



wwPDB EM Validation Summary Report ⓘ

Nov 24, 2024 – 02:25 AM JST

PDB ID : 8IC4
EMDB ID : EMD-35354
Title : Respiratory complex Membrane domain of CI, focus-refined of type I, PERK
-/- mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.20 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:

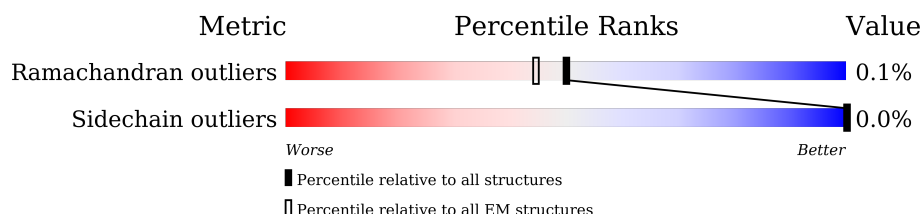
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	 9% 91%
2	J	172	 28% 90% 10%
3	K	98	 7% 96%
4	L	607	 97%
5	M	459	 97%
6	N	345	 98%
7	O	355	 15% 88% 10%
8	U	156	 54% 44%
9	X	172	 16% 84%

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Mol	Chain	Length	Quality of chain
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	

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 31638 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
			355	231	59	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- 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	318	Total	C	N	O	S	0	0
			2588	1662	426	490	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	87	Total	C	N	O	S	0	0
			700	450	103	142	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	103	Total	C	N	O	S	0	0
			859	544	157	150	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	99	Total	C	N	O	S	0	0
			835	541	134	156	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	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	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	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

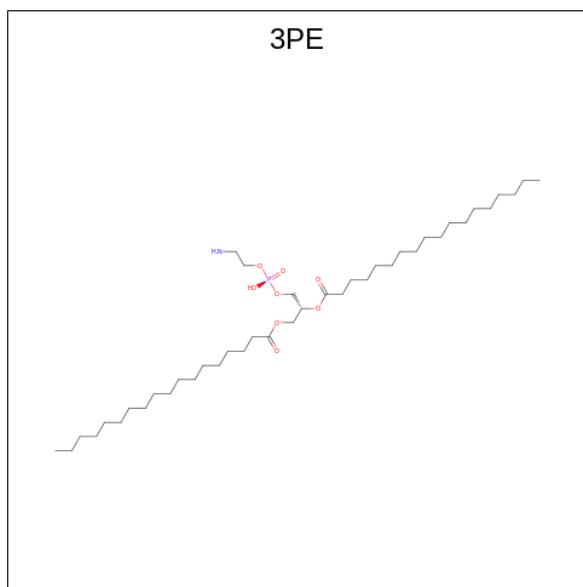
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

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

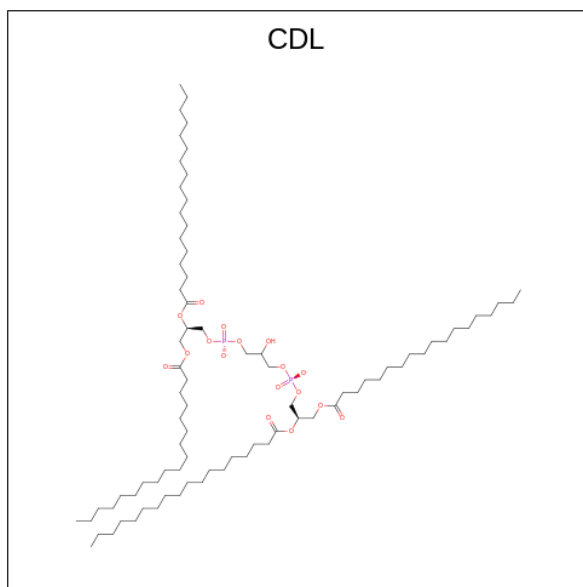
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

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



Mol	Chain	Residues	Atoms					AltConf
25	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	J	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
			44	34	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
			49	39	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
			41	31	1	8	1	

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

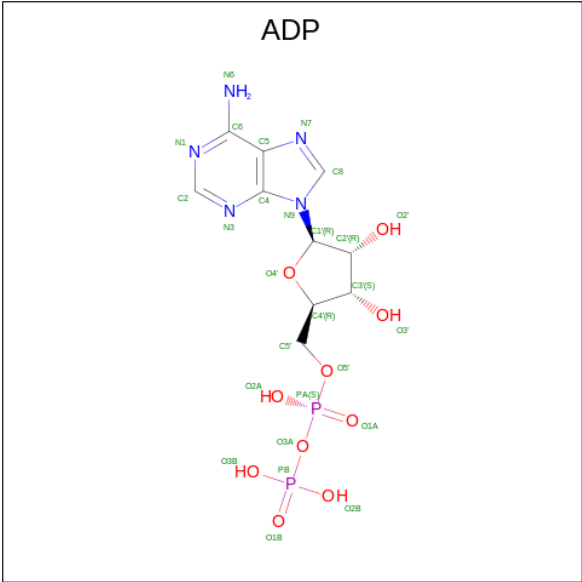


Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			73	54	17	2	
26	M	1	Total	C	O	P	0
			82	63	17	2	
26	Y	1	Total	C	O	P	0
			71	52	17	2	
26	d	1	Total	C	O	P	0
			65	46	17	2	
26	h	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

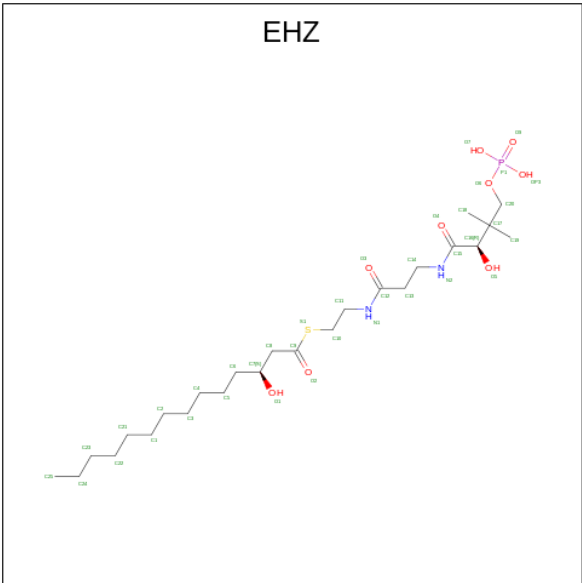
Mol	Chain	Residues	Atoms		AltConf
27	L	1	Total	Zn	0
			1	1	

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

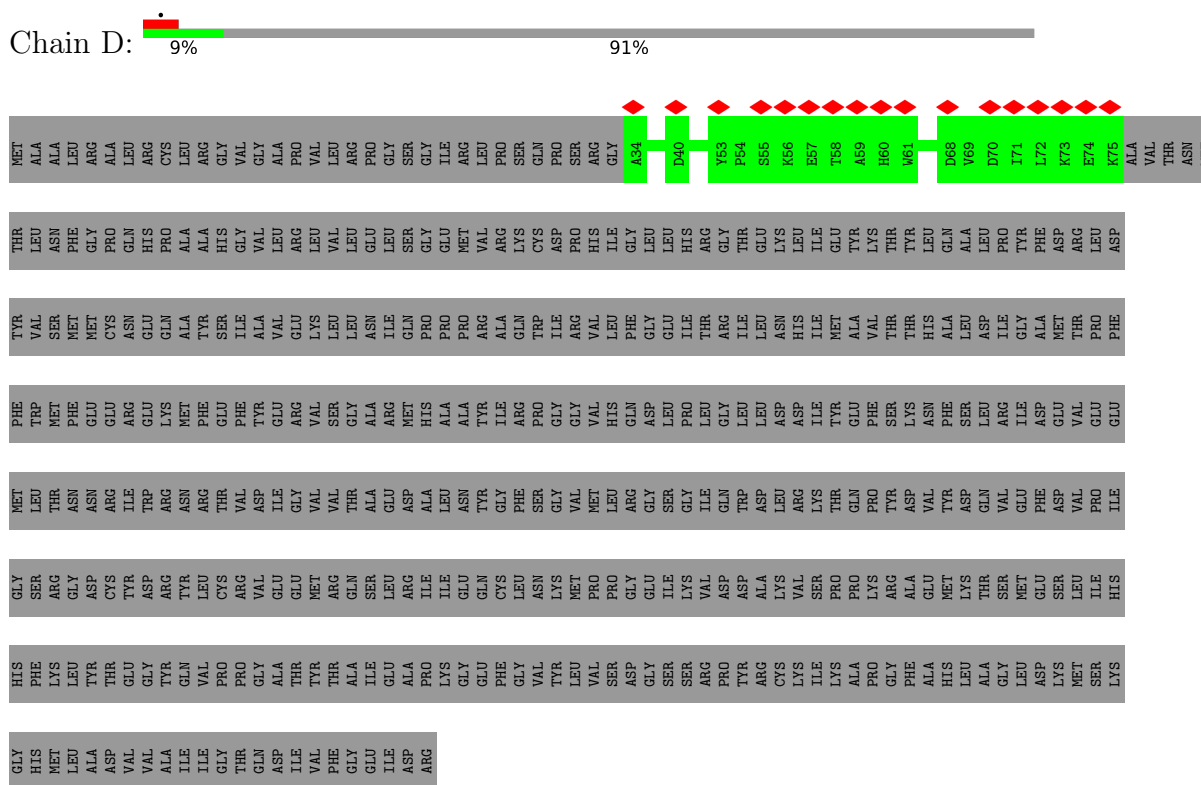
- Molecule 29 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



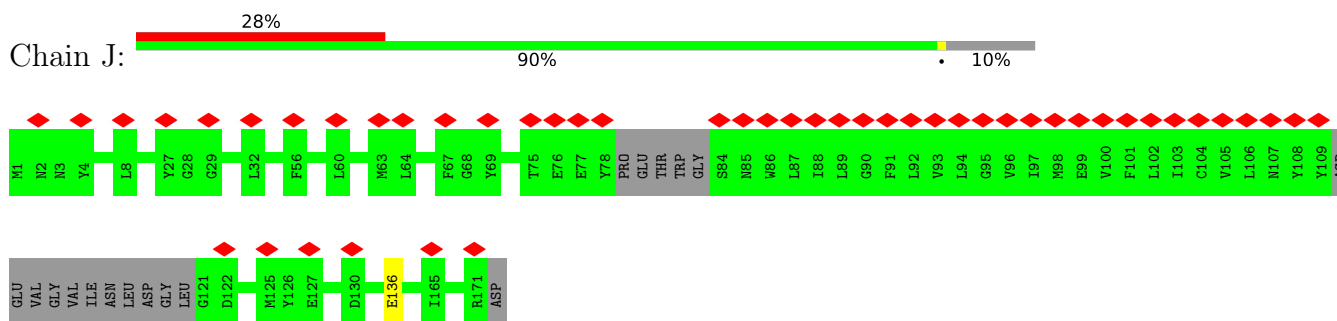
3 Residue-property plots

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.

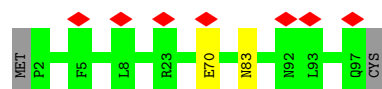
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



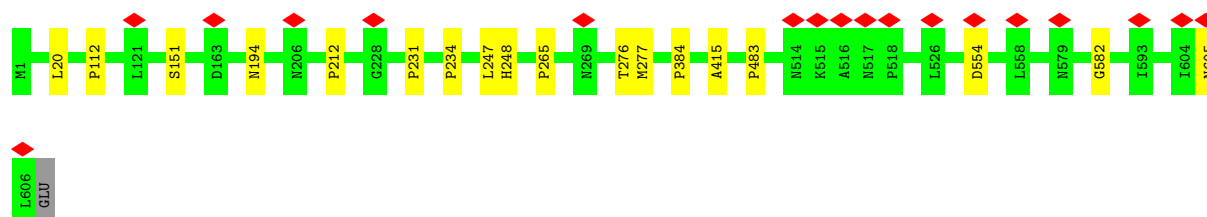
- Molecule 2: NADH-ubiquinone oxidoreductase chain 6



- Molecule 3: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 4: NADH-ubiquinone oxidoreductase chain 5



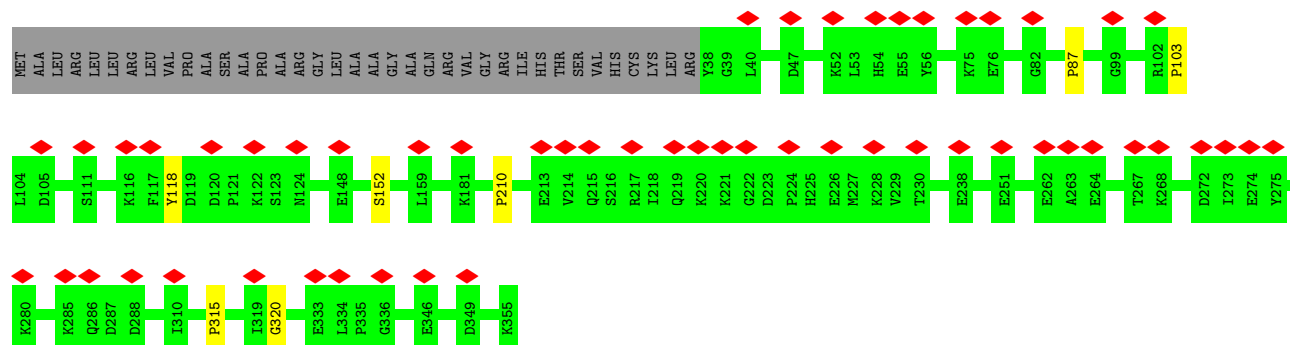
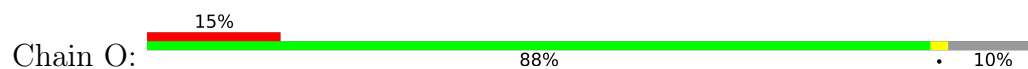
- Molecule 5: NADH-ubiquinone oxidoreductase chain 4



