wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 09:37 PM UTC

PDB ID	:	7VWL / pdb_00007vwl
EMDB ID	:	EMD-32155
Title	:	Membrane arm of deactive state CI from rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-11
Resolution	:	2.70 Å(reported)

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

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

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

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

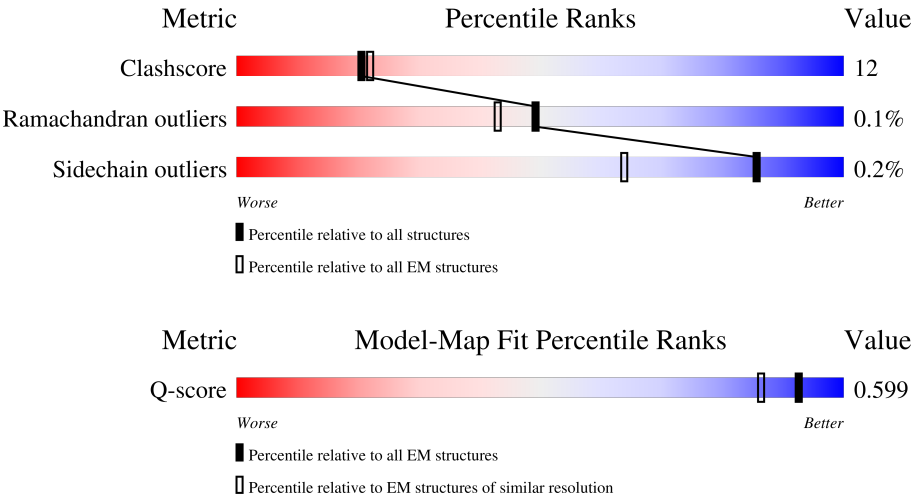
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	40	22% 75% 25%
2	S	70	81% 19%
3	U	83	6% 88% 12%
4	V	140	21% 74% 25%

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Mol	Chain	Length	Quality of chain
5	W	113	82% 18%
6	X	88	7% 77% 23%
7	Y	70	19% 79% 21%
8	Z	84	21% 87% 13%
9	a	140	80% 20%
10	b	126	11% 68% 13% 18%
11	c	156	5% 79% 21%
12	d	175	6% 79% 21%
13	e	107	12% 79% 21%
14	f	42	12% 88% 12%
15	g	121	88% 12%
16	h	105	70% 30%
17	i	347	73% 27%
18	j	113	17% 59% 27% 12%
19	k	98	5% 78% 22%
20	l	603	73% 27%
21	m	175	8% 52% 22% 26%
22	n	56	18% 70% 27%
23	o	128	5% 89% 11%
24	p	178	83% 17%
25	r	459	80% 20%
26	s	318	73% 21% 5%
27	u	171	70% 30%
28	v	131	15% 60% 34% 5%
29	w	320	9% 78% 22%

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
30	CDL	a	201	-	-	X	-
30	CDL	i	401	-	-	X	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 39049 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	Q	40	Total	C	N	O	S	0	0
			333	217	56	59	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			702	452	103	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			343	225	58	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	603	Total	C	N	O	S	0	0
			4773	3164	740	819	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			448	291	81	75	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	o	128	Total	C	N	O	0	0
			1062	691	182	189		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			1032	644	195	184	9		

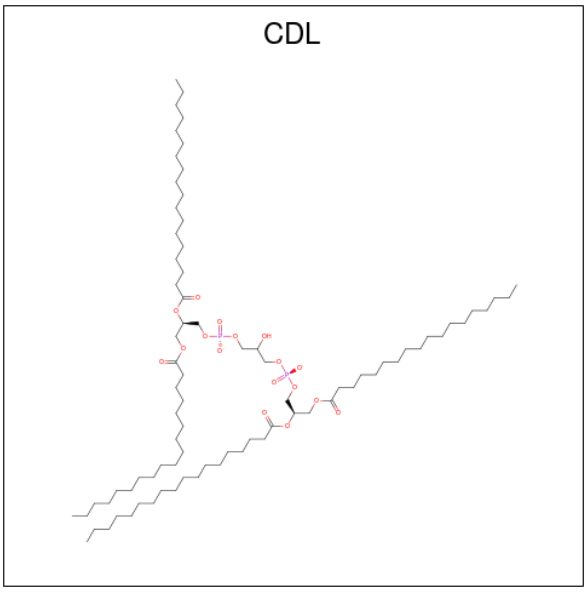
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

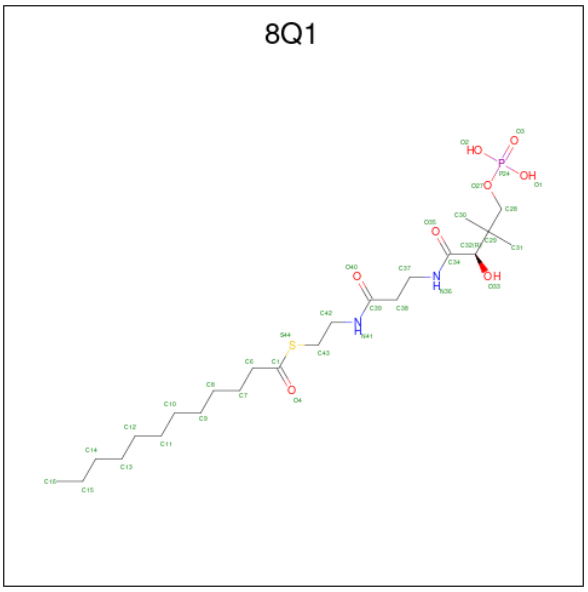
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2576	1640	435	491	10		

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



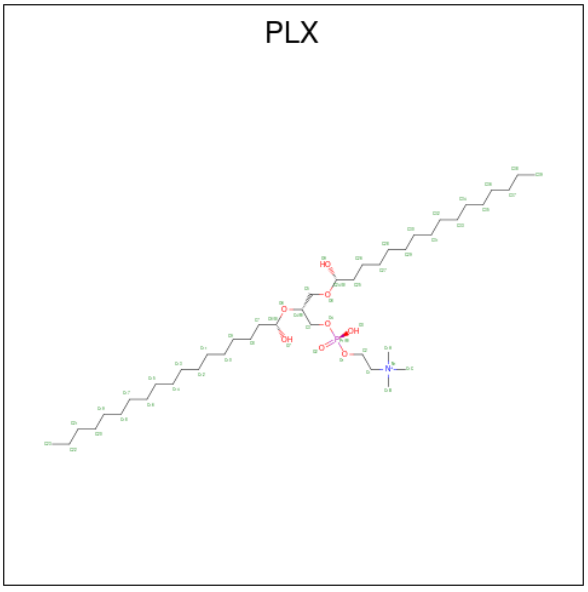
Mol	Chain	Residues	Atoms				AltConf
30	V	1	Total	C	O	P	0
			71	52	17	2	
30	a	1	Total	C	O	P	0
			91	72	17	2	
30	i	1	Total	C	O	P	0
			66	47	17	2	
30	l	1	Total	C	O	P	0
			65	46	17	2	
30	r	1	Total	C	O	P	0
			99	80	17	2	
30	r	1	Total	C	O	P	0
			100	81	17	2	
30	u	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 31 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
31	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 32 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



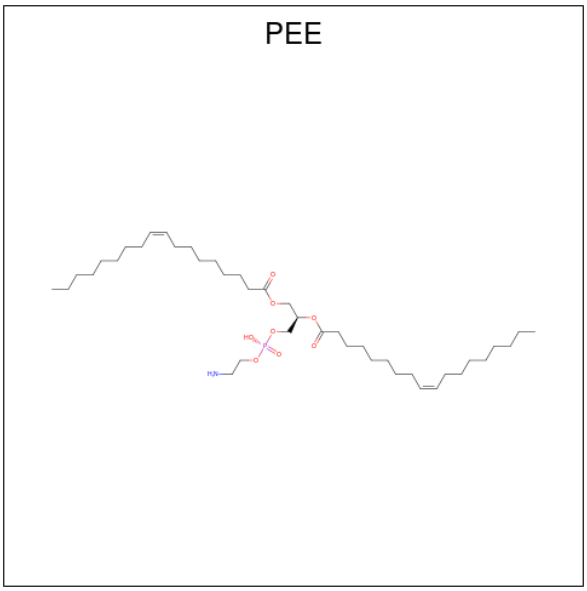
Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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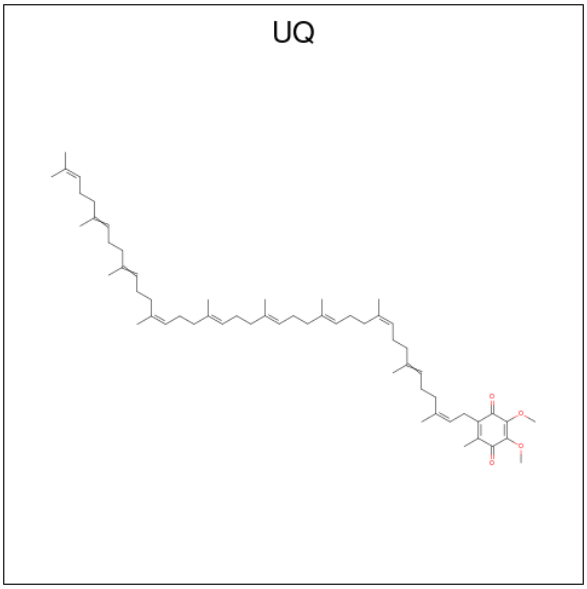
Mol	Chain	Residues	Atoms					AltConf
32	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 33 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



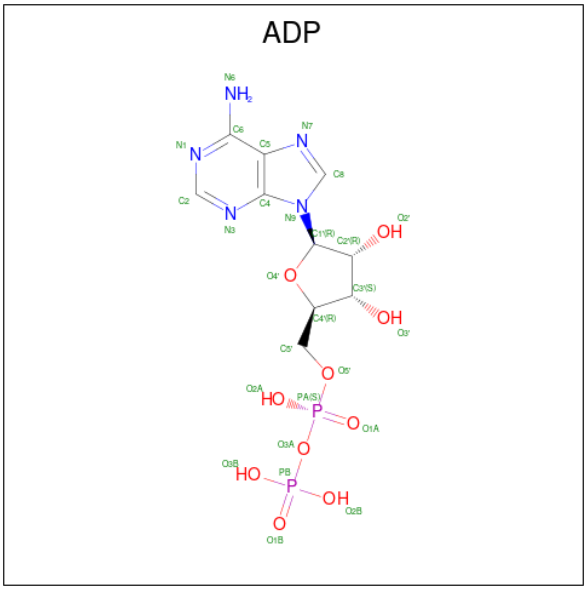
Mol	Chain	Residues	Atoms					AltConf
33	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
33	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
33	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
33	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
33	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			28	24	4	

- Molecule 35 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
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	Q	6	Total O 6 6	0
36	S	1	Total O 1 1	0
36	U	3	Total O 3 3	0
36	V	2	Total O 2 2	0
36	a	4	Total O 4 4	0
36	b	1	Total O 1 1	0
36	c	5	Total O 5 5	0
36	d	2	Total O 2 2	0
36	e	2	Total O 2 2	0
36	h	4	Total O 4 4	0
36	i	62	Total O 62 62	0
36	j	14	Total O 14 14	0
36	k	15	Total O 15 15	0
36	l	53	Total O 53 53	0
36	m	14	Total O 14 14	0
36	n	2	Total O 2 2	0
36	p	2	Total O 2 2	0
36	r	84	Total O 84 84	0
36	s	65	Total O 65 65	0
36	u	1	Total O 1 1	0
36	w	3	Total O 3 3	0

3 Residue-property plots (i)

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

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

Chain Q:





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

Chain S:

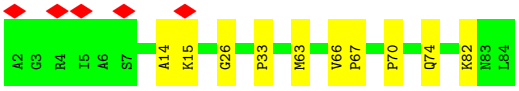




• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:

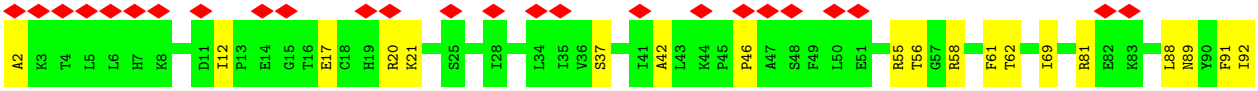


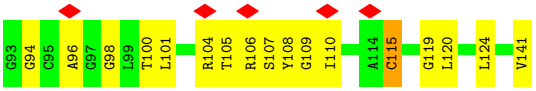


• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:







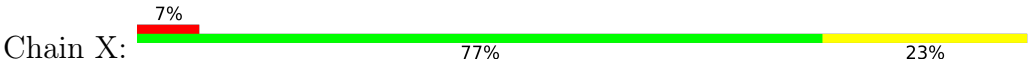
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

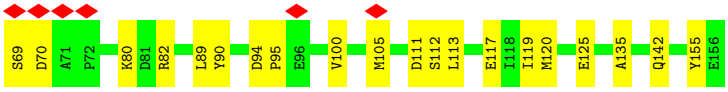
Chain W:



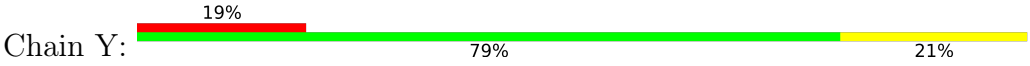


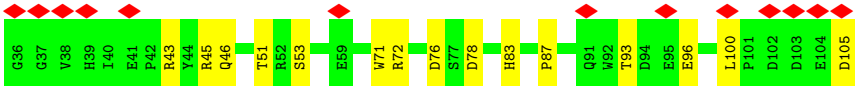
• Molecule 6: Acyl carrier protein, mitochondrial



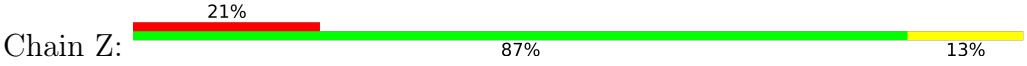


• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



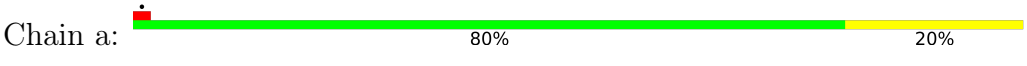


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3





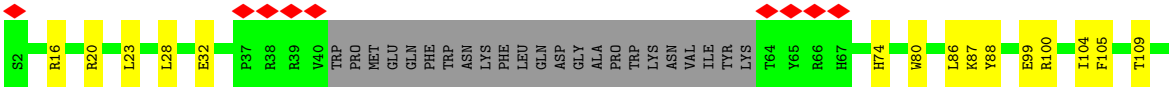
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

