wwPDB EM Validation Summary Report

Nov 28, 2022 – 11:09 PM JST

PDB ID	:	7VC0
EMDB ID	:	EMD-31887
Title	:	Membrane arm of active state CI from Rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-09-01
Resolution	:	2.60 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:

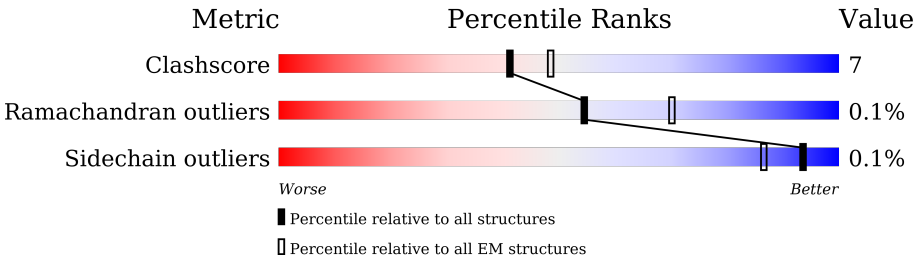
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	44	16% 84% 16%
2	S	70	. 91% 9%
3	U	83	8% 95% 5%
4	V	140	7% 92% 8%
5	W	113	6% 88% 12%
6	X	88	5% 94% 6%
7	Y	67	19% 87% 13%
8	Z	80	16% 96% .

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Mol	Chain	Length	Quality of chain
9	a	138	100%
10	b	126	10% 77% 22%
11	c	156	6% 100%
12	d	175	7% 100%
13	e	104	11% 99%
14	f	49	29% 100%
15	g	122	100%
16	h	105	10% 100%
17	i	347	100%
18	j	115	99%
19	k	98	100%
20	l	606	100%
21	m	175	18% 100%
22	n	56	23% 100%
23	o	128	5% 100%
24	p	178	99%
25	r	459	100%
26	s	318	99%
27	u	171	6% 99%
28	v	125	18% 100%
29	w	320	11% 100%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 40048 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
			703	454	104	140	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
			378	246	65	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	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
			4807	3188	744	824	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
			1298	867	188	230	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	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	318	Total	C	N	O	S	0	0
			2508	1678	385	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	125	Total	C	N	O	S	0	0
			1062	665	200	188	9		

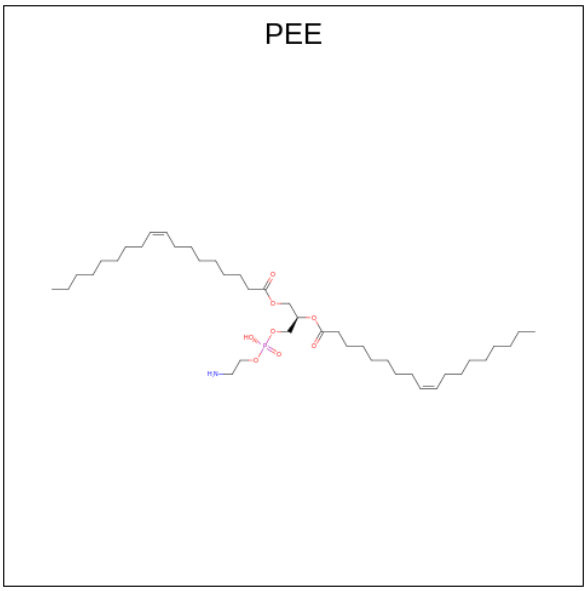
There is a discrepancy between the modelled and reference sequences:

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.

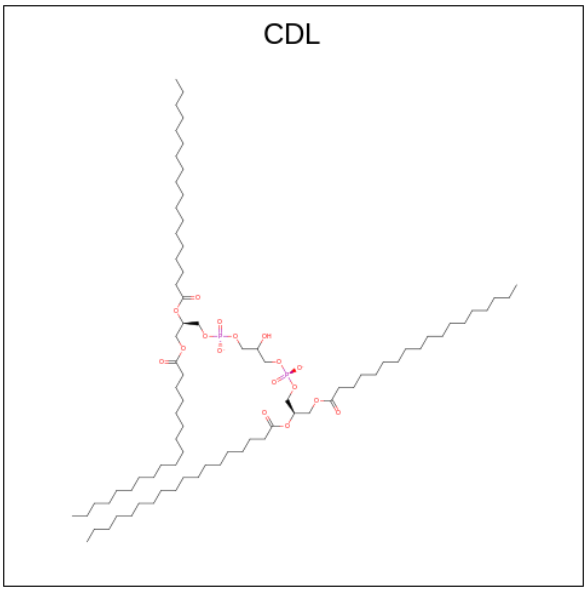
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



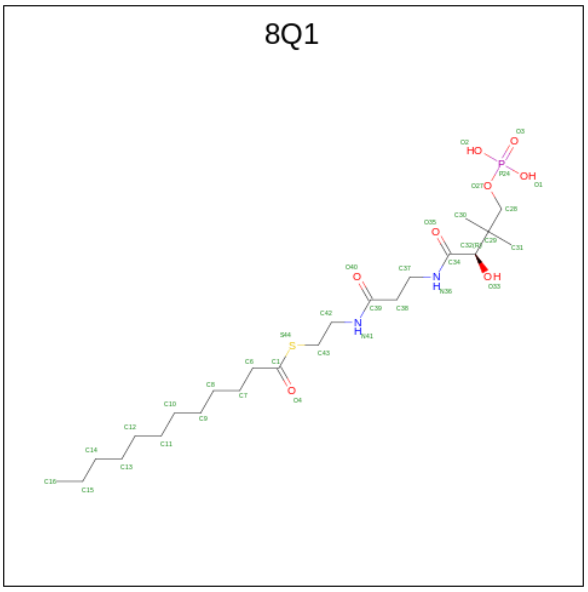
Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			96	76	2	16	2	
30	l	1	Total	C	N	O	P	0
			96	76	2	16	2	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



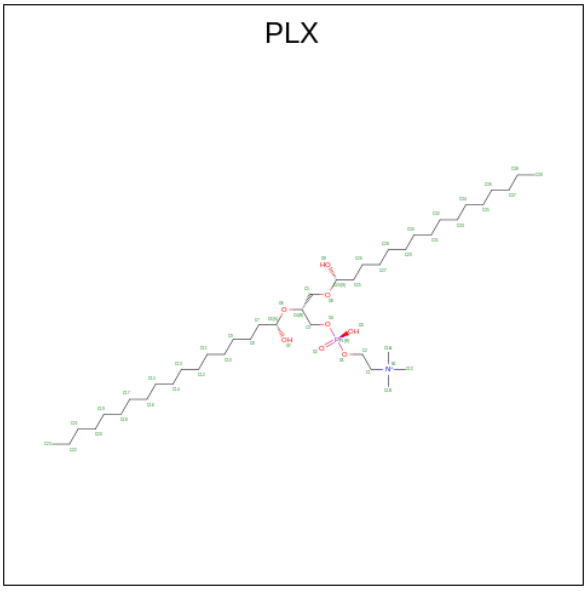
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	a	1	Total	C	O	P	0
			100	81	17	2	
31	k	1	Total	C	O	P	0
			100	81	17	2	
31	l	1	Total	C	O	P	0
			88	69	17	2	
31	o	1	Total	C	O	P	0
			100	81	17	2	
31	r	1	Total	C	O	P	0
			175	137	34	4	
31	r	1	Total	C	O	P	0
			175	137	34	4	
31	s	1	Total	C	O	P	0
			89	70	17	2	
31	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 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-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

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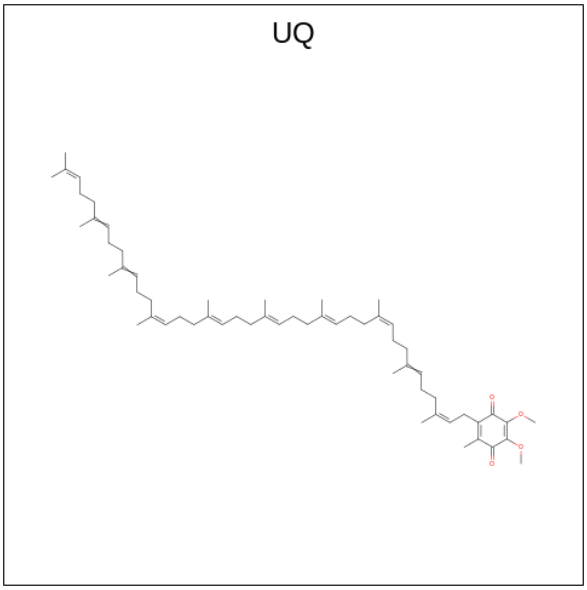
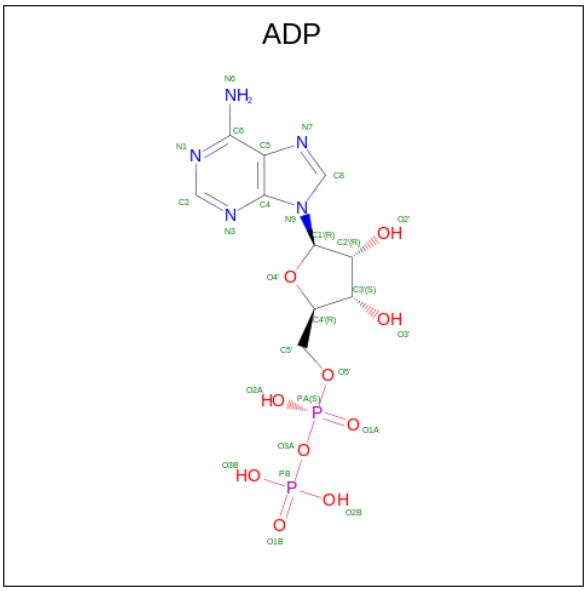
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			104	84	2	16	2	
33	j	1	Total	C	N	O	P	0
			104	84	2	16	2	
33	n	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: 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
			38	34	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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	5	Total	O	0
			5	5	
36	S	5	Total	O	0
			5	5	
36	U	3	Total	O	0
			3	3	
36	V	2	Total	O	0
			2	2	
36	W	2	Total	O	0
			2	2	
36	Y	1	Total	O	0
			1	1	
36	a	1	Total	O	0
			1	1	
36	b	1	Total	O	0
			1	1	
36	c	3	Total	O	0
			3	3	
36	d	1	Total	O	0
			1	1	
36	e	2	Total	O	0
			2	2	

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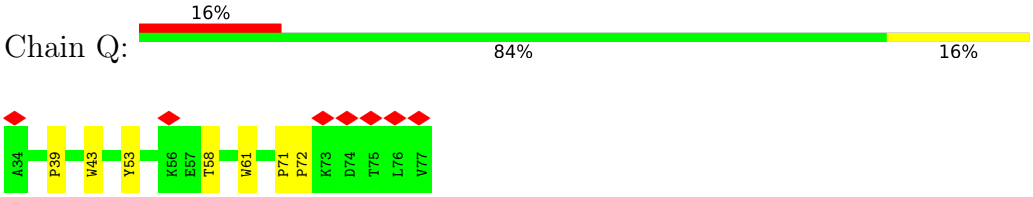
Mol	Chain	Residues	Atoms	AltConf
36	h	5	Total O 5 5	0
36	i	72	Total O 72 72	0
36	j	27	Total O 27 27	0
36	k	29	Total O 29 29	0
36	l	63	Total O 63 63	0
36	m	18	Total O 18 18	0
36	n	2	Total O 2 2	0
36	p	2	Total O 2 2	0
36	r	85	Total O 85 85	0
36	s	92	Total O 92 92	0
36	u	1	Total O 1 1	0
36	w	2	Total O 2 2	0

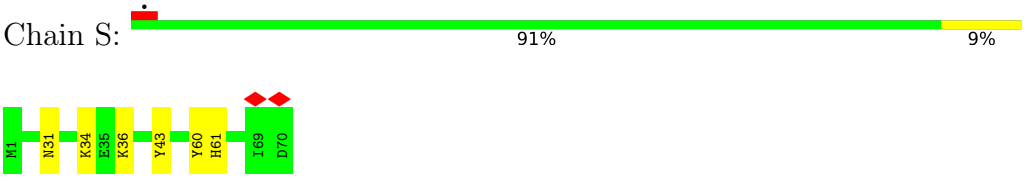
3 Residue-property plots (i)

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.

