C14-C15	-2.32	122.08	127.66
77	m	401	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
79	A9	601	HEA	CAD-C3D-C4D	2.31	128.69	124.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	A9	602	HEA	C25-C23-C24	2.29	119.67	114.60
77	y	401	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
70	B	501	3PE	O31-C31-O32	-2.26	117.89	123.59
70	B	501	3PE	C23-C22-C21	-2.26	105.42	113.62
73	8	501	FMN	C4'-C3'-C2'	-2.25	108.68	113.36
71	J	101	CDL	CA4-OA6-CA5	-2.24	112.27	117.79
73	8	501	FMN	C9A-N10-C10	-2.22	117.31	120.77
78	o	301	HEC	CAD-CBD-CGD	-2.21	107.57	113.76
78	z	301	HEC	CAD-CBD-CGD	-2.21	107.57	113.76
79	A9	602	HEA	C26-C15-C16	2.20	118.97	115.27
79	A9	601	HEA	C4A-CHB-C1B	2.20	125.45	122.56
79	A9	601	HEA	C12-C13-C14	-2.18	106.49	112.23
79	A9	601	HEA	C4B-C3B-C2B	-2.16	103.73	107.41
73	8	501	FMN	C6-C5A-C9A	2.10	121.90	118.94
76	R	601	NAP	O3B-C3B-C2B	-2.08	105.27	111.17
79	A9	601	HEA	C27-C19-C18	-2.07	118.36	123.68
78	z	301	HEC	CMB-C2B-C1B	-2.07	125.29	128.46
79	A9	602	HEA	CBD-CAD-C3D	2.06	118.34	112.63
78	o	301	HEC	CMB-C2B-C1B	-2.05	125.32	128.46
79	A9	601	HEA	C3C-C4C-NC	2.04	111.85	109.21
72	L	200	PC1	O31-C31-C32	2.04	118.30	111.91

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	A9	601	HEA	NB
79	A9	601	HEA	NA
79	A9	601	HEA	ND
79	A9	602	HEA	NB
79	A9	602	HEA	NA
79	A9	602	HEA	ND

All (385) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	4	501	3PE	C11-O13-P-O11
70	4	501	3PE	C11-O13-P-O12
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	O13-C11-C12-N
70	4	501	3PE	C22-C21-O21-C2
70	4	503	3PE	C11-O13-P-O14
70	4	503	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	2	401	3PE	C11-O13-P-O12
70	2	401	3PE	C11-O13-P-O14
70	2	401	3PE	O13-C11-C12-N
70	B	501	3PE	C1-O11-P-O14
70	B	501	3PE	O22-C21-O21-C2
70	B	501	3PE	C22-C21-O21-C2
71	4	502	CDL	CA2-OA2-PA1-OA3
71	6	701	CDL	CA3-OA5-PA1-OA4
71	6	701	CDL	CB2-OB2-PB2-OB3
71	6	701	CDL	CB2-OB2-PB2-OB4
71	6	701	CDL	CB3-OB5-PB2-OB3
71	J	101	CDL	CA2-OA2-PA1-OA3
71	J	101	CDL	CA2-OA2-PA1-OA5
71	J	101	CDL	C11-CA5-OA6-CA4
71	J	101	CDL	CB2-OB2-PB2-OB3
71	J	101	CDL	CB2-OB2-PB2-OB4
71	J	101	CDL	OB5-CB3-CB4-OB6
72	4	504	PC1	C11-O13-P-O12
72	4	504	PC1	C1-O11-P-O12
72	4	504	PC1	C1-O11-P-O13
72	4	504	PC1	O13-C11-C12-N
72	4	504	PC1	C22-C21-O21-C2
72	2	402	PC1	C1-O11-P-O12
72	2	402	PC1	C1-O11-P-O14
72	L	200	PC1	C22-C21-O21-C2
72	S	401	PC1	C11-O13-P-O12
72	S	401	PC1	C11-O13-P-O14
72	S	401	PC1	O13-C11-C12-N
72	j	201	PC1	C11-O13-P-O12
72	j	201	PC1	C1-O11-P-O13
72	j	201	PC1	O13-C11-C12-N
72	j	201	PC1	O22-C21-O21-C2
72	j	201	PC1	C22-C21-O21-C2
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	O4'-C4'-C5'-O5'
73	8	501	FMN	C5'-O5'-P-O1P
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P
76	R	601	NAP	C5B-O5B-PA-O2A
76	R	601	NAP	C5B-O5B-PA-O3
76	R	601	NAP	C1B-C2B-O2B-P2B
76	R	601	NAP	C5D-O5D-PN-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
76	R	601	NAP	C5D-O5D-PN-O1N
76	R	601	NAP	C5D-O5D-PN-O2N
76	R	601	NAP	C2D-C1D-N1N-C2N
76	R	601	NAP	C2D-C1D-N1N-C6N
79	A9	601	HEA	C12-C11-C3B-C2B
70	2	401	3PE	O32-C31-O31-C3
71	4	502	CDL	OA9-CA7-OA8-CA6
71	6	701	CDL	OA9-CA7-OA8-CA6
70	2	401	3PE	C32-C31-O31-C3
71	6	701	CDL	C31-CA7-OA8-CA6
71	4	502	CDL	OB9-CB7-OB8-CB6
70	4	501	3PE	O22-C21-O21-C2
71	J	101	CDL	OA7-CA5-OA6-CA4
72	4	504	PC1	O22-C21-O21-C2
72	2	402	PC1	O22-C21-O21-C2
72	L	200	PC1	O22-C21-O21-C2
71	4	502	CDL	C31-CA7-OA8-CA6
71	J	101	CDL	OA9-CA7-OA8-CA6
71	4	502	CDL	C71-CB7-OB8-CB6
71	J	101	CDL	C71-CB7-OB8-CB6
70	4	503	3PE	O22-C21-O21-C2
71	J	101	CDL	OB9-CB7-OB8-CB6
70	4	501	3PE	C32-C31-O31-C3
72	2	402	PC1	C22-C21-O21-C2
76	R	601	NAP	O4D-C4D-C5D-O5D
71	J	101	CDL	C31-CA7-OA8-CA6
70	4	503	3PE	C2-C1-O11-P
72	2	402	PC1	C36-C37-C38-C39
72	2	402	PC1	C26-C27-C28-C29
79	A9	601	HEA	C15-C16-C17-C18
72	S	401	PC1	C23-C24-C25-C26
70	4	501	3PE	C2E-C2F-C2G-C2H
70	4	501	3PE	O32-C31-O31-C3
72	2	402	PC1	C32-C33-C34-C35
72	4	504	PC1	C32-C31-O31-C3
72	L	200	PC1	C32-C31-O31-C3
72	j	201	PC1	C32-C31-O31-C3
72	L	200	PC1	C34-C35-C36-C37
71	4	502	CDL	C12-C13-C14-C15
72	S	401	PC1	C3B-C3C-C3D-C3E
72	2	402	PC1	C21-C22-C23-C24
72	j	201	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
72	L	200	PC1	C21-C22-C23-C24
70	4	503	3PE	C2B-C2C-C2D-C2E
70	4	503	3PE	C31-C32-C33-C34
70	2	401	3PE	C31-C32-C33-C34
72	4	504	PC1	C21-C22-C23-C24
77	m	401	HEM	C3D-CAD-CBD-CGD
77	y	401	HEM	C3D-CAD-CBD-CGD
70	4	501	3PE	C33-C34-C35-C36
72	4	504	PC1	O32-C31-O31-C3
71	6	701	CDL	C32-C33-C34-C35
71	J	101	CDL	CA7-C31-C32-C33
72	4	504	PC1	C24-C25-C26-C27
72	L	200	PC1	O32-C31-O31-C3
70	4	503	3PE	C1-O11-P-O13
70	2	401	3PE	C11-O13-P-O11
70	B	501	3PE	C1-O11-P-O13
71	4	502	CDL	CB2-OB2-PB2-OB5
71	6	701	CDL	CB2-OB2-PB2-OB5
71	6	701	CDL	CB3-OB5-PB2-OB2
71	J	101	CDL	CB2-OB2-PB2-OB5
72	2	402	PC1	C1-O11-P-O13
72	S	401	PC1	C11-O13-P-O11
72	j	201	PC1	C11-O13-P-O11
70	4	503	3PE	C27-C28-C29-C2A
70	4	501	3PE	C21-C22-C23-C24
71	6	701	CDL	OB7-CB5-OB6-CB4
72	S	401	PC1	C34-C35-C36-C37
71	6	701	CDL	C51-CB5-OB6-CB4
72	S	401	PC1	C22-C21-O21-C2
70	4	501	3PE	C2C-C2D-C2E-C2F
70	4	503	3PE	C2E-C2F-C2G-C2H
70	B	501	3PE	C2B-C2C-C2D-C2E
71	4	502	CDL	C60-C61-C62-C63
72	4	504	PC1	C26-C27-C28-C29
72	L	200	PC1	C3C-C3D-C3E-C3F
70	4	501	3PE	C27-C28-C29-C2A
70	B	501	3PE	C2A-C2B-C2C-C2D
72	L	200	PC1	C3B-C3C-C3D-C3E
72	S	401	PC1	C24-C25-C26-C27
72	j	201	PC1	C3B-C3C-C3D-C3E
72	S	401	PC1	O22-C21-O21-C2
72	j	201	PC1	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	J	101	CDL	C14-C15-C16-C17
71	4	502	CDL	O1-C1-CA2-OA2
71	4	502	CDL	C13-C14-C15-C16
71	4	502	CDL	C11-C12-C13-C14
72	j	201	PC1	C3D-C3E-C3F-C3G
72	2	402	PC1	C2C-C2D-C2E-C2F
70	B	501	3PE	C35-C36-C37-C38
72	S	401	PC1	C37-C38-C39-C3A
70	B	501	3PE	C37-C38-C39-C3A
70	4	501	3PE	C32-C33-C34-C35
70	4	503	3PE	C23-C24-C25-C26
70	2	401	3PE	C35-C36-C37-C38
72	S	401	PC1	C32-C31-O31-C3
70	2	401	3PE	C22-C23-C24-C25
70	B	501	3PE	C39-C3A-C3B-C3C
71	J	101	CDL	C15-C16-C17-C18
72	2	402	PC1	C28-C29-C2A-C2B
72	j	201	PC1	C33-C34-C35-C36
70	4	503	3PE	C2A-C2B-C2C-C2D
70	4	503	3PE	C2C-C2D-C2E-C2F
70	4	503	3PE	C32-C31-O31-C3
72	S	401	PC1	C35-C36-C37-C38
71	4	502	CDL	C81-C82-C83-C84
72	L	200	PC1	C3A-C3B-C3C-C3D
72	j	201	PC1	C31-C32-C33-C34
70	2	401	3PE	C28-C29-C2A-C2B
70	B	501	3PE	C28-C29-C2A-C2B
71	4	502	CDL	CA5-C11-C12-C13
70	B	501	3PE	C2D-C2E-C2F-C2G
72	L	200	PC1	C32-C33-C34-C35
72	4	504	PC1	C33-C34-C35-C36
72	2	402	PC1	C23-C24-C25-C26
72	L	200	PC1	C22-C23-C24-C25
72	L	200	PC1	C11-C12-N-C13
71	6	701	CDL	C11-CA5-OA6-CA4
72	4	504	PC1	C27-C28-C29-C2A
72	2	402	PC1	C22-C23-C24-C25
70	4	501	3PE	C25-C26-C27-C28
70	4	503	3PE	O32-C31-O31-C3
72	S	401	PC1	O32-C31-O31-C3
70	4	503	3PE	C21-C22-C23-C24
71	6	701	CDL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	J	101	CDL	CB5-C51-C52-C53
70	2	401	3PE	C22-C21-O21-C2
70	B	501	3PE	O11-C1-C2-O21
72	L	200	PC1	O11-C1-C2-O21
70	B	501	3PE	C23-C24-C25-C26
70	2	401	3PE	O22-C21-O21-C2
72	L	200	PC1	C11-C12-N-C14
72	L	200	PC1	C11-C12-N-C15
72	2	402	PC1	C25-C26-C27-C28
71	4	502	CDL	C31-C32-C33-C34
71	6	701	CDL	OA7-CA5-OA6-CA4
71	4	502	CDL	C51-CB5-OB6-CB4
70	2	401	3PE	C2D-C2E-C2F-C2G
71	4	502	CDL	CA2-OA2-PA1-OA5
71	6	701	CDL	CA3-OA5-PA1-OA2
72	4	504	PC1	C11-O13-P-O11
72	2	402	PC1	C11-O13-P-O11
71	4	502	CDL	C76-C77-C78-C79
77	m	401	HEM	C2A-CAA-CBA-CGA
77	y	401	HEM	C2A-CAA-CBA-CGA
70	4	501	3PE	C1-C2-C3-O31
71	6	701	CDL	C34-C35-C36-C37
72	4	504	PC1	C1-C2-C3-O31
70	2	401	3PE	C3A-C3B-C3C-C3D
70	B	501	3PE	C3B-C3C-C3D-C3E
72	4	504	PC1	C2A-C2B-C2C-C2D
70	4	503	3PE	C35-C36-C37-C38
70	2	401	3PE	C34-C35-C36-C37
70	4	503	3PE	C33-C34-C35-C36
72	2	402	PC1	C24-C25-C26-C27
70	4	501	3PE	C3-C2-O21-C21
70	2	401	3PE	C36-C37-C38-C39
71	J	101	CDL	C51-C52-C53-C54
71	4	502	CDL	OB6-CB4-CB6-OB8
71	4	502	CDL	C59-C60-C61-C62
71	4	502	CDL	OB7-CB5-OB6-CB4
71	6	701	CDL	C72-C73-C74-C75
70	4	501	3PE	C2F-C2G-C2H-C2I
70	4	501	3PE	O11-C1-C2-C3
70	B	501	3PE	O11-C1-C2-C3
71	J	101	CDL	OB5-CB3-CB4-CB6
72	L	200	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	B	501	3PE	C38-C39-C3A-C3B
71	4	502	CDL	C57-C58-C59-C60
73	8	501	FMN	C2'-C1'-N10-C10
70	B	501	3PE	C3C-C3D-C3E-C3F
72	L	200	PC1	C1-C2-C3-O31
71	6	701	CDL	CA5-C11-C12-C13
72	2	402	PC1	C39-C3A-C3B-C3C
72	S	401	PC1	C3C-C3D-C3E-C3F
72	L	200	PC1	O31-C31-C32-C33
71	J	101	CDL	OA5-CA3-CA4-OA6
71	4	502	CDL	OA6-CA4-CA6-OA8
72	L	200	PC1	O21-C2-C3-O31
72	S	401	PC1	O21-C2-C3-O31
71	6	701	CDL	C51-C52-C53-C54
71	4	502	CDL	OA7-CA5-OA6-CA4
72	2	402	PC1	C37-C38-C39-C3A
71	4	502	CDL	C11-CA5-OA6-CA4
76	R	601	NAP	PN-O3-PA-O5B
72	S	401	PC1	O11-C1-C2-C3
72	4	504	PC1	C2B-C2C-C2D-C2E
76	R	601	NAP	C3D-C4D-C5D-O5D
70	4	503	3PE	C24-C25-C26-C27
70	B	501	3PE	C3A-C3B-C3C-C3D
70	4	503	3PE	C1-C2-O21-C21
71	6	701	CDL	C71-C72-C73-C74
72	2	402	PC1	C32-C31-O31-C3
70	4	501	3PE	C26-C27-C28-C29
72	S	401	PC1	O11-C1-C2-O21
72	j	201	PC1	O11-C1-C2-O21
70	4	501	3PE	O21-C2-C3-O31
70	2	401	3PE	O21-C2-C3-O31
76	R	601	NAP	C2B-O2B-P2B-O3X
71	4	502	CDL	C34-C35-C36-C37
70	4	503	3PE	C11-O13-P-O11
70	2	401	3PE	C2E-C2F-C2G-C2H
71	6	701	CDL	C1-CA2-OA2-PA1
72	4	504	PC1	C2-C1-O11-P
70	4	503	3PE	C1-O11-P-O12
70	4	503	3PE	C1-O11-P-O14
70	B	501	3PE	C1-O11-P-O12
71	4	502	CDL	CA2-OA2-PA1-OA4
71	4	502	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	6	701	CDL	CA2-OA2-PA1-OA3
71	6	701	CDL	CA3-OA5-PA1-OA3
71	J	101	CDL	CA3-OA5-PA1-OA4
72	4	504	PC1	C11-O13-P-O14
72	4	504	PC1	C1-O11-P-O14
72	2	402	PC1	C11-O13-P-O12
72	j	201	PC1	C11-O13-P-O14
72	j	201	PC1	C1-O11-P-O12
76	R	601	NAP	C5B-O5B-PA-O1A
71	4	502	CDL	OB5-CB3-CB4-CB6
72	j	201	PC1	C12-C11-O13-P
73	8	501	FMN	C1'-C2'-C3'-O3'
72	2	402	PC1	C38-C39-C3A-C3B
72	L	200	PC1	C26-C27-C28-C29
70	4	501	3PE	O11-C1-C2-O21
70	B	501	3PE	C24-C25-C26-C27
71	4	502	CDL	CB3-CB4-CB6-OB8
72	2	402	PC1	O13-C11-C12-N
72	L	200	PC1	O13-C11-C12-N
72	S	401	PC1	C1-C2-C3-O31
72	4	504	PC1	O21-C2-C3-O31
72	S	401	PC1	C32-C33-C34-C35
70	2	401	3PE	O21-C21-C22-C23
70	B	501	3PE	C2C-C2D-C2E-C2F
72	2	402	PC1	O32-C31-O31-C3
71	4	502	CDL	C63-C64-C65-C66
70	B	501	3PE	C29-C2A-C2B-C2C
71	4	502	CDL	C77-C78-C79-C80
71	J	101	CDL	OA5-CA3-CA4-CA6
72	j	201	PC1	C38-C39-C3A-C3B
70	4	501	3PE	C29-C2A-C2B-C2C
71	J	101	CDL	CB3-OB5-PB2-OB2
72	S	401	PC1	C1-O11-P-O13
72	j	201	PC1	C3F-C3G-C3H-C3I
71	6	701	CDL	CA4-CA3-OA5-PA1
72	2	402	PC1	C31-C32-C33-C34
70	B	501	3PE	C31-C32-C33-C34
78	o	301	HEC	C3D-CAD-CBD-CGD
78	z	301	HEC	C3D-CAD-CBD-CGD
71	4	502	CDL	CA2-C1-CB2-OB2
79	A9	601	HEA	CAD-CBD-CGD-O1D
71	4	502	CDL	CB3-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
71	6	701	CDL	CB3-CB4-OB6-CB5
72	2	402	PC1	C1-C2-O21-C21
72	4	504	PC1	C38-C39-C3A-C3B
71	4	502	CDL	C71-C72-C73-C74
73	8	501	FMN	C3'-C4'-C5'-O5'
70	B	501	3PE	C26-C27-C28-C29
72	j	201	PC1	O11-C1-C2-C3
79	A9	602	HEA	CAD-CBD-CGD-O1D
71	6	701	CDL	O1-C1-CB2-OB2
71	6	701	CDL	OA6-CA4-CA6-OA8
79	A9	602	HEA	CAD-CBD-CGD-O2D
71	4	502	CDL	CB2-C1-CA2-OA2
71	J	101	CDL	CA2-C1-CB2-OB2
79	A9	601	HEA	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O2D
70	4	503	3PE	C22-C23-C24-C25
78	o	301	HEC	CAD-CBD-CGD-O2D
78	z	301	HEC	CAD-CBD-CGD-O2D
70	2	401	3PE	C21-C22-C23-C24
72	S	401	PC1	C28-C29-C2A-C2B
72	2	402	PC1	C29-C2A-C2B-C2C
72	S	401	PC1	C21-C22-C23-C24
70	B	501	3PE	C32-C33-C34-C35
70	4	501	3PE	O31-C31-C32-C33
71	6	701	CDL	C72-C71-CB7-OB8
72	L	200	PC1	O32-C31-C32-C33
71	6	701	CDL	C15-C16-C17-C18
78	o	301	HEC	CAA-CBA-CGA-O1A
78	z	301	HEC	CAA-CBA-CGA-O1A
77	m	402	HEM	CAA-CBA-CGA-O1A
77	y	402	HEM	CAA-CBA-CGA-O1A
71	4	502	CDL	C12-C11-CA5-OA6
71	4	502	CDL	OB5-CB3-CB4-OB6
72	2	402	PC1	C2D-C2E-C2F-C2G
70	B	501	3PE	O31-C31-C32-C33
78	o	301	HEC	CAA-CBA-CGA-O2A
78	z	301	HEC	CAA-CBA-CGA-O2A
79	A9	602	HEA	CAA-CBA-CGA-O2A
71	6	701	CDL	CA7-C31-C32-C33
77	m	402	HEM	CAA-CBA-CGA-O2A
77	y	402	HEM	CAA-CBA-CGA-O2A
72	2	402	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