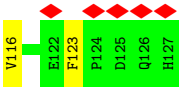




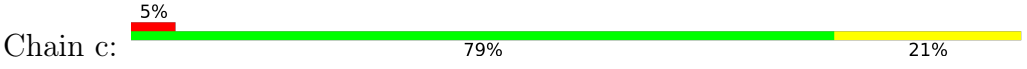
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

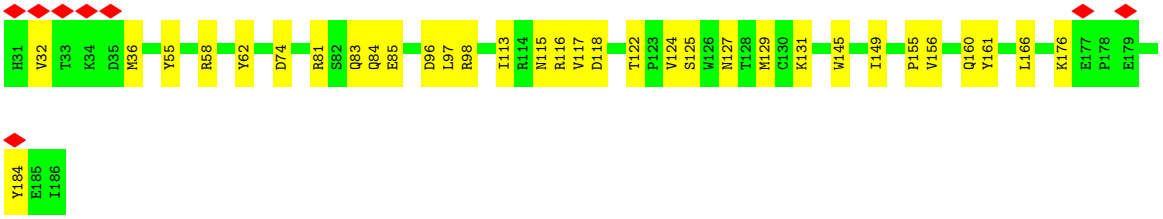




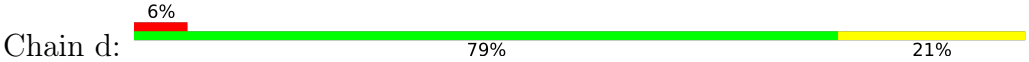


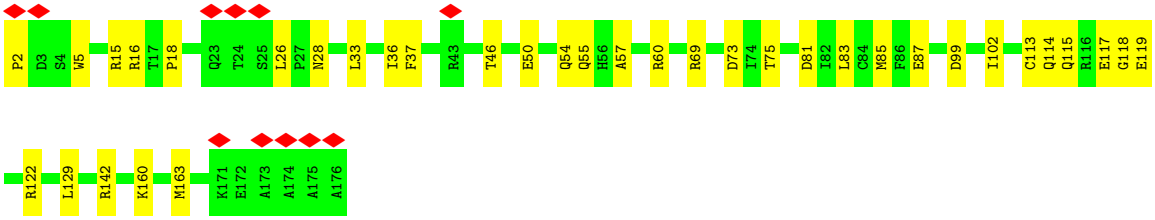
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



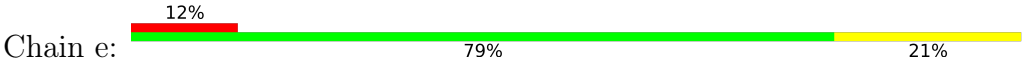


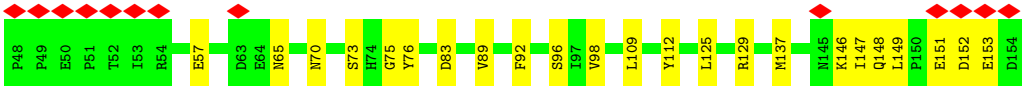
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



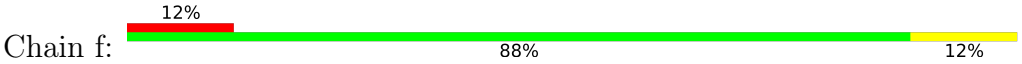


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



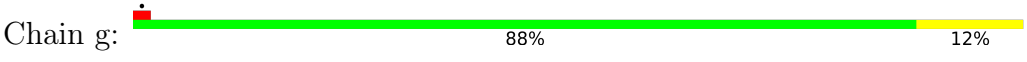


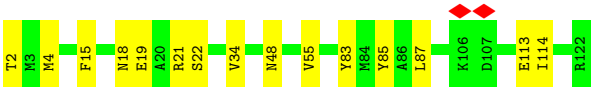
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial





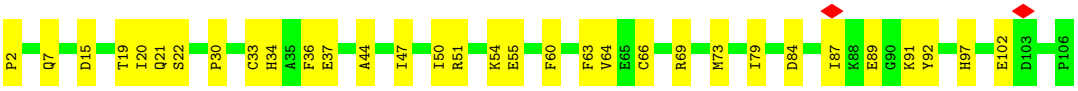
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2





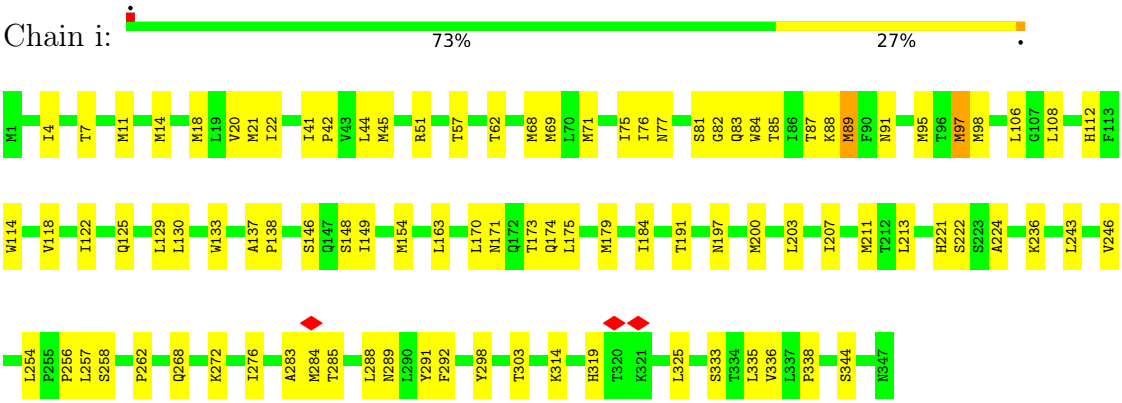
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5





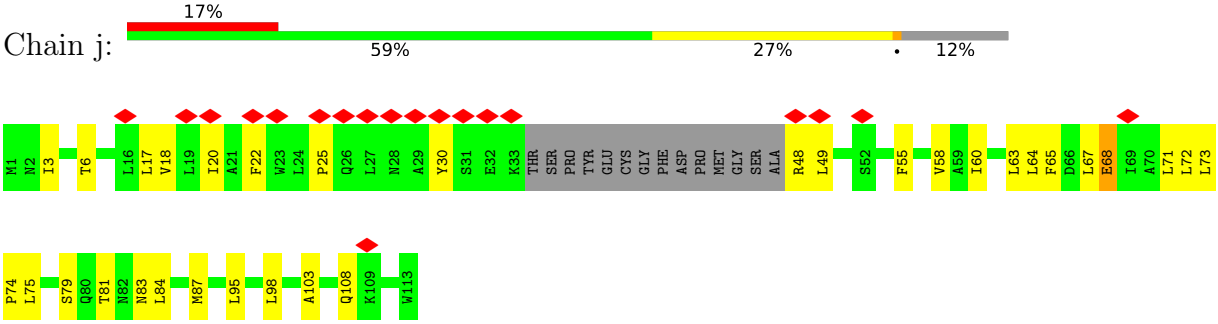
• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i:



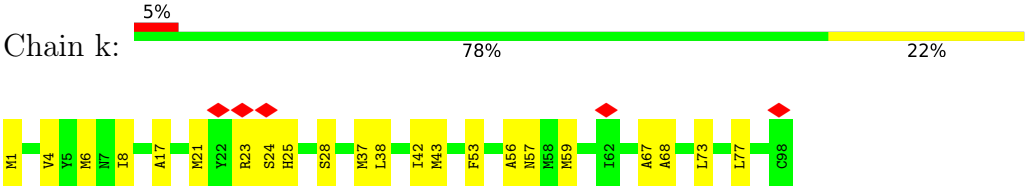
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:



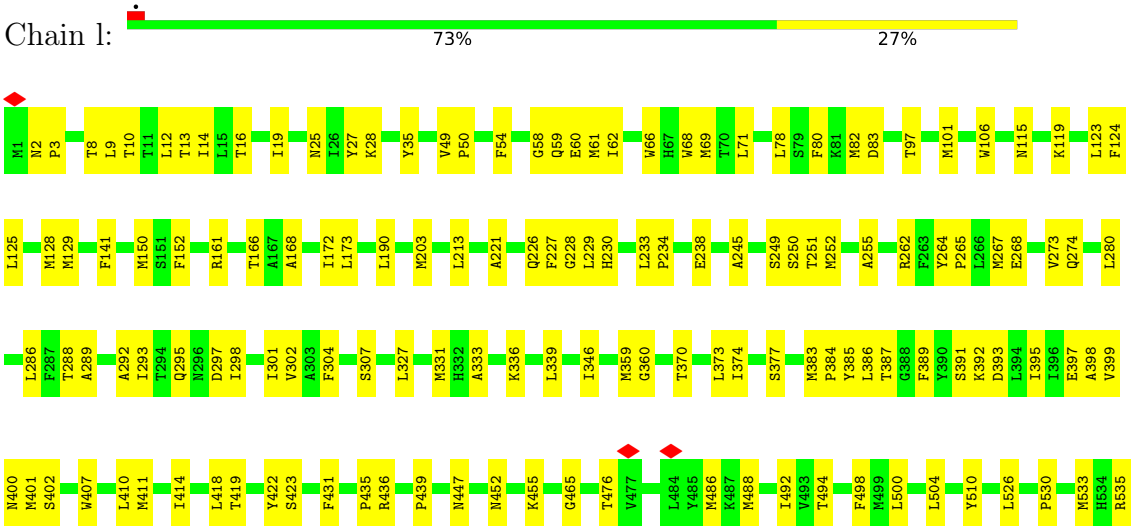
• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

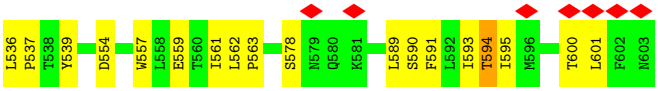
Chain k:



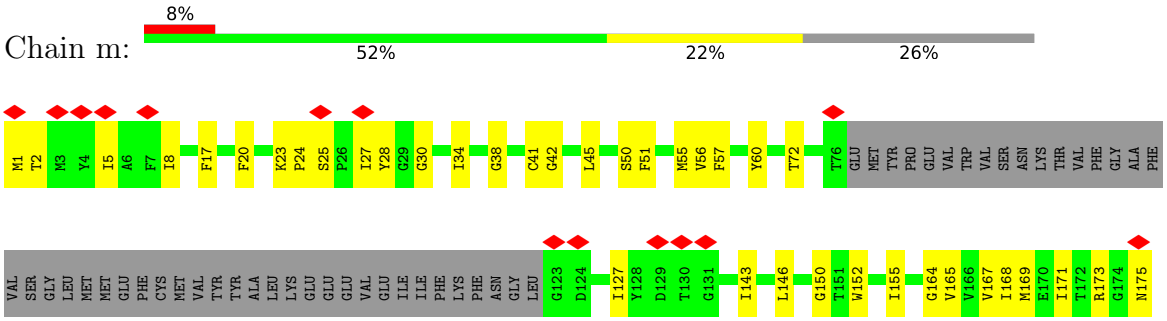
• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:

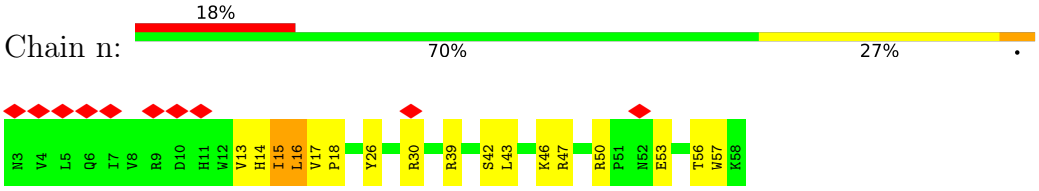




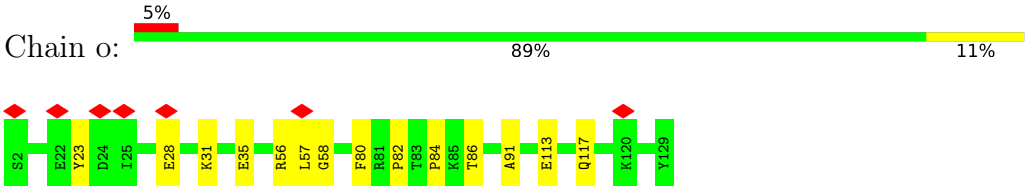
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6



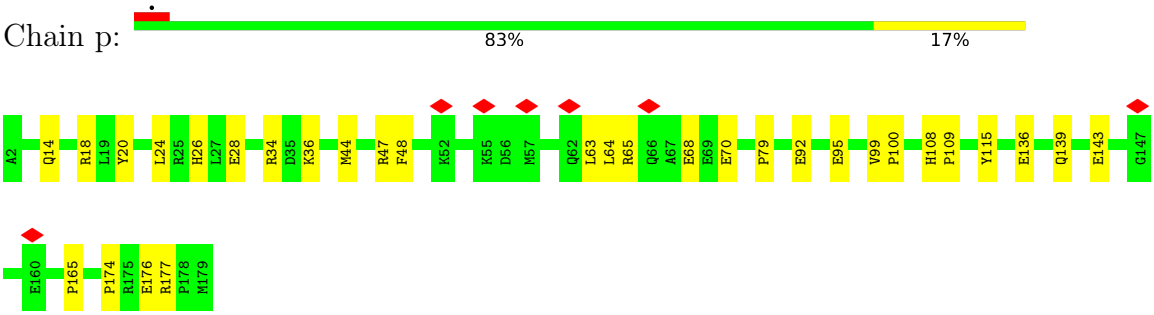
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



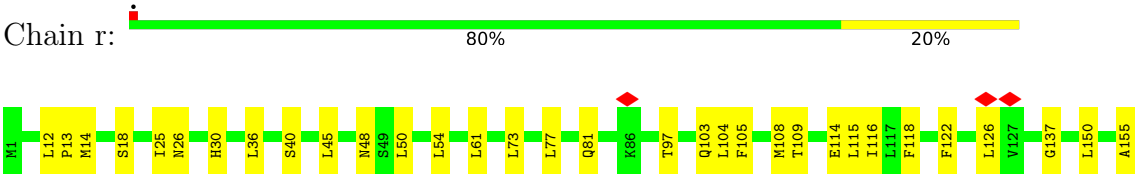
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