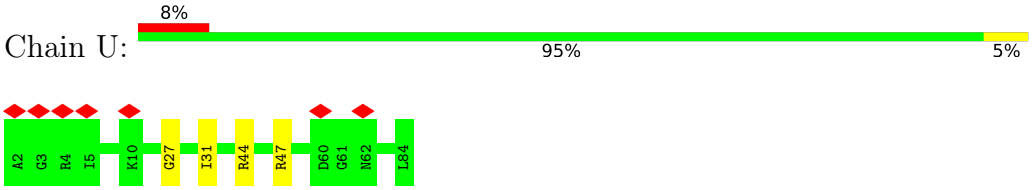
• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



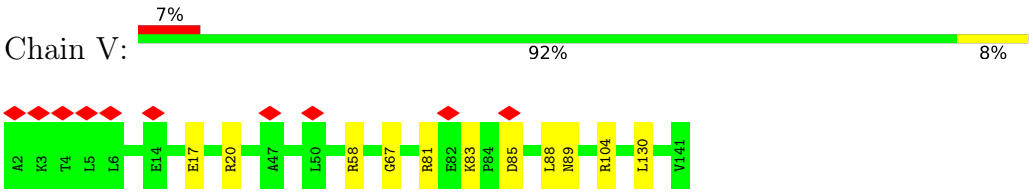
• Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



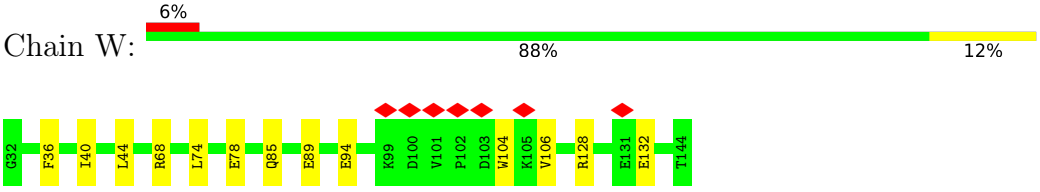
• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

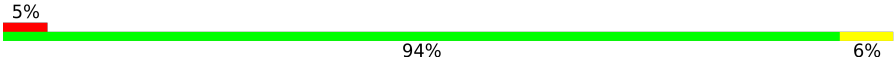


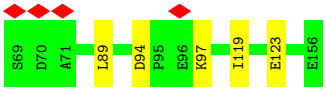
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



• Molecule 6: Acyl carrier protein, mitochondrial

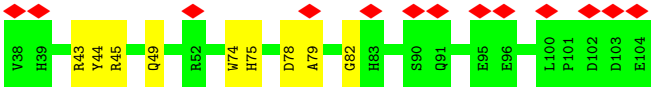
Chain X:





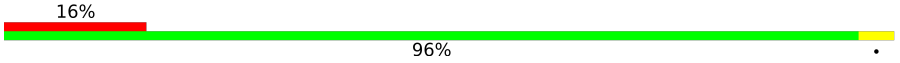
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

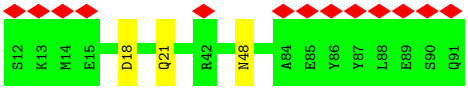
Chain Y:



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

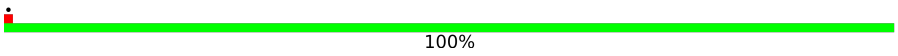
Chain Z:





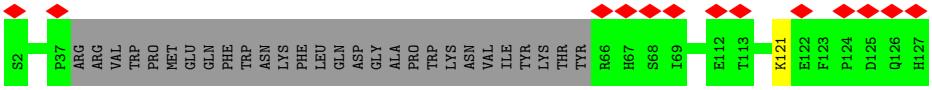
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:



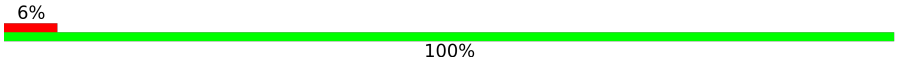
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

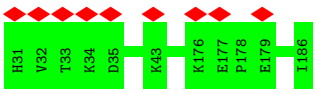
Chain b:



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

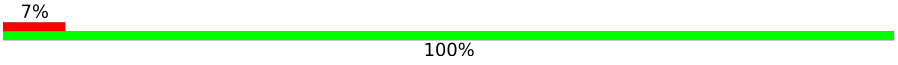
Chain c:

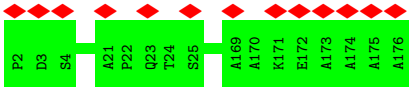




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

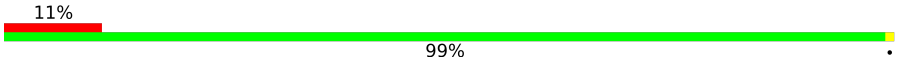
Chain d:

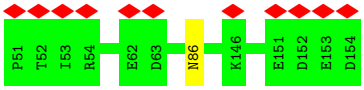




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

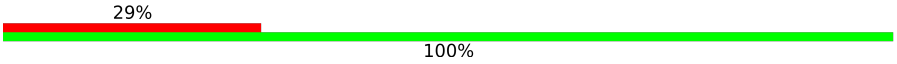
Chain e:

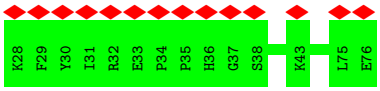




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

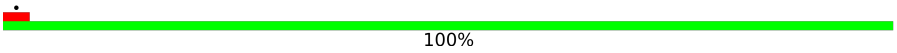
Chain f:





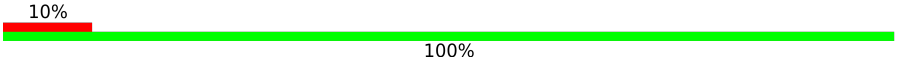
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

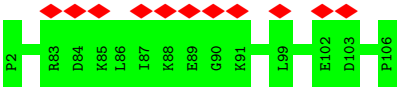
Chain g:



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

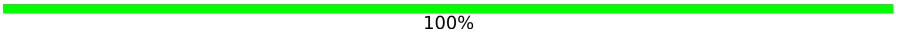
Chain h:

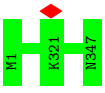




• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

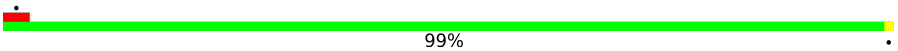
Chain i:

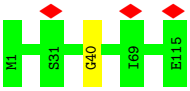




• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

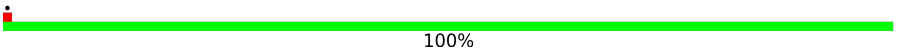
Chain j:

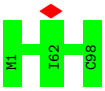




• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

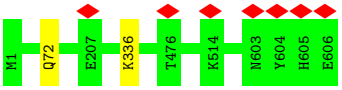
Chain k:





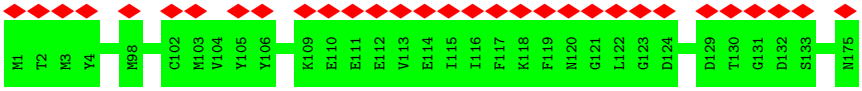
• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:



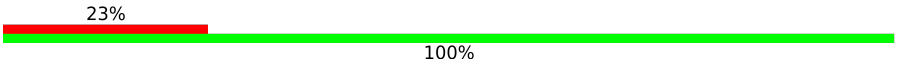
• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

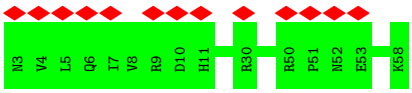
Chain m:



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

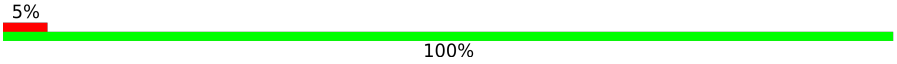
Chain n:

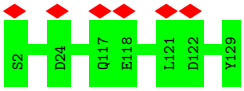




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

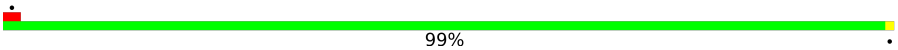
Chain o:

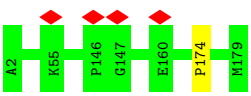




• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

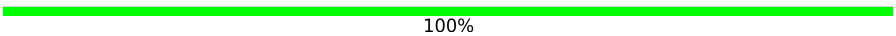
Chain p:

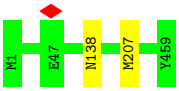




• Molecule 25: NADH-ubiquinone oxidoreductase chain 4

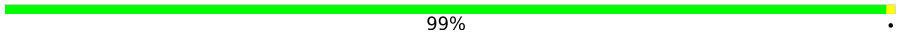
Chain r:

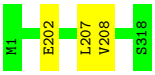




• Molecule 26: NADH-ubiquinone oxidoreductase chain 1

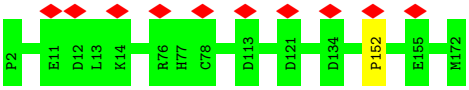
Chain s:





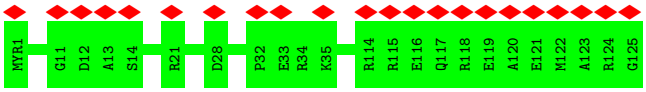
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:



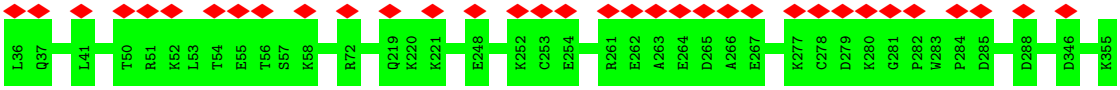
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:



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

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	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	0.082	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0152	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	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: 8Q1, UQ, PLX, ADP, PEE, CDL, MYR

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	0.27	0/380	0.44	0/525
2	S	0.27	0/581	0.52	0/781
3	U	0.26	0/664	0.43	0/912
4	V	0.26	0/1042	0.48	0/1411
5	W	0.28	0/973	0.51	0/1312
6	X	0.27	0/715	0.40	0/967
7	Y	0.26	0/610	0.49	0/836
8	Z	0.26	0/660	0.45	0/892
9	a	0.28	0/1184	0.51	0/1603
10	b	0.26	0/844	0.52	0/1149
11	c	0.29	0/1371	0.48	0/1875
12	d	0.27	0/1494	0.50	0/2015
13	e	0.27	0/891	0.51	0/1210
14	f	0.26	0/386	0.43	0/523
15	g	0.30	0/1036	0.51	0/1401
16	h	0.26	0/889	0.51	0/1190
17	i	0.28	0/2773	0.46	0/3768
18	j	0.25	0/938	0.47	0/1281
19	k	0.28	0/759	0.50	0/1029
20	l	0.28	0/4937	0.46	0/6715
21	m	0.29	0/1331	0.47	0/1808
22	n	0.25	0/491	0.53	0/663
23	o	0.28	0/1092	0.51	0/1481
24	p	0.29	0/1590	0.53	0/2155
25	r	0.27	0/3723	0.47	0/5078
26	s	0.29	0/2581	0.48	0/3529
27	u	0.27	0/1436	0.50	0/1938
28	v	0.28	0/1071	0.54	0/1434
29	w	0.27	0/2650	0.49	0/3588
All	All	0.28	0/39092	0.48	0/53069

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
10	b	0	1
25	r	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	b	121	LYS	Peptide
25	r	207	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	363	0	332	9	0
2	S	566	0	561	4	0
3	U	643	0	642	3	0
4	V	1021	0	1025	8	0
5	W	949	0	935	8	0
6	X	703	0	692	3	0
7	Y	584	0	529	5	0
8	Z	641	0	620	2	0
9	a	1151	0	1164	0	0
10	b	819	0	835	0	0
11	c	1315	0	1208	0	0
12	d	1461	0	1429	0	0
13	e	867	0	817	0	0
14	f	378	0	356	0	0
15	g	1005	0	999	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	h	867	0	871	0	0
17	i	2710	0	2874	0	0
18	j	914	0	951	0	0
19	k	748	0	799	0	0
20	l	4807	0	4946	0	0
21	m	1298	0	1272	0	0
22	n	479	0	486	0	0
23	o	1062	0	1072	0	0
24	p	1534	0	1470	0	0
25	r	3631	0	3839	0	0
26	s	2508	0	2607	0	0
27	u	1398	0	1374	0	0
28	v	1062	0	1036	0	0
29	w	2590	0	2553	0	0
30	Q	47	0	71	14	0
30	U	51	0	82	0	0
30	W	41	0	59	3	0
30	j	51	0	82	0	0
30	l	96	0	146	0	0
30	r	51	0	82	0	0
31	V	94	0	138	3	0
31	a	100	0	156	0	0
31	k	100	0	156	0	0
31	l	88	0	129	0	0
31	o	100	0	156	0	0
31	r	175	0	253	0	0
31	s	89	0	125	0	0
31	u	55	0	54	0	0
32	X	35	0	0	0	0
33	e	52	0	88	0	0
33	g	52	0	88	0	0
33	j	104	0	176	0	0
33	n	52	0	88	0	0
33	r	52	0	88	0	0
34	s	38	0	47	0	0
35	w	27	0	11	0	0
36	Q	5	0	0	0	0
36	S	5	0	0	0	0
36	U	3	0	0	0	0
36	V	2	0	0	0	0
36	W	2	0	0	0	0
36	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
36	b	1	0	0	0	0
36	c	3	0	0	0	0
36	d	1	0	0	0	0
36	e	2	0	0	0	0
36	h	5	0	0	0	0
36	i	72	0	0	0	0
36	j	27	0	0	0	0
36	k	29	0	0	0	0
36	l	63	0	0	0	0
36	m	18	0	0	0	0
36	n	2	0	0	0	0
36	p	2	0	0	0	0
36	r	85	0	0	0	0
36	s	92	0	0	0	0
36	u	1	0	0	0	0
36	w	2	0	0	0	0
All	All	40048	0	40569	53	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 7.

