



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2026 – 09:19 AM UTC

PDB ID : 7VYG / pdb_00007vyg
EMDB ID : EMD-32204
Title : Membrane arm of active state CI from rotenone dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-14
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

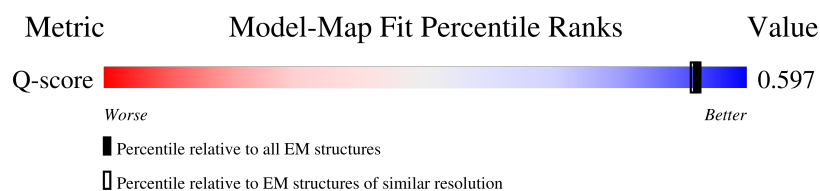
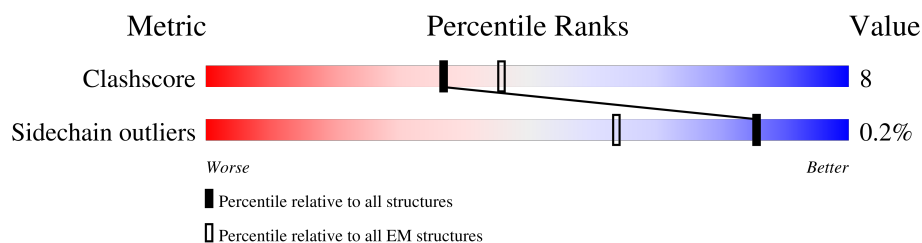
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	Q	44	
2	S	70	
3	U	83	
4	V	140	
5	W	113	

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Mol	Chain	Length	Quality of chain
6	X	88	
7	Y	67	
8	Z	80	
9	a	138	
10	b	126	
11	c	156	
12	d	175	
13	e	104	
14	f	49	
15	g	121	
16	h	105	
17	i	347	
18	j	115	
19	k	98	
20	l	606	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	125	
29	w	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CDL	m	201	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 39639 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	44	Total	C	N	O	S	0	0
			363	236	60	66	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
			566	364	103	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
			699	450	103	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	98	Total	C	N	O	S	0	0
			819	537	144	137	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	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	49	Total	C	N	O	0	0
			377	246	65	66		

- 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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	13		

- 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
			479	311	88	79	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	S	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
			1530	980	278	264	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	318	Total	C	N	O	S	0	0
			2502	1675	382	424	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
			1028	642	195	182	9		

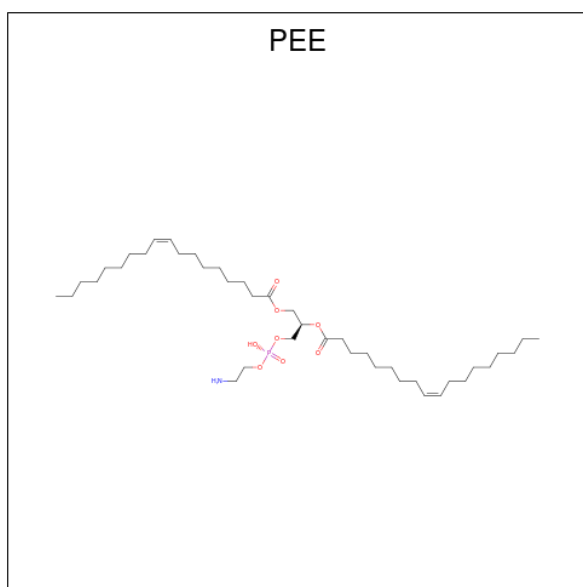
There is a discrepancy between the modelled and reference sequences:

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.

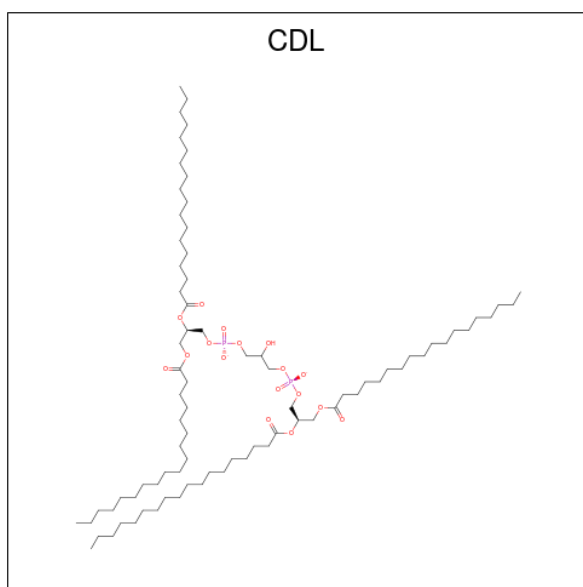
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2583	1645	439	489	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



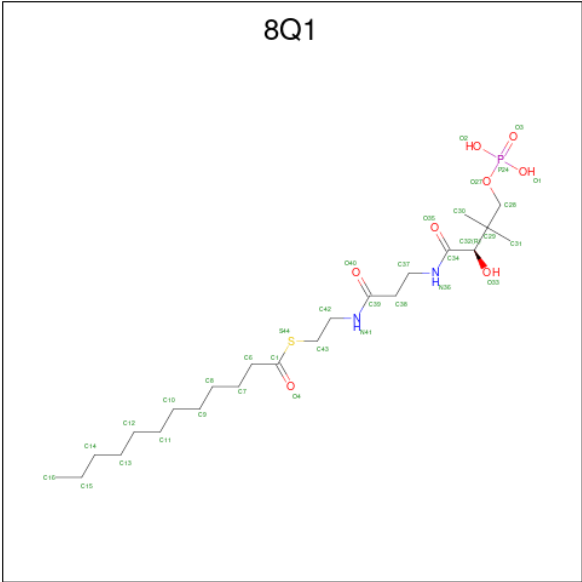
Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	f	1	Total	N				0
			1	1				
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	j	1	Total	N				0
			1	1				
30	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	v	1	Total	N				0
			1	1				

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



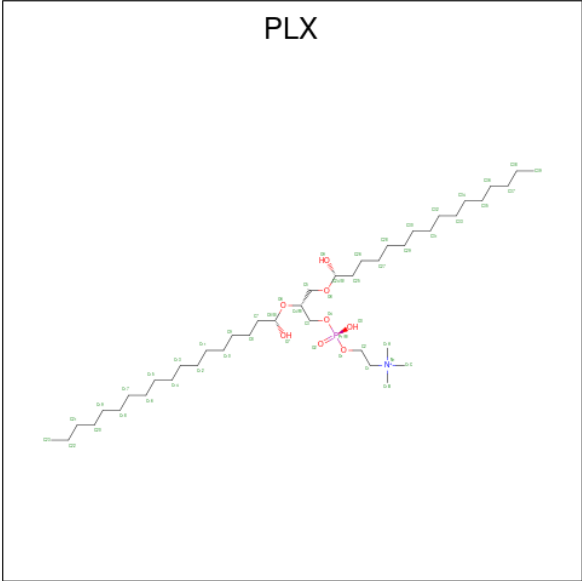
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	V	1	Total	C	O	P	0
			100	81	17	2	
31	a	1	Total	C	O	P	0
			100	81	17	2	
31	l	1	Total	C	O	P	0
			99	80	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	m	1	Total	C	O	P	0
			95	76	17	2	
31	n	1	Total	C	O	P	0
			55	36	17	2	
31	r	1	Total	C	O	P	0
			99	80	17	2	
31	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 32 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
32	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 33 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-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



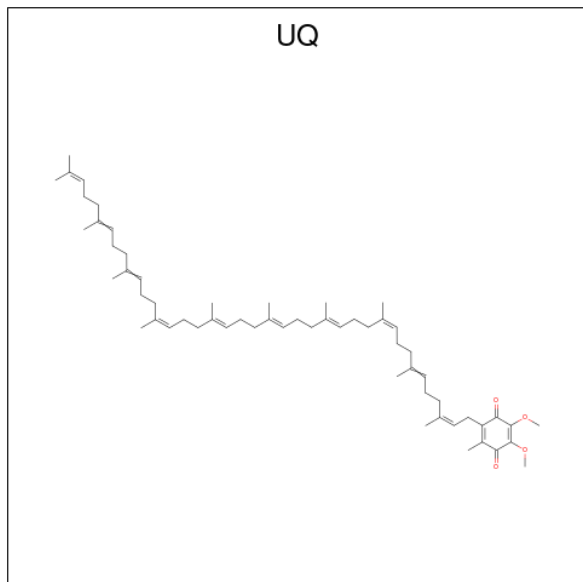
Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	P	
			52	42	1	8	1	0

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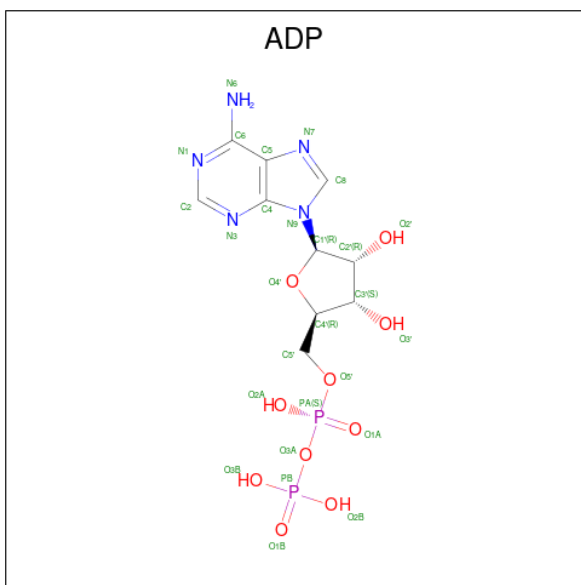
Mol	Chain	Residues	Atoms					AltConf
33	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			38	34	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

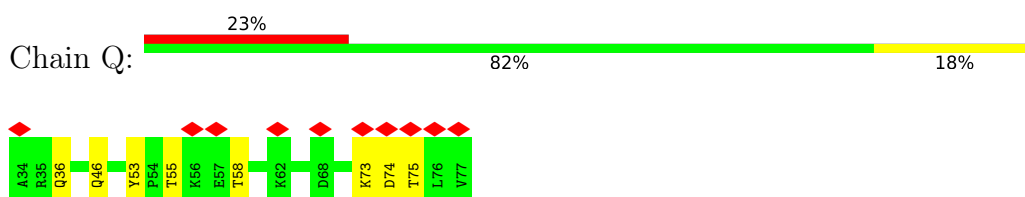


Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

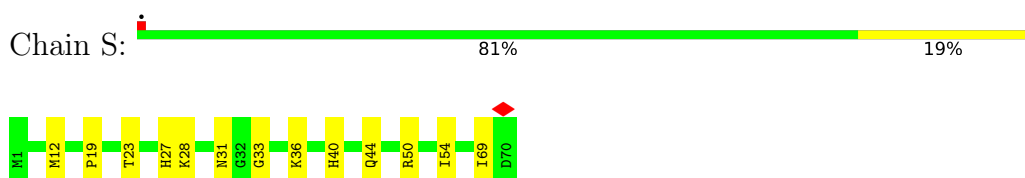
3 Residue-property plots [i](#)

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.

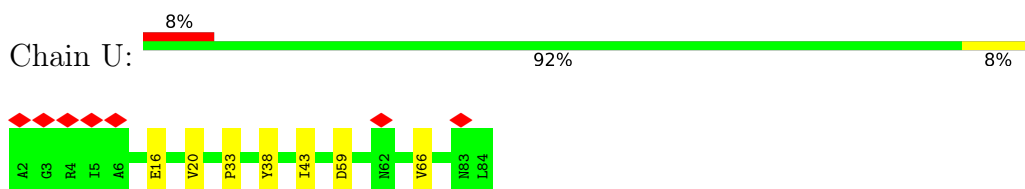
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



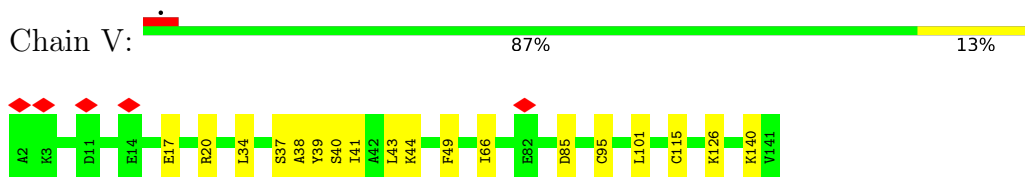
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



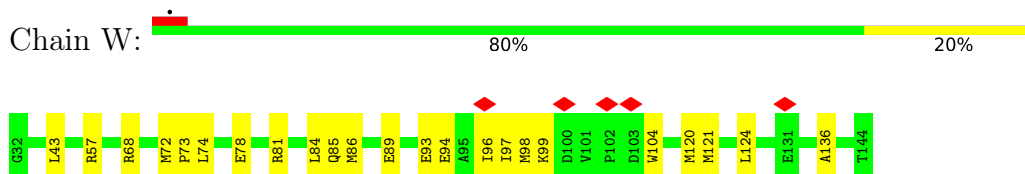
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



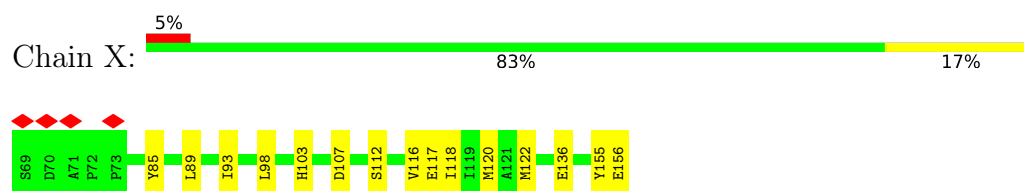
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



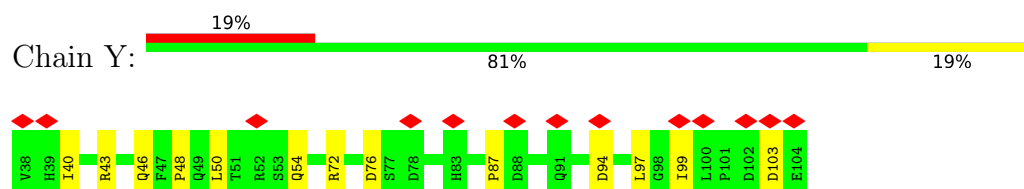
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