- Molecule 6: NADH-ubiquinone oxidoreductase chain 2

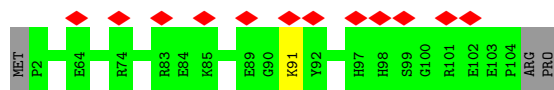


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

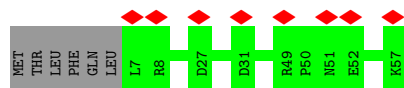
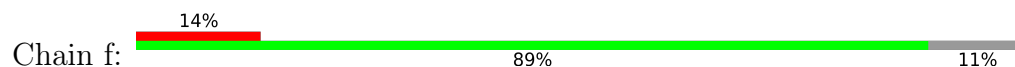


- Molecule 8: Acyl carrier protein, mitochondrial





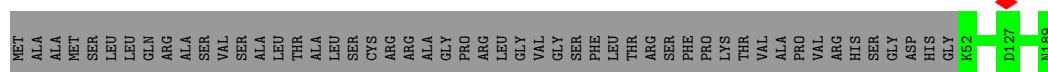
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



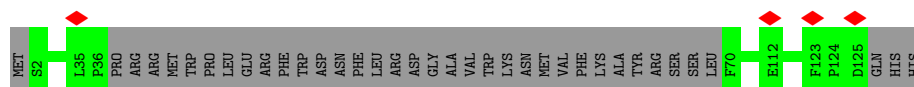
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



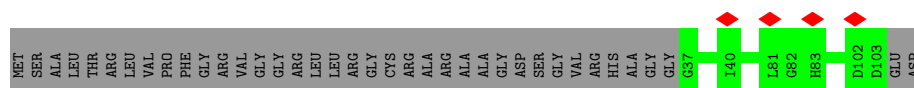
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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



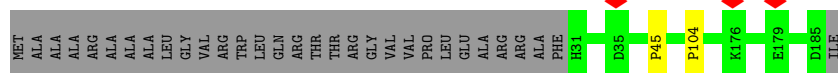
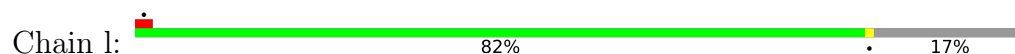
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



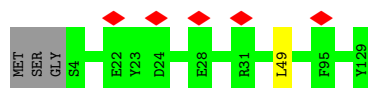
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



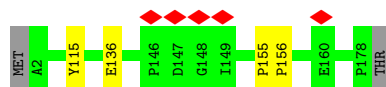
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



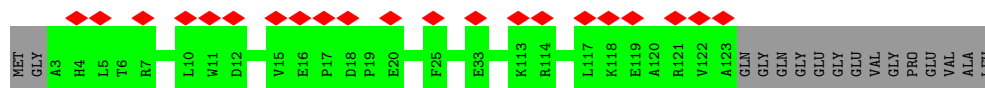
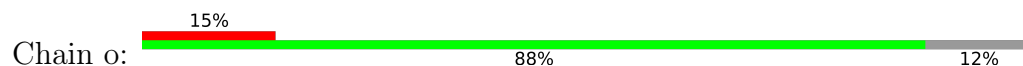
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



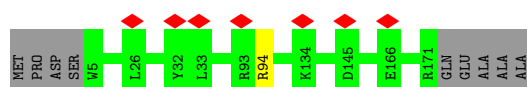
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- 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	45095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.164	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CDL, ZN, EHZ, 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	0.39	0/370	0.59	0/506
2	J	0.39	0/1205	0.59	1/1633 (0.1%)
3	K	0.57	0/732	0.79	2/994 (0.2%)
4	L	0.67	5/4921 (0.1%)	0.90	19/6696 (0.3%)
5	M	0.69	4/3717 (0.1%)	0.90	10/5062 (0.2%)
6	N	0.67	2/2756 (0.1%)	0.85	7/3751 (0.2%)
7	O	0.63	4/2655 (0.2%)	0.74	8/3601 (0.2%)
8	U	0.61	0/712	0.79	2/962 (0.2%)
9	X	0.54	0/230	0.72	0/313
10	Y	0.52	0/1054	0.59	0/1429
11	c	0.46	0/400	0.76	1/544 (0.2%)
12	d	0.61	1/1028 (0.1%)	0.63	2/1387 (0.1%)
13	e	0.51	1/881 (0.1%)	0.64	1/1173 (0.1%)
14	f	0.40	0/451	0.44	0/607
15	g	0.63	1/863 (0.1%)	0.92	3/1175 (0.3%)
16	h	0.52	0/1197	0.74	0/1621
17	i	0.56	0/790	0.74	0/1074
18	j	0.51	0/599	0.69	0/820
19	k	0.82	1/578 (0.2%)	0.94	3/782 (0.4%)
20	l	0.69	2/1359 (0.1%)	0.76	1/1855 (0.1%)
21	m	0.55	0/1079	0.75	0/1463
22	n	0.64	1/1589 (0.1%)	0.74	2/2152 (0.1%)
23	o	0.50	0/1063	0.63	0/1427
24	p	0.53	0/1448	0.71	1/1957 (0.1%)
All	All	0.61	22/31677 (0.1%)	0.79	63/42984 (0.1%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.75	1.67	1.47
19	k	50	PRO	N-CD	-13.70	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	255	PRO	N-CD	-13.52	1.28	1.47
7	O	315	PRO	N-CD	-12.22	1.30	1.47
7	O	210	PRO	N-CD	-11.38	1.31	1.47

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	50	PRO	CA-N-CD	9.93	125.61	111.70
6	N	255	PRO	CA-N-CD	9.86	125.50	111.70
7	O	315	PRO	CA-N-CD	8.77	123.98	111.70
19	k	50	PRO	N-CA-CB	-8.13	93.54	103.30
7	O	210	PRO	CA-N-CD	7.79	122.60	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	40/463 (9%)	36 (90%)	4 (10%)	0	100	100
2	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
3	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
4	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
5	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
8	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
9	X	25/172 (14%)	23 (92%)	2 (8%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
13	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
14	f	49/57 (86%)	49 (100%)	0	0	100	100
15	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
16	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
17	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
18	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
19	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
20	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	22	57
23	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
24	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
All	All	3750/4813 (78%)	3569 (95%)	179 (5%)	2 (0%)	50	80

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	37/395 (9%)	37 (100%)	0	100	100
2	J	124/138 (90%)	124 (100%)	0	100	100
3	K	86/88 (98%)	86 (100%)	0	100	100
4	L	549/550 (100%)	549 (100%)	0	100	100
5	M	415/415 (100%)	415 (100%)	0	100	100
6	N	307/308 (100%)	307 (100%)	0	100	100
7	O	282/309 (91%)	282 (100%)	0	100	100
8	U	80/135 (59%)	80 (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	91/94 (97%)	91 (100%)	0	100	100
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	90/129 (70%)	90 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	86/120 (72%)	86 (100%)	0	100	100
18	j	62/87 (71%)	62 (100%)	0	100	100
19	k	54/78 (69%)	54 (100%)	0	100	100
20	l	140/161 (87%)	140 (100%)	0	100	100
21	m	112/114 (98%)	111 (99%)	1 (1%)	75	89
22	n	162/164 (99%)	162 (100%)	0	100	100
23	o	111/121 (92%)	111 (100%)	0	100	100
24	p	152/158 (96%)	152 (100%)	0	100	100
All	All	3385/4214 (80%)	3384 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	m	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
16	h	170	GLN
22	n	76	HIS
17	i	83	HIS
21	m	75	ASN
24	p	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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$
25	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.08	3 (6%)
25	3PE	L	701	-	39,39,50	1.02	2 (5%)	42,44,55	1.06	2 (4%)
25	3PE	J	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.06	3 (6%)
25	3PE	m	201	-	40,40,50	1.01	2 (5%)	43,45,55	1.15	3 (6%)
25	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.14	3 (7%)
26	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.14	6 (7%)
25	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.14	3 (5%)
26	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.20	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.15	6 (8%)
26	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.14	6 (6%)
28	ADP	O	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	4 (13%)
25	3PE	M	501	-	36,36,50	1.08	2 (5%)	39,41,55	1.05	3 (7%)
29	EHZ	n	201	-	27,31,37	1.91	7 (25%)	37,41,47	1.56	4 (10%)
25	3PE	D	501	-	37,37,50	1.06	2 (5%)	40,42,55	1.08	3 (7%)
26	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.16	7 (9%)
25	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.10	3 (5%)

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	705	-	-	13/47/47/54	-
25	3PE	L	701	-	-	9/43/43/54	-
25	3PE	J	201	-	-	13/49/49/54	-
25	3PE	m	201	-	-	11/44/44/54	-
25	3PE	i	201	-	-	9/43/43/54	-
26	CDL	L	703	-	-	20/83/83/110	-
25	3PE	M	502	-	-	14/52/52/54	-
26	CDL	d	201	-	-	27/75/75/110	-
26	CDL	h	201	-	-	19/78/78/110	-
26	CDL	M	503	-	-	24/92/92/110	-
28	ADP	O	401	-	-	2/12/32/32	0/3/3/3
25	3PE	M	501	-	-	10/40/40/54	-
29	EHZ	n	201	-	-	21/39/39/45	-
25	3PE	D	501	-	-	10/41/41/54	-
26	CDL	Y	201	-	-	16/81/81/110	-
25	3PE	L	702	-	-	13/52/52/54	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C12-N1	5.51	1.45	1.33
29	n	201	EHZ	C15-N2	5.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	201	CDL	OA8-CA7	4.30	1.45	1.33
25	M	501	3PE	O31-C31	4.30	1.45	1.33
25	J	201	3PE	O31-C31	4.29	1.45	1.33

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	201	EHZ	C8-C9-S1	5.56	120.50	113.63
26	M	503	CDL	OA6-CA5-C11	4.63	121.47	111.50
26	L	703	CDL	OB6-CB5-C51	4.23	120.61	111.50
26	h	201	CDL	OB6-CB5-C51	4.21	120.57	111.50
25	M	502	3PE	O21-C21-C22	4.14	120.42	111.50

There are no chirality outliers.

