



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 29, 2016 – 11:02 AM EST

PDB ID : 5LNK
EMDB ID: : EMD-4093
Title : Entire ovine respiratory complex I
Authors : Fiedorczuk, K.; Letts, J.A.; Kaszuba, K.; Sazanov, L.A.
Deposited on : 2016-08-04
Resolution : 3.90 Å(reported)
Based on PDB ID : 4HEA

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

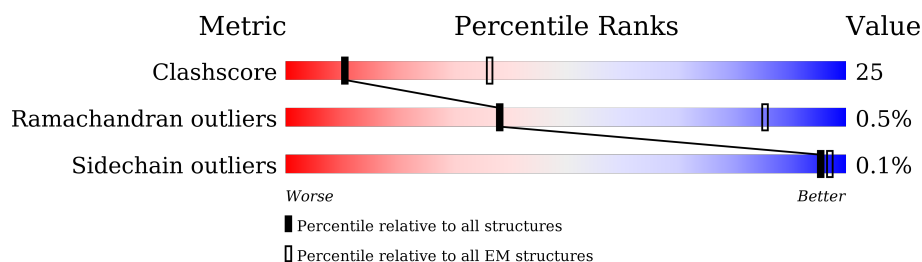
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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






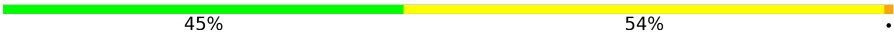


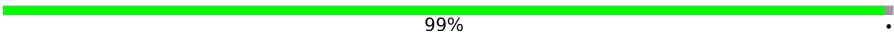

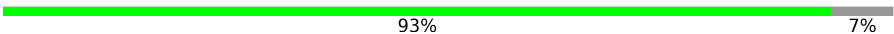

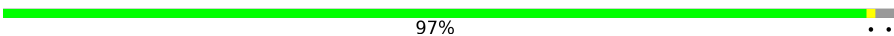


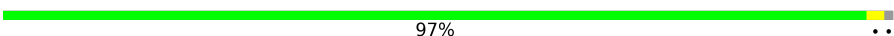

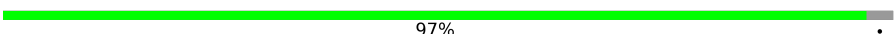
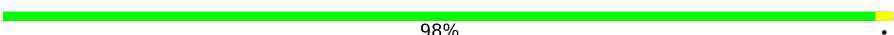

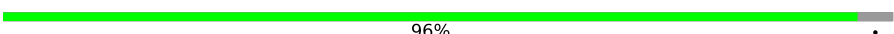

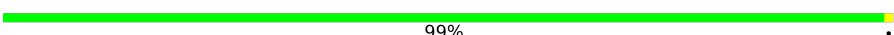

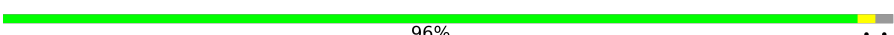


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	445	
2	2	217	
3	3	704	
4	4	412	
5	5	228	
6	6	179	
7	9	176	
8	H	318	
9	N	347	

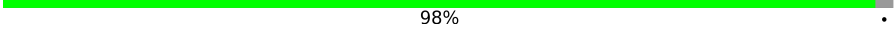
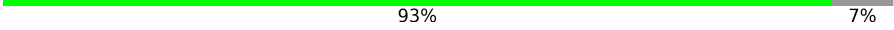

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Mol	Chain	Length	Quality of chain
10	A	115	
11	M	459	
12	K	98	
13	L	599	
14	J	175	
15	a	75	
16	b	96	
17	c	133	
18	d	338	
19	e	98	
20	f	115	
21	g	127	
22	h	112	
23	i	145	
24	X	88	
24	j	88	
25	k	320	
26	l	105	
27	m	83	
28	n	97	
29	o	120	
30	p	128	
31	q	143	
32	r	127	
33	s	136	

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Mol	Chain	Length	Quality of chain
34	t	178	 90% 7%
35	u	72	 92% 8%
36	v	158	 84% 5% 9%
37	w	125	 67% 31%
38	x	49	 98%
39	y	57	 93% 7%
40	z	70	 99%
41	Z	175	 61% 35%
42	Y	171	 47% 53%
43	W	143	 62% 35%
44	V	119	 86% 14%

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
45	SF4	1	500	-	-	X	-
45	SF4	6	300	-	-	X	-
45	SF4	9	502	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 63760 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 Mitochondrial complex I, 51 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	432	Total	C	N	O	S	0	0
			3328	2097	596	615	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	214	Total	C	N	O	S	0	0
			1655	1056	279	310	10		

- Molecule 3 is a protein called Mitochondrial complex I, 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	387	Total	C	N	O	S	0	0
			3098	1974	535	565	24		

- Molecule 5 is a protein called Mitochondrial complex I, 30 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called Mitochondrial complex I, ND1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

- Molecule 9 is a protein called Mitochondrial complex I, ND2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 10 is a protein called Mitochondrial complex I, ND3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

- Molecule 11 is a protein called Mitochondrial complex I, ND4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	459	Total	C	N	O	S	0	0
			3645	2428	571	606	40		

- Molecule 12 is a protein called Mitochondrial complex I, ND4L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	86	Total	C	N	O	S	0	0
			649	428	96	111	14		

- Molecule 13 is a protein called Mitochondrial complex I, ND5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	599	Total	C	N	O	S	0	0
			4456	2926	714	777	39		

- Molecule 14 is a protein called Mitochondrial complex I, ND6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	175	Total	C	N	O	S	0	0
			1188	780	184	214	10		

- Molecule 15 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	41	Total	C	N	O	S	0	0
			343	213	61	68	1		

- Molecule 16 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 17 is a protein called Mitochondrial complex I, 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	123	Total	C	N	O	S	0	0
			1000	631	178	188	3		

- Molecule 18 is a protein called Mitochondrial complex I, 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	314	Total	C	N	O	S	0	0
			2473	1585	448	435	5		

- Molecule 19 is a protein called Mitochondrial complex I, B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

- Molecule 20 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	112	Total	C	N	O	S	0	0
			909	589	152	166	2		

- Molecule 21 is a protein called Mitochondrial complex I, B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 22 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 23 is a protein called Mitochondrial complex I, B17.2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	144	Total	C	N	O	S	0	0
			1200	772	214	209	5		

- Molecule 24 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	85	Total	C	N	O	S	0	0
			684	442	101	136	5		
24	X	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 25 is a protein called Mitochondrial complex I, 42 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	320	Total	C	N	O	S	0	0
			2268	1430	394	435	9		

- Molecule 26 is a protein called Mitochondrial complex I, 15 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	95	Total	C	N	O	S	0	0
			792	503	146	137	6		

- Molecule 27 is a protein called Mitochondrial complex I, B9 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 28 is a protein called Mitochondrial complex I, B12 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	74	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 29 is a protein called Mitochondrial complex I, B14.5b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 30 is a protein called Mitochondrial complex I, B15 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	112	Total	C	N	O	S	0	0
			841	526	162	152	1		

- Molecule 31 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	140	Total	C	N	O	S	0	0
			1151	739	202	201	9		

- Molecule 32 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	93	Total	C	N	O	S	0	0
			752	491	131	130			

- Molecule 33 is a protein called Mitochondrial complex I, B18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	s	118	Total	C	N	O	S	0	0
			988	616	187	176	9		

- Molecule 34 is a protein called Mitochondrial complex I, B22 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	166	Total	C	N	O	S	0	0
			1434	916	265	247	6		

- Molecule 35 is a protein called Mitochondrial complex I, AGGG subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	66	Total	C	N	O	S	0	0
			563	372	94	96	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	v	143	Total	C	N	O	S	0	0
			861	544	155	158	4		

- Molecule 37 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	w	86	Total	C	N	O	S	0	0
			715	462	119	130	4		

- Molecule 38 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	x	48	Total	C	N	O	0	0
			403	266	69	68		

- Molecule 39 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	y	53	Total	C	N	O	0	0
			457	301	80	76		

- Molecule 40 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	z	69	Total	C	N	O	S	0	0
			568	364	105	95	4		

- Molecule 41 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 42 is a protein called Mitochondrial complex I, PGIV subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

