



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:46 PM UTC

PDB ID : 5O31 / pdb_00005o31
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

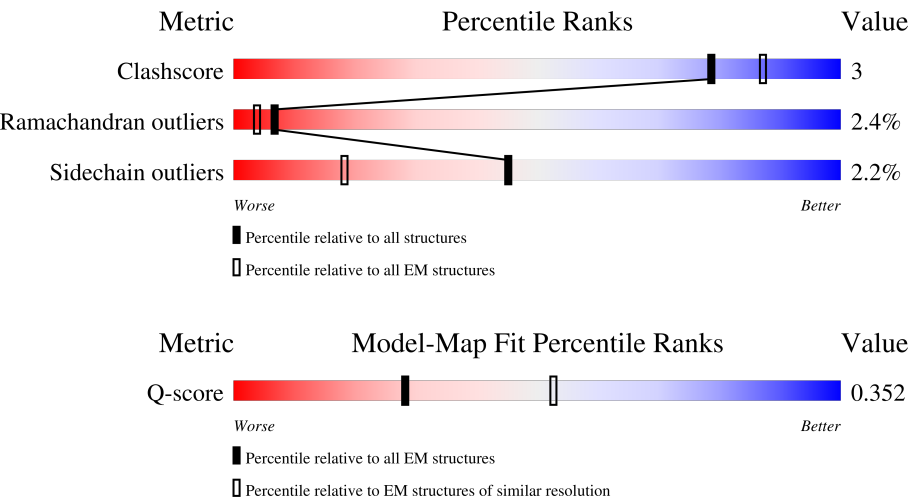
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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.



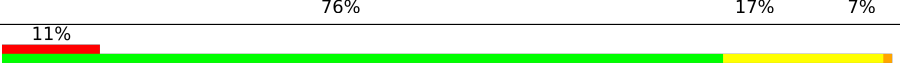
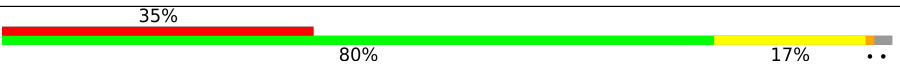
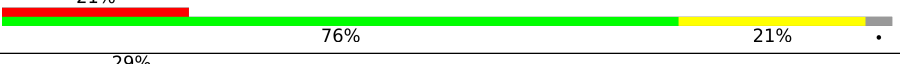
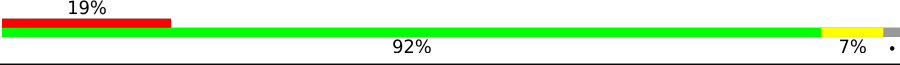
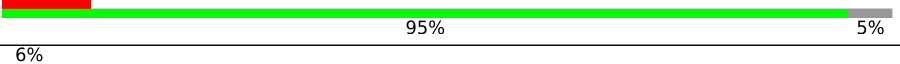
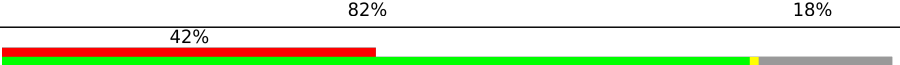
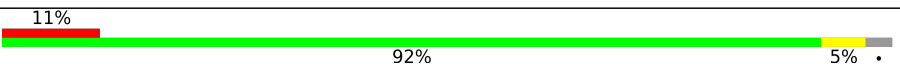
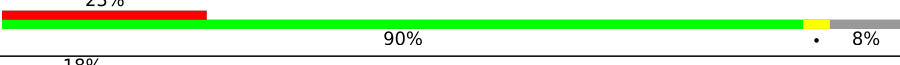
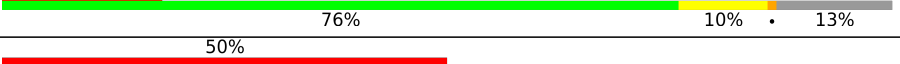
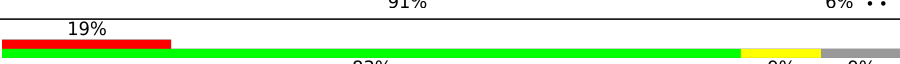
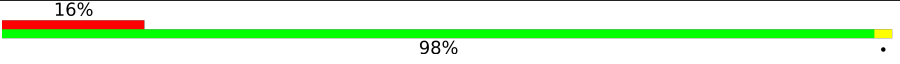
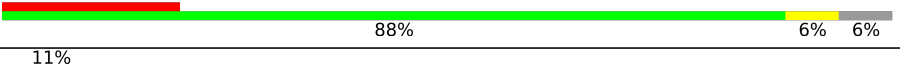
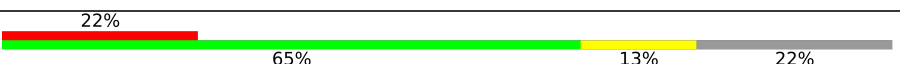
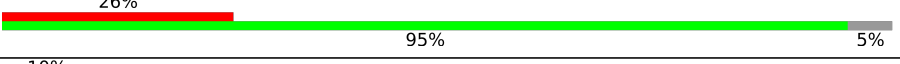
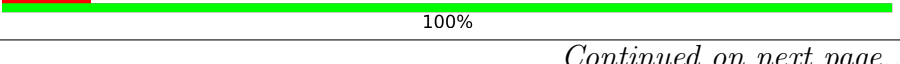
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5607 (3.63 - 4.63)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	23% 63% 13% • 23%
2	B	179	8% 72% 8% • 18%
3	C	228	11% 75% 14% 11%
4	D	430	18% 83% 13% ••

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Mol	Chain	Length	Quality of chain
5	E	217	
6	F	464	
7	H	318	
8	I	176	
9	J	175	
10	K	98	
11	L	606	
12	M	459	
13	N	347	
14	O	320	
15	P	297	
16	S	98	
17	T	88	
17	U	88	
18	V	115	
19	W	128	
20	Y	141	
21	a	70	
22	b	80	
23	c	49	
24	e	105	
25	f	57	
26	g	125	
27	i	111	
28	j	52	

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Mol	Chain	Length	Quality of chain
29	k	74	
30	l	120	
31	o	136	
32	p	169	
33	q	145	
34	G	704	
35	s	75	
36	Q	133	
37	R	96	
38	r	112	
39	h	143	
40	d	116	
41	X	171	
42	m	128	
43	n	178	
44	Z	144	

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		

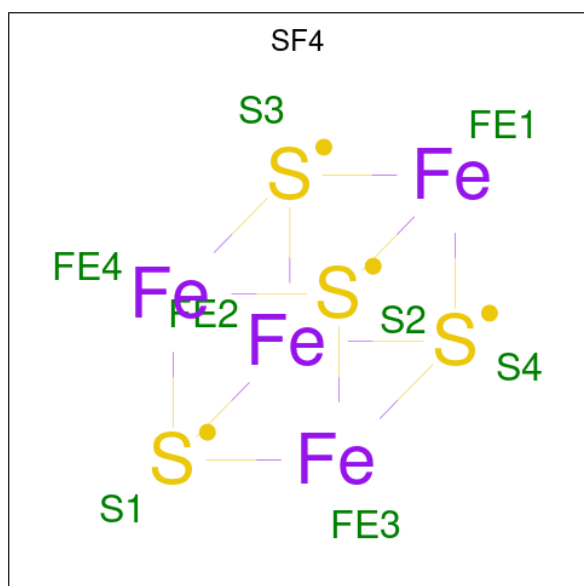
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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 (CCD ID: SF4) (formula: Fe₄S₄).



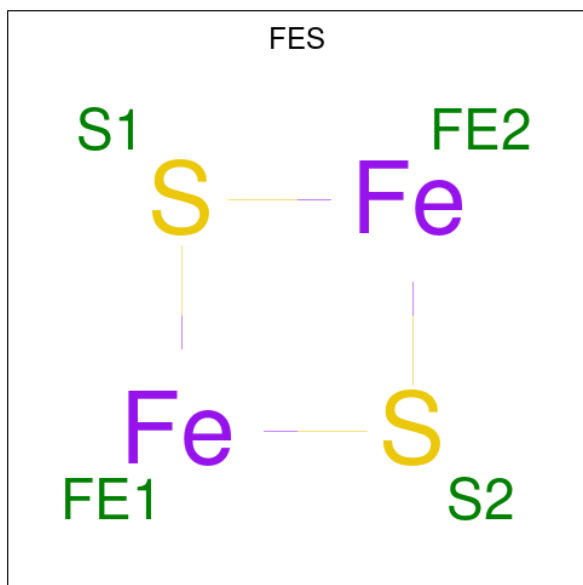
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

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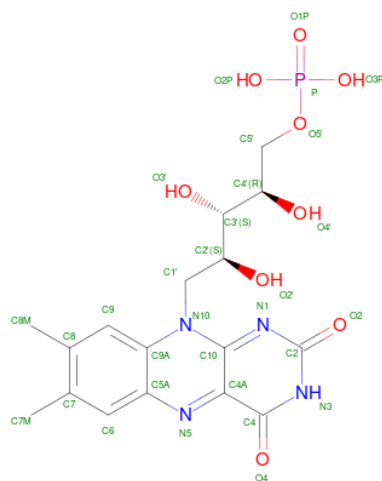
Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



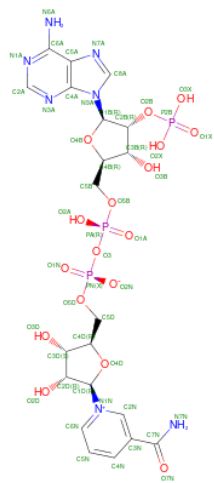
Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (CCD ID: 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 31	C 17	N 4	O 9	P 1	0

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



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

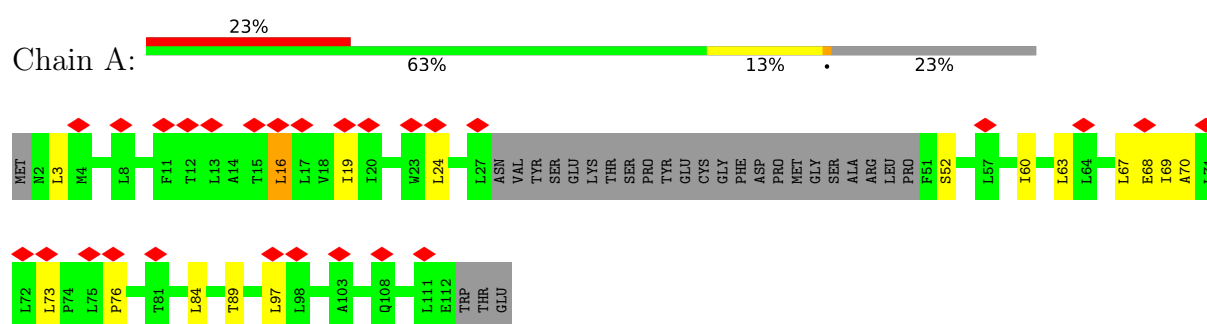
- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

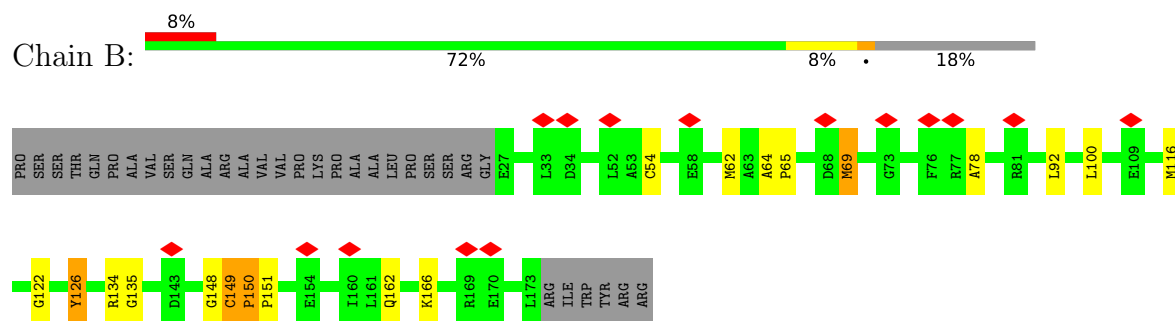
3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

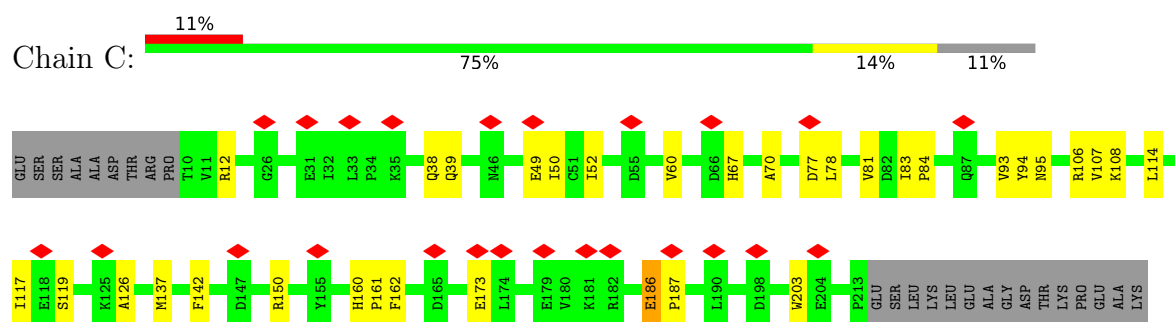
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



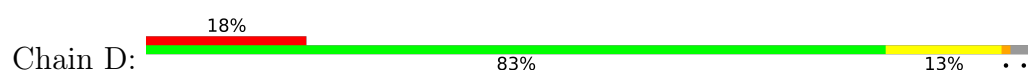
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

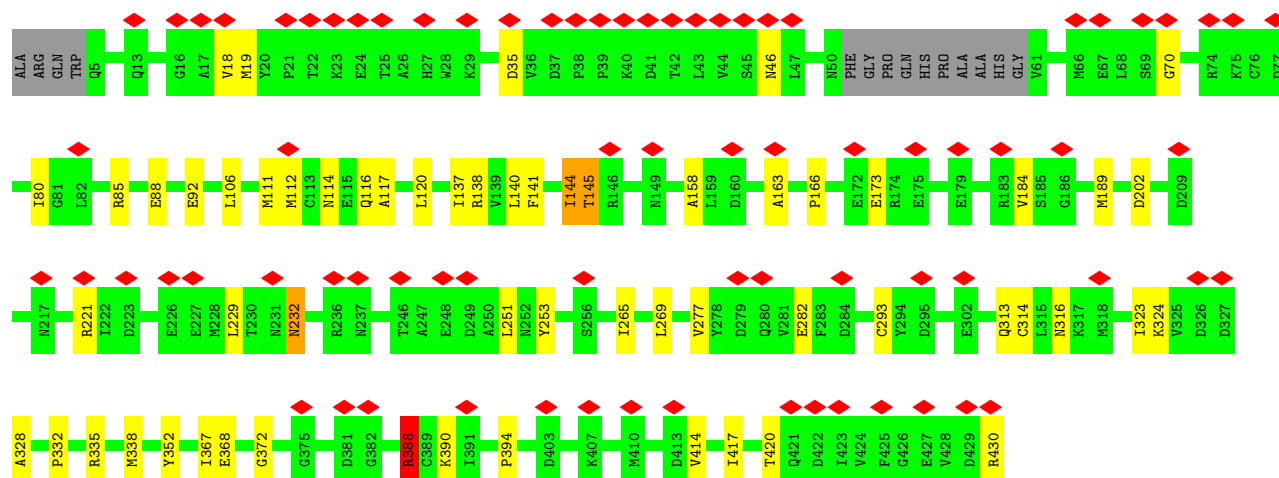


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

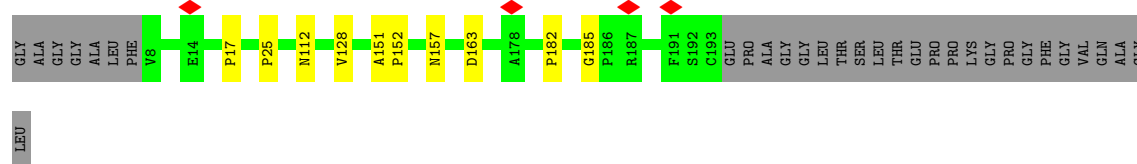
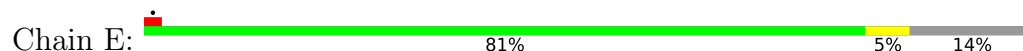


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

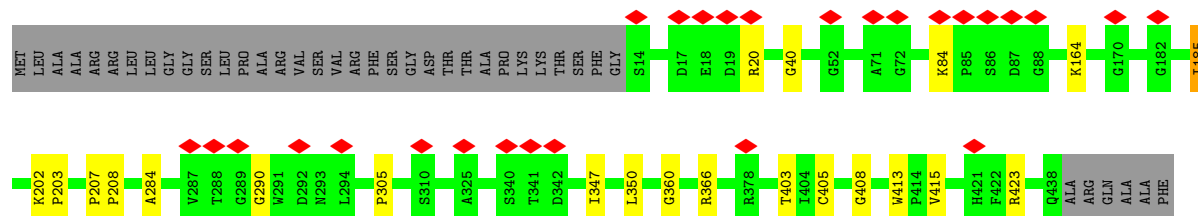
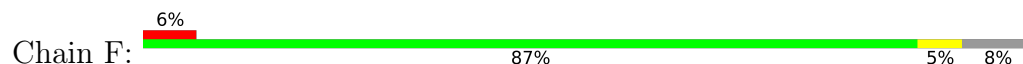