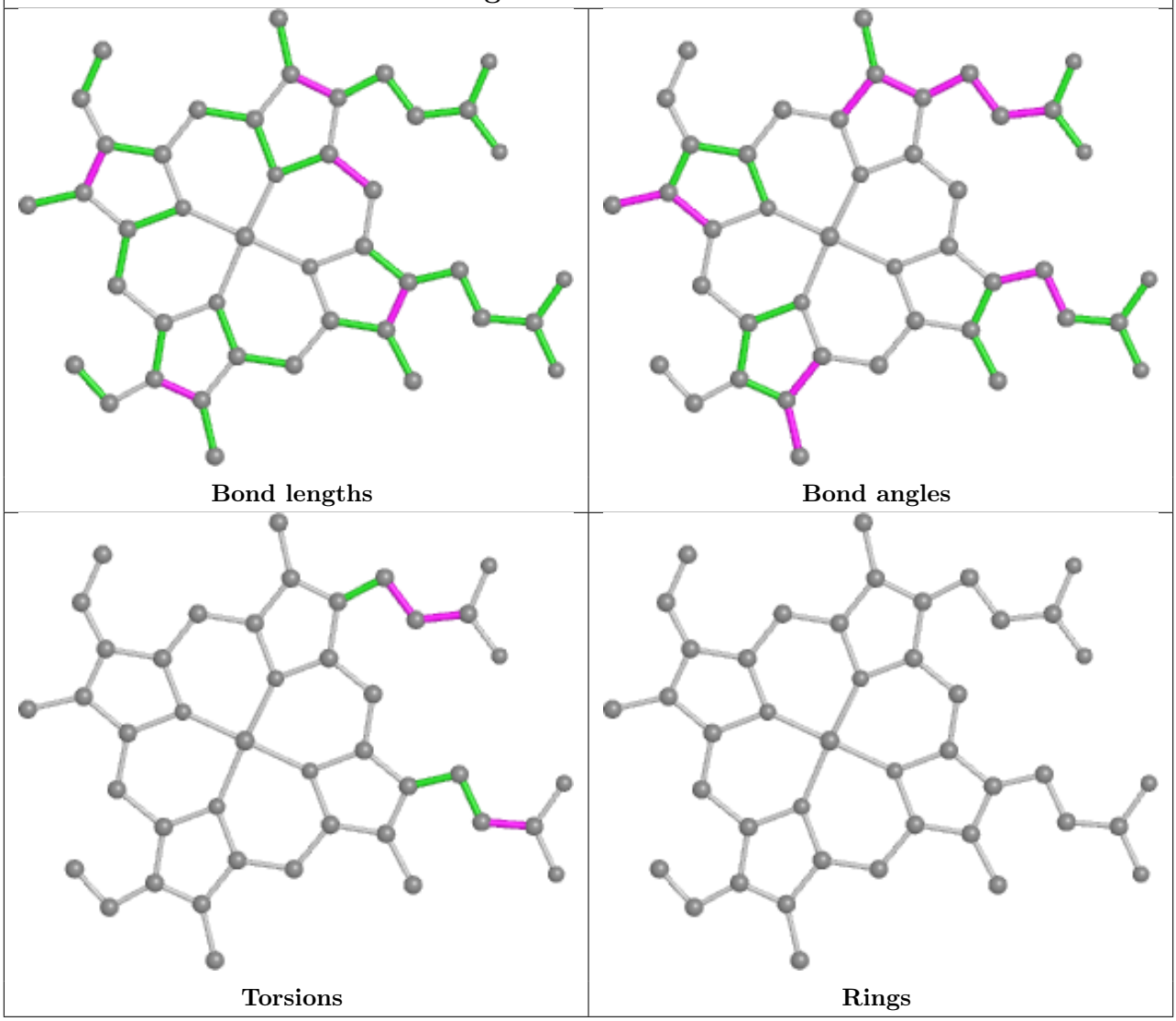
Mol	Chain	Res	Type	Atoms
79	A9	602	HEA	CAA-CBA-CGA-O1A
70	4	501	3PE	C35-C36-C37-C38
70	4	501	3PE	C2-C1-O11-P
76	R	601	NAP	O4B-C4B-C5B-O5B
78	o	301	HEC	CAD-CBD-CGD-O1D
78	z	301	HEC	CAD-CBD-CGD-O1D
70	4	501	3PE	C23-C24-C25-C26
71	4	502	CDL	CA3-CA4-CA6-OA8
71	6	701	CDL	CA3-CA4-CA6-OA8
70	B	501	3PE	C25-C26-C27-C28
72	S	401	PC1	C27-C28-C29-C2A
70	4	501	3PE	O32-C31-C32-C33
71	4	502	CDL	C12-C11-CA5-OA7
71	J	101	CDL	C55-C56-C57-C58
71	6	701	CDL	C72-C71-CB7-OB9
79	A9	601	HEA	CAA-CBA-CGA-O2A
71	4	502	CDL	CB2-OB2-PB2-OB4
71	4	502	CDL	CB3-OB5-PB2-OB3
72	2	402	PC1	C11-O13-P-O14
70	B	501	3PE	O32-C31-C32-C33
72	2	402	PC1	O32-C31-C32-C33
72	S	401	PC1	O31-C31-C32-C33
72	L	200	PC1	C38-C39-C3A-C3B
70	4	501	3PE	C12-C11-O13-P
70	4	503	3PE	C12-C11-O13-P
72	S	401	PC1	C12-C11-O13-P
72	S	401	PC1	C1-C2-O21-C21
70	4	503	3PE	C26-C27-C28-C29
72	S	401	PC1	C33-C34-C35-C36
77	m	401	HEM	CAD-CBD-CGD-O1D
77	y	401	HEM	CAD-CBD-CGD-O1D
72	j	201	PC1	C36-C37-C38-C39
79	A9	602	HEA	C26-C15-C16-C17
73	8	501	FMN	N10-C1'-C2'-O2'
79	A9	601	HEA	O11-C11-C3B-C2B
71	6	701	CDL	C32-C31-CA7-OA8
72	4	504	PC1	O31-C31-C32-C33
71	6	701	CDL	C74-C75-C76-C77
77	m	401	HEM	CAD-CBD-CGD-O2D
77	y	401	HEM	CAD-CBD-CGD-O2D
72	S	401	PC1	O32-C31-C32-C33
72	S	401	PC1	C11-C12-N-C13