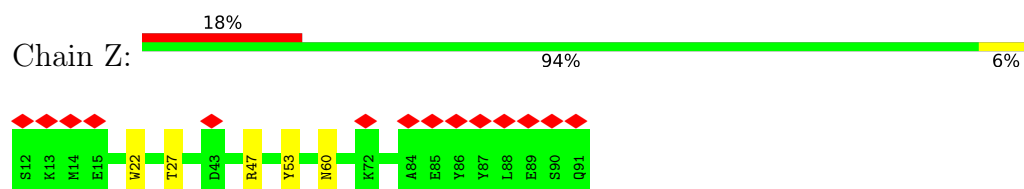
- Molecule 6: Acyl carrier protein, mitochondrial



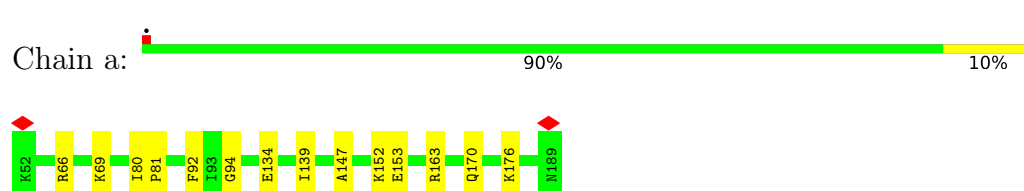
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



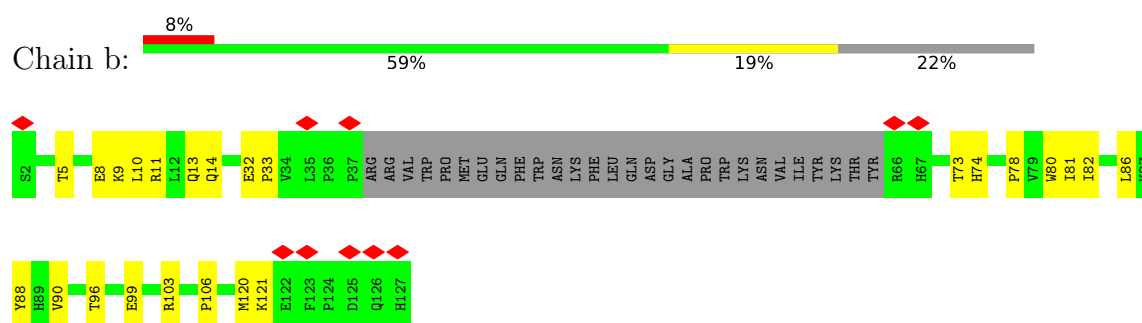
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



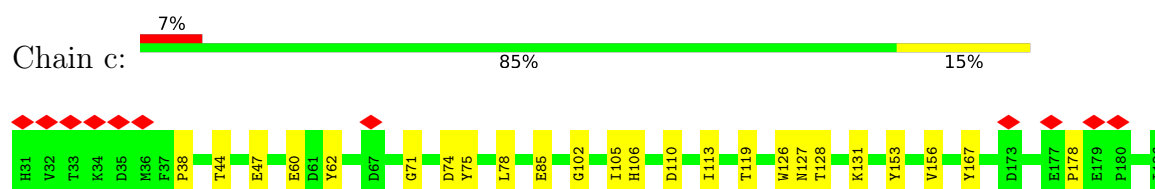
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



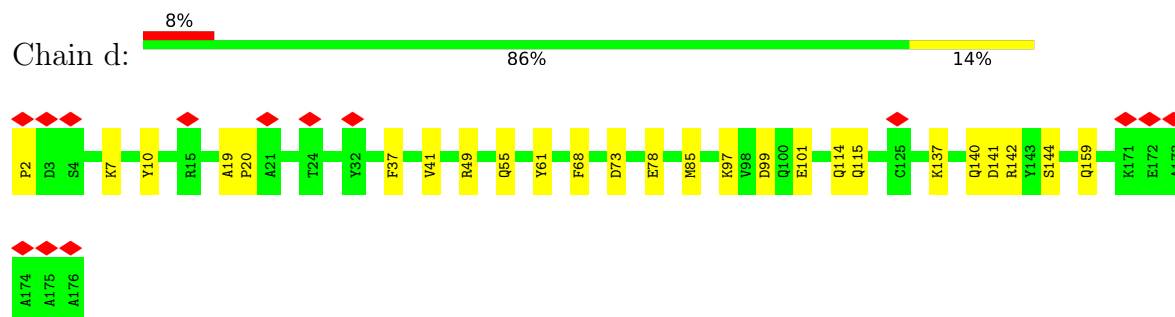
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



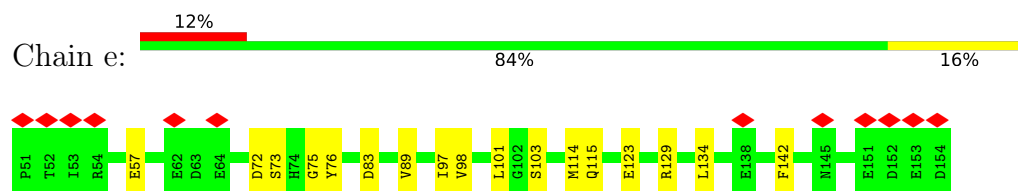
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



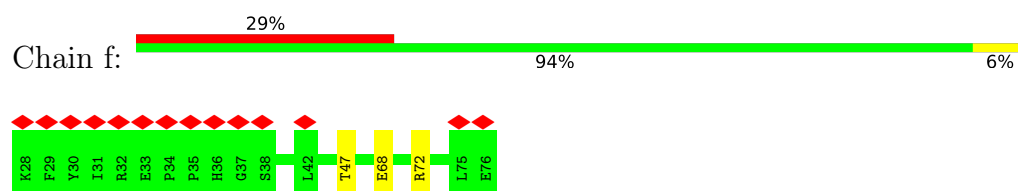
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



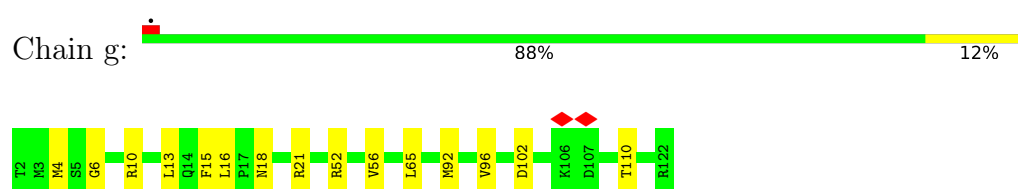
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



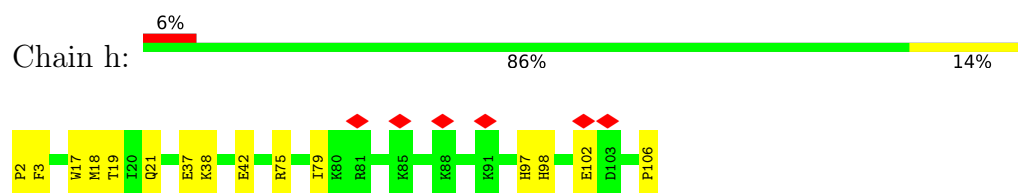
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



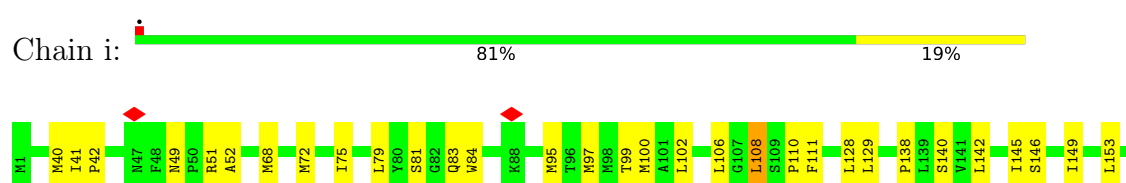
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

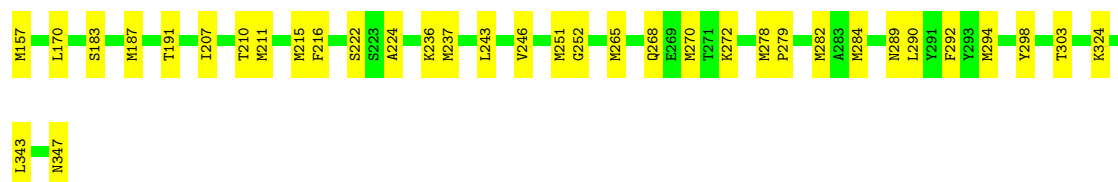


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

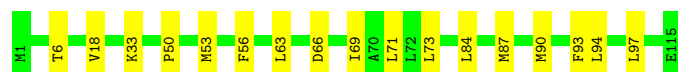
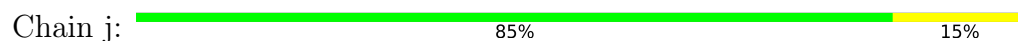


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

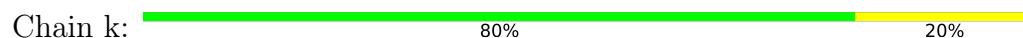




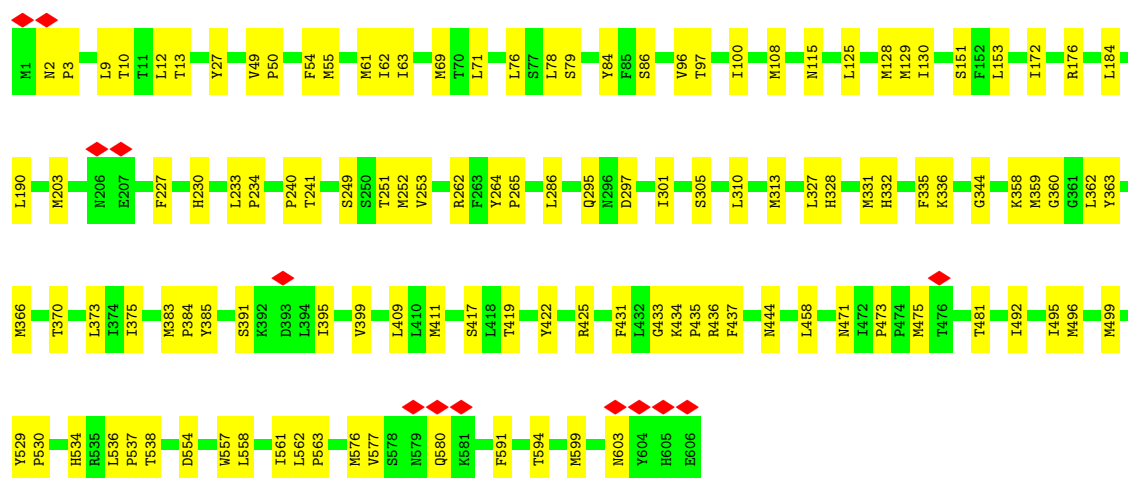
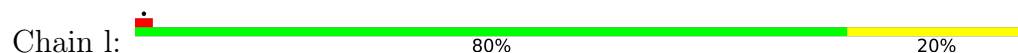
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



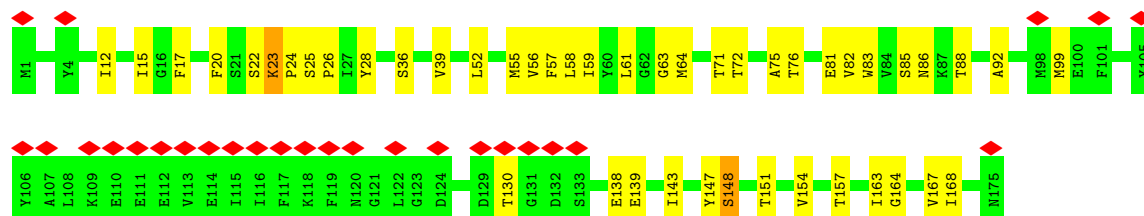
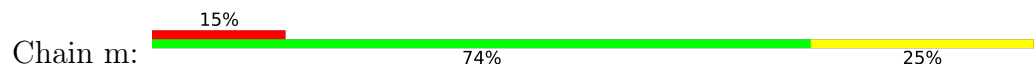
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



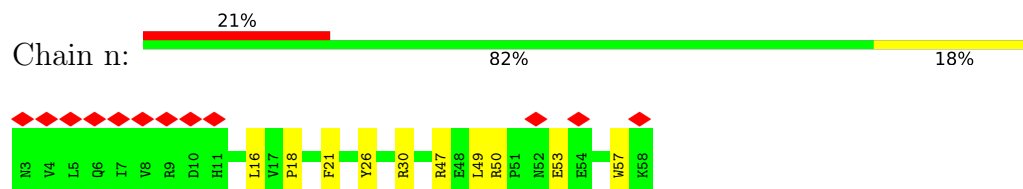
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5



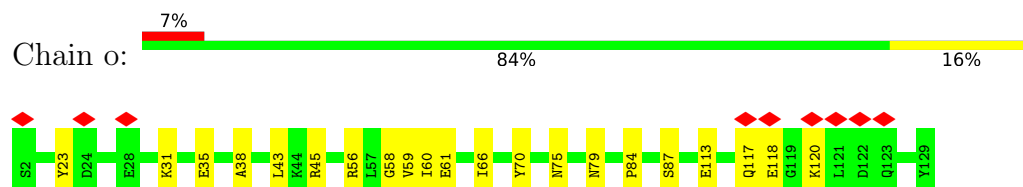
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



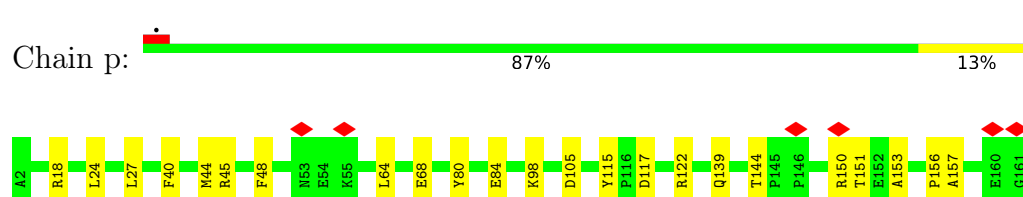
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