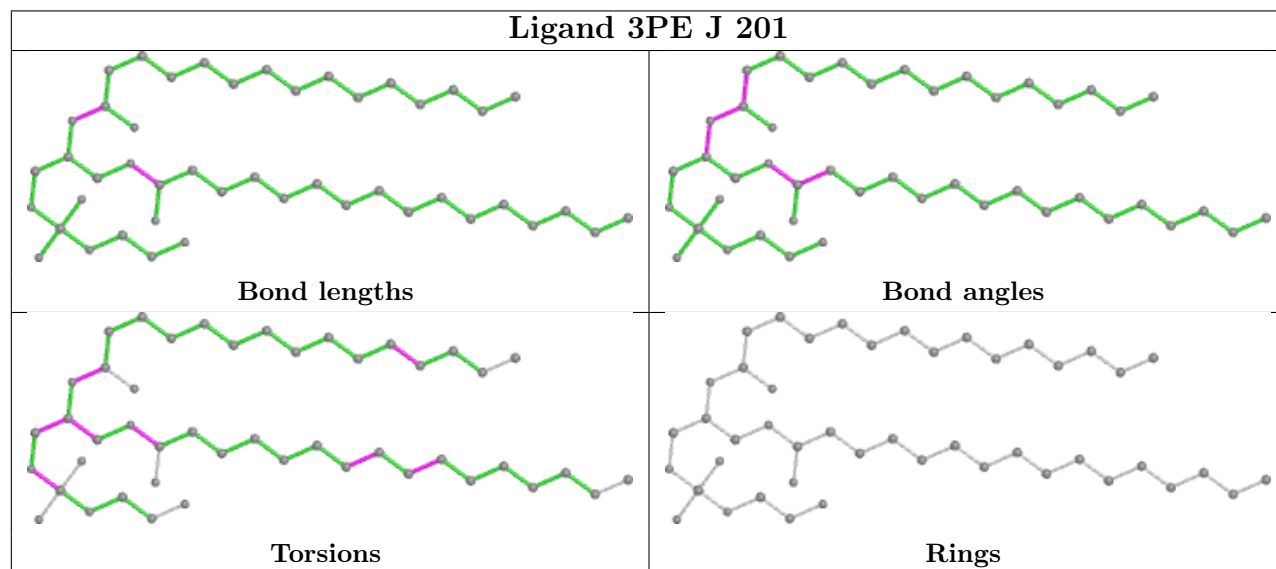
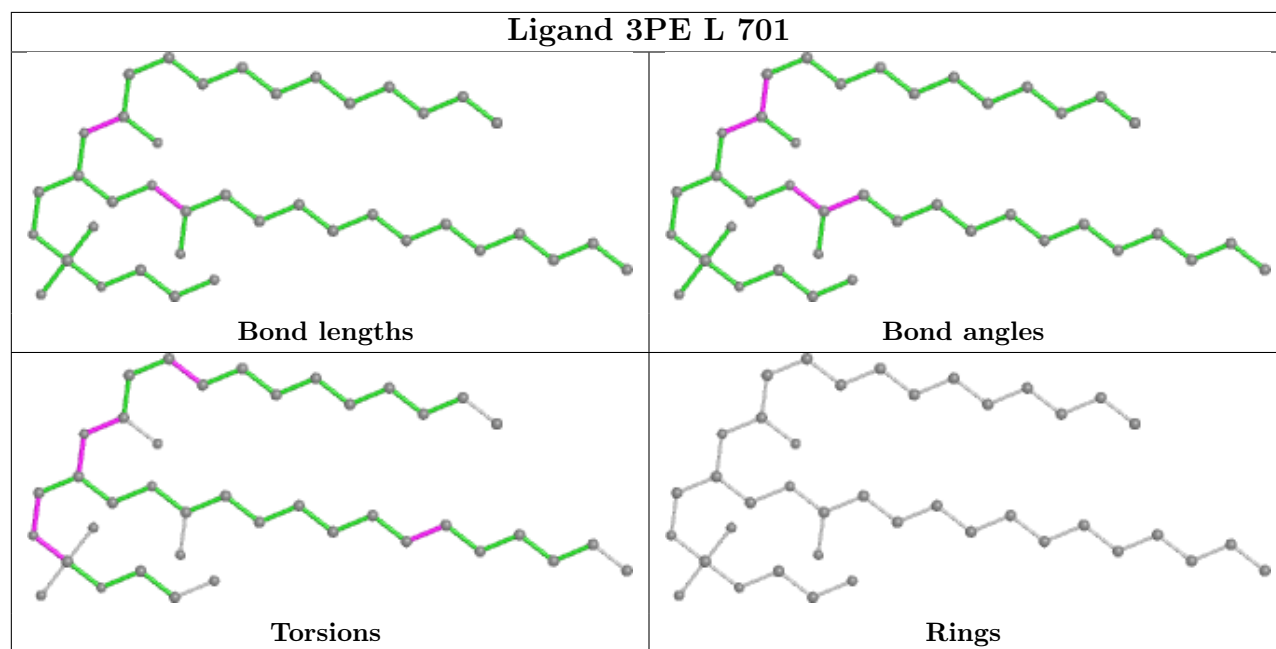
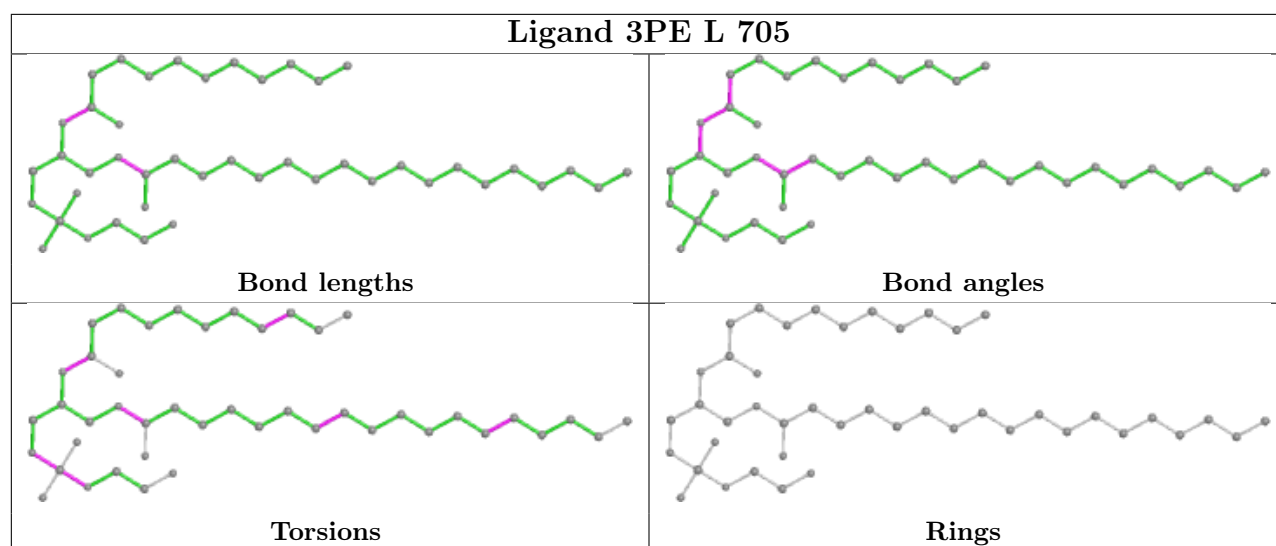
5 of 231 torsion outliers are listed below:

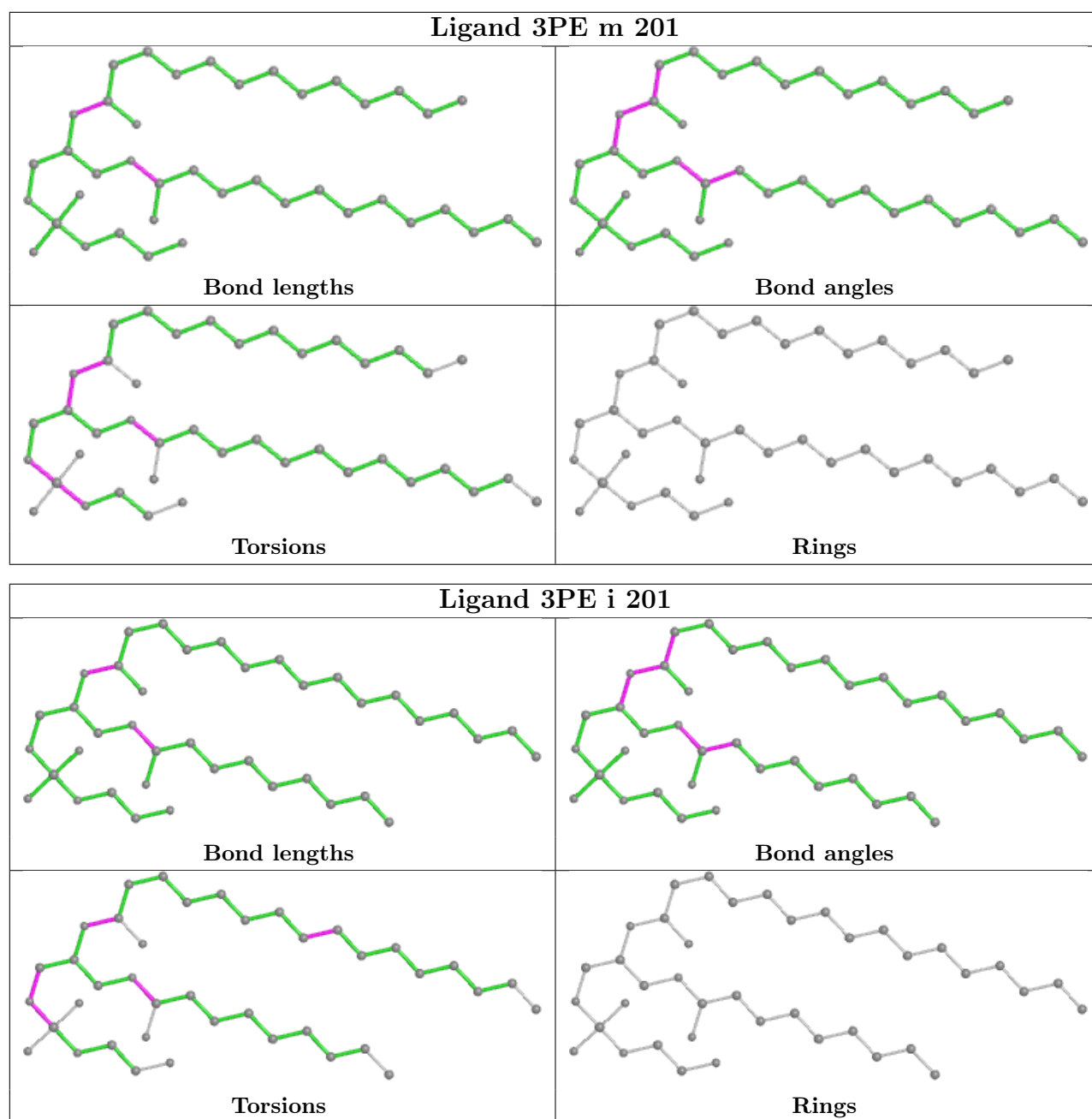
Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O14
25	J	201	3PE	C1-O11-P-O12
25	J	201	3PE	C1-O11-P-O13
25	J	201	3PE	C1-O11-P-O14
25	L	701	3PE	C1-O11-P-O12

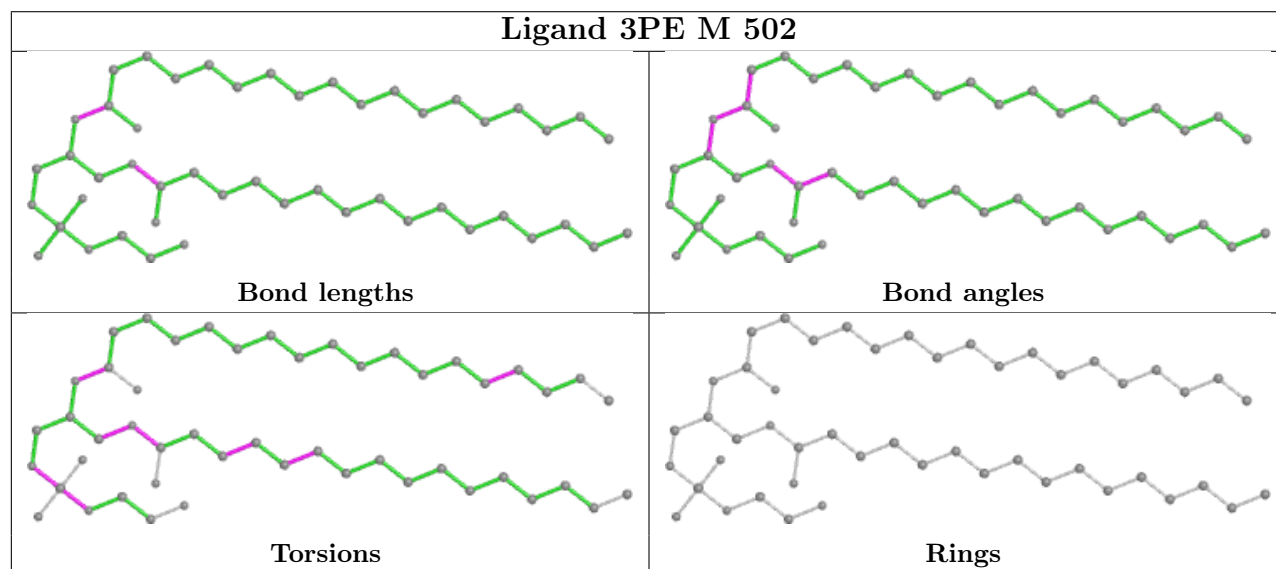
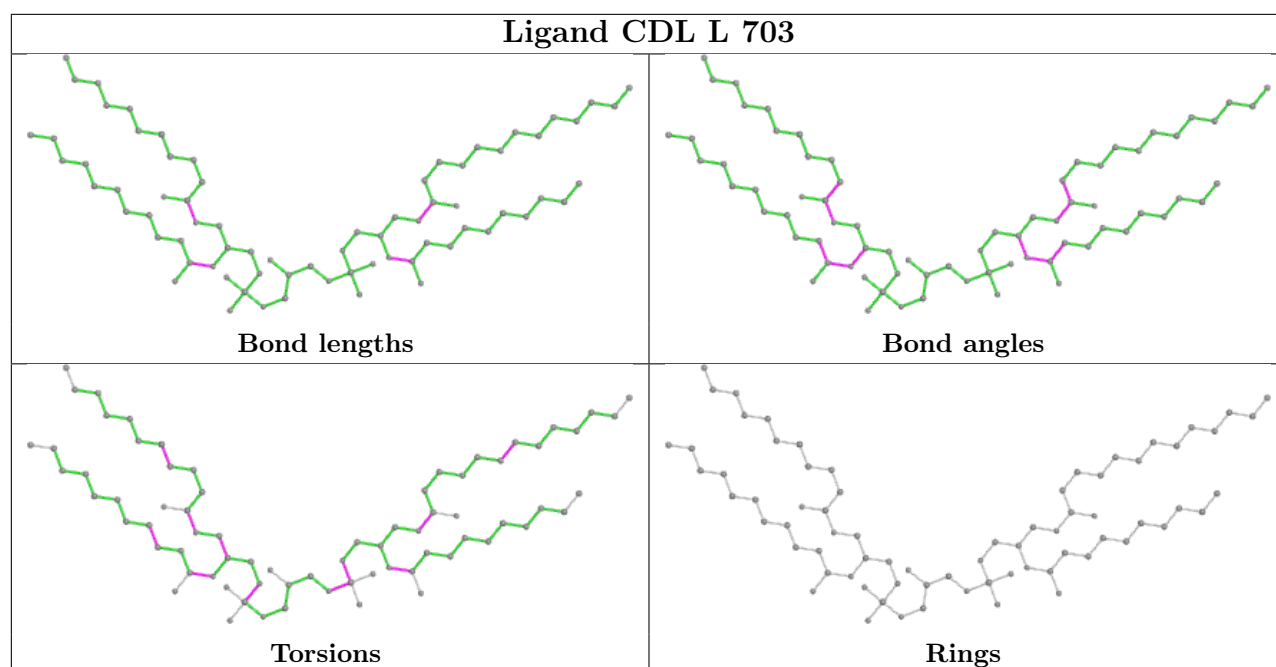
There are no ring outliers.