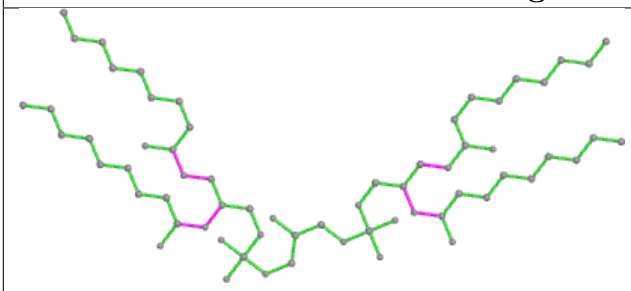
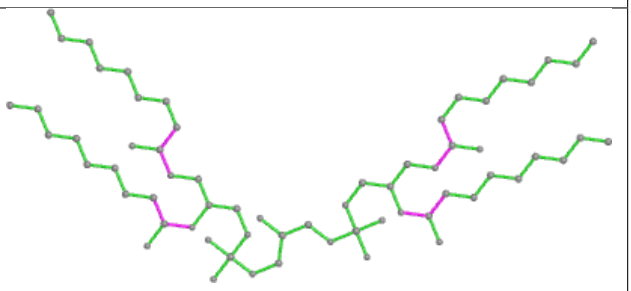
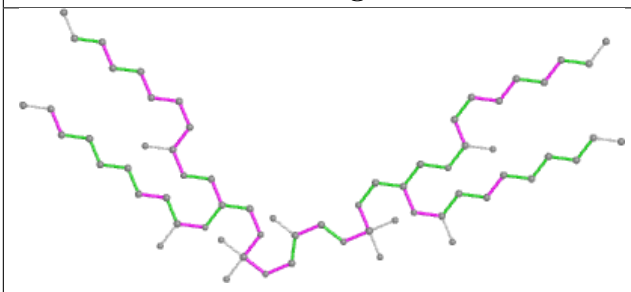
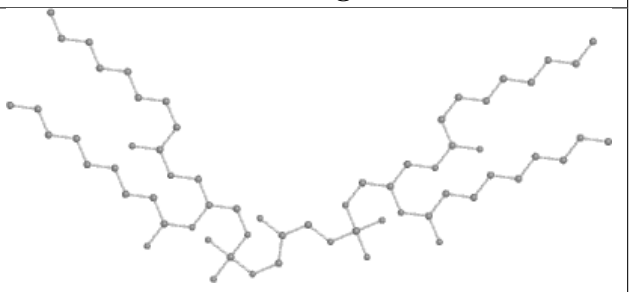
There are no ring outliers.

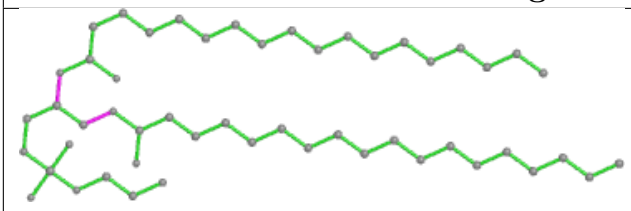
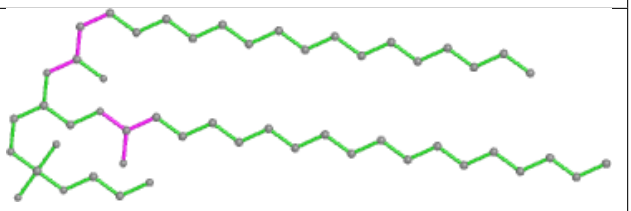
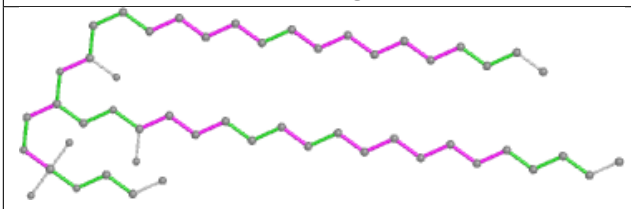
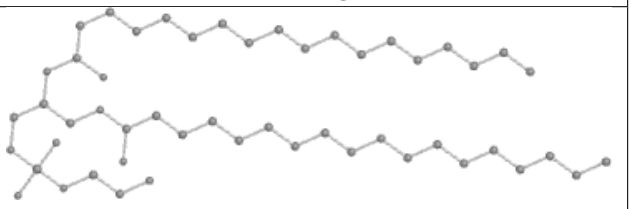
No monomer is involved in short contacts.

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.

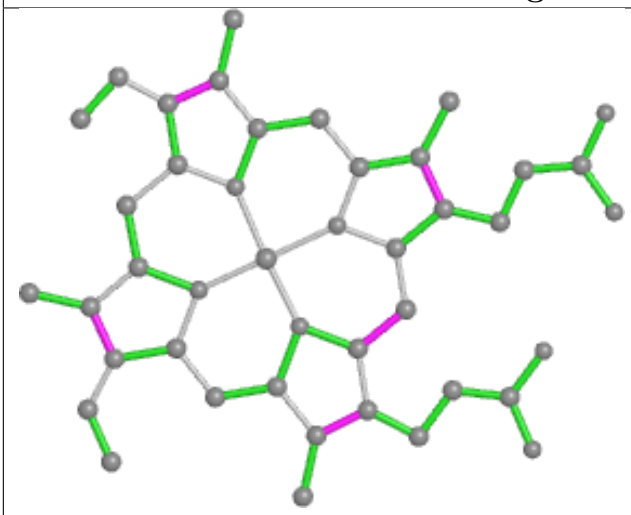
Ligand HEC z 301



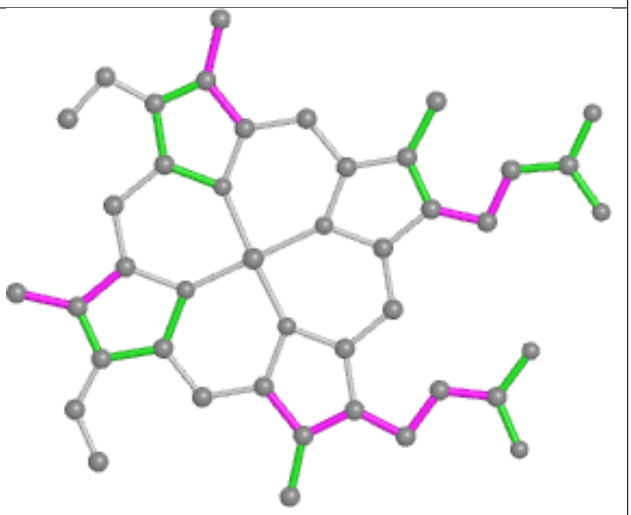
Ligand CDL 6 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