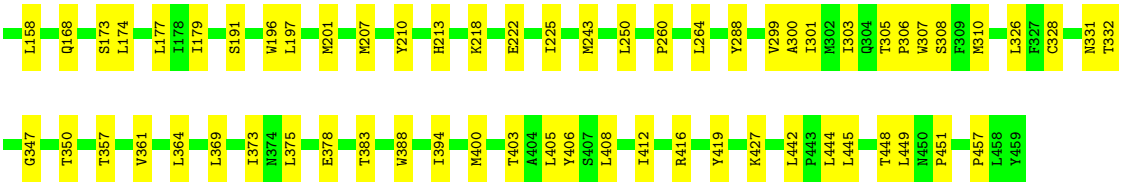


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



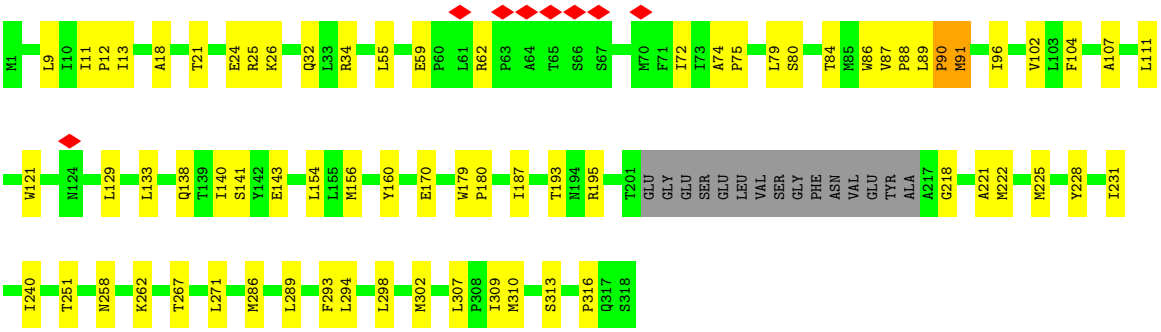
• Molecule 25: NADH-ubiquinone oxidoreductase chain 4





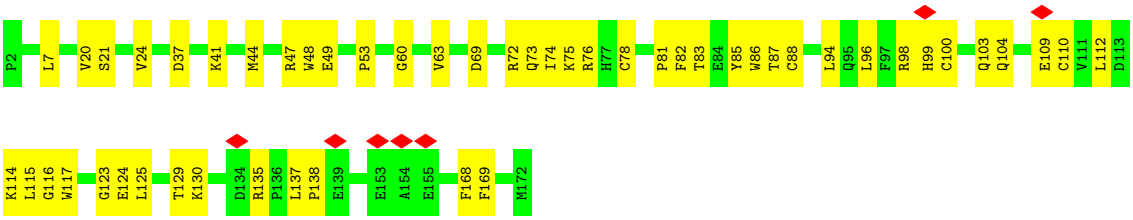
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1





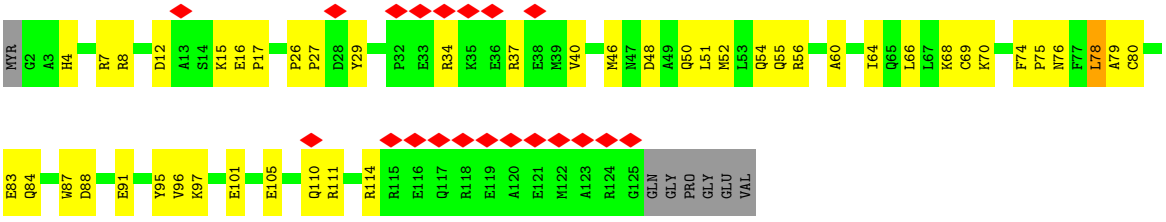
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



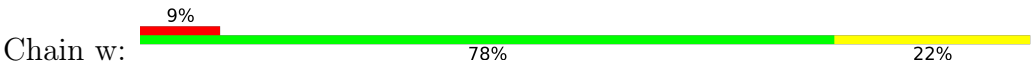


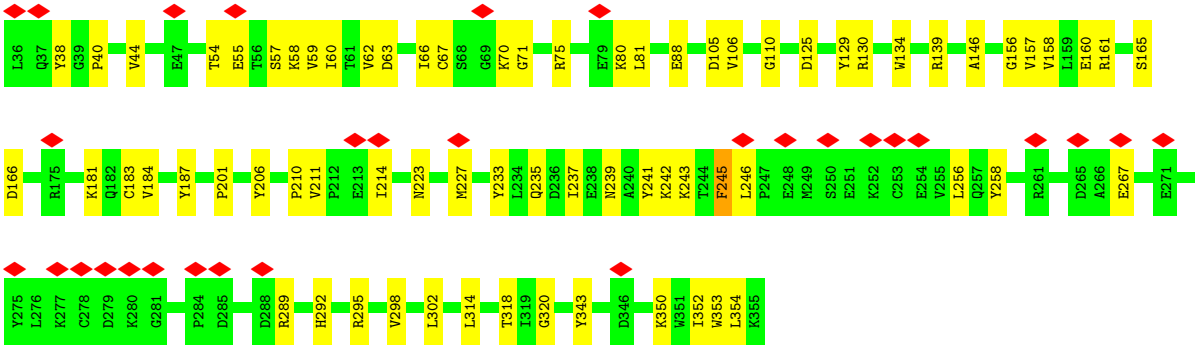
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





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




L36 Q37 Y38 G39 P40 V44 E47 T54 E55 T56 S57 K58 V59 I60 T61 V62 D63 I66 C67 S68 G69 K70 G71 R75 E79 K80 L81 E88 D105 V106 G110 D125 Y129 R130 W134 R139 A146 G156 V157 V158 L159 E160 R161 S165
D166 R175 K181 Q182 C183 V184 Y187 P201 Y206 P210 V211 P212 E213 I214 N223 M227 Y233 L234 Q235 D236 I237 E238 N239 A240 Y241 K242 K243 T244 F245 L246 P247 E248 M249 S250 E251 K252 C253 E254 V255 L256 Q257 Y258 R261 D265 A266 E267 E271
Y275 L276 K277 C278 D279 K280 G281 P284 D285 D288 R289 H292 R295 V298 L302 L314 T318 I319 G320 Y343 D346 K350 W351 I352 W353 L354 K355

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169835	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	257.808, 257.808, 257.808	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, 8Q1, ADP, CDL, UQ, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	Q	0.24	0/350	0.42	0/483
2	S	0.16	0/582	0.37	0/783
3	U	0.13	0/664	0.31	0/912
4	V	0.19	0/1042	0.46	0/1411
5	W	0.16	0/973	0.31	0/1312
6	X	0.14	0/714	0.36	0/967
7	Y	0.14	0/626	0.36	0/857
8	Z	0.12	0/695	0.31	0/939
9	a	0.19	0/1199	0.41	1/1623 (0.1%)
10	b	0.16	0/906	0.37	0/1232
11	c	0.17	0/1371	0.36	0/1875
12	d	0.15	0/1494	0.32	0/2015
13	e	0.16	0/916	0.40	0/1246
14	f	0.17	0/351	0.33	0/474
15	g	0.15	0/1031	0.32	0/1394
16	h	0.18	0/889	0.42	0/1190
17	i	0.18	0/2773	0.39	1/3768 (0.0%)
18	j	0.22	0/819	0.51	0/1117
19	k	0.21	0/759	0.42	0/1029
20	l	0.18	0/4901	0.42	1/6667 (0.0%)
21	m	0.21	0/973	0.50	0/1320
22	n	0.22	0/459	0.62	1/621 (0.2%)
23	o	0.15	0/1092	0.36	0/1481
24	p	0.16	0/1590	0.34	0/2155
25	r	0.18	0/3723	0.38	0/5078
26	s	0.20	0/2464	0.48	0/3369
27	u	0.19	0/1436	0.52	2/1938 (0.1%)
28	v	0.20	0/1056	0.56	1/1416 (0.1%)
29	w	0.17	0/2636	0.44	4/3573 (0.1%)
All	All	0.18	0/38484	0.41	11/52245 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	s	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	i	89	MET	N-CA-C	7.24	119.17	111.28
9	a	91	VAL	N-CA-C	6.65	116.78	110.53
20	l	600	THR	N-CA-C	6.18	118.09	111.36
29	w	243	LYS	N-CA-C	5.73	117.61	111.36
22	n	16	LEU	N-CA-C	5.64	117.43	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	s	91	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	333	0	301	9	0
2	S	567	0	565	14	0
3	U	643	0	642	9	0
4	V	1021	0	1027	42	0
5	W	949	0	935	19	0
6	X	702	0	683	17	0
7	Y	600	0	539	12	0
8	Z	674	0	643	8	0
9	a	1165	0	1174	27	0
10	b	879	0	899	20	0
11	c	1315	0	1208	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	d	1461	0	1429	34	0
13	e	890	0	837	22	0
14	f	343	0	344	4	0
15	g	1000	0	994	14	0
16	h	867	0	873	26	0
17	i	2710	0	2874	99	0
18	j	800	0	855	50	0
19	k	748	0	799	23	0
20	l	4773	0	4915	135	0
21	m	951	0	962	51	0
22	n	448	0	426	22	0
23	o	1062	0	1072	12	0
24	p	1534	0	1470	19	0
25	r	3631	0	3839	81	0
26	s	2394	0	2508	72	0
27	u	1398	0	1380	57	0
28	v	1032	0	986	46	0
29	w	2576	0	2520	55	0
30	V	71	0	92	16	0
30	a	91	0	132	35	0
30	i	66	0	76	21	0
30	l	65	0	74	7	0
30	r	199	0	307	19	0
30	u	63	0	70	18	0
31	X	35	0	0	1	0
32	a	52	0	88	10	0
32	e	52	0	88	5	0
32	i	52	0	88	4	0
32	j	52	0	88	6	0
32	r	52	0	88	10	0
33	i	47	0	71	16	0
33	j	51	0	82	9	0
33	l	92	0	138	25	0
33	m	41	0	59	16	0
33	r	51	0	82	12	0
33	s	51	0	82	2	0
34	s	28	0	31	7	0
35	w	27	0	11	1	0
36	Q	6	0	0	0	0
36	S	1	0	0	0	0
36	U	3	0	0	0	0
36	V	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	4	0	0	0	0
36	b	1	0	0	0	0
36	c	5	0	0	0	0
36	d	2	0	0	0	0
36	e	2	0	0	0	0
36	h	4	0	0	2	0
36	i	62	0	0	9	0
36	j	14	0	0	1	0
36	k	15	0	0	0	0
36	l	53	0	0	3	0
36	m	14	0	0	2	0
36	n	2	0	0	3	0
36	p	2	0	0	0	0
36	r	84	0	0	5	0
36	s	65	0	0	5	0
36	u	1	0	0	0	0
36	w	3	0	0	0	0
All	All	39049	0	39446	942	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 12.

The worst 5 of 942 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)
28:v:69:CYS:SG	28:v:80:CYS:HB3	1.56	1.45
27:u:78:CYS:HB3	27:u:110:CYS:SG	1.71	1.30
28:v:69:CYS:SG	28:v:80:CYS:CB	2.30	1.19
29:w:66:ILE:O	29:w:214:ILE:HD11	1.40	1.18
18:j:3:ILE:HG21	33:m:201:PEE:H13	1.23	1.11

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
4	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	41
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
9	a	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	b	99/126 (79%)	92 (93%)	7 (7%)	0	100	100
11	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
12	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
13	e	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
14	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
15	g	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
16	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
19	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
20	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
21	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
24	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	44
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	36	60
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/131 (93%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	303 (95%)	14 (4%)	1 (0%)	36	60
All	All	4586/4757 (96%)	4399 (96%)	183 (4%)	4 (0%)	49	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	w	67	CYS
4	V	46	PRO
26	s	90	PRO
24	p	174	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	58 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	100 (99%)	1 (1%)	68	86
5	W	10/99 (10%)	10 (100%)	0	100	100
8	Z	16/65 (25%)	16 (100%)	0	100	100
9	a	122/122 (100%)	122 (100%)	0	100	100
10	b	40/119 (34%)	40 (100%)	0	100	100
12	d	2/155 (1%)	2 (100%)	0	100	100
13	e	45/99 (46%)	45 (100%)	0	100	100
14	f	36/38 (95%)	36 (100%)	0	100	100
15	g	108/108 (100%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	310 (100%)	1 (0%)	86	94
18	j	88/99 (89%)	87 (99%)	1 (1%)	65	85
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	534/537 (99%)	533 (100%)	1 (0%)	87	95
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	44/53 (83%)	43 (98%)	1 (2%)	44	73
23	o	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	p	159/159 (100%)	159 (100%)	0	100 100
25	r	410/410 (100%)	410 (100%)	0	100 100
26	s	263/275 (96%)	263 (100%)	0	100 100
27	u	153/153 (100%)	152 (99%)	1 (1%)	76 90
28	v	105/115 (91%)	103 (98%)	2 (2%)	50 77
29	w	280/283 (99%)	280 (100%)	0	100 100
All	All	3378/3894 (87%)	3370 (100%)	8 (0%)	85 95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	v	78	LEU
28	v	8	ARG
22	n	15	ILE
20	l	594	THR
27	u	109	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
27	u	99	HIS
28	v	4	HIS
20	l	192	HIS
20	l	175	ASN
28	v	85	HIS

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)

22 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	$\#\|Z\| > 2$
30	CDL	u	201	-	62,62,99	1.14	4 (6%)	68,74,111	1.14	4 (5%)
32	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
30	CDL	V	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.11	6 (7%)
33	PEE	l	702	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
32	PLX	i	402	-	51,51,51	1.21	3 (5%)	53,59,59	0.62	1 (1%)
30	CDL	i	401	-	65,65,99	1.13	4 (6%)	71,77,111	1.23	8 (11%)
30	CDL	l	701	-	64,64,99	1.30	9 (14%)	70,76,111	1.01	4 (5%)
33	PEE	r	501	-	50,50,50	1.17	6 (12%)	53,55,55	0.98	2 (3%)
35	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.90	8 (18%)
34	UQ	s	402	-	28,28,63	3.32	9 (32%)	36,37,79	2.70	12 (33%)
33	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
30	CDL	r	503	-	98,98,99	1.11	9 (9%)	104,110,111	0.90	4 (3%)
33	PEE	i	403	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	2 (4%)
33	PEE	s	401	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
30	CDL	r	504	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
32	PLX	e	201	-	51,51,51	1.20	5 (9%)	53,59,59	0.64	1 (1%)
31	8Q1	X	201	-	32,34,34	2.23	7 (21%)	39,43,43	1.83	12 (30%)
32	PLX	r	502	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
30	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.11	6 (6%)
33	PEE	m	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
32	PLX	a	202	-	51,51,51	0.60	0	53,59,59	0.69	0
33	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)

