



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 10:03 AM JST

PDB ID : 5XTD / pdb_00005xtd
EMDB ID : EMD-6773
Title : Cryo-EM structure of human respiratory complex I
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

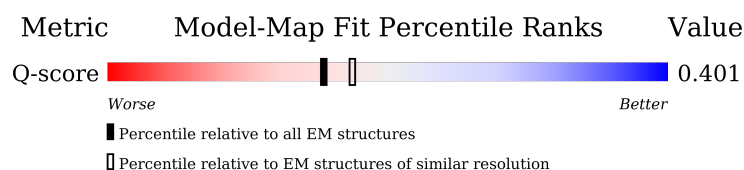
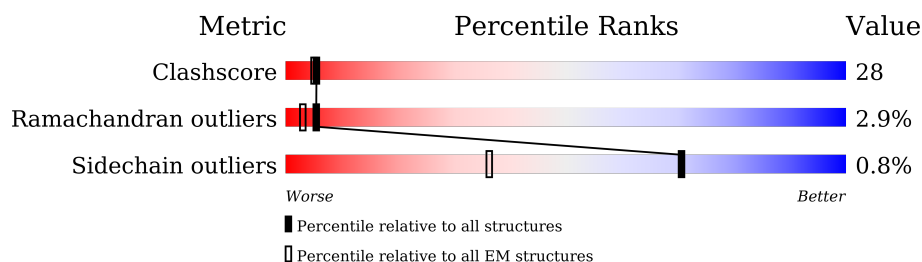
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	113	

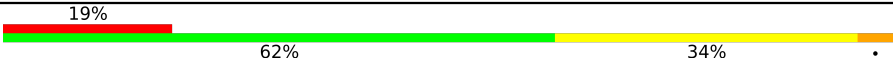
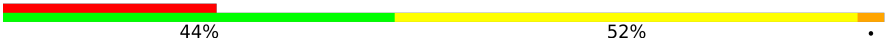
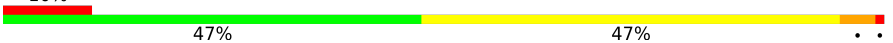
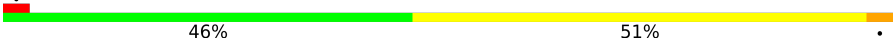
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Mol	Chain	Length	Quality of chain
5	F	83	
6	G	85	
6	X	85	
7	H	112	
8	I	110	
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	128	
26	c	153	
27	d	171	
28	e	97	

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Mol	Chain	Length	Quality of chain
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	137	
44	w	320	

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
45	SF4	A	501	-	-	X	-
45	SF4	B	302	-	-	X	-
45	SF4	M	801	-	-	X	-
46	FMN	A	502	-	-	X	-
47	PLX	b	201	-	-	X	-
49	NDP	J	401	-	-	X	-
50	FES	O	301	-	-	X	-
52	PEE	V	202	-	-	X	-
52	PEE	l	701	-	-	X	-

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 66789 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 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

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

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

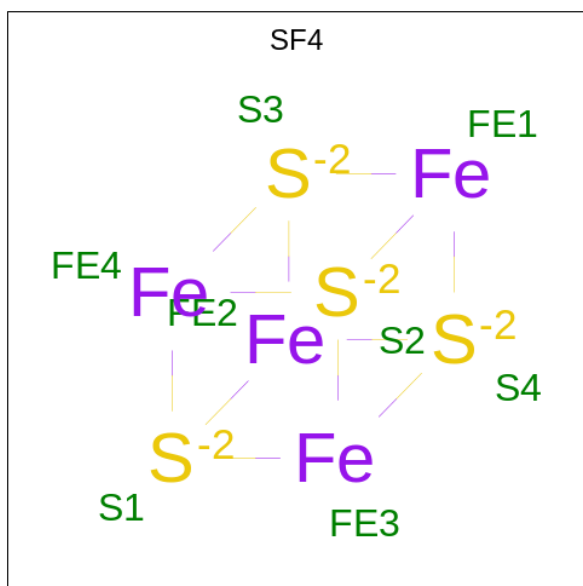
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

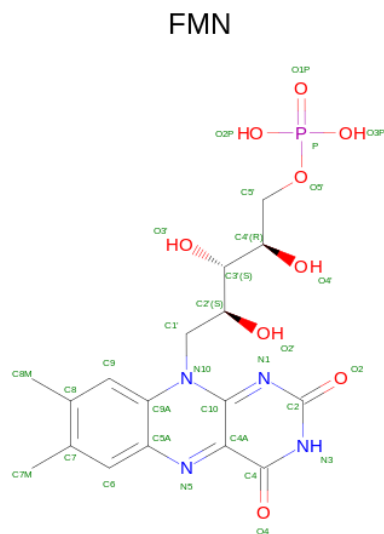
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



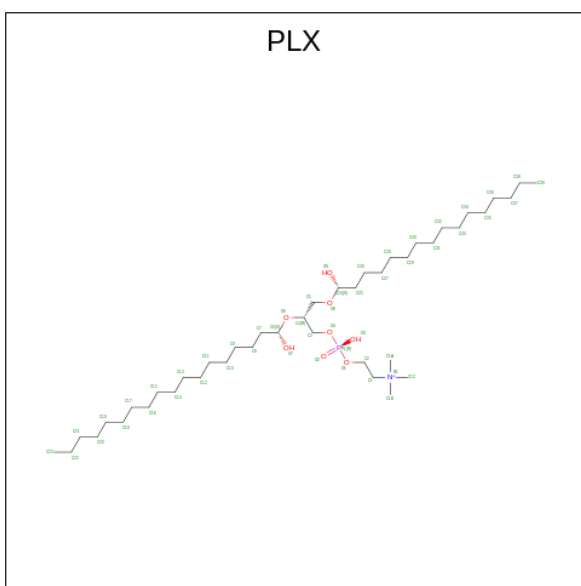
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 47 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: C₄₂H₈₉NO₈P).



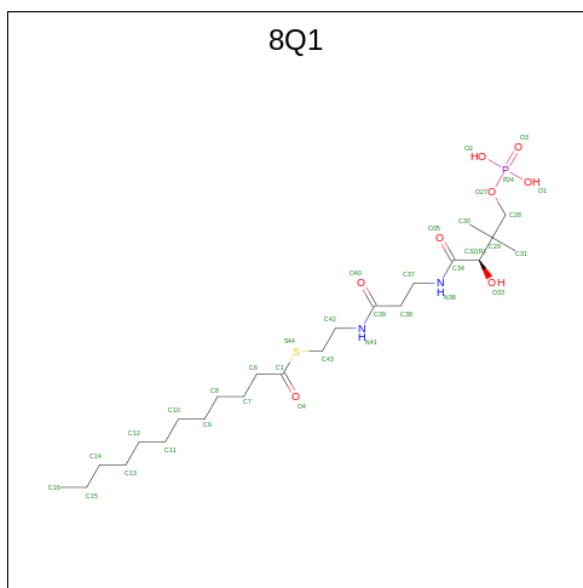
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total 52	C 42	N 1	O 8	P 1	0
47	U	1	Total 52	C 42	N 1	O 8	P 1	0

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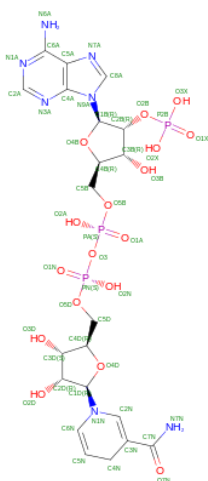
Mol	Chain	Residues	Atoms					AltConf
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



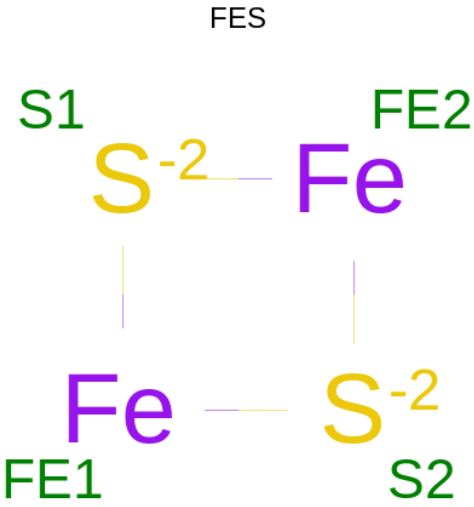
Mol	Chain	Residues	Atoms						AltConf
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



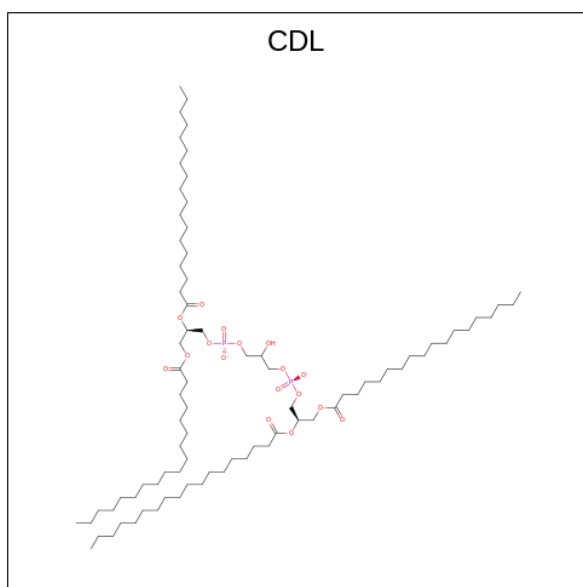
Mol	Chain	Residues	Atoms					AltConf
49	J	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



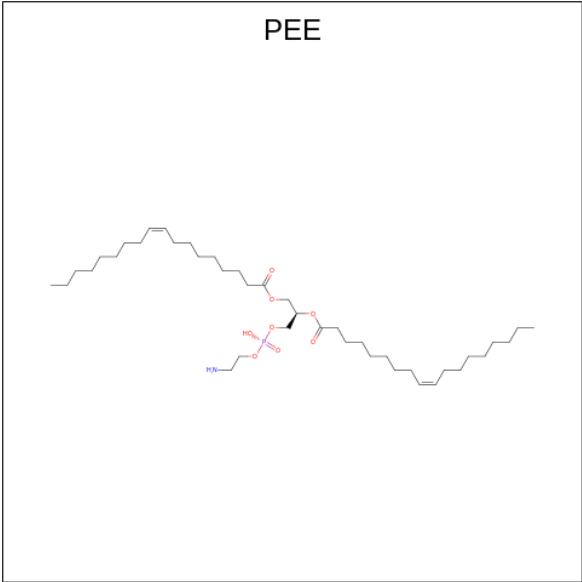
Mol	Chain	Residues	Atoms			AltConf
50	M	1	Total 4	Fe 2	S 2	0
50	O	1	Total 4	Fe 2	S 2	0

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			63	44	17	2	
51	i	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	n	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 52 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

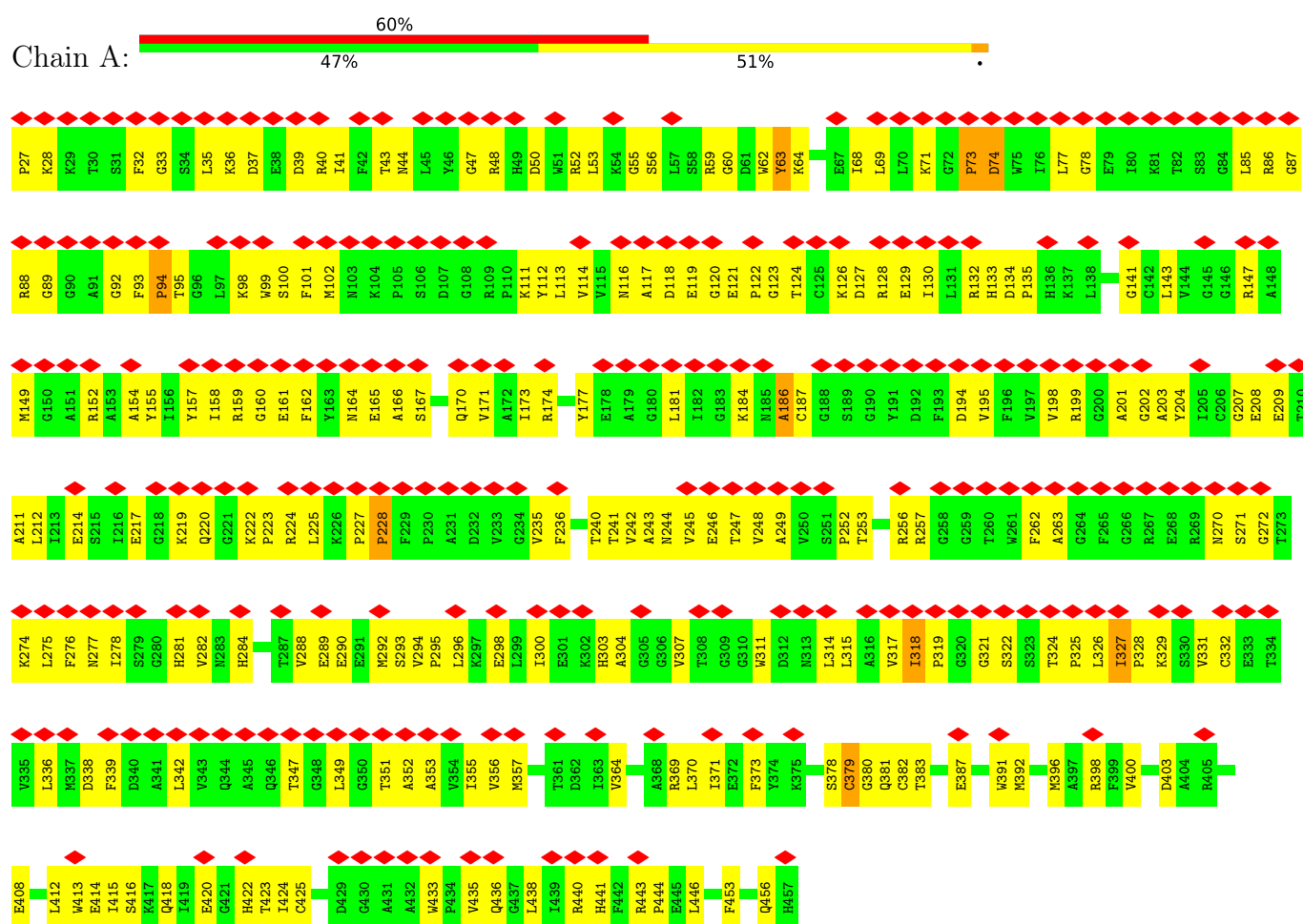


Mol	Chain	Residues	Atoms					AltConf
52	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	1	1	Total	C	N	O	P	0
			51	41	1	8	1	