The worst 5 of 53 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)
30:Q:101:PEE:H37	30:Q:101:PEE:C37	1.94	0.98
1:Q:53:TYR:CE1	30:Q:101:PEE:H2	2.02	0.95
30:Q:101:PEE:H42	30:Q:101:PEE:H34	1.48	0.94
30:Q:101:PEE:H37	30:Q:101:PEE:H60	1.57	0.86
1:Q:53:TYR:CE1	30:Q:101:PEE:C1	2.67	0.77

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	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
3	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
4	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
5	W	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
10	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
11	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
12	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
13	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
14	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
15	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
16	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
17	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
18	j	113/115 (98%)	107 (95%)	5 (4%)	1 (1%)	17	35
19	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
20	l	604/606 (100%)	589 (98%)	14 (2%)	1 (0%)	47	71
21	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	176/178 (99%)	172 (98%)	3 (2%)	1 (1%)	25	47
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	316/318 (99%)	302 (96%)	13 (4%)	1 (0%)	41	64
27	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	25	47
28	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
29	w	318/320 (99%)	310 (98%)	8 (2%)	0	100	100
All	All	4667/4756 (98%)	4506 (97%)	156 (3%)	5 (0%)	54	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	l	72	GLN
26	s	208	VAL
18	j	40	GLY
24	p	174	PRO
27	u	152	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	38/38 (100%)	38 (100%)	0	100	100
2	S	57/58 (98%)	57 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	101 (100%)	0	100	100
5	W	99/99 (100%)	99 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	Y	62/62 (100%)	62 (100%)	0	100	100
8	Z	62/62 (100%)	62 (100%)	0	100	100
9	a	121/121 (100%)	121 (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	155/155 (100%)	155 (100%)	0	100	100
13	e	96/96 (100%)	95 (99%)	1 (1%)	76	90
14	f	36/45 (80%)	36 (100%)	0	100	100
15	g	108/109 (99%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	311 (100%)	0	100	100
18	j	100/100 (100%)	100 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	l	538/540 (100%)	537 (100%)	1 (0%)	93 98
21	m	131/141 (93%)	131 (100%)	0	100 100
22	n	53/53 (100%)	53 (100%)	0	100 100
23	o	113/113 (100%)	113 (100%)	0	100 100
24	p	159/159 (100%)	159 (100%)	0	100 100
25	r	410/410 (100%)	409 (100%)	1 (0%)	93 98
26	s	275/275 (100%)	273 (99%)	2 (1%)	84 94
27	u	153/153 (100%)	153 (100%)	0	100 100
28	v	108/111 (97%)	108 (100%)	0	100 100
29	w	283/283 (100%)	283 (100%)	0	100 100
All	All	4125/4183 (99%)	4120 (100%)	5 (0%)	93 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	e	86	ASN
20	l	336	LYS
25	r	138	ASN
26	s	202	GLU
26	s	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
17	i	289	ASN
20	l	580	GLN
29	w	219	GLN
22	n	11	HIS
17	i	268	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

25 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	$\#\|Z\| > 2$
31	CDL	s	401	-	88,88,99	1.13	8 (9%)	94,100,111	0.92	4 (4%)
30	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)
31	CDL	V	201	-	93,93,99	1.12	9 (9%)	99,105,111	0.84	4 (4%)
31	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.90	4 (3%)
31	CDL	o	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.88	4 (3%)
30	PEE	Q	101	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
33	PLX	j	202	-	51,51,51	1.14	3 (5%)	55,59,59	0.62	1 (1%)
32	8Q1	X	201	-	31,34,34	2.07	6 (19%)	40,43,43	1.74	12 (30%)
30	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
31	CDL	u	201	-	54,54,99	1.23	4 (7%)	60,66,111	1.26	5 (8%)
33	PLX	g	201	-	51,51,51	1.14	3 (5%)	55,59,59	0.62	1 (1%)
33	PLX	r	502	-	51,51,51	1.14	5 (9%)	55,59,59	0.63	1 (1%)
35	ADP	w	401	-	24,29,29	3.11	6 (25%)	29,45,45	1.37	3 (10%)
30	PEE	l	702	-	49,49,50	1.16	6 (12%)	52,54,55	0.95	2 (3%)
30	PEE	U	401	-	50,50,50	1.15	6 (12%)	53,55,55	0.99	2 (3%)
31	CDL	r	504	-	75,75,99	1.20	8 (10%)	81,87,111	0.96	4 (4%)
30	PEE	l	703	-	45,45,50	1.23	5 (11%)	48,50,55	0.98	2 (4%)
33	PLX	n	101	-	51,51,51	1.16	4 (7%)	55,59,59	0.59	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.60	1 (1%)
34	UQ	s	402	-	38,38,63	3.54	9 (23%)	46,49,79	2.85	16 (34%)
30	PEE	j	201	-	50,50,50	1.15	5 (10%)	53,55,55	0.91	2 (3%)
31	CDL	r	503	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
33	PLX	e	201	-	51,51,51	0.64	0	55,59,59	0.62	0
31	CDL	k	101	-	99,99,99	1.09	8 (8%)	105,111,111	0.81	4 (3%)
31	CDL	l	701	-	87,87,99	1.13	8 (9%)	93,99,111	0.89	4 (4%)

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
31	CDL	s	401	-	-	43/99/99/110	-
30	PEE	r	501	-	-	29/54/54/54	-
31	CDL	V	201	-	-	57/104/104/110	-
31	CDL	a	201	-	-	65/110/110/110	-
31	CDL	o	201	-	-	55/110/110/110	-
30	PEE	Q	101	-	-	28/50/50/54	-
33	PLX	j	202	-	-	25/55/55/55	-
32	8Q1	X	201	-	-	11/41/41/41	-
30	PEE	W	201	-	-	23/44/44/54	-
31	CDL	u	201	-	-	19/65/65/110	-
33	PLX	g	201	-	-	27/55/55/55	-
33	PLX	r	502	-	-	25/55/55/55	-
35	ADP	w	401	-	-	5/12/32/32	0/3/3/3
30	PEE	l	702	-	-	22/53/53/54	-
30	PEE	U	401	-	-	26/54/54/54	-
31	CDL	r	504	-	-	43/86/86/110	-
30	PEE	l	703	-	-	22/49/49/54	-
33	PLX	n	101	-	-	30/55/55/55	-
33	PLX	j	203	-	-	27/55/55/55	-
34	UQ	s	402	-	-	14/33/57/87	0/1/1/1
30	PEE	j	201	-	-	25/54/54/54	-
31	CDL	r	503	-	-	58/109/109/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PLX	e	201	-	-	17/55/55/55	-
31	CDL	k	101	-	-	57/110/110/110	-
31	CDL	l	701	-	-	44/98/98/110	-

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C18-C19	9.63	1.56	1.33
34	s	402	UQ	C13-C14	9.29	1.55	1.33
34	s	402	UQ	C23-C24	9.07	1.54	1.33
35	w	401	ADP	C3'-C4'	-9.01	1.30	1.53
34	s	402	UQ	C8-C9	8.95	1.54	1.33

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	s	402	UQ	C7-C8-C9	-8.47	112.70	126.79
34	s	402	UQ	C17-C18-C19	-5.98	113.26	127.66
34	s	402	UQ	C12-C13-C14	-5.71	113.91	127.66
34	s	402	UQ	C22-C23-C24	-5.67	114.00	127.66
35	w	401	ADP	N3-C2-N1	-4.52	121.61	128.68

There are no chirality outliers.

5 of 797 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C11-C10-O2-C2
30	Q	101	PEE	C4-O4P-P-O2P
30	Q	101	PEE	C4-O4P-P-O1P
30	Q	101	PEE	C5-C4-O4P-P
30	W	201	PEE	C1-O3P-P-O2P

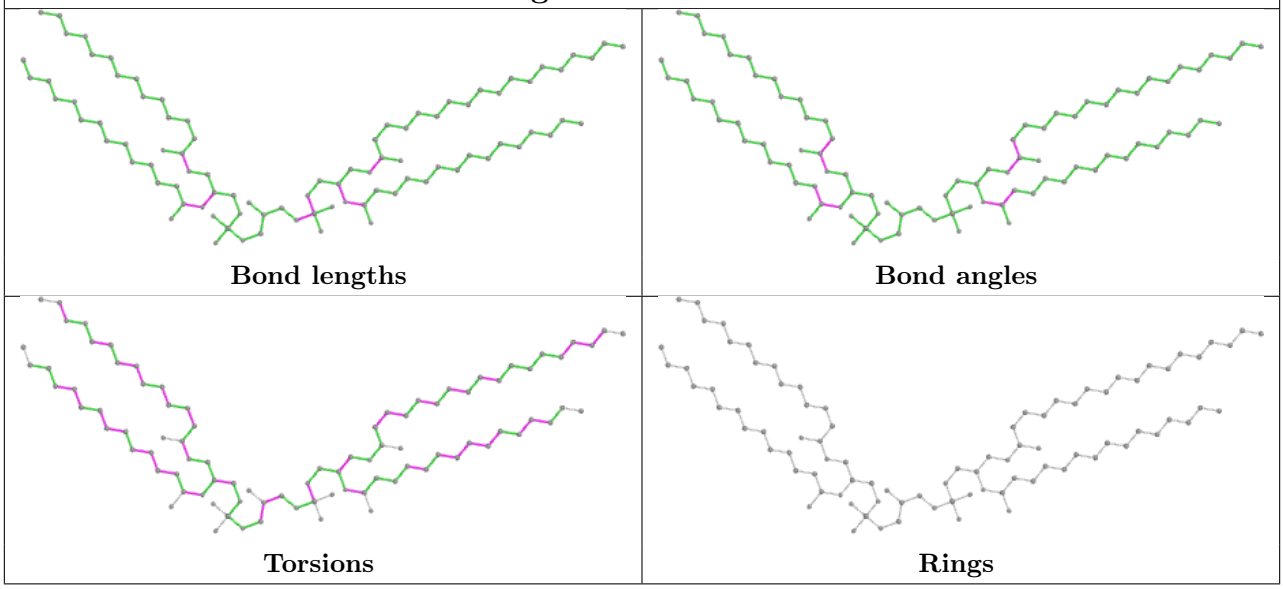
There are no ring outliers.

3 monomers are involved in 20 short contacts:

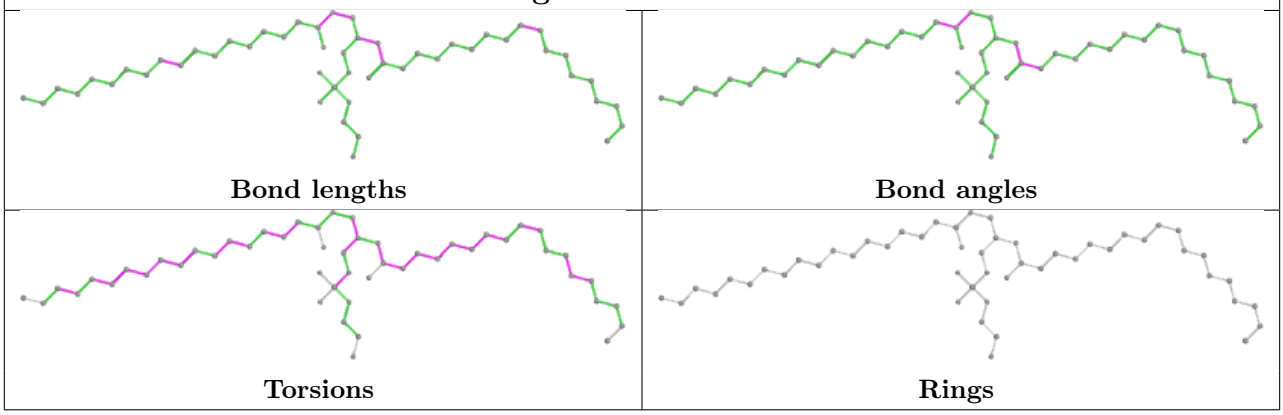
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	V	201	CDL	3	0
30	Q	101	PEE	14	0
30	W	201	PEE	3	0

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.