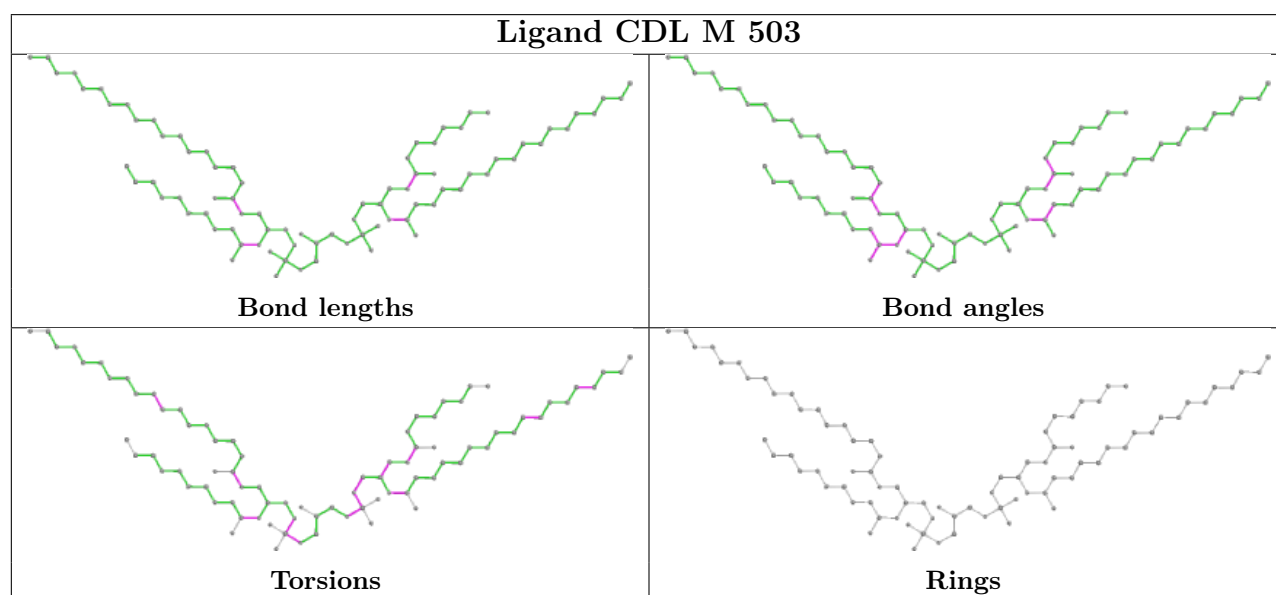
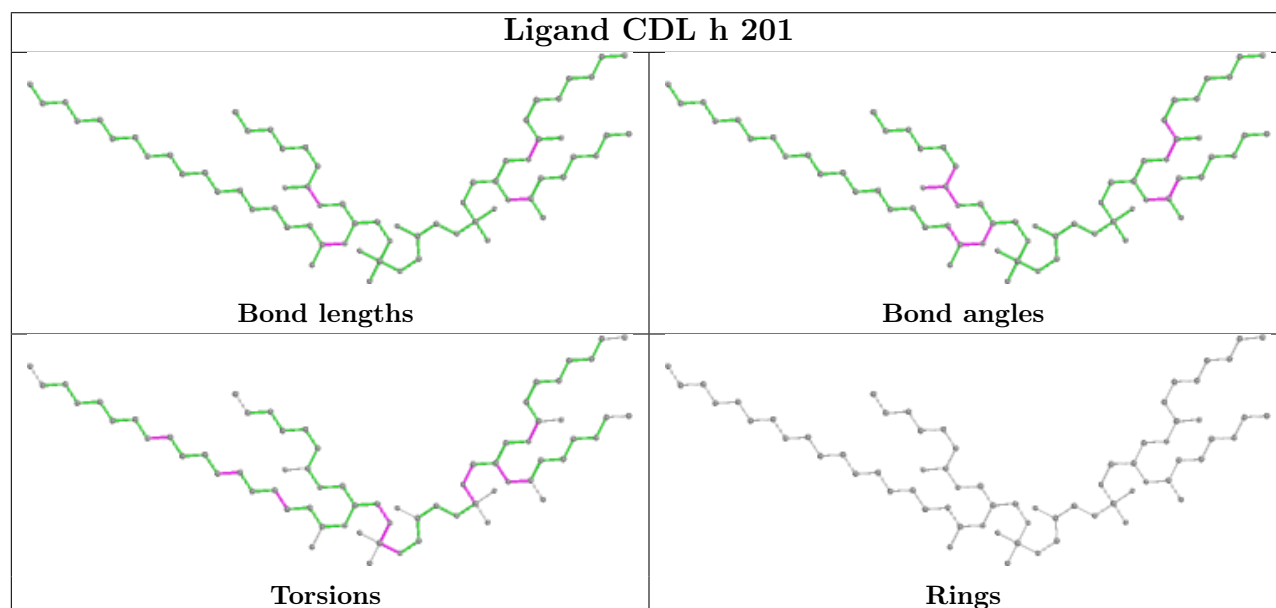
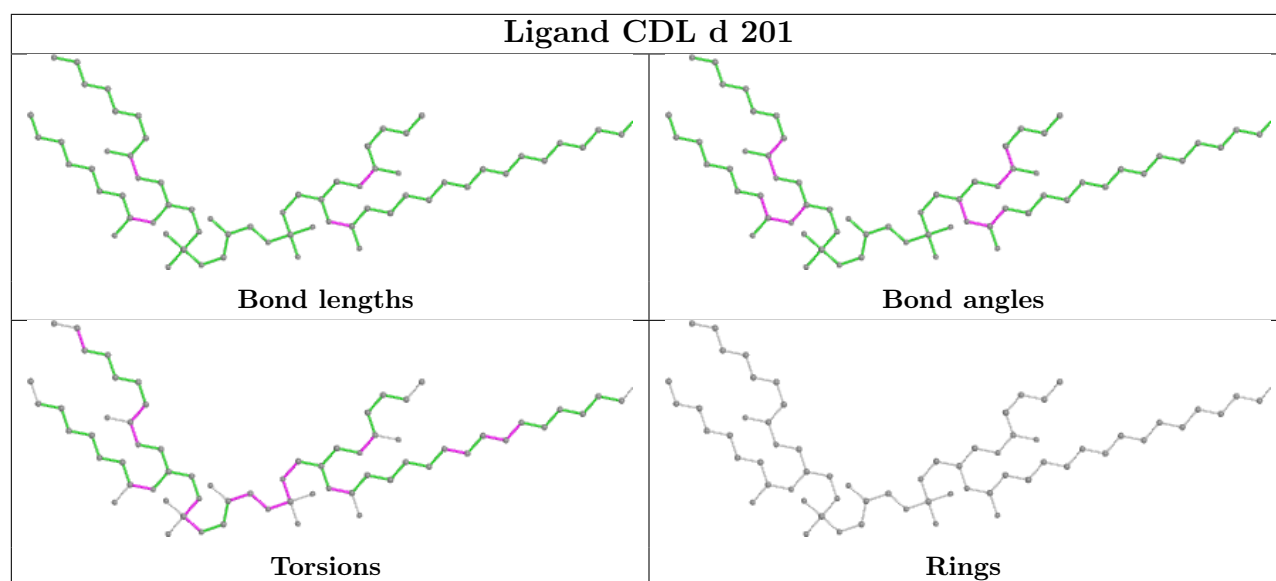
No monomer is involved in short contacts.

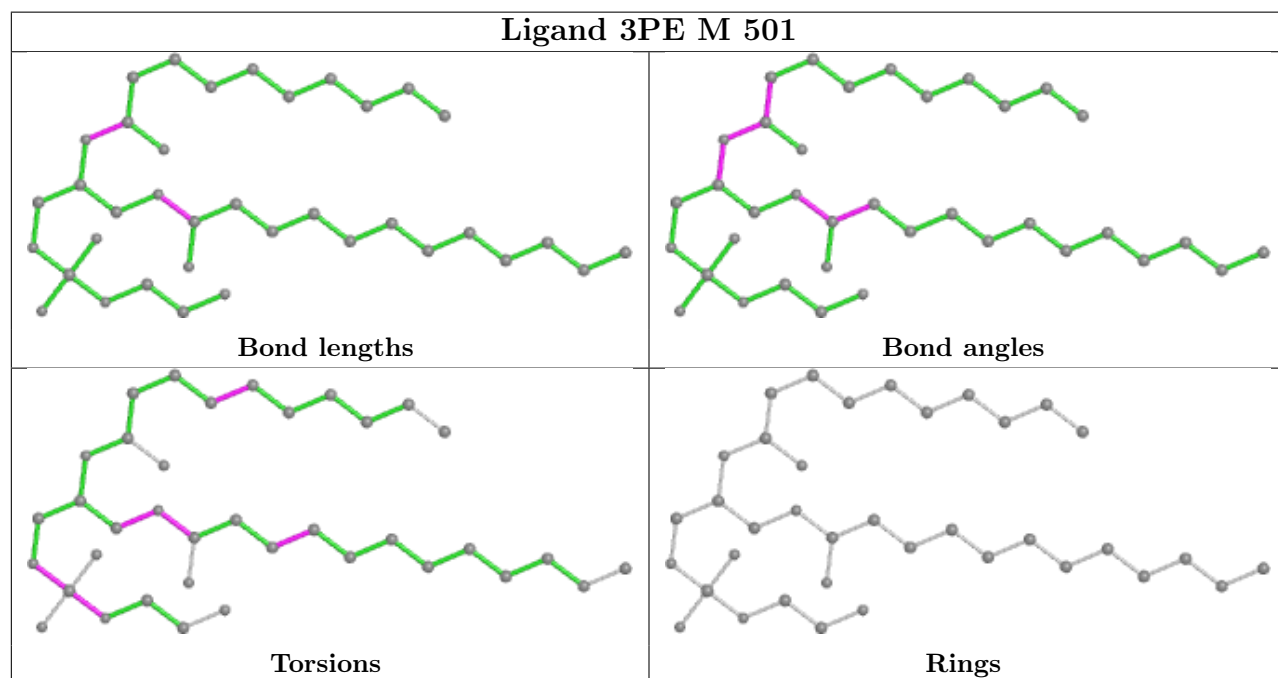
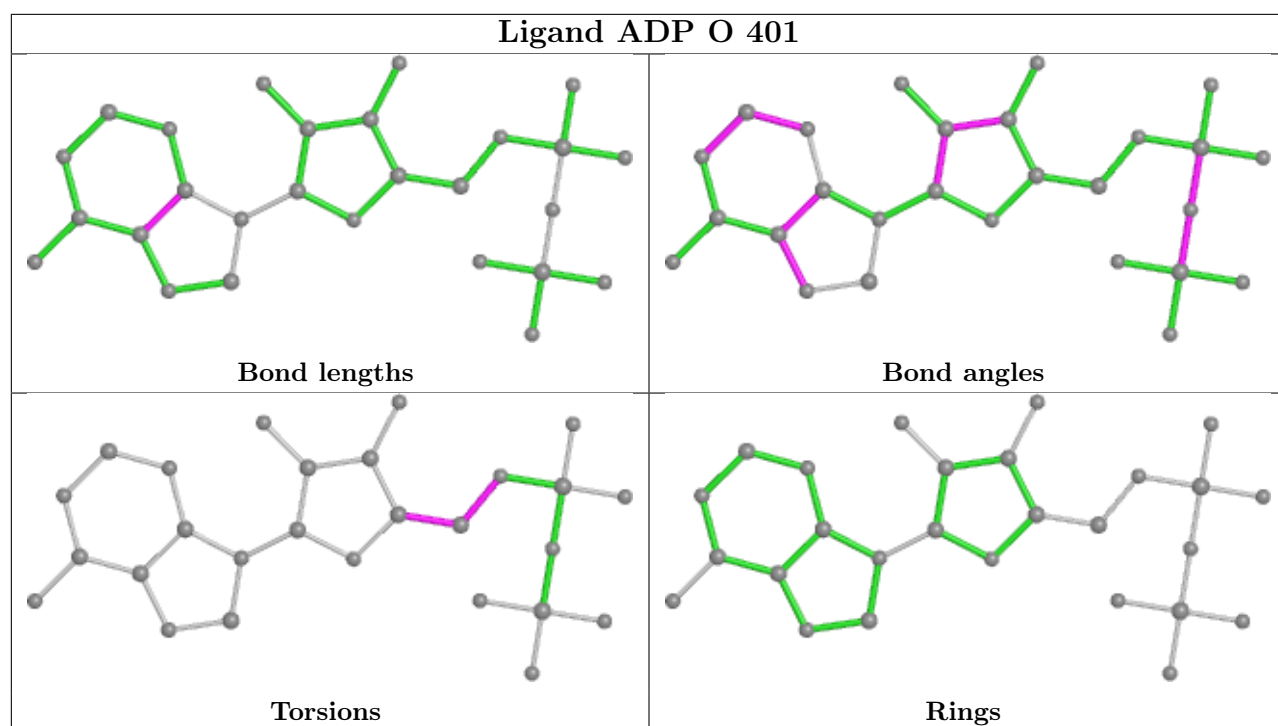
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