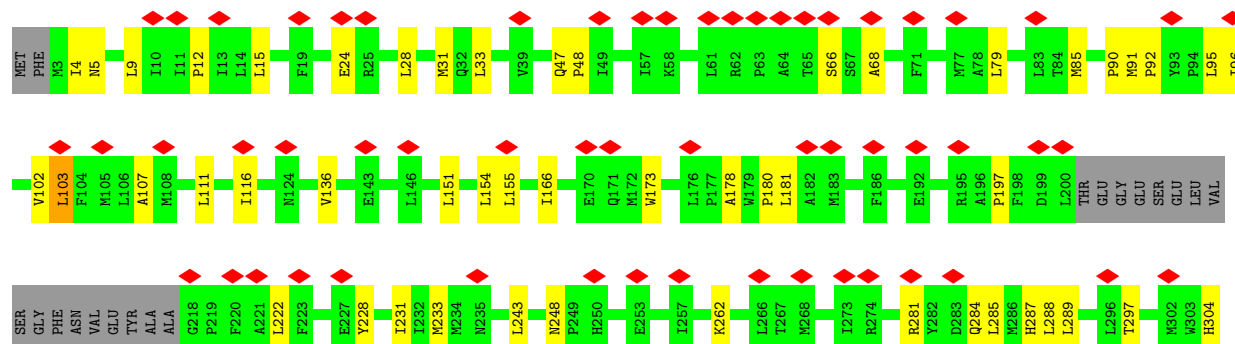
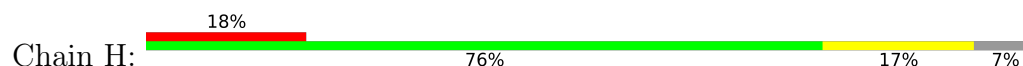
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



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

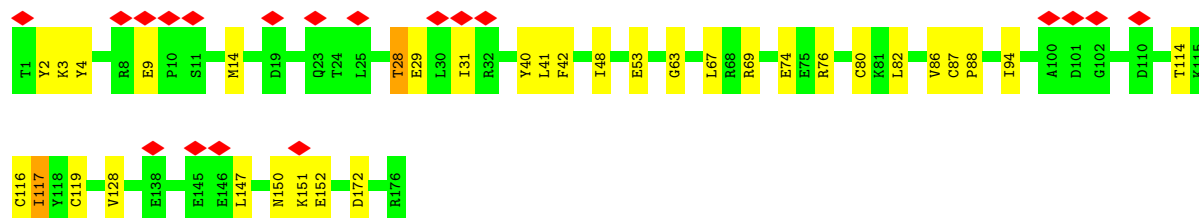
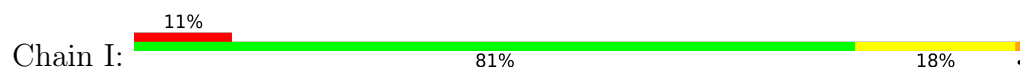


- Molecule 7: NADH-ubiquinone oxidoreductase chain 1

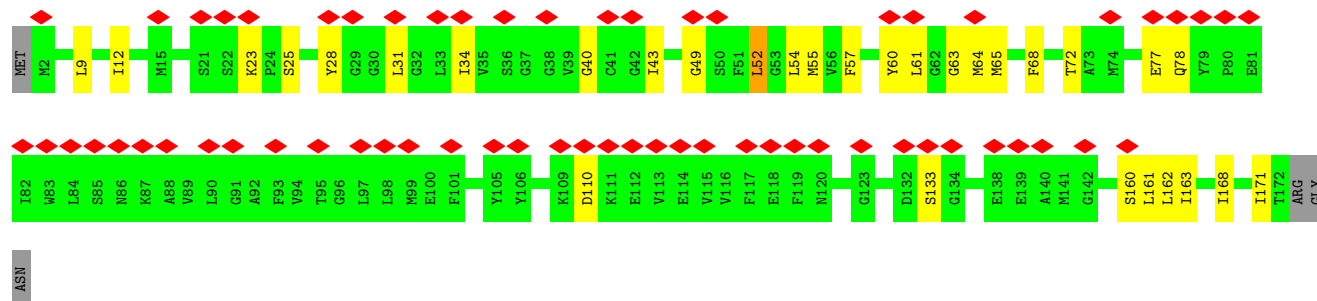
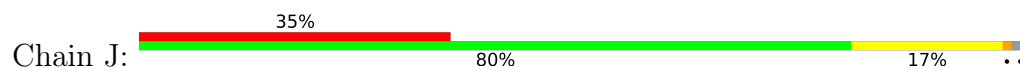




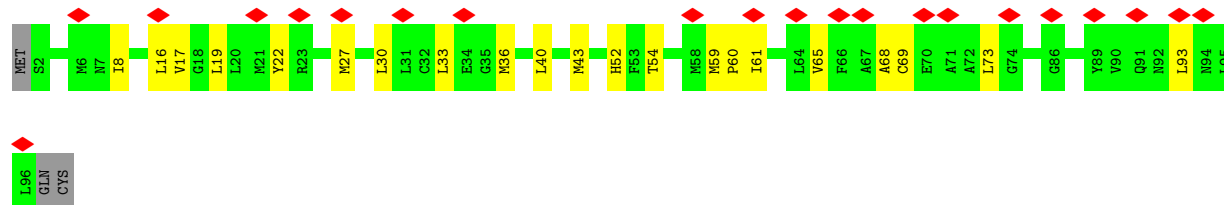
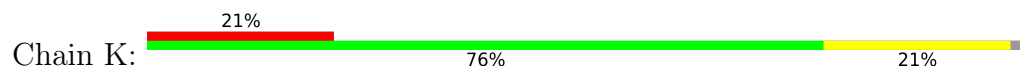
- Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



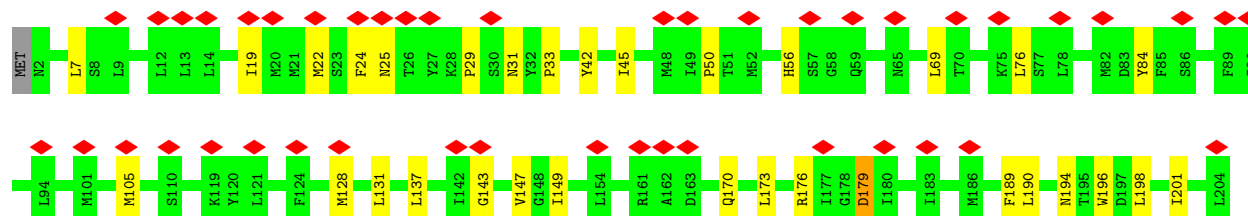
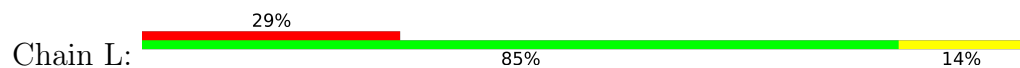
- Molecule 9: NADH-ubiquinone oxidoreductase chain 6

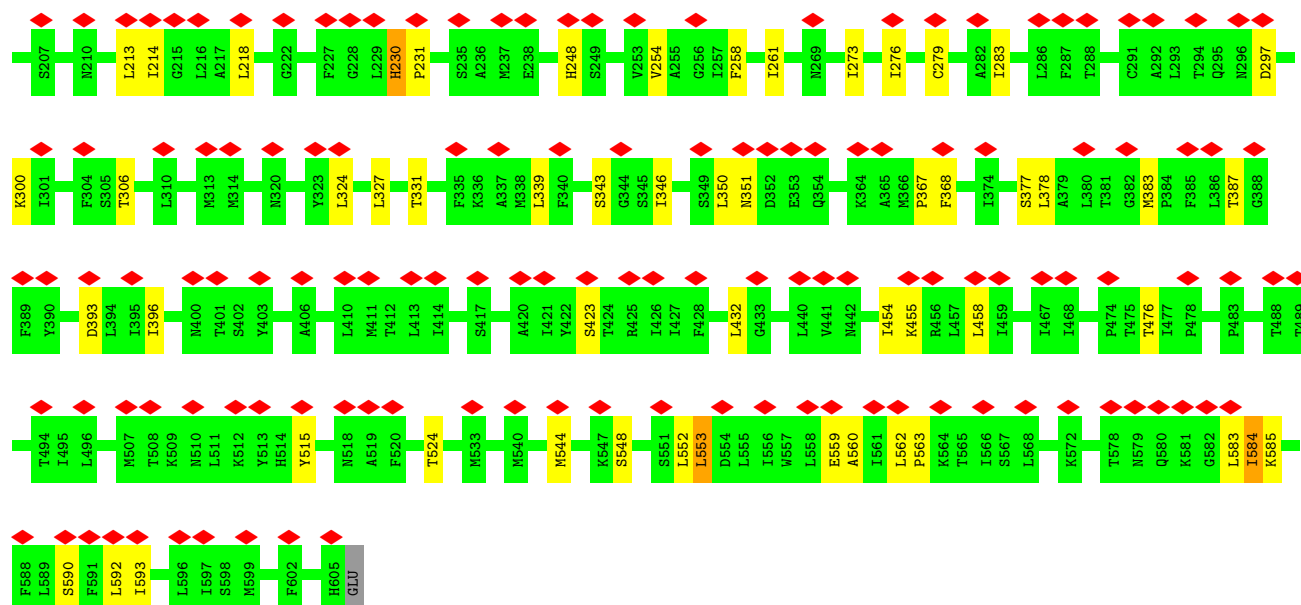


- Molecule 10: NADH-ubiquinone oxidoreductase chain 4L

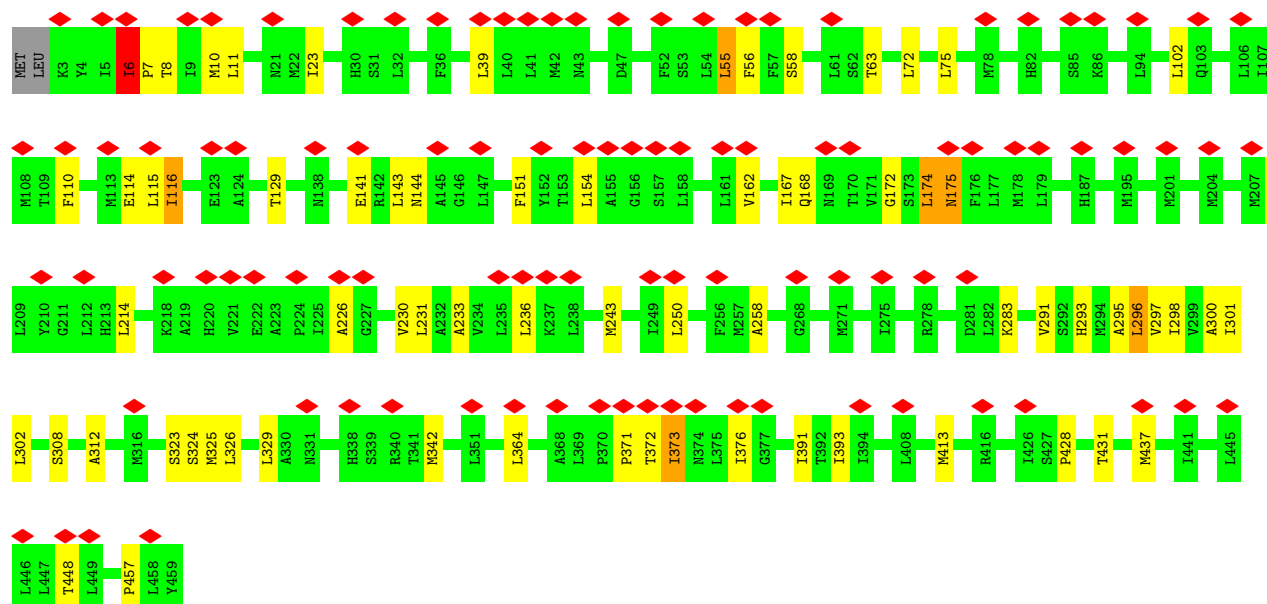
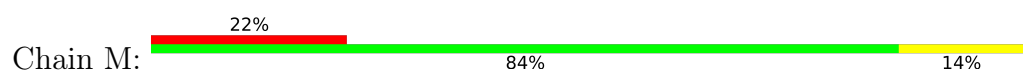


- Molecule 11: NADH-ubiquinone oxidoreductase chain 5

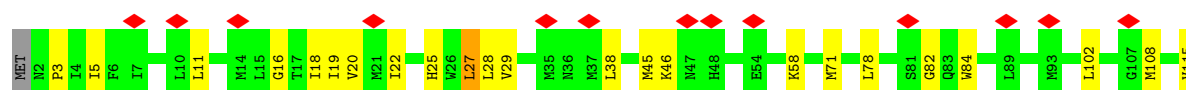
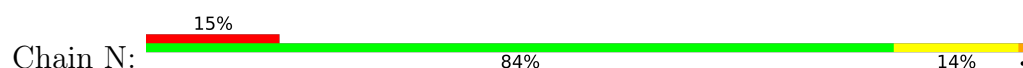


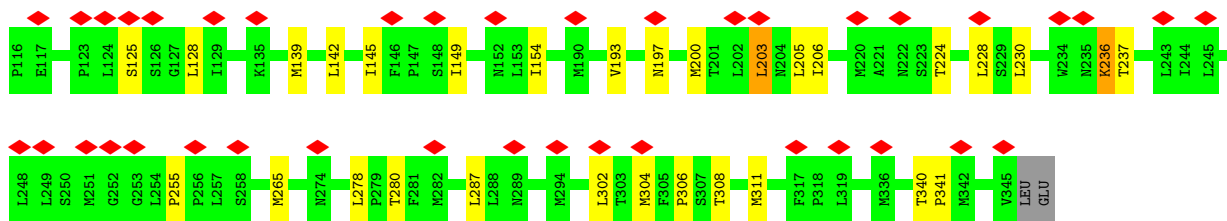


• Molecule 12: NADH-ubiquinone oxidoreductase chain 4

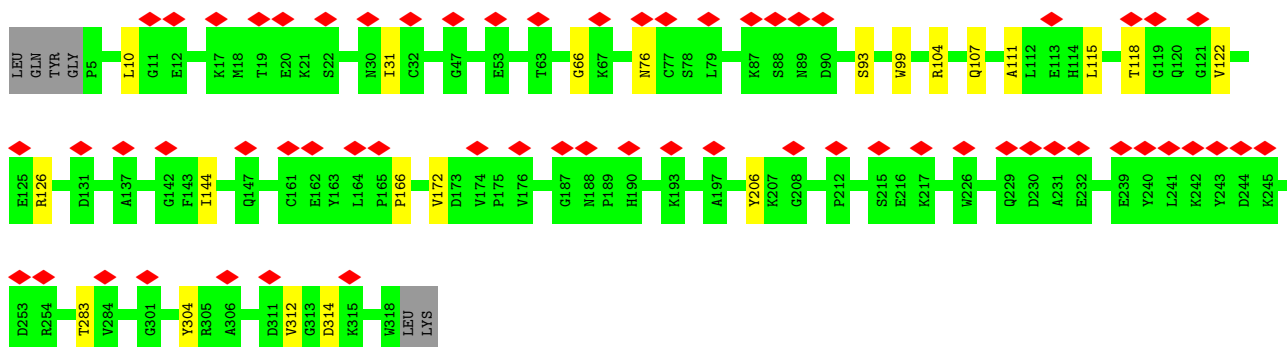
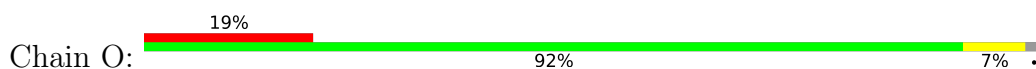


• Molecule 13: NADH-ubiquinone oxidoreductase chain 2

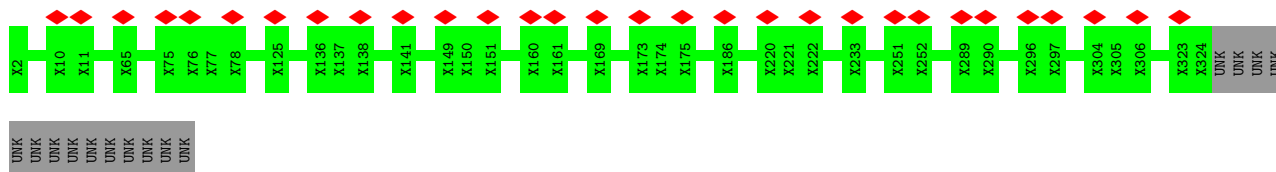




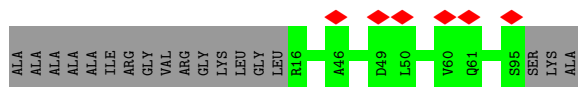
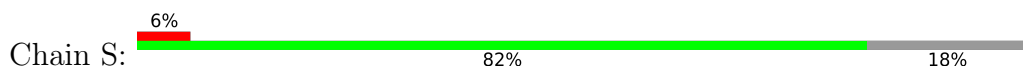
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



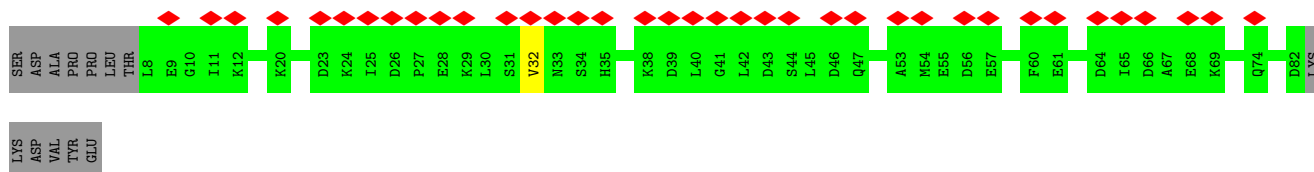
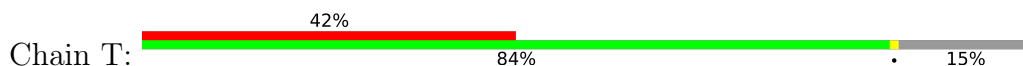
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9



