wwPDB EM Validation Summary Report

Nov 21, 2022 – 12:19 pm GMT

PDB ID	:	7ZKP
EMDB ID	:	EMD-14764
Title	:	Late assembly intermediate of the proximal proton pumping module of complex I with assembly factors NDUFAF1 and CIA84
Authors	:	Schiller, J.; Laube, E.; Vonck, J.; Zickermann, V.
Deposited on	:	2022-04-13
Resolution	:	3.20 Å(reported)
Based on initial model	:	7O71

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

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

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

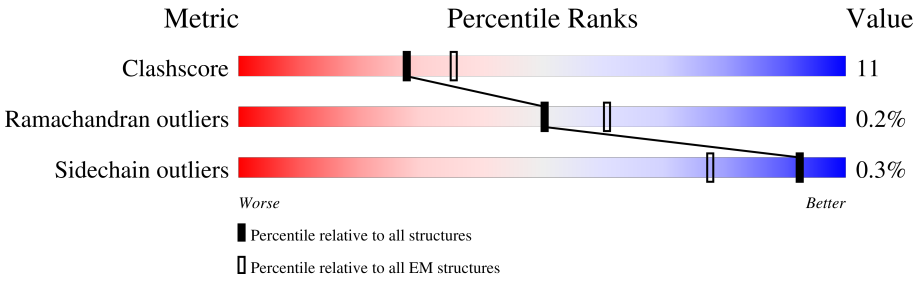
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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%

Mol	Chain	Length	Quality of chain
1	D	87	77% 22% .
2	L	89	54% 45% .
3	U	172	72% 26% ..
4	W	123	67% 7% 25%
5	X	169	74% 21% .. .
6	1	341	65% 24% 11%
7	2	469	77% 23%
8	3	128	50% 39% 11%
9	6	185	69% 31% .

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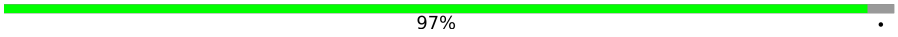
Mol	Chain	Length	Quality of chain
10	g	78	
11	b	74	
12	9	89	
13	C	852	
14	A	290	

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

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

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 19929 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 Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	89	Total	C	N	O	S	0	0
			693	465	109	116	3		

- Molecule 3 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 4 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	92	Total	C	N	O	S	0	0
			744	476	133	130	5		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit -domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	164	Total	C	N	O	S	0	0
			1274	828	216	226	4		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	303	Total	C	N	O	S	0	0
			2426	1664	347	408	7		

- Molecule 7 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	469	Total	C	N	O	S	0	0
			3776	2558	550	656	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	114	Total	C	N	O	S	0	0
			909	626	131	150	2		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	184	Total	C	N	O	S	0	0
			1453	985	208	251	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	1	FME	-	insertion	UNP S5U3X7

- Molecule 10 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	76	Total	C	N	O	0	0
			622	408	113	101		

- Molecule 11 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
11	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 12 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 13 is a protein called assembly factor CIA84.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	337	Total	C	N	O	S	0	0
			2763	1754	471	525	13		

- Molecule 14 is a protein called CIA30 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	216	Total	C	N	O	S	0	0
			1749	1119	296	328	6		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	-	expression tag	UNP A0A1D8NEL0
A	239	ASN	-	expression tag	UNP A0A1D8NEL0
A	240	LEU	-	expression tag	UNP A0A1D8NEL0
A	241	TYR	-	expression tag	UNP A0A1D8NEL0
A	242	PHE	-	expression tag	UNP A0A1D8NEL0
A	243	GLN	-	expression tag	UNP A0A1D8NEL0
A	244	GLY	-	expression tag	UNP A0A1D8NEL0
A	245	ALA	-	expression tag	UNP A0A1D8NEL0
A	246	GLU	-	expression tag	UNP A0A1D8NEL0
A	247	ALA	-	expression tag	UNP A0A1D8NEL0
A	248	ALA	-	expression tag	UNP A0A1D8NEL0
A	249	ALA	-	expression tag	UNP A0A1D8NEL0
A	250	LYS	-	expression tag	UNP A0A1D8NEL0
A	251	GLU	-	expression tag	UNP A0A1D8NEL0
A	252	ALA	-	expression tag	UNP A0A1D8NEL0
A	253	ALA	-	expression tag	UNP A0A1D8NEL0
A	254	ALA	-	expression tag	UNP A0A1D8NEL0
A	255	LYS	-	expression tag	UNP A0A1D8NEL0
A	256	ALA	-	expression tag	UNP A0A1D8NEL0
A	257	TRP	-	expression tag	UNP A0A1D8NEL0
A	258	SER	-	expression tag	UNP A0A1D8NEL0
A	259	HIS	-	expression tag	UNP A0A1D8NEL0
A	260	PRO	-	expression tag	UNP A0A1D8NEL0
A	261	GLN	-	expression tag	UNP A0A1D8NEL0
A	262	PHE	-	expression tag	UNP A0A1D8NEL0