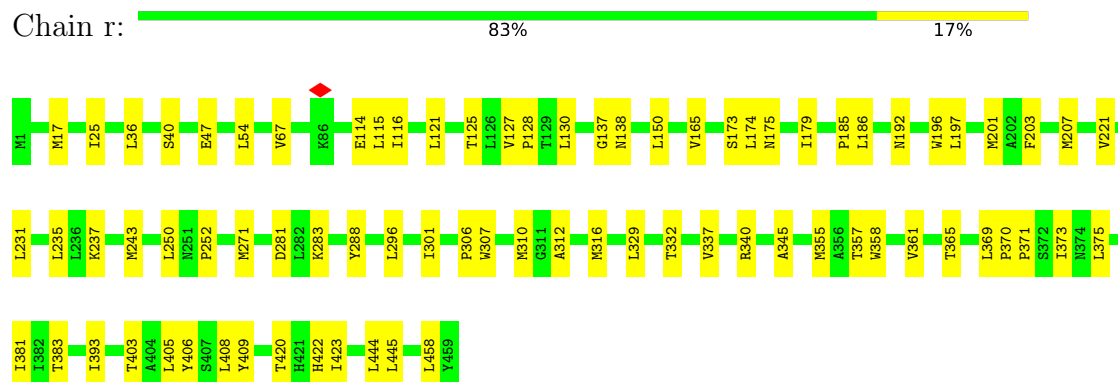
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



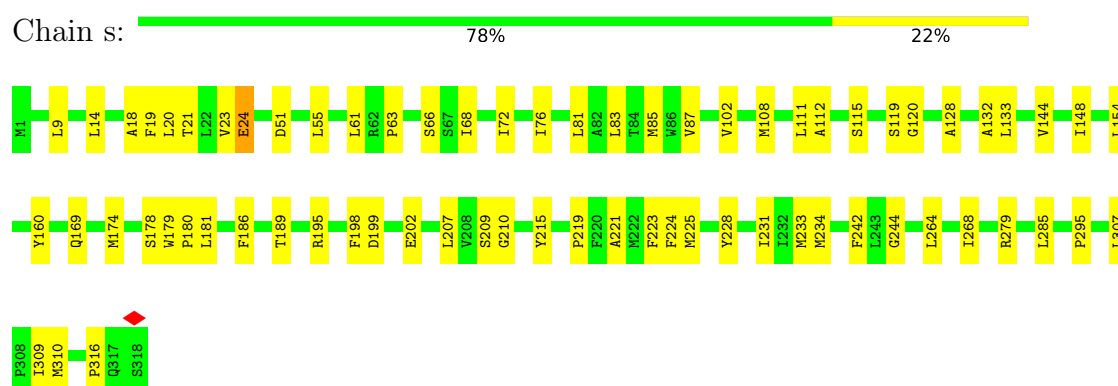
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

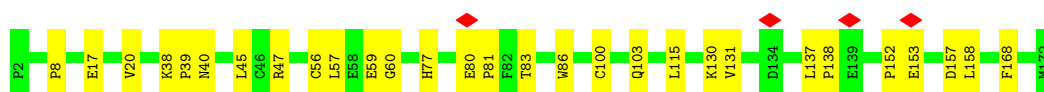


- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



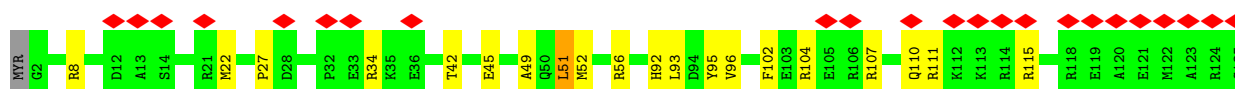
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  83% 17%



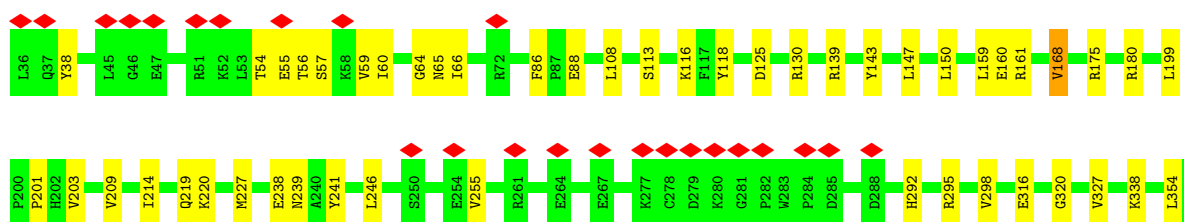
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  18% 83% 15% ..



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

Chain w:  8% 85% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111024	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 ($e^-/\text{\AA}^2$)	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	0.197	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.14	0/380	0.34	0/525
2	S	0.14	0/581	0.39	0/781
3	U	0.12	0/664	0.28	0/912
4	V	0.13	0/1042	0.26	0/1411
5	W	0.16	0/973	0.34	0/1312
6	X	0.12	0/711	0.28	0/963
7	Y	0.13	0/610	0.31	0/836
8	Z	0.11	0/660	0.28	0/892
9	a	0.13	0/1184	0.30	0/1603
10	b	0.15	0/844	0.39	0/1149
11	c	0.12	0/1371	0.32	0/1875
12	d	0.13	0/1494	0.29	0/2015
13	e	0.13	0/891	0.29	0/1210
14	f	0.10	0/385	0.25	0/522
15	g	0.13	0/1031	0.30	0/1394
16	h	0.13	0/889	0.31	0/1190
17	i	0.18	0/2773	0.36	0/3768
18	j	0.18	0/938	0.36	0/1281
19	k	0.18	0/759	0.40	0/1029
20	l	0.15	0/4947	0.34	0/6728
21	m	0.25	0/1325	0.54	1/1800 (0.1%)
22	n	0.13	0/491	0.29	0/663
23	o	0.14	0/1092	0.31	0/1481
24	p	0.13	0/1586	0.29	0/2150
25	r	0.17	0/3723	0.34	0/5078
26	s	0.20	0/2575	0.42	0/3522
27	u	0.14	0/1436	0.34	0/1938
28	v	0.12	0/1052	0.35	2/1411 (0.1%)
29	w	0.13	0/2643	0.29	0/3580
All	All	0.15	0/39050	0.34	3/53019 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
28	v	51	LEU	CA-C-N	5.26	133.41	122.41
28	v	51	LEU	C-N-CA	5.26	133.41	122.41
21	m	148	SER	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	363	0	332	9	0
2	S	566	0	561	8	0
3	U	643	0	642	6	0
4	V	1021	0	1025	13	0
5	W	949	0	935	21	0
6	X	699	0	682	10	0
7	Y	584	0	529	11	0
8	Z	641	0	620	6	0
9	a	1151	0	1164	12	0
10	b	819	0	835	21	0
11	c	1315	0	1208	15	0
12	d	1461	0	1429	21	0
13	e	867	0	817	13	0
14	f	377	0	353	4	0
15	g	1000	0	994	15	0
16	h	867	0	871	15	0
17	i	2710	0	2874	51	0
18	j	914	0	951	18	0
19	k	748	0	799	23	0
20	l	4816	0	4955	93	0
21	m	1292	0	1261	52	0
22	n	479	0	486	8	0
23	o	1062	0	1072	16	0
24	p	1530	0	1464	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	r	3631	0	3839	61	0
26	s	2502	0	2596	52	0
27	u	1398	0	1374	22	0
28	v	1028	0	982	15	0
29	w	2583	0	2540	33	0
30	Q	47	0	71	7	0
30	U	51	0	82	2	0
30	W	41	0	59	1	0
30	f	1	0	0	0	0
30	j	52	0	82	3	0
30	l	136	0	200	11	0
30	r	51	0	82	5	0
30	v	1	0	0	0	0
31	V	194	0	294	15	0
31	a	100	0	156	3	0
31	l	199	0	307	16	0
31	m	95	0	143	34	0
31	n	55	0	54	1	0
31	r	99	0	151	7	0
31	s	89	0	125	7	0
32	X	35	0	0	0	0
33	a	52	0	88	2	0
33	e	52	0	88	5	0
33	g	52	0	88	7	0
33	j	104	0	176	5	0
33	r	52	0	88	4	0
34	s	38	0	47	3	0
35	w	27	0	11	1	0
All	All	39639	0	40582	612	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 8.

The worst 5 of 612 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)
31:m:201:CDL:C39	31:m:201:CDL:H272	1.90	1.00
21:m:55:MET:HE3	21:m:55:MET:HA	1.43	0.98
21:m:64:MET:HE2	21:m:64:MET:HA	1.52	0.91
21:m:23:LYS:HZ3	31:m:201:CDL:H711	1.34	0.91
18:j:63:LEU:HD21	21:m:63:GLY:HA2	1.51	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
9	a	63/121 (52%)	63 (100%)	0	100	100
10	b	90/119 (76%)	90 (100%)	0	100	100
11	c	141/141 (100%)	141 (100%)	0	100	100
12	d	75/155 (48%)	75 (100%)	0	100	100
13	e	72/96 (75%)	72 (100%)	0	100	100
14	f	35/45 (78%)	35 (100%)	0	100	100
15	g	108/108 (100%)	108 (100%)	0	100	100
16	h	87/93 (94%)	87 (100%)	0	100	100
17	i	268/311 (86%)	267 (100%)	1 (0%)	84	94
18	j	100/100 (100%)	100 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	540/540 (100%)	540 (100%)	0	100	100
21	m	129/141 (92%)	126 (98%)	3 (2%)	44	76
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	158/159 (99%)	158 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	274/275 (100%)	273 (100%)	1 (0%)	84	94
27	u	153/153 (100%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	v	104/111 (94%)	104 (100%)	0	100	100
29	w	281/283 (99%)	280 (100%)	1 (0%)	84	94
All	All	3339/3612 (92%)	3333 (100%)	6 (0%)	85	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	m	148	SER
26	s	24	GLU
29	w	168	VAL
21	m	22	SER
17	i	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
20	l	135	ASN
29	w	188	ASN
20	l	470	ASN
28	v	44	GLN
20	l	199	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 29 ligands modelled in this entry, 3 are modelled with single atom - leaving 26 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	$\# Z > 2$
33	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.61	1 (1%)
31	CDL	l	702	-	98,98,99	1.11	8 (8%)	104,110,111	0.91	4 (3%)
31	CDL	r	503	-	98,98,99	1.11	8 (8%)	104,110,111	0.87	4 (3%)
30	PEE	l	704	-	49,49,50	1.19	6 (12%)	52,54,55	0.95	2 (3%)
30	PEE	U	401	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
33	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
33	PLX	j	204	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
30	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	0.97	2 (4%)
31	CDL	n	101	-	54,54,99	1.38	9 (16%)	60,66,111	1.11	4 (6%)
34	UQ	s	402	-	38,38,63	3.63	11 (28%)	48,49,79	2.75	17 (35%)
31	CDL	m	201	-	94,94,99	0.94	4 (4%)	100,106,111	1.04	7 (7%)
31	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
33	PLX	j	203	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
31	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.89	4 (4%)
30	PEE	Q	101	-	46,46,50	1.23	6 (13%)	49,51,55	1.04	2 (4%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
33	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
30	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
33	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
30	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
32	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.59	6 (15%)
35	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.91	9 (20%)
31	CDL	s	401	-	88,88,99	1.16	9 (10%)	94,100,111	0.94	4 (4%)
30	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
31	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
31	CDL	l	703	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (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
33	PLX	r	502	-	-	22/55/55/55	-
31	CDL	l	702	-	-	54/109/109/110	-
31	CDL	r	503	-	-	55/109/109/110	-
30	PEE	l	704	-	-	28/53/53/54	-
30	PEE	U	401	-	-	22/54/54/54	-
33	PLX	e	201	-	-	30/55/55/55	-
33	PLX	j	204	-	-	31/55/55/55	-
30	PEE	l	705	-	-	26/49/49/54	-
31	CDL	n	101	-	-	29/65/65/110	-
34	UQ	s	402	-	-	12/33/57/87	0/1/1/1
31	CDL	m	201	-	-	59/105/105/110	-
31	CDL	V	202	-	-	59/110/110/110	-
33	PLX	j	203	-	-	27/55/55/55	-
31	CDL	V	201	-	-	61/104/104/110	-
30	PEE	Q	101	-	-	23/50/50/54	-
30	PEE	r	501	-	-	25/54/54/54	-
33	PLX	a	202	-	-	30/55/55/55	-
30	PEE	l	701	-	-	24/43/43/54	-
33	PLX	g	201	-	-	36/55/55/55	-
30	PEE	j	201	-	-	24/54/54/54	-
32	8Q1	X	201	-	-	21/41/41/41	-
35	ADP	w	401	-	-	6/16/32/32	0/3/3/3
31	CDL	s	401	-	-	49/99/99/110	-
30	PEE	W	201	-	-	25/44/44/54	-
31	CDL	a	201	-	-	58/110/110/110	-
31	CDL	l	703	-	-	47/110/110/110	-

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C18-C19	10.03	1.56	1.33
34	s	402	UQ	C13-C14	9.61	1.55	1.33
34	s	402	UQ	C23-C24	9.38	1.54	1.33
34	s	402	UQ	C8-C9	9.29	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.98	1.30	1.53

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	402	UQ	C7-C8-C9	-8.02	113.01	126.83
34	s	402	UQ	C22-C23-C24	-6.28	113.26	127.62
34	s	402	UQ	C12-C13-C14	-6.26	113.29	127.62
34	s	402	UQ	C17-C18-C19	-5.95	114.00	127.62
32	X	201	8Q1	C6-C1-S44	5.87	120.40	113.40

There are no chirality outliers.

5 of 883 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C11-C10-O2-C2
30	Q	101	PEE	O4-C10-O2-C2
30	Q	101	PEE	C1-O3P-P-O2P
30	Q	101	PEE	C1-O3P-P-O1P
30	Q	101	PEE	C1-O3P-P-O4P

There are no ring outliers.