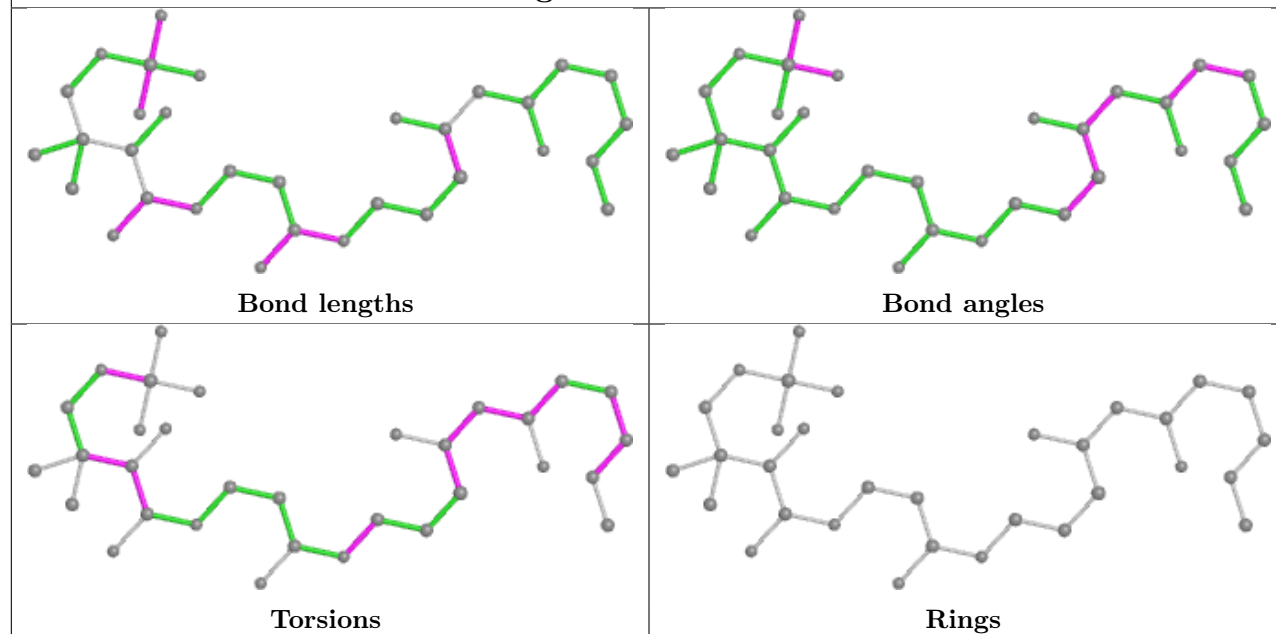




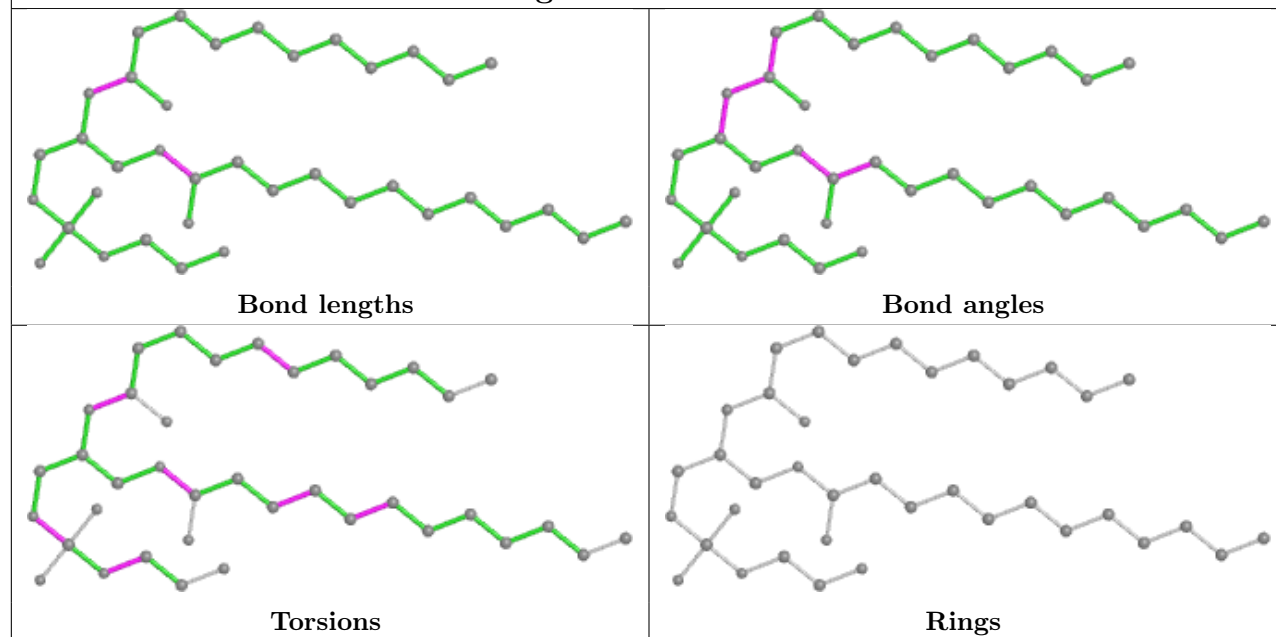


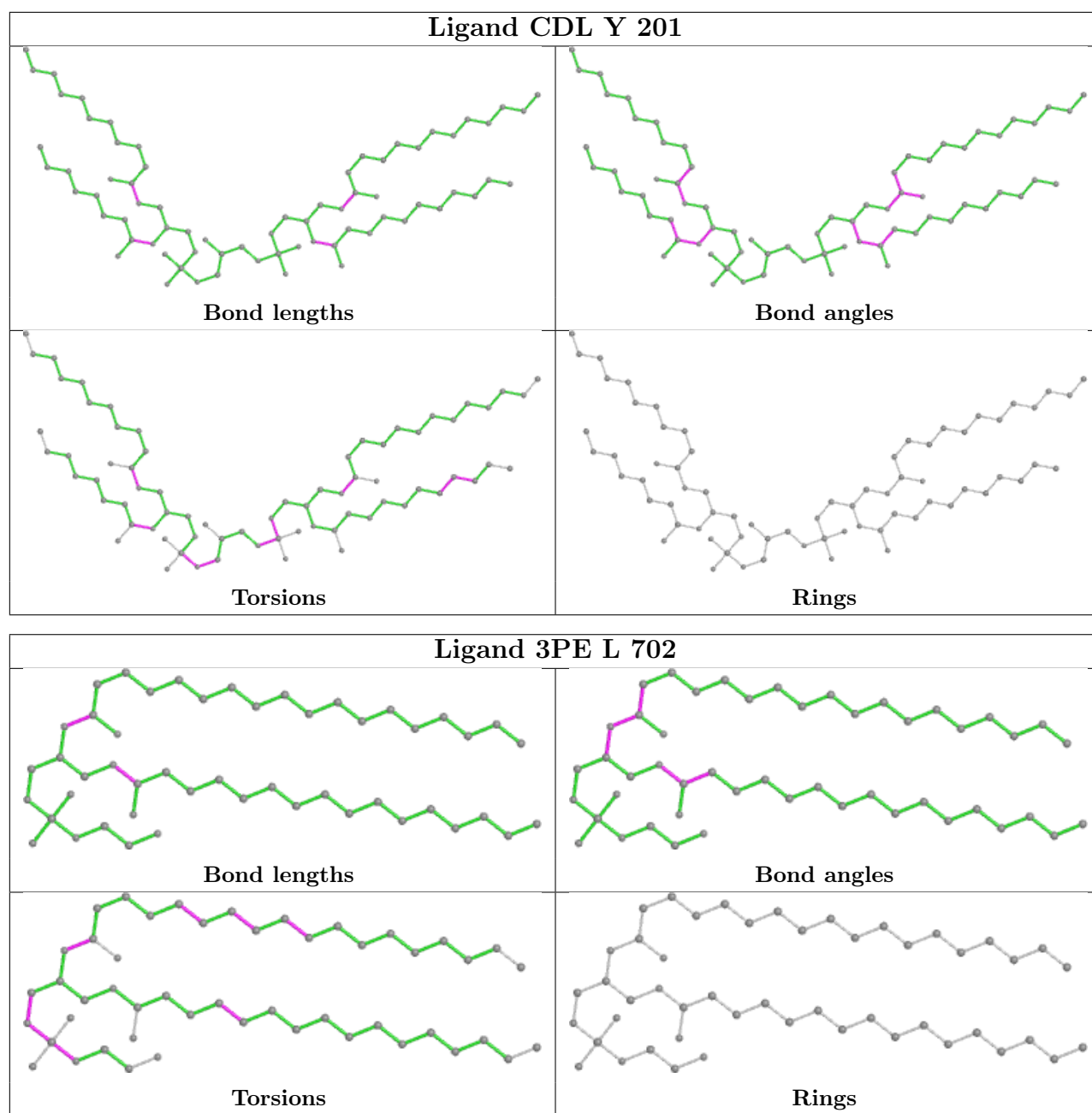


Ligand EHZ n 201



Ligand 3PE D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

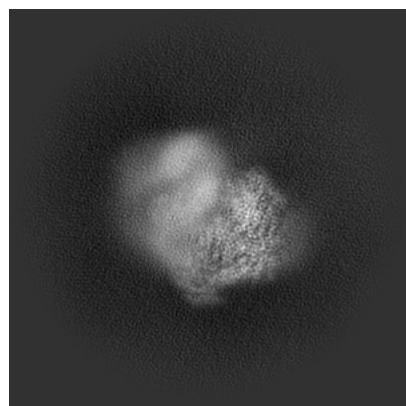
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35354. These allow visual inspection of the internal detail of the map and identification of artifacts.

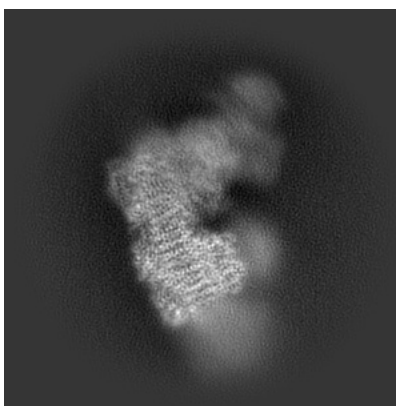
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

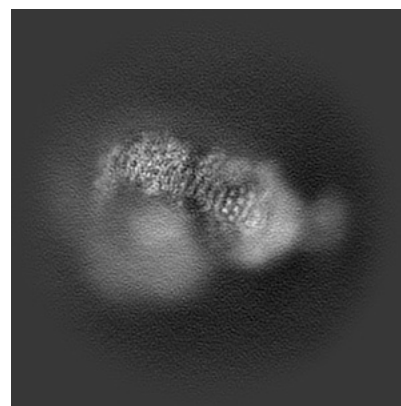
6.1.1 Primary map



X

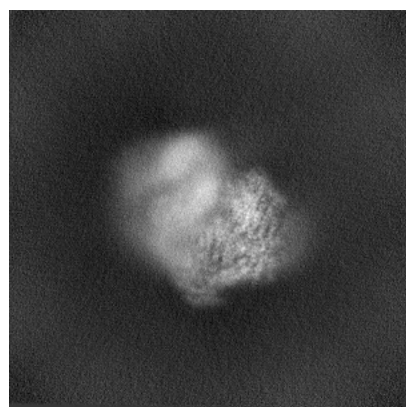


Y



Z

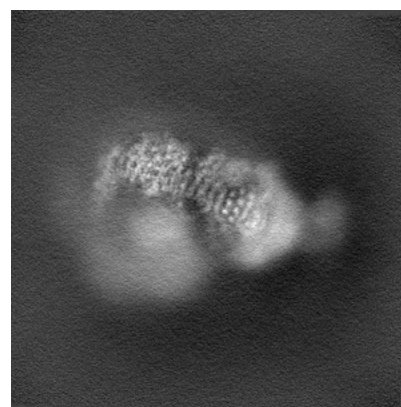
6.1.2 Raw map



X



Y

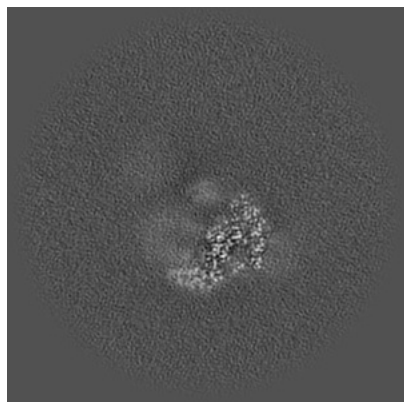


Z

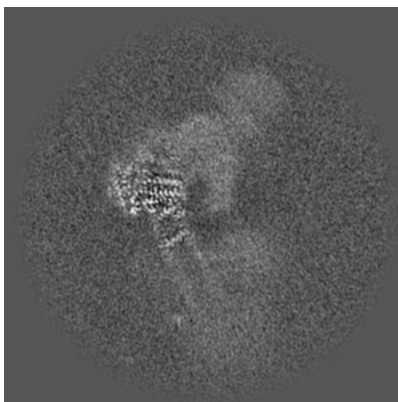
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