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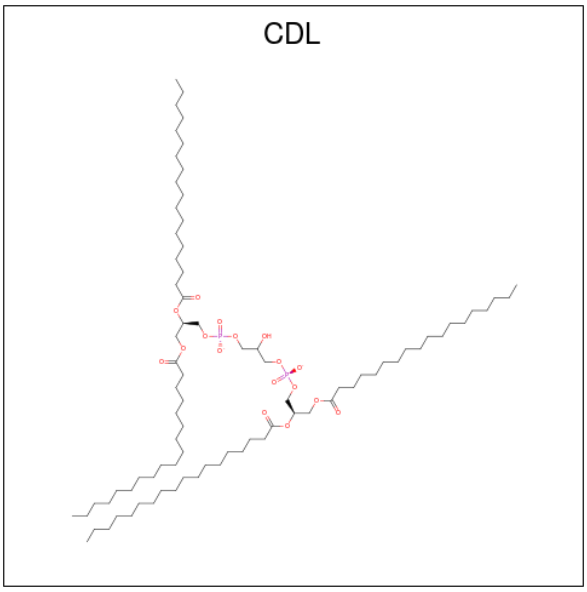
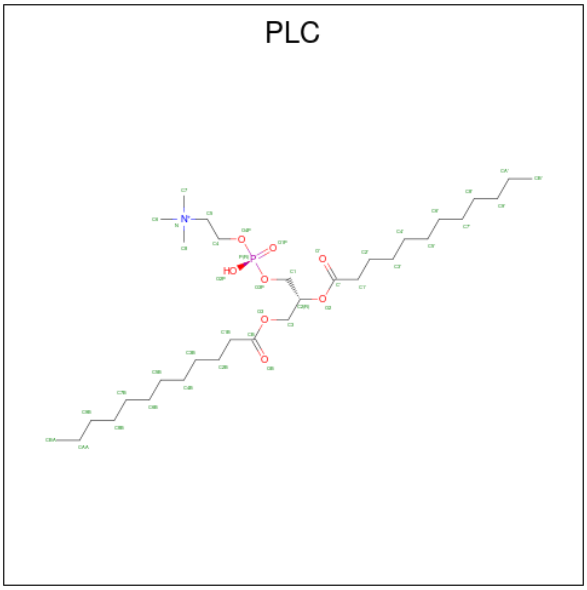
Chain	Residue	Modelled	Actual	Comment	Reference
A	263	GLU	-	expression tag	UNP A0A1D8NEL0
A	264	LYS	-	expression tag	UNP A0A1D8NEL0
A	265	GLY	-	expression tag	UNP A0A1D8NEL0
A	266	GLY	-	expression tag	UNP A0A1D8NEL0
A	267	GLY	-	expression tag	UNP A0A1D8NEL0
A	268	SER	-	expression tag	UNP A0A1D8NEL0
A	269	GLY	-	expression tag	UNP A0A1D8NEL0
A	270	GLY	-	expression tag	UNP A0A1D8NEL0
A	271	GLY	-	expression tag	UNP A0A1D8NEL0
A	272	SER	-	expression tag	UNP A0A1D8NEL0
A	273	GLY	-	expression tag	UNP A0A1D8NEL0
A	274	GLY	-	expression tag	UNP A0A1D8NEL0
A	275	SER	-	expression tag	UNP A0A1D8NEL0
A	276	ALA	-	expression tag	UNP A0A1D8NEL0
A	277	TRP	-	expression tag	UNP A0A1D8NEL0
A	278	SER	-	expression tag	UNP A0A1D8NEL0
A	279	HIS	-	expression tag	UNP A0A1D8NEL0
A	280	PRO	-	expression tag	UNP A0A1D8NEL0
A	281	GLN	-	expression tag	UNP A0A1D8NEL0
A	282	PHE	-	expression tag	UNP A0A1D8NEL0
A	283	GLU	-	expression tag	UNP A0A1D8NEL0
A	284	LYS	-	expression tag	UNP A0A1D8NEL0

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



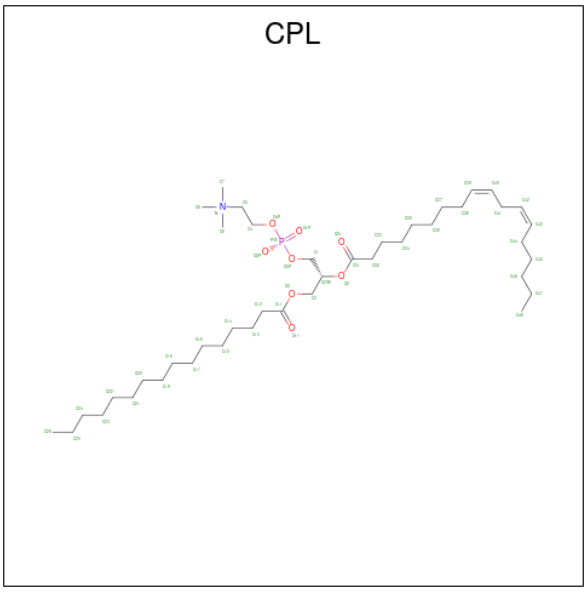
Mol	Chain	Residues	Atoms				AltConf
15	X	1	Total	C	O	P	0
			64	46	16	2	
15	g	1	Total	C	O	P	0
			83	64	17	2	

- Molecule 16 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



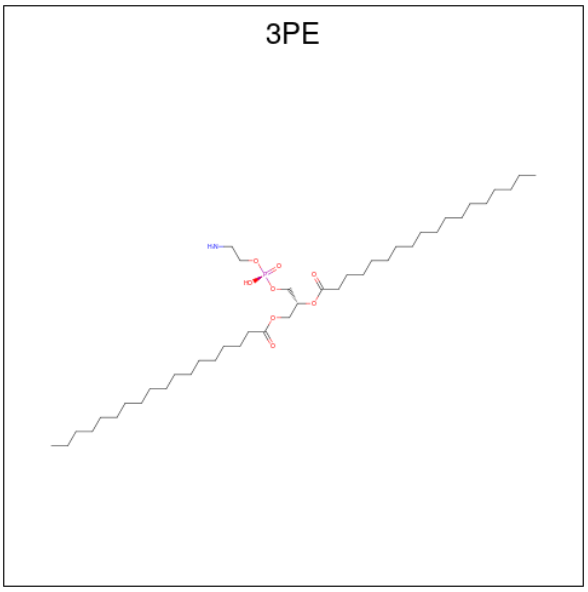
Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 17 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



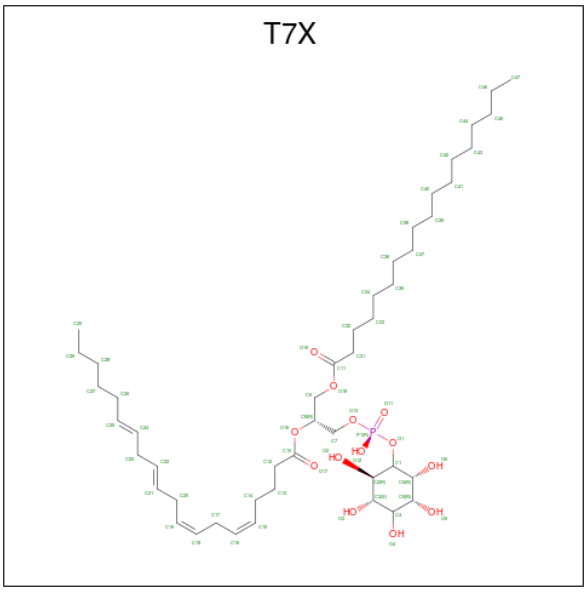
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	g	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 19 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



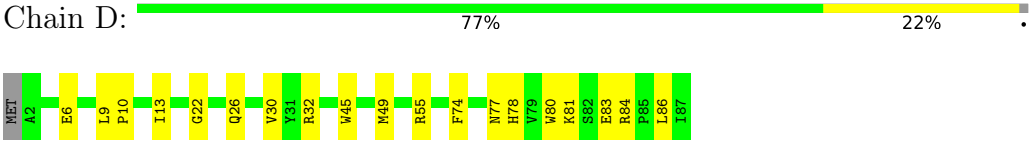
Mol	Chain	Residues	Atoms				AltConf
19	b	1	Total	C	O	P	0
			48	34	13	1	

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. 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. 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.