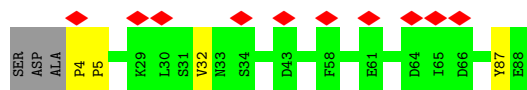
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



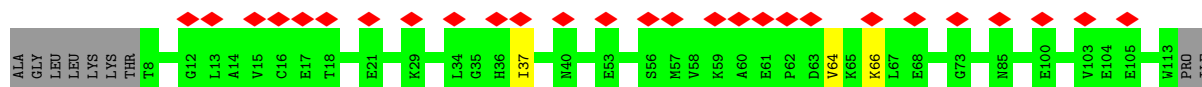
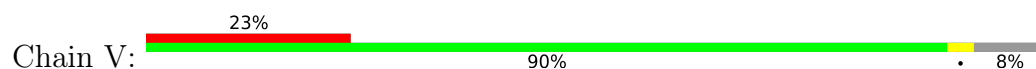
- Molecule 17: Acyl carrier protein, mitochondrial



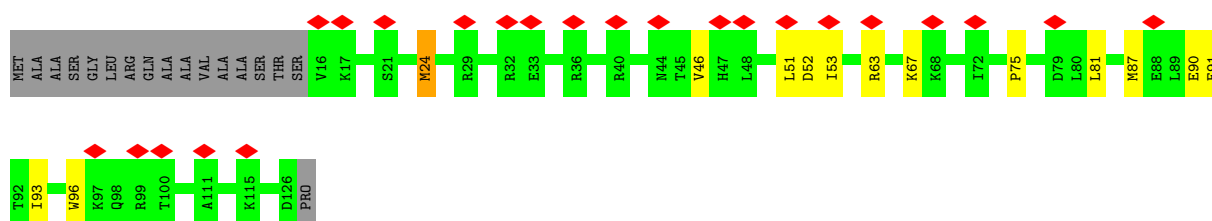
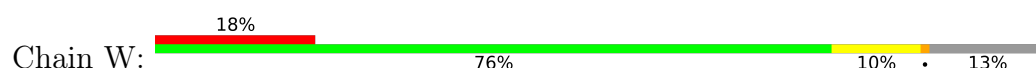
- Molecule 17: Acyl carrier protein, mitochondrial



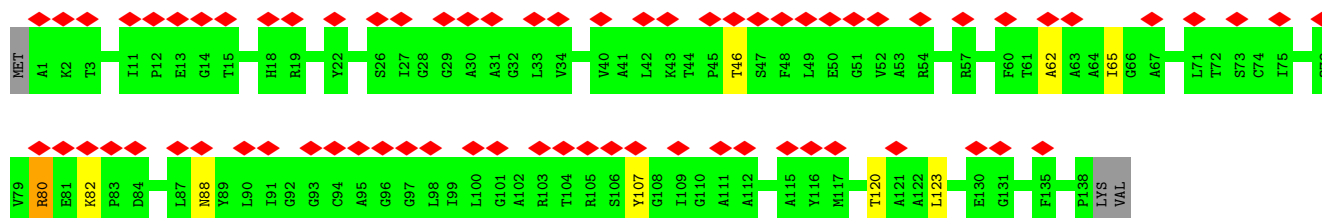
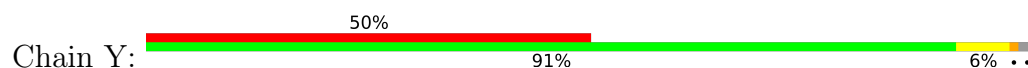
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



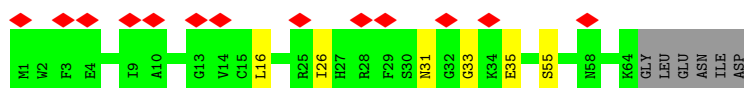
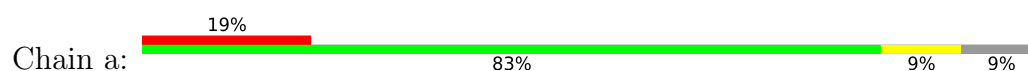
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

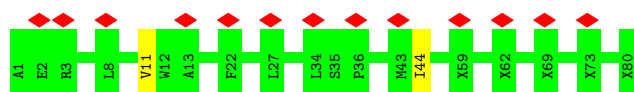


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

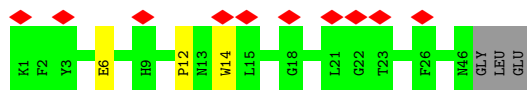
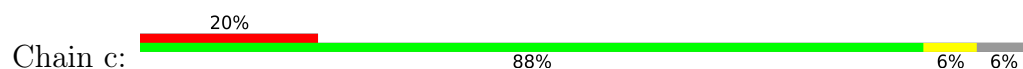


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

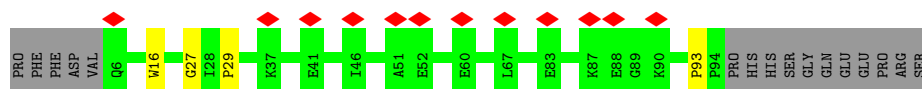
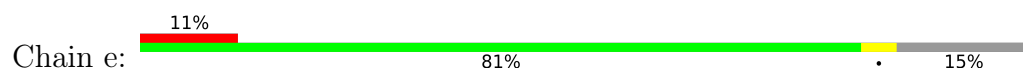




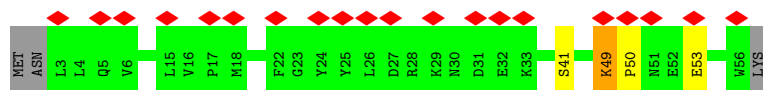
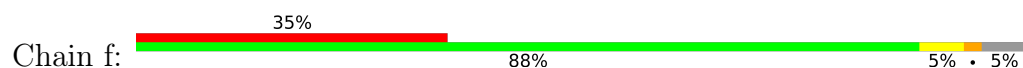
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



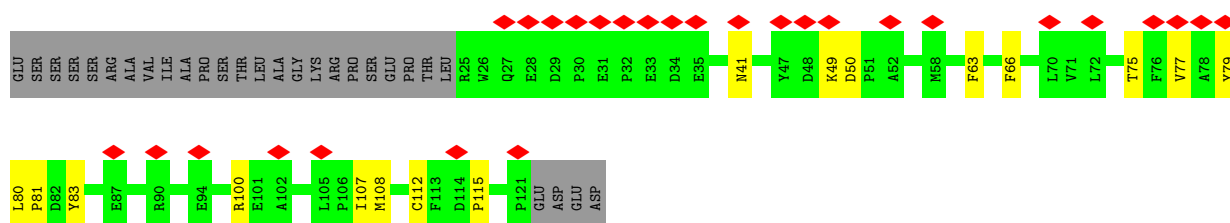
- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



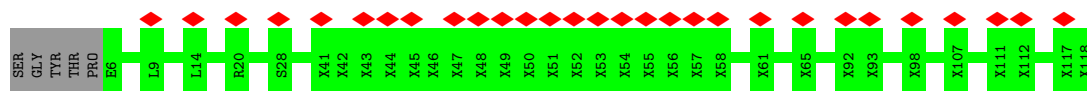
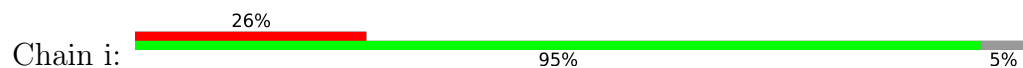
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



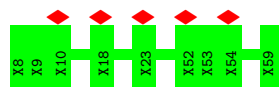
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



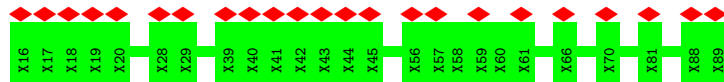
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



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



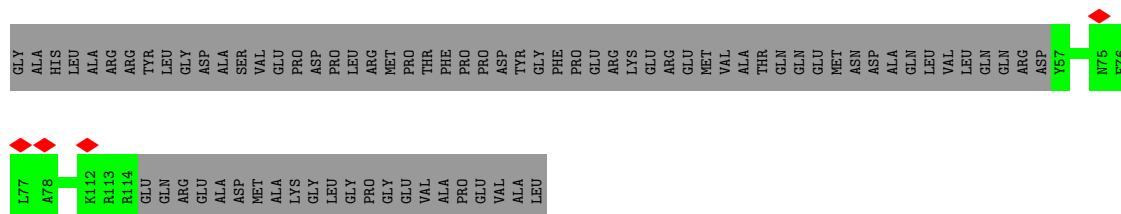
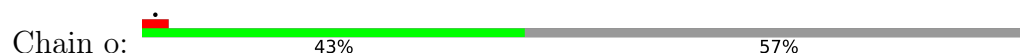
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



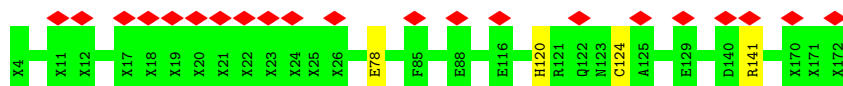
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8



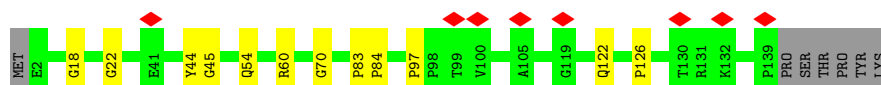
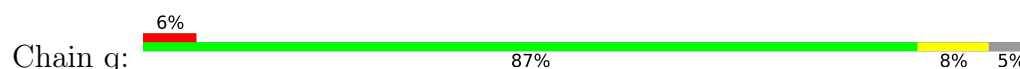
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



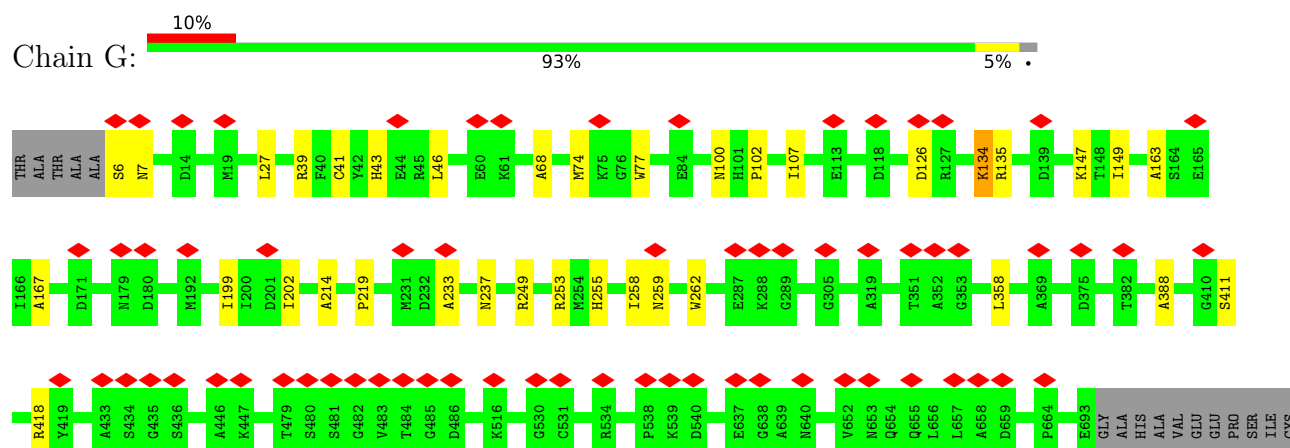
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



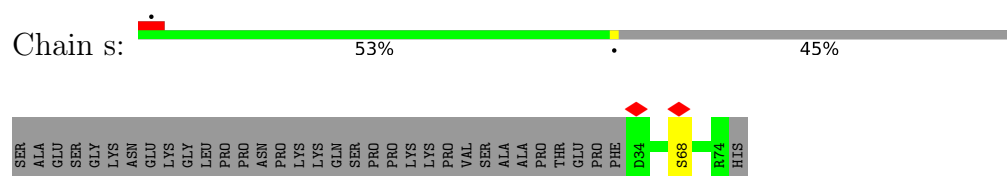
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



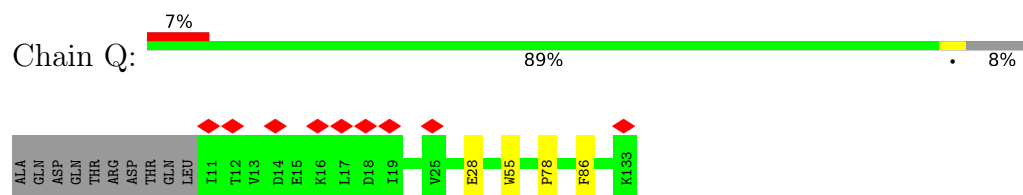
- Molecule 34: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



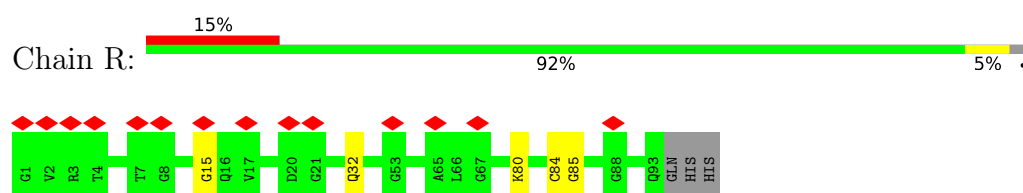
- Molecule 35: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



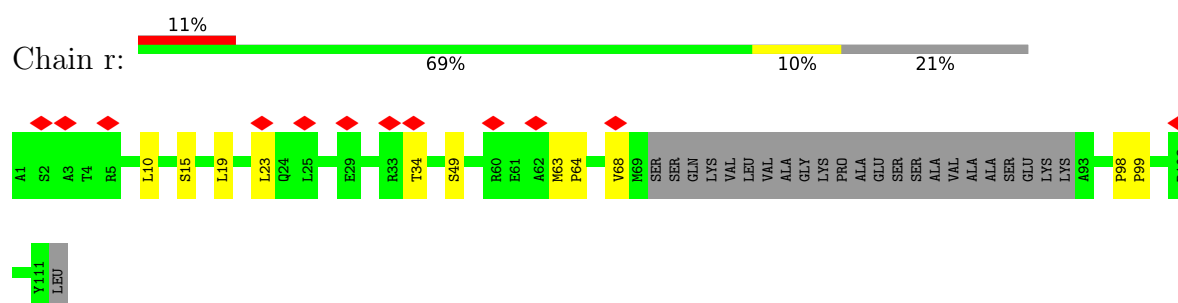
- Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



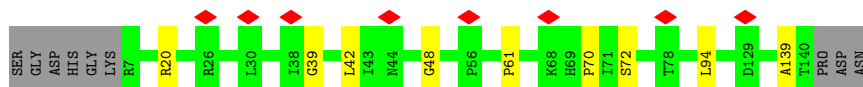
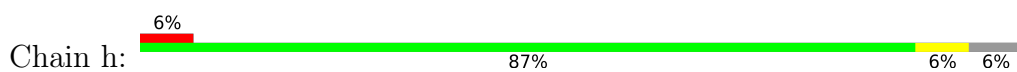
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



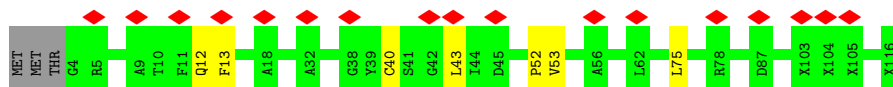
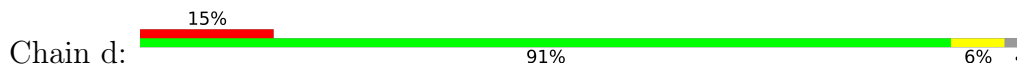
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



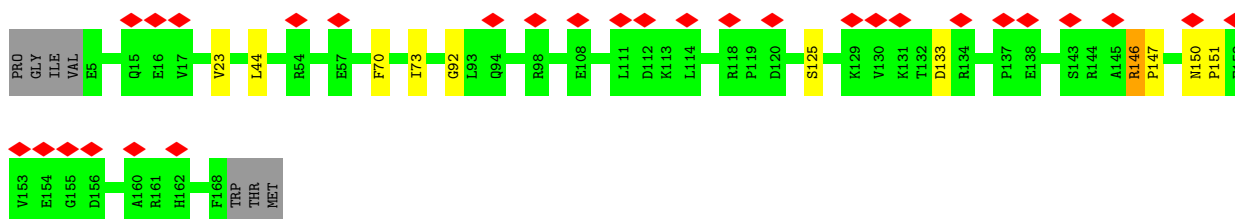
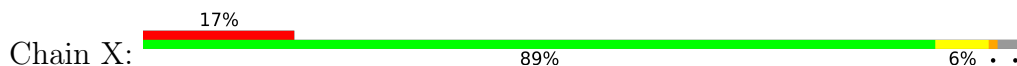
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



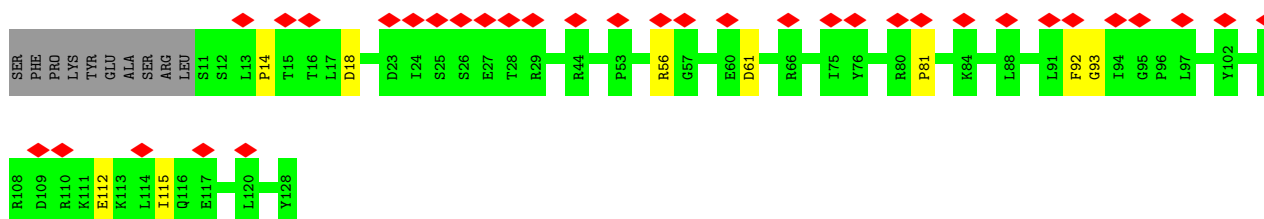
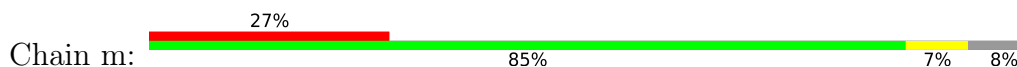
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2,NADH dehydrogenase [ubiquinone] 1 subunit C2