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
30	CDL	u	201	-	-	17/73/73/110	-
32	PLX	j	202	-	-	30/55/55/55	-
30	CDL	V	201	-	-	28/81/81/110	-
33	PEE	l	702	-	-	18/49/49/54	-
32	PLX	i	402	-	-	27/55/55/55	-
30	CDL	i	401	-	-	29/76/76/110	-
30	CDL	l	701	-	-	36/75/75/110	-
33	PEE	r	501	-	-	22/54/54/54	-
35	ADP	w	401	-	-	4/16/32/32	0/3/3/3
34	UQ	s	402	-	-	9/21/45/87	0/1/1/1
33	PEE	l	703	-	-	24/49/49/54	-
30	CDL	r	503	-	-	56/109/109/110	-
33	PEE	i	403	-	-	19/50/50/54	-
33	PEE	s	401	-	-	26/54/54/54	-
30	CDL	r	504	-	-	66/110/110/110	-
32	PLX	e	201	-	-	33/55/55/55	-
31	8Q1	X	201	-	-	19/41/41/41	-
32	PLX	r	502	-	-	24/55/55/55	-
30	CDL	a	201	-	-	26/101/101/110	-
33	PEE	m	201	-	-	17/44/44/54	-
32	PLX	a	202	-	-	13/55/55/55	-
33	PEE	j	201	-	-	22/54/54/54	-

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C13-C14	9.67	1.55	1.33
34	s	402	UQ	C8-C9	9.30	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.94	1.30	1.53
34	s	402	UQ	C18-C19	7.90	1.56	1.32
35	w	401	ADP	O4'-C4'	7.76	1.62	1.45

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	s	402	UQ	C7-C8-C9	-8.91	111.49	126.83
34	s	402	UQ	C12-C13-C14	-6.04	113.80	127.62
31	X	201	8Q1	C6-C1-S44	5.59	120.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	w	401	ADP	C5-C4-N3	-5.46	119.20	126.72
35	w	401	ADP	N3-C2-N1	-4.54	121.70	128.58

There are no chirality outliers.

5 of 565 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	V	201	CDL	CA2-OA2-PA1-OA4
30	V	201	CDL	CA2-OA2-PA1-OA5
30	V	201	CDL	CB2-OB2-PB2-OB4
30	V	201	CDL	CB2-OB2-PB2-OB5
30	V	201	CDL	CB3-OB5-PB2-OB2

There are no ring outliers.

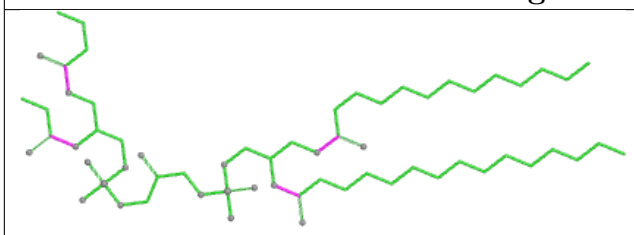
22 monomers are involved in 224 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	u	201	CDL	18	0
32	j	202	PLX	6	0
30	V	201	CDL	16	0
33	l	702	PEE	6	0
32	i	402	PLX	4	0
30	i	401	CDL	21	0
30	l	701	CDL	7	0
33	r	501	PEE	12	0
35	w	401	ADP	1	0
34	s	402	UQ	7	0
33	l	703	PEE	19	0
30	r	503	CDL	9	0
33	i	403	PEE	16	0
33	s	401	PEE	2	0
30	r	504	CDL	10	0
32	e	201	PLX	5	0
31	X	201	8Q1	1	0
32	r	502	PLX	10	0
30	a	201	CDL	35	0
33	m	201	PEE	16	0
32	a	202	PLX	10	0
33	j	201	PEE	9	0

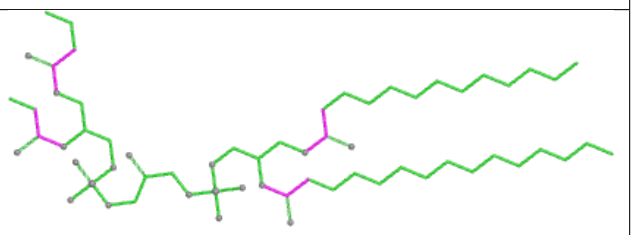
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

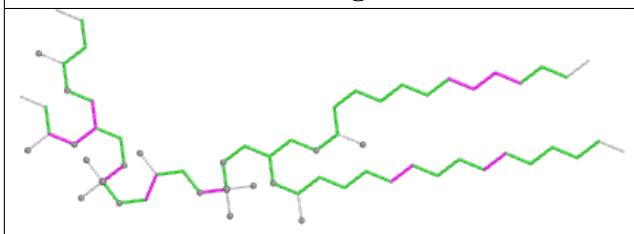
Ligand CDL u 201



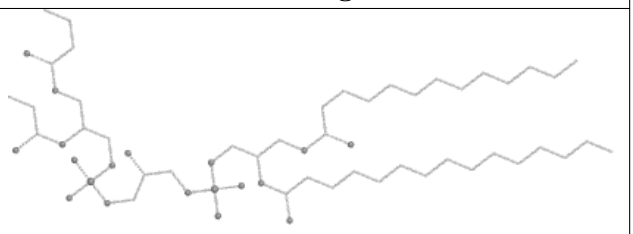
Bond lengths



Bond angles

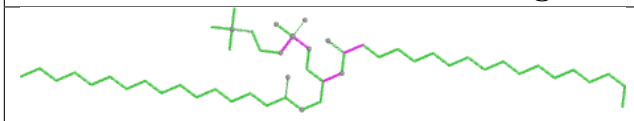


Torsions

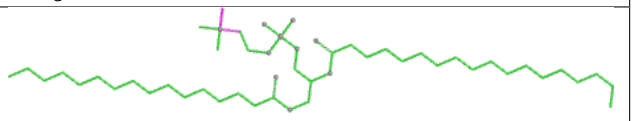


Rings

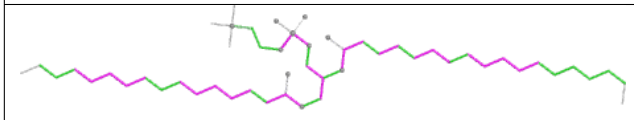
Ligand PLX j 202



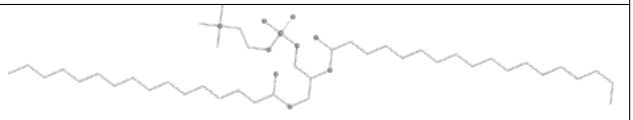
Bond lengths



Bond angles

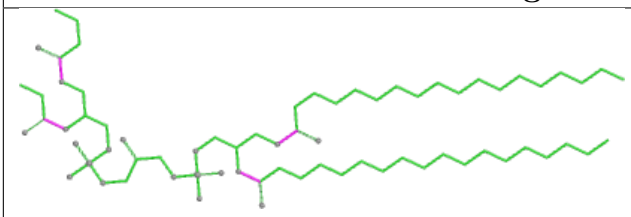


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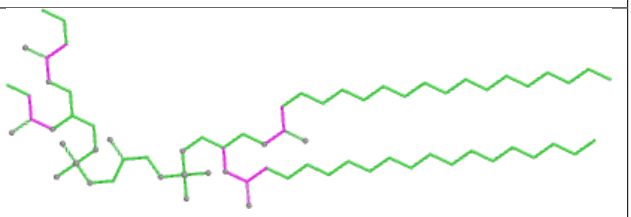