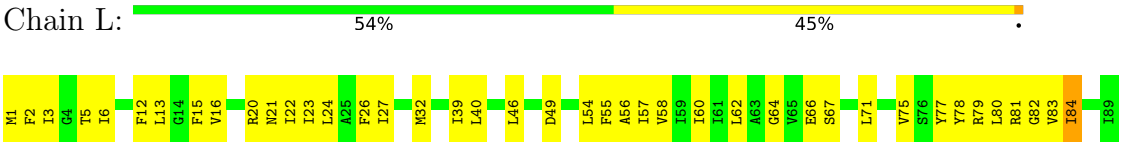
• Molecule 1: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain D:



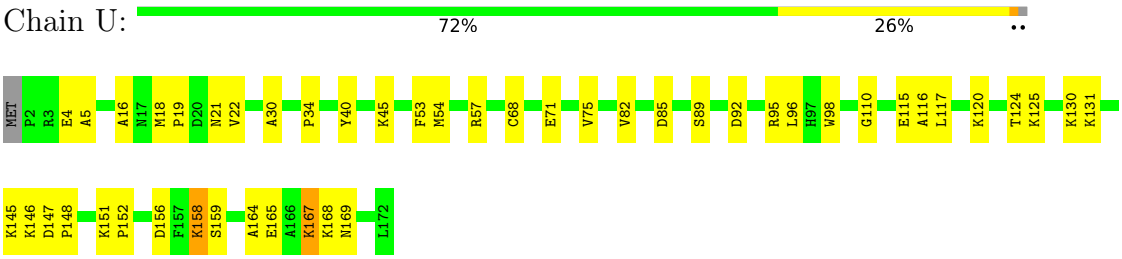
• Molecule 2: NADH-ubiquinone oxidoreductase chain 4L

Chain L:



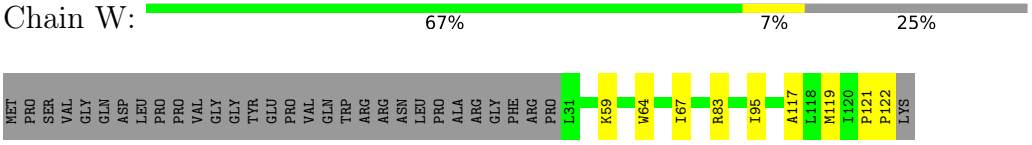
• Molecule 3: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain U:



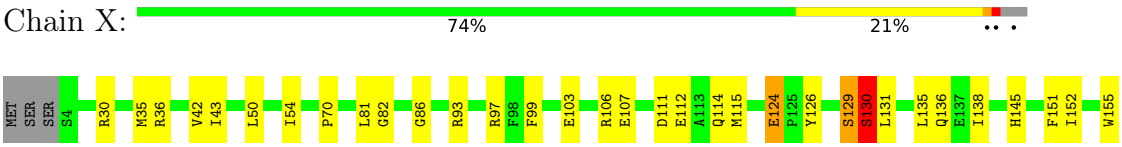
• Molecule 4: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

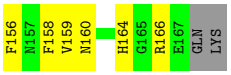
Chain W:



• Molecule 5: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit-domain-containing protein

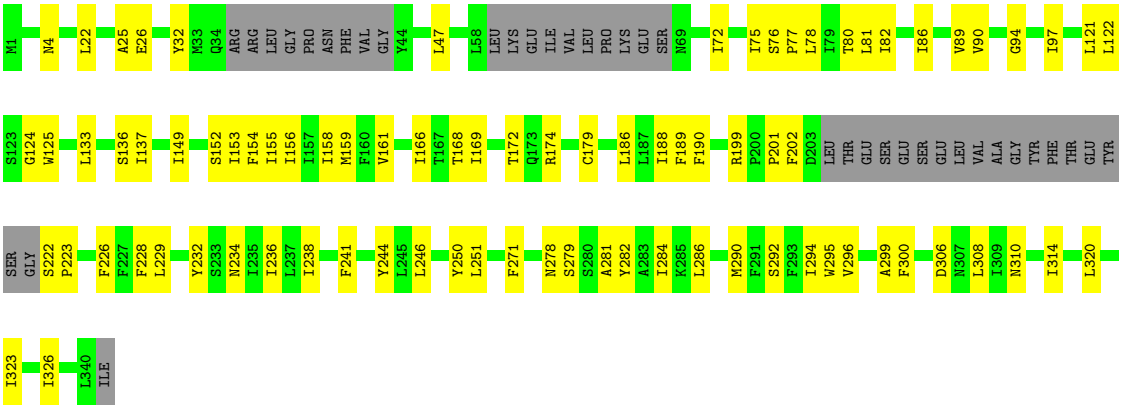
Chain X:





• Molecule 6: NADH-ubiquinone oxidoreductase chain 1

Chain 1:

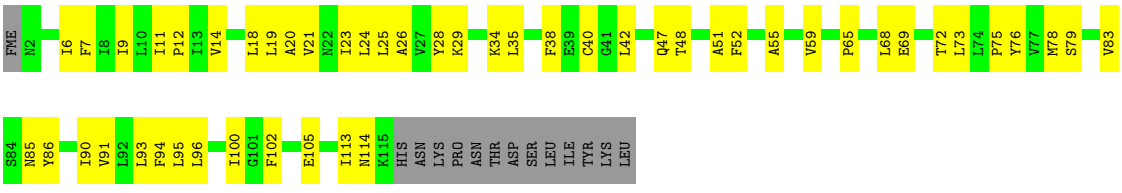


• Molecule 7: NADH dehydrogenase subunit 2

Chain 2:

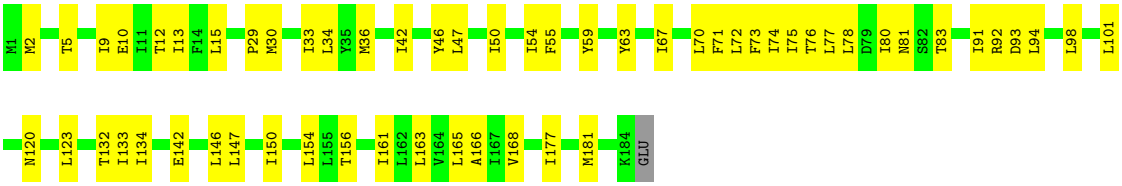
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain 3:



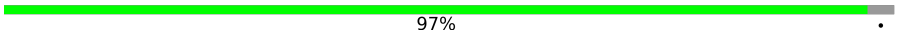
• Molecule 9: NADH-ubiquinone oxidoreductase chain 6

Chain 6:



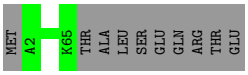
• Molecule 10: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain g:



• Molecule 11: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:

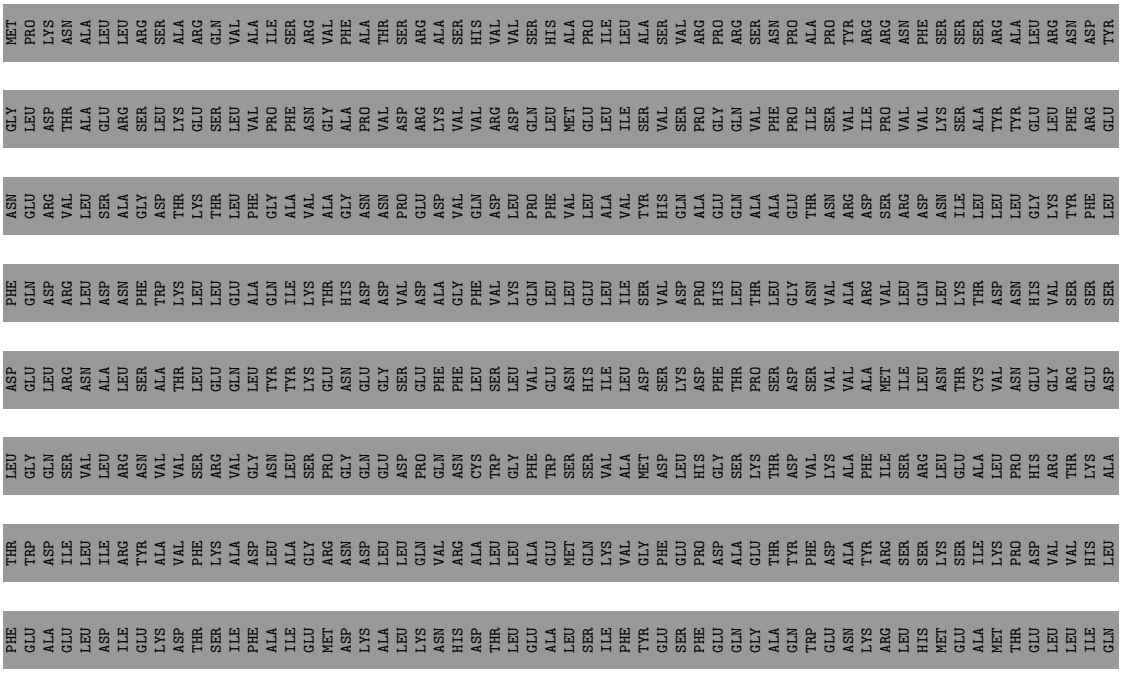


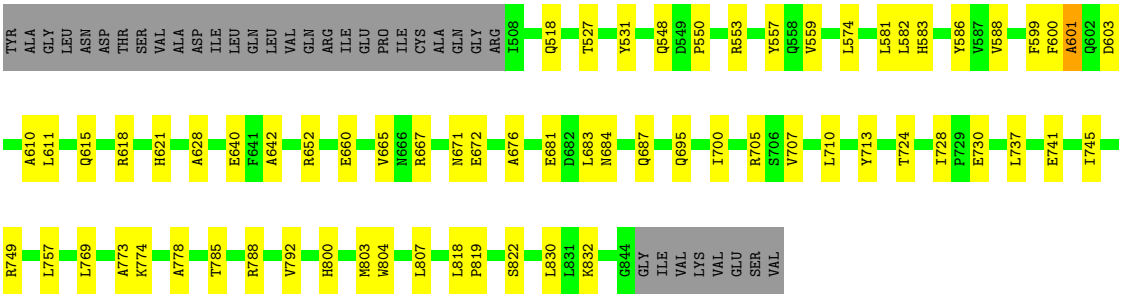
• Molecule 12: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 9:

• Molecule 13: assembly factor CIA84

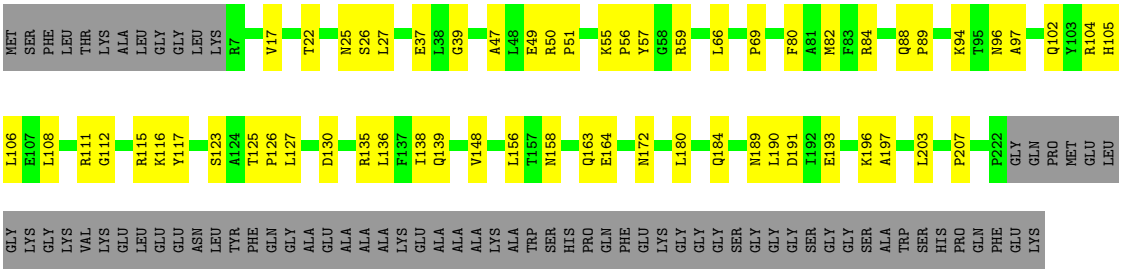
Chain C:





• Molecule 14: CIA30 domain-containing protein

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, CPL, 3PE, CDL, T7X, PLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	D	0.24	0/697	0.49	0/940
2	L	0.26	0/692	0.49	0/937
3	U	0.26	0/1374	0.51	0/1856
4	W	0.24	0/758	0.47	0/1017
5	X	0.34	0/1313	0.55	1/1782 (0.1%)
6	1	0.27	0/2482	0.44	0/3389
7	2	0.27	0/3846	0.42	0/5242
8	3	0.32	0/930	0.49	0/1269
9	6	0.26	0/1468	0.46	0/2003
10	g	0.25	0/648	0.49	0/887
11	b	0.25	0/503	0.38	0/679
12	9	0.24	0/684	0.45	0/918
13	C	0.25	0/2828	0.45	0/3832
14	A	0.26	0/1791	0.56	0/2435
All	All	0.27	0/20014	0.47	1/27186 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	130	SER	N-CA-CB	-5.17	102.74	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	681	0	671	16	0
2	L	693	0	753	44	0
3	U	1345	0	1327	28	0
4	W	744	0	761	7	0
5	X	1274	0	1245	46	0
6	1	2426	0	2522	56	0
7	2	3776	0	4004	85	0
8	3	909	0	970	35	0
9	6	1453	0	1576	54	0
10	g	622	0	602	0	0
11	b	490	0	509	0	0
12	9	672	0	683	8	0
13	C	2763	0	2672	47	0
14	A	1749	0	1731	45	0
15	X	64	0	78	26	0
15	g	83	0	116	0	0
16	1	42	0	64	2	0
17	2	52	0	79	4	0
18	g	43	0	63	0	0
19	b	48	0	0	0	0
All	All	19929	0	20426	400	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 11.

