wwPDB EM Validation Summary Report (i)

Aug 23, 2026 – 05:03 pm BST

PDB ID	:	9I4I / pdb_00009i4i
EMDB ID	:	EMD-52619
Title	:	High resolution Cryo-EM structure of human complex I in mitochondria
Authors	:	Nguyen, M.D.; Singh, V.; Rorbach, J.
Deposited on	:	2025-01-24
Resolution	:	2.63 Å(reported)

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

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

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

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

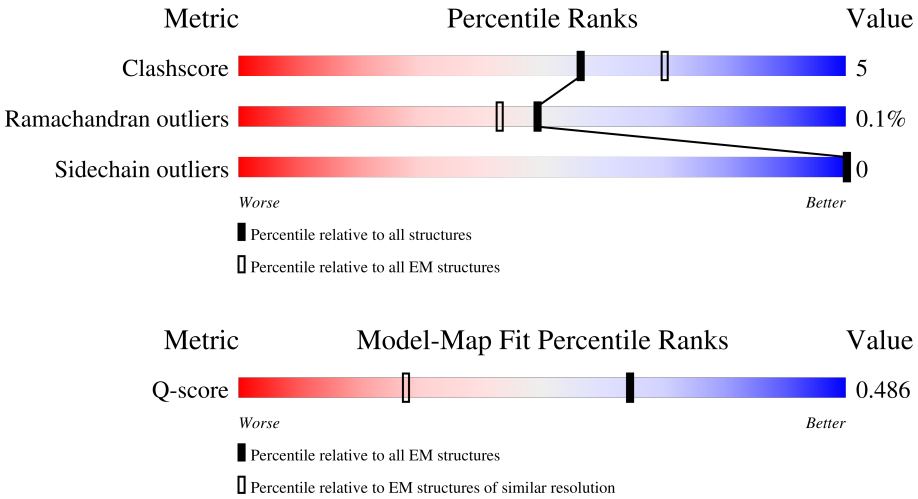
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.63 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



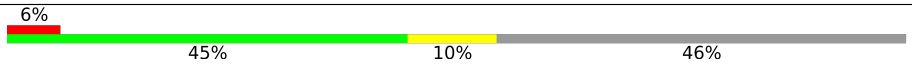
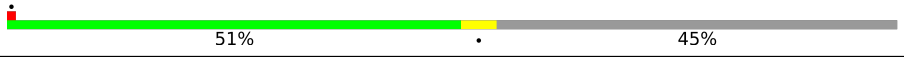
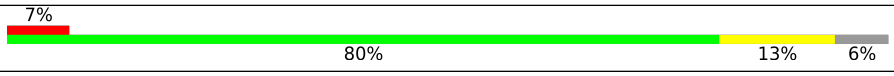
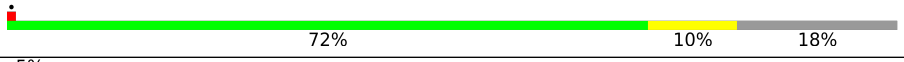
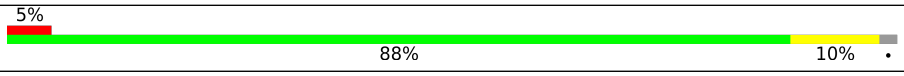
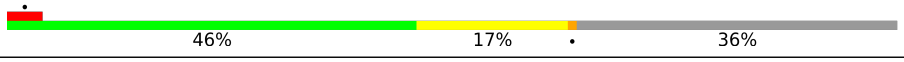
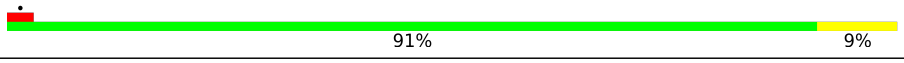
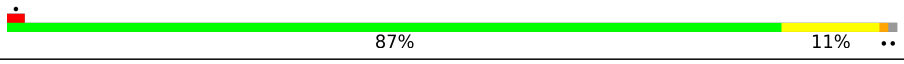
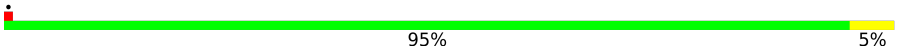
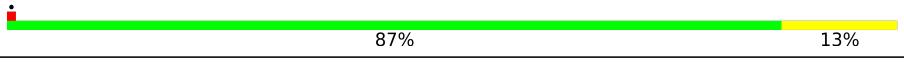
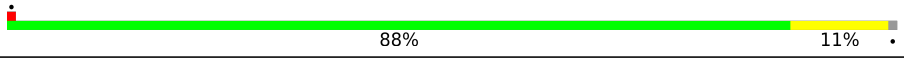
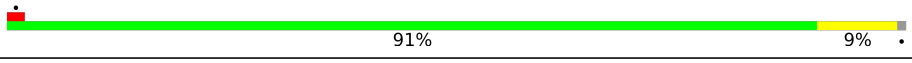
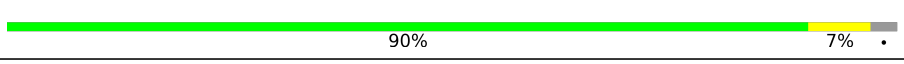
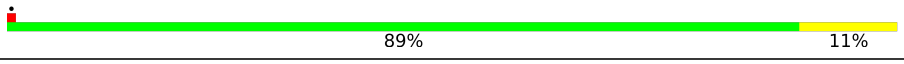
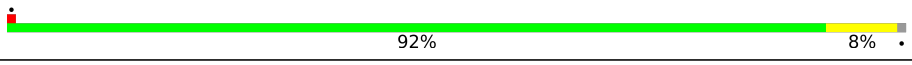
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	Q	463	83% 10% 7%
2	S	70	84% 16%
3	U	84	87% 11%
4	V	141	93% 6%

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Mol	Chain	Length	Quality of chain
5	W	144	
6	H	156	
6	X	156	
7	Y	105	
8	Z	98	
9	a	189	
10	b	128	
11	c	186	
12	d	172	
13	e	153	
14	f	76	
15	g	119	
16	h	106	
17	i	347	
18	j	115	
19	k	98	
20	l	603	
21	m	174	
22	n	58	
23	o	129	
24	p	179	
25	r	459	
26	s	318	
27	u	172	
28	v	137	

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Mol	Chain	Length	Quality of chain
29	w	355	83% 7% 10%
30	C	464	5% 76% 17% 6%
31	D	210	75% 9% 16%
32	E	213	67% 8% 24%
33	F	128	88% 5% 8%
34	G	99	73% 13% 14%
35	I	116	89% 8%
36	J	377	81% 9% 10%
37	K	108	30% 6% 64%
38	L	175	61% 9% 31%
39	M	727	81% 13% 6%
40	N	145	93% 6%
41	O	249	74% 11% 15%
42	P	264	72% 7% 21%
43	T	124	68% 10% 23%
44	t	113	78% 8% 14%

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
51	SF4	C	501	-	-	X	-
52	FMN	C	502	X	X	X	-

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 136393 atoms, of which 68697 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Q	430	6894	2215	3433	599	624	23	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	S	70	1138	367	570	101	96	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	U	83	1302	427	655	105	113	2	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	V	140	2069	668	1031	178	187	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	W	140	2304	738	1153	205	202	6	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	X	86	Total	C	H	N	O	S	0	0
			1386	448	690	102	140	6		
6	H	85	Total	C	H	N	O	S	0	0
			1369	443	681	101	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Y	61	Total	C	H	N	O	S	0	0
			1035	361	491	89	93	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Z	83	Total	C	H	N	O	S	0	0
			1339	447	660	115	115	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	a	138	Total	C	H	N	O	S	0	0
			2356	771	1182	199	202	2		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	b	120	Total	C	H	N	O	S	0	0
			2070	672	1049	176	169	4		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	c	152	Total	C	H	N	O	S	0	0
			2453	819	1180	215	227	12		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	169	Total	C	H	N	O	S	0	0
			2837	895	1404	262	264	12		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	e	107	Total	C	H	N	O	S	0	0
			1737	569	850	146	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	49	Total	C	H	N	O	0	0
			844	278	425	71	70		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	g	119	Total	C	H	N	O	S	1	0
			2035	663	1023	176	169	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	h	105	Total	C	H	N	O	S	0	0
			1747	551	876	162	151	7		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	i	347	Total	C	H	N	O	S	0	0
			5626	1818	2893	420	470	25		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	j	115	Total	C	H	N	O	S	0	0
			1890	631	964	132	154	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	k	98	Total	C	H	N	O	S	0	0
			1530	488	787	114	128	13		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	l	601	Total	C	H	N	O	S	0	0
			9583	3110	4880	739	823	31		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	m	173	Total	C	H	N	O	S	0	0
			2619	872	1317	192	227	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	n	54	Total	C	H	N	O	S	0	0
			923	295	466	82	77	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	o	128	Total	C	H	N	O	S	0	0
			2154	685	1088	192	187	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	p	173	Total	C	H	N	O	S	0	0
			2947	963	1448	266	262	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	r	459	Total	C	H	N	O	S	0	0
			7444	2404	3821	569	620	30		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	s	316	Total	C	H	N	O	S	0	0
			5091	1672	2593	376	435	15		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	u	171	Total	C	H	N	O	S	0	0
			2791	893	1386	249	254	9		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	v	121	Total	C	H	N	O	S	0	0
			2069	647	1032	200	180	10		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	w	320	Total	C	H	N	O	S	0	0
			5221	1680	2598	447	487	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	C	434	Total	C	H	N	O	S	0	0
			6668	2110	3321	601	616	20		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	D	176	Total	C	H	N	O	S	0	0
			2787	893	1367	243	271	13		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
32	E	161	Total	C	H	N	O	P	S	0	0
			2577	816	1290	233	223	1	14		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	F	118	Total	C	H	N	O	S	0	0
			2016	640	1017	183	171	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	G	85	Total	C	H	N	O	S	0	0
			1380	430	697	127	124	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	I	112	Total	C	H	N	O	S	0	0
			1875	593	953	157	169	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	J	341	Total	C	H	N	O	S	0	0
			5547	1780	2802	490	467	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	K	39	Total	C	H	N	O	S	0	0
			586	191	282	53	59	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	L	121	Total	C	H	N	O	S	0	0
			1954	617	975	176	182	4		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	M	687	Total	C	H	N	O	S	0	0
			10596	3310	5321	917	1009	39		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	N	144	Total	C	H	N	O	S	0	0
			2375	775	1172	211	213	4		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	O	212	Total	C	H	N	O	S	0	0
			3291	1047	1648	276	310	10		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	P	208	Total	C	H	N	O	S	0	0
			3421	1117	1691	297	313	3		

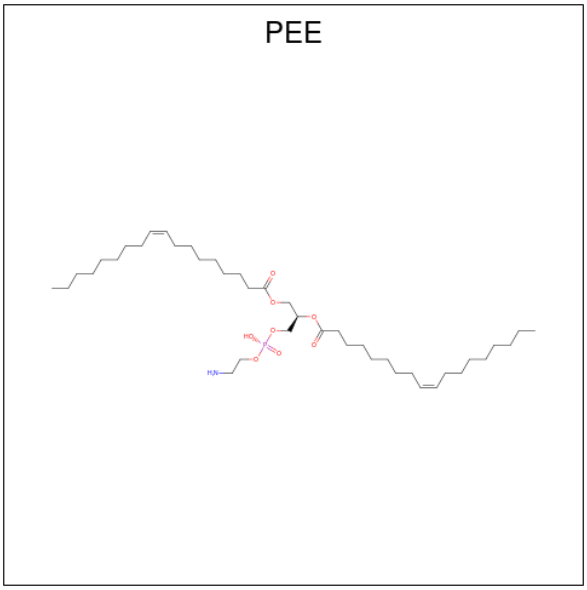
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	T	96	Total	C	H	N	O	S	0	0
			1484	465	732	141	143	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

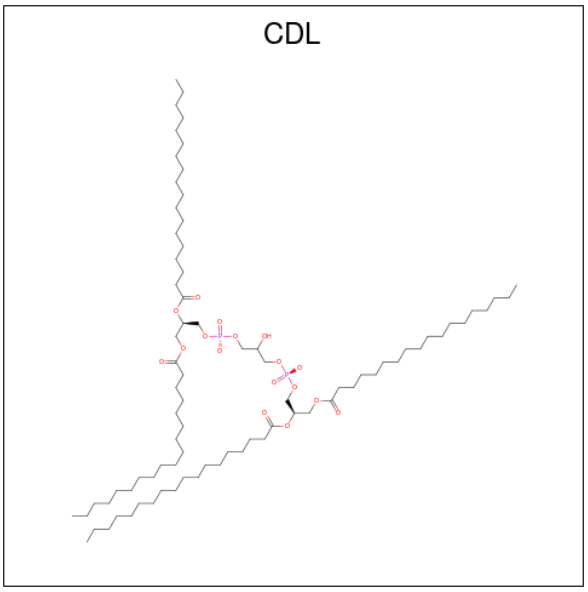
Mol	Chain	Residues	Atoms						AltConf	Trace
44	t	97	Total	C	H	N	O	S	0	0
			1582	489	802	148	141	2		

- Molecule 45 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



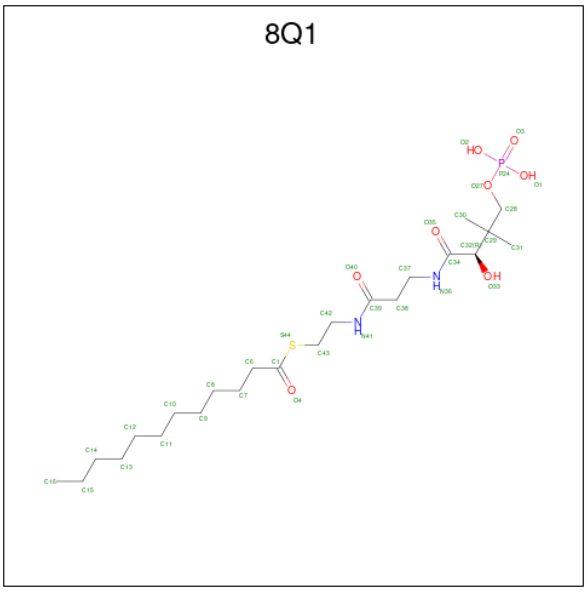
Mol	Chain	Residues	Atoms						AltConf
45	V	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	W	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	i	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	i	1	Total	C	H	N	O	P	0
			121	39	72	1	8	1	
45	l	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	E	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
45	J	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



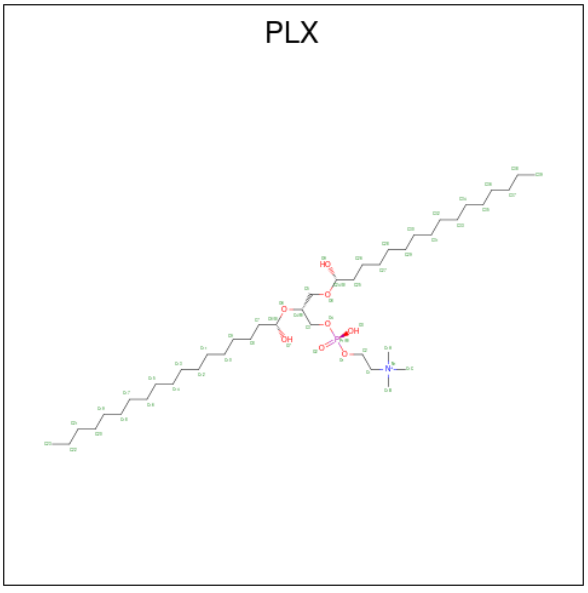
Mol	Chain	Residues	Atoms					AltConf
46	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	V	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	i	1	Total	C	H	O	P	0
			144	45	80	17	2	
46	l	1	Total	C	H	O	P	0
			144	45	80	17	2	
46	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
46	u	1	Total	C	H	O	P	0
			144	45	80	17	2	

- Molecule 47 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
47	X	1	Total	C	H	N	O	P	S	0
			78	23	43	2	8	1	1	
47	F	1	Total	C	H	N	O	P	S	0
			78	23	43	2	8	1	1	

- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



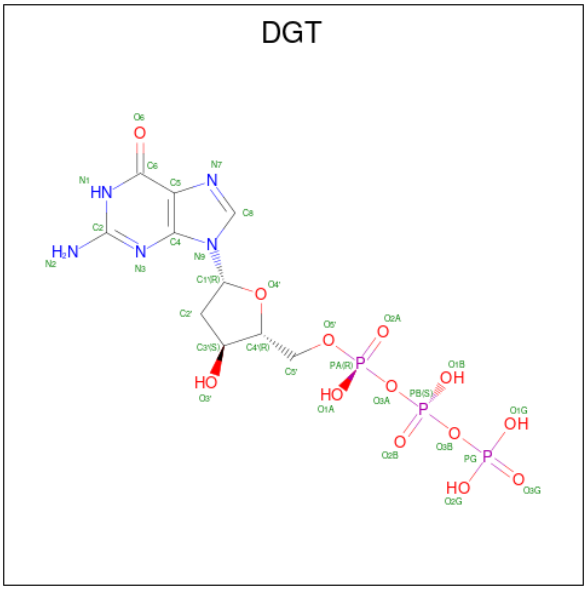
Mol	Chain	Residues	Atoms						AltConf
48	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
48	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	j	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	o	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	r	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	s	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
48	N	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	

- Molecule 49 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

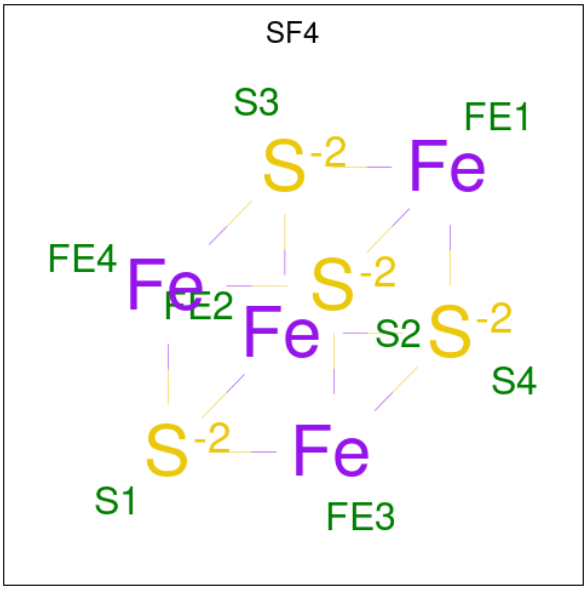


Mol	Chain	Residues	Atoms						AltConf
49	w	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

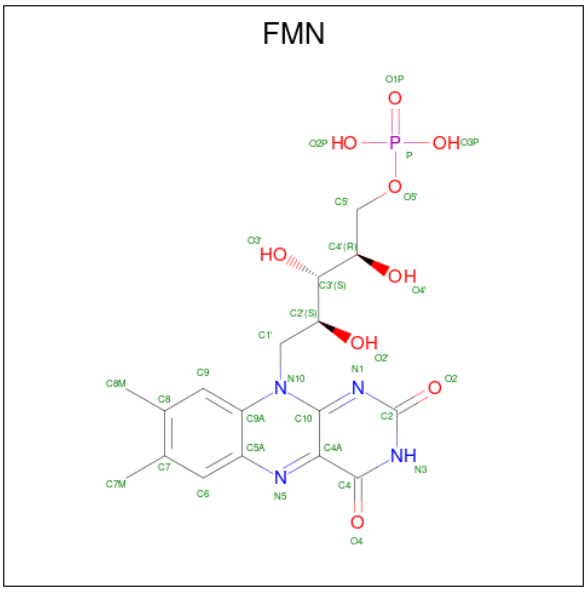
Mol	Chain	Residues	Atoms		AltConf
50	w	1	Total	Mg	0
			1	1	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



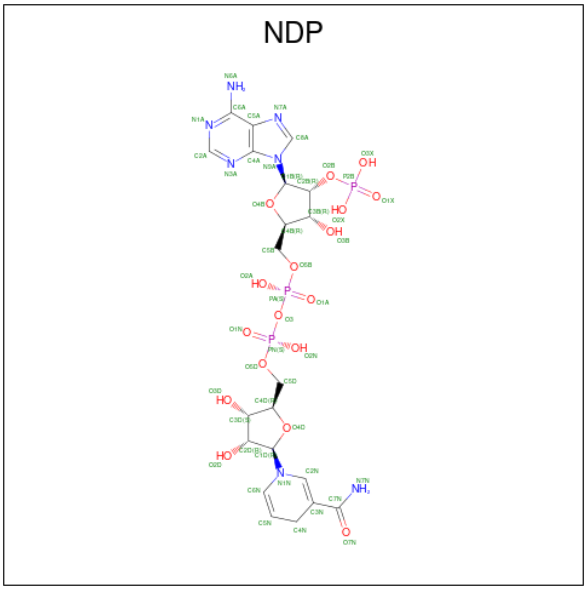
Mol	Chain	Residues	Atoms	AltConf
51	C	1	Total Fe S 8 4 4	0
51	D	1	Total Fe S 8 4 4	0
51	D	1	Total Fe S 8 4 4	0
51	E	1	Total Fe S 8 4 4	0
51	M	1	Total Fe S 8 4 4	0
51	M	1	Total Fe S 8 4 4	0

- Molecule 52 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
52	C	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

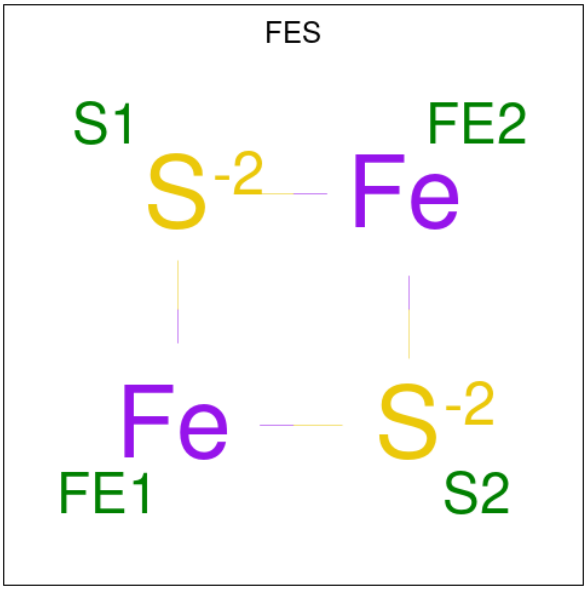
- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
54	M	1	Total Fe S 4 2 2	0
54	O	1	Total Fe S 4 2 2	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	T	1	Total Zn 1 1	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	AltConf
56	X	1	Total O 1 1	0

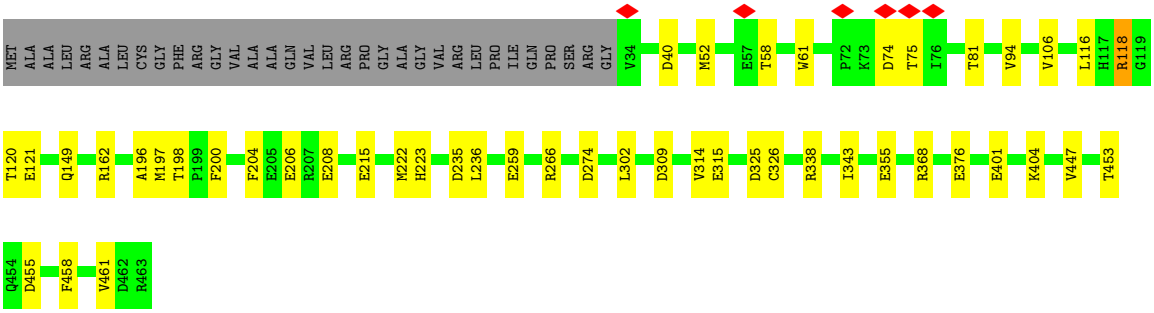
3 Residue-property plots (i)

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] iron-sulfur protein 2, mitochondrial

Chain Q:

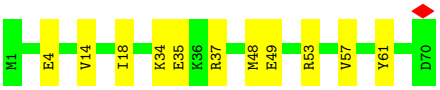




• Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:

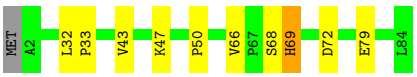




• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

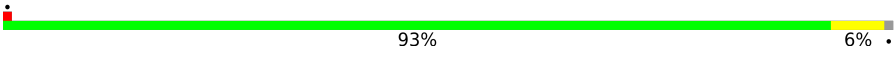
Chain U:

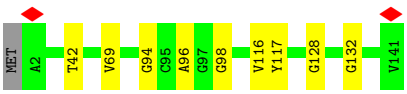




• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

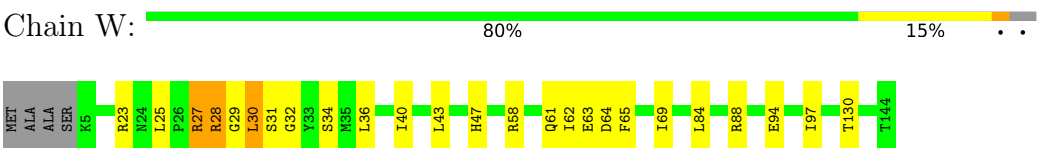
Chain V:





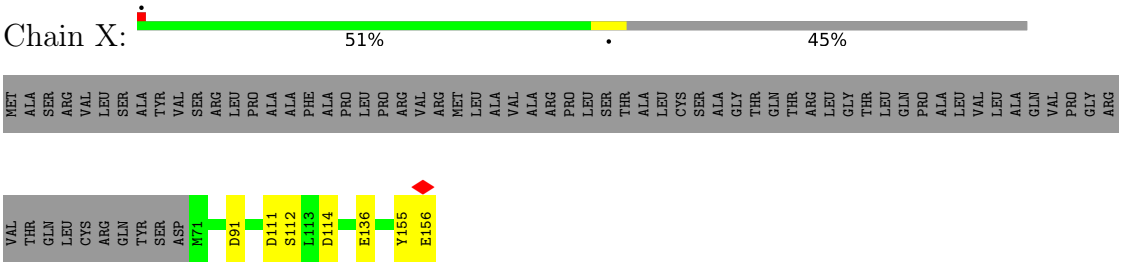
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



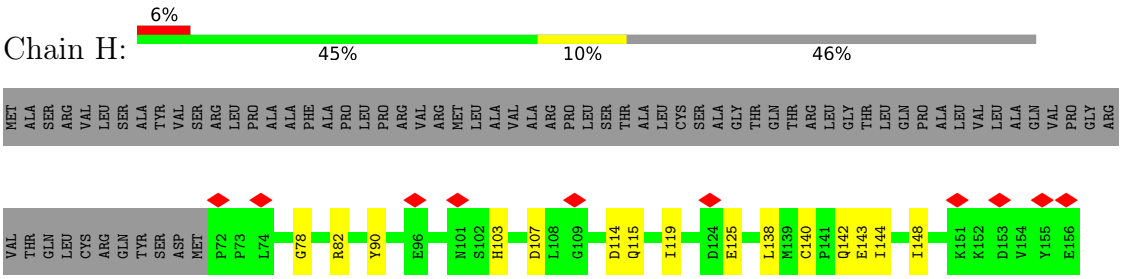
• Molecule 6: Acyl carrier protein, mitochondrial

Chain X:



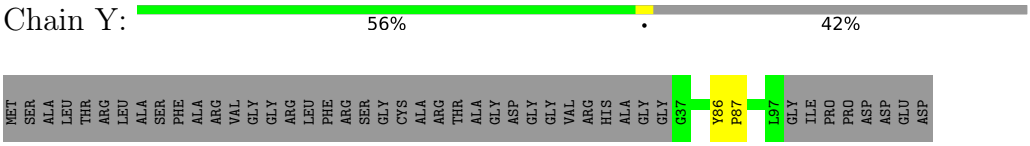
• Molecule 6: Acyl carrier protein, mitochondrial

Chain H:



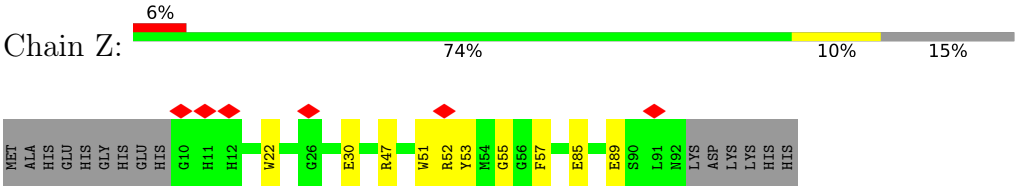
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



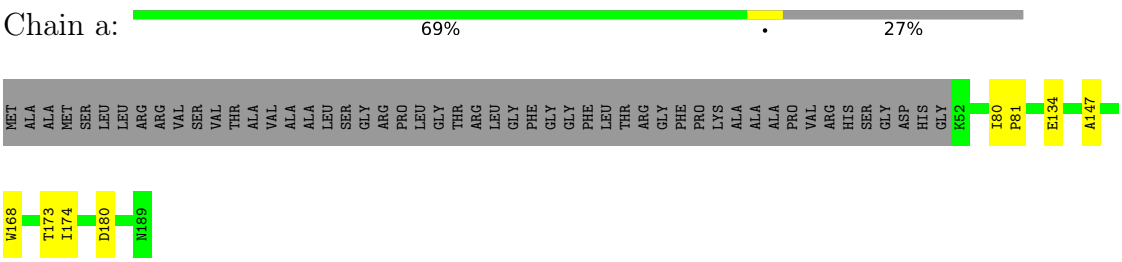
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

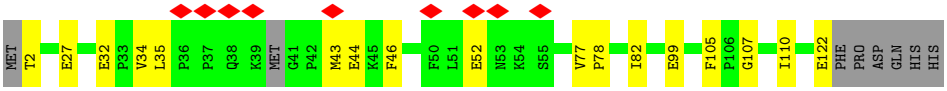
Chain a:



• Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:

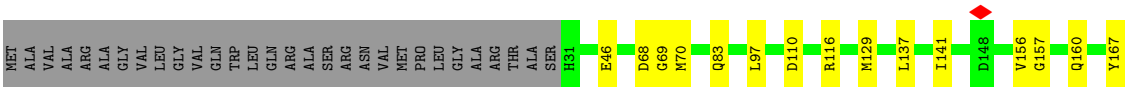


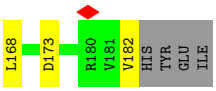


• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:



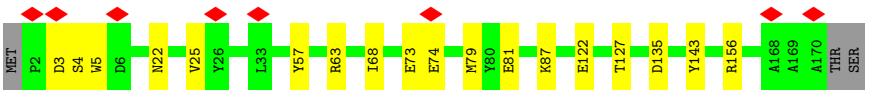




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:

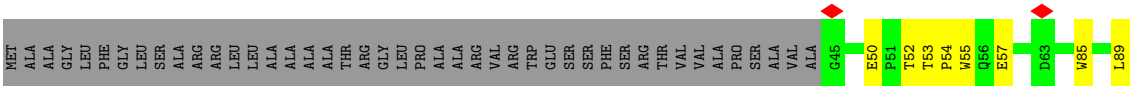




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:

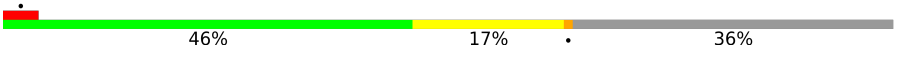


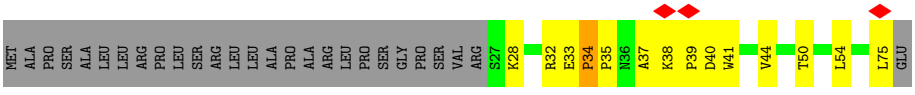




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

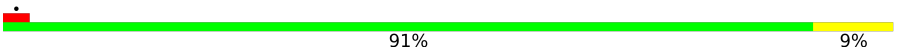
Chain f:

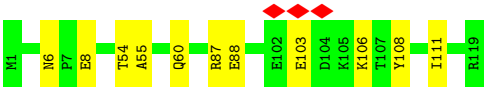




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:

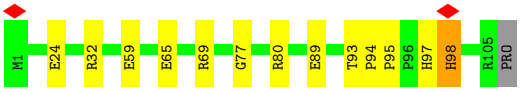




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:

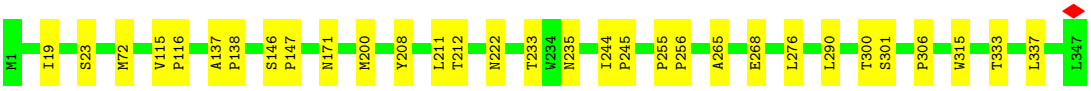




• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

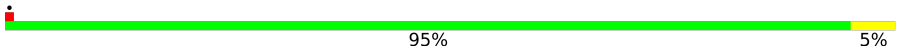
Chain i:

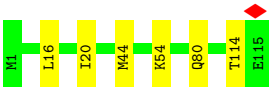




• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:

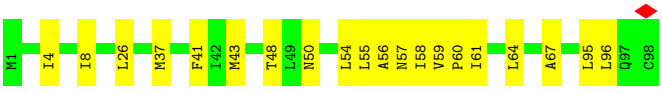




• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

Chain k:

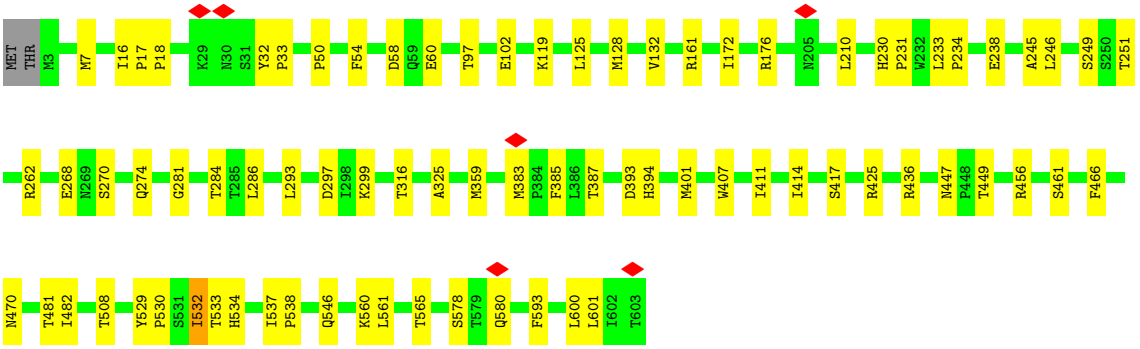




• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

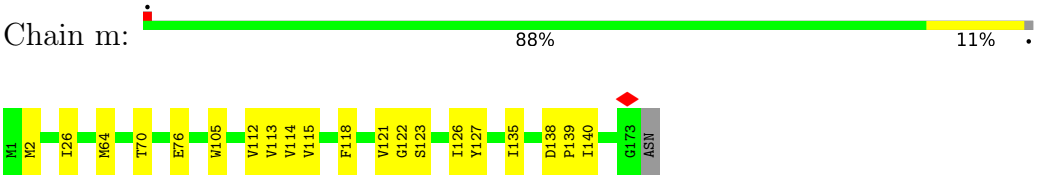
Chain l:





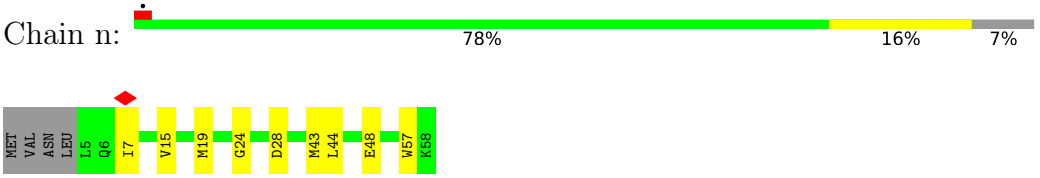
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m:



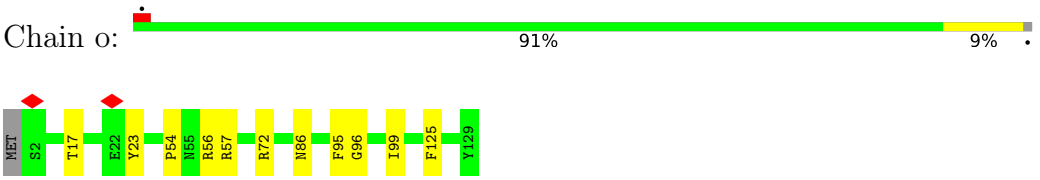
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



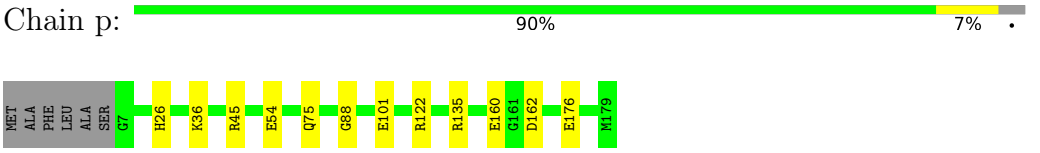
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:



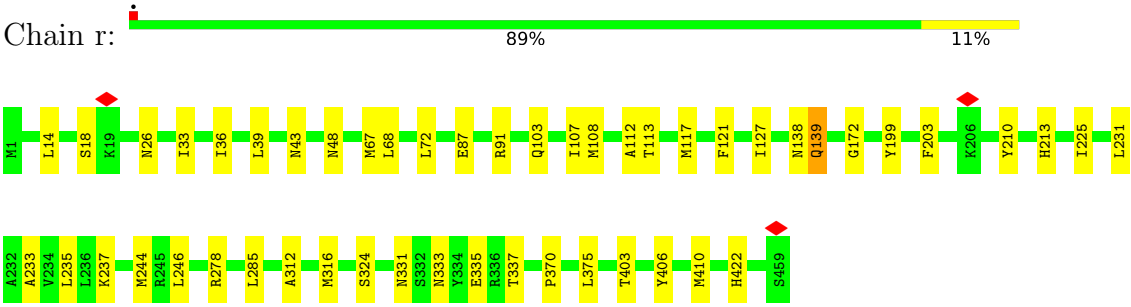
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



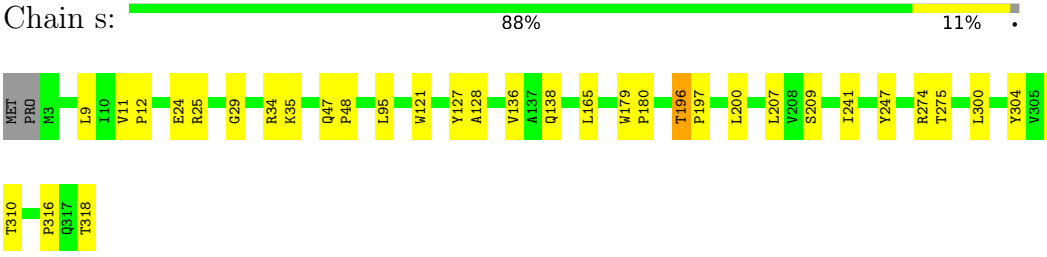
• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain r:



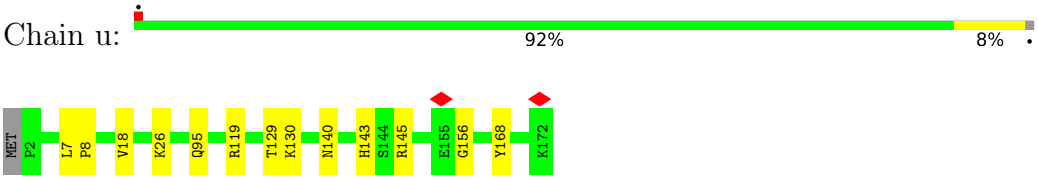
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s:



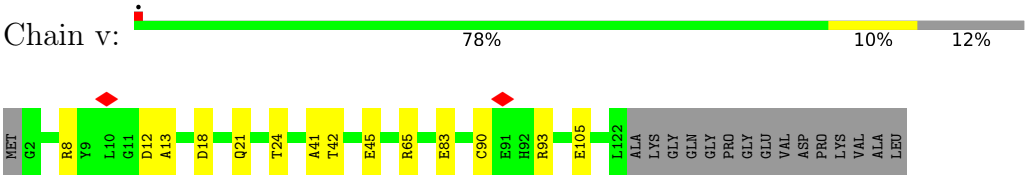
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:



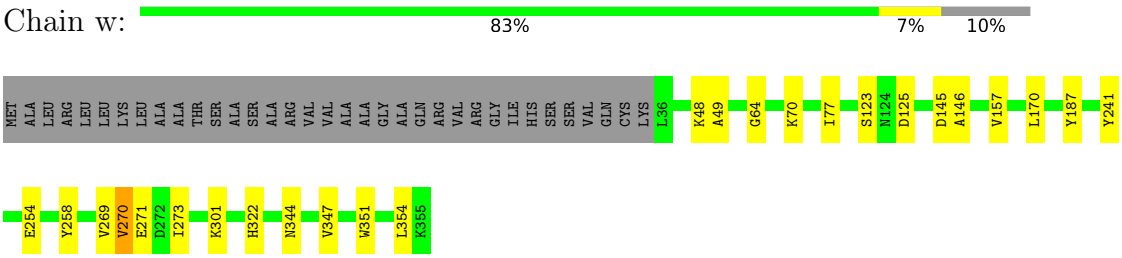
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



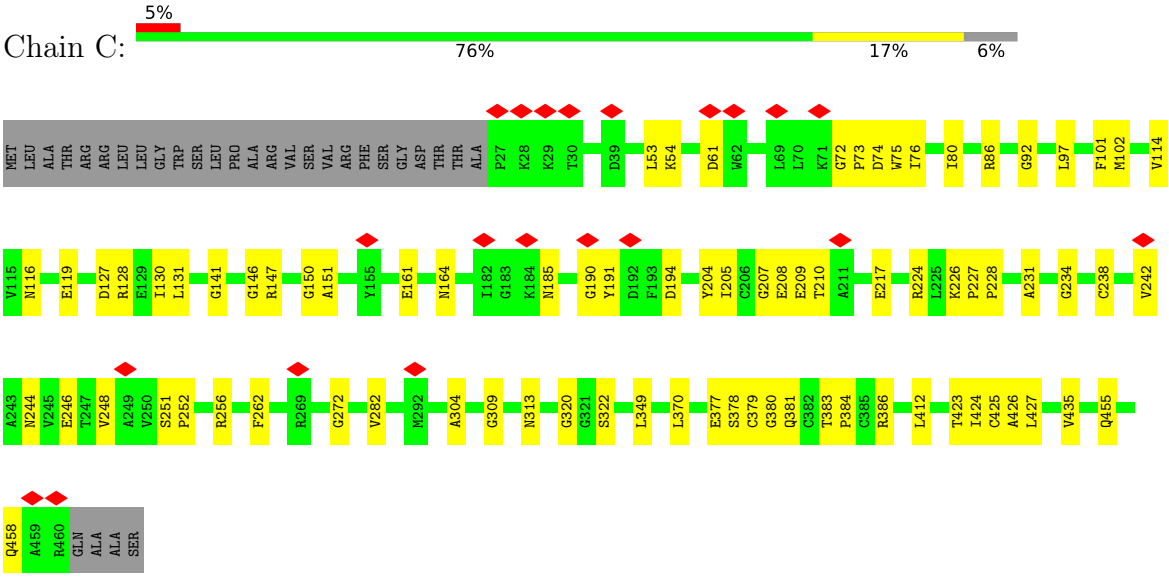
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:



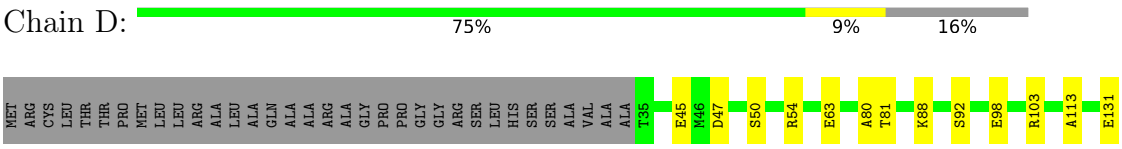
• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

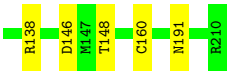
Chain C:



• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain D:



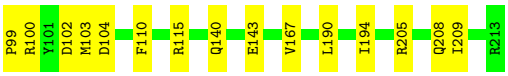


• Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain E:



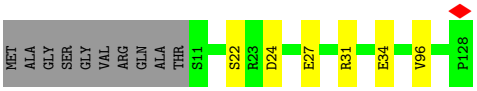




• Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain F:





• Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain G:

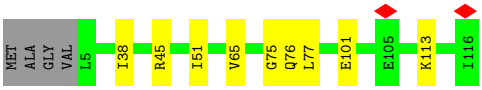




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain I:





• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:

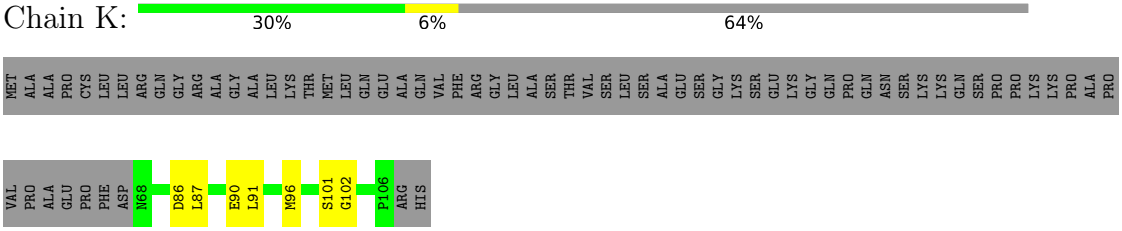






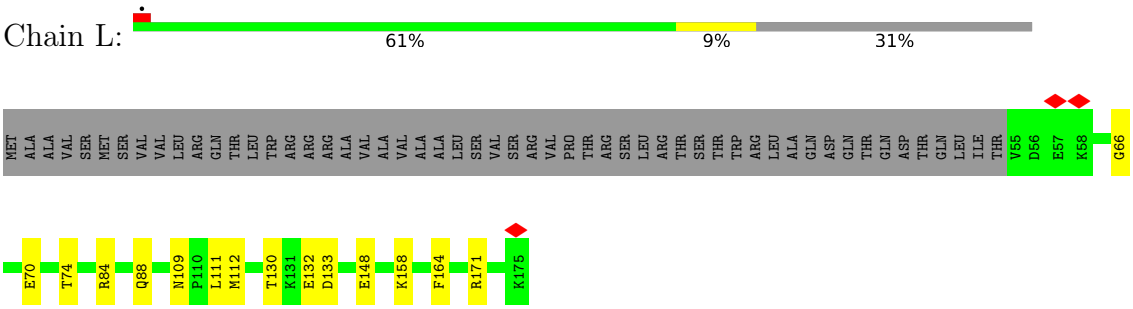
• Molecule 37: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



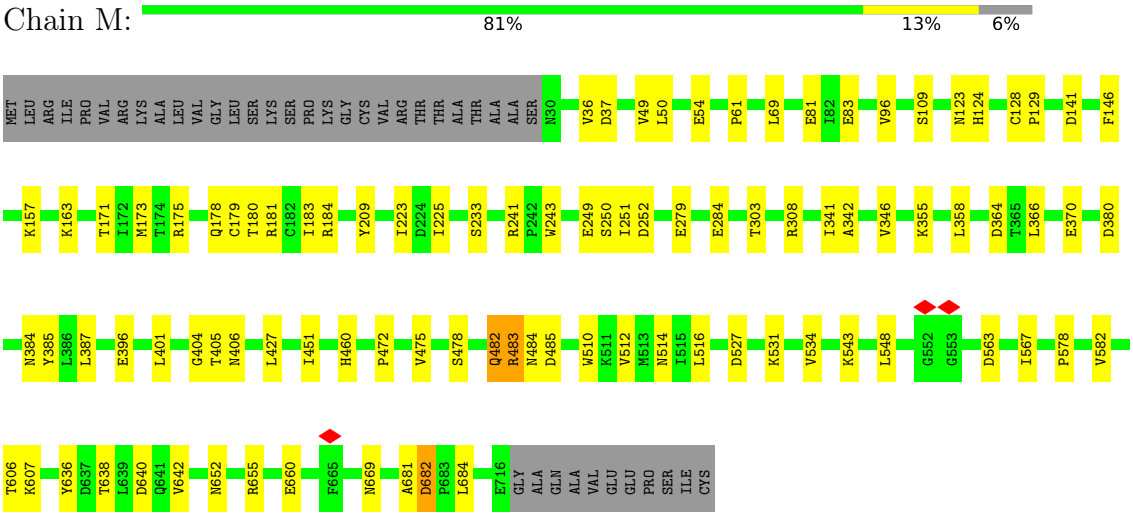
• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