25 monomers are involved in 133 short contacts:

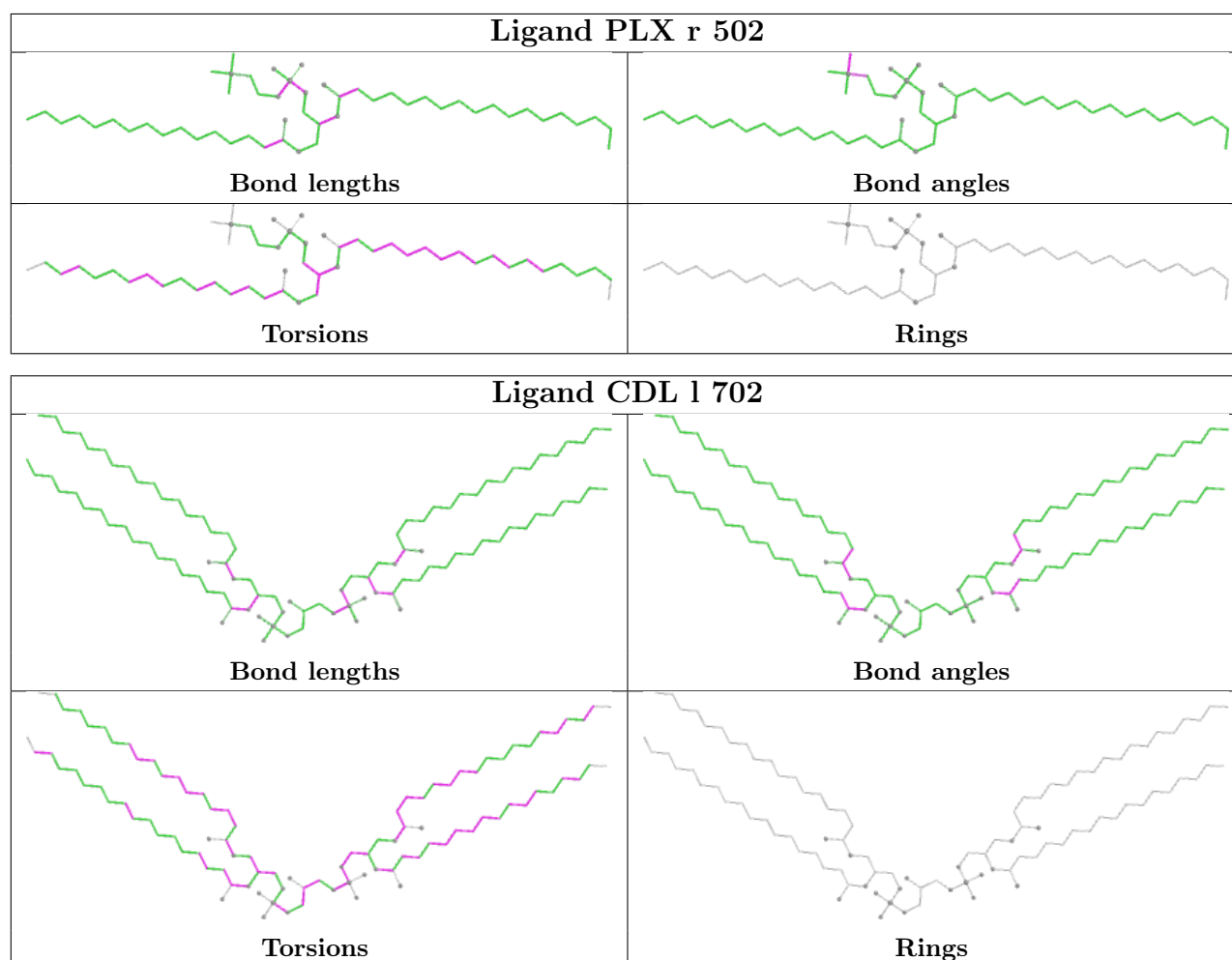
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	r	502	PLX	4	0
31	l	702	CDL	11	0
31	r	503	CDL	7	0
30	l	704	PEE	5	0
30	U	401	PEE	2	0
33	e	201	PLX	5	0
33	j	204	PLX	2	0
30	l	705	PEE	5	0
31	n	101	CDL	1	0
34	s	402	UQ	3	0
31	m	201	CDL	34	0
31	V	202	CDL	7	0
33	j	203	PLX	3	0
31	V	201	CDL	8	0
30	Q	101	PEE	7	0
30	r	501	PEE	5	0
33	a	202	PLX	2	0
30	l	701	PEE	1	0
33	g	201	PLX	7	0
30	j	201	PEE	3	0
35	w	401	ADP	1	0

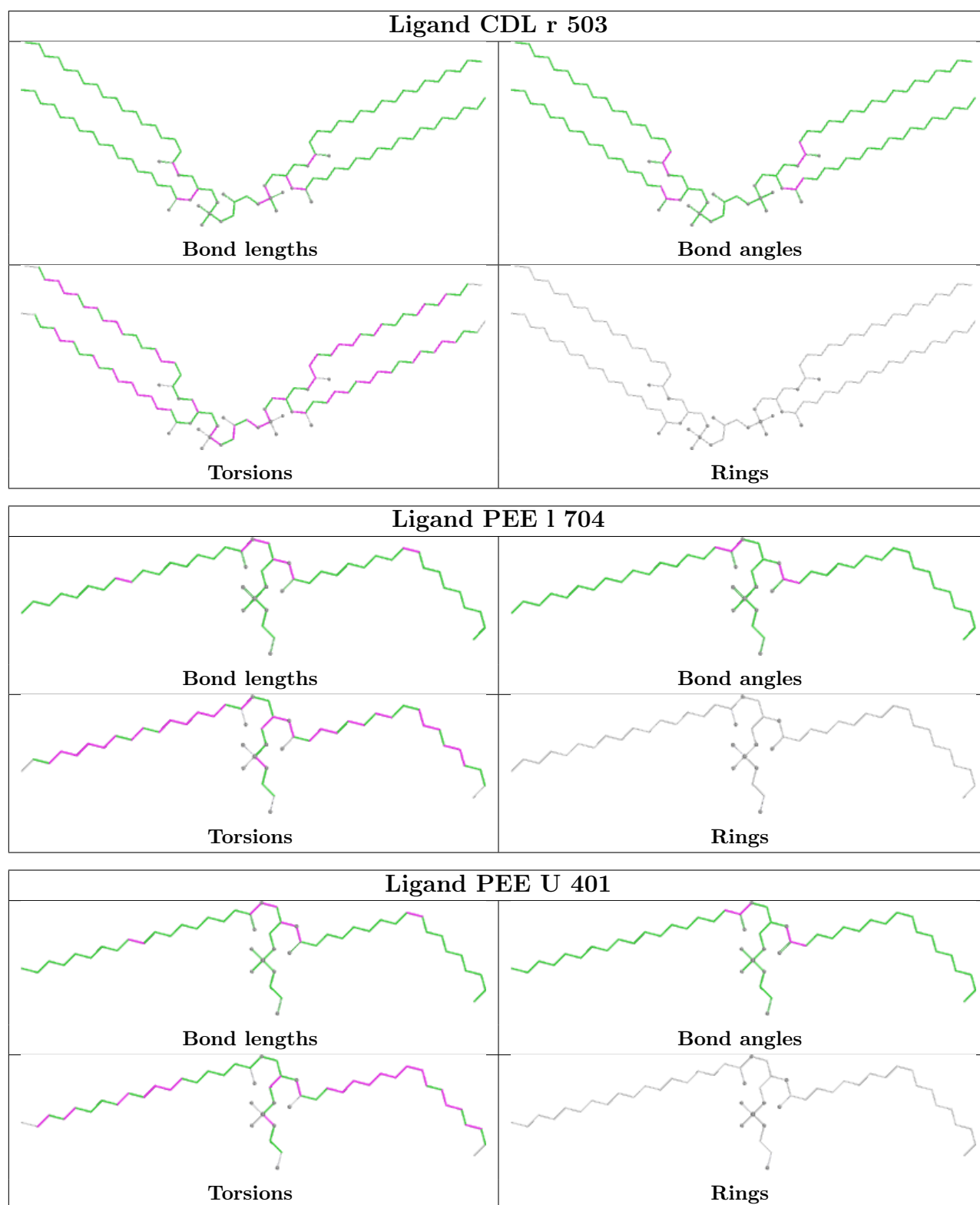
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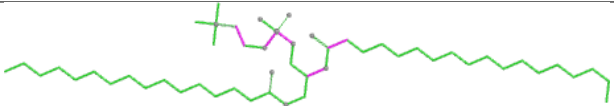
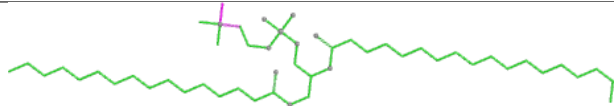
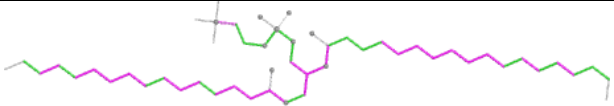
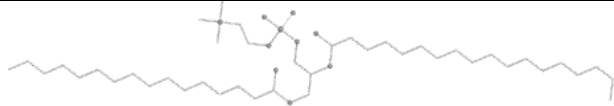
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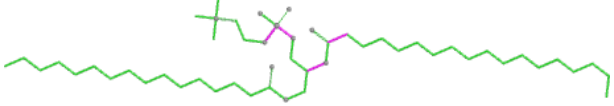
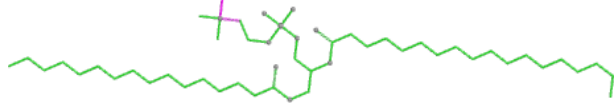
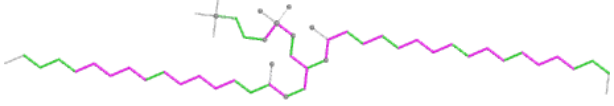
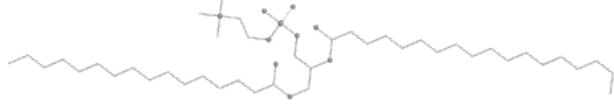
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	s	401	CDL	7	0
30	W	201	PEE	1	0
31	a	201	CDL	3	0
31	l	703	CDL	5	0

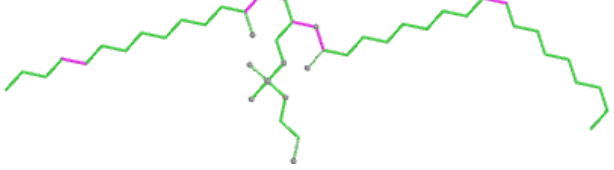
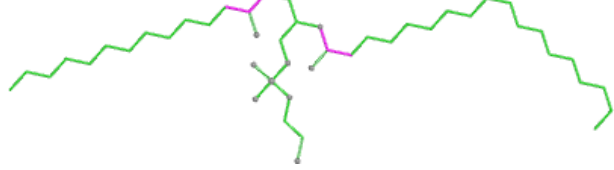
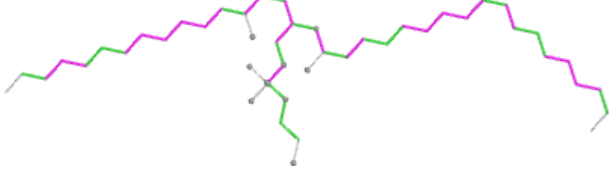
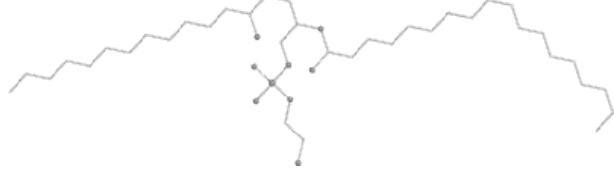
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