The worst 5 of 400 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)
5:X:160:ASN:ND2	15:X:201:CDL:HA21	1.87	0.90
5:X:159:VAL:HG22	15:X:201:CDL:HA31	1.58	0.83
7:2:9:LEU:HD11	7:2:28:ILE:HD11	1.61	0.82
5:X:30:ARG:NH2	5:X:111:ASP:OD1	2.15	0.80
5:X:129:SER:HB2	5:X:136:GLN:NE2	1.96	0.79

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	D	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
2	L	87/89 (98%)	81 (93%)	5 (6%)	1 (1%)	14	51
3	U	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
4	W	90/123 (73%)	89 (99%)	1 (1%)	0	100	100
5	X	162/169 (96%)	159 (98%)	3 (2%)	0	100	100
6	1	295/341 (86%)	286 (97%)	9 (3%)	0	100	100
7	2	467/469 (100%)	457 (98%)	10 (2%)	0	100	100
8	3	112/128 (88%)	94 (84%)	18 (16%)	0	100	100
9	6	182/185 (98%)	173 (95%)	9 (5%)	0	100	100
10	g	74/78 (95%)	70 (95%)	4 (5%)	0	100	100
11	b	62/74 (84%)	62 (100%)	0	0	100	100
12	9	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
13	C	335/852 (39%)	318 (95%)	16 (5%)	1 (0%)	41	74
14	A	214/290 (74%)	190 (89%)	22 (10%)	2 (1%)	17	56
All	All	2417/3146 (77%)	2309 (96%)	104 (4%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	A	26	SER
13	C	601	ALA
14	A	96	ASN
2	L	84	ILE

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	D	68/69 (99%)	68 (100%)	0	100 100
2	L	76/76 (100%)	76 (100%)	0	100 100
3	U	147/148 (99%)	143 (97%)	4 (3%)	44 75
4	W	76/102 (74%)	76 (100%)	0	100 100
5	X	127/133 (96%)	124 (98%)	3 (2%)	49 77
6	1	268/301 (89%)	268 (100%)	0	100 100
7	2	432/432 (100%)	432 (100%)	0	100 100
8	3	100/113 (88%)	100 (100%)	0	100 100
9	6	165/166 (99%)	165 (100%)	0	100 100
10	g	63/65 (97%)	63 (100%)	0	100 100
11	b	50/59 (85%)	50 (100%)	0	100 100
12	9	73/76 (96%)	73 (100%)	0	100 100
13	C	297/745 (40%)	297 (100%)	0	100 100
14	A	193/245 (79%)	193 (100%)	0	100 100
All	All	2135/2730 (78%)	2128 (100%)	7 (0%)	92 96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	U	167	LYS
5	X	124	GLU
5	X	130	SER
5	X	129	SER
3	U	158	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	2	29	ASN
8	3	107	ASN
13	C	583	HIS
13	C	695	GLN
13	C	739	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	FME	L	1	2	8,9,10	0.91	0	7,9,11	0.90	0
6	FME	1	1	6	8,9,10	0.93	0	7,9,11	0.88	0
7	FME	2	1	7	8,9,10	0.93	0	7,9,11	0.86	0
9	FME	6	1	9	8,9,10	0.92	0	7,9,11	0.90	0

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
2	FME	L	1	2	-	2/7/9/11	-
6	FME	1	1	6	-	0/7/9/11	-
7	FME	2	1	7	-	3/7/9/11	-
9	FME	6	1	9	-	5/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	1	FME	N-CA-CB-CG
7	2	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
9	6	1	FME	O1-CN-N-CA
9	6	1	FME	N-CA-CB-CG
9	6	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
16	PLC	1	401	-	41,41,41	1.19	3 (7%)	47,49,49	1.10	3 (6%)
17	CPL	2	501	-	51,51,51	1.14	3 (5%)	57,59,59	1.16	4 (7%)
18	3PE	g	102	-	42,42,50	0.55	0	45,47,55	0.55	1 (2%)
15	CDL	g	101	-	82,82,99	0.30	0	88,94,111	0.38	0
15	CDL	X	201	-	63,63,99	0.47	0	68,74,111	0.77	2 (2%)
19	T7X	b	501	-	48,48,61	0.55	0	57,60,73	0.78	1 (1%)

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
16	PLC	1	401	-	-	25/45/45/45	-
17	CPL	2	501	-	-	25/55/55/55	-
18	3PE	g	102	-	-	21/46/46/54	-
15	CDL	g	101	-	-	30/93/93/110	-
15	CDL	X	201	-	-	41/73/73/110	-
19	T7X	b	501	-	-	15/43/67/80	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	401	PLC	O3-CB	3.05	1.42	1.33
17	2	501	CPL	O3-C11	3.00	1.42	1.33
16	1	401	PLC	O2-C'	2.94	1.42	1.34
16	1	401	PLC	O2-C2	-2.45	1.40	1.46
17	2	501	CPL	O2-C2	-2.43	1.40	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	501	CPL	O2-C31-C32	4.11	120.35	111.50
16	1	401	PLC	O2-C'-C1'	4.08	120.30	111.50
17	2	501	CPL	C8-N-C7	3.96	119.16	108.97
16	1	401	PLC	C7-N-C6	3.84	118.84	108.97
17	2	501	CPL	C41-C40-C39	3.43	152.51	123.57

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	X	201	CDL	CA3-OA5-PA1-OA4
15	X	201	CDL	OA7-CA5-OA6-CA4
15	X	201	CDL	C11-CA5-OA6-CA4
15	X	201	CDL	CB4-CB3-OB5-PB2
15	X	201	CDL	CB3-CB4-CB6-OB8

There are no ring outliers.