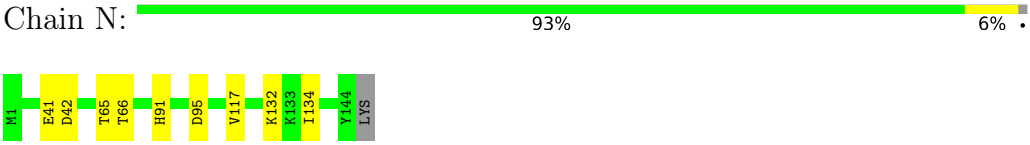
• Molecule 39: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



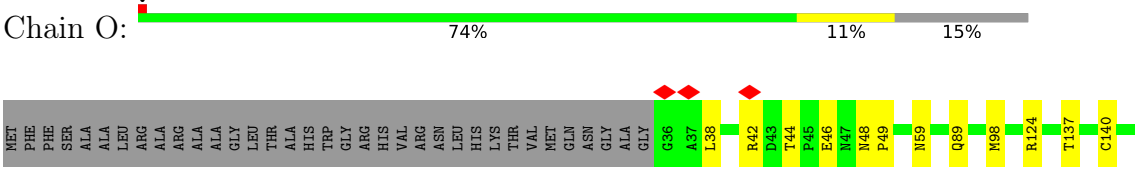
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

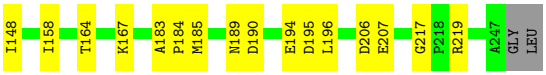
Chain N:



• Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

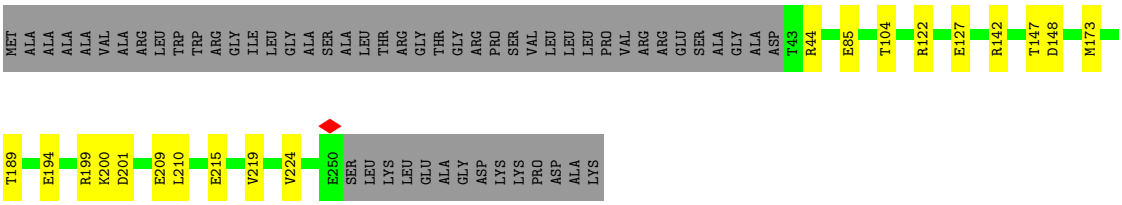
Chain O:





• Molecule 42: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



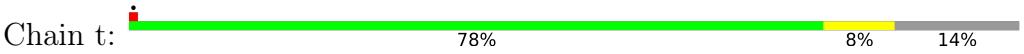


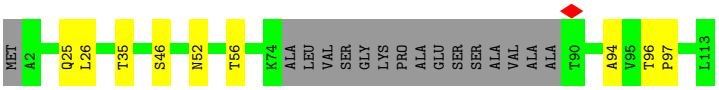
• Molecule 43: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.381	Depositor
Minimum map value	-1.294	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.477	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.875, 0.875, 0.875	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: FMN, 8Q1, DGT, SF4, ZN, PEE, PLX, SEP, FES, CDL, NMM, MG, NDP

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	Q	0.22	0/3540	0.27	0/4798
2	S	0.18	0/583	0.25	0/785
3	U	0.18	0/670	0.34	0/920
4	V	0.17	0/1065	0.23	0/1450
5	W	0.18	0/1182	0.29	0/1600
6	H	0.13	0/700	0.27	0/945
6	X	0.15	0/708	0.23	0/956
7	Y	0.14	0/570	0.31	0/778
8	Z	0.15	0/702	0.33	0/945
9	a	0.16	0/1209	0.22	0/1639
10	b	0.15	0/1054	0.29	0/1423
11	c	0.16	0/1326	0.26	0/1809
12	d	0.15	0/1463	0.24	0/1968
13	e	0.21	0/915	0.37	0/1245
14	f	0.17	0/432	0.29	0/585
15	g	0.17	0/1046	0.23	0/1412
16	h	0.18	0/892	0.30	0/1193
17	i	0.20	0/2806	0.30	0/3840
18	j	0.21	0/952	0.30	0/1301
19	k	0.26	0/754	0.39	0/1024
20	l	0.16	0/4826	0.26	0/6594
21	m	0.20	0/1334	0.31	0/1816
22	n	0.14	0/468	0.26	0/630
23	o	0.16	0/1093	0.25	0/1479
24	p	0.16	0/1553	0.24	0/2104
25	r	0.18	0/3717	0.25	0/5082
26	s	0.22	0/2568	0.33	0/3523
27	u	0.15	0/1445	0.27	0/1953
28	v	0.13	0/1060	0.27	0/1417
29	w	0.19	0/2689	0.27	0/3637
30	C	0.15	0/3422	0.28	0/4620
31	D	0.22	0/1452	0.29	0/1964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	E	0.25	0/1309	0.33	0/1771
33	F	0.19	0/1024	0.25	0/1378
34	G	0.14	0/695	0.26	0/938
35	I	0.19	0/941	0.26	0/1275
36	J	0.19	0/2820	0.26	0/3819
37	K	0.11	0/312	0.27	0/423
38	L	0.19	0/1002	0.25	0/1352
39	M	0.18	0/5363	0.29	0/7267
40	N	0.19	0/1244	0.29	0/1691
41	O	0.14	0/1682	0.28	0/2289
42	P	0.23	0/1780	0.29	0/2424
43	T	0.19	0/766	0.24	0/1032
44	t	0.20	0/799	0.29	0/1081
All	All	0.18	0/67933	0.28	0/92175

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
3	U	0	1
5	W	0	1
13	e	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	U	69	HIS	Peptide
5	W	27	ARG	Sidechain
13	e	120	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	3461	3433	3418	36	0
2	S	568	570	567	9	0
3	U	647	655	653	13	0
4	V	1038	1031	1027	5	0
5	W	1151	1153	1151	18	0
6	H	688	681	680	10	0
6	X	696	690	688	5	0
7	Y	544	491	487	1	0
8	Z	679	660	657	8	0
9	a	1174	1182	1177	7	0
10	b	1021	1049	1043	14	0
11	c	1273	1180	1174	13	0
12	d	1433	1404	1402	18	0
13	e	887	850	848	15	0
14	f	419	425	423	11	0
15	g	1012	1023	1021	12	0
16	h	871	876	872	11	0
17	i	2733	2893	2892	20	0
18	j	926	964	978	4	0
19	k	743	787	794	17	0
20	l	4703	4880	4878	55	0
21	m	1302	1317	1326	15	0
22	n	457	466	463	7	0
23	o	1066	1088	1086	8	0
24	p	1499	1448	1442	9	0
25	r	3623	3821	3817	35	0
26	s	2498	2593	2602	33	0
27	u	1405	1386	1378	15	0
28	v	1037	1032	1026	10	0
29	w	2623	2598	2587	25	0
30	C	3347	3321	3310	57	0
31	D	1420	1367	1364	14	0
32	E	1287	1290	1286	16	0
33	F	999	1017	1011	4	0
34	G	683	697	695	10	0
35	I	922	953	950	7	0
36	J	2745	2802	2787	23	0
37	K	304	282	269	6	0
38	L	979	975	968	12	0
39	M	5275	5321	5311	69	0
40	N	1203	1172	1167	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	O	1643	1648	1644	22	0
42	P	1730	1691	1685	14	0
43	T	752	732	727	8	0
44	t	780	802	798	7	0
45	E	51	77	80	3	0
45	J	51	77	80	0	0
45	V	51	77	80	2	0
45	W	51	77	80	0	0
45	i	100	149	151	2	0
45	l	51	77	80	2	0
46	V	200	312	312	0	0
46	i	64	80	72	0	0
46	l	164	236	228	2	0
46	u	64	80	72	0	0
47	F	35	43	0	1	0
47	X	35	43	0	0	0
48	N	52	88	88	0	0
48	g	104	176	176	1	0
48	j	52	88	88	0	0
48	o	52	88	88	0	0
48	r	52	88	88	0	0
48	s	52	88	88	1	0
49	w	31	12	12	1	0
50	w	1	0	0	0	0
51	C	8	0	0	3	0
51	D	16	0	0	0	0
51	E	8	0	0	1	0
51	M	16	0	0	2	0
52	C	31	19	14	32	0
53	J	48	26	24	1	0
54	M	4	0	0	0	0
54	O	4	0	0	1	0
55	T	1	0	0	0	0
56	X	1	0	0	0	0
All	All	67696	68697	68430	672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 672 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:C:502:FMN:C4A	52:C:502:FMN:N5	1.70	1.54
52:C:502:FMN:C10	52:C:502:FMN:N1	1.71	1.50
52:C:502:FMN:C7	52:C:502:FMN:C7M	2.00	1.38
52:C:502:FMN:O5'	52:C:502:FMN:C5'	1.77	1.32
52:C:502:FMN:O2'	52:C:502:FMN:C3'	1.85	1.25

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	427/463 (92%)	405 (95%)	22 (5%)	0	100	100
2	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
3	U	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
4	V	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
5	W	138/144 (96%)	130 (94%)	5 (4%)	3 (2%)	5	7
6	H	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
6	X	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
7	Y	59/105 (56%)	54 (92%)	5 (8%)	0	100	100
8	Z	81/98 (83%)	70 (86%)	11 (14%)	0	100	100
9	a	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
10	b	116/128 (91%)	102 (88%)	14 (12%)	0	100	100
11	c	150/186 (81%)	137 (91%)	13 (9%)	0	100	100
12	d	167/172 (97%)	166 (99%)	1 (1%)	0	100	100
13	e	105/153 (69%)	94 (90%)	11 (10%)	0	100	100
14	f	47/76 (62%)	44 (94%)	2 (4%)	1 (2%)	5	7
15	g	118/119 (99%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	h	103/106 (97%)	91 (88%)	11 (11%)	1 (1%)	12	18
17	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
18	j	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
19	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
20	l	599/603 (99%)	561 (94%)	37 (6%)	1 (0%)	43	58
21	m	171/174 (98%)	155 (91%)	16 (9%)	0	100	100
22	n	52/58 (90%)	47 (90%)	5 (10%)	0	100	100
23	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	171/179 (96%)	161 (94%)	10 (6%)	0	100	100
25	r	457/459 (100%)	441 (96%)	15 (3%)	1 (0%)	43	58
26	s	314/318 (99%)	294 (94%)	19 (6%)	1 (0%)	36	50
27	u	169/172 (98%)	156 (92%)	13 (8%)	0	100	100
28	v	119/137 (87%)	110 (92%)	9 (8%)	0	100	100
29	w	318/355 (90%)	303 (95%)	14 (4%)	1 (0%)	36	50
30	C	430/464 (93%)	392 (91%)	38 (9%)	0	100	100
31	D	174/210 (83%)	169 (97%)	5 (3%)	0	100	100
32	E	158/213 (74%)	147 (93%)	11 (7%)	0	100	100
33	F	116/128 (91%)	110 (95%)	6 (5%)	0	100	100
34	G	83/99 (84%)	74 (89%)	9 (11%)	0	100	100
35	I	110/116 (95%)	102 (93%)	8 (7%)	0	100	100
36	J	339/377 (90%)	316 (93%)	23 (7%)	0	100	100
37	K	37/108 (34%)	31 (84%)	6 (16%)	0	100	100
38	L	119/175 (68%)	113 (95%)	6 (5%)	0	100	100
39	M	685/727 (94%)	620 (90%)	62 (9%)	3 (0%)	30	42
40	N	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
41	O	210/249 (84%)	187 (89%)	23 (11%)	0	100	100
42	P	206/264 (78%)	189 (92%)	17 (8%)	0	100	100
43	T	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
44	t	93/113 (82%)	83 (89%)	10 (11%)	0	100	100
All	All	8147/9202 (88%)	7597 (93%)	538 (7%)	12 (0%)	49	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	W	28	ARG
16	h	98	HIS
26	s	196	THR
29	w	270	VAL
39	M	483	ARG

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	Q	370/392 (94%)	370 (100%)	0	100	100
2	S	59/59 (100%)	59 (100%)	0	100	100
3	U	72/73 (99%)	72 (100%)	0	100	100
4	V	102/103 (99%)	102 (100%)	0	100	100
5	W	121/123 (98%)	121 (100%)	0	100	100
6	H	79/136 (58%)	79 (100%)	0	100	100
6	X	80/136 (59%)	80 (100%)	0	100	100
7	Y	58/87 (67%)	58 (100%)	0	100	100
8	Z	66/79 (84%)	66 (100%)	0	100	100
9	a	124/159 (78%)	124 (100%)	0	100	100
10	b	113/122 (93%)	113 (100%)	0	100	100
11	c	136/161 (84%)	136 (100%)	0	100	100
12	d	152/155 (98%)	152 (100%)	0	100	100
13	e	99/130 (76%)	99 (100%)	0	100	100
14	f	45/67 (67%)	45 (100%)	0	100	100
15	g	106/105 (101%)	106 (100%)	0	100	100
16	h	91/92 (99%)	91 (100%)	0	100	100
17	i	314/314 (100%)	314 (100%)	0	100	100
18	j	104/104 (100%)	104 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	l	531/533 (100%)	531 (100%)	0	100	100
21	m	136/137 (99%)	136 (100%)	0	100	100
22	n	51/55 (93%)	51 (100%)	0	100	100
23	o	114/115 (99%)	114 (100%)	0	100	100
24	p	157/161 (98%)	157 (100%)	0	100	100
25	r	416/416 (100%)	416 (100%)	0	100	100
26	s	277/279 (99%)	277 (100%)	0	100	100
27	u	154/155 (99%)	154 (100%)	0	100	100
28	v	110/121 (91%)	110 (100%)	0	100	100
29	w	288/313 (92%)	288 (100%)	0	100	100
30	C	348/371 (94%)	348 (100%)	0	100	100
31	D	151/174 (87%)	151 (100%)	0	100	100
32	E	135/173 (78%)	135 (100%)	0	100	100
33	F	110/116 (95%)	110 (100%)	0	100	100
34	G	75/80 (94%)	75 (100%)	0	100	100
35	I	100/102 (98%)	100 (100%)	0	100	100
36	J	295/323 (91%)	295 (100%)	0	100	100
37	K	32/93 (34%)	32 (100%)	0	100	100
38	L	107/157 (68%)	107 (100%)	0	100	100
39	M	577/608 (95%)	577 (100%)	0	100	100
40	N	130/131 (99%)	130 (100%)	0	100	100
41	O	181/206 (88%)	181 (100%)	0	100	100
42	P	190/229 (83%)	190 (100%)	0	100	100
43	T	80/100 (80%)	80 (100%)	0	100	100
44	t	88/98 (90%)	88 (100%)	0	100	100
All	All	7209/7928 (91%)	7209 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
36	J	323	HIS

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Mol	Chain	Res	Type
40	N	116	ASN
36	J	356	HIS
39	M	148	ASN
41	O	59	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NMM	Q	118	1	9,11,12	1.74	1 (11%)	6,12,14	1.36	1 (16%)
32	SEP	E	58	32	8,9,10	1.55	1 (12%)	8,12,14	1.51	2 (25%)

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
1	NMM	Q	118	1	-	1/9/11/13	-
32	SEP	E	58	32	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	118	NMM	CZ-NH2	4.61	1.45	1.34
32	E	58	SEP	P-O1P	3.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	E	58	SEP	P-OG-CB	-2.89	110.33	118.30
1	Q	118	NMM	NE-CZ-NH2	2.75	122.00	119.48
32	E	58	SEP	OG-CB-CA	2.54	110.61	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Q	118	NMM	O-C-CA-CB
32	E	58	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Q	118	NMM	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
53	NDP	J	401	-	49,52,52	3.97	22 (44%)	66,80,80	1.81	13 (19%)
48	PLX	g	202	-	51,51,51	1.01	3 (5%)	55,59,59	0.61	0
46	CDL	l	703	-	99,99,99	1.20	7 (7%)	105,111,111	0.92	2 (1%)
45	PEE	W	201	-	50,50,50	1.13	3 (6%)	53,55,55	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	8Q1	X	201	-	31,34,34	1.73	6 (19%)	40,43,43	1.29	4 (10%)
45	PEE	i	402	-	50,50,50	1.14	3 (6%)	53,55,55	1.15	3 (5%)
48	PLX	g	201	-	51,51,51	0.98	2 (3%)	55,59,59	0.69	0
45	PEE	E	301	-	50,50,50	1.12	3 (6%)	53,55,55	1.09	2 (3%)
48	PLX	r	501	-	51,51,51	1.00	4 (7%)	55,59,59	0.68	0
46	CDL	V	202	-	99,99,99	1.22	7 (7%)	105,111,111	1.25	5 (4%)
45	PEE	V	201	-	50,50,50	1.12	3 (6%)	53,55,55	1.05	2 (3%)
49	DGT	w	401	50	29,33,33	3.56	14 (48%)	44,52,52	2.14	13 (29%)
51	SF4	M	801	39	0,12,12	-	-	-		
51	SF4	M	802	39	0,12,12	-	-	-		
52	FMN	C	502	-	33,33,33	22.73	32 (96%)	48,50,50	7.20	26 (54%)
51	SF4	D	301	31	0,12,12	-	-	-		
46	CDL	i	401	-	63,63,99	1.37	7 (11%)	69,75,111	0.93	3 (4%)
54	FES	O	301	41	0,4,4	-	-	-		
48	PLX	N	201	-	51,51,51	0.99	3 (5%)	55,59,59	0.71	0
46	CDL	l	702	-	63,63,99	1.37	7 (11%)	69,75,111	0.96	3 (4%)
48	PLX	o	201	-	51,51,51	1.01	4 (7%)	55,59,59	0.68	1 (1%)
45	PEE	l	701	-	50,50,50	1.14	3 (6%)	53,55,55	1.28	3 (5%)
51	SF4	D	302	31	0,12,12	-	-	-		
45	PEE	J	402	-	50,50,50	1.13	3 (6%)	53,55,55	1.29	4 (7%)
48	PLX	s	401	-	51,51,51	0.97	3 (5%)	55,59,59	0.73	0
45	PEE	i	403	-	48,48,50	1.15	3 (6%)	51,53,55	1.04	3 (5%)
46	CDL	u	201	-	63,63,99	1.38	7 (11%)	69,75,111	0.82	2 (2%)
51	SF4	E	302	1,32	0,12,12	-	-	-		
51	SF4	C	501	30	0,12,12	-	-	-		
48	PLX	j	201	-	51,51,51	0.96	4 (7%)	55,59,59	0.76	2 (3%)
47	8Q1	F	201	-	31,34,34	1.73	6 (19%)	40,43,43	1.41	5 (12%)
54	FES	M	803	39	0,4,4	-	-	-		
46	CDL	V	203	-	99,99,99	1.21	7 (7%)	105,111,111	0.85	3 (2%)

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
53	NDP	J	401	-	-	5/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLX	g	202	-	-	12/55/55/55	-
46	CDL	l	703	-	-	14/110/110/110	-
45	PEE	W	201	-	-	15/54/54/54	-
45	PEE	i	402	-	-	15/54/54/54	-
47	8Q1	X	201	-	-	4/41/41/41	-
48	PLX	g	201	-	-	15/55/55/55	-
45	PEE	E	301	-	-	14/54/54/54	-
48	PLX	r	501	-	-	16/55/55/55	-
46	CDL	V	202	-	-	26/110/110/110	-
45	PEE	V	201	-	-	30/54/54/54	-
49	DGT	w	401	50	-	5/22/34/34	0/3/3/3
51	SF4	M	801	39	-	-	0/6/5/5
51	SF4	M	802	39	-	-	0/6/5/5
52	FMN	C	502	-	1/1/4/4	6/18/18/18	0/3/3/3
51	SF4	D	301	31	-	-	0/6/5/5
46	CDL	i	401	-	-	14/74/74/110	-
54	FES	O	301	41	-	-	0/1/1/1
48	PLX	N	201	-	-	13/55/55/55	-
46	CDL	l	702	-	-	22/74/74/110	-
48	PLX	o	201	-	-	12/55/55/55	-
45	PEE	l	701	-	-	20/54/54/54	-
51	SF4	D	302	31	-	-	0/6/5/5
45	PEE	J	402	-	-	13/54/54/54	-
48	PLX	s	401	-	-	18/55/55/55	-
45	PEE	i	403	-	-	14/52/52/54	-
46	CDL	u	201	-	-	12/74/74/110	-
51	SF4	E	302	1,32	-	-	0/6/5/5
51	SF4	C	501	30	-	-	0/6/5/5
48	PLX	j	201	-	-	18/55/55/55	-
47	8Q1	F	201	-	-	8/41/41/41	-
54	FES	M	803	39	-	-	0/1/1/1
46	CDL	V	203	-	-	25/110/110/110	-

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	C	502	FMN	C8M-C8	52.75	2.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	C	502	FMN	C9-C9A	52.75	2.25	1.39
52	C	502	FMN	C1'-C2'	50.06	2.23	1.52
52	C	502	FMN	O4'-C4'	-49.06	0.39	1.43
52	C	502	FMN	C5A-N5	37.04	2.10	1.39

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	C	502	FMN	C5A-C9A-N10	22.74	141.43	117.95
52	C	502	FMN	C4A-C10-N1	-20.90	76.23	124.73
52	C	502	FMN	N10-C10-N1	17.30	168.11	118.35
52	C	502	FMN	C8M-C8-C7	-15.51	88.95	120.74
52	C	502	FMN	C8M-C8-C9	11.96	141.60	119.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	C	502	FMN	C4'

5 of 366 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	V	201	PEE	C2-C1-O3P-P
45	V	201	PEE	C1-O3P-P-O2P
45	V	201	PEE	O4P-C4-C5-N
45	W	201	PEE	C1-O3P-P-O1P
45	W	201	PEE	C4-O4P-P-O2P

There are no ring outliers.

