



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 06:36 PM UTC

PDB ID : 8IBF / pdb_00008ibf
EMDB ID : EMD-35342
Title : Respiratory complex Membrane domain of CI, focus-refined of type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.30 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

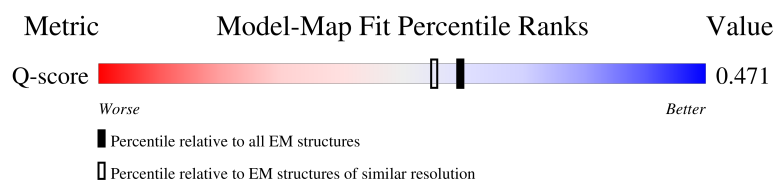
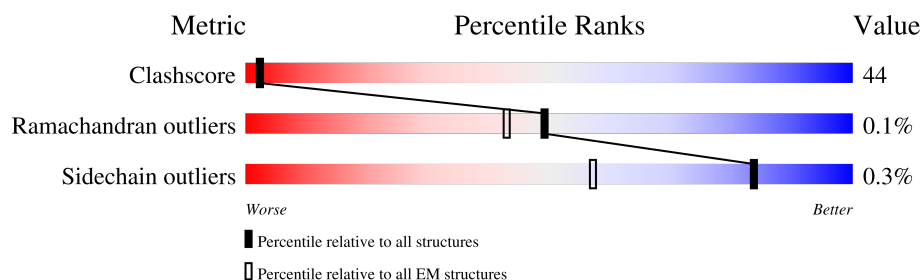
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	D	463	
2	J	172	
3	K	98	
4	L	607	

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Mol	Chain	Length	Quality of chain
5	M	459	
6	N	345	
7	O	355	
8	U	156	
9	X	172	
10	Y	143	
11	c	76	
12	d	120	
13	e	106	
14	f	57	
15	g	151	
16	h	189	
17	i	128	
18	j	105	
19	k	104	
20	l	186	
21	m	129	
22	n	179	
23	o	137	
24	p	176	

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
27	ADP	O	401	-	-	X	-

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 31948 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	42	Total	C	N	O	S	0	0
			350	227	58	64	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	163	Total	C	N	O	S	0	0
			1229	828	175	211	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	116	LEU	ASN	conflict	UNP P03925
J	117	GLY	LEU	conflict	UNP P03925

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 8 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	89	Total	C	N	O	S	0	0
			718	462	105	146	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	27	Total	C	N	O	0	0
			221	146	39	36		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	95	Total	C	N	O	S	0	0
			802	523	140	136	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	73	Total	C	N	O	S	0	0
			582	383	102	95	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	126	Total	C	N	O	S	0	0
			1050	676	189	185			

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

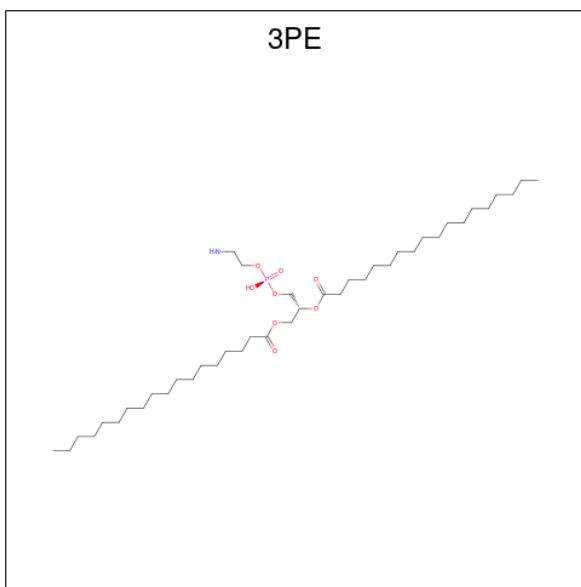
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

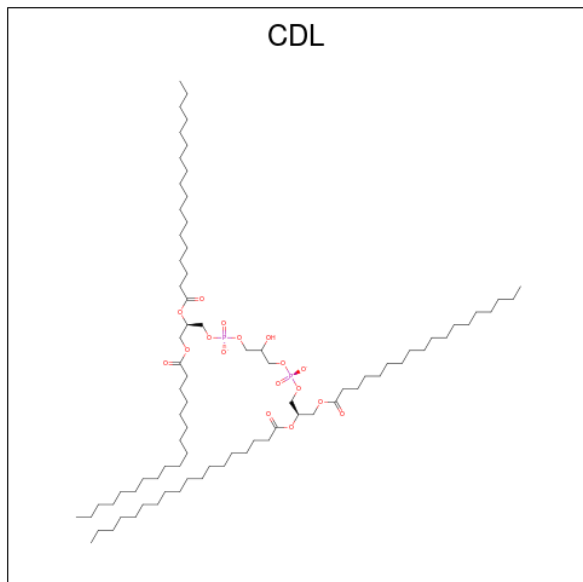
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



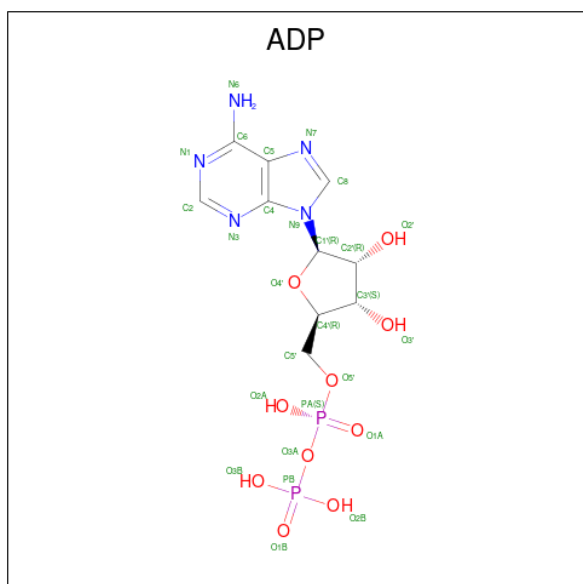
Mol	Chain	Residues	Atoms					AltConf
25	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
25	d	1	Total	C	N	O	P	0
			31	21	1	8	1	
25	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	m	1	Total	C	N	O	P	0
			47	37	1	8	1	
25	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



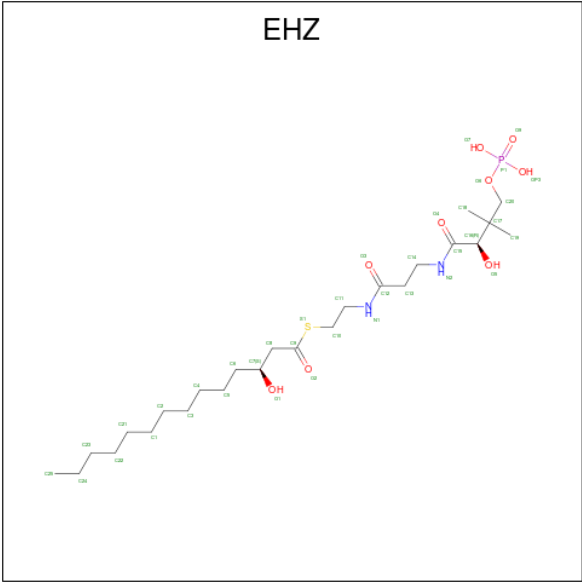
Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			78	59	17	2	
26	X	1	Total	C	O	P	0
			67	48	17	2	
26	h	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 27 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 28 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

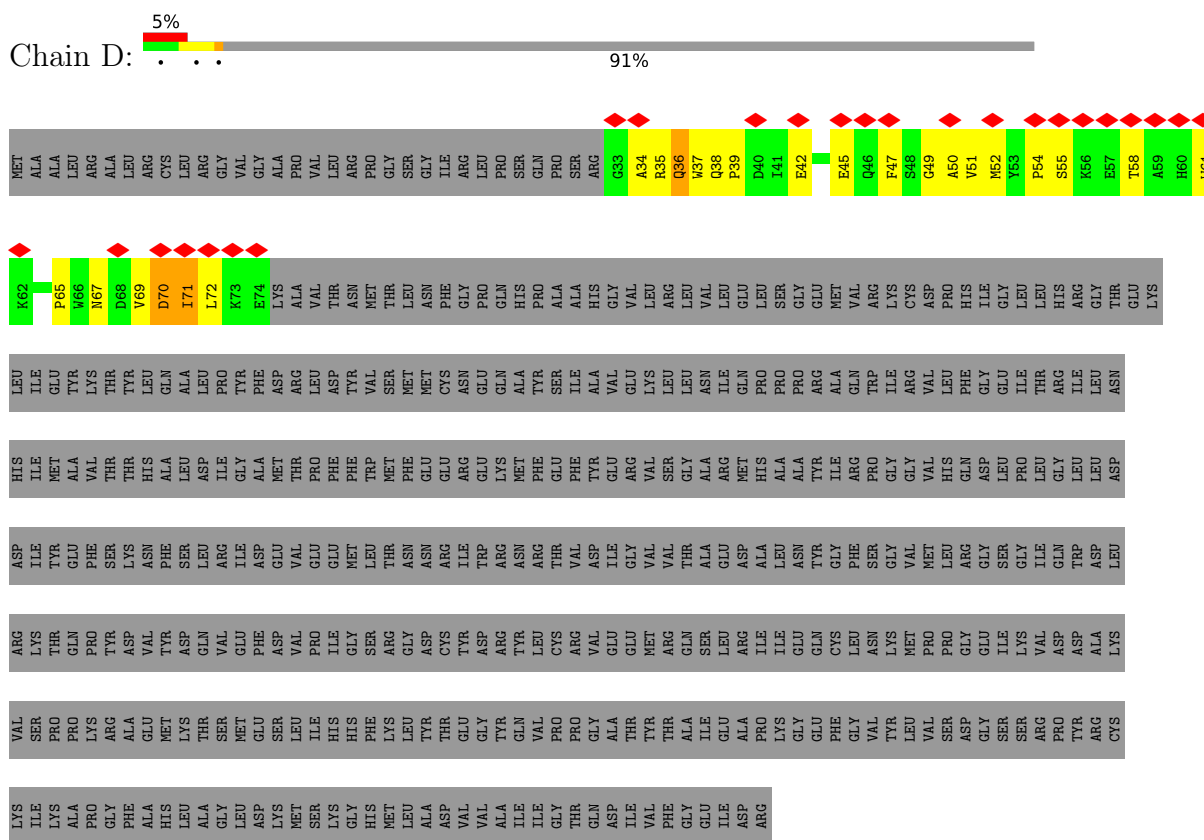


Mol	Chain	Residues	Atoms						AltConf
28	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

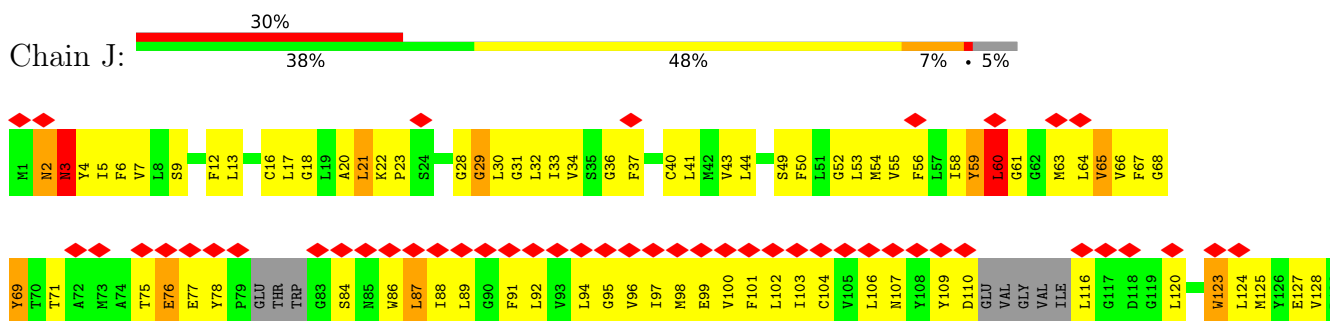
3 Residue-property plots

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] iron-sulfur protein 2, mitochondrial

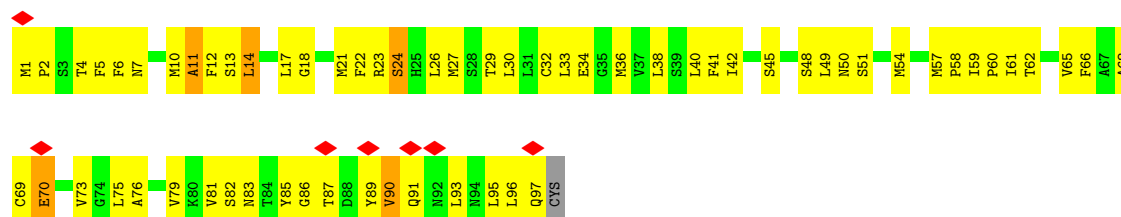


- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

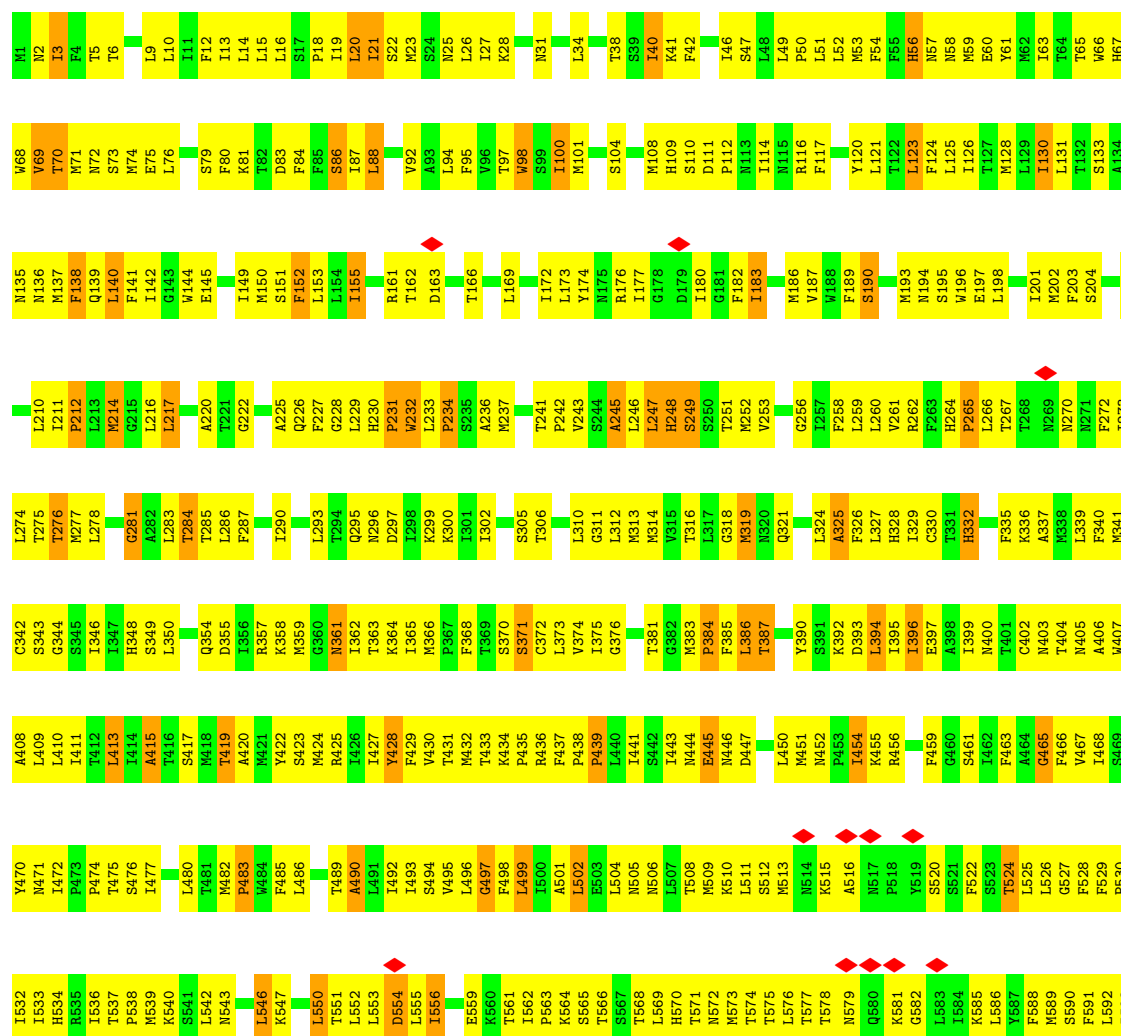


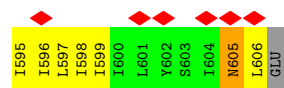


• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L



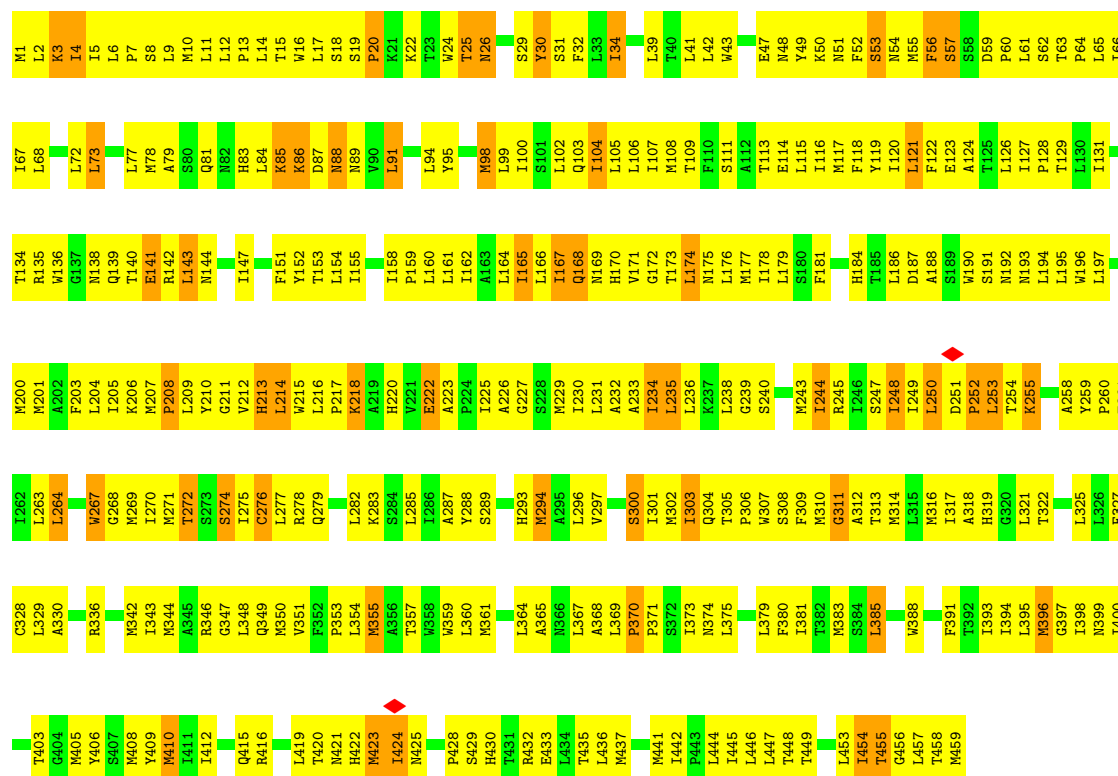
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5