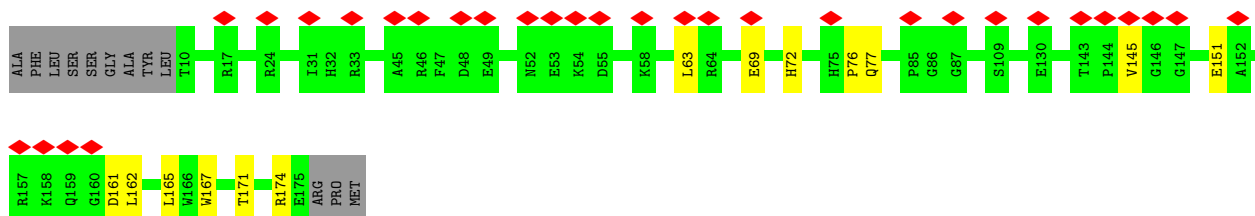
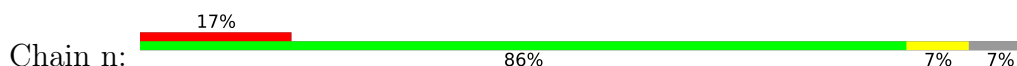
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



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

[illegible]

4 Experimental information

Property	Value	Source
EM 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
Maximum map value	1.450	Depositor
Minimum map value	-0.316	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, NAP, SF4, ZN, FMN

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	A	0.56	0/706	1.03	0/967
2	B	0.54	0/1187	1.01	1/1607 (0.1%)
3	C	0.58	0/1728	0.93	3/2353 (0.1%)
4	D	0.53	0/3304	0.95	0/4478
5	E	0.58	0/1062	1.05	0/1484
6	F	0.55	0/2488	1.03	1/3434 (0.0%)
7	H	0.56	0/2378	0.98	2/3250 (0.1%)
8	I	0.55	0/1419	0.92	0/1925
9	J	0.58	0/1239	1.05	0/1688
10	K	0.51	0/730	0.98	0/988
11	L	0.57	0/4653	0.99	0/6350
12	M	0.55	0/3638	0.98	1/4967 (0.0%)
13	N	0.59	1/2656 (0.0%)	1.03	1/3630 (0.0%)
14	O	0.54	0/1983	0.99	0/2742
16	S	0.52	0/408	1.02	0/571
17	T	0.50	0/380	1.14	0/531
17	U	0.51	0/436	1.12	0/610
18	V	0.56	0/713	1.06	0/977
19	W	0.57	0/831	0.95	0/1128
20	Y	0.58	0/1031	0.98	0/1400
21	a	0.62	0/494	0.98	0/669
22	b	0.57	0/352	0.95	0/481
23	c	0.64	0/330	1.08	0/455
24	e	0.54	0/630	0.96	1/851 (0.1%)
25	f	0.57	0/356	0.99	0/488
26	g	0.65	0/696	1.02	1/957 (0.1%)
27	i	0.48	0/224	0.88	0/300
31	o	0.48	0/296	1.16	0/412
32	p	0.49	0/535	0.99	0/718
33	q	0.63	0/704	1.16	5/984 (0.5%)
34	G	0.52	0/4212	0.94	0/5789
35	s	0.54	0/238	0.94	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	Q	0.49	0/768	0.87	0/1066
37	R	0.53	0/649	0.85	0/879
38	r	0.67	0/594	1.02	0/824
39	h	0.57	0/837	0.98	0/1157
40	d	0.59	0/730	0.99	0/992
41	X	0.55	0/1200	0.98	0/1634
42	m	0.57	0/926	0.96	0/1260
43	n	0.52	0/1163	0.96	0/1586
44	Z	0.52	0/718	1.00	0/967
All	All	0.56	1/49622 (0.0%)	0.99	16/67881 (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
2	B	0	1
12	M	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	115	VAL	CA-CB	5.05	1.56	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	255	PRO	N-CA-C	7.88	120.31	110.70
3	C	160	HIS	CA-C-N	7.30	128.96	119.84
3	C	160	HIS	C-N-CA	7.30	128.96	119.84
6	F	207	PRO	N-CA-C	6.59	118.75	110.70
7	H	91	MET	CA-C-N	6.50	127.96	119.84
7	H	91	MET	C-N-CA	6.50	127.96	119.84
12	M	56	PHE	N-CA-C	-6.47	104.44	112.72
33	q	83	PRO	CA-C-N	6.17	127.55	119.84
33	q	83	PRO	C-N-CA	6.17	127.55	119.84
33	q	97	PRO	N-CA-C	6.16	118.22	110.70
3	C	38	GLN	N-CA-C	5.80	117.29	110.97
24	e	93	PRO	N-CA-C	5.67	117.61	110.70
26	g	107	ILE	N-CA-C	5.50	112.09	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	GLY	N-CA-C	5.33	118.49	111.03
33	q	97	PRO	CA-C-N	-5.15	115.07	120.94
33	q	97	PRO	C-N-CA	-5.15	115.07	120.94

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	10	0
2	B	1159	0	1166	10	0
3	C	1678	0	1612	18	0
4	D	3229	0	3123	32	0
5	E	1038	0	623	2	0
6	F	2441	0	1628	5	0
7	H	2312	0	2426	25	0
8	I	1388	0	1323	20	0
9	J	1211	0	1165	18	0
10	K	720	0	761	15	0
11	L	4538	0	4480	39	0
12	M	3549	0	3674	36	0
13	N	2592	0	2632	23	0
14	O	1941	0	1366	5	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	6	0
20	Y	1011	0	1020	3	0
21	a	480	0	440	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	519	0	408	0	0
23	c	320	0	277	0	0
24	e	619	0	513	1	0
25	f	350	0	260	1	0
26	g	677	0	559	6	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	1	0
33	q	696	0	338	4	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	2	0
38	r	575	0	425	10	0
39	h	822	0	644	5	0
40	d	803	0	659	2	0
41	X	1170	0	969	3	0
42	m	904	0	832	3	0
43	n	1124	0	862	1	0
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	270	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.

All (270) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:42:PHE:CZ	38:r:10:LEU:CD2	2.74	0.70
8:I:42:PHE:CE1	38:r:10:LEU:HD21	2.27	0.70
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
8:I:42:PHE:CZ	38:r:10:LEU:HD21	2.35	0.62
12:M:143:LEU:HD21	13:N:302:LEU:HD11	1.82	0.61
4:D:221:ARG:HH22	38:r:23:LEU:HA	1.67	0.60
12:M:372:THR:HA	12:M:448:THR:HG22	1.84	0.60
14:O:304:TYR:HB3	40:d:52:PRO:HB3	1.83	0.59
3:C:137:MET:HA	3:C:161:PRO:HG2	1.84	0.59
3:C:52:ILE:HD13	3:C:107:VAL:HG13	1.84	0.59
11:L:230:HIS:N	11:L:231:PRO:HD3	2.18	0.58
2:B:62:MET:HB3	2:B:69:MET:HG2	1.87	0.57
3:C:126:ALA:HB2	4:D:253:TYR:HA	1.86	0.57
4:D:282:GLU:HB2	4:D:313:GLN:HE22	1.69	0.56
43:n:69:GLU:H	43:n:72:HIS:HD2	1.53	0.56
1:A:67:LEU:HD22	10:K:65:VAL:HA	1.87	0.56
9:J:60:TYR:HA	9:J:64:MET:HB2	1.87	0.56
7:H:85:MET:HB3	7:H:233:MET:HE2	1.87	0.56
34:G:233:ALA:HB3	34:G:388:ALA:HB2	1.87	0.56
13:N:230:LEU:HD11	13:N:304:MET:HG2	1.88	0.55
10:K:19:LEU:HD11	10:K:36:MET:HG3	1.89	0.55
34:G:255:HIS:HD2	34:G:258:ILE:H	1.53	0.55
6:F:360:GLY:HA2	6:F:366:ARG:HB3	1.89	0.55
13:N:236:LYS:HD3	13:N:237:THR:H	1.71	0.55
8:I:42:PHE:CE1	38:r:10:LEU:CD2	2.89	0.54
5:E:151:ALA:HB3	5:E:152:PRO:HD3	1.89	0.54
11:L:69:LEU:HD13	11:L:76:LEU:HB2	1.89	0.54
13:N:125:SER:HA	13:N:128:LEU:HD12	1.89	0.54
34:G:100:ASN:HB3	34:G:135:ARG:HG2	1.90	0.54
1:A:68:GLU:HG3	9:J:161:LEU:HD13	1.89	0.54
26:g:80:LEU:HB3	39:h:72:SER:HB3	1.89	0.54
4:D:269:LEU:HB2	4:D:368:GLU:HB2	1.89	0.54
1:A:97:LEU:HD22	9:J:162:LEU:HD11	1.91	0.53
7:H:102:VAL:HG21	7:H:154:LEU:HD11	1.91	0.53
12:M:55:LEU:HD13	12:M:58:SER:HB2	1.91	0.53
10:K:59:MET:HB3	13:N:27:LEU:HD13	1.90	0.53
34:G:6:SER:O	34:G:7:ASN:HB2	2.09	0.53
12:M:129:THR:HG21	12:M:236:LEU:HD11	1.91	0.53
13:N:200:MET:HE2	13:N:265:MET:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:559:GLU:O	11:L:563:PRO:HD2	2.09	0.52
3:C:94:TYR:HB2	3:C:107:VAL:HB	1.91	0.52
6:F:305:PRO:HD3	6:F:413:TRP:HB3	1.91	0.52
34:G:74:MET:HB2	34:G:77:TRP:HE1	1.73	0.52
7:H:47:GLN:N	7:H:48:PRO:HD2	2.25	0.52
4:D:202:ASP:HB3	4:D:323:ILE:HG13	1.91	0.52
12:M:6:ILE:HG22	12:M:10:MET:HG2	1.91	0.52
11:L:368:PHE:HE2	11:L:454:ILE:HB	1.76	0.51
7:H:107:ALA:HB1	9:J:57:PHE:HB3	1.91	0.51
11:L:149:ILE:HD11	12:M:364:LEU:HD22	1.93	0.51
19:W:91:GLU:HG2	19:W:96:TRP:HD1	1.75	0.51
33:q:18:GLY:HA3	33:q:22:GLY:HA3	1.92	0.51
2:B:149:CYS:SG	2:B:150:PRO:HD2	2.50	0.51
34:G:237:ASN:HB3	34:G:253:ARG:HE	1.74	0.51
2:B:126:TYR:CZ	4:D:85:ARG:HD3	2.45	0.51
7:H:79:LEU:HD11	7:H:222:LEU:HB2	1.91	0.51
12:M:114:GLU:HG2	12:M:116:ILE:H	1.75	0.51
12:M:168:GLN:HB3	12:M:174:LEU:HG	1.93	0.51
1:A:63:LEU:HD21	10:K:68:ALA:HB1	1.93	0.50
3:C:81:VAL:HA	4:D:388:ARG:HE	1.76	0.50
3:C:150:ARG:H	19:W:87:MET:HE2	1.76	0.50
6:F:403:THR:HG21	6:F:408:GLY:HA3	1.93	0.50
12:M:325:MET:HE1	12:M:437:MET:HG3	1.94	0.50
4:D:111:MET:HE3	4:D:189:MET:HB3	1.93	0.50
2:B:122:GLY:HA2	2:B:135:GLY:HA3	1.92	0.50
19:W:24:MET:H	19:W:75:PRO:HB3	1.76	0.50
26:g:112:CYS:H	32:p:141:ARG:HE	1.58	0.50
39:h:48:GLY:HA2	39:h:70:PRO:HD3	1.92	0.50
4:D:173:GLU:HG3	4:D:221:ARG:HG2	1.94	0.50
11:L:455:LYS:HA	11:L:458:LEU:HD12	1.93	0.50
12:M:258:ALA:HB1	12:M:302:LEU:HB3	1.94	0.49
8:I:69:ARG:HA	8:I:76:ARG:HB2	1.94	0.49
10:K:22:TYR:HB2	11:L:585:LYS:HG3	1.93	0.49
11:L:377:SER:HB2	11:L:423:SER:HB2	1.94	0.49
12:M:72:LEU:HA	12:M:75:LEU:HB2	1.94	0.49
19:W:63:ARG:HG2	19:W:67:LYS:HE2	1.95	0.49
4:D:116:GLN:HE22	4:D:138:ARG:HD3	1.77	0.49
10:K:8:ILE:HD12	10:K:43:MET:HG2	1.95	0.49
13:N:149:ILE:HB	13:N:154:ILE:HD11	1.94	0.49
10:K:17:VAL:HA	11:L:592:LEU:HD21	1.93	0.48
10:K:69:CYS:HB3	13:N:38:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Z:39:ILE:HA	44:Z:42:LEU:HD12	1.95	0.48
11:L:297:ASP:HB2	11:L:300:LYS:HB2	1.95	0.48
11:L:343:SER:HA	11:L:346:ILE:HD12	1.94	0.48
11:L:590:SER:HA	11:L:593:ILE:HD12	1.94	0.48
11:L:214:ILE:HG23	11:L:218:LEU:HD13	1.96	0.48
26:g:100:ARG:HD2	26:g:108:MET:HA	1.94	0.48
12:M:114:GLU:HG3	12:M:175:ASN:HA	1.96	0.48
34:G:27:LEU:HB2	34:G:68:ALA:HB1	1.96	0.48
1:A:76:PRO:HB3	7:H:155:LEU:HA	1.95	0.48
3:C:81:VAL:HG13	4:D:388:ARG:HD2	1.95	0.48
4:D:92:GLU:HG2	4:D:388:ARG:H	1.79	0.48
4:D:324:LYS:HE2	4:D:332:PRO:HG2	1.96	0.48
8:I:3:LYS:O	8:I:4:TYR:HB2	2.14	0.48
12:M:8:THR:HA	12:M:11:LEU:HD12	1.95	0.47
8:I:53:GLU:HG2	33:q:60:ARG:HA	1.96	0.47
3:C:52:ILE:HG21	3:C:60:VAL:HG21	1.97	0.47
3:C:119:SER:HB3	3:C:142:PHE:HB3	1.96	0.47
11:L:254:VAL:HG22	11:L:258:PHE:HB2	1.97	0.47
14:O:104:ARG:HA	14:O:107:GLN:HG2	1.97	0.47
20:Y:80:ARG:HH21	20:Y:88:ASN:HA	1.78	0.47
1:A:84:LEU:HD22	7:H:309:ILE:HG12	1.96	0.47
11:L:230:HIS:H	11:L:231:PRO:HD3	1.78	0.47
2:B:116:MET:HE3	2:B:151:PRO:HG2	1.97	0.47
3:C:162:PHE:CZ	4:D:388:ARG:HB3	2.49	0.47
7:H:90:PRO:HB2	7:H:166:ILE:HD11	1.96	0.47
9:J:40:GLY:HA2	9:J:43:ILE:HD12	1.97	0.47
44:Z:56:ARG:HA	44:Z:59:LEU:HD12	1.97	0.47
9:J:171:ILE:HG23	13:N:45:MET:HE2	1.97	0.47
8:I:67:LEU:HD21	8:I:152:GLU:HG2	1.96	0.47
4:D:293:CYS:HB3	4:D:420:THR:HG21	1.97	0.46
4:D:316:ASN:HA	44:Z:10:PRO:HB3	1.97	0.46
8:I:42:PHE:CE2	38:r:10:LEU:HD23	2.51	0.46
13:N:78:LEU:HA	13:N:82:GLY:HA2	1.96	0.46
7:H:178:ALA:HB1	7:H:181:LEU:HB2	1.98	0.46
34:G:43:HIS:HB3	34:G:46:LEU:HB2	1.98	0.46
12:M:162:VAL:HG21	13:N:280:THR:HG22	1.97	0.46
20:Y:62:ALA:HA	20:Y:65:ILE:HD12	1.98	0.46
42:m:112:GLU:HA	42:m:115:ILE:HD12	1.97	0.46
7:H:284:GLN:HA	7:H:287:HIS:HB2	1.97	0.46
11:L:378:LEU:HD22	11:L:383:MET:HE3	1.97	0.46
9:J:28:TYR:HA	9:J:31:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:G:219:PRO:HA	34:G:249:ARG:HH21	1.80	0.46
11:L:19:ILE:HA	11:L:22:MET:HE3	1.98	0.46
12:M:102:LEU:HD21	12:M:129:THR:HG23	1.98	0.46
7:H:111:LEU:HD13	9:J:61:LEU:HB3	1.97	0.46
14:O:172:VAL:HG13	14:O:206:TYR:HE2	1.81	0.46
17:U:4:PRO:HA	17:U:5:PRO:HD3	1.88	0.46
1:A:16:LEU:HA	1:A:19:ILE:HD12	1.97	0.46
11:L:7:LEU:HD23	11:L:50:PRO:HD3	1.97	0.46
40:d:40:CYS:HA	40:d:43:LEU:HD12	1.98	0.46
1:A:73:LEU:HD23	7:H:151:LEU:HD21	1.98	0.45
12:M:342:MET:HE3	12:M:413:MET:HE2	1.97	0.45
12:M:39:LEU:HD11	26:g:77:VAL:HG22	1.98	0.45
13:N:102:LEU:HD13	13:N:142:LEU:HG	1.97	0.45
3:C:83:ILE:HA	3:C:84:PRO:HD3	1.83	0.45
3:C:93:VAL:HG22	3:C:108:LYS:HG2	1.97	0.45
9:J:65:MET:HA	9:J:68:PHE:HB2	1.98	0.45
13:N:203:LEU:HA	13:N:206:ILE:HD12	1.97	0.45
7:H:33:LEU:HB2	8:I:40:TYR:CE2	2.52	0.45
10:K:30:LEU:HA	10:K:33:LEU:HD12	1.97	0.45
12:M:233:ALA:HA	12:M:236:LEU:HD12	1.98	0.45
36:Q:55:TRP:HB2	36:Q:86:PHE:HB2	1.98	0.45
2:B:122:GLY:HA3	8:I:114:THR:HB	1.97	0.45
4:D:114:ASN:C	4:D:116:GLN:H	2.25	0.45
11:L:33:PRO:HB2	11:L:105:MET:HE1	1.99	0.45
11:L:42:TYR:HA	11:L:45:ILE:HD12	1.99	0.45
3:C:49:GLU:HG3	3:C:106:ARG:HD2	1.98	0.45
7:H:285:LEU:HA	7:H:288:LEU:HD12	1.99	0.45
9:J:72:THR:HG23	10:K:27:MET:HE2	1.98	0.45
7:H:12:PRO:HA	7:H:15:LEU:HD12	1.99	0.44
12:M:323:SER:HA	12:M:326:LEU:HD12	1.99	0.44
26:g:75:THR:HA	26:g:79:TYR:HB3	1.98	0.44
4:D:414:VAL:HA	4:D:417:ILE:HD12	1.99	0.44
20:Y:120:THR:HA	20:Y:123:LEU:HD12	1.99	0.44
8:I:117:ILE:HD12	8:I:119:CYS:HB3	1.99	0.44
9:J:23:LYS:HE3	10:K:22:TYR:HA	2.00	0.44
11:L:548:SER:HA	11:L:552:LEU:HD12	1.98	0.44
13:N:16:GLY:HA2	13:N:19:ILE:HD12	1.98	0.44
4:D:117:ALA:HA	4:D:367:ILE:HD12	2.00	0.44
8:I:42:PHE:CE2	38:r:10:LEU:CD2	3.01	0.44
11:L:258:PHE:HA	11:L:261:ILE:HD12	1.99	0.44
9:J:9:LEU:HA	9:J:12:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:87:CYS:HA	8:I:88:PRO:HD3	1.84	0.44
14:O:111:ALA:HB1	14:O:122:VAL:HG11	1.99	0.44
4:D:158:ALA:HB1	4:D:163:ALA:HB3	2.00	0.44
11:L:324:LEU:HA	11:L:327:LEU:HD12	2.00	0.44
25:f:49:LYS:H	25:f:50:PRO:HD2	1.82	0.44
11:L:190:LEU:HD13	11:L:196:TRP:HE1	1.83	0.44
38:r:98:PRO:HA	38:r:99:PRO:HD3	1.94	0.43
4:D:141:PHE:HA	4:D:144:ILE:HG22	2.01	0.43
7:H:173:TRP:HD1	7:H:243:LEU:HA	1.83	0.43
11:L:248:HIS:HB3	11:L:306:THR:HG21	2.00	0.43
19:W:46:VAL:HG13	19:W:51:LEU:HA	1.99	0.43
1:A:70:ALA:HB1	9:J:55:MET:HE1	2.01	0.43
9:J:55:MET:HE2	10:K:61:ILE:HG23	2.01	0.43
12:M:295:ALA:HA	12:M:298:ILE:HD12	2.01	0.43
34:G:163:ALA:HA	34:G:167:ALA:HB3	2.00	0.43
12:M:300:ALA:HB1	12:M:308:SER:HB2	2.00	0.43
7:H:31:MET:HG2	8:I:41:LEU:HD12	2.00	0.43
12:M:230:VAL:HG21	12:M:283:LYS:HZ1	1.83	0.43
13:N:224:THR:H	13:N:228:LEU:HD23	1.82	0.43
13:N:340:THR:N	13:N:341:PRO:HD2	2.33	0.43
8:I:82:LEU:O	8:I:86:VAL:HG23	2.19	0.43
13:N:311:MET:H	14:O:99:TRP:HZ3	1.66	0.43
34:G:202:ILE:HD11	34:G:262:TRP:HE1	1.84	0.43
2:B:162:GLN:HG3	2:B:166:LYS:HE2	2.00	0.43
6:F:202:LYS:HA	6:F:203:PRO:HD3	1.90	0.43
11:L:128:MET:HE2	11:L:147:VAL:HG21	2.00	0.43
13:N:18:ILE:HG23	13:N:22:ILE:HD12	2.00	0.43
2:B:92:LEU:HD21	2:B:100:LEU:HD13	2.01	0.42
4:D:328:ALA:HB3	34:G:126:ASP:HB2	2.00	0.42
4:D:352:TYR:HB3	8:I:86:VAL:HG22	2.01	0.42
9:J:52:LEU:HD11	10:K:60:PRO:HG2	2.00	0.42
19:W:90:GLU:HA	19:W:93:ILE:HD12	2.01	0.42
3:C:67:HIS:HD2	3:C:70:ALA:H	1.67	0.42
7:H:304:HIS:HA	7:H:307:LEU:HD12	2.00	0.42
11:L:176:ARG:HA	11:L:179:ASP:HB2	2.00	0.42
11:L:198:LEU:HD23	11:L:201:ILE:HD11	2.02	0.42
12:M:154:LEU:HB3	13:N:287:LEU:HD21	2.02	0.42
13:N:25:HIS:HB3	13:N:28:LEU:HB2	2.01	0.42
21:a:31:ASN:HD22	21:a:35:GLU:H	1.66	0.42
11:L:393:ASP:HA	11:L:396:ILE:HD12	2.01	0.42
12:M:167:ILE:HD13	12:M:250:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD12	9:J:168:ILE:HD13	2.00	0.42
7:H:243:LEU:HD13	7:H:262:LYS:HB3	2.01	0.42
33:q:122:GLN:HA	37:R:32:GLN:HB2	2.01	0.42
3:C:186:GLU:H	3:C:187:PRO:CD	2.32	0.42
4:D:372:GLY:HA3	4:D:394:PRO:HB3	2.01	0.42
9:J:160:SER:HA	9:J:163:ILE:HD12	2.02	0.42
12:M:293:HIS:HA	12:M:296:LEU:HD12	2.01	0.42
4:D:390:LYS:HA	4:D:430:ARG:HD3	2.01	0.42
7:H:5:ASN:HD21	21:a:26:ILE:HG12	1.85	0.42
11:L:170:GLN:HA	11:L:173:LEU:HB3	2.02	0.42
12:M:141:GLU:HB2	12:M:144:ASN:HD22	1.85	0.42
4:D:232:ASN:HD22	4:D:232:ASN:HA	1.67	0.41
44:Z:72:PRO:HA	44:Z:75:GLN:HB3	2.01	0.41
12:M:115:LEU:HD12	12:M:174:LEU:HB3	2.02	0.41
12:M:243:MET:HG2	12:M:301:ILE:HG21	2.02	0.41
34:G:27:LEU:HD21	34:G:39:ARG:HD3	2.02	0.41
7:H:116:ILE:HG23	7:H:136:VAL:HG22	2.02	0.41
11:L:562:LEU:HB3	12:M:151:PHE:HE2	1.86	0.41
44:Z:71:MET:N	44:Z:72:PRO:HD2	2.29	0.41
7:H:24:GLU:O	7:H:28:LEU:HB3	2.21	0.41
8:I:150:ASN:HB3	33:q:126:PRO:HA	2.02	0.41
12:M:231:LEU:HD22	12:M:324:SER:HB2	2.01	0.41
2:B:64:ALA:HA	2:B:65:PRO:HD3	1.88	0.41
2:B:134:ARG:HH12	3:C:173:GLU:HB2	1.84	0.41
3:C:77:ASP:HB2	3:C:95:ASN:HB3	2.01	0.41
3:C:117:ILE:HG22	3:C:142:PHE:CD1	2.56	0.41
7:H:103:LEU:HB3	9:J:54:LEU:HD13	2.02	0.41
7:H:228:TYR:HA	7:H:231:ILE:HD12	2.01	0.41
11:L:276:ILE:HA	11:L:279:CYS:HB2	2.02	0.41
12:M:297:VAL:HG13	12:M:312:ALA:HB1	2.03	0.41
24:e:29:PRO:HG3	39:h:139:ALA:HA	2.03	0.41
34:G:107:ILE:HD13	37:R:85:GLY:HA3	2.03	0.41
34:G:147:LYS:HE3	34:G:149:ILE:HD11	2.01	0.41
39:h:39:GLY:HA2	39:h:42:LEU:HD12	2.03	0.41
4:D:166:PRO:HG3	4:D:229:LEU:HD21	2.03	0.41
6:F:347:ILE:HA	6:F:350:LEU:HD12	2.02	0.41
10:K:93:LEU:HD11	11:L:584:ILE:HG13	2.02	0.41
11:L:29:PRO:C	11:L:31:ASN:H	2.29	0.41
12:M:329:LEU:HD23	12:M:437:MET:HE3	2.03	0.41
12:M:373:ILE:HA	12:M:376:ILE:HD12	2.03	0.41
34:G:102:PRO:HA	34:G:134:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:LEU:HD12	4:D:314:CYS:HB3	2.03	0.41
11:L:131:LEU:HB2	11:L:143:GLY:HA3	2.01	0.41
11:L:553:LEU:HD11	42:m:93:GLY:HA2	2.03	0.41
8:I:42:PHE:CD2	38:r:10:LEU:HD23	2.55	0.40
11:L:544:MET:HE3	42:m:92:PHE:HZ	1.87	0.40
41:X:70:PHE:HA	41:X:73:ILE:HD12	2.02	0.40
41:X:146:ARG:HA	41:X:147:PRO:HD3	1.96	0.40
12:M:431:THR:HG23	39:h:20:ARG:HH21	1.86	0.40
4:D:88:GLU:OE1	4:D:390:LYS:HG2	2.21	0.40
4:D:335:ARG:HA	4:D:338:MET:HG2	2.03	0.40
10:K:40:LEU:HD22	13:N:71:MET:HG3	2.03	0.40
13:N:20:VAL:HA	13:N:29:VAL:HG12	2.02	0.40
18:V:64:VAL:HG12	18:V:66:LYS:H	1.86	0.40
26:g:63:PHE:HA	26:g:66:PHE:HB3	2.04	0.40
4:D:251:LEU:HD21	4:D:265:ILE:HG12	2.03	0.40
7:H:180:PRO:HD3	44:Z:42:LEU:HD21	2.02	0.40
11:L:137:LEU:HB3	11:L:196:TRP:HE3	1.86	0.40
12:M:63:THR:HG21	12:M:110:PHE:HB3	2.04	0.40
12:M:208:PRO:HB2	12:M:291:VAL:HG13	2.02	0.40
38:r:63:MET:HA	38:r:64:PRO:HD3	1.94	0.40
41:X:150:ASN:HA	41:X:151:PRO:HD3	1.93	0.40
8:I:28:THR:HA	8:I:31:ILE:HD12	2.02	0.40
13:N:139:MET:HG2	13:N:205:LEU:HD11	2.03	0.40

