



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:47 PM UTC

PDB ID : 9TI4 / pdb_00009ti4
EMDB ID : EMD-54784
Title : High resolution Cryo-EM structure of human complex I in mitochondria
Authors : Nguyen, M.D.; Singh, V.; Rorbach, J.
Deposited on : 2025-12-04
Resolution : 2.66 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:

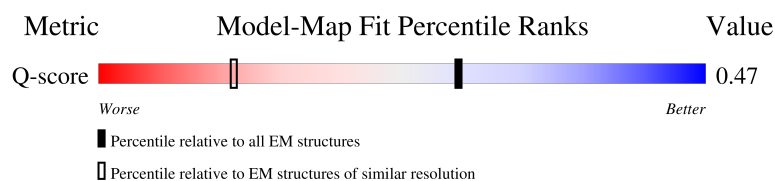
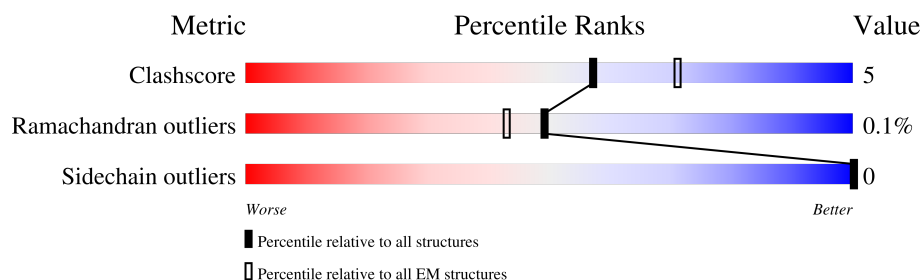
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 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.



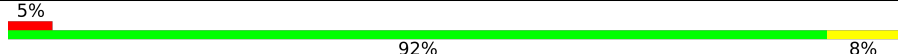
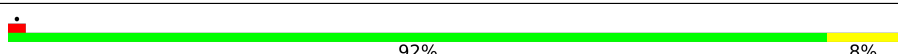
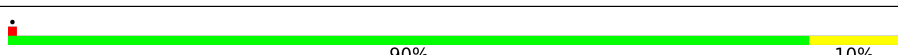
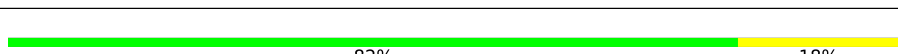
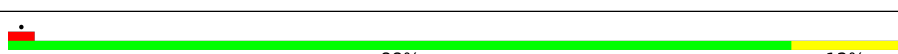
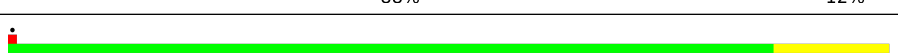
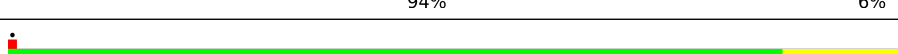
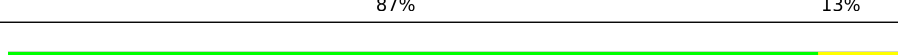
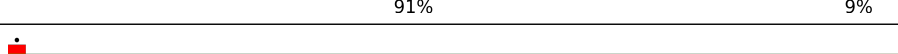
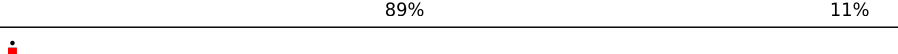
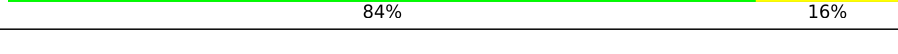
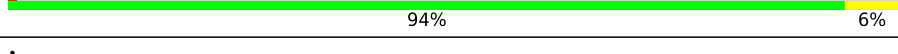
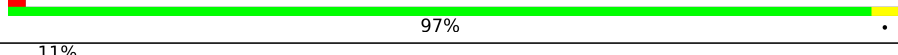
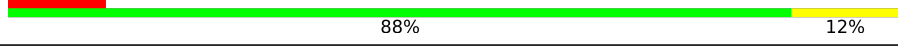
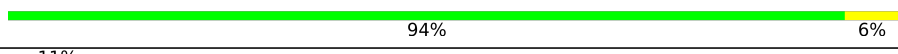
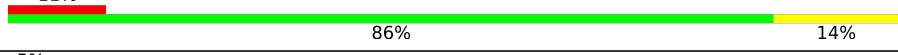
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	C	434	
2	D	176	
3	E	161	
4	F	118	

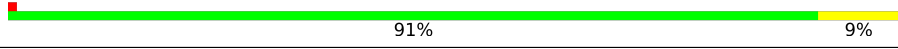
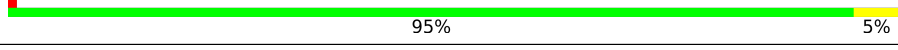
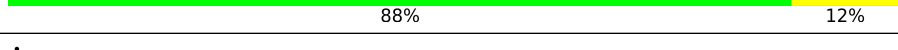
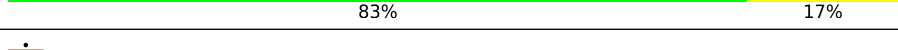
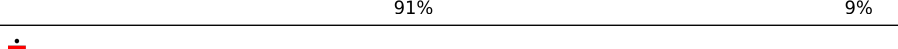
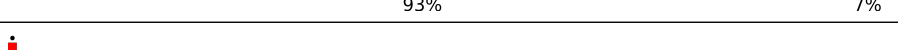
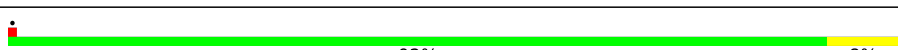
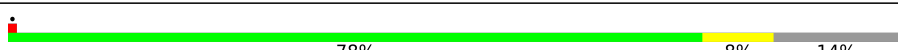
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Mol	Chain	Length	Quality of chain
5	G	85	
6	H	86	
6	X	86	
7	I	112	
8	J	341	
9	K	39	
10	L	121	
11	M	687	
12	N	144	
13	O	212	
14	P	208	
15	Q	430	
16	S	70	
17	T	96	
18	U	83	
19	V	140	
20	W	140	
21	Y	61	
22	Z	83	
23	a	138	
24	b	120	
25	c	152	
26	d	169	
27	e	107	
28	f	49	

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Mol	Chain	Length	Quality of chain
29	g	119	 91% 9%
30	h	105	 88% 11%
31	i	347	 91% 9%
32	j	115	 95% 5%
33	k	98	 80% 20%
34	l	601	 87% 13%
35	m	173	 88% 12%
36	n	54	 83% 17%
37	o	128	 91% 9%
38	p	173	 93% 7%
39	r	459	 89% 11%
40	s	316	 89% 11%
41	u	171	 92% 8%
42	v	121	 7% 88% 12%
43	w	320	 92% 8%
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
45	SF4	C	501	-	-	X	-
46	FMN	C	502	-	-	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] flavoprotein 1, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	71	MET	-	initiating methionine	UNP O14561
X	71	MET	-	initiating methionine	UNP O14561

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

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

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

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	?	-	MET	deletion	UNP O95139

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

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

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

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

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

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

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

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

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

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

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

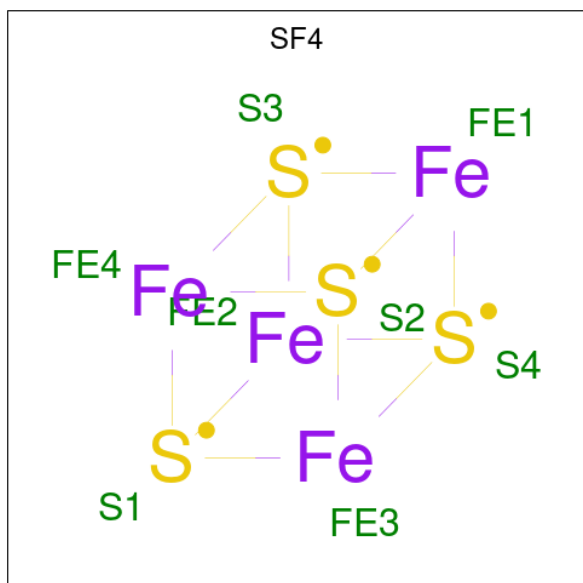
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

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

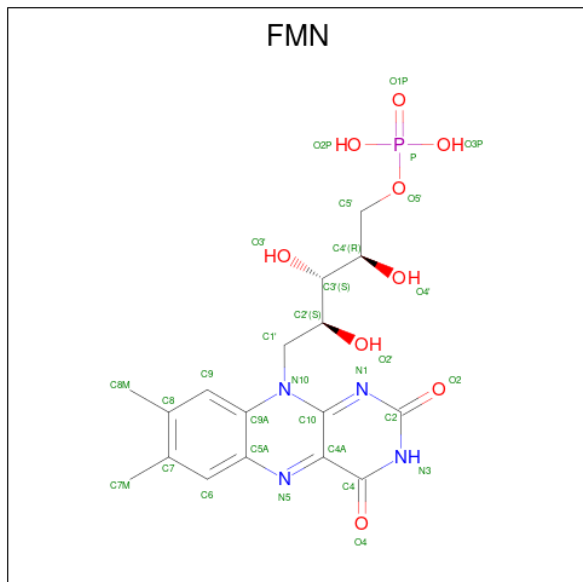
Mol	Chain	Residues	Atoms						AltConf	Trace
44	t	97	Total	C	H	N	O	S	0	0
			1582	489	802	148	141	2		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



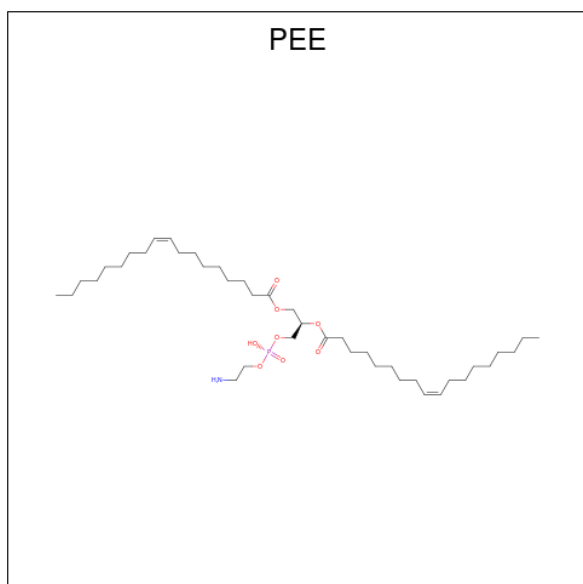
Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	Fe	S	0
			8	4	4	
45	D	1	Total	Fe	S	0
			8	4	4	
45	D	1	Total	Fe	S	0
			8	4	4	
45	E	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



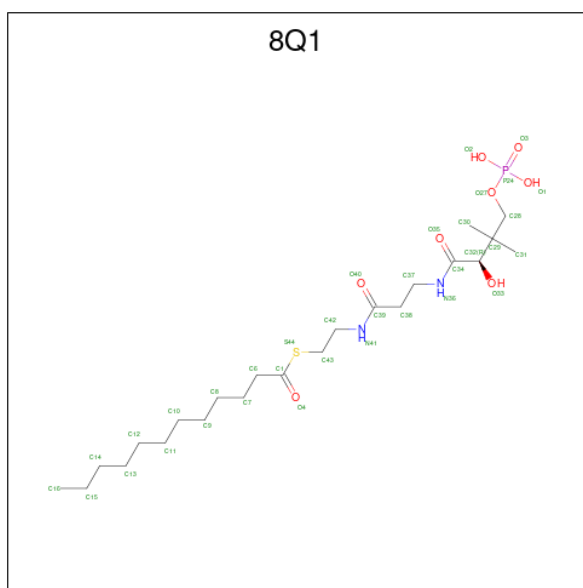
Mol	Chain	Residues	Atoms					AltConf	
47	E	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	

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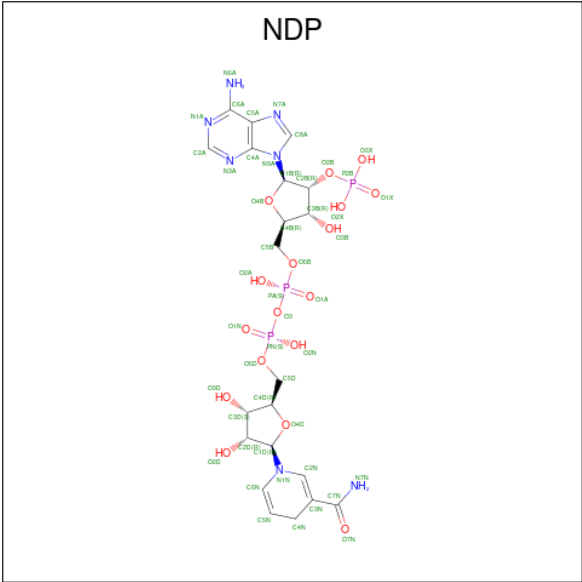
Mol	Chain	Residues	Atoms						AltConf
47	J	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
47	V	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
47	W	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
47	i	1	Total	C	H	N	O	P	0
			128	41	77	1	8	1	
47	i	1	Total	C	H	N	O	P	0
			121	39	72	1	8	1	
47	l	1	Total	C	H	N	O	P	0
			128	41	77	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: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



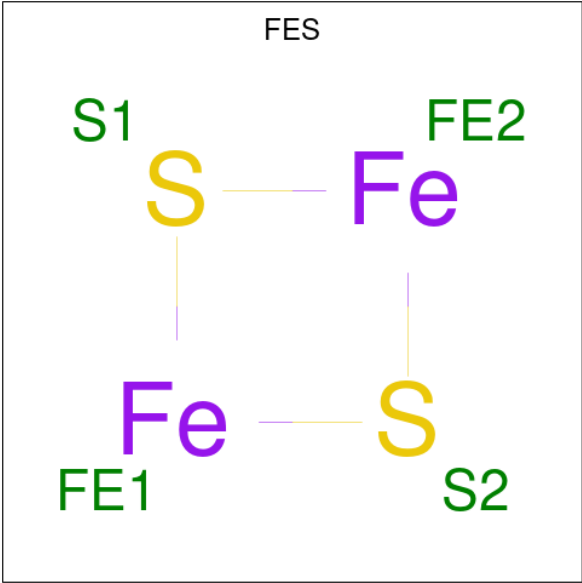
Mol	Chain	Residues	Atoms							AltConf
48	F	1	Total 78	C 23	H 43	N 2	O 8	P 1	S 1	0
48	X	1	Total 78	C 23	H 43	N 2	O 8	P 1	S 1	0

- Molecule 49 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).



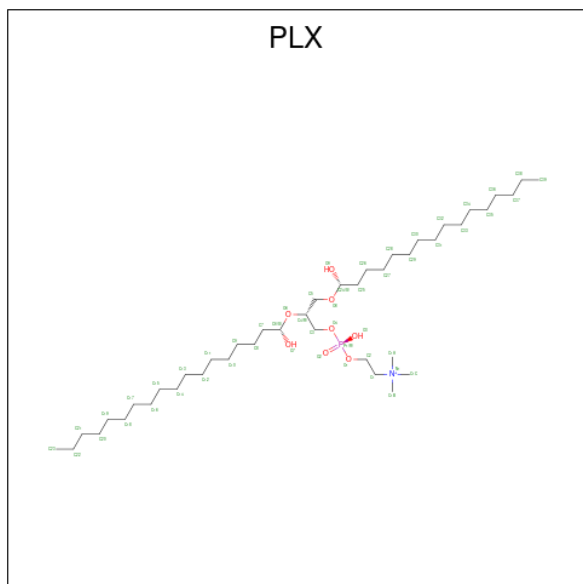
Mol	Chain	Residues	Atoms						AltConf
49	J	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 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).

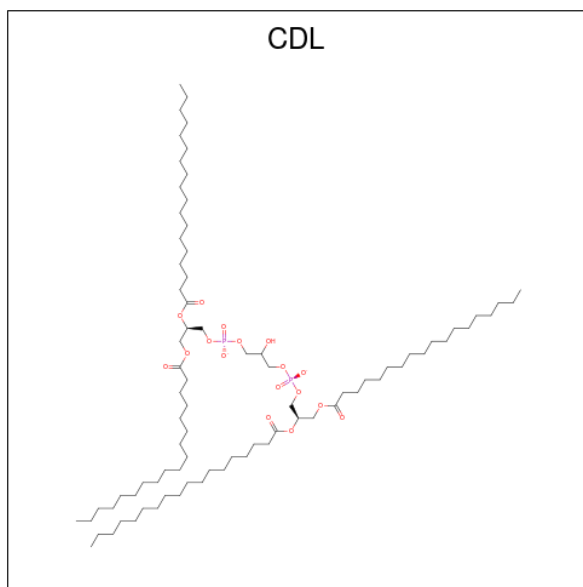


Mol	Chain	Residues	Atoms						AltConf
51	N	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
51	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
51	g	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
51	j	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
51	o	1	Total	C	H	N	O	P	0
			140	42	88	1	8	1	
51	r	1	Total	C	H	N	O	P	0
			140	42	88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

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

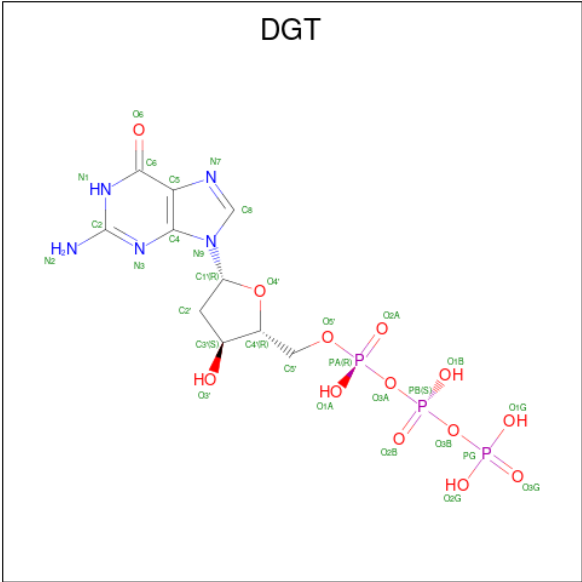
Mol	Chain	Residues	Atoms		AltConf
52	T	1	Total	Zn	0
			1	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 54 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
54	w	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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

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

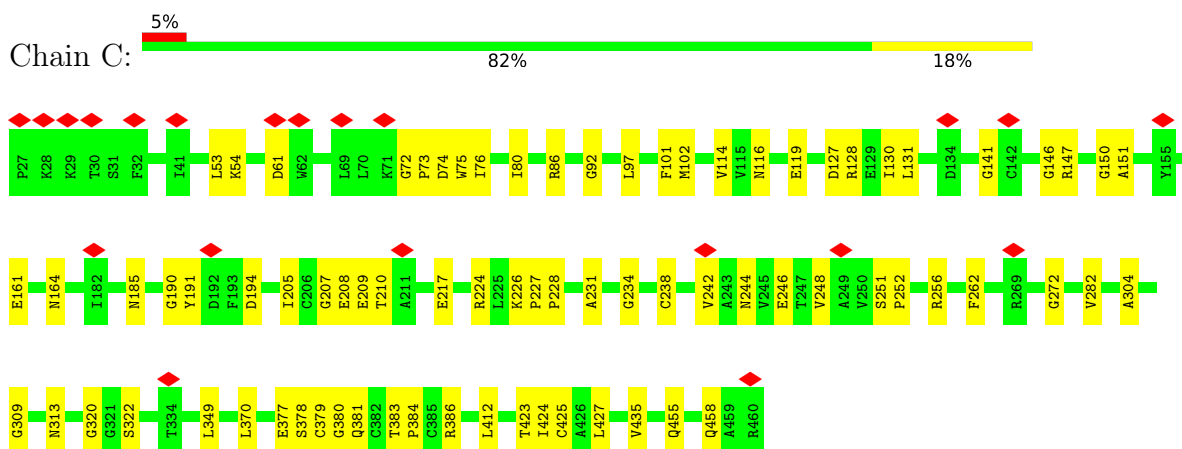
- Molecule 56 is water.