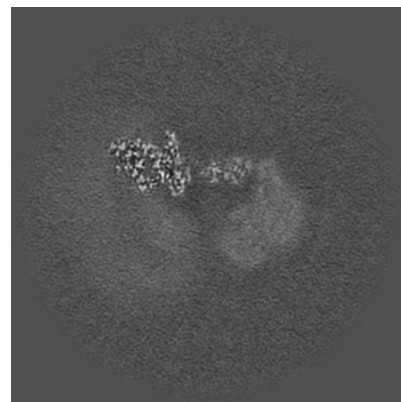
6.2.1 Primary map



X Index: 256

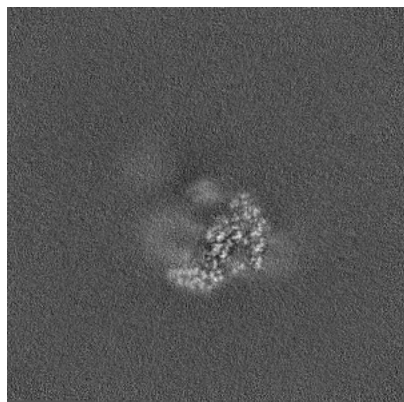


Y Index: 256

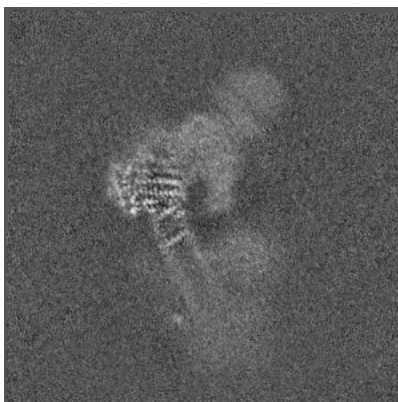


Z Index: 256

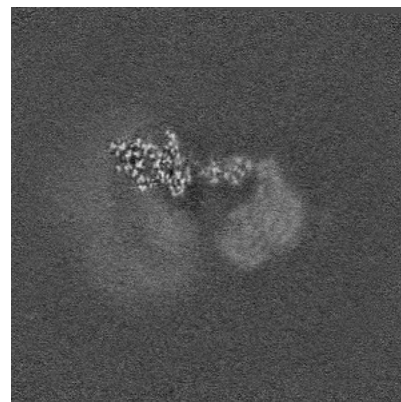
6.2.2 Raw map



X Index: 256



Y Index: 256

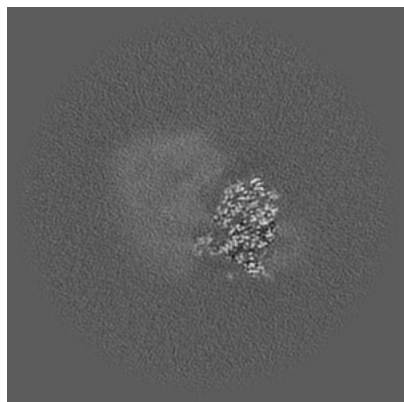


Z Index: 256

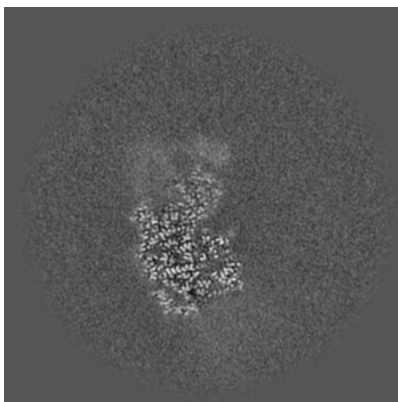
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

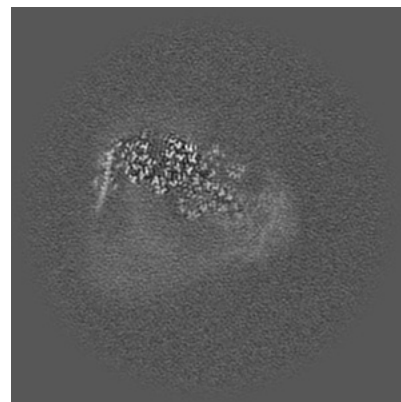
6.3.1 Primary map



X Index: 211

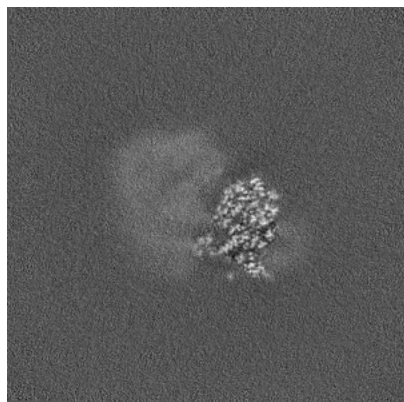


Y Index: 300

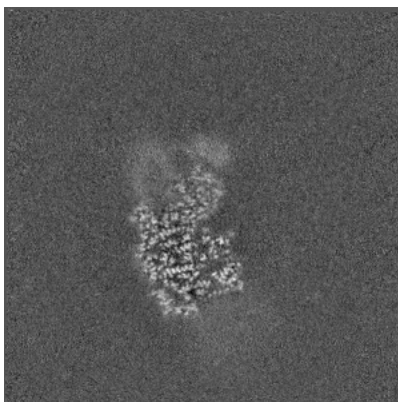


Z Index: 224

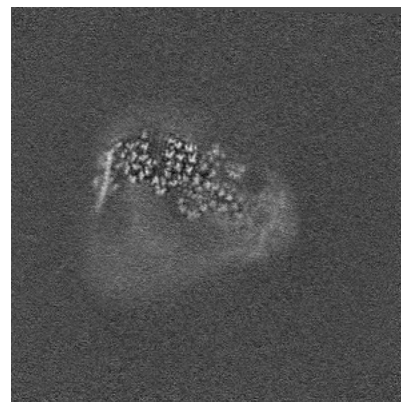
6.3.2 Raw map



X Index: 211



Y Index: 300

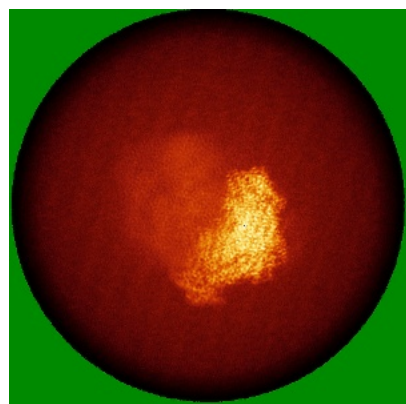


Z Index: 224

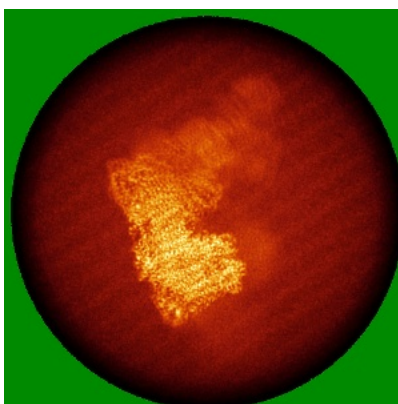
The images above show the largest variance slices of the map in three orthogonal directions.

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

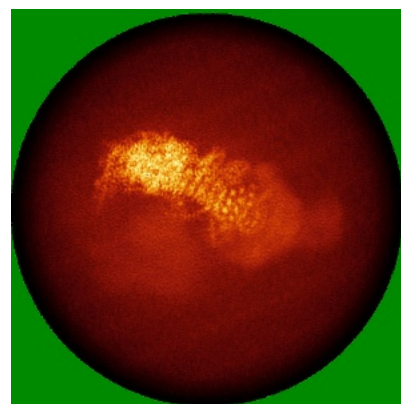
6.4.1 Primary map



X

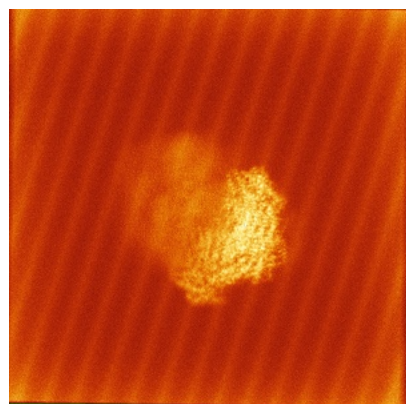


Y

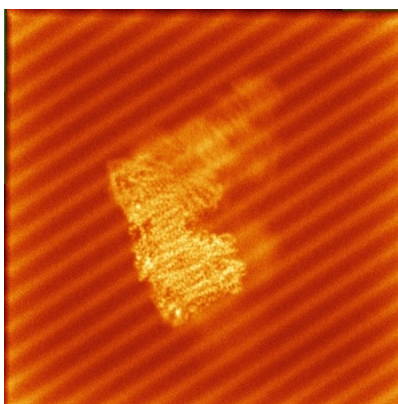


Z

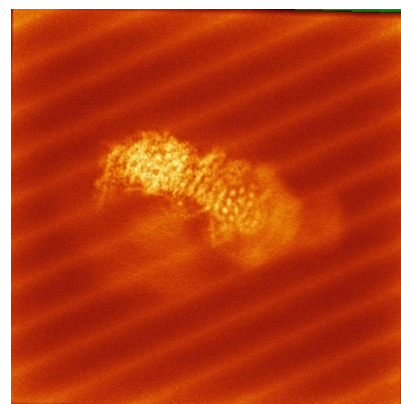
6.4.2 Raw map



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.

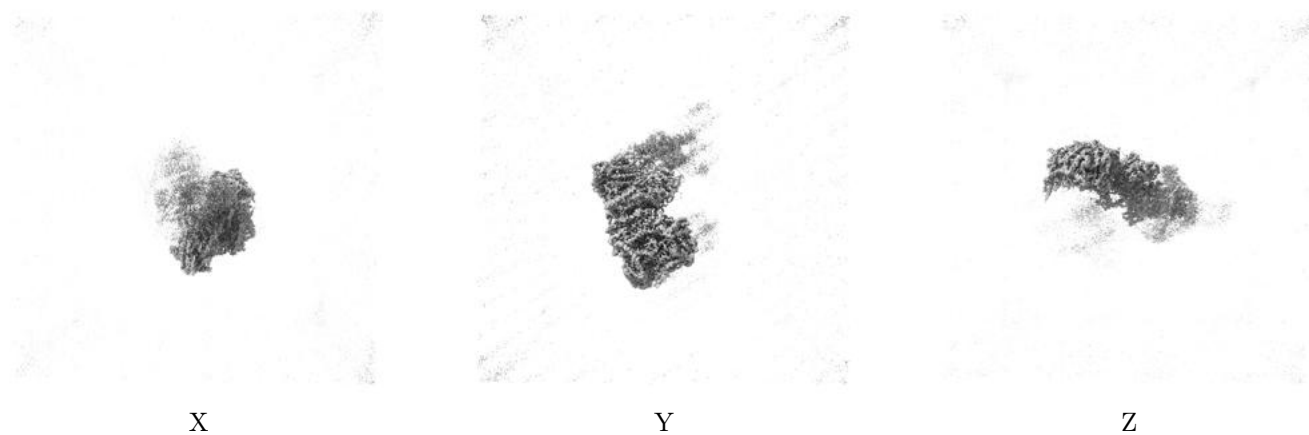
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

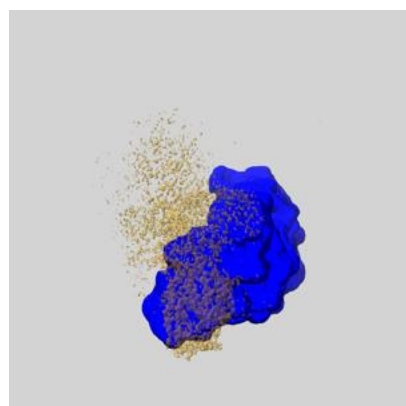
6.6 Mask visualisation [i](#)

