wwPDB EM Validation Summary Report (i)

Nov 10, 2024 – 03:38 pm GMT

PDB ID	:	6RFS
EMDB ID	:	EMD-4874
Title	:	Cryo-EM structure of a respiratory complex I mutant lacking NDUFS4
Authors	:	Parey, K.; Vonck, J.
Deposited on	:	2019-04-16
Resolution	:	4.04 Å(reported)

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

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

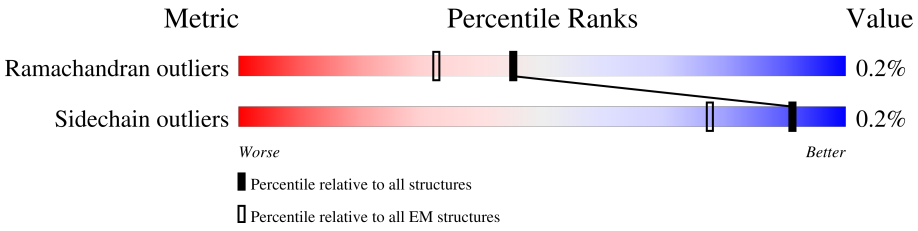
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.04 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	728	14% 94% • 5%
2	B	488	17% 93% • 7%
3	C	466	9% 81% • 17%
4	D	87	22% 99% •
5	E	375	25% 88% 12%
6	F	144	9% 84% 16%
7	G	281	12% 84% • 15%
8	H	243	17% 87% • 12%
9	I	229	10% 82% • 17%

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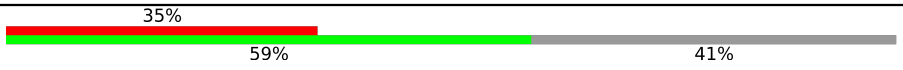
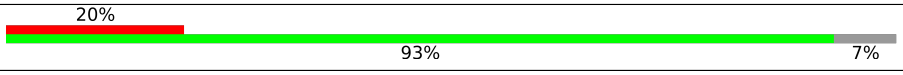
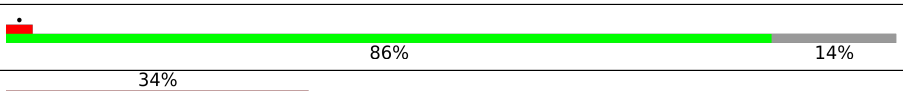
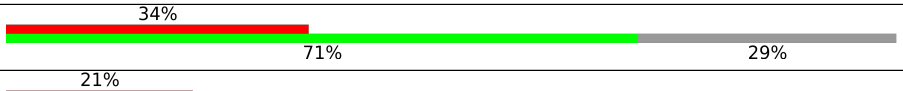
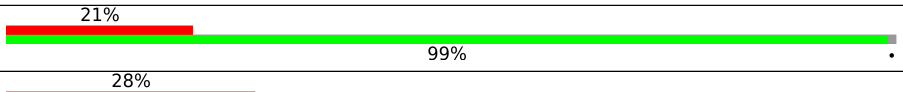
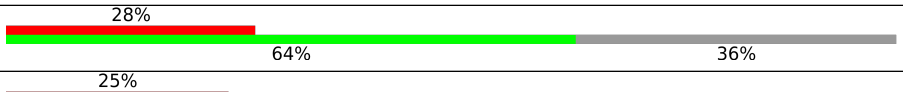
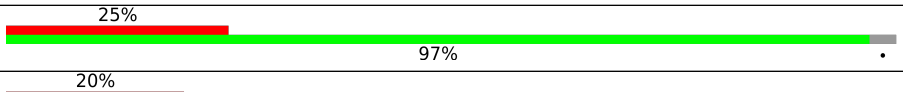
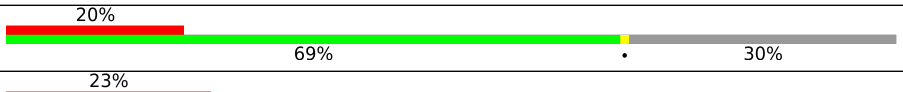
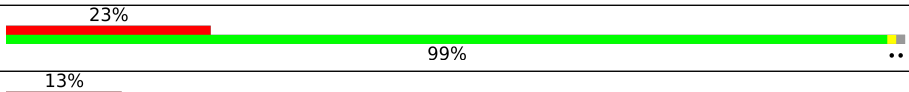
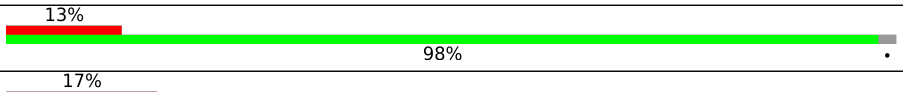
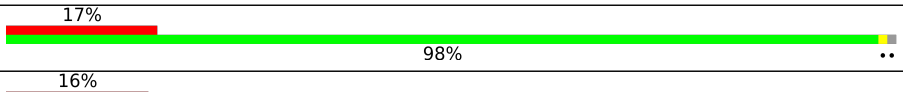
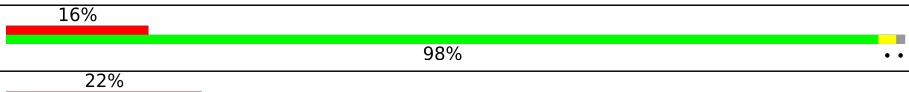
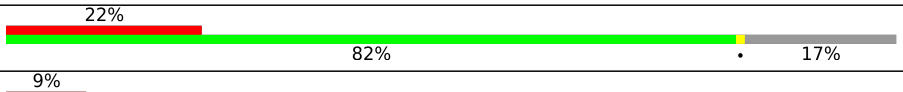
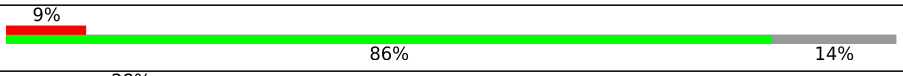
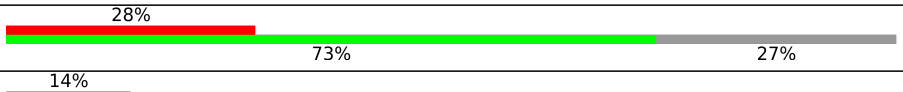
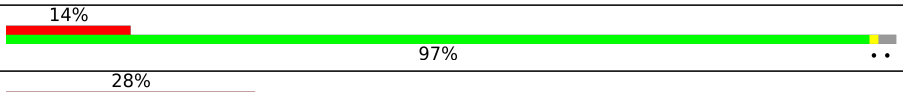
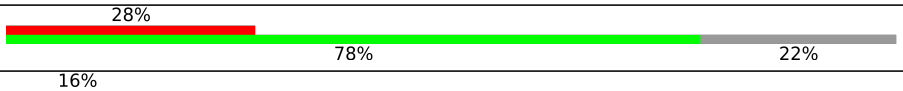
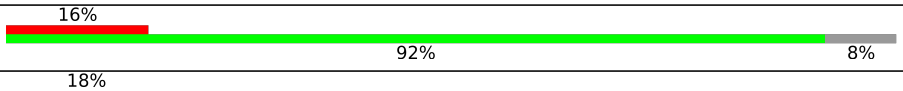
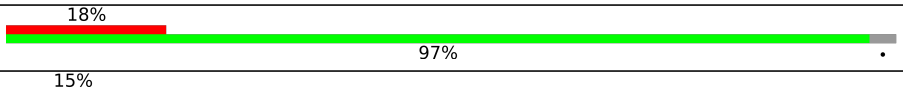
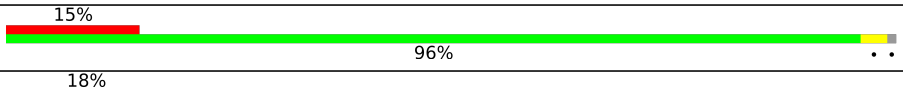
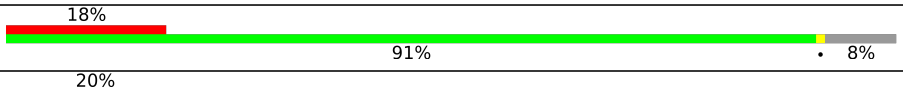
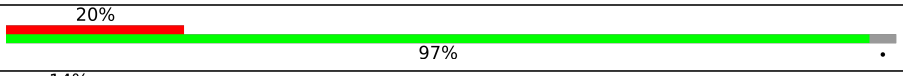
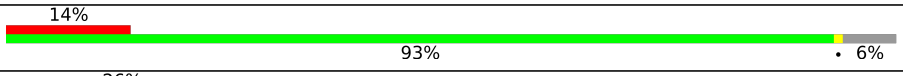
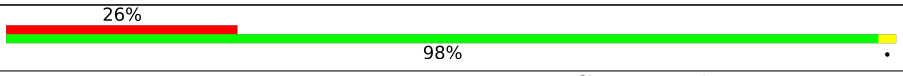
Mol	Chain	Length	Quality of chain
10	J	198	
11	K	210	
12	L	89	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	249	
19	U	172	
20	W	123	
21	X	169	
22	Z	182	
23	a	149	
24	b	74	
25	c	60	
26	d	92	
27	e	67	
28	f	87	
29	g	78	
30	h	138	
31	i	90	
32	j	93	
33	n	120	
34	1	341	

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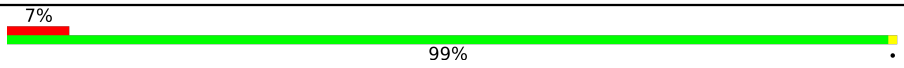
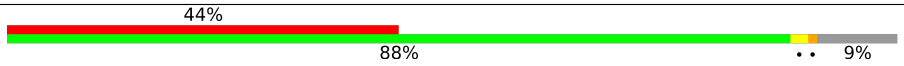
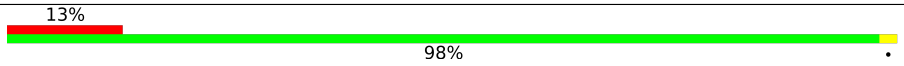
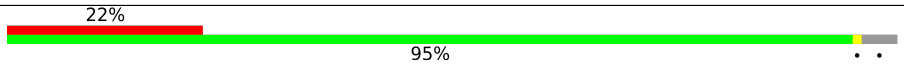
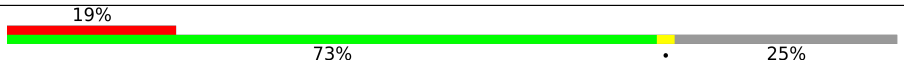
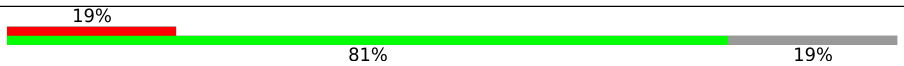
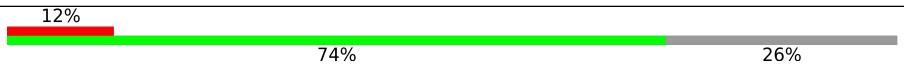
Mol	Chain	Length	Quality of chain
35	2	469	
36	3	128	
37	4	486	
38	5	655	
39	6	185	
40	8	99	
41	9	89	

2 Entry composition (i)

There are 47 unique types of molecules in this entry. The entry contains 60966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	692	5258	3263	926	1040	29	0	0

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	456	3528	2229	621	654	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	387	3052	1948	522	561	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	86	682	432	127	120	3	0	0

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	331	2650	1683	464	494	9	0	0

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Com-

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total 990	C 629	N 166	O 193	S 2	0	0

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total 1978	C 1272	N 336	O 366	S 4	0	0

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	213	Total 1664	C 1043	N 279	O 324	S 18	0	0

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total 1519	C 966	N 254	O 289	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	116	Total 790	C 495	N 146	O 147	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	170	Total 1347	C 857	N 236	O 239	S 15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	83	Total	C	N	O	S	0	0
			645	434	102	106	3		

- Molecule 13 is a protein called Subunit NUMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1037	667	182	186	2		

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	106	Total	C	N	O	S	0	0
			885	562	168	152	3		

- Molecule 18 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 19 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	171	Total	C	N	O	S	0	0
			1346	847	236	253	10		

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 21 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1300	842	222	232	4		

- Molecule 22 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	181	Total	C	N	O	S	0	0
			1390	893	240	256	1		

- Molecule 23 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 24 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

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

- Molecule 25 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 26 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	90	Total	C	N	O	S	0	0
			761	472	137	149	3		

- Molecule 27 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 28 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 29 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
29	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 30 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 31 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 32 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
32	j	90	Total	C	N	O	0	0
			724	465	132	127		

- Molecule 33 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	113	Total	C	N	O	S	0	0
			904	582	153	168	1		

- Molecule 34 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	340	Total	C	N	O	S	0	0
			2682	1826	393	456	7		

- Molecule 35 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	469	Total	C	N	O	S	0	0
			3775	2557	550	656	12		

- Molecule 36 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	116	Total	C	N	O	S	0	0
			911	623	136	150	2		

- Molecule 37 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	486	Total	C	N	O	S	0	0
			3856	2600	586	655	15		

- Molecule 38 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	632	Total	C	N	O	S	0	0
			4954	3306	756	867	25		

- Molecule 39 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6	138	Total	C	N	O	S	0	0
			1096	752	154	183	7		

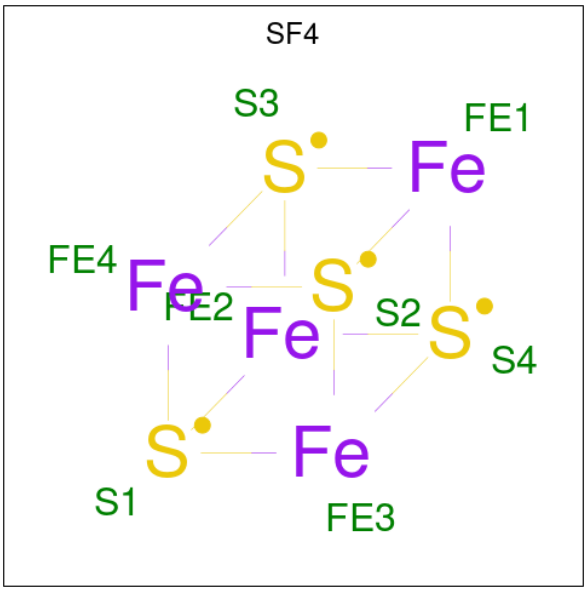
- Molecule 40 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	8	80	Total	C	N	O	S	0	0
			662	420	120	114	8		