17 monomers are involved in 55 short contacts:

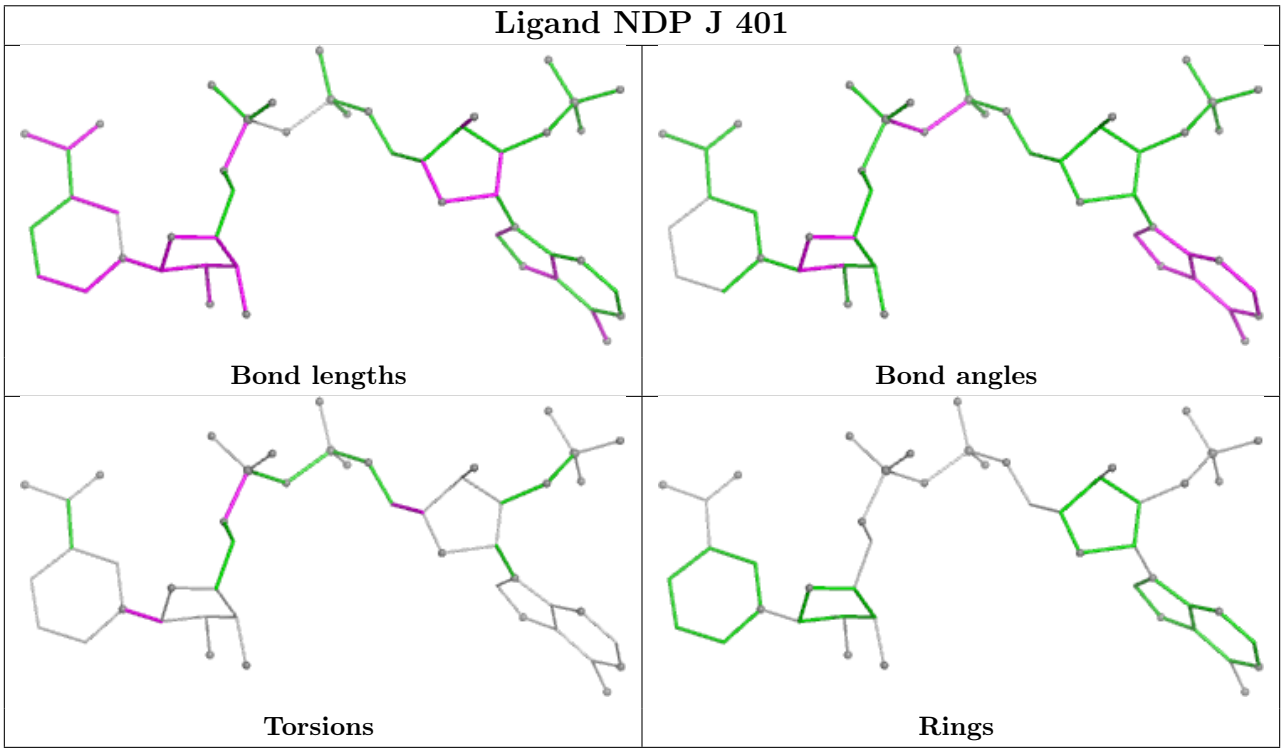
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	J	401	NDP	1	0
46	l	703	CDL	1	0
45	i	402	PEE	2	0
48	g	201	PLX	1	0
45	E	301	PEE	3	0
45	V	201	PEE	2	0
49	w	401	DGT	1	0
51	M	801	SF4	1	0
51	M	802	SF4	1	0

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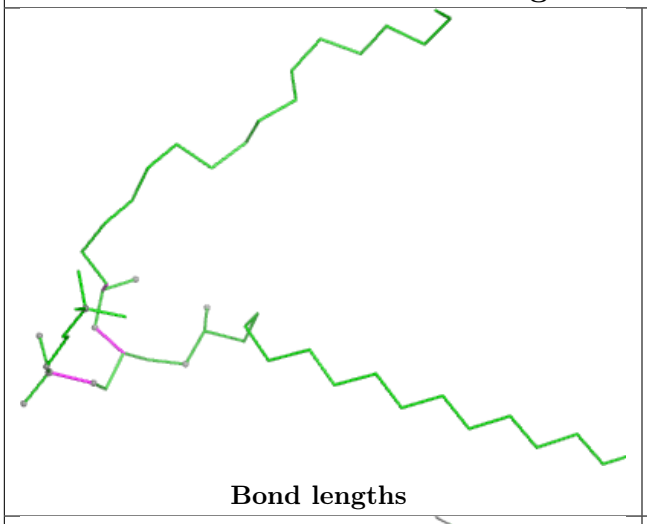
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	C	502	FMN	32	0
54	O	301	FES	1	0
46	l	702	CDL	1	0
45	l	701	PEE	2	0
48	s	401	PLX	1	0
51	E	302	SF4	1	0
51	C	501	SF4	3	0
47	F	201	8Q1	1	0

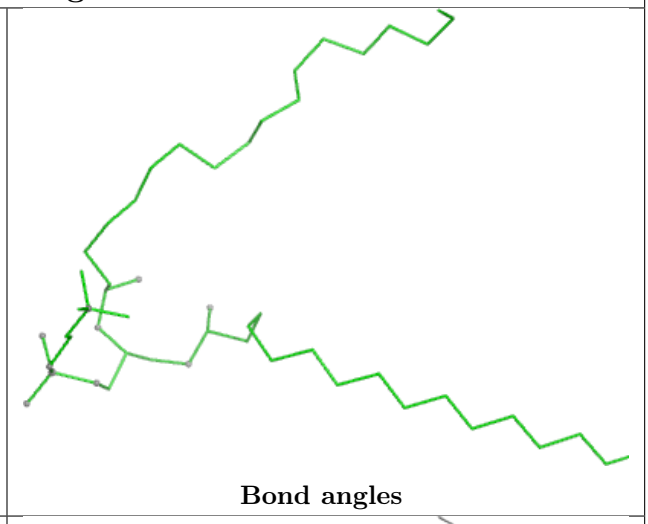
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



