



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 13, 2018 – 02:03 PM EDT

PDB ID : 5O31
EMDB ID: : EMD-3731
Title : Mitochondrial complex I in the deactive state
Authors : Blaza, J.N.; Vinothkumar, K.R.; Hirst, J.
Deposited on : 2017-05-23
Resolution : 4.13 Å(reported)

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 : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

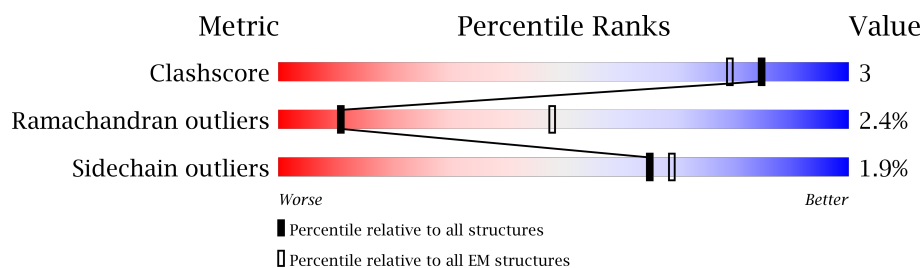
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.13 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.








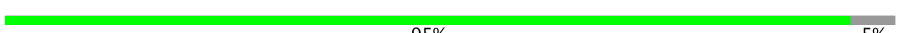













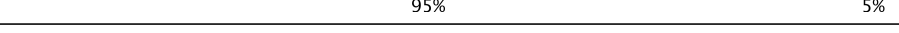
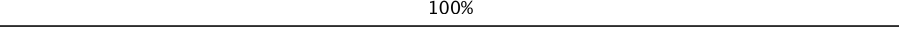
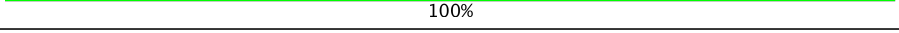
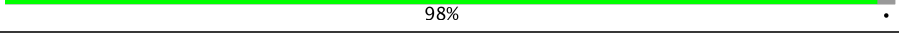

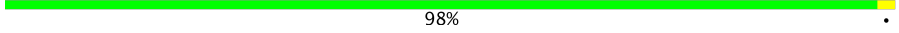
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	A	115	64% 11% • 23%
2	B	179	71% 8% • 18%
3	C	228	75% 14% 11%
4	D	430	84% 12% •
5	E	217	81% 5% 14%
6	F	464	87% • 8%
7	H	318	79% 14% 7%
8	I	176	84% 16% •
9	J	175	82% 15% ••




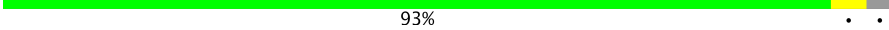


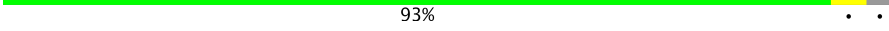




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Mol	Chain	Length	Quality of chain
10	K	98	 79% 18% .
11	L	606	 88% 11% .
12	M	459	 86% 12% .
13	N	347	 87% 12% .
14	O	320	 92% 6% .
15	P	297	 95% 5%
16	S	98	 82% 18%
17	T	88	 84% . 15%
17	U	88	 92% 5% .
18	V	115	 89% . 8%
19	W	128	 78% 8% . 13%
20	Y	141	 91% 6% ..
21	a	70	 89% . 9%
22	b	80	 99% .
23	c	49	 88% 6% 6%
24	e	105	 82% . 15%
25	f	57	 89% 5% 5%
26	g	125	 73% 5% 22%
27	i	111	 95% 5%
28	j	52	 100%
29	k	74	 100%
30	l	120	 98% .
31	o	136	 43% 57%
32	p	169	 98% .
33	q	145	 92% . 5%

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Mol	Chain	Length	Quality of chain
34	G	704	 92% 5% •
35	s	75	 53% • 45%
36	Q	133	 89% • 8%
37	R	96	 93% • •
38	r	112	 72% 6% 21%
39	h	143	 92% • 6%
40	d	116	 93% • •
41	X	171	 91% 5% • •
42	m	128	 87% 5% 8%
43	n	178	 88% 6% 7%
44	Z	144	 88% 6% • 5%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 52703 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	88	Total	C	N	O	S	0	0
			691	474	100	114	3		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	147	Total	C	N	O	S	0	0
			1159	740	203	202	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	204	Total	C	N	O	S	0	0
			1678	1086	286	303	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	416	Total	C	N	O	S	0	0
			3229	2056	560	589	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	conflict	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	186	Total	C	N	O	S	0	0
			1038	645	196	193	4		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	425	Total	C	N	O	S	0	0
			2441	1508	467	460	6		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	296	Total	C	N	O	S	0	0
			2312	1557	357	376	22		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	176	Total	C	N	O	S	0	0
			1388	875	239	264	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	171	Total	C	N	O	S	0	0
			1211	814	179	207	11		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	95	Total	C	N	O	S	0	0
			720	472	108	126	14		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	604	Total	C	N	O	S	0	0
			4538	3005	708	787	38		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	457	Total	C	N	O	S	0	0
			3549	2363	556	592	38		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	344	Total	C	N	O	S	0	0
			2592	1713	405	440	34		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	314	Total	C	N	O	S	0	0
			1941	1225	353	360	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	283	Total	C	N	O		0	0
			1415	849	283	283			

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	80	Total	C	N	O		0	0
			405	245	80	80			

- Molecule 17 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	75	Total	C	N	O		0	0
			378	228	75	75			
17	U	85	Total	C	N	O		0	0
			432	262	85	85			

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	106	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	111	Total	C	N	O	S	0	0
			817	516	154	144	3		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	138	Total	C	N	O	S	0	0
			1011	644	173	188	6		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	64	Total	C	N	O	S	0	0
			480	312	86	77	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	80	Total	C	N	O	S	0	0
			519	336	89	93	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	c	46	Total	C	N	O	0	0
			320	211	56	53		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	89	Total	C	N	O	S	0	0
			619	383	122	109	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	27	GLY	LYS	conflict	UNP Q02379

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	54	Total	C	N	O	S	0	0
			350	223	62	64	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	97	Total	C	N	O	S	0	0
			677	438	120	117	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	106	Total	C	N	O		0	0
			616	376	126	114			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	52	Total	C	N	O		0	0
			260	156	52	52			

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	k	74	Total	C	N	O		0	0
			370	222	74	74			

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	l	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	58	Total	C	N	O	S	0	0
			296	176	58	58	4		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	p	169	Total	C	N	O	S	0	0
			1039	633	198	202	6		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	q	138	Total	C	N	O	0	0
			696	420	138	138		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	G	688	Total	C	N	O	S	0	0
			4151	2549	792	786	24		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	s	41	Total	C	N	O	0	0
			234	148	42	44		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Q	123	Total	C	N	O	0	0
			749	476	143	130		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	93	Total	C	N	O	S	0	0
			638	399	124	112	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	r	88	Total	C	N	O	0	0
			575	363	116	96		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	h	134	Total	C	N	O	0	0
			822	527	153	142		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	113	Total	C	N	O	S	0	0
			803	519	145	136	3		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	X	164	Total	C	N	O	S	0	0
			1170	736	216	209	9		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	m	118	Total	C	N	O	0	0
			904	579	168	157		

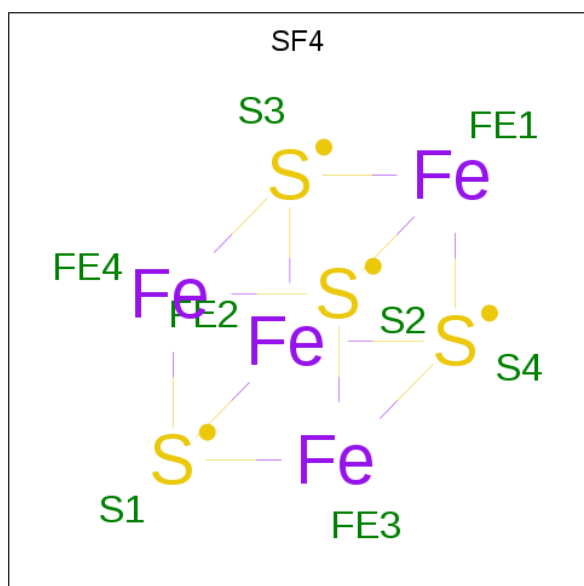
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	166	Total	C	N	O	S	0	0
			1124	707	217	197	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	137	Total	C	N	O	S	0	0
			920	575	171	167	7		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



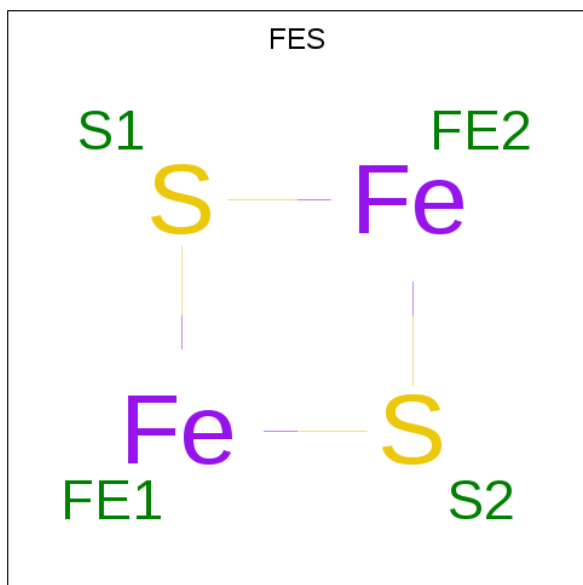
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			16	8	8	

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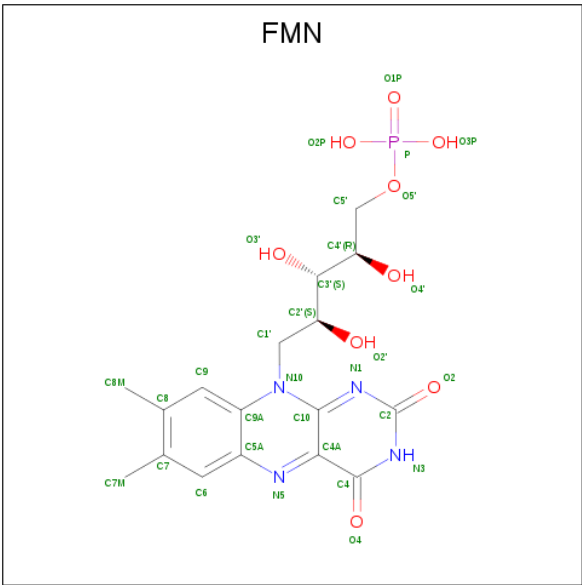
Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	Fe	S	0
			16	8	8	
45	G	1	Total	Fe	S	0
			16	8	8	
45	G	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



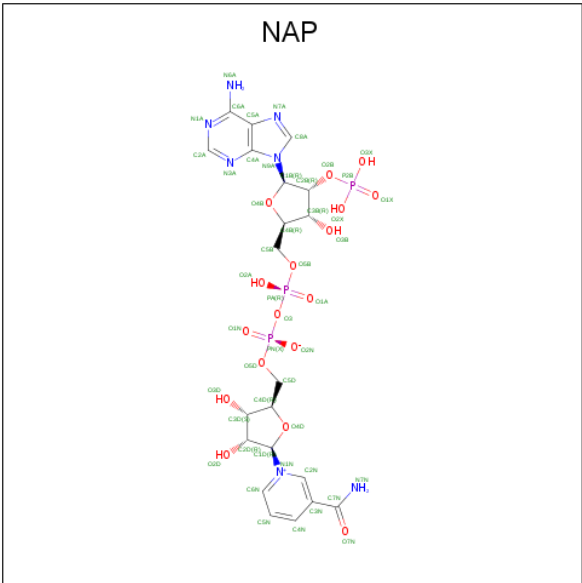
Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



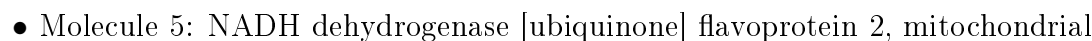
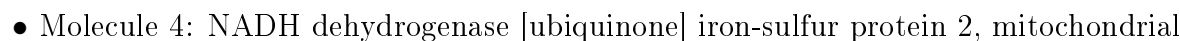
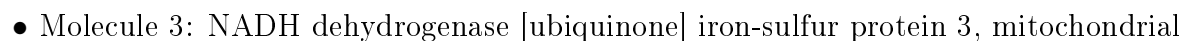
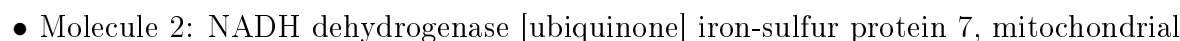
Mol	Chain	Residues	Atoms					AltConf
47	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms		AltConf
49	R	1	Total 1	Zn 1	0

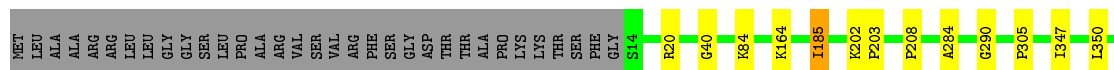
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3





- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 87% 8%



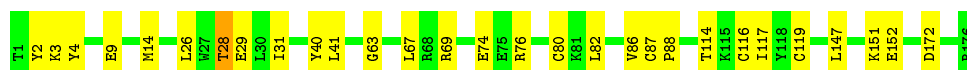
- Molecule 7: NADH-ubiquinone oxidoreductase chain 1

Chain H: 79% 14% 7%



- Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I: 84% 16%



- Molecule 9: NADH-ubiquinone oxidoreductase chain 6

Chain J: 82% 15%



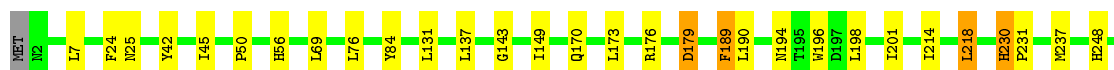
- Molecule 10: NADH-ubiquinone oxidoreductase chain 4L

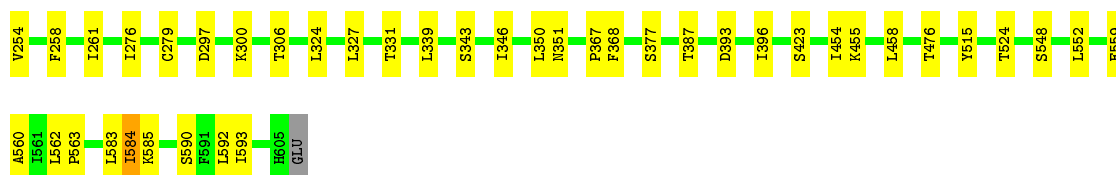
Chain K: 79% 18%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 5

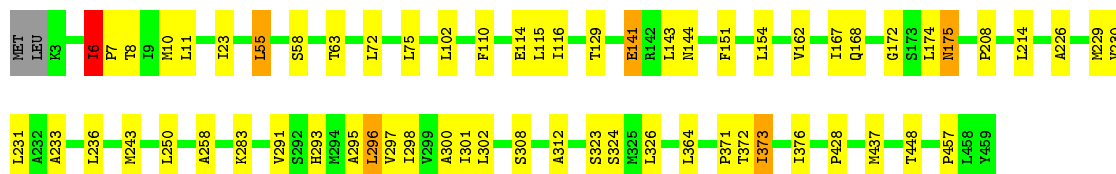
Chain L: 88% 11%





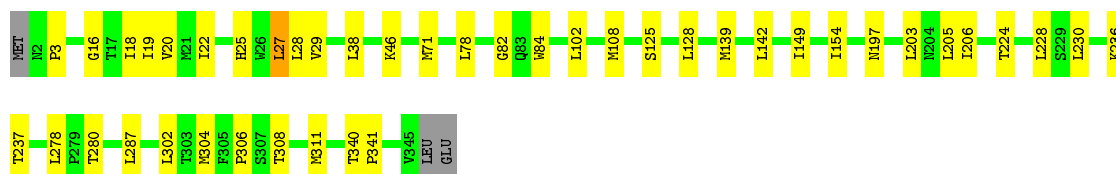
- Molecule 12: NADH-ubiquinone oxidoreductase chain 4

Chain M: 86% 12%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 2

Chain N: 87% 12%



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 92% 6%



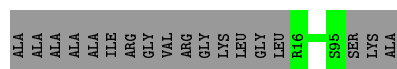
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9

Chain P: 95% 5%



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 82% 18%



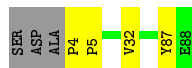
- Molecule 17: Acyl carrier protein, mitochondrial

Chain T: 84% 15%



- Molecule 17: Acyl carrier protein, mitochondrial

Chain U: 92% 5%



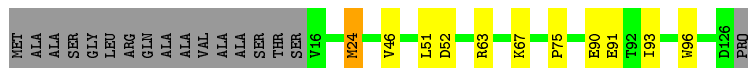
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V: 89% 8%



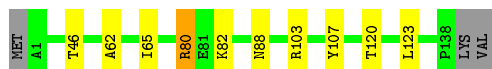
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W: 78% 8% 13%



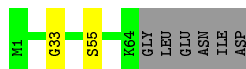
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y: 91% 6%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a: 89% 9%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 99%



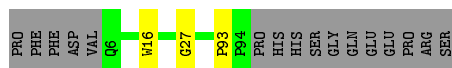
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c: 88% 6% 6%



- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 82% 15%



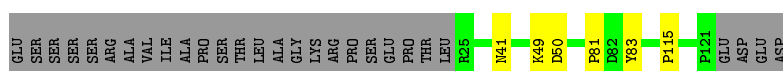
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 89% 5% 5%



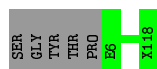
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 73% 5% 22%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 95% 5%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

Chain j: 100%

There are no outlier residues recorded for this chain.

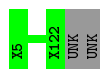
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8

Chain l: 98%



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  43% 57%

GLY ALA HIS LEU LEU ALA ARG ARG TYR GLY GLY ASP GLY ALA SER VAL GLU PRO ALA ASP PRO GLU LEU ARG MET THR PRO PHE PRO ASP TYR GLY PHE PRO GLU ARG LYS GLU ARG GLU MET VAL ALA THR GLN GLN MET ASP ASP ALA GLN LEU VAL GLN GLN ASP ASP Y67 R114 GLU

GLN ARG GLU ALA ASP MET LYS LYS GLY GLY PRO GLY GLU VAL ALA PRO GLU VAL ALA LEU

- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  98% .

Y4 E78 H120 G124 X172

- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  92% 5% .

MET E2 Y44 G45 Q54 G70 P84 P139 PRO SER THR PRO TYR LYS

- Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  92% 5% .

THR ALA THR ALA S6 N7 L27 K32 R39 F40 C41 Y42 H43 L46 A68 M74 M77 N100 H101 P102 I107 D126 R129 K134 R135 K147 T148 I149 A163 A167 I202 A214 F215 P219 A233 N237 R249


R253 R254 R255 I258 N259 W262 L358 A388 R396 S411 R418 E693 GLY ALA HIS LYS VAL GLU GLU PRO SER ILE CYS

- Molecule 35: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  53% 45% .

SER ALA GLU SER GLY LYS ASN GLU LYS GLY LEU PRO PRO ASN PRO LYS LYS GLN SER PRO PRO PHE D34 S68 F74 HIS

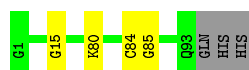
- Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  89% 8% .

ALA GLN ASP GLN THR ARG ASP THR GLN LEU I111 E28 R55 P78 P86 K133

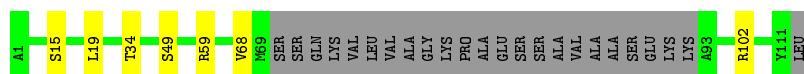
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  93%



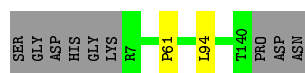
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  72% 6% 21%



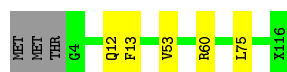
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:  92% 6%




- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  93%




- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  91% 5%




- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  87% 5% 8%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  88% 6% 7%

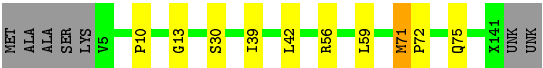


- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

88%

6% • 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	125006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was done per particle after the CTF was estimated on the whole micrograph.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	101499	Depositor
Image detector	FEI FALCON II (4k x 4k)	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: FMN, ZN, SF4, NAP, FES

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	A	0.43	0/706	0.63	0/967
10	K	0.39	0/730	0.64	0/988
11	L	0.43	0/4653	0.59	0/6350
12	M	0.41	0/3638	0.62	0/4967
13	N	0.41	0/2656	0.61	0/3630
14	O	0.39	0/1983	0.53	0/2742
16	S	0.32	0/408	0.49	0/571
17	T	0.31	0/380	0.49	0/531
17	U	0.31	0/436	0.50	0/610
18	V	0.37	0/713	0.53	0/977
19	W	0.39	0/831	0.56	0/1128
2	B	0.39	0/1187	0.63	0/1607
20	Y	0.42	0/1031	0.55	0/1400
21	a	0.44	0/494	0.56	0/669
22	b	0.43	0/352	0.56	0/481
23	c	0.44	0/330	0.58	0/455
24	e	0.38	0/630	0.55	0/851
25	f	0.42	0/356	0.56	0/488
26	g	0.46	0/696	0.63	0/957
27	i	0.36	0/224	0.57	0/300
3	C	0.43	0/1728	0.61	0/2353
31	o	0.32	0/296	0.48	0/412
32	p	0.38	0/535	0.53	0/718
33	q	0.36	0/704	0.59	0/984
34	G	0.36	0/4212	0.53	0/5789
35	s	0.40	0/238	0.55	0/332
36	Q	0.39	0/768	0.52	0/1066
37	R	0.39	0/649	0.52	0/879
38	r	0.43	0/594	0.58	0/824
39	h	0.38	0/837	0.53	0/1157
4	D	0.39	0/3304	0.59	0/4478
40	d	0.45	0/730	0.54	0/992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
41	X	0.41	0/1200	0.56	0/1634
42	m	0.42	0/926	0.58	0/1260
43	n	0.39	0/1163	0.52	0/1586
44	Z	0.39	0/718	0.55	0/967
5	E	0.38	0/1062	0.54	0/1484
6	F	0.37	0/2488	0.51	0/3434
7	H	0.42	0/2378	0.60	0/3250
8	I	0.41	0/1419	0.63	0/1925
9	J	0.45	0/1239	0.55	0/1688
All	All	0.40	0/49622	0.57	0/67881

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
12	M	0	1
2	B	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
2	B	149	CYS	Peptide
12	M	6	ILE	Peptide

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	A	691	0	728	9	0
2	B	1159	0	1166	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1678	0	1612	17	0
4	D	3229	0	3123	30	0
5	E	1038	0	623	2	0
6	F	2441	0	1628	5	0
7	H	2312	0	2426	23	0
8	I	1388	0	1323	11	0
9	J	1211	0	1165	14	0
10	K	720	0	761	13	0
11	L	4538	0	4480	32	0
12	M	3549	0	3674	31	0
13	N	2592	0	2632	21	0
14	O	1941	0	1366	4	0
15	P	1415	0	303	0	0
16	S	405	0	197	0	0
17	T	378	0	176	0	0
17	U	432	0	207	1	0
18	V	700	0	582	1	0
19	W	817	0	743	5	0
20	Y	1011	0	1020	3	0
21	a	480	0	440	0	0
22	b	519	0	408	0	0
23	c	320	0	277	0	0
24	e	619	0	513	0	0
25	f	350	0	260	0	0
26	g	677	0	559	0	0
27	i	616	0	300	0	0
28	j	260	0	58	0	0
29	k	370	0	77	0	0
30	l	590	0	125	0	0
31	o	296	0	134	0	0
32	p	1039	0	582	0	0
33	q	696	0	338	0	0
34	G	4151	0	3048	16	0
35	s	234	0	138	0	0
36	Q	749	0	496	1	0
37	R	638	0	565	1	0
38	r	575	0	425	0	0
39	h	822	0	644	0	0
40	d	803	0	659	0	0
41	X	1170	0	969	3	0
42	m	904	0	832	0	0
43	n	1124	0	862	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Z	920	0	704	7	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	E	4	0	0	0	0
46	G	4	0	0	0	0
47	F	31	0	19	0	0
48	P	48	0	25	0	0
49	R	1	0	0	0	0
All	All	52703	0	43392	220	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 3.

The worst 5 of 220 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)
44:Z:71:MET:H	44:Z:72:PRO:HD2	1.55	0.71
4:D:112:MET:H	4:D:145:THR:HG21	1.59	0.68
11:L:189:PHE:HB3	11:L:196:TRP:HB3	1.77	0.66
5:E:152:PRO:HD2	5:E:163:ASP:HA	1.81	0.62
12:M:143:LEU:HD21	13:N:302:LEU:HD11	1.82	0.61

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	A	84/115 (73%)	79 (94%)	4 (5%)	1 (1%)	15 57
2	B	145/179 (81%)	124 (86%)	19 (13%)	2 (1%)	13 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	202/228 (89%)	175 (87%)	23 (11%)	4 (2%)	9	48
4	D	412/430 (96%)	364 (88%)	41 (10%)	7 (2%)	11	51
5	E	184/217 (85%)	157 (85%)	20 (11%)	7 (4%)	4	34
6	F	423/464 (91%)	381 (90%)	33 (8%)	9 (2%)	8	47
7	H	292/318 (92%)	264 (90%)	20 (7%)	8 (3%)	6	41
8	I	174/176 (99%)	144 (83%)	22 (13%)	8 (5%)	3	30
9	J	169/175 (97%)	150 (89%)	13 (8%)	6 (4%)	4	35
10	K	93/98 (95%)	87 (94%)	5 (5%)	1 (1%)	17	59
11	L	602/606 (99%)	535 (89%)	54 (9%)	13 (2%)	8	46
12	M	455/459 (99%)	412 (90%)	32 (7%)	11 (2%)	7	44
13	N	342/347 (99%)	311 (91%)	26 (8%)	5 (2%)	12	53
14	O	312/320 (98%)	277 (89%)	24 (8%)	11 (4%)	4	36
16	S	78/98 (80%)	75 (96%)	3 (4%)	0	100	100
17	T	73/88 (83%)	66 (90%)	6 (8%)	1 (1%)	13	53
17	U	83/88 (94%)	72 (87%)	9 (11%)	2 (2%)	7	44
18	V	104/115 (90%)	88 (85%)	15 (14%)	1 (1%)	18	61
19	W	109/128 (85%)	93 (85%)	14 (13%)	2 (2%)	10	50
20	Y	136/141 (96%)	125 (92%)	7 (5%)	4 (3%)	5	40
21	a	62/70 (89%)	58 (94%)	2 (3%)	2 (3%)	5	38
22	b	44/80 (55%)	38 (86%)	6 (14%)	0	100	100
23	c	44/49 (90%)	41 (93%)	0	3 (7%)	1	21
24	e	87/105 (83%)	78 (90%)	7 (8%)	2 (2%)	7	45
25	f	52/57 (91%)	46 (88%)	3 (6%)	3 (6%)	2	25
26	g	95/125 (76%)	72 (76%)	17 (18%)	6 (6%)	1	24
27	i	25/111 (22%)	23 (92%)	2 (8%)	0	100	100
31	o	56/136 (41%)	50 (89%)	6 (11%)	0	100	100
32	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	3	30
33	q	136/145 (94%)	111 (82%)	20 (15%)	5 (4%)	4	35
34	G	686/704 (97%)	621 (90%)	59 (9%)	6 (1%)	20	62
35	s	39/75 (52%)	34 (87%)	4 (10%)	1 (3%)	6	42
36	Q	121/133 (91%)	107 (88%)	12 (10%)	2 (2%)	11	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	R	91/96 (95%)	79 (87%)	10 (11%)	2 (2%)	8	46
38	r	84/112 (75%)	66 (79%)	13 (16%)	5 (6%)	2	24
39	h	132/143 (92%)	111 (84%)	20 (15%)	1 (1%)	22	65
40	d	93/116 (80%)	84 (90%)	6 (6%)	3 (3%)	5	38
41	X	162/171 (95%)	142 (88%)	16 (10%)	4 (2%)	6	43
42	m	116/128 (91%)	93 (80%)	18 (16%)	5 (4%)	3	31
43	n	164/178 (92%)	135 (82%)	19 (12%)	10 (6%)	2	24
44	Z	93/144 (65%)	82 (88%)	8 (9%)	3 (3%)	5	38
All	All	6921/7837 (88%)	6110 (88%)	642 (9%)	169 (2%)	11	44

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	PRO
3	C	12	ARG
4	D	388	ARG
6	F	423	ARG
7	H	92	PRO

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	A	73/101 (72%)	69 (94%)	4 (6%)	25	61
2	B	124/150 (83%)	116 (94%)	8 (6%)	20	55
3	C	179/204 (88%)	175 (98%)	4 (2%)	57	80
4	D	332/371 (90%)	327 (98%)	5 (2%)	70	86
5	E	36/183 (20%)	36 (100%)	0	100	100
6	F	97/368 (26%)	92 (95%)	5 (5%)	27	62
7	H	250/275 (91%)	248 (99%)	2 (1%)	85	92
8	I	143/151 (95%)	138 (96%)	5 (4%)	41	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	112/142 (79%)	109 (97%)	3 (3%)	50	75
10	K	83/86 (96%)	81 (98%)	2 (2%)	54	78
11	L	463/534 (87%)	454 (98%)	9 (2%)	62	83
12	M	387/413 (94%)	381 (98%)	6 (2%)	68	85
13	N	277/316 (88%)	273 (99%)	4 (1%)	71	86
14	O	102/283 (36%)	101 (99%)	1 (1%)	80	90
16	S	4/81 (5%)	4 (100%)	0	100	100
17	T	3/81 (4%)	3 (100%)	0	100	100
17	U	5/81 (6%)	5 (100%)	0	100	100
18	V	49/101 (48%)	48 (98%)	1 (2%)	60	82
19	W	71/114 (62%)	71 (100%)	0	100	100
20	Y	99/102 (97%)	98 (99%)	1 (1%)	80	90
21	a	41/59 (70%)	41 (100%)	0	100	100
22	b	36/36 (100%)	35 (97%)	1 (3%)	49	74
23	c	26/45 (58%)	26 (100%)	0	100	100
24	e	46/94 (49%)	45 (98%)	1 (2%)	57	80
25	f	22/54 (41%)	22 (100%)	0	100	100
26	g	51/112 (46%)	51 (100%)	0	100	100
27	i	20/31 (64%)	20 (100%)	0	100	100
31	o	5/119 (4%)	5 (100%)	0	100	100
32	p	50/62 (81%)	50 (100%)	0	100	100
33	q	9/131 (7%)	9 (100%)	0	100	100
34	G	226/588 (38%)	221 (98%)	5 (2%)	57	80
35	s	9/69 (13%)	9 (100%)	0	100	100
36	Q	31/119 (26%)	31 (100%)	0	100	100
37	R	52/79 (66%)	51 (98%)	1 (2%)	62	83
38	r	32/96 (33%)	30 (94%)	2 (6%)	21	56
39	h	45/124 (36%)	44 (98%)	1 (2%)	57	80
40	d	62/84 (74%)	60 (97%)	2 (3%)	44	72
41	X	95/154 (62%)	95 (100%)	0	100	100
42	m	79/114 (69%)	77 (98%)	2 (2%)	53	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	n	78/160 (49%)	78 (100%)	0	100	100
44	Z	63/83 (76%)	63 (100%)	0	100	100
All	All	3967/6550 (61%)	3892 (98%)	75 (2%)	65	83

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	52	LEU
11	L	237	MET
38	r	102	ARG
9	J	77	GLU
11	L	179	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	248	HIS
13	N	289	ASN
42	m	78	ASN
12	M	144	ASN
13	N	36	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	B	201	2	0,12,12	0.00	-	0,24,24	0.00	-
46	FES	E	301	5	0,4,4	0.00	-	0,4,4	0.00	-
47	FMN	F	501	-	31,33,33	1.83	6 (19%)	38,50,50	2.12	8 (21%)
45	SF4	F	502	6	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	G	801	34	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	G	802	34	0,12,12	0.00	-	0,24,24	0.00	-
46	FES	G	803	34	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	I	201	8	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	I	202	8	0,12,12	0.00	-	0,24,24	0.00	-
48	NAP	P	501	-	44,52,52	0.93	2 (4%)	51,80,80	1.39	5 (9%)

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	B	201	2	-	0/0/48/48	0/6/5/5
46	FES	E	301	5	-	0/0/4/4	0/1/1/1
47	FMN	F	501	-	-	0/16/18/18	0/3/3/3
45	SF4	F	502	6	-	0/0/48/48	0/6/5/5
45	SF4	G	801	34	-	0/0/48/48	0/6/5/5
45	SF4	G	802	34	-	0/0/48/48	0/6/5/5
46	FES	G	803	34	-	0/0/4/4	0/1/1/1
45	SF4	I	201	8	-	0/0/48/48	0/6/5/5
45	SF4	I	202	8	-	0/0/48/48	0/6/5/5
48	NAP	P	501	-	-	0/27/67/67	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	P	501	NAP	C2A-N3A	2.02	1.35	1.32
47	F	501	FMN	C10-N1	2.21	1.36	1.33
48	P	501	NAP	C5A-C4A	3.37	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	501	FMN	C9A-N10	3.56	1.43	1.38
47	F	501	FMN	C8-C7	3.80	1.50	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	P	501	NAP	N3A-C2A-N1A	-6.70	123.03	128.86
47	F	501	FMN	C4-C4A-C10	-3.70	116.97	119.96
47	F	501	FMN	C4A-C4-N3	-3.43	118.59	123.48
48	P	501	NAP	C4A-C5A-N7A	-2.80	106.70	109.41
48	P	501	NAP	C4B-O4B-C1B	2.08	111.98	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
15	P	2
27	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	186:UNK	C	200:UNK	N	21.75
1	P	252:UNK	C	280:UNK	N	19.92
1	i	32:PRO	C	40:UNK	N	15.54