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%)	10 42
2	B	145/179 (81%)	124 (86%)	19 (13%)	2 (1%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	202/228 (89%)	175 (87%)	23 (11%)	4 (2%)	6	33
4	D	412/430 (96%)	364 (88%)	41 (10%)	7 (2%)	7	36
5	E	184/217 (85%)	157 (85%)	20 (11%)	7 (4%)	2	21
6	F	423/464 (91%)	381 (90%)	33 (8%)	9 (2%)	5	32
7	H	292/318 (92%)	264 (90%)	20 (7%)	8 (3%)	4	27
8	I	174/176 (99%)	144 (83%)	22 (13%)	8 (5%)	2	19
9	J	169/175 (97%)	150 (89%)	13 (8%)	6 (4%)	2	22
10	K	93/98 (95%)	87 (94%)	5 (5%)	1 (1%)	11	44
11	L	602/606 (99%)	535 (89%)	54 (9%)	13 (2%)	5	31
12	M	455/459 (99%)	412 (90%)	32 (7%)	11 (2%)	4	29
13	N	342/347 (99%)	311 (91%)	26 (8%)	5 (2%)	8	38
14	O	312/320 (98%)	277 (89%)	24 (8%)	11 (4%)	3	23
16	S	78/98 (80%)	75 (96%)	3 (4%)	0	100	100
17	T	73/88 (83%)	66 (90%)	6 (8%)	1 (1%)	9	39
17	U	83/88 (94%)	72 (87%)	9 (11%)	2 (2%)	4	29
18	V	104/115 (90%)	88 (85%)	15 (14%)	1 (1%)	12	46
19	W	109/128 (85%)	93 (85%)	14 (13%)	2 (2%)	6	34
20	Y	136/141 (96%)	125 (92%)	7 (5%)	4 (3%)	3	26
21	a	62/70 (89%)	58 (94%)	2 (3%)	2 (3%)	3	24
22	b	44/80 (55%)	38 (86%)	6 (14%)	0	100	100
23	c	44/49 (90%)	41 (93%)	0	3 (7%)	1	14
24	e	87/105 (83%)	78 (90%)	7 (8%)	2 (2%)	5	30
25	f	52/57 (91%)	46 (88%)	3 (6%)	3 (6%)	1	16
26	g	95/125 (76%)	72 (76%)	17 (18%)	6 (6%)	1	15
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%)	2	19
33	q	136/145 (94%)	111 (82%)	20 (15%)	5 (4%)	2	22
34	G	686/704 (97%)	621 (90%)	59 (9%)	6 (1%)	14	48
35	s	39/75 (52%)	34 (87%)	4 (10%)	1 (3%)	4	28
36	Q	121/133 (91%)	107 (88%)	12 (10%)	2 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	R	91/96 (95%)	79 (87%)	10 (11%)	2 (2%)	5	31
38	r	84/112 (75%)	66 (79%)	13 (16%)	5 (6%)	1	15
39	h	132/143 (92%)	111 (84%)	20 (15%)	1 (1%)	16	52
40	d	93/116 (80%)	84 (90%)	6 (6%)	3 (3%)	3	24
41	X	162/171 (95%)	142 (88%)	16 (10%)	4 (2%)	4	29
42	m	116/128 (91%)	93 (80%)	18 (16%)	5 (4%)	2	20
43	n	164/178 (92%)	135 (82%)	19 (12%)	10 (6%)	1	15
44	Z	93/144 (65%)	82 (88%)	8 (9%)	3 (3%)	3	24
All	All	6921/7837 (88%)	6110 (88%)	642 (9%)	169 (2%)	7	29

All (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
11	L	194	ASN
12	M	226	ALA
26	g	41	ASN
33	q	45	GLY
33	q	84	PRO
43	n	145	VAL
43	n	151	GLU
43	n	161	ASP
43	n	165	LEU
43	n	171	THR
43	n	174	ARG
4	D	70	GLY
7	H	68	ALA
8	I	14	MET
8	I	151	LYS
9	J	133	SER
10	K	52	HIS
11	L	24	PHE
11	L	25	ASN
11	L	84	TYR
12	M	7	PRO

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Mol	Chain	Res	Type
12	M	373	ILE
13	N	3	PRO
13	N	46	LYS
13	N	308	THR
14	O	93	SER
14	O	166	PRO
19	W	52	ASP
20	Y	80	ARG
21	a	55	SER
23	c	12	PRO
33	q	54	GLN
34	G	214	ALA
34	G	259	ASN
38	r	34	THR
38	r	68	VAL
41	X	133	ASP
43	n	162	LEU
44	Z	13	GLY
44	Z	30	SER
1	A	52	SER
3	C	39	GLN
3	C	203	TRP
4	D	35	ASP
4	D	46	ASN
5	E	157	ASN
6	F	20	ARG
6	F	284	ALA
8	I	74	GLU
8	I	116	CYS
9	J	78	GLN
9	J	110	ASP
11	L	56	HIS
11	L	476	THR
11	L	583	LEU
12	M	55	LEU
12	M	428	PRO
13	N	197	ASN
13	N	306	PRO
14	O	118	THR
14	O	126	ARG
14	O	283	THR
20	Y	46	THR

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Mol	Chain	Res	Type
20	Y	107	TYR
32	p	124	CYS
33	q	70	GLY
34	G	358	LEU
34	G	418	ARG
37	R	80	LYS
38	r	15	SER
38	r	19	LEU
40	d	53	VAL
42	m	14	PRO
42	m	18	ASP
43	n	167	TRP
3	C	186	GLU
6	F	164	LYS
7	H	197	PRO
7	H	281	ARG
8	I	2	TYR
8	I	63	GLY
11	L	351	ASN
11	L	387	THR
11	L	560	ALA
12	M	23	ILE
14	O	10	LEU
17	U	87	TYR
21	a	33	GLY
24	e	16	TRP
25	f	41	SER
25	f	53	GLU
26	g	49	LYS
26	g	83	TYR
32	p	78	GLU
32	p	120	HIS
33	q	44	TYR
34	G	134	LYS
34	G	411	SER
35	s	68	SER
36	Q	28	GLU
38	r	49	SER
40	d	13	PHE
41	X	146	ARG
42	m	56	ARG
2	B	78	ALA