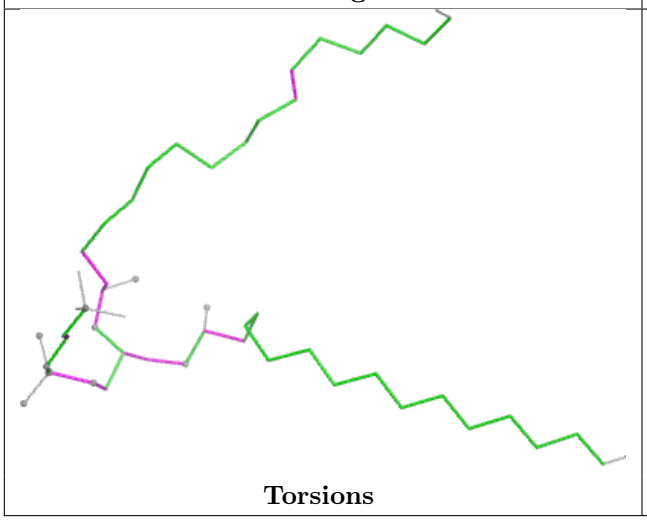
Ligand PLX g 202



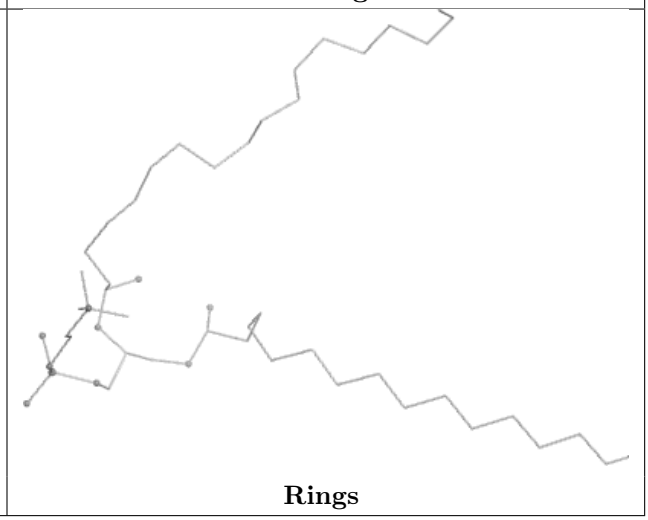
Bond lengths



Bond angles

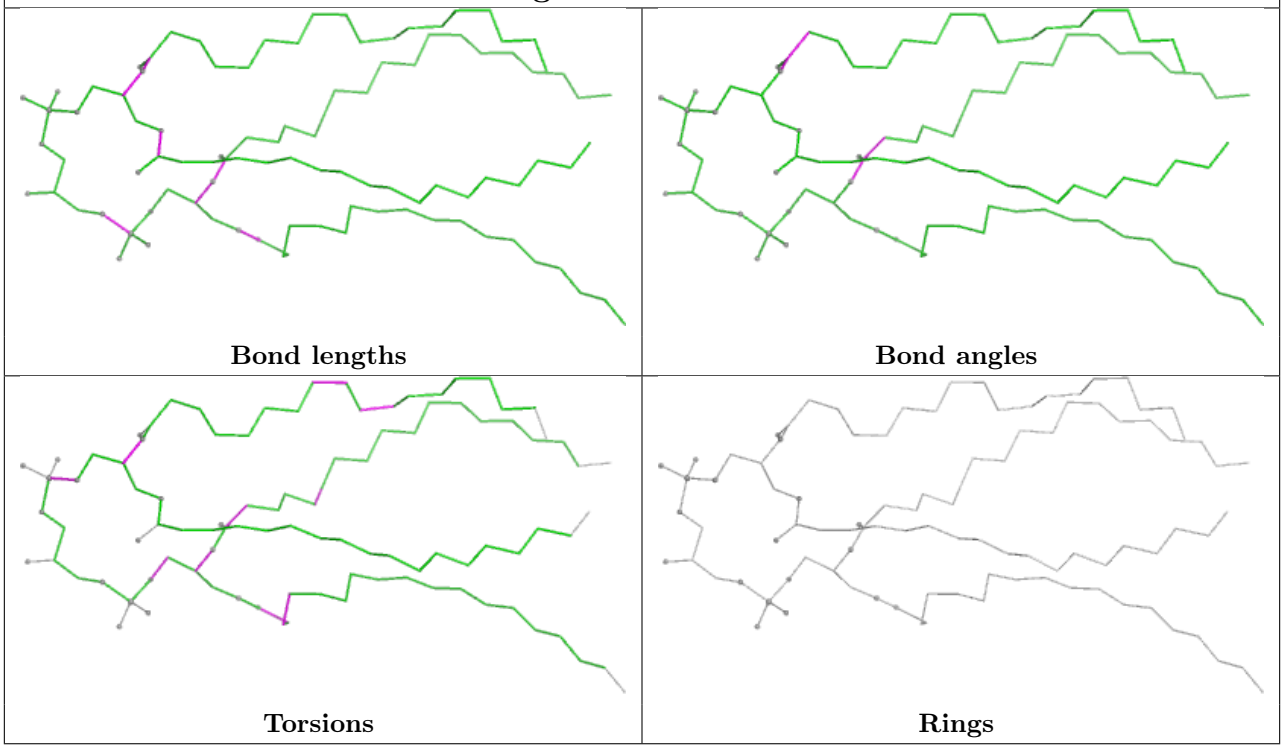


Torsions

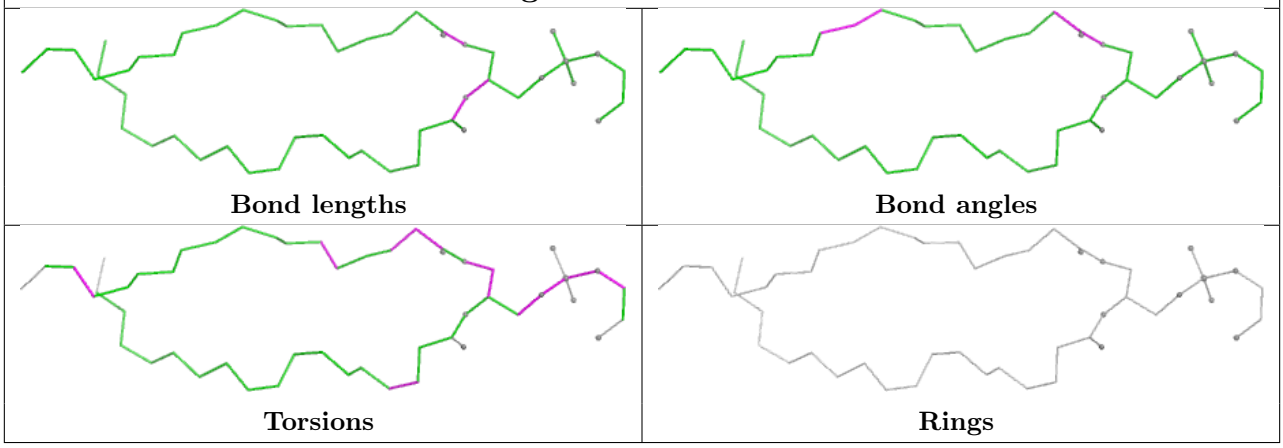


Rings

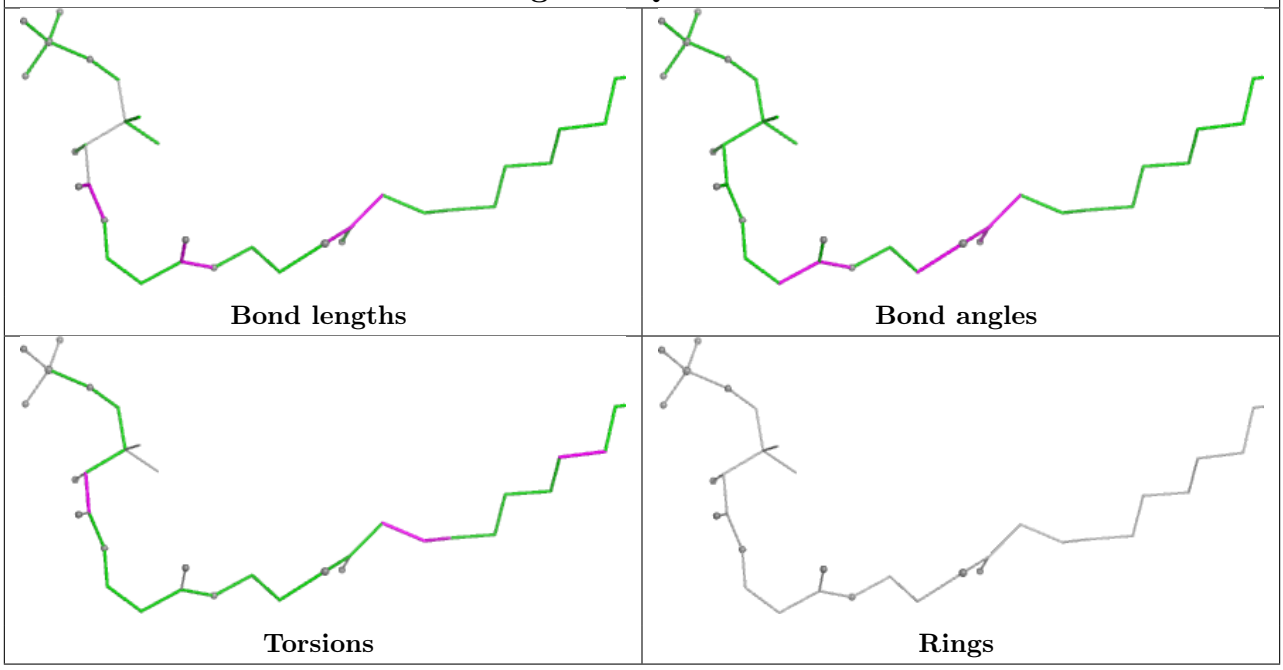
Ligand CDL l 703



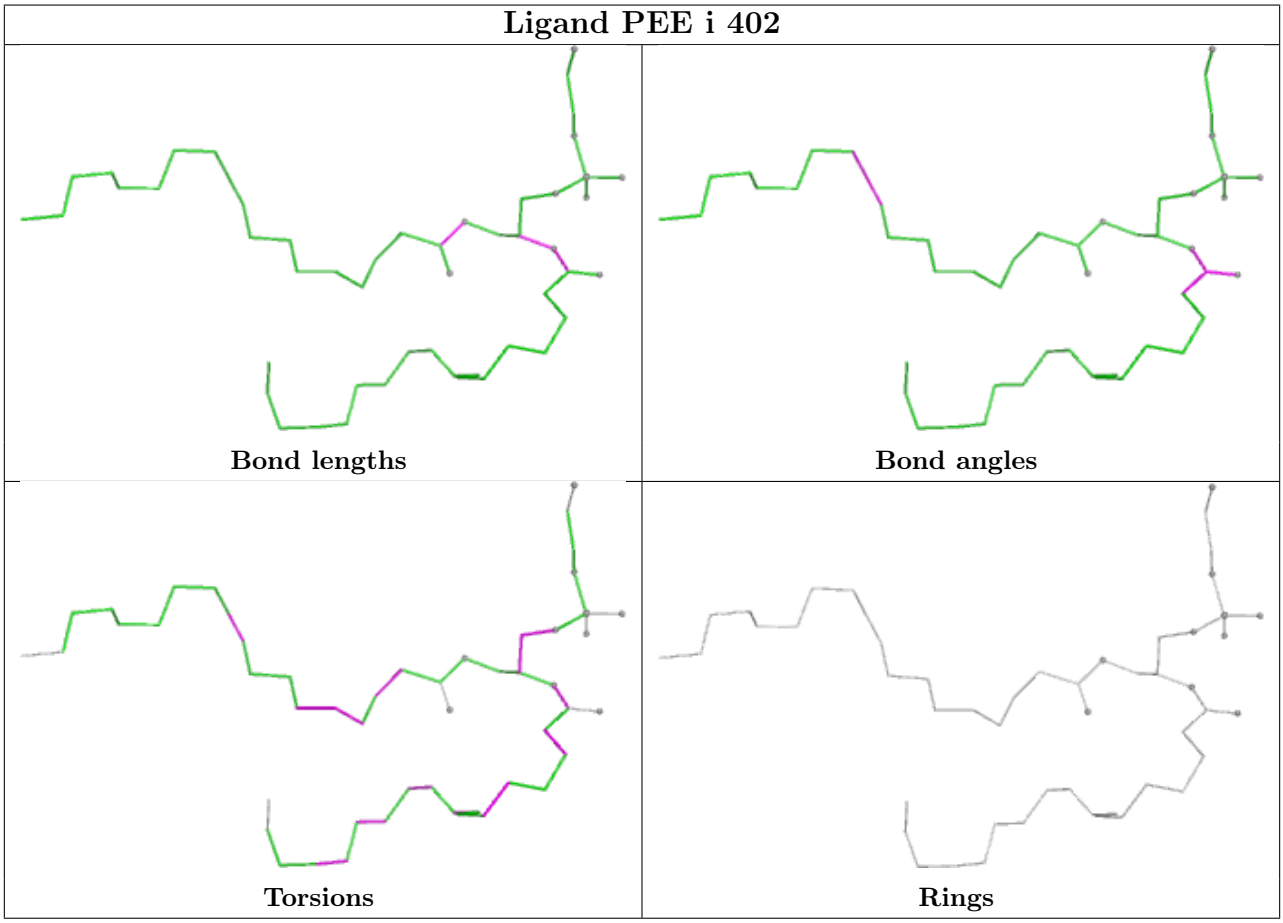
Ligand PEE W 201



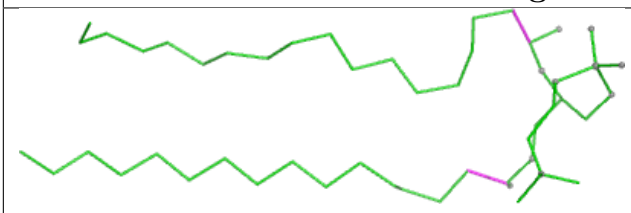
Ligand 8Q1 X 201



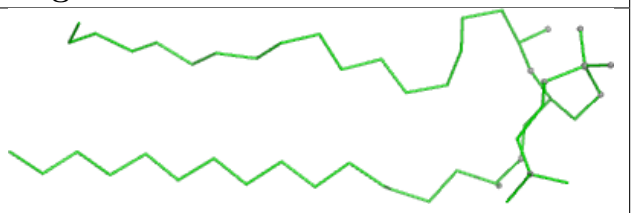
Ligand PEE i 402



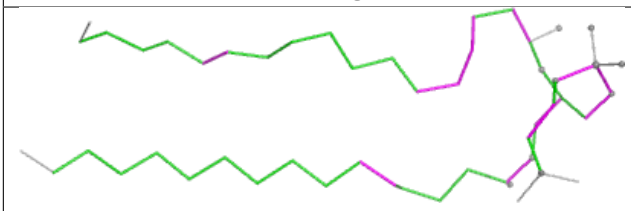
Ligand PLX g 201



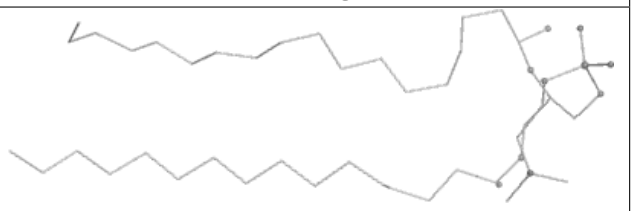
Bond lengths



Bond angles

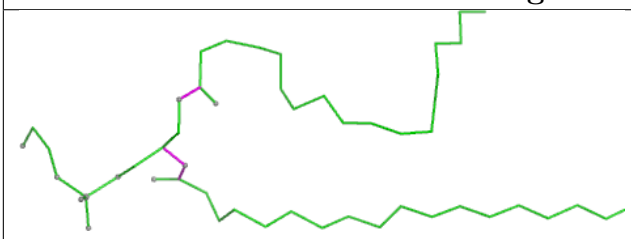


Torsions

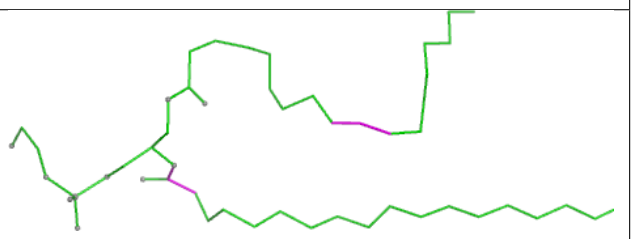


Rings

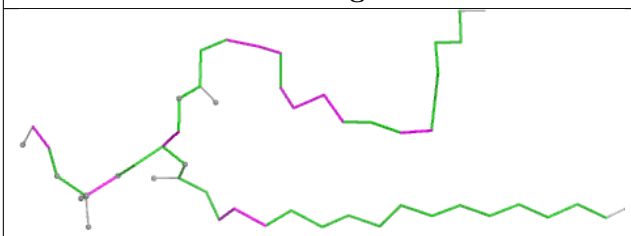
Ligand PEE E 301



Bond lengths



Bond angles

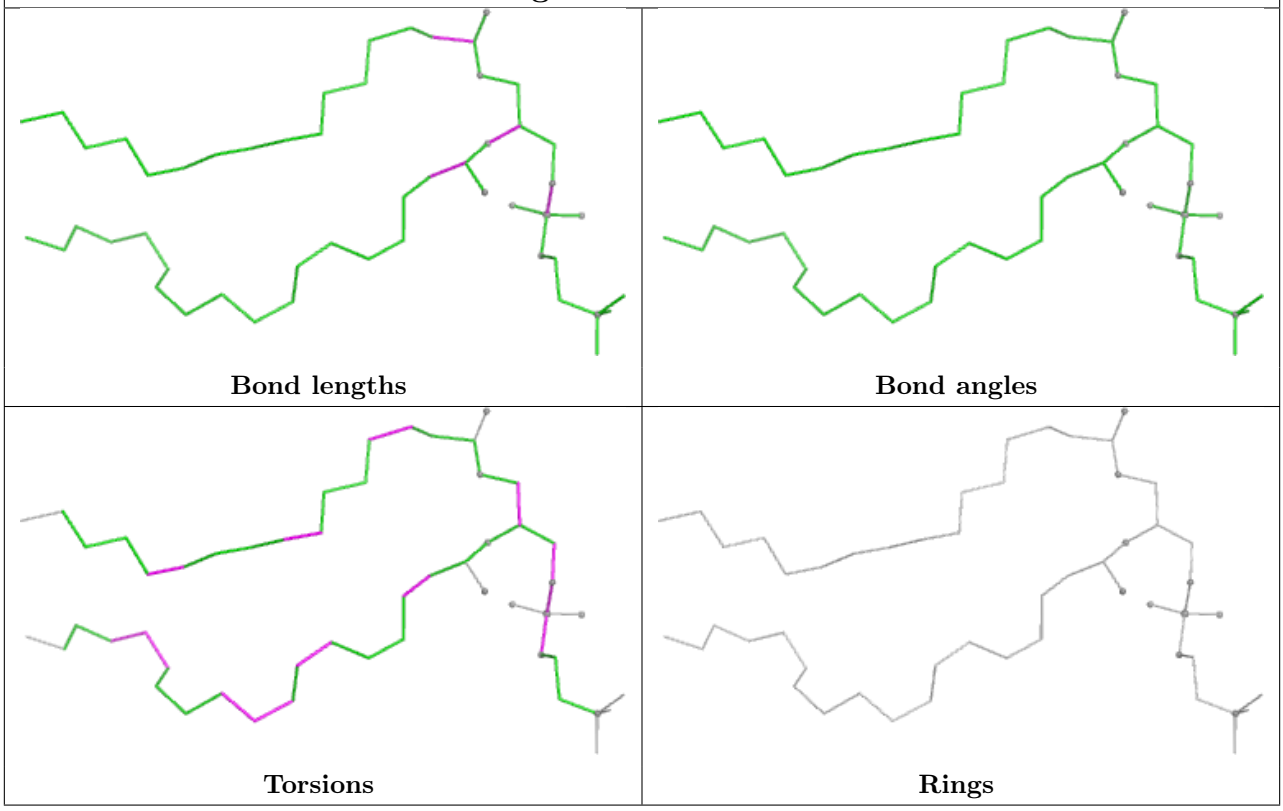


Torsions

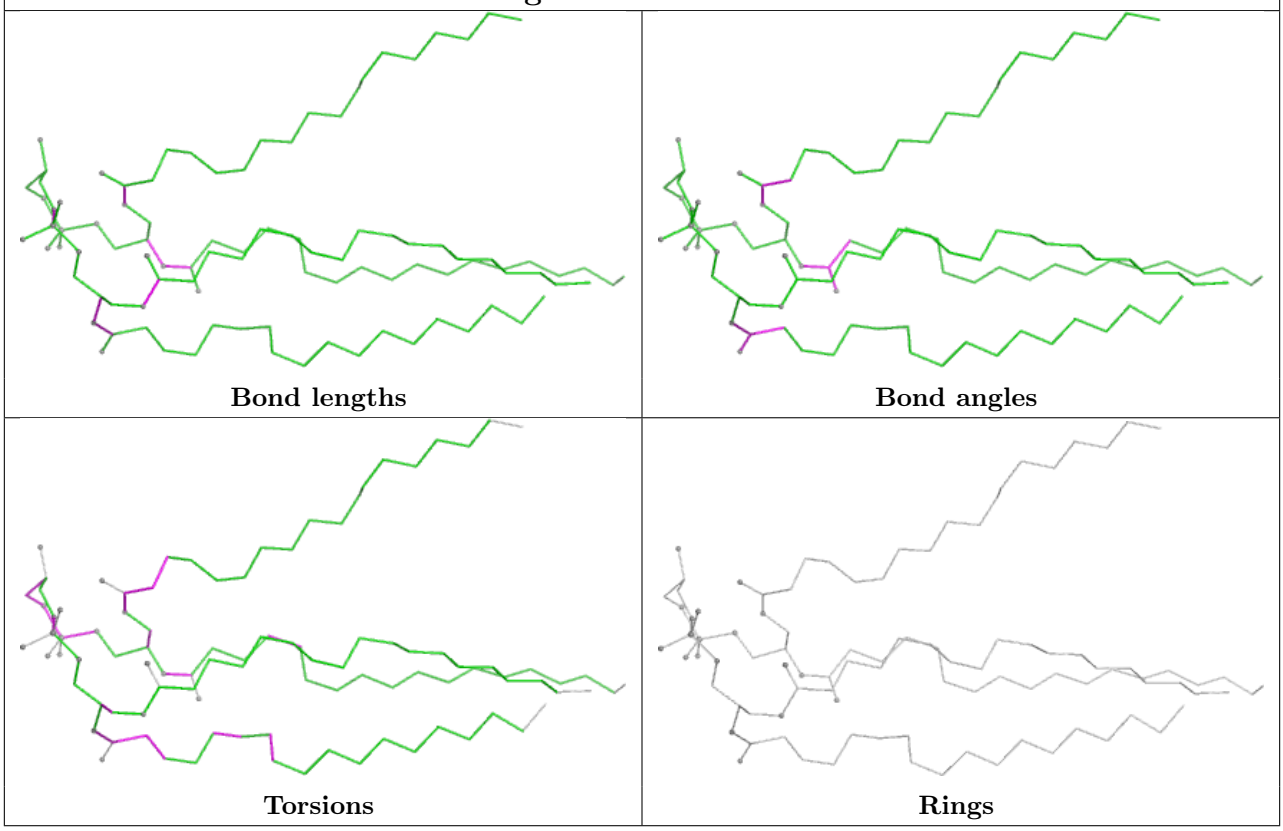


Rings

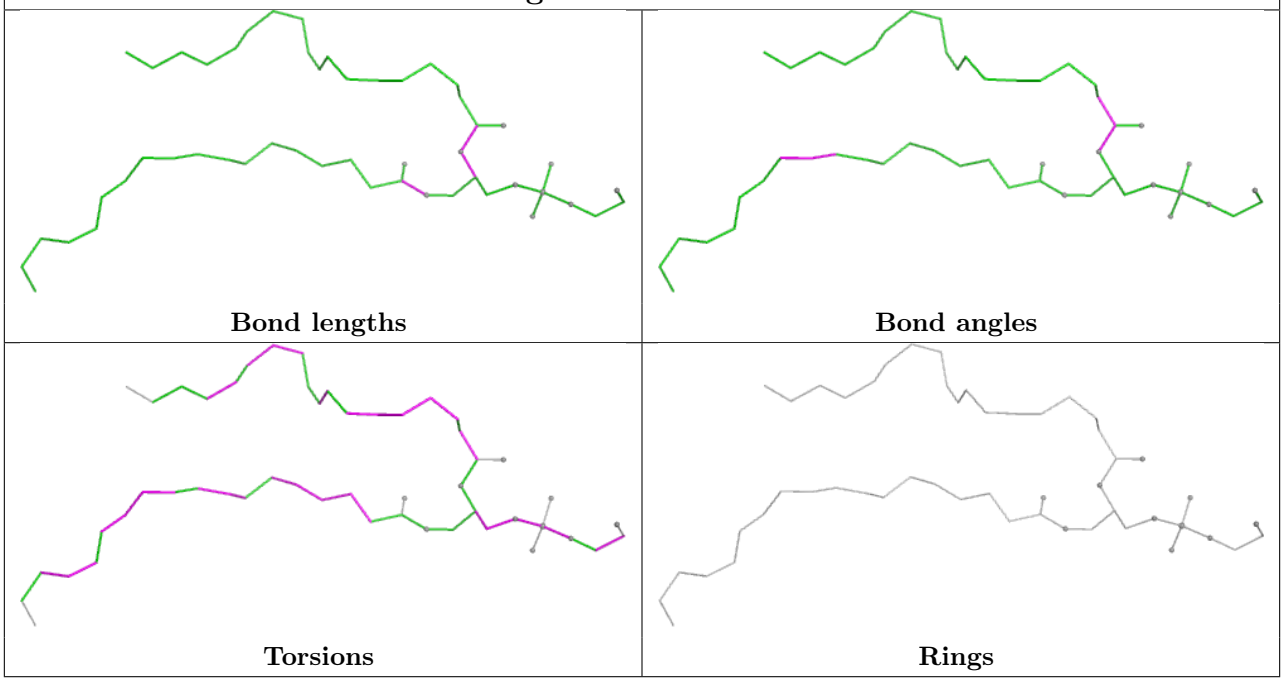
Ligand PLX r 501



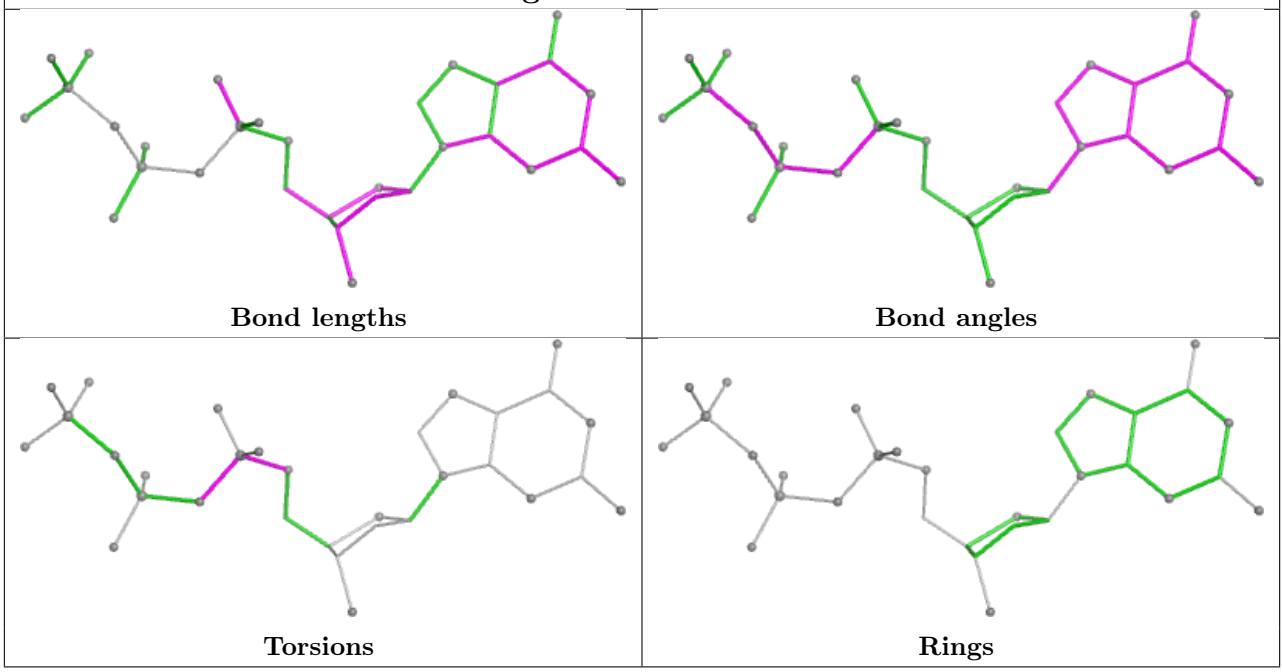
Ligand CDL V 202



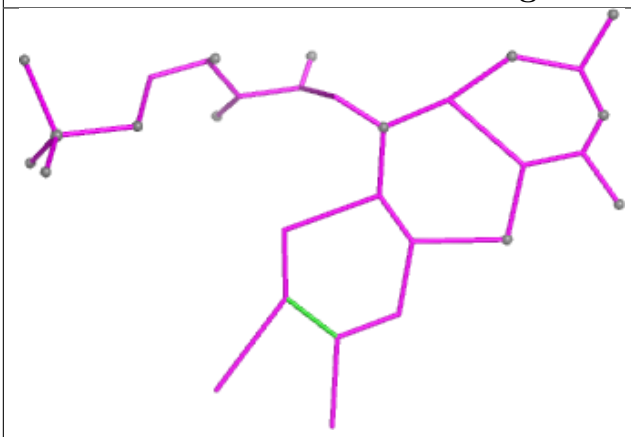
Ligand PEE V 201



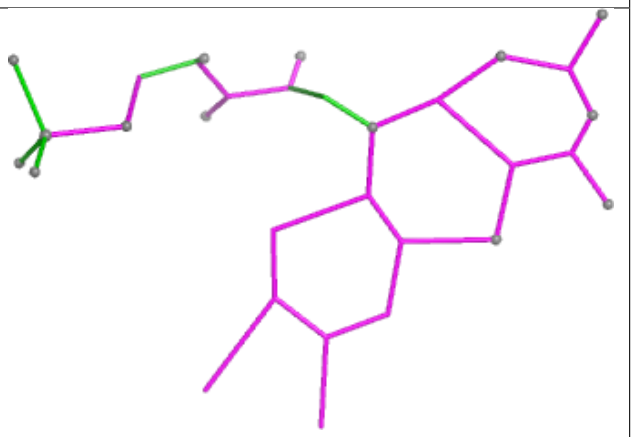
Ligand DGT w 401



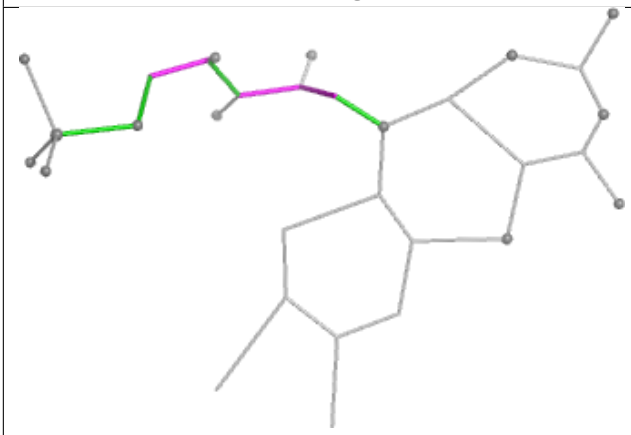
Ligand FMN C 502



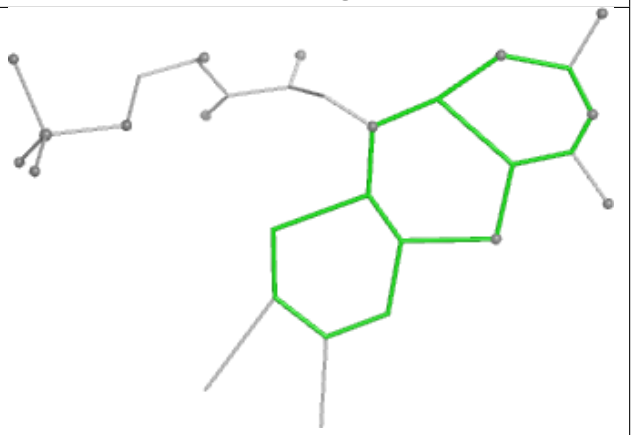
Bond lengths



Bond angles

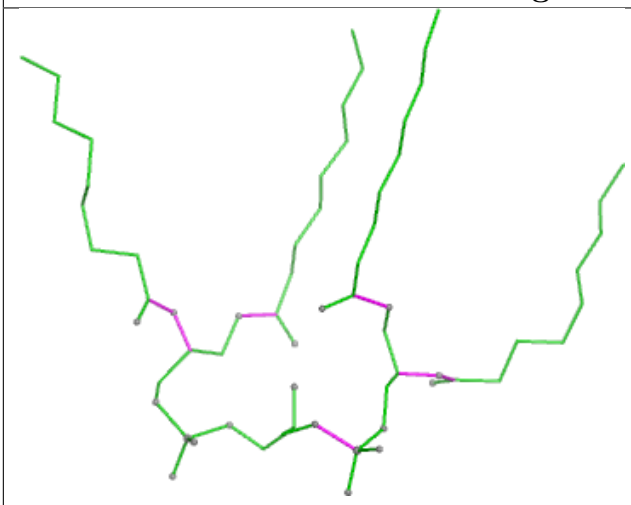


Torsions

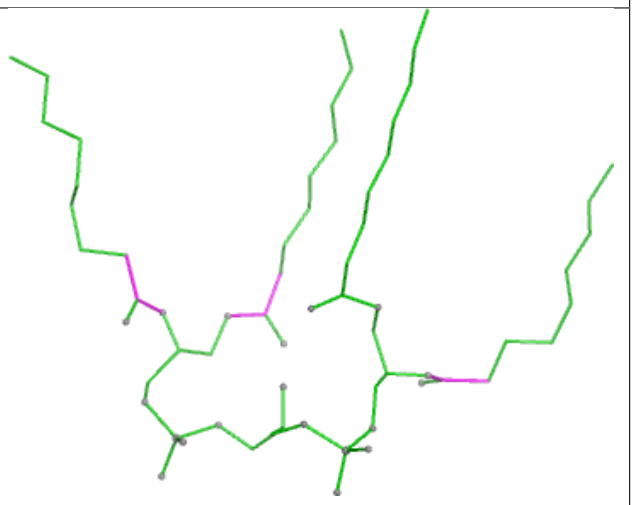


Rings

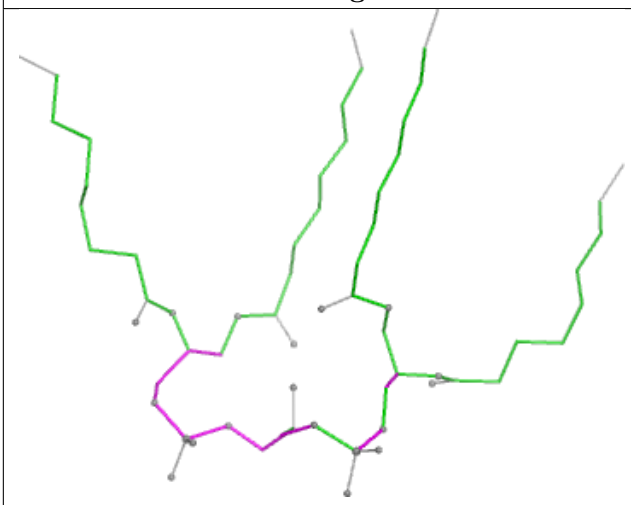
Ligand CDL i 401



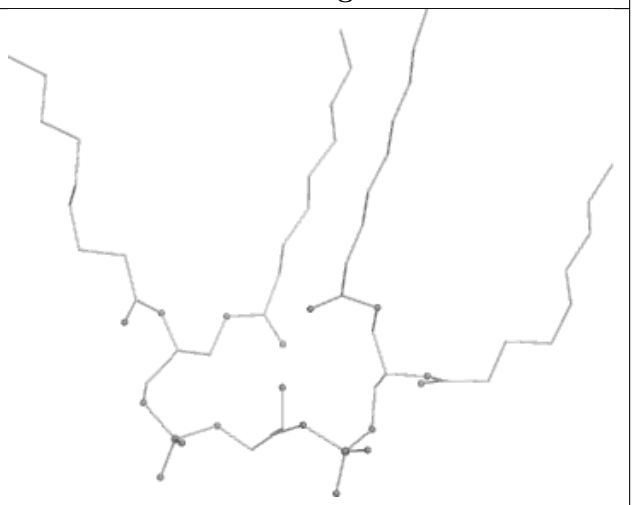
Bond lengths



Bond angles

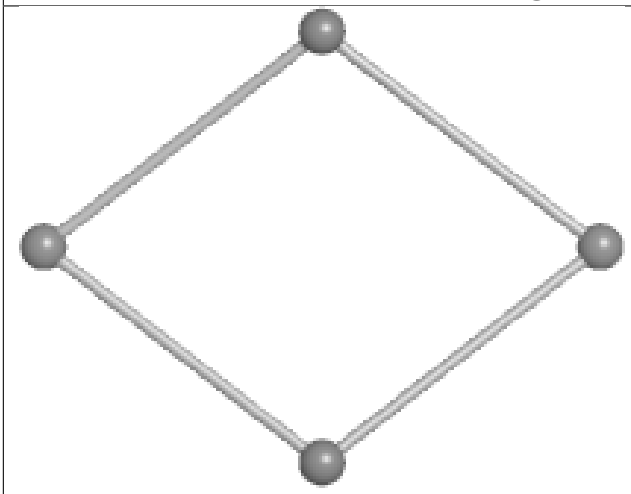


Torsions

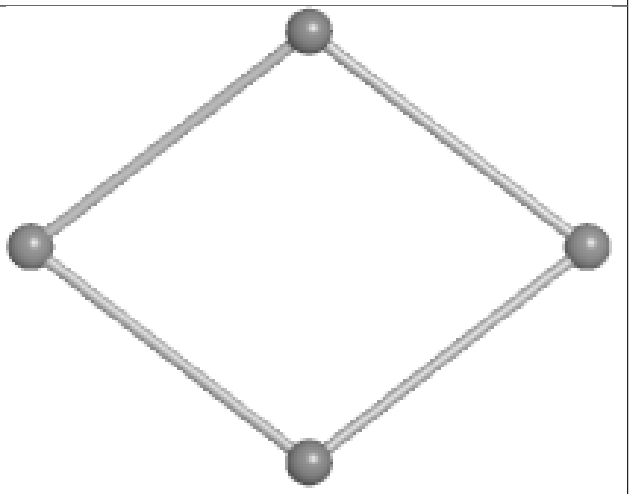


Rings

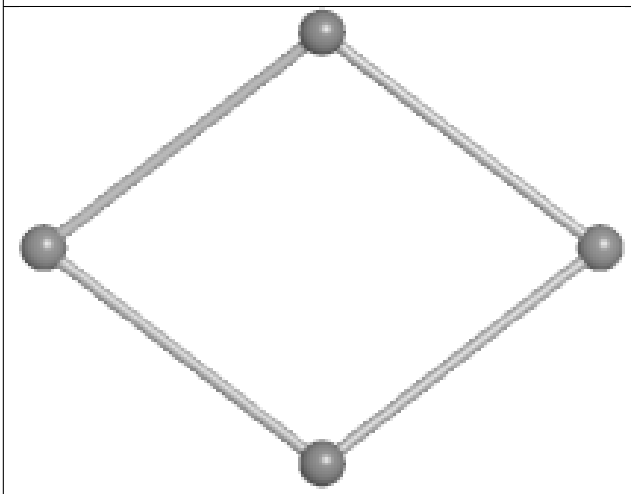
Ligand FES O 301



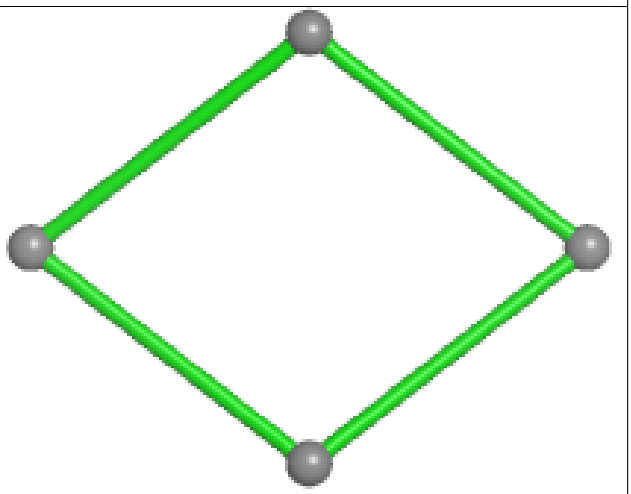
Bond lengths



Bond angles

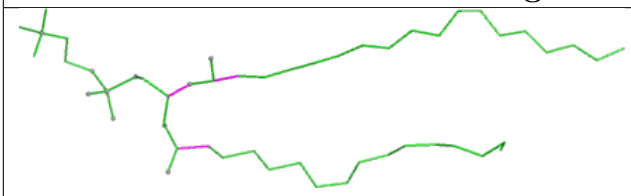