Rings

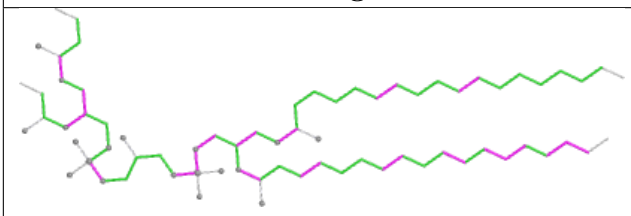
Ligand CDL V 201



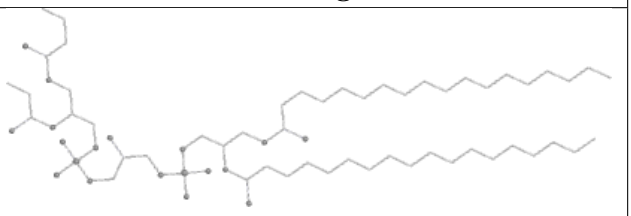
Bond lengths



Bond angles

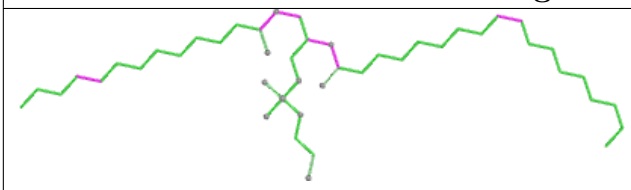


Torsions

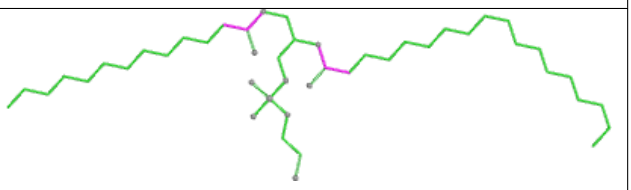


Rings

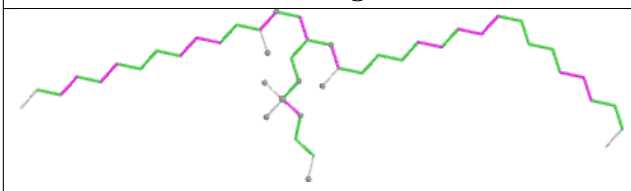
Ligand PEE l 702



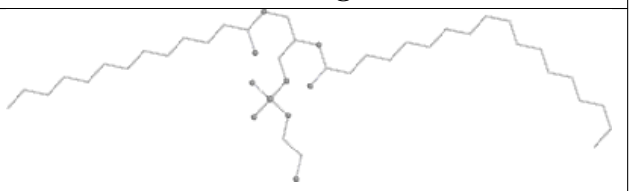
Bond lengths



Bond angles

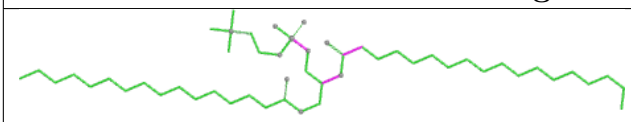


Torsions

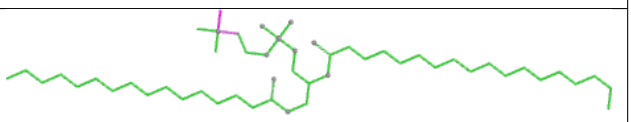


Rings

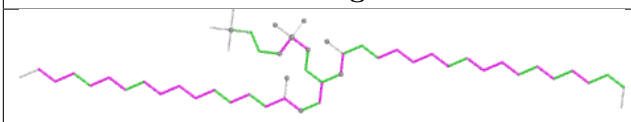
Ligand PLX i 402



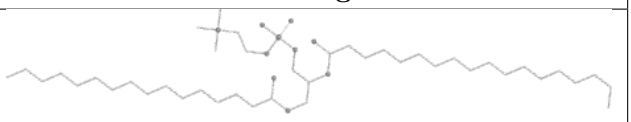
Bond lengths



Bond angles

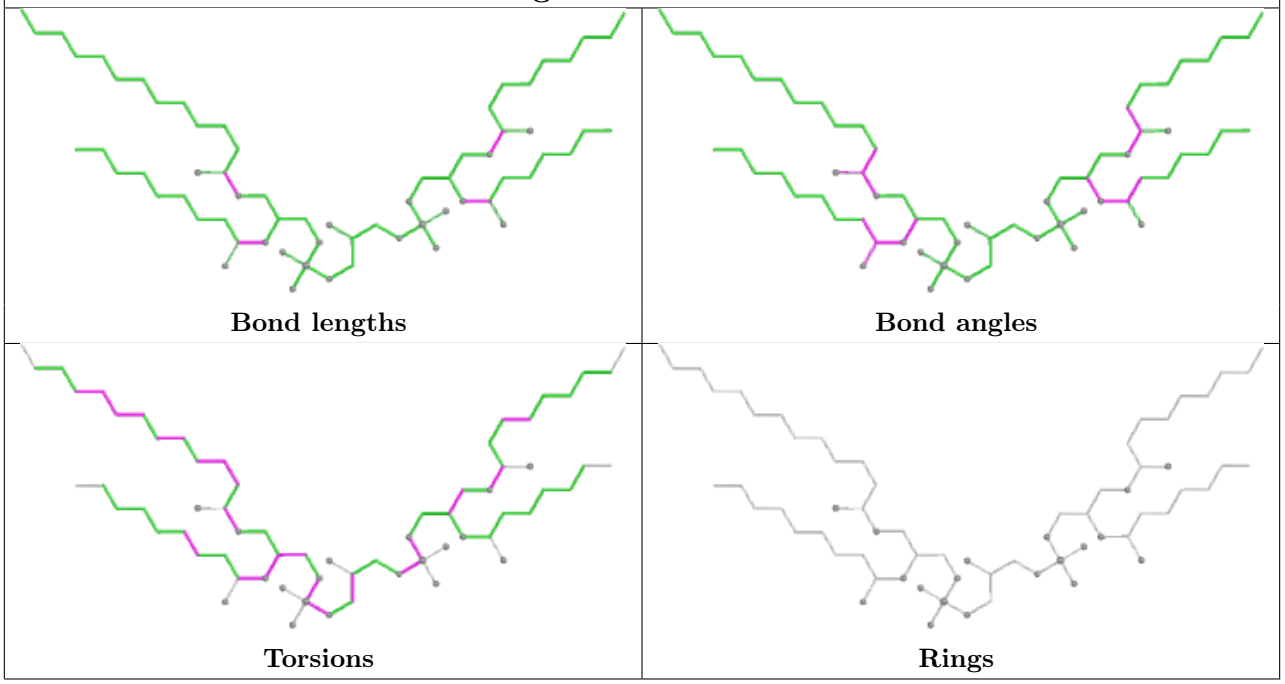


Torsions

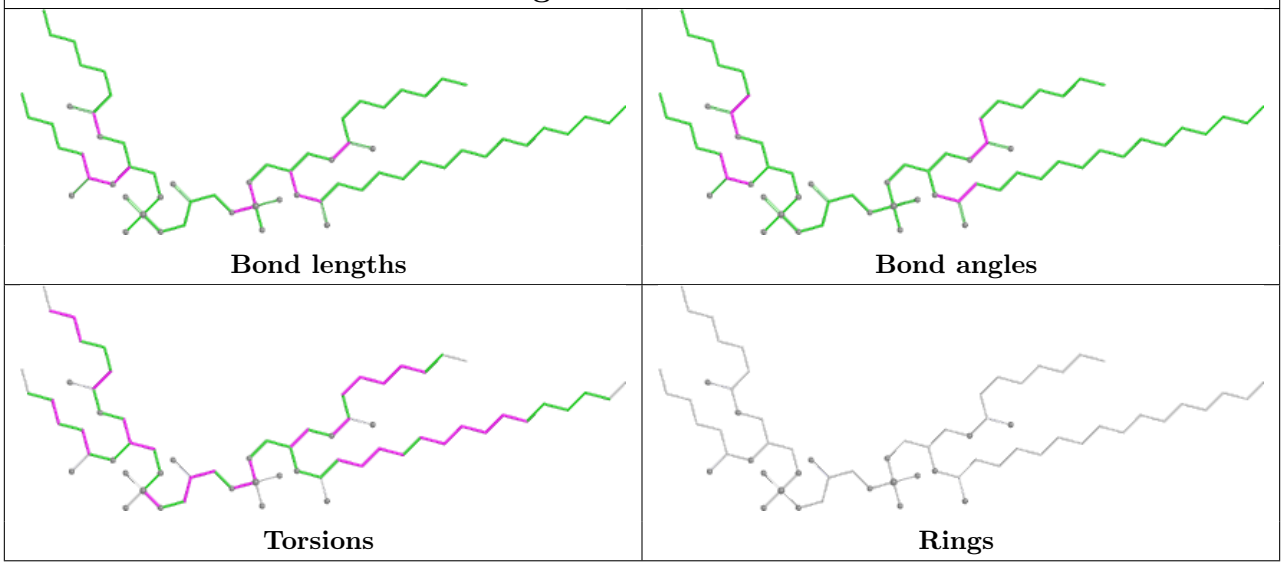


Rings

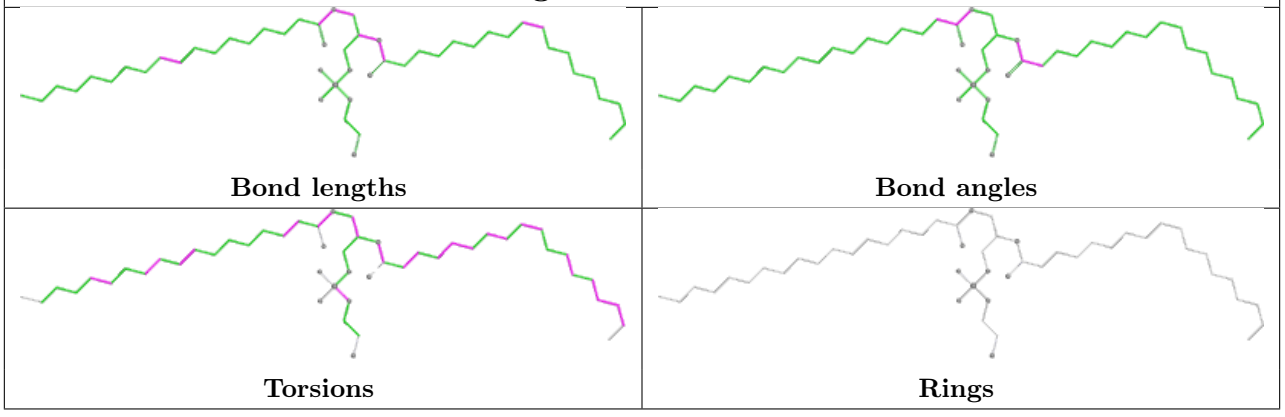
Ligand CDL i 401



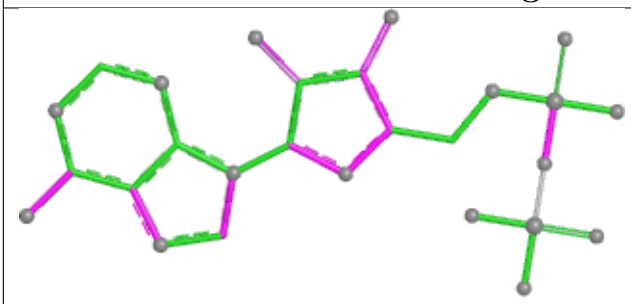
Ligand CDL l 701



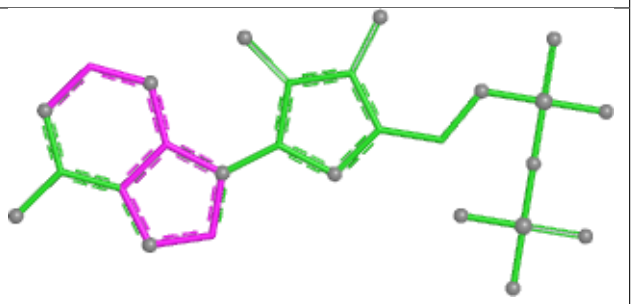
Ligand PEE r 501



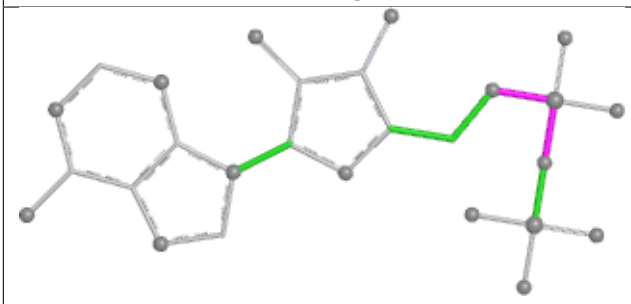
Ligand ADP w 401