- Molecule 41 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

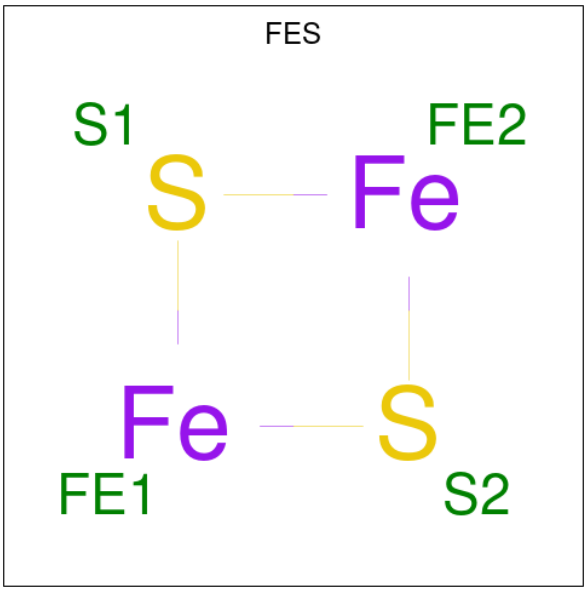
Mol	Chain	Residues	Atoms					AltConf	Trace
41	9	66	Total	C	N	O	S	0	0
			528	325	99	98	6		

- Molecule 42 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



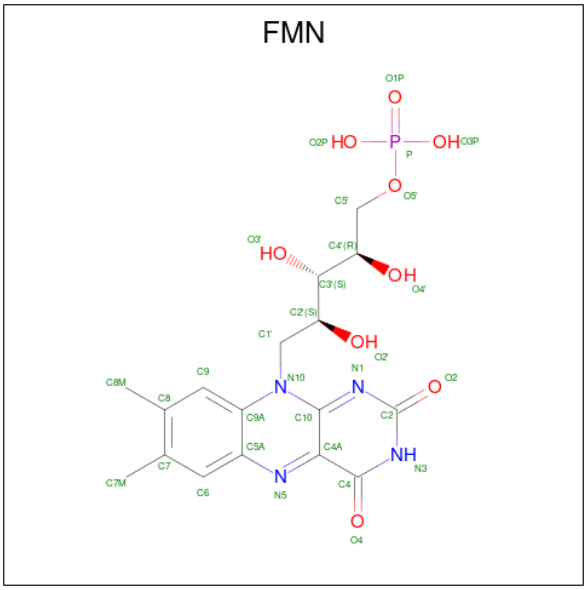
Mol	Chain	Residues	Atoms	AltConf
42	A	1	Total Fe S 8 4 4	0
42	A	1	Total Fe S 8 4 4	0
42	B	1	Total Fe S 8 4 4	0
42	I	1	Total Fe S 8 4 4	0
42	I	1	Total Fe S 8 4 4	0
42	K	1	Total Fe S 8 4 4	0

- Molecule 43 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			4	2	2	
43	H	1	Total	Fe	S	0
			4	2	2	

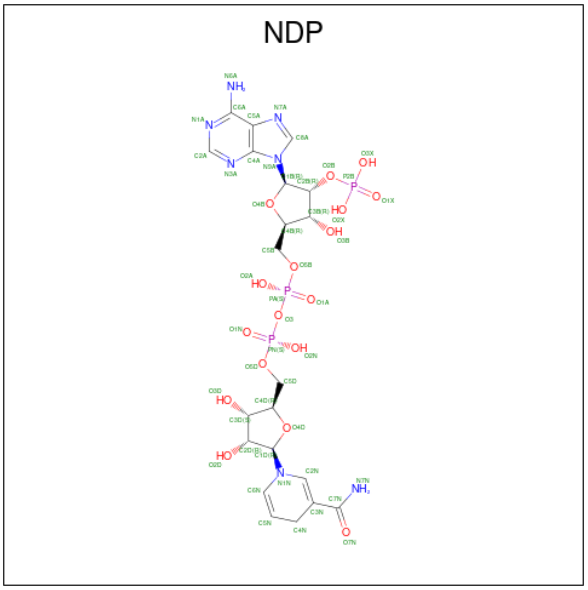
- Molecule 44 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 45 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	M	1	Total	Zn	0
			1	1	

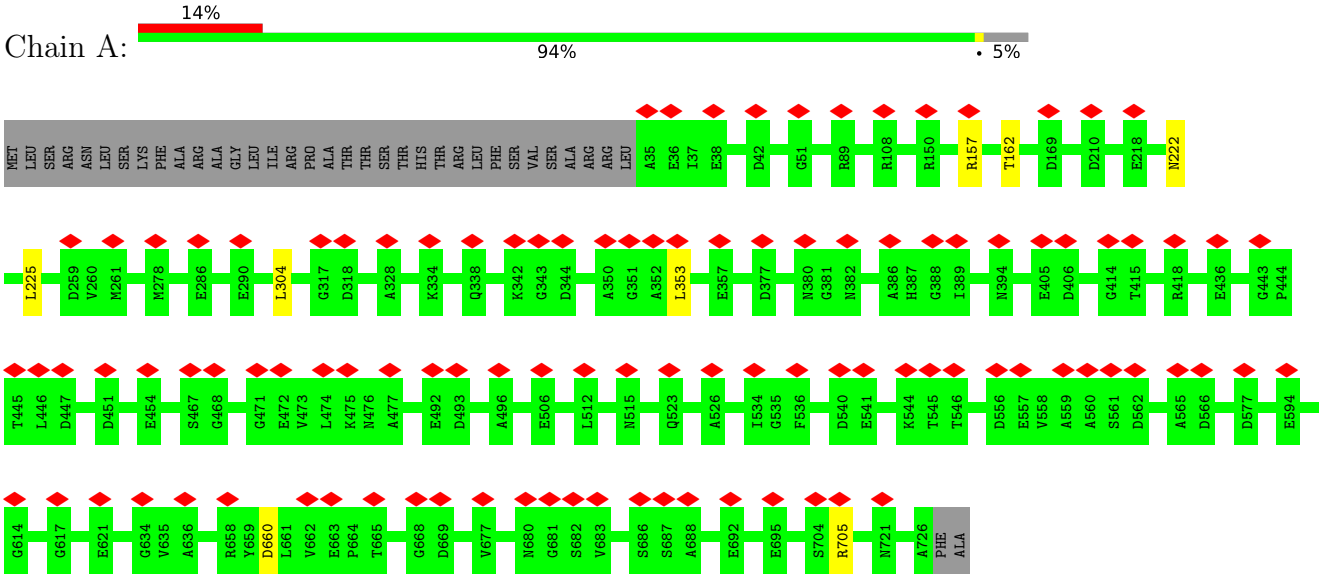
- Molecule 47 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

Mol	Chain	Residues	Atoms						AltConf
47	O	1	Total	C	N	O	P	S	0
			30	19	2	7	1	1	

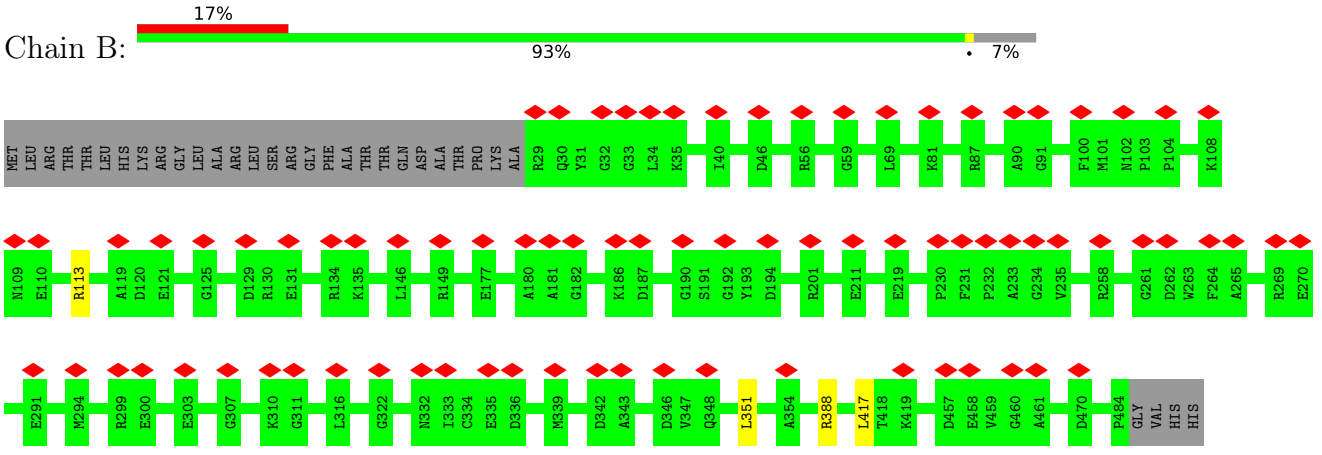
3 Residue-property plots (i)

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.

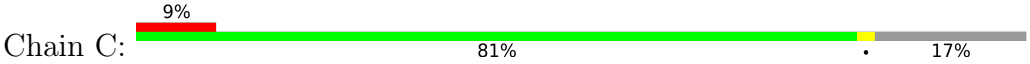
• Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

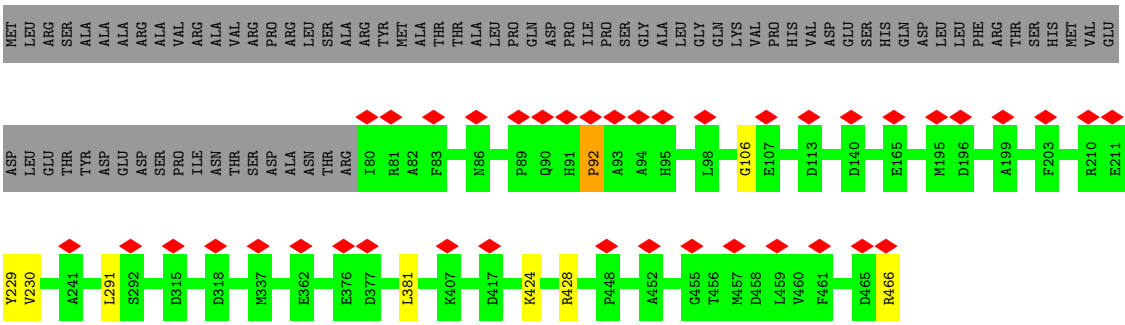


• Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)



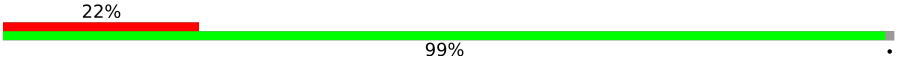
• Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

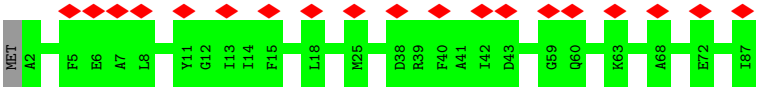




• Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

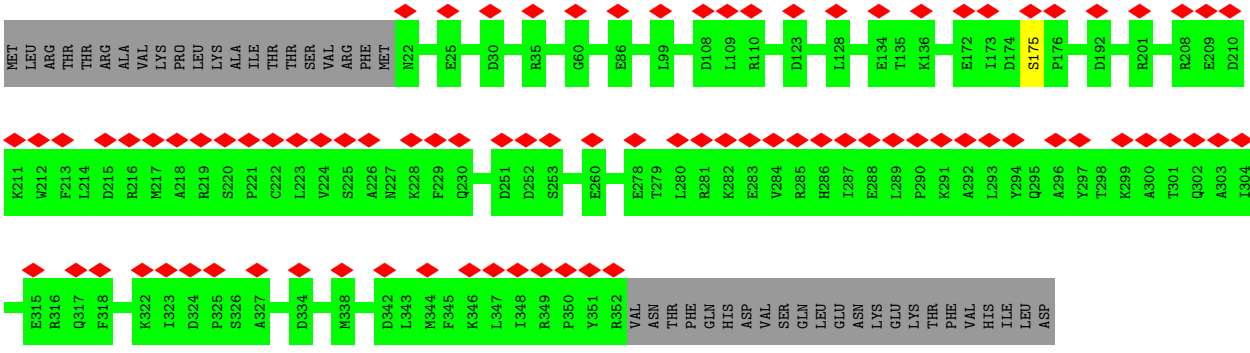
Chain D:





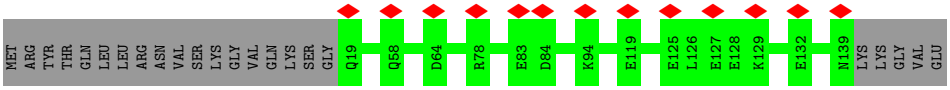
• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain E:



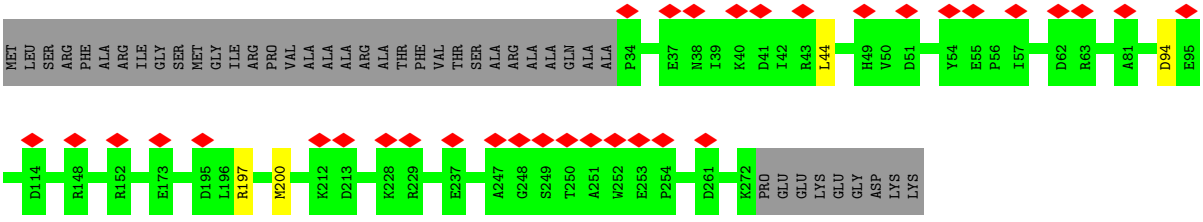
• Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain F:



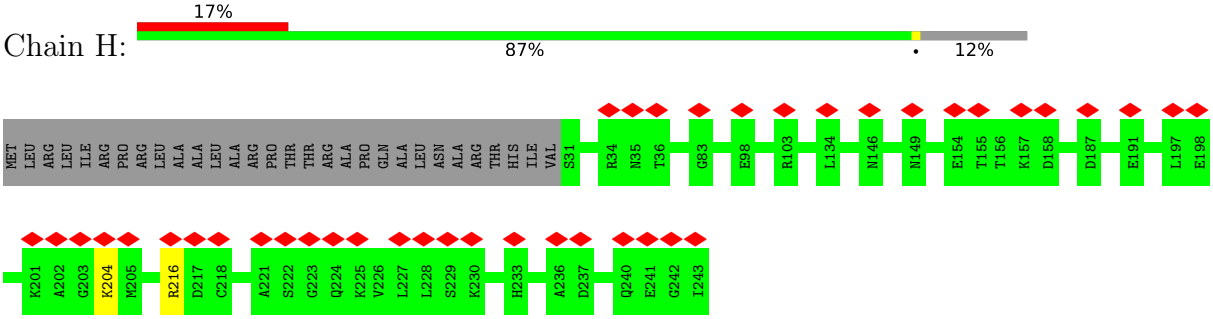
• Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain G:



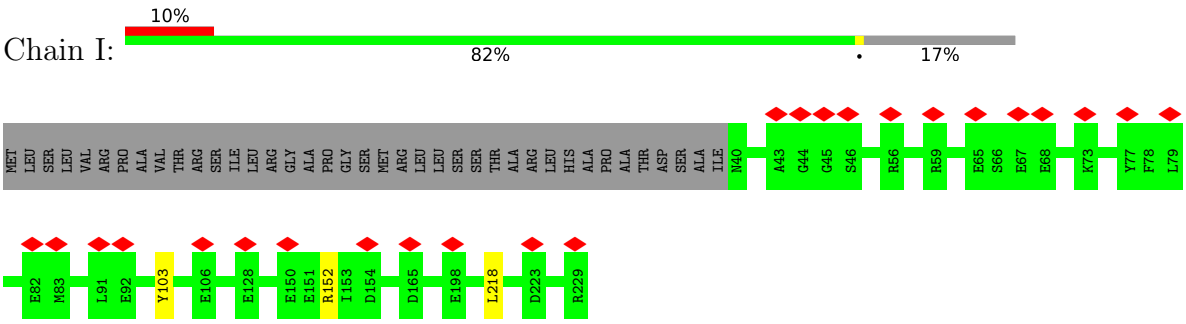
• Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain H:



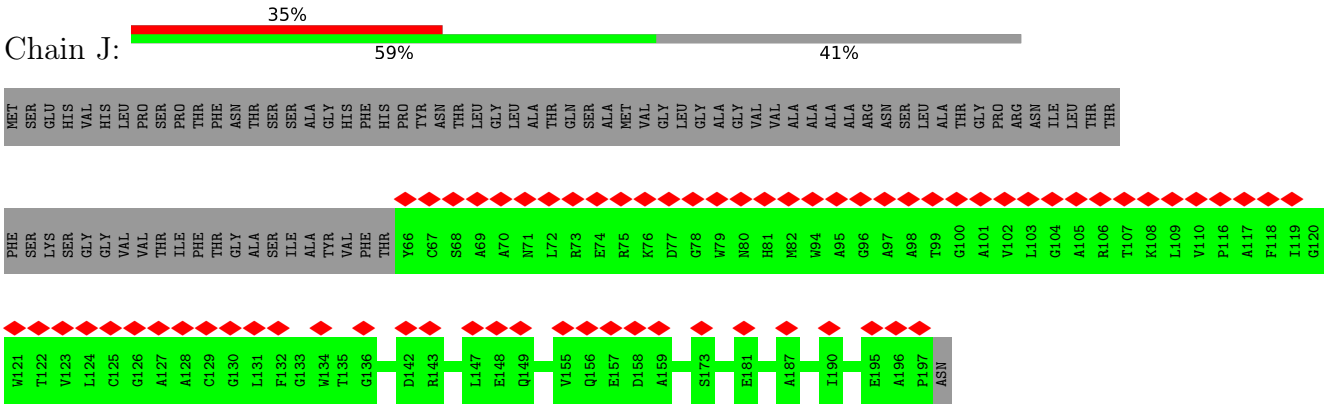
• Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain I:



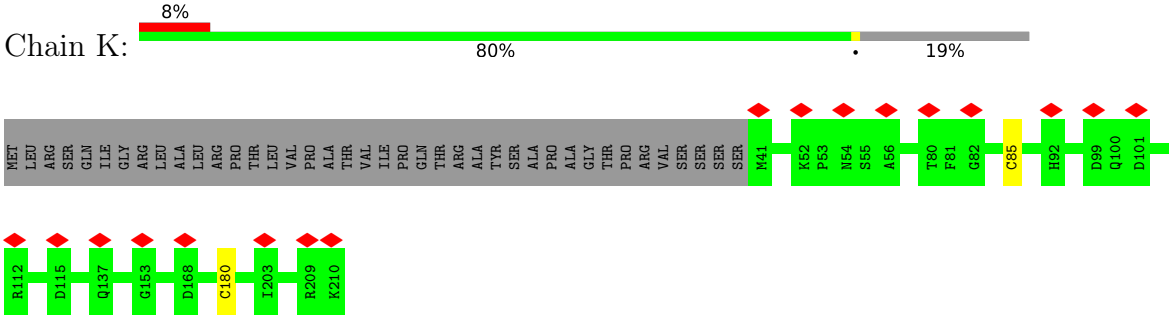
• Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain J:



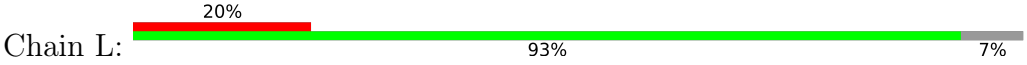
• Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

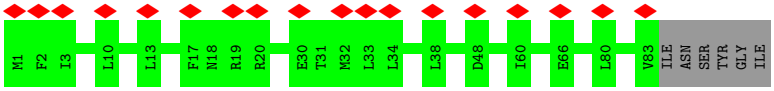
Chain K:



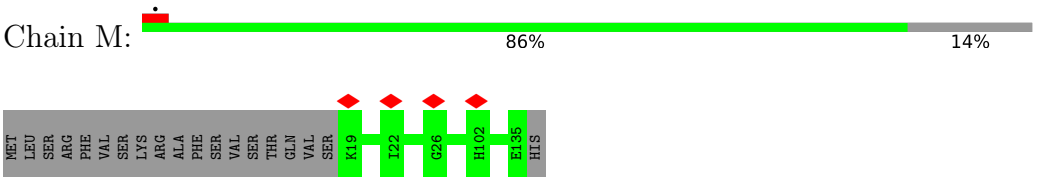
• Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain L:

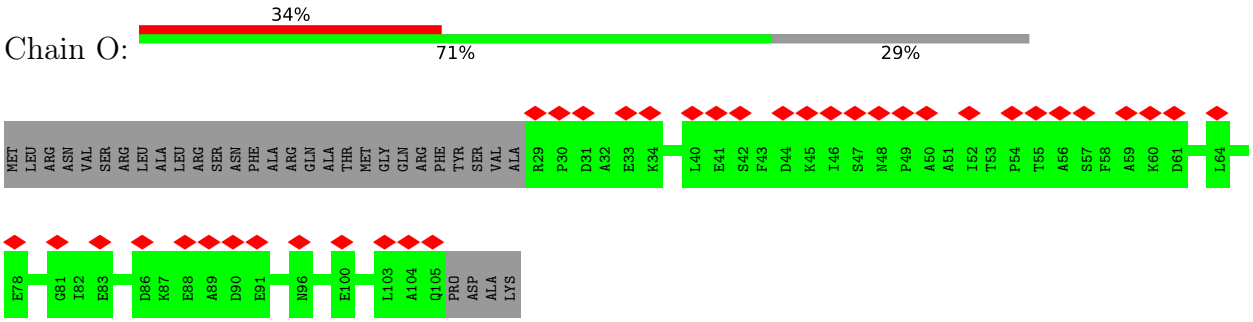




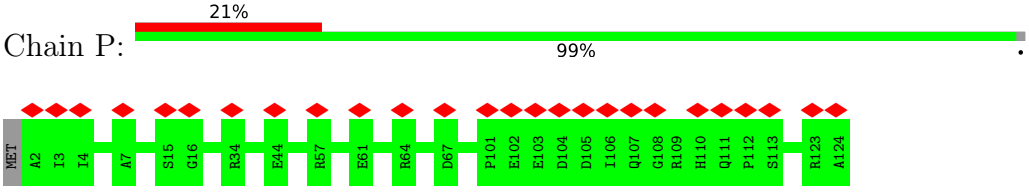
• Molecule 13: Subunit NUMM of NADH:Ubiquinone Oxidoreductase (Complex I)



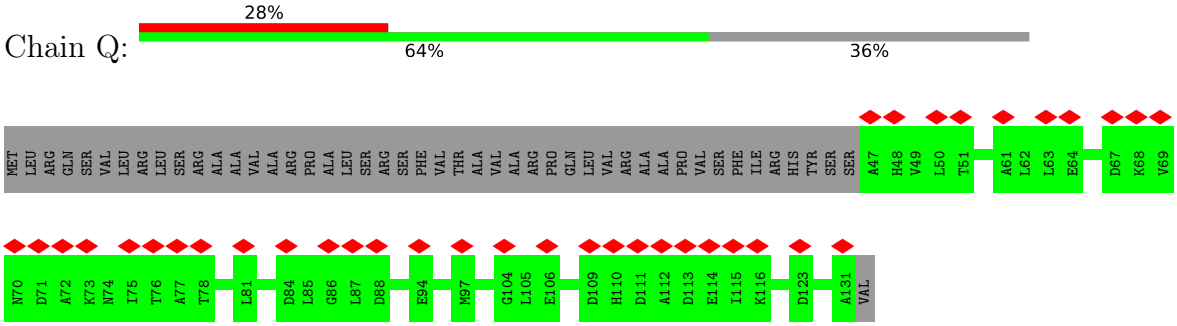
• Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



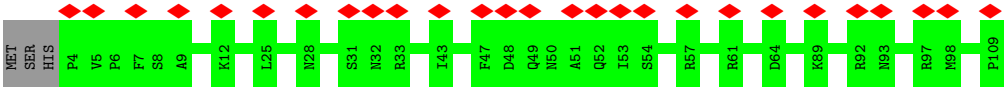
• Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



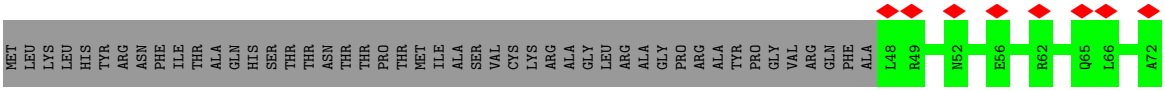
• Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

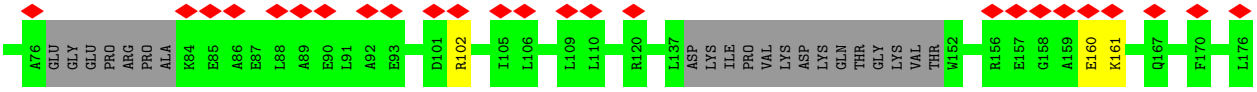


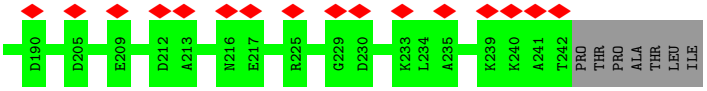
• Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



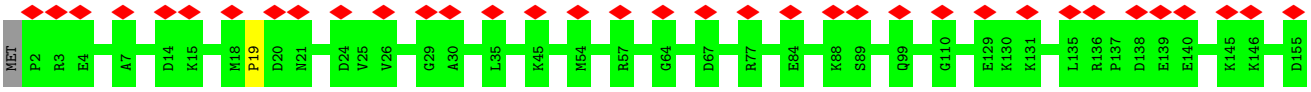
• Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

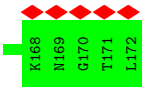




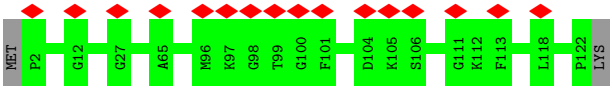


• Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

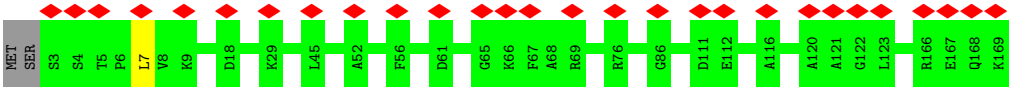




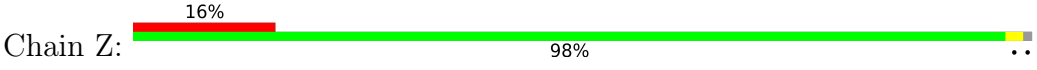
• Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

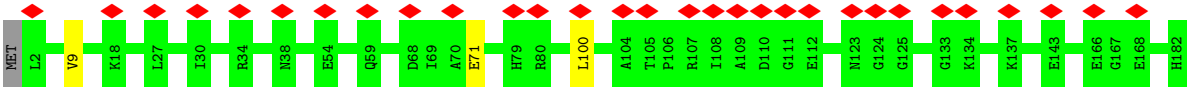


• Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)



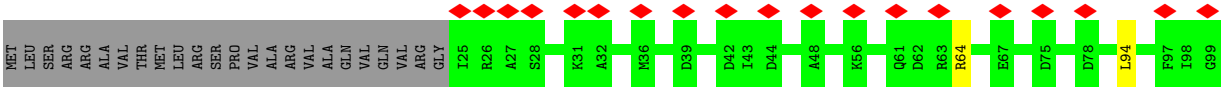
• Molecule 22: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