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

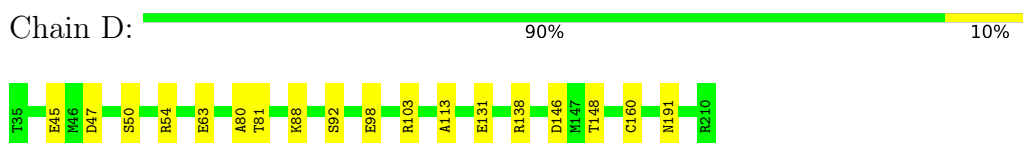
3 Residue-property plots

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.

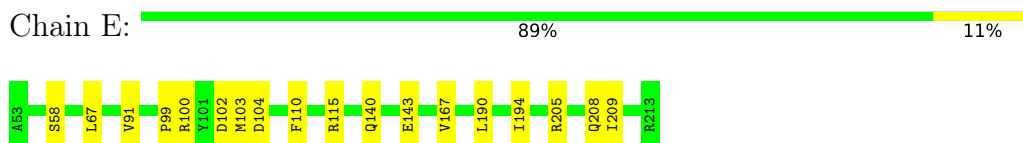
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



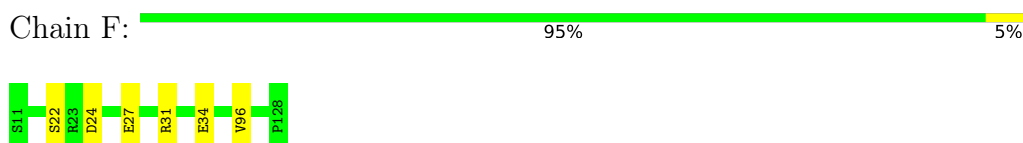
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- 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

Chain G:  85% 15%

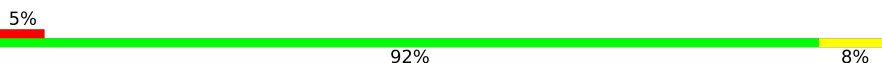


- Molecule 6: Acyl carrier protein, mitochondrial

Chain H:  16% 81% 17%



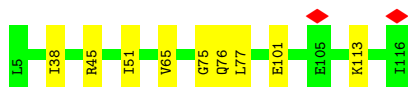
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  5% 92% 8%



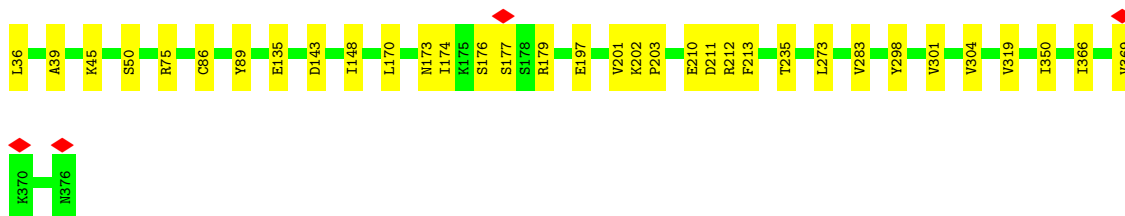
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain I:  92% 8%



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J:  90% 10%

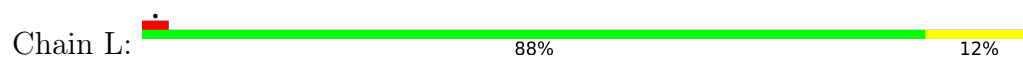


- Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

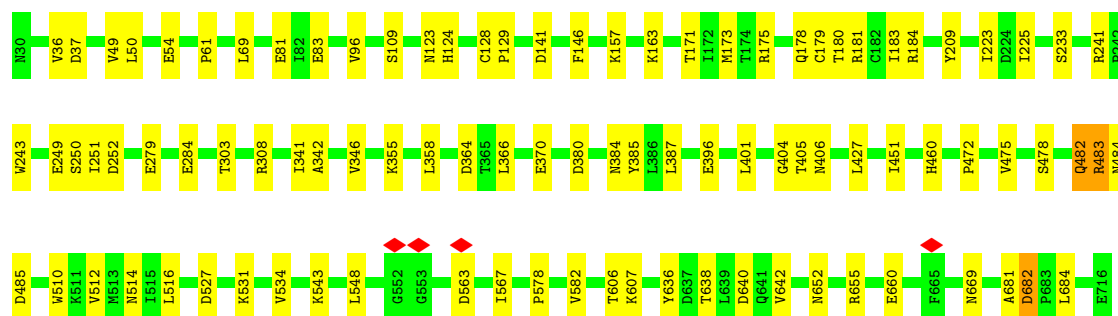
Chain K:  82% 18%



- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



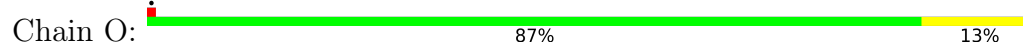
- Molecule 11: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



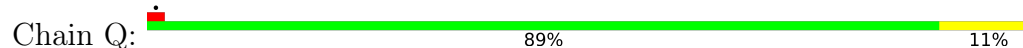
- Molecule 13: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

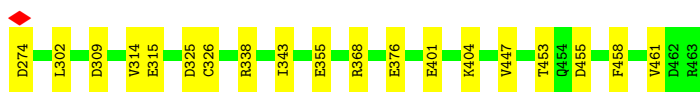


- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

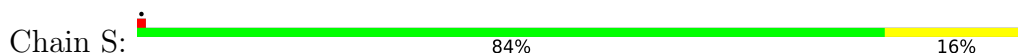


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

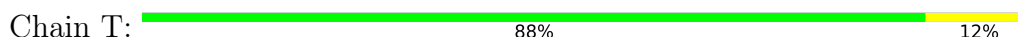




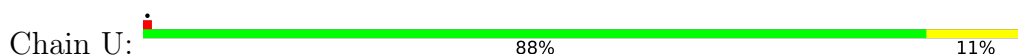
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



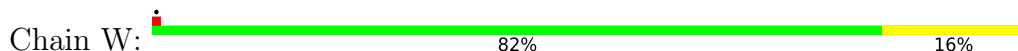
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



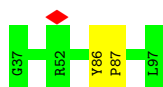
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



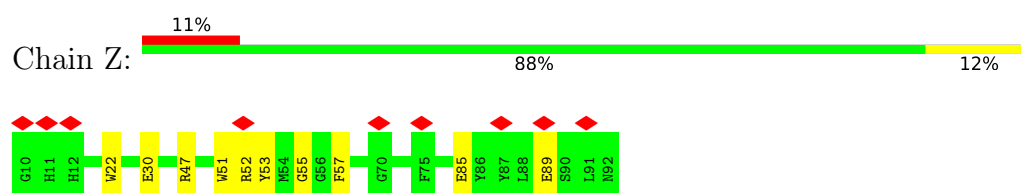
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



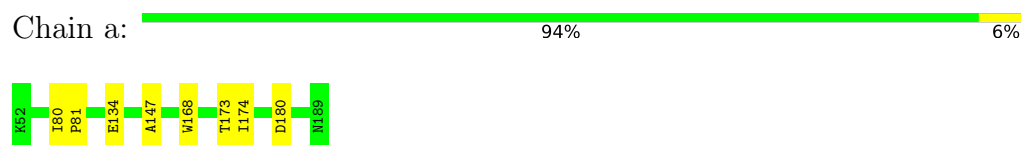
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



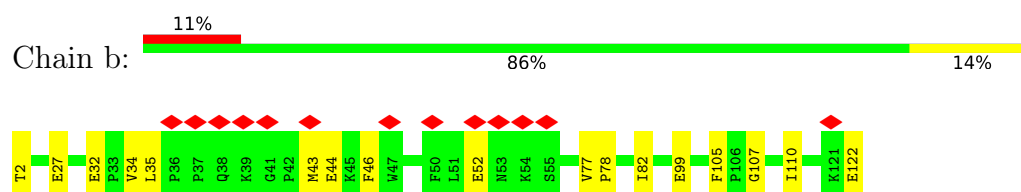
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



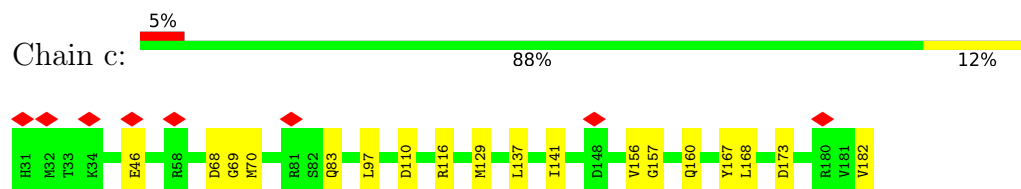
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



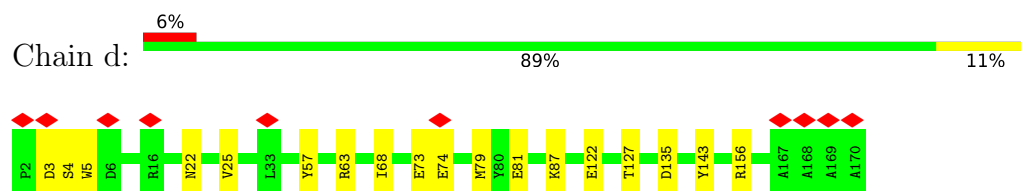
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



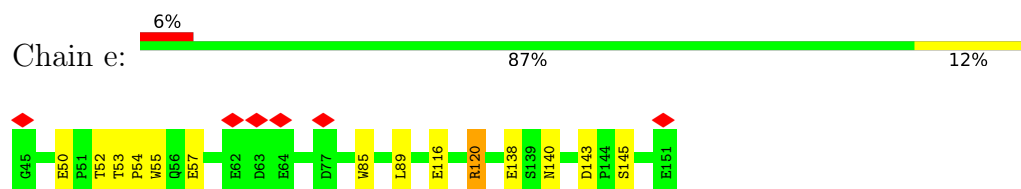
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

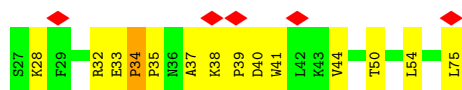


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

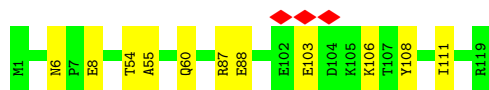
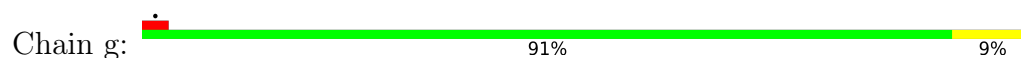


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

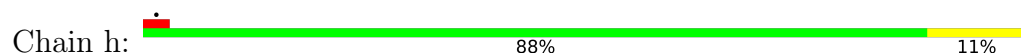




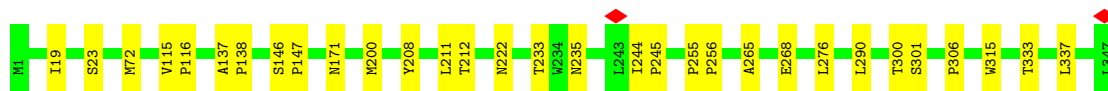
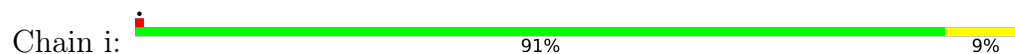
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



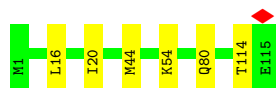
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



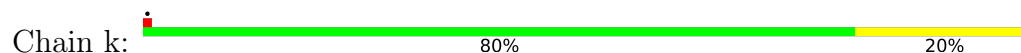
- Molecule 31: NADH-ubiquinone oxidoreductase chain 2



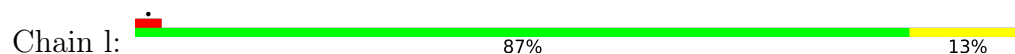
- Molecule 32: NADH-ubiquinone oxidoreductase chain 3

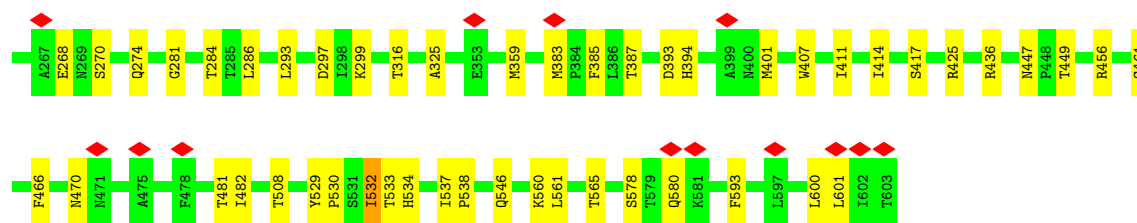


- Molecule 33: NADH-ubiquinone oxidoreductase chain 4L

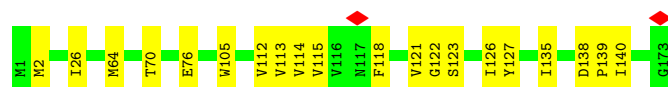
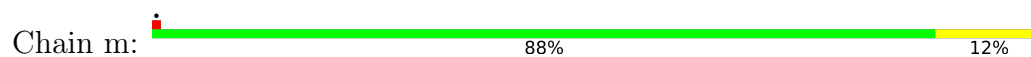


- Molecule 34: NADH-ubiquinone oxidoreductase chain 5

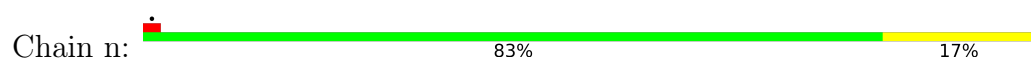




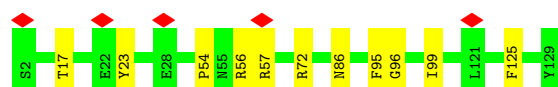
- Molecule 35: NADH-ubiquinone oxidoreductase chain 6



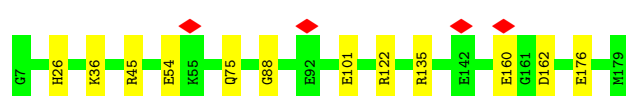
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



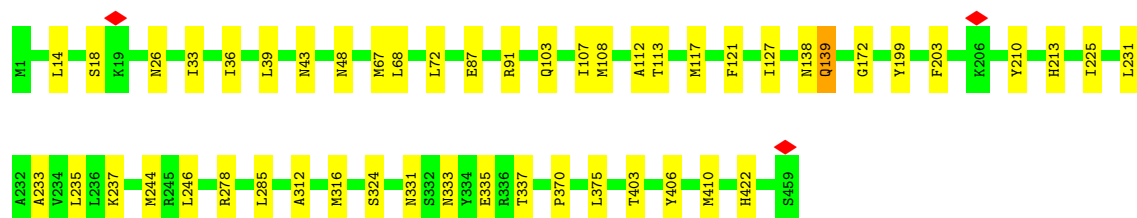
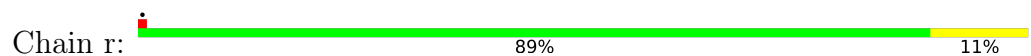
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 39: NADH-ubiquinone oxidoreductase chain 4

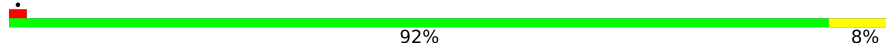


- Molecule 40: NADH-ubiquinone oxidoreductase chain 1

Chain s:  89% 11%



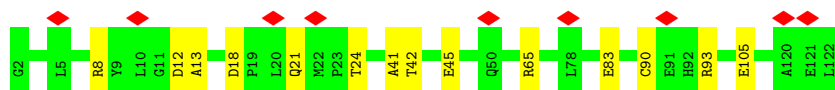
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  92% 8%

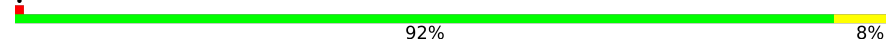


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  7% 88% 12%



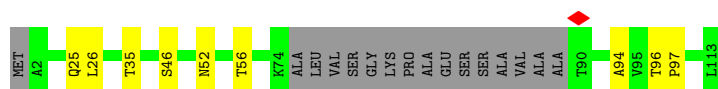
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  92% 8%



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

Chain t:  78% 8% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	236346	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.496	Depositor
Minimum map value	-1.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.477	Depositor
Map size (Å)	230400.0, 230400.0, 230400.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, CDL, FMN, MG, PEE, SF4, NDP, DGT, ZN, NMM, 8Q1, FES, PLX