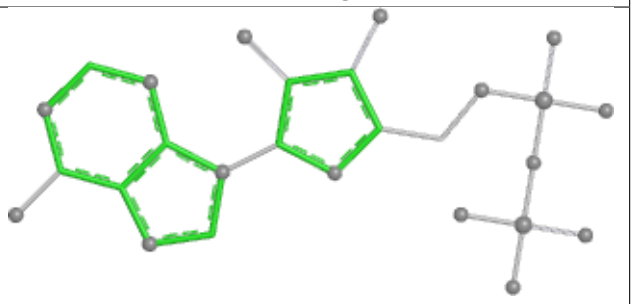
Bond lengths



Bond angles

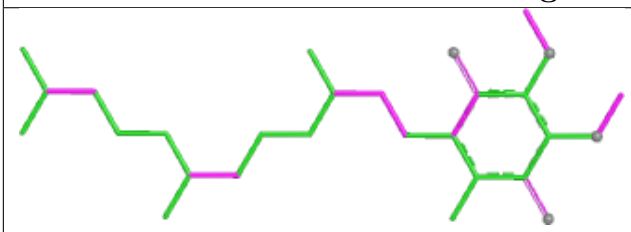


Torsions

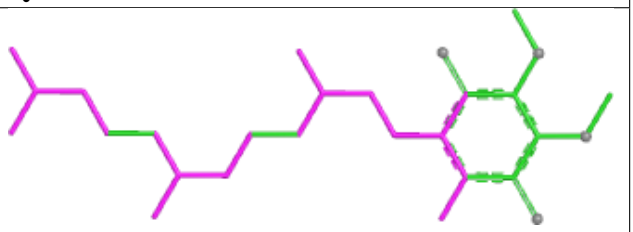


Rings

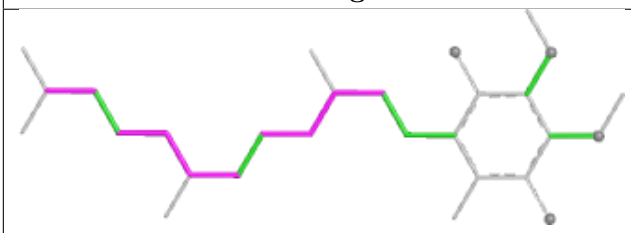
Ligand UQ s 402



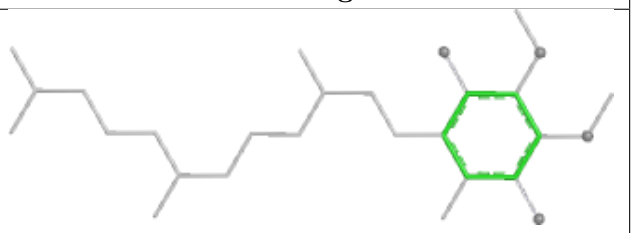
Bond lengths



Bond angles

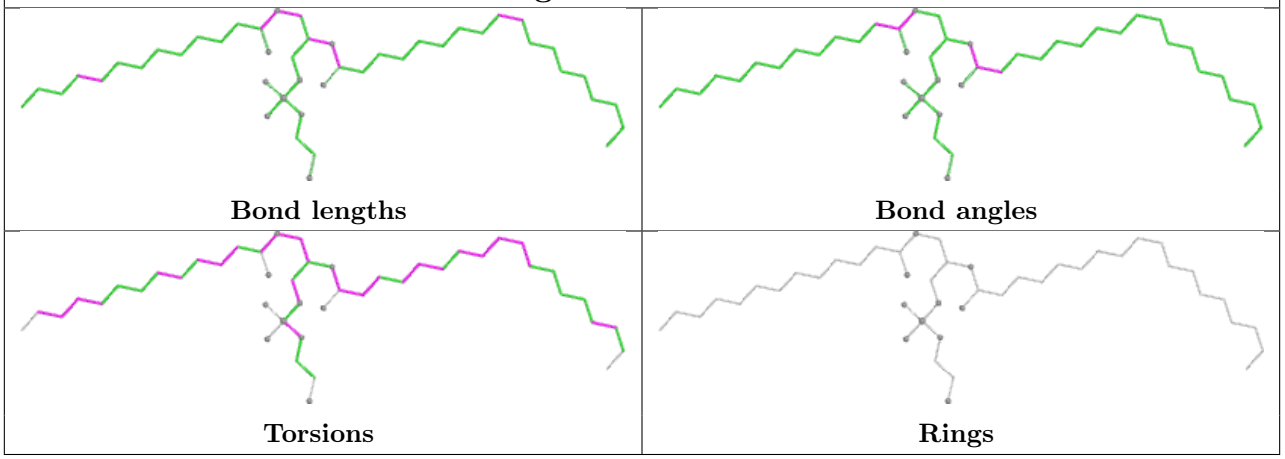


Torsions

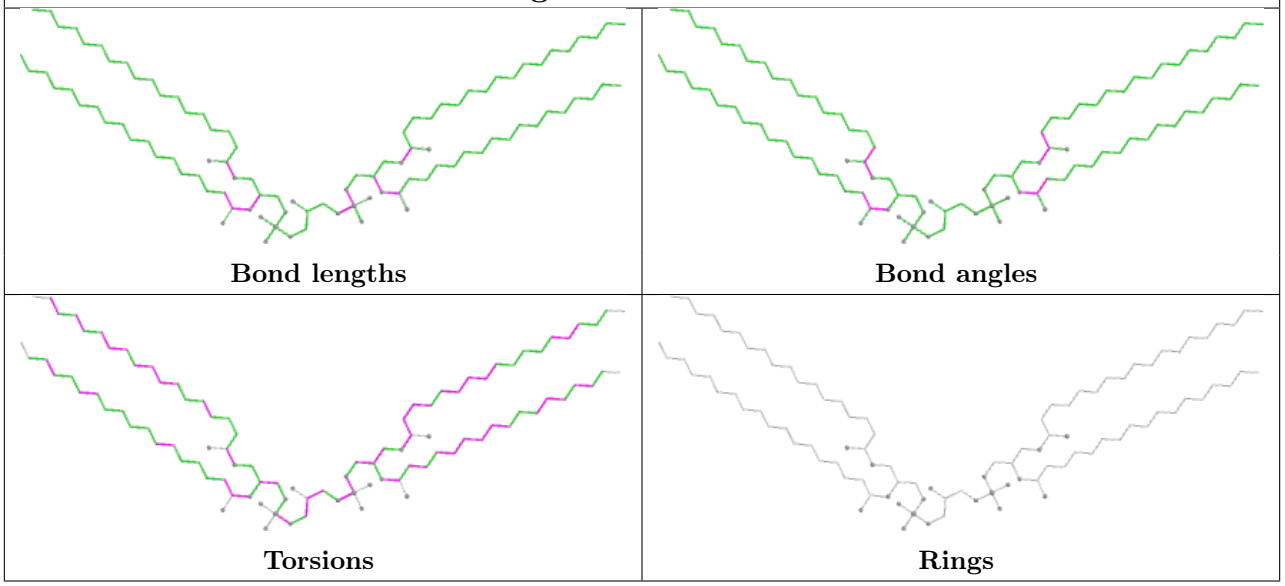


Rings

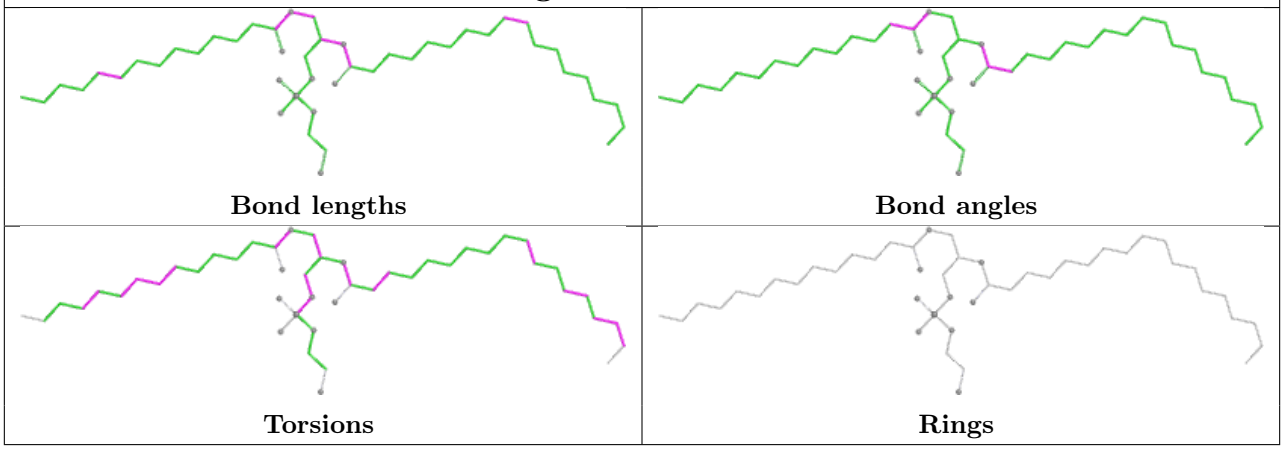
Ligand PEE l 703



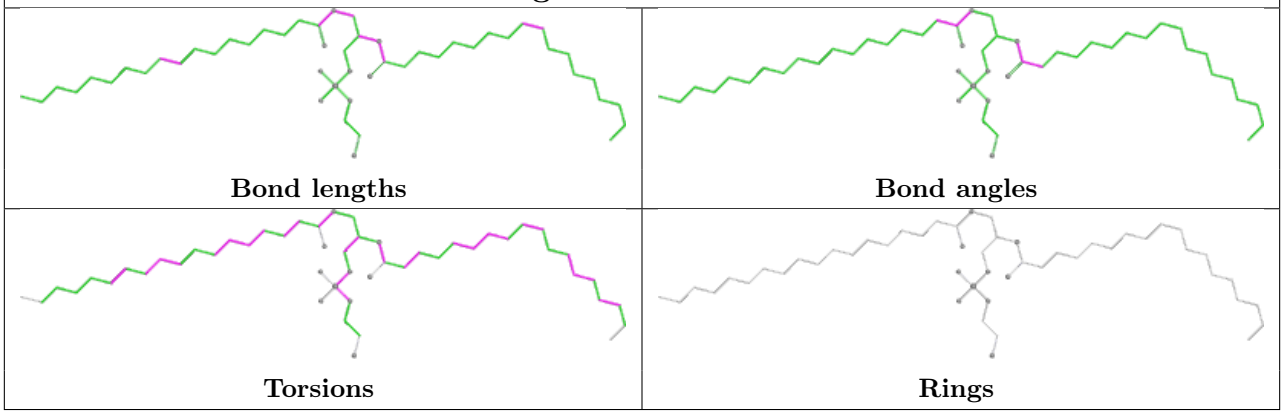
Ligand CDL r 503



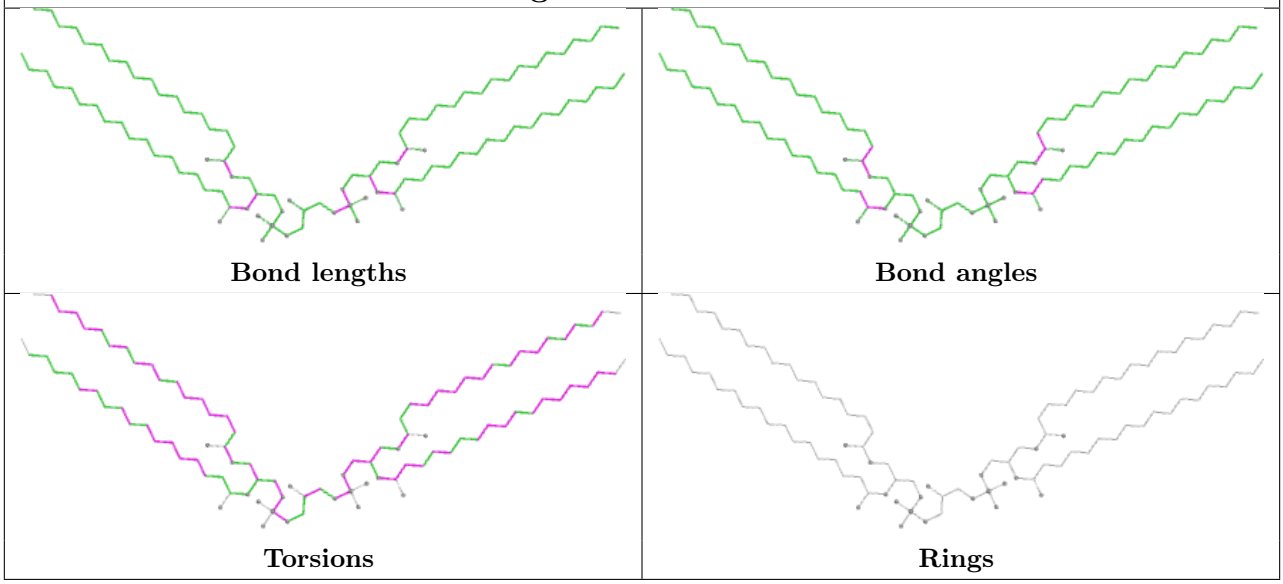
Ligand PEE i 403



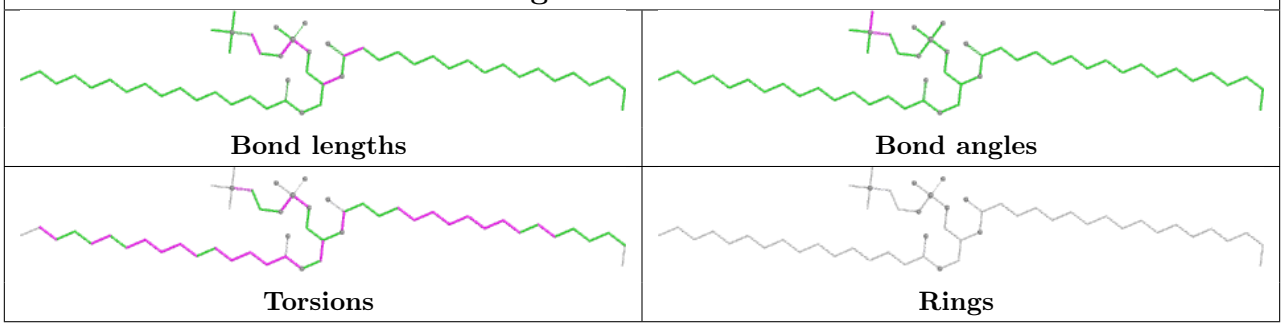
Ligand PEE s 401



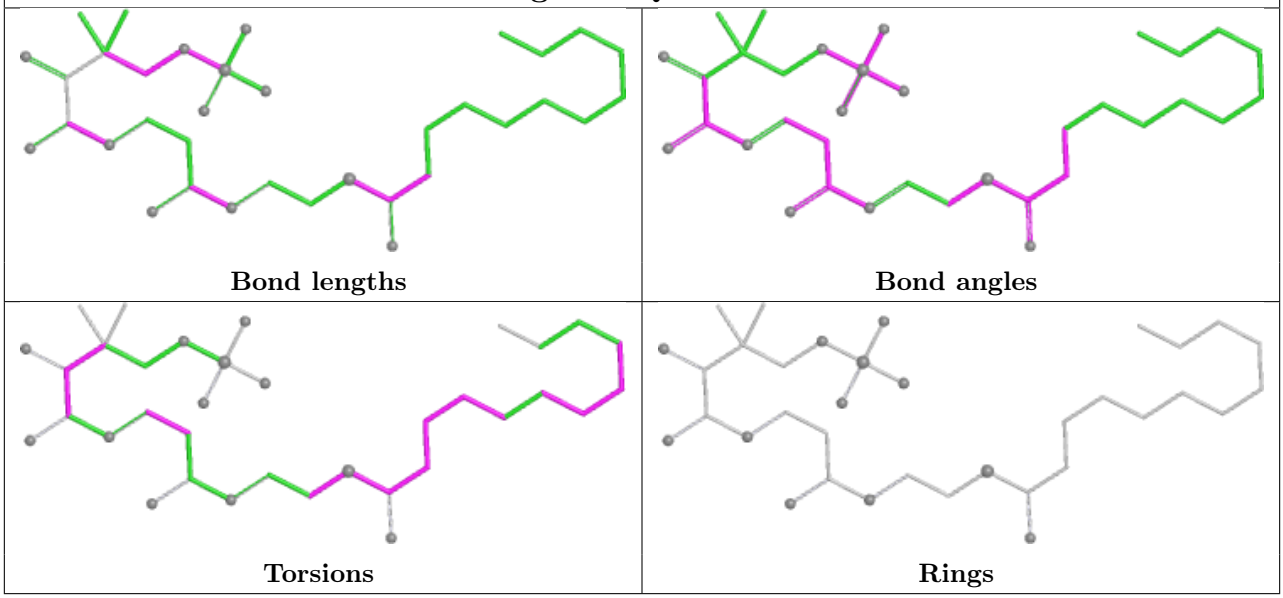
Ligand CDL r 504



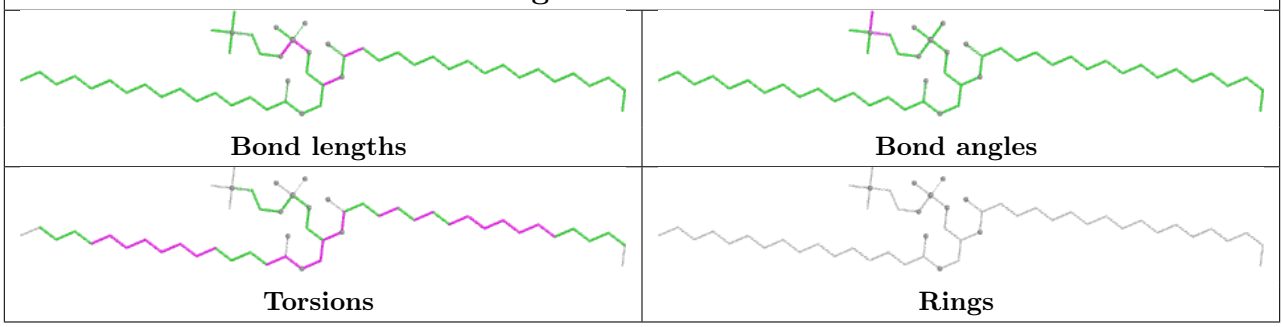
Ligand PLX e 201



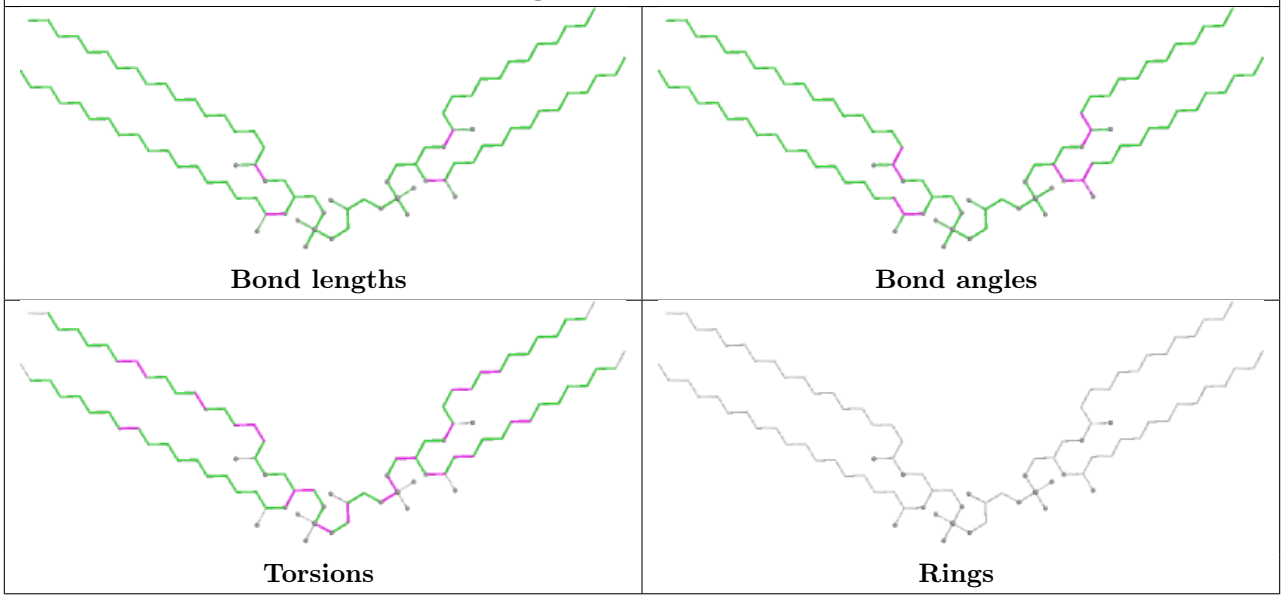
Ligand 8Q1 X 201

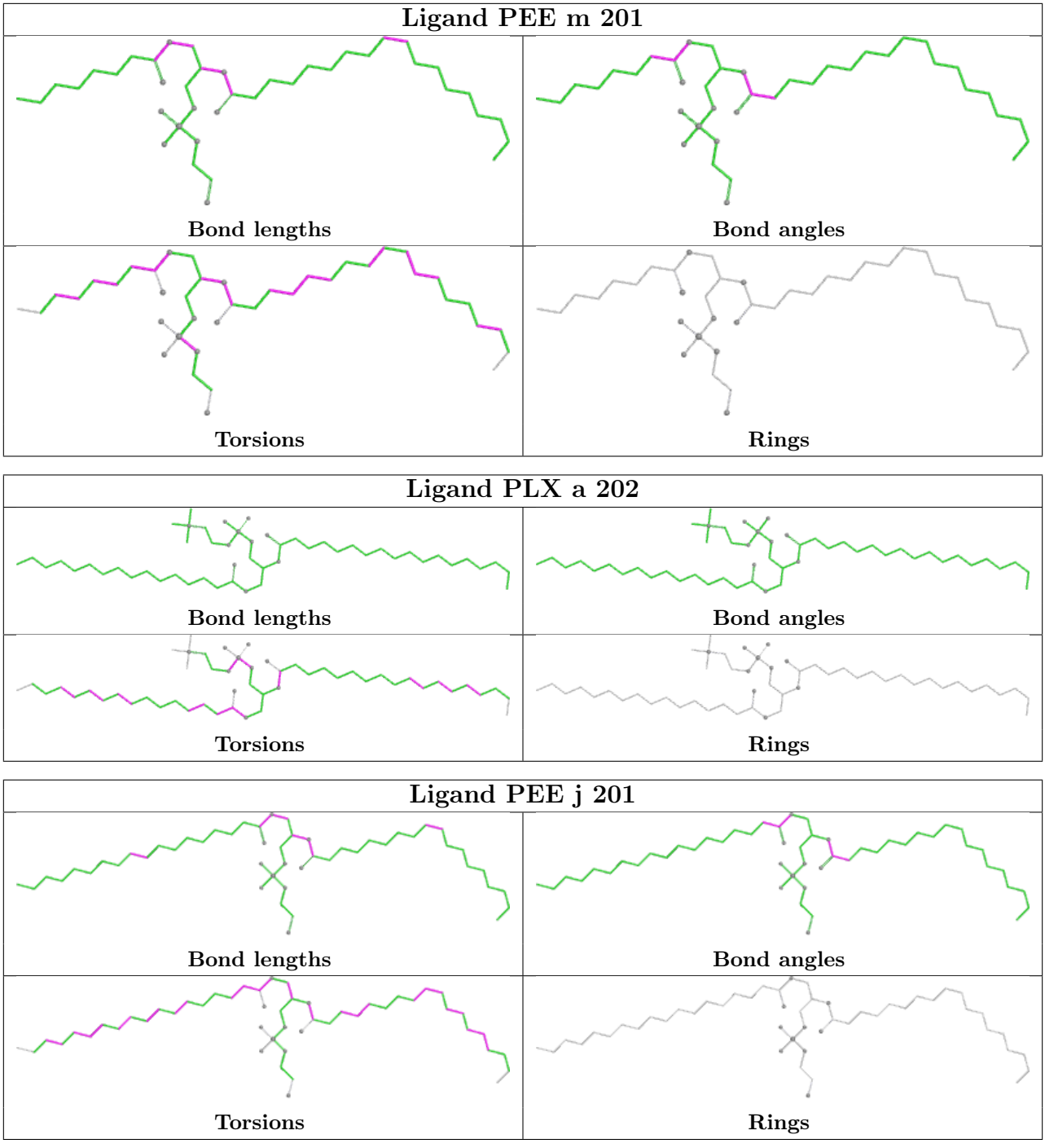


Ligand PLX r 502



Ligand CDL a 201





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.