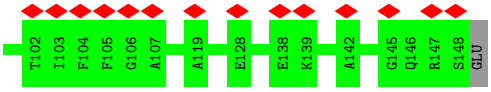




• Molecule 23: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)

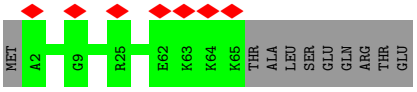
Chain a:





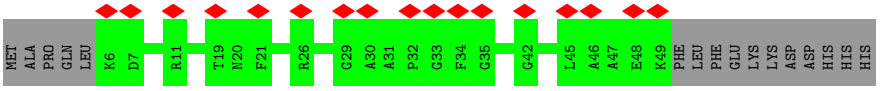
• Molecule 24: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:



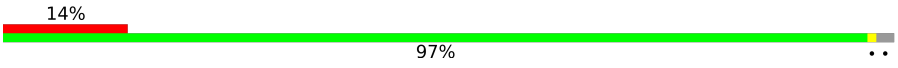
• Molecule 25: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

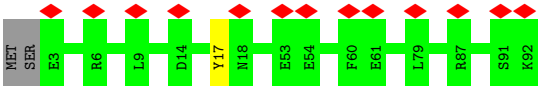
Chain c:



• Molecule 26: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

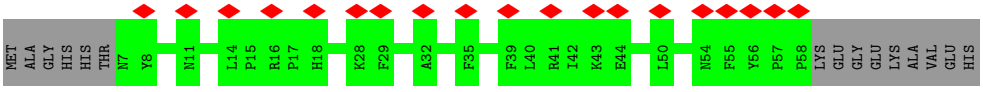
Chain d:





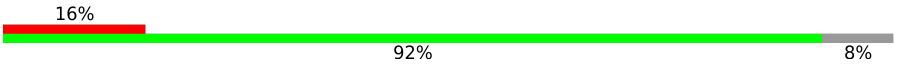
• Molecule 27: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

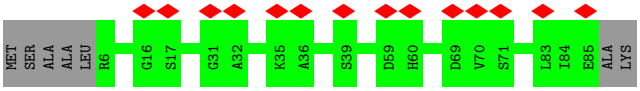
Chain e:



• Molecule 28: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

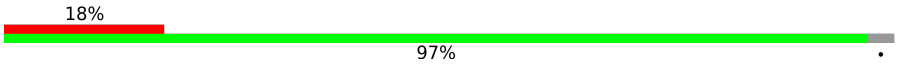
Chain f:

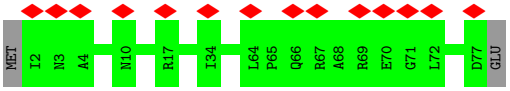




• Molecule 29: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)

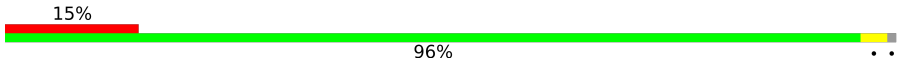
Chain g:

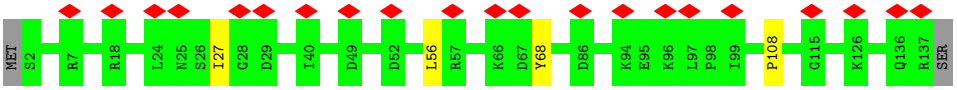




• Molecule 30: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

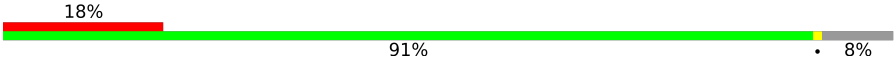
Chain h:

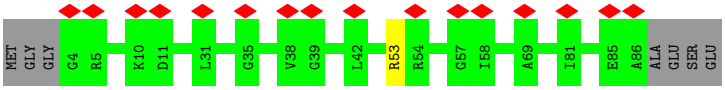




• Molecule 31: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

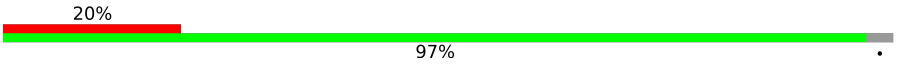
Chain i:

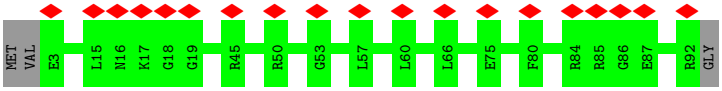




• Molecule 32: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

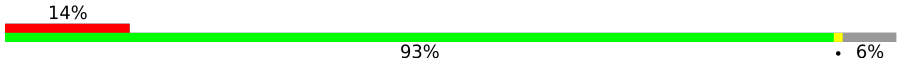
Chain j:

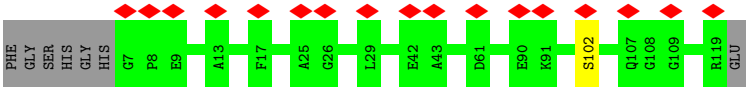




• Molecule 33: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)

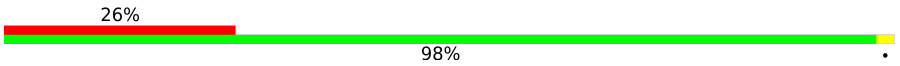
Chain n:

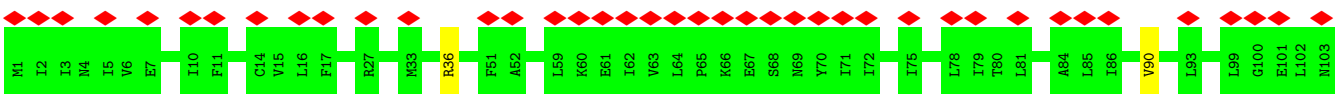


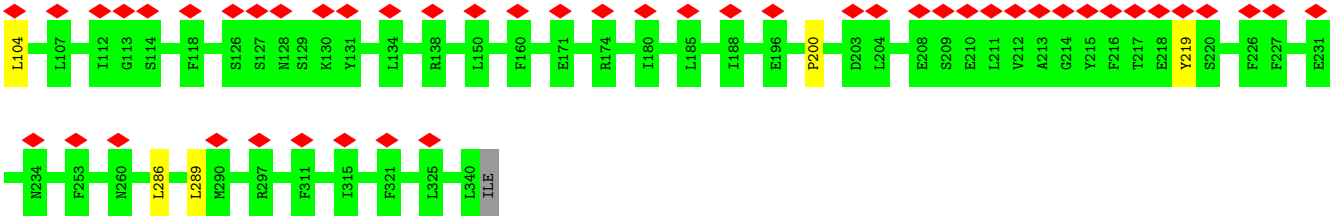


• Molecule 34: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

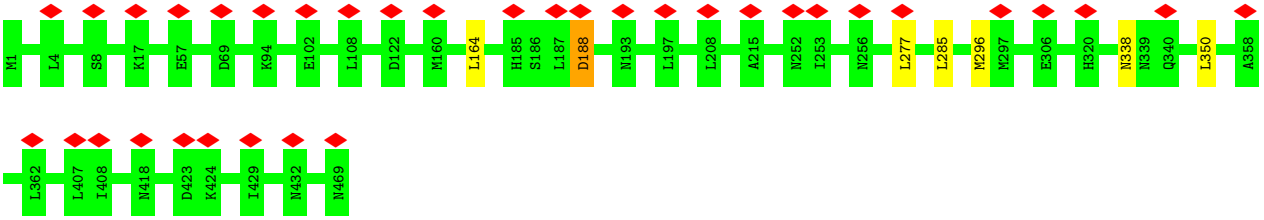
Chain 1:



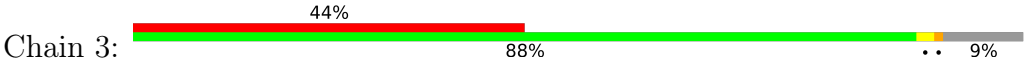


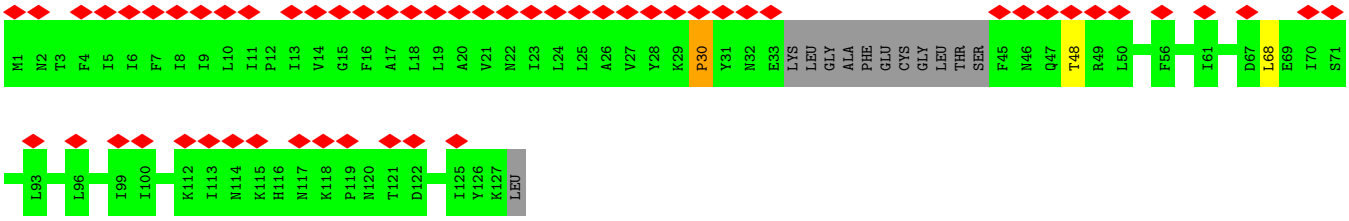


• Molecule 35: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

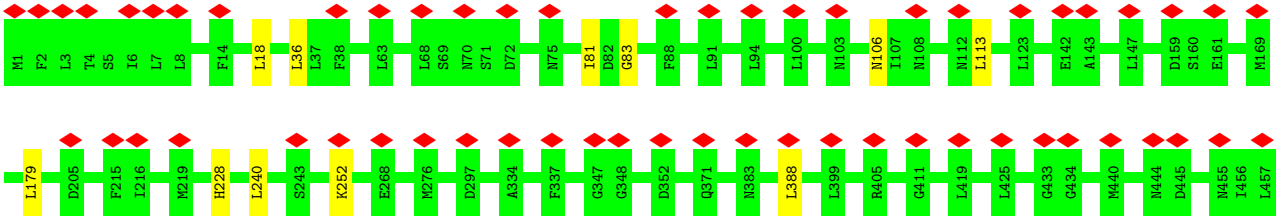


• Molecule 36: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

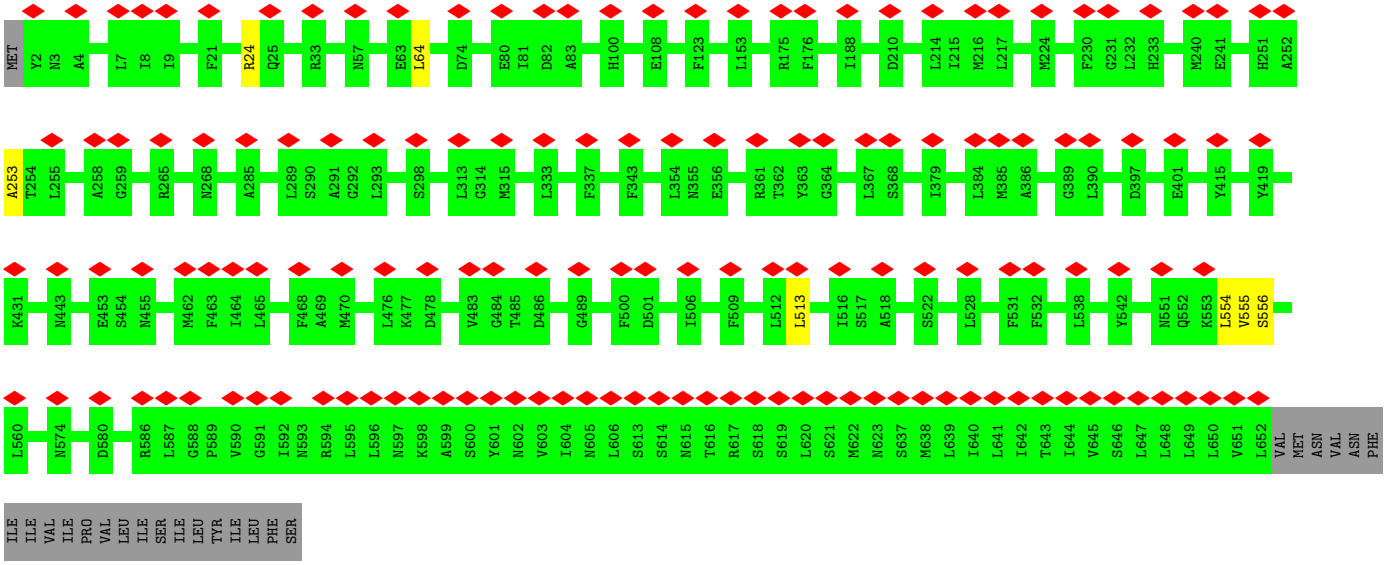




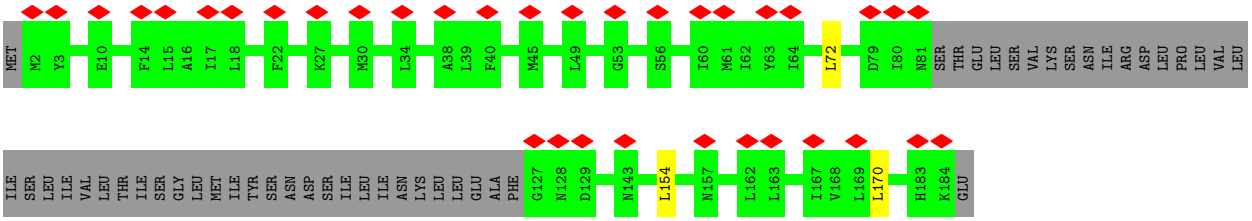
• Molecule 37: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)



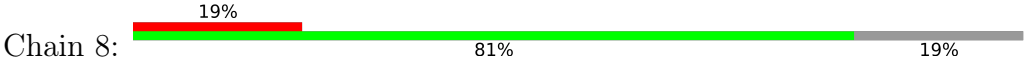
• Molecule 38: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

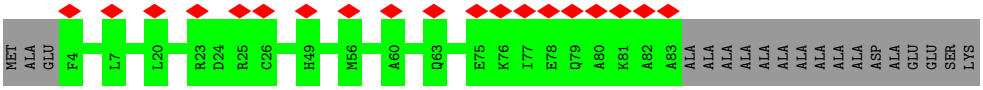


• Molecule 39: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)