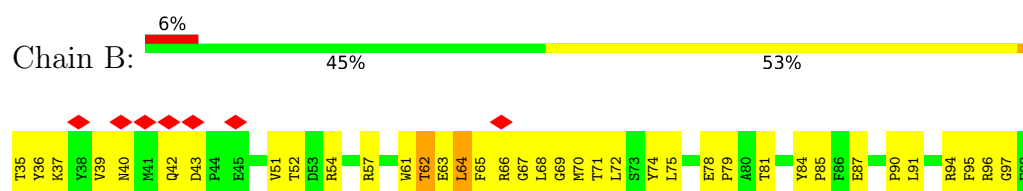
3 Residue-property plots

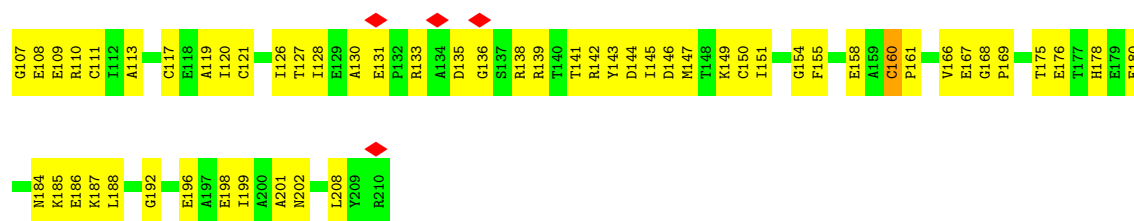
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

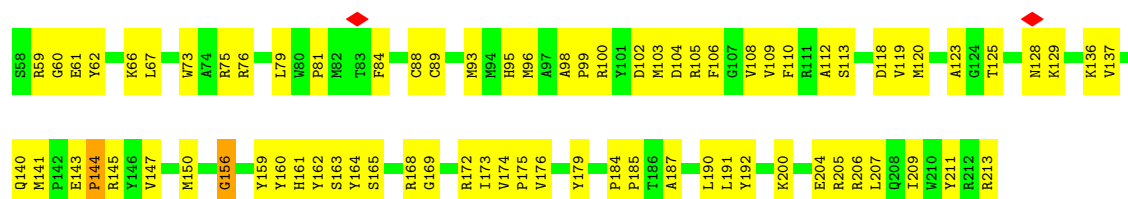


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

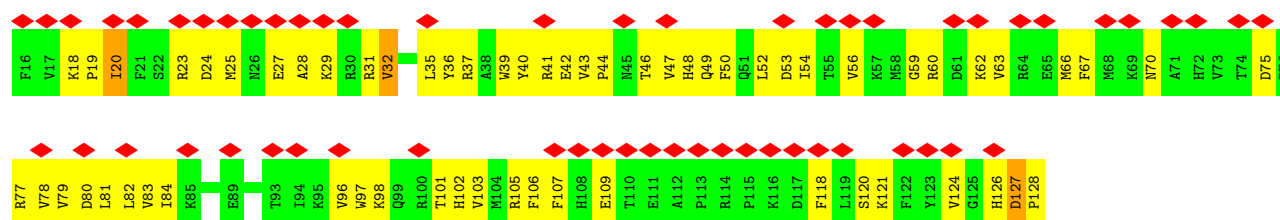




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial





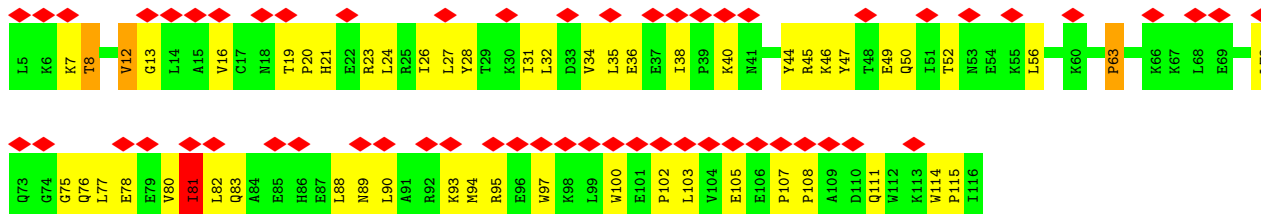
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 53% 44%



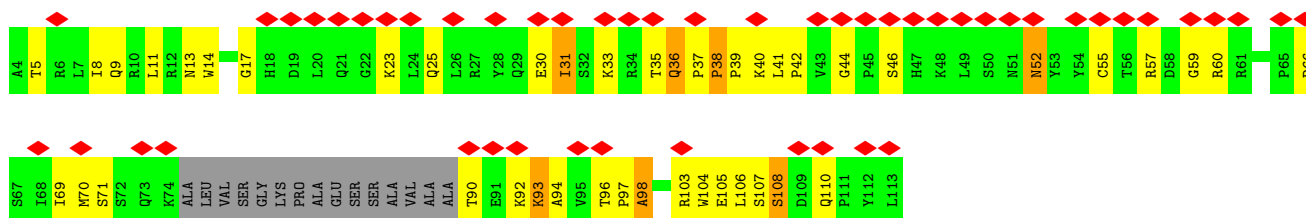
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 51% 52% 45%



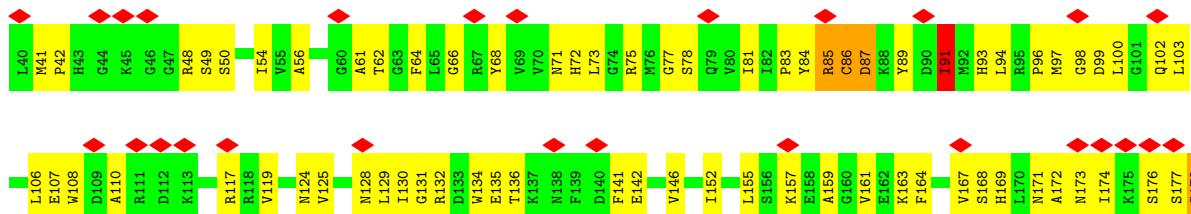
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 45% 45% 35% 6% 14%



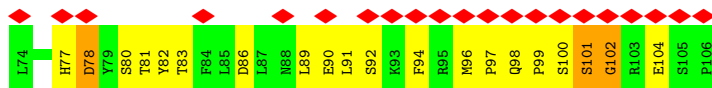
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J: 32% 45% 51%

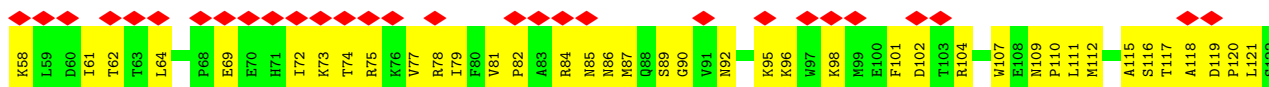
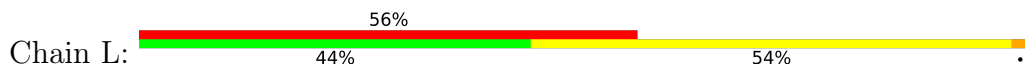




- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

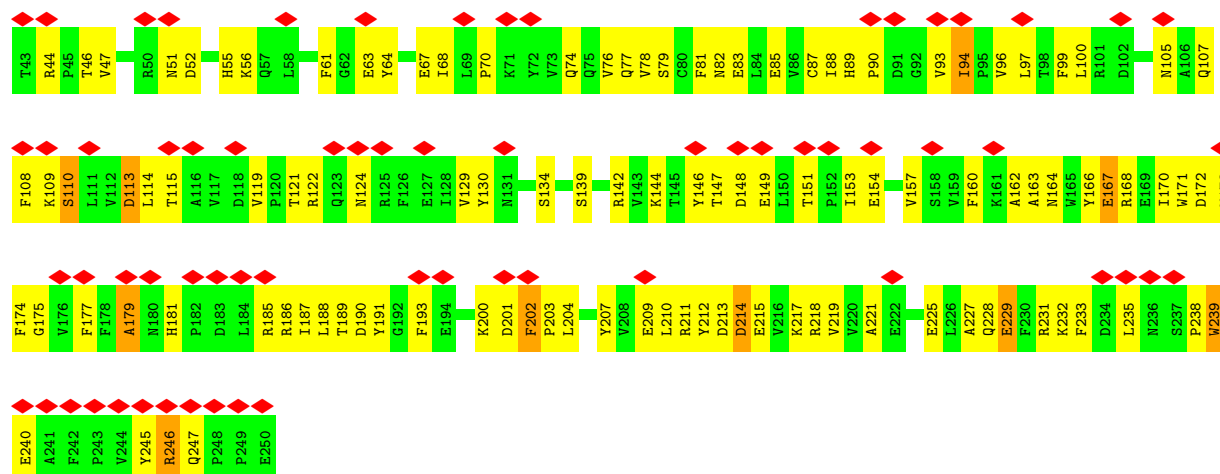


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

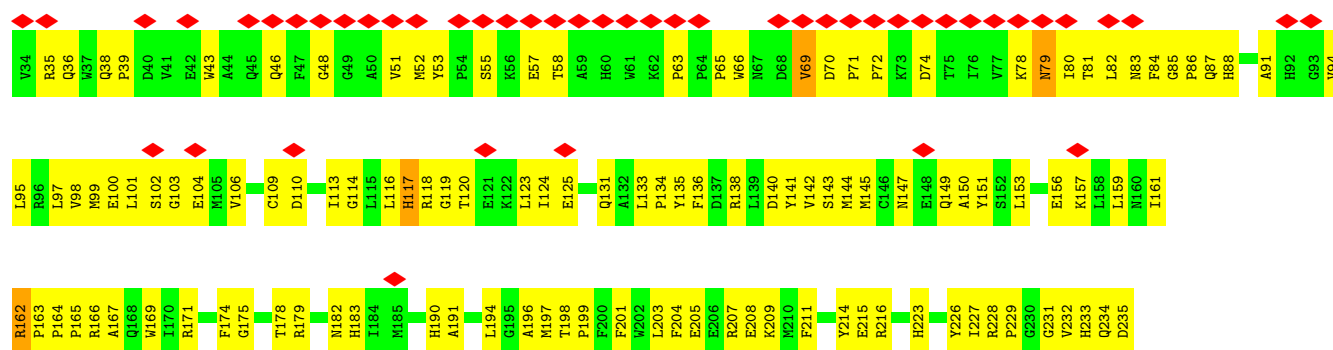


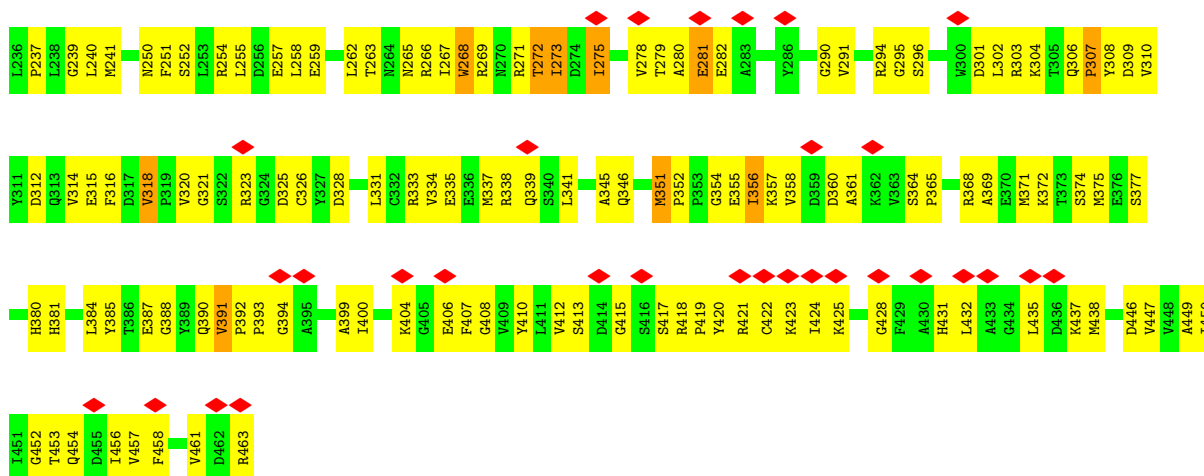


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

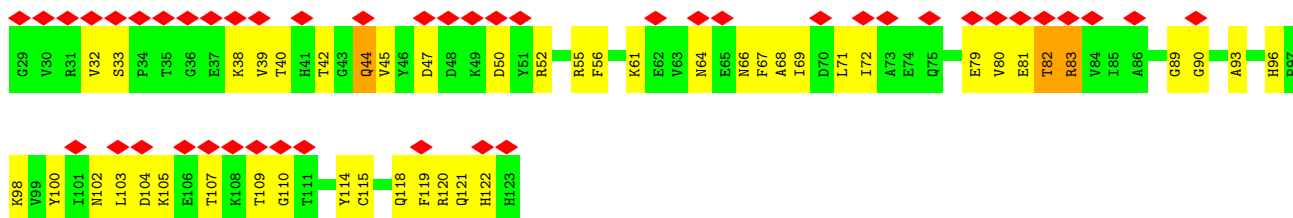




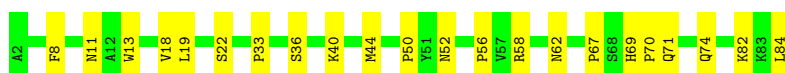
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



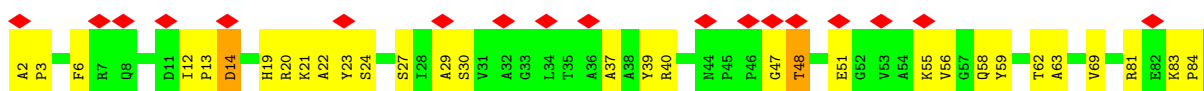
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

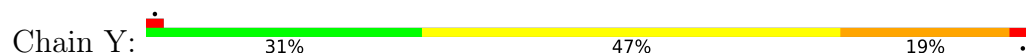




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



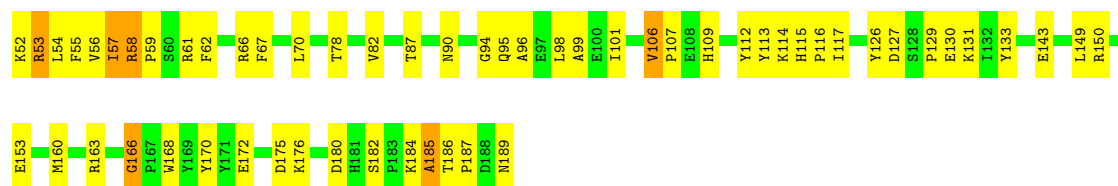
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



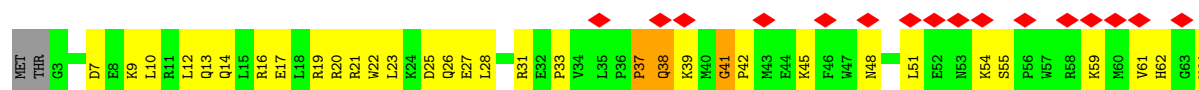
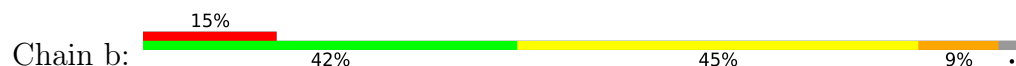
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

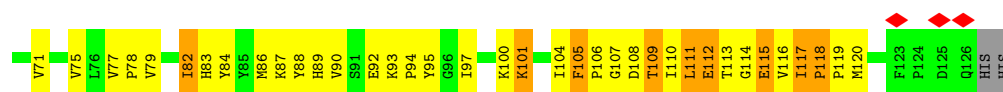


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

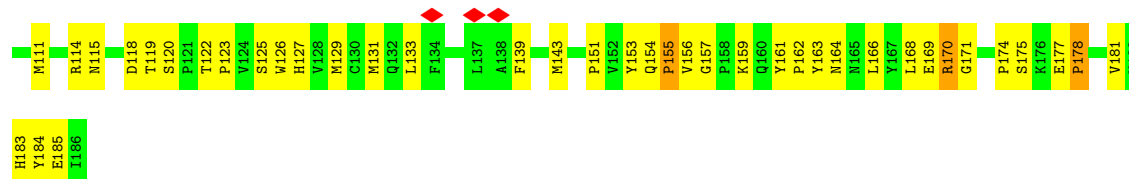
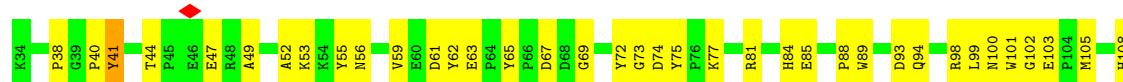