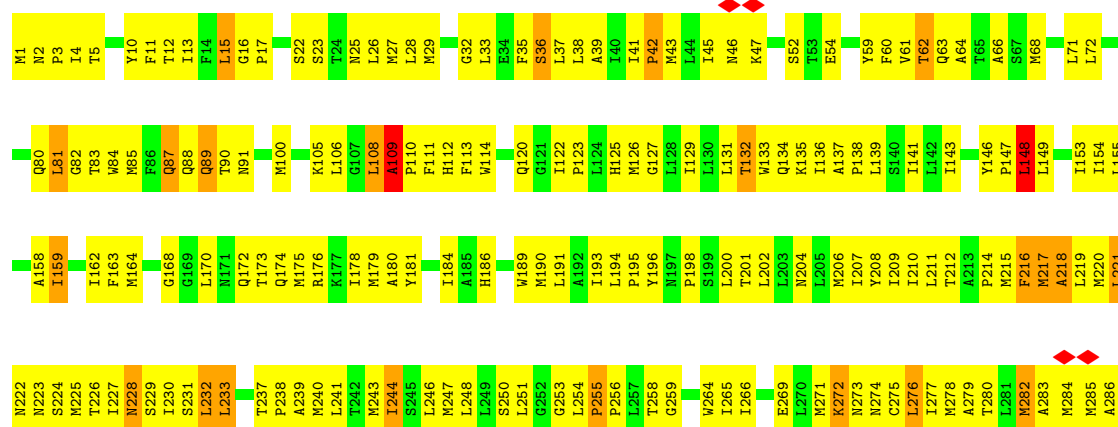
• Molecule 5: NADH-ubiquinone oxidoreductase chain 4

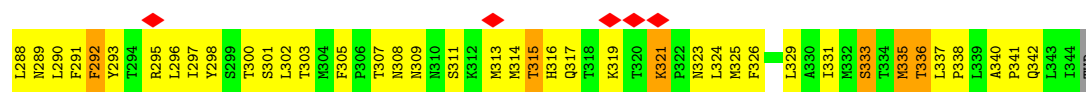
Chain M: 28% 60% 12%



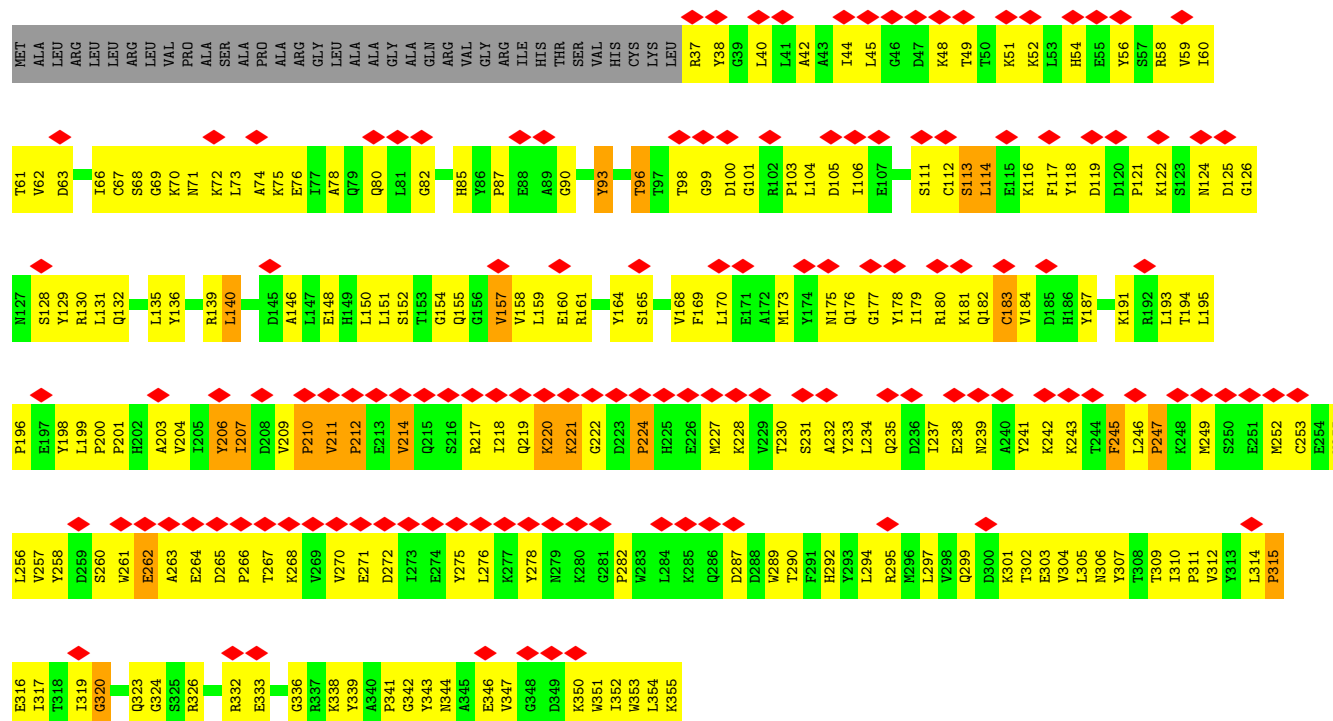
• Molecule 6: NADH-ubiquinone oxidoreductase chain 2

Chain N: 34% 57% 8%

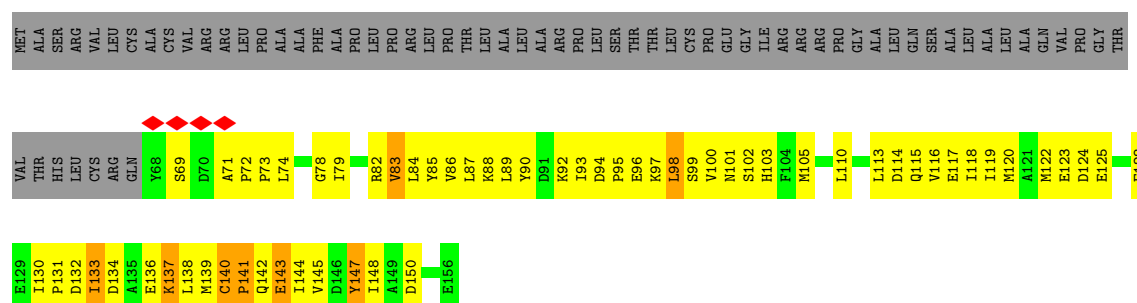




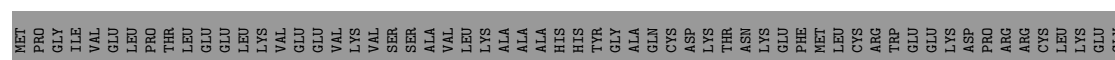
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 8: Acyl carrier protein, mitochondrial



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



LYS LEU VAL ASN GLY CYS ALA LEU ASN PHE LYS PHE ARG GLN TLE LYS SER PRO HIS CYS VAL ALA GLU PRO PHE THR SER GLU TYR ARG TRP THR CYS LEU ASP TYR SER ASN MET GLN PHE ARG HIS CYS ARG GLN GLN ALA LYS PHE ASP GLN VAL CYS VAL LEU LYS ASP LYS LEU GLY TRP VAL ARG PRO

ASP LEU GLY VAL SER LYS VAL THR LYS VAL THR ASP ARG PRO LEU PRO GLU ASN ARG A146 R147 P148 N151 P152 V153 I154 E155 L158 K159 P160 A161 H163 G164 T165 R166 F167 F168 F169 W170 T171 V172

- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y: 32% 52% 44% . .

MET ALA VAL K5 R6 F7 F8 E9 A80 Y11 H12 E13 V14 P15 D16 G17 T18 Q19 C20 H21 R22 K23 I26 L30 G31 G35 I36 I37 G38 S39 V43 S44 L45 M46 P47 A48 D49 S50 T51 L52 E53 A56 R57 V58 G59 R60 F63 T64 A65 A66 A67 I68

M71 F72 G73 L74 T75 T76 C77 V78 S79 Q81 R82 R83 E84 D87 D88 P89 N91 Y92 Y93 I94 G95 C97 A98 L101 T102 H103 S109 Y110 A114 M115 G116 Y119 M120 G121 A124 F127 K128 I129 G130 K131 L137 F138 P139 T140 P141 K142 V143

- Molecule 11: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c: 18% 25% 32% 5% 38%

MET ALA PRO VAL LEU ARG SER PHE SER ARG LEU ALA PRO ALA ARG LEU PRO SER CYS SER SER THR ARG SER LYS F29 Y30 R32 E33 P34 V35 N36 A37 K38 P39 M40 W41 V44 G45 L46 S47 A50 F53 M54 W55 Y57 Q60 T61 H62 E64

D65 V66 L67 E68 Y69 K70 R71 R72 N73 G74 L75 GLU

- Molecule 12: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d: 11% 38% 59% .

M1 M2 N3 G4 R5 P6 G7 H8 E9 P10 L11 K12 L13 L14 P15 D16 E17 A18 S19 S20 L21 P22 P23 P24 K25 L26 N27 D28 P29 R30 Y33 L37 G38 Y39 C40 L43 M44 D45 M46 M47 L48 R49 M50 R51 P52 V53 M54 R55 A56 G57 L58 H59 R60 D61 L62 L63 F64

V65 T66 F70 A71 G72 Y73 K77 R78 Q79 R80 Y81 L82 D87 H88 D89 M90 F91 G92 Y93 I94 E99 D100 F101 P102 E103 K104 E105 K106 T107 T108 Y109 A110 E111 I112 L113 E114 F115 H117 P118 V119 R120

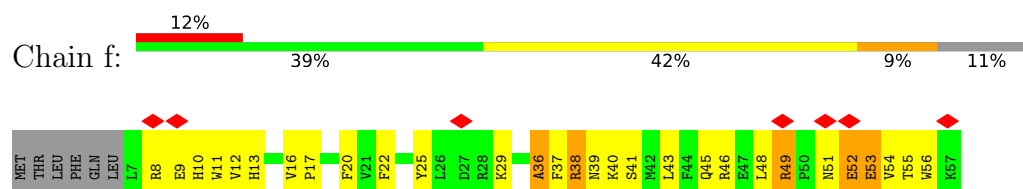
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 13% 47% 46% 6% .

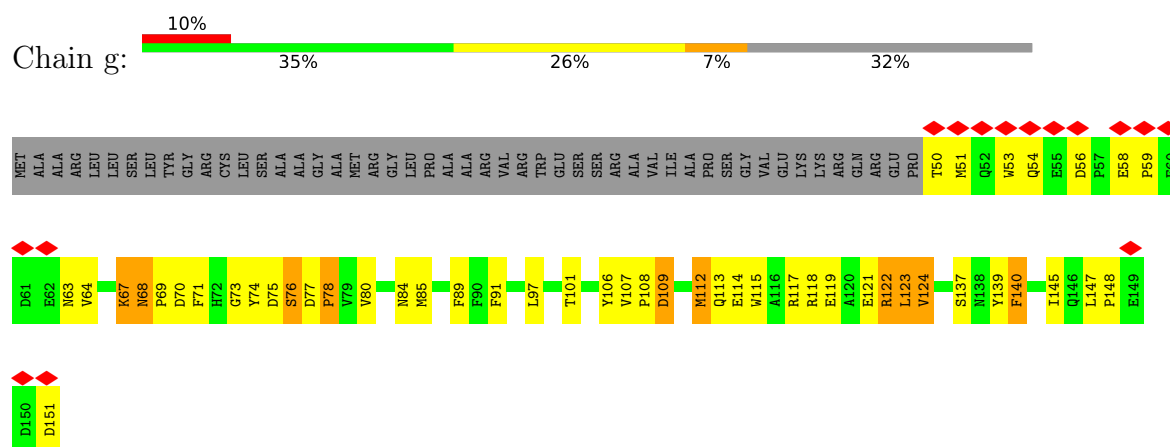
MET F2 F3 L4 D5 I6 L14 D15 R16 H17 F18 M19 F20 L21 R32 C33 H34 A35 F36 E37 K38 E39 V40 T41 E42 C43 A44 H45 G46 T47 G48 G49 T50 R51 B51 A52 F60 D61 E65 R69 Y70 K71 T72 W73 R74 R75 I79 Q82 L86 M87 R88 E89 G90

K91 Y92 T93 F94 P95 P96 H97 H98 S99 G100 R101 E102 E103 P104 R105 P106

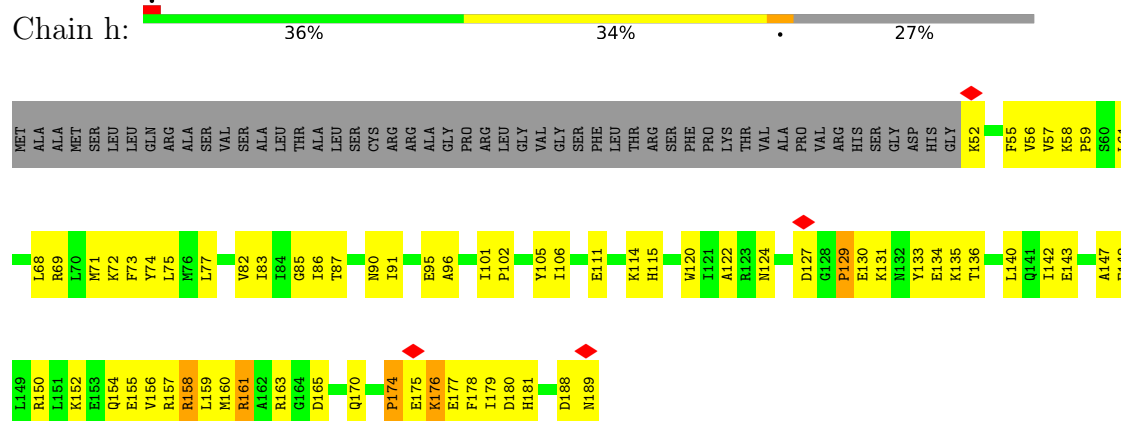
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



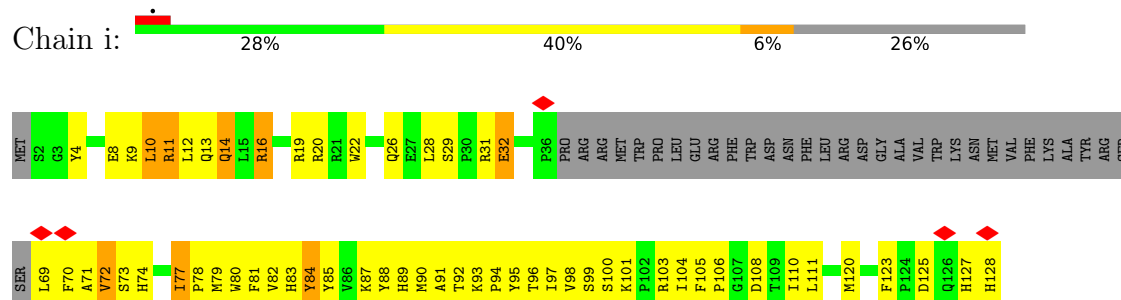
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