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	C	0.15	0/3422	0.28	0/4620
2	D	0.22	0/1452	0.29	0/1964
3	E	0.25	0/1309	0.33	0/1771
4	F	0.19	0/1024	0.25	0/1378
5	G	0.14	0/695	0.26	0/938
6	H	0.13	0/700	0.27	0/945
6	X	0.15	0/708	0.23	0/956
7	I	0.19	0/941	0.26	0/1275
8	J	0.19	0/2820	0.26	0/3819
9	K	0.11	0/312	0.27	0/423
10	L	0.19	0/1002	0.25	0/1352
11	M	0.18	0/5363	0.29	0/7267
12	N	0.19	0/1244	0.29	0/1691
13	O	0.14	0/1682	0.28	0/2289
14	P	0.23	0/1780	0.29	0/2424
15	Q	0.22	0/3540	0.27	0/4798
16	S	0.18	0/583	0.25	0/785
17	T	0.19	0/766	0.24	0/1032
18	U	0.18	0/670	0.34	0/920
19	V	0.17	0/1065	0.23	0/1450
20	W	0.18	0/1182	0.29	0/1600
21	Y	0.14	0/570	0.31	0/778
22	Z	0.15	0/702	0.33	0/945
23	a	0.16	0/1209	0.22	0/1639
24	b	0.15	0/1054	0.29	0/1423
25	c	0.16	0/1326	0.26	0/1809
26	d	0.15	0/1463	0.24	0/1968
27	e	0.21	0/915	0.37	0/1245
28	f	0.17	0/432	0.29	0/585
29	g	0.17	0/1046	0.23	0/1412
30	h	0.18	0/892	0.30	0/1193
31	i	0.20	0/2806	0.30	0/3840

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	j	0.21	0/952	0.30	0/1301
33	k	0.26	0/754	0.39	0/1024
34	l	0.16	0/4826	0.26	0/6594
35	m	0.20	0/1334	0.31	0/1816
36	n	0.14	0/468	0.26	0/630
37	o	0.16	0/1093	0.25	0/1479
38	p	0.16	0/1553	0.24	0/2104
39	r	0.18	0/3717	0.25	0/5082
40	s	0.22	0/2568	0.33	0/3523
41	u	0.15	0/1445	0.27	0/1953
42	v	0.13	0/1060	0.27	0/1417
43	w	0.19	0/2689	0.27	0/3637
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
18	U	0	1
20	W	0	1
27	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
18	U	69	HIS	Peptide
20	W	27	ARG	Sidechain
27	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	C	3347	3321	3310	54	0
2	D	1420	1367	1364	14	0
3	E	1287	1290	1286	16	0
4	F	999	1017	1011	4	0
5	G	683	697	695	10	0
6	H	688	681	680	10	0
6	X	696	690	688	5	0
7	I	922	953	950	7	0
8	J	2745	2802	2787	23	0
9	K	304	282	269	6	0
10	L	979	975	968	12	0
11	M	5275	5321	5311	69	0
12	N	1203	1172	1167	7	0
13	O	1643	1648	1644	22	0
14	P	1730	1691	1685	14	0
15	Q	3461	3433	3418	36	0
16	S	568	570	567	9	0
17	T	752	732	727	8	0
18	U	647	655	653	13	0
19	V	1038	1031	1027	5	0
20	W	1151	1153	1151	18	0
21	Y	544	491	487	1	0
22	Z	679	660	657	8	0
23	a	1174	1182	1177	7	0
24	b	1021	1049	1043	14	0
25	c	1273	1180	1174	13	0
26	d	1433	1404	1402	18	0
27	e	887	850	848	15	0
28	f	419	425	423	11	0
29	g	1012	1023	1021	12	0
30	h	871	876	872	11	0
31	i	2733	2893	2892	20	0
32	j	926	964	978	4	0
33	k	743	787	794	17	0
34	l	4703	4880	4878	55	0
35	m	1302	1317	1326	15	0
36	n	457	466	463	7	0
37	o	1066	1088	1086	8	0
38	p	1499	1448	1442	9	0
39	r	3623	3821	3817	35	0
40	s	2498	2593	2602	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	u	1405	1386	1378	15	0
42	v	1037	1032	1026	10	0
43	w	2623	2598	2587	25	0
44	t	780	802	798	7	0
45	C	8	0	0	3	0
45	D	16	0	0	0	0
45	E	8	0	0	1	0
45	M	16	0	0	2	0
46	C	31	19	19	9	0
47	E	51	77	80	3	0
47	J	51	77	80	0	0
47	V	51	77	80	2	0
47	W	51	77	80	0	0
47	i	100	149	151	2	0
47	l	51	77	80	2	0
48	F	35	43	0	1	0
48	X	35	43	0	0	0
49	J	48	26	24	1	0
50	M	4	0	0	0	0
50	O	4	0	0	1	0
51	N	52	88	88	0	0
51	g	104	176	176	1	0
51	j	52	88	88	0	0
51	o	52	88	88	0	0
51	r	52	88	88	0	0
51	s	52	88	88	1	0
52	T	1	0	0	0	0
53	V	200	312	312	0	0
53	i	64	80	72	0	0
53	l	164	236	228	2	0
53	u	64	80	72	0	0
54	w	31	12	12	1	0
55	w	1	0	0	0	0
56	X	1	0	0	0	0
All	All	67696	68697	68435	649	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 649 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)
40:s:196:THR:HG23	40:s:197:PRO:CD	1.89	1.03
11:M:124:HIS:CE1	45:M:801:SF4:S2	2.57	0.97
40:s:196:THR:HG23	40:s:197:PRO:HD3	1.49	0.93
34:l:529:TYR:O	34:l:533:THR:HG22	1.69	0.92
34:l:119:LYS:NZ	53:l:702:CDL:OB4	2.09	0.85

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	C	430/434 (99%)	392 (91%)	38 (9%)	0	100	100
2	D	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	E	158/161 (98%)	147 (93%)	11 (7%)	0	100	100
4	F	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
5	G	83/85 (98%)	74 (89%)	9 (11%)	0	100	100
6	H	83/86 (96%)	77 (93%)	6 (7%)	0	100	100
6	X	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
7	I	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	J	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
9	K	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
10	L	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
11	M	685/687 (100%)	620 (90%)	62 (9%)	3 (0%)	30	45
12	N	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
13	O	210/212 (99%)	187 (89%)	23 (11%)	0	100	100
14	P	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
15	Q	427/430 (99%)	405 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
17	T	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
18	U	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
19	V	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
20	W	138/140 (99%)	130 (94%)	5 (4%)	3 (2%)	5	9
21	Y	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
22	Z	81/83 (98%)	70 (86%)	11 (14%)	0	100	100
23	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
24	b	116/120 (97%)	102 (88%)	14 (12%)	0	100	100
25	c	150/152 (99%)	137 (91%)	13 (9%)	0	100	100
26	d	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
27	e	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
28	f	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	5	9
29	g	118/119 (99%)	116 (98%)	2 (2%)	0	100	100
30	h	103/105 (98%)	91 (88%)	11 (11%)	1 (1%)	12	20
31	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
32	j	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
33	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
34	l	599/601 (100%)	561 (94%)	37 (6%)	1 (0%)	43	60
35	m	171/173 (99%)	155 (91%)	16 (9%)	0	100	100
36	n	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
37	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
38	p	171/173 (99%)	161 (94%)	10 (6%)	0	100	100
39	r	457/459 (100%)	441 (96%)	15 (3%)	1 (0%)	43	60
40	s	314/316 (99%)	294 (94%)	19 (6%)	1 (0%)	36	52
41	u	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
42	v	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
43	w	318/320 (99%)	303 (95%)	14 (4%)	1 (0%)	36	52
44	t	93/113 (82%)	83 (89%)	10 (11%)	0	100	100
All	All	8147/8261 (99%)	7597 (93%)	538 (7%)	12 (0%)	49	66

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	W	28	ARG
30	h	98	HIS
40	s	196	THR
11	M	483	ARG
11	M	682	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	C	348/348 (100%)	348 (100%)	0	100	100
2	D	151/151 (100%)	151 (100%)	0	100	100
3	E	135/135 (100%)	135 (100%)	0	100	100
4	F	110/110 (100%)	110 (100%)	0	100	100
5	G	75/75 (100%)	75 (100%)	0	100	100
6	H	79/80 (99%)	79 (100%)	0	100	100
6	X	80/80 (100%)	80 (100%)	0	100	100
7	I	100/100 (100%)	100 (100%)	0	100	100
8	J	295/295 (100%)	295 (100%)	0	100	100
9	K	32/38 (84%)	32 (100%)	0	100	100
10	L	107/110 (97%)	107 (100%)	0	100	100
11	M	577/577 (100%)	577 (100%)	0	100	100
12	N	130/130 (100%)	130 (100%)	0	100	100
13	O	181/181 (100%)	181 (100%)	0	100	100
14	P	190/190 (100%)	190 (100%)	0	100	100
15	Q	370/370 (100%)	370 (100%)	0	100	100
16	S	59/59 (100%)	59 (100%)	0	100	100
17	T	80/80 (100%)	80 (100%)	0	100	100
18	U	72/72 (100%)	72 (100%)	0	100	100
19	V	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	W	121/121 (100%)	121 (100%)	0	100	100
21	Y	58/58 (100%)	58 (100%)	0	100	100
22	Z	66/66 (100%)	66 (100%)	0	100	100
23	a	124/124 (100%)	124 (100%)	0	100	100
24	b	113/114 (99%)	113 (100%)	0	100	100
25	c	136/136 (100%)	136 (100%)	0	100	100
26	d	152/152 (100%)	152 (100%)	0	100	100
27	e	99/99 (100%)	99 (100%)	0	100	100
28	f	45/45 (100%)	45 (100%)	0	100	100
29	g	106/105 (101%)	106 (100%)	0	100	100
30	h	91/91 (100%)	91 (100%)	0	100	100
31	i	314/314 (100%)	314 (100%)	0	100	100
32	j	104/104 (100%)	104 (100%)	0	100	100
33	k	85/85 (100%)	85 (100%)	0	100	100
34	l	531/531 (100%)	531 (100%)	0	100	100
35	m	136/136 (100%)	136 (100%)	0	100	100
36	n	51/51 (100%)	51 (100%)	0	100	100
37	o	114/114 (100%)	114 (100%)	0	100	100
38	p	157/157 (100%)	157 (100%)	0	100	100
39	r	416/416 (100%)	416 (100%)	0	100	100
40	s	277/277 (100%)	277 (100%)	0	100	100
41	u	154/154 (100%)	154 (100%)	0	100	100
42	v	110/110 (100%)	110 (100%)	0	100	100
43	w	288/288 (100%)	288 (100%)	0	100	100
44	t	88/98 (90%)	88 (100%)	0	100	100
All	All	7209/7229 (100%)	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
32	j	10	ASN

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Mol	Chain	Res	Type
39	r	169	ASN
33	k	7	ASN
37	o	24	ASN
40	s	230	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
3	SEP	E	58	3	8,9,10	1.61	1 (12%)	7,12,14	1.20	1 (14%)
15	NMM	Q	118	15	8,11,12	1.85	1 (12%)	7,12,14	1.25	1 (14%)

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
3	SEP	E	58	3	-	2/6/8/10	-
15	NMM	Q	118	15	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	118	NMM	CZ-NH2	4.84	1.45	1.34
3	E	58	SEP	P-O1P	3.51	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	118	NMM	NE-CZ-NH2	2.76	122.01	119.48
3	E	58	SEP	OG-CB-CA	2.51	110.59	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	58	SEP	C-CA-CB-OG
15	Q	118	NMM	O-C-CA-CB
3	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
15	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	$\# Z > 2$
45	SF4	D	301	2	0,12,12	-	-	-		
53	CDL	l	702	-	63,63,99	1.40	7 (11%)	69,75,111	0.97	3 (4%)
46	FMN	C	502	-	33,33,33	0.86	1 (3%)	48,50,50	1.06	4 (8%)
48	8Q1	X	201	-	32,34,34	1.66	6 (18%)	39,43,43	1.33	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	PLX	o	201	-	51,51,51	1.04	4 (7%)	53,59,59	0.67	1 (1%)
47	PEE	l	701	-	50,50,50	1.16	3 (6%)	53,55,55	1.29	3 (5%)
47	PEE	V	201	-	50,50,50	1.15	3 (6%)	53,55,55	1.06	2 (3%)
53	CDL	i	401	-	63,63,99	1.40	7 (11%)	69,75,111	0.94	3 (4%)
50	FES	M	803	11	0,4,4	-	-	-		
45	SF4	M	802	11	0,12,12	-	-	-		
53	CDL	l	703	-	99,99,99	1.24	8 (8%)	105,111,111	0.93	4 (3%)
48	8Q1	F	201	-	32,34,34	1.65	5 (15%)	39,43,43	1.44	6 (15%)
45	SF4	M	801	11	0,12,12	-	-	-		
47	PEE	W	201	-	50,50,50	1.16	3 (6%)	53,55,55	1.03	2 (3%)
51	PLX	g	202	-	51,51,51	1.05	3 (5%)	53,59,59	0.61	0
47	PEE	i	403	-	48,48,50	1.17	3 (6%)	51,53,55	1.05	3 (5%)
51	PLX	N	201	-	51,51,51	1.02	4 (7%)	53,59,59	0.71	0
47	PEE	i	402	-	50,50,50	1.17	3 (6%)	53,55,55	1.16	3 (5%)
45	SF4	D	302	2	0,12,12	-	-	-		
51	PLX	r	501	-	51,51,51	1.04	4 (7%)	53,59,59	0.68	0
51	PLX	s	401	-	51,51,51	1.00	3 (5%)	53,59,59	0.73	0
54	DGT	w	401	55	32,33,33	3.75	17 (53%)	48,52,52	2.00	12 (25%)
49	NDP	J	401	-	51,52,52	3.96	24 (47%)	71,80,80	1.71	12 (16%)
53	CDL	u	201	-	63,63,99	1.42	7 (11%)	69,75,111	0.83	3 (4%)
53	CDL	V	203	-	99,99,99	1.25	8 (8%)	105,111,111	0.86	4 (3%)
47	PEE	E	301	-	50,50,50	1.14	3 (6%)	53,55,55	1.10	2 (3%)
45	SF4	E	302	15,3	0,12,12	-	-	-		
51	PLX	g	201	-	51,51,51	1.01	3 (5%)	53,59,59	0.68	0
45	SF4	C	501	1	0,12,12	-	-	-		
50	FES	O	301	13	0,4,4	-	-	-		
51	PLX	j	201	-	51,51,51	0.99	4 (7%)	53,59,59	0.76	2 (3%)
53	CDL	V	202	-	99,99,99	1.26	7 (7%)	105,111,111	1.26	6 (5%)
47	PEE	J	402	-	50,50,50	1.15	4 (8%)	53,55,55	1.29	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	D	301	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	l	702	-	-	20/74/74/110	-
46	FMN	C	502	-	-	11/18/18/18	0/3/3/3
48	8Q1	X	201	-	-	4/41/41/41	-
51	PLX	o	201	-	-	12/55/55/55	-
47	PEE	l	701	-	-	18/54/54/54	-
47	PEE	V	201	-	-	28/54/54/54	-
53	CDL	i	401	-	-	11/74/74/110	-
50	FES	M	803	11	-	-	0/1/1/1
45	SF4	M	802	11	-	-	0/6/5/5
53	CDL	l	703	-	-	12/110/110/110	-
48	8Q1	F	201	-	-	8/41/41/41	-
45	SF4	M	801	11	-	-	0/6/5/5
47	PEE	W	201	-	-	15/54/54/54	-
51	PLX	g	202	-	-	11/55/55/55	-
47	PEE	i	403	-	-	13/52/52/54	-
51	PLX	N	201	-	-	12/55/55/55	-
47	PEE	i	402	-	-	15/54/54/54	-
51	PLX	r	501	-	-	15/55/55/55	-
51	PLX	s	401	-	-	17/55/55/55	-
54	DGT	w	401	55	-	5/22/34/34	0/3/3/3
45	SF4	D	302	2	-	-	0/6/5/5
49	NDP	J	401	-	-	4/34/77/77	0/5/5/5
53	CDL	u	201	-	-	11/74/74/110	-
53	CDL	V	203	-	-	24/110/110/110	-
47	PEE	E	301	-	-	14/54/54/54	-
51	PLX	g	201	-	-	14/55/55/55	-
45	SF4	E	302	15,3	-	-	0/6/5/5
45	SF4	C	501	1	-	-	0/6/5/5
50	FES	O	301	13	-	-	0/1/1/1
51	PLX	j	201	-	-	17/55/55/55	-
53	CDL	V	202	-	-	24/110/110/110	-
47	PEE	J	402	-	-	12/54/54/54	-

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	401	NDP	C2D-C3D	-11.17	1.23	1.53

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	401	NDP	PN-O3	8.94	1.69	1.59
49	J	401	NDP	C2B-C1B	-8.60	1.31	1.53
49	J	401	NDP	O4B-C1B	8.20	1.60	1.42
54	w	401	DGT	O4'-C4'	7.54	1.61	1.45

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	w	401	DGT	C1'-N9-C8	-7.02	112.18	127.91
53	V	202	CDL	OB6-CB5-C51	6.31	125.13	111.48
49	J	401	NDP	N3A-C2A-N1A	-5.60	120.10	128.58
49	J	401	NDP	N6A-C6A-N1A	-5.56	105.99	118.38
47	E	301	PEE	C40-C39-C38	5.17	163.55	124.83

There are no chirality outliers.

5 of 347 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	C	502	FMN	C2'-C1'-N10-C10
46	C	502	FMN	N10-C1'-C2'-O2'
46	C	502	FMN	N10-C1'-C2'-C3'
46	C	502	FMN	C1'-C2'-C3'-O3'
46	C	502	FMN	C1'-C2'-C3'-C4'

There are no ring outliers.