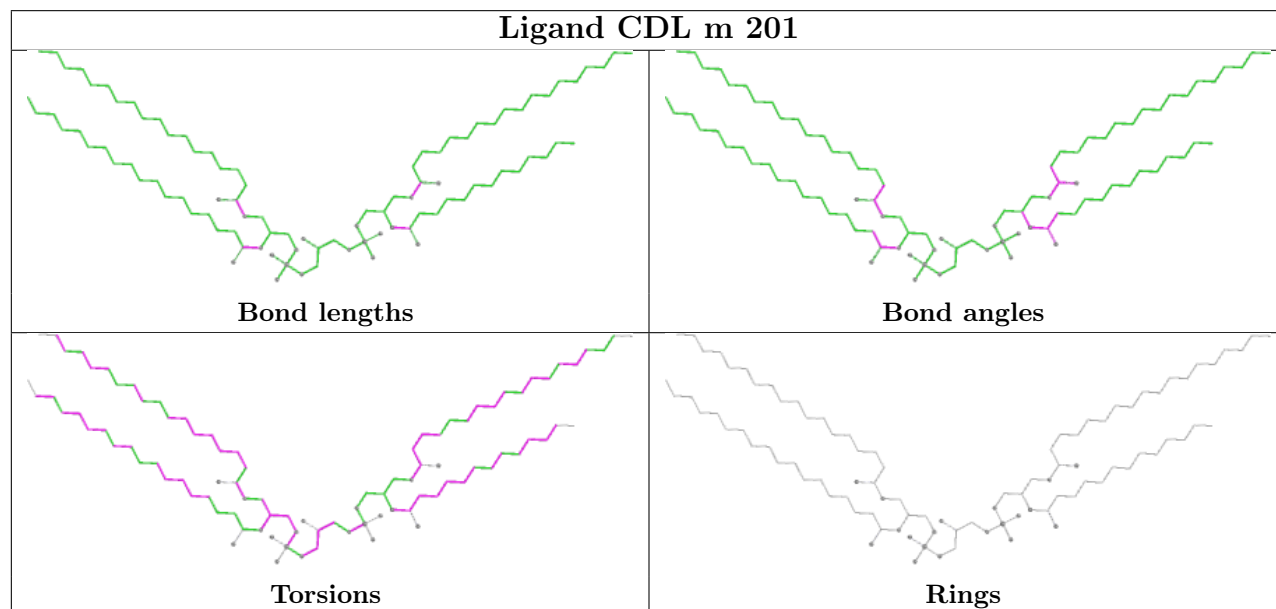
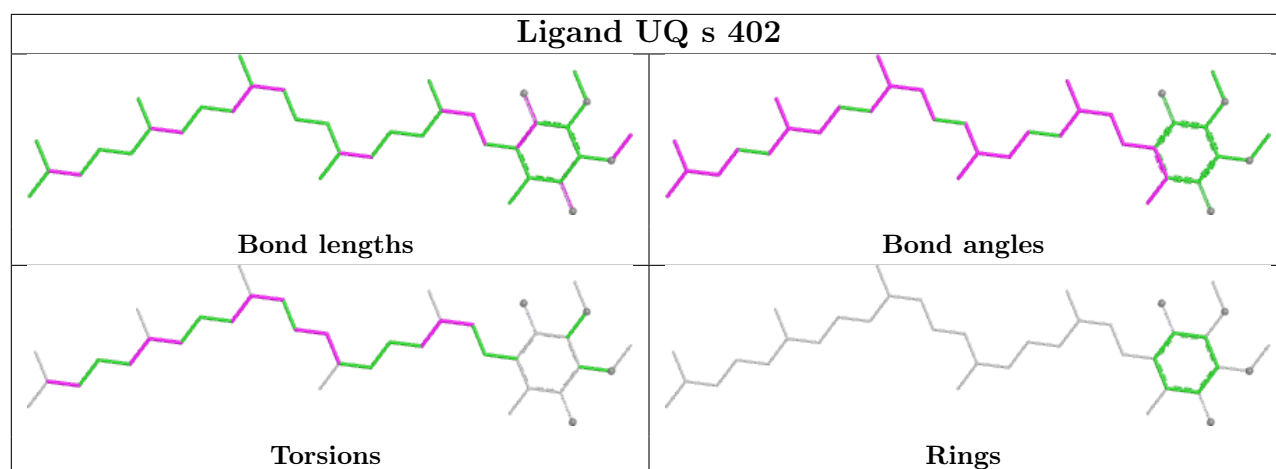
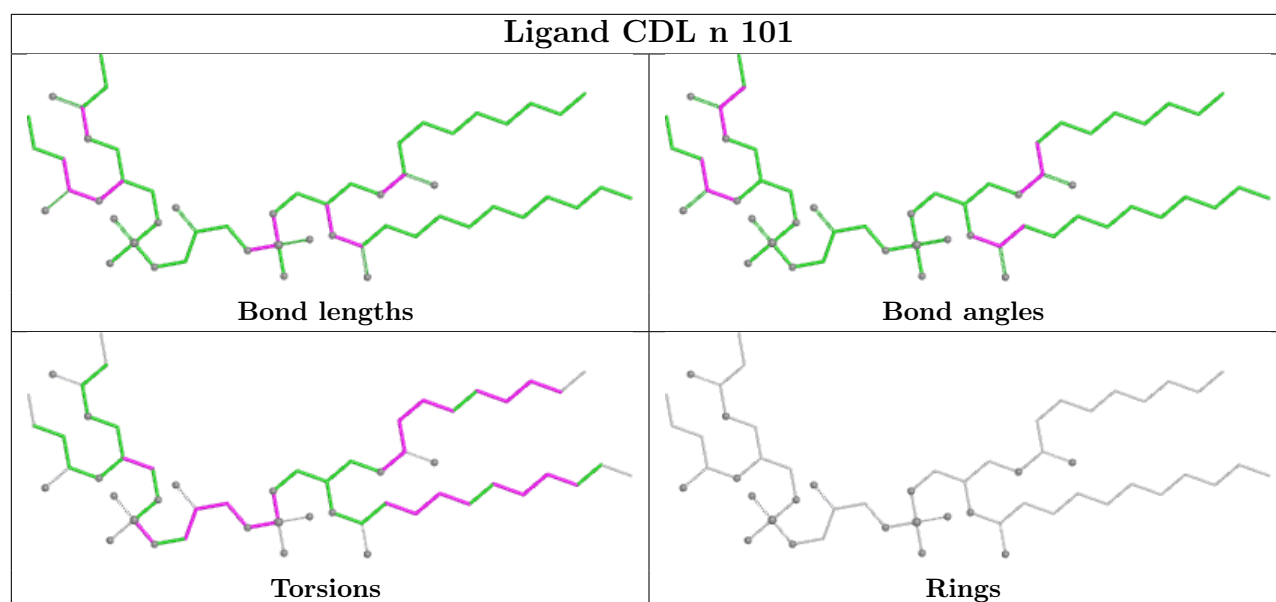


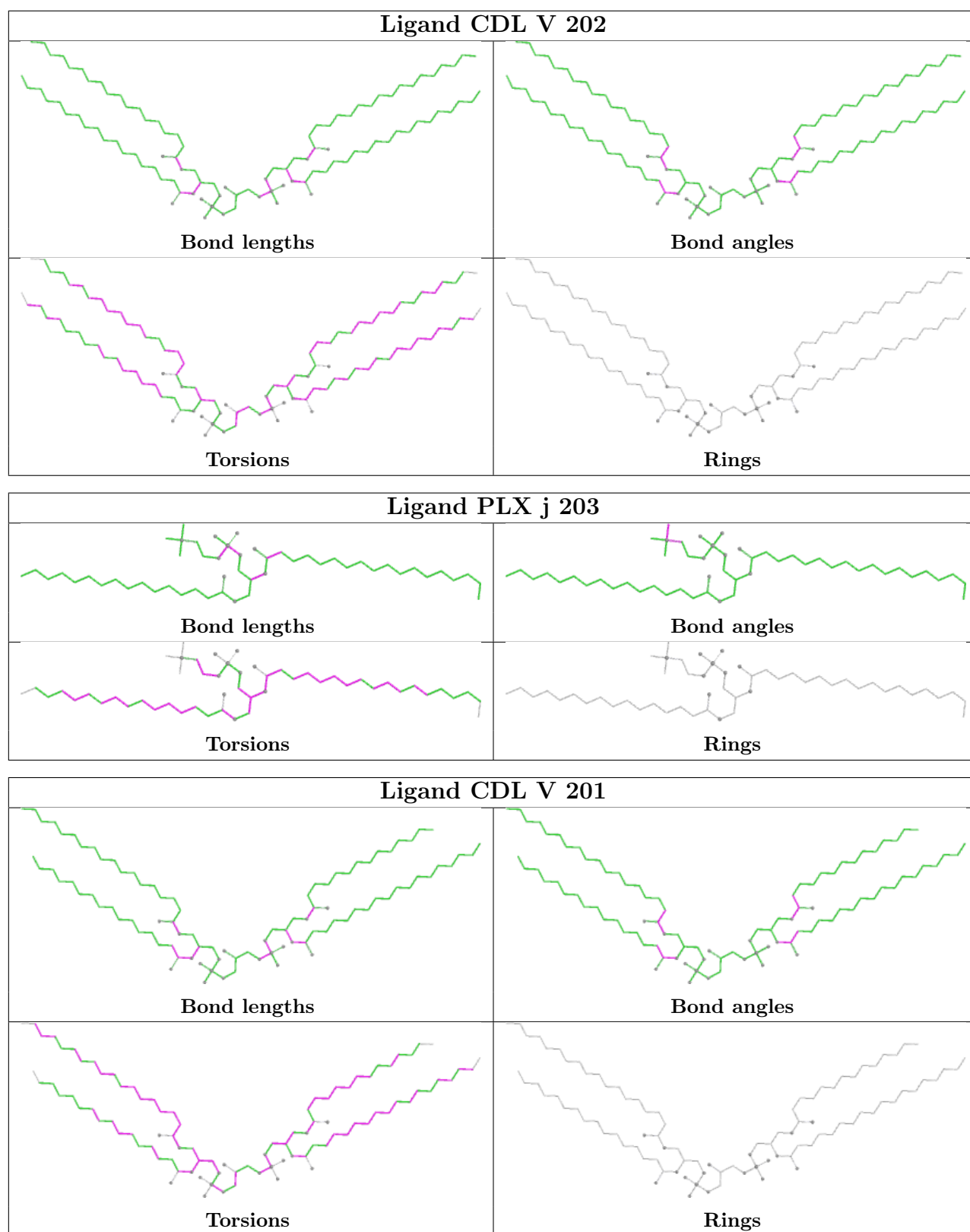


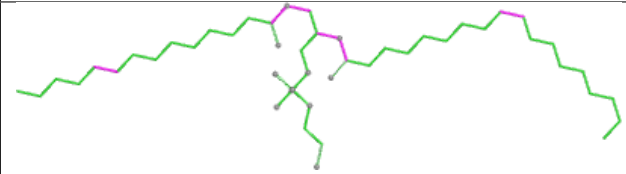
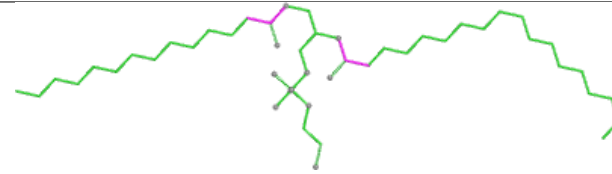
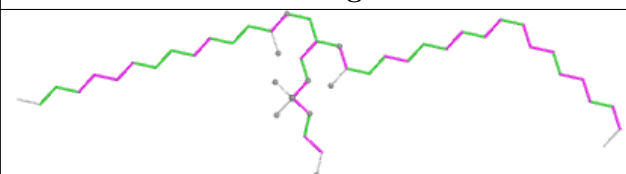
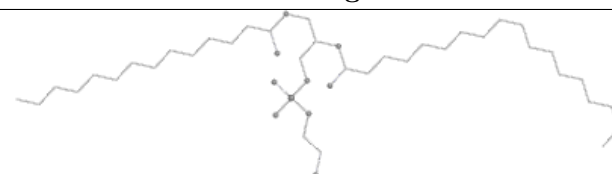
Ligand PLX e 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

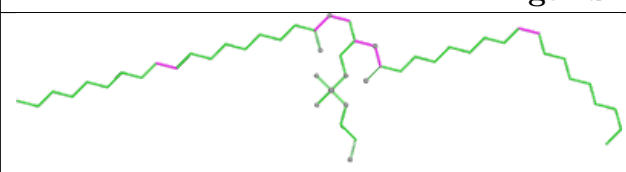
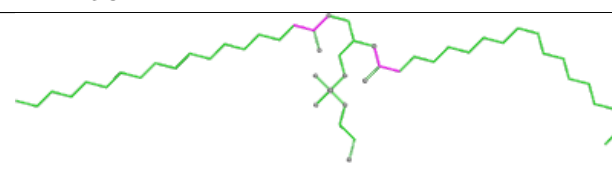
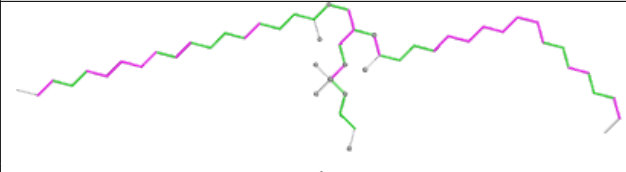
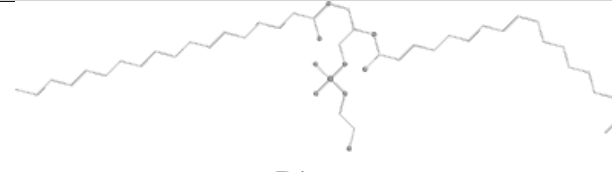
Ligand PLX j 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

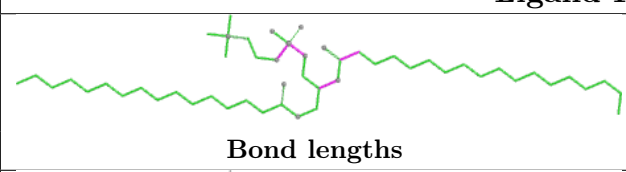
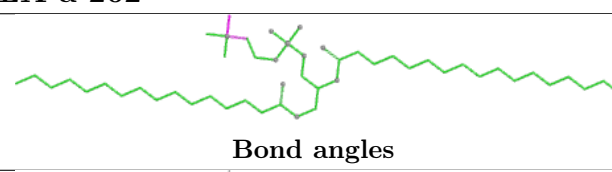
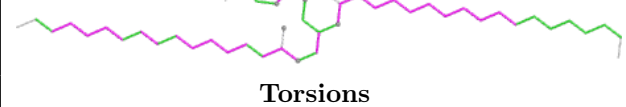
Ligand PEE l 705	
	