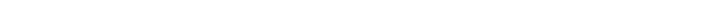


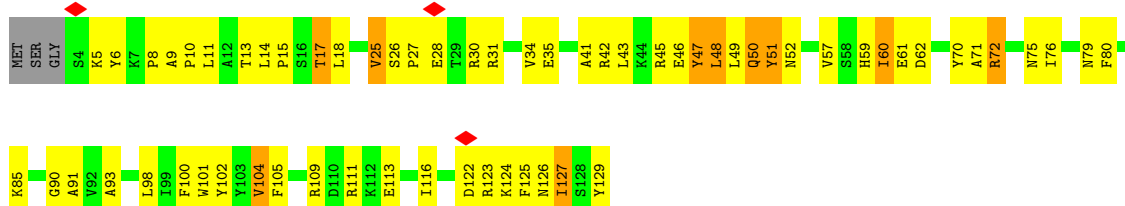
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



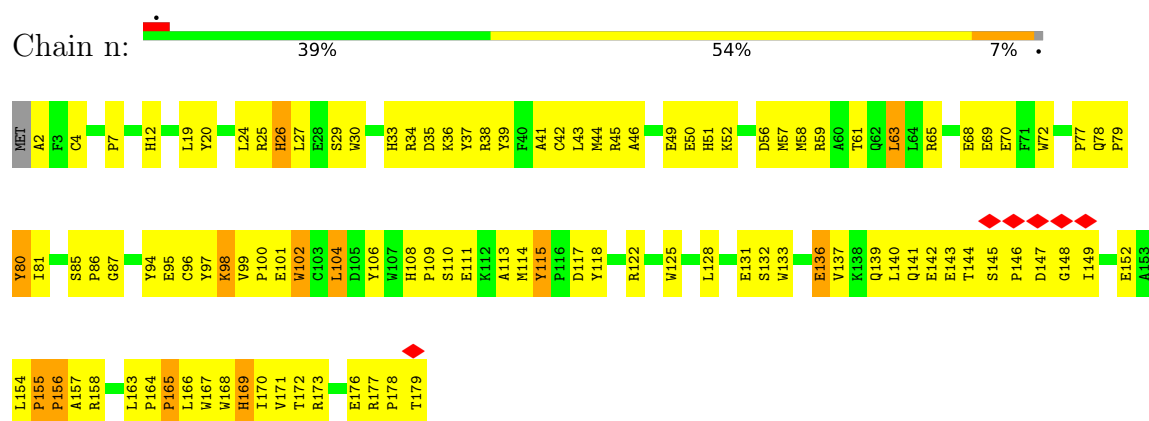
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



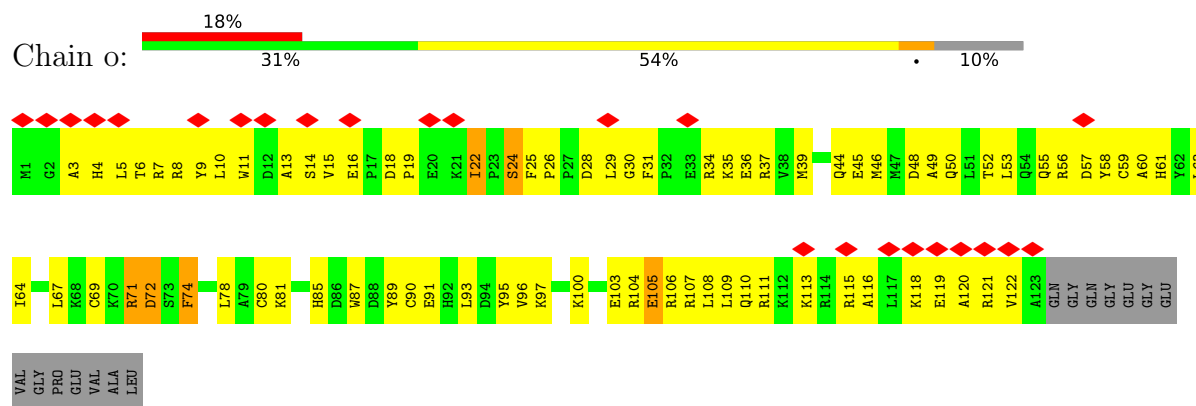
- Chain j: 



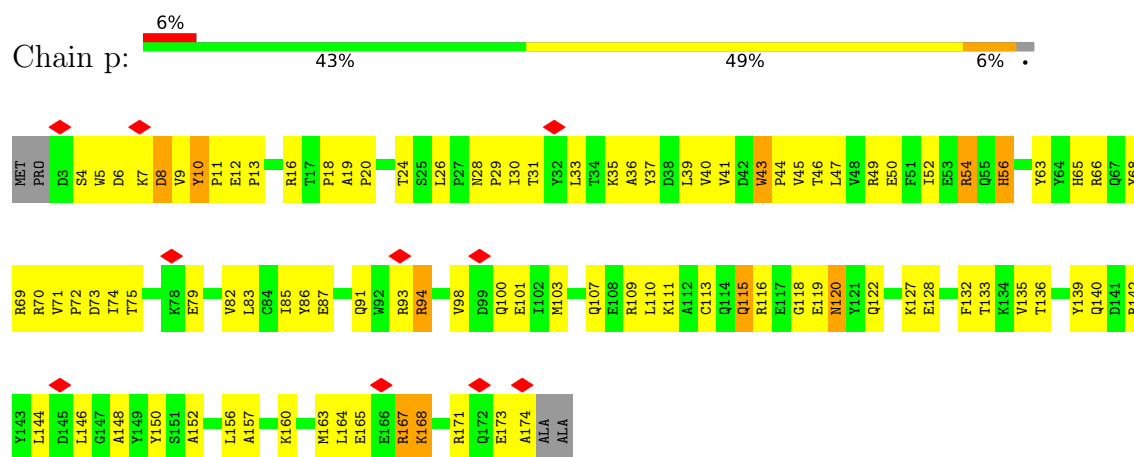
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.050	Depositor
Minimum map value	-1.895	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, EH2, ADP

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	D	0.64	0/365	1.06	3/500 (0.6%)
2	J	0.84	1/1257 (0.1%)	1.26	20/1704 (1.2%)
3	K	0.90	0/740	1.54	13/1005 (1.3%)
4	L	0.99	7/4921 (0.1%)	1.57	107/6696 (1.6%)
5	M	1.01	7/3717 (0.2%)	1.57	86/5062 (1.7%)
6	N	1.01	3/2756 (0.1%)	1.44	51/3751 (1.4%)
7	O	1.00	8/2666 (0.3%)	1.40	41/3615 (1.1%)
8	U	0.98	1/731 (0.1%)	1.30	14/988 (1.4%)
9	X	0.72	0/230	0.98	0/313
10	Y	0.86	0/1054	0.98	2/1429 (0.1%)
11	c	0.93	1/400 (0.2%)	1.49	12/544 (2.2%)
12	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
13	e	0.69	1/900 (0.1%)	1.01	5/1199 (0.4%)
14	f	0.95	1/451 (0.2%)	1.38	12/607 (2.0%)
15	g	0.89	3/886 (0.3%)	1.35	19/1207 (1.6%)
16	h	0.77	1/1197 (0.1%)	1.26	8/1621 (0.5%)
17	i	0.84	0/829	1.35	14/1127 (1.2%)
18	j	0.80	0/588	1.32	8/805 (1.0%)
19	k	0.98	2/600 (0.3%)	1.44	14/810 (1.7%)
20	l	0.98	3/1367 (0.2%)	1.22	9/1866 (0.5%)
21	m	0.92	2/1079 (0.2%)	1.24	17/1463 (1.2%)
22	n	0.94	2/1596 (0.1%)	1.32	18/2162 (0.8%)
23	o	0.82	1/1075 (0.1%)	1.14	10/1442 (0.7%)
24	p	0.71	1/1485 (0.1%)	1.05	15/2007 (0.7%)
All	All	0.93	47/31918 (0.1%)	1.37	509/43310 (1.2%)

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	247	PRO	N-CD	16.66	1.71	1.47
12	d	115	PRO	N-CD	-14.15	1.27	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.84	1.67	1.47
6	N	255	PRO	N-CD	-13.65	1.28	1.47
11	c	39	PRO	N-CD	-13.22	1.29	1.47

The worst 5 of 509 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	370	PRO	N-CA-C	14.57	128.48	110.70
6	N	255	PRO	N-CA-C	14.50	128.39	110.70
7	O	118	TYR	N-CA-C	13.84	125.88	111.07
22	n	165	PRO	N-CA-C	13.34	130.41	111.33
7	O	222	GLY	N-CA-C	13.25	129.73	112.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	350	0	320	40	0
2	J	1229	0	1250	130	0
3	K	729	0	764	96	0
4	L	4798	0	4986	608	0
5	M	3630	0	3854	544	0
6	N	2694	0	2896	336	0
7	O	2599	0	2552	306	0
8	U	718	0	705	89	0
9	X	221	0	215	34	0
10	Y	1030	0	1015	74	0
11	c	389	0	385	48	0
12	d	996	0	1001	93	0
13	e	877	0	869	92	0
14	f	439	0	433	37	0
15	g	858	0	787	75	0
16	h	1162	0	1163	134	0
17	i	802	0	802	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	j	563	0	510	72	0
19	k	582	0	584	46	0
20	l	1312	0	1204	103	0
21	m	1050	0	1061	109	0
22	n	1541	0	1470	151	0
23	o	1050	0	1045	103	0
24	p	1452	0	1413	140	0
25	K	46	0	66	9	0
25	L	167	0	233	28	0
25	M	88	0	130	8	0
25	N	51	0	82	11	0
25	Y	41	0	56	8	0
25	d	31	0	36	8	0
25	i	40	0	54	19	0
25	m	139	0	209	23	0
26	L	78	0	100	16	0
26	X	67	0	81	9	0
26	h	70	0	87	17	0
27	O	27	0	12	11	0
28	n	32	0	0	0	0
All	All	31948	0	32430	2862	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 44.

The worst 5 of 2862 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)
7:O:247:PRO:CD	7:O:247:PRO:N	1.71	1.38
7:O:168:VAL:HG21	7:O:241:TYR:CZ	1.66	1.29
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.20
4:L:141:PHE:CE2	5:M:375:LEU:HD21	1.81	1.16
4:L:466:PHE:HB2	18:j:68:TRP:HZ2	1.11	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	40/463 (9%)	38 (95%)	2 (5%)	0	100	100
2	J	157/172 (91%)	148 (94%)	9 (6%)	0	100	100
3	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
4	L	604/607 (100%)	573 (95%)	31 (5%)	0	100	100
5	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	65
7	O	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
8	U	87/156 (56%)	81 (93%)	6 (7%)	0	100	100
9	X	25/172 (14%)	21 (84%)	4 (16%)	0	100	100
10	Y	137/143 (96%)	132 (96%)	5 (4%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
13	e	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
14	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
15	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
16	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
17	i	91/128 (71%)	81 (89%)	10 (11%)	0	100	100
18	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
19	k	71/104 (68%)	68 (96%)	3 (4%)	0	100	100
20	l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	176/179 (98%)	165 (94%)	10 (6%)	1 (1%)	21	52
23	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
24	p	170/176 (97%)	153 (90%)	17 (10%)	0	100	100
All	All	3782/4813 (79%)	3590 (95%)	190 (5%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	109	ALA
22	n	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	36/395 (9%)	36 (100%)	0	100	100
2	J	129/137 (94%)	126 (98%)	3 (2%)	44	66
3	K	87/88 (99%)	87 (100%)	0	100	100
4	L	549/550 (100%)	547 (100%)	2 (0%)	84	84
5	M	415/415 (100%)	414 (100%)	1 (0%)	87	88
6	N	307/308 (100%)	305 (99%)	2 (1%)	76	80
7	O	283/309 (92%)	283 (100%)	0	100	100
8	U	82/135 (61%)	82 (100%)	0	100	100
9	X	23/154 (15%)	23 (100%)	0	100	100
10	Y	104/107 (97%)	104 (100%)	0	100	100
11	c	41/67 (61%)	41 (100%)	0	100	100
12	d	107/107 (100%)	107 (100%)	0	100	100
13	e	93/94 (99%)	92 (99%)	1 (1%)	65	76
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	93/129 (72%)	93 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	90/120 (75%)	89 (99%)	1 (1%)	65	76
18	j	61/87 (70%)	61 (100%)	0	100	100
19	k	55/78 (70%)	55 (100%)	0	100	100
20	l	141/161 (88%)	141 (100%)	0	100	100
21	m	112/114 (98%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	n	163/164 (99%)	162 (99%)	1 (1%)	78	81
23	o	112/121 (93%)	112 (100%)	0	100	100
24	p	156/158 (99%)	156 (100%)	0	100	100
All	All	3409/4213 (81%)	3398 (100%)	11 (0%)	84	86

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	159	ILE
13	e	91	LYS
22	n	98	LYS
17	i	72	VAL
4	L	69	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
14	f	13	HIS
20	l	115	ASN
16	h	154	GLN
18	j	83	HIS
22	n	12	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 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$
25	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.15	3 (7%)
25	3PE	L	703	-	39,39,50	1.02	2 (5%)	42,44,55	1.16	3 (7%)
25	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.14	4 (7%)
25	3PE	m	202	-	50,50,50	0.91	2 (4%)	53,55,55	1.15	4 (7%)
26	CDL	L	704	-	77,77,99	1.01	4 (5%)	83,89,111	1.14	6 (7%)
28	EHZ	n	201	-	29,31,37	1.78	7 (24%)	37,41,47	1.65	7 (18%)
25	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.06	2 (4%)
25	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.12	4 (8%)
25	3PE	m	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.14	3 (6%)
25	3PE	m	201	-	46,46,50	0.97	2 (4%)	49,51,55	1.12	3 (6%)
25	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.22	4 (10%)
25	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.16	5 (9%)
27	ADP	O	401	-	28,29,29	1.36	4 (14%)	43,45,45	1.87	10 (23%)
25	3PE	N	401	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	4 (7%)
26	CDL	h	201	-	69,69,99	1.09	4 (5%)	75,81,111	1.23	7 (9%)
26	CDL	X	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
25	3PE	Y	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.19	5 (11%)
25	3PE	L	705	-	37,37,50	1.04	2 (5%)	40,42,55	1.14	3 (7%)
25	3PE	d	201	-	30,30,50	1.15	2 (6%)	33,35,55	1.33	5 (15%)

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
25	3PE	L	701	-	-	5/43/43/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	L	703	-	-	6/43/43/54	-
25	3PE	L	702	-	-	13/52/52/54	-
25	3PE	m	202	-	-	9/54/54/54	-
26	CDL	L	704	-	-	27/88/88/110	-
28	EHZ	n	201	-	-	13/39/39/45	-
25	3PE	i	201	-	-	15/43/43/54	-
25	3PE	K	101	-	-	16/49/49/54	-
25	3PE	m	203	-	-	7/44/44/54	-
25	3PE	m	201	-	-	10/50/50/54	-
25	3PE	M	501	-	-	13/40/40/54	-
25	3PE	M	502	-	-	12/54/54/54	-
27	ADP	O	401	-	-	2/16/32/32	0/3/3/3
25	3PE	N	401	-	-	10/54/54/54	-
26	CDL	h	201	-	-	24/80/80/110	-
26	CDL	X	201	-	-	22/77/77/110	-
25	3PE	Y	201	-	-	10/44/44/54	-
25	3PE	L	705	-	-	14/41/41/54	-
25	3PE	d	201	-	-	7/34/34/54	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	201	EHZ	C12-N1	4.92	1.45	1.33
28	n	201	EHZ	C15-N2	4.87	1.45	1.33
27	O	401	ADP	C5-C4	4.35	1.46	1.39
26	X	201	CDL	OB8-CB7	4.28	1.45	1.33
25	K	101	3PE	O31-C31	4.25	1.45	1.33

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	401	ADP	C5-C4-N3	-5.69	118.88	126.72
28	n	201	EHZ	C8-C9-S1	4.96	119.83	113.56
25	m	201	3PE	O21-C21-C22	4.68	121.62	111.48
25	M	501	3PE	O21-C21-C22	4.64	121.52	111.48
27	O	401	ADP	N3-C4-N9	4.59	134.97	127.17

There are no chirality outliers.