17 monomers are involved in 32 short contacts:

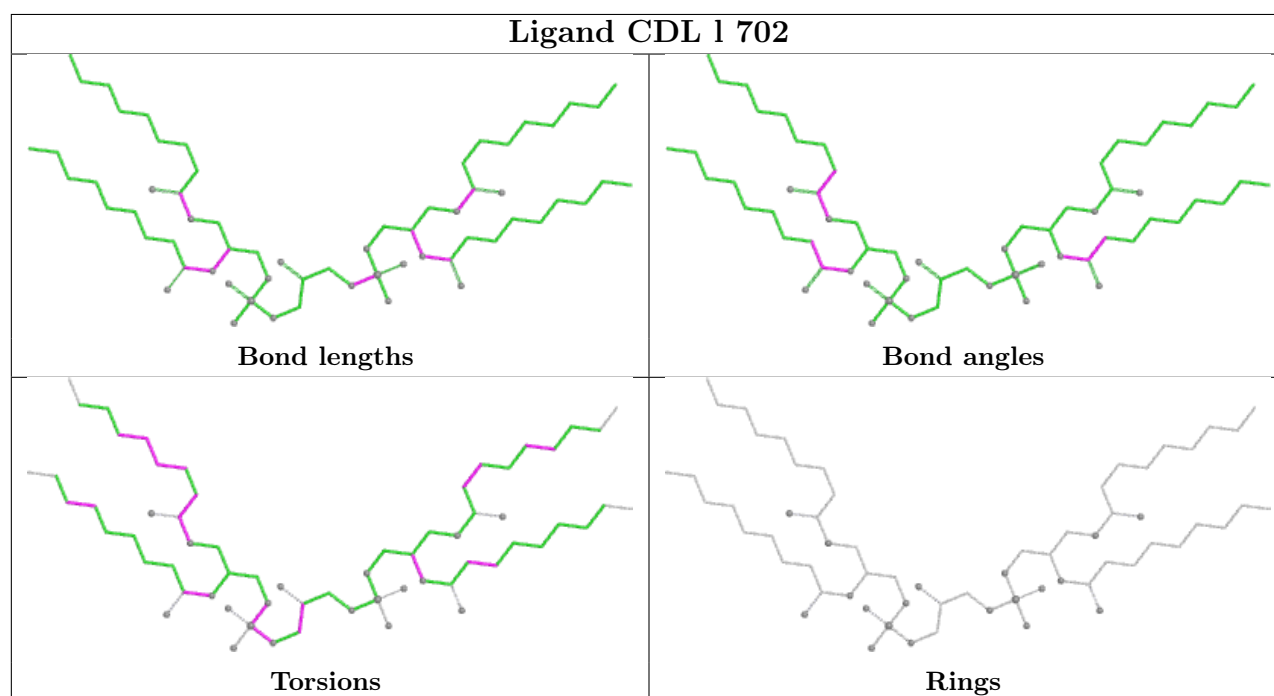
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	l	702	CDL	1	0
46	C	502	FMN	9	0
47	l	701	PEE	2	0
47	V	201	PEE	2	0
45	M	802	SF4	1	0
53	l	703	CDL	1	0
48	F	201	8Q1	1	0
45	M	801	SF4	1	0
47	i	402	PEE	2	0
51	s	401	PLX	1	0
54	w	401	DGT	1	0
49	J	401	NDP	1	0
47	E	301	PEE	3	0

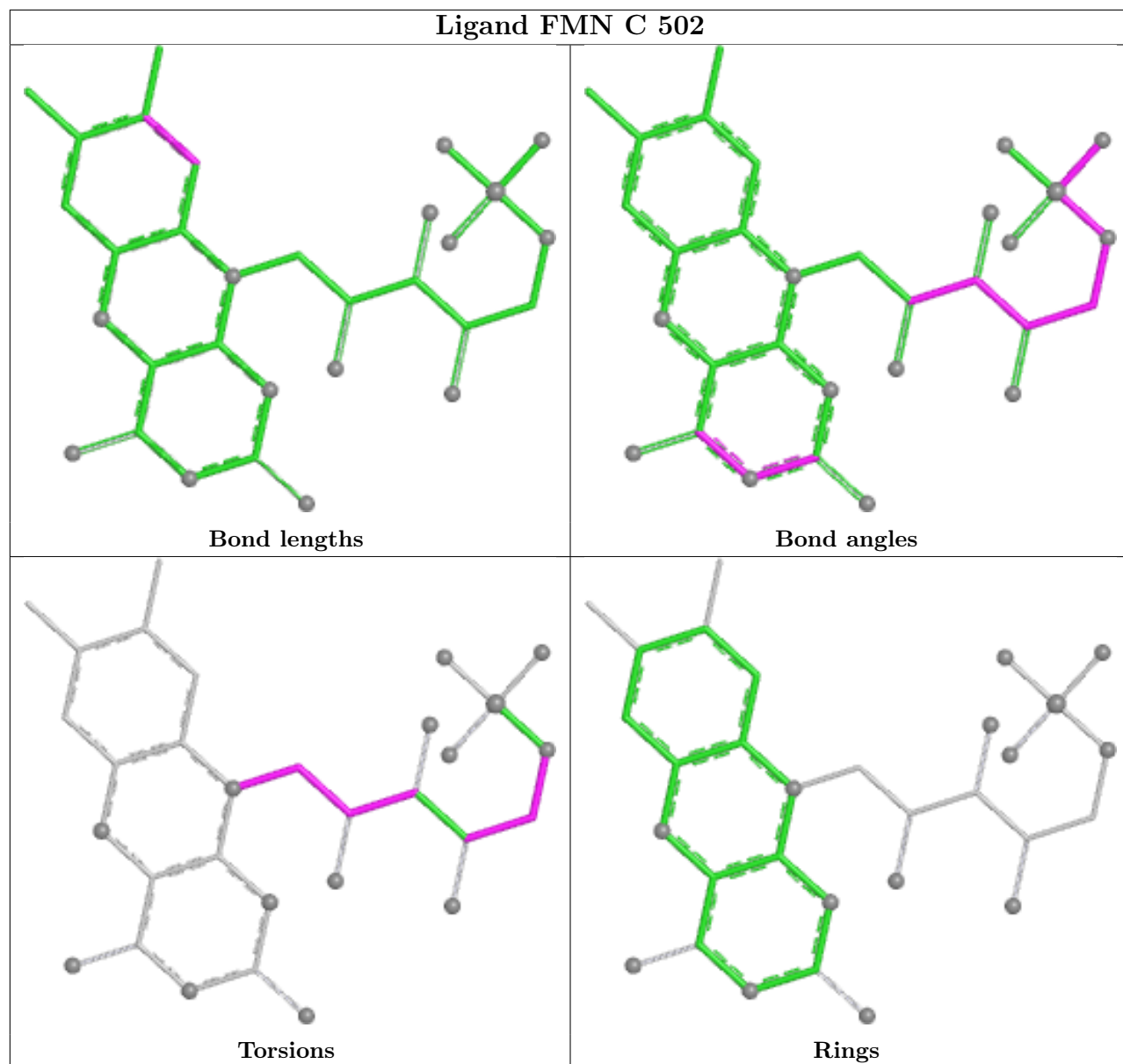
Continued on next page...

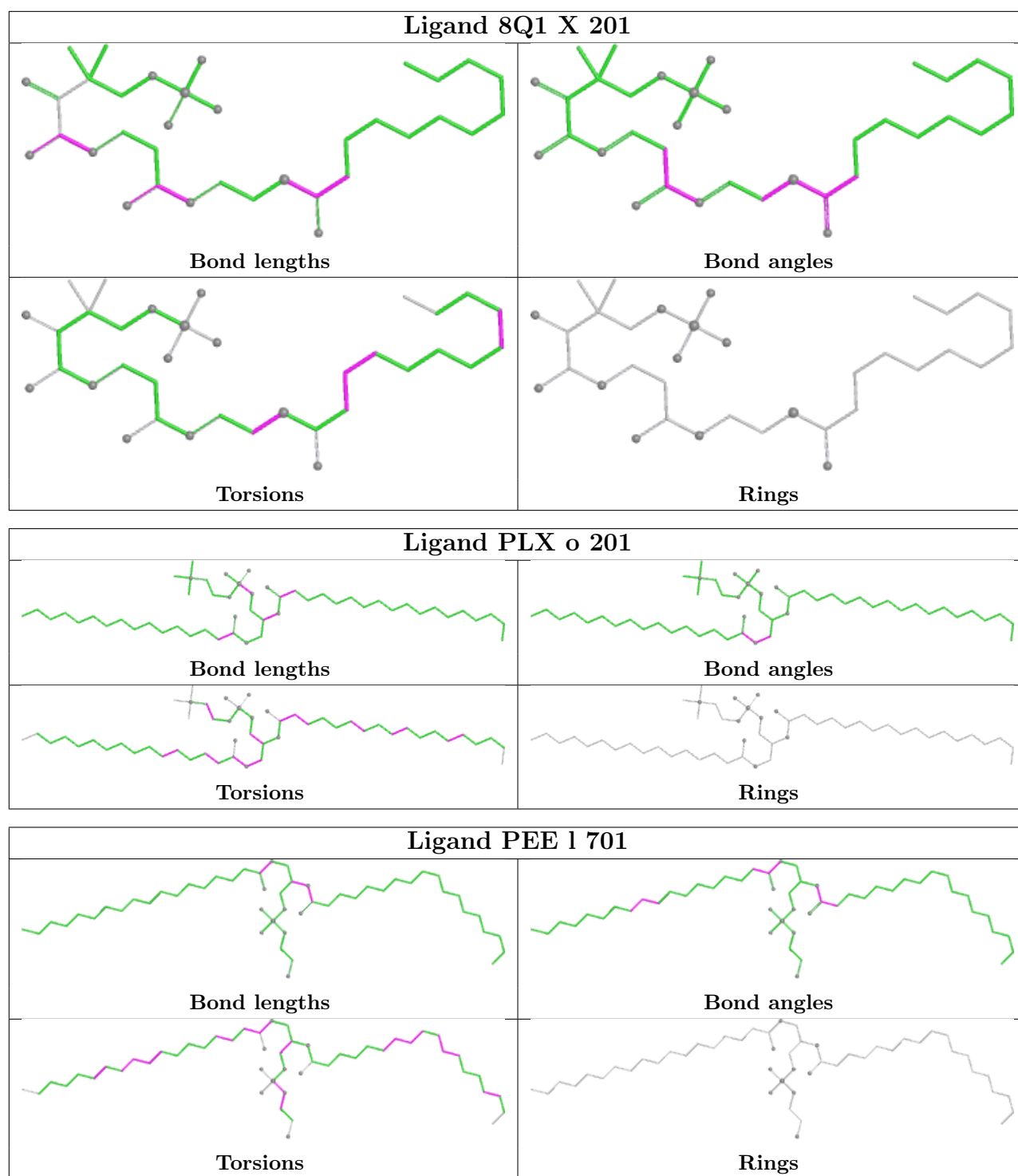
Continued from previous page...

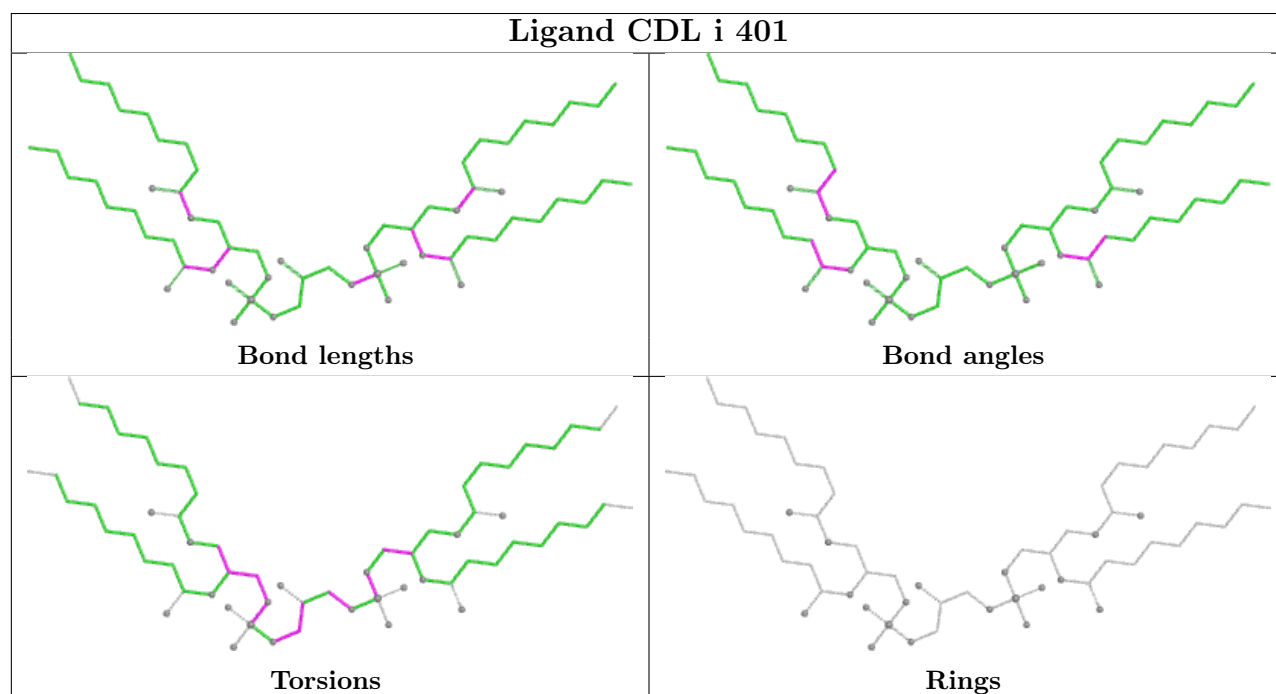
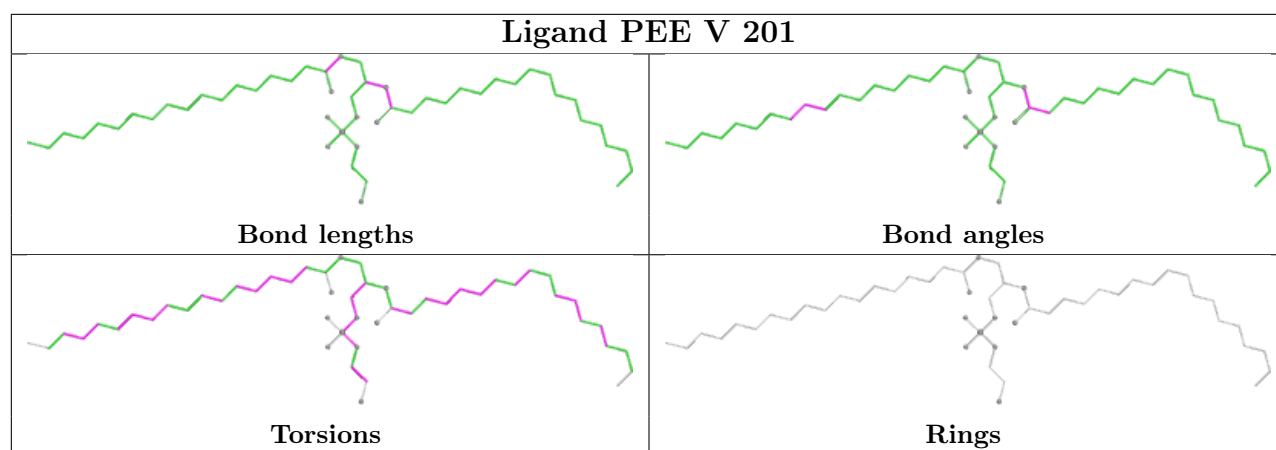
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	E	302	SF4	1	0
51	g	201	PLX	1	0
45	C	501	SF4	3	0
50	O	301	FES	1	0

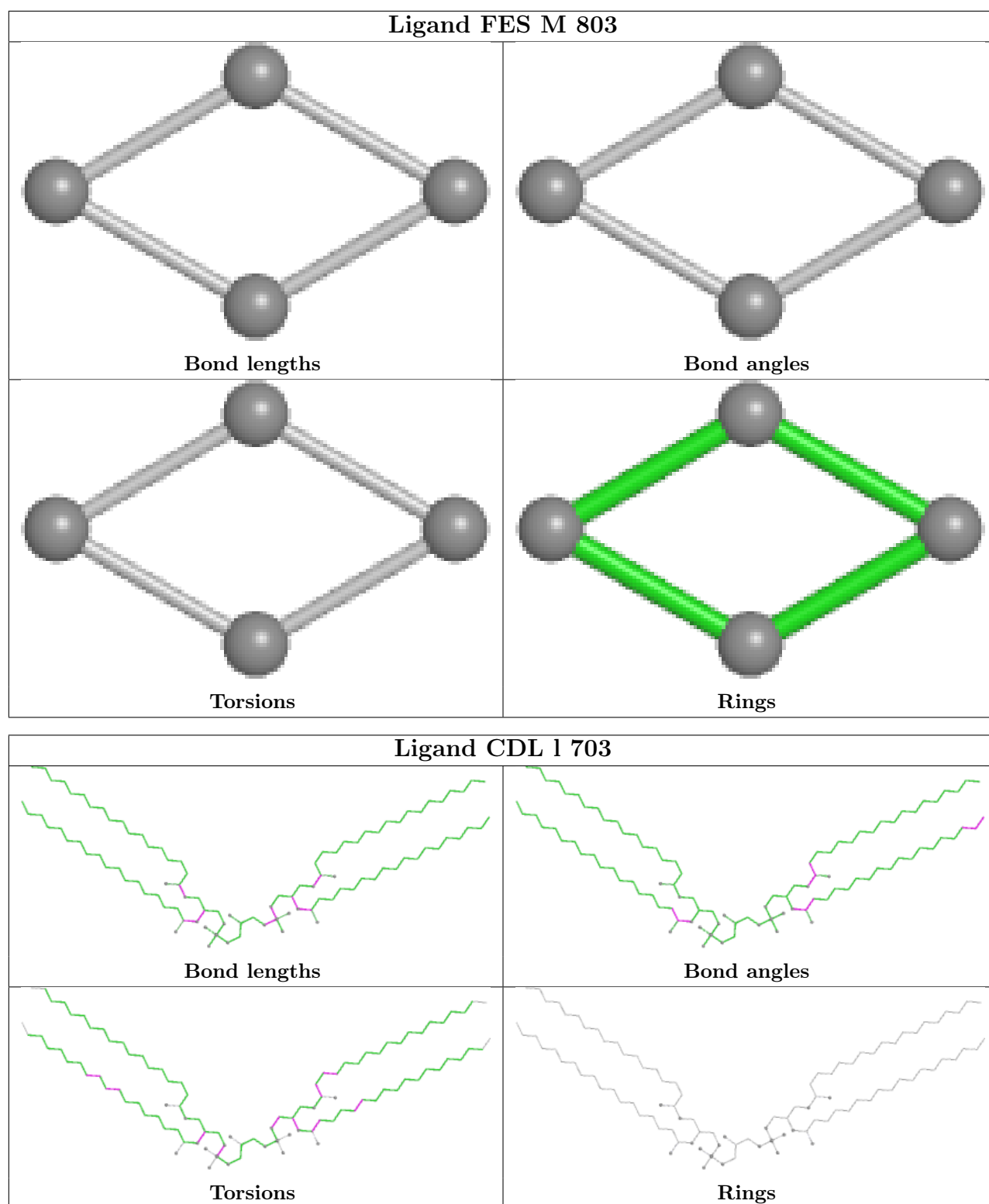
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