3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	401	PLC	2	0

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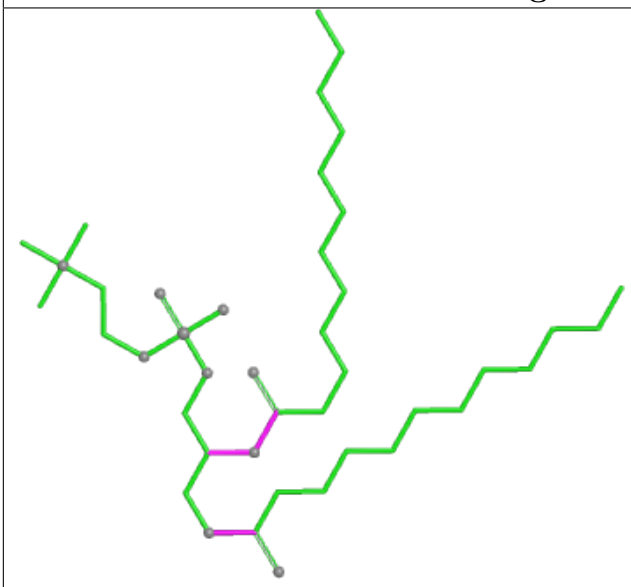
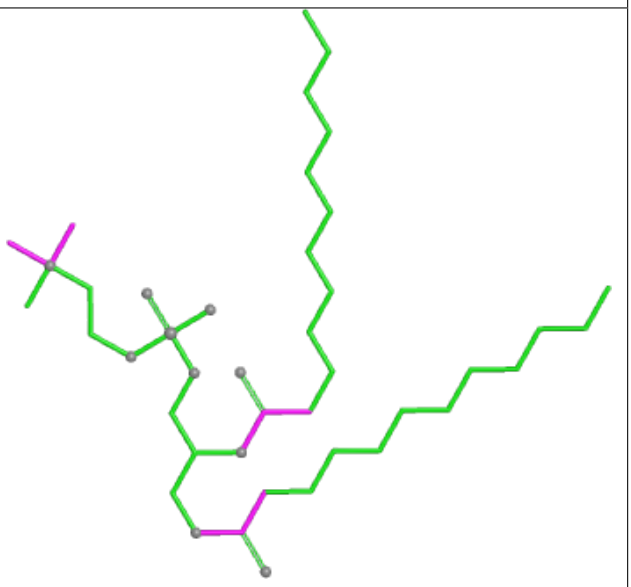
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	501	CPL	4	0
15	X	201	CDL	26	0

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.