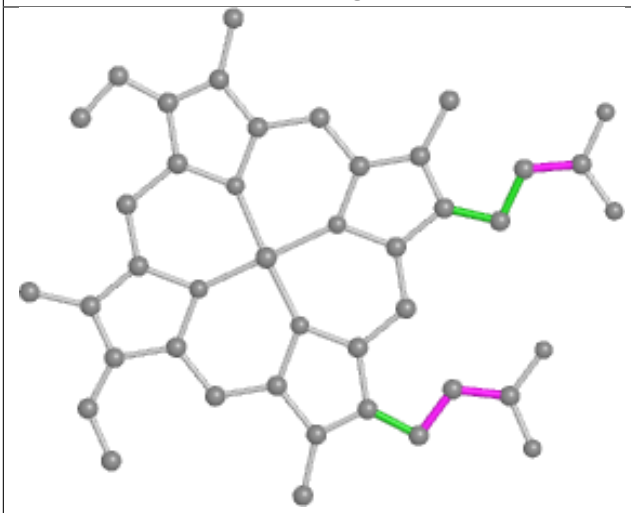
Ligand HEC o 301



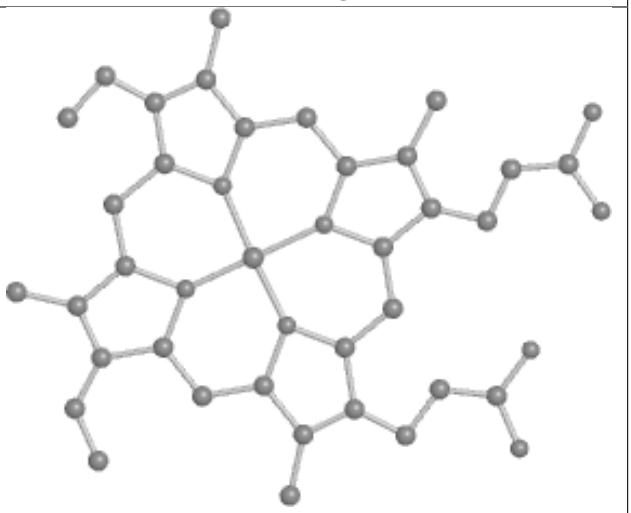
Bond lengths



Bond angles

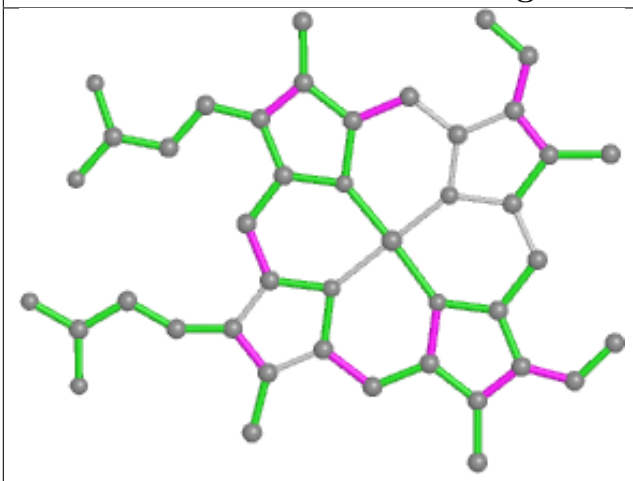


Torsions

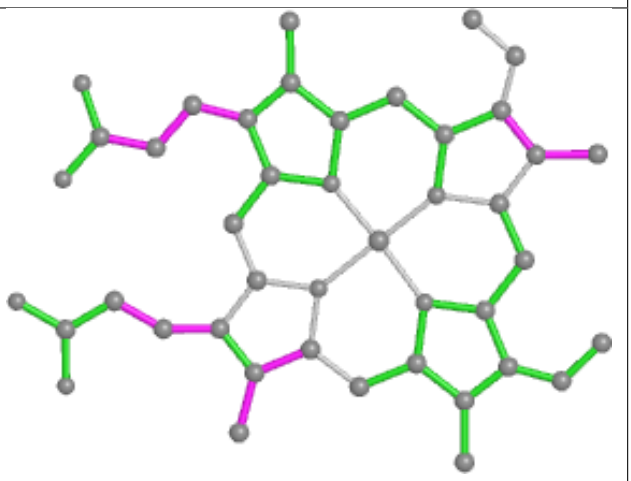


Rings

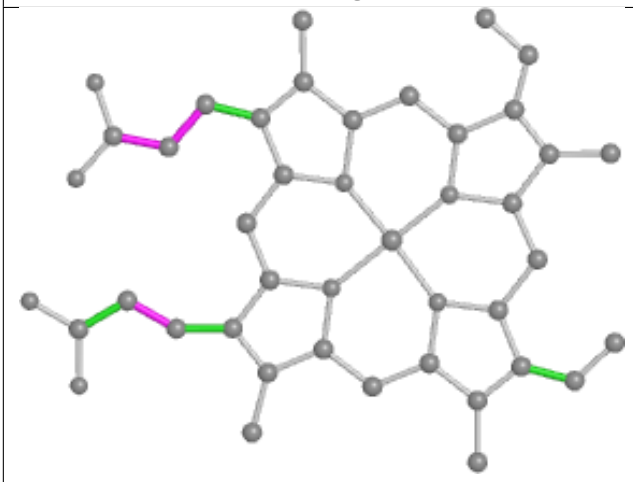
Ligand HEM m 401



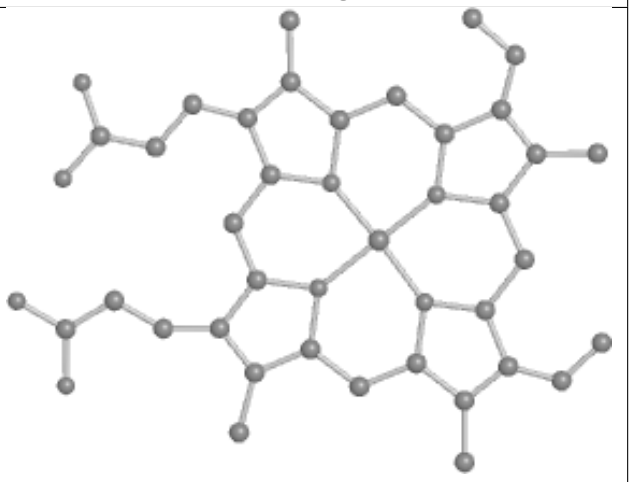
Bond lengths



Bond angles

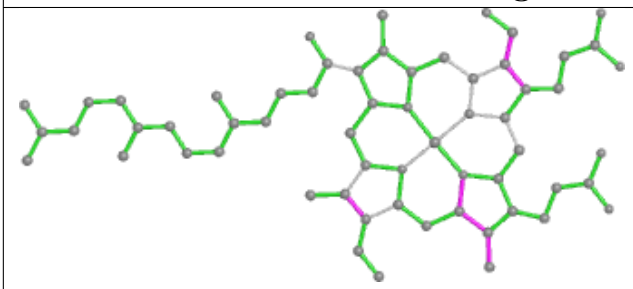


Torsions

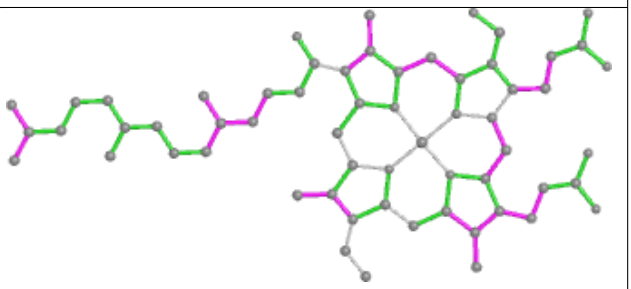


Rings

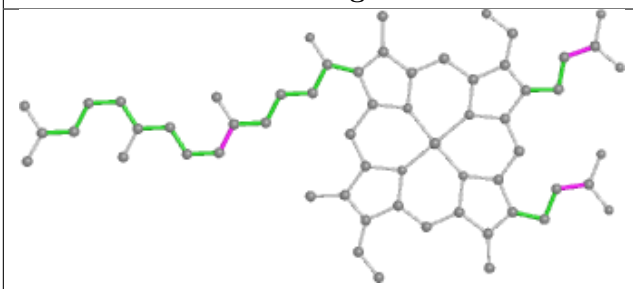
Ligand HEA A9 602



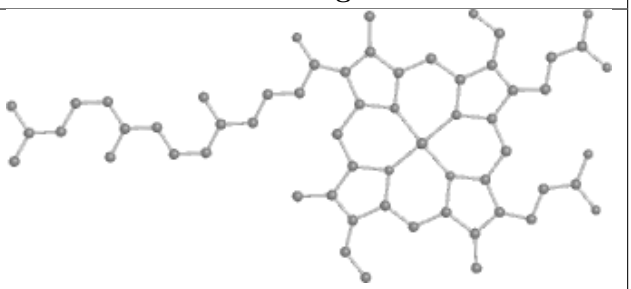
Bond lengths



Bond angles

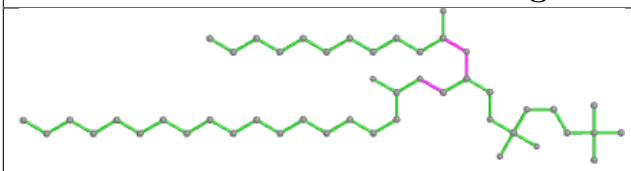


Torsions

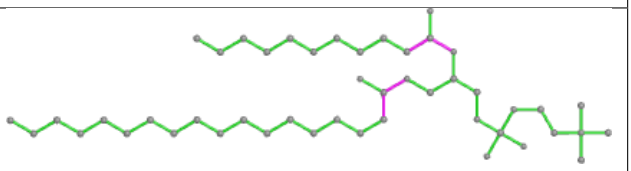


Rings

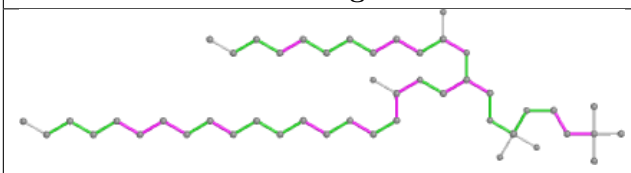
Ligand PC1 L 200



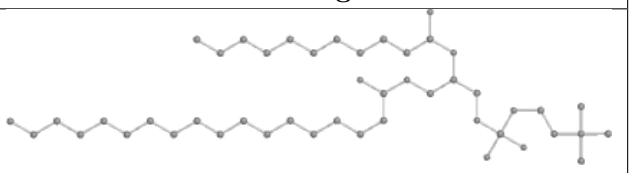
Bond lengths



Bond angles

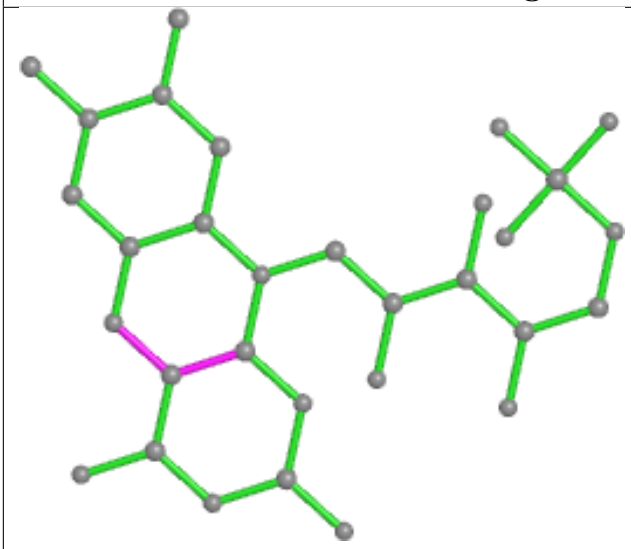


Torsions

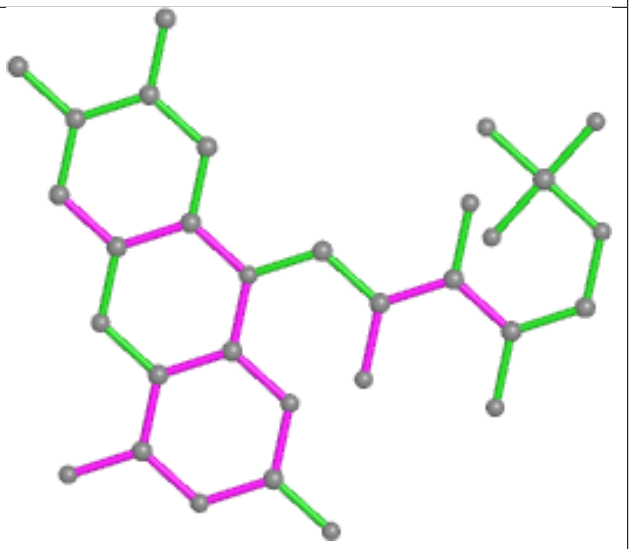


Rings

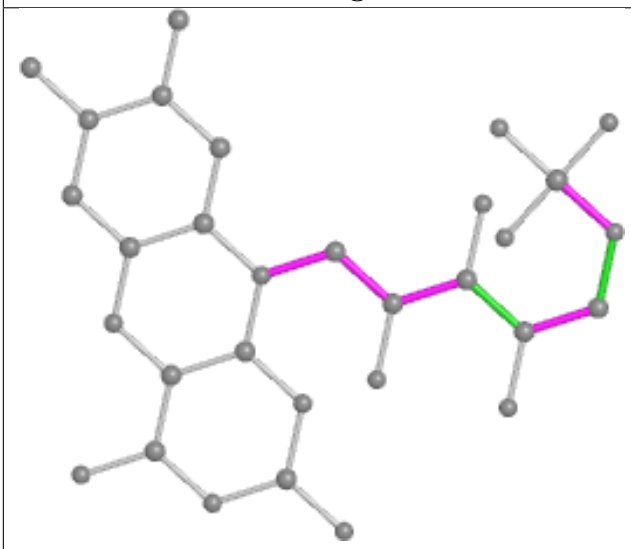
Ligand FMN 8 501



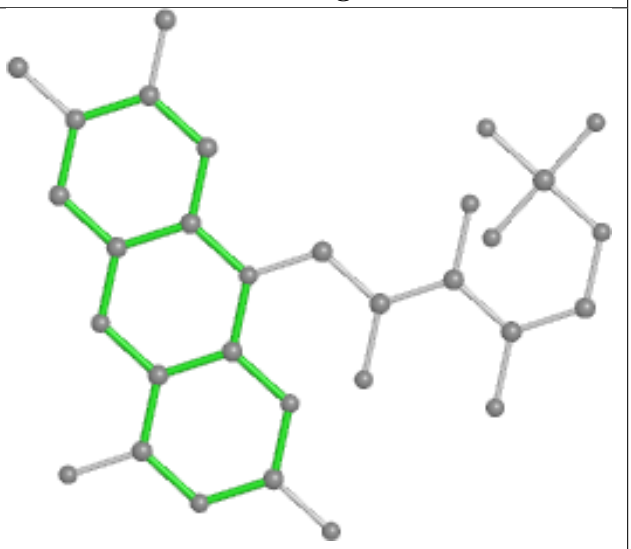
Bond lengths



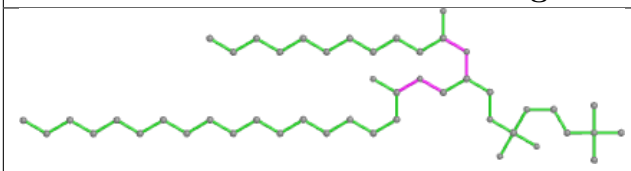
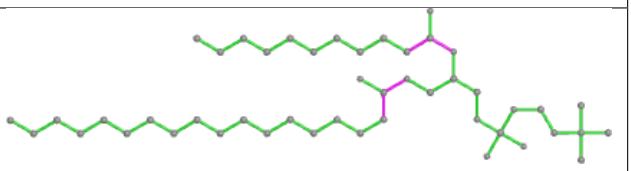
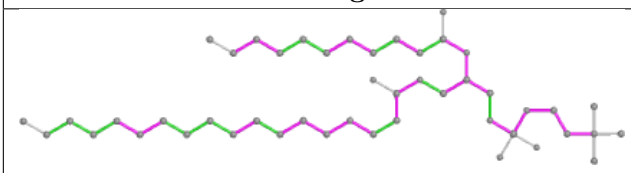
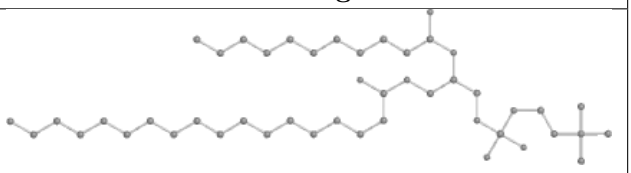
Bond angles

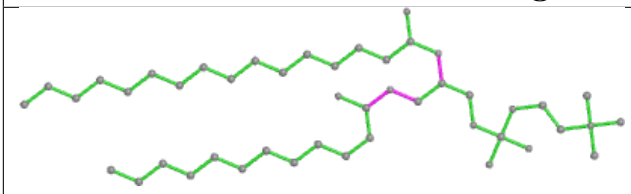
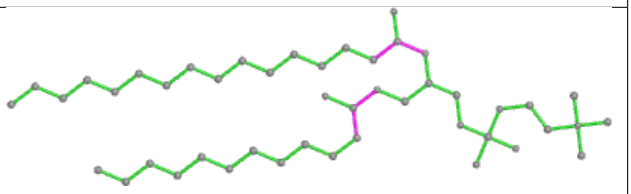
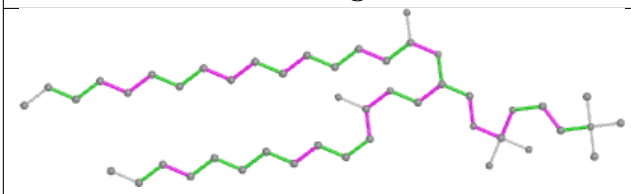
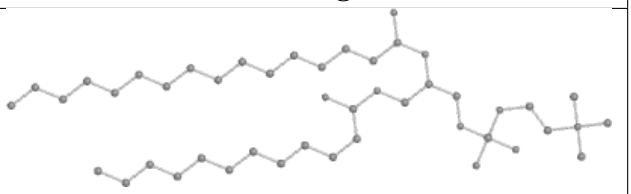


Torsions

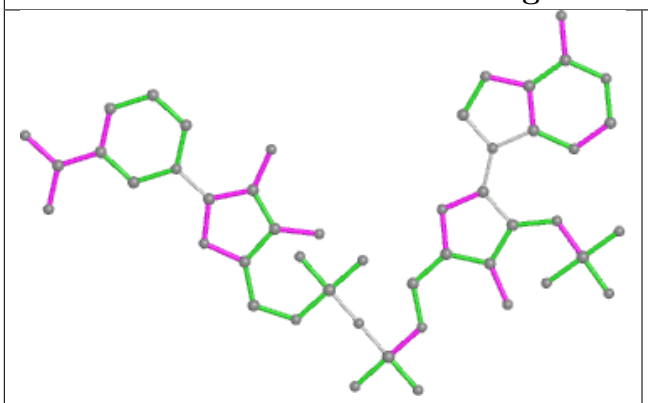


Rings

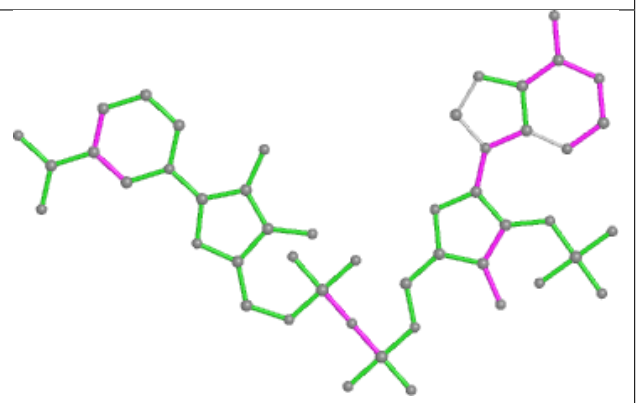
Ligand PC1 S 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 4 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