Torsions

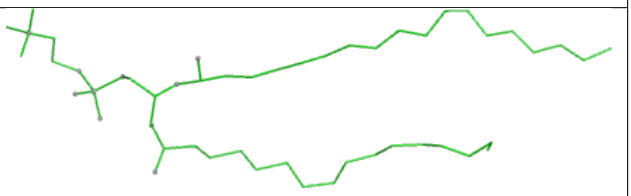


Rings

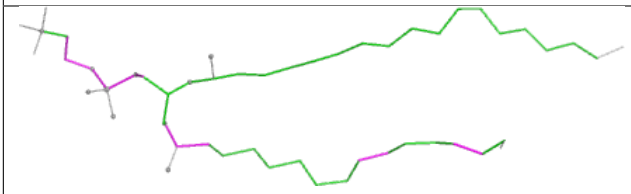
Ligand PLX N 201



Bond lengths



Bond angles

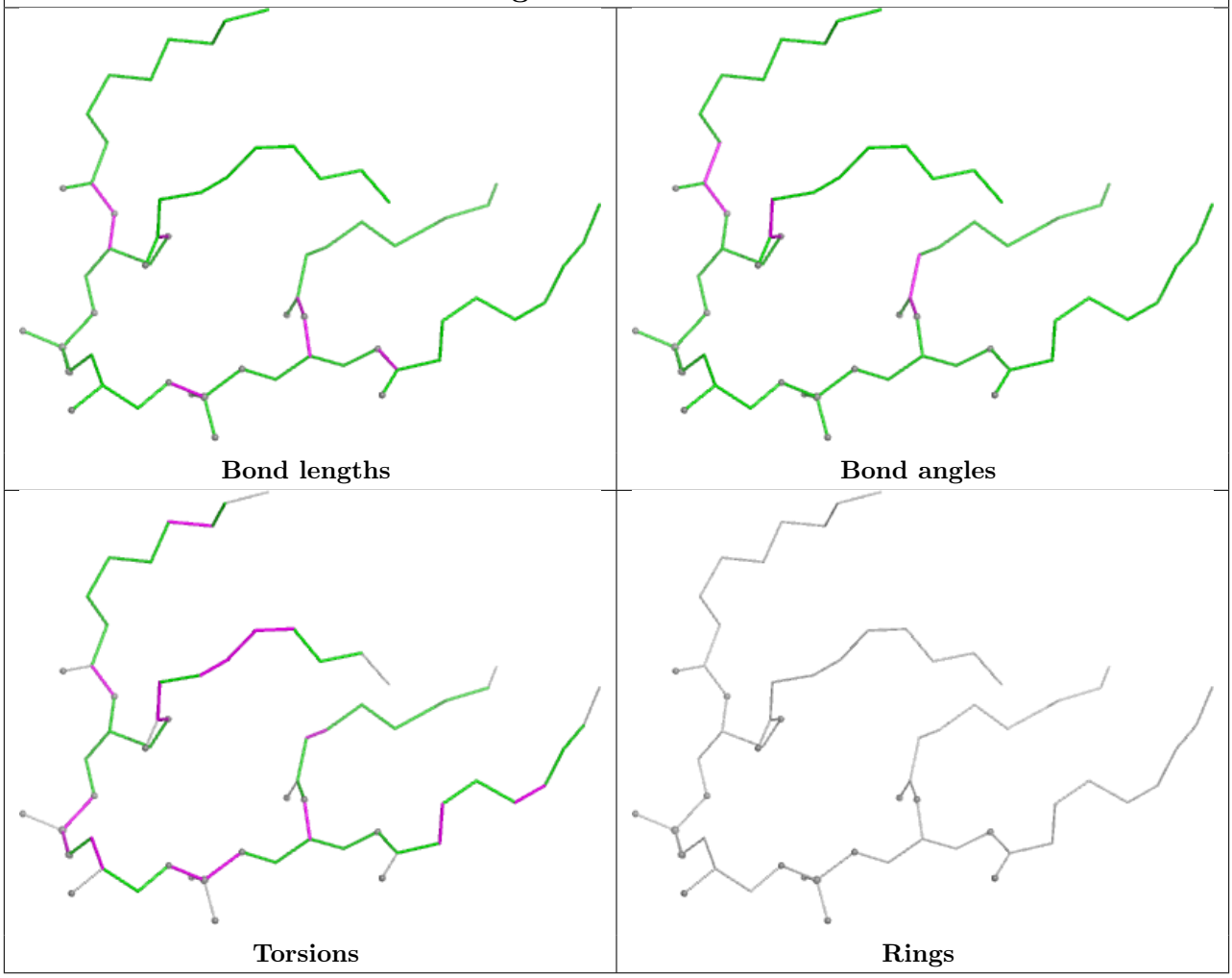


Torsions

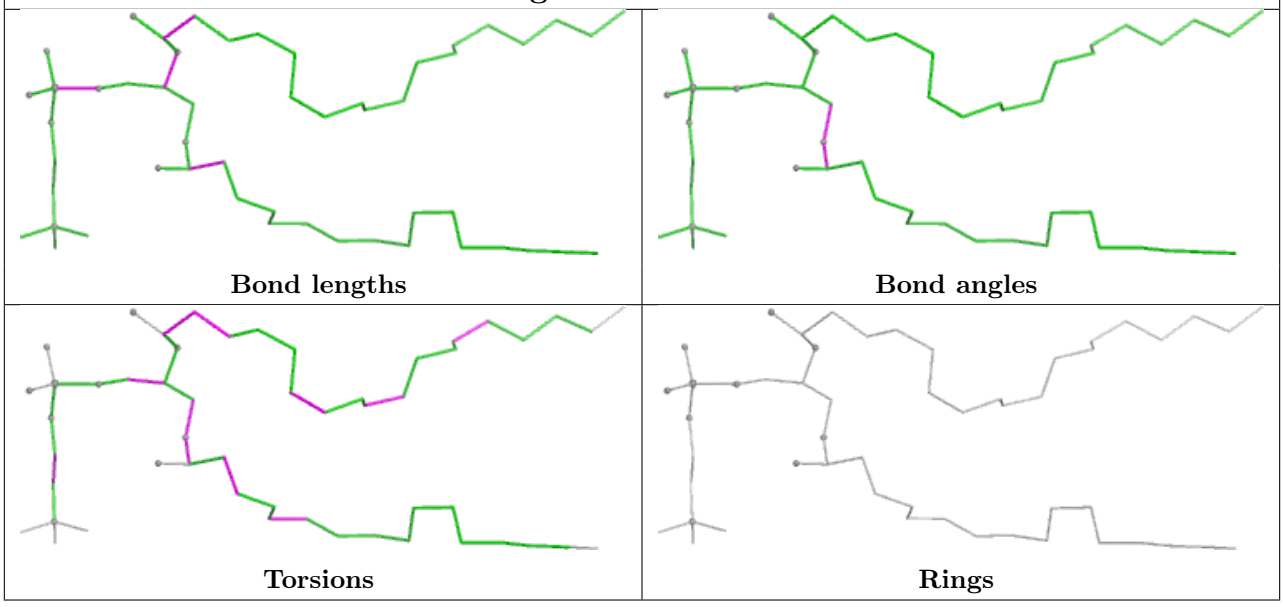


Rings

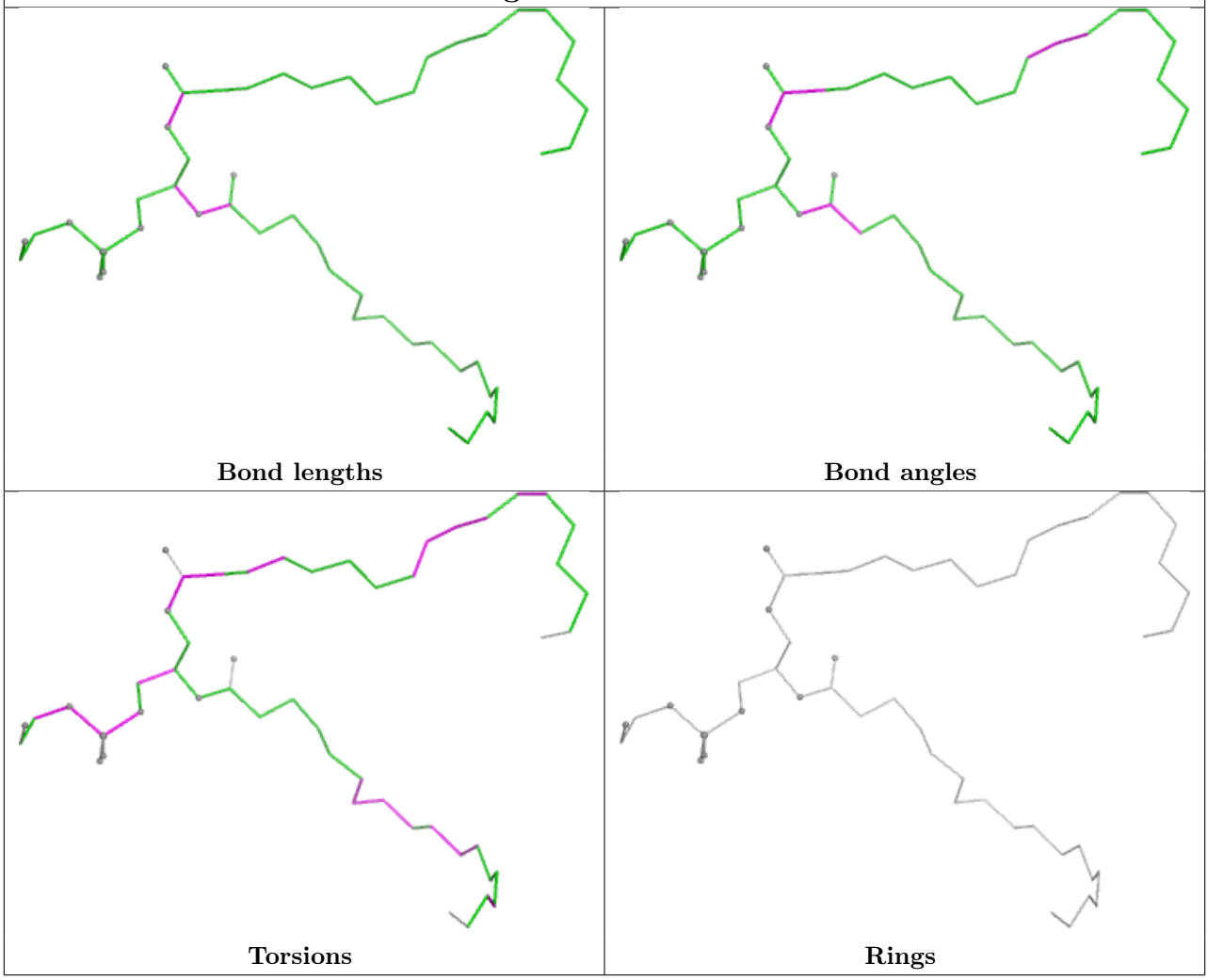
Ligand CDL l 702



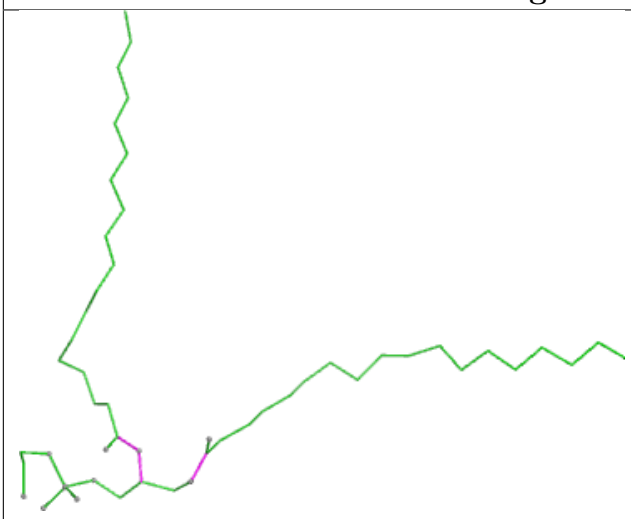
Ligand PLX o 201



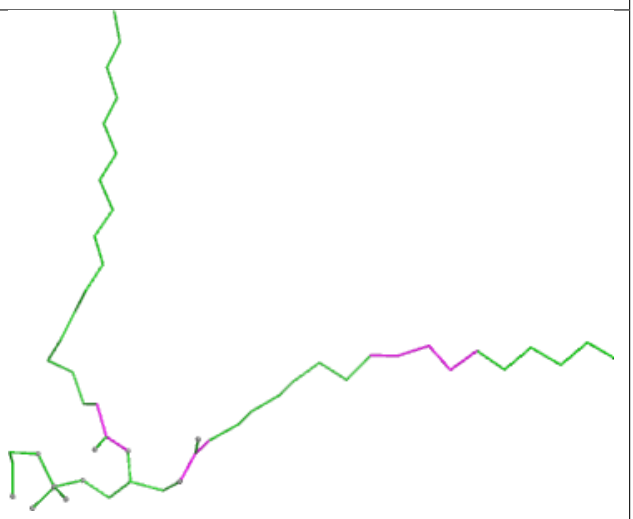
Ligand PEE l 701



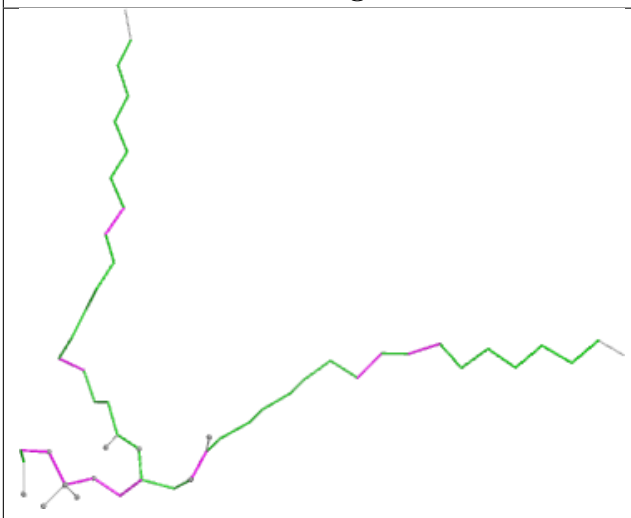
Ligand PEE J 402



Bond lengths



Bond angles



Torsions



Rings

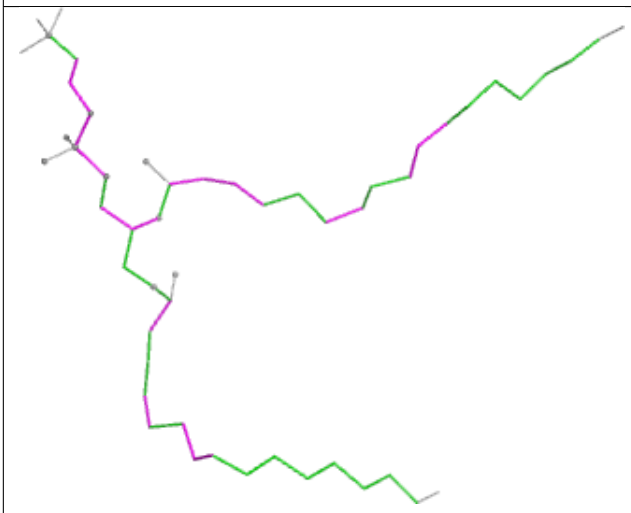
Ligand PLX s 401



Bond lengths



Bond angles

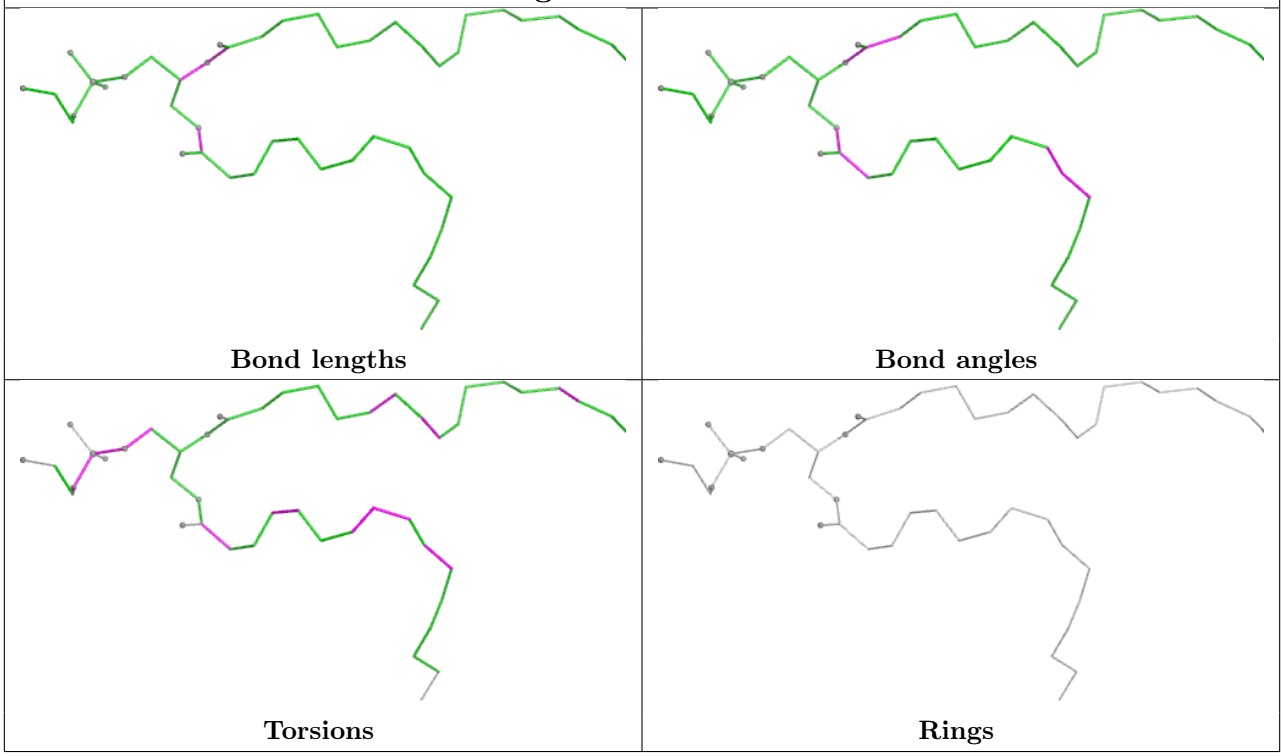


Torsions

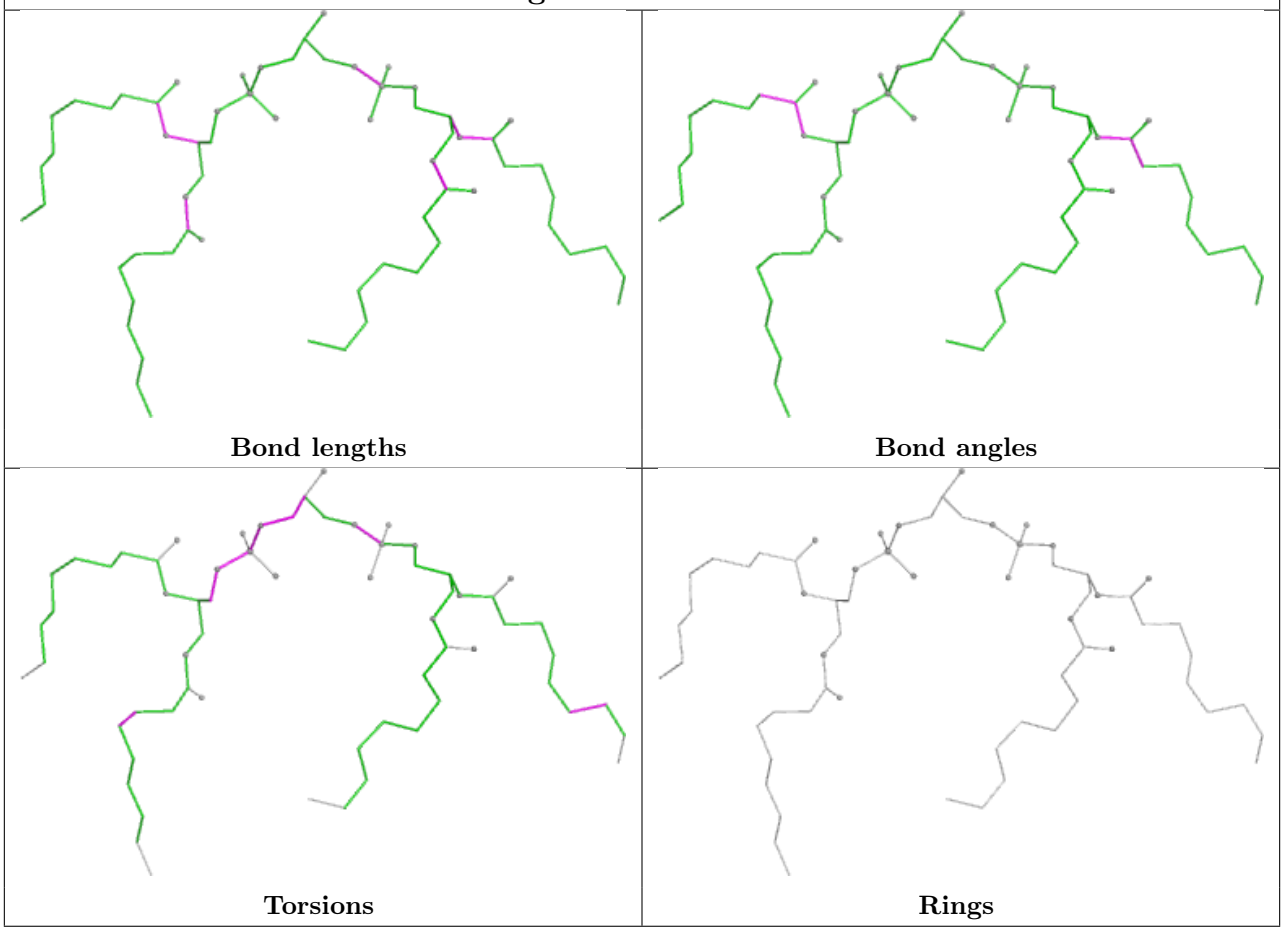


Rings

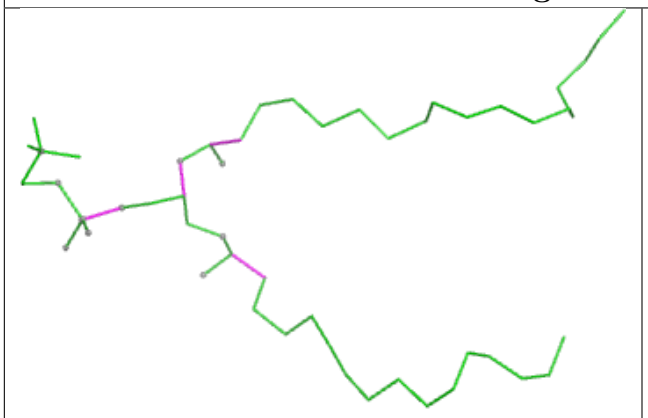
Ligand PEE i 403



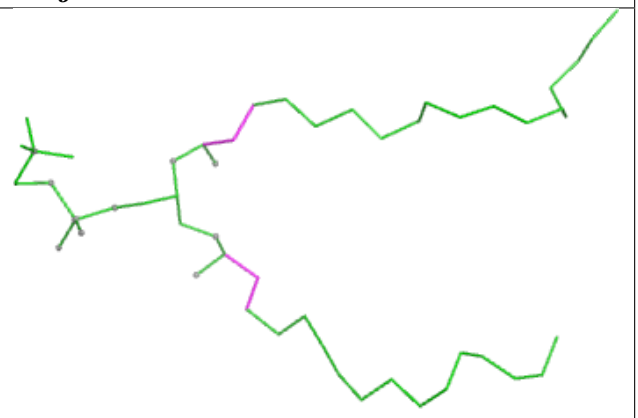
Ligand CDL u 201



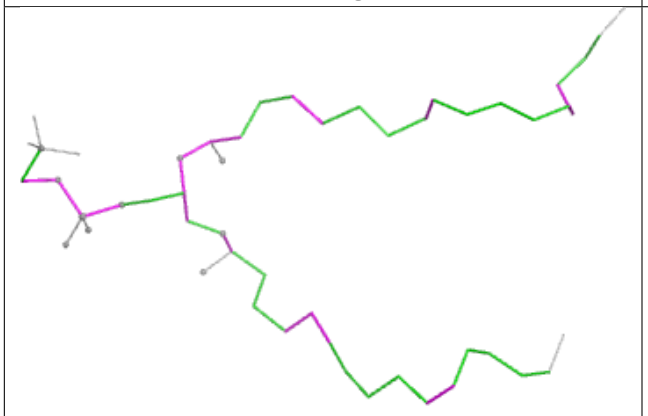
Ligand PLX j 201



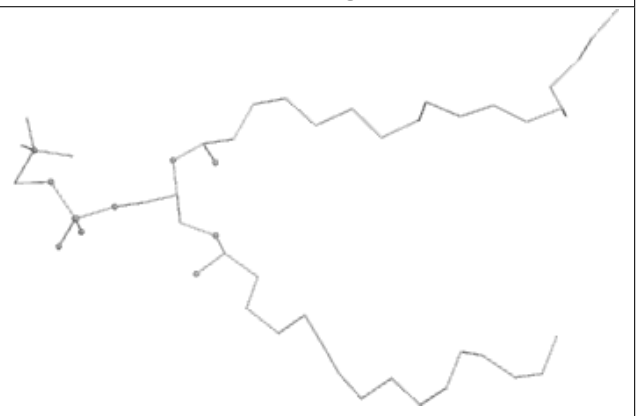
Bond lengths



Bond angles

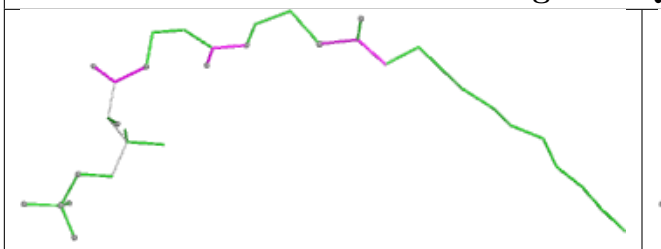


Torsions

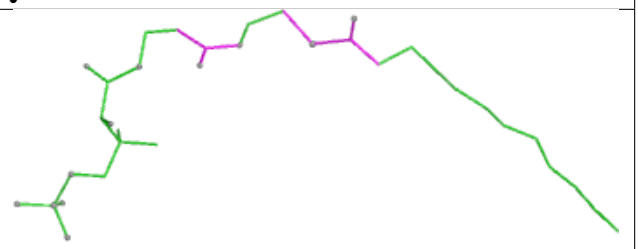


Rings

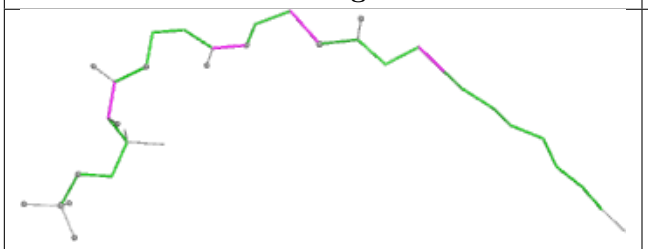
Ligand 8Q1 F 201



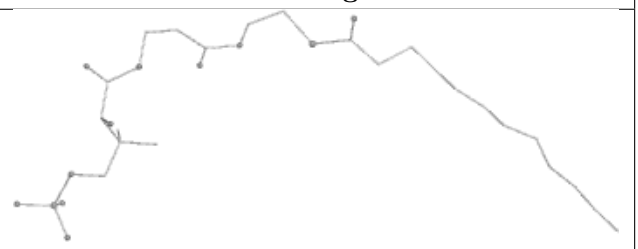
Bond lengths



Bond angles

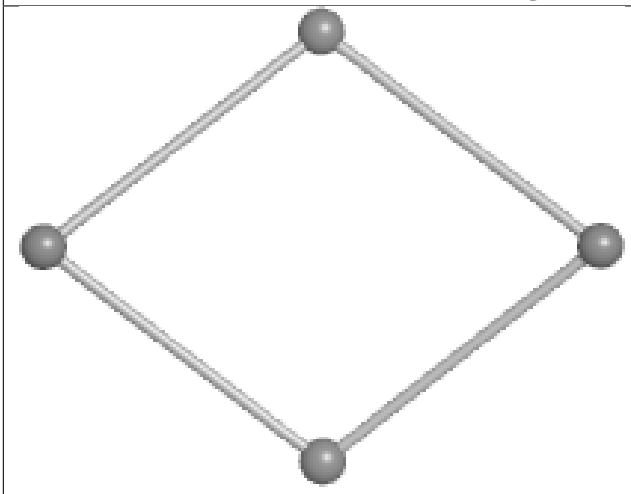


Torsions

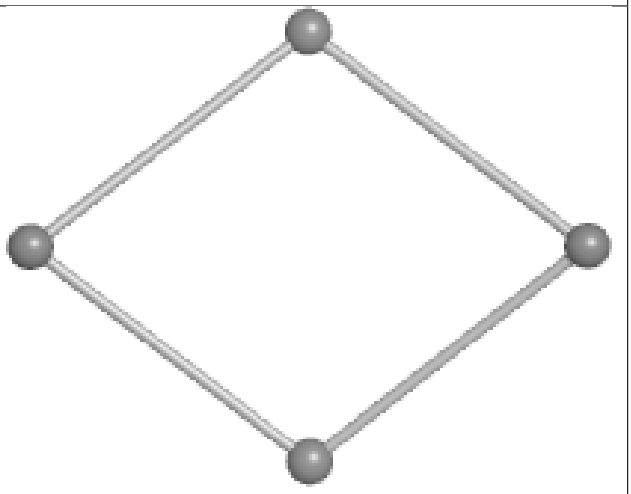


Rings

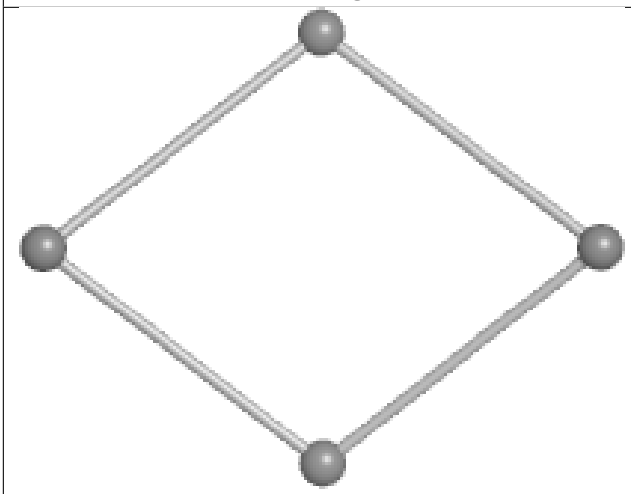
Ligand FES M 803



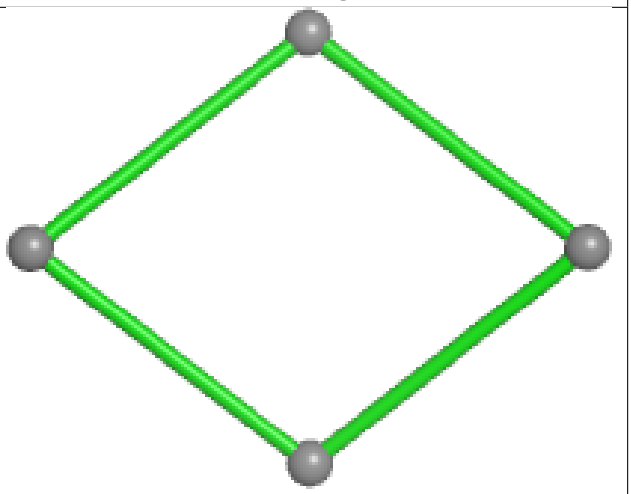
Bond lengths



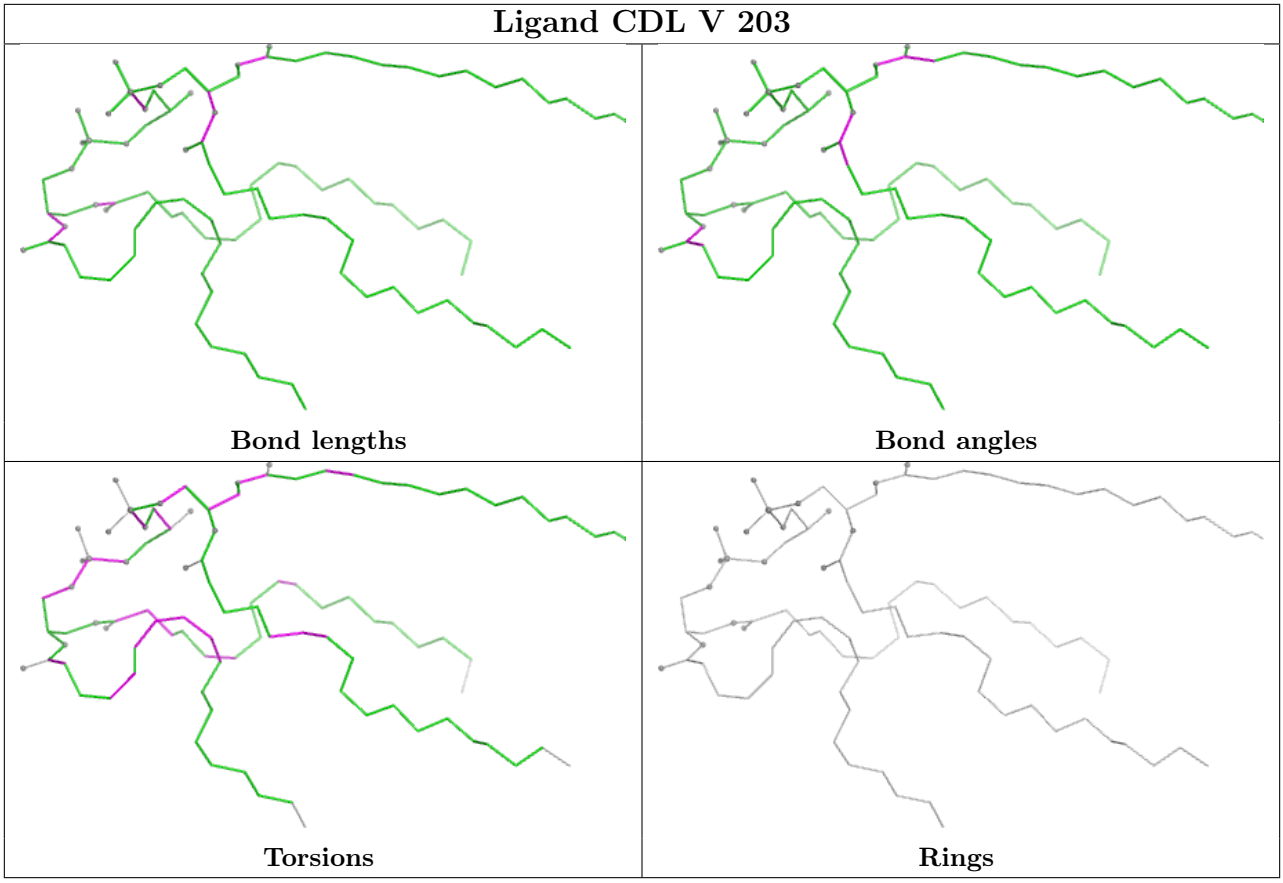
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	457:HIS	C	458:GLN	N	3.27

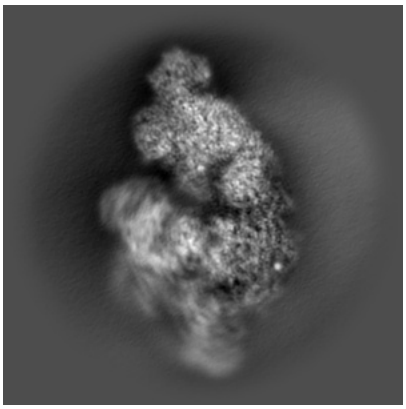
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52619. These allow visual inspection of the internal detail of the map and identification of artifacts.

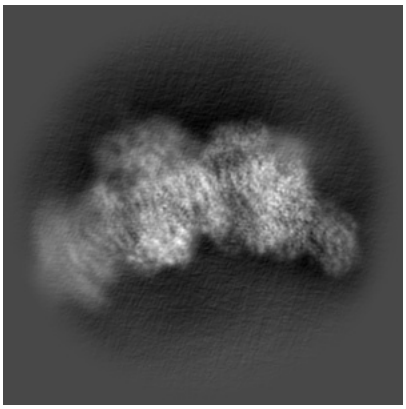