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6





- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



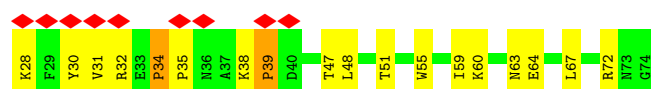
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

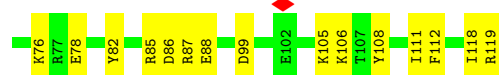
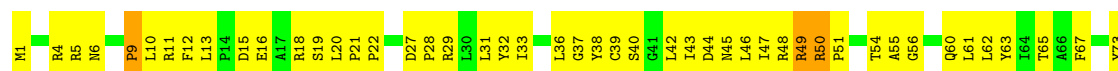


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

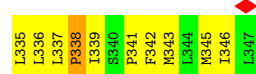
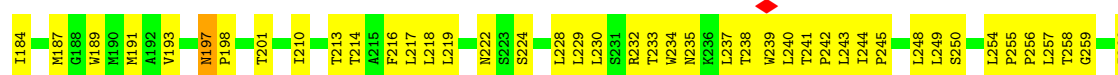
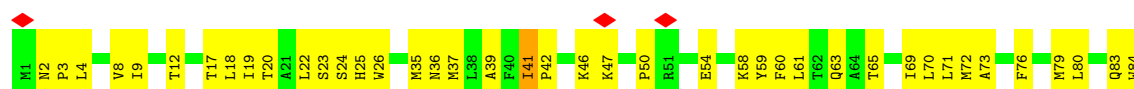




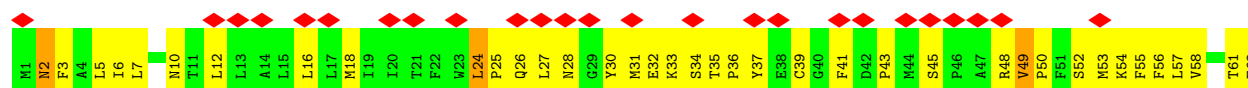
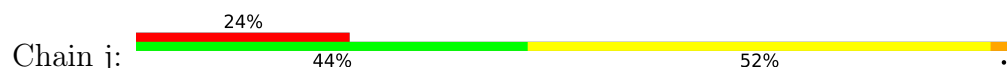
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



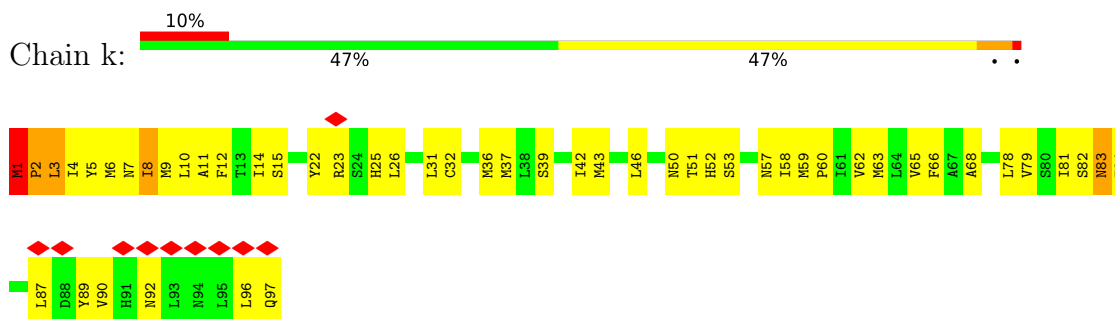
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2



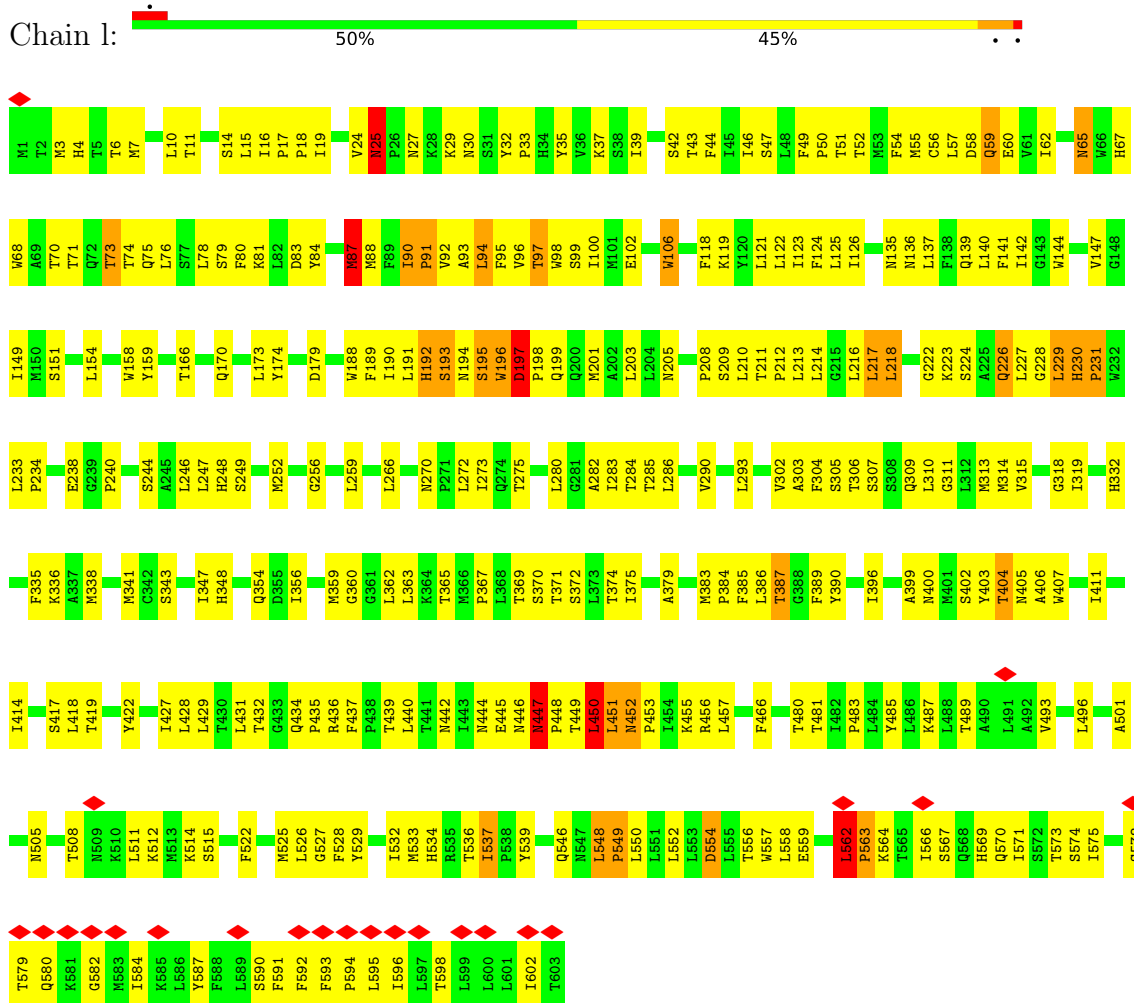
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



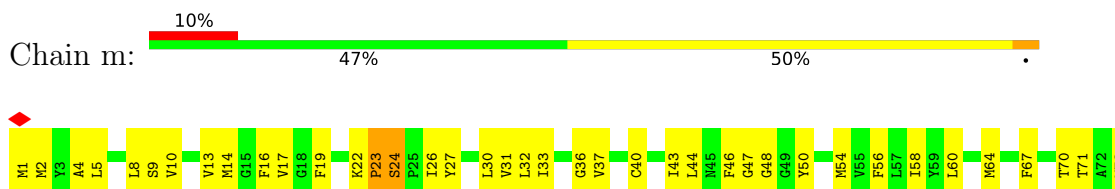
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

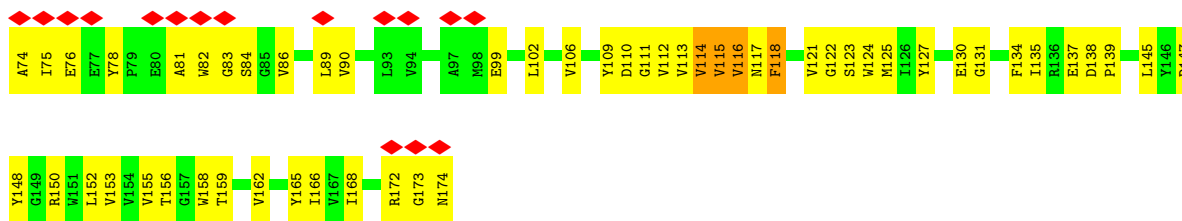


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

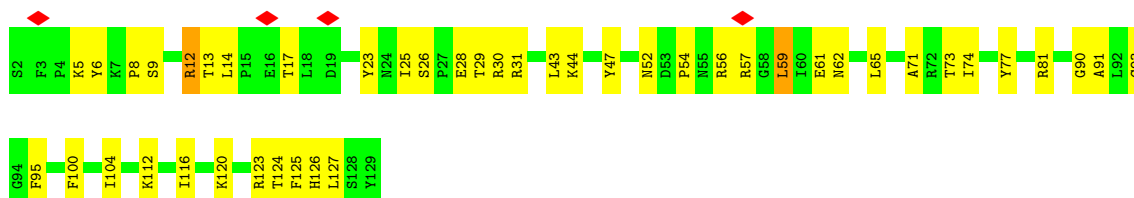




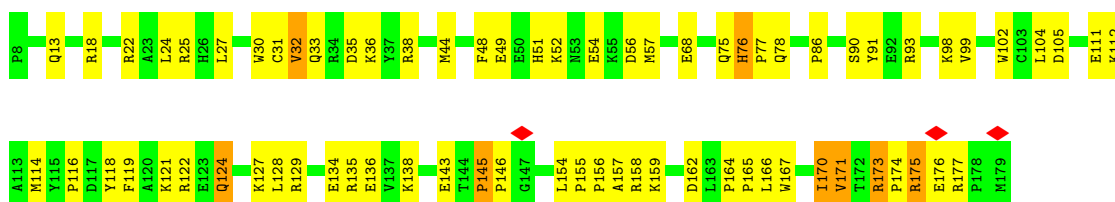
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



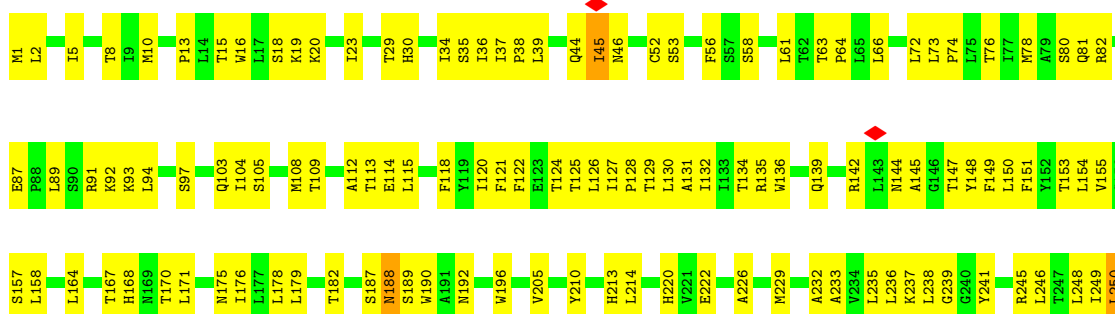
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

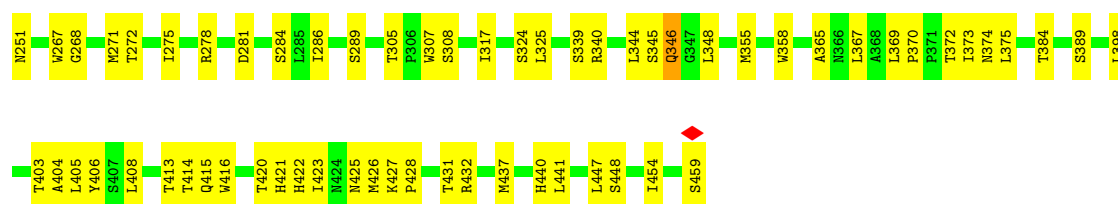


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

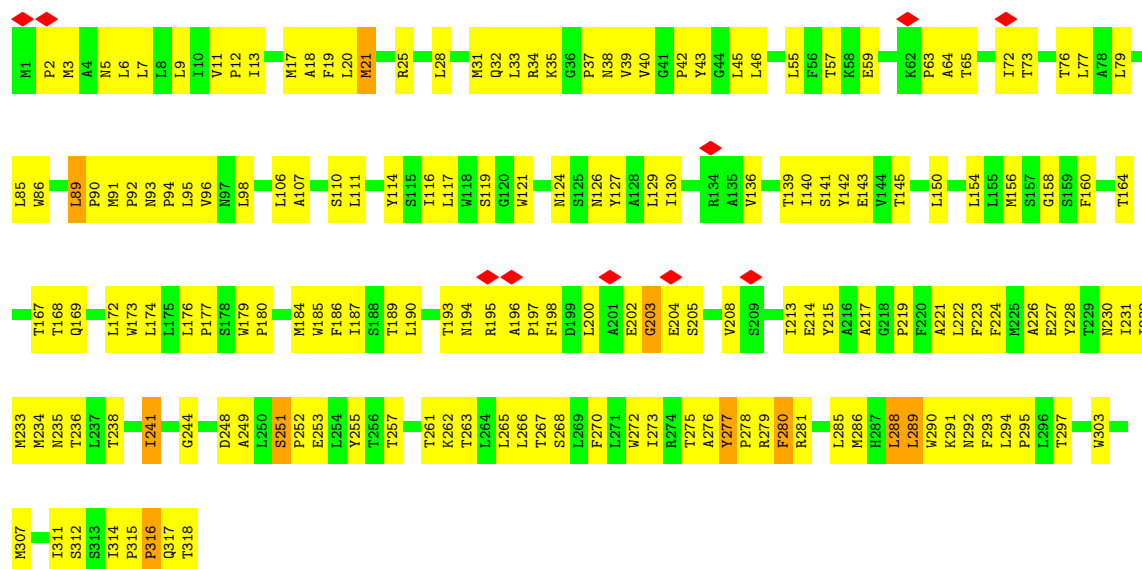


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

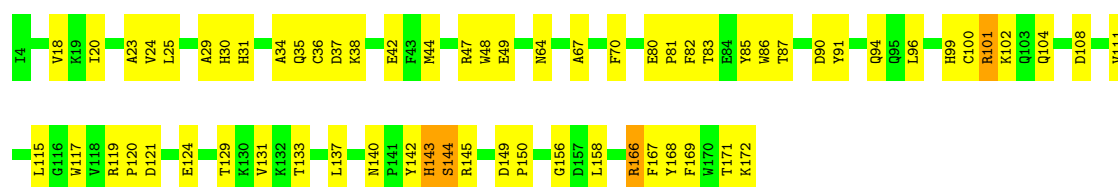




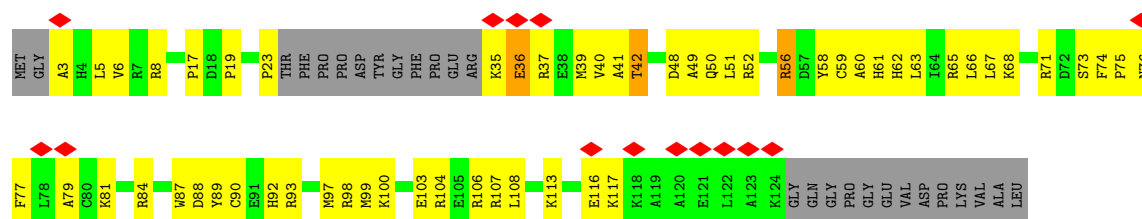
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