Bond lengths	Bond angles
	
Torsions	Rings

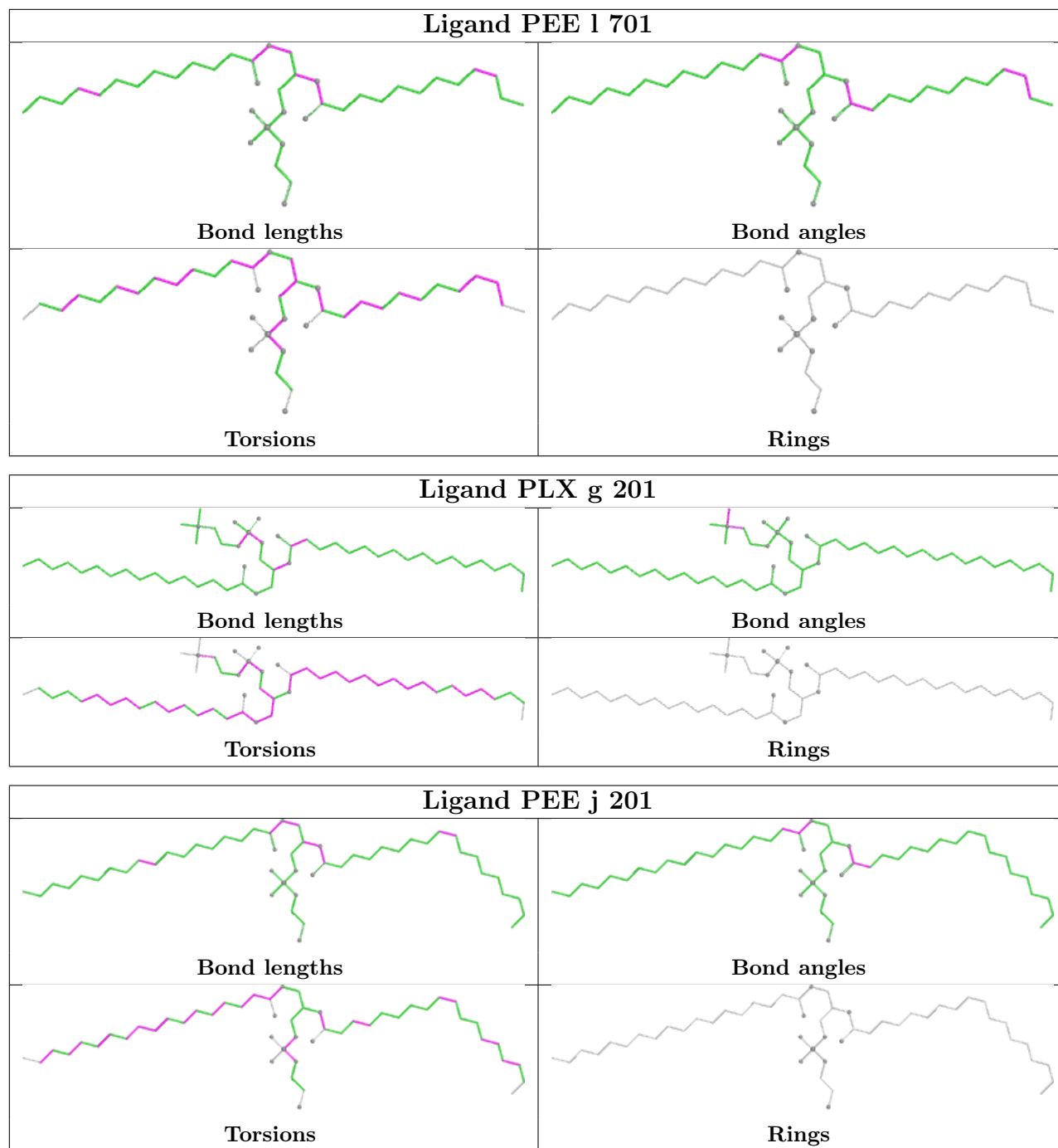


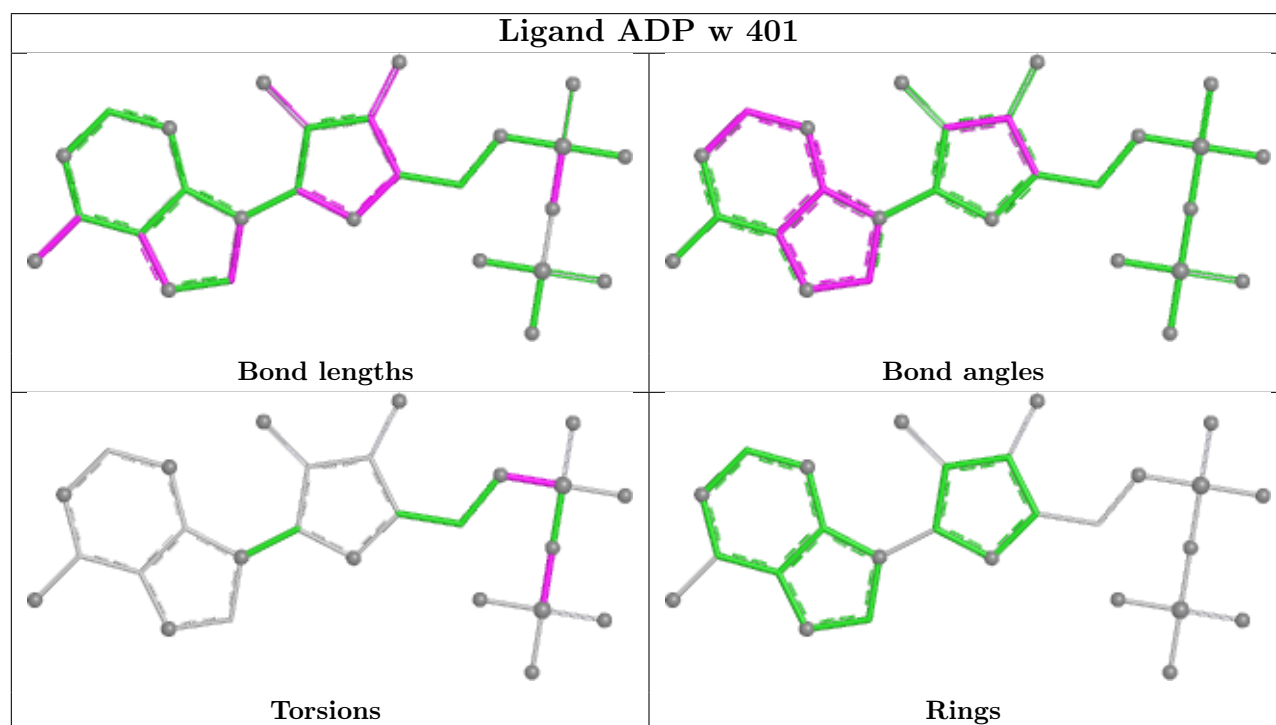
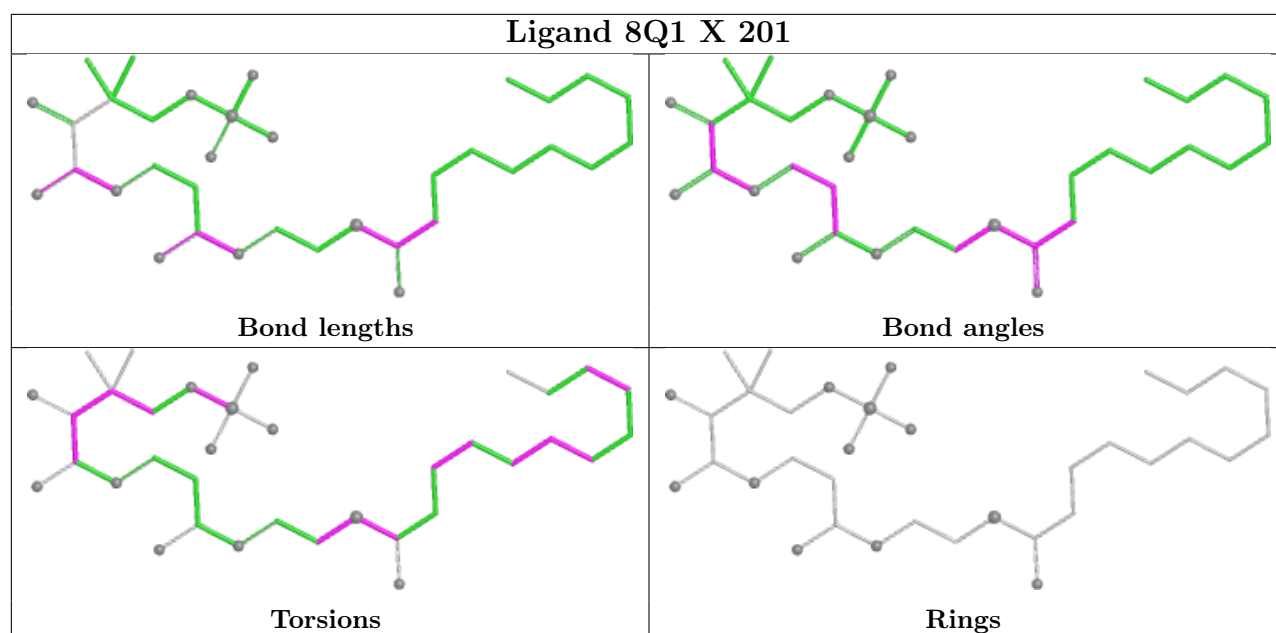


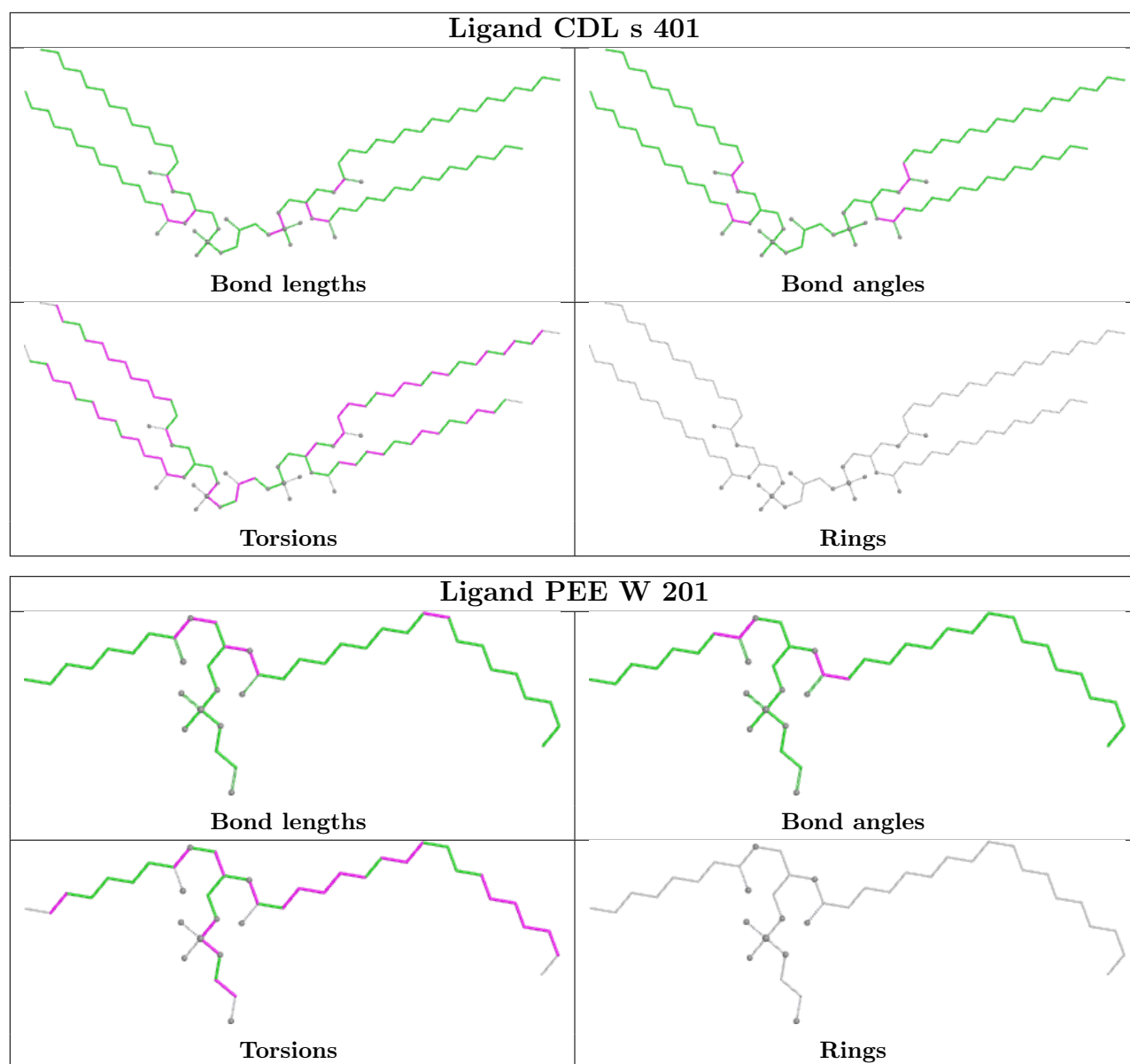
Ligand PEE Q 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

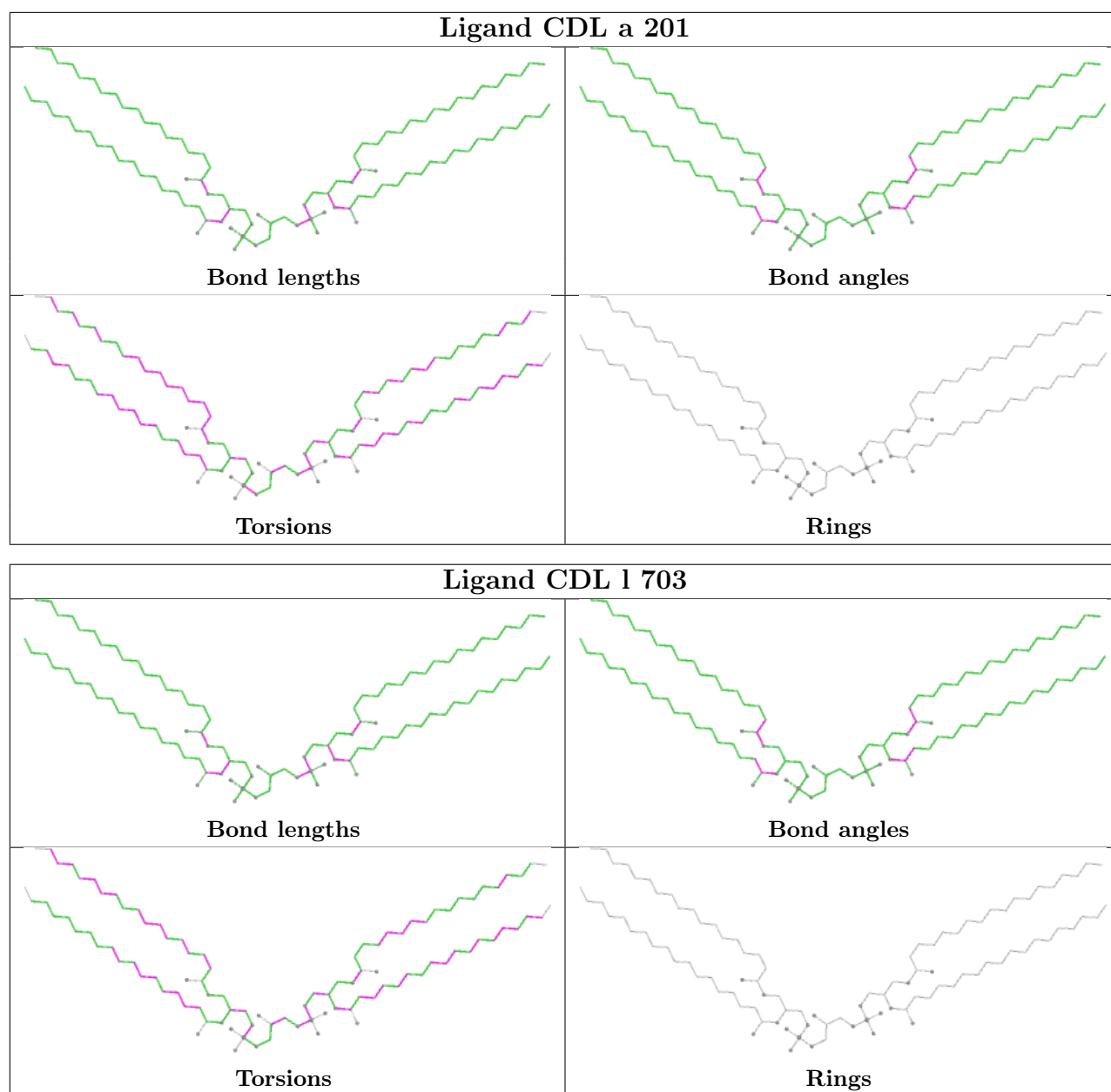
Ligand PEE r 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX a 202	
	
Bond lengths	Bond angles
	
Torsions	Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

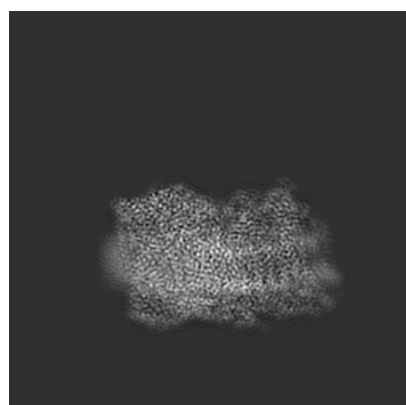
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32204. These allow visual inspection of the internal detail of the map and identification of artifacts.