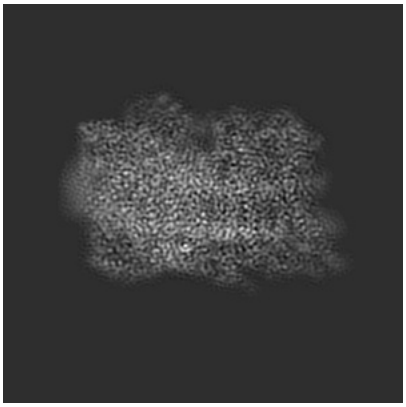
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32155. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

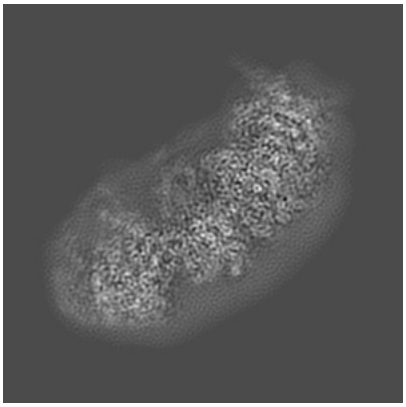
6.1.1 Primary map



X



Y

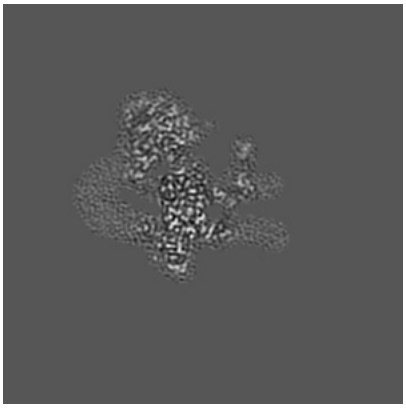


Z

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

6.2 Central slices

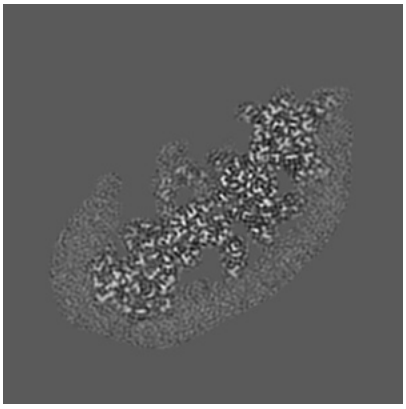
6.2.1 Primary map



X Index: 240



Y Index: 240

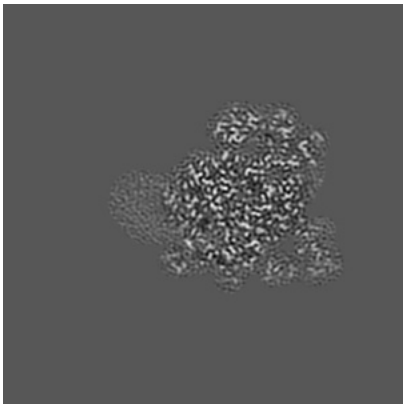


Z Index: 240

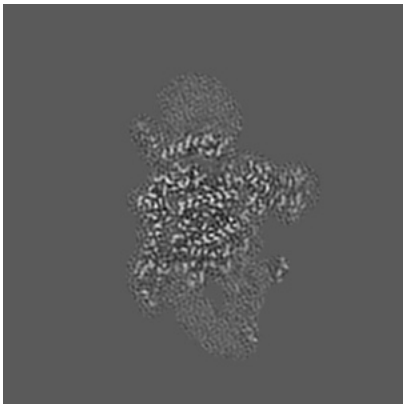
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

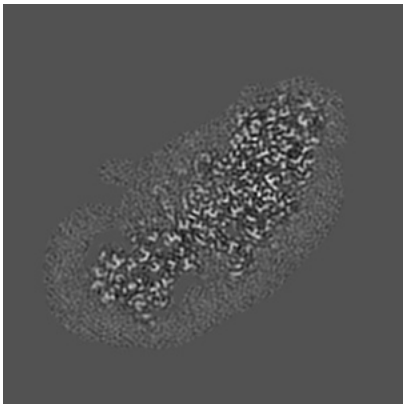
6.3.1 Primary map



X Index: 321



Y Index: 202

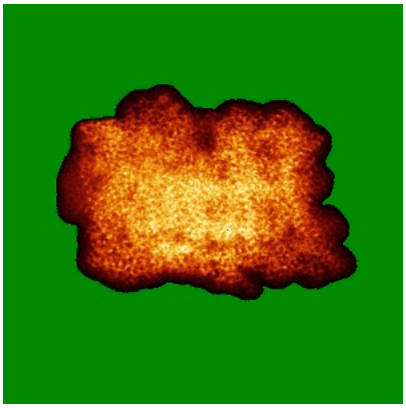


Z Index: 258

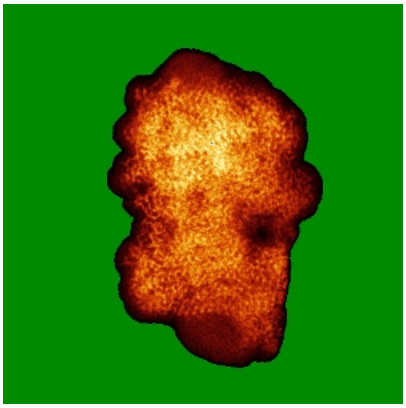
The images above show the largest variance slices of the map in three orthogonal directions.

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

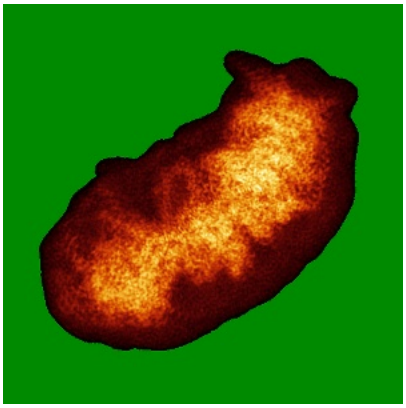
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

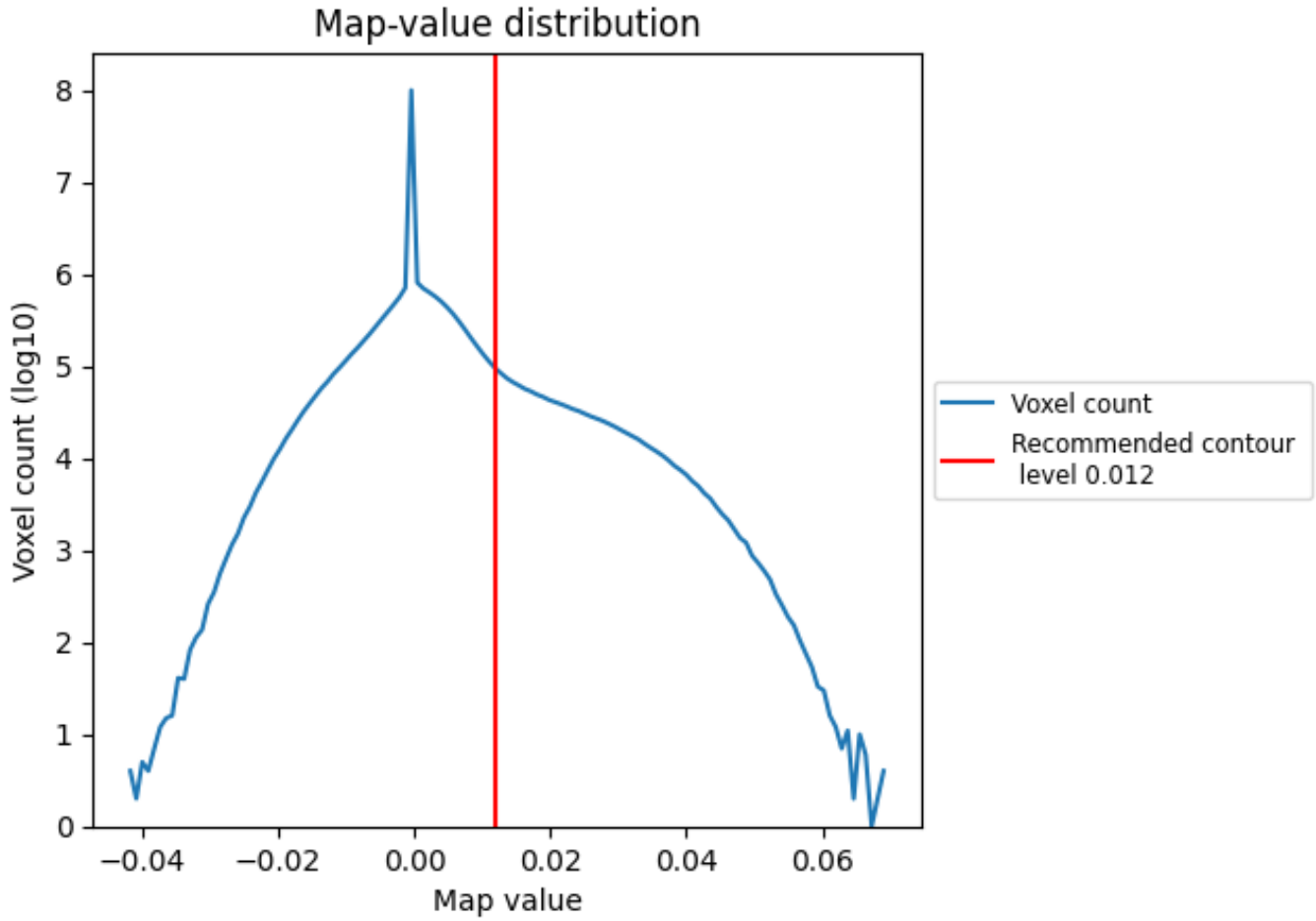
6.6 Mask visualisation (i)

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

7 Map analysis

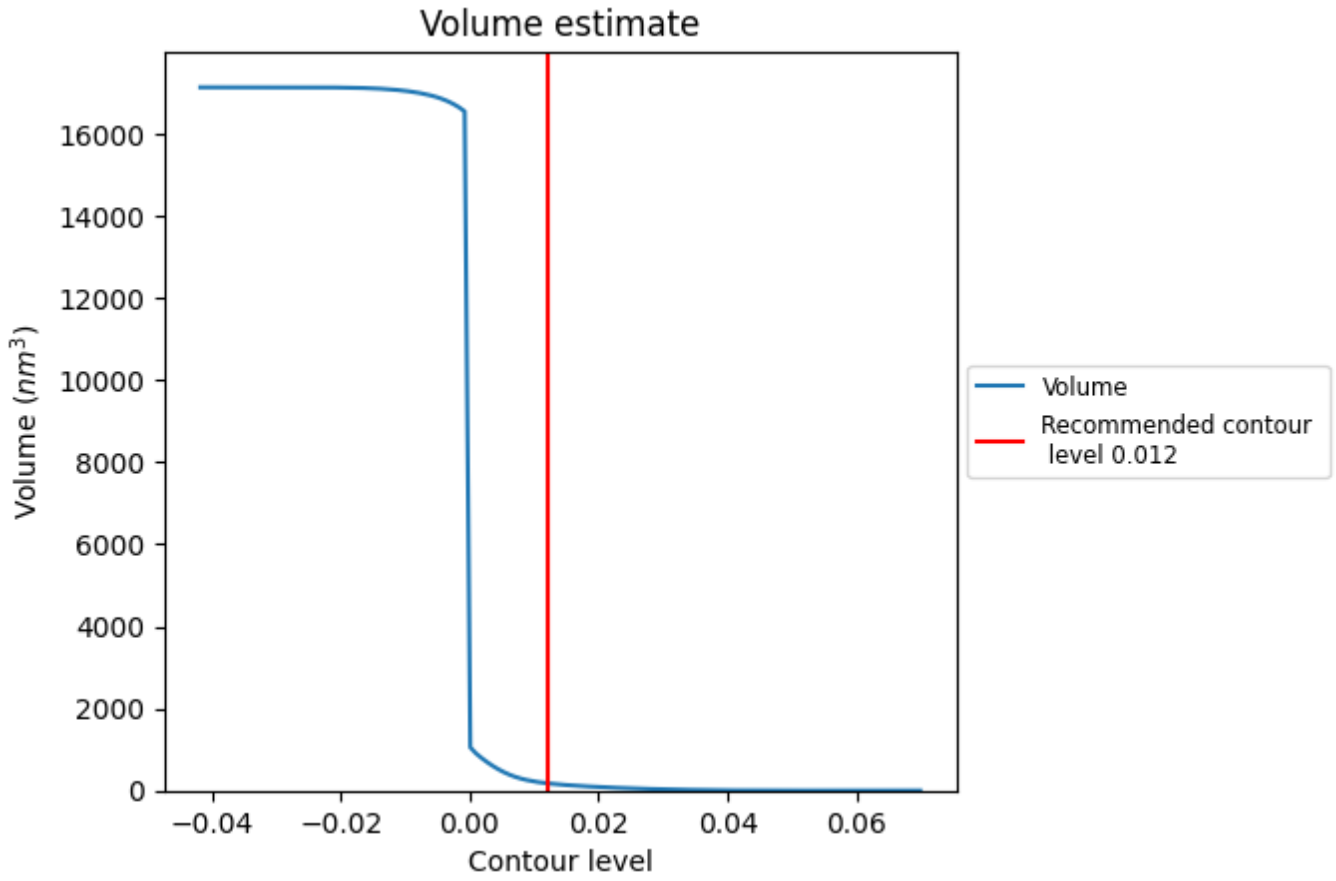
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