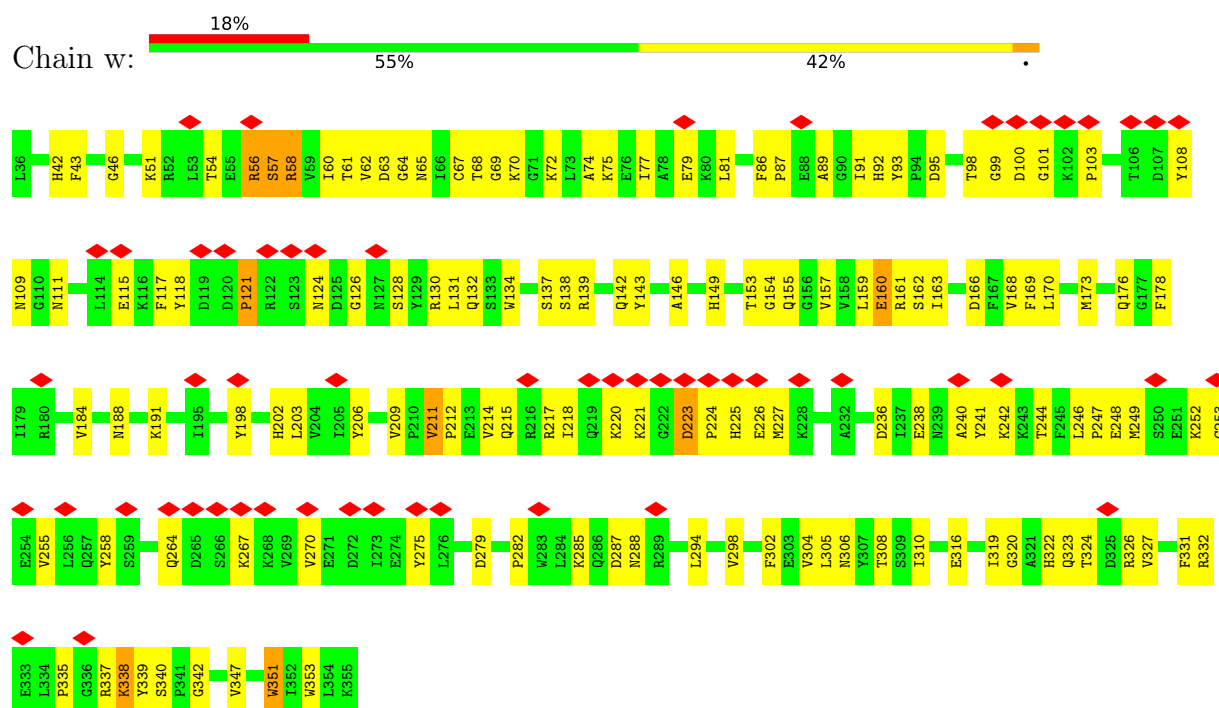
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	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 ($e^-/\text{\AA}^2$)	1.25	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	0.325	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0525	Depositor
Map size ($\text{\AA}$)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	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: 8Q1, PEE, PLX, NDP, SF4, CDL, FMN, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3398	0.87	5/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.36	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	H	0.45	0/941	0.87	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	7/1681 (0.4%)
14	O	0.39	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.55	0/3552	1.01	15/4815 (0.3%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	T	0.38	0/755	0.79	0/1017
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	W	0.74	1/1166 (0.1%)	1.05	5/1579 (0.3%)
22	Y	0.61	0/559	1.16	7/763 (0.9%)
23	Z	0.56	0/669	0.82	0/899
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	d	0.78	0/1445	0.97	3/1945 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	l	0.84	4/4840 (0.1%)	1.03	29/6611 (0.4%)
36	m	0.82	0/1346	0.99	5/1832 (0.3%)
37	n	0.63	0/484	0.99	0/652
38	o	0.71	0/1093	0.89	0/1479
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	v	0.63	0/934	1.00	4/1241 (0.3%)
44	w	0.53	1/2533 (0.0%)	0.91	7/3440 (0.2%)
All	All	0.67	12/67276 (0.0%)	0.96	232/91300 (0.3%)

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
44	w	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.58	1.50	1.54
25	b	117	ILE	C-N	6.56	1.41	1.33
21	W	117	VAL	CA-CB	-6.07	1.49	1.54
40	r	37	ILE	CA-CB	-5.94	1.51	1.54
25	b	105	PHE	C-N	5.80	1.41	1.33

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	10	MET	CA-C-N	-10.85	109.21	120.38
21	W	10	MET	C-N-CA	-10.85	109.21	120.38
8	I	38	PRO	CA-C-N	10.35	130.66	119.28
8	I	38	PRO	C-N-CA	10.35	130.66	119.28
16	Q	162	ARG	CA-C-N	10.24	127.03	119.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	213	0
2	B	1420	0	1371	119	0
3	C	1249	0	1253	82	0
4	E	968	0	982	63	0
5	F	670	0	679	38	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	H	922	0	950	58	0
8	I	769	0	788	46	0
9	J	2712	0	2757	235	0
10	K	274	0	257	25	0
11	L	964	0	962	63	0
12	M	5274	0	5312	339	0
13	N	1195	0	1155	50	0
14	O	1643	0	1646	113	0
15	P	1730	0	1685	115	0
16	Q	3460	0	3419	310	0
17	S	568	0	567	39	0
18	T	742	0	723	40	0
19	U	647	0	653	17	0
20	V	1038	0	1027	36	0
21	W	1135	0	1129	56	0
22	Y	533	0	475	97	0
23	Z	648	0	627	19	0
24	a	1174	0	1177	105	0
25	b	1059	0	1079	126	0
26	c	1236	0	1092	81	0
27	d	1418	0	1375	120	0
28	e	810	0	772	35	0
29	f	405	0	407	19	0
30	g	1004	0	1008	64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	h	863	0	861	66	0
32	i	2735	0	2893	185	0
33	j	919	0	968	76	0
34	k	740	0	792	89	0
35	l	4717	0	4893	400	0
36	m	1313	0	1330	122	0
37	n	473	0	480	30	0
38	o	1066	0	1086	52	0
39	p	1495	0	1440	94	0
40	r	3629	0	3825	164	0
41	s	2509	0	2617	170	0
42	u	1394	0	1367	60	0
43	v	921	0	892	90	0
44	w	2474	0	2304	116	0
45	A	8	0	0	6	0
45	B	16	0	0	3	0
45	C	8	0	0	0	0
45	M	16	0	0	3	0
46	A	31	0	19	16	0
47	B	52	0	88	4	0
47	U	52	0	88	3	0
47	V	52	0	88	5	0
47	b	52	0	88	38	0
47	g	156	0	264	13	0
47	r	104	0	176	23	0
48	E	35	0	0	4	0
48	p	35	0	0	12	0
49	J	48	0	26	26	0
50	M	4	0	0	1	0
50	O	4	0	0	2	0
51	V	63	0	68	8	0
51	i	64	0	72	3	0
51	l	128	0	144	4	0
51	n	64	0	72	10	0
52	V	51	0	82	21	0
52	W	51	0	82	19	0
52	l	100	0	157	68	0
All	All	66789	0	67204	3729	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 28.

The worst 5 of 3729 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)
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.65
35:l:533:MET:CE	52:l:702:PEE:H36	1.25	1.58
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.57
24:a:55:PHE:HE2	39:p:118:TYR:CE2	1.17	1.56
24:a:55:PHE:CE2	39:p:118:TYR:CD2	1.91	1.55

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	31
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	52
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	25
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	29
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	17
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	18
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	13
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	31
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	25
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	25
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	17
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	25
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	428/430 (100%)	397 (93%)	24 (6%)	7 (2%)	7	35
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	26
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	19
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	40
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	31
21	W	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	3	26
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	5
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	31
25	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	2	20
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	18
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	52
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	25
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	31
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	17
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	15
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	34
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	27
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	25
35	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	6	32
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	15
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	22
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	25
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	32
41	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	4	27
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	26
43	v	107/137 (78%)	90 (84%)	14 (13%)	3 (3%)	4	27
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	27
All	All	8097/8236 (98%)	7338 (91%)	526 (6%)	233 (3%)	5	26

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	77 (99%)	1 (1%)	61	71
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	74
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	70
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	83
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	76
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	22
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	76
25	b	118/122 (97%)	113 (96%)	5 (4%)	26	51
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	46
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	83
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	74
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	48
35	l	531/532 (100%)	512 (96%)	19 (4%)	31	54
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	71
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/121 (74%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
All	All	7093/7209 (98%)	7034 (99%)	59 (1%)	70	76

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	d	61	GLN
35	l	450	LEU
34	k	3	LEU

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Mol	Chain	Res	Type
35	l	447	ASN
35	l	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
35	l	248	HIS
41	s	169	GLN
35	l	332	HIS
38	o	52	ASN
42	u	104	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 ligands 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	$\# Z > 2$
47	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	A	501	1	0,12,12	-	-	-		
47	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
47	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
52	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
47	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
48	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
51	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
47	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
52	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
49	NDP	J	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.75	11 (16%)
46	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
47	PLX	g	202	-	51,51,51	0.75	1 (1%)	55,59,59	0.61	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
45	SF4	M	802	12	0,12,12	-	-	-		
50	FES	M	803	-	0,4,4	-	-	-		
47	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
47	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
51	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
51	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
52	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
52	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
47	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.59	1 (1%)
51	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
48	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
50	FES	O	301	14	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	B	303	-	-	21/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	b	201	-	-	27/55/55/55	-
47	PLX	U	101	-	-	22/55/55/55	-
52	PEE	W	201	-	-	32/54/54/54	-
47	PLX	r	502	-	-	36/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
48	8Q1	E	201	-	-	18/41/41/41	-
51	CDL	l	703	-	-	38/74/74/110	-
47	PLX	r	501	-	-	28/55/55/55	-
52	PEE	l	702	-	-	27/54/54/54	-
49	NDP	J	401	-	-	15/34/77/77	0/5/5/5
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
47	PLX	g	202	-	-	25/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
51	CDL	l	704	-	-	44/74/74/110	-
45	SF4	M	802	12	-	-	0/6/5/5
50	FES	M	803	-	-	-	0/1/1/1
47	PLX	g	201	-	-	25/55/55/55	-
47	PLX	g	203	-	-	24/55/55/55	-
51	CDL	n	101	-	-	33/74/74/110	-
51	CDL	i	401	-	-	39/74/74/110	-
52	PEE	V	202	-	-	27/54/54/54	-
52	PEE	l	701	-	-	32/52/52/54	-
47	PLX	V	203	-	-	26/55/55/55	-
51	CDL	V	201	-	-	42/69/69/110	-
45	SF4	B	302	2	-	-	0/6/5/5
48	8Q1	p	201	-	-	19/41/41/41	-
50	FES	O	301	14	-	-	0/1/1/1

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	201	8Q1	C34-N36	5.30	1.45	1.33
48	E	201	8Q1	C34-N36	5.24	1.45	1.33
48	p	201	8Q1	C39-N41	5.24	1.45	1.33
48	E	201	8Q1	C39-N41	4.93	1.44	1.33
46	A	502	FMN	C9A-C5A	4.42	1.48	1.41

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	J	401	NDP	C5A-C4A-N3A	-6.19	118.68	126.75
48	p	201	8Q1	C6-C1-S44	6.03	120.47	113.46
49	J	401	NDP	PN-O3-PA	-5.21	114.94	132.83
49	J	401	NDP	N3A-C4A-N9A	4.96	135.26	127.08
48	E	201	8Q1	C6-C1-S44	4.56	118.77	113.46

There are no chirality outliers.

5 of 607 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	B	303	PLX	C2-O1-P1-O2

There are no ring outliers.

28 monomers are involved in 285 short contacts:

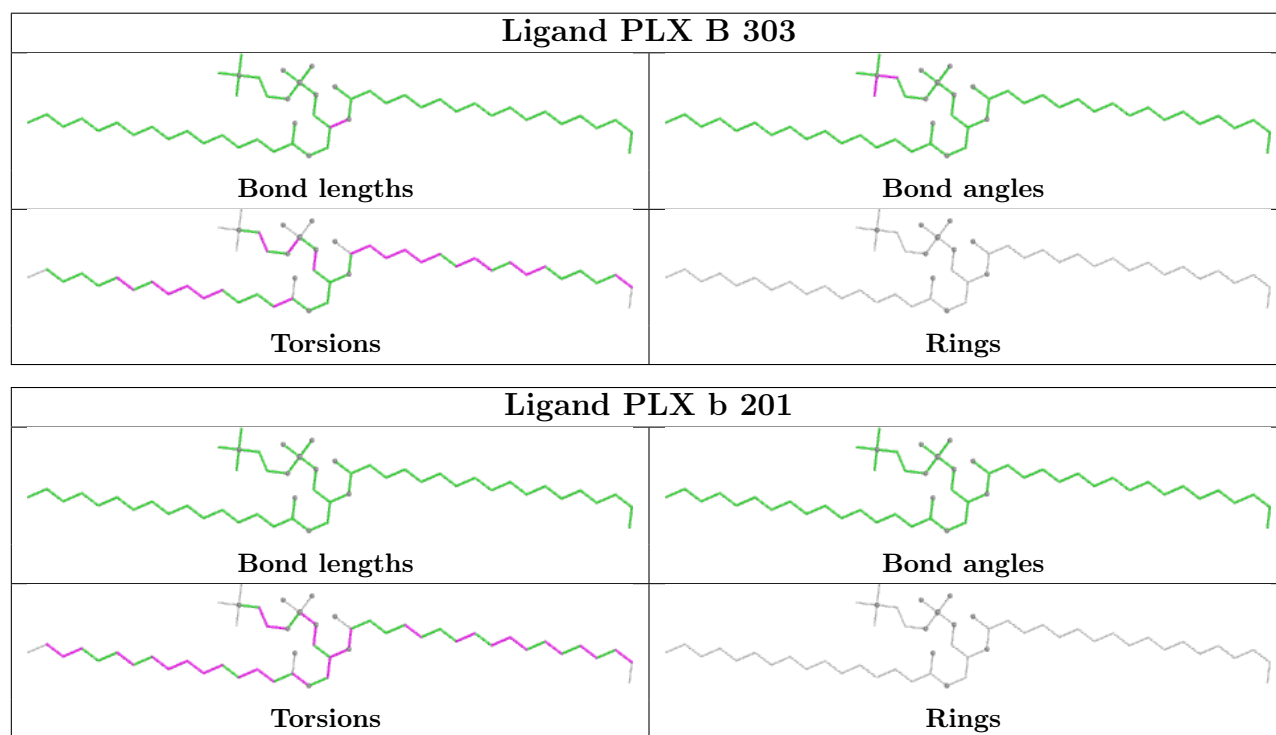
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	B	303	PLX	4	0
45	A	501	SF4	6	0
47	b	201	PLX	38	0
47	U	101	PLX	3	0
52	W	201	PEE	19	0
45	B	301	SF4	1	0
47	r	502	PLX	17	0
48	E	201	8Q1	4	0
51	l	703	CDL	2	0
47	r	501	PLX	6	0
52	l	702	PEE	18	0
49	J	401	NDP	26	0
46	A	502	FMN	16	0
47	g	202	PLX	3	0
45	M	801	SF4	3	0
51	l	704	CDL	2	0
50	M	803	FES	1	0
47	g	201	PLX	2	0
47	g	203	PLX	8	0
51	n	101	CDL	10	0
51	i	401	CDL	3	0