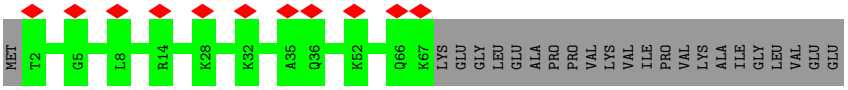


• Molecule 40: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)





• Molecule 41: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	-2000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	45872	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	497.04, 497.04, 497.04	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: FES, FMN, NDP, ZN, ZMP, SF4

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	0.48	0/5351	0.66	3/7262 (0.0%)
2	B	0.47	0/3605	0.67	4/4865 (0.1%)
3	C	0.59	0/3122	0.76	5/4225 (0.1%)
4	D	0.45	0/698	0.55	0/940
5	E	0.42	0/2709	0.65	0/3671
6	F	0.41	0/1011	0.64	0/1371
7	G	0.54	0/2040	0.69	3/2781 (0.1%)
8	H	0.39	0/1700	0.66	0/2307
9	I	0.62	0/1557	0.72	2/2110 (0.1%)
10	J	0.39	0/805	0.66	0/1096
11	K	0.61	0/1385	0.67	0/1883
12	L	0.49	0/653	0.73	0/883
13	M	0.47	0/935	0.60	0/1268
14	O	0.36	0/598	0.56	0/813
15	P	0.47	0/1062	0.62	0/1427
16	Q	0.37	0/654	0.57	0/890
17	R	0.39	0/910	0.60	0/1229
18	S	0.42	0/1454	0.68	0/1960
19	U	0.49	0/1375	0.69	0/1856
20	W	0.41	0/998	0.61	0/1346
21	X	0.44	0/1339	0.63	1/1814 (0.1%)
22	Z	0.43	0/1431	0.68	2/1955 (0.1%)
23	a	0.46	0/1064	0.63	1/1439 (0.1%)
24	b	0.43	0/503	0.59	0/679
25	c	0.36	0/364	0.52	0/491
26	d	0.47	0/777	0.58	0/1043
27	e	0.39	0/456	0.56	0/619
28	f	0.39	0/639	0.66	0/856
29	g	0.45	0/643	0.56	0/880
30	h	0.52	0/1168	0.73	2/1589 (0.1%)
31	i	0.38	0/666	0.51	0/907
32	j	0.44	0/745	0.58	0/1006

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	n	0.45	0/932	0.64	1/1264 (0.1%)
34	1	0.52	0/2755	0.78	3/3764 (0.1%)
35	2	0.60	0/3855	0.76	7/5252 (0.1%)
36	3	0.47	0/930	0.76	2/1269 (0.2%)
37	4	0.53	0/3950	0.78	7/5392 (0.1%)
38	5	0.46	0/5078	0.67	1/6934 (0.0%)
39	6	0.46	0/1117	0.76	3/1524 (0.2%)
40	8	0.38	0/676	0.65	0/904
41	9	0.45	0/537	0.60	0/717
All	All	0.49	0/62247	0.68	47/84481 (0.1%)

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
1	A	0	2
3	C	0	3
5	E	0	1
8	H	0	1
11	K	0	1
18	S	0	1
22	Z	0	1
30	h	0	1
34	1	0	3
35	2	0	1
36	3	0	1
37	4	0	3
38	5	0	3
All	All	0	22

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	56	LEU	CA-CB-CG	8.38	134.58	115.30
3	C	381	LEU	CB-CG-CD1	-7.91	97.55	111.00
37	4	36	LEU	CB-CG-CD1	-7.42	98.39	111.00
2	B	417	LEU	CA-CB-CG	-7.41	98.26	115.30
35	2	285	LEU	CB-CG-CD2	-7.15	98.85	111.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	THR	Peptide
1	A	222	ASN	Peptide
3	C	106	GLY	Peptide
3	C	222	GLY	Peptide
3	C	229	TYR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	690/728 (95%)	628 (91%)	61 (9%)	1 (0%)	48 81
2	B	454/488 (93%)	414 (91%)	40 (9%)	0	100 100
3	C	385/466 (83%)	347 (90%)	35 (9%)	3 (1%)	16 53
4	D	84/87 (97%)	74 (88%)	10 (12%)	0	100 100
5	E	329/375 (88%)	307 (93%)	22 (7%)	0	100 100
6	F	119/144 (83%)	108 (91%)	11 (9%)	0	100 100
7	G	237/281 (84%)	221 (93%)	16 (7%)	0	100 100
8	H	211/243 (87%)	184 (87%)	26 (12%)	1 (0%)	25 61
9	I	188/229 (82%)	171 (91%)	17 (9%)	0	100 100
10	J	110/198 (56%)	99 (90%)	11 (10%)	0	100 100
11	K	168/210 (80%)	149 (89%)	19 (11%)	0	100 100
12	L	81/89 (91%)	80 (99%)	1 (1%)	0	100 100
13	M	115/136 (85%)	97 (84%)	18 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	75/109 (69%)	70 (93%)	5 (7%)	0	100	100
15	P	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
16	Q	83/132 (63%)	78 (94%)	5 (6%)	0	100	100
17	R	104/109 (95%)	92 (88%)	12 (12%)	0	100	100
18	S	168/249 (68%)	155 (92%)	12 (7%)	1 (1%)	22	58
19	U	169/172 (98%)	151 (89%)	17 (10%)	1 (1%)	22	58
20	W	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
21	X	165/169 (98%)	155 (94%)	10 (6%)	0	100	100
22	Z	179/182 (98%)	160 (89%)	19 (11%)	0	100	100
23	a	122/149 (82%)	108 (88%)	14 (12%)	0	100	100
24	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100
25	c	42/60 (70%)	36 (86%)	6 (14%)	0	100	100
26	d	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	12	45
27	e	50/67 (75%)	46 (92%)	4 (8%)	0	100	100
28	f	78/87 (90%)	69 (88%)	9 (12%)	0	100	100
29	g	74/78 (95%)	61 (82%)	13 (18%)	0	100	100
30	h	134/138 (97%)	124 (92%)	9 (7%)	1 (1%)	19	55
31	i	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
32	j	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
33	n	111/120 (92%)	99 (89%)	12 (11%)	0	100	100
34	1	338/341 (99%)	303 (90%)	35 (10%)	0	100	100
35	2	467/469 (100%)	429 (92%)	37 (8%)	1 (0%)	44	76
36	3	112/128 (88%)	97 (87%)	14 (12%)	1 (1%)	14	49
37	4	484/486 (100%)	460 (95%)	23 (5%)	1 (0%)	44	76
38	5	626/655 (96%)	587 (94%)	37 (6%)	2 (0%)	37	70
39	6	134/185 (72%)	123 (92%)	11 (8%)	0	100	100
40	8	78/99 (79%)	72 (92%)	6 (8%)	0	100	100
41	9	64/89 (72%)	60 (94%)	4 (6%)	0	100	100
All	All	7587/8543 (89%)	6943 (92%)	630 (8%)	14 (0%)	45	76

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	3	30	PRO
38	5	555	VAL
1	A	660	ASP
18	S	161	LYS
3	C	92	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	565/595 (95%)	563 (100%)	2 (0%)	89 91
2	B	364/389 (94%)	364 (100%)	0	100 100
3	C	321/394 (82%)	319 (99%)	2 (1%)	84 88
4	D	68/69 (99%)	68 (100%)	0	100 100
5	E	287/329 (87%)	287 (100%)	0	100 100
6	F	109/129 (84%)	109 (100%)	0	100 100
7	G	216/245 (88%)	215 (100%)	1 (0%)	86 90
8	H	188/212 (89%)	188 (100%)	0	100 100
9	I	156/187 (83%)	155 (99%)	1 (1%)	84 88
10	J	62/147 (42%)	62 (100%)	0	100 100
11	K	147/180 (82%)	146 (99%)	1 (1%)	81 86
12	L	72/77 (94%)	72 (100%)	0	100 100
13	M	97/115 (84%)	97 (100%)	0	100 100
14	O	65/91 (71%)	65 (100%)	0	100 100
15	P	109/110 (99%)	109 (100%)	0	100 100
16	Q	72/111 (65%)	72 (100%)	0	100 100
17	R	97/100 (97%)	97 (100%)	0	100 100
18	S	149/211 (71%)	148 (99%)	1 (1%)	81 86
19	U	147/148 (99%)	147 (100%)	0	100 100
20	W	100/102 (98%)	100 (100%)	0	100 100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	X	131/133 (98%)	131 (100%)	0	100 100
22	Z	147/148 (99%)	147 (100%)	0	100 100
23	a	108/129 (84%)	107 (99%)	1 (1%)	75 83
24	b	50/59 (85%)	50 (100%)	0	100 100
25	c	30/45 (67%)	30 (100%)	0	100 100
26	d	83/85 (98%)	83 (100%)	0	100 100
27	e	44/55 (80%)	44 (100%)	0	100 100
28	f	69/73 (94%)	69 (100%)	0	100 100
29	g	62/64 (97%)	62 (100%)	0	100 100
30	h	121/123 (98%)	121 (100%)	0	100 100
31	i	64/68 (94%)	63 (98%)	1 (2%)	58 74
32	j	71/73 (97%)	71 (100%)	0	100 100
33	n	97/102 (95%)	97 (100%)	0	100 100
34	1	292/302 (97%)	291 (100%)	1 (0%)	91 92
35	2	433/433 (100%)	433 (100%)	0	100 100
36	3	98/114 (86%)	98 (100%)	0	100 100
37	4	434/434 (100%)	434 (100%)	0	100 100
38	5	530/580 (91%)	529 (100%)	1 (0%)	92 94
39	6	122/167 (73%)	122 (100%)	0	100 100
40	8	69/76 (91%)	69 (100%)	0	100 100
41	9	57/76 (75%)	57 (100%)	0	100 100
All	All	6503/7280 (89%)	6491 (100%)	12 (0%)	91 94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	102	ARG
23	a	64	ARG
38	5	24	ARG
31	i	53	ARG
3	C	466	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
36	3	85	ASN
38	5	335	HIS
37	4	26	HIS
37	4	480	ASN
38	5	574	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\#\|Z\| > 2$
42	SF4	B	501	2	0,12,12	-	-	-		
42	SF4	I	302	9	0,12,12	-	-	-		
42	SF4	A	802	1	0,12,12	-	-	-		
47	ZMP	O	201	14	23,29,36	1.95	6 (26%)	28,36,45	2.08	8 (28%)
42	SF4	A	801	1	0,12,12	-	-	-		
43	FES	A	803	1	0,4,4	-	-	-		
45	NDP	E	401	-	45,52,52	3.94	18 (40%)	53,80,80	2.35	6 (11%)
42	SF4	I	301	9	0,12,12	-	-	-		
44	FMN	B	502	-	33,33,33	2.86	12 (36%)	48,50,50	1.57	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	FES	H	301	8	0,4,4	-	-	-		
42	SF4	K	301	11	0,12,12	-	-	-		

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
42	SF4	B	501	2	-	-	0/6/5/5
47	ZMP	O	201	14	-	17/34/36/43	-
42	SF4	A	802	1	-	-	0/6/5/5
42	SF4	I	302	9	-	-	0/6/5/5
42	SF4	A	801	1	-	-	0/6/5/5
43	FES	A	803	1	-	-	0/1/1/1
45	NDP	E	401	-	-	14/30/77/77	0/5/5/5
42	SF4	I	301	9	-	-	0/6/5/5
44	FMN	B	502	-	-	6/18/18/18	0/3/3/3
43	FES	H	301	8	-	-	0/1/1/1
42	SF4	K	301	11	-	-	0/6/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	401	NDP	O4B-C1B	13.38	1.59	1.41
45	E	401	NDP	C6N-C5N	12.39	1.55	1.33
44	B	502	FMN	C4A-N5	7.64	1.45	1.30
45	E	401	NDP	O4D-C1D	7.44	1.59	1.42
45	E	401	NDP	C2D-C1D	-7.30	1.30	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	E	401	NDP	C5A-C6A-N6A	9.98	135.52	120.35
45	E	401	NDP	C1B-N9A-C4A	-8.85	111.09	126.64
47	O	201	ZMP	C9-C10-S1	7.00	121.61	113.46
45	E	401	NDP	N6A-C6A-N1A	-6.94	104.18	118.57
45	E	401	NDP	N3A-C2A-N1A	-5.70	119.77	128.68

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

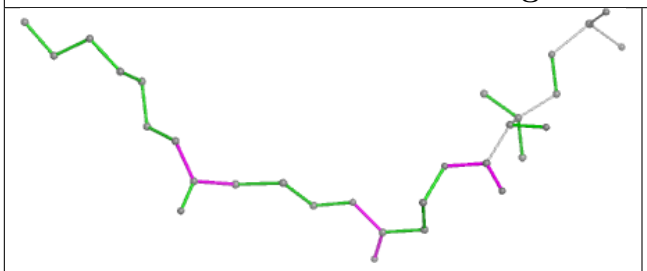
Mol	Chain	Res	Type	Atoms
44	B	502	FMN	N10-C1'-C2'-O2'
44	B	502	FMN	N10-C1'-C2'-C3'
44	B	502	FMN	C1'-C2'-C3'-O3'
44	B	502	FMN	C1'-C2'-C3'-C4'
44	B	502	FMN	O2'-C2'-C3'-O3'

There are no ring outliers.