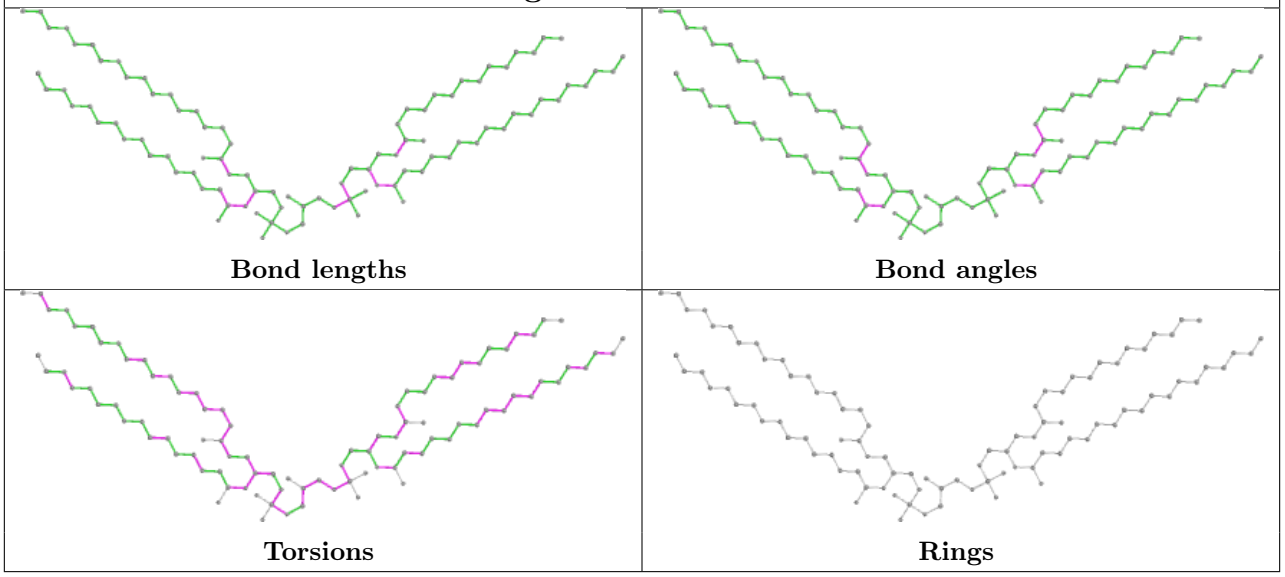
Ligand CDL s 401



Ligand PEE r 501



Ligand CDL V 201



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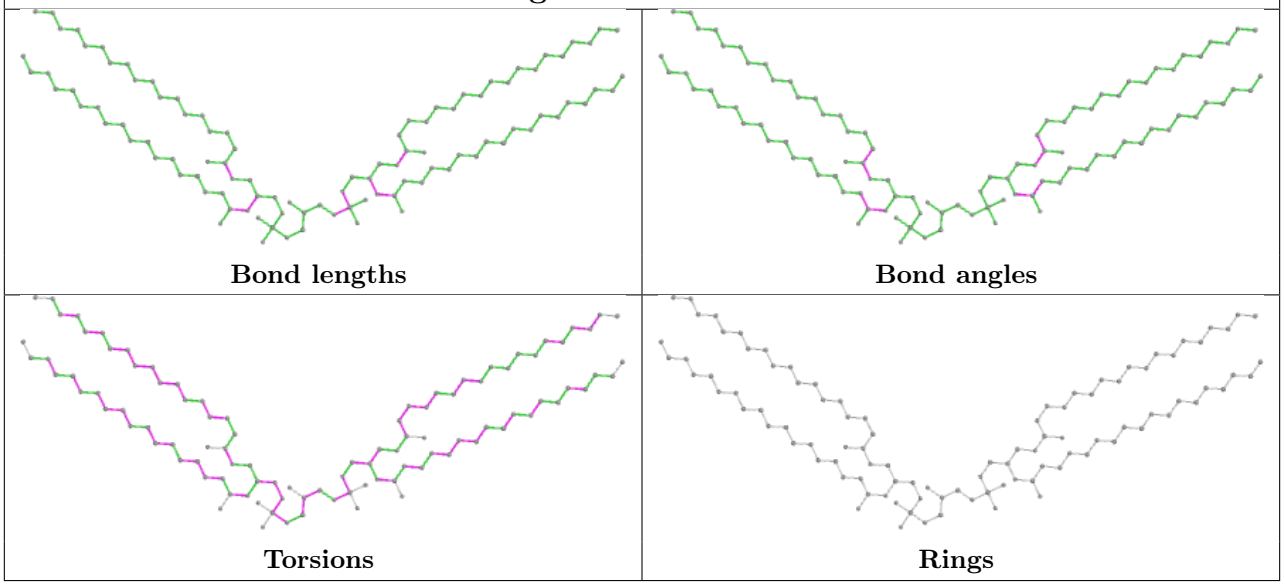

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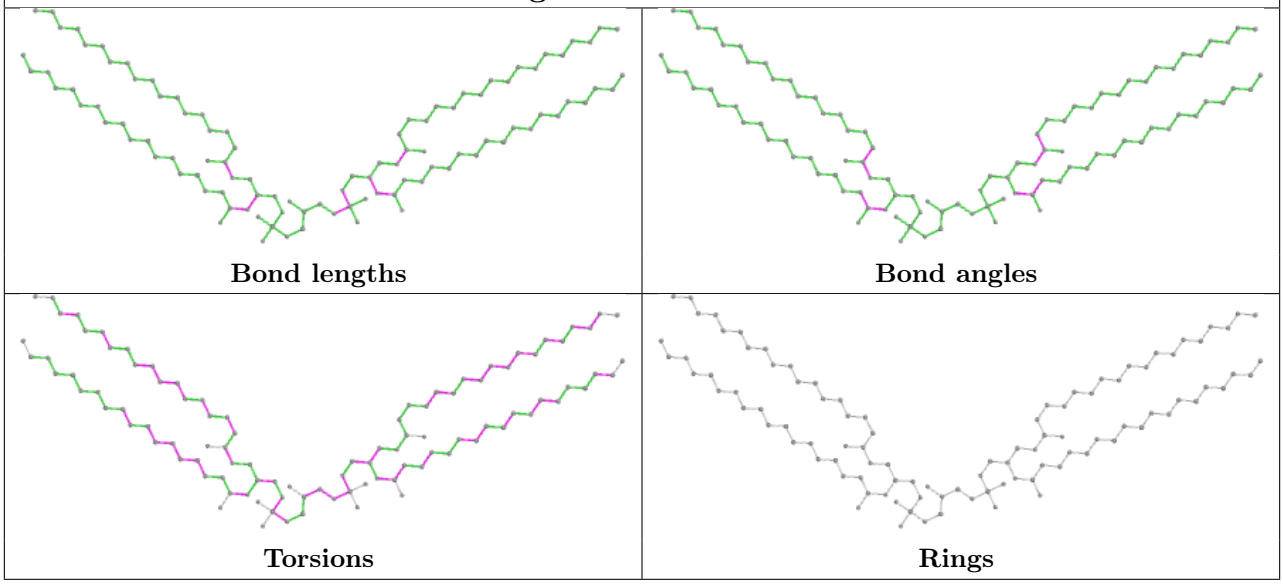

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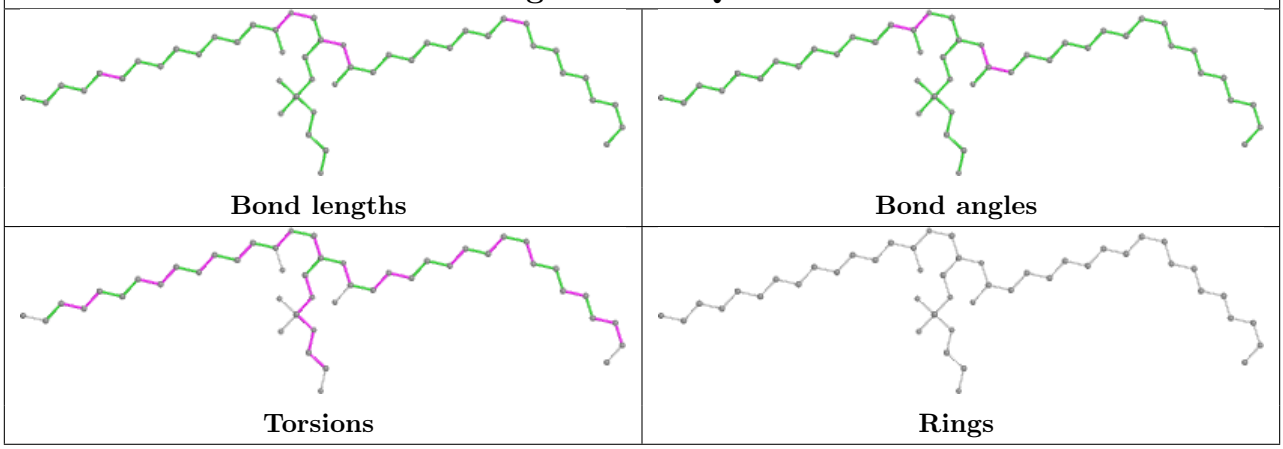

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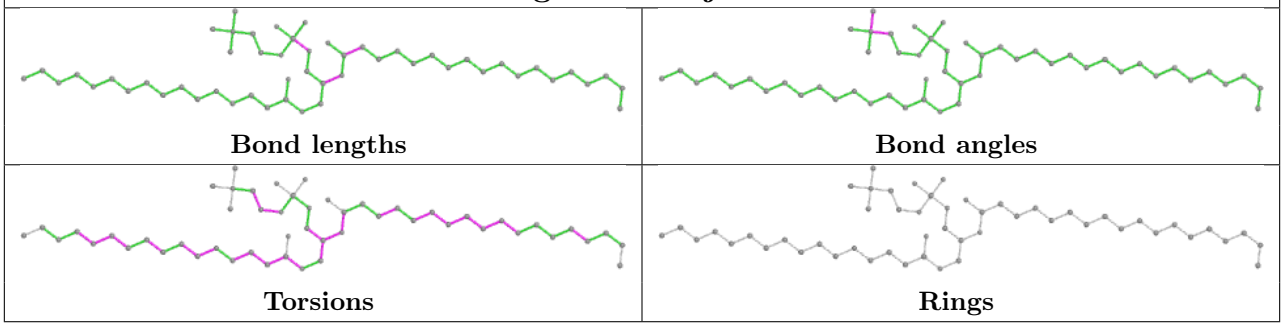
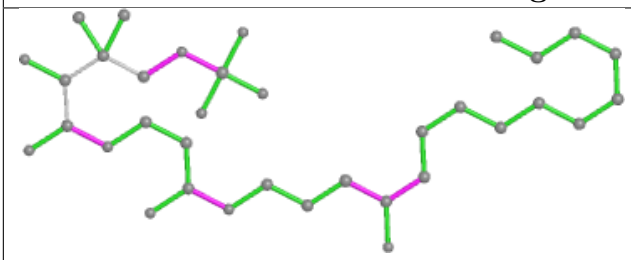
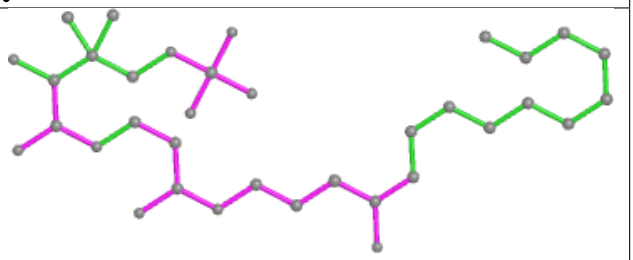