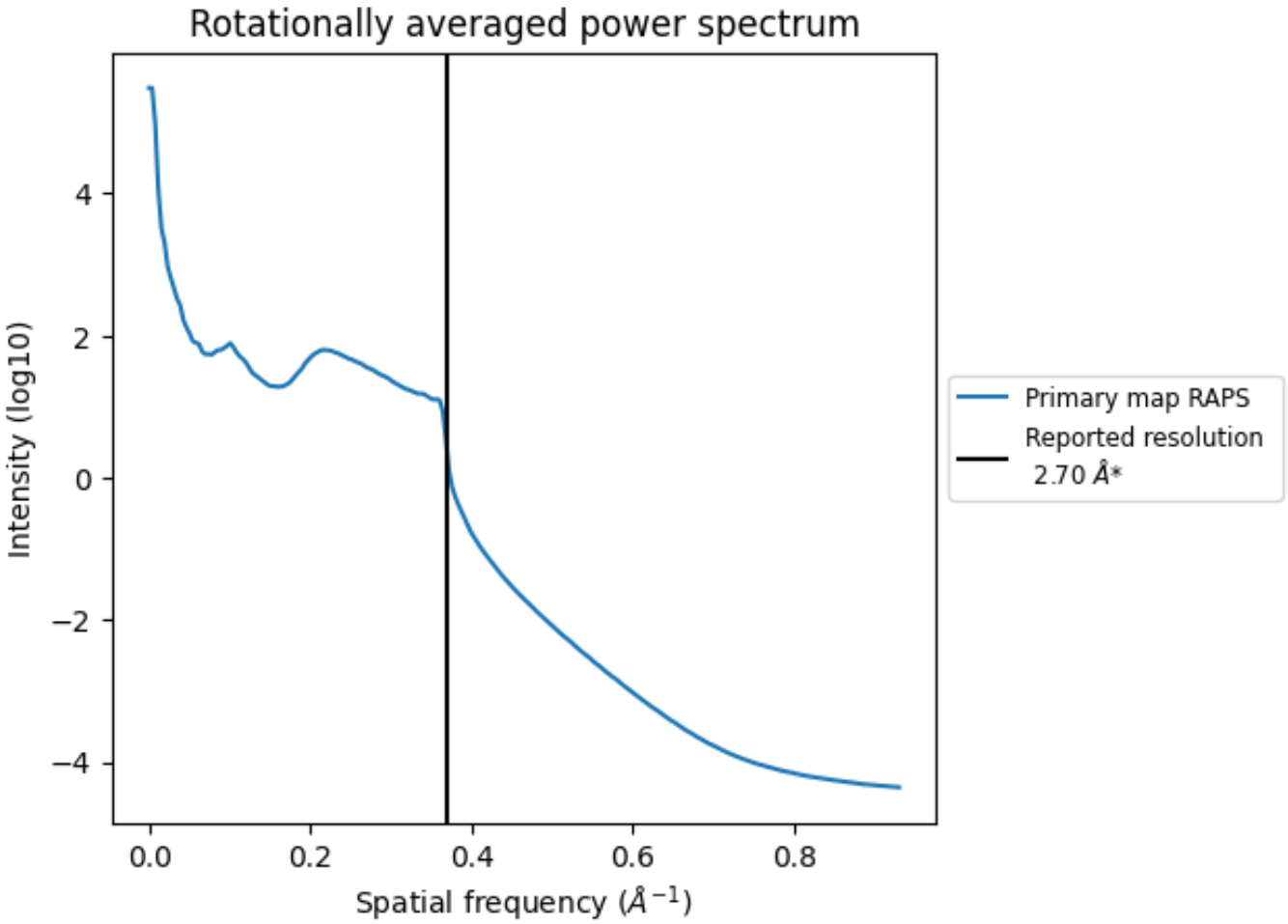
7.2 Volume estimate (i)



The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 161 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 0.370 $Å^{-1}$

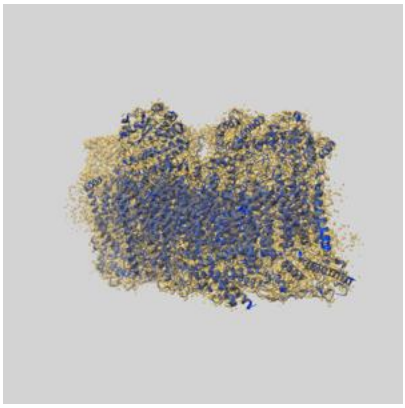
8 Fourier-Shell correlation (i)

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

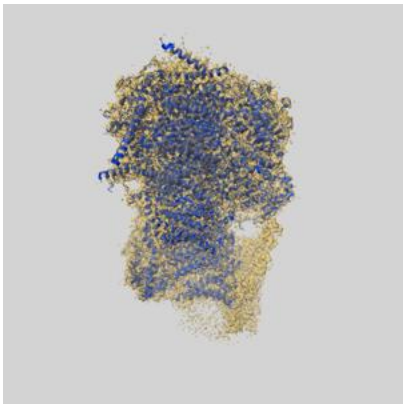
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32155 and PDB model 7VWL. Per-residue inclusion information can be found in section 3 on page 15.

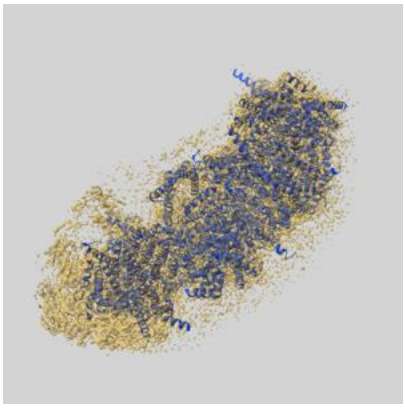
9.1 Map-model overlay



X



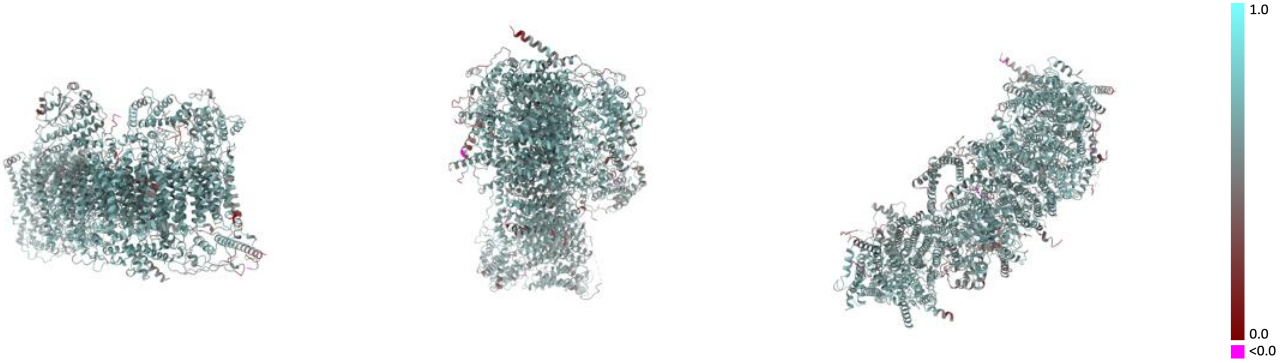
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

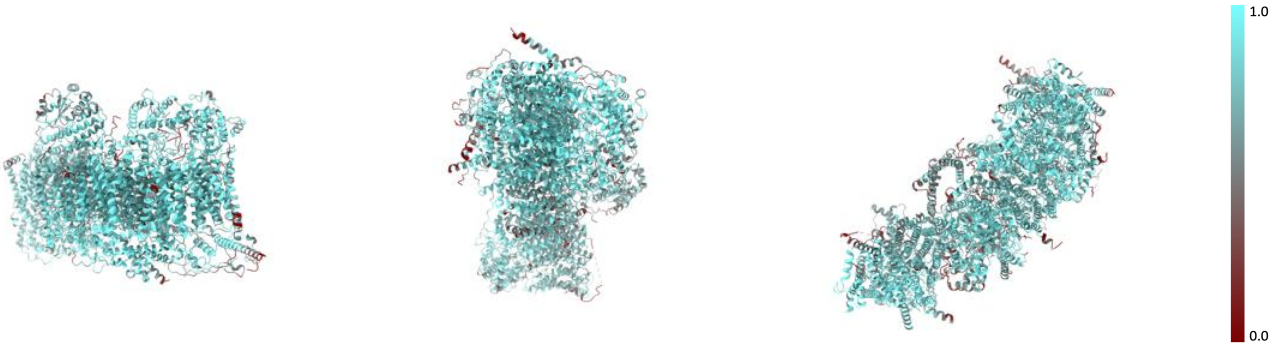
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

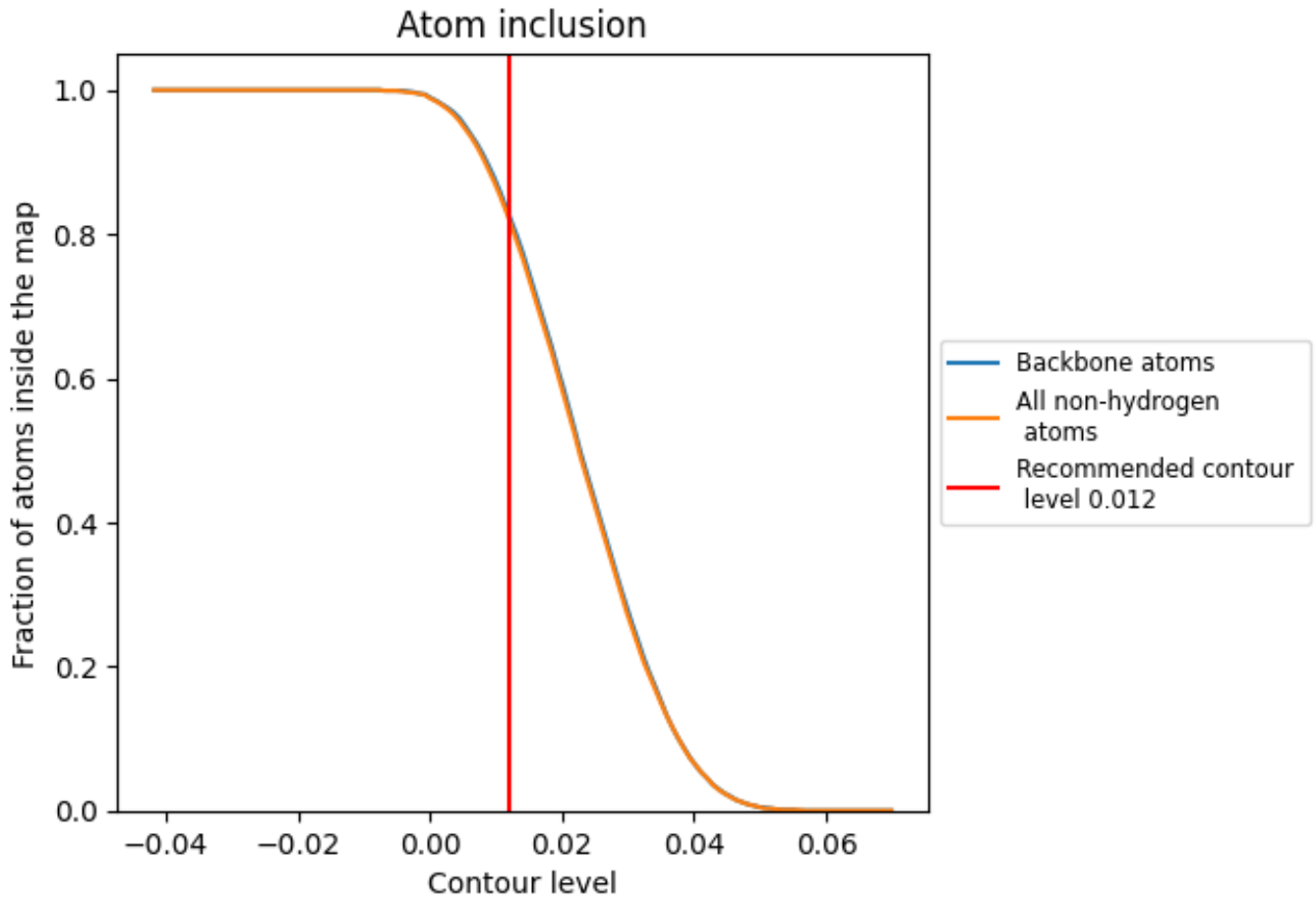
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.5990
Q	0.6410	0.5390
S	0.8610	0.6060
U	0.8080	0.5850
V	0.5990	0.5300
W	0.8580	0.6160
X	0.7800	0.5690
Y	0.6870	0.5400
Z	0.6460	0.5100
a	0.8690	0.6300
b	0.7160	0.5440
c	0.8410	0.6040
d	0.8320	0.6060
e	0.7610	0.5650
f	0.7340	0.5530
g	0.9030	0.6290
h	0.8610	0.6100
i	0.9080	0.6370
j	0.6850	0.5540
k	0.8140	0.5920
l	0.8830	0.6320
m	0.7560	0.5640
n	0.7470	0.5730
o	0.8310	0.5990
p	0.8440	0.6100
r	0.9080	0.6360
s	0.8560	0.6100
u	0.8150	0.5960
v	0.7150	0.5410
w	0.7400	0.5620