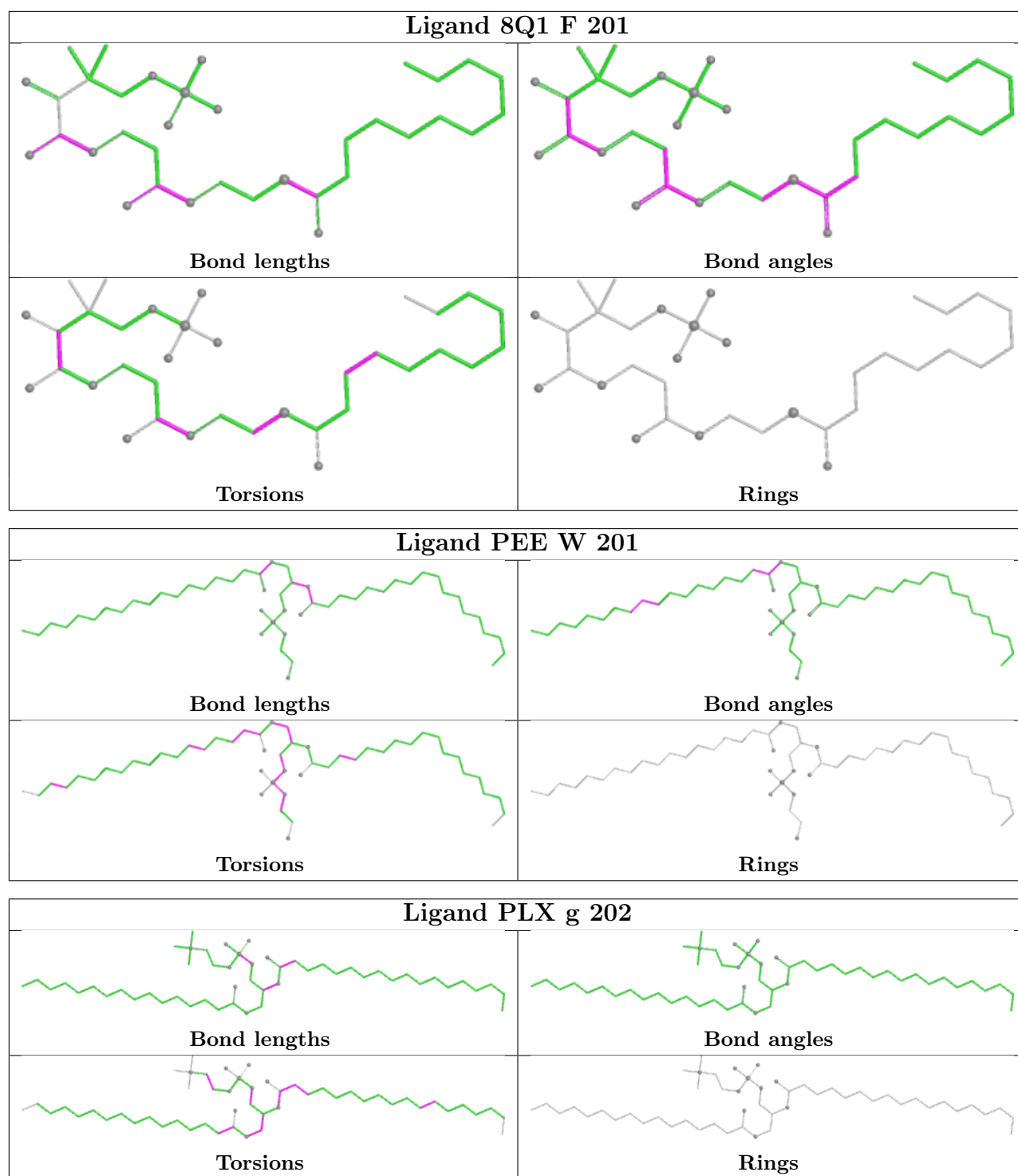


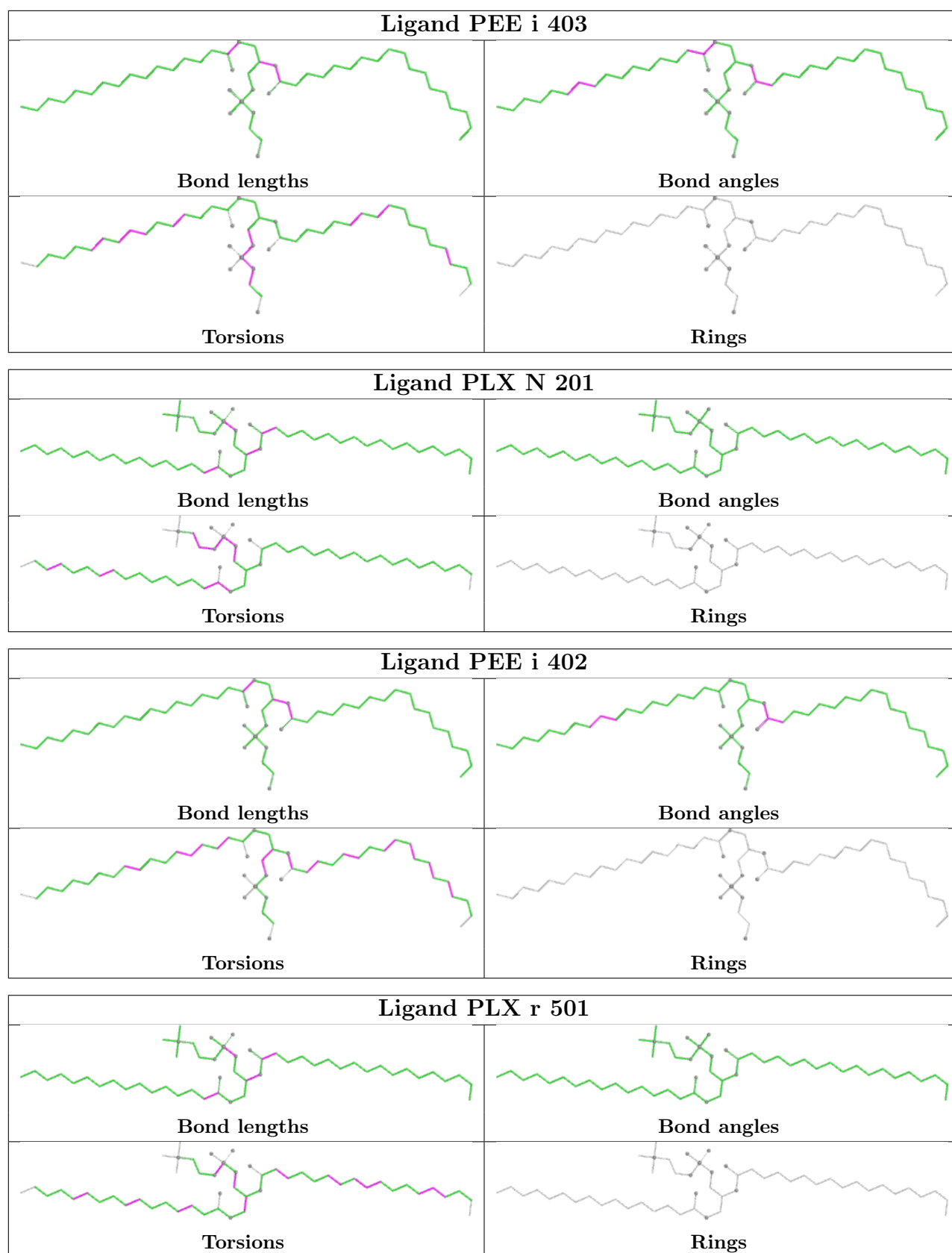


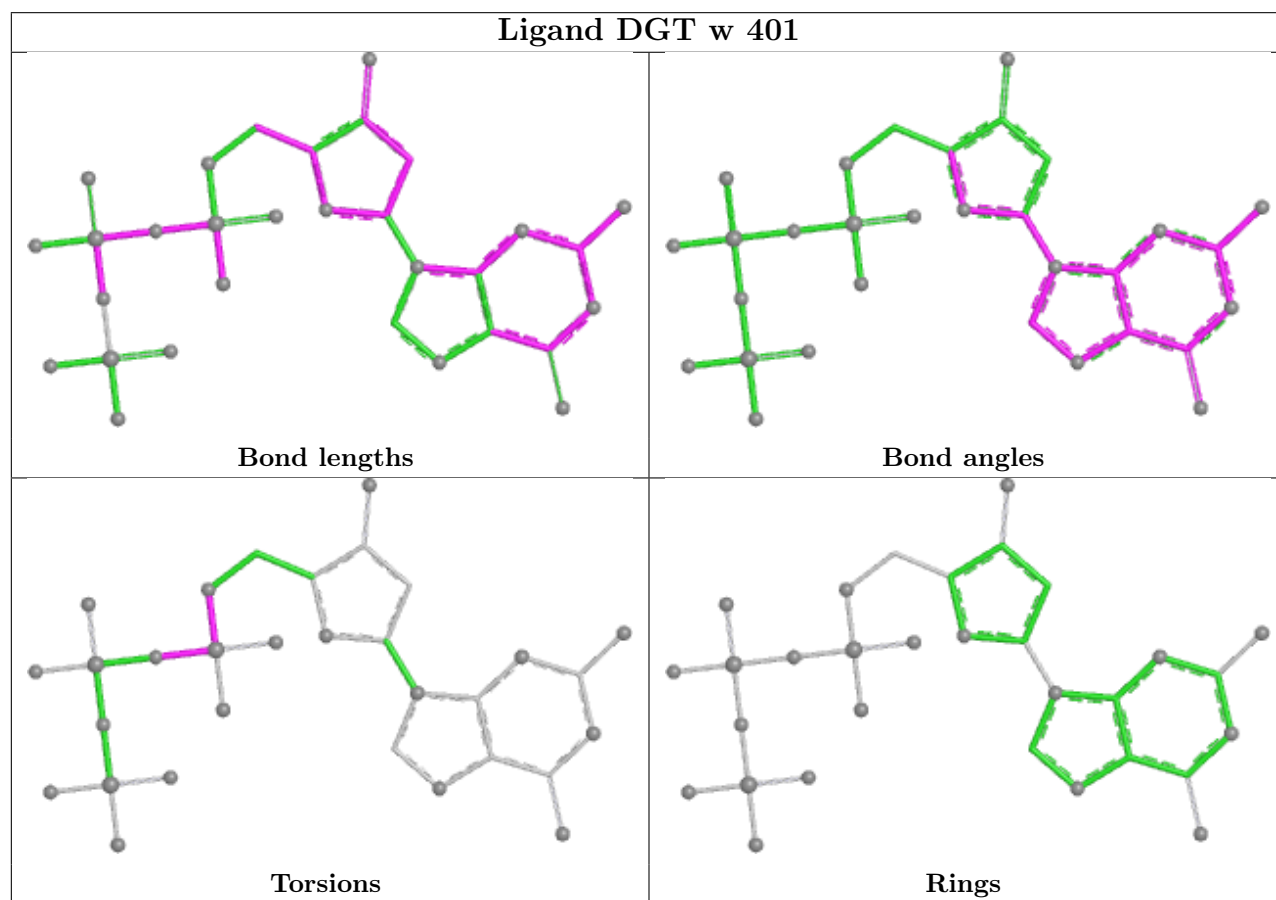
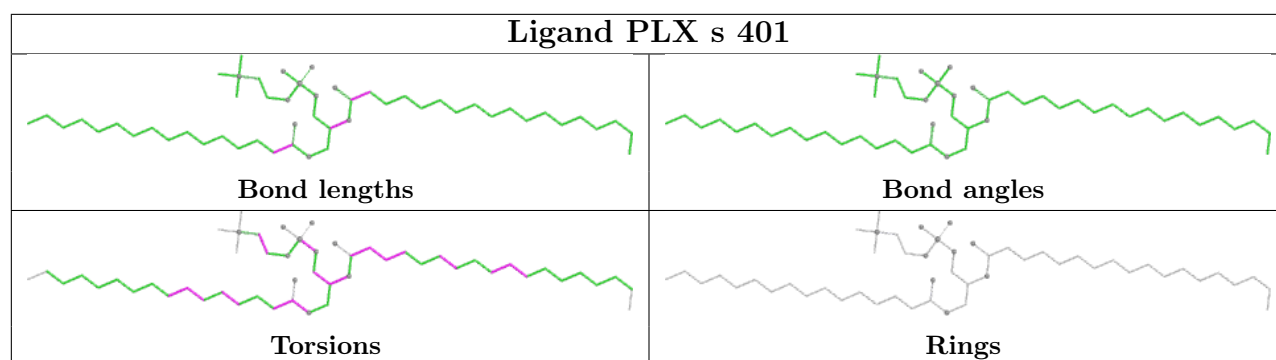


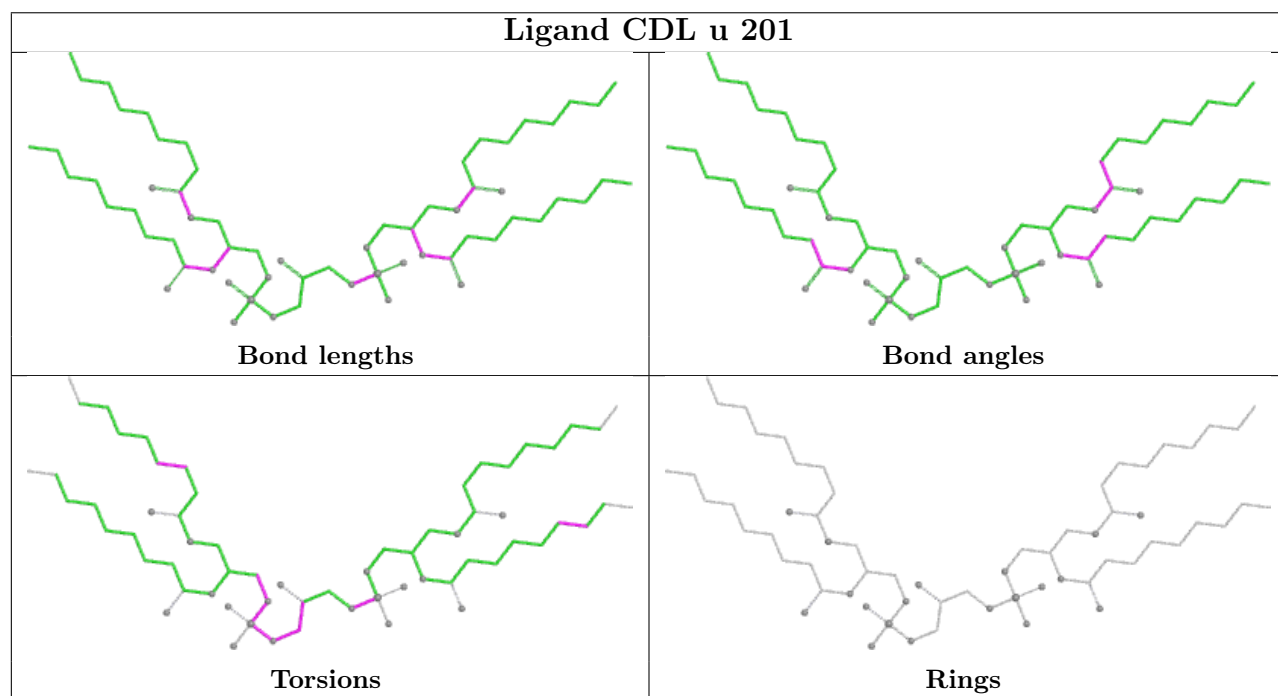
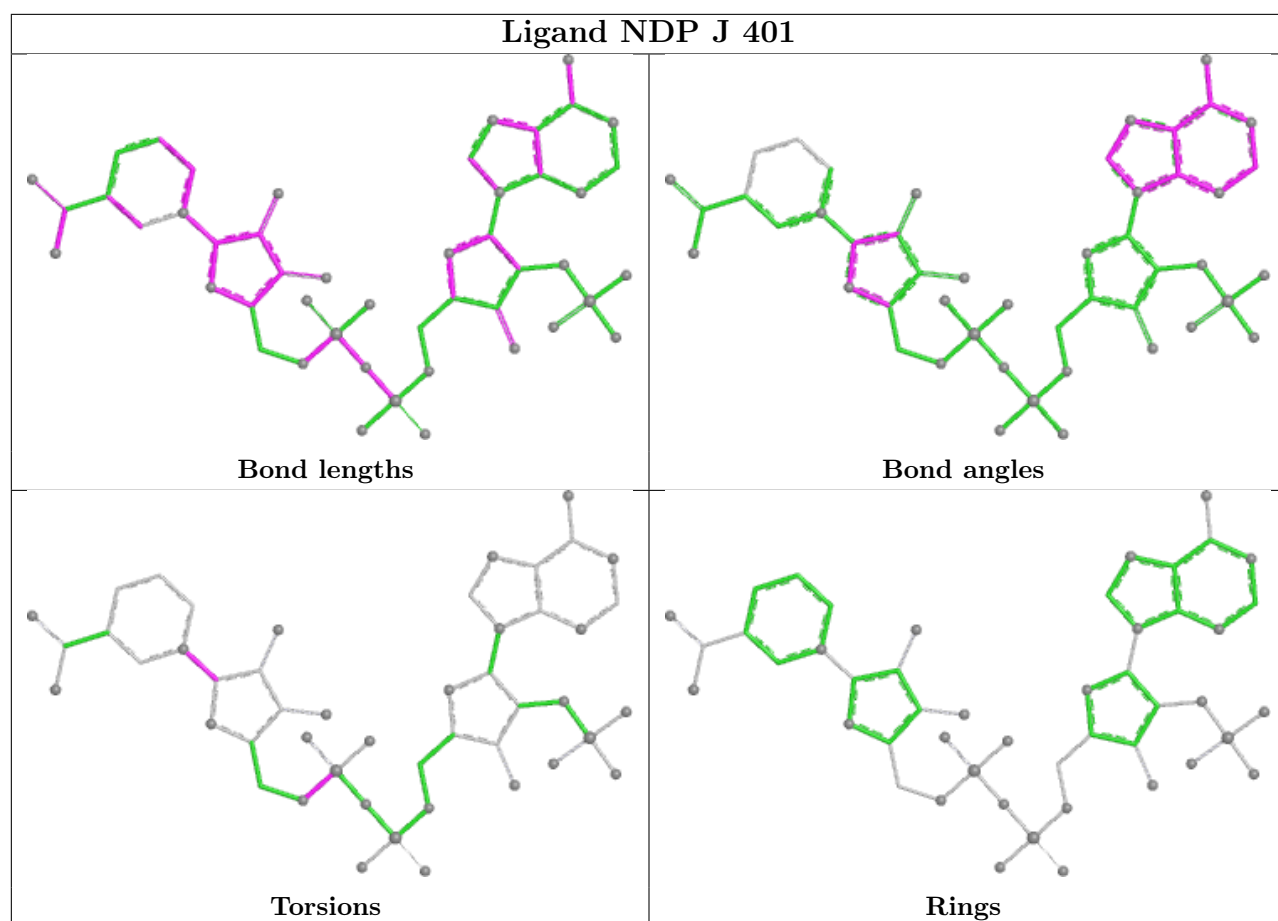