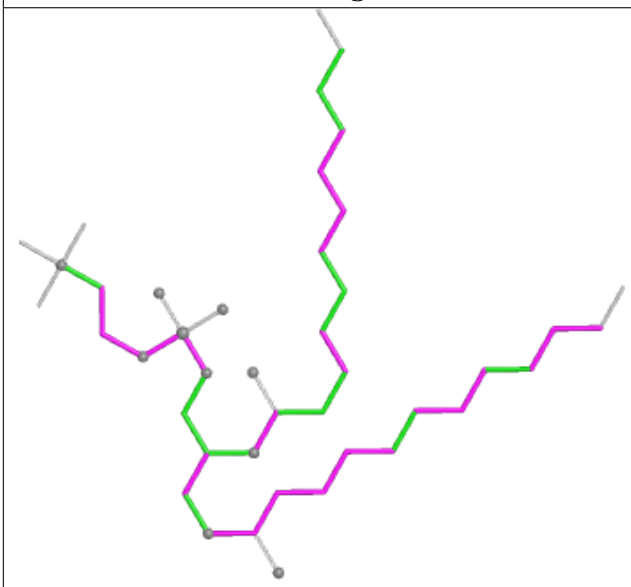
Ligand PLC 1 401



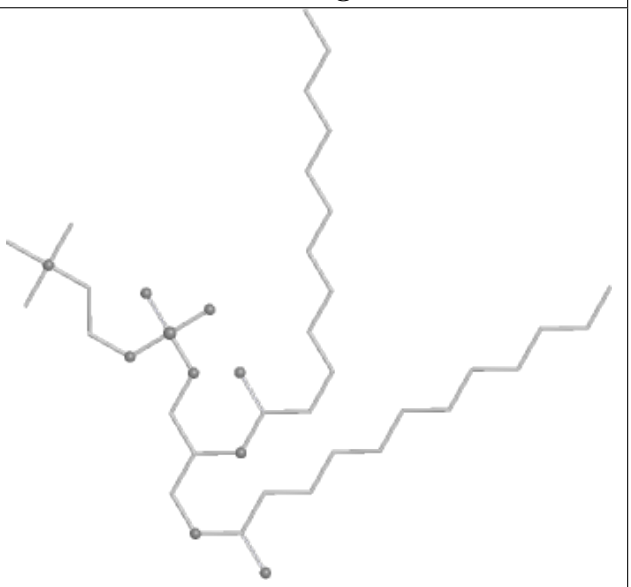
Bond lengths



Bond angles

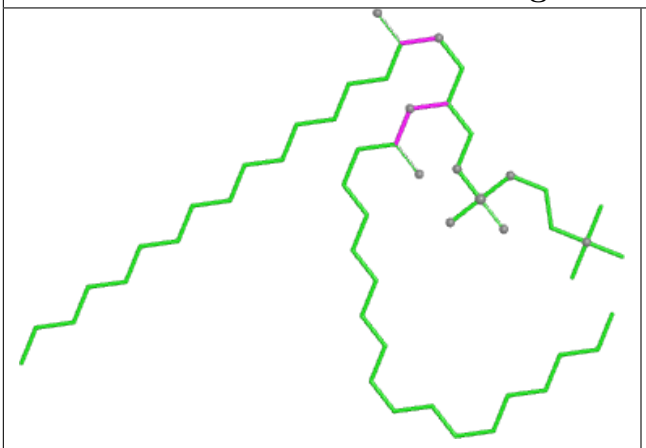


Torsions

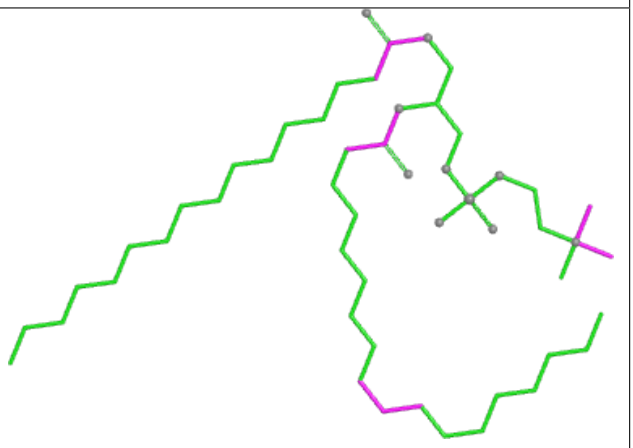


Rings

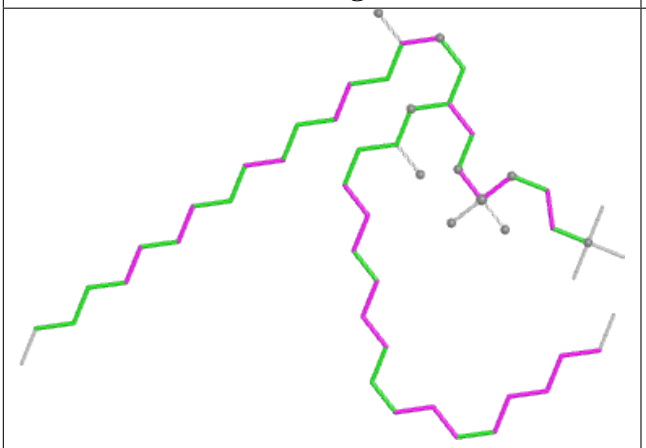
Ligand CPL 2 501



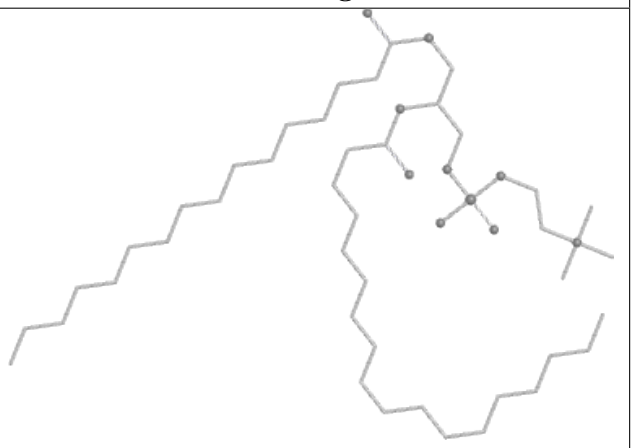
Bond lengths



Bond angles

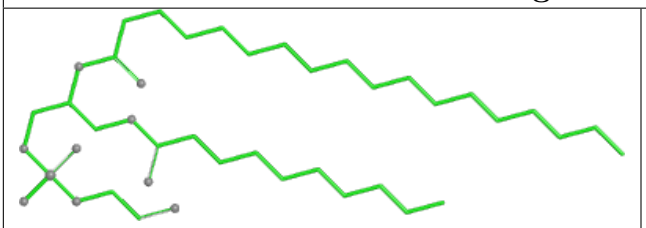


Torsions

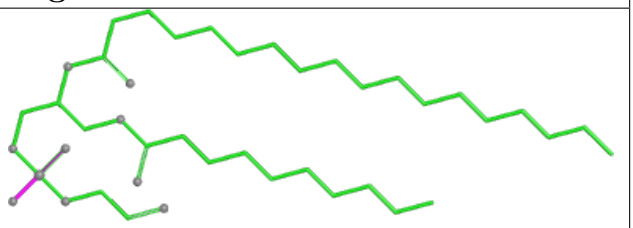


Rings

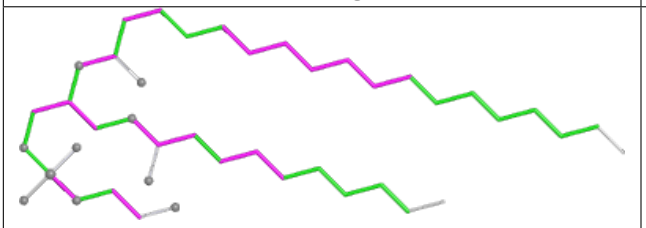
Ligand 3PE g 102



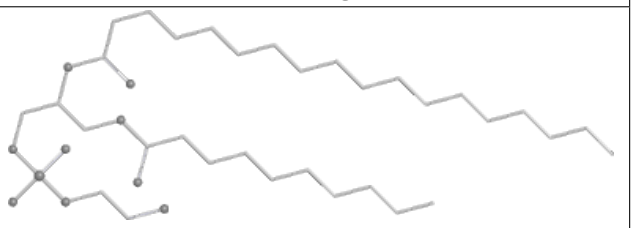
Bond lengths



Bond angles

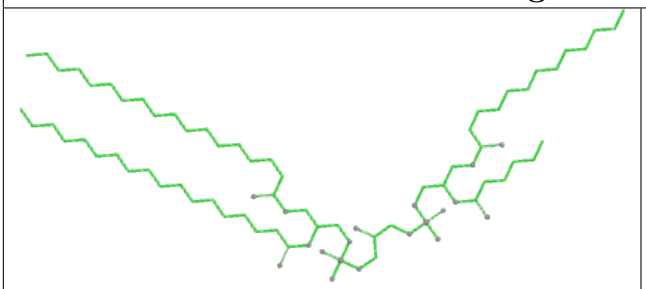