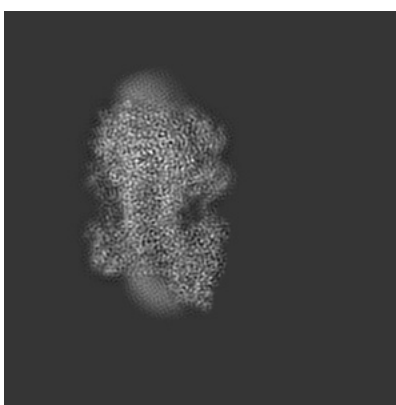
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

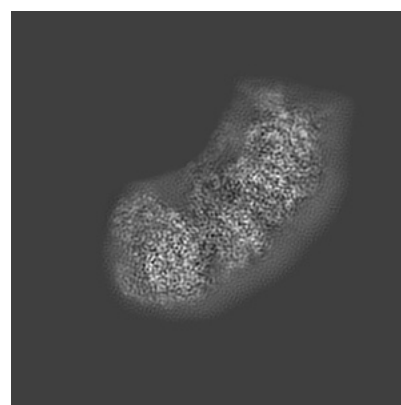
6.1.1 Primary map



X



Y

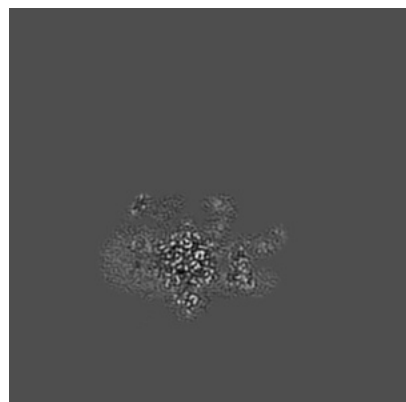


Z

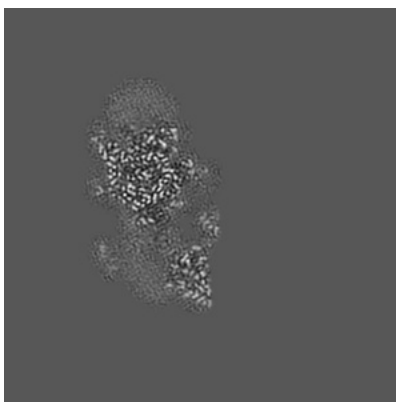
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

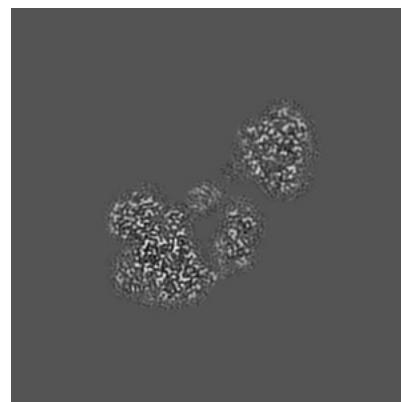
6.2.1 Primary map



X Index: 155



Y Index: 155

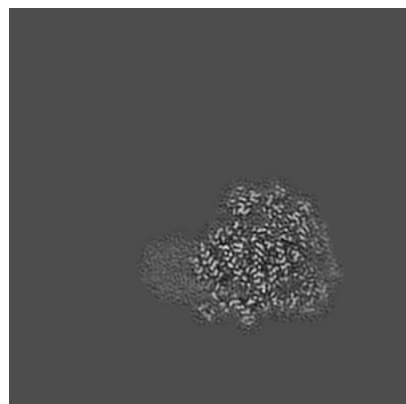


Z Index: 155

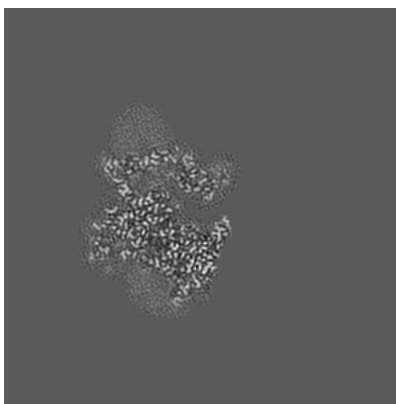
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

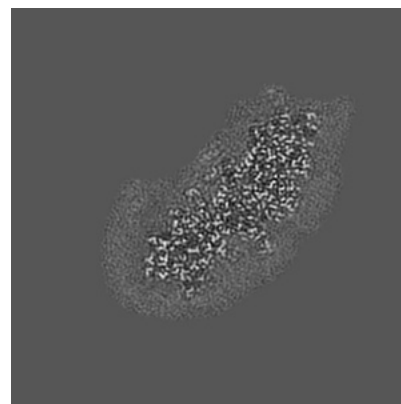
6.3.1 Primary map



X Index: 208



Y Index: 129

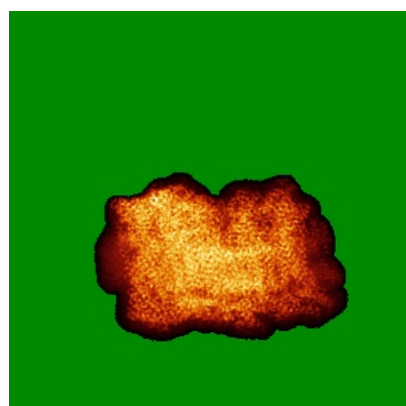


Z Index: 123

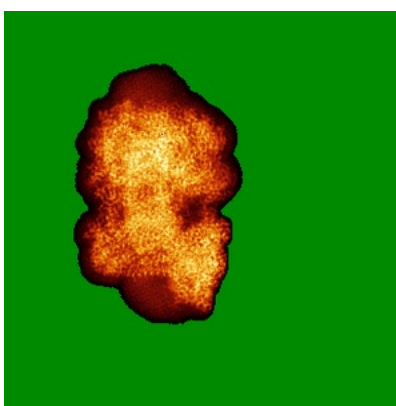
The images above show the largest variance slices of the map in three orthogonal directions.

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

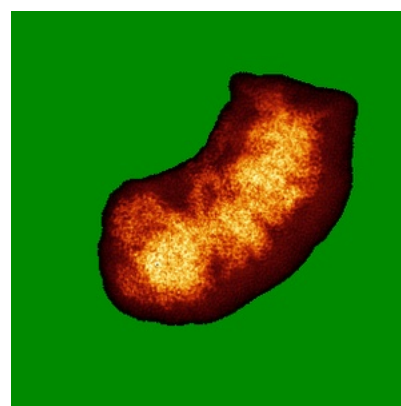
6.4.1 Primary map



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

This section was not generated.

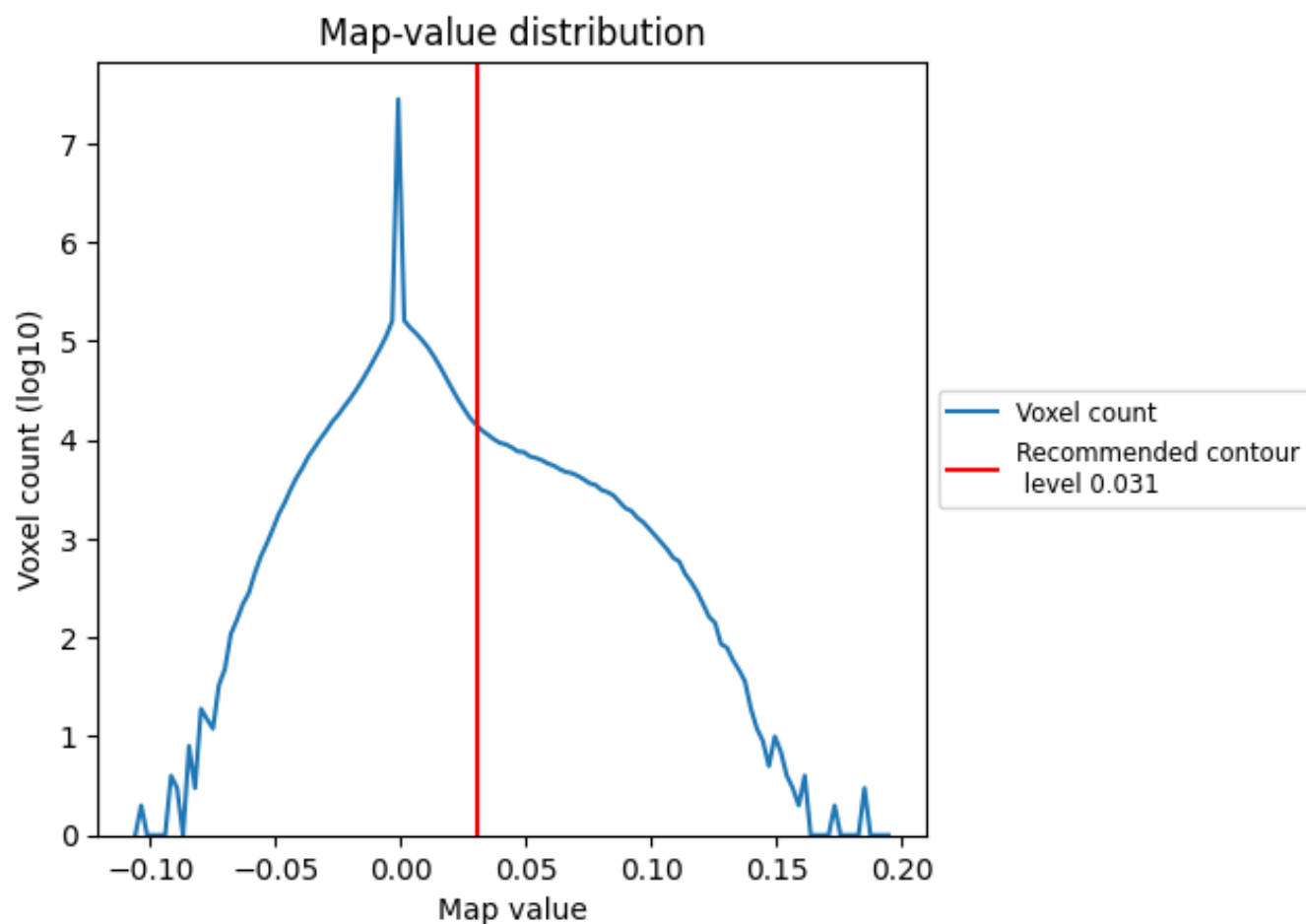
6.6 Mask visualisation

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

7 Map analysis [i](#)

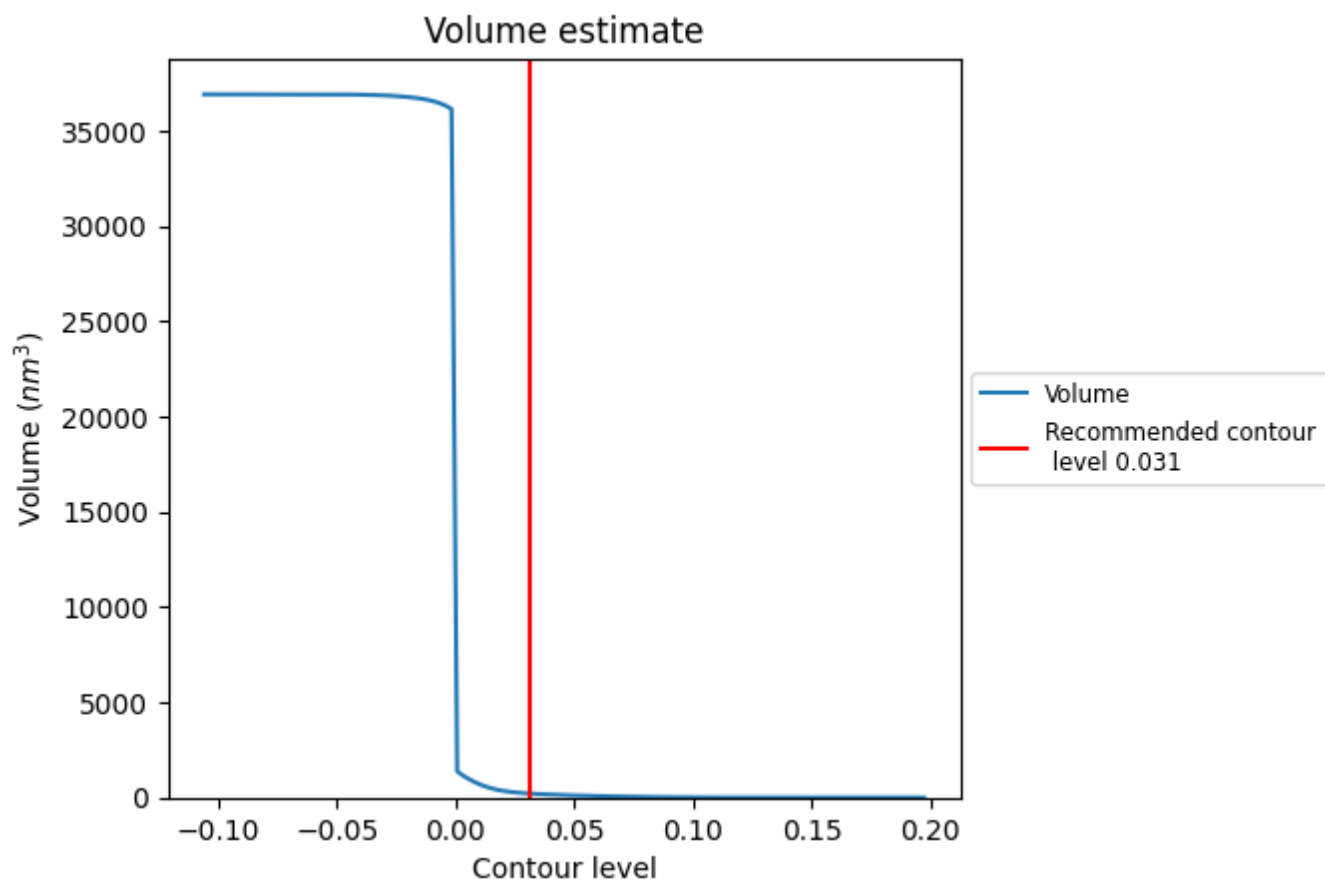
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