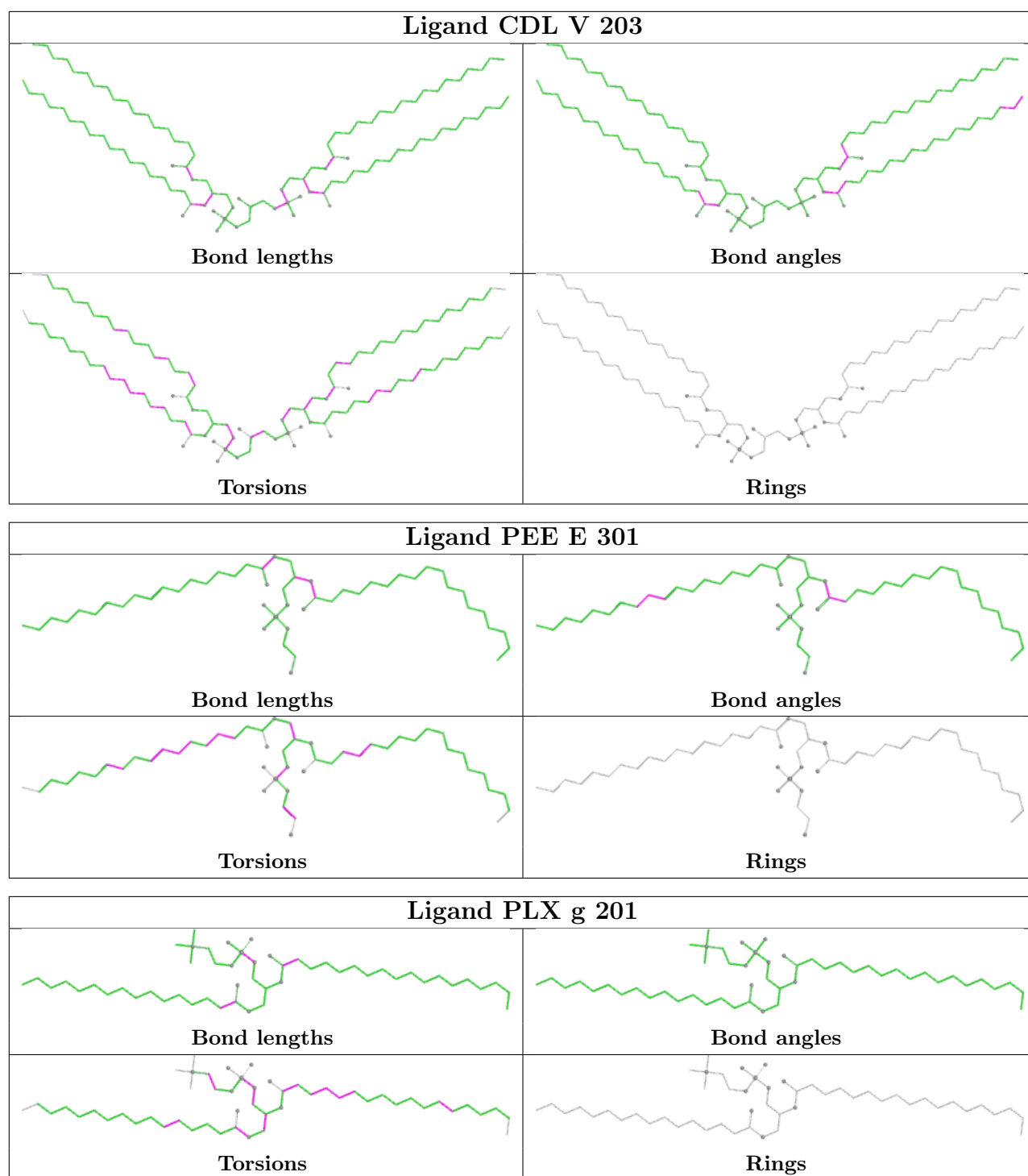


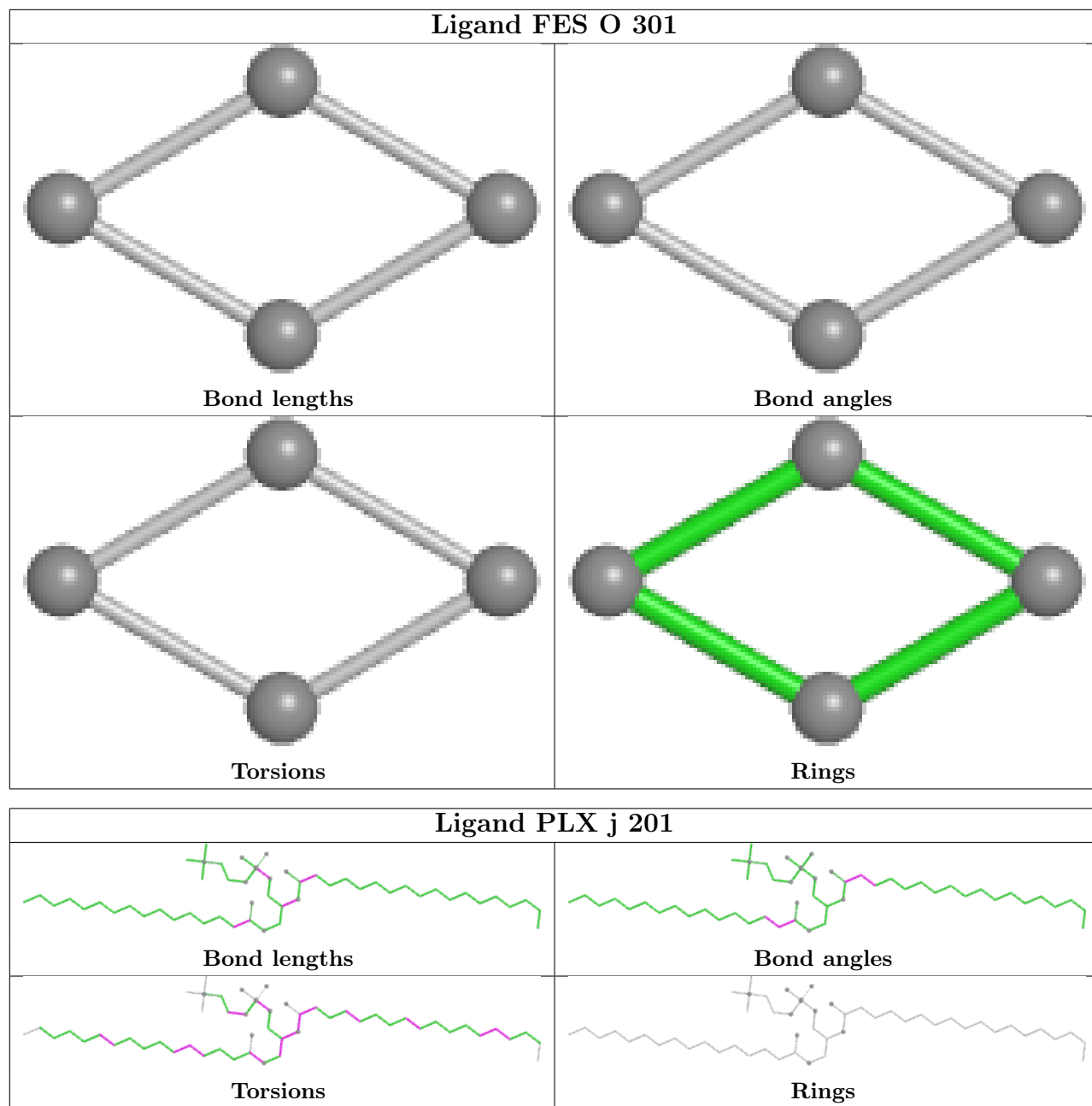


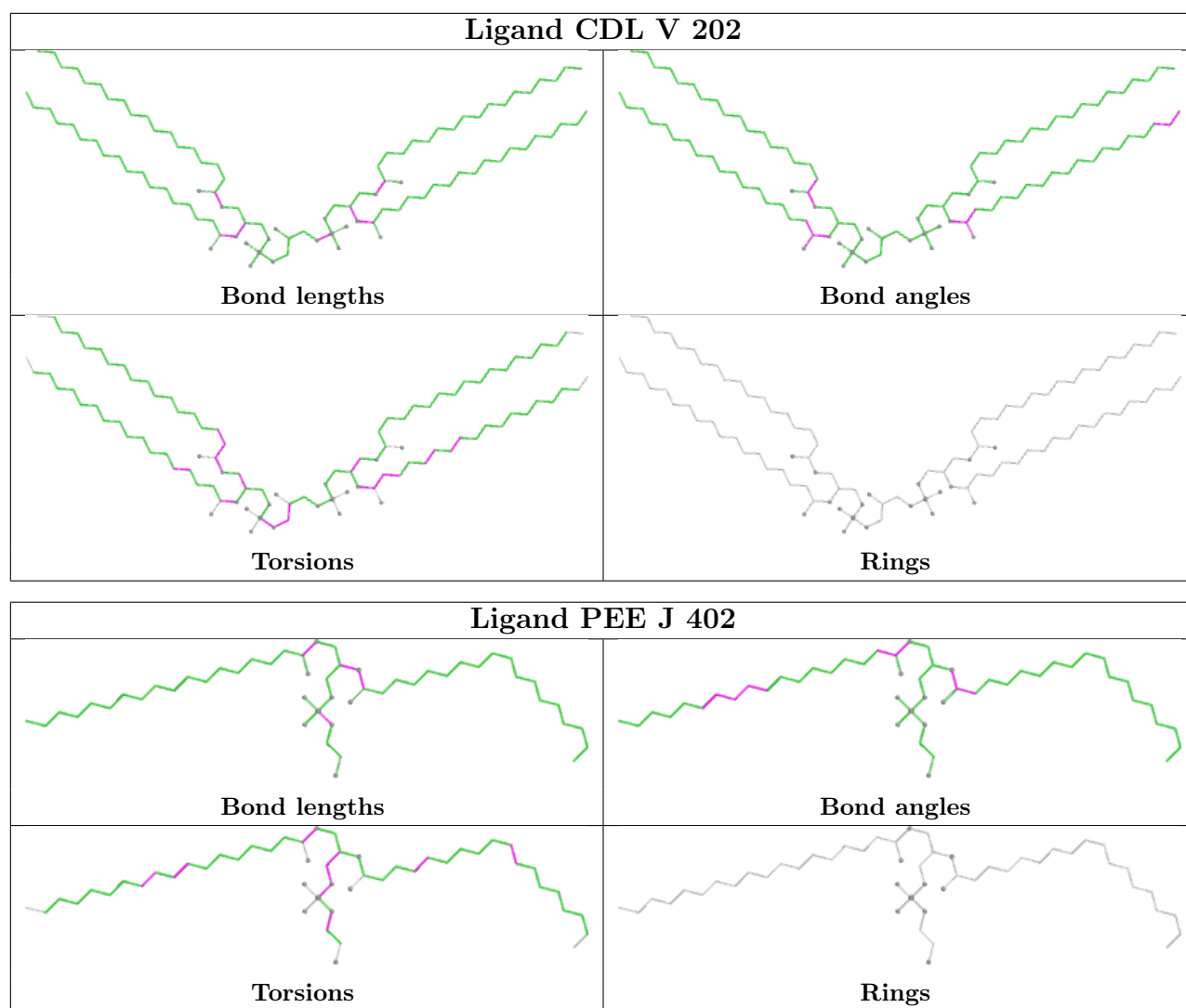












5.7 Other polymers [i](#)

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
24	b	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	39:LYS	C	41:GLY	N	4.62
1	C	457:HIS	C	458:GLN	N	3.27

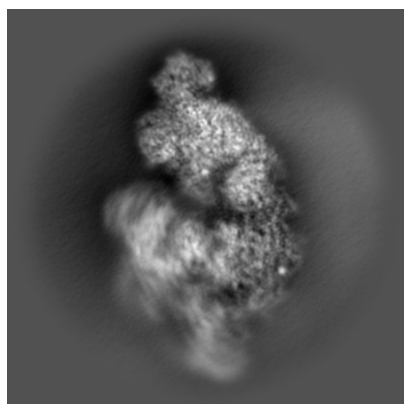
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54784. These allow visual inspection of the internal detail of the map and identification of artifacts.

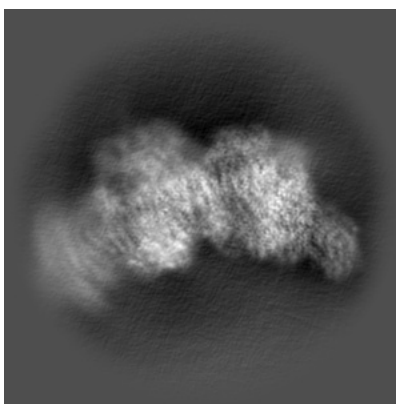
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

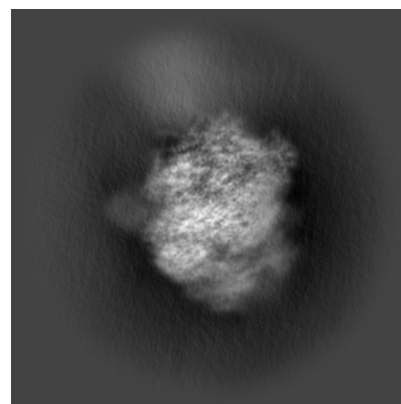
6.1.1 Primary map



X

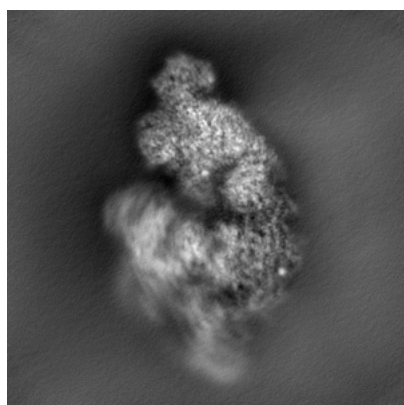


Y

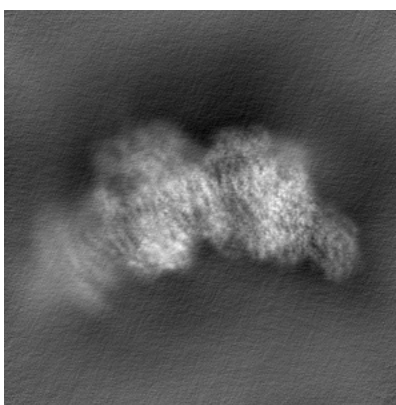


Z

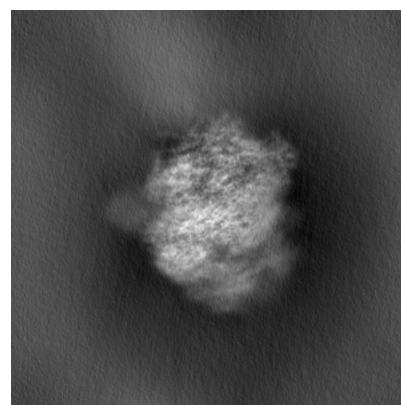
6.1.2 Raw map



X



Y

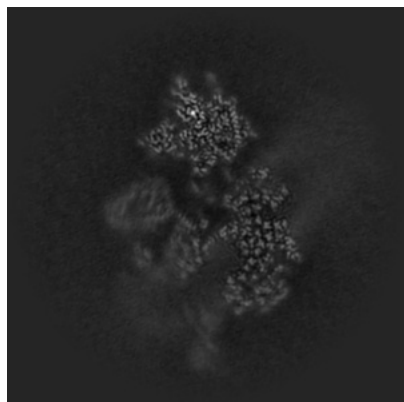


Z

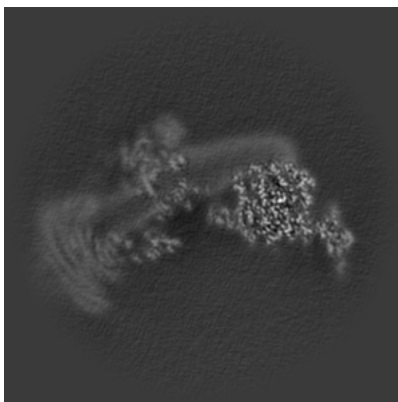
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