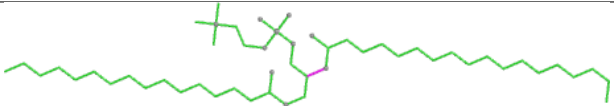
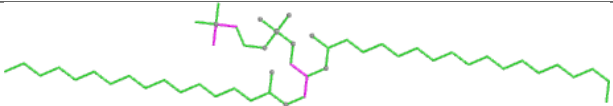
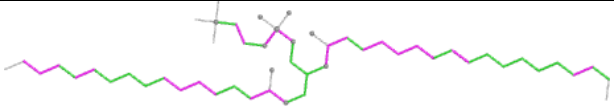
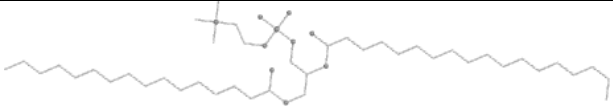
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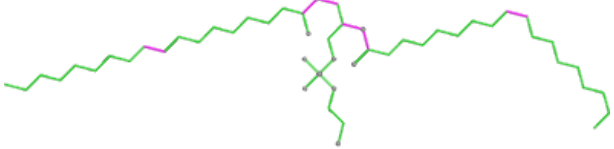
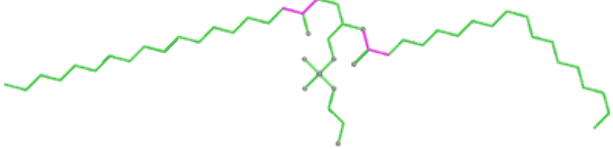
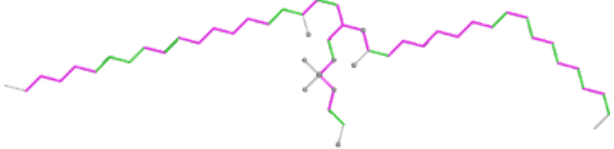
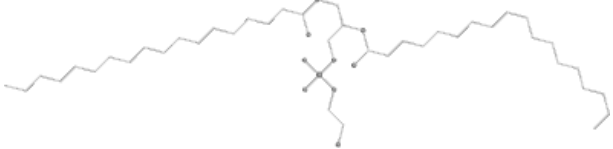
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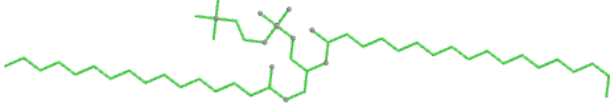
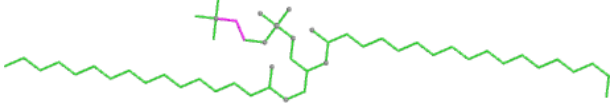
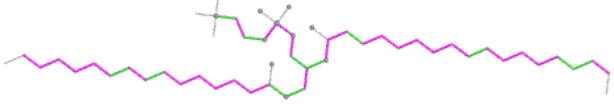
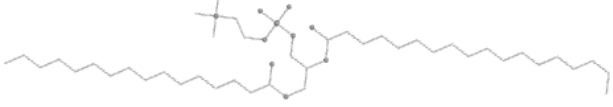
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	V	202	PEE	21	0
52	I	701	PEE	50	0
47	V	203	PLX	5	0
51	V	201	CDL	8	0
45	B	302	SF4	2	0
48	p	201	8Q1	12	0
50	O	301	FES	2	0

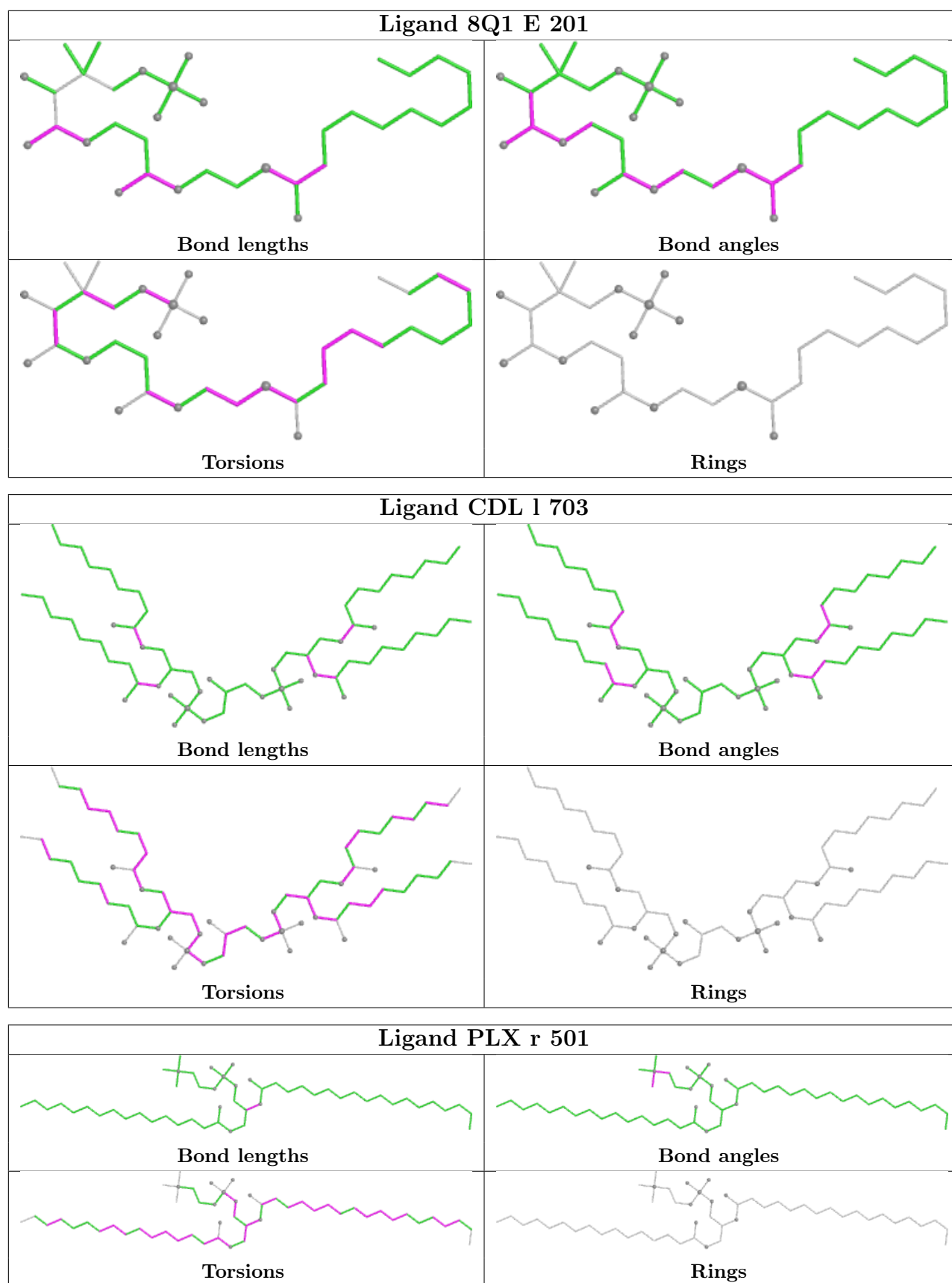
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

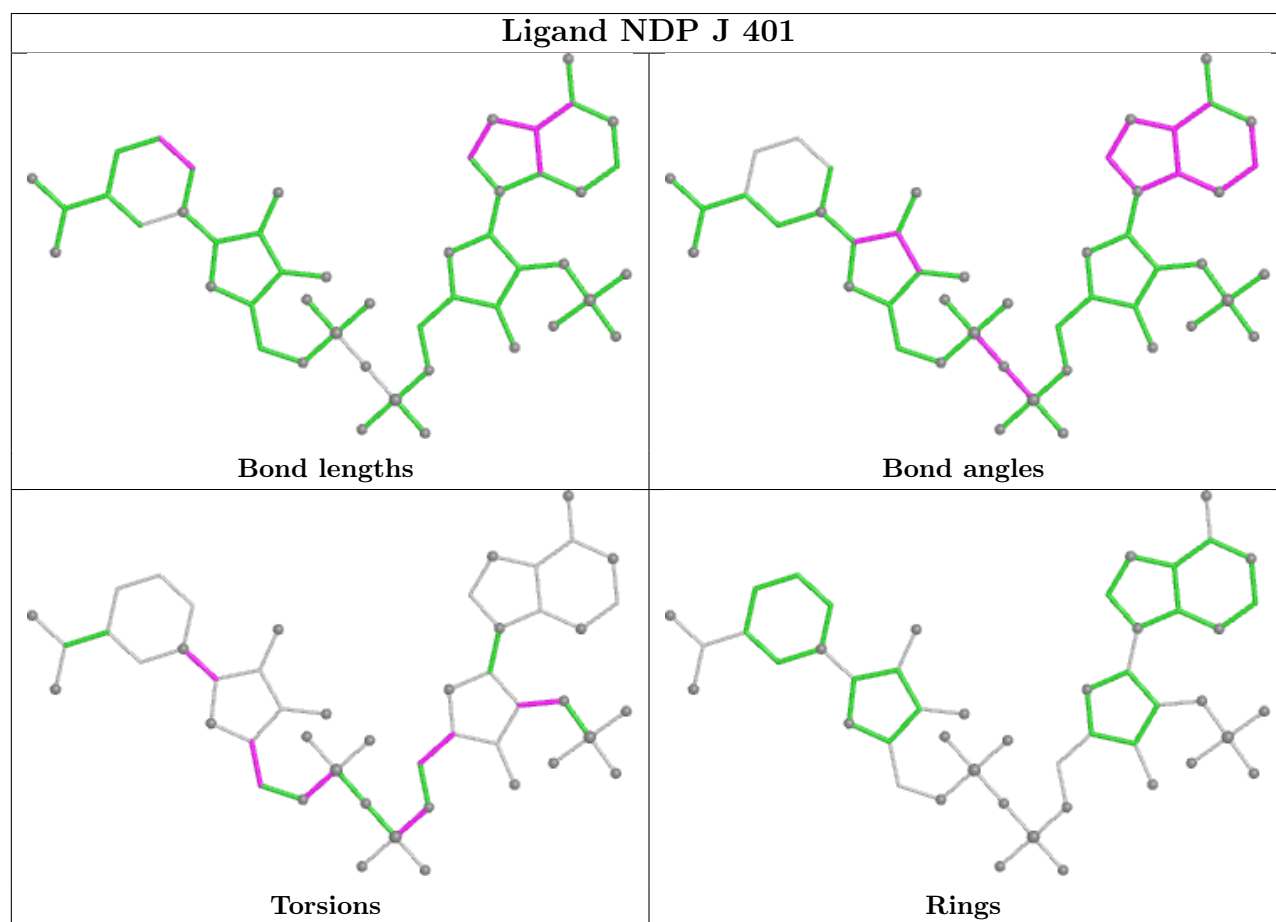
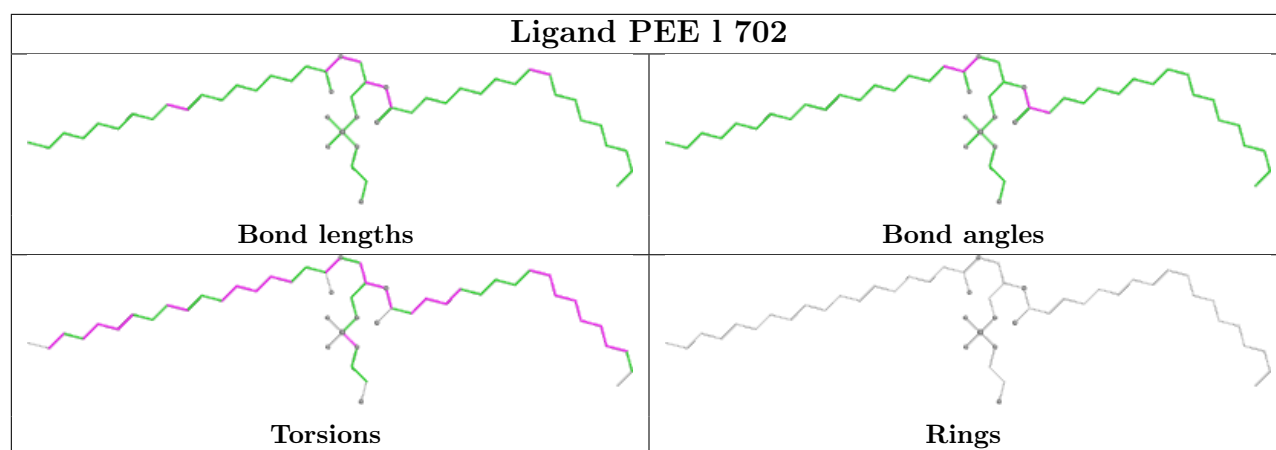