5 of 235 torsion outliers are listed below:

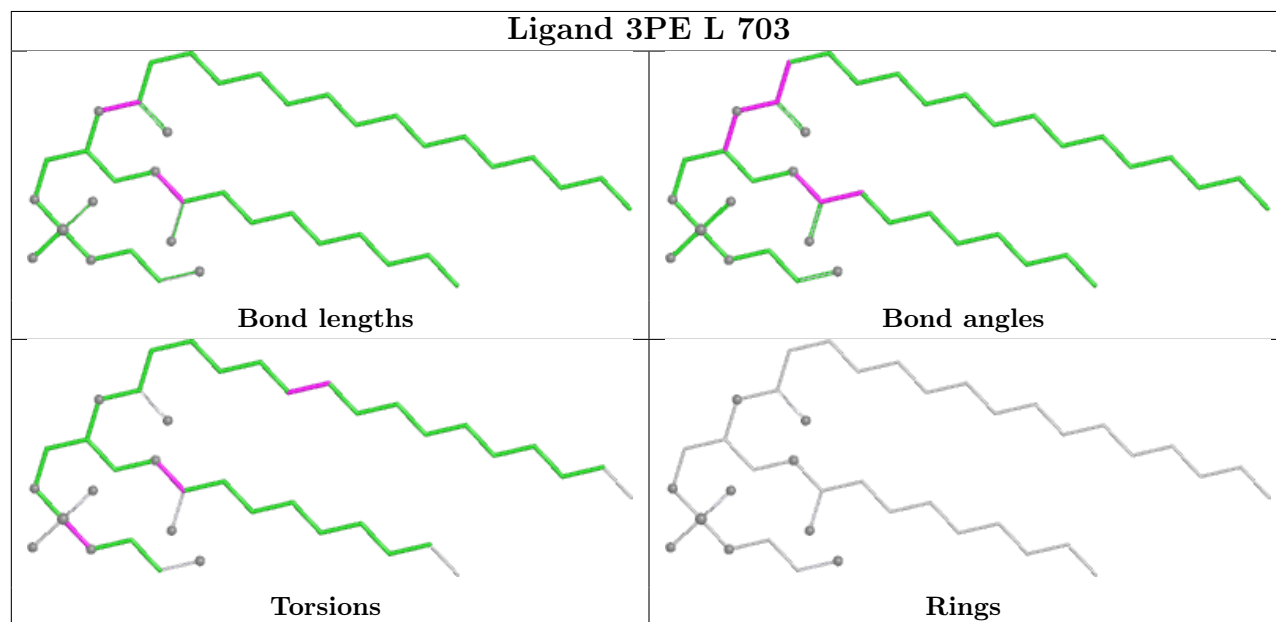
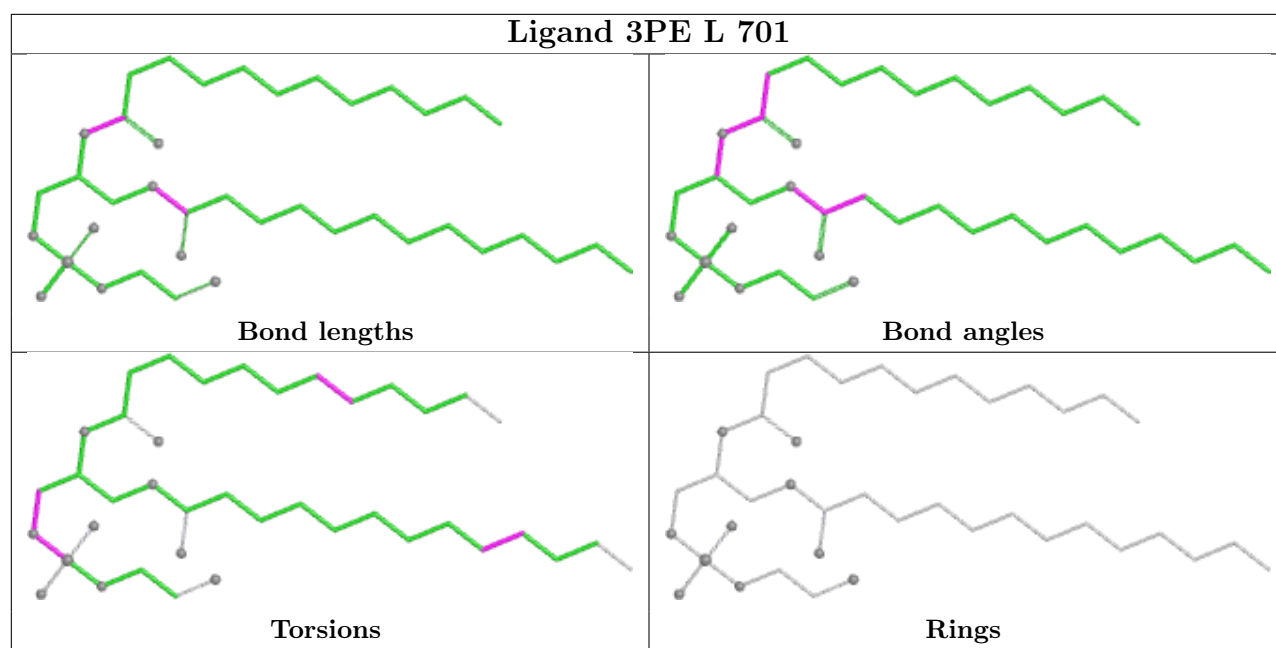
Mol	Chain	Res	Type	Atoms
25	K	101	3PE	C11-O13-P-O12
25	L	701	3PE	C1-O11-P-O12
25	L	701	3PE	C1-O11-P-O13
25	L	701	3PE	C2-C1-O11-P
25	L	702	3PE	C1-O11-P-O12

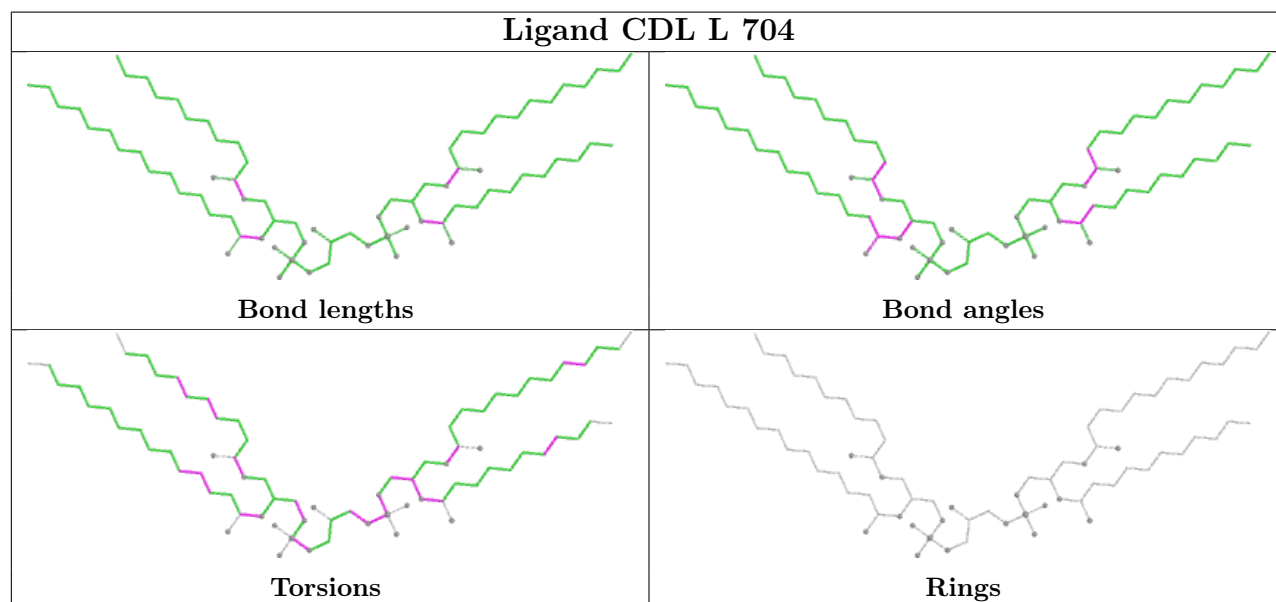
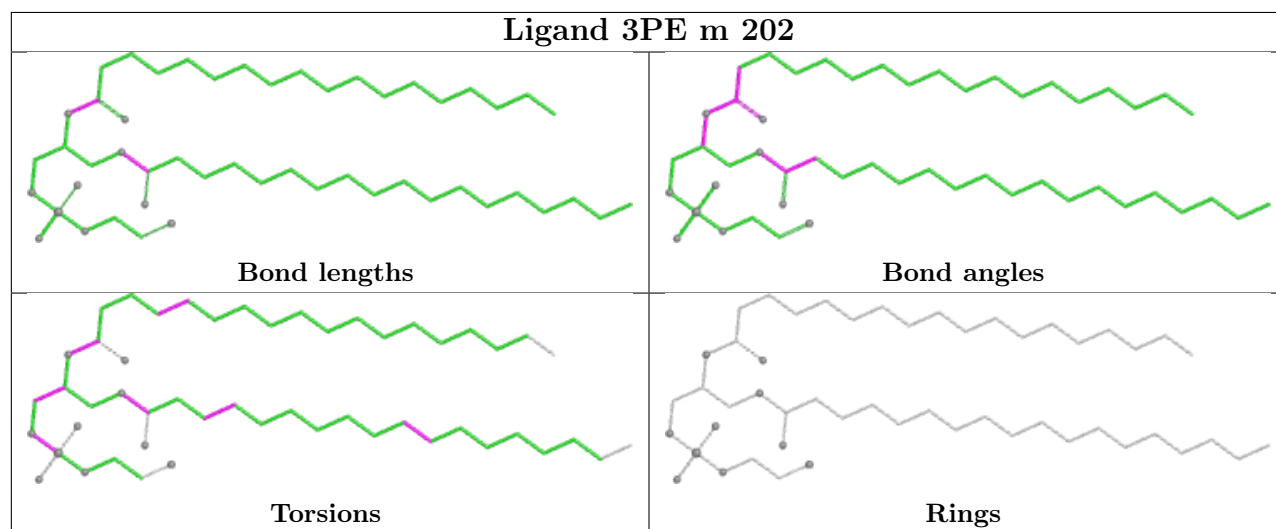
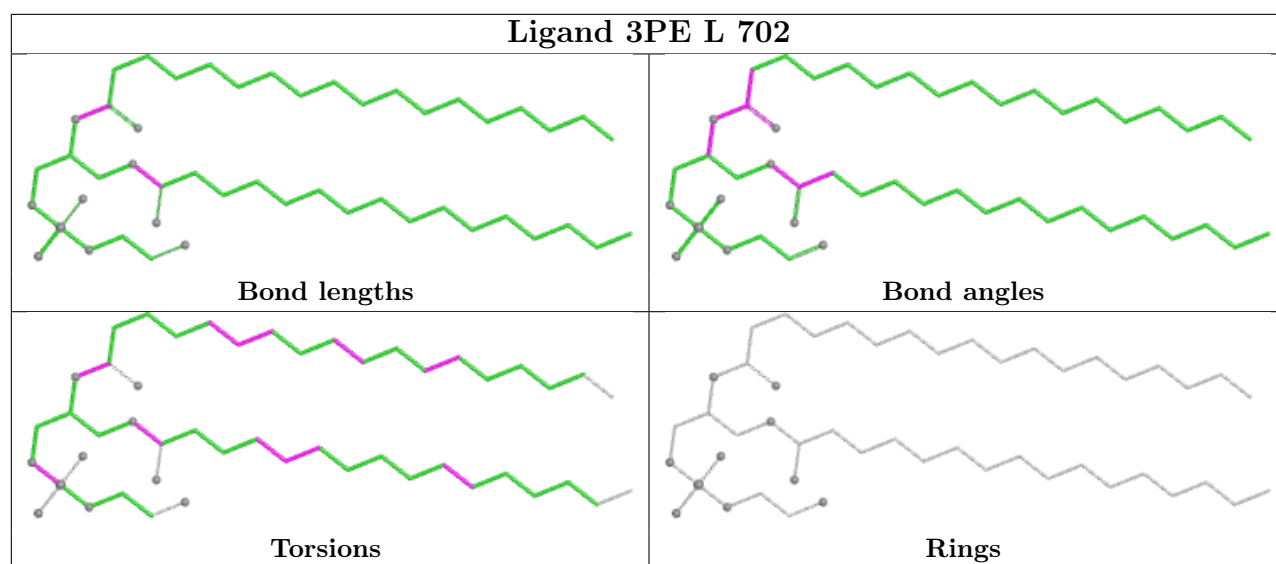
There are no ring outliers.

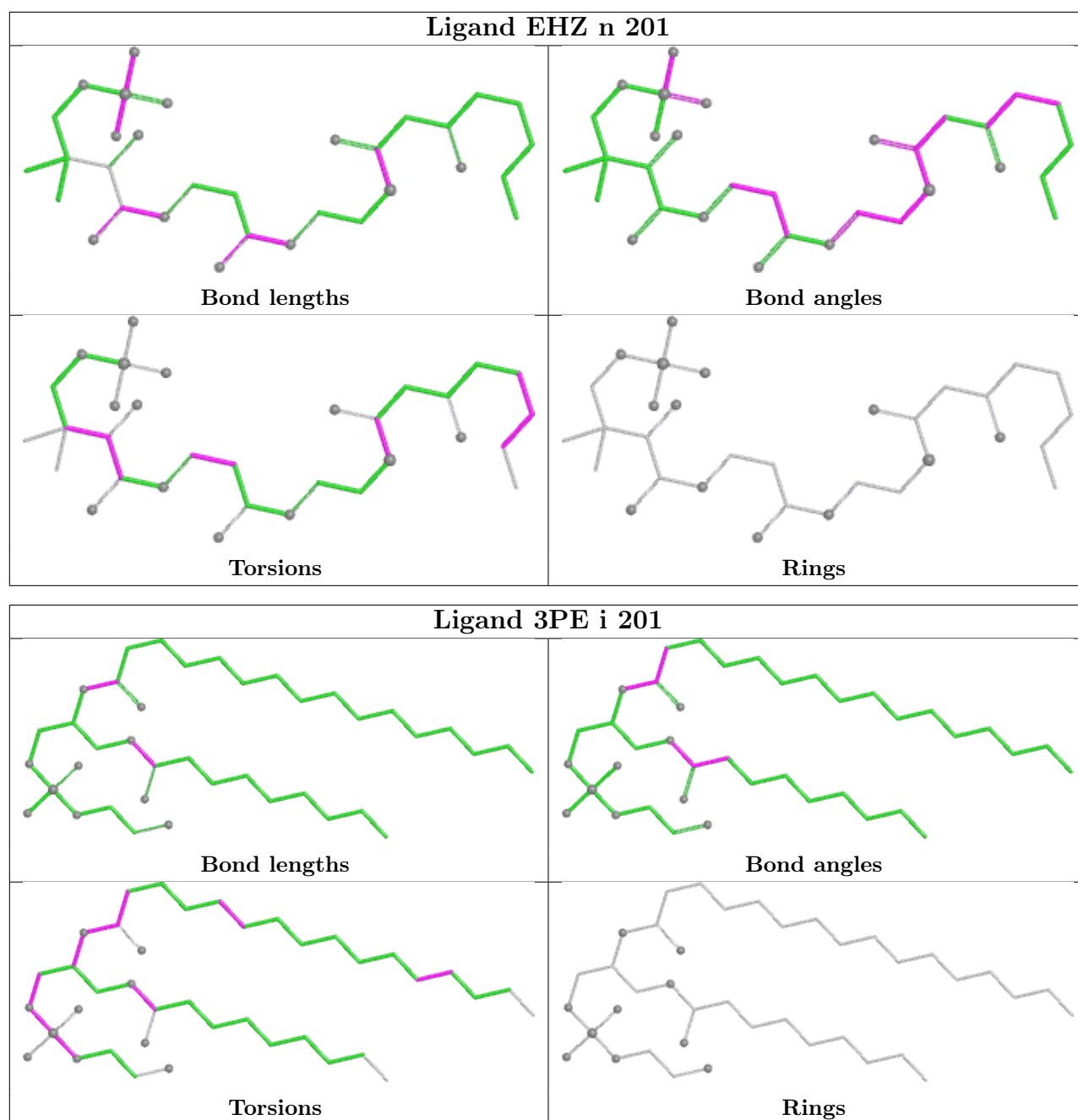
18 monomers are involved in 160 short contacts:

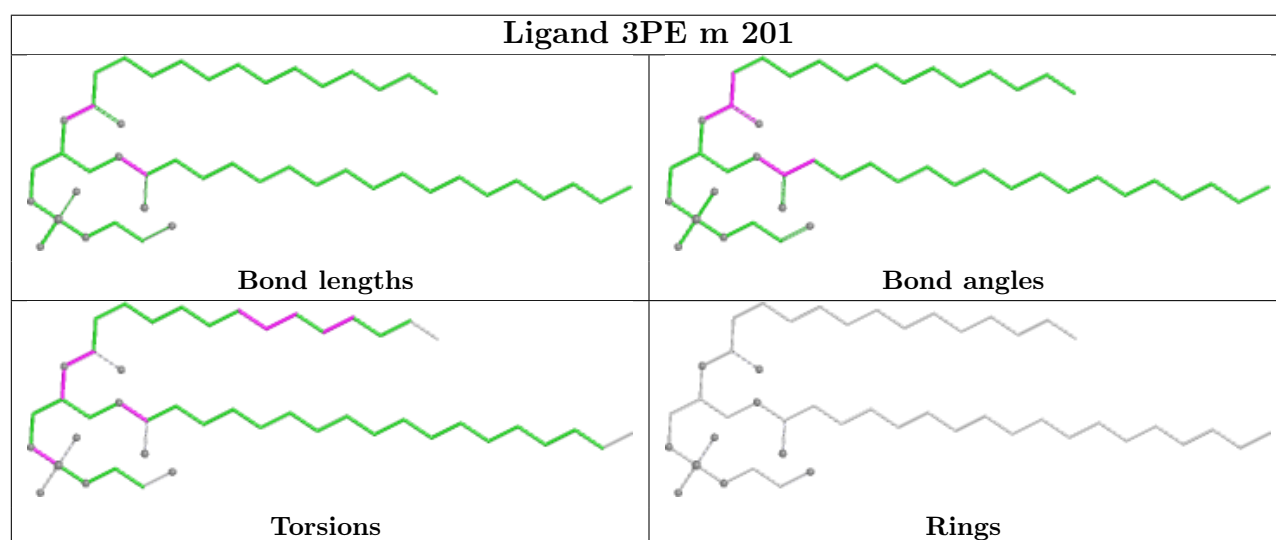
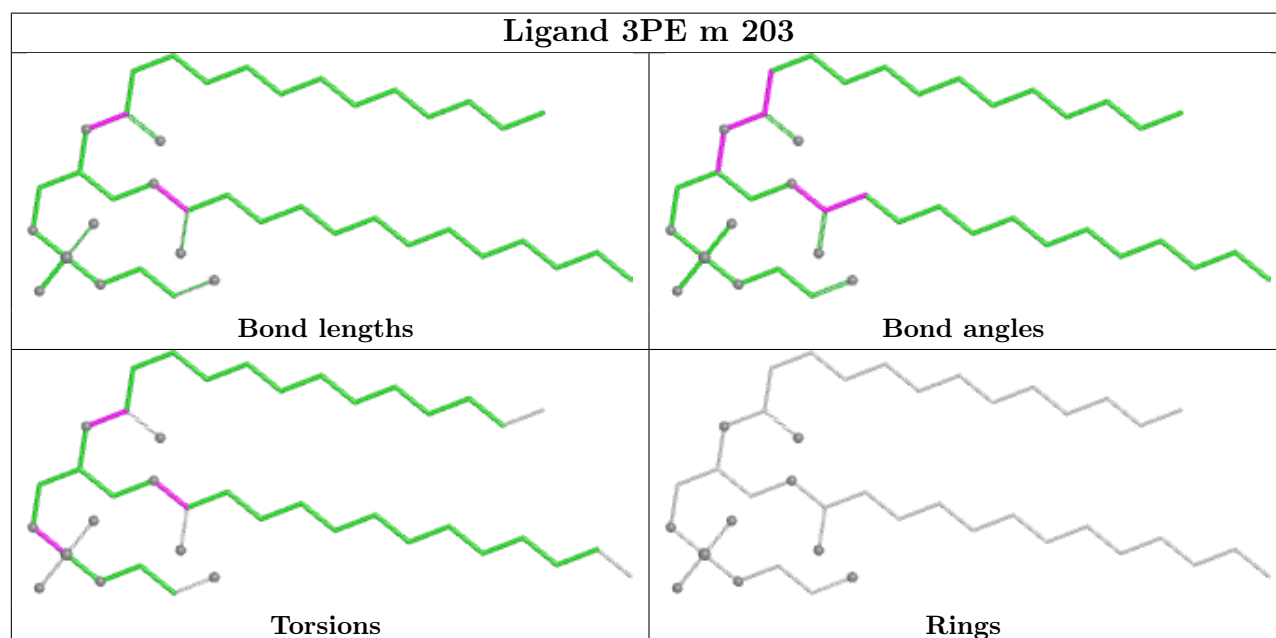
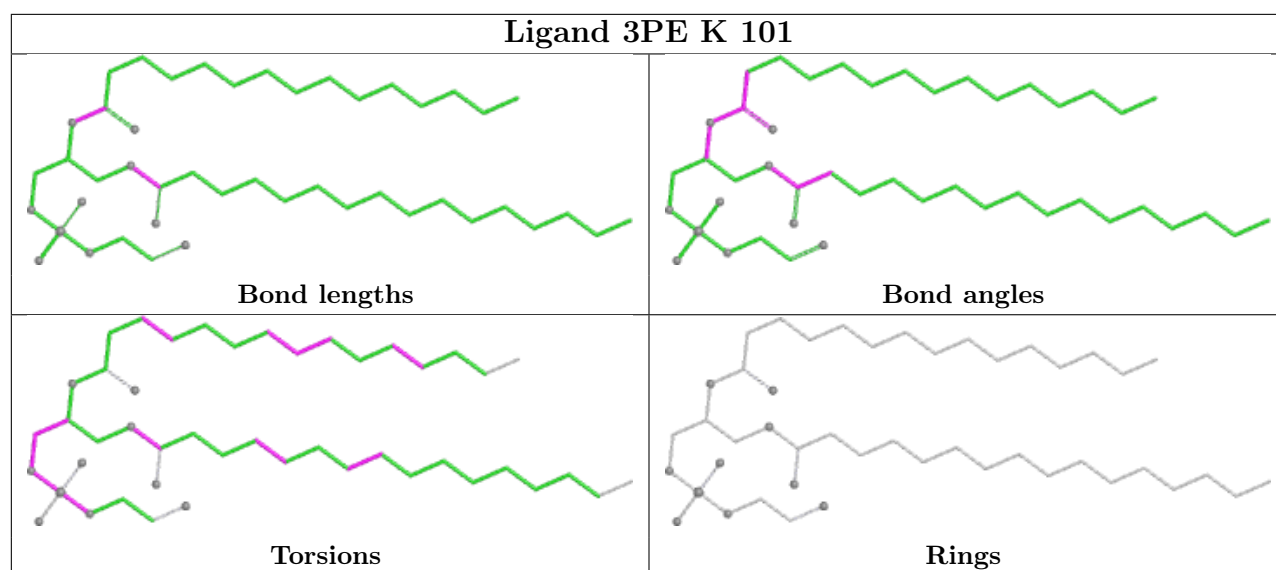
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	701	3PE	8	0
25	L	703	3PE	6	0
25	L	702	3PE	9	0
25	m	202	3PE	10	0
26	L	704	CDL	16	0
25	i	201	3PE	19	0
25	K	101	3PE	9	0
25	m	203	3PE	4	0
25	m	201	3PE	12	0
25	M	501	3PE	3	0
25	M	502	3PE	5	0
27	O	401	ADP	11	0
25	N	401	3PE	11	0
26	h	201	CDL	17	0
26	X	201	CDL	9	0
25	Y	201	3PE	8	0
25	L	705	3PE	5	0
25	d	201	3PE	8	0

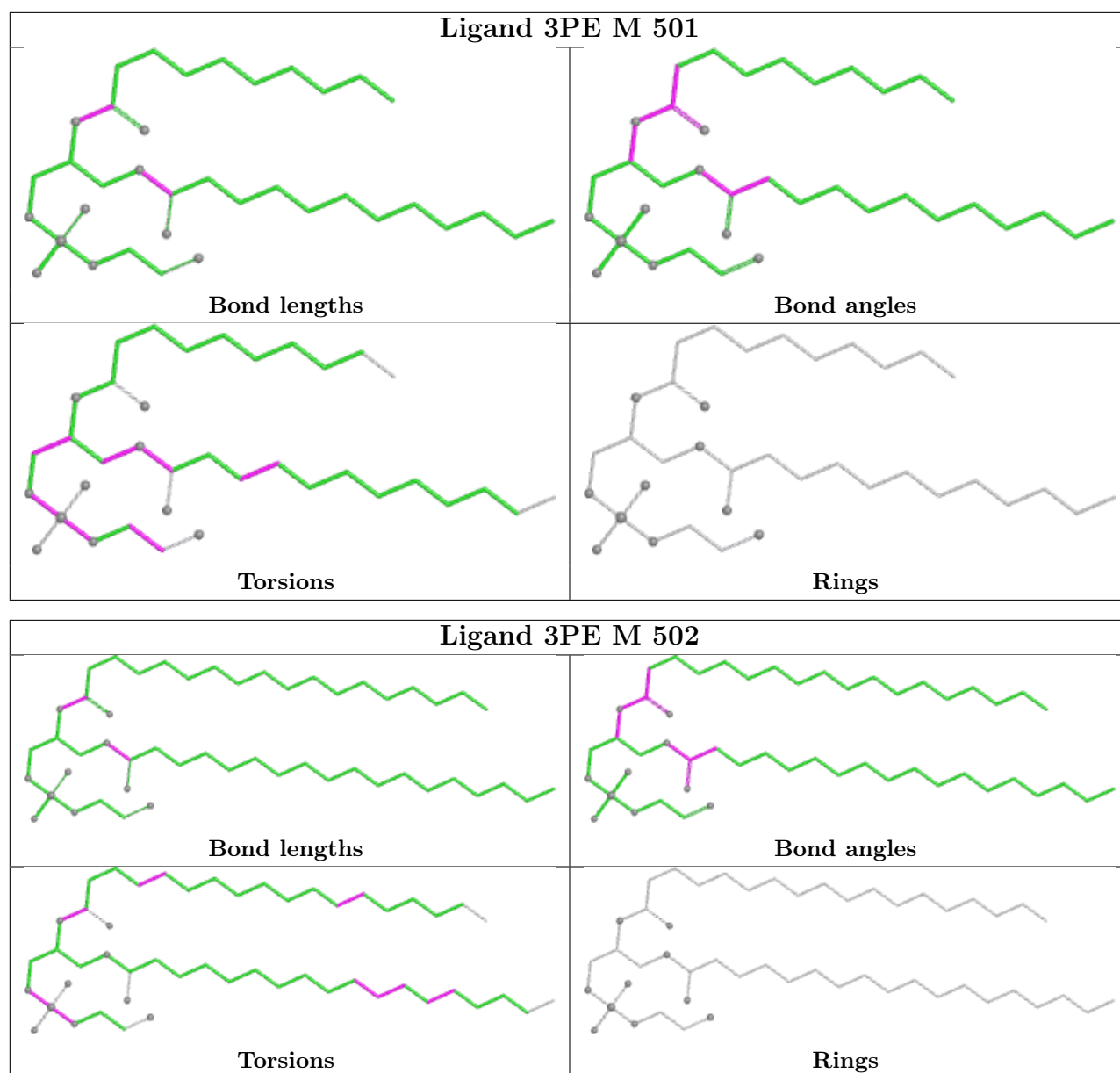
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

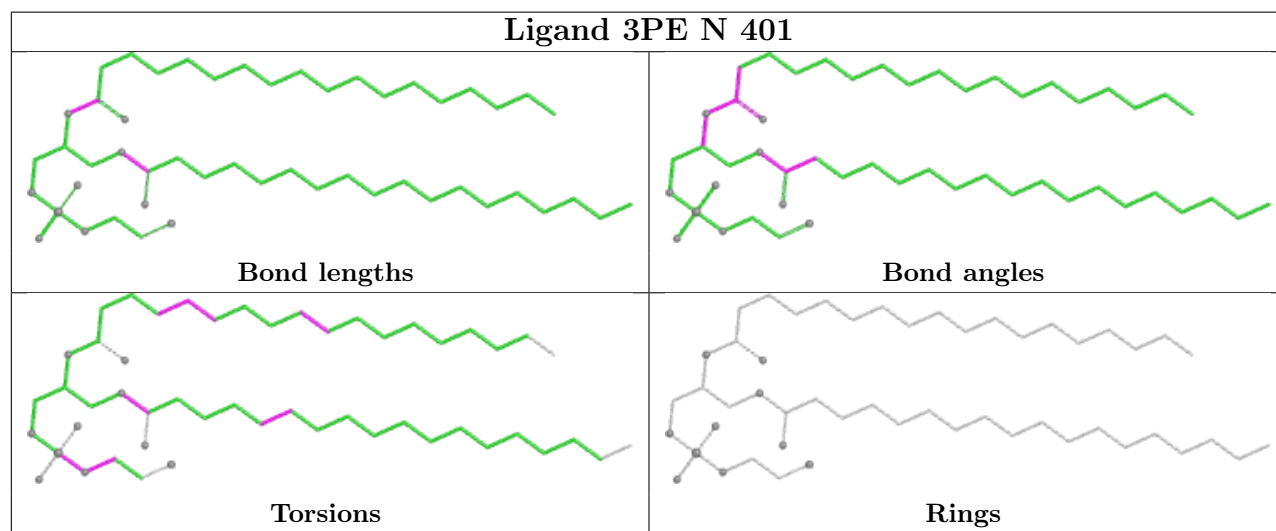
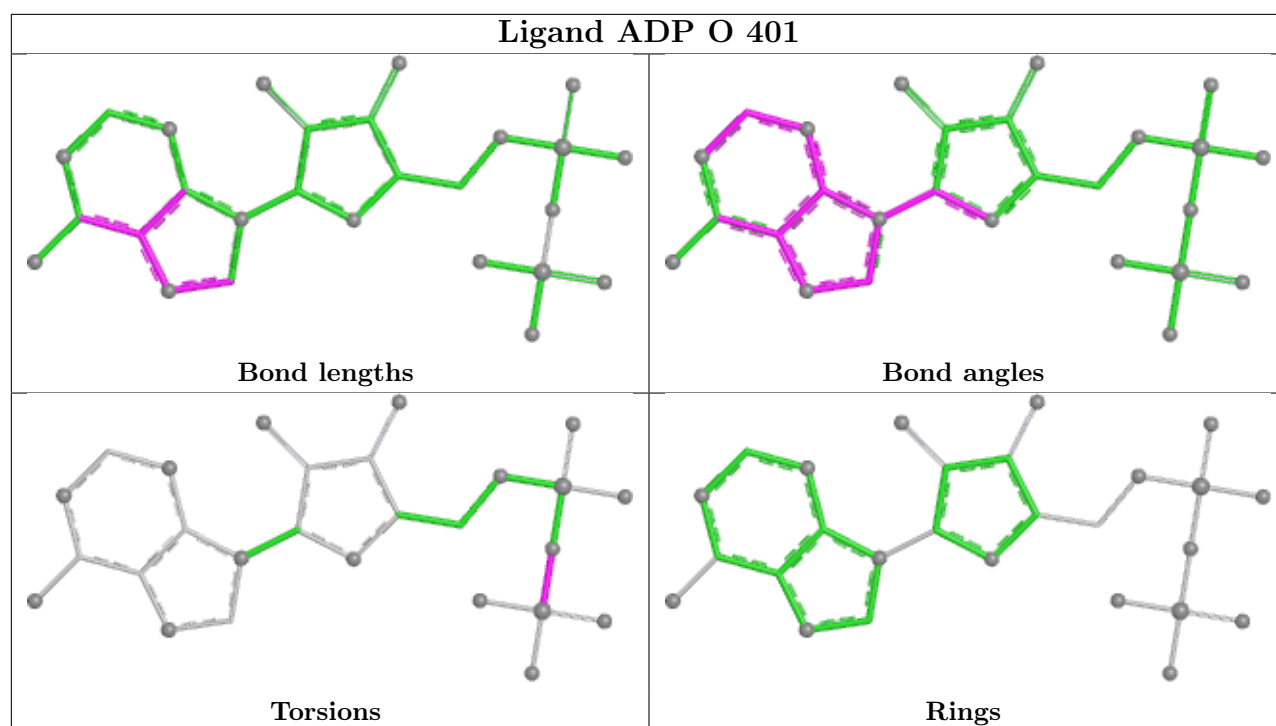


