



wwPDB EM Validation Summary Report ⓘ

Aug 22, 2026 – 07:20 am BST

PDB ID : 5LDW / pdb_00005ldw
EMDB ID : EMD-4040
Title : Structure of mammalian respiratory Complex I, class1
Authors : Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on : 2016-06-28
Resolution : 4.27 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 ⓘ 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:

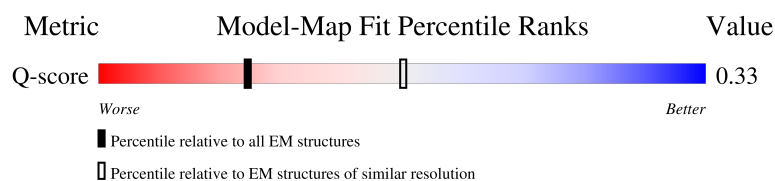
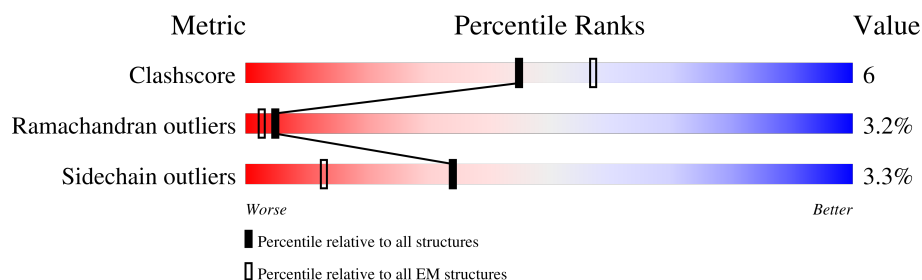
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 4.27 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	4567 (3.77 - 4.76)

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	13% 63% 12% 23%
2	B	179	7% 65% 15% 18%
3	C	228	15% 75% 13% 10%
4	D	429	12% 78% 15% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	217	
6	F	444	
7	G	785	
8	H	318	
9	I	176	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	316	
16	P	300	
17	Q	113	
18	R	89	
19	S	99	
20	T	88	
20	U	88	
21	V	115	
22	W	128	
23	X	169	
24	Y	141	
25	Z	138	
26	a	70	
27	b	80	
28	c	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	d	114	
30	e	105	
31	f	57	
32	g	125	
33	h	134	
34	i	106	
35	j	52	
36	k	74	
37	l	118	
38	m	118	
39	n	166	
40	o	136	
41	p	169	
42	q	145	
43	r	87	
44	s	35	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 51181 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
			687	472	99	113	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	206	Total	C	N	O	S	0	0
			1684	1091	285	305	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
			959	583	186	186	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
			2356	1432	463	455	6		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	685	Total	C	N	O	S	0	0
			3614	2172	715	712	15		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	296	Total	C	N	O	S	0	0
			2306	1551	357	376	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1366	857	238	261	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	457	Total	C	N	O	S	0	0
			3536	2352	555	591	38		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	314	Total	C	N	O	S	0	0
			1851	1148	347	353	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUFA9.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUFS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	113	Total	C	N	O	0	0
			565	339	113	113		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, NDUFS6,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial,NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			501	304	99	95	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	106	Total	C	N	O	S	0	0
			685	430	126	128	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NDUFA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1133	703	213	208	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total	C	N	O	S	0	0
			921	573	172	170	6		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NDUFA3.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	114	Total	C	N	O	S	0	0
			790	504	146	137	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	89	Total	C	N	O	S	0	0
			616	382	121	108	5		

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

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, NDUF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	134	Total	C	N	O		0	0
			770	486	143	141			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NDUF6.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUF2.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4, NDUFB4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4, NDUFB4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	118	Total	C	N	O	0	0
			887	566	165	156		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NDUFB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	166	Total	C	N	O	S	0	0
			1088	677	212	196	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10,NADH dehydroge-

nase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

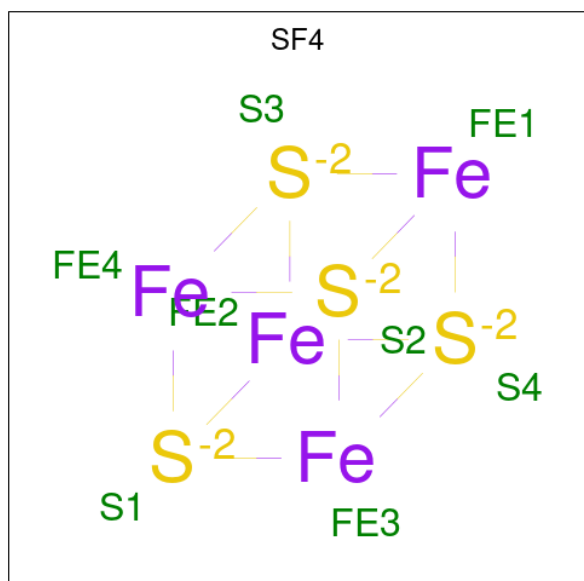
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUF7.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	r	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3.

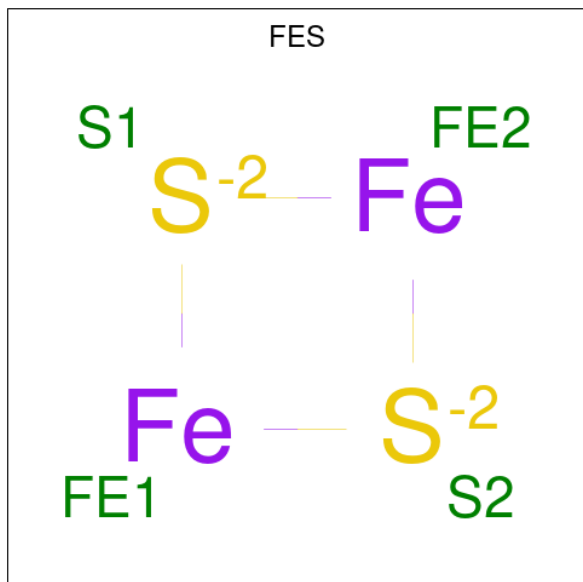
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



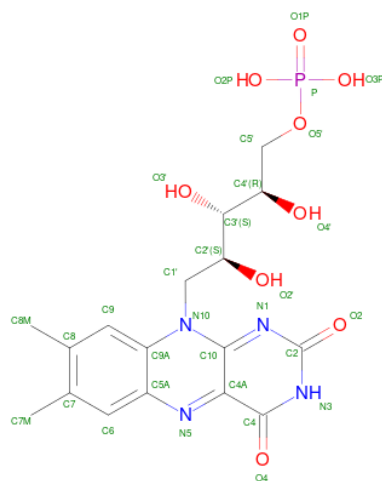
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

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



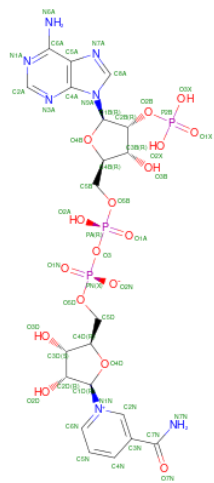
Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- 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

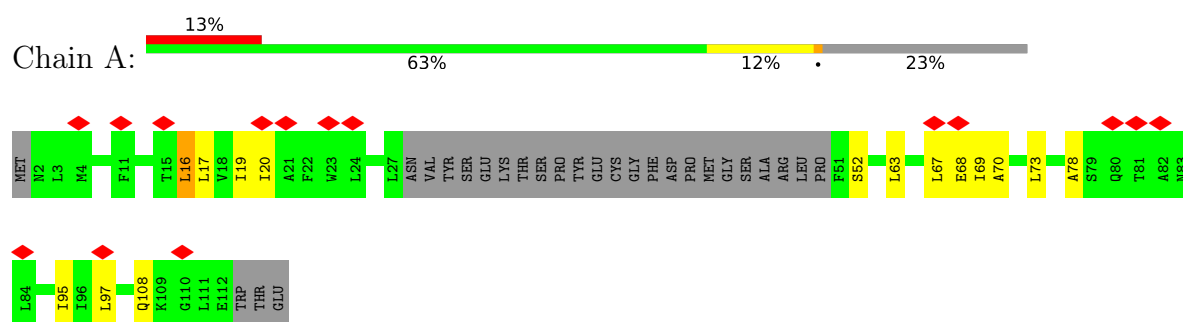
- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

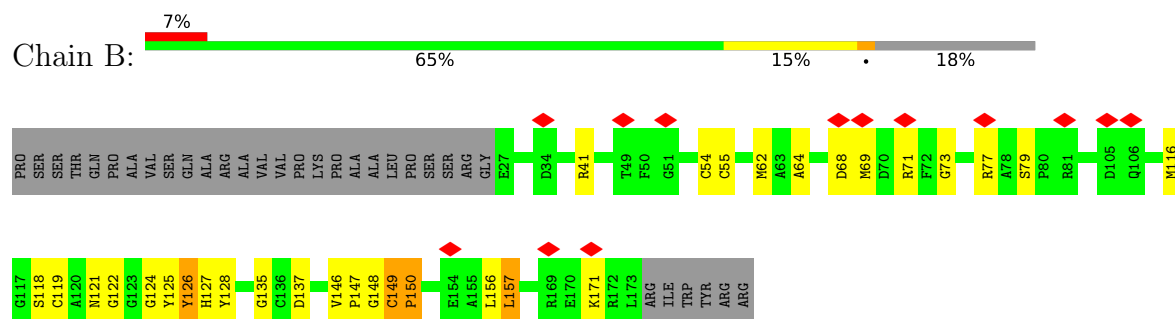
3 Residue-property plots [i](#)

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.

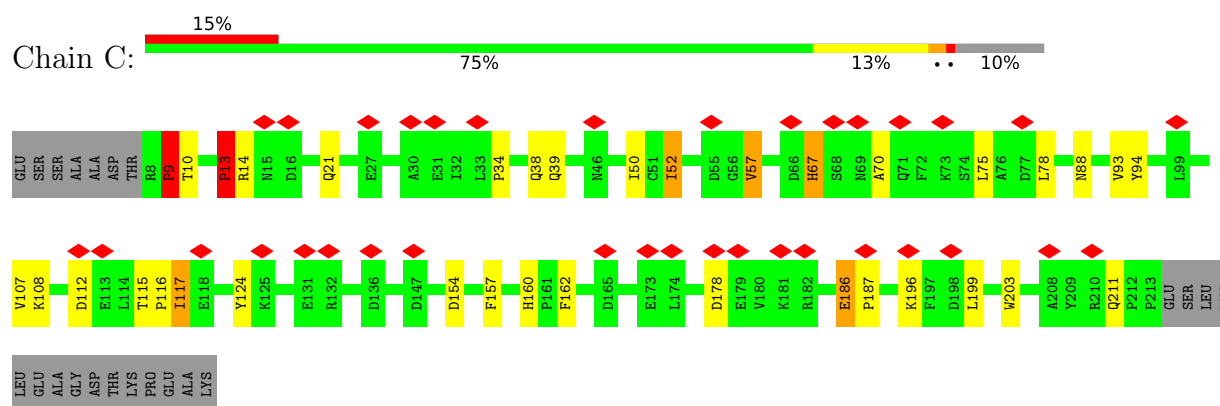
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



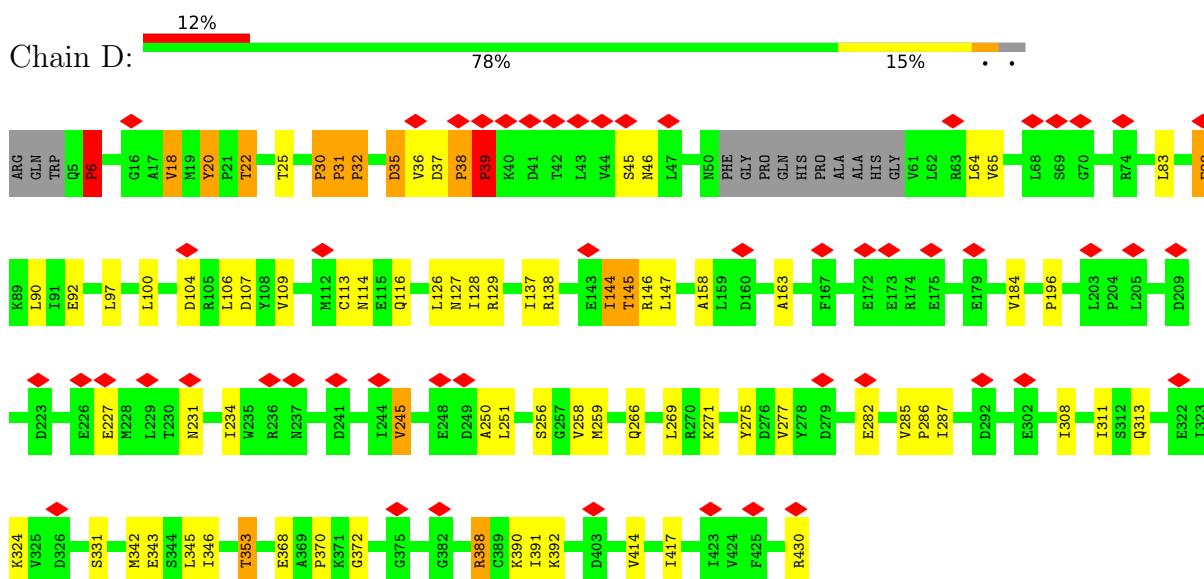
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



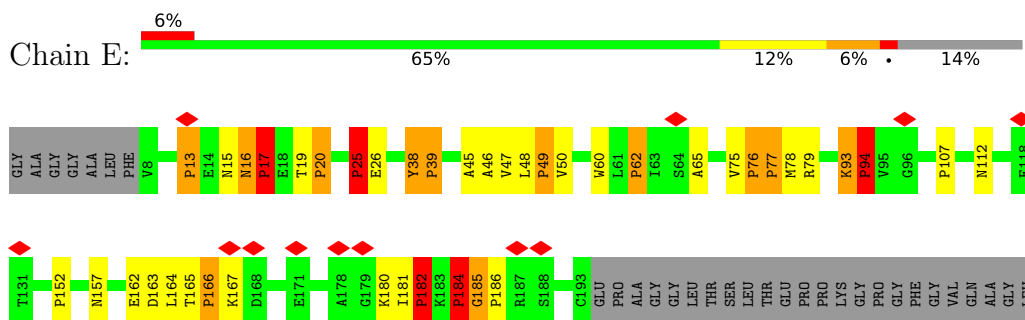
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



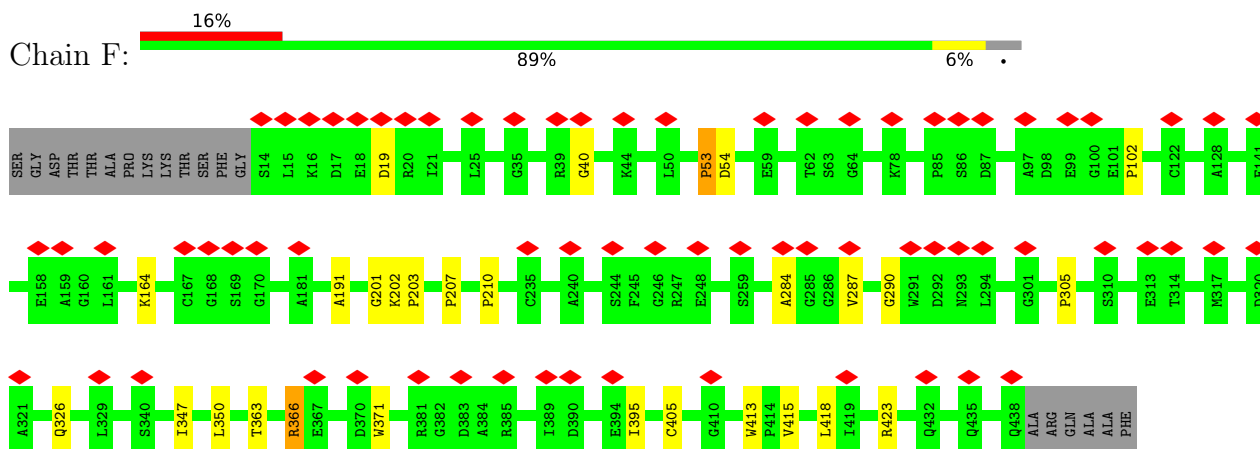
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



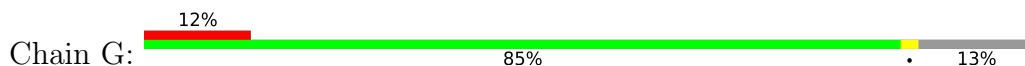
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

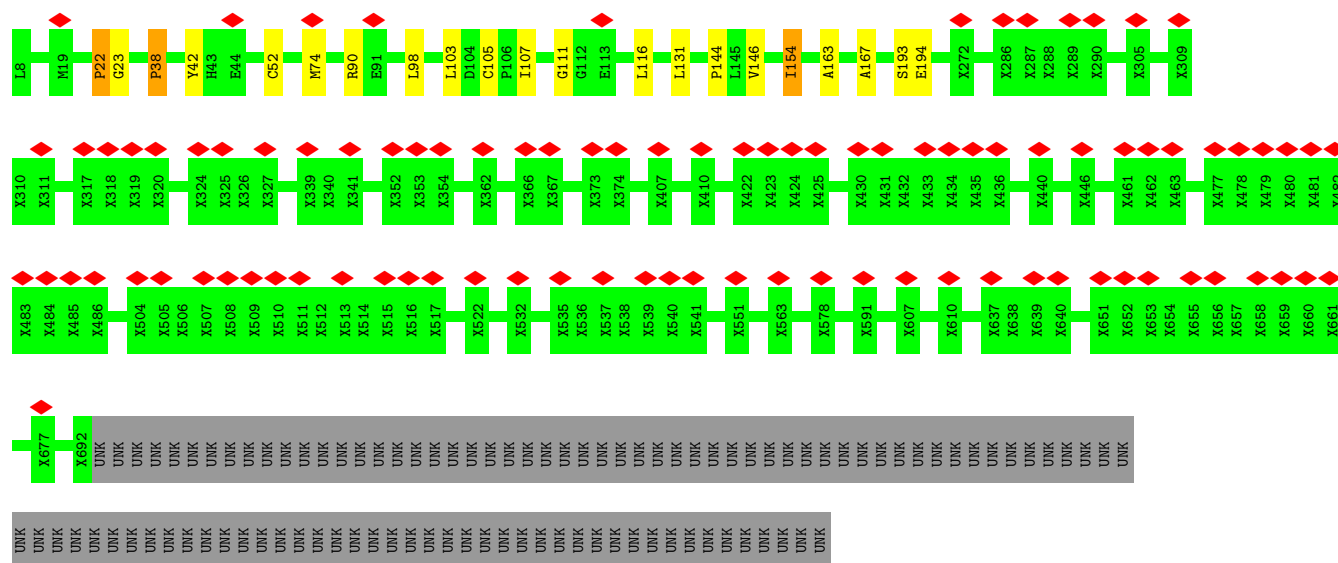


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

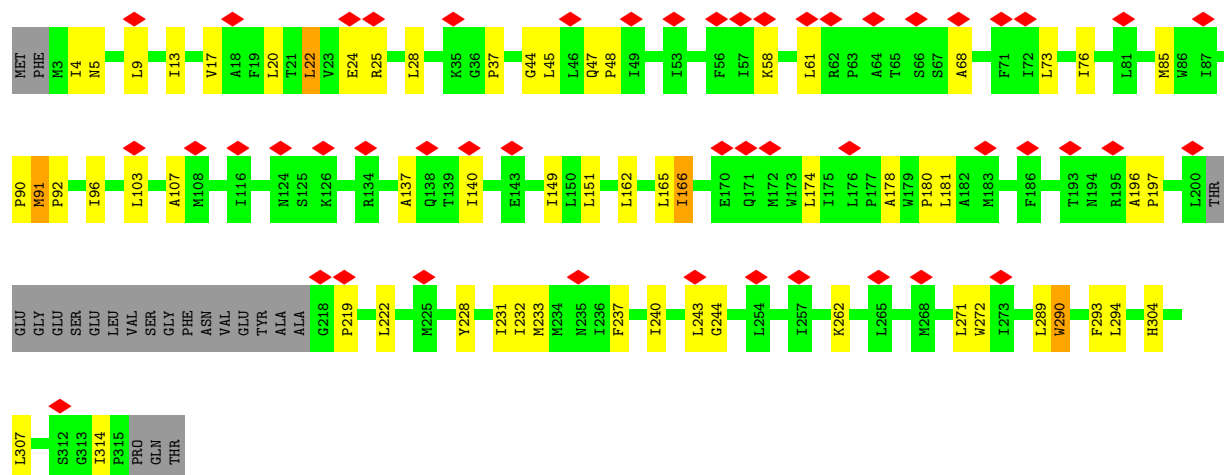
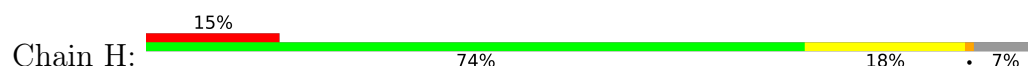


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

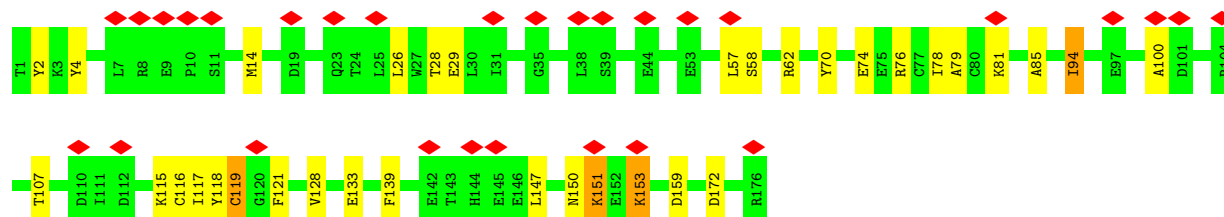
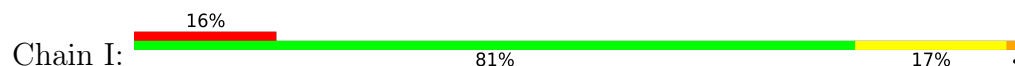




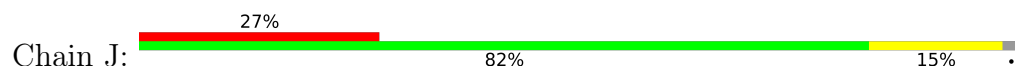
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

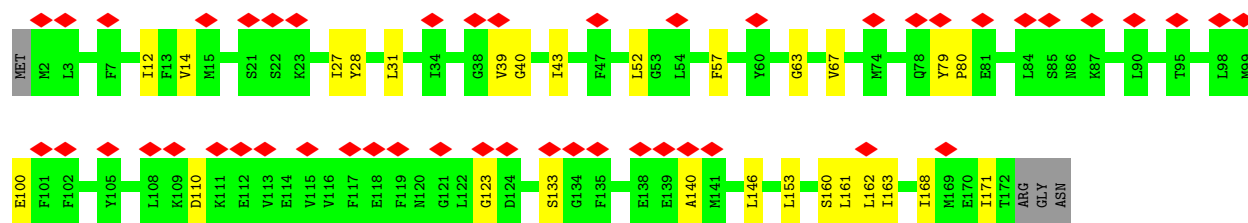


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

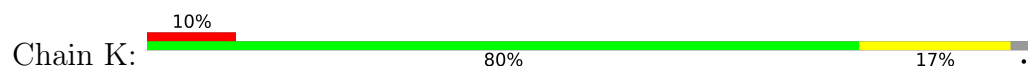


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

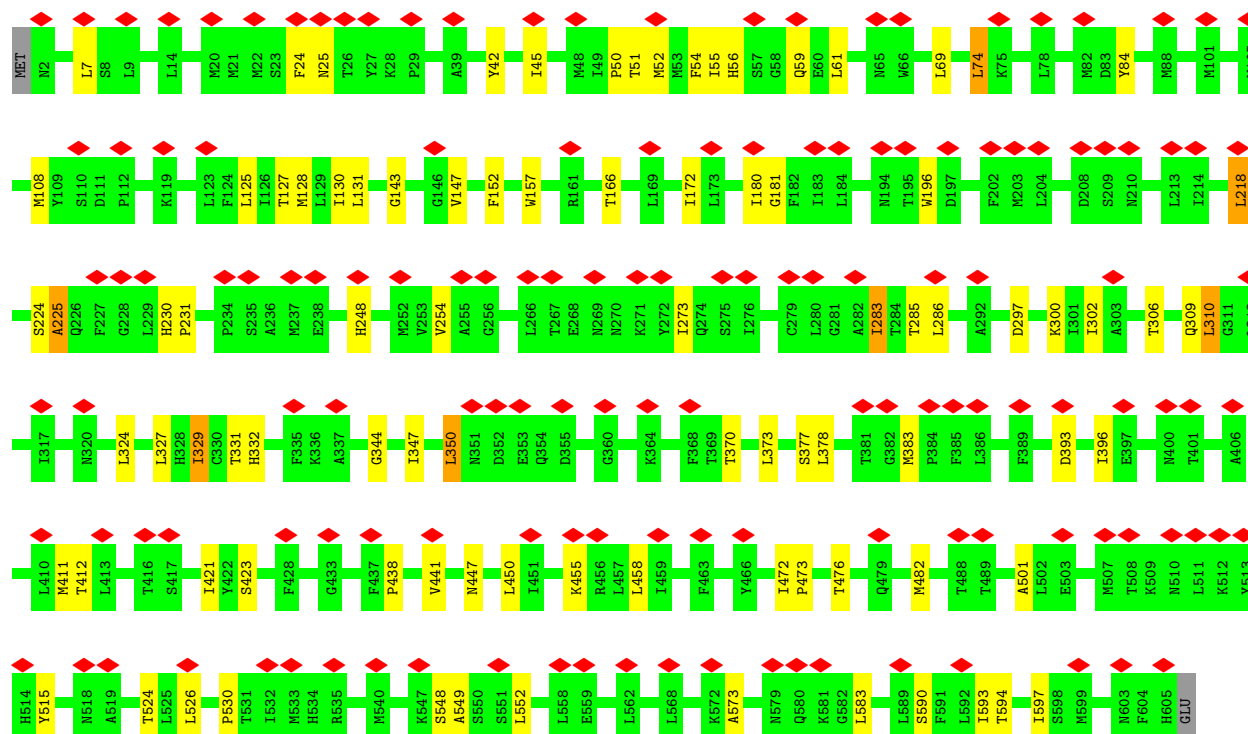
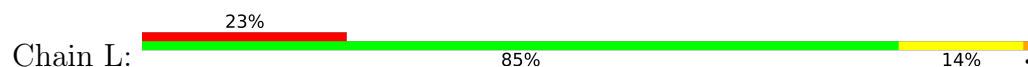




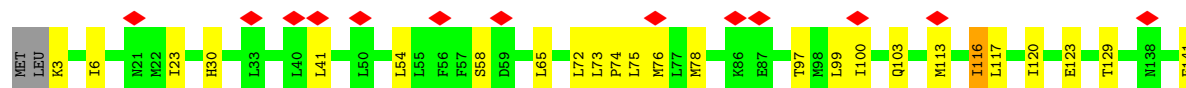
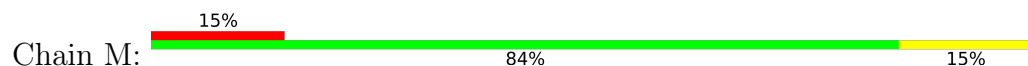
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

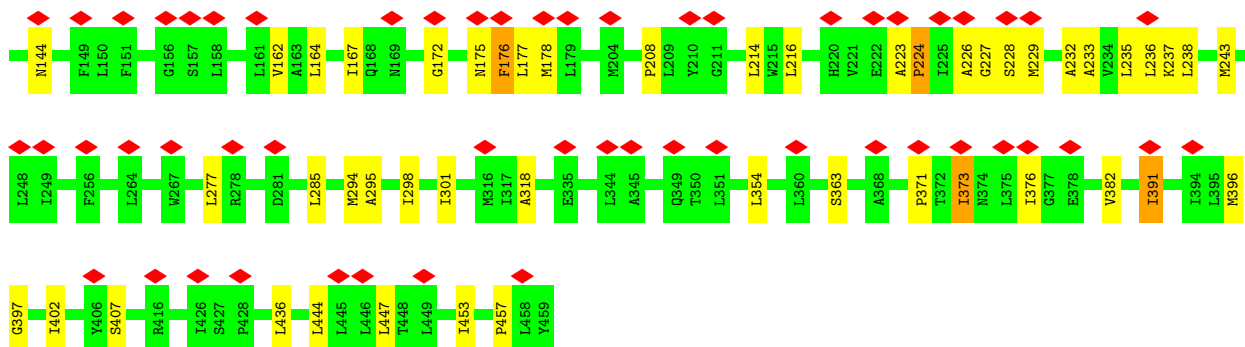


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

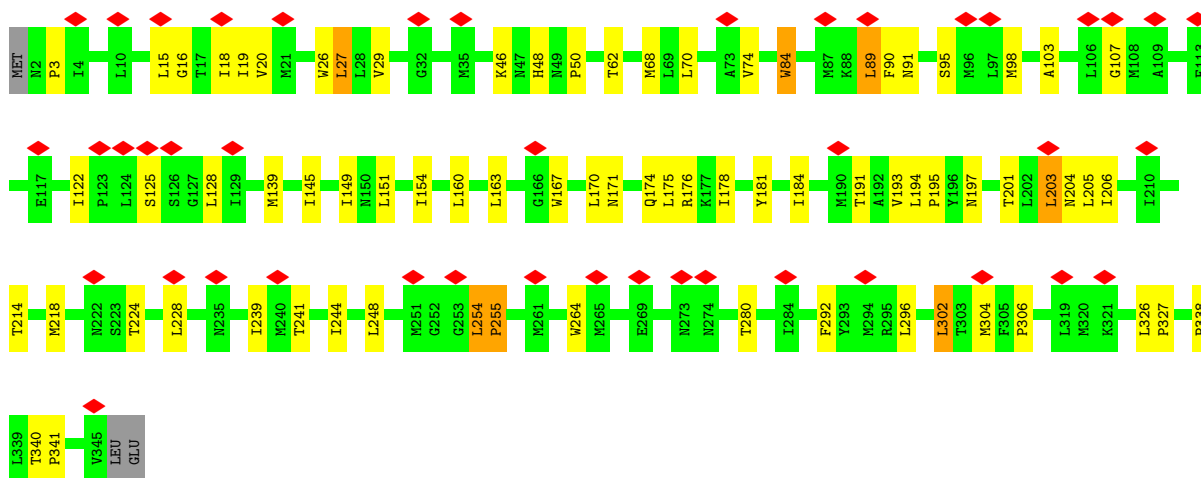
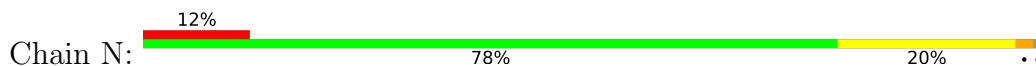


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

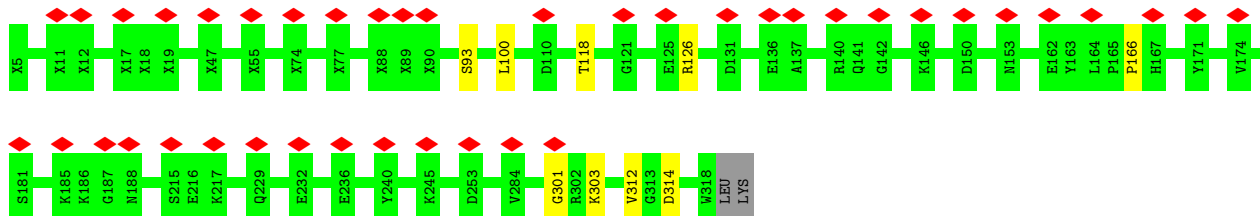




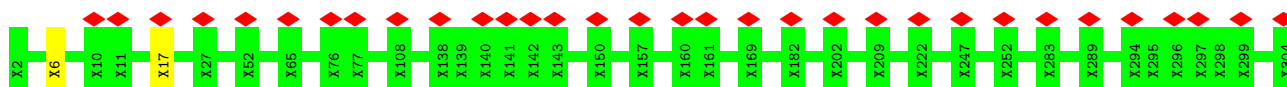
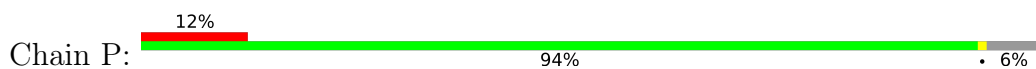
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, NDUFA9

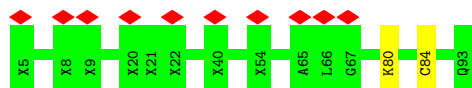




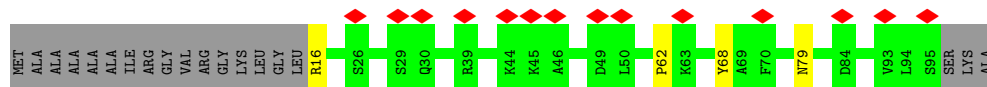
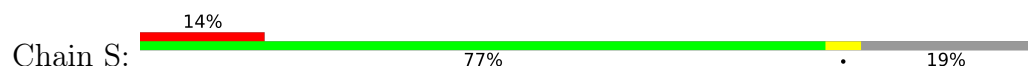
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, NDUF54



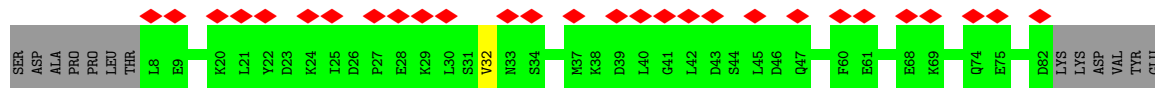
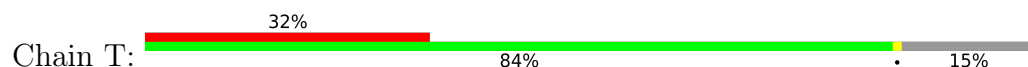
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, NDUF56, NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial, NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



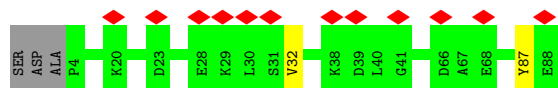
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



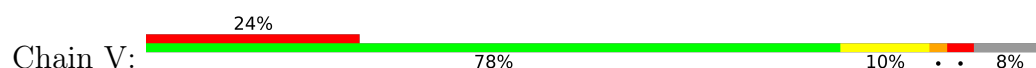
- Molecule 20: Acyl carrier protein, mitochondrial

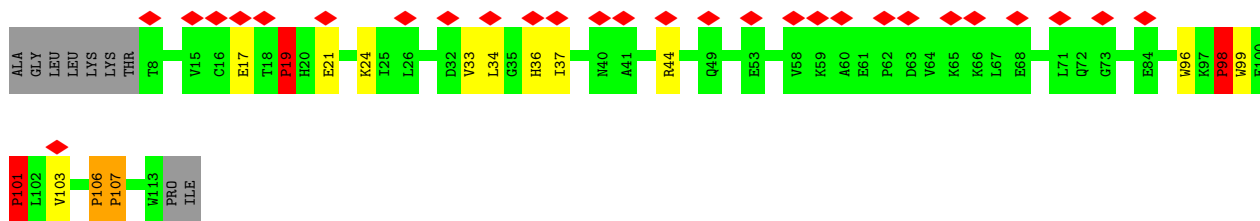


- Molecule 20: Acyl carrier protein, mitochondrial

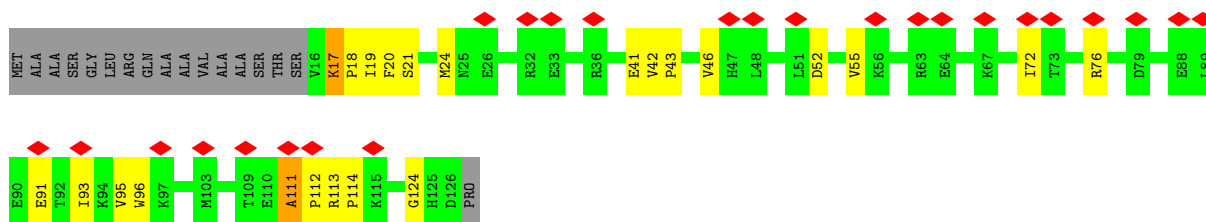


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

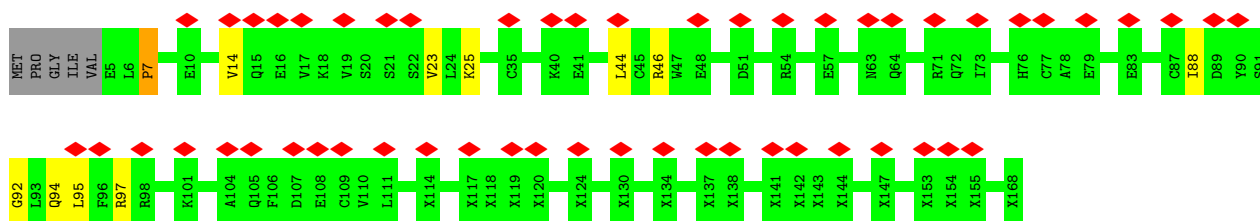




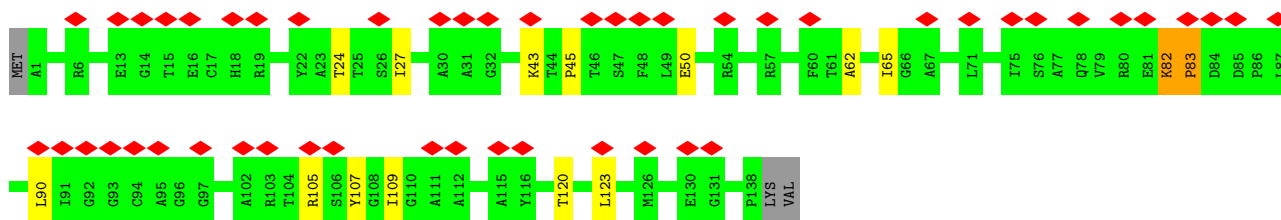
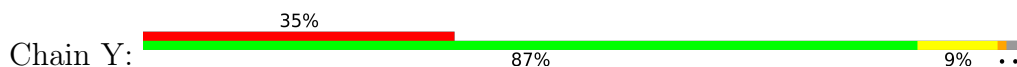
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



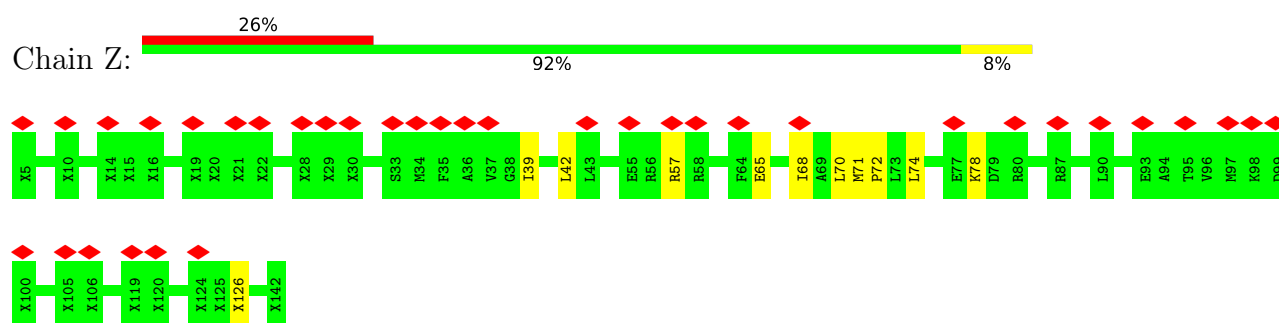
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NDUFA8



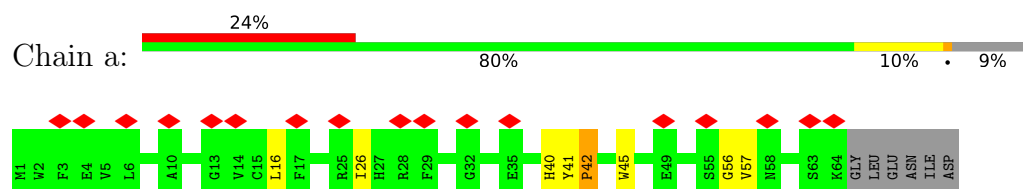
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



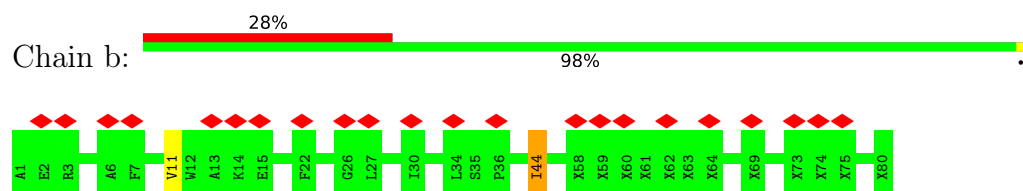
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NDUFA13



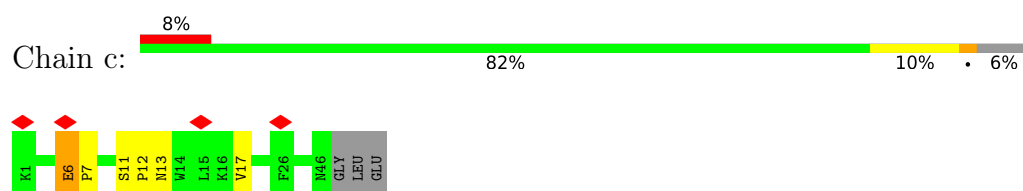
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



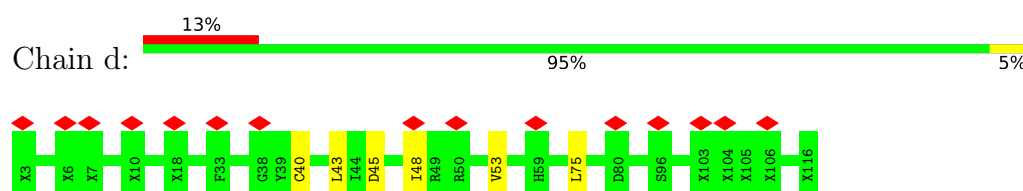
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3, NDUFA3



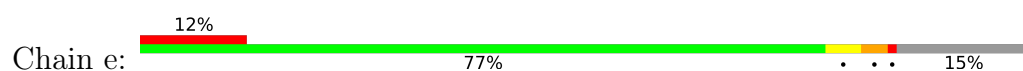
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

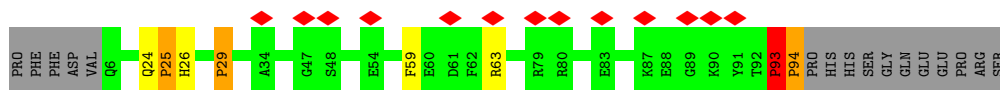


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NADH dehydrogenase [ubiquinone] 1 subunit C2, NDUFC2

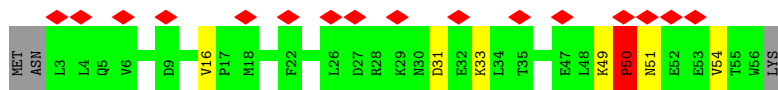
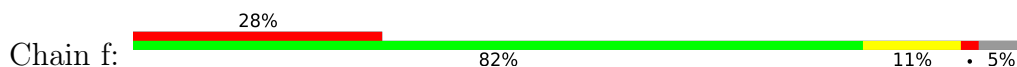


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

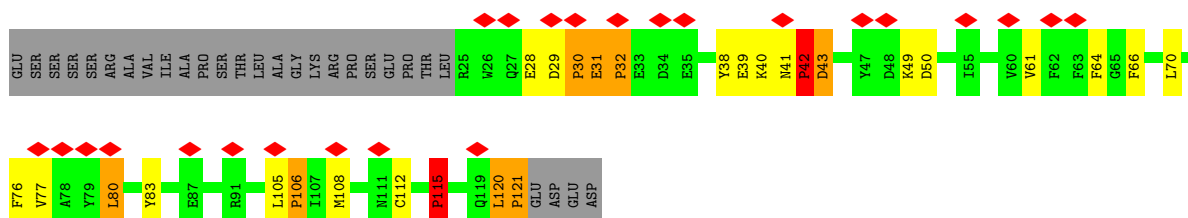




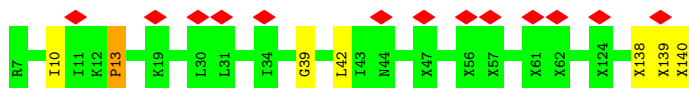
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



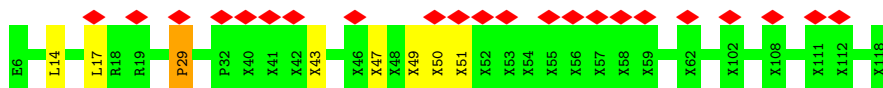
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



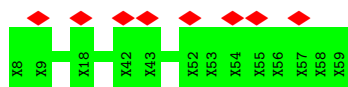
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, NDUF5



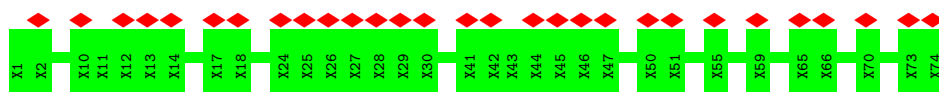
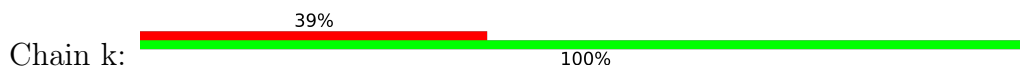
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6, NDUF6



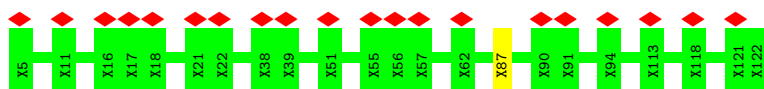
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUF2



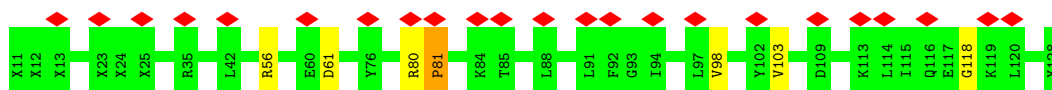
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUFB3



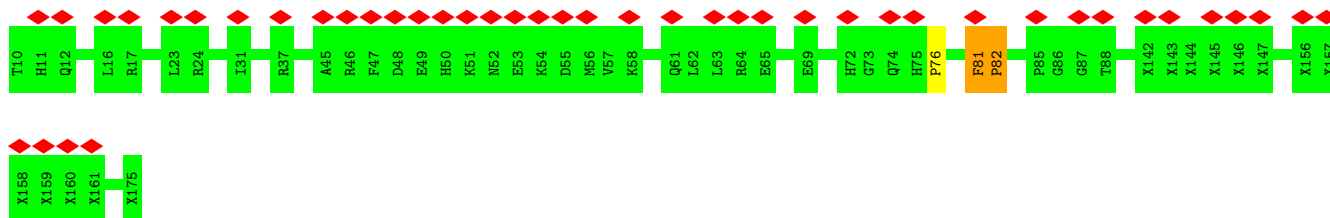
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUFB8



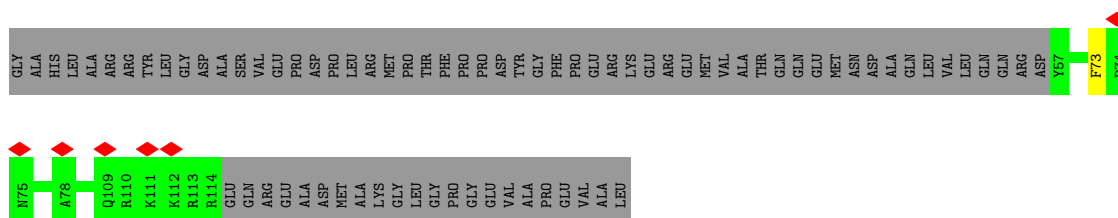
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4, NDUFB4, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4, NDUFB4, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

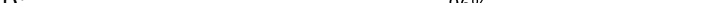


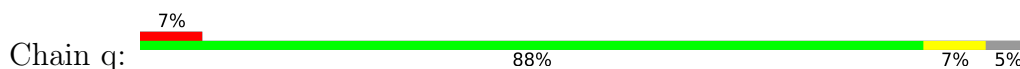
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NDUFB9



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Chain p:  14% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48033	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; 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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.318	Depositor
Minimum map value	-0.301	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	478.80002, 478.80002, 478.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FES, SF4, NAP, 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	0/702	1.00	0/962
2	B	0.53	0/1187	0.99	3/1607 (0.2%)
3	C	0.58	0/1735	0.98	6/2365 (0.3%)
4	D	0.57	0/3304	1.02	9/4478 (0.2%)
5	E	0.79	0/975	1.44	14/1370 (1.0%)
6	F	0.58	0/2389	1.06	2/3299 (0.1%)
7	G	0.57	0/1213	1.04	2/1658 (0.1%)
8	H	0.57	0/2371	0.99	0/3241
9	I	0.53	0/1395	0.93	0/1893
10	J	0.59	0/1239	1.07	0/1688
11	K	0.49	0/730	1.02	0/988
12	L	0.55	0/4653	0.98	0/6350
13	M	0.54	0/3624	0.98	1/4949 (0.0%)
14	N	0.57	0/2656	1.04	3/3630 (0.1%)
15	O	0.52	0/1446	1.01	0/1997
18	R	0.48	0/235	0.79	0/316
19	S	0.50	0/408	1.07	0/571
20	T	0.50	0/380	1.15	0/531
20	U	0.49	0/436	1.12	0/610
21	V	0.68	0/696	1.23	5/954 (0.5%)
22	W	0.65	0/831	1.15	4/1128 (0.4%)
23	X	0.55	0/877	1.00	1/1181 (0.1%)
24	Y	0.57	0/1031	1.02	0/1400
25	Z	0.46	0/585	0.97	0/781
26	a	0.61	0/494	0.97	2/669 (0.3%)
27	b	0.57	0/352	0.93	0/481
28	c	0.64	0/330	1.13	0/455
29	d	0.47	0/581	0.95	0/782
30	e	0.63	0/627	1.18	4/848 (0.5%)
31	f	0.67	0/356	1.08	1/488 (0.2%)
32	g	0.71	0/696	1.25	8/957 (0.8%)
33	h	0.62	0/301	1.11	1/409 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	i	0.65	0/224	1.09	1/300 (0.3%)
38	m	0.56	0/801	0.92	0/1085
39	n	0.50	0/914	0.98	0/1247
40	o	0.49	0/296	1.12	0/412
41	p	0.48	0/535	1.01	0/718
42	q	0.62	0/704	1.11	3/984 (0.3%)
All	All	0.57	0/42309	1.04	70/57782 (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
2	B	0	1

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	19	ILE	N-CA-C	11.72	121.67	110.42
7	G	22	PRO	CA-N-CD	-9.60	98.56	112.00
6	F	53	PRO	CA-N-CD	-9.49	98.71	112.00
5	E	77	PRO	CA-N-CD	-9.47	98.74	112.00
4	D	32	PRO	CA-N-CD	-9.41	98.83	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	CYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	687	0	722	11	0
2	B	1159	0	1166	15	0
3	C	1684	0	1610	37	0
4	D	3229	0	3123	87	0
5	E	959	0	509	84	0
6	F	2356	0	1535	12	0
7	G	3614	0	1341	16	0
8	H	2306	0	2419	31	0
9	I	1366	0	1286	11	0
10	J	1211	0	1165	15	0
11	K	720	0	761	20	0
12	L	4538	0	4480	40	0
13	M	3536	0	3652	36	0
14	N	2592	0	2631	61	0
15	O	1851	0	1131	0	0
16	P	1415	0	303	1	0
17	Q	565	0	122	1	0
18	R	501	0	246	0	0
19	S	405	0	197	3	0
20	T	378	0	176	0	0
20	U	432	0	207	0	0
21	V	685	0	563	19	0
22	W	817	0	743	32	0
23	X	1133	0	837	7	0
24	Y	1011	0	1018	5	0
25	Z	921	0	655	9	0
26	a	480	0	440	2	0
27	b	519	0	408	1	0
28	c	320	0	277	2	0
29	d	790	0	597	2	0
30	e	616	0	506	40	0
31	f	350	0	260	6	0
32	g	677	0	559	41	0
33	h	770	0	404	15	0
34	i	616	0	302	7	0
35	j	260	0	57	0	0
36	k	370	0	78	0	0
37	l	590	0	125	1	0
38	m	887	0	781	2	0
39	n	1088	0	769	2	0
40	o	296	0	134	0	0
41	p	1039	0	583	2	0
42	q	696	0	338	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	435	0	96	1	0
44	s	175	0	40	0	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	51181	0	39396	568	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 6.

The worst 5 of 568 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)
4:D:38:PRO:HG3	14:N:50:PRO:CG	1.23	1.61
30:e:93:PRO:CD	30:e:94:PRO:HD3	1.24	1.61
30:e:93:PRO:HD2	30:e:94:PRO:CD	1.23	1.60
4:D:38:PRO:CG	14:N:50:PRO:CB	1.78	1.58
4:D:38:PRO:CD	14:N:50:PRO:HG3	1.06	1.50

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%)	3 (4%)	2 (2%)	4 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	145/179 (81%)	128 (88%)	10 (7%)	7 (5%)	2	16
3	C	204/228 (90%)	174 (85%)	23 (11%)	7 (3%)	3	21
4	D	412/429 (96%)	360 (87%)	37 (9%)	15 (4%)	2	20
5	E	184/217 (85%)	151 (82%)	18 (10%)	15 (8%)	0	9
6	F	423/444 (95%)	375 (89%)	38 (9%)	10 (2%)	4	27
7	G	201/785 (26%)	168 (84%)	26 (13%)	7 (4%)	3	20
8	H	292/318 (92%)	270 (92%)	16 (6%)	6 (2%)	5	30
9	I	174/176 (99%)	144 (83%)	19 (11%)	11 (6%)	1	13
10	J	169/175 (97%)	150 (89%)	14 (8%)	5 (3%)	3	23
11	K	93/98 (95%)	88 (95%)	5 (5%)	0	100	100
12	L	602/606 (99%)	539 (90%)	52 (9%)	11 (2%)	6	33
13	M	455/459 (99%)	411 (90%)	33 (7%)	11 (2%)	4	27
14	N	342/347 (99%)	309 (90%)	26 (8%)	7 (2%)	6	31
15	O	227/316 (72%)	199 (88%)	20 (9%)	8 (4%)	3	20
18	R	34/89 (38%)	30 (88%)	3 (9%)	1 (3%)	3	24
19	S	78/99 (79%)	73 (94%)	5 (6%)	0	100	100
20	T	73/88 (83%)	69 (94%)	3 (4%)	1 (1%)	9	39
20	U	83/88 (94%)	74 (89%)	7 (8%)	2 (2%)	4	27
21	V	104/115 (90%)	91 (88%)	8 (8%)	5 (5%)	2	16
22	W	109/128 (85%)	90 (83%)	12 (11%)	7 (6%)	1	13
23	X	108/169 (64%)	94 (87%)	11 (10%)	3 (3%)	4	24
24	Y	136/141 (96%)	124 (91%)	8 (6%)	4 (3%)	3	24
25	Z	69/138 (50%)	65 (94%)	4 (6%)	0	100	100
26	a	62/70 (89%)	54 (87%)	4 (6%)	4 (6%)	1	13
27	b	44/80 (55%)	40 (91%)	4 (9%)	0	100	100
28	c	44/49 (90%)	39 (89%)	2 (4%)	3 (7%)	1	12
29	d	69/114 (60%)	64 (93%)	4 (6%)	1 (1%)	9	39
30	e	87/105 (83%)	76 (87%)	10 (12%)	1 (1%)	11	45
31	f	52/57 (91%)	44 (85%)	5 (10%)	3 (6%)	1	14
32	g	95/125 (76%)	67 (70%)	15 (16%)	13 (14%)	0	3
33	h	38/134 (28%)	35 (92%)	1 (3%)	2 (5%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	25/106 (24%)	24 (96%)	1 (4%)	0	100	100
38	m	96/118 (81%)	84 (88%)	8 (8%)	4 (4%)	2	18
39	n	126/166 (76%)	113 (90%)	10 (8%)	3 (2%)	4	27
40	o	56/136 (41%)	52 (93%)	3 (5%)	1 (2%)	6	33
41	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	2	17
42	q	136/145 (94%)	110 (81%)	21 (15%)	5 (4%)	2	20
All	All	5798/7521 (77%)	5117 (88%)	493 (8%)	188 (3%)	5	21

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	HIS
2	B	150	PRO
3	C	9	PRO
4	D	38	PRO
5	E	16	ASN

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	72/101 (71%)	69 (96%)	3 (4%)	26	48
2	B	124/150 (83%)	118 (95%)	6 (5%)	23	45
3	C	179/204 (88%)	172 (96%)	7 (4%)	28	50
4	D	332/371 (90%)	317 (96%)	15 (4%)	24	47
5	E	21/183 (12%)	20 (95%)	1 (5%)	23	45
6	F	84/353 (24%)	81 (96%)	3 (4%)	31	52
7	G	64/172 (37%)	60 (94%)	4 (6%)	16	38
8	H	249/275 (90%)	237 (95%)	12 (5%)	23	45
9	I	138/151 (91%)	128 (93%)	10 (7%)	13	35
10	J	112/142 (79%)	111 (99%)	1 (1%)	70	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	83/86 (96%)	81 (98%)	2 (2%)	43	63
12	L	463/534 (87%)	449 (97%)	14 (3%)	36	57
13	M	384/413 (93%)	373 (97%)	11 (3%)	37	58
14	N	277/316 (88%)	262 (95%)	15 (5%)	20	43
15	O	83/207 (40%)	82 (99%)	1 (1%)	63	73
18	R	17/26 (65%)	16 (94%)	1 (6%)	18	41
19	S	4/82 (5%)	4 (100%)	0	100	100
20	T	3/81 (4%)	3 (100%)	0	100	100
20	U	5/81 (6%)	5 (100%)	0	100	100
21	V	47/101 (46%)	47 (100%)	0	100	100
22	W	71/114 (62%)	70 (99%)	1 (1%)	59	71
23	X	83/103 (81%)	82 (99%)	1 (1%)	63	73
24	Y	99/102 (97%)	96 (97%)	3 (3%)	36	57
25	Z	59/59 (100%)	58 (98%)	1 (2%)	53	67
26	a	41/59 (70%)	40 (98%)	1 (2%)	43	63
27	b	36/36 (100%)	34 (94%)	2 (6%)	19	42
28	c	26/45 (58%)	26 (100%)	0	100	100
29	d	56/60 (93%)	55 (98%)	1 (2%)	51	66
30	e	45/95 (47%)	45 (100%)	0	100	100
31	f	22/54 (41%)	21 (96%)	1 (4%)	24	47
32	g	51/112 (46%)	51 (100%)	0	100	100
33	h	28/35 (80%)	28 (100%)	0	100	100
34	i	20/27 (74%)	20 (100%)	0	100	100
38	m	75/86 (87%)	74 (99%)	1 (1%)	61	71
39	n	65/117 (56%)	65 (100%)	0	100	100
40	o	5/119 (4%)	5 (100%)	0	100	100
41	p	50/62 (81%)	49 (98%)	1 (2%)	48	66
42	q	9/131 (7%)	9 (100%)	0	100	100
All	All	3582/5445 (66%)	3463 (97%)	119 (3%)	34	55

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	119	CYS
24	Y	107	TYR
12	L	283	ILE
24	Y	105	ARG
41	p	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	415	GLN
22	W	57	GLN
14	N	36	ASN
15	O	107	GLN
23	X	76	HIS

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
46	FES	G	803	7	0,4,4	-	-	-		
46	FES	E	301	5	0,4,4	-	-	-		
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
48	NAP	P	501	-	49,52,52	1.17	5 (10%)	69,80,80	1.69	12 (17%)
45	SF4	I	202	9	0,12,12	-	-	-		
45	SF4	G	801	7	0,12,12	-	-	-		
47	FMN	F	501	-	33,33,33	1.65	5 (15%)	48,50,50	1.41	8 (16%)
45	SF4	G	802	7	0,12,12	-	-	-		
45	SF4	I	201	9	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
46	FES	G	803	7	-	-	0/1/1/1
46	FES	E	301	5	-	-	0/1/1/1
45	SF4	B	201	2	-	-	0/6/5/5
45	SF4	F	502	6	-	-	0/6/5/5
48	NAP	P	501	-	-	6/35/67/67	0/5/5/5
45	SF4	I	202	9	-	-	0/6/5/5
45	SF4	G	801	7	-	-	0/6/5/5
47	FMN	F	501	-	-	12/18/18/18	0/3/3/3
45	SF4	G	802	7	-	-	0/6/5/5
45	SF4	I	201	9	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	501	FMN	C9A-C5A	5.82	1.50	1.41
48	P	501	NAP	C5A-C4A	4.82	1.48	1.39
47	F	501	FMN	C8-C7	3.98	1.50	1.40
48	P	501	NAP	C5A-C6A	2.97	1.49	1.41
47	F	501	FMN	C4A-N5	2.56	1.35	1.30

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	P	501	NAP	C5A-C4A-N3A	-6.22	118.63	126.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	P	501	NAP	N3A-C4A-N9A	4.85	135.07	127.08
48	P	501	NAP	C2A-N3A-C4A	4.08	121.39	111.75
48	P	501	NAP	N3A-C2A-N1A	-3.55	123.06	128.60
48	P	501	NAP	C3D-C2D-C1D	3.41	106.11	100.98

There are no chirality outliers.

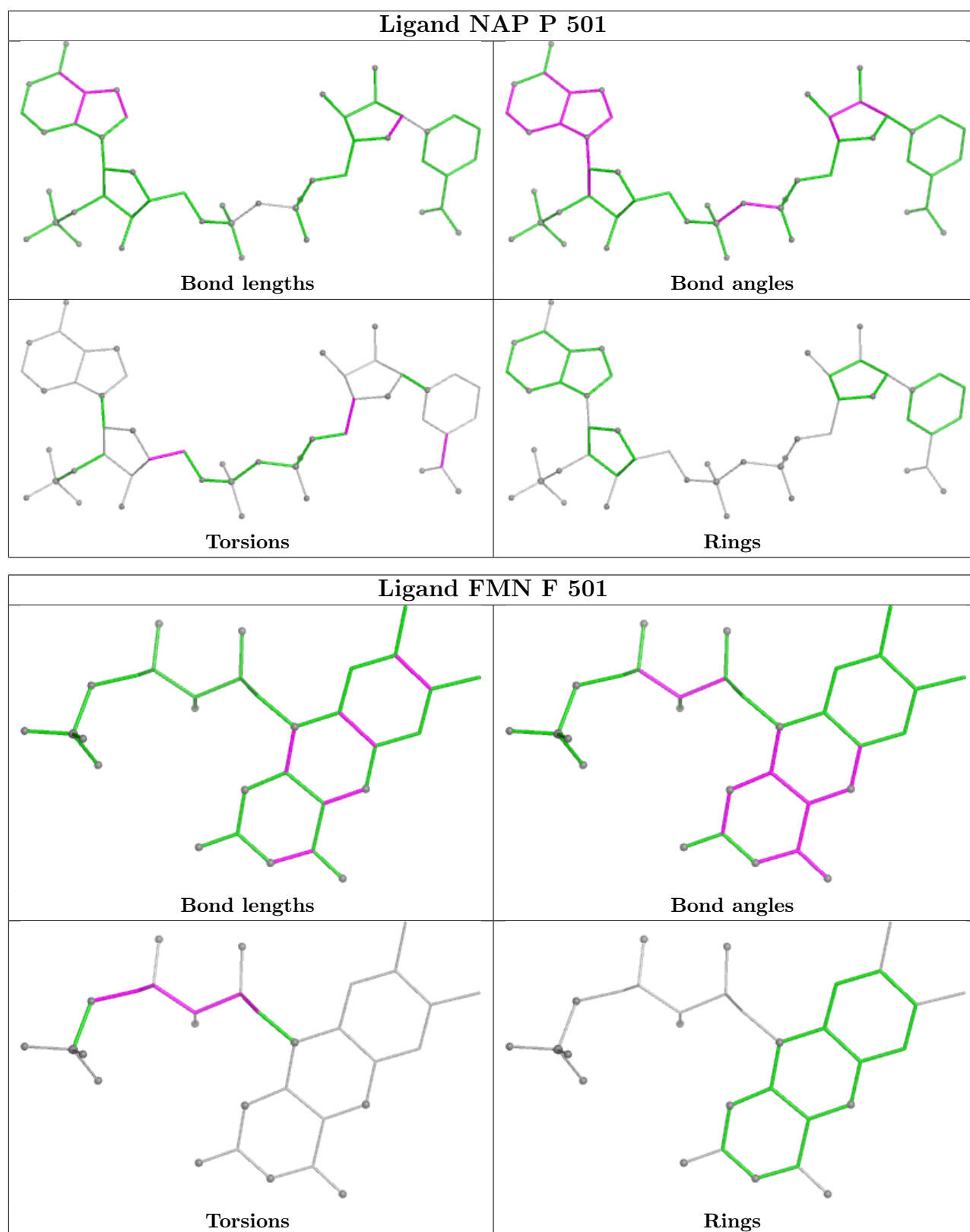
5 of 18 torsion outliers are listed below:

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	C3'-C4'-C5'-O5'

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	2
43	r	1
34	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	70:UNK	C	100:UNK	N	22.99
1	P	252:UNK	C	280:UNK	N	21.70
1	P	186:UNK	C	200:UNK	N	21.19
1	i	32:PRO	C	40:UNK	N	15.55

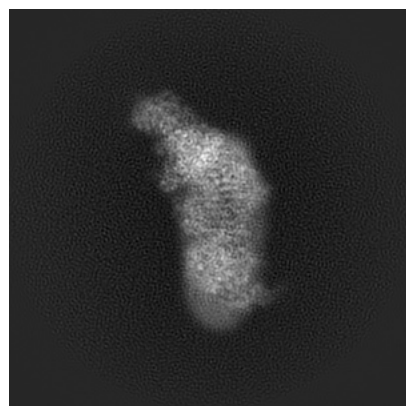
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4040. These allow visual inspection of the internal detail of the map and identification of artifacts.

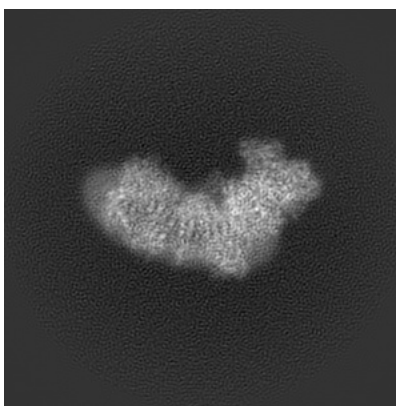
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

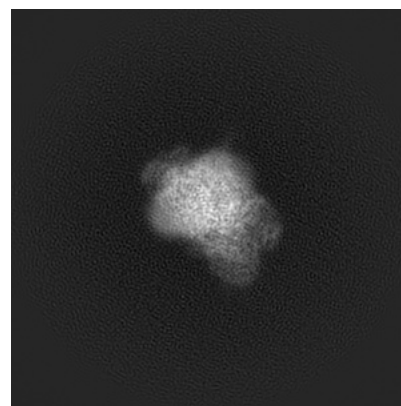
6.1.1 Primary map



X

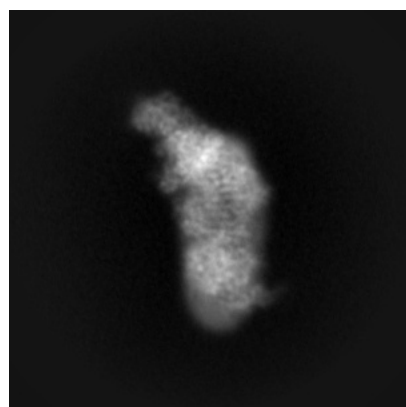


Y

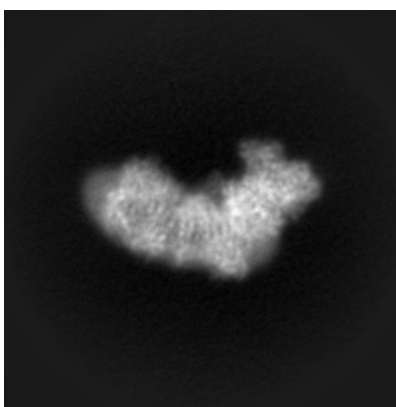


Z

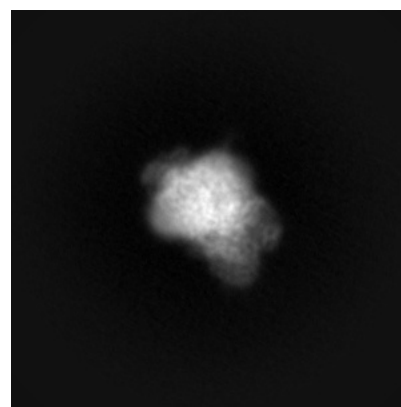
6.1.2 Raw map



X



Y

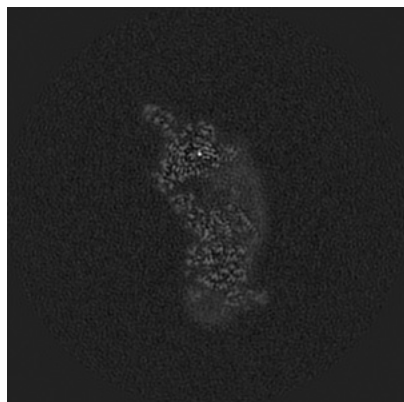


Z

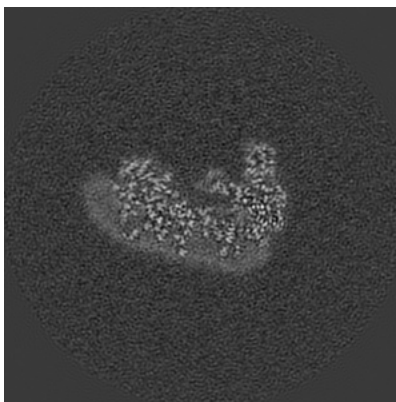
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

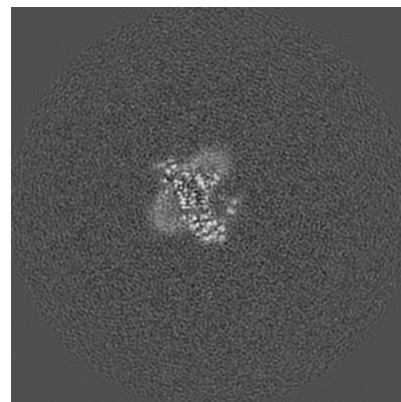
6.2.1 Primary map



X Index: 180

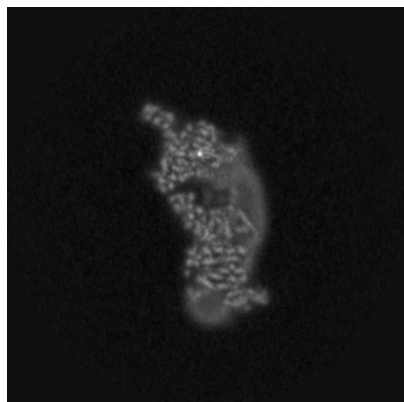


Y Index: 180

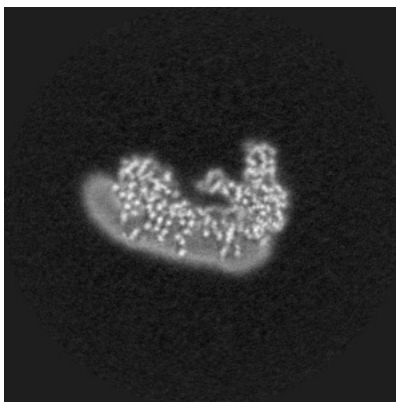


Z Index: 180

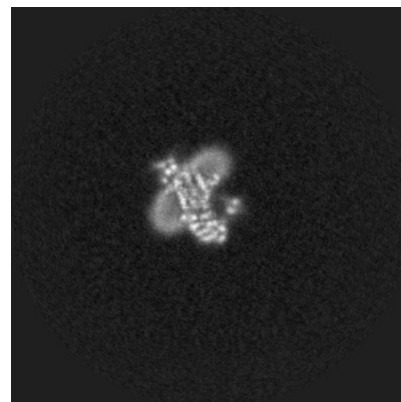
6.2.2 Raw map



X Index: 180



Y Index: 180

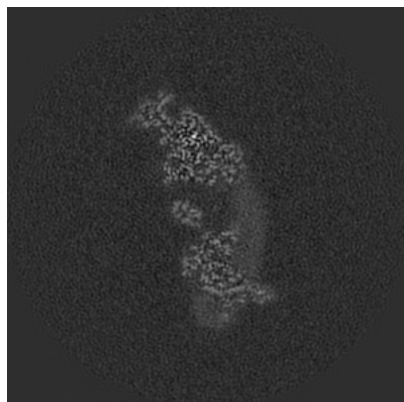


Z Index: 180

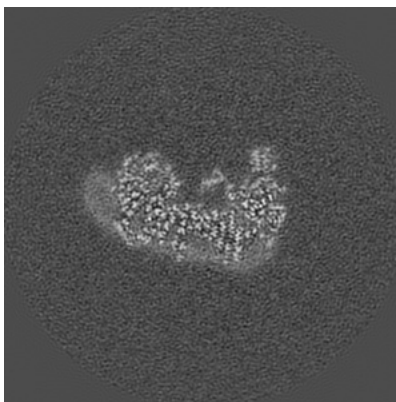
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

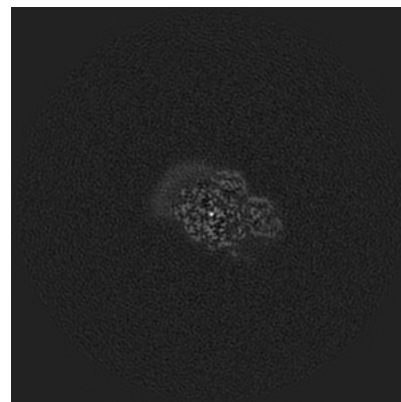
6.3.1 Primary map



X Index: 190

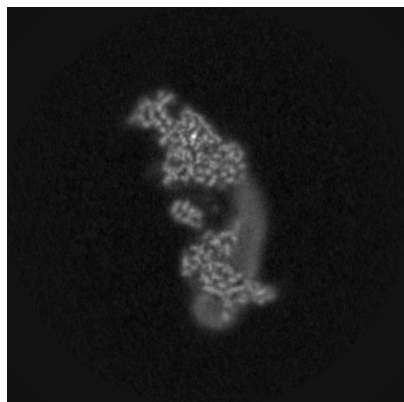


Y Index: 185

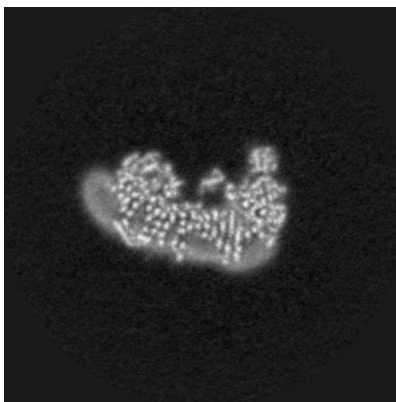


Z Index: 227

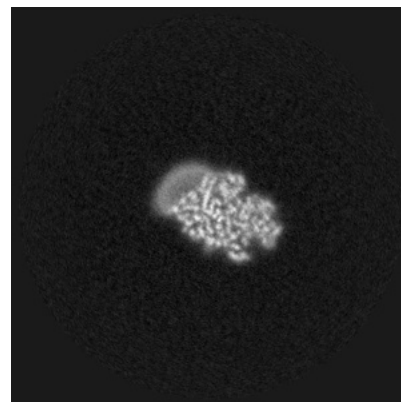
6.3.2 Raw map



X Index: 190



Y Index: 185

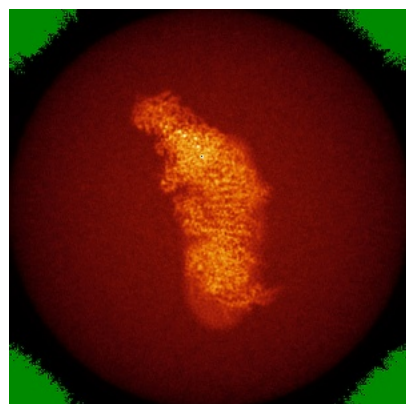


Z Index: 232

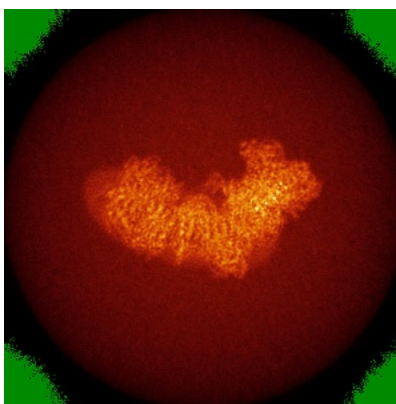
The images above show the largest variance slices of the map in three orthogonal directions.

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

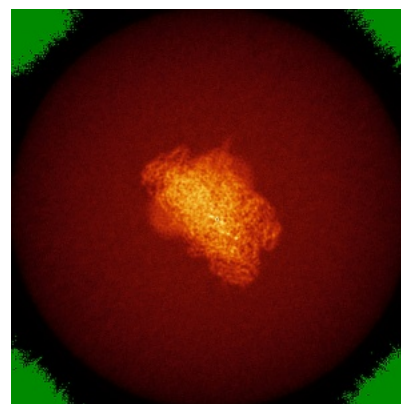
6.4.1 Primary map



X

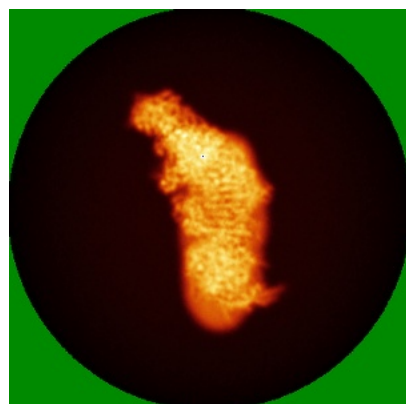


Y



Z

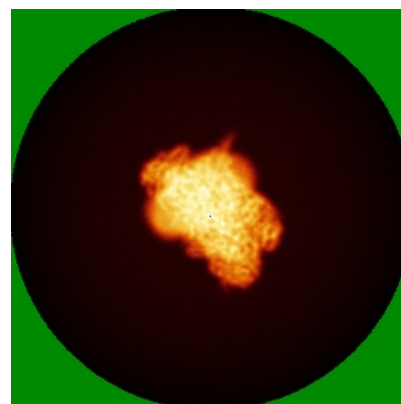
6.4.2 Raw map



X



Y

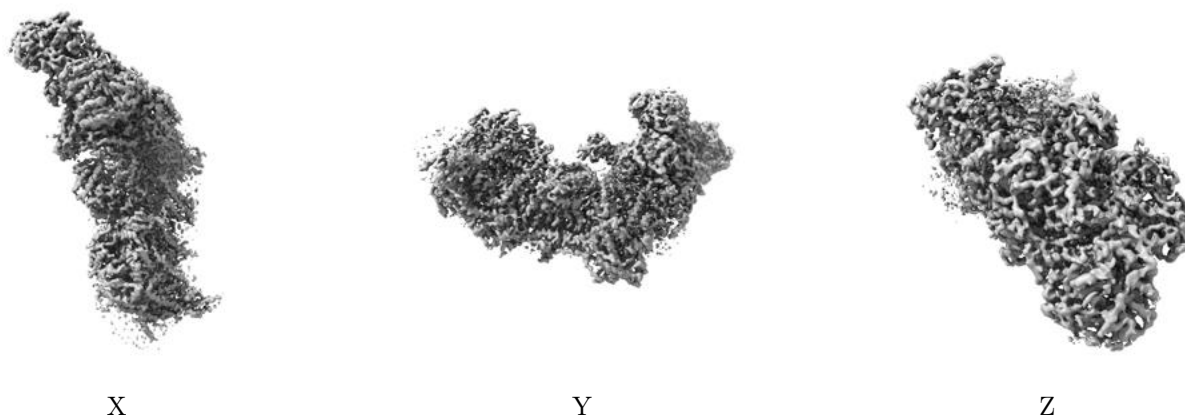


Z

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.