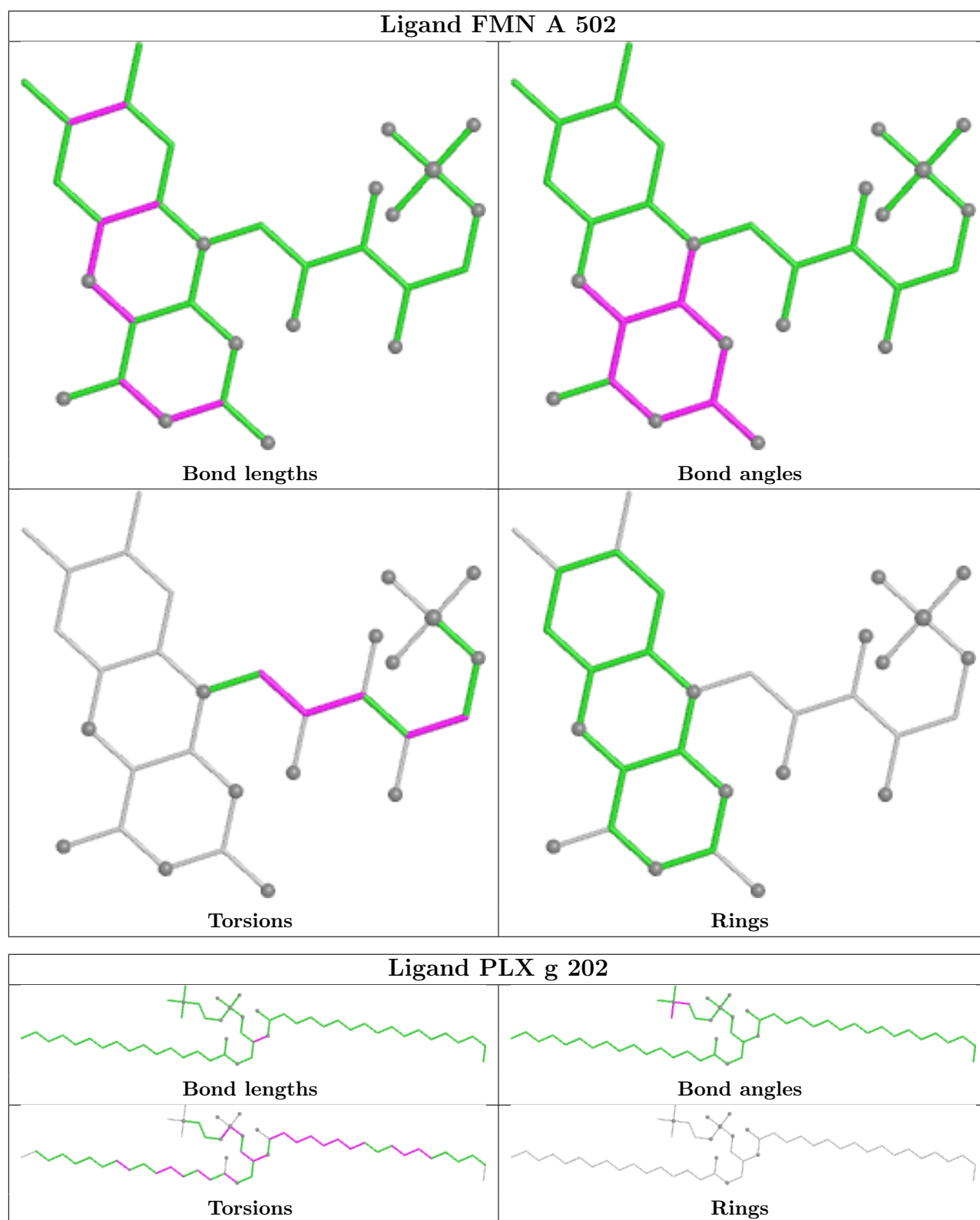
Ligand PLX U 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

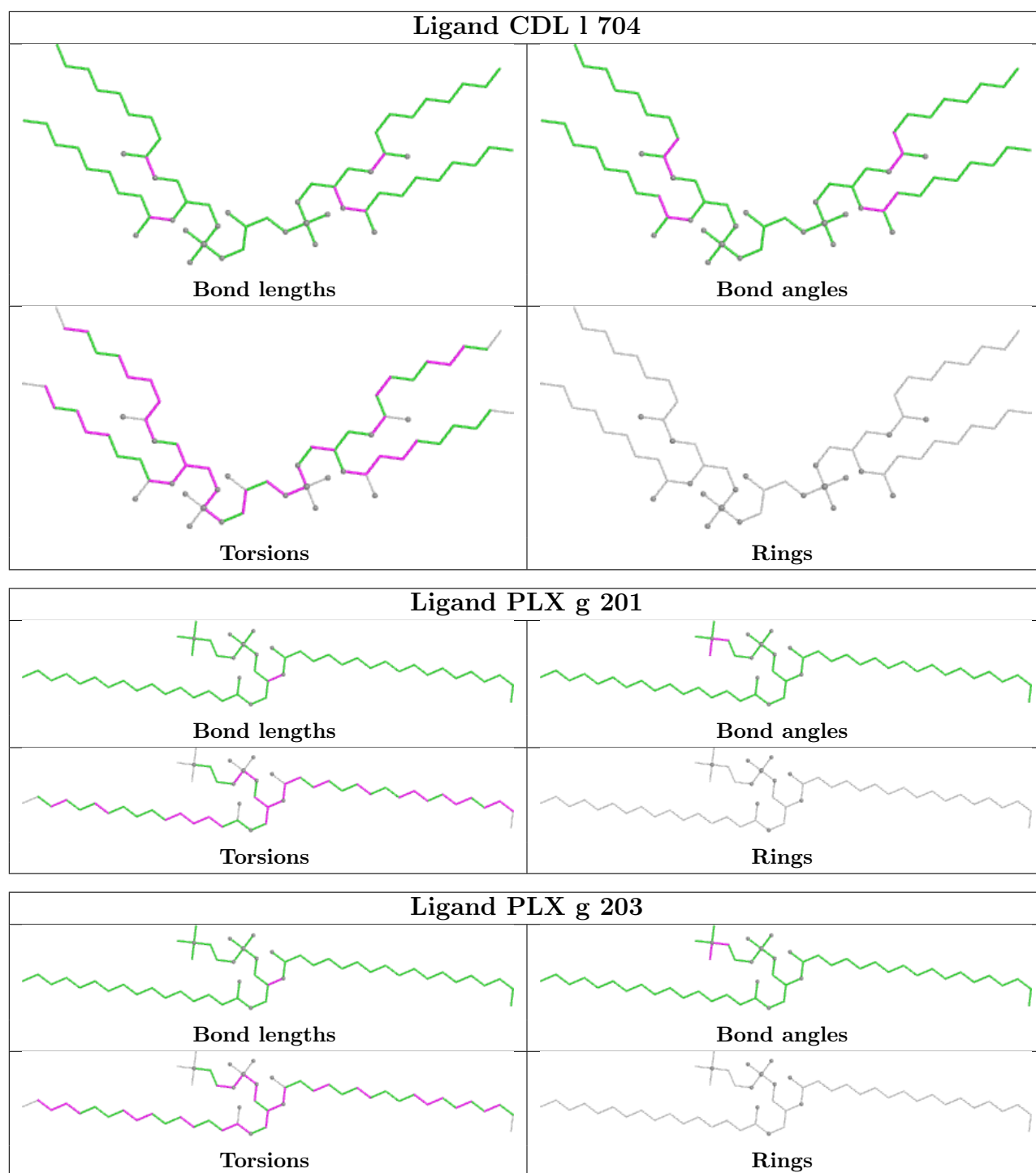
Ligand PEE W 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

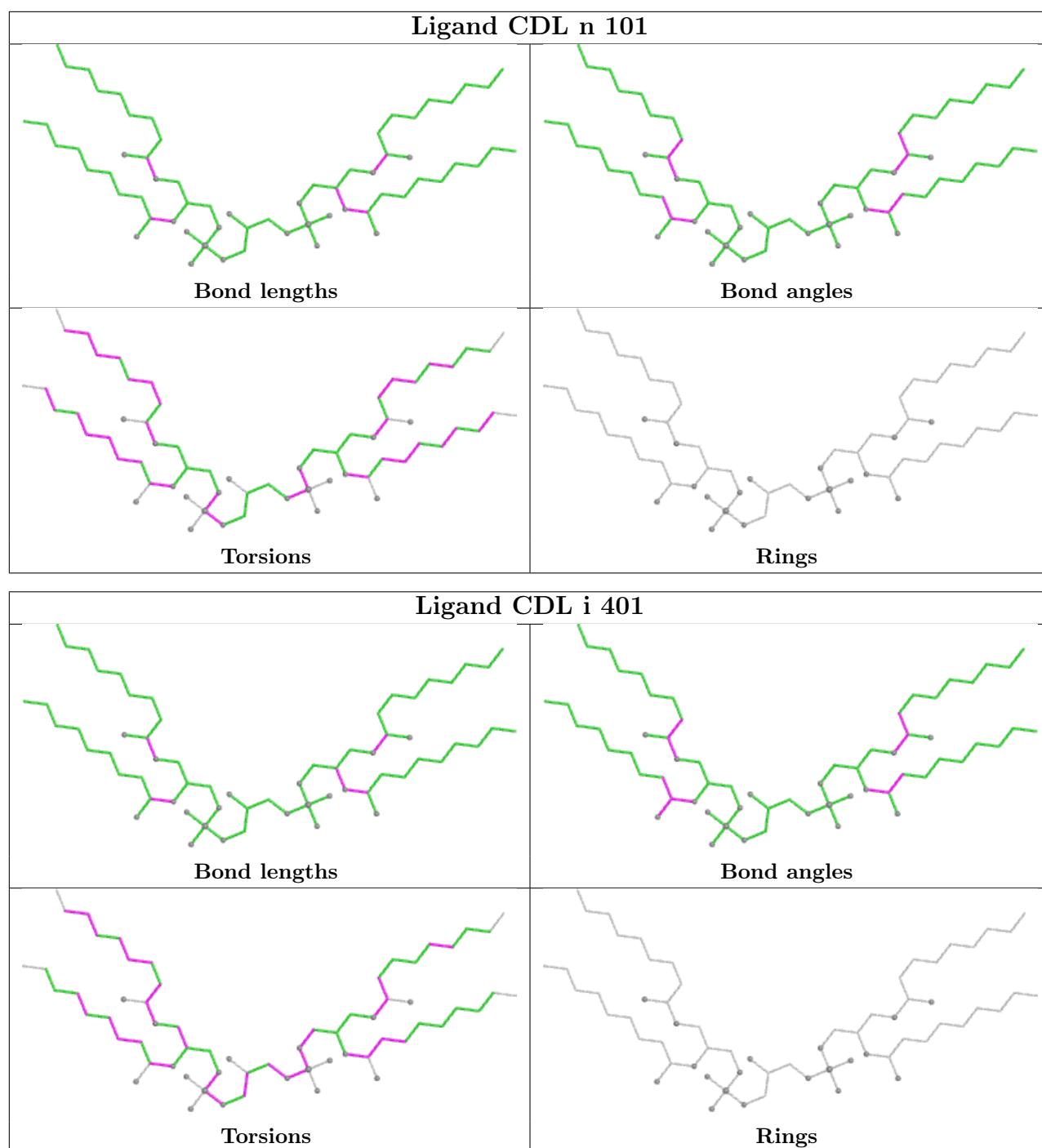
Ligand PLX r 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

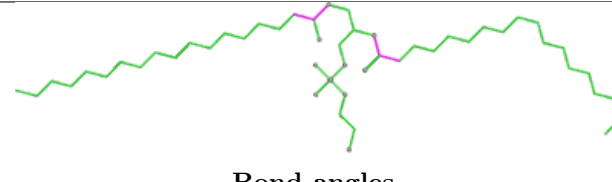
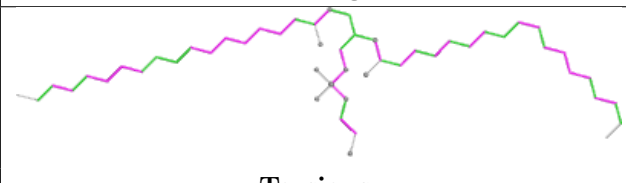
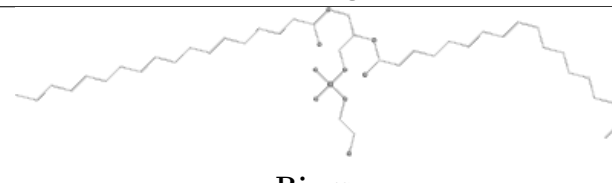


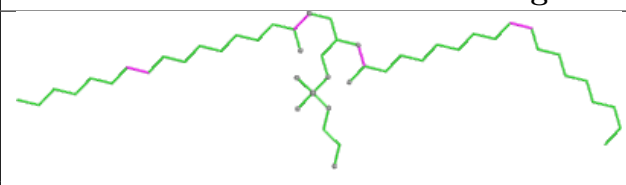
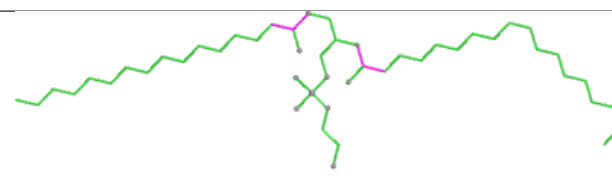
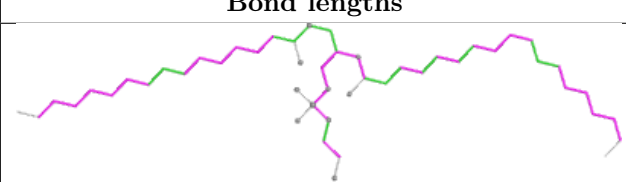
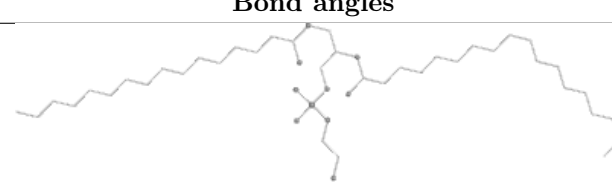


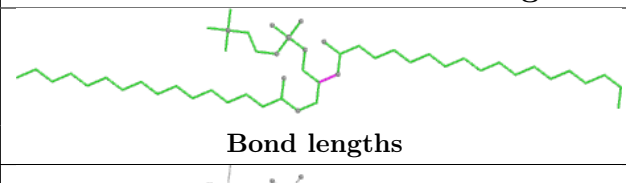
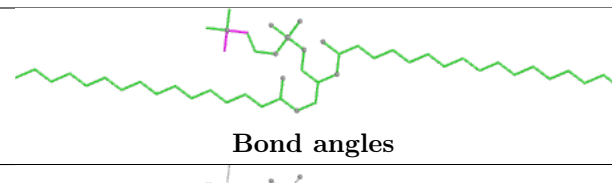
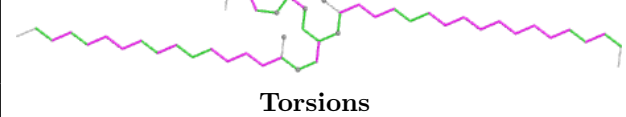


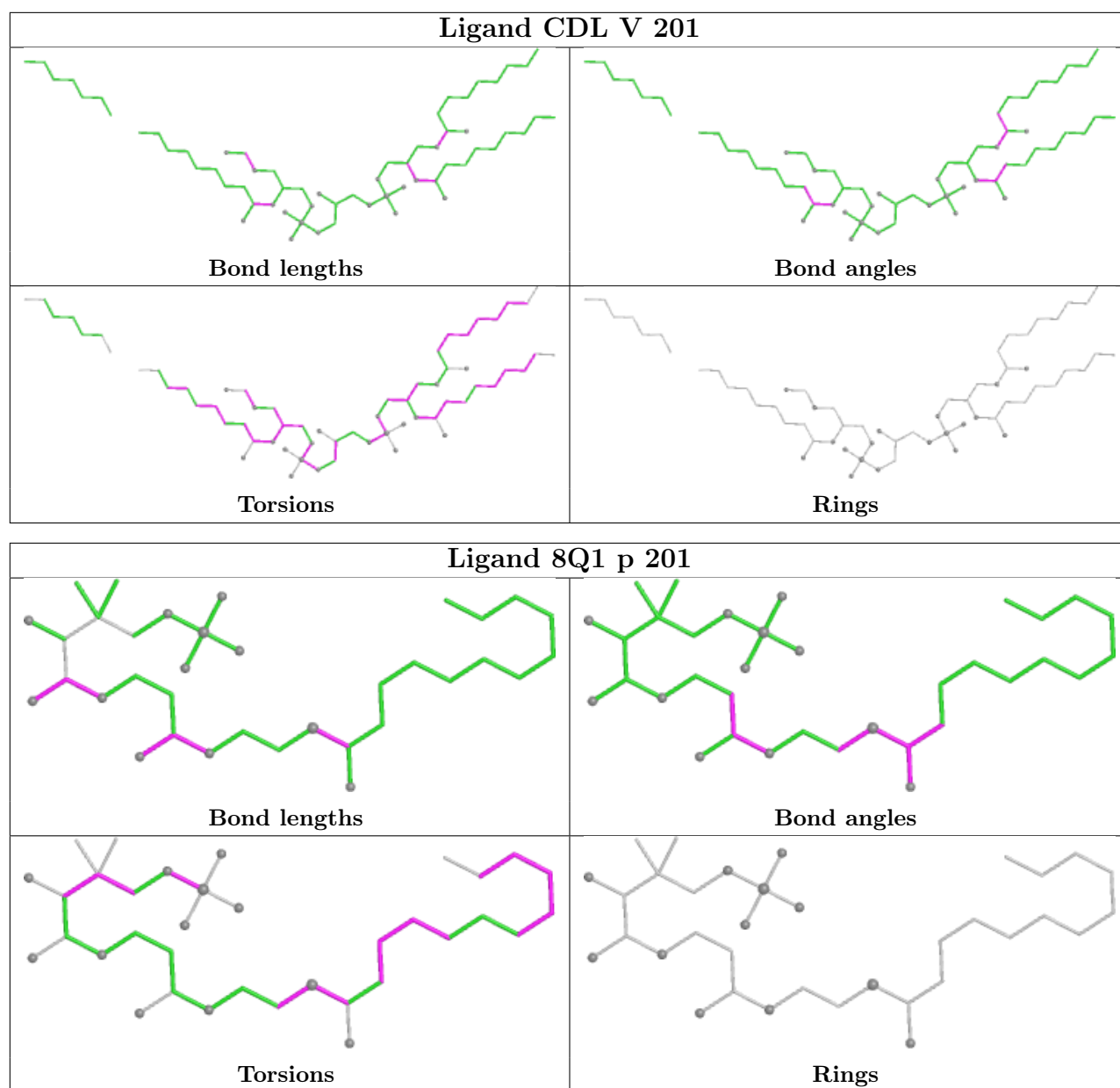




Ligand PEE V 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE I 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX V 203	
	
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.