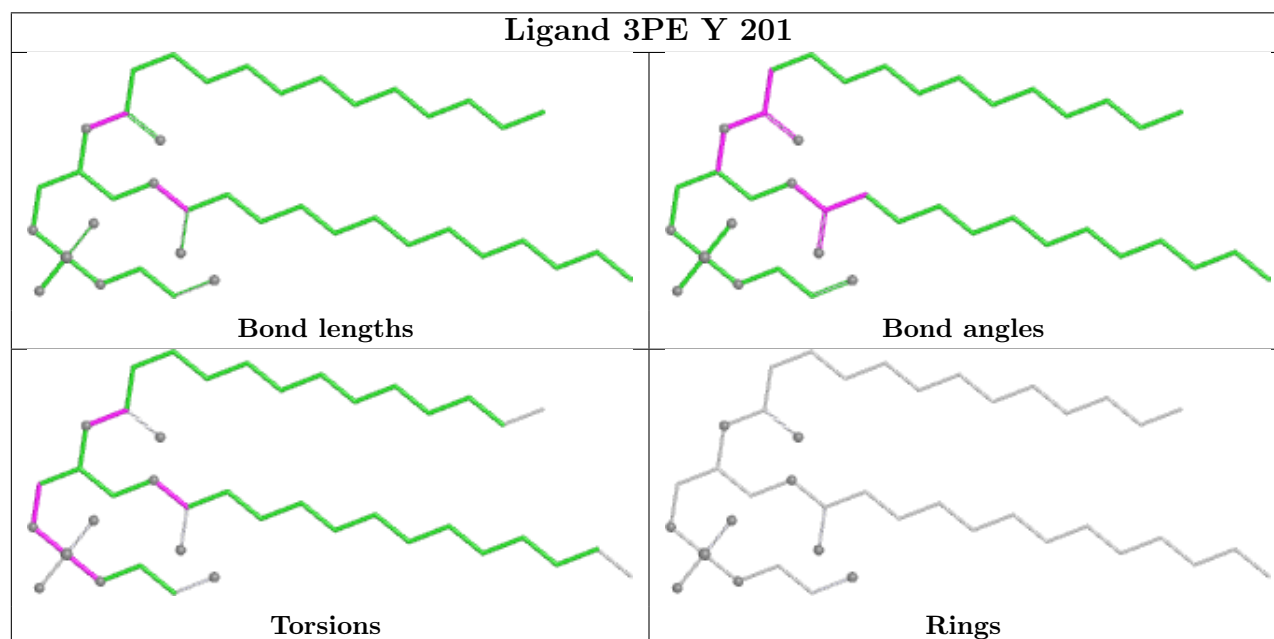
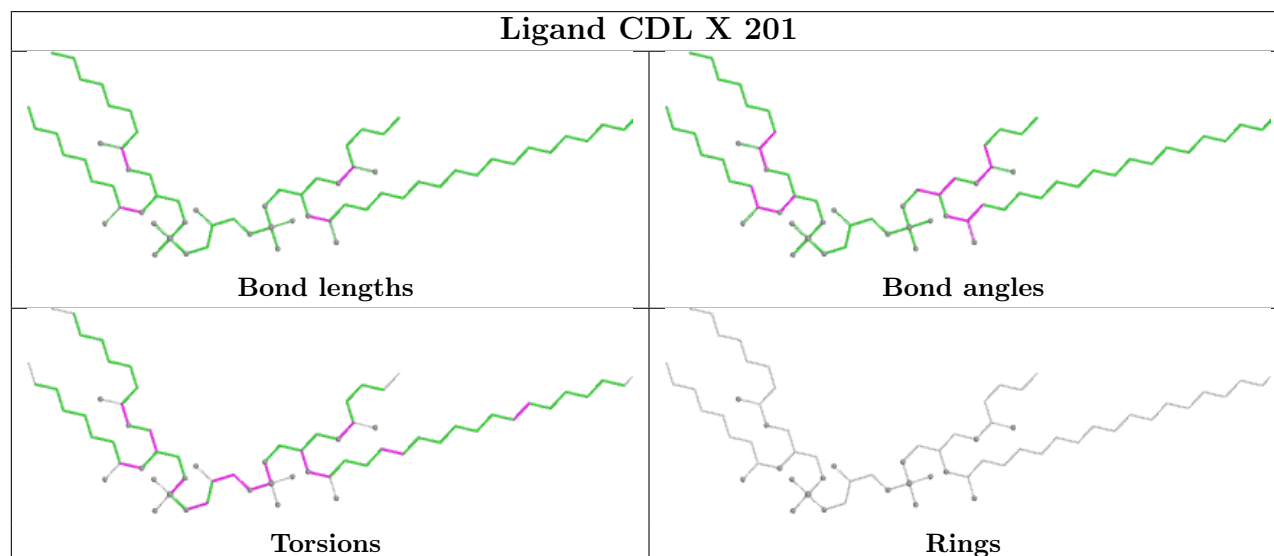
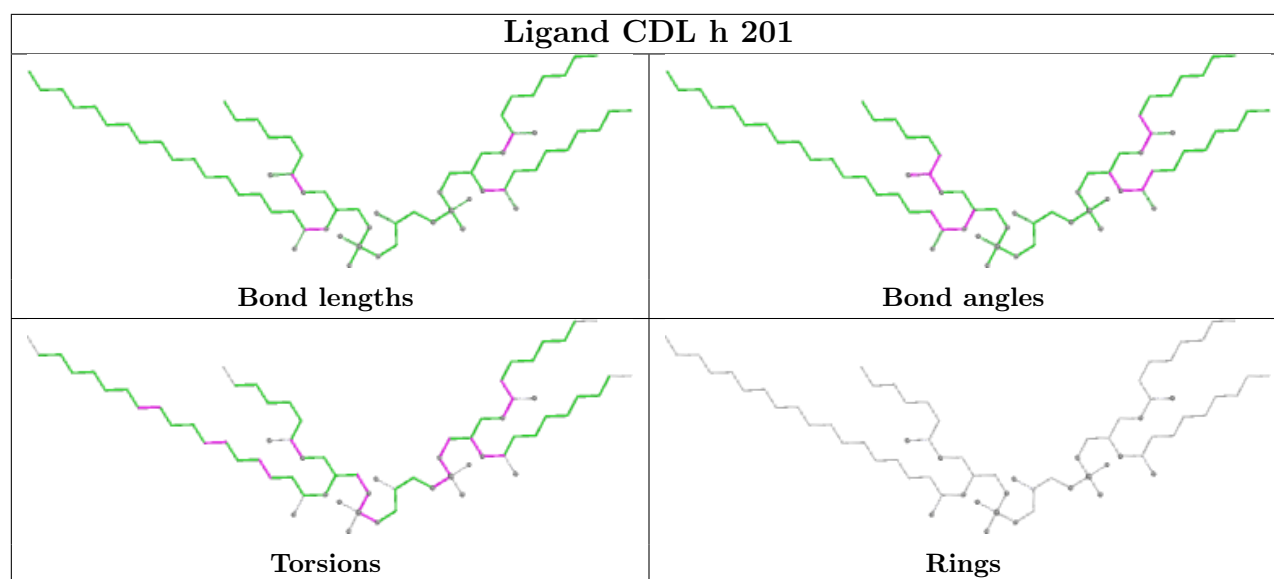


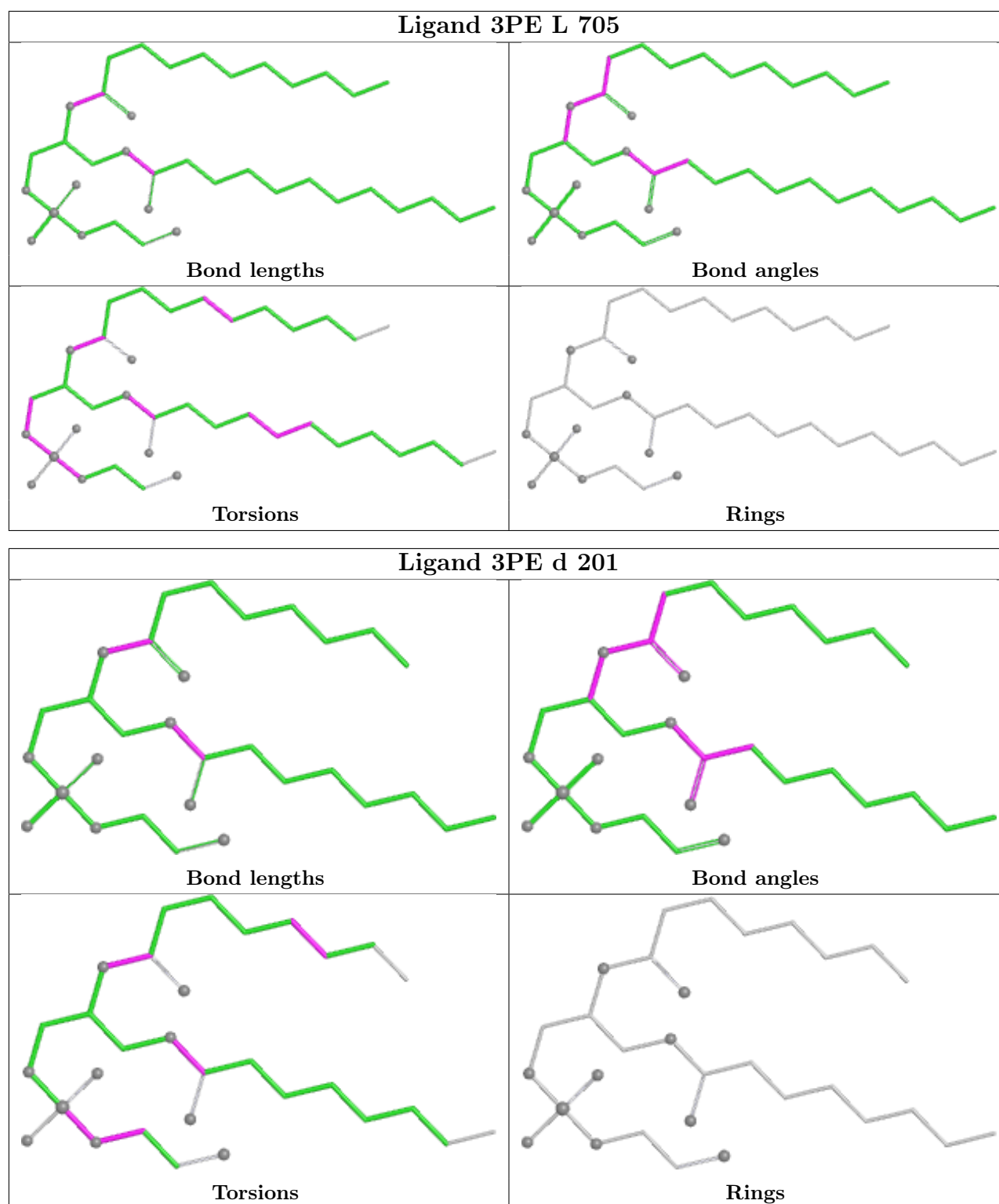












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

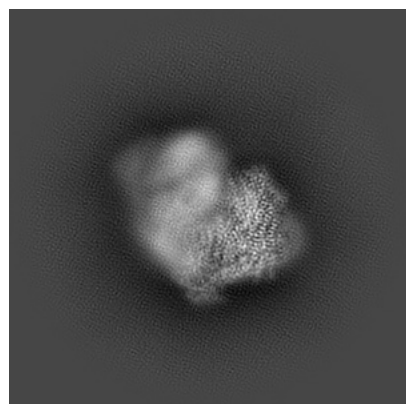
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35342. These allow visual inspection of the internal detail of the map and identification of artifacts.

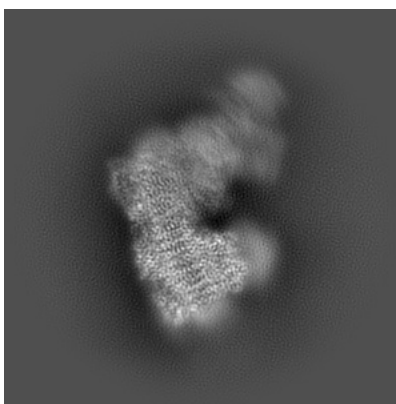
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

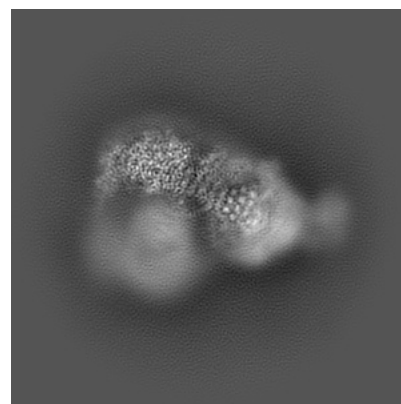
6.1.1 Primary map



X

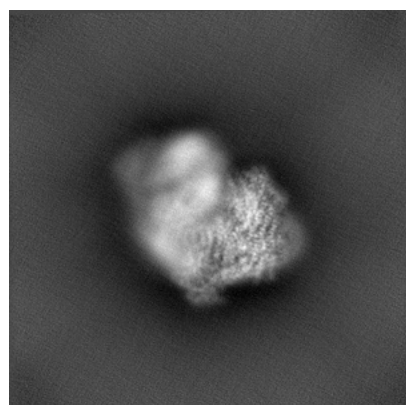


Y

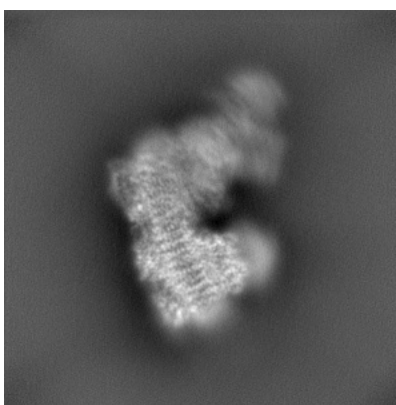


Z

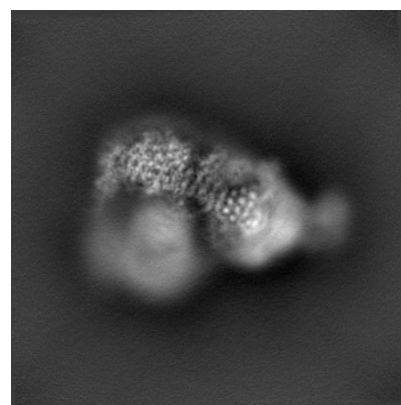
6.1.2 Raw map



X



Y

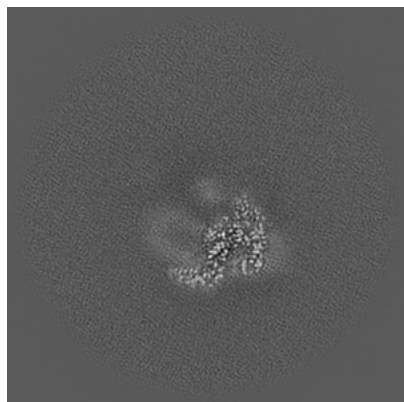


Z

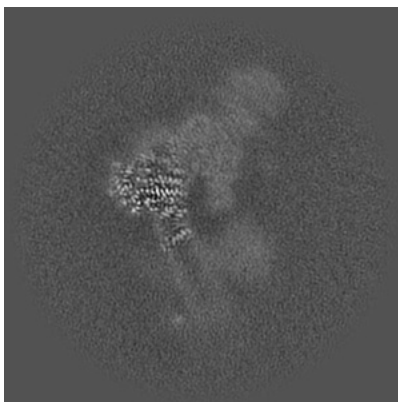
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

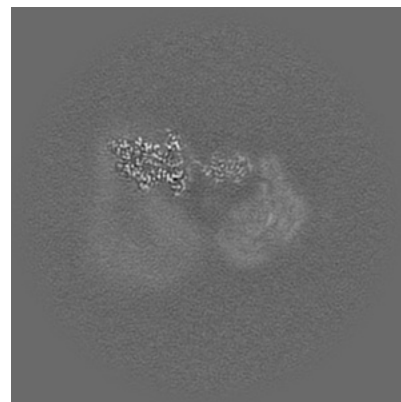
6.2.1 Primary map



X Index: 192

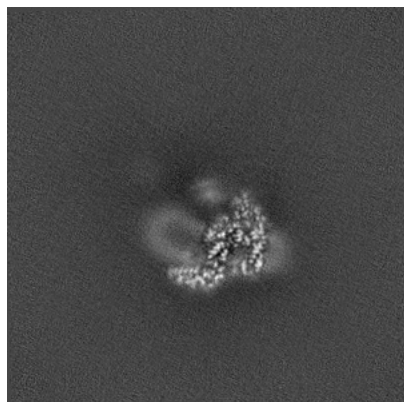


Y Index: 192

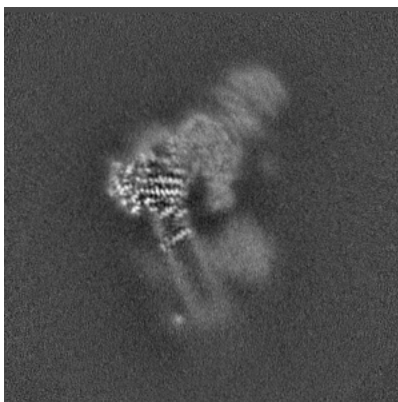


Z Index: 192

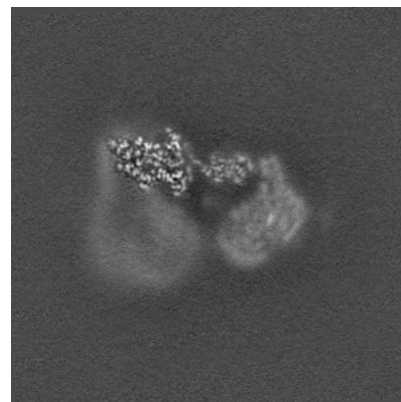
6.2.2 Raw map



X Index: 192



Y Index: 192

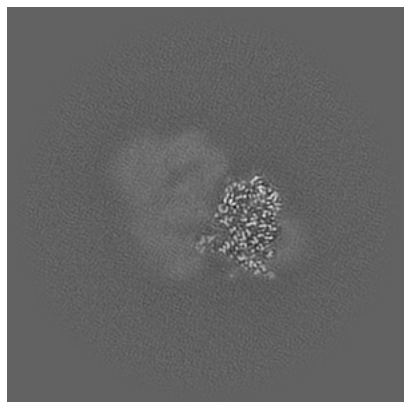


Z Index: 192

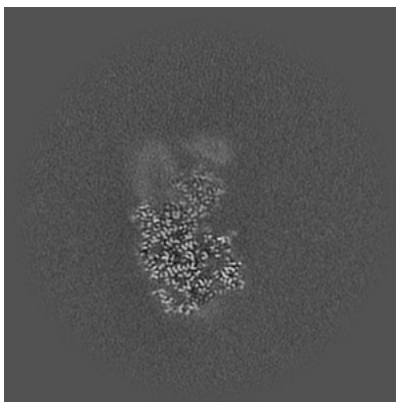
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