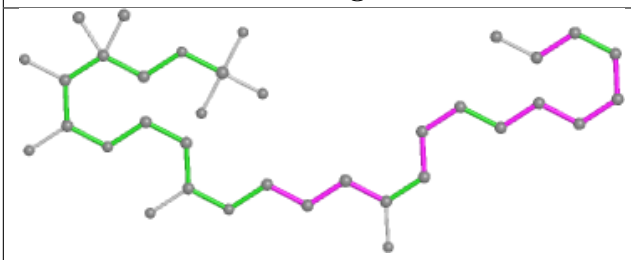
Ligand 8Q1 X 201



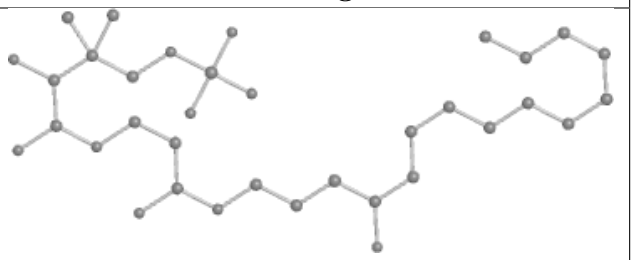
Bond lengths



Bond angles

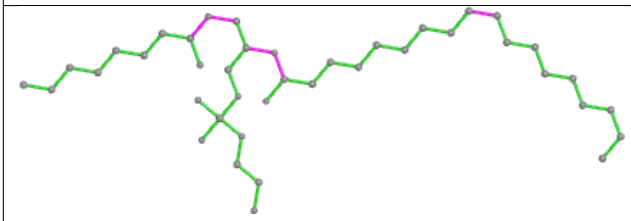


Torsions

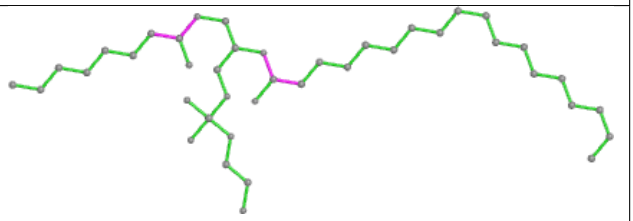


Rings

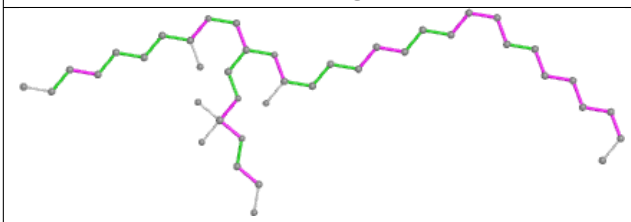
Ligand PEE W 201



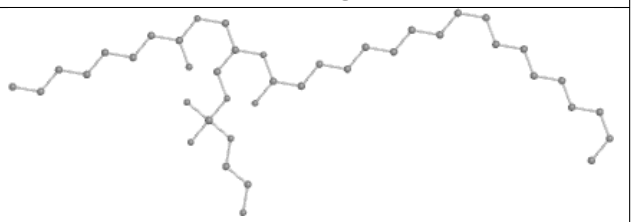
Bond lengths



Bond angles

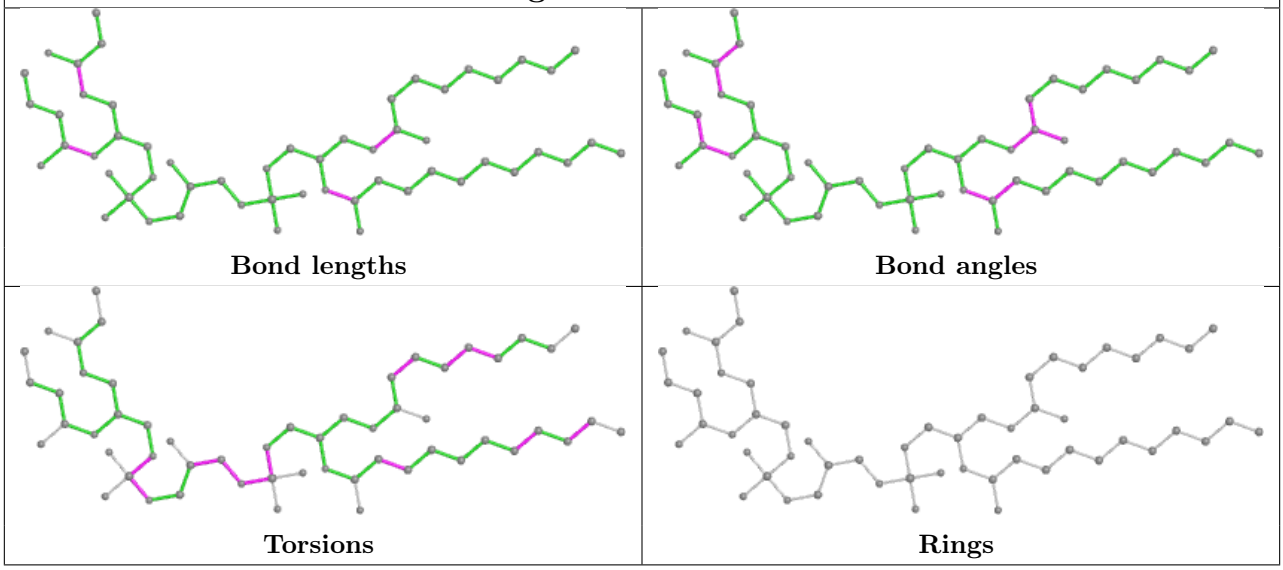


Torsions

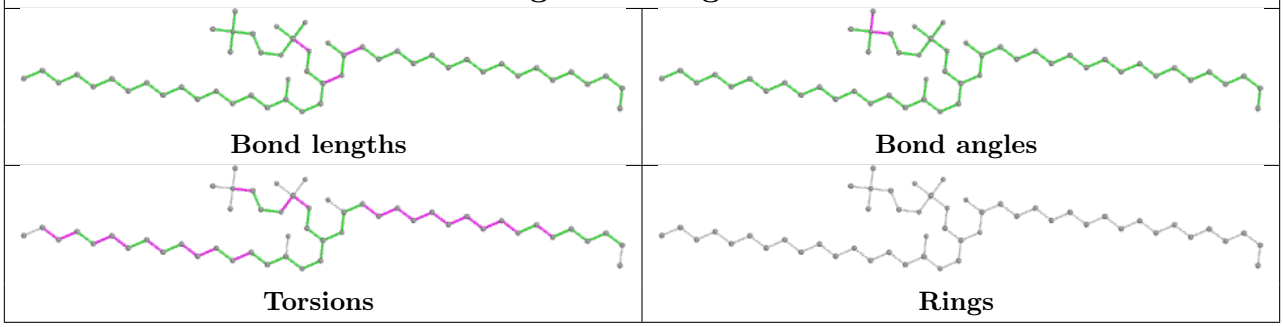


Rings

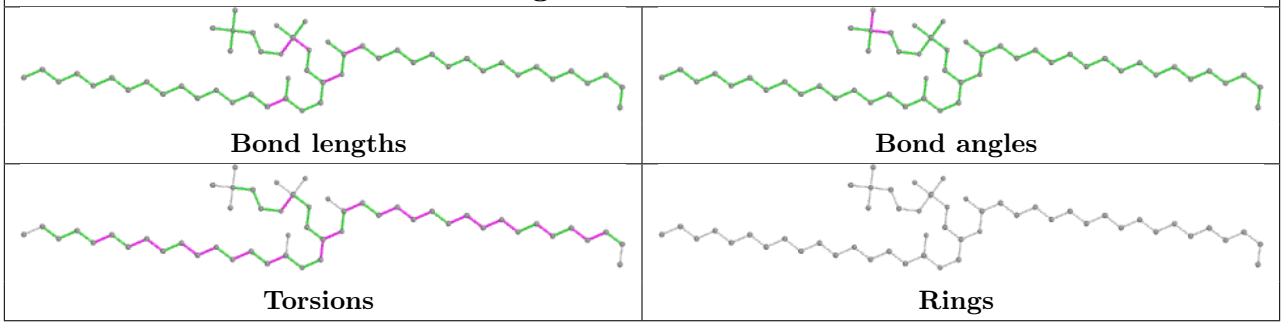
Ligand CDL u 201



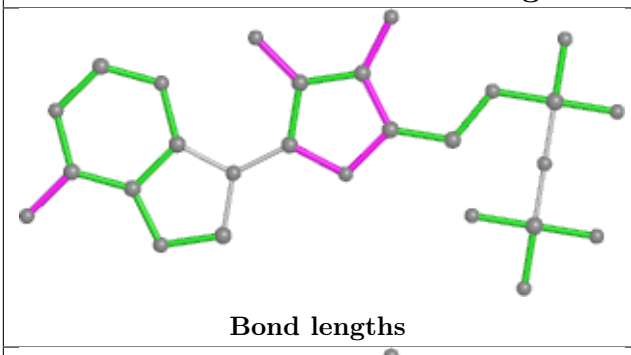
Ligand PLX g 201

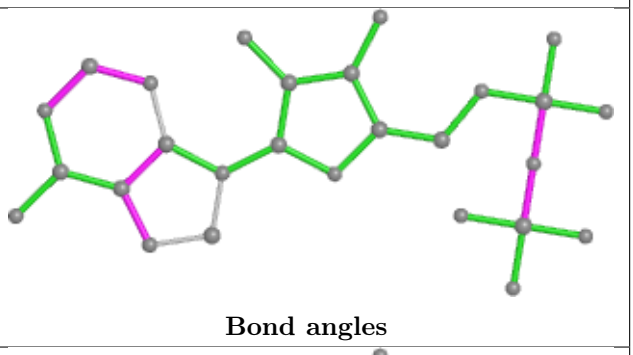


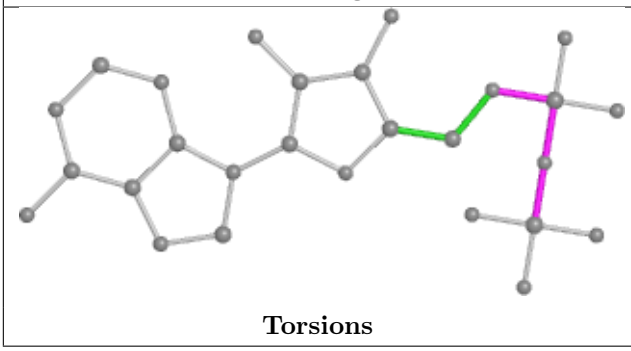
Ligand PLX r 502

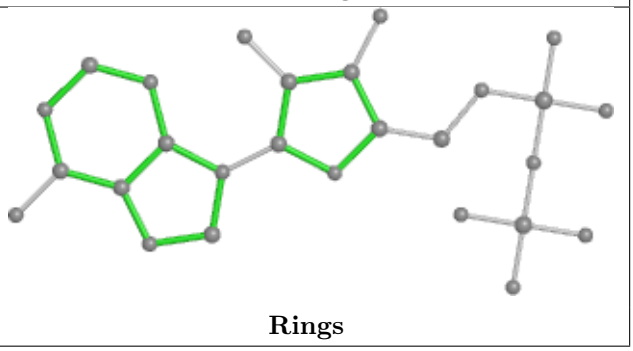


Ligand ADP w 401

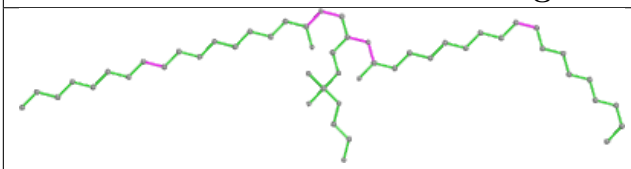

Bond lengths

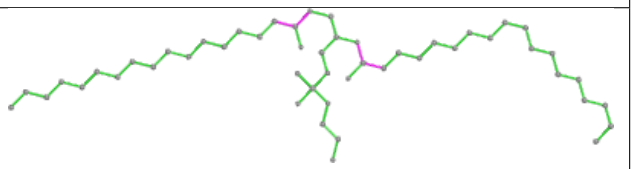

Bond angles