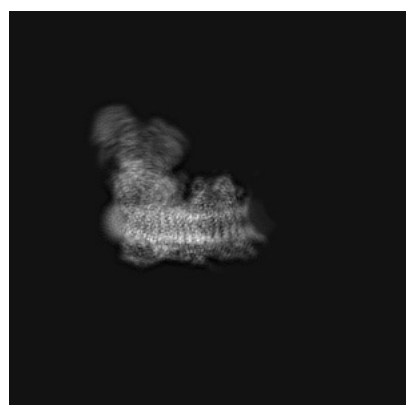
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6773. These allow visual inspection of the internal detail of the map and identification of artifacts.

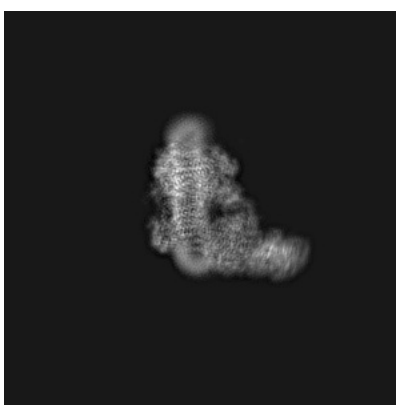
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

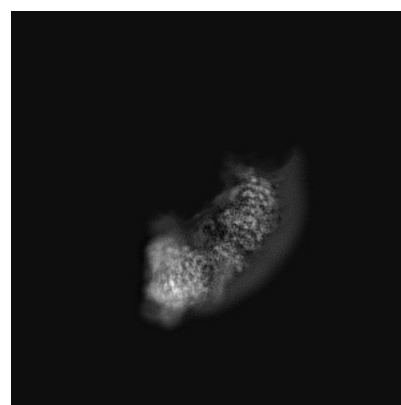
6.1.1 Primary map



X



Y



Z

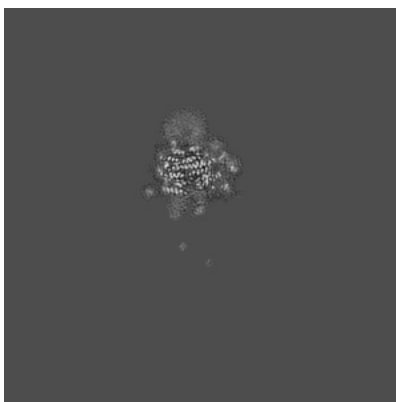
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

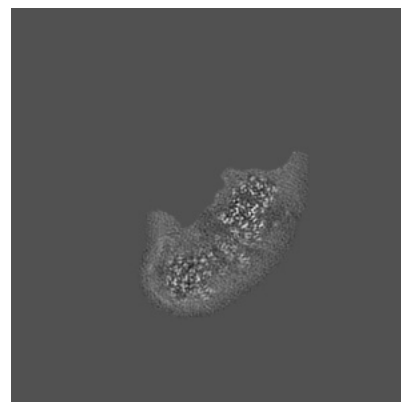
6.2.1 Primary map



X Index: 240



Y Index: 240

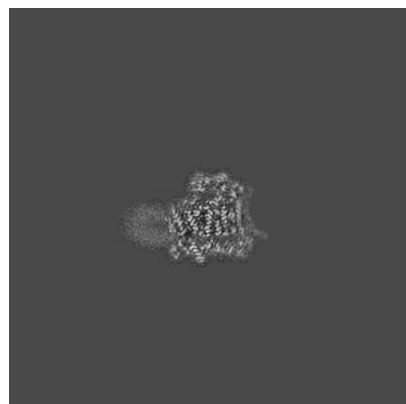


Z Index: 240

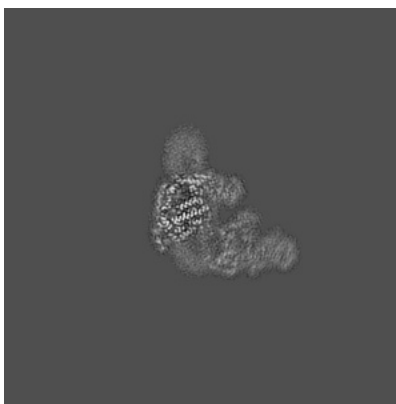
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

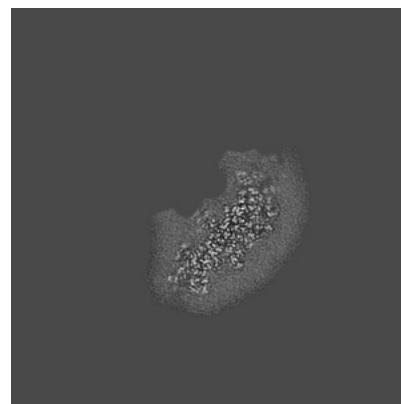
6.3.1 Primary map



X Index: 290



Y Index: 183

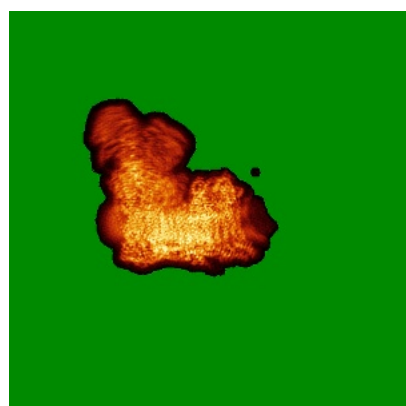


Z Index: 208

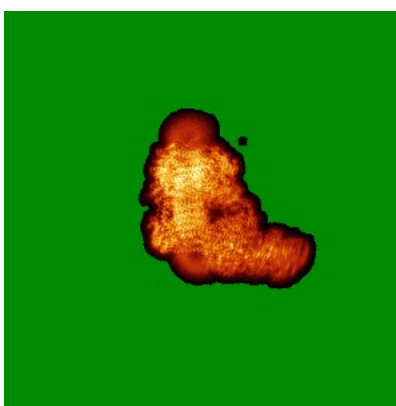
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

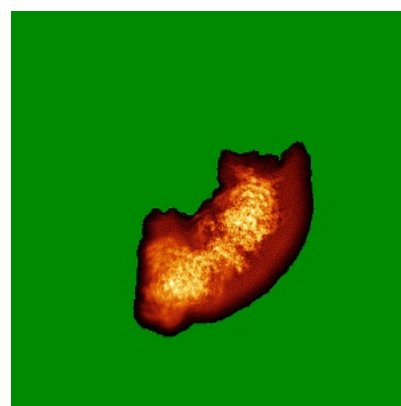
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0525. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

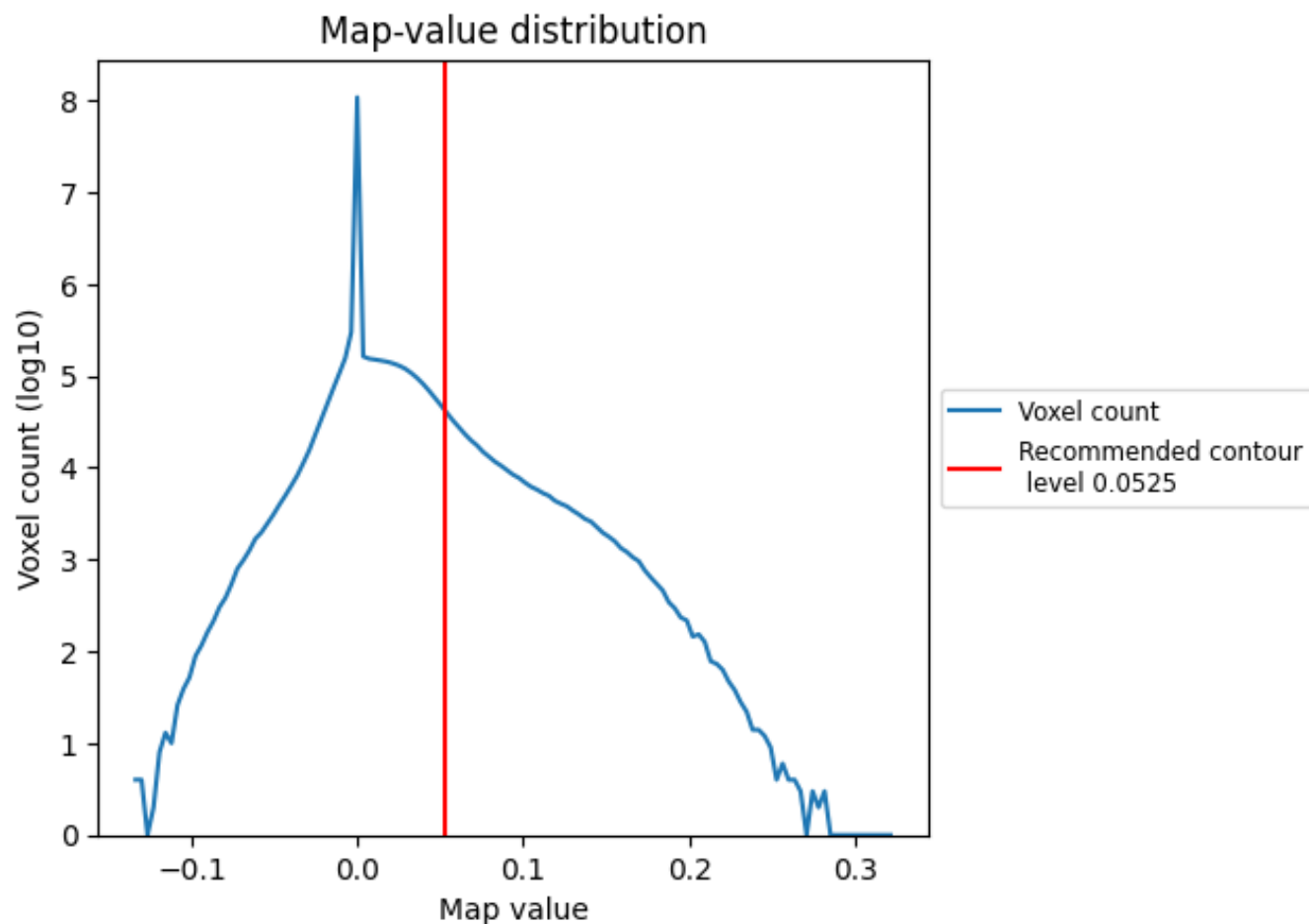
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

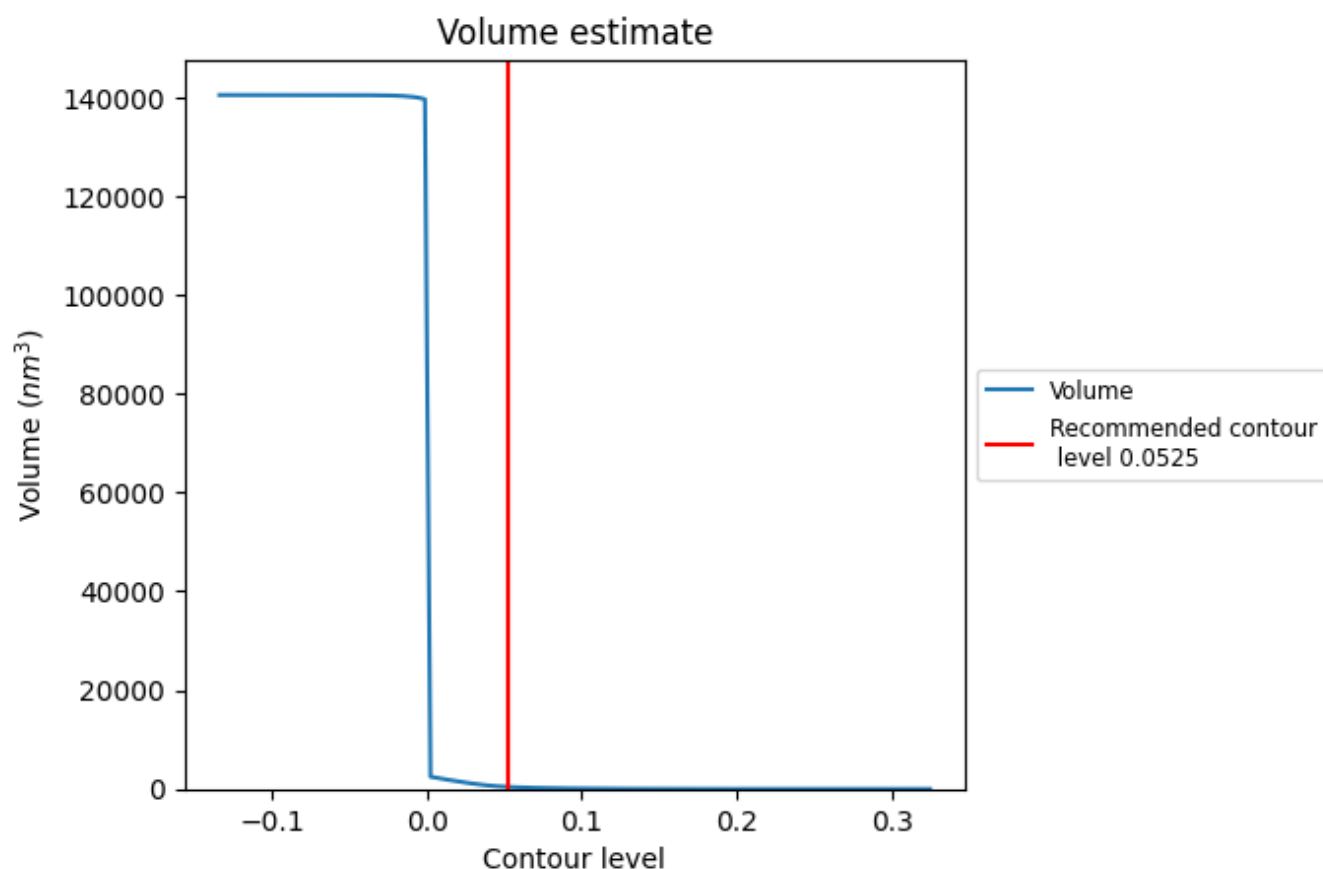
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