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

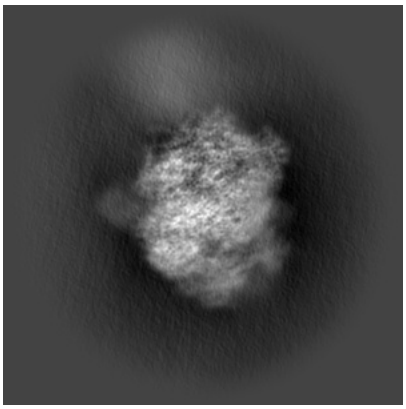
6.1.1 Primary map



X

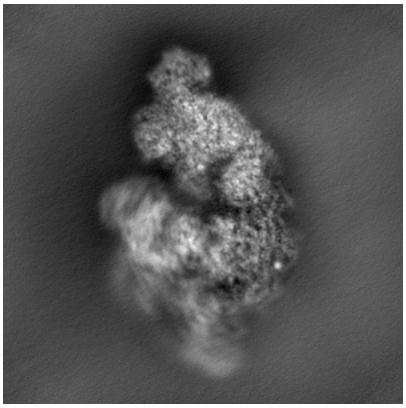


Y

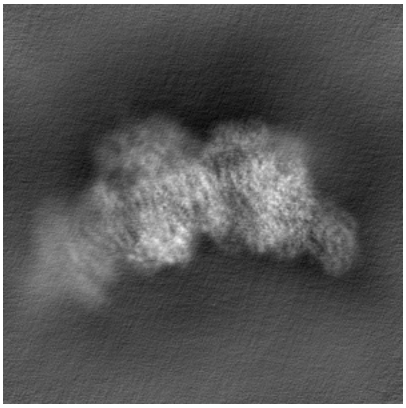


Z

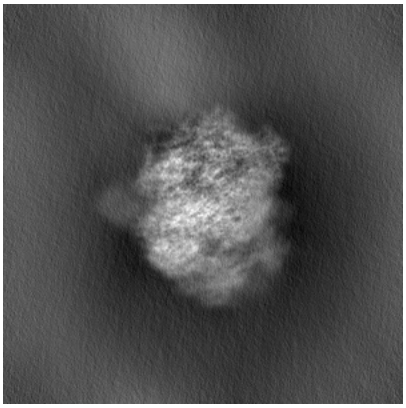
6.1.2 Raw map



X



Y

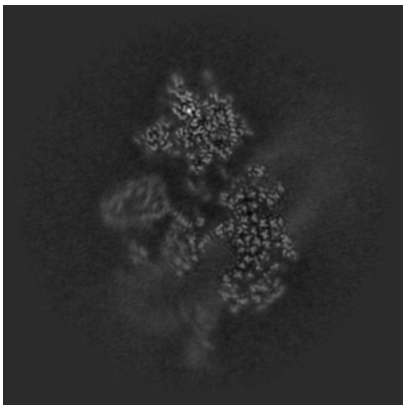


Z

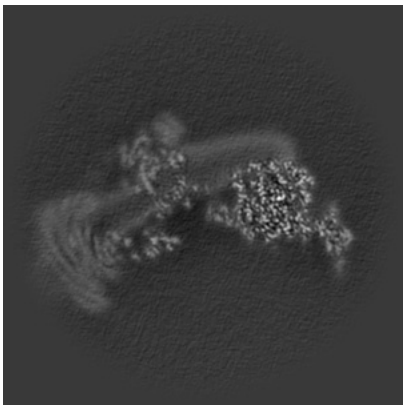
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

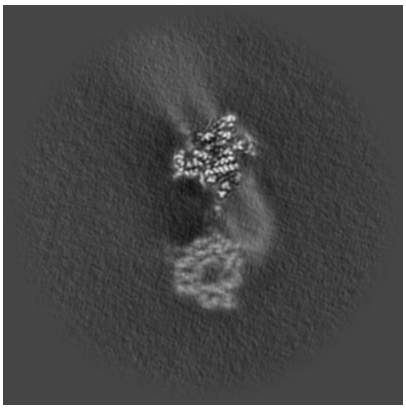
6.2.1 Primary map



X Index: 240

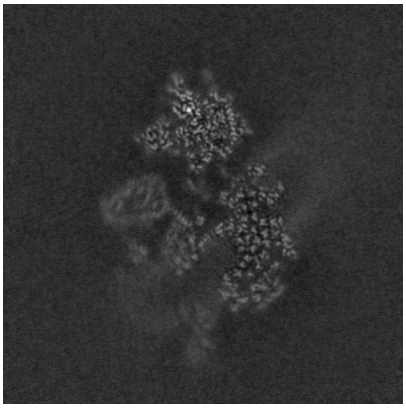


Y Index: 240

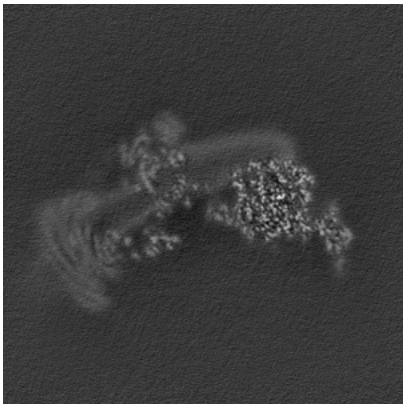


Z Index: 240

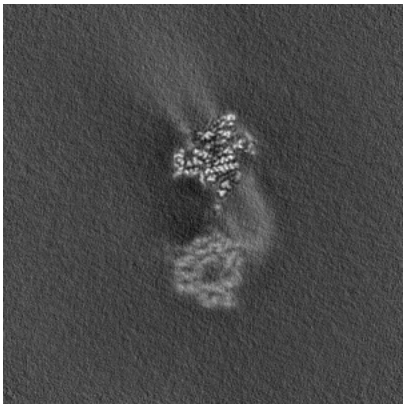
6.2.2 Raw map



X Index: 240



Y Index: 240

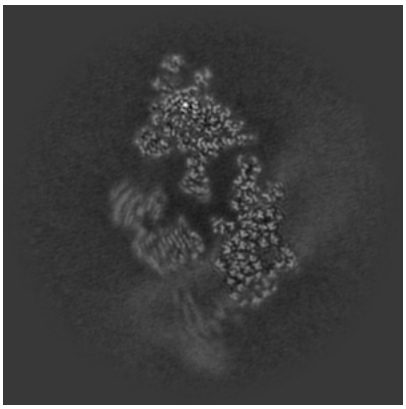


Z Index: 240

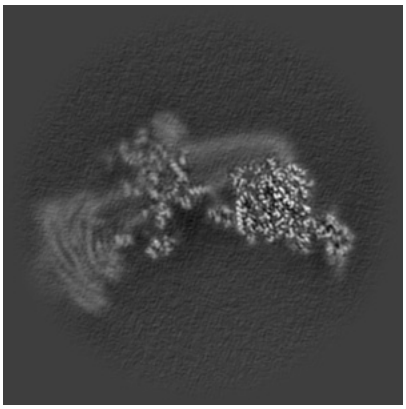
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

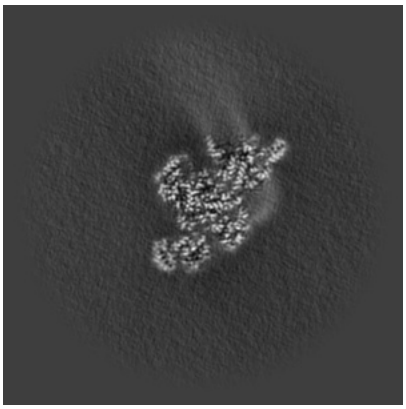
6.3.1 Primary map



X Index: 225

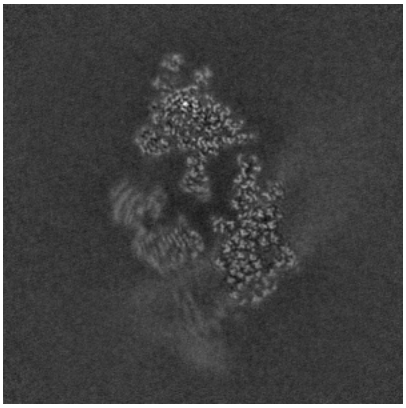


Y Index: 236

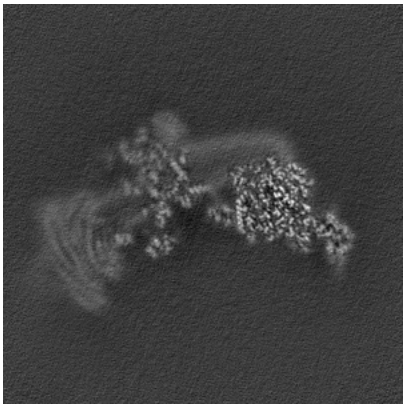


Z Index: 311

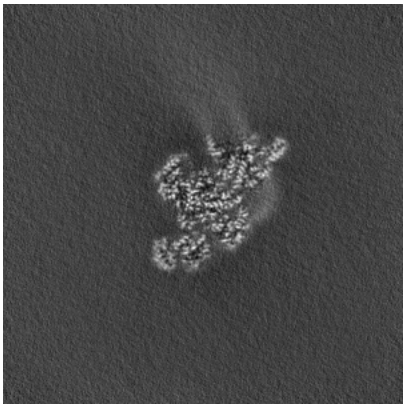
6.3.2 Raw map



X Index: 225



Y Index: 236

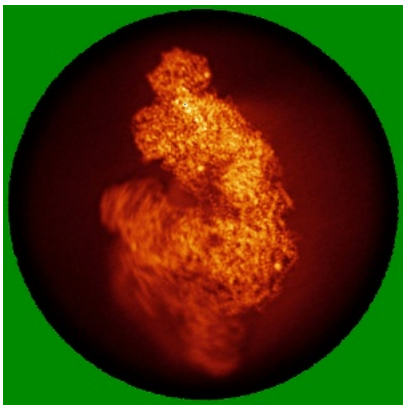


Z Index: 311

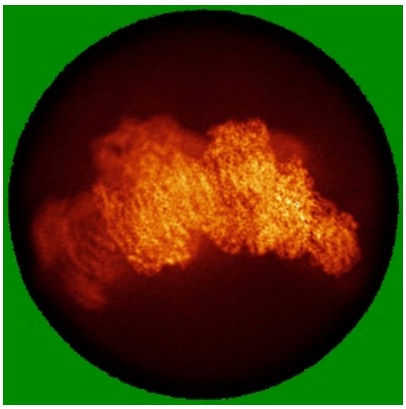
The images above show the largest variance slices of the map in three orthogonal directions.

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

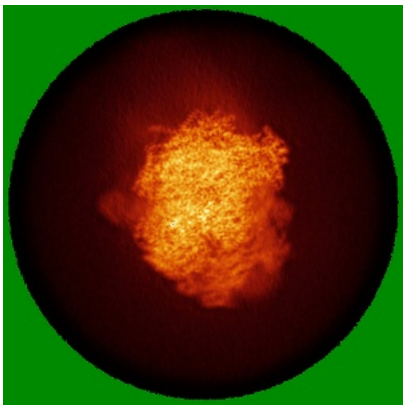
6.4.1 Primary map



X

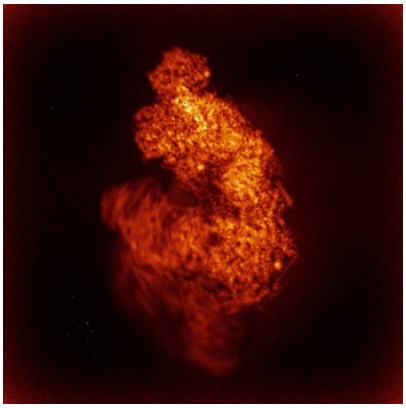


Y

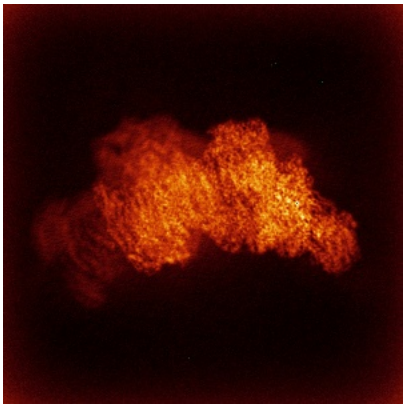


Z

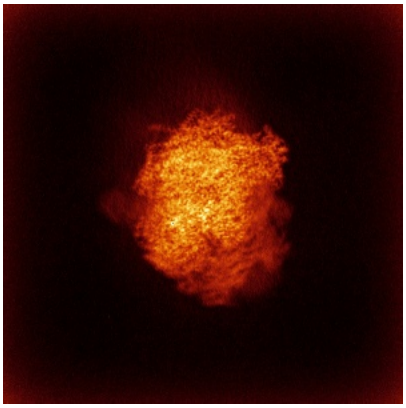
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

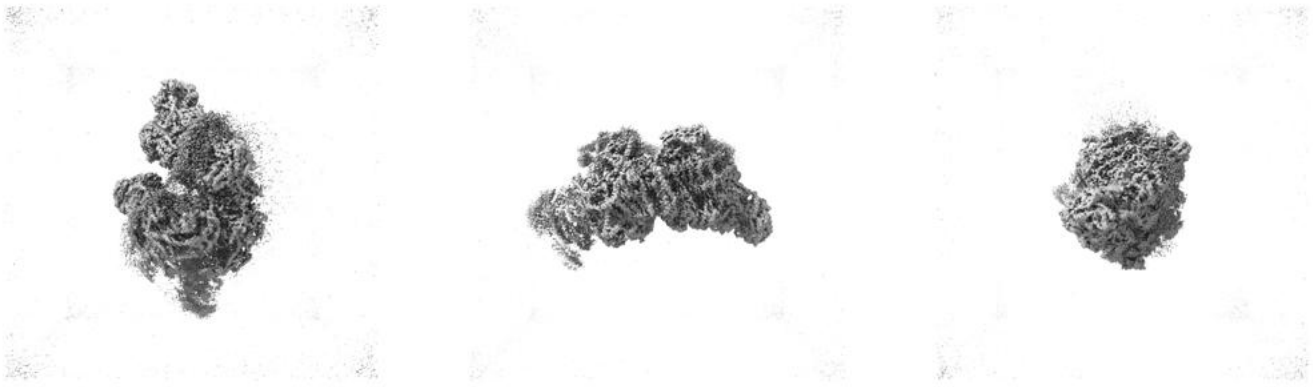
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.477. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