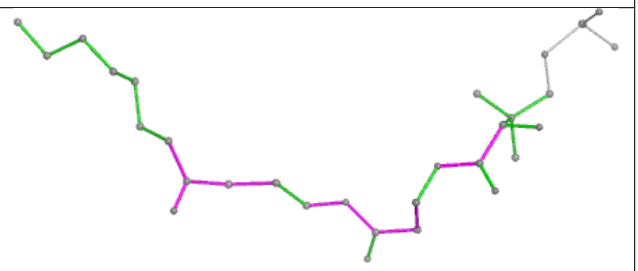
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

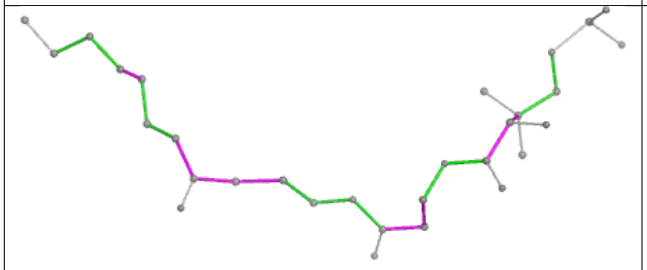
Ligand ZMP O 201



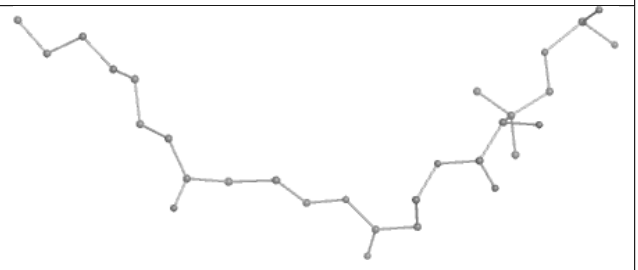
Bond lengths



Bond angles

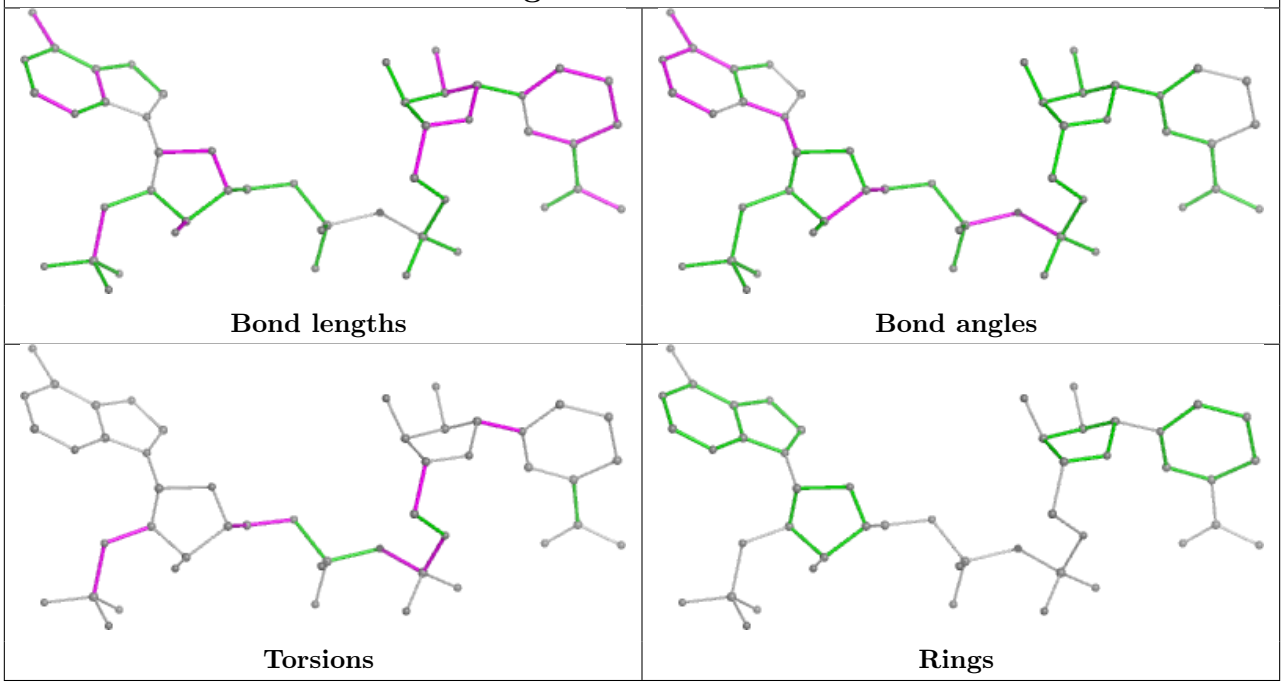


Torsions

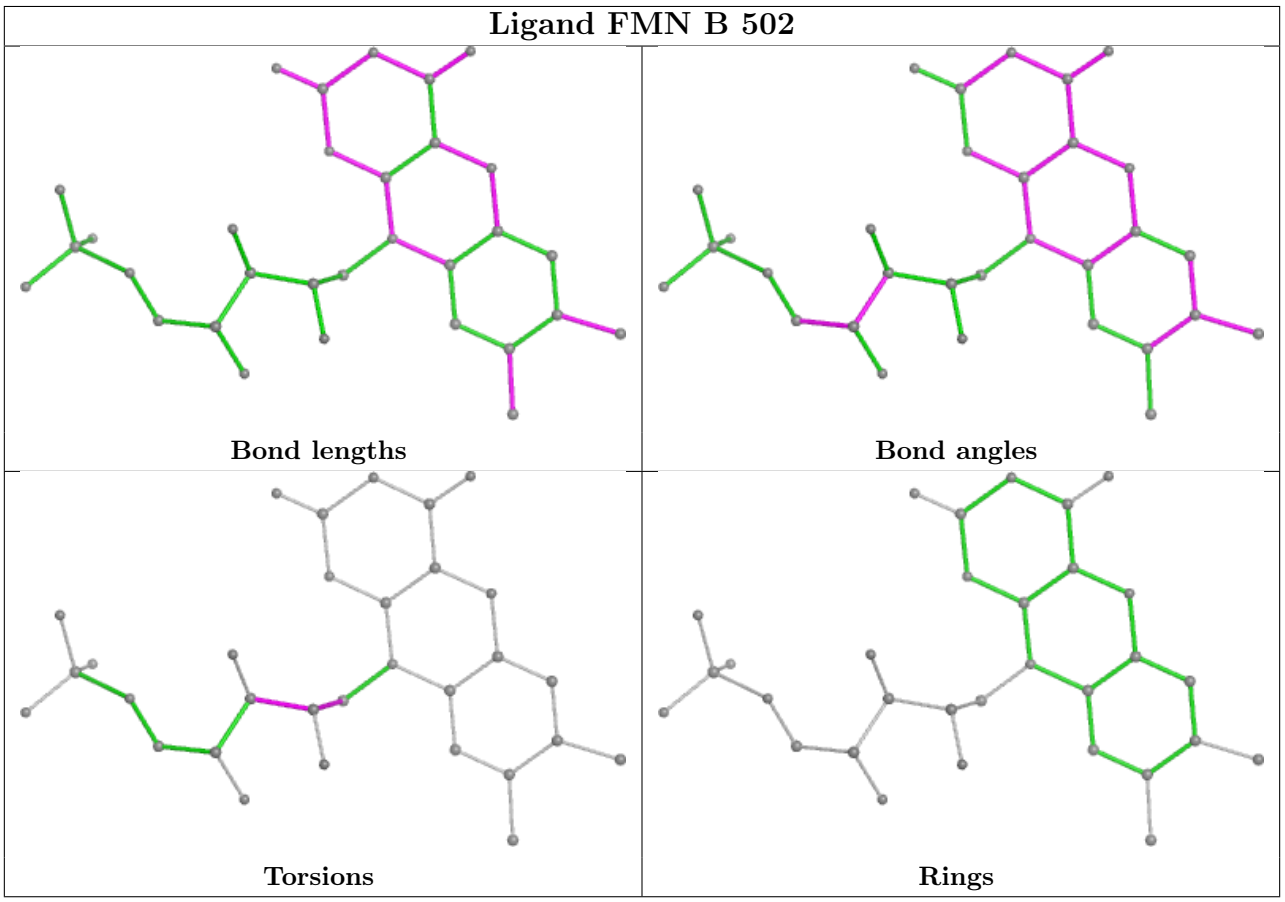


Rings

Ligand NDP E 401



Ligand FMN B 502



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
38	5	2
10	J	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	623:ASN	C	637:SER	N	19.55
1	J	110:VAL	C	116:PRO	N	11.30
1	J	82:MET	C	94:TRP	N	10.82
1	5	606:LEU	C	613:SER	N	9.79

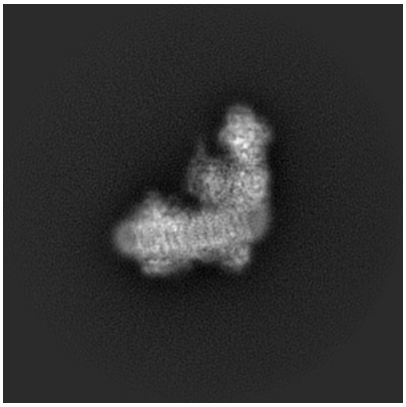
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4874. These allow visual inspection of the internal detail of the map and identification of artifacts.

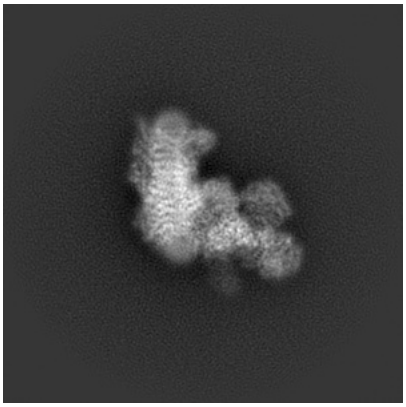
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

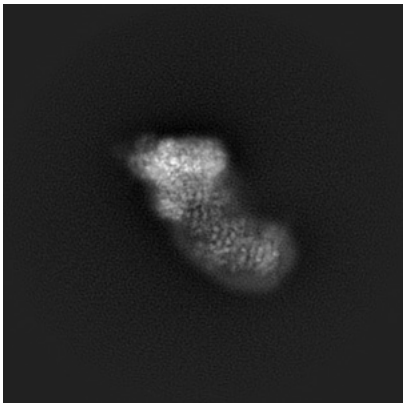
6.1.1 Primary map



X



Y

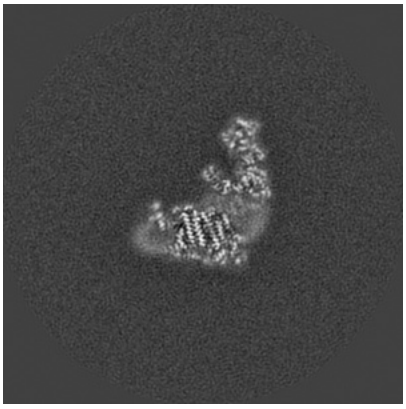


Z

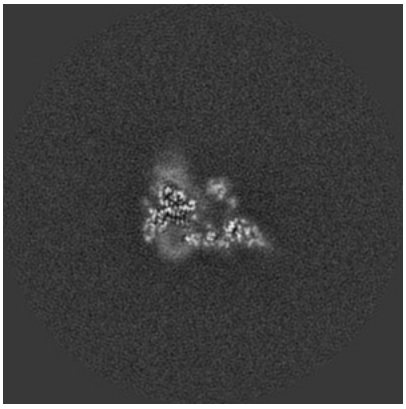
The images above show the map projected in three orthogonal directions.

6.2 Central slices

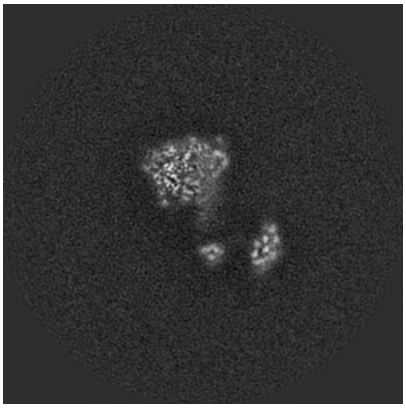
6.2.1 Primary map



X Index: 228



Y Index: 228

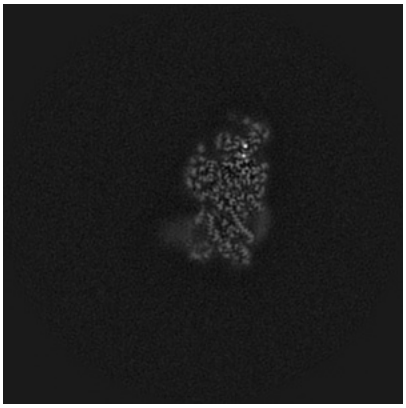


Z Index: 228

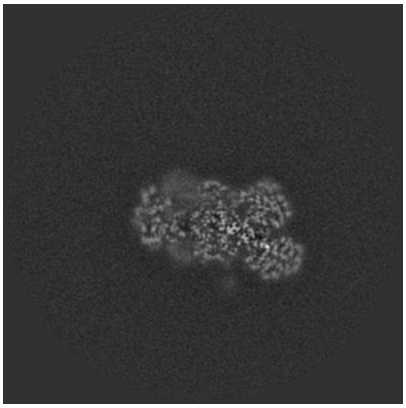
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

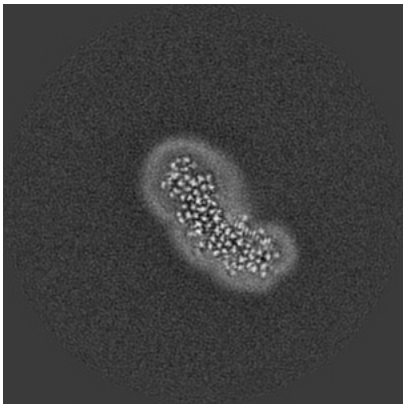
6.3.1 Primary map



X Index: 193



Y Index: 270

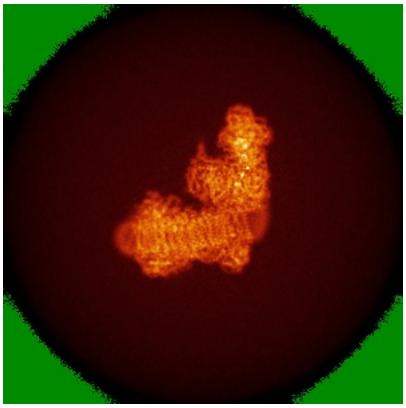


Z Index: 201

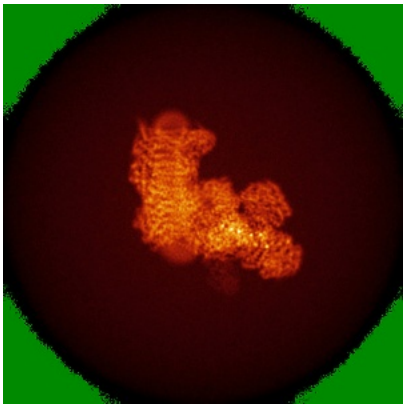
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