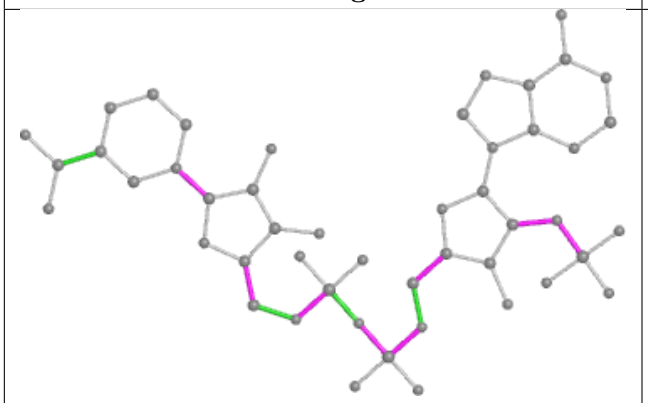
Ligand NAP R 601



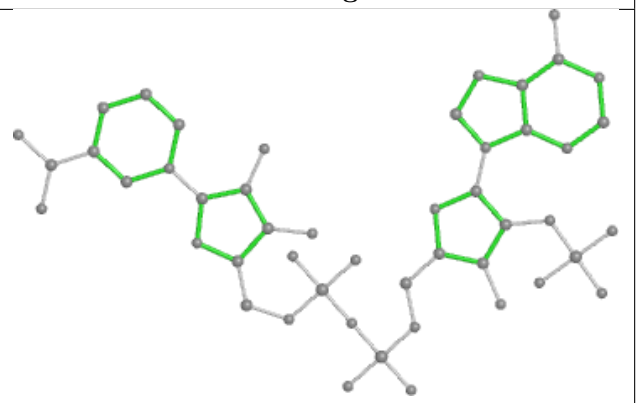
Bond lengths



Bond angles

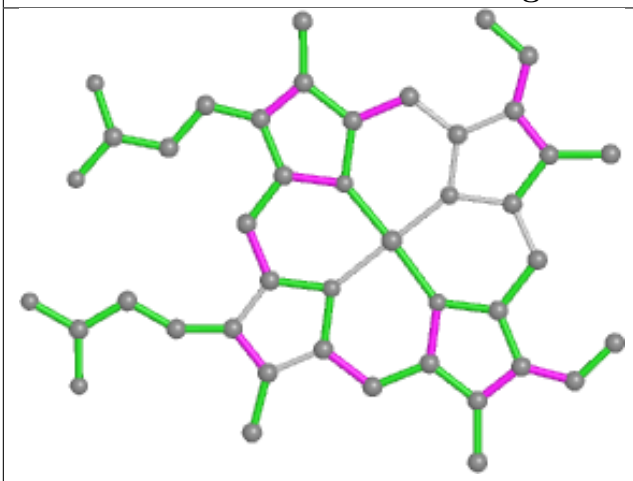


Torsions

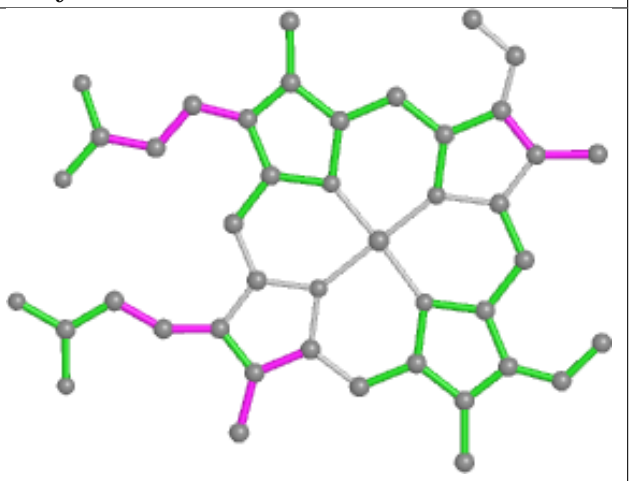


Rings

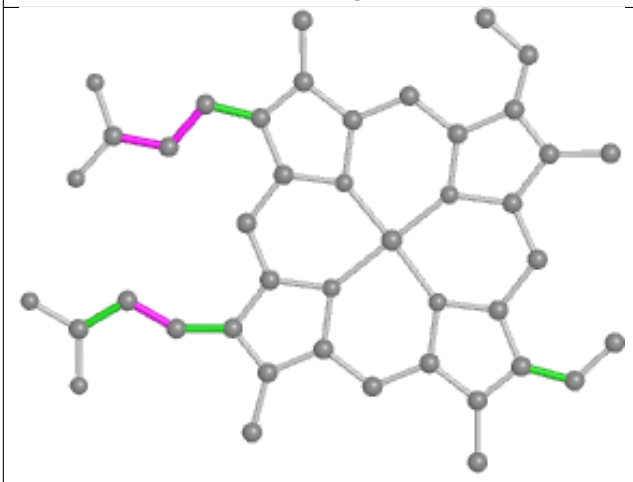
Ligand HEM y 401



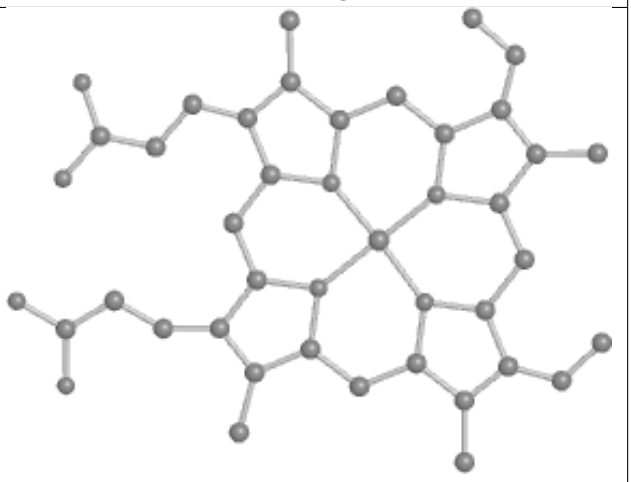
Bond lengths



Bond angles

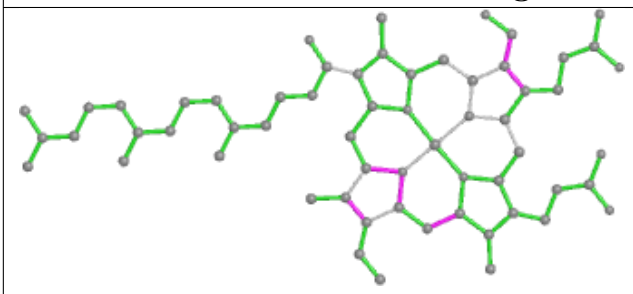


Torsions

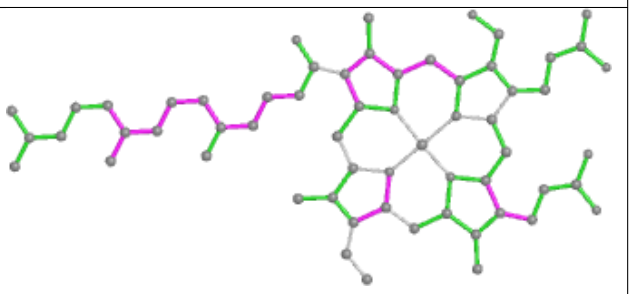


Rings

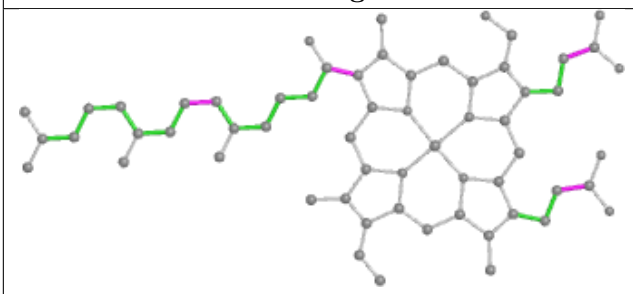
Ligand HEA A9 601



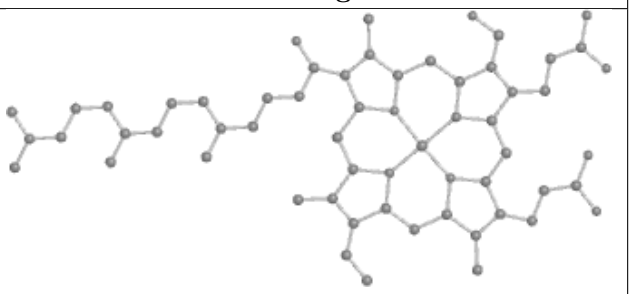
Bond lengths



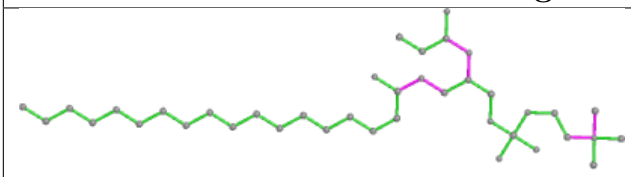
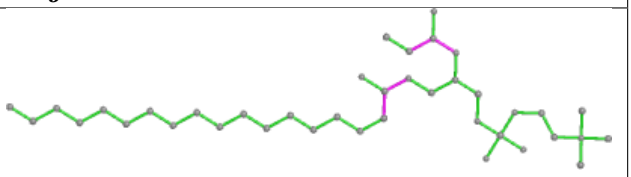
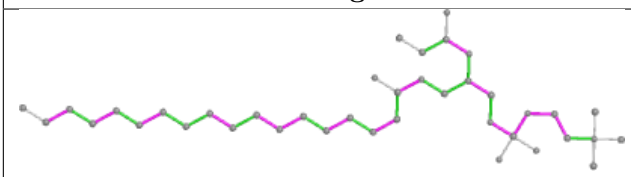
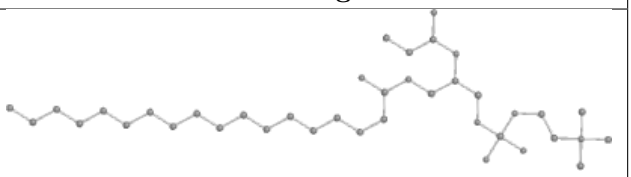
Bond angles

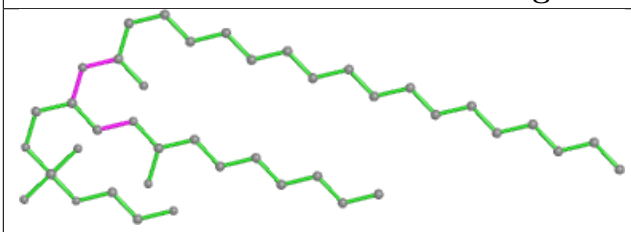
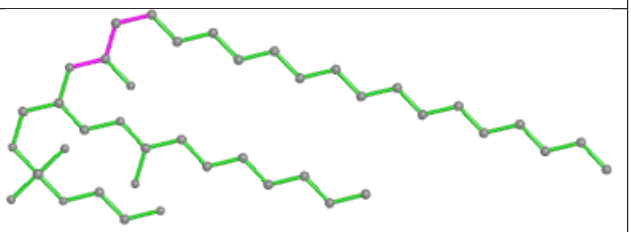
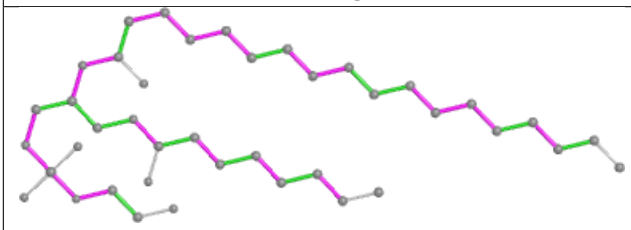
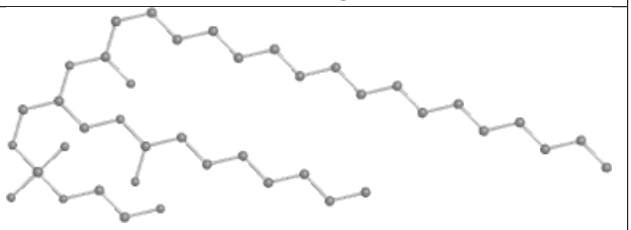


Torsions

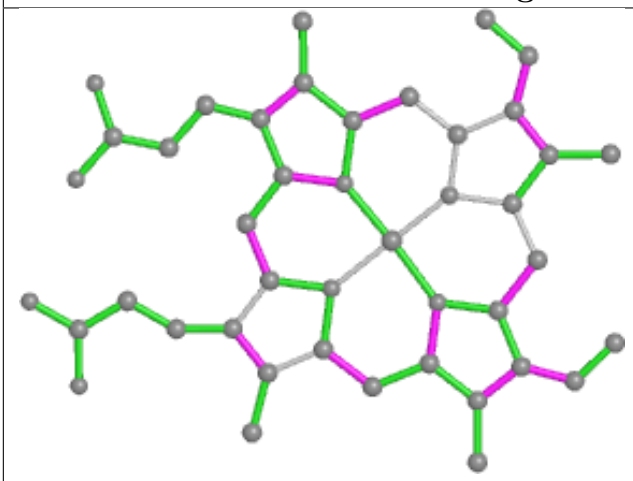


Rings

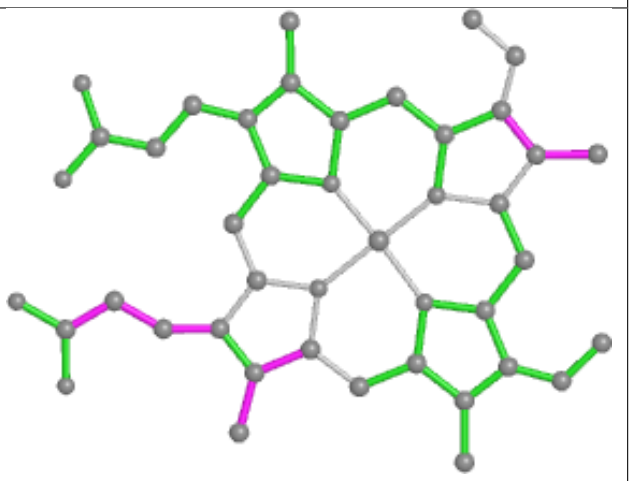
Ligand PC1 j 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE 4 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