Torsions

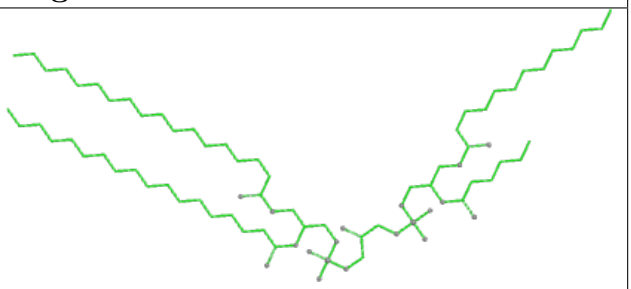


Rings

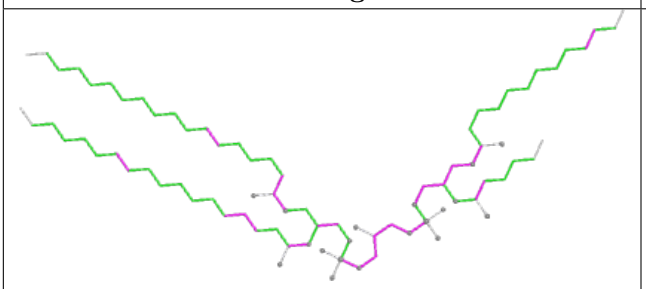
Ligand CDL g 101



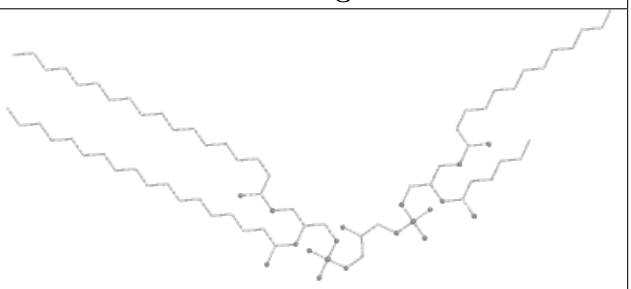
Bond lengths



Bond angles

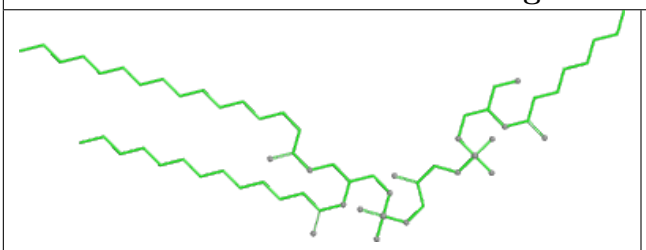


Torsions

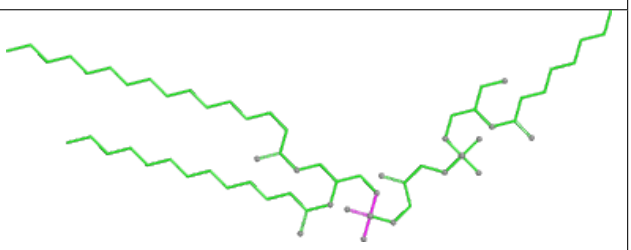


Rings

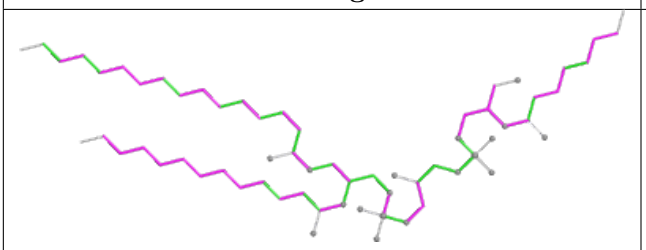
Ligand CDL X 201



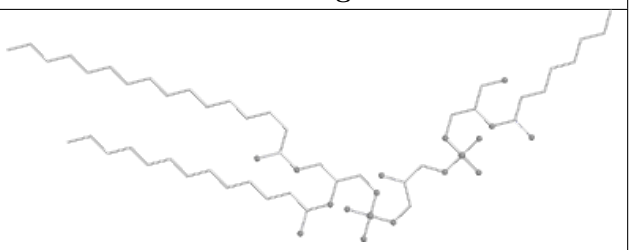
Bond lengths



Bond angles

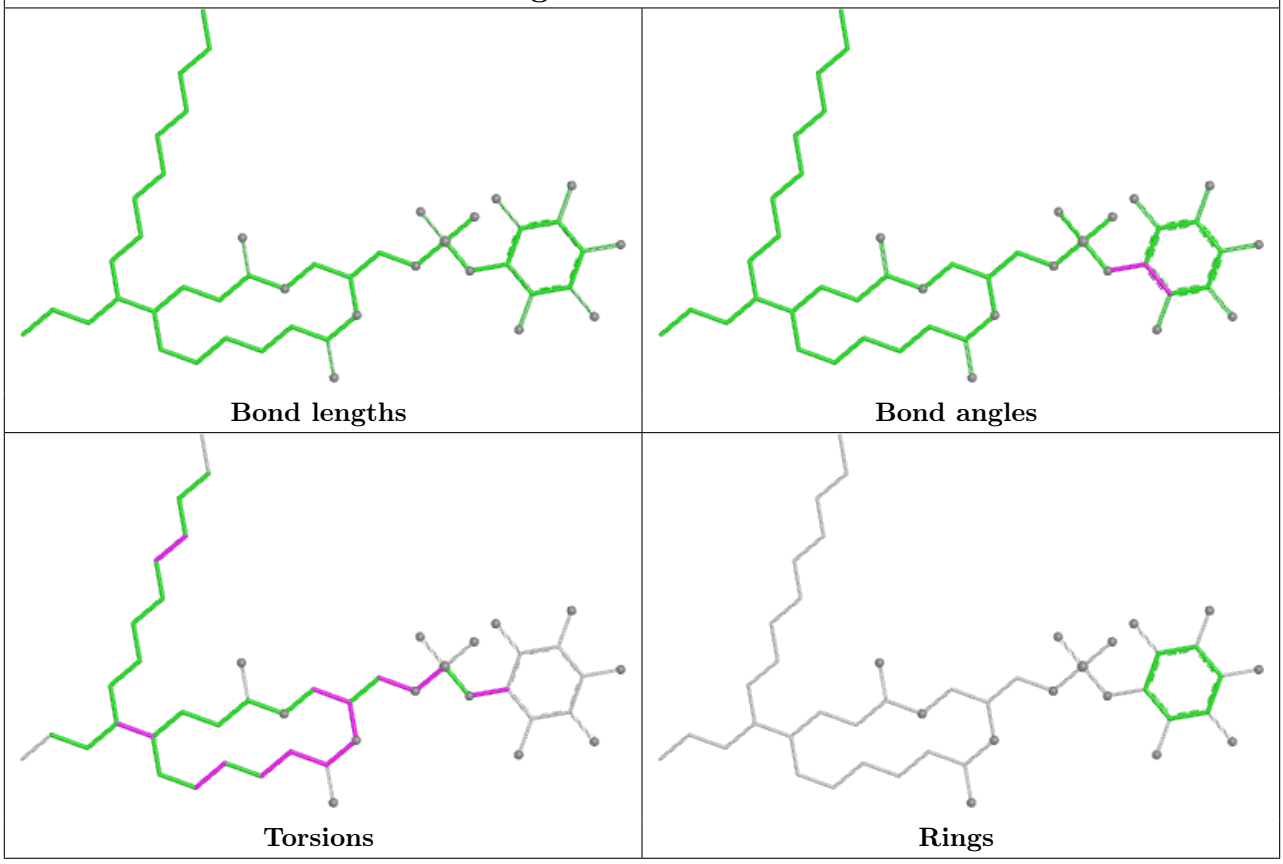


Torsions



Rings

Ligand T7X b 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14764. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.