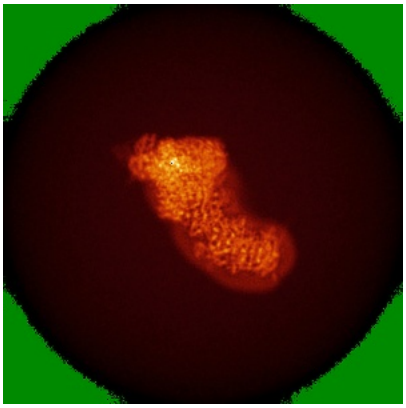
6.4.1 Primary map



X



Y

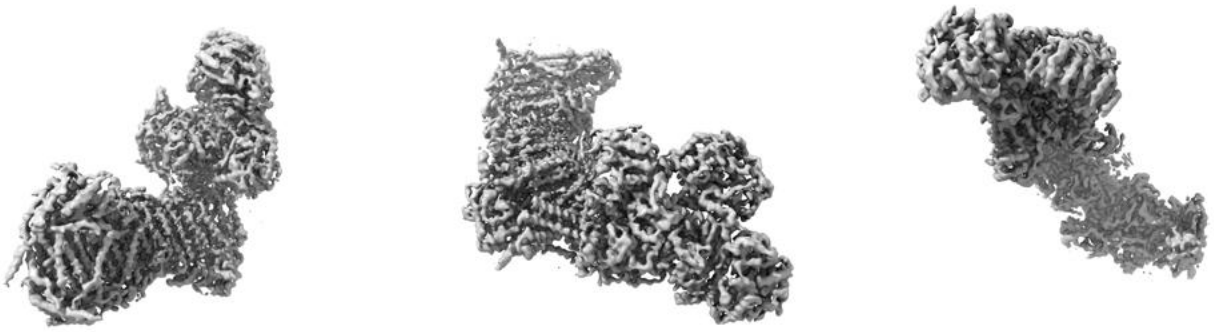


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

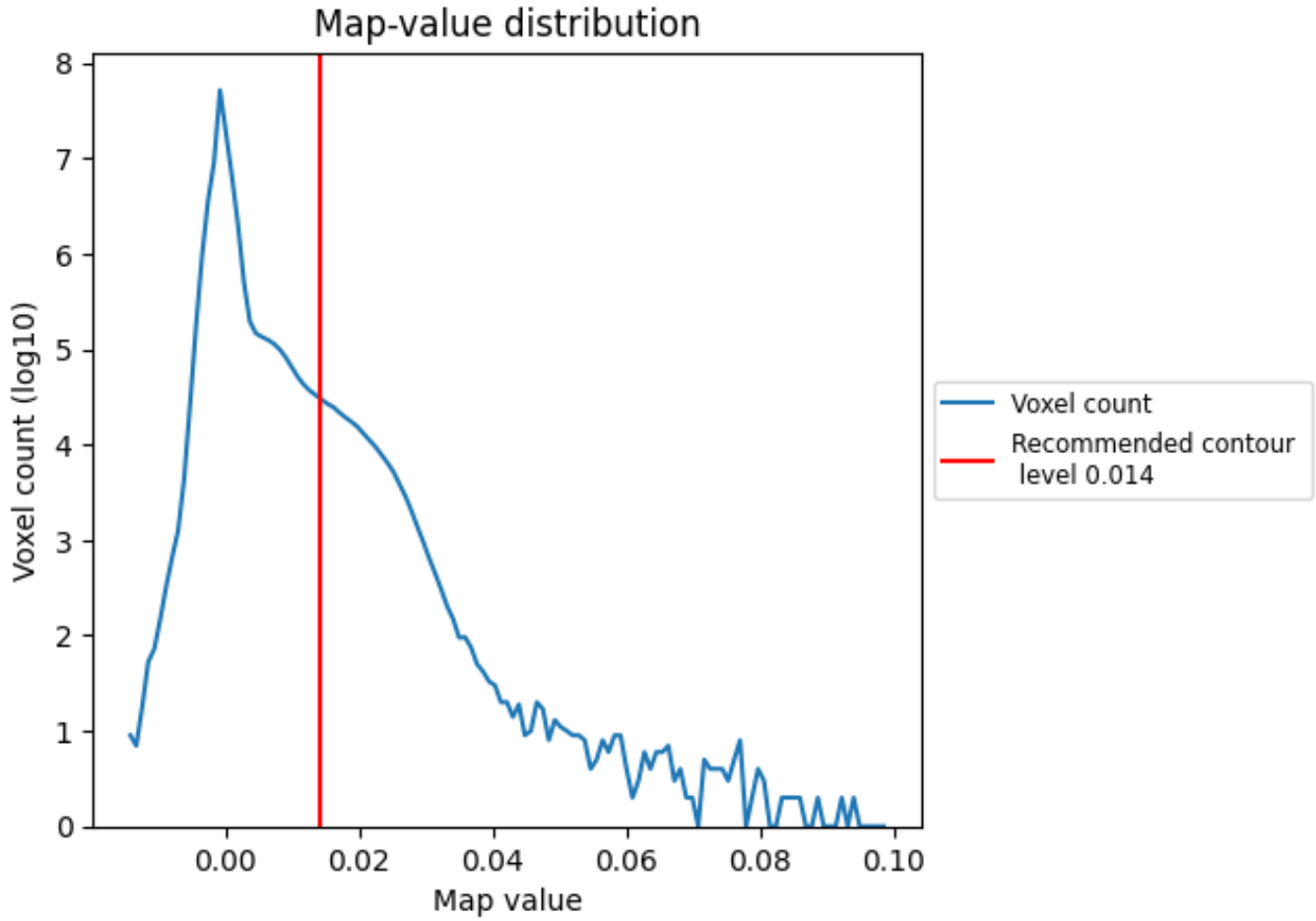
6.6 Mask visualisation (i)

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

7 Map analysis

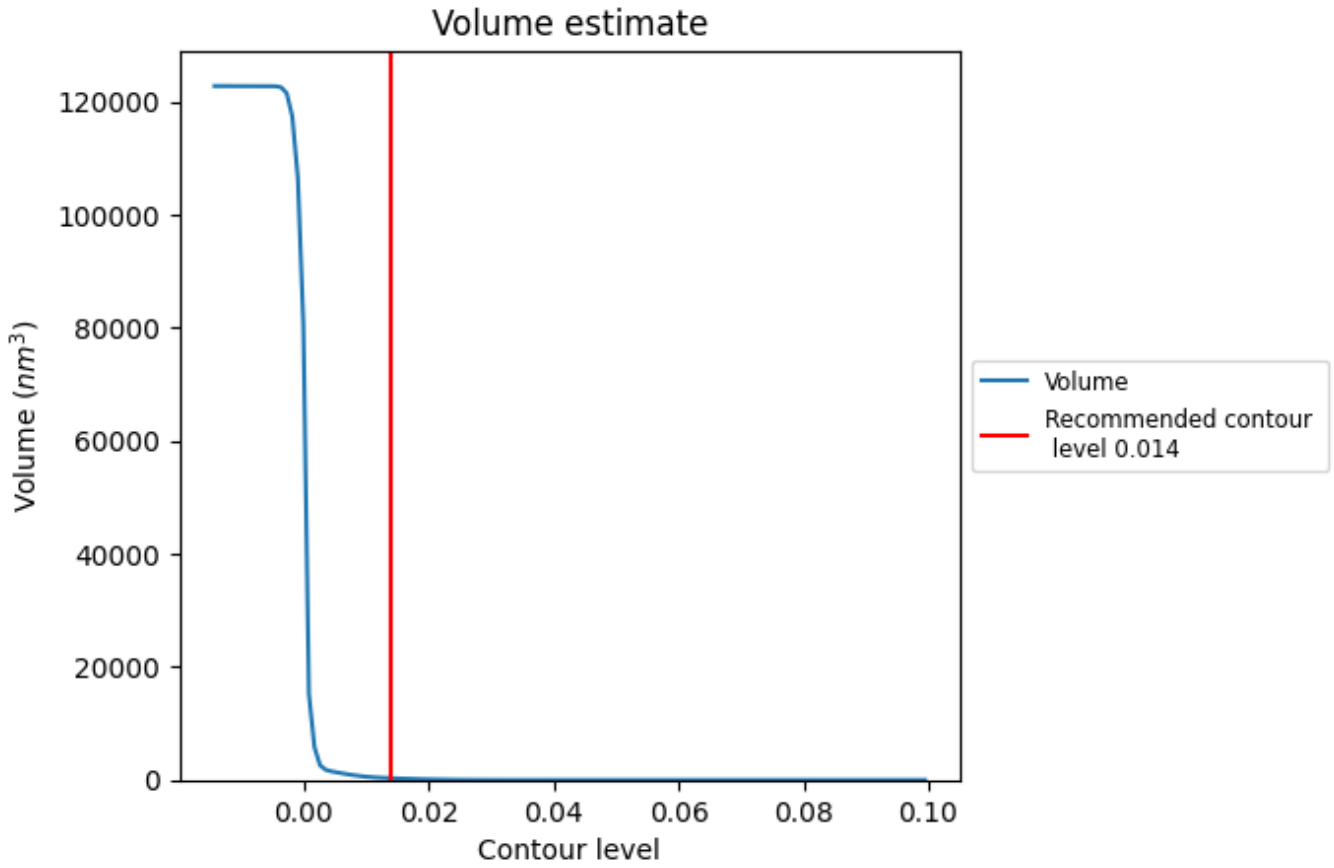
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

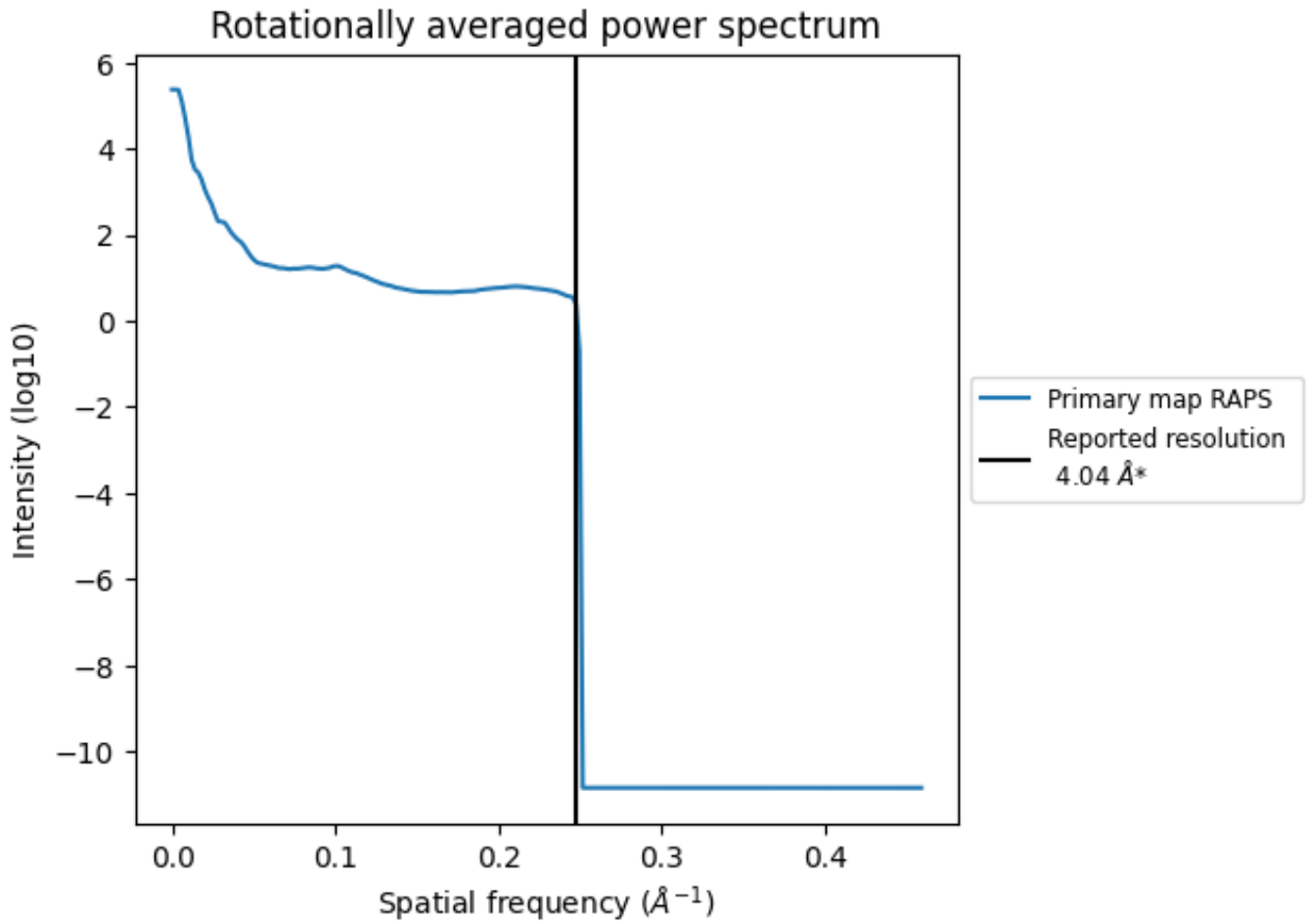
7.2 Volume estimate



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 275 kDa.