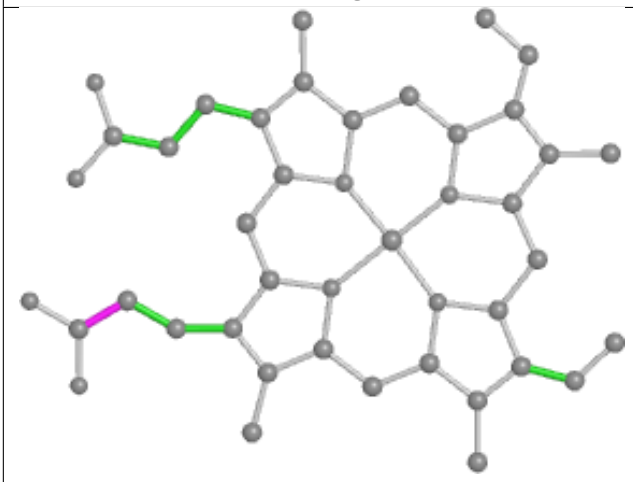
Ligand HEM m 402



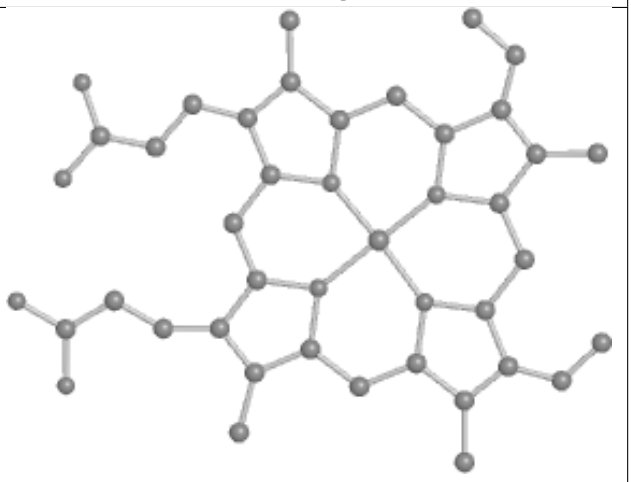
Bond lengths



Bond angles

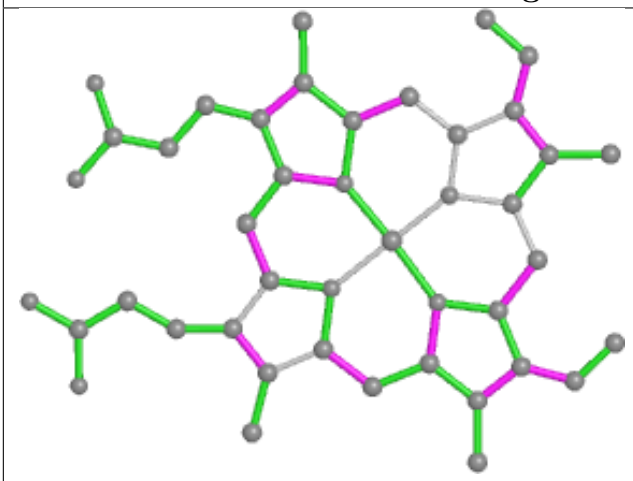


Torsions

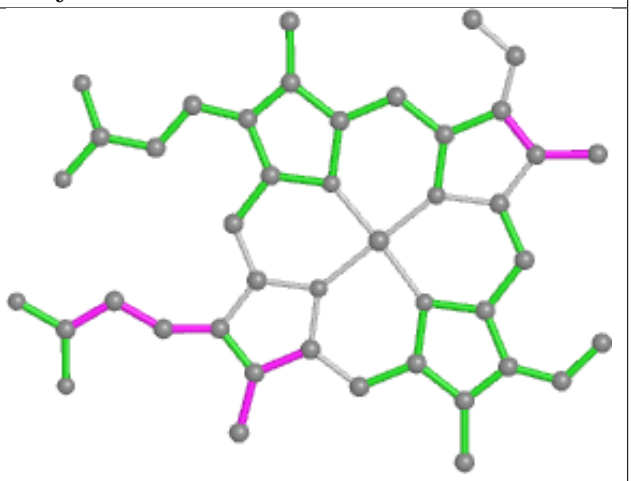


Rings

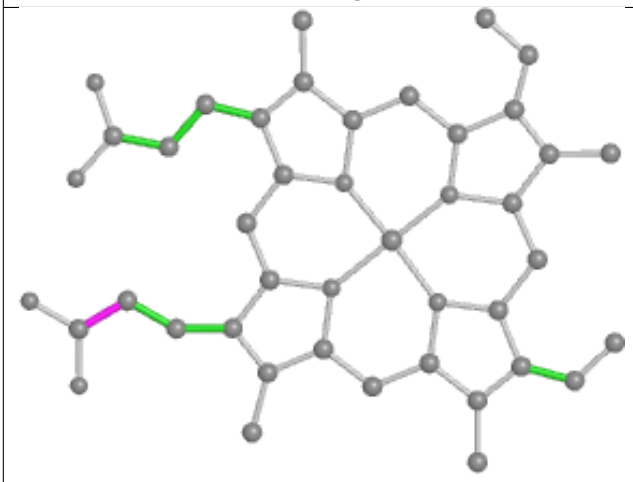
Ligand HEM y 402



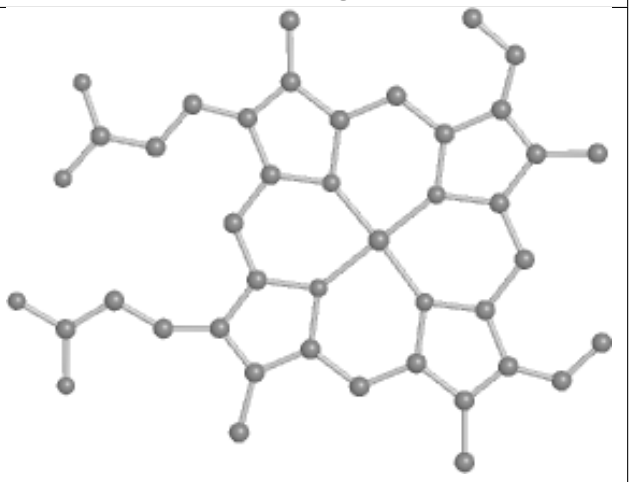
Bond lengths



Bond angles

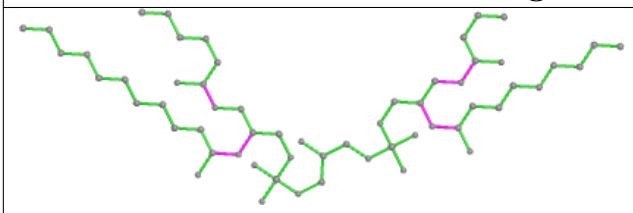


Torsions

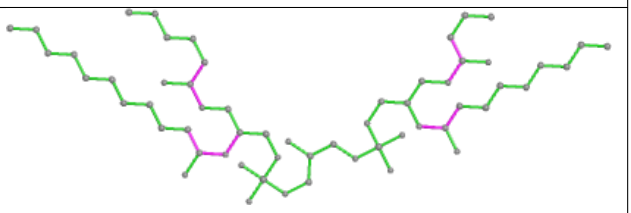


Rings

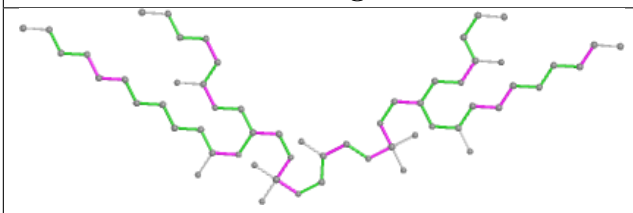
Ligand CDL J 101



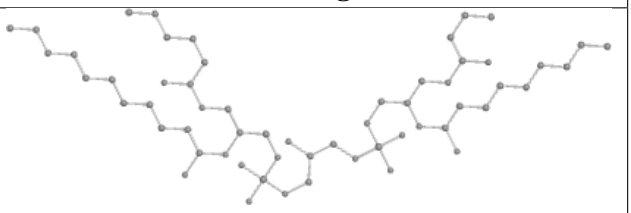
Bond lengths



Bond angles

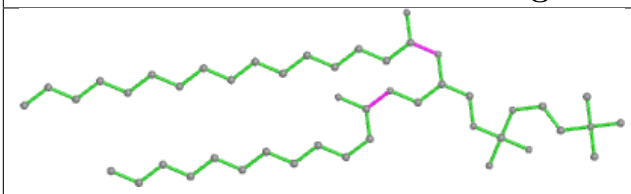


Torsions

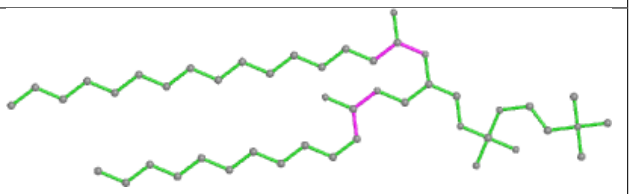


Rings

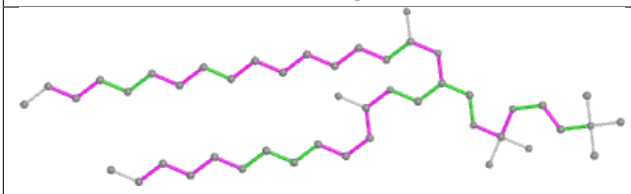
Ligand PC1 2 402



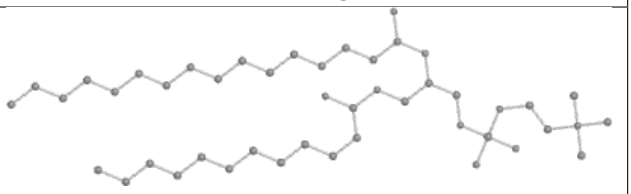
Bond lengths



Bond angles

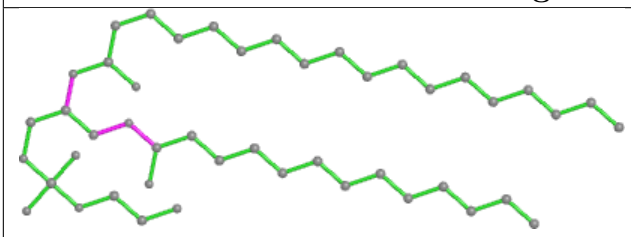


Torsions

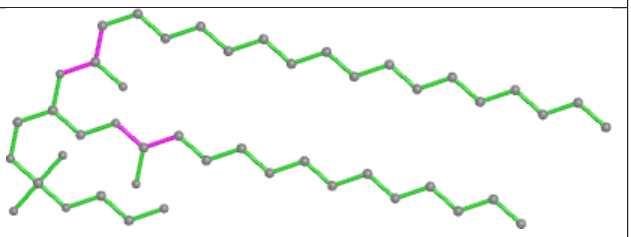


Rings

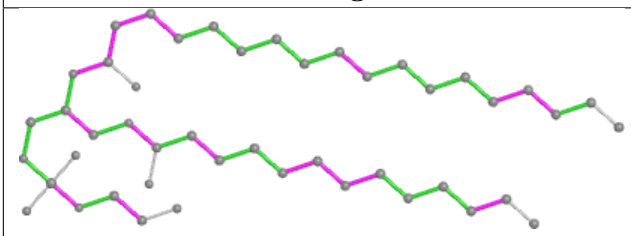
Ligand 3PE 2 401



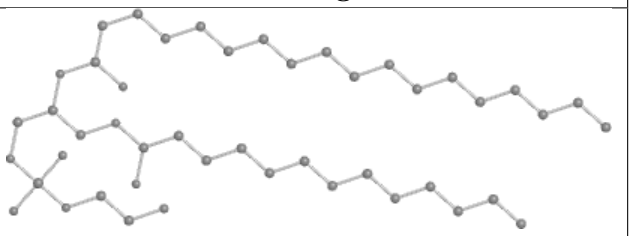
Bond lengths



Bond angles

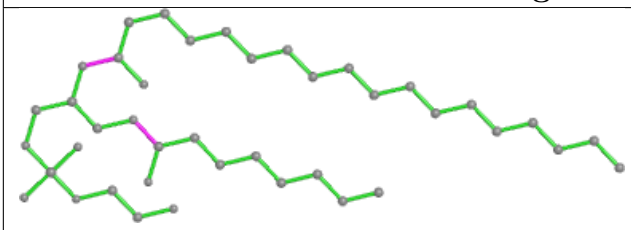


Torsions

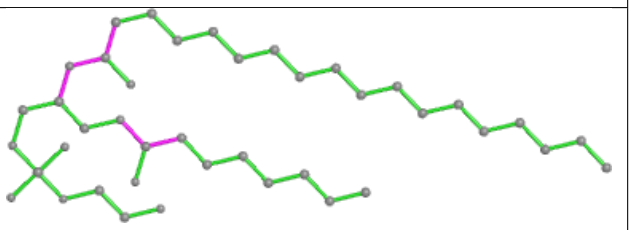


Rings

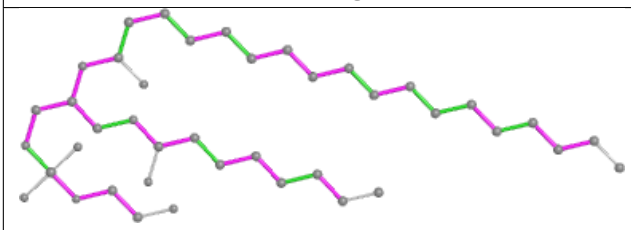
Ligand 3PE 4 501



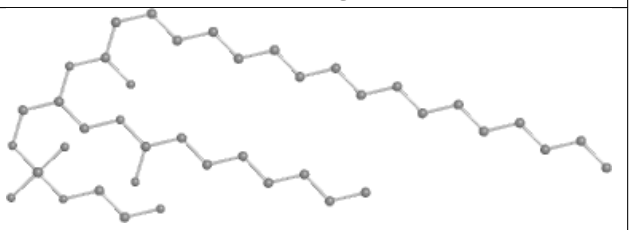
Bond lengths



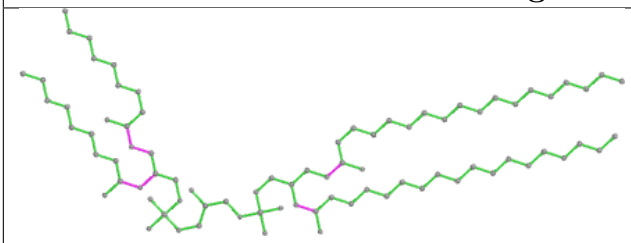
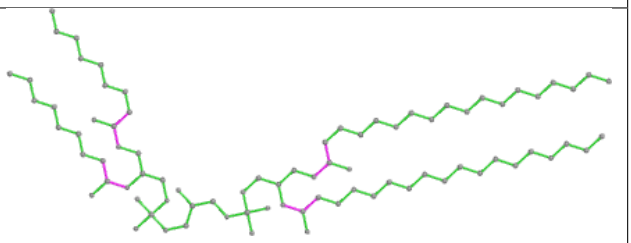
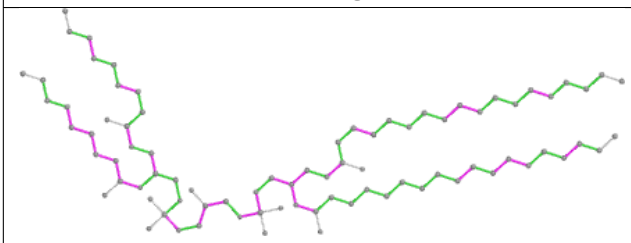
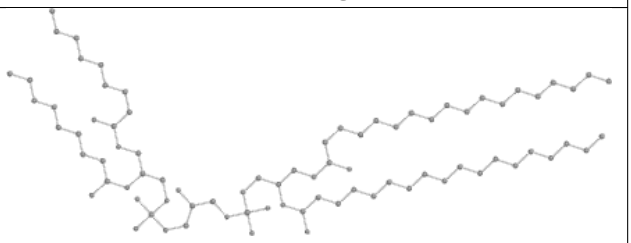
Bond angles