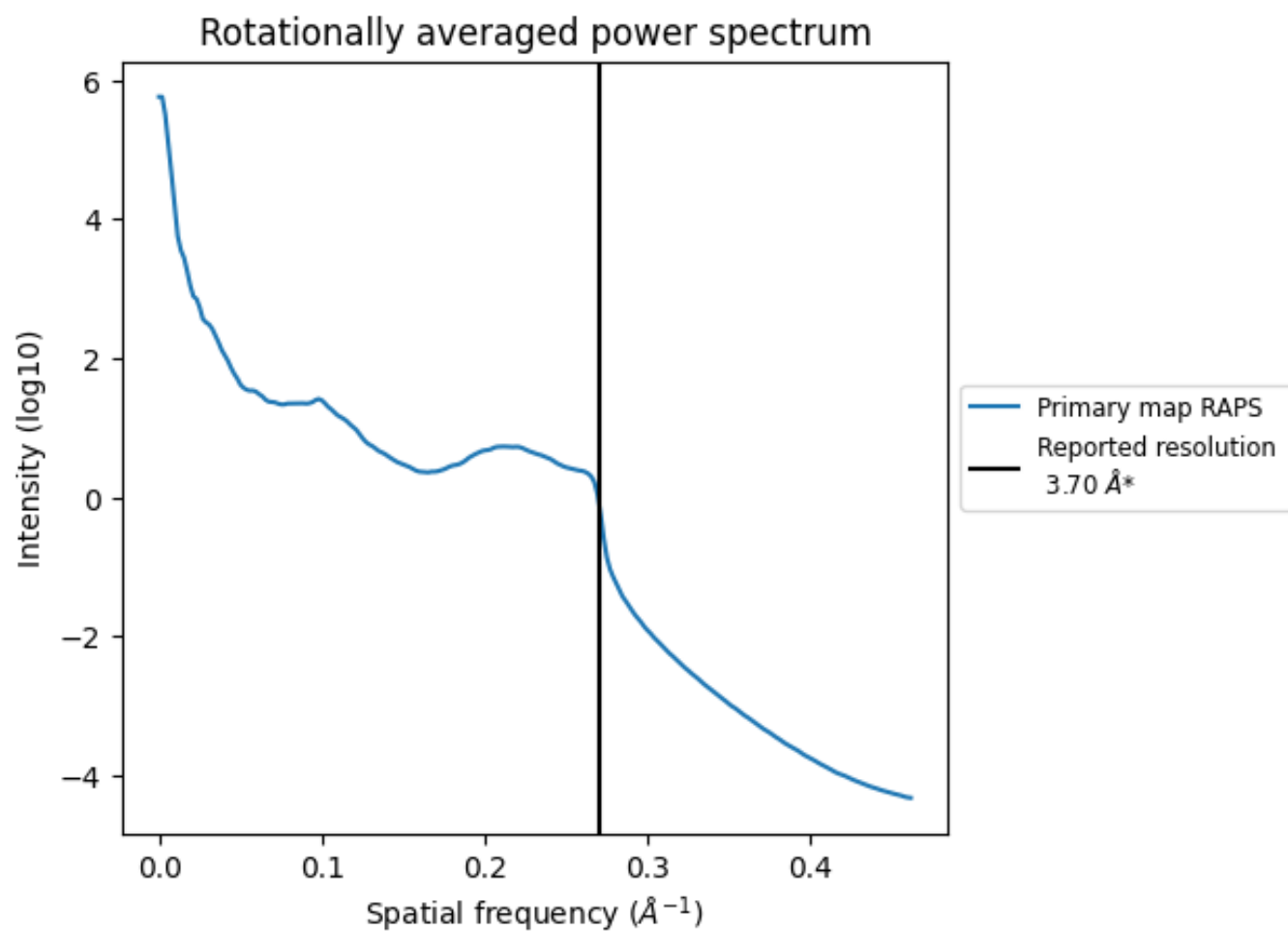
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 372 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

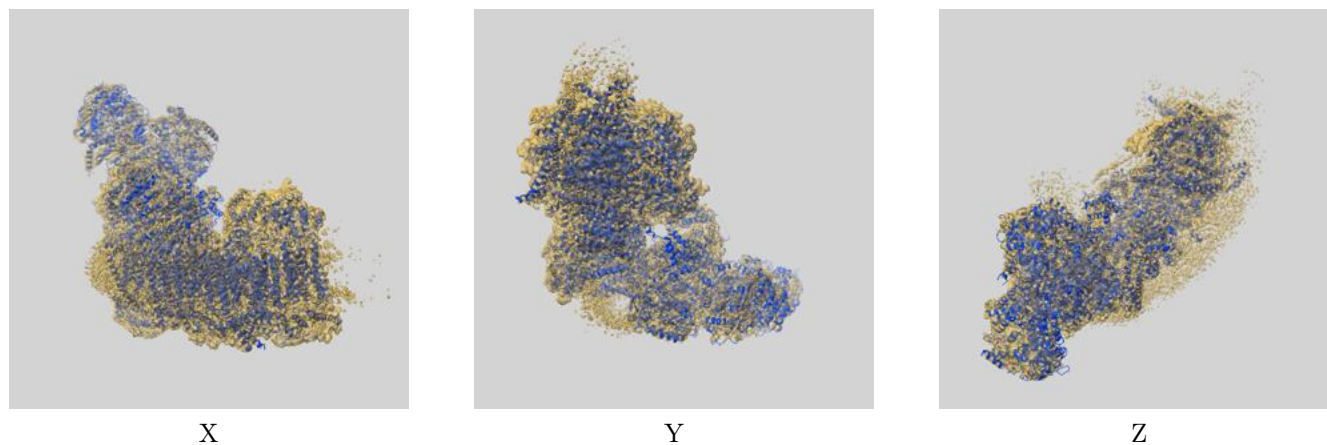
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

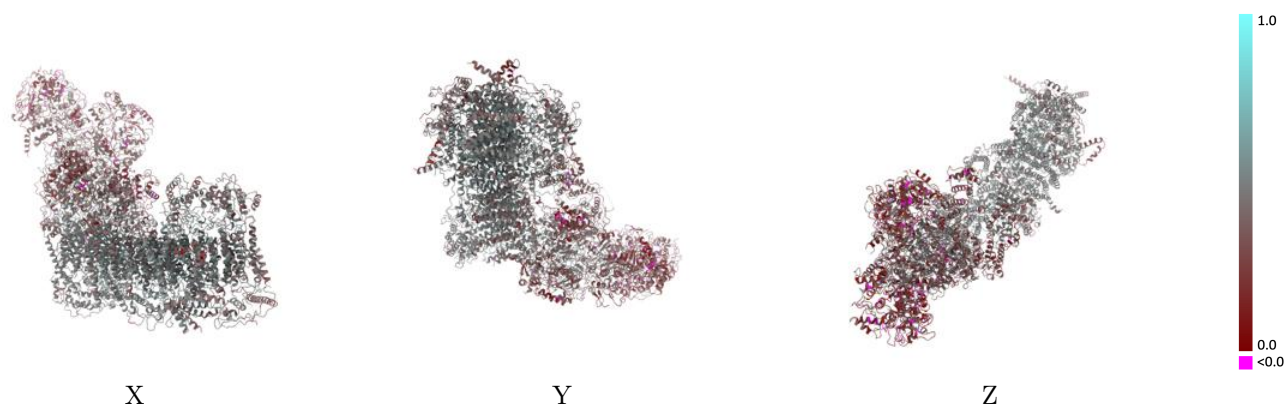
This section contains information regarding the fit between EMDB map EMD-6773 and PDB model 5XTD. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



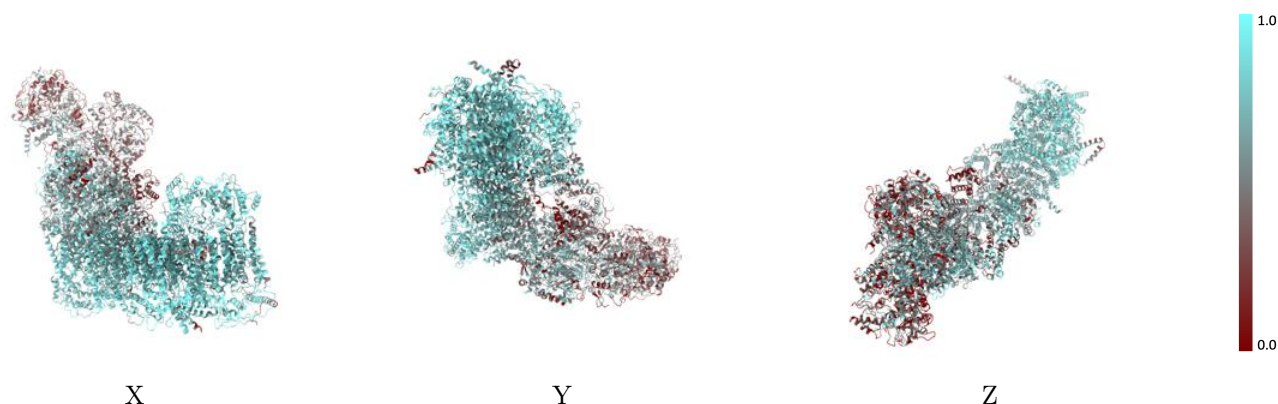
The images above show the 3D surface view of the map at the recommended contour level 0.0525 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



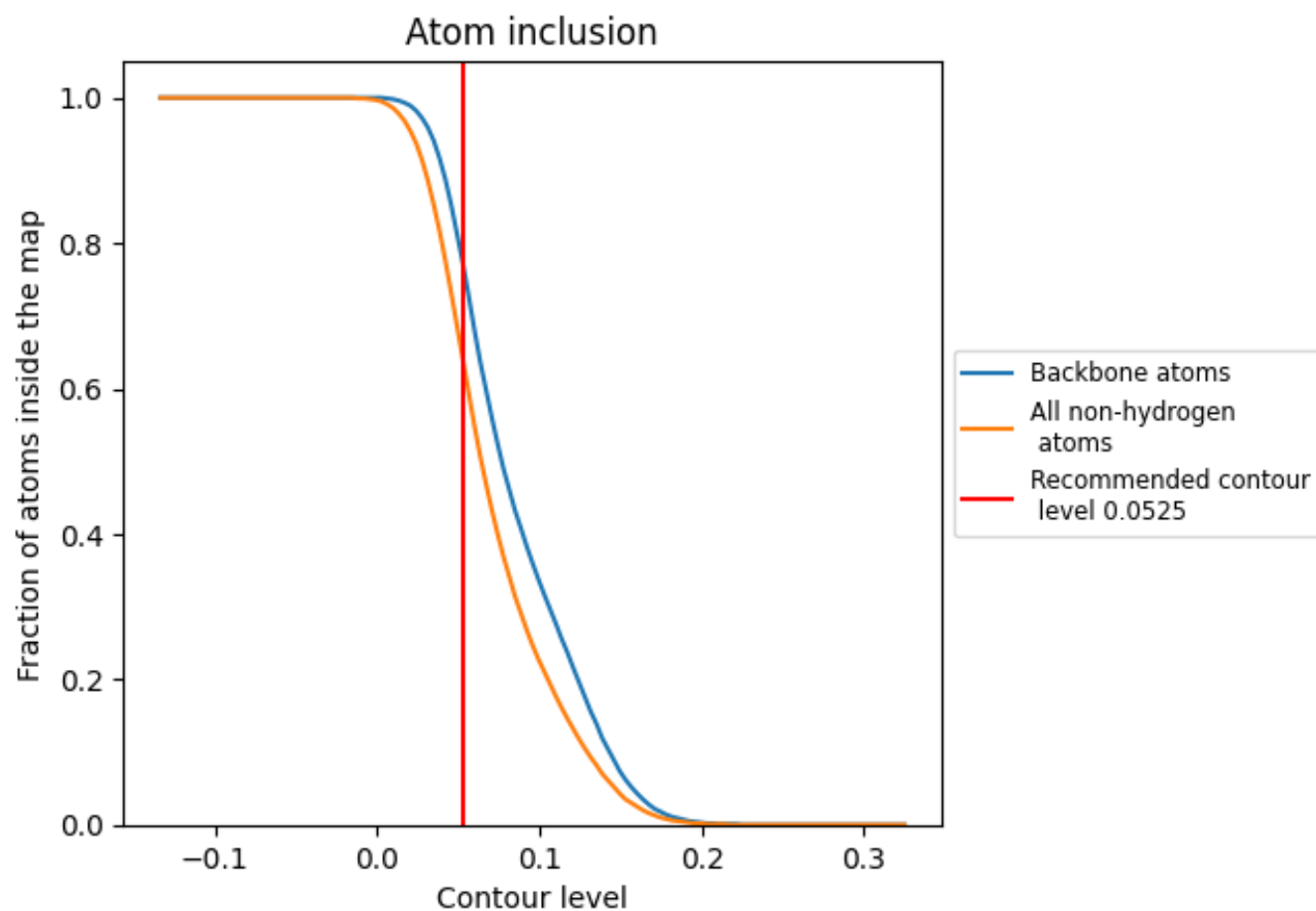
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0525).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0525) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.4010
A	 0.3440	 0.2340
B	 0.7530	 0.4320
C	 0.7910	 0.4590
E	 0.3910	 0.3140
F	 0.3690	 0.2200
G	 0.1290	 0.2310
H	 0.4360	 0.2870
I	 0.4070	 0.3250
J	 0.5260	 0.3290
K	 0.3020	 0.2340
L	 0.3510	 0.2970
M	 0.4030	 0.2840
N	 0.5340	 0.3760
O	 0.3390	 0.2460
P	 0.5330	 0.3350
Q	 0.6230	 0.3820
S	 0.8200	 0.4740
T	 0.4140	 0.3560
U	 0.7870	 0.4510
V	 0.6180	 0.4430
W	 0.8030	 0.4550
X	 0.7880	 0.4390
Y	 0.8360	 0.4350
Z	 0.7600	 0.4170
a	 0.8660	 0.5000
b	 0.7050	 0.3980
c	 0.8320	 0.4840
d	 0.8260	 0.4620
e	 0.7660	 0.4730
f	 0.6670	 0.3950
g	 0.7960	 0.4890
h	 0.8170	 0.4660
i	 0.7810	 0.5020
j	 0.6040	 0.4120



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Chain	Atom inclusion	Q-score
k	 0.7110	 0.4750
l	 0.7560	 0.4770
m	 0.7010	 0.4490
n	 0.7370	 0.4510
o	 0.7890	 0.4710
p	 0.8180	 0.4600
r	 0.8290	 0.5080
s	 0.7680	 0.4730
u	 0.8410	 0.4560
v	 0.7170	 0.3930
w	 0.6340	 0.3910