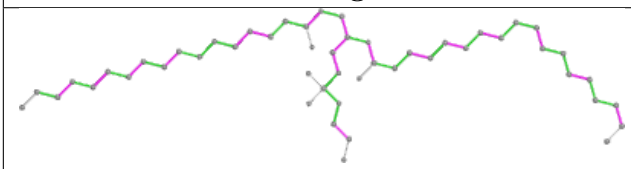

Torsions

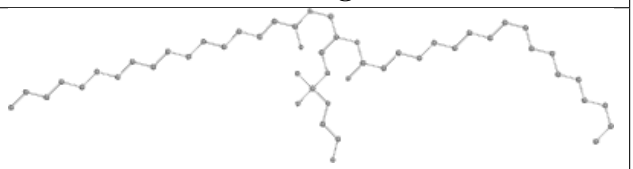

Rings

Ligand PEE l 702


Bond lengths

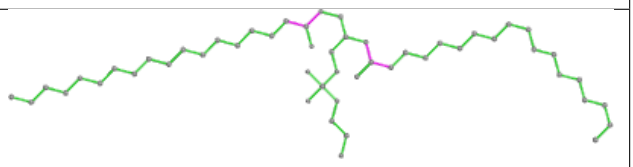

Bond angles

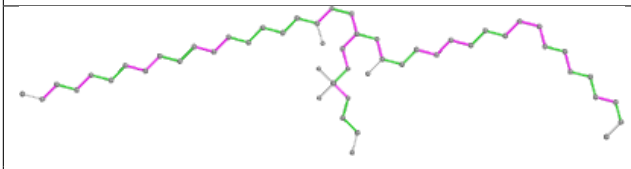

Torsions

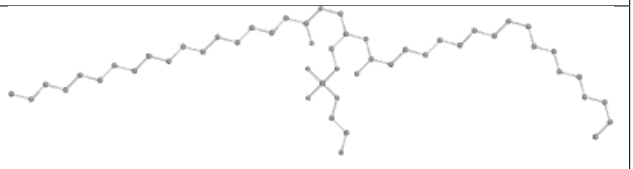

Rings

Ligand PEE U 401

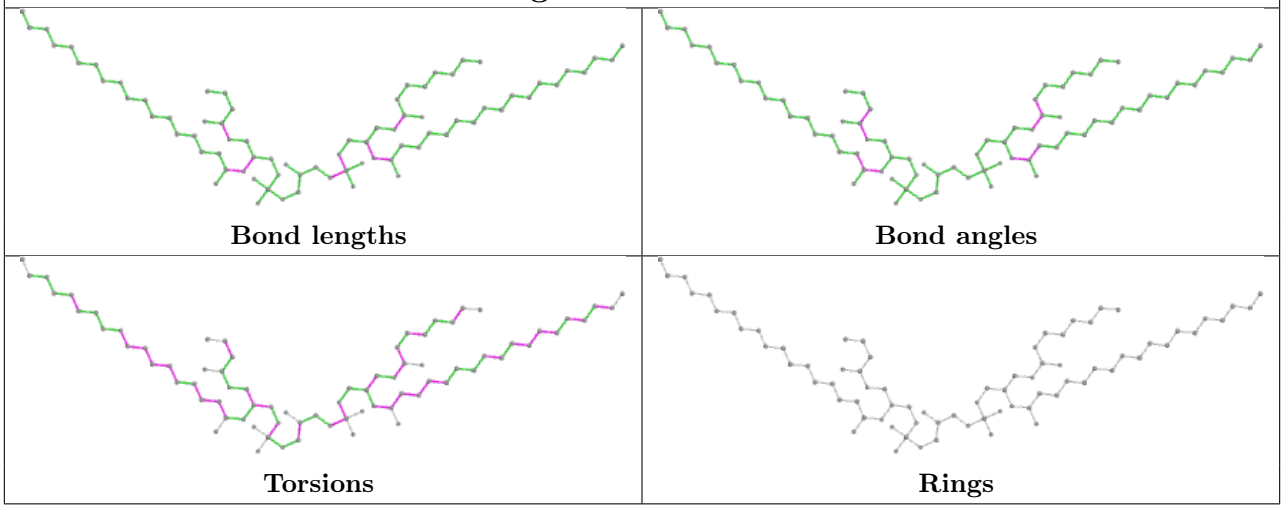

Bond lengths


Bond angles

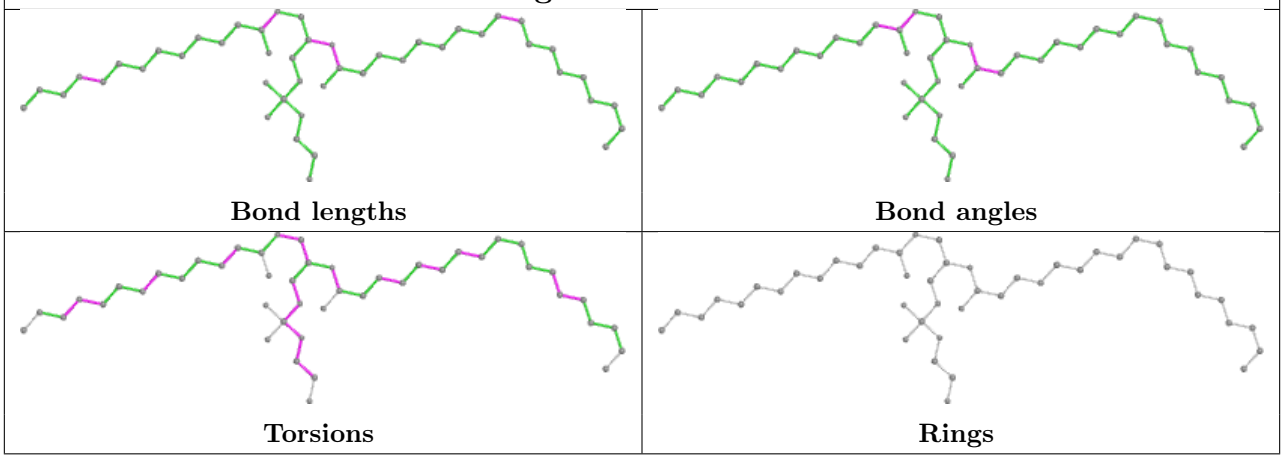

Torsions


Rings

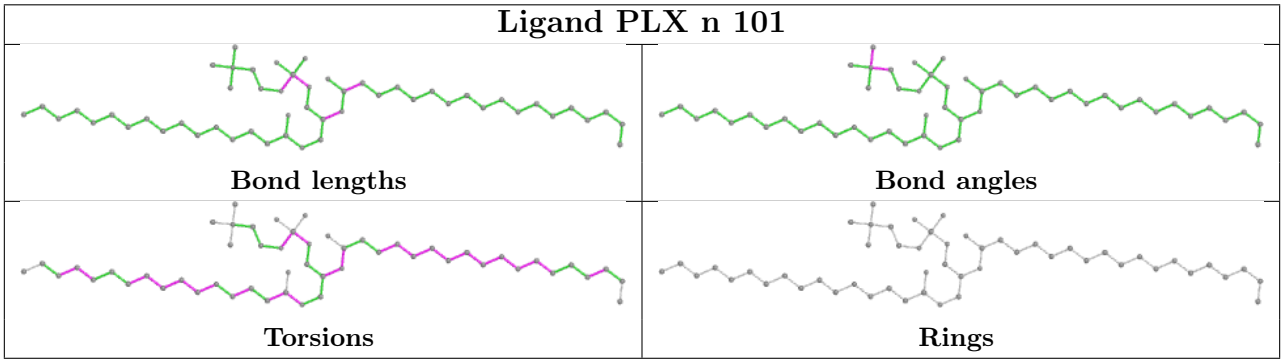
Ligand CDL r 504



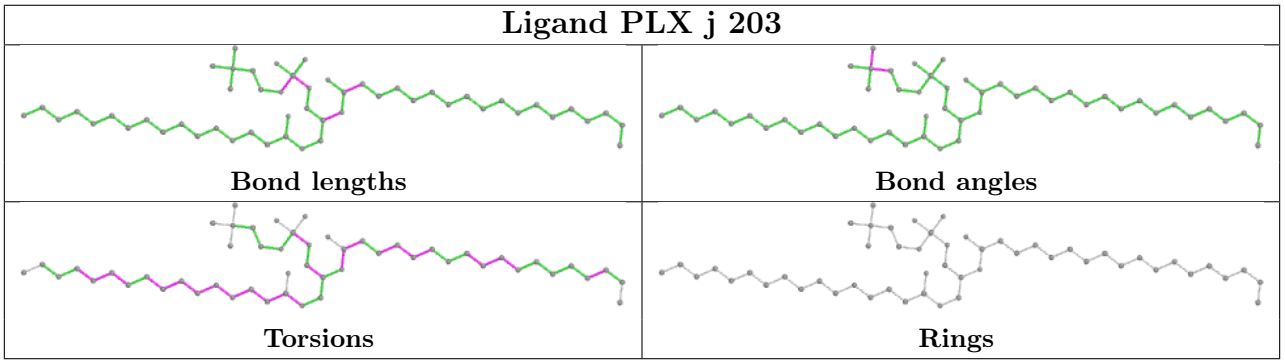
Ligand PEE l 703



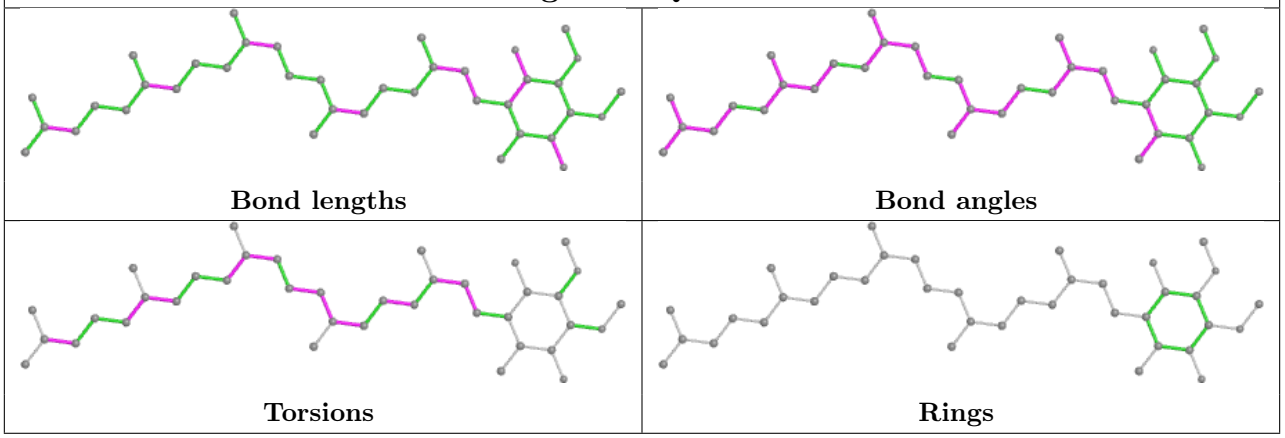
Ligand PLX n 101



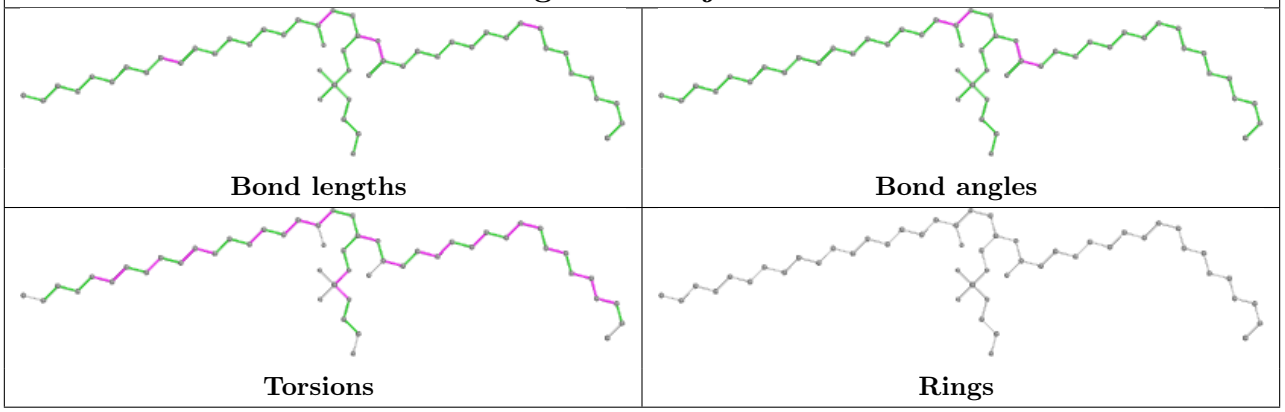
Ligand PLX j 203



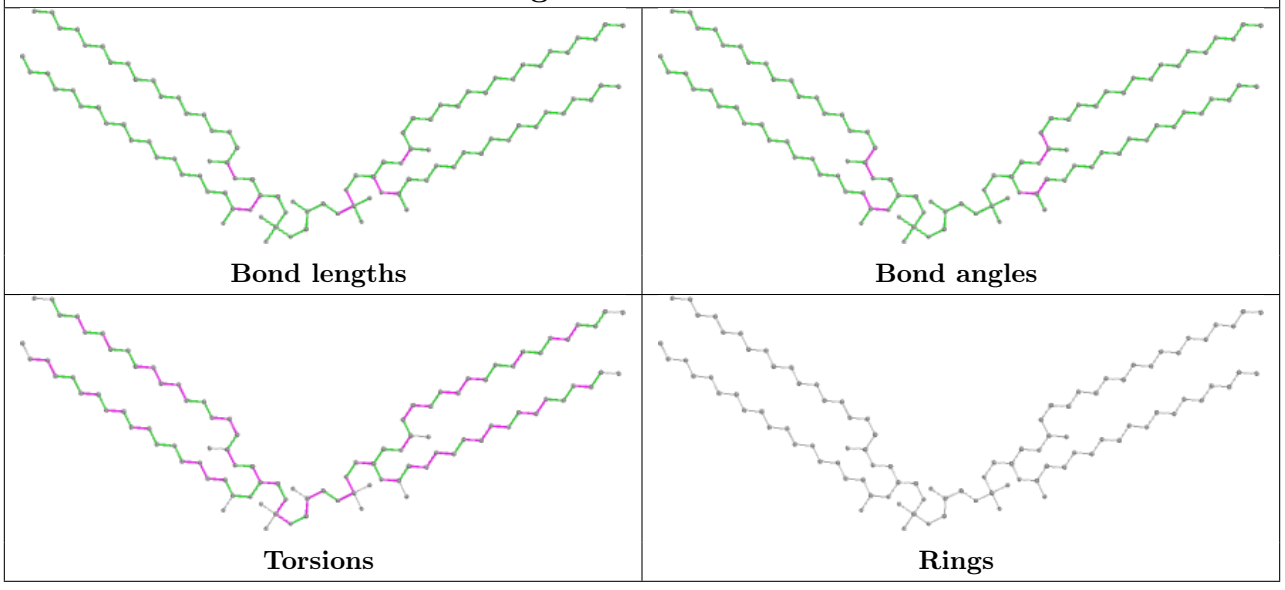
Ligand UQ s 402

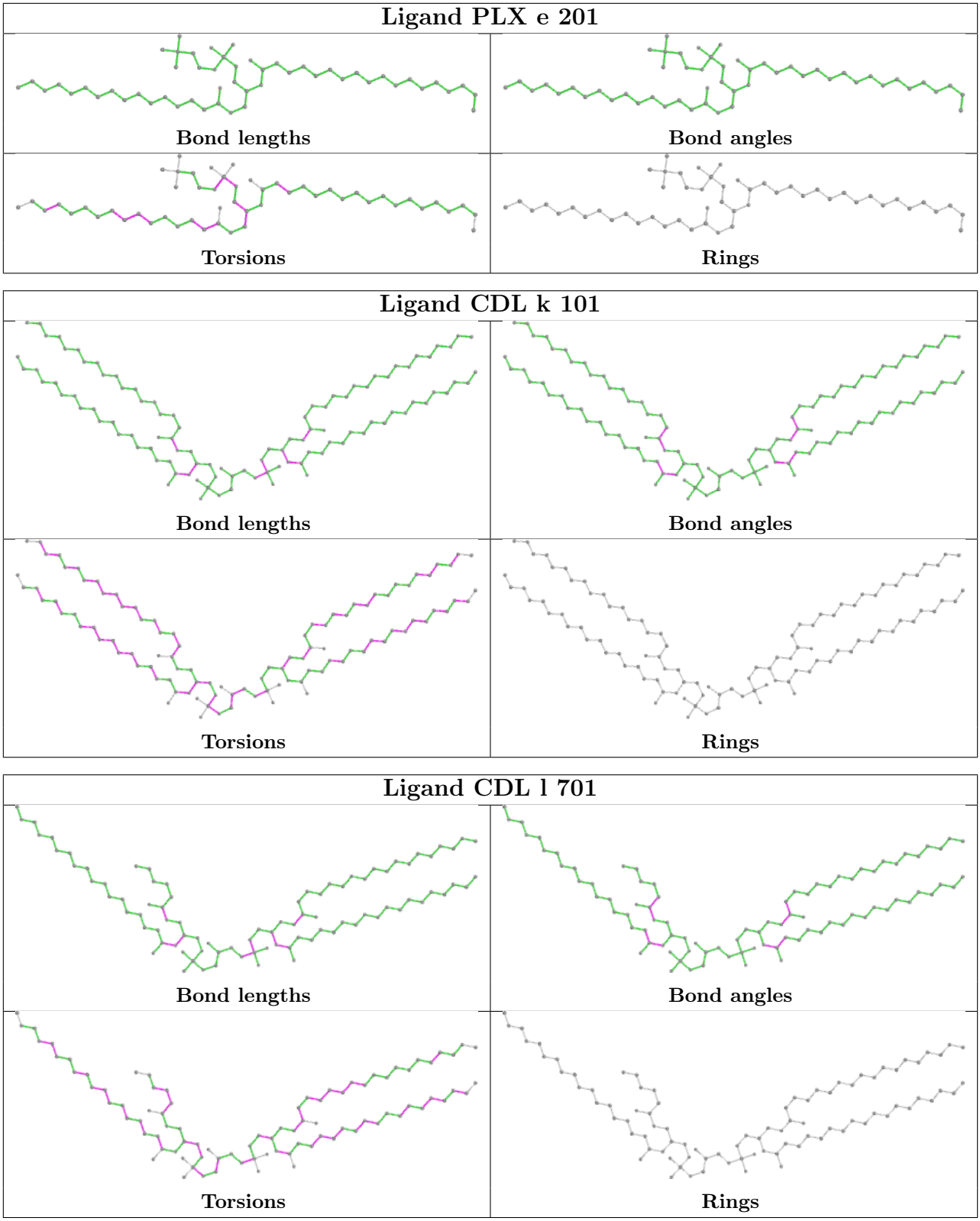


Ligand PEE j 201



Ligand CDL r 503





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.