Torsions



Rings

Ligand CDL 4 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

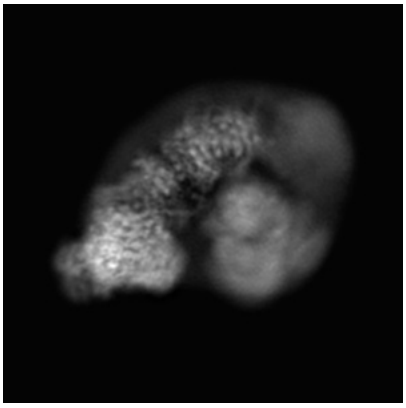
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30674. These allow visual inspection of the internal detail of the map and identification of artifacts.

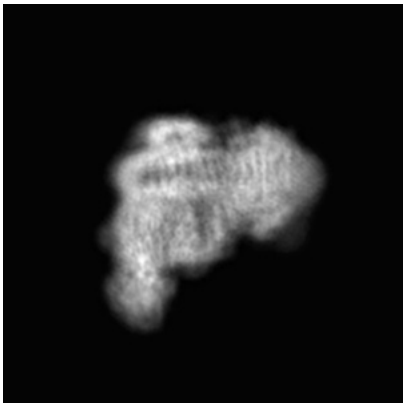
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

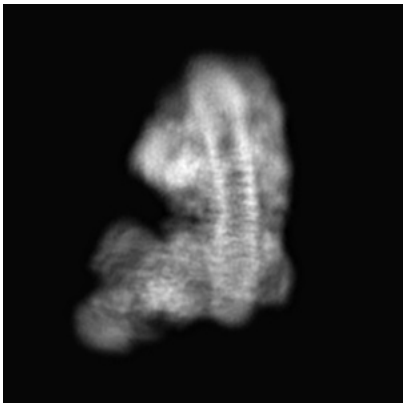
6.1.1 Primary map



X



Y

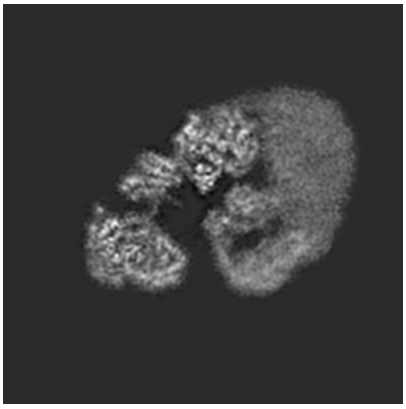


Z

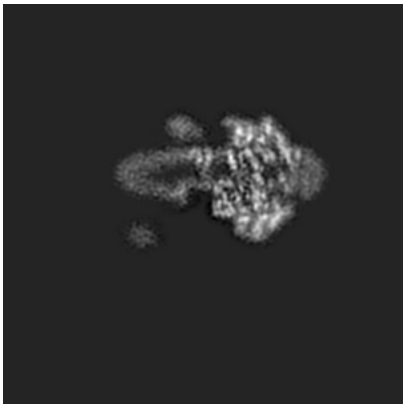
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

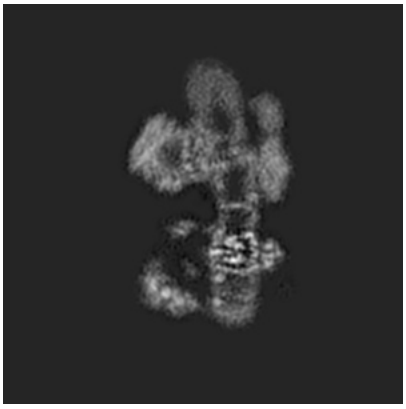
6.2.1 Primary map



X Index: 140



Y Index: 140

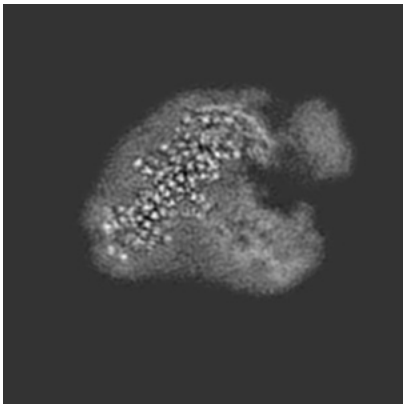


Z Index: 140

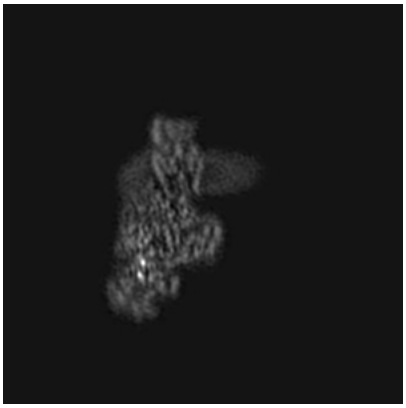
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

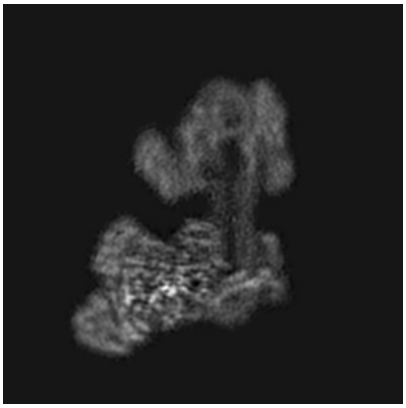
6.3.1 Primary map



X Index: 173



Y Index: 75



Z Index: 103

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

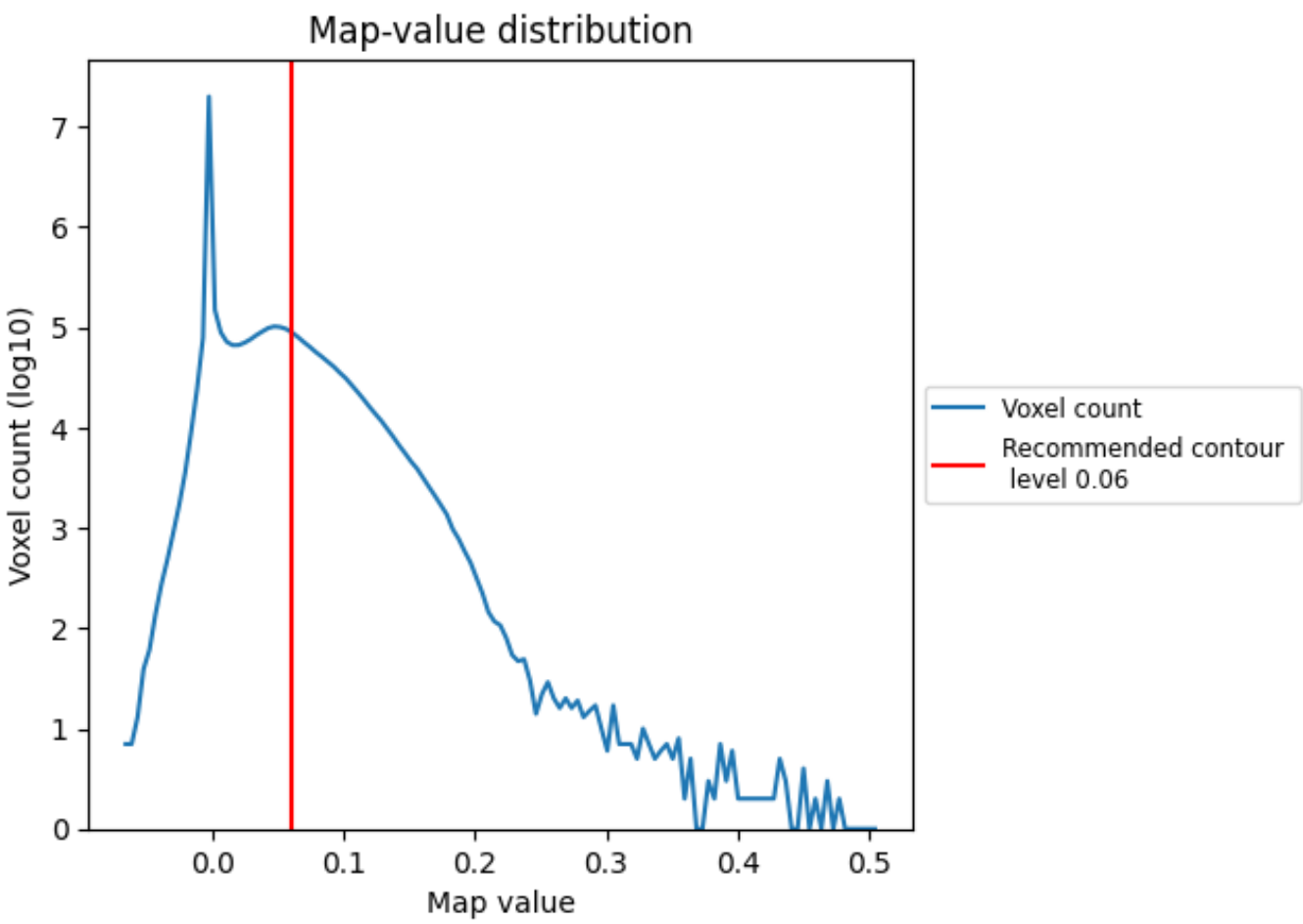
6.5 Mask visualisation (i)

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

7 Map analysis (i)

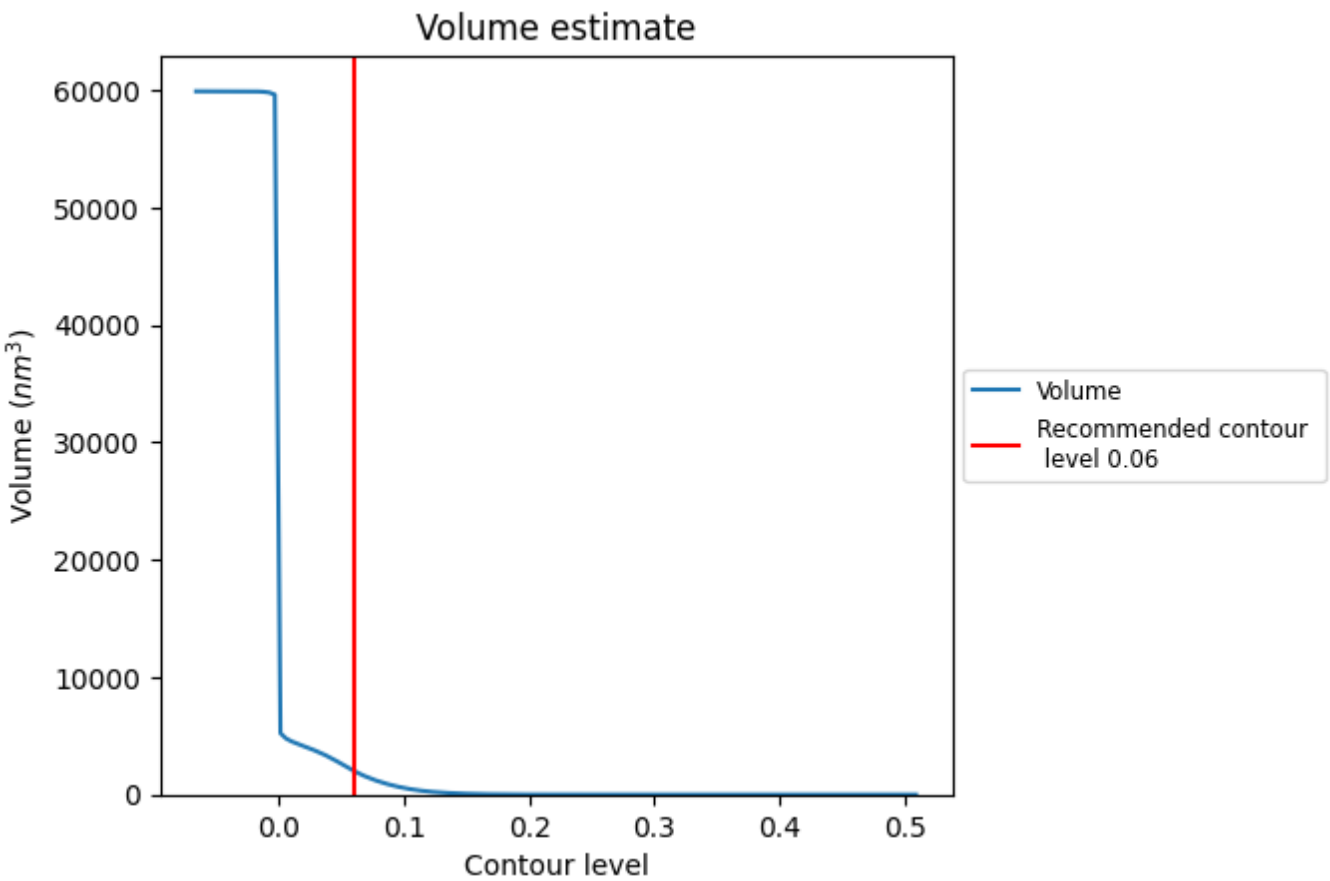
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