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

7.3 Rotationally averaged power spectrum (i)

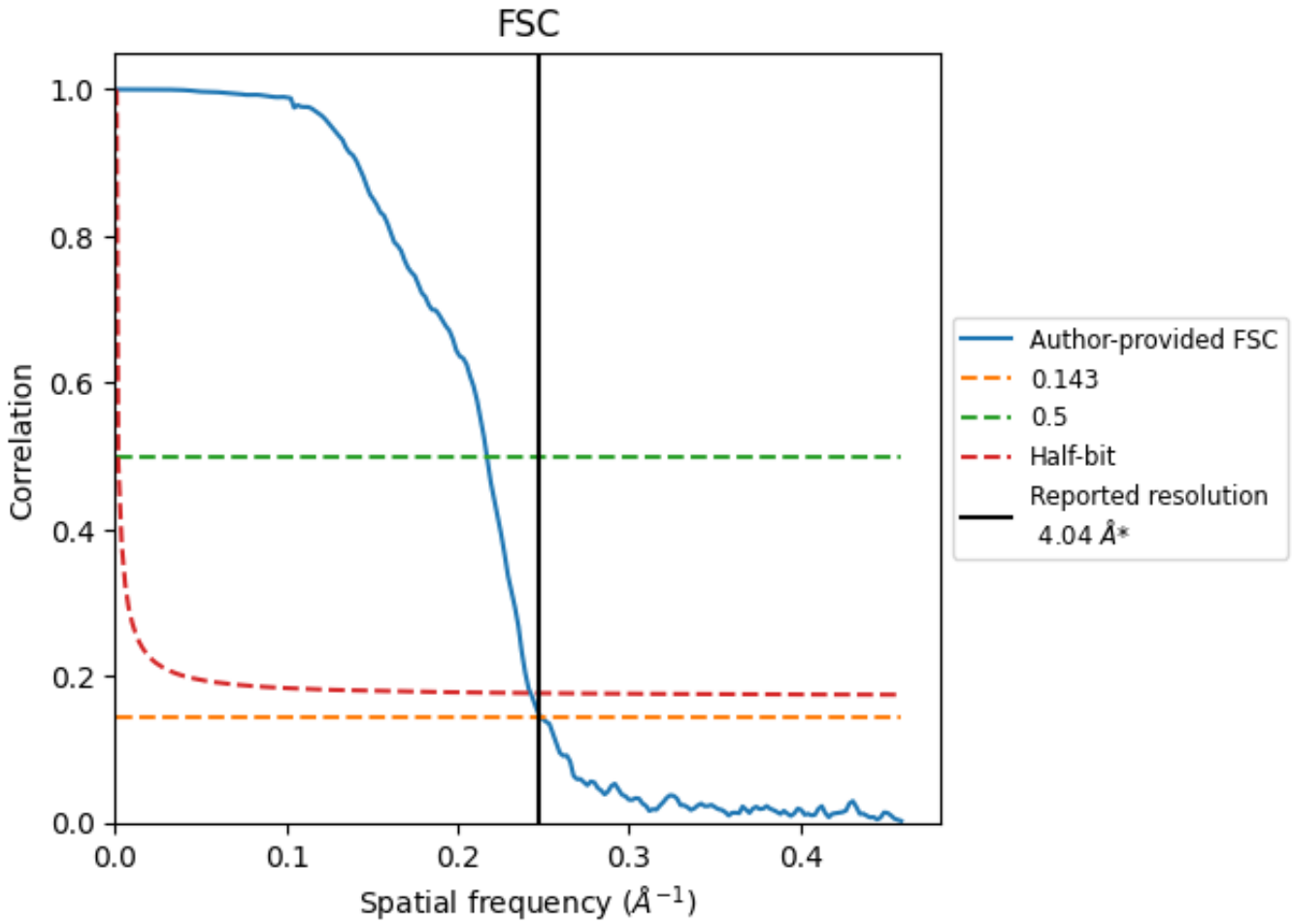


*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8.2 Resolution estimates (i)

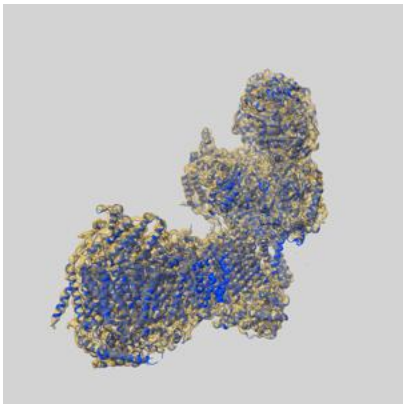
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.04	-	-
Author-provided FSC curve	4.02	4.61	4.12
Unmasked-calculated*	-	-	-

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

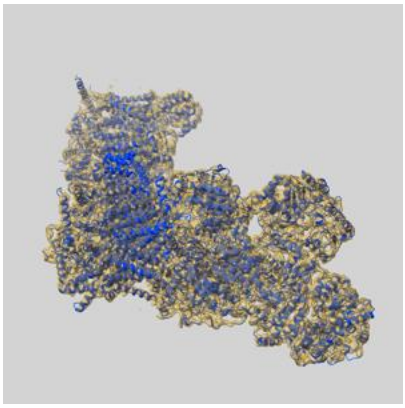
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4874 and PDB model 6RFS. Per-residue inclusion information can be found in section 3 on page 16.

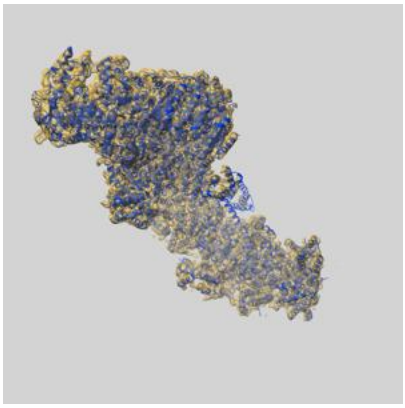
9.1 Map-model overlay



X



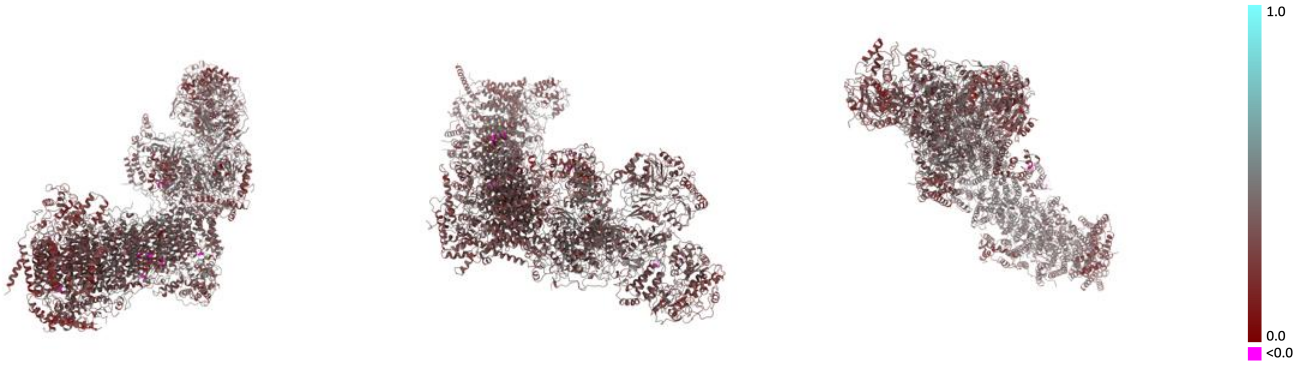
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

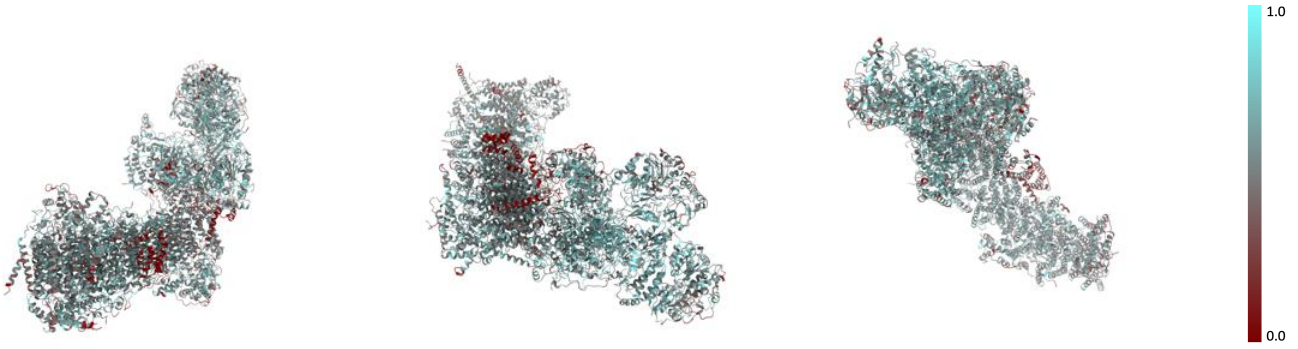
9.2 Q-score mapped to coordinate model



X Y Z

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

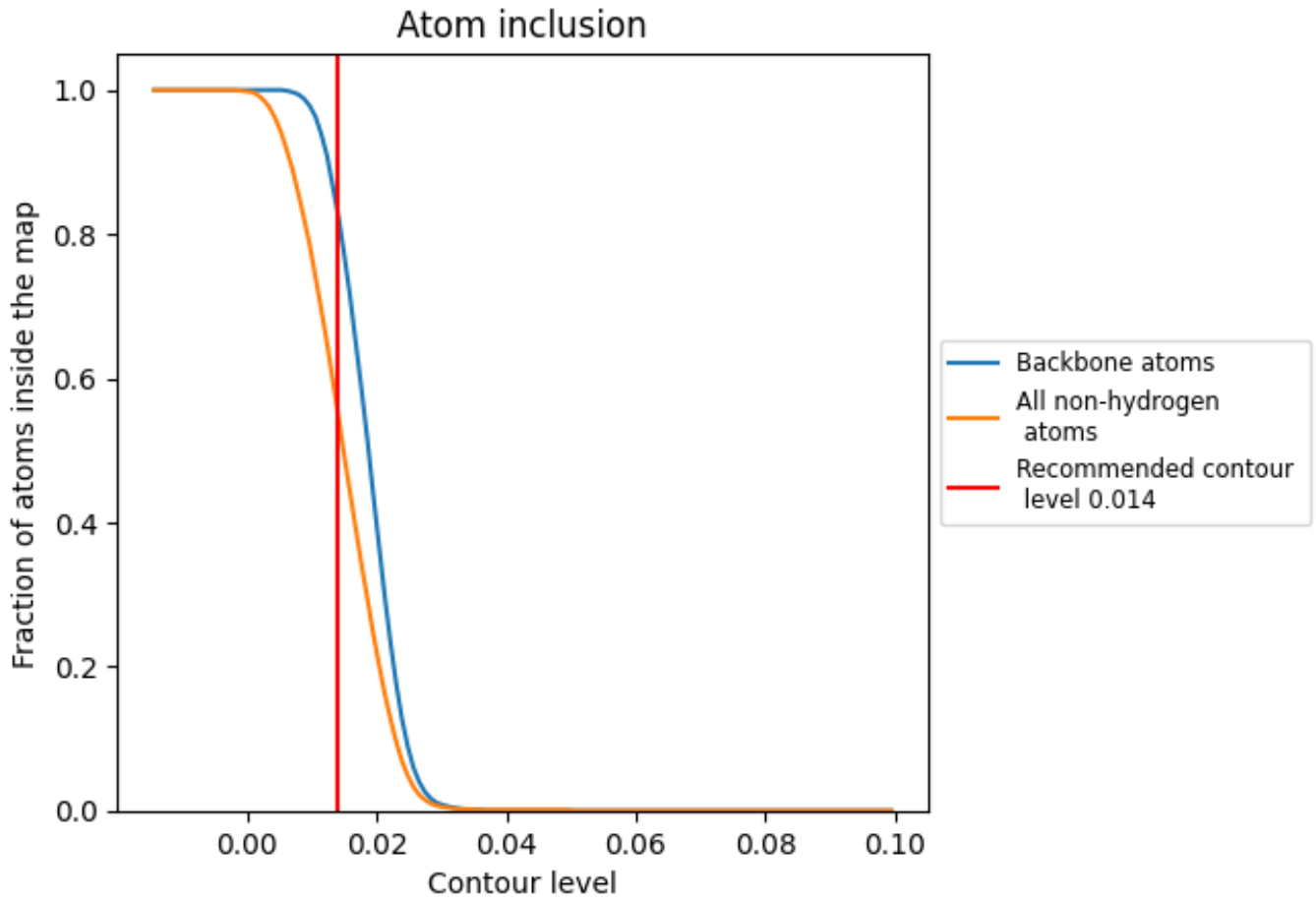
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 55% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5540	0.3420
1	0.5010	0.3370
2	0.5930	0.3710
3	0.3790	0.3330
4	0.5700	0.3560
5	0.5090	0.3130
6	0.4980	0.3420
8	0.4850	0.2730
9	0.5620	0.3300
A	0.5960	0.3520
B	0.5750	0.3170
C	0.6110	0.3760
D	0.5410	0.3360
E	0.4980	0.3230
F	0.5970	0.3390
G	0.6100	0.3890
H	0.5580	0.3250
I	0.6390	0.3740
J	0.3550	0.3110
K	0.6280	0.3780
L	0.5260	0.3380
M	0.6550	0.3920
O	0.3830	0.2810
P	0.5550	0.3370
Q	0.4260	0.2770
R	0.5310	0.3110
S	0.5080	0.3010
U	0.5390	0.3260
W	0.5900	0.3420
X	0.5630	0.3500
Z	0.5930	0.3710
a	0.5040	0.3220
b	0.5930	0.3470
c	0.4780	0.2980
d	0.5870	0.3230

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Chain	Atom inclusion	Q-score
e	0.4730	0.2970
f	0.5220	0.3010
g	0.5700	0.3620
h	0.6140	0.3780
i	0.5670	0.3340
j	0.5460	0.3780
n	0.5640	0.3390