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

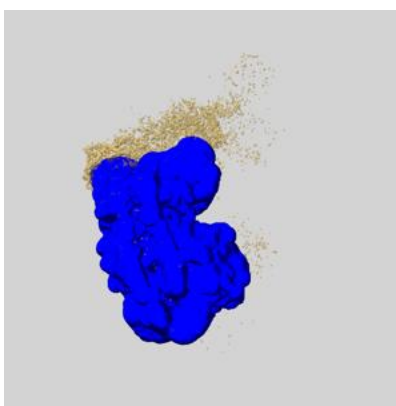
A mask typically either:

- 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_35354_msk_1.map [i](#)



X



Y

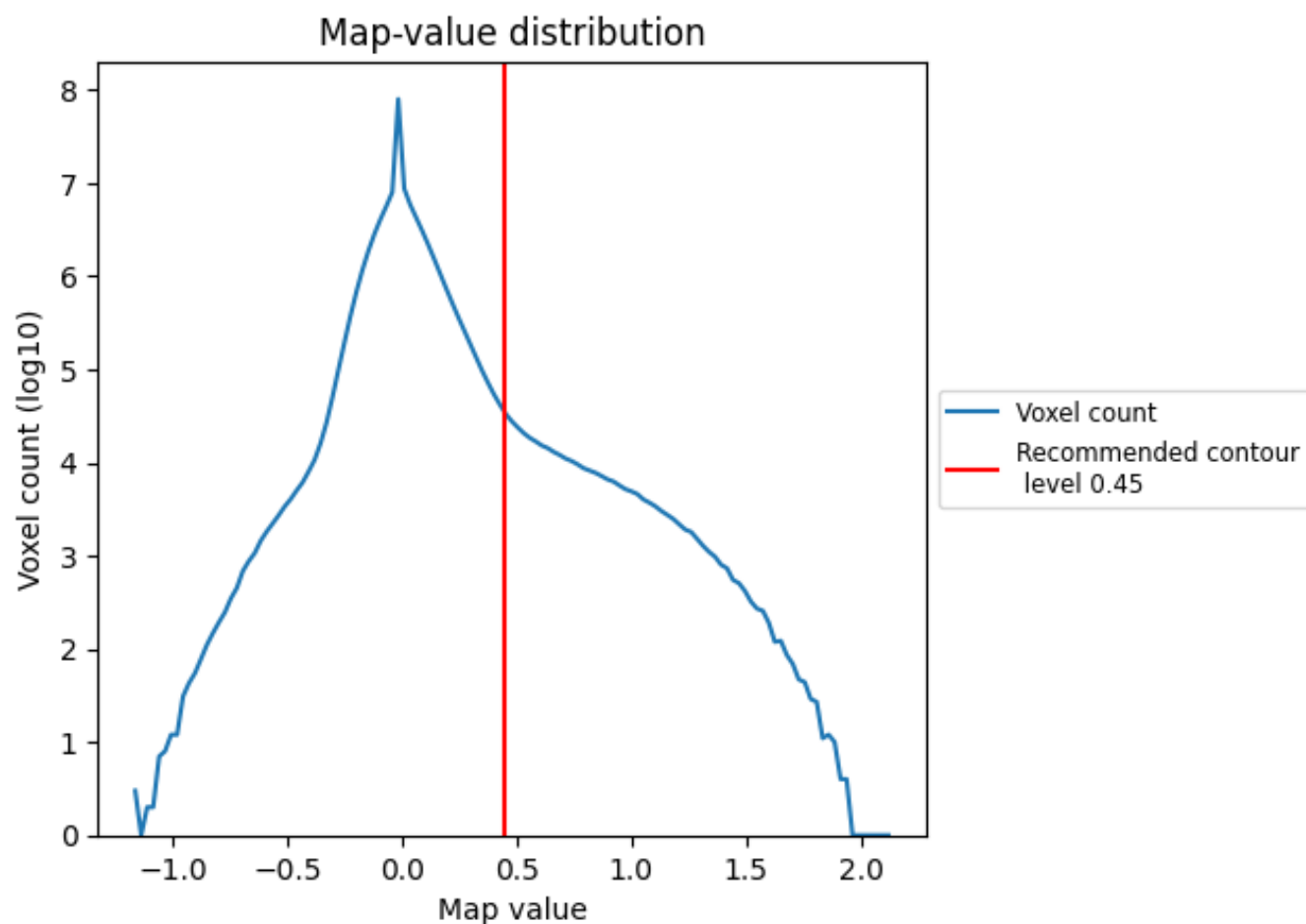


Z

7 Map analysis [i](#)

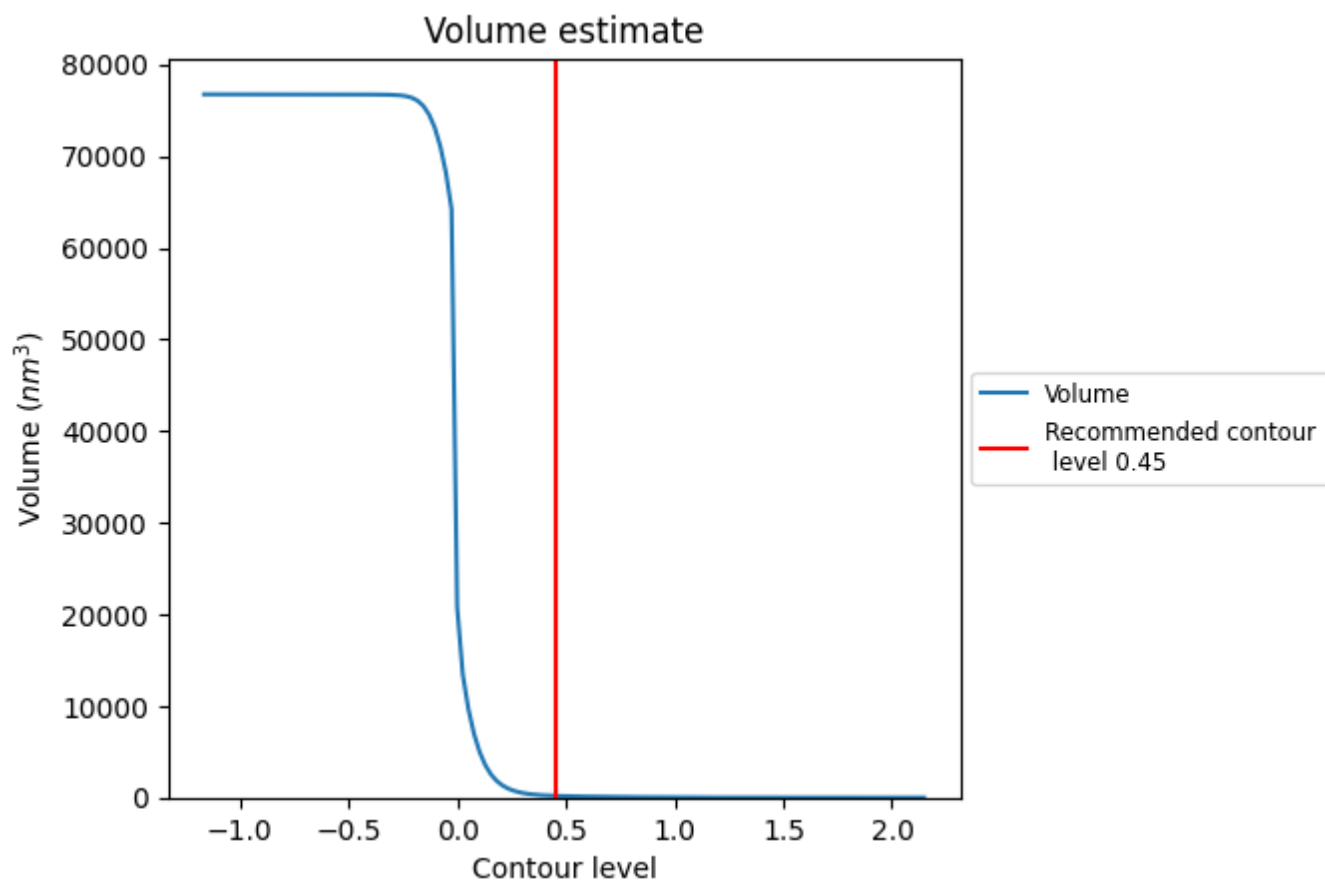
This section contains the results of statistical analysis of the map.

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.

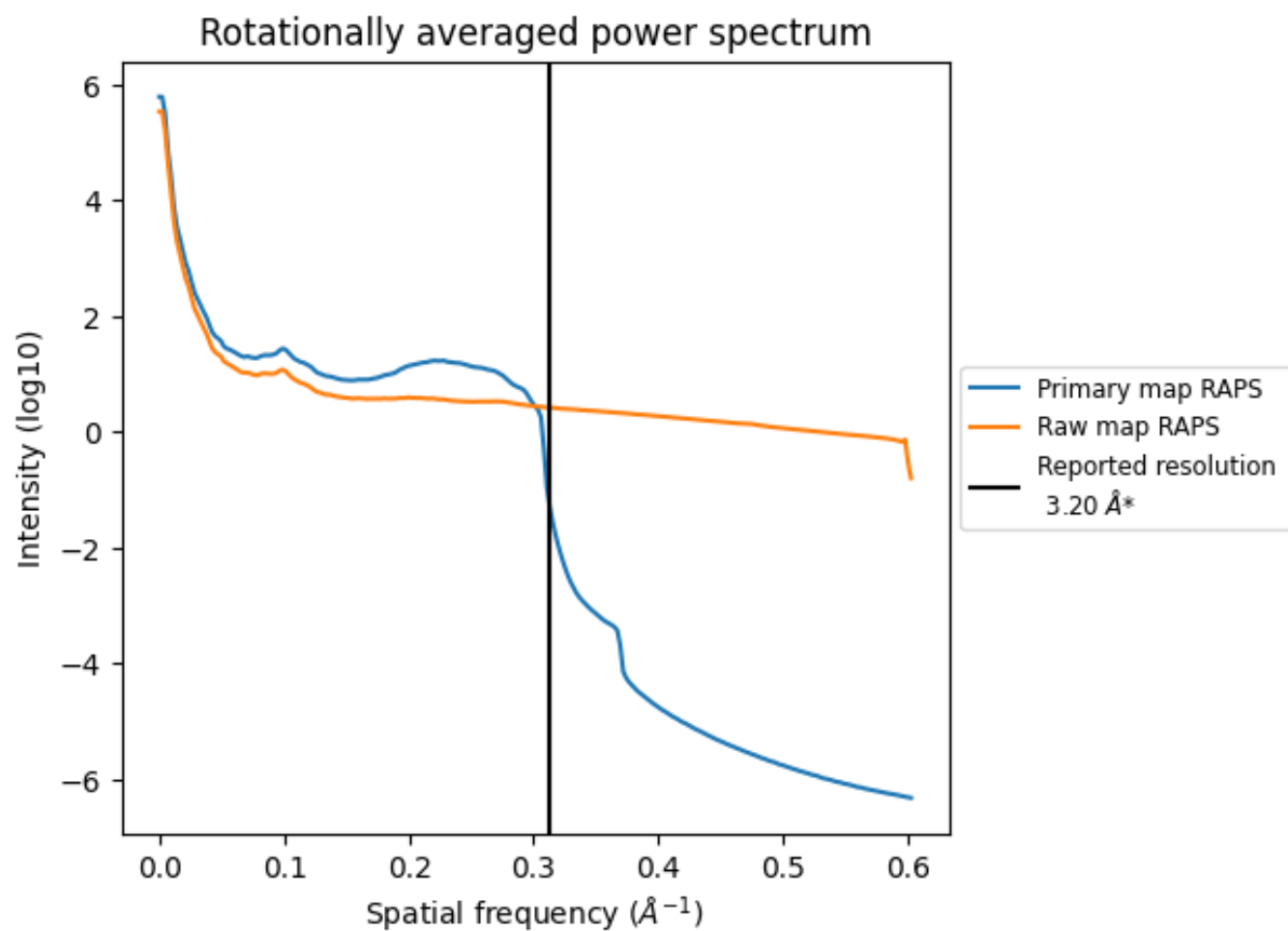
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 171 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