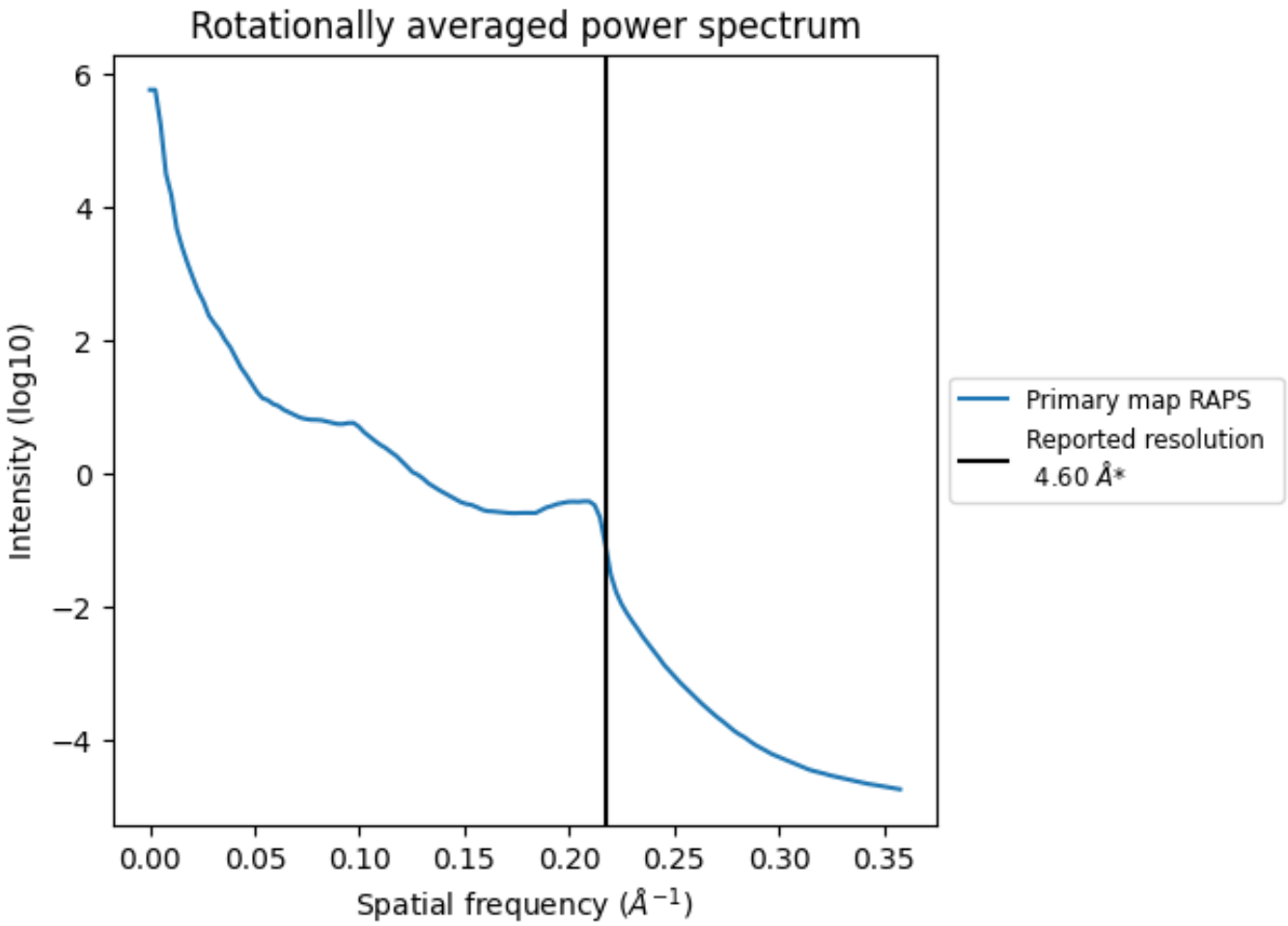
7.2 Volume estimate (i)



The volume at the recommended contour level is 2007 nm^3; this corresponds to an approximate mass of 1813 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

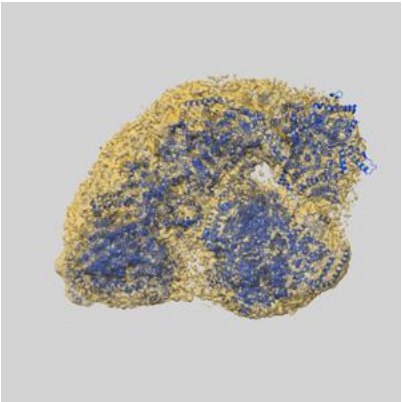
8 Fourier-Shell correlation (i)

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

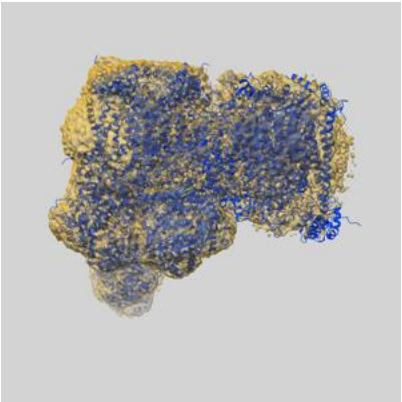
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30674 and PDB model 7DGR. Per-residue inclusion information can be found in section 3 on page 24.

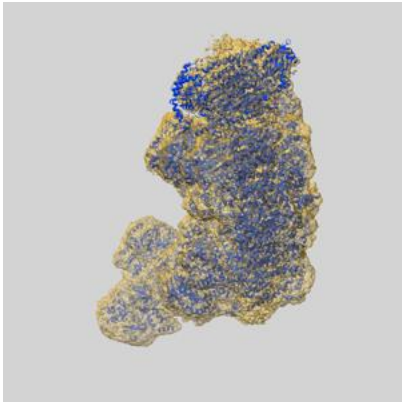
9.1 Map-model overlay (i)



X



Y



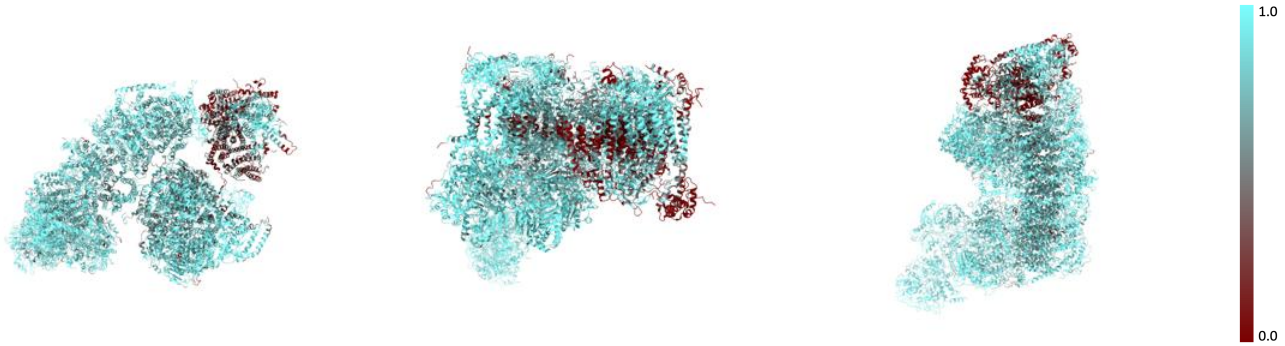
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

This section was not generated.

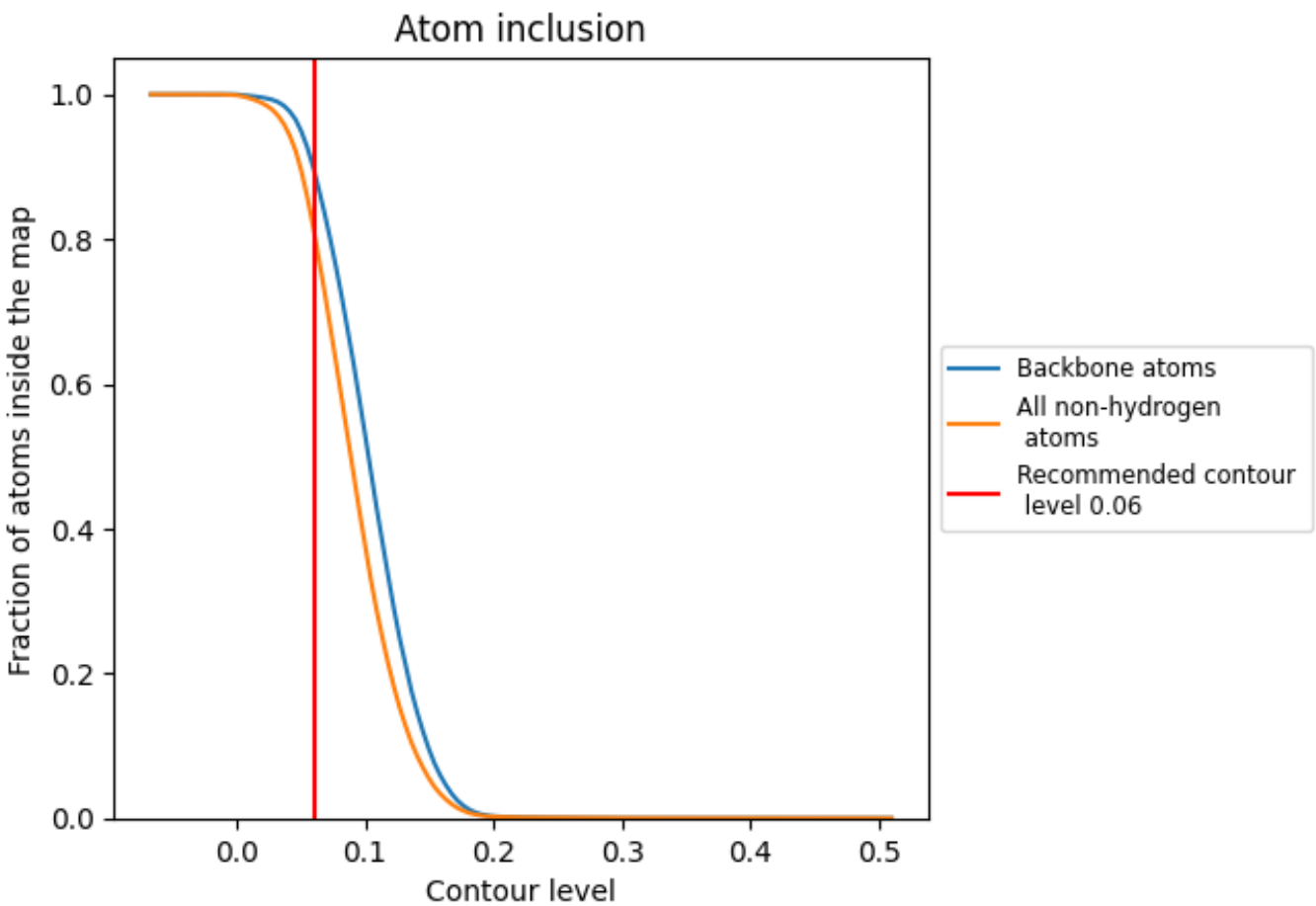
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8142
1	0.8293
2	0.8068
3	0.7049
4	0.7842
5	0.7907
6	0.7761
7	0.7749
8	0.9829
9	0.9634
A	0.9669
A0	0.7870
A1	0.7438
A2	0.6871
A3	0.6471
A4	0.1933
A5	0.5644
A6	0.3284
A7	0.2773
A8	0.2681
A9	0.5823
B	0.8676
B0	0.3547
B1	0.8125
B2	0.5711
B3	0.7509
B4	0.3914
C	0.9196
C0	0.1480
C1	0.3263
C2	0.4266
C3	0.1824
C4	0.7762
D	0.9029
E	0.9122

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
F	0.9121
G	0.9283
H	0.9526
I	0.8983
J	0.9353
K	0.9733
L	0.8103
M	0.8681
N	0.9162
O	0.8667
P	0.8341
Q	0.9566
R	0.8841
S	0.9044
T	0.8077
U	0.6761
V	0.9460
W	0.9804
X	0.8989
Y	0.9504
Z	0.9277
a	0.7954
b	0.9462
c	0.9536
d	0.9771
e	0.9168
f	0.9647
g	0.9346
h	0.9234
i	0.9231
j	0.7833
k	0.9267
l	0.9113
m	0.7760
o	0.9361
p	0.8967
q	0.8844
r	0.7957
s	0.8787
t	0.7312
u	0.8397
v	0.8393

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
w	0.8908
x	0.9434
y	0.7238
z	0.8809