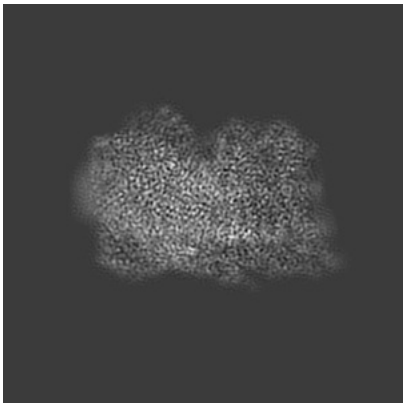
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31887. 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.

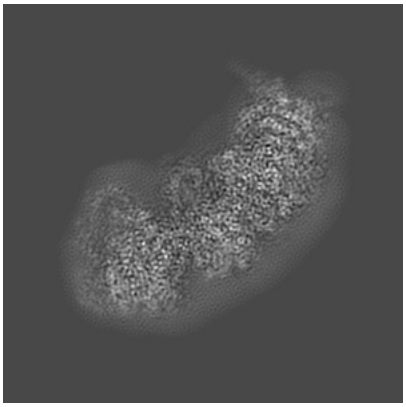
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

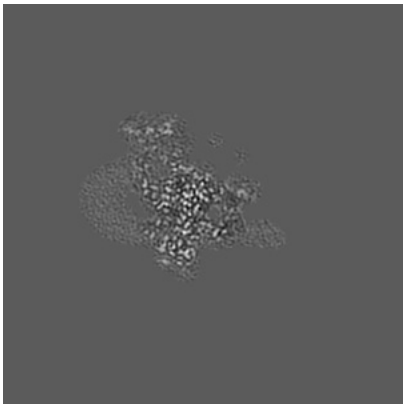


Z

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

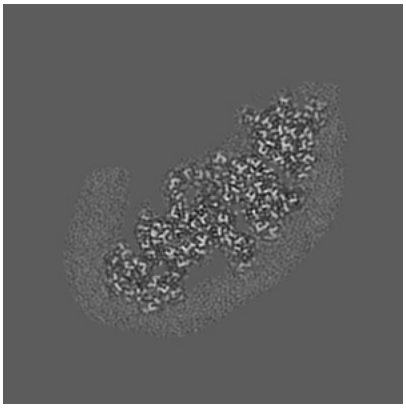
6.2 Central slices

6.2.1 Primary map



X Index: 256

Y Index: 256

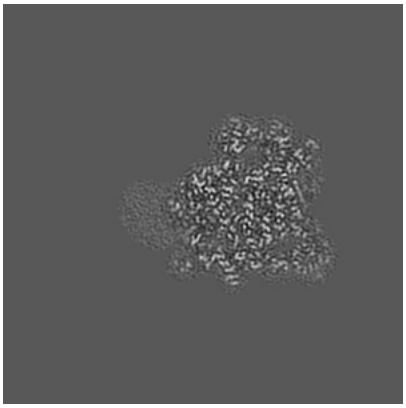


Z Index: 256

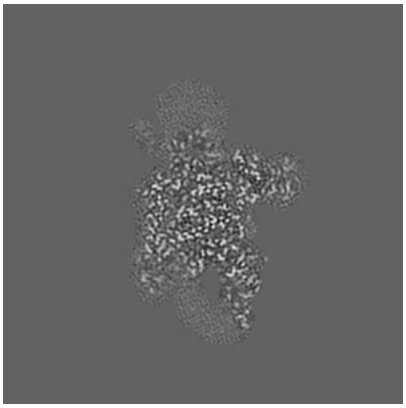
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

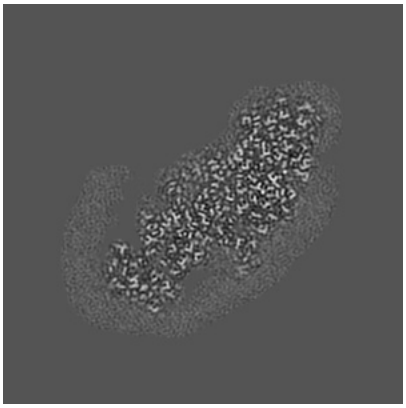
6.3.1 Primary map



X Index: 347



Y Index: 217

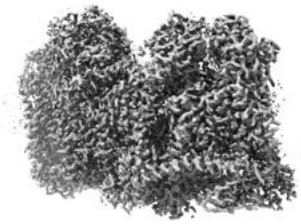


Z Index: 267

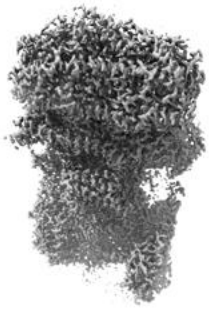
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

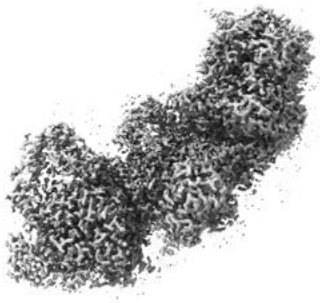
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

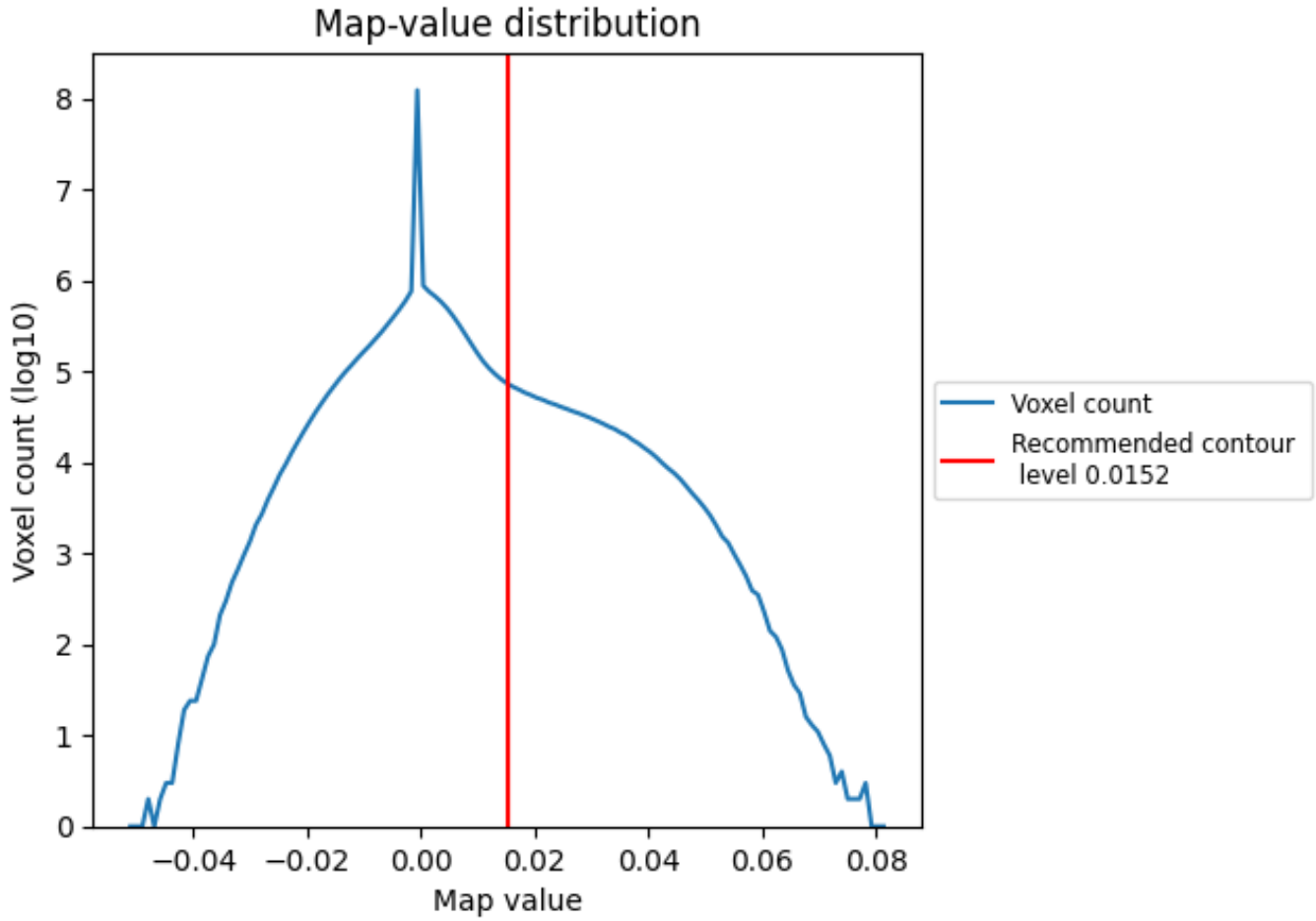
6.5 Mask visualisation (i)

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

7 Map analysis

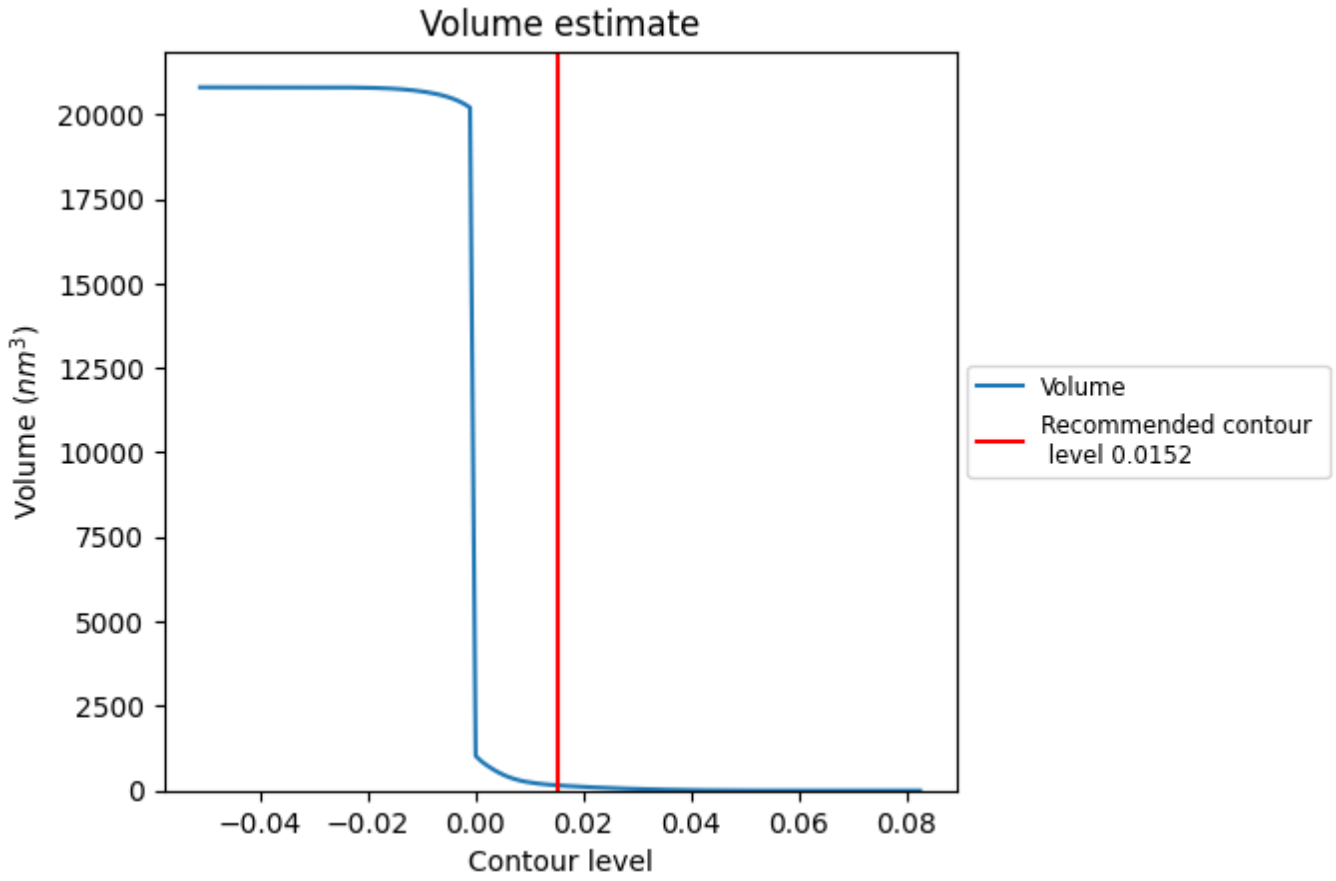
This section contains the results of statistical analysis of the map.