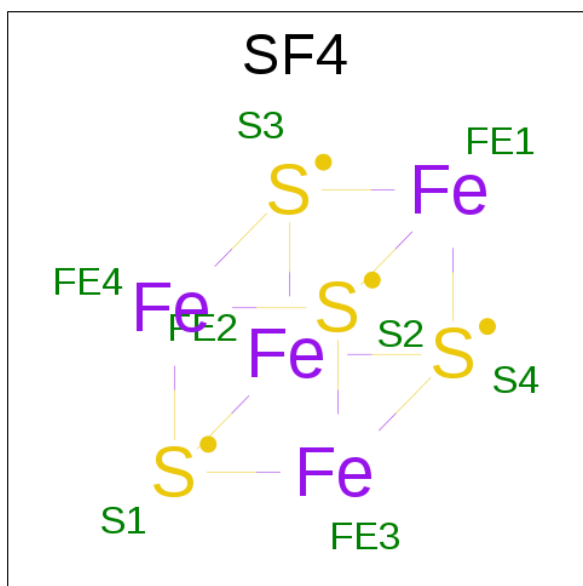
- Molecule 43 is a protein called Mitochondrial complex I, SGD1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 44 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	119	Total	C	N	O	S	0	0
			595	357	119	119			

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



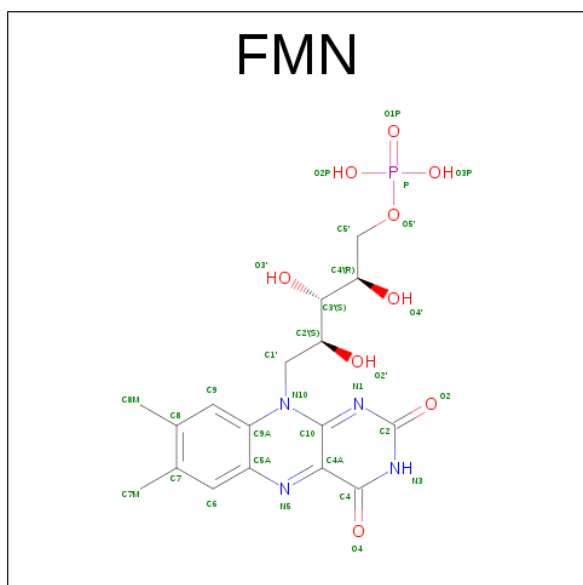
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			16	8	8	
45	3	1	Total	Fe	S	0
			16	8	8	
45	6	1	Total	Fe	S	0
			8	4	4	

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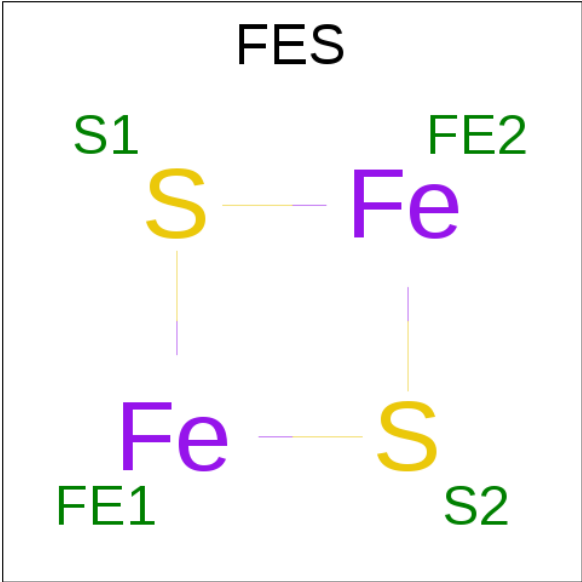
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			16	8	8	
45	9	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



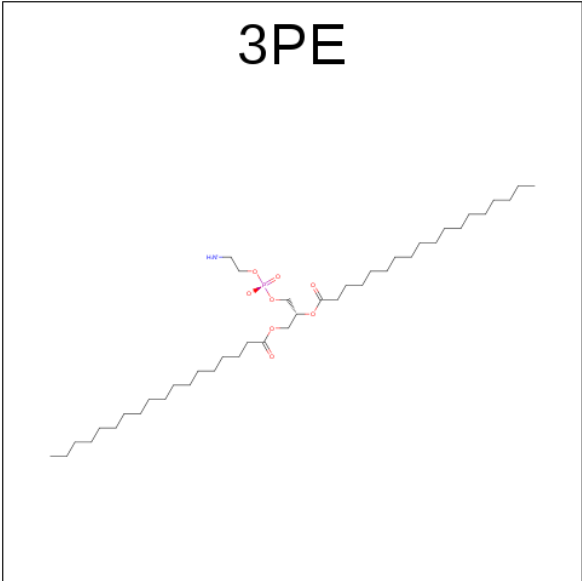
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	2	1	Total	Fe	S	0
			4	2	2	
47	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



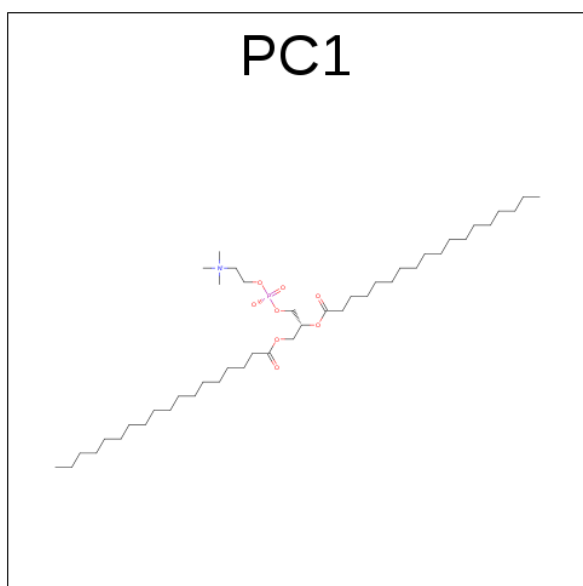
Mol	Chain	Residues	Atoms					AltConf
48	9	1	Total	C	N	O	P	0
			51	41	1	8	1	

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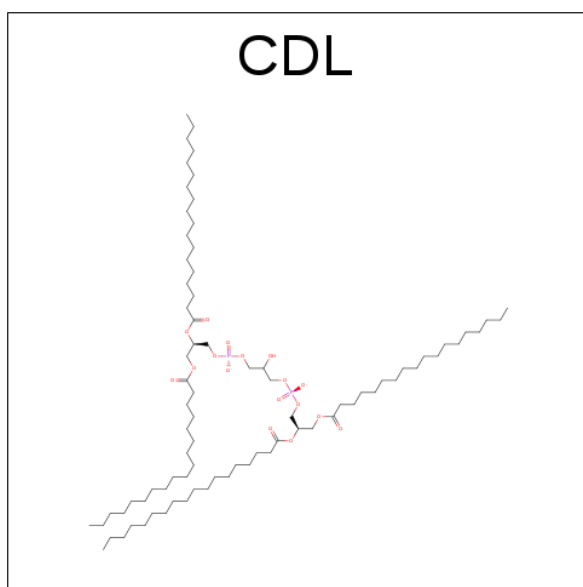
Mol	Chain	Residues	Atoms					AltConf
48	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	o	1	Total	C	N	O	P	0
			87	67	2	16	2	
48	o	1	Total	C	N	O	P	0
			87	67	2	16	2	

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
49	N	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	o	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

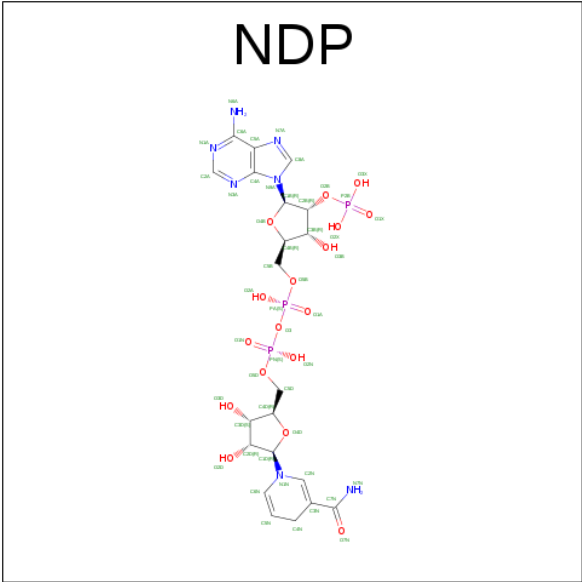


Mol	Chain	Residues	Atoms				AltConf
50	M	1	Total	C	O	P	0
			82	63	17	2	
50	L	1	Total	C	O	P	0
			84	65	17	2	
50	J	1	Total	C	O	P	0
			79	60	17	2	
50	i	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

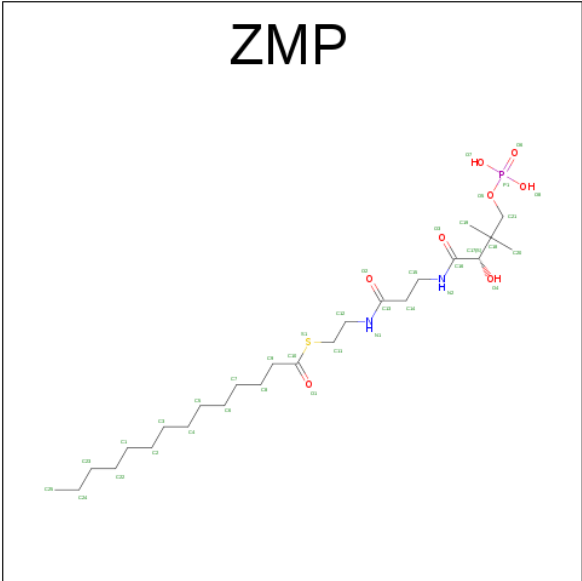
Mol	Chain	Residues	Atoms		AltConf
51	b	1	Total	Zn	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



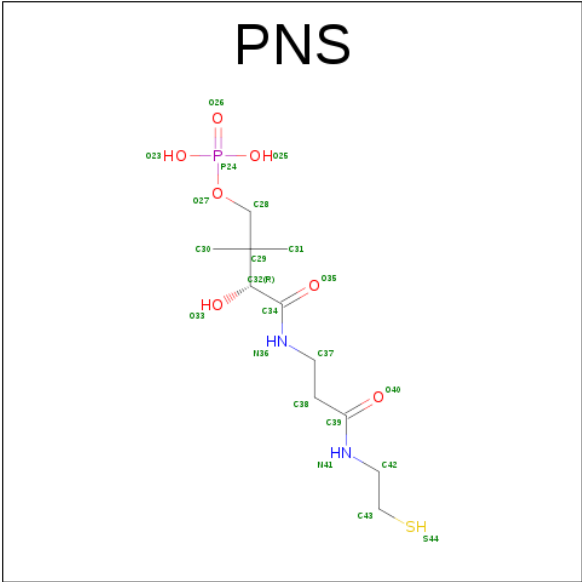
Mol	Chain	Residues	Atoms					AltConf
52	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
53	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 54 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).

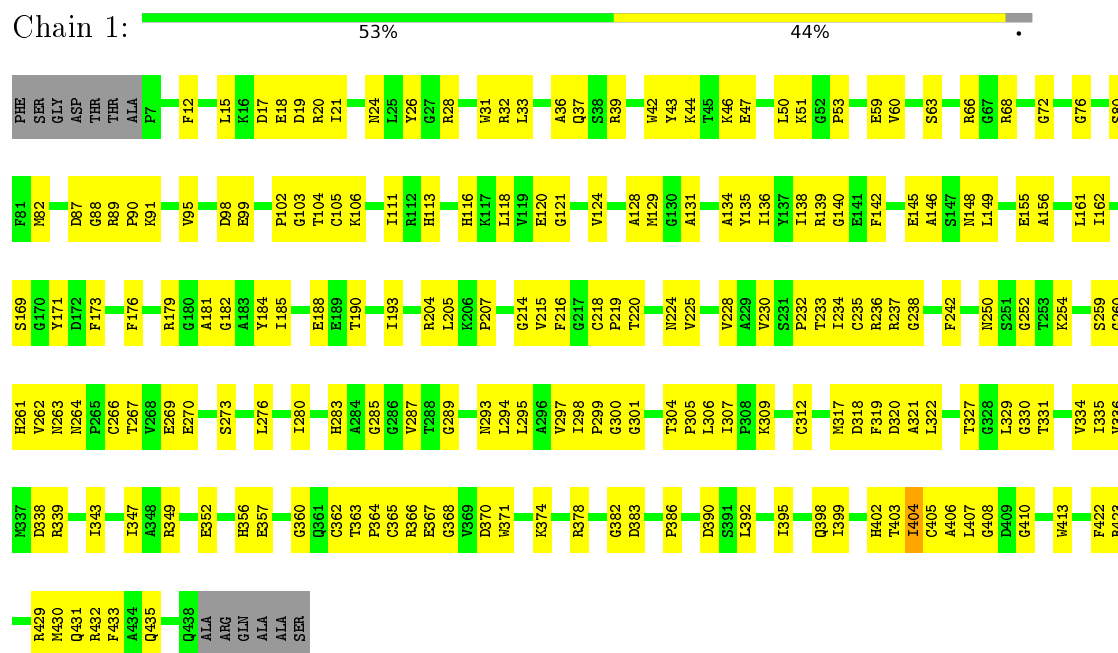


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

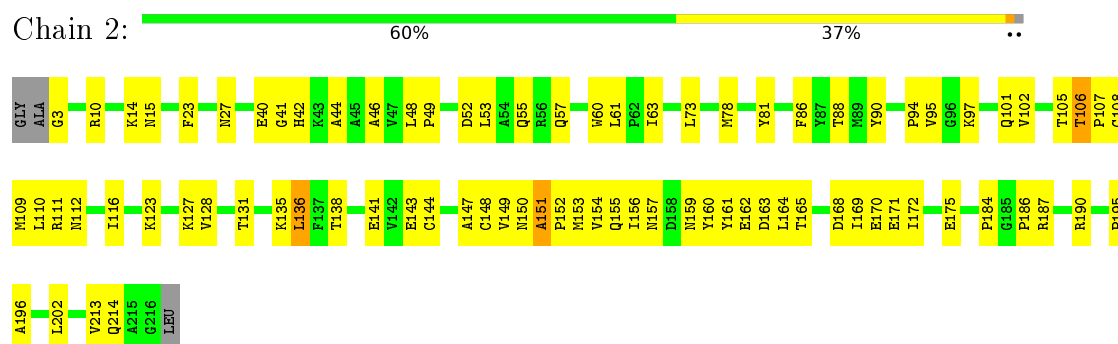
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Mitochondrial complex I, 51 kDa subunit

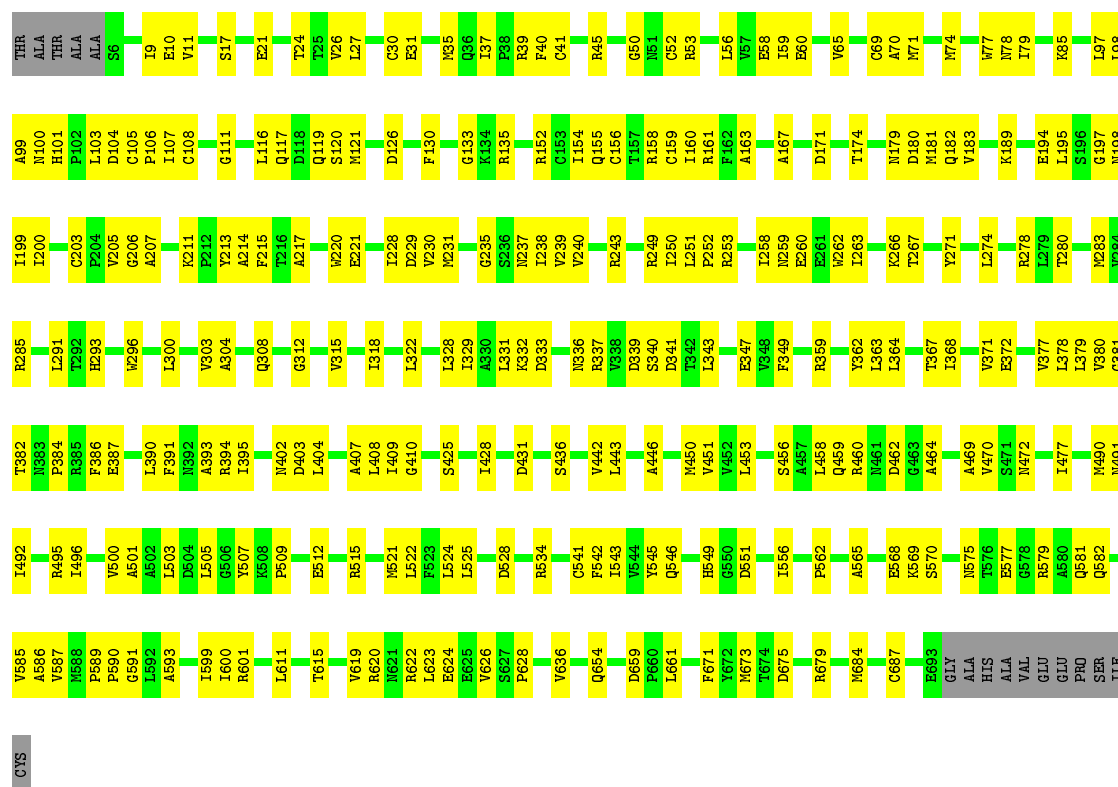


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

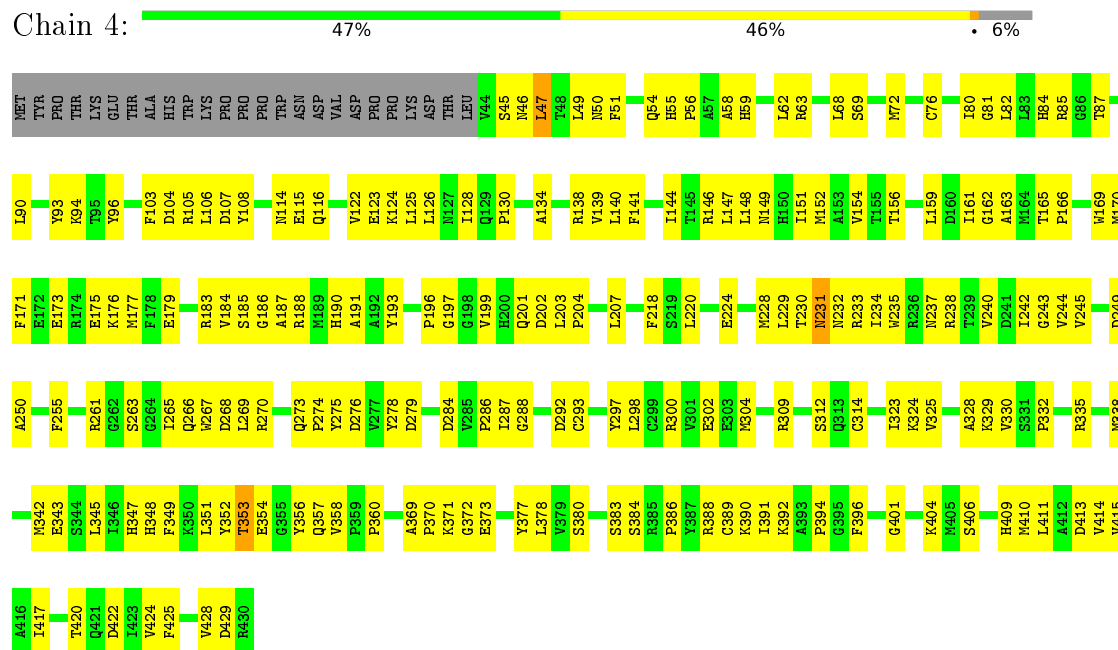


- Molecule 3: Mitochondrial complex I, 75 kDa subunit

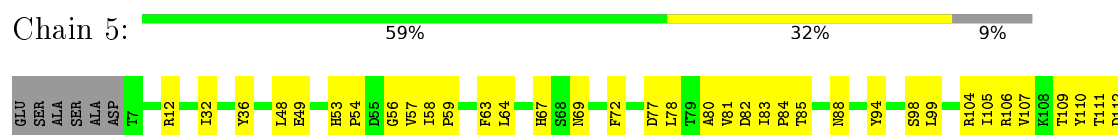


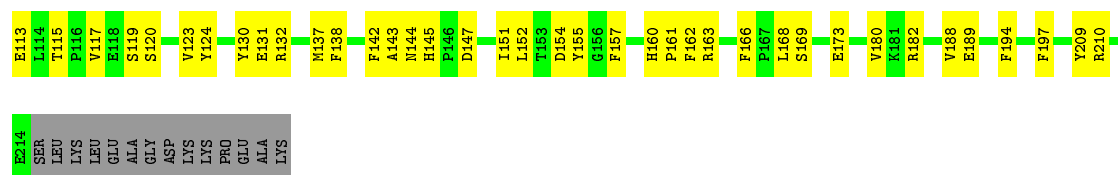


• Molecule 4: Mitochondrial complex I, 49 kDa subunit

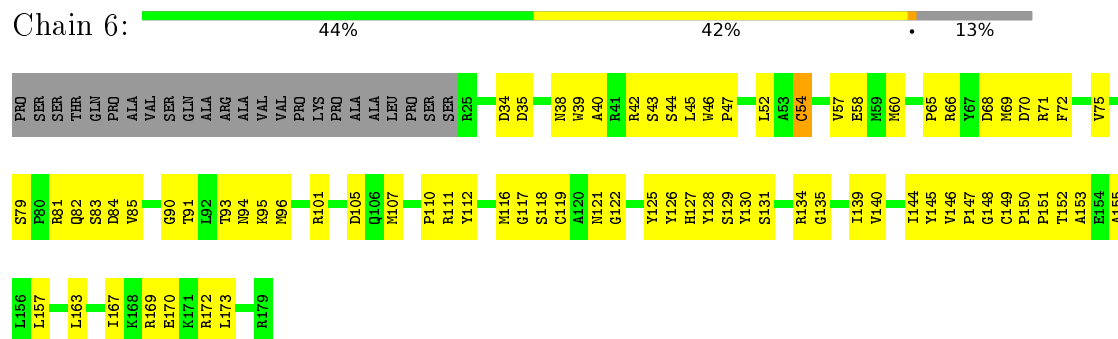


• Molecule 5: Mitochondrial complex I, 30 kDa subunit

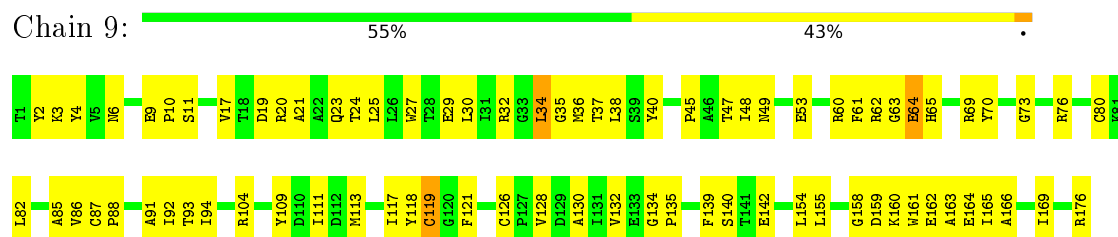




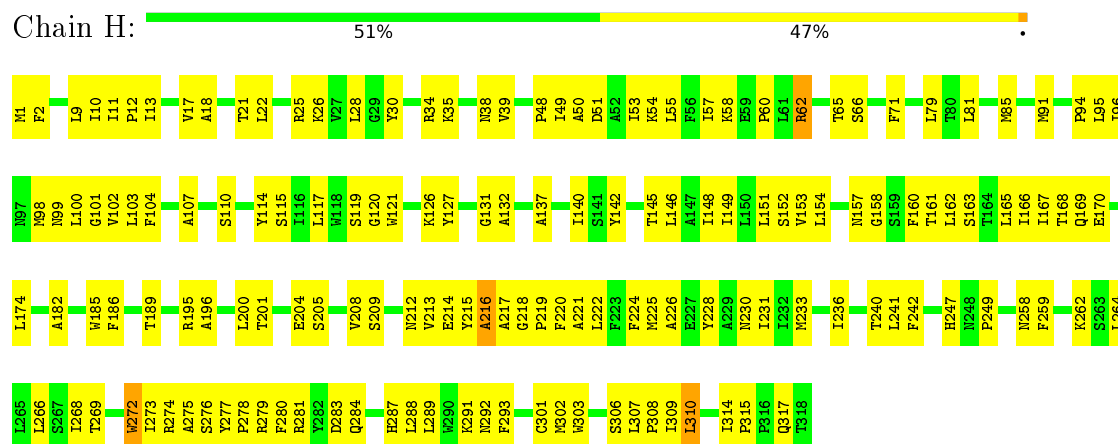
• Molecule 6: Mitochondrial complex I, PSST subunit



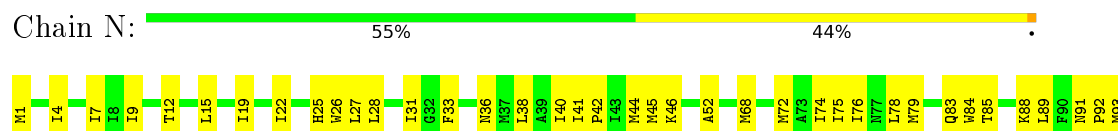
• Molecule 7: Mitochondrial complex I, TYKY subunit

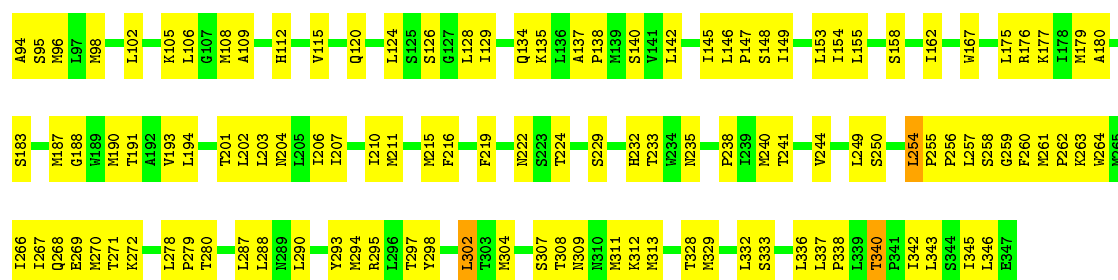


• Molecule 8: Mitochondrial complex I, ND1 subunit

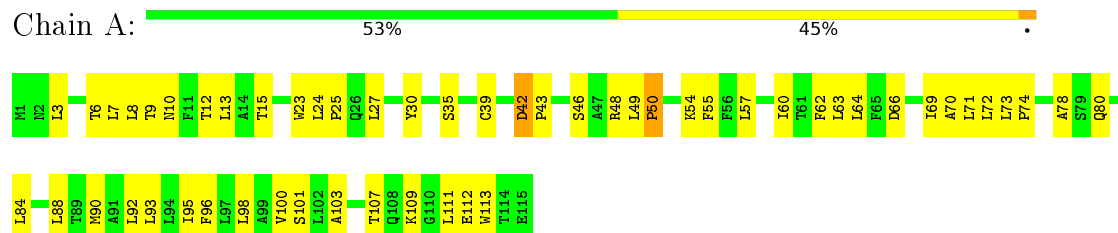


• Molecule 9: Mitochondrial complex I, ND2 subunit

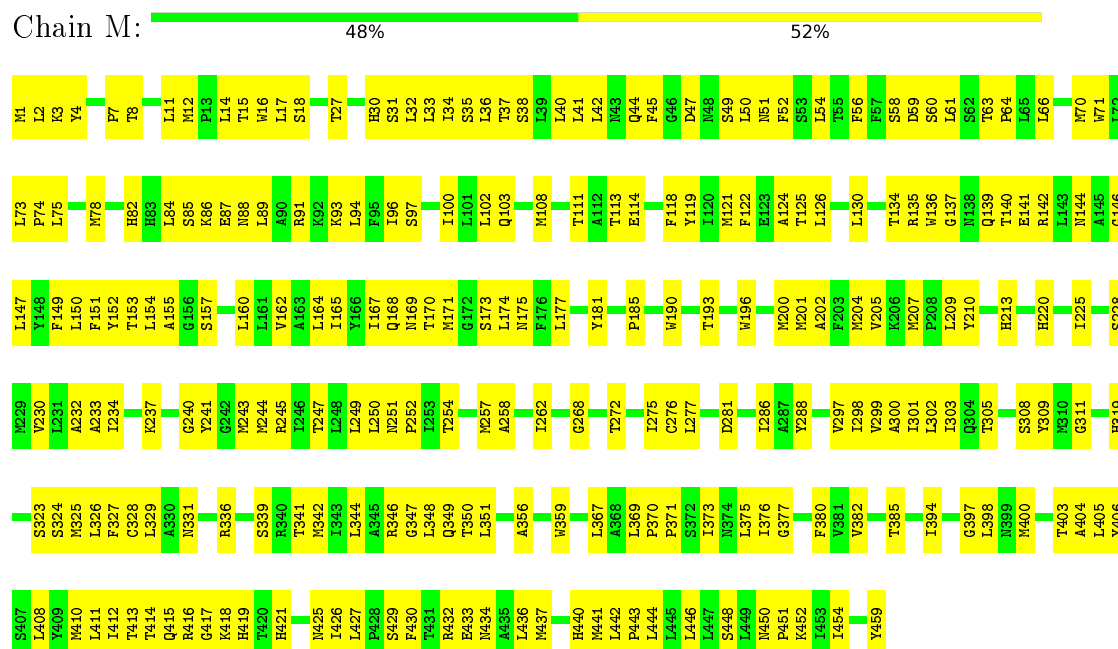




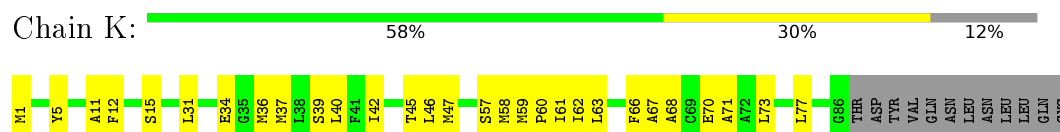
• Molecule 10: Mitochondrial complex I, ND3 subunit



• Molecule 11: Mitochondrial complex I, ND4 subunit

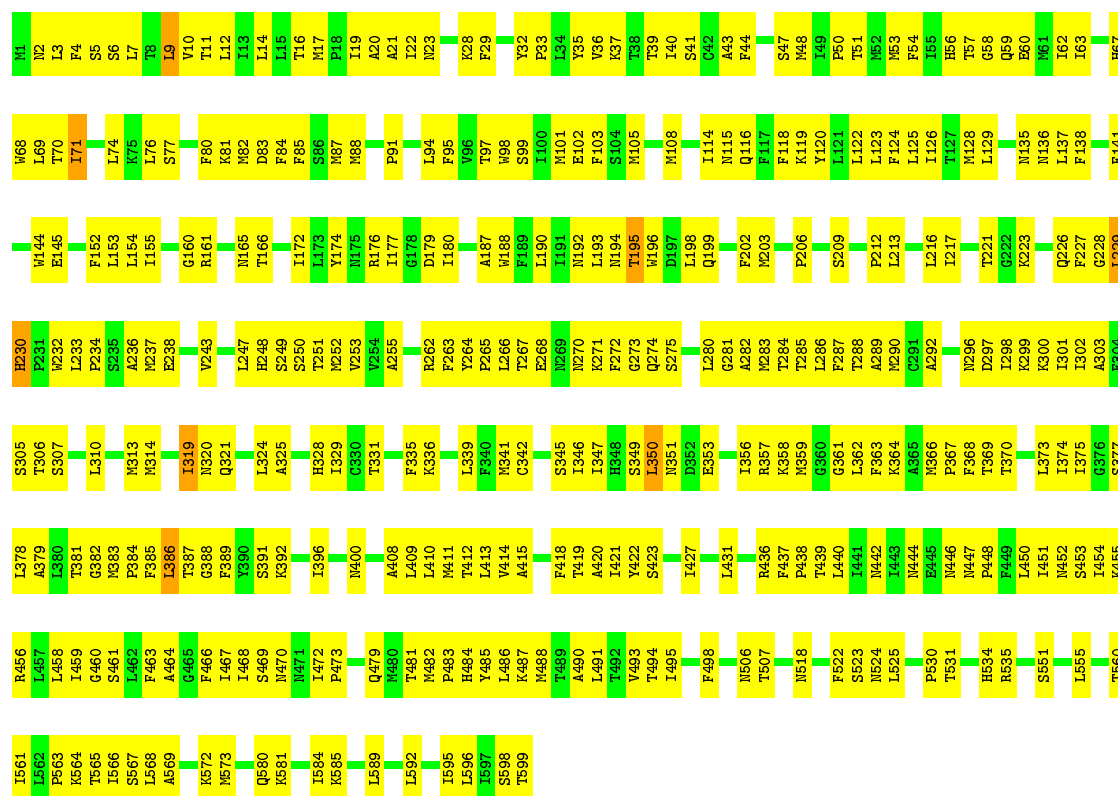


• Molecule 12: Mitochondrial complex I, ND4L subunit



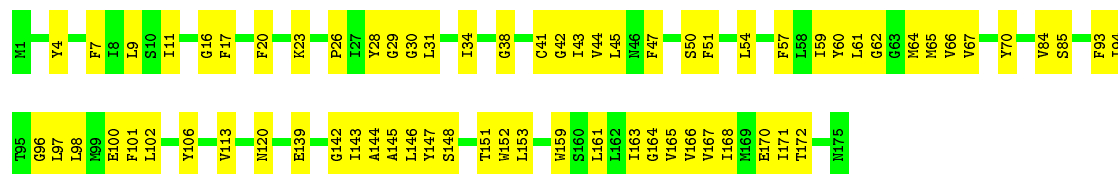
• Molecule 13: Mitochondrial complex I, ND5 subunit





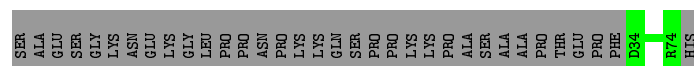
• Molecule 14: Mitochondrial complex I, ND6 subunit

Chain J: 61% 39%



• Molecule 15: Mitochondrial complex I, 10 kDa subunit

Chain a: 55% 45%



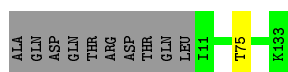
• Molecule 16: Mitochondrial complex I, 13 kDa subunit

Chain b: 99%



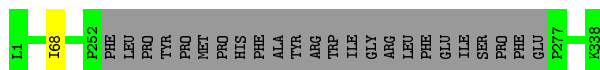
• Molecule 17: Mitochondrial complex I, 18 kDa subunit

Chain c: 92% 8%



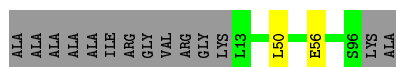
- Molecule 18: Mitochondrial complex I, 39 kDa subunit

Chain d: 93% 7%



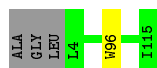
- Molecule 19: Mitochondrial complex I, B8 subunit

Chain e: 84% 14%



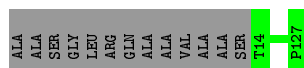
- Molecule 20: Mitochondrial complex I, B13 subunit

Chain f: 97% 2%



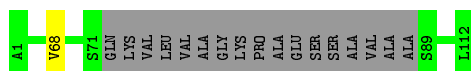
- Molecule 21: Mitochondrial complex I, B14 subunit

Chain g: 90% 10%



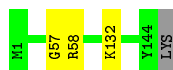
- Molecule 22: Mitochondrial complex I, B14.5a subunit

Chain h: 84% 15%



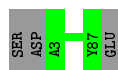
- Molecule 23: Mitochondrial complex I, B17.2 subunit

Chain i: 97% 2%



- Molecule 24: Acyl carrier protein

Chain j: 97% 2%



- Molecule 24: Acyl carrier protein

Chain X:  57% 43%

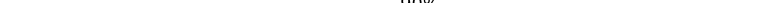


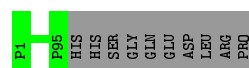
- Molecule 25: Mitochondrial complex I, 42 kDa subunit

Chain k: 98%



- Molecule 26: Mitochondrial complex I, 15 kDa subunit

Chain 1:  90% 10%



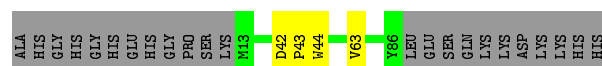
- Molecule 27: Mitochondrial complex I, B9 subunit

Chain m: 96%



- Molecule 28: Mitochondrial complex I, B12 subunit

Chain n:  72% 24%



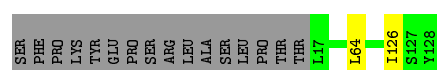
- Molecule 29: Mitochondrial complex I, B14.5b subunit

Chain o: 99%



- Molecule 30: Mitochondrial complex I, B15 subunit

Chain p: 86% • 13%



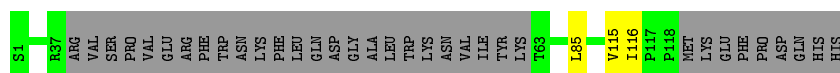
- Molecule 31: Mitochondrial complex I, B16.6 subunit

Chain q:  96% ..




- Molecule 32: Mitochondrial complex I, B17 subunit

Chain r:  71% . 27%



- Molecule 33: Mitochondrial complex I, B18 subunit

Chain s:  85% .. 13%



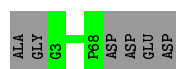
- Molecule 34: Mitochondrial complex I, B22 subunit

Chain t:  90% . 7%




- Molecule 35: Mitochondrial complex I, AGGG subunit

Chain u:  92% 8%



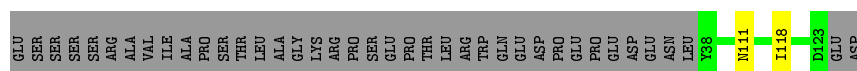
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:  84% 5% . 9%



- Molecule 37: Mitochondrial complex I, ESSS subunit

Chain w:  67% . 31%



- Molecule 38: Mitochondrial complex I, KFYI subunit

Chain x:  98% .



- Molecule 39: Mitochondrial complex I, MNLL subunit

Chain y: 93% 7%



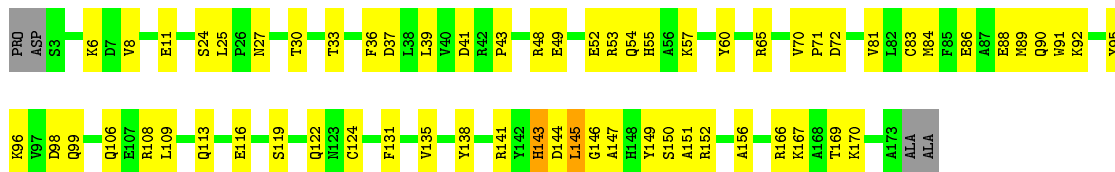
- Molecule 40: Mitochondrial complex I, MWFE subunit

Chain z: 99% .



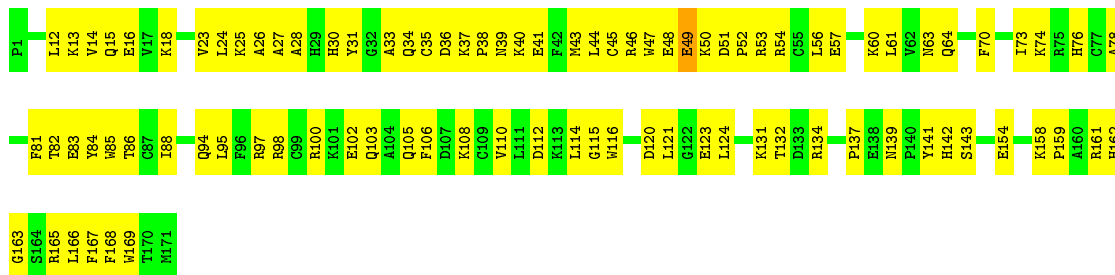
- Molecule 41: Mitochondrial complex I, PDSW subunit

Chain Z: 61% 35% ..



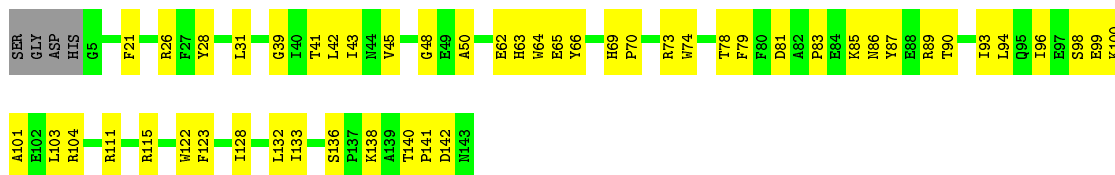
- Molecule 42: Mitochondrial complex I, PGIV subunit

Chain Y: 47% 53% .



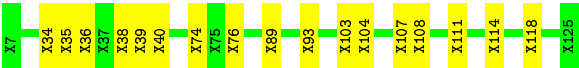
- Molecule 43: Mitochondrial complex I, SGDHI subunit

Chain W: 62% 35% .



- Molecule 44: Mitochondrial complex I, B14.7 subunit

Chain V: 86% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	82000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	100720	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CDL, PNS, PC1, FMN, FES, SF4, NDP, ZMP, 3PE

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 >2	RMSZ	# Z >2
1	1	0.34	0/3403	0.52	0/4597
10	A	0.42	1/947 (0.1%)	0.61	0/1296
11	M	0.38	0/3739	0.62	0/5095
12	K	0.36	0/658	0.62	0/888
13	L	0.37	0/4563	0.64	3/6227 (0.0%)
14	J	0.41	0/1212	0.57	0/1652
15	a	0.29	0/352	0.53	0/476
16	b	0.38	0/749	0.50	0/1009
17	c	0.36	0/1023	0.56	0/1382
18	d	0.33	0/2532	0.59	0/3430
19	e	0.47	1/688 (0.1%)	0.53	0/927
2	2	0.35	0/1695	0.59	1/2305 (0.0%)
20	f	0.32	0/929	0.51	0/1260
21	g	0.34	0/993	0.49	0/1336
22	h	0.33	0/775	0.61	0/1048
23	i	0.32	0/1241	0.54	0/1687
24	X	0.32	0/719	0.55	0/971
24	j	0.30	0/696	0.53	0/940
25	k	0.34	1/2309 (0.0%)	0.56	0/3141
26	l	0.36	0/811	0.57	0/1085
27	m	0.34	0/647	0.49	0/890
28	n	0.34	0/595	0.66	0/805
29	o	0.38	0/1035	0.55	0/1398
3	3	0.34	0/5362	0.53	0/7266
30	p	0.30	0/855	0.54	1/1155 (0.1%)
31	q	0.36	0/1180	0.63	1/1590 (0.1%)
32	r	0.37	0/774	0.62	1/1058 (0.1%)
33	s	0.32	0/1011	0.58	0/1356
34	t	0.41	1/1483 (0.1%)	0.56	1/2006 (0.0%)
35	u	0.35	0/590	0.59	0/809
36	v	0.30	0/877	0.65	0/1208
37	w	0.38	0/737	0.57	0/999

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	x	0.31	0/416	0.46	0/564
39	y	0.34	0/470	0.47	0/636
4	4	0.41	0/3172	0.57	1/4288 (0.0%)
40	z	0.38	0/583	0.55	0/785
41	Z	0.38	0/1475	0.55	0/1989
42	Y	0.39	0/1440	0.68	0/1942
43	W	0.39	0/1188	0.54	0/1607
5	5	0.40	0/1776	0.52	0/2417
6	6	0.42	0/1272	0.54	0/1720
7	9	0.45	1/1445 (0.1%)	0.64	1/1956 (0.1%)
8	H	0.43	0/2603	0.63	1/3561 (0.0%)
9	N	0.42	1/2787 (0.0%)	0.62	0/3795
All	All	0.37	6/63807 (0.0%)	0.58	11/86552 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	A	0	2
13	L	0	6
17	c	0	1
19	e	0	1
2	2	0	1
20	f	0	1
23	i	0	1
25	k	0	3
29	o	0	1
31	q	0	2
33	s	0	2
34	t	0	1
36	v	0	7
4	4	0	1
42	Y	0	1
7	9	0	1
8	H	0	3
9	N	0	3
All	All	0	38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	50	LEU	C-N	-9.90	1.15	1.34
34	t	163	PRO	C-N	9.08	1.51	1.34
25	k	174	VAL	C-N	-8.55	1.18	1.34
9	N	304	MET	C-N	-7.74	1.16	1.34
10	A	42	ASP	C-N	5.94	1.45	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	74	GLN	C-N-CA	-6.59	105.21	121.70
4	4	47	LEU	CA-CB-CG	6.59	130.45	115.30
7	9	34	LEU	CA-CB-CG	-6.21	101.03	115.30
13	L	9	LEU	CA-CB-CG	6.18	129.52	115.30
30	p	64	LEU	CA-CB-CG	5.77	128.57	115.30

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	151	ALA	Peptide
4	4	54	GLN	Peptide
7	9	64	GLU	Peptide
8	H	216	ALA	Peptide
8	H	62	ARG	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	1	3328	0	3287	166	0
2	2	1655	0	1663	75	0
3	3	5275	0	5300	209	0
4	4	3098	0	3068	199	0
5	5	1726	0	1676	66	0
6	6	1241	0	1251	82	0
7	9	1414	0	1370	93	0
8	H	2528	0	2641	153	0
9	N	2723	0	2929	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	922	0	953	56	0
11	M	3645	0	3850	208	0
12	K	649	0	699	37	0
13	L	4456	0	4298	310	0
14	J	1188	0	1068	72	0
15	a	343	0	320	0	0
16	b	737	0	710	0	0
17	c	1000	0	997	0	0
18	d	2473	0	2461	0	0
19	e	677	0	686	0	0
20	f	909	0	947	0	0
21	g	969	0	980	0	0
22	h	757	0	771	0	0
23	i	1200	0	1169	0	0
24	X	707	0	700	27	0
24	j	684	0	682	0	0
25	k	2268	0	1995	0	0
26	l	792	0	798	0	0
27	m	626	0	635	0	0
28	n	578	0	558	0	0
29	o	1004	0	995	0	0
30	p	841	0	760	0	0
31	q	1151	0	1150	0	0
32	r	752	0	752	0	0
33	s	988	0	930	0	0
34	t	1434	0	1392	0	0
35	u	563	0	511	0	0
36	v	861	0	557	0	0
37	w	715	0	679	0	0
38	x	403	0	405	0	0
39	y	457	0	459	0	0
40	z	568	0	558	0	0
41	Z	1441	0	1416	49	0
42	Y	1403	0	1384	84	0
43	W	1155	0	1177	54	0
44	V	595	0	127	9	0
45	1	8	0	0	2	0
45	3	16	0	0	2	0
45	6	8	0	0	2	0
45	9	16	0	0	4	0
46	1	31	0	19	8	0
47	2	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	3	4	0	0	0	0
48	9	51	0	82	9	0
48	J	51	0	82	6	0
48	o	87	0	128	0	0
49	A	47	0	71	3	0
49	M	46	0	66	2	0
49	N	46	0	66	2	0
49	o	39	0	55	0	0
50	J	79	0	108	1	0
50	L	84	0	118	13	0
50	M	82	0	114	2	0
50	i	58	0	60	0	0
51	b	1	0	0	0	0
52	d	48	0	26	0	0
53	j	34	0	40	0	0
54	X	21	0	21	0	0
All	All	63760	0	62770	1861	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 25.

The worst 5 of 1861 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)
13:L:451:ILE:O	13:L:455:LYS:HB2	1.43	1.15
13:L:374:ILE:O	13:L:378:LEU:HB3	1.62	0.98
11:M:254:THR:O	11:M:258:ALA:HB2	1.64	0.97
13:L:232:TRP:HD1	13:L:233:LEU:HD12	1.33	0.93
9:N:311:MET:HG2	9:N:312:LYS:H	1.32	0.93

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	1	430/445 (97%)	405 (94%)	24 (6%)	1 (0%)	52	86
2	2	212/217 (98%)	189 (89%)	22 (10%)	1 (0%)	34	76
3	3	686/704 (97%)	616 (90%)	70 (10%)	0	100	100
4	4	385/412 (93%)	337 (88%)	46 (12%)	2 (0%)	34	76
5	5	206/228 (90%)	183 (89%)	23 (11%)	0	100	100
6	6	153/179 (86%)	138 (90%)	15 (10%)	0	100	100
7	9	174/176 (99%)	150 (86%)	24 (14%)	0	100	100
8	H	316/318 (99%)	278 (88%)	37 (12%)	1 (0%)	46	82
9	N	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
10	A	113/115 (98%)	97 (86%)	15 (13%)	1 (1%)	21	65
11	M	457/459 (100%)	392 (86%)	64 (14%)	1 (0%)	52	86
12	K	84/98 (86%)	72 (86%)	12 (14%)	0	100	100
13	L	597/599 (100%)	518 (87%)	75 (13%)	4 (1%)	26	70
14	J	173/175 (99%)	142 (82%)	29 (17%)	2 (1%)	16	61
15	a	39/75 (52%)	33 (85%)	6 (15%)	0	100	100
16	b	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
17	c	121/133 (91%)	109 (90%)	12 (10%)	0	100	100
18	d	310/338 (92%)	253 (82%)	56 (18%)	1 (0%)	46	82
19	e	82/98 (84%)	74 (90%)	8 (10%)	0	100	100
20	f	110/115 (96%)	95 (86%)	15 (14%)	0	100	100
21	g	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
22	h	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	17	63
23	i	142/145 (98%)	116 (82%)	24 (17%)	2 (1%)	14	58
24	X	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
24	j	83/88 (94%)	70 (84%)	13 (16%)	0	100	100
25	k	318/320 (99%)	263 (83%)	50 (16%)	5 (2%)	12	56
26	l	93/105 (89%)	83 (89%)	10 (11%)	0	100	100
27	m	78/83 (94%)	72 (92%)	6 (8%)	0	100	100
28	n	72/97 (74%)	50 (69%)	18 (25%)	4 (6%)	2	29
29	o	118/120 (98%)	105 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	p	110/128 (86%)	83 (76%)	26 (24%)	1 (1%)	21	65
31	q	138/143 (96%)	126 (91%)	12 (9%)	0	100	100
32	r	89/127 (70%)	75 (84%)	12 (14%)	2 (2%)	8	50
33	s	116/136 (85%)	93 (80%)	21 (18%)	2 (2%)	11	55
34	t	164/178 (92%)	142 (87%)	22 (13%)	0	100	100
35	u	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
36	v	141/158 (89%)	103 (73%)	33 (23%)	5 (4%)	4	41
37	w	84/125 (67%)	67 (80%)	15 (18%)	2 (2%)	7	49
38	x	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
39	y	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
40	z	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
41	Z	169/175 (97%)	147 (87%)	21 (12%)	1 (1%)	30	73
42	Y	169/171 (99%)	137 (81%)	32 (19%)	0	100	100
43	W	137/143 (96%)	115 (84%)	21 (15%)	1 (1%)	26	70
All	All	7824/8344 (94%)	6800 (87%)	984 (13%)	40 (0%)	38	76

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	106	THR
28	n	63	VAL
33	s	14	VAL
13	L	71	ILE
13	L	319	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	346/354 (98%)	346 (100%)	0	100	100
2	2	182/183 (100%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	578/588 (98%)	578 (100%)	0	100	100
4	4	334/358 (93%)	334 (100%)	0	100	100
5	5	189/204 (93%)	189 (100%)	0	100	100
6	6	131/150 (87%)	130 (99%)	1 (1%)	86	93
7	9	151/151 (100%)	151 (100%)	0	100	100
8	H	278/278 (100%)	278 (100%)	0	100	100
9	N	315/315 (100%)	315 (100%)	0	100	100
10	A	103/103 (100%)	103 (100%)	0	100	100
11	M	412/412 (100%)	412 (100%)	0	100	100
12	K	75/87 (86%)	75 (100%)	0	100	100
13	L	445/532 (84%)	445 (100%)	0	100	100
14	J	101/144 (70%)	101 (100%)	0	100	100
15	a	40/68 (59%)	40 (100%)	0	100	100
16	b	79/80 (99%)	79 (100%)	0	100	100
17	c	110/119 (92%)	110 (100%)	0	100	100
18	d	257/292 (88%)	257 (100%)	0	100	100
19	e	75/81 (93%)	75 (100%)	0	100	100
20	f	100/101 (99%)	100 (100%)	0	100	100
21	g	107/113 (95%)	107 (100%)	0	100	100
22	h	83/94 (88%)	83 (100%)	0	100	100
23	i	130/131 (99%)	130 (100%)	0	100	100
24	X	81/81 (100%)	81 (100%)	0	100	100
24	j	78/81 (96%)	78 (100%)	0	100	100
25	k	199/284 (70%)	199 (100%)	0	100	100
26	l	85/94 (90%)	85 (100%)	0	100	100
27	m	69/71 (97%)	69 (100%)	0	100	100
28	n	53/75 (71%)	53 (100%)	0	100	100
29	o	107/107 (100%)	107 (100%)	0	100	100
30	p	71/114 (62%)	71 (100%)	0	100	100
31	q	120/121 (99%)	120 (100%)	0	100	100
32	r	80/121 (66%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	s	100/119 (84%)	100 (100%)	0	100	100
34	t	151/160 (94%)	149 (99%)	2 (1%)	76	89
35	u	58/62 (94%)	58 (100%)	0	100	100
36	v	38/142 (27%)	38 (100%)	0	100	100
37	w	77/112 (69%)	77 (100%)	0	100	100
38	x	43/44 (98%)	43 (100%)	0	100	100
39	y	49/53 (92%)	49 (100%)	0	100	100
40	z	58/59 (98%)	58 (100%)	0	100	100
41	Z	155/157 (99%)	154 (99%)	1 (1%)	90	95
42	Y	154/154 (100%)	154 (100%)	0	100	100
43	W	122/125 (98%)	122 (100%)	0	100	100
All	All	6569/7274 (90%)	6565 (100%)	4 (0%)	95	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
34	t	153	LEU
34	t	165	LEU
41	Z	145	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
16	b	13	HIS
18	d	250	HIS
37	w	45	HIS
17	c	44	ASN
18	d	37	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	SF4	1	500	1	0,12,12	0.00	-	0,24,24	0.00	-
46	FMN	1	501	-	32,33,33	1.10	2 (6%)	34,50,50	2.94	5 (14%)
47	FES	2	300	2	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	3	801	3	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	3	802	3	0,12,12	0.00	-	0,24,24	0.00	-
47	FES	3	803	3	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	6	300	6	0,12,12	0.00	-	0,24,24	0.00	-
48	3PE	9	501	-	50,50,50	0.32	0	52,55,55	0.41	0
45	SF4	9	502	7	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	9	503	7	0,12,12	0.00	-	0,24,24	0.00	-
49	PC1	A	200	-	46,46,53	0.34	0	50,54,61	0.32	0
50	CDL	J	300	-	78,78,99	0.36	0	80,90,111	0.37	0
48	3PE	J	301	-	50,50,50	0.33	0	52,55,55	0.31	0
50	CDL	L	601	-	83,83,99	0.34	0	85,95,111	0.40	0
49	PC1	M	501	-	45,45,53	0.33	0	49,53,61	0.31	0
50	CDL	M	502	-	81,81,99	0.35	0	83,93,111	0.36	0
49	PC1	N	401	-	45,45,53	0.34	0	49,53,61	0.35	0
54	PNS	X	401	24	13,20,21	0.51	0	16,26,29	0.91	1 (6%)
52	NDP	d	401	-	44,52,52	0.48	0	55,80,80	0.65	1 (1%)
50	CDL	i	201	-	57,57,99	0.41	0	59,69,111	0.36	0
53	ZMP	j	101	24	26,33,36	1.07	2 (7%)	31,40,45	1.41	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PC1	o	201	-	38,38,53	0.36	0	42,46,61	0.31	0
48	3PE	o	202	-	40,40,50	0.38	0	42,45,55	0.34	0
48	3PE	o	203	-	45,45,50	0.35	0	47,50,55	0.38	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
45	SF4	1	500	1	-	0/0/48/48	0/6/5/5
46	FMN	1	501	-	-	0/18/18/18	0/3/3/3
47	FES	2	300	2	-	0/0/4/4	0/1/1/1
45	SF4	3	801	3	-	0/0/48/48	0/6/5/5
45	SF4	3	802	3	-	0/0/48/48	0/6/5/5
47	FES	3	803	3	-	0/0/4/4	0/1/1/1
45	SF4	6	300	6	-	0/0/48/48	0/6/5/5
48	3PE	9	501	-	-	0/54/54/54	0/0/0/0
45	SF4	9	502	7	-	0/0/48/48	0/6/5/5
45	SF4	9	503	7	-	0/0/48/48	0/6/5/5
49	PC1	A	200	-	-	0/50/50/57	0/0/0/0
50	CDL	J	300	-	-	0/89/89/110	0/0/0/0
48	3PE	J	301	-	-	0/54/54/54	0/0/0/0
50	CDL	L	601	-	-	0/94/94/110	0/0/0/0
49	PC1	M	501	-	-	0/49/49/57	0/0/0/0
50	CDL	M	502	-	-	0/92/92/110	0/0/0/0
49	PC1	N	401	-	-	0/49/49/57	0/0/0/0
54	PNS	X	401	24	-	0/24/26/27	0/0/0/0
52	NDP	d	401	-	-	0/30/77/77	0/5/5/5
50	CDL	i	201	-	-	0/68/68/110	0/0/0/0
53	ZMP	j	101	24	-	0/38/40/43	0/0/0/0
49	PC1	o	201	-	-	0/42/42/57	0/0/0/0
48	3PE	o	202	-	-	0/44/44/54	0/0/0/0
48	3PE	o	203	-	-	0/49/49/54	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	j	101	ZMP	C10-S1	-4.27	1.70	1.76
46	1	501	FMN	C5A-N5	2.26	1.38	1.35
53	j	101	ZMP	C9-C10	2.60	1.53	1.50
46	1	501	FMN	C4-N3	3.07	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	501	FMN	C4A-C4-N3	-7.33	113.93	123.52
46	1	501	FMN	C4A-C10-N10	-5.37	116.62	120.52
46	1	501	FMN	N3-C2-N1	-4.72	119.75	127.69
53	j	101	ZMP	O1-C10-C9	-4.69	120.71	123.94
46	1	501	FMN	C4-C4A-C10	-3.97	117.40	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1	500	SF4	2	0
46	1	501	FMN	8	0
45	3	801	SF4	1	0
45	3	802	SF4	1	0
45	6	300	SF4	2	0
48	9	501	3PE	9	0
45	9	502	SF4	3	0
45	9	503	SF4	1	0
49	A	200	PC1	3	0
50	J	300	CDL	1	0
48	J	301	3PE	6	0
50	L	601	CDL	13	0
49	M	501	PC1	2	0
50	M	502	CDL	2	0
49	N	401	PC1	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	k	1
9	N	1

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Mol	Chain	Number of breaks
19	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	174:VAL	C	175:PRO	N	1.18
1	N	304:MET	C	305:PHE	N	1.16
1	e	50:LEU	C	51:PRO	N	1.15