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Mol	Chain	Res	Type
4	D	18	VAL
4	D	19	MET
4	D	277	VAL
5	E	17	PRO
5	E	112	ASN
5	E	182	PRO
6	F	185	ILE
6	F	290	GLY
7	H	66	SER
7	H	96	ILE
8	I	28	THR
12	M	371	PRO
12	M	457	PRO
14	O	314	ASP
19	W	24	MET
23	c	6	GLU
23	c	14	TRP
26	g	50	ASP
36	Q	78	PRO
40	d	12	GLN
41	X	125	SER
43	n	76	PRO
5	E	128	VAL
11	L	515	TYR
12	M	175	ASN
14	O	31	ILE
14	O	76	ASN
17	T	32	VAL
17	U	32	VAL
37	R	15	GLY
42	m	61	ASP
5	E	25	PRO
6	F	84	LYS
9	J	25	SER
18	V	37	ILE
25	f	49	LYS
26	g	81	PRO
26	g	115	PRO
43	n	77	GLN
6	F	40	GLY
6	F	208	PRO
7	H	248	ASN

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Mol	Chain	Res	Type
9	J	49	GLY
11	L	230	HIS
11	L	367	PRO
12	M	172	GLY
20	Y	82	LYS
41	X	92	GLY
5	E	185	GLY
7	H	313	GLY
42	m	81	PRO
44	Z	71	MET
8	I	9	GLU
9	J	63	GLY
14	O	66	GLY
14	O	312	VAL
24	e	27	GLY
12	M	6	ILE
39	h	61	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%)	68 (93%)	5 (7%)	14	38
2	B	124/150 (83%)	121 (98%)	3 (2%)	43	63
3	C	179/204 (88%)	176 (98%)	3 (2%)	53	68
4	D	332/371 (90%)	323 (97%)	9 (3%)	39	60
5	E	36/183 (20%)	36 (100%)	0	100	100
6	F	97/368 (26%)	94 (97%)	3 (3%)	35	56
7	H	250/275 (91%)	243 (97%)	7 (3%)	38	59
8	I	143/151 (95%)	135 (94%)	8 (6%)	19	43
9	J	112/142 (79%)	109 (97%)	3 (3%)	39	60
10	K	83/86 (96%)	80 (96%)	3 (4%)	31	53
11	L	463/534 (87%)	452 (98%)	11 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	387/413 (94%)	380 (98%)	7 (2%)	51	67
13	N	277/316 (88%)	266 (96%)	11 (4%)	28	50
14	O	102/283 (36%)	100 (98%)	2 (2%)	48	66
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%)	49 (100%)	0	100	100
19	W	71/114 (62%)	69 (97%)	2 (3%)	38	59
20	Y	99/102 (97%)	99 (100%)	0	100	100
21	a	41/59 (70%)	40 (98%)	1 (2%)	43	63
22	b	36/36 (100%)	34 (94%)	2 (6%)	19	43
23	c	26/45 (58%)	26 (100%)	0	100	100
24	e	46/94 (49%)	46 (100%)	0	100	100
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%)	224 (99%)	2 (1%)	70	76
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%)	50	66
38	r	32/96 (33%)	32 (100%)	0	100	100
39	h	45/124 (36%)	44 (98%)	1 (2%)	45	64
40	d	62/84 (74%)	61 (98%)	1 (2%)	55	69
41	X	95/154 (62%)	93 (98%)	2 (2%)	47	65
42	m	79/114 (69%)	79 (100%)	0	100	100
43	n	78/160 (49%)	77 (99%)	1 (1%)	61	72
44	Z	63/83 (76%)	63 (100%)	0	100	100
All	All	3967/6550 (61%)	3879 (98%)	88 (2%)	45	64

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	16	LEU
1	A	24	LEU
1	A	69	ILE
1	A	89	THR
2	B	54	CYS
2	B	69	MET
2	B	126	TYR
3	C	50	ILE
3	C	78	LEU
3	C	114	LEU
4	D	80	ILE
4	D	106	LEU
4	D	120	LEU
4	D	137	ILE
4	D	144	ILE
4	D	145	THR
4	D	184	VAL
4	D	232	ASN
4	D	388	ARG
6	F	185	ILE
6	F	405	CYS
6	F	415	VAL
7	H	4	ILE
7	H	9	LEU
7	H	95	LEU
7	H	103	LEU
7	H	289	LEU
7	H	297	THR
7	H	314	ILE
8	I	29	GLU
8	I	48	ILE
8	I	80	CYS
8	I	94	ILE
8	I	117	ILE
8	I	128	VAL
8	I	147	LEU
8	I	172	ASP
9	J	34	ILE
9	J	52	LEU
9	J	77	GLU
10	K	16	LEU

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Mol	Chain	Res	Type
10	K	54	THR
10	K	73	LEU
11	L	179	ASP
11	L	213	LEU
11	L	273	ILE
11	L	283	ILE
11	L	331	THR
11	L	339	LEU
11	L	350	LEU
11	L	432	LEU
11	L	524	THR
11	L	553	LEU
11	L	584	ILE
12	M	6	ILE
12	M	116	ILE
12	M	174	LEU
12	M	214	LEU
12	M	296	LEU
12	M	391	ILE
12	M	393	ILE
13	N	5	ILE
13	N	11	LEU
13	N	27	LEU
13	N	58	LYS
13	N	84	TRP
13	N	108	MET
13	N	145	ILE
13	N	193	VAL
13	N	203	LEU
13	N	236	LYS
13	N	278	LEU
14	O	115	LEU
14	O	144	ILE
19	W	53	ILE
19	W	81	LEU
21	a	16	LEU
22	b	11	VAL
22	b	44	ILE
34	G	41	CYS
34	G	199	ILE
37	R	84	CYS
39	h	94	LEU

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Mol	Chain	Res	Type
40	d	75	LEU
41	X	23	VAL
41	X	44	LEU
43	n	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	80	GLN
2	B	94	ASN
2	B	121	ASN
3	C	41	GLN
3	C	46	ASN
3	C	69	ASN
4	D	114	ASN
4	D	116	GLN
4	D	200	HIS
4	D	232	ASN
4	D	266	GLN
6	F	373	ASN
6	F	398	GLN
6	F	416	GLN
7	H	5	ASN
7	H	169	GLN
7	H	171	GLN
7	H	248	ASN
7	H	250	HIS
7	H	284	GLN
8	I	49	ASN
8	I	123	GLN
8	I	144	HIS
10	K	50	ASN
10	K	83	ASN
11	L	67	HIS
11	L	113	ASN
11	L	115	ASN
11	L	192	ASN
11	L	194	ASN
11	L	199	GLN
11	L	248	HIS
11	L	270	ASN

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Mol	Chain	Res	Type
11	L	274	GLN
11	L	320	ASN
11	L	321	GLN
11	L	332	HIS
11	L	400	ASN
11	L	405	ASN
11	L	580	GLN
12	M	30	HIS
12	M	83	HIS
12	M	138	ASN
12	M	144	ASN
12	M	251	ASN
12	M	304	GLN
12	M	331	ASN
12	M	399	ASN
13	N	36	ASN
13	N	48	HIS
13	N	77	ASN
13	N	144	GLN
13	N	186	HIS
13	N	273	ASN
13	N	289	ASN
14	O	92	ASN
14	O	120	GLN
19	W	57	GLN
21	a	31	ASN
22	b	45	ASN
23	c	34	GLN
23	c	35	HIS
25	f	13	HIS
26	g	86	GLN
32	p	103	ASN
32	p	106	GLN
32	p	139	GLN
34	G	28	GLN
34	G	78	ASN
34	G	100	ASN
34	G	110	GLN
34	G	255	HIS
36	Q	81	ASN
37	R	51	GLN
37	R	90	GLN

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Mol	Chain	Res	Type
37	R	93	GLN
40	d	97	HIS
41	X	76	HIS
41	X	102	GLN
42	m	82	ASN
43	n	11	HIS
43	n	32	HIS
43	n	50	HIS
43	n	72	HIS
44	Z	53	ASN
44	Z	60	GLN
44	Z	75	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	-	-		
48	NAP	P	501	-	50,52,52	1.26	6 (12%)	71,80,80	1.59	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	G	802	34	0,12,12	-	-	-		
46	FES	G	803	34	0,4,4	-	-	-		
47	FMN	F	501	-	33,33,33	1.67	5 (15%)	48,50,50	1.40	8 (16%)
45	SF4	G	801	34	0,12,12	-	-	-		
45	SF4	I	202	8	0,12,12	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
45	SF4	I	201	8	0,12,12	-	-	-		
46	FES	E	301	5	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	B	201	2	-	-	0/6/5/5
48	NAP	P	501	-	-	6/35/67/67	0/5/5/5
45	SF4	G	802	34	-	-	0/6/5/5
46	FES	G	803	34	-	-	0/1/1/1
47	FMN	F	501	-	-	9/18/18/18	0/3/3/3
45	SF4	G	801	34	-	-	0/6/5/5
45	SF4	I	202	8	-	-	0/6/5/5
45	SF4	F	502	6	-	-	0/6/5/5
45	SF4	I	201	8	-	-	0/6/5/5
46	FES	E	301	5	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	501	FMN	C9A-C5A	6.07	1.50	1.41
48	P	501	NAP	C5A-C4A	5.05	1.48	1.39
47	F	501	FMN	C8-C7	4.00	1.50	1.40
48	P	501	NAP	C5A-C6A	2.96	1.49	1.41
47	F	501	FMN	C10-N10	2.48	1.42	1.37
48	P	501	NAP	O4D-C1D	2.35	1.44	1.40
47	F	501	FMN	C4A-N5	2.34	1.35	1.30
48	P	501	NAP	C8A-N7A	2.33	1.36	1.31
48	P	501	NAP	C5A-N7A	-2.29	1.34	1.39
47	F	501	FMN	C4-N3	-2.24	1.34	1.38
48	P	501	NAP	PA-O3	2.05	1.61	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	P	501	NAP	C5A-C4A-N3A	-5.82	118.71	126.72
48	P	501	NAP	N3A-C4A-N9A	4.65	135.08	127.17
48	P	501	NAP	C2A-N3A-C4A	3.89	121.34	111.83
48	P	501	NAP	N3A-C2A-N1A	-3.67	123.03	128.58
48	P	501	NAP	C4A-C5A-N7A	-3.39	106.70	110.58
47	F	501	FMN	C4'-C3'-C2'	3.20	118.89	113.57
47	F	501	FMN	C4A-C10-N1	-2.89	117.52	124.59
47	F	501	FMN	C4-C4A-N5	2.67	121.89	118.21
48	P	501	NAP	C4D-O4D-C1D	2.56	112.27	109.92
48	P	501	NAP	C5A-N7A-C8A	2.48	107.36	103.45
48	P	501	NAP	C2B-C1B-N9A	-2.46	109.71	113.75
47	F	501	FMN	C10-N1-C2	2.44	122.12	116.85
48	P	501	NAP	C4A-N9A-C8A	2.34	108.19	105.74
48	P	501	NAP	C6A-C5A-N7A	2.21	136.36	132.09
47	F	501	FMN	C4A-C10-N10	2.14	119.55	116.48
48	P	501	NAP	C2D-C3D-C4D	2.13	106.72	102.61
47	F	501	FMN	C4A-C4-N3	2.10	118.59	113.25
47	F	501	FMN	O4-C4-C4A	-2.07	121.06	126.53
47	F	501	FMN	C5A-N5-C4A	2.06	121.42	118.09

There are no chirality outliers.

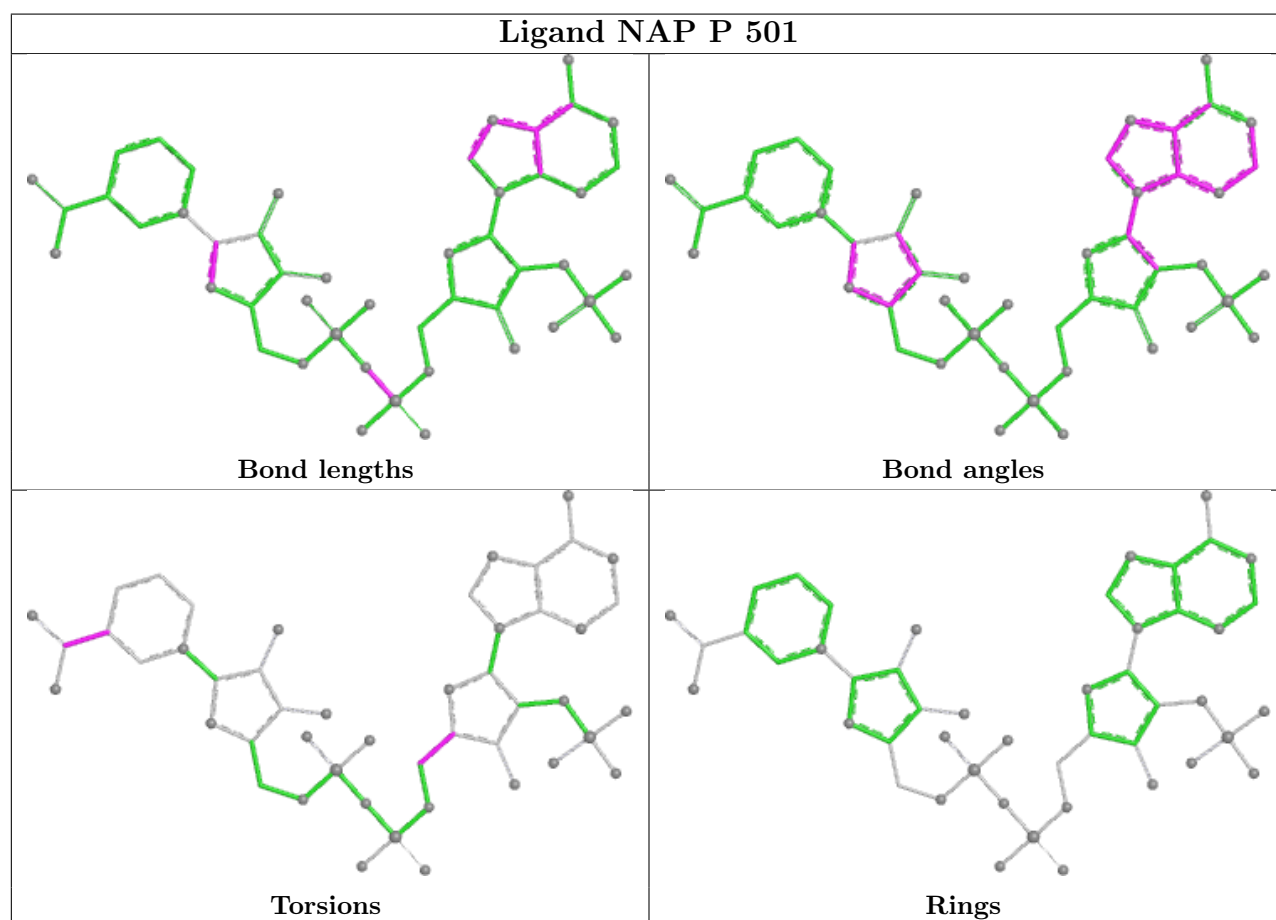
All (15) torsion outliers are listed below:

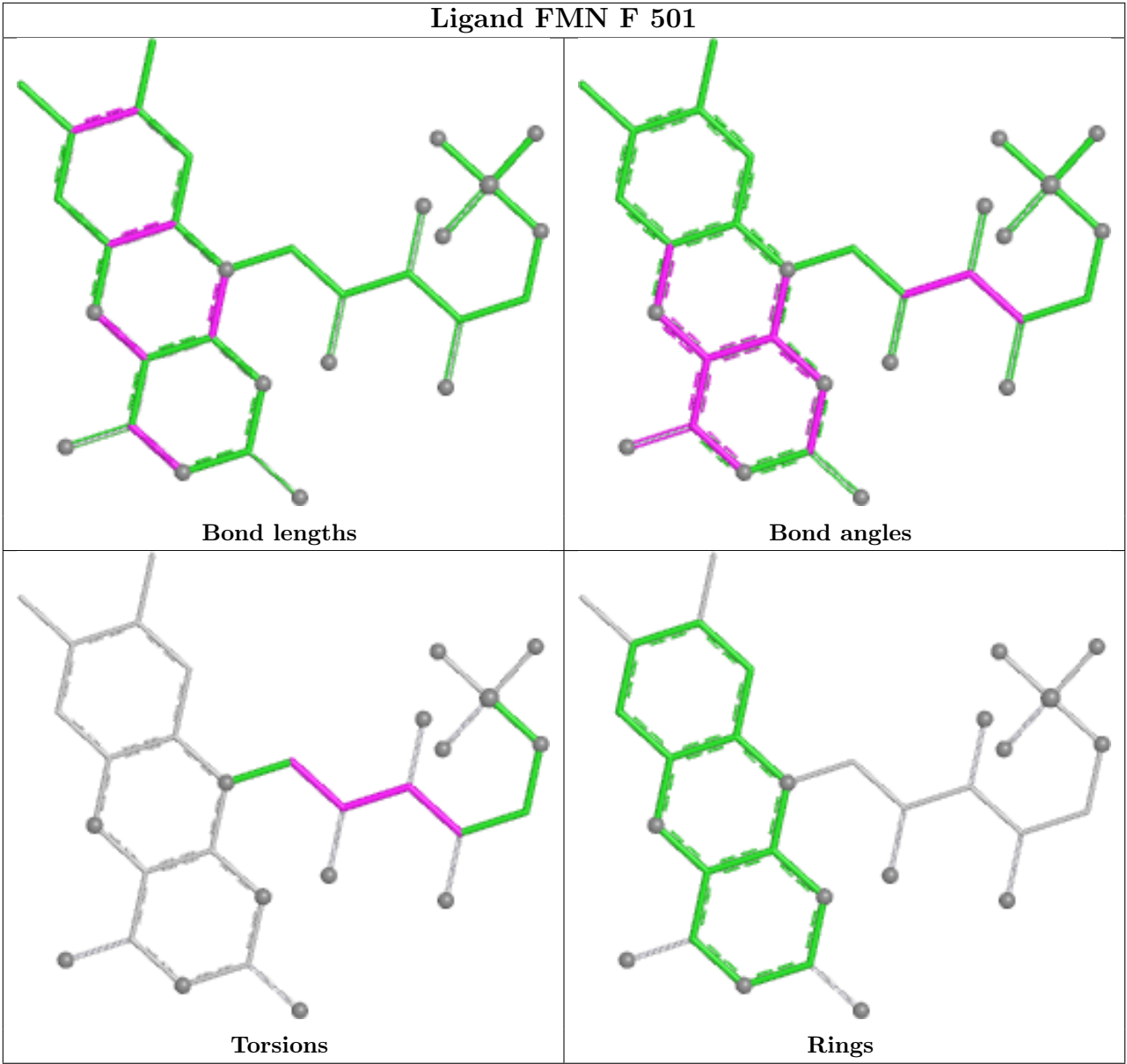
Mol	Chain	Res	Type	Atoms
47	F	501	FMN	N10-C1'-C2'-O2'
47	F	501	FMN	N10-C1'-C2'-C3'
47	F	501	FMN	C1'-C2'-C3'-O3'
47	F	501	FMN	C1'-C2'-C3'-C4'
47	F	501	FMN	C2'-C3'-C4'-C5'
47	F	501	FMN	O3'-C3'-C4'-C5'
48	P	501	NAP	C2N-C3N-C7N-O7N
48	P	501	NAP	C2N-C3N-C7N-N7N
48	P	501	NAP	C4N-C3N-C7N-O7N
48	P	501	NAP	C4N-C3N-C7N-N7N
47	F	501	FMN	O3'-C3'-C4'-O4'
47	F	501	FMN	C2'-C3'-C4'-O4'
48	P	501	NAP	O4B-C4B-C5B-O5B
48	P	501	NAP	C3B-C4B-C5B-O5B
47	F	501	FMN	O2'-C2'-C3'-O3'

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

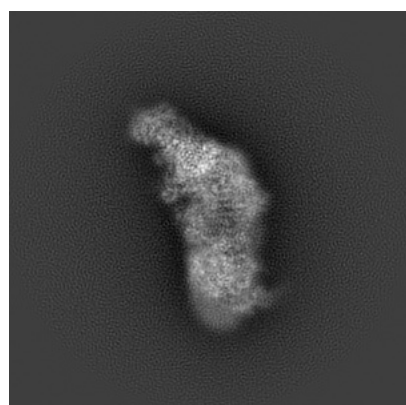
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3731. These allow visual inspection of the internal detail of the map and identification of artifacts.