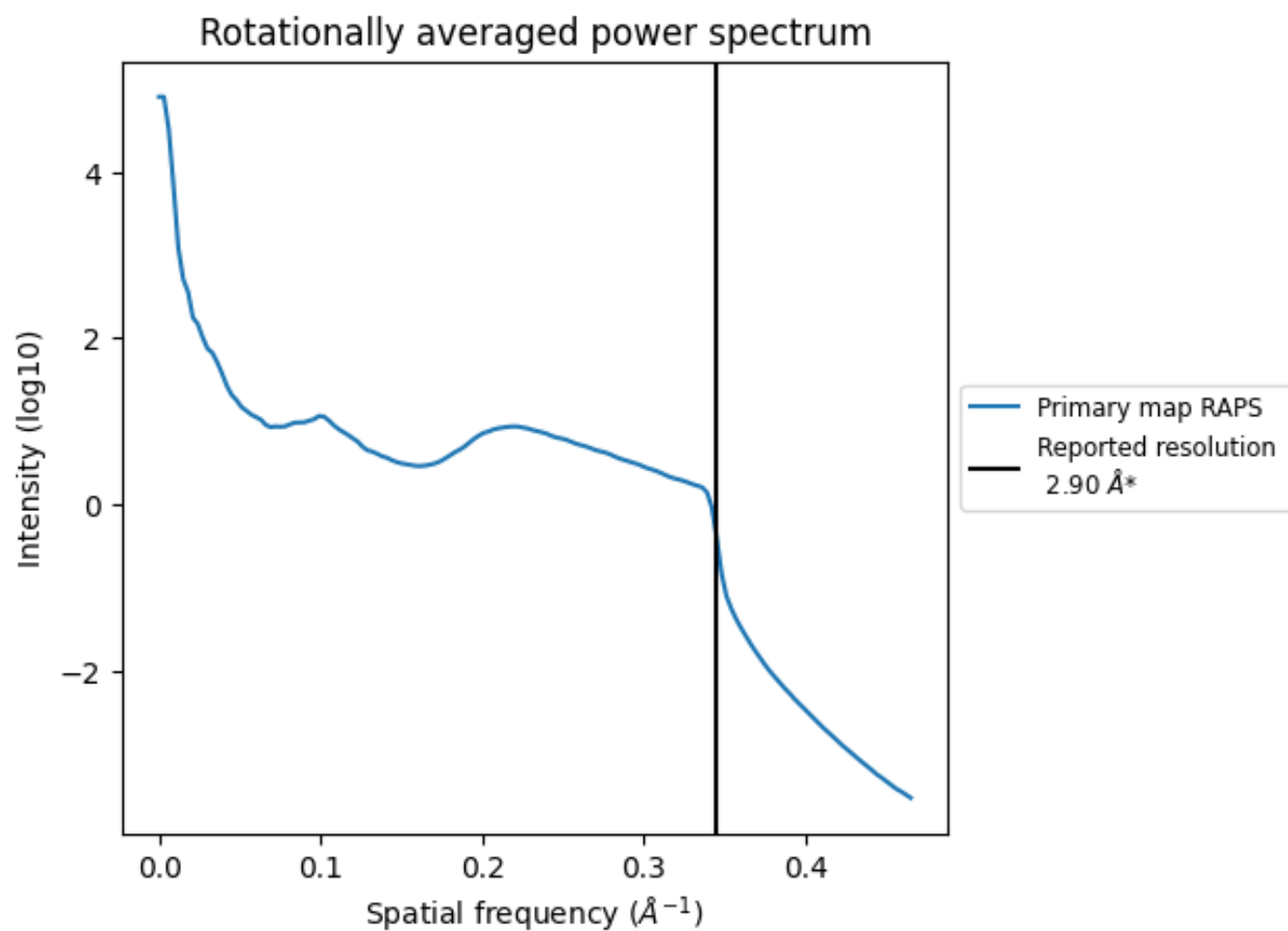
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

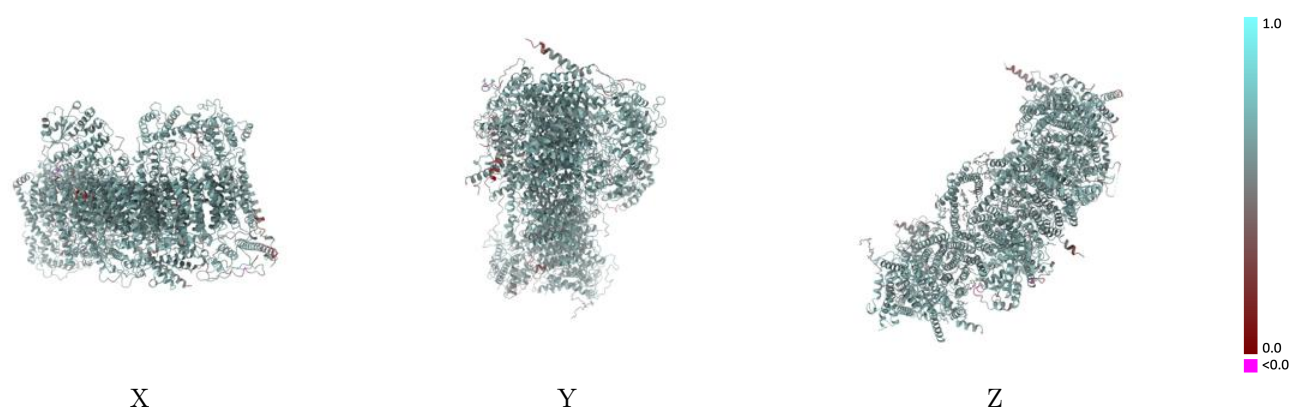
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32204 and PDB model 7VYG. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)

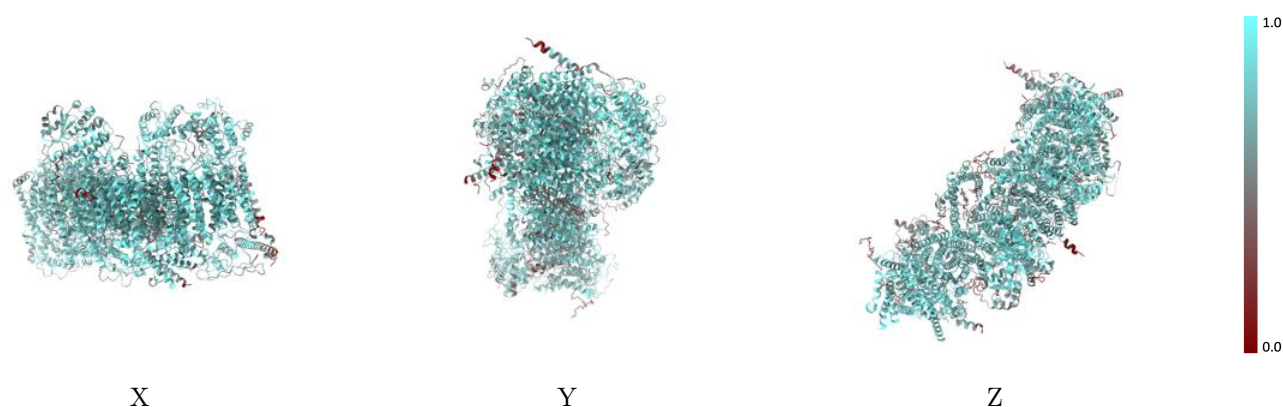
This section was not generated.

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



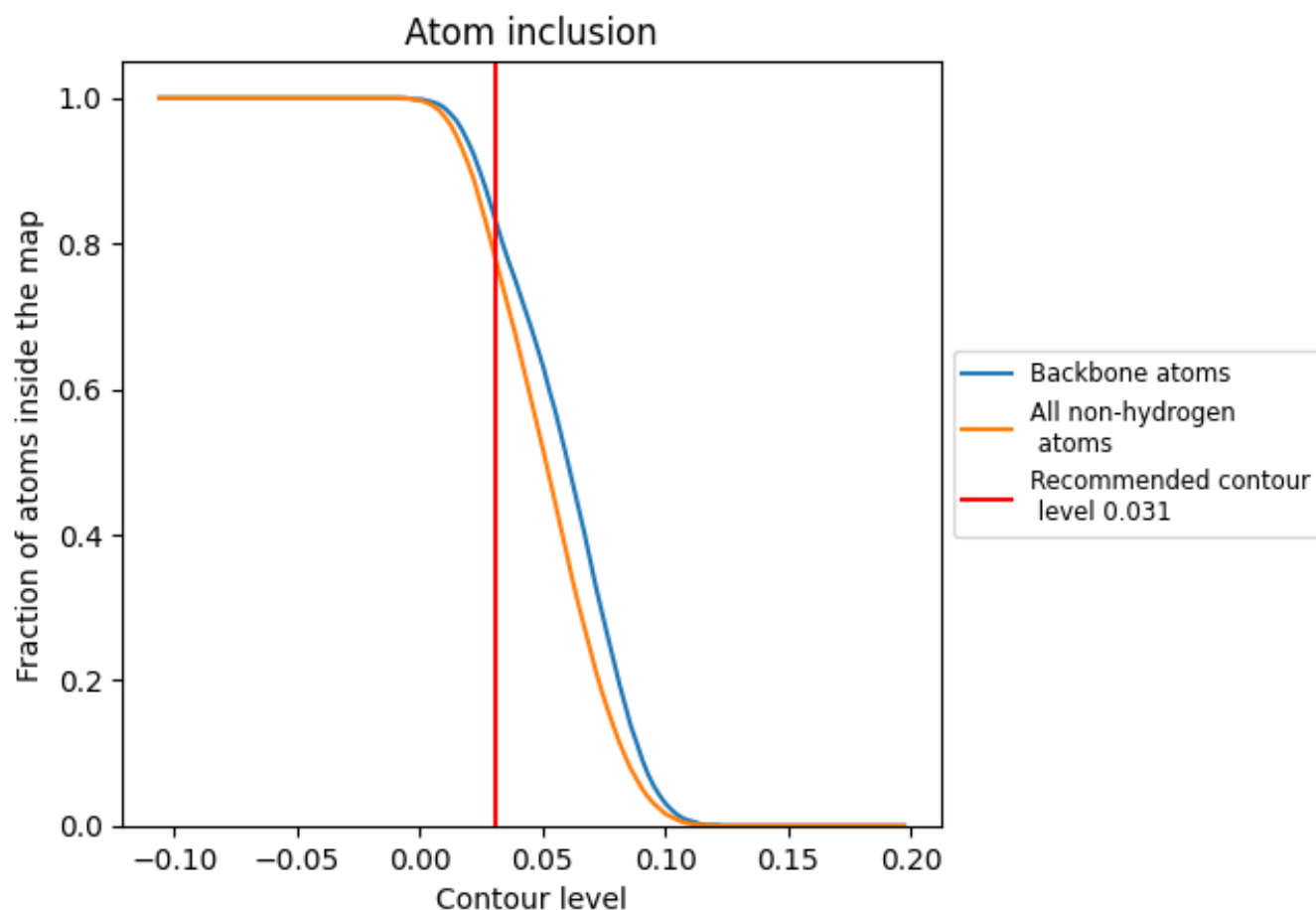
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.5970
Q	 0.6450	 0.5710
S	 0.8370	 0.6080
U	 0.7370	 0.5900
V	 0.6620	 0.5830
W	 0.7810	 0.5960
X	 0.7340	 0.5850
Y	 0.6680	 0.5480
Z	 0.6210	 0.5340
a	 0.7990	 0.6160
b	 0.7230	 0.5670
c	 0.7790	 0.5980
d	 0.7390	 0.5820
e	 0.7170	 0.5880
f	 0.6000	 0.5310
g	 0.8200	 0.6070
h	 0.7620	 0.5820
i	 0.8770	 0.6260
j	 0.7430	 0.6030
k	 0.8560	 0.6180
l	 0.8060	 0.6080
m	 0.6830	 0.5680
n	 0.6320	 0.5490
o	 0.7520	 0.5930
p	 0.8040	 0.6070
r	 0.8490	 0.6210
s	 0.8340	 0.6160
u	 0.7800	 0.5890
v	 0.6780	 0.5540
w	 0.7400	 0.5850