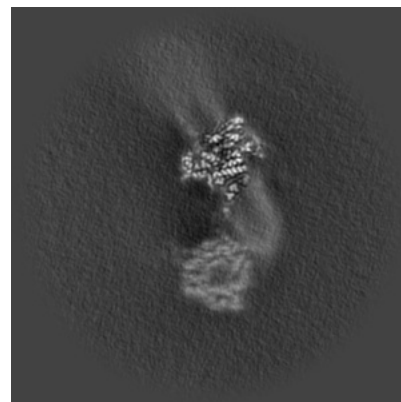
6.2.1 Primary map



X Index: 240

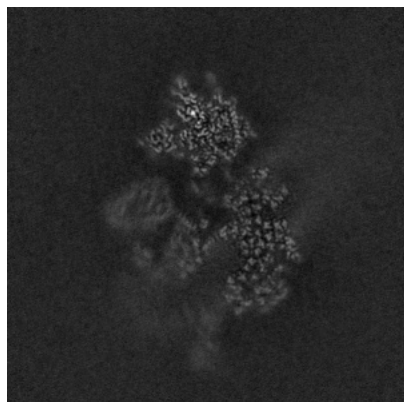


Y Index: 240

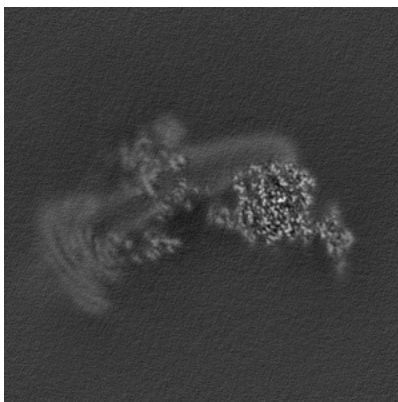


Z Index: 240

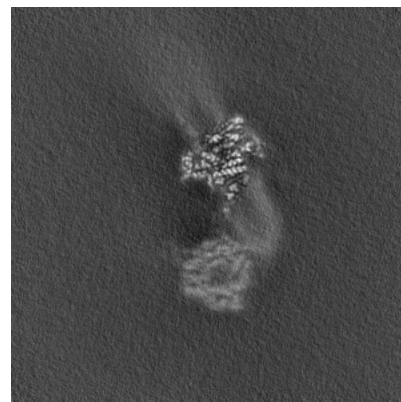
6.2.2 Raw map



X Index: 240



Y Index: 240

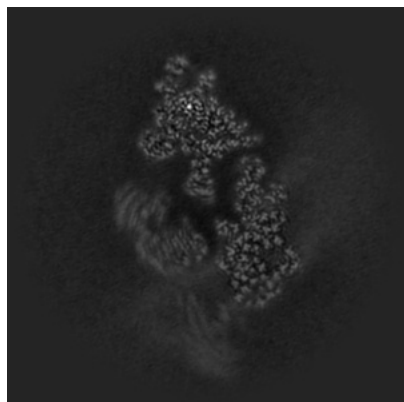


Z Index: 240

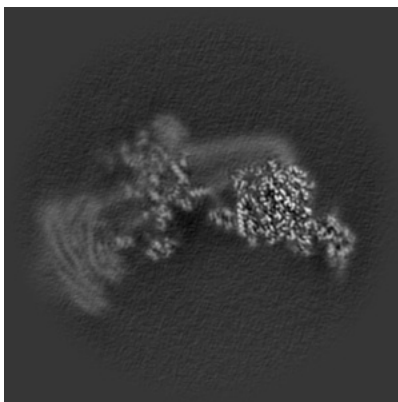
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

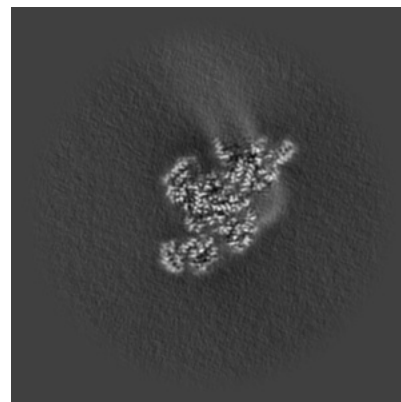
6.3.1 Primary map



X Index: 224

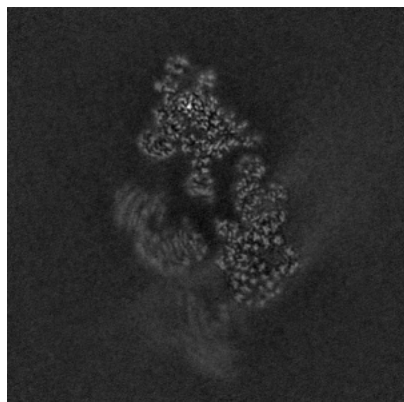


Y Index: 236

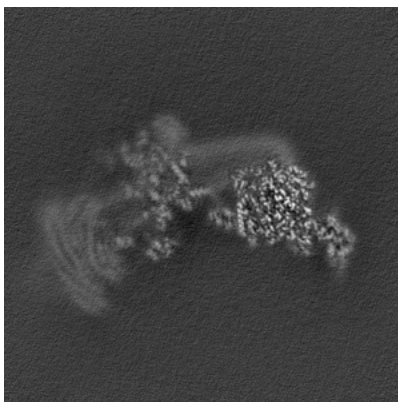


Z Index: 311

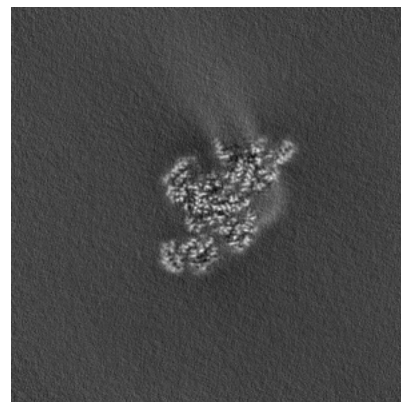
6.3.2 Raw map



X Index: 223



Y Index: 236

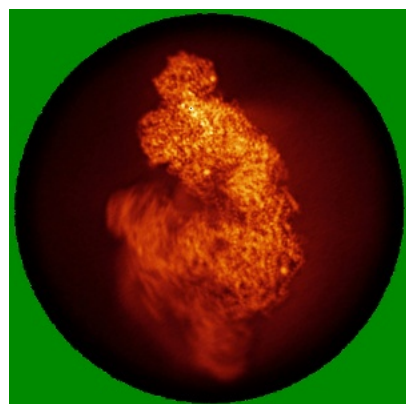


Z Index: 311

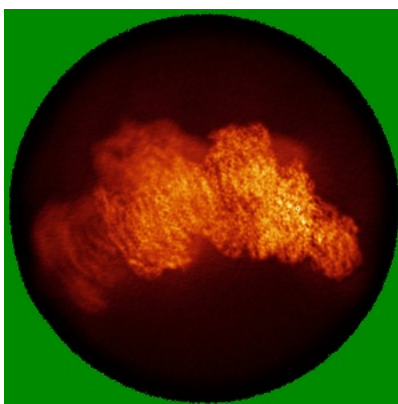
The images above show the largest variance slices of the map in three orthogonal directions.

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

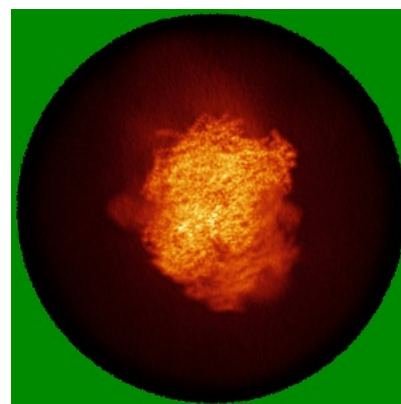
6.4.1 Primary map



X

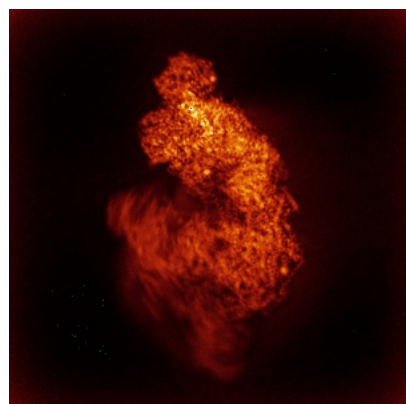


Y

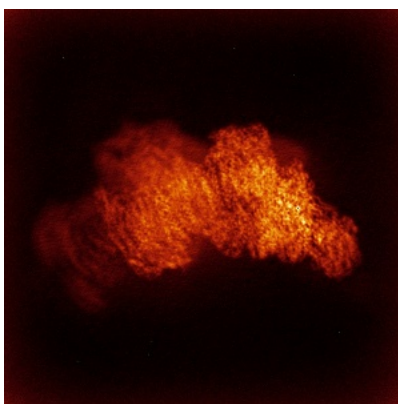


Z

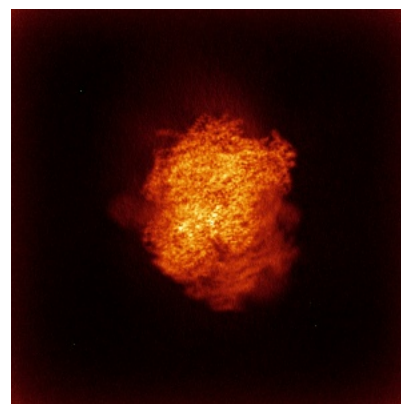
6.4.2 Raw map



X



Y

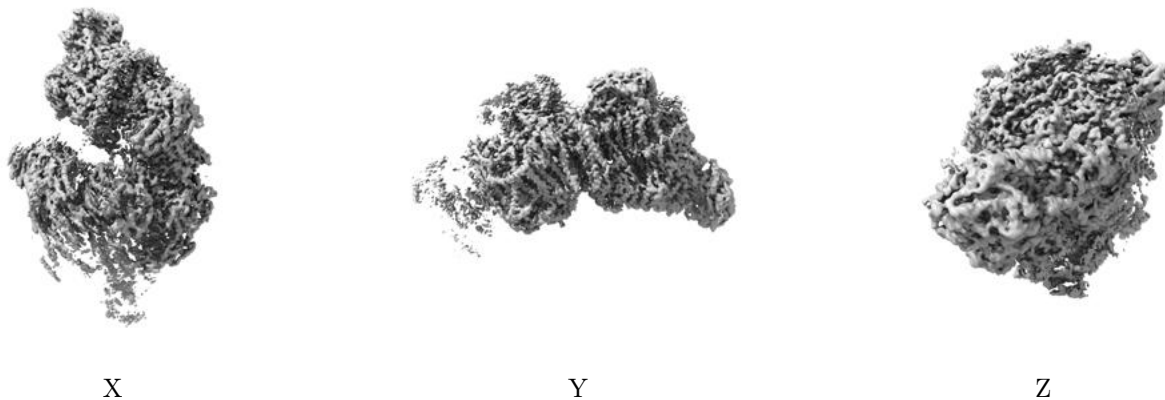


Z

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.

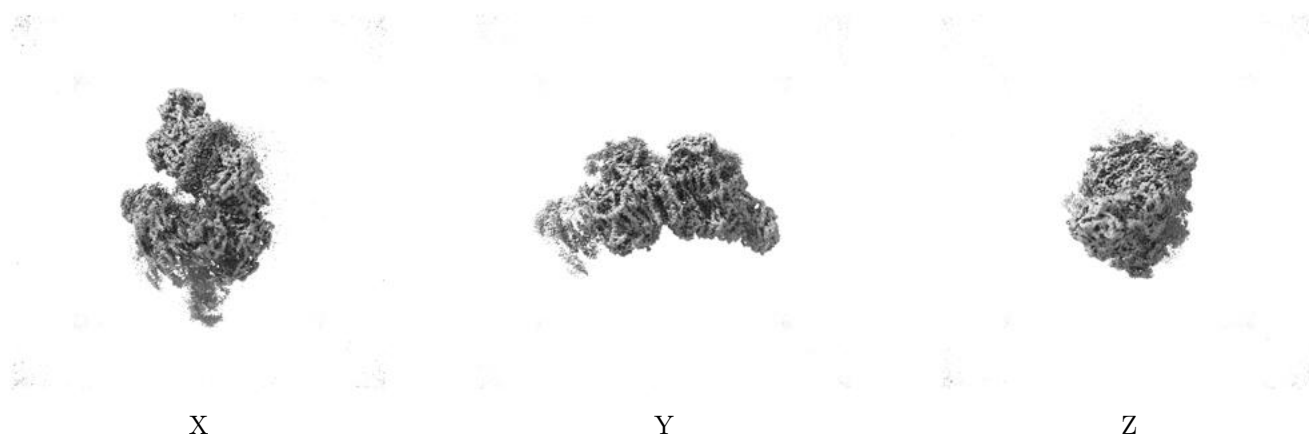
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

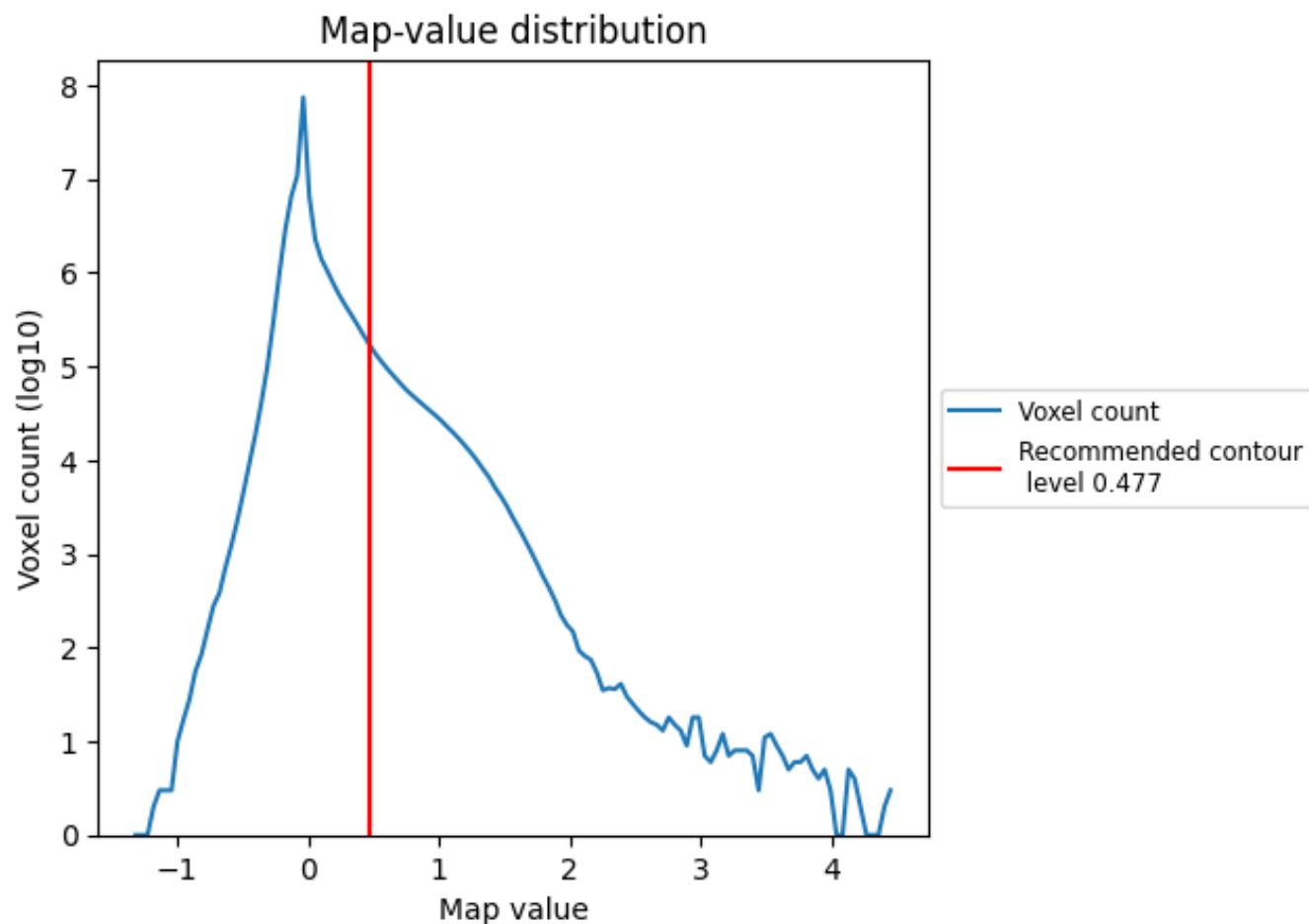
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

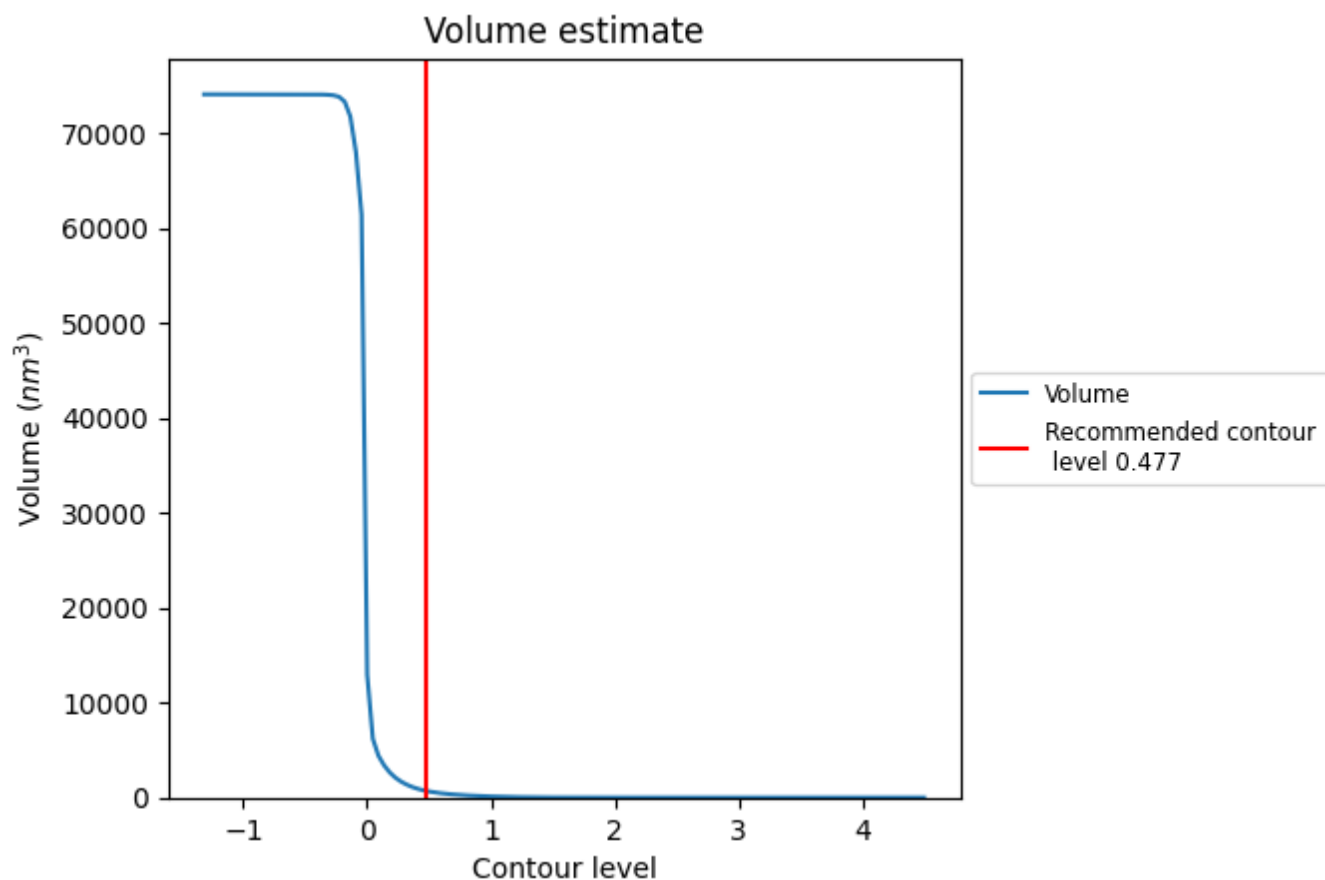
This section contains the results of statistical analysis of the map.