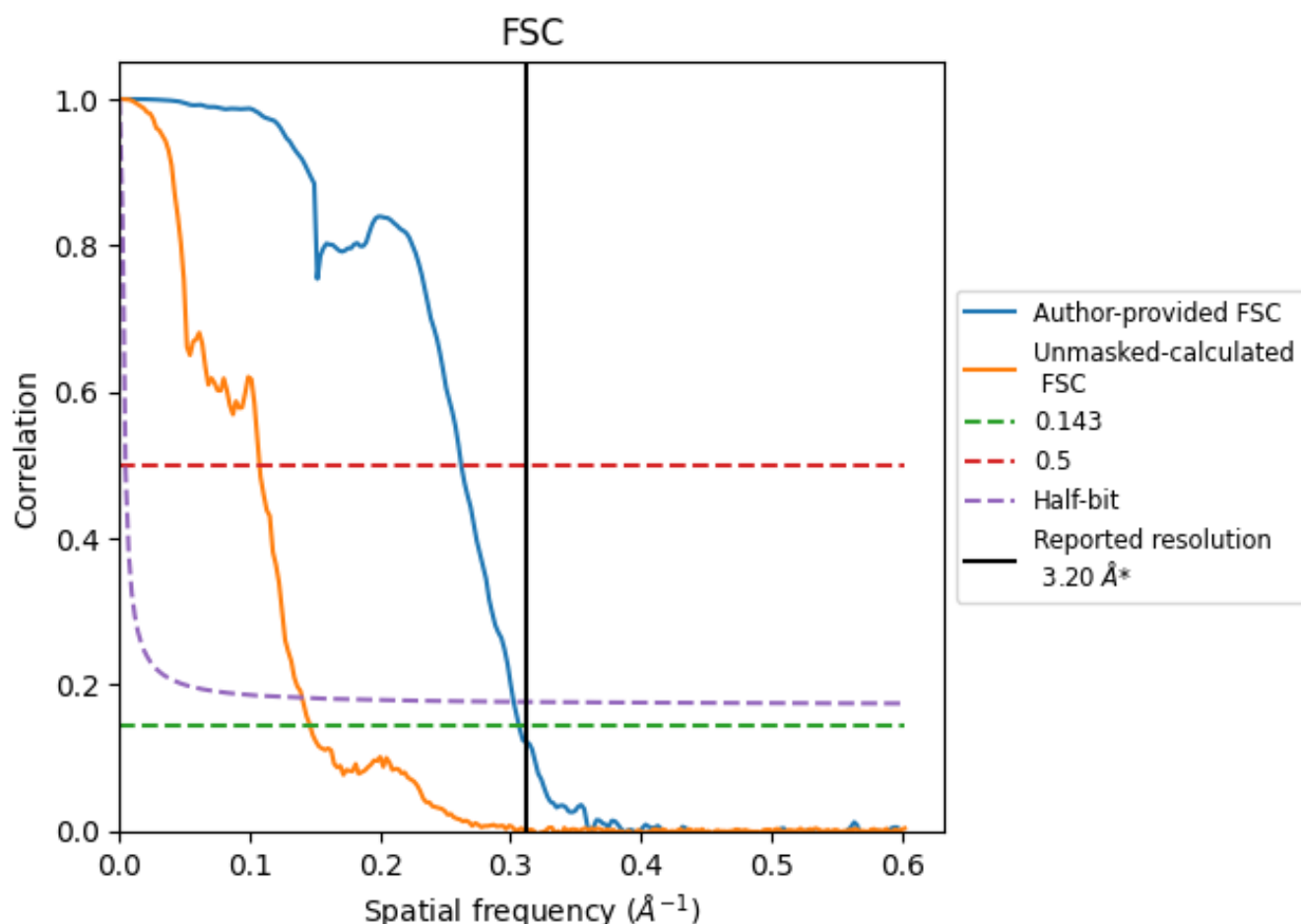


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

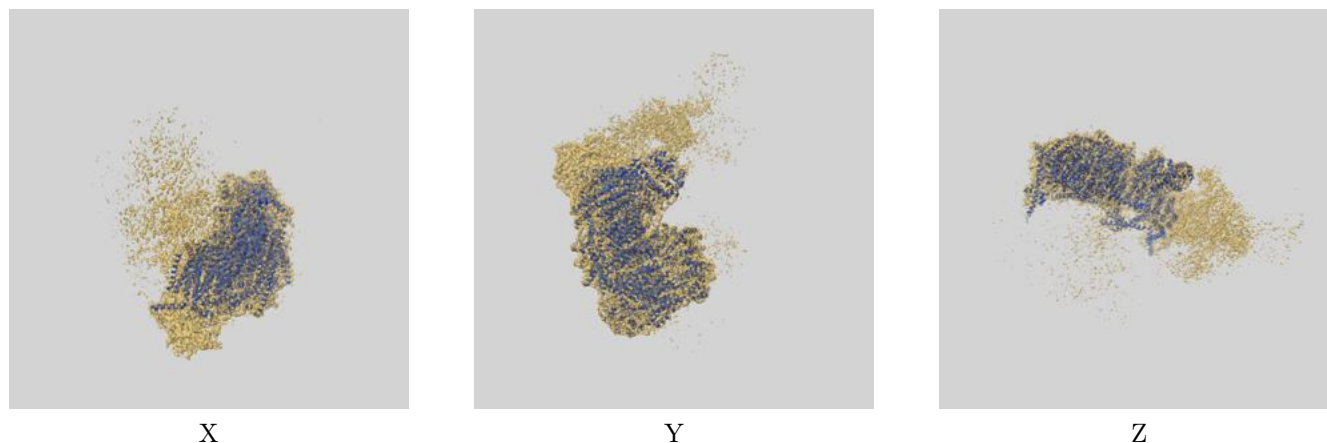
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.81	3.31
Unmasked-calculated*	6.84	9.31	7.14

*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 6.84 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

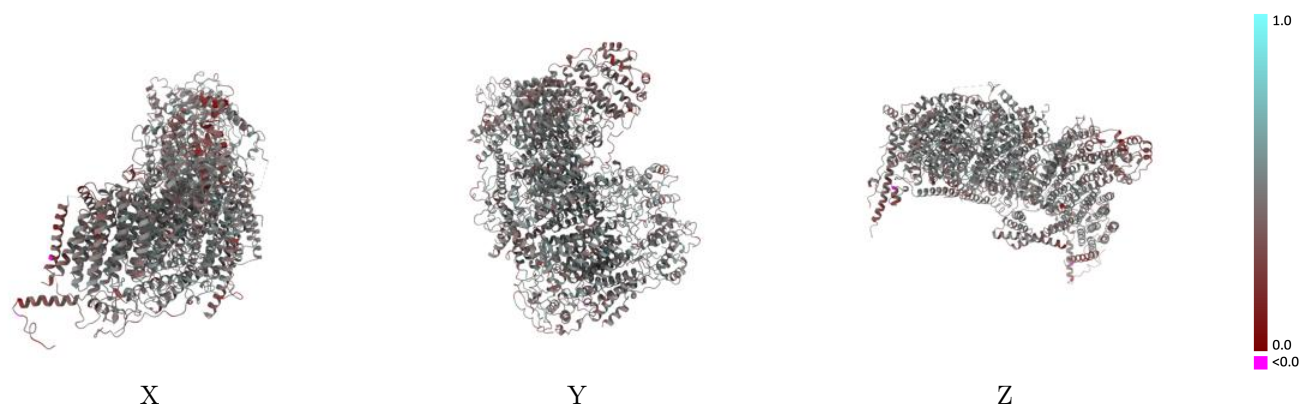
This section contains information regarding the fit between EMDB map EMD-35354 and PDB model 8IC4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



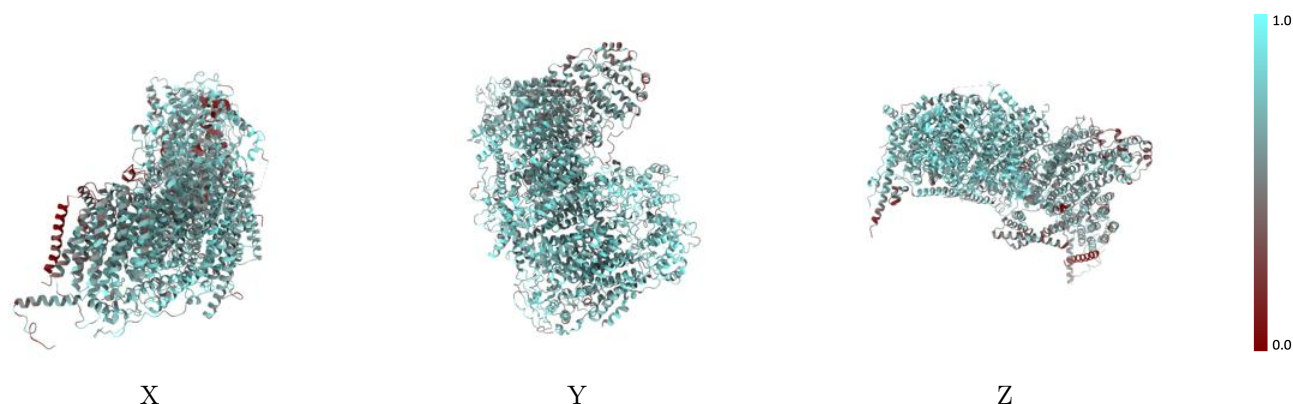
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



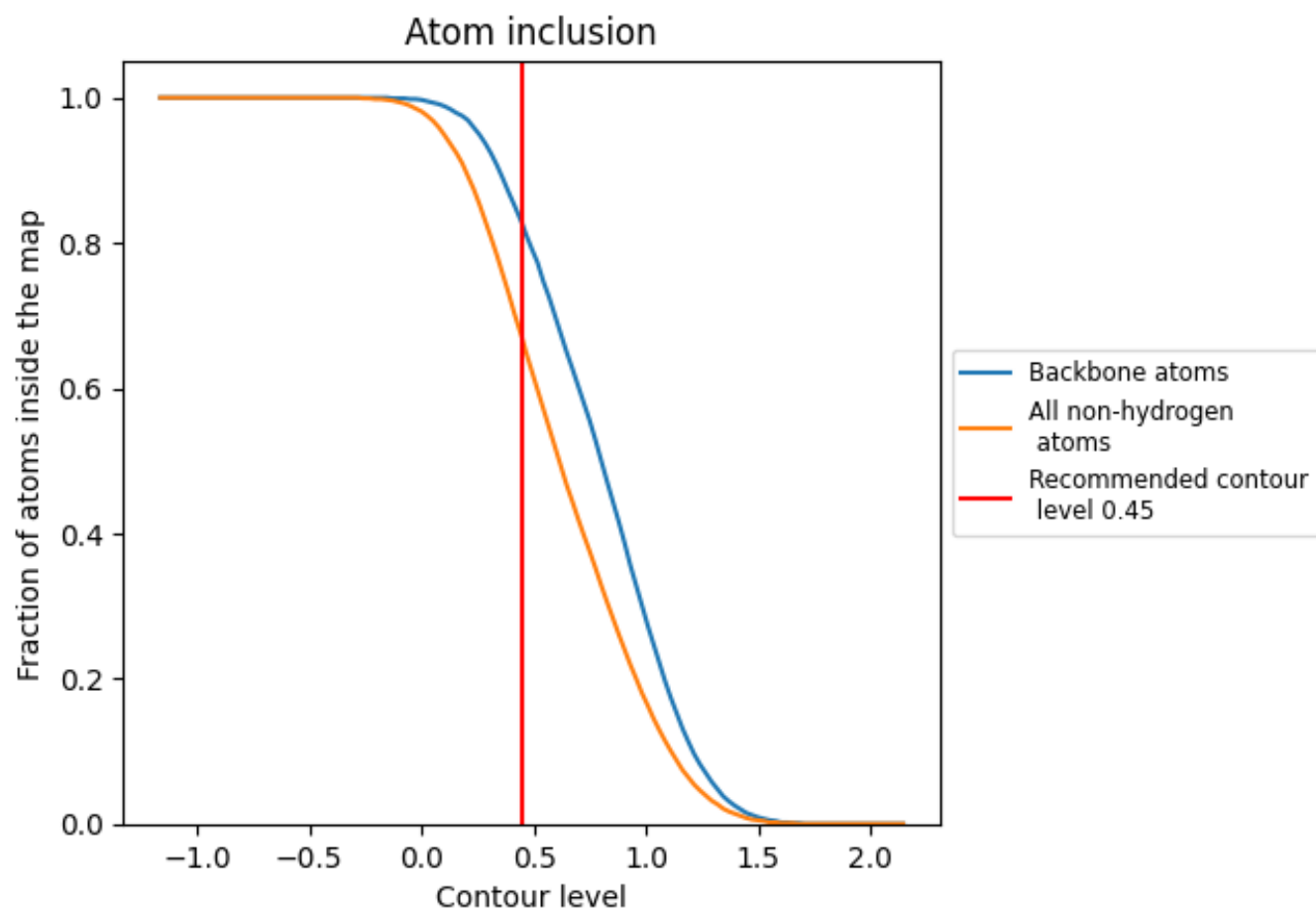
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 67% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.4500
D	 0.4170	 0.4180
J	 0.4460	 0.4010
K	 0.6210	 0.4630
L	 0.6960	 0.4680
M	 0.7040	 0.4860
N	 0.6940	 0.4770
O	 0.5680	 0.3830
U	 0.7420	 0.4720
X	 0.7450	 0.4480
Y	 0.4880	 0.4150
c	 0.5820	 0.4040
d	 0.7030	 0.4670
e	 0.6030	 0.3850
f	 0.6640	 0.4600
g	 0.7100	 0.4560
h	 0.7180	 0.4630
i	 0.7060	 0.4560
j	 0.6920	 0.4160
k	 0.7520	 0.4620
l	 0.7480	 0.4710
m	 0.6850	 0.4550
n	 0.7610	 0.4750
o	 0.6540	 0.4080
p	 0.7070	 0.4380