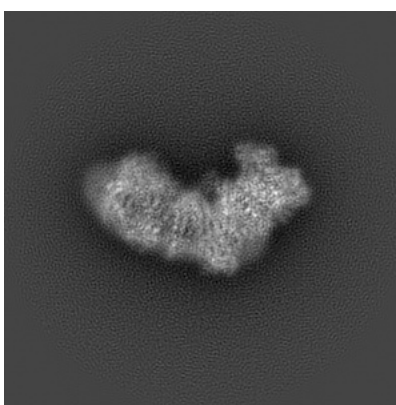
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

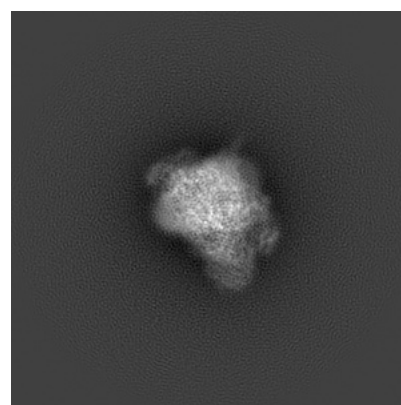
6.1.1 Primary map



X



Y

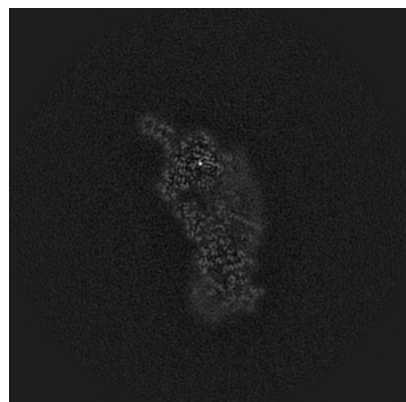


Z

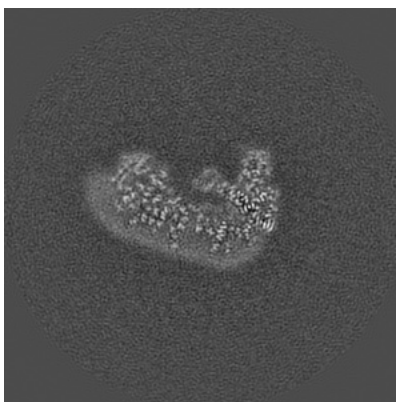
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

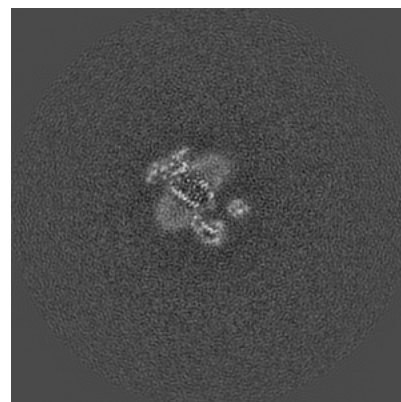
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

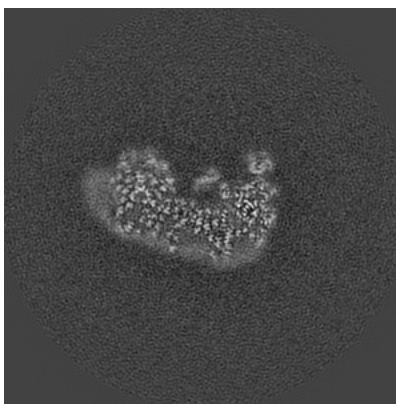
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

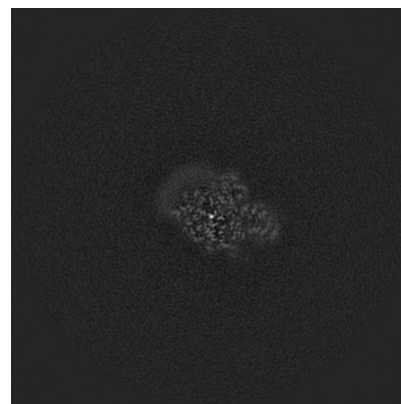
6.3.1 Primary map



X Index: 185



Y Index: 184

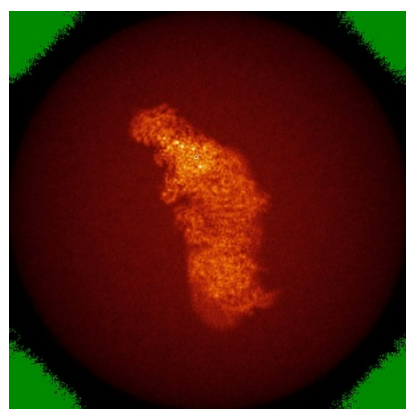


Z Index: 219

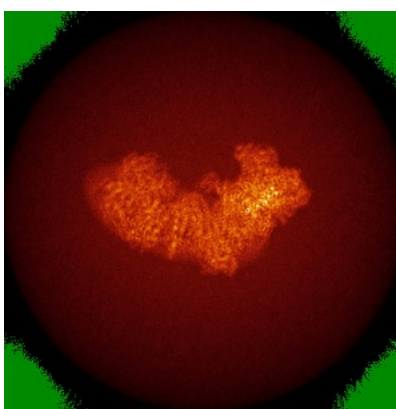
The images above show the largest variance slices of the map in three orthogonal directions.

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

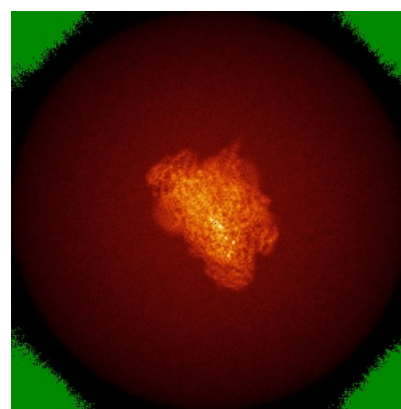
6.4.1 Primary map



X



Y

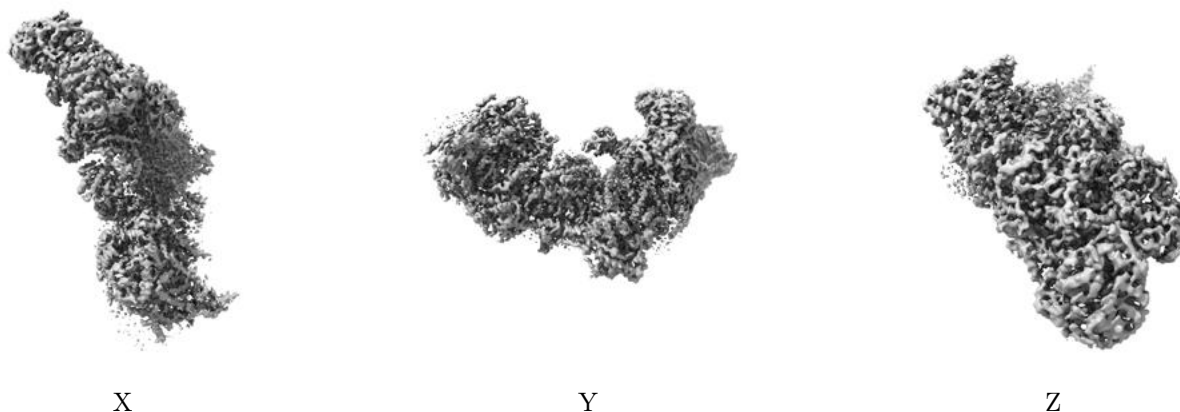


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

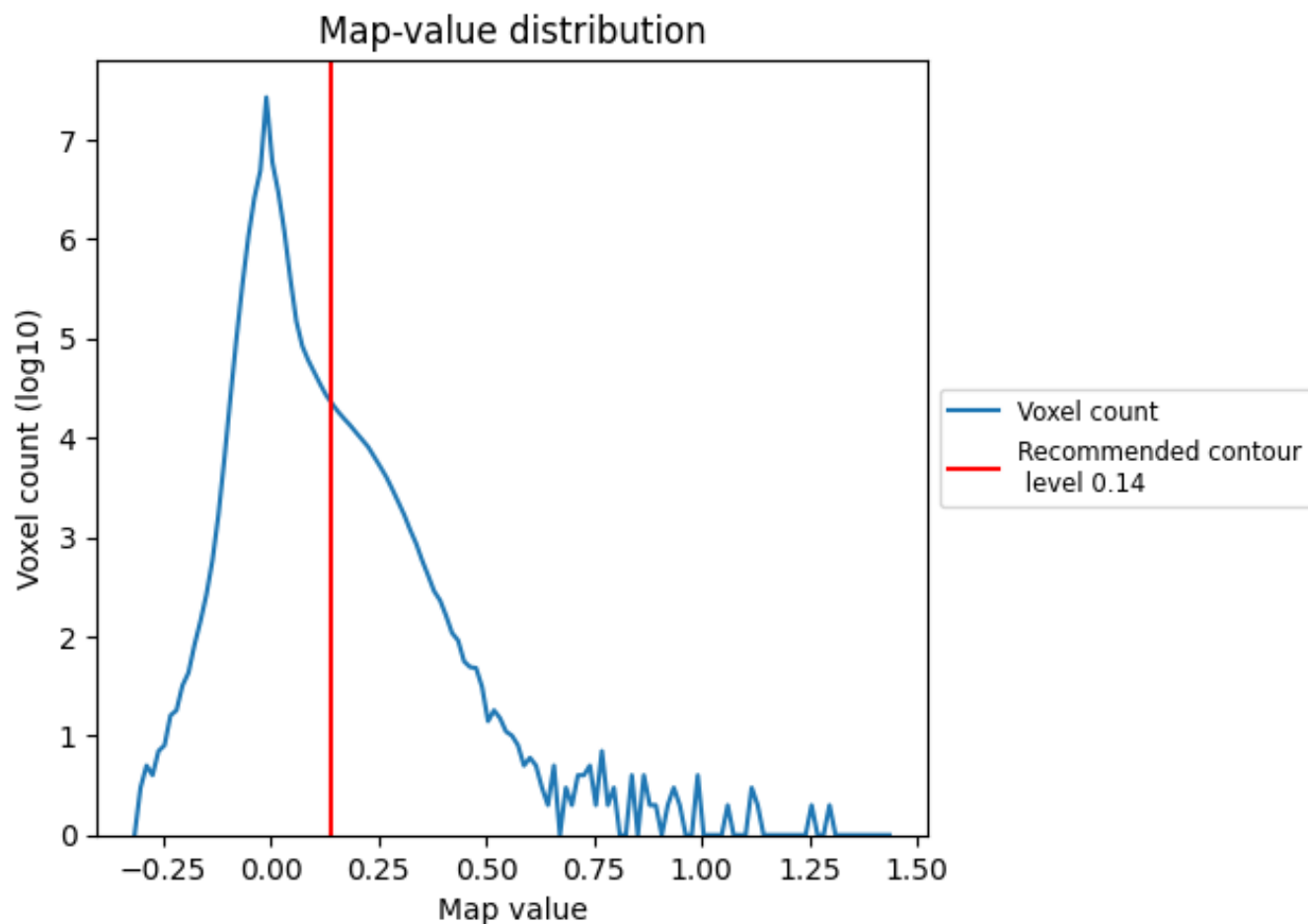
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

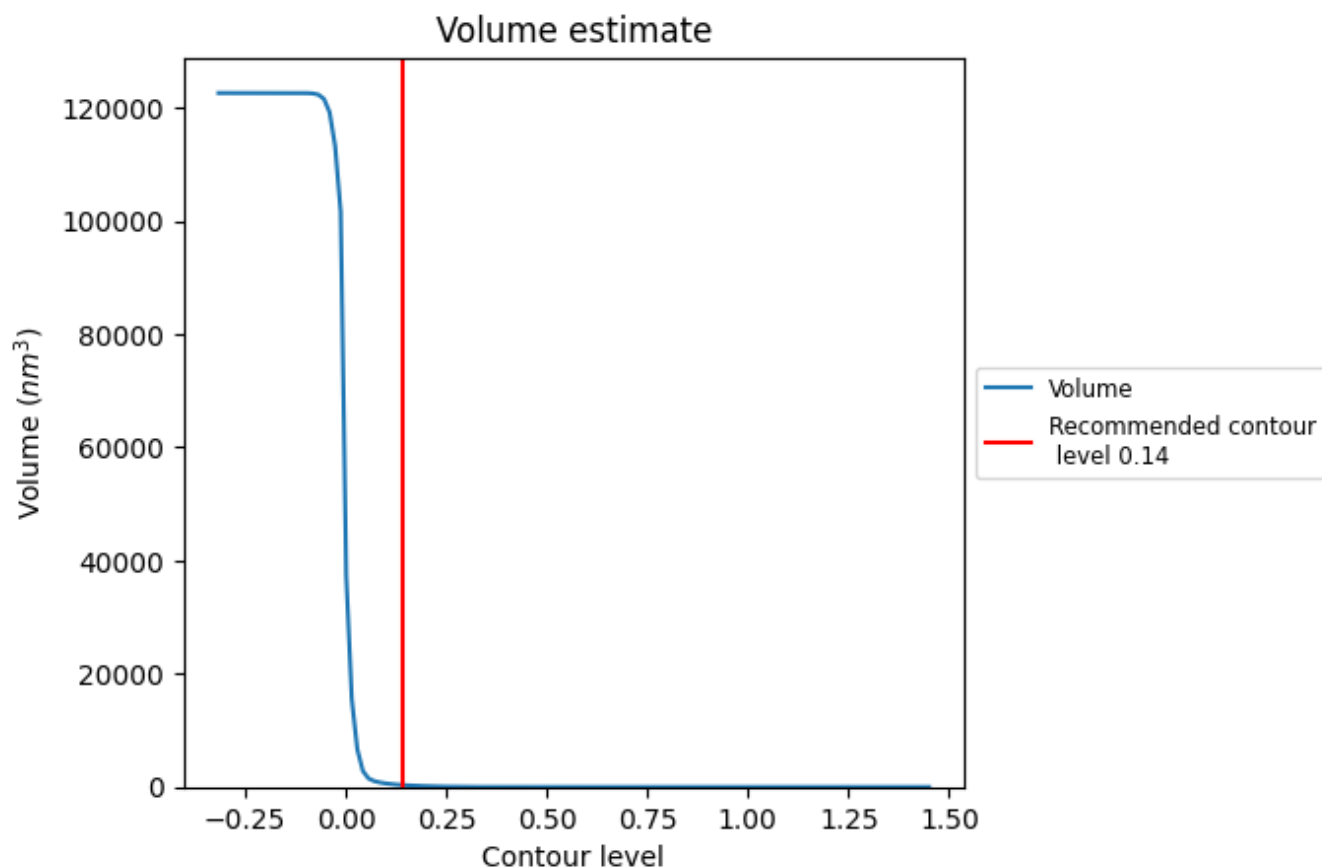
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