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.

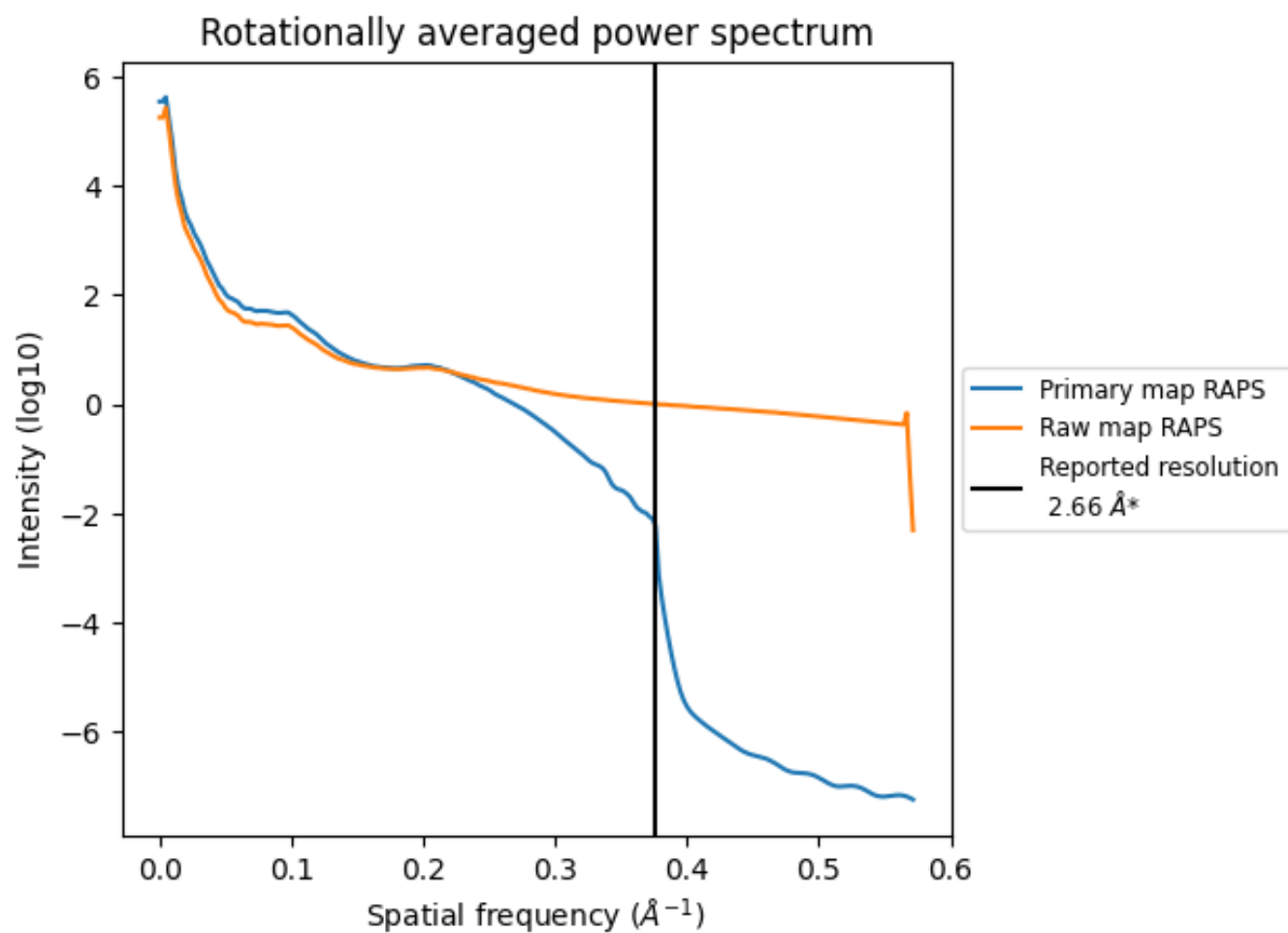
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 704 nm³; this corresponds to an approximate mass of 636 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 ⓘ

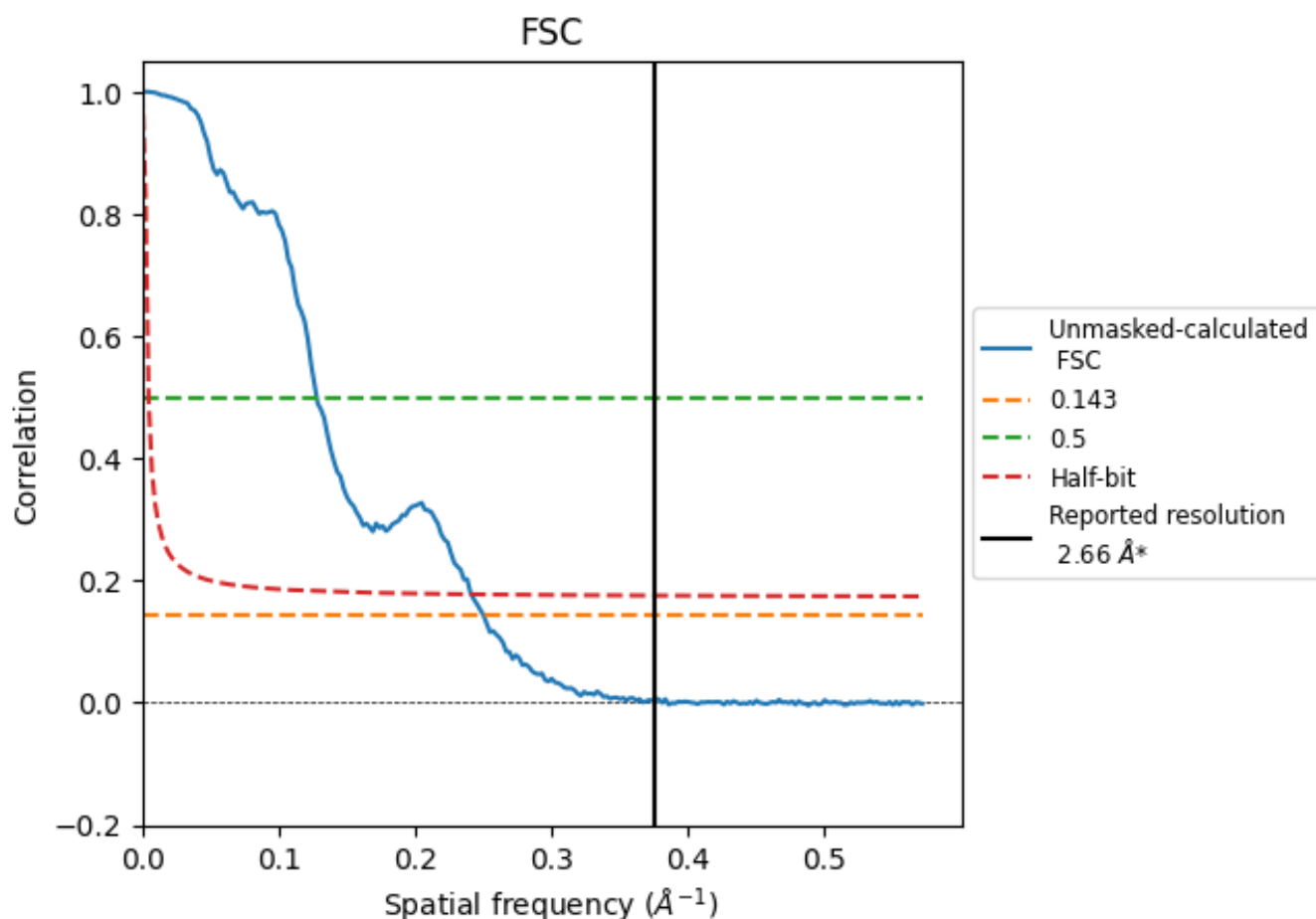


*Reported resolution corresponds to spatial frequency of $0.376 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

8.2 Resolution estimates [i](#)

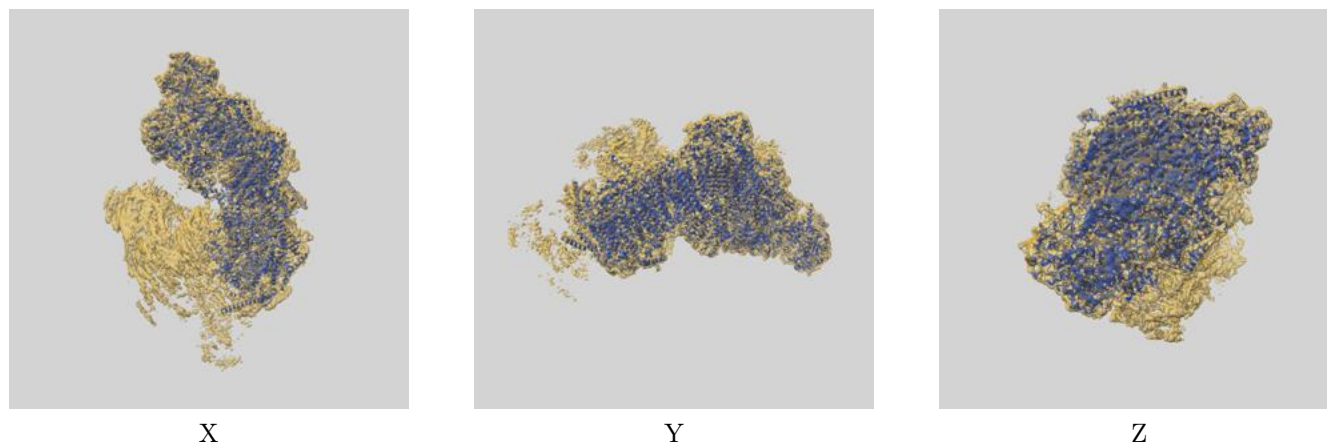
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	7.82	4.15

*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 4.00 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

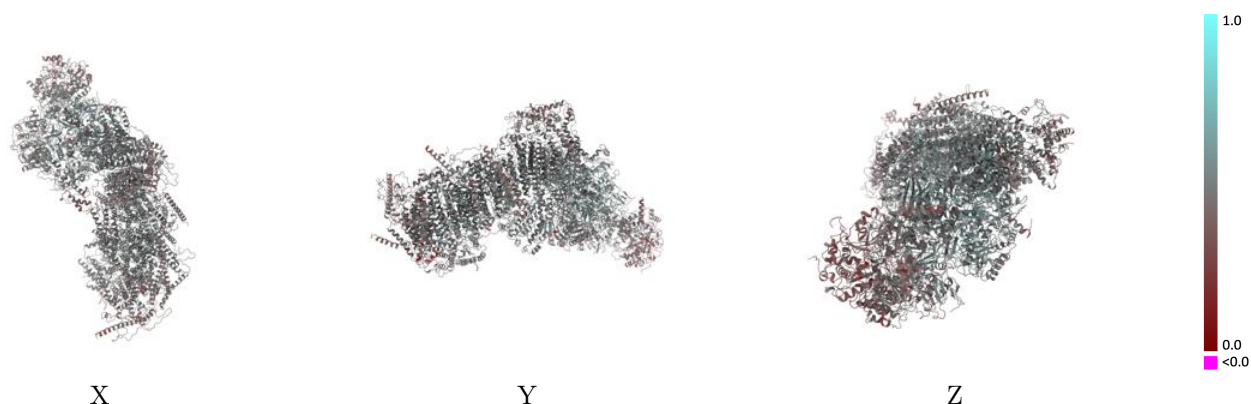
This section contains information regarding the fit between EMDB map EMD-54784 and PDB model 9TI4. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



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](#)

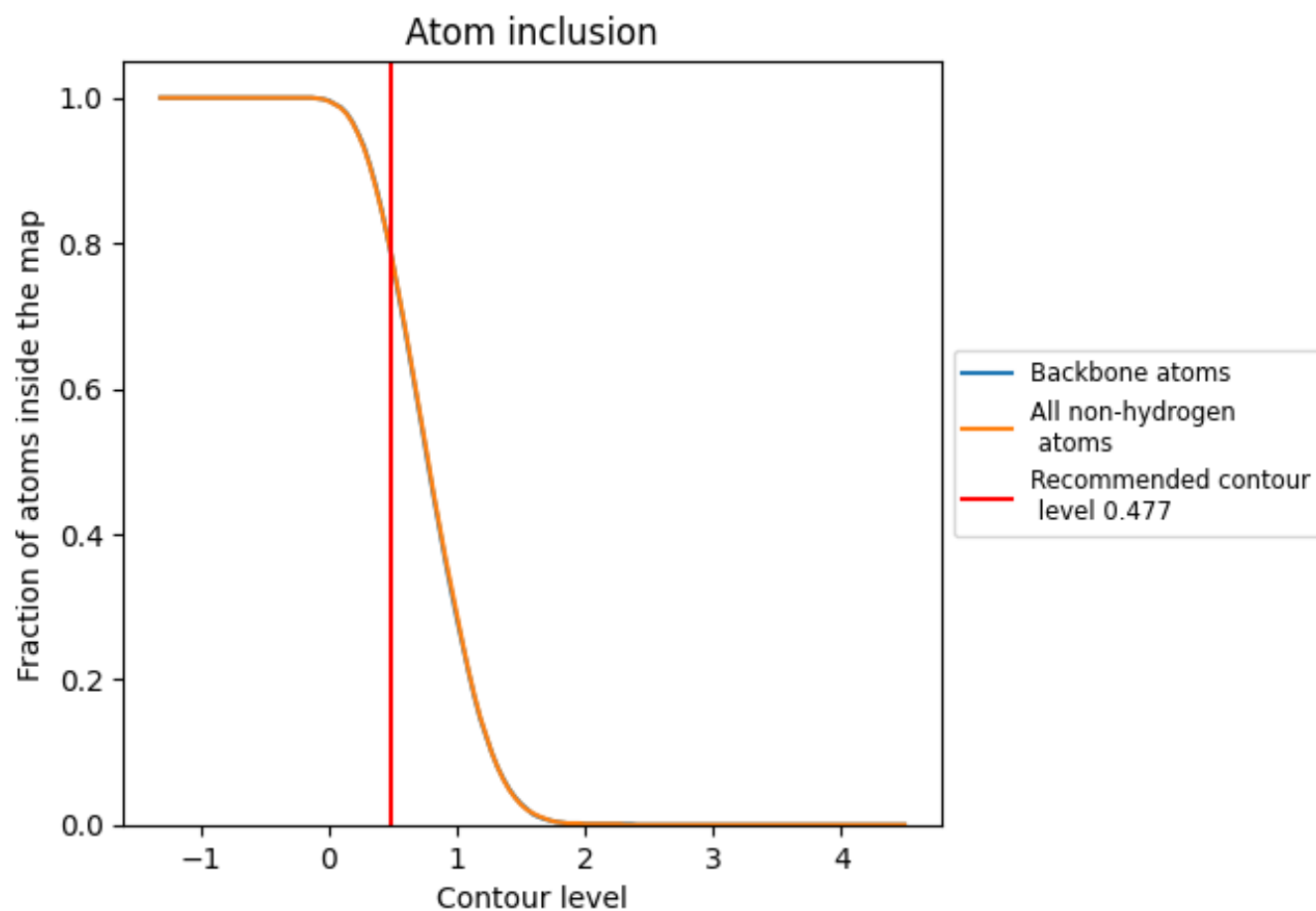


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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	 0.7930	 0.4700
C	 0.7830	 0.3810
D	 0.9360	 0.5320
E	 0.9010	 0.5240
F	 0.8380	 0.4950
G	 0.8330	 0.4180
H	 0.6250	 0.3770
I	 0.7960	 0.4550
J	 0.8890	 0.5030
K	 0.8120	 0.3790
L	 0.8300	 0.5030
M	 0.8500	 0.4590
N	 0.9180	 0.5000
O	 0.8210	 0.3990
P	 0.8650	 0.5190
Q	 0.8580	 0.5260
S	 0.8670	 0.4540
T	 0.9200	 0.5040
U	 0.8270	 0.4580
V	 0.6490	 0.4710
W	 0.8440	 0.4570
X	 0.7160	 0.4420
Y	 0.7110	 0.4170
Z	 0.6710	 0.4020
a	 0.8230	 0.4780
b	 0.6840	 0.3930
c	 0.7610	 0.4780
d	 0.7360	 0.4400
e	 0.7330	 0.4480
f	 0.6620	 0.3810
g	 0.7460	 0.4720
h	 0.8380	 0.4570
i	 0.7670	 0.5040
j	 0.7840	 0.4970
k	 0.8070	 0.4920



Continued on next page...

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Chain	Atom inclusion	Q-score
l	 0.7090	 0.4670
m	 0.8080	 0.4670
n	 0.7280	 0.4350
o	 0.7240	 0.4760
p	 0.7920	 0.4750
r	 0.7740	 0.5020
s	 0.8780	 0.5080
t	 0.8690	 0.4880
u	 0.8100	 0.4380
v	 0.6920	 0.3940
w	 0.8210	 0.4920