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.

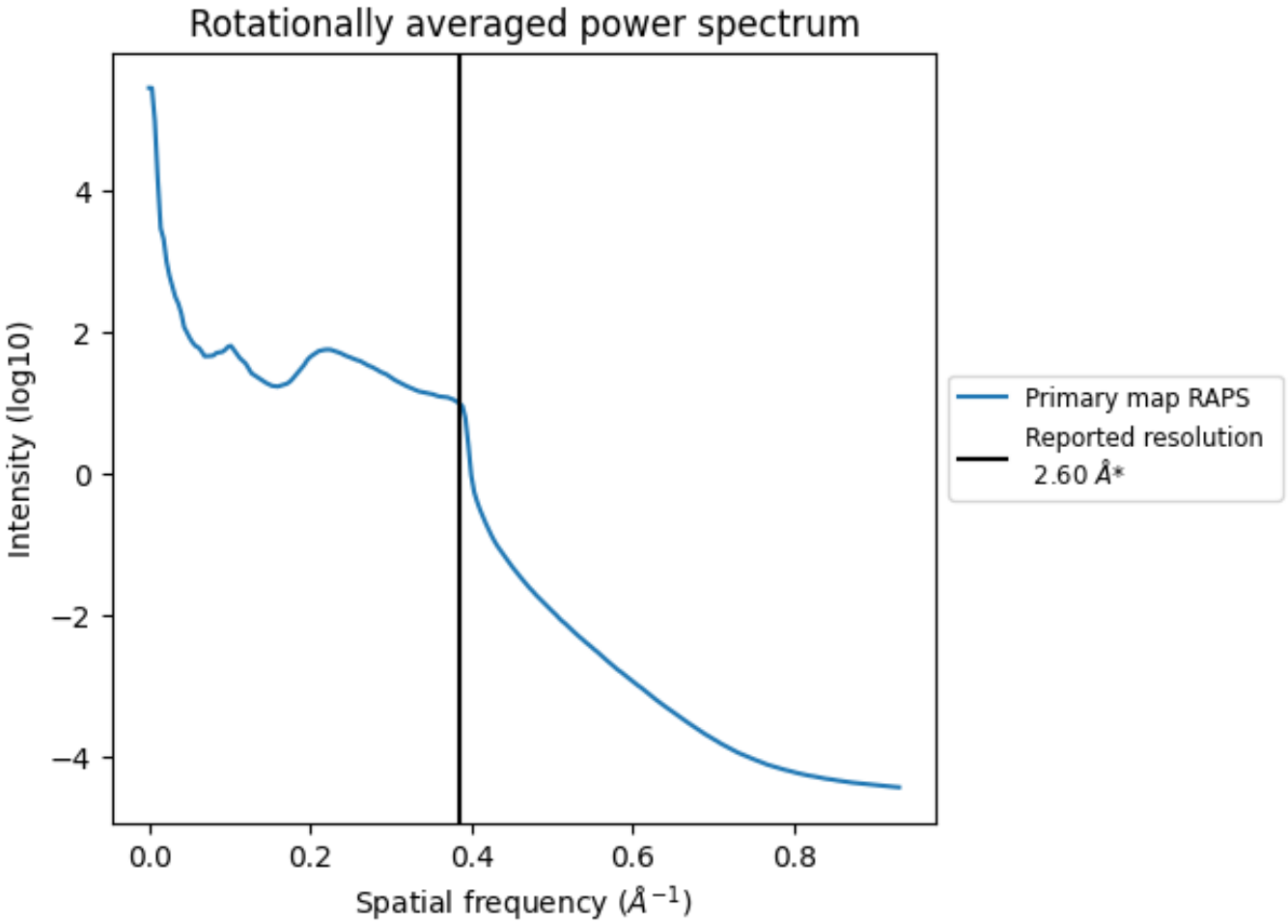
7.2 Volume estimate (i)



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 140 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 0.385 $Å^{-1}$

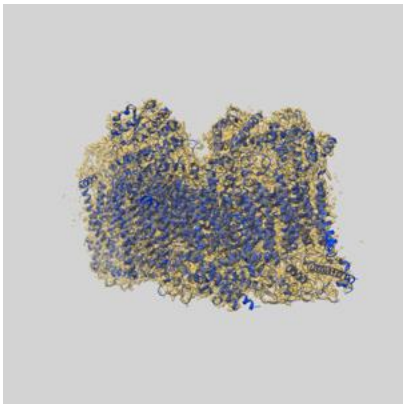
8 Fourier-Shell correlation (i)

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

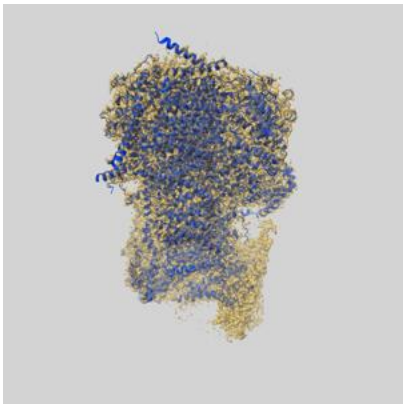
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31887 and PDB model 7VC0. Per-residue inclusion information can be found in section 3 on page 15.

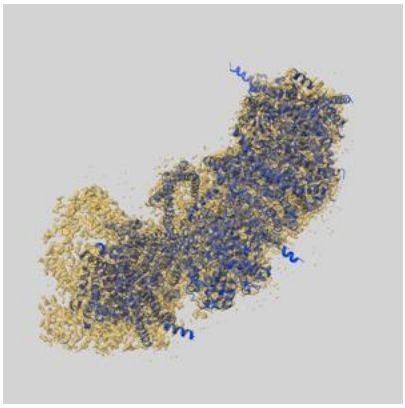
9.1 Map-model overlay



X



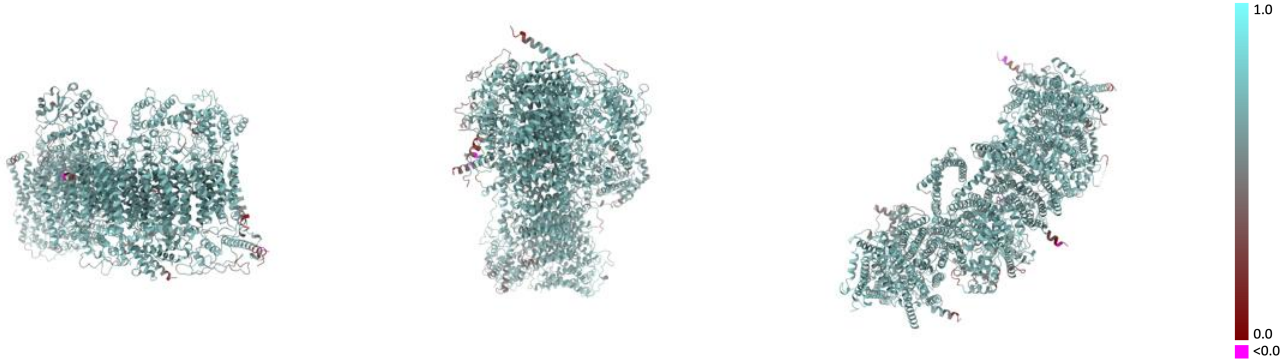
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0152 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.

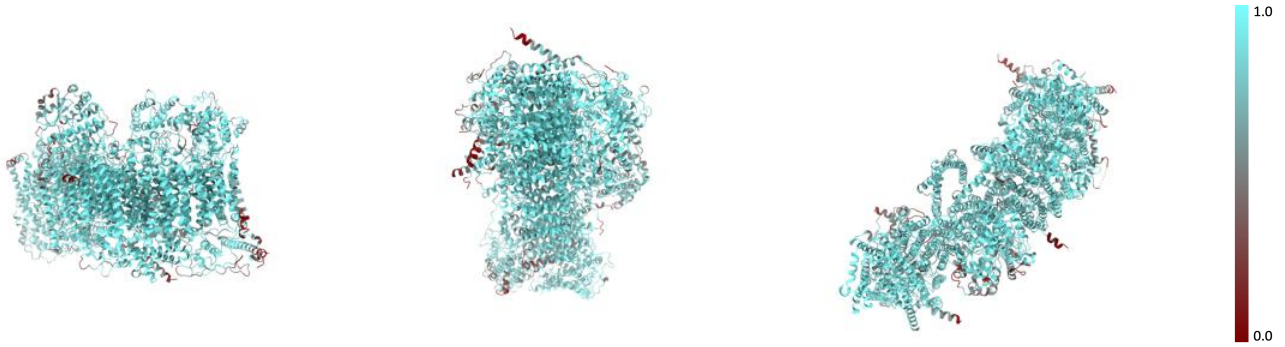
9.2 Q-score mapped to coordinate model (i)



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.

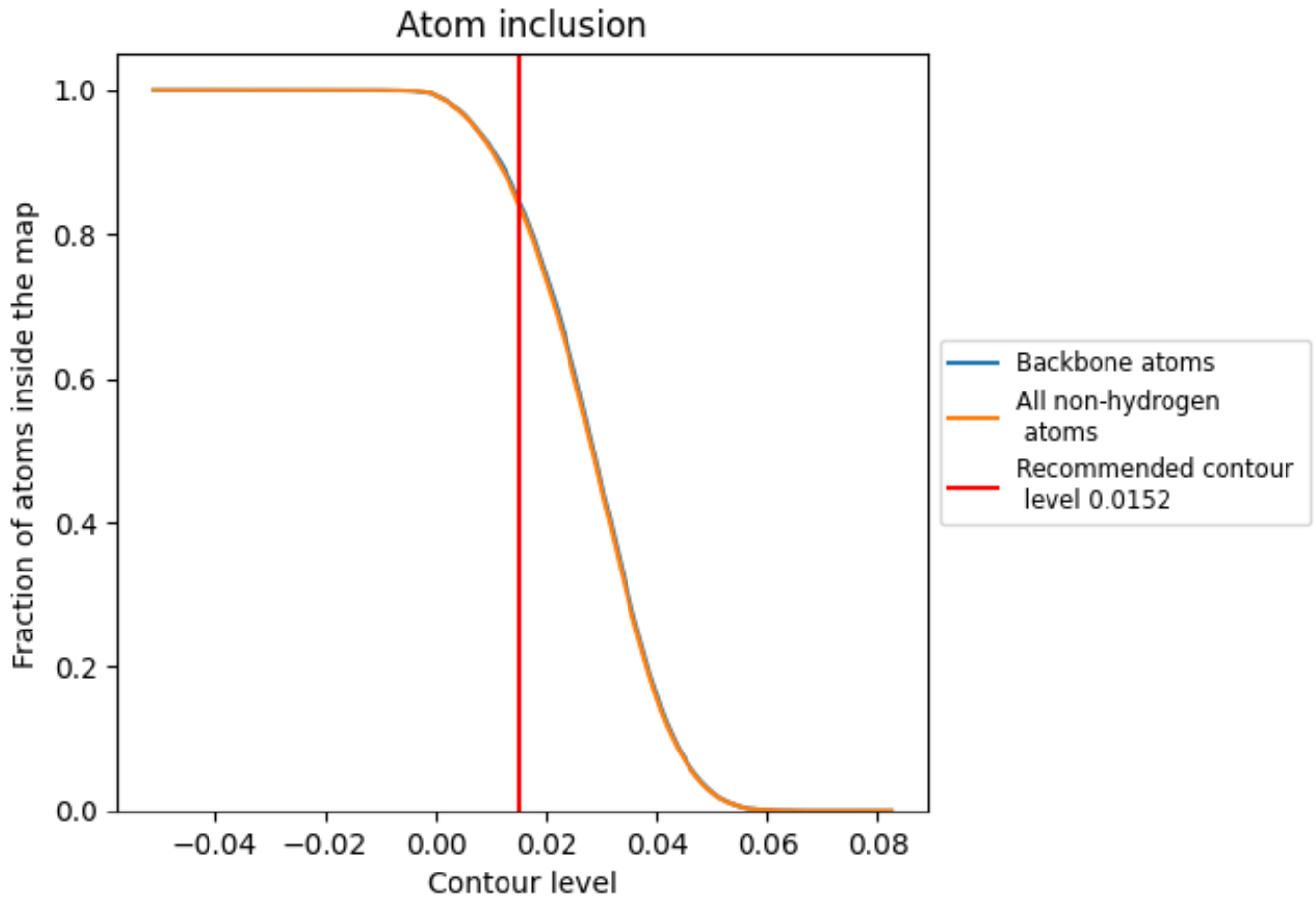
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0152).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.0152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.6470
Q	0.7444	0.6210
S	0.8895	0.6580
U	0.7559	0.6100
V	0.7644	0.6290
W	0.8146	0.6300
X	0.8224	0.6480
Y	0.7223	0.6050
Z	0.6752	0.5700
a	0.8818	0.6660
b	0.7771	0.6200
c	0.8632	0.6570
d	0.8226	0.6440
e	0.7806	0.6200
f	0.6405	0.5690
g	0.8840	0.6620
h	0.7955	0.6280
i	0.9538	0.6910
j	0.7887	0.6370
k	0.8694	0.6530
l	0.9042	0.6750
m	0.7785	0.6160
n	0.6550	0.5680
o	0.7972	0.6380
p	0.8531	0.6540
r	0.9251	0.6760
s	0.8968	0.6670
u	0.7825	0.6350
v	0.7063	0.5770
w	0.7793	0.6260