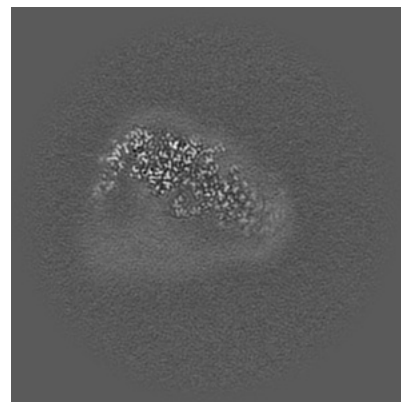
6.3.1 Primary map



X Index: 158

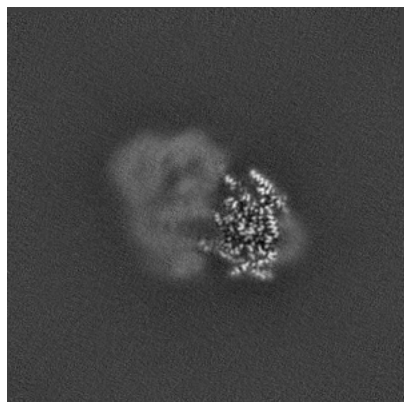


Y Index: 226

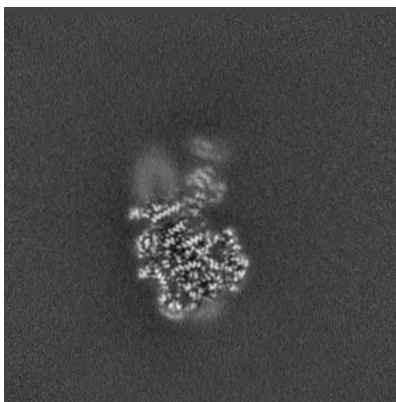


Z Index: 162

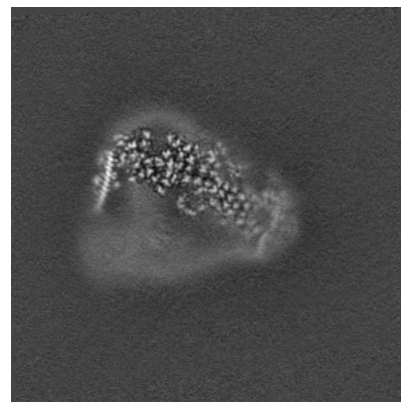
6.3.2 Raw map



X Index: 153



Y Index: 237

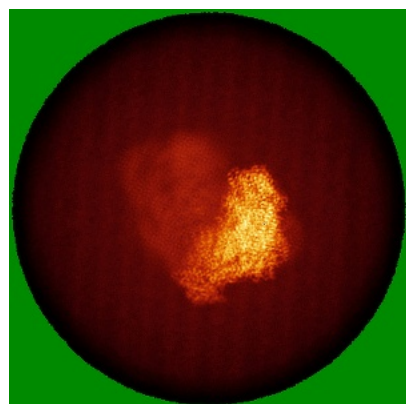


Z Index: 167

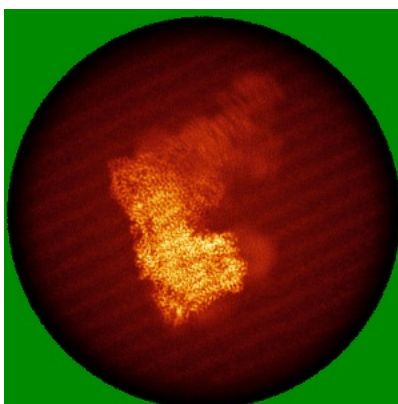
The images above show the largest variance slices of the map in three orthogonal directions.

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

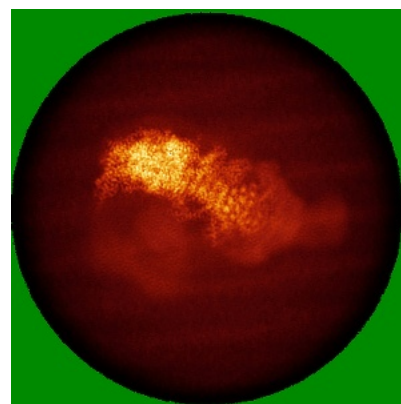
6.4.1 Primary map



X

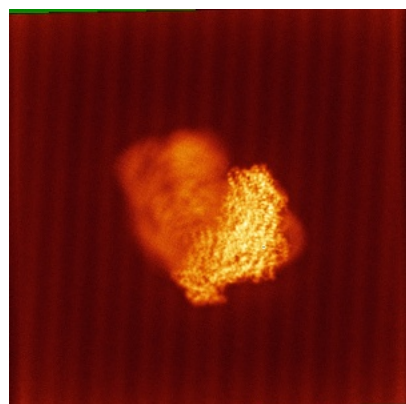


Y

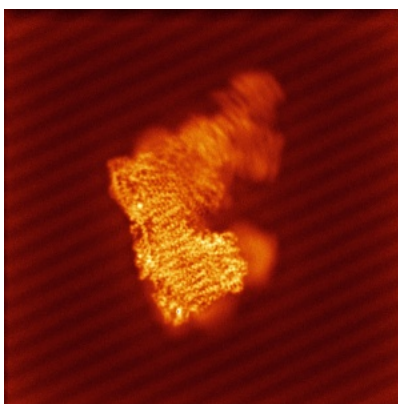


Z

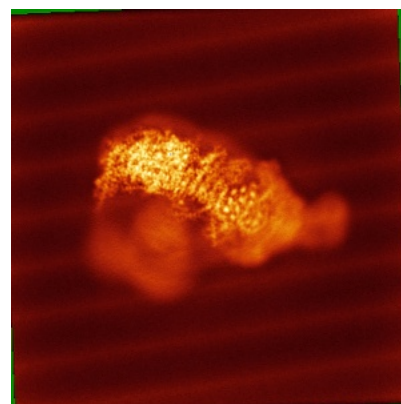
6.4.2 Raw map



X



Y



Z

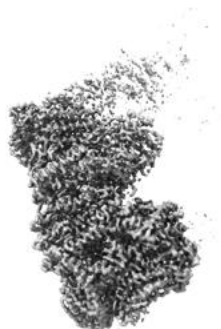
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

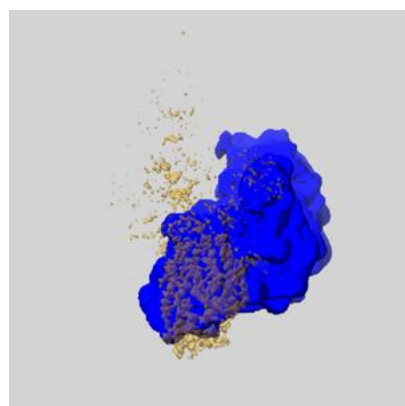
6.6 Mask visualisation [i](#)

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

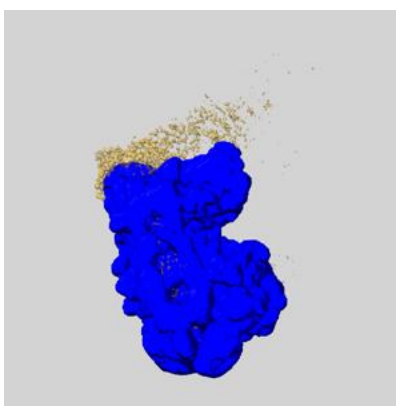
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

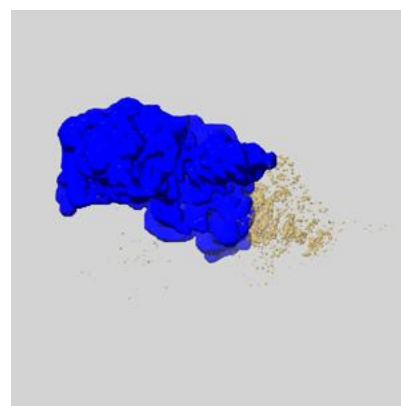
6.6.1 emd_35342_msk_1.map [i](#)



X



Y

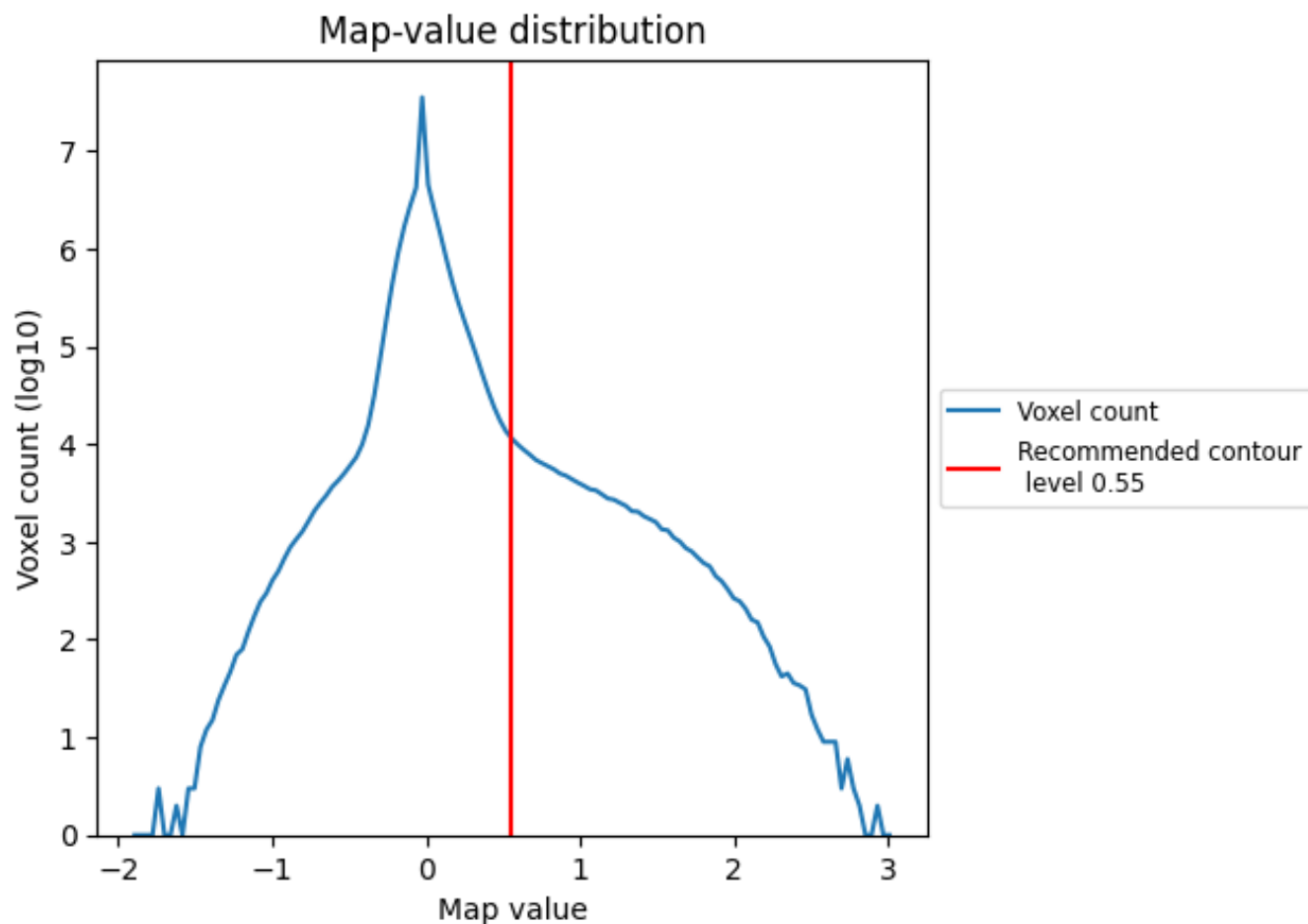


Z

7 Map analysis [i](#)

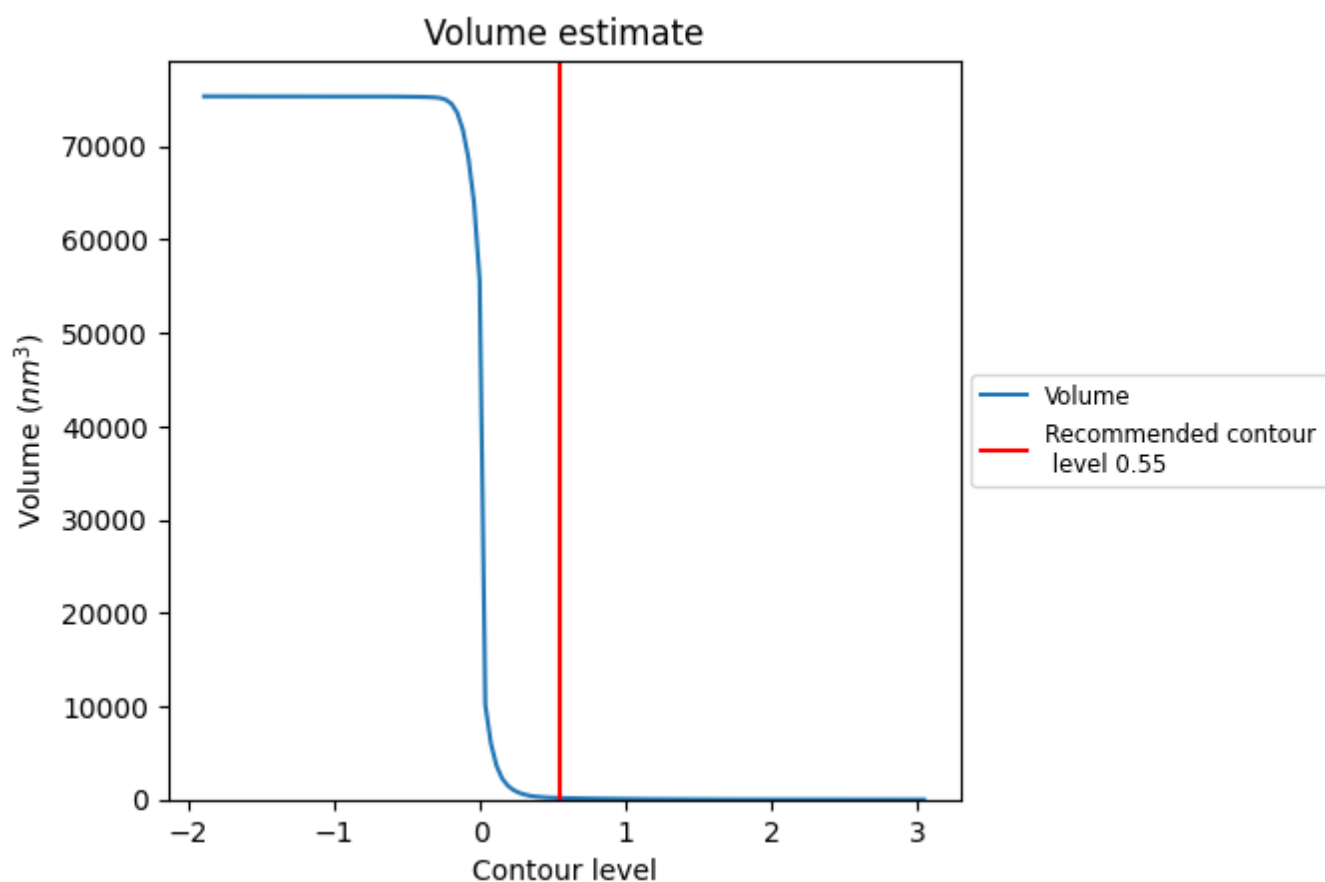
This section contains the results of statistical analysis of the map.

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.

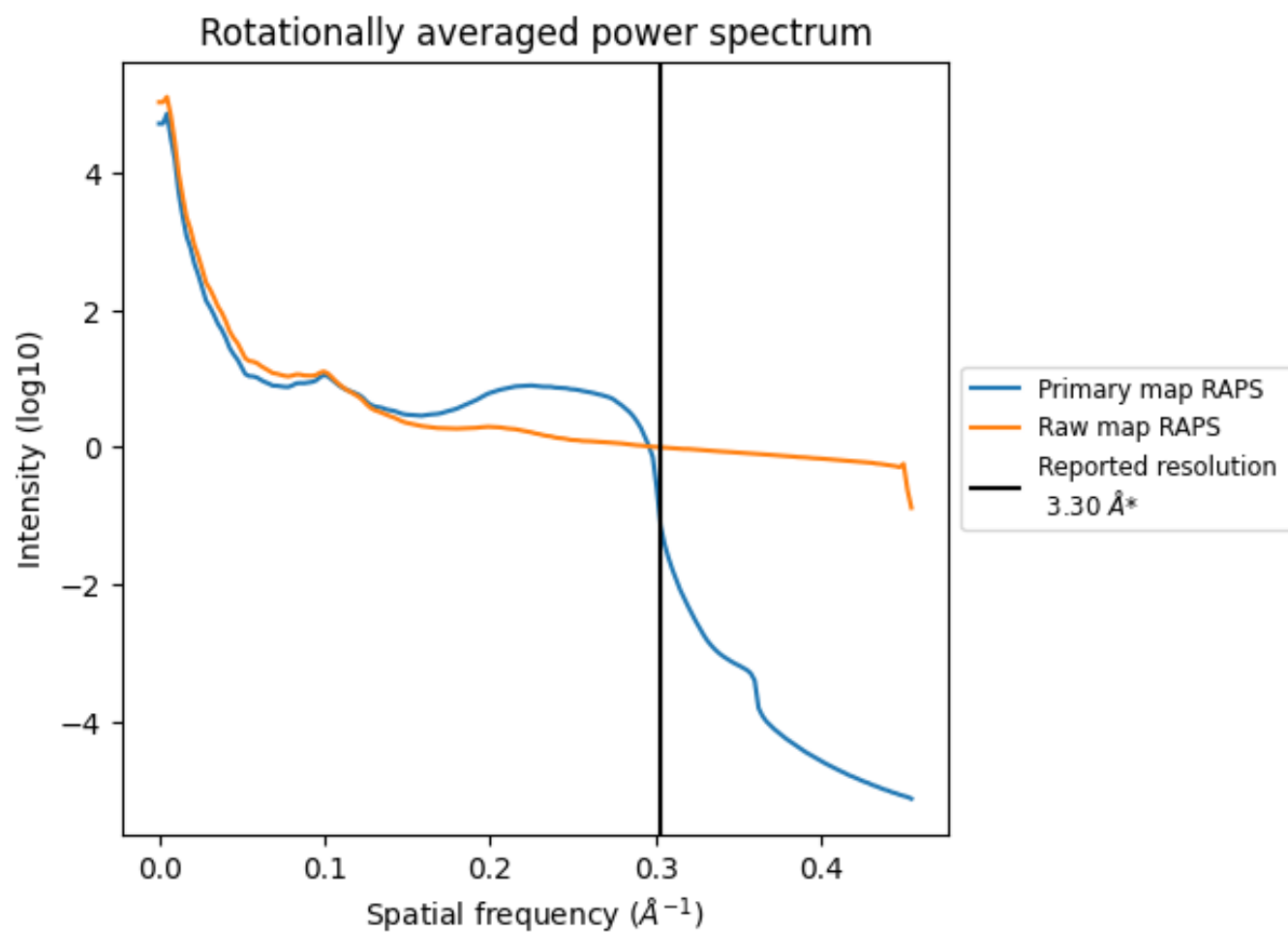
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 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 ⓘ

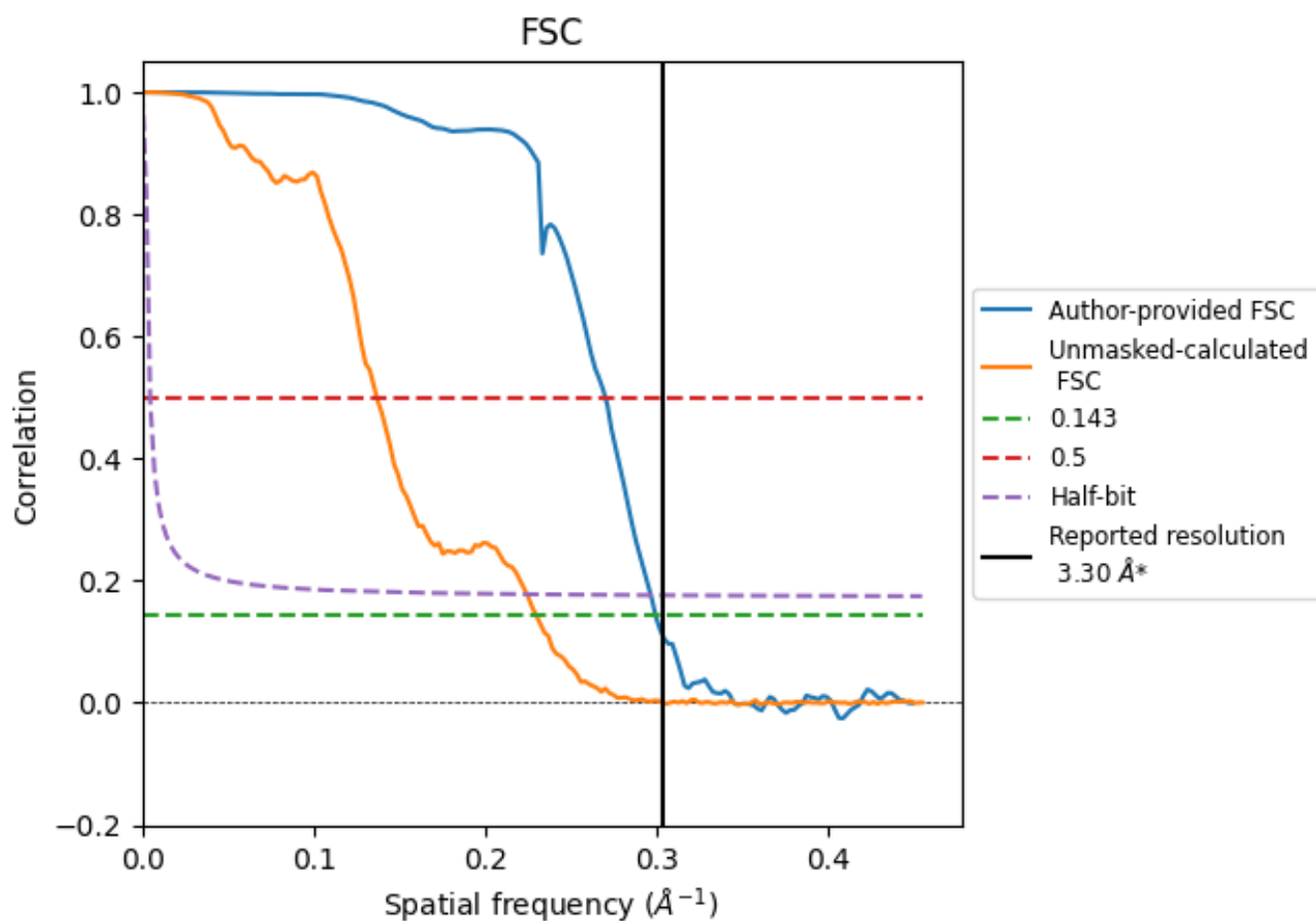


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

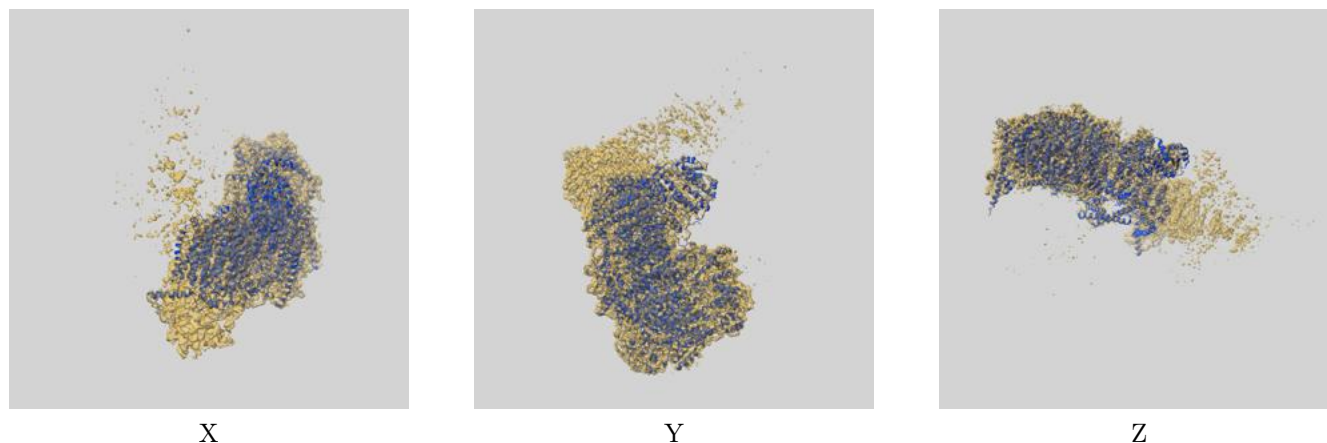
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.71	3.37
Unmasked-calculated*	4.35	7.31	4.46

*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 4.35 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

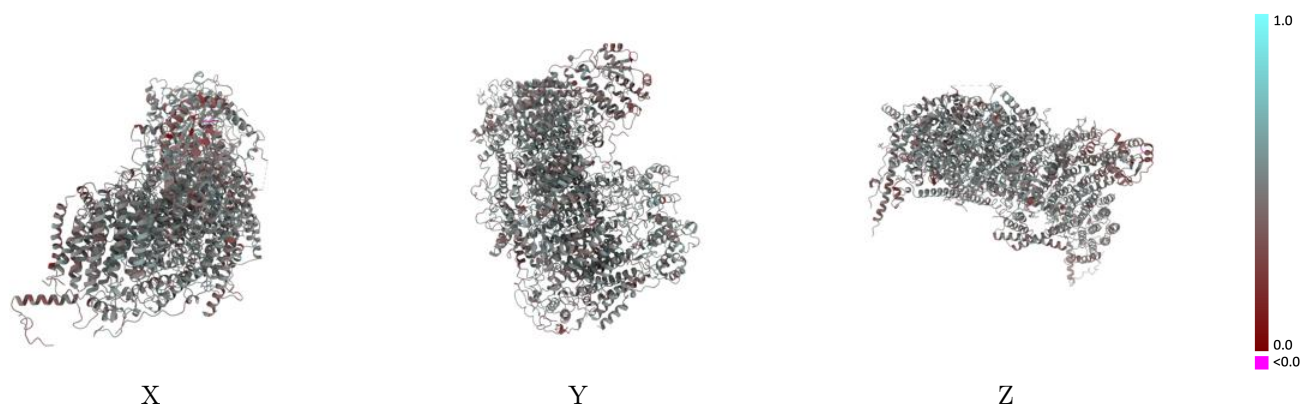
This section contains information regarding the fit between EMDB map EMD-35342 and PDB model 8IBF. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



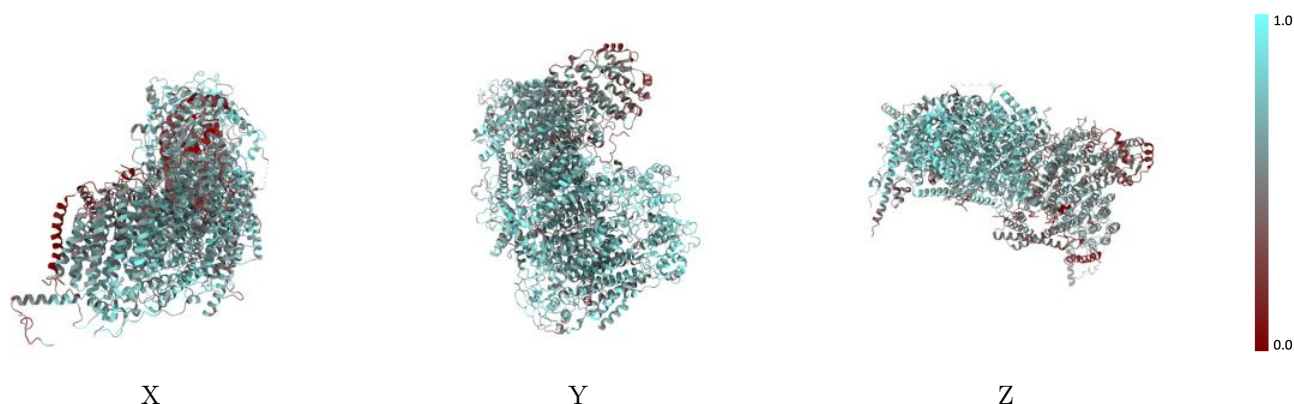
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



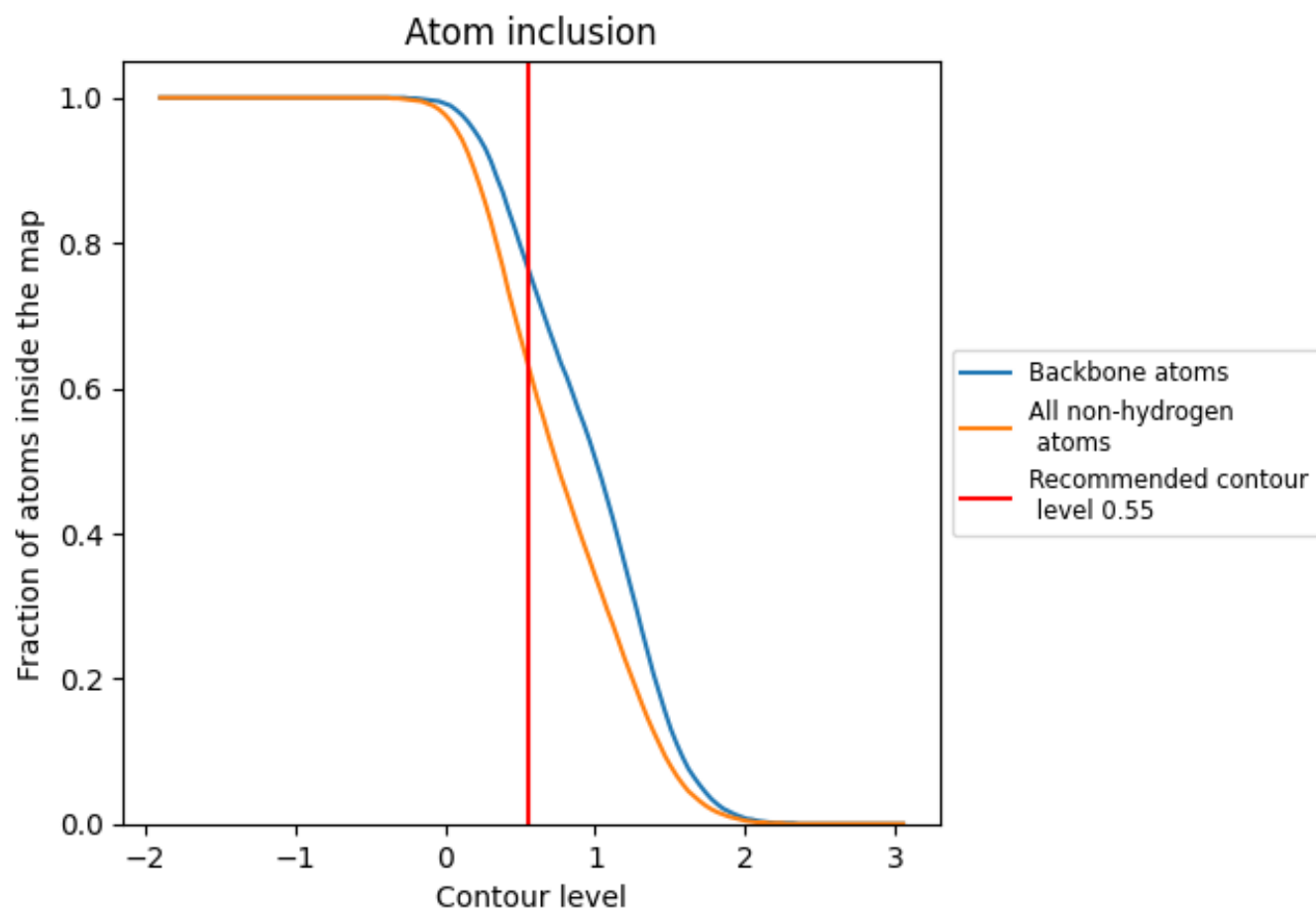
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6350	 0.4710
D	 0.3180	 0.4700
J	 0.4500	 0.4350
K	 0.5620	 0.4800
L	 0.6700	 0.4800
M	 0.6990	 0.4960
N	 0.6570	 0.4930
O	 0.4340	 0.4140
U	 0.7270	 0.4810
X	 0.6470	 0.4890
Y	 0.4580	 0.4380
c	 0.5160	 0.4070
d	 0.6720	 0.4970
e	 0.5930	 0.4310
f	 0.6290	 0.4650
g	 0.6610	 0.4610
h	 0.6960	 0.4730
i	 0.7010	 0.4960
j	 0.6930	 0.4550
k	 0.7190	 0.4850
l	 0.7340	 0.4930
m	 0.6250	 0.4810
n	 0.7600	 0.5010
o	 0.6480	 0.4350
p	 0.6780	 0.4590