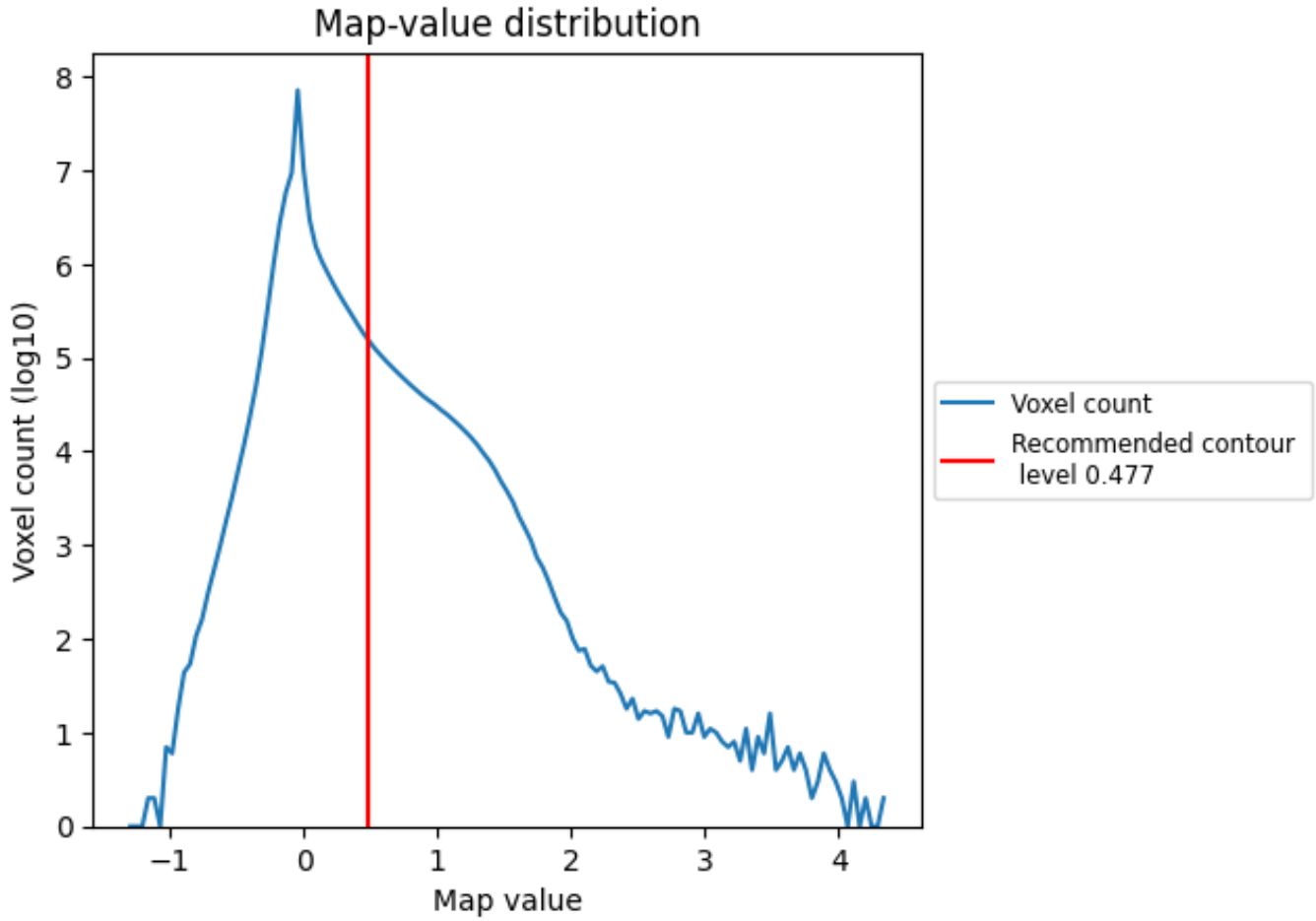
6.6 Mask visualisation (i)

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

7 Map analysis

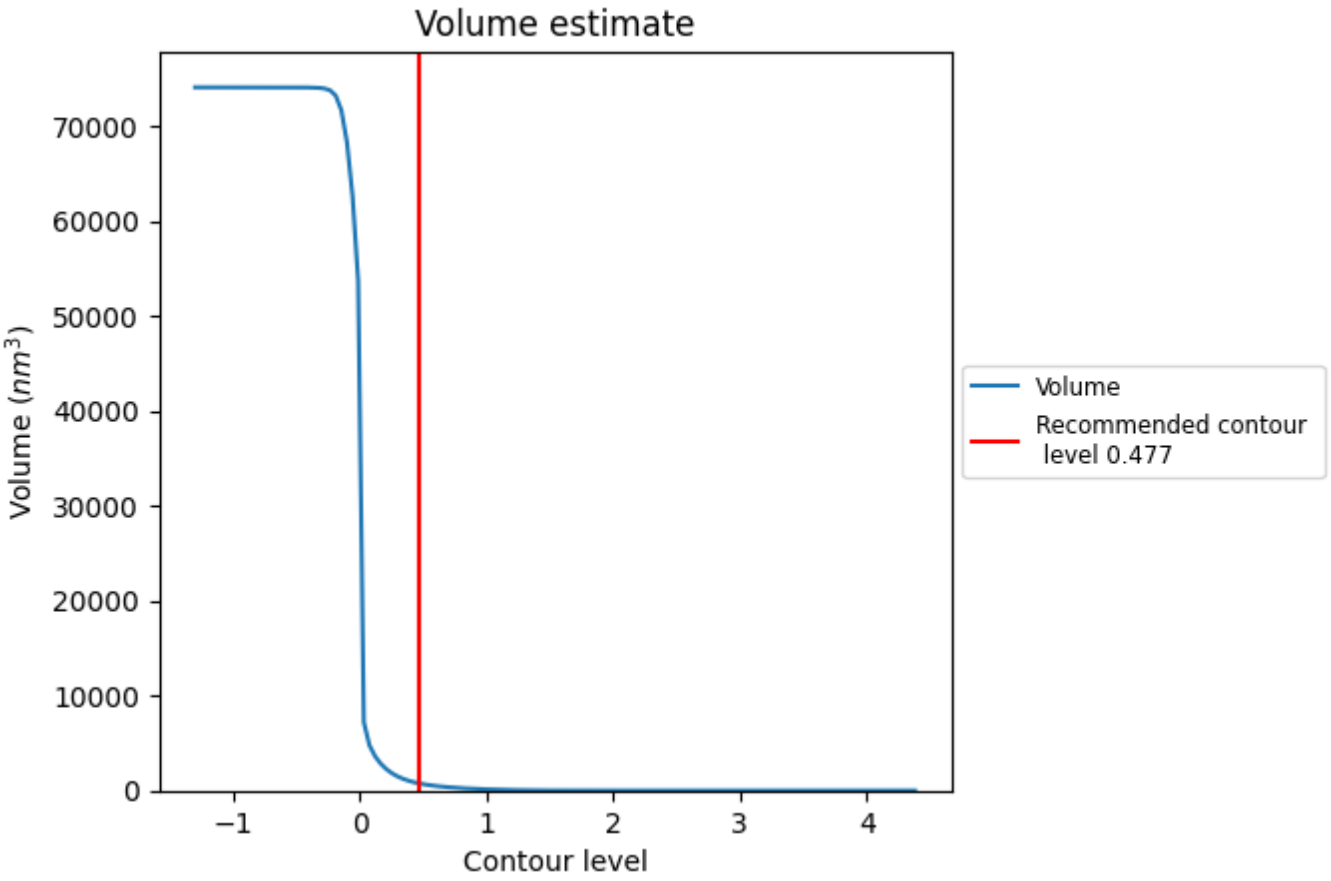
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

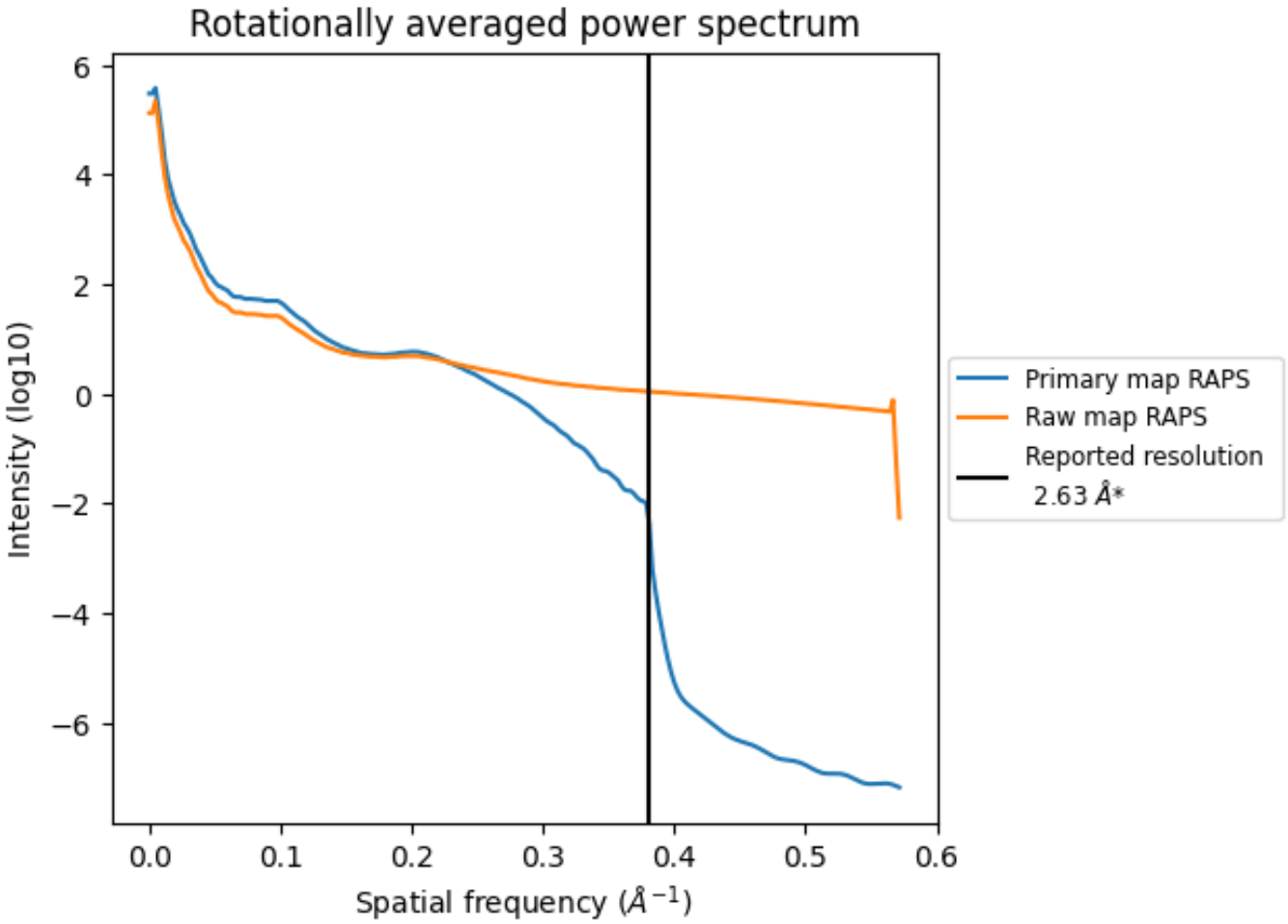
7.2 Volume estimate (i)



The volume at the recommended contour level is 741 nm^3; this corresponds to an approximate mass of 669 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)

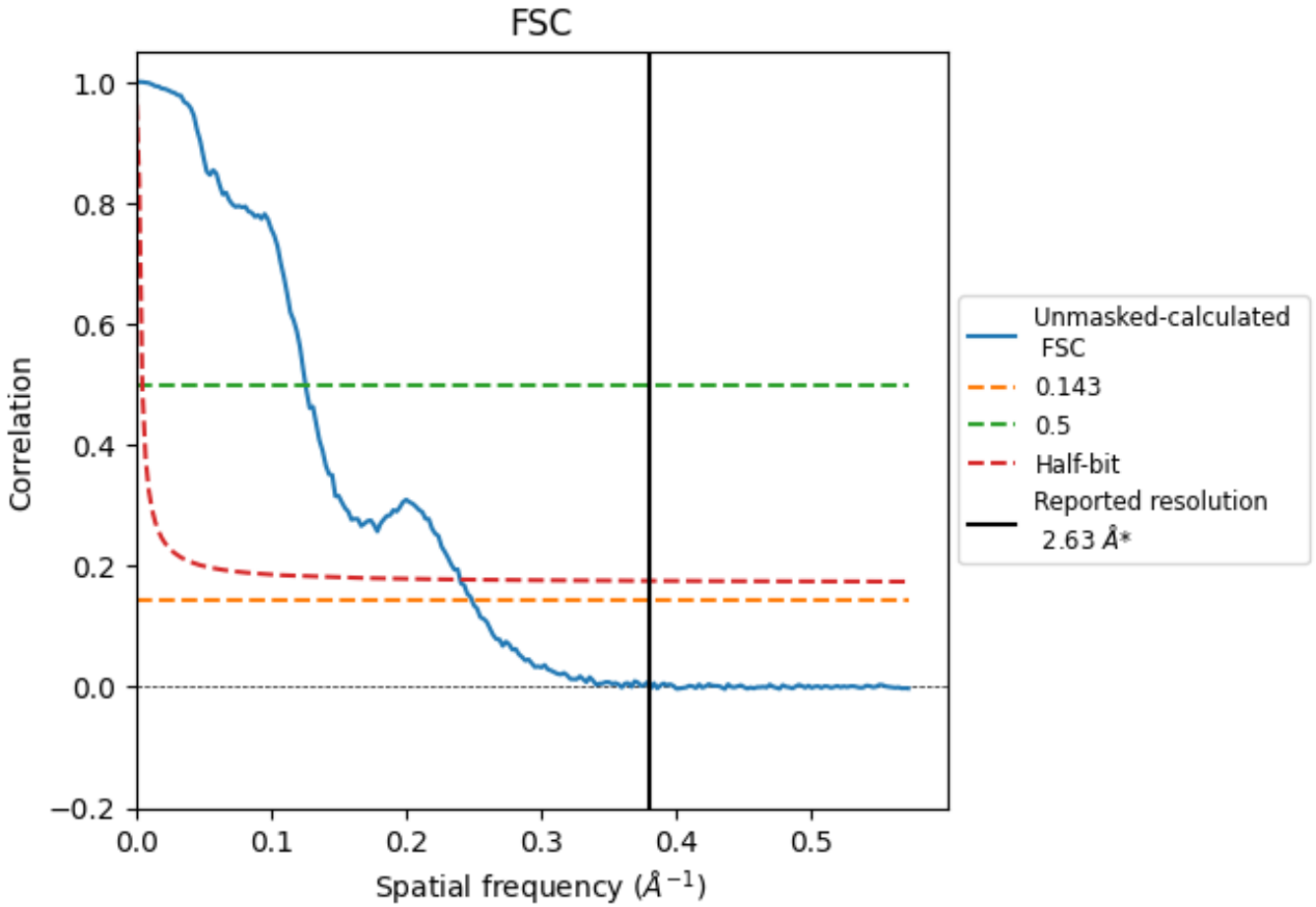


*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

8.2 Resolution estimates (i)

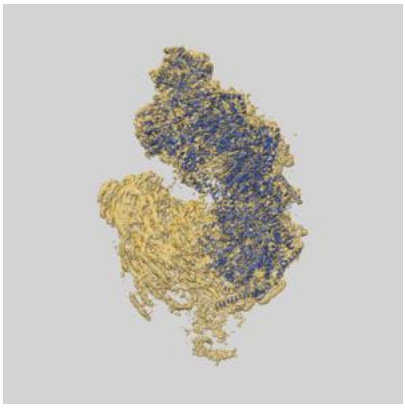
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.97	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.63 by more than 10 %

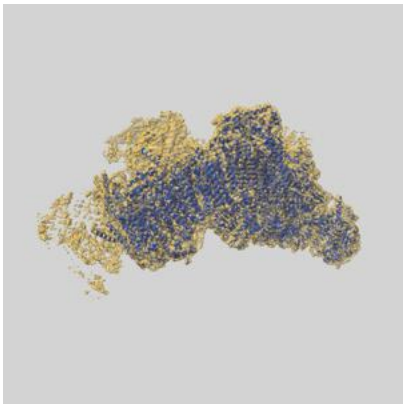
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52619 and PDB model 9I4I. Per-residue inclusion information can be found in section 3 on page 19.

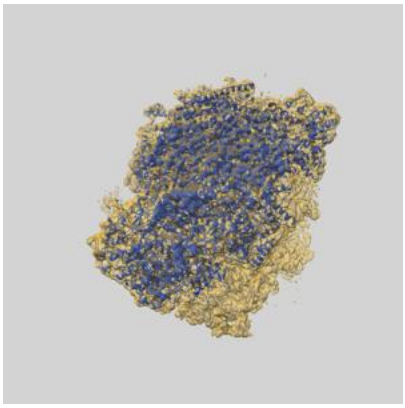
9.1 Map-model overlay



X



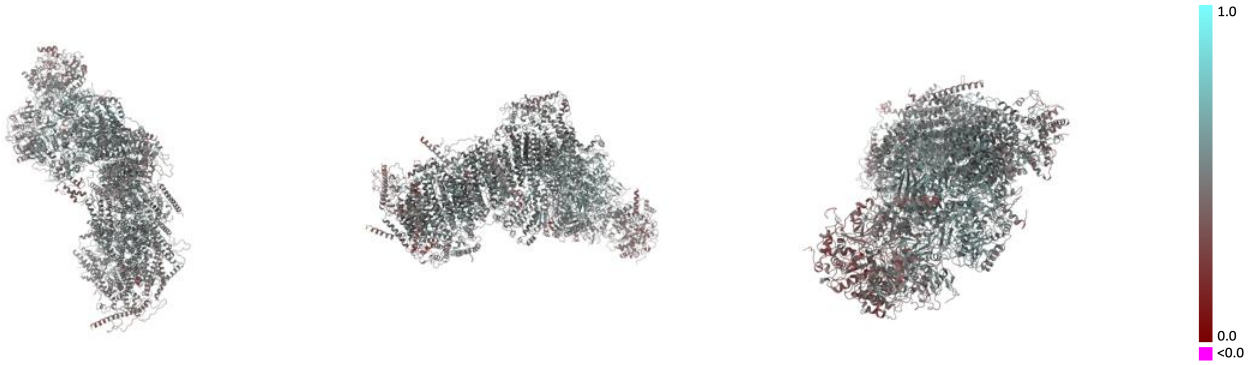
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.477 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

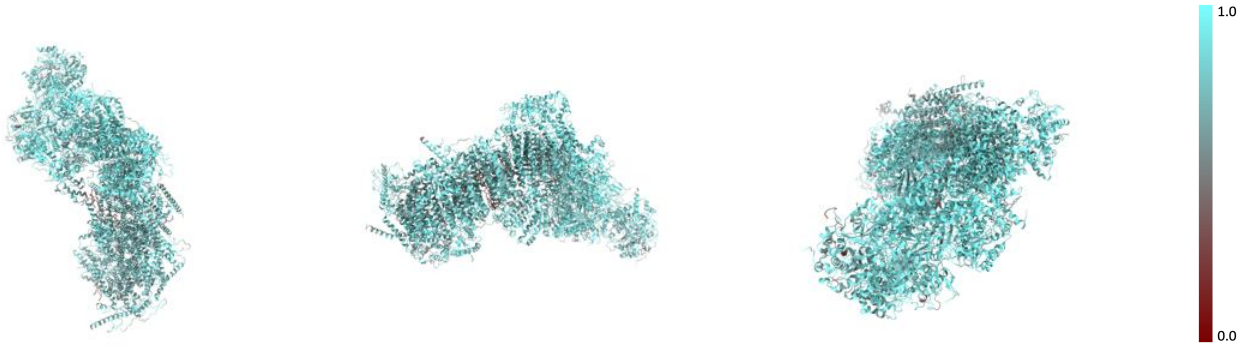
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

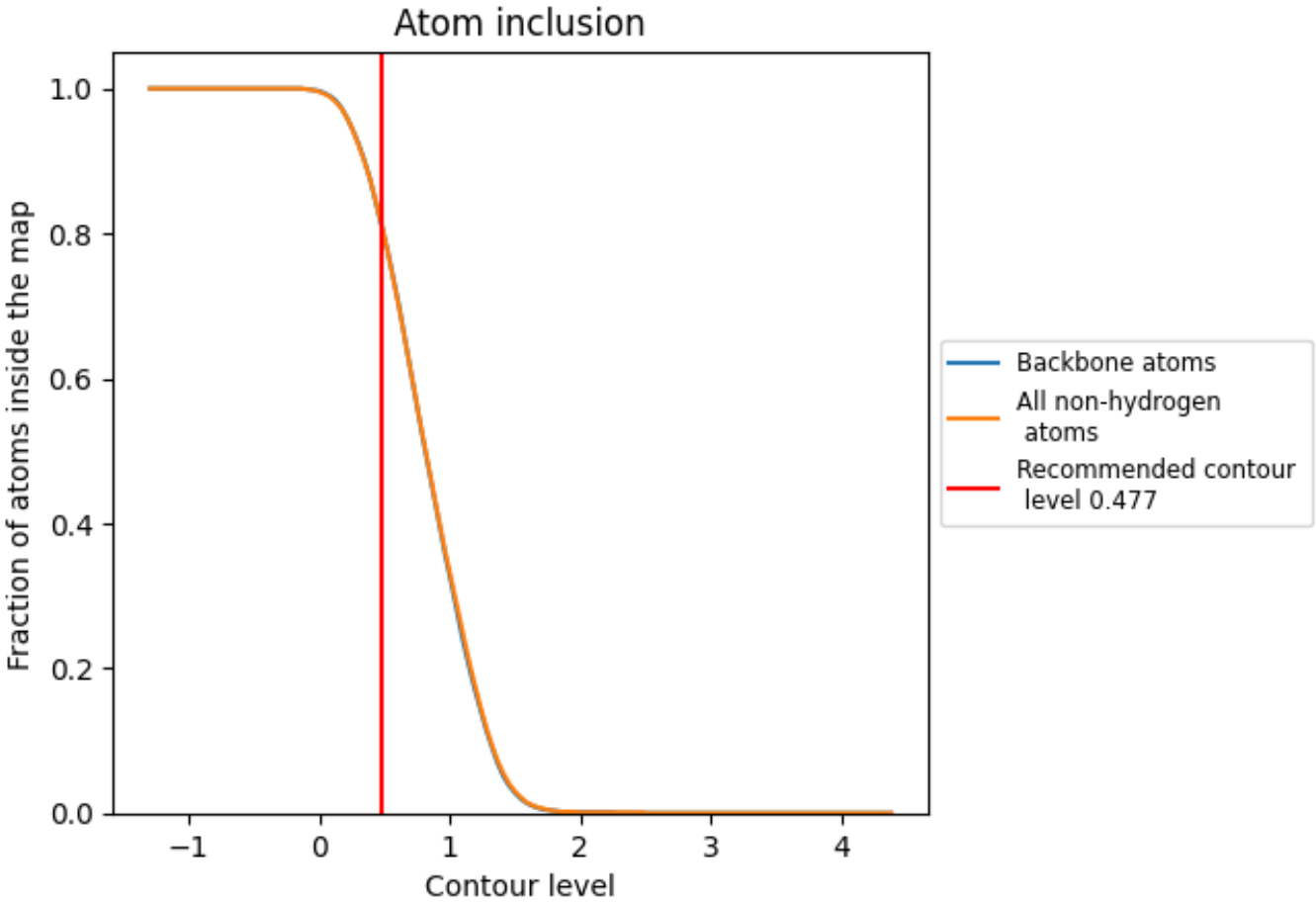
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.477).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.477) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.4860
C	0.7860	0.3970
D	0.9300	0.5380
E	0.9070	0.5330
F	0.8530	0.5100
G	0.8270	0.4240
H	0.6730	0.3870
I	0.8250	0.4800
J	0.8900	0.5160
K	0.8150	0.3870
L	0.8300	0.5120
M	0.8450	0.4660
N	0.9120	0.5070
O	0.8210	0.4090
P	0.8690	0.5350
Q	0.8750	0.5390
S	0.8840	0.4830
T	0.9240	0.5140
U	0.8450	0.4820
V	0.6960	0.4890
W	0.8540	0.4900
X	0.7850	0.4540
Y	0.7690	0.4360
Z	0.7070	0.4190
a	0.8450	0.5020
b	0.7270	0.4070
c	0.8140	0.4960
d	0.7780	0.4610
e	0.7930	0.4670
f	0.7030	0.3960
g	0.7770	0.4980
h	0.8570	0.4820
i	0.7940	0.5220
j	0.7950	0.5150
k	0.8260	0.5100



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Chain	Atom inclusion	Q-score
l	0.7500	0.4860
m	0.8290	0.4900
n	0.7720	0.4650
o	0.7870	0.4880
p	0.8490	0.4890
r	0.8100	0.5200
s	0.8830	0.5250
t	0.8760	0.5070
u	0.8360	0.4680
v	0.7520	0.4030
w	0.8490	0.4990