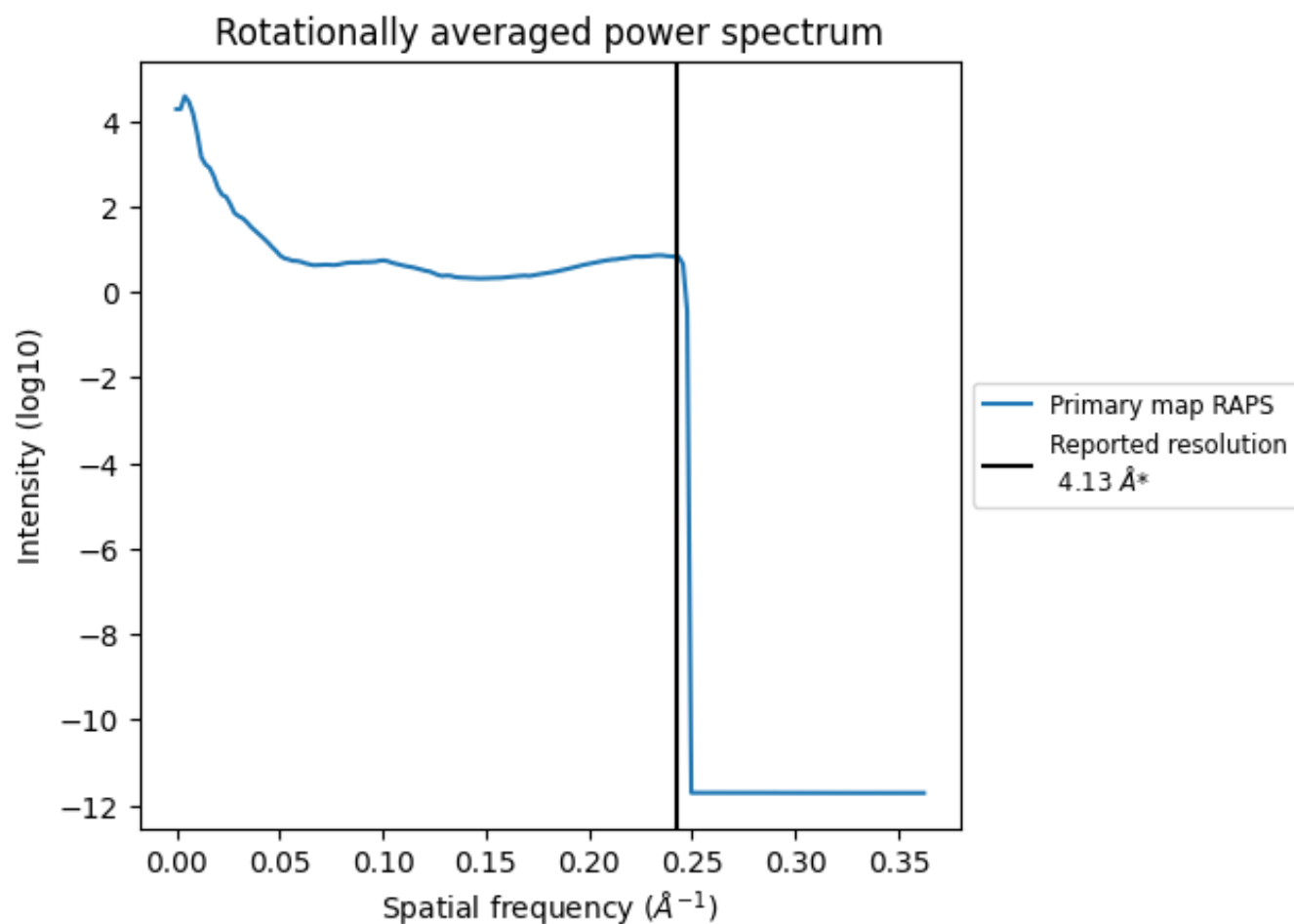
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 341 nm³; this corresponds to an approximate mass of 308 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

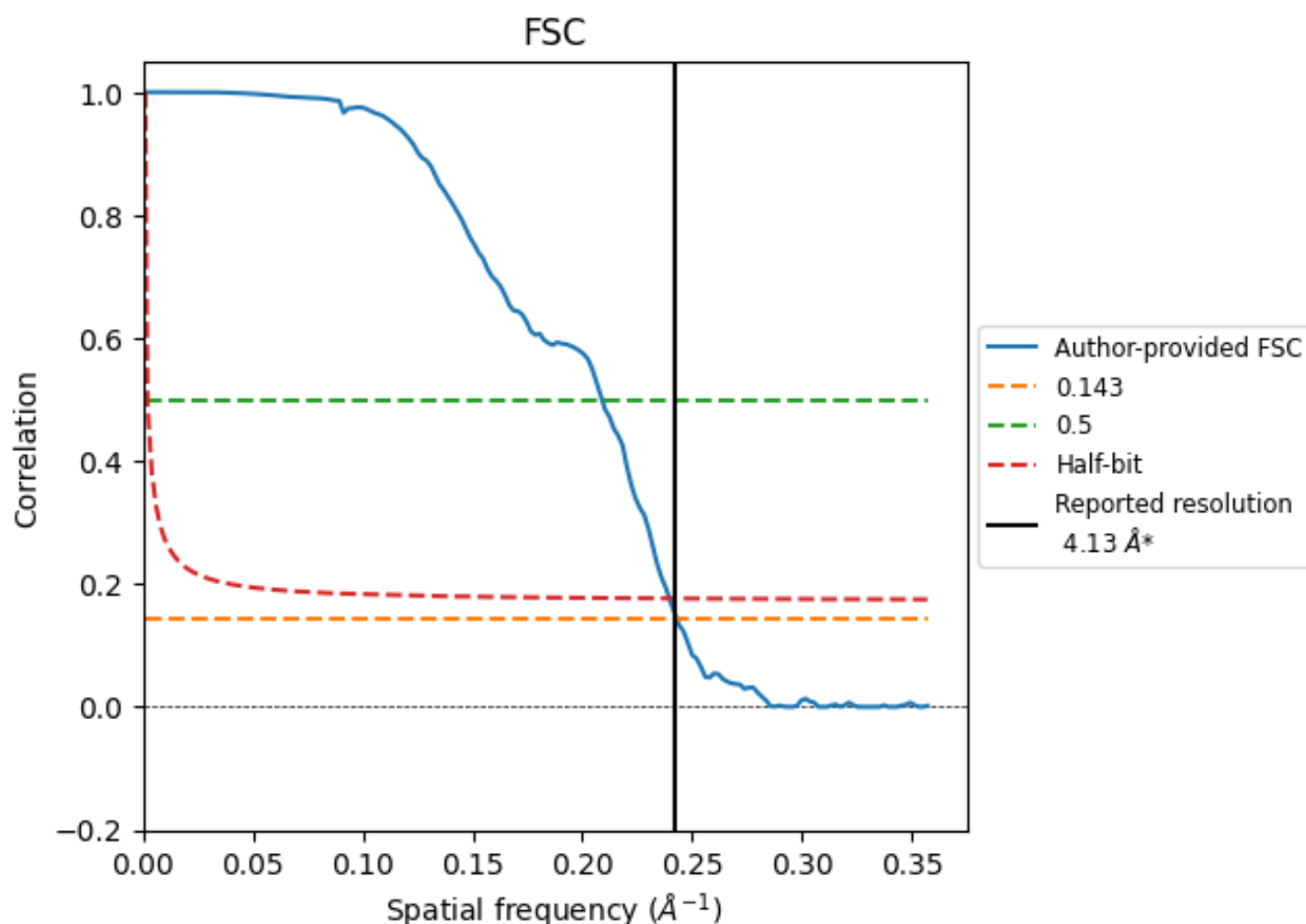


*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.242 Å⁻¹

8.2 Resolution estimates [i](#)

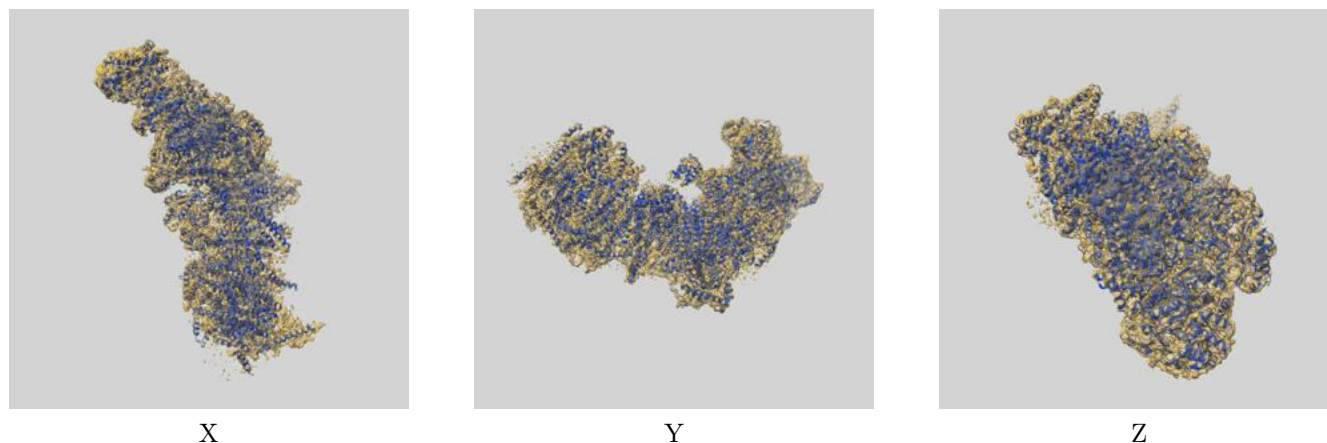
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.13	-	-
Author-provided FSC curve	4.12	4.79	4.17
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

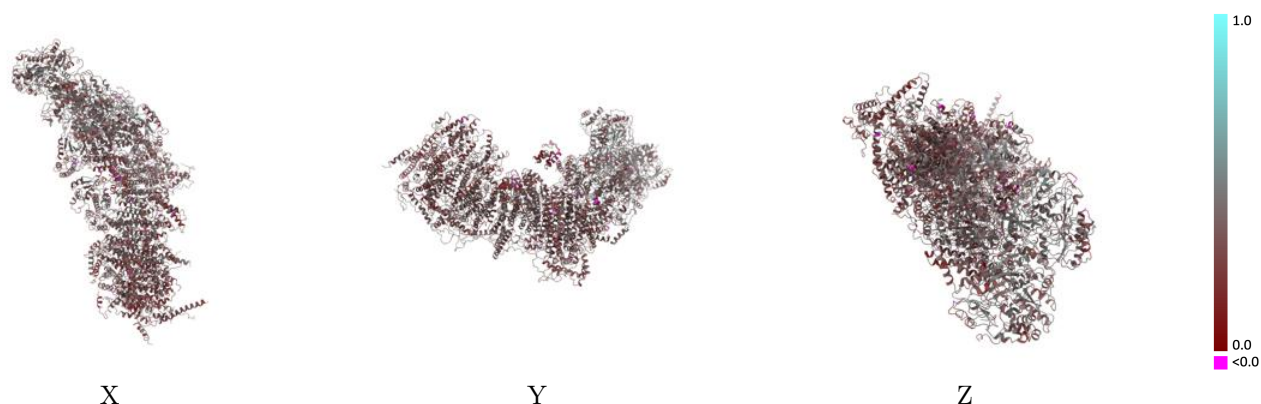
This section contains information regarding the fit between EMDB map EMD-3731 and PDB model 5O31. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



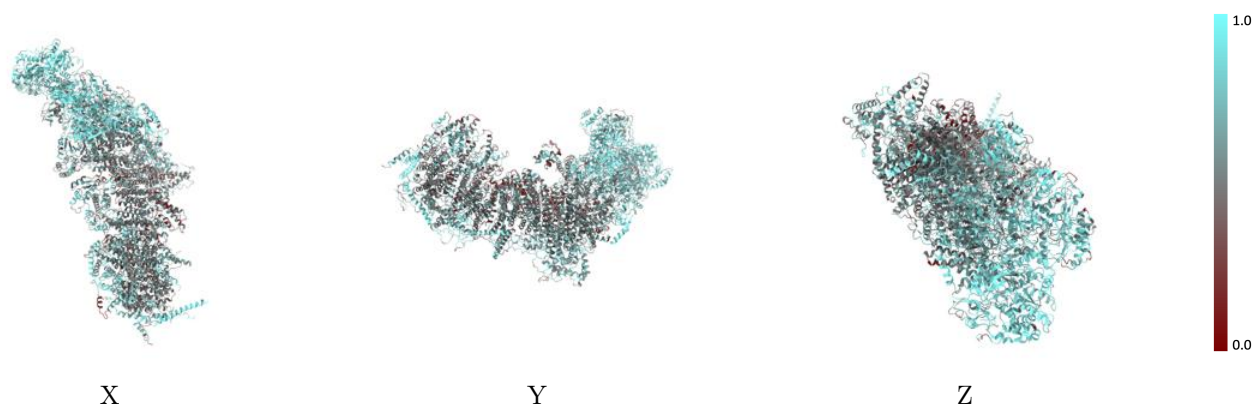
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



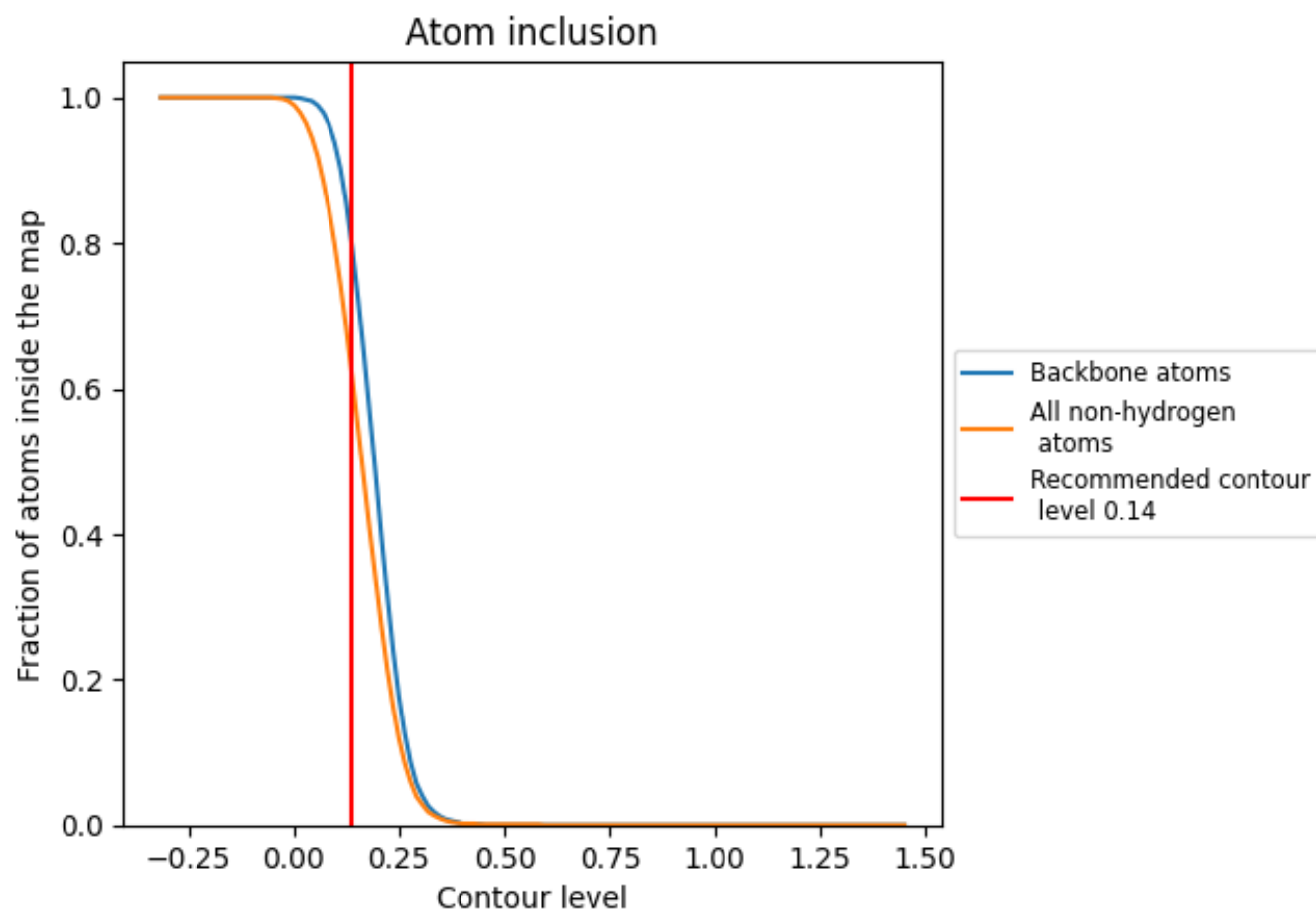
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.3520
A	 0.4960	 0.3340
B	 0.6270	 0.3750
C	 0.6200	 0.3630
D	 0.5790	 0.3670
E	 0.8250	 0.3910
F	 0.7540	 0.3810
G	 0.7150	 0.4050
H	 0.5480	 0.3440
I	 0.6600	 0.3640
J	 0.4490	 0.3140
K	 0.5040	 0.3370
L	 0.5000	 0.3090
M	 0.5320	 0.3380
N	 0.5570	 0.3570
O	 0.6280	 0.3600
P	 0.7590	 0.3960
Q	 0.7600	 0.4360
R	 0.6500	 0.3840
S	 0.8000	 0.3670
T	 0.4730	 0.2310
U	 0.7080	 0.3610
V	 0.6000	 0.3240
W	 0.5680	 0.3170
X	 0.6160	 0.3260
Y	 0.3870	 0.2820
Z	 0.6200	 0.3070
a	 0.5780	 0.3040
b	 0.5900	 0.3400
c	 0.5680	 0.3070
d	 0.6090	 0.3510
e	 0.6270	 0.3740
f	 0.5350	 0.3320
g	 0.5290	 0.3170
h	 0.7120	 0.3780



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Chain	Atom inclusion	Q-score
i	 0.6000	 0.3200
j	 0.7610	 0.3600
k	 0.6190	 0.3300
l	 0.7030	 0.3560
m	 0.5360	 0.3130
n	 0.6340	 0.3350
o	 0.8350	 0.3210
p	 0.6790	 0.3570
q	 0.7960	 0.4070
r	 0.7190	 0.3920
s	 0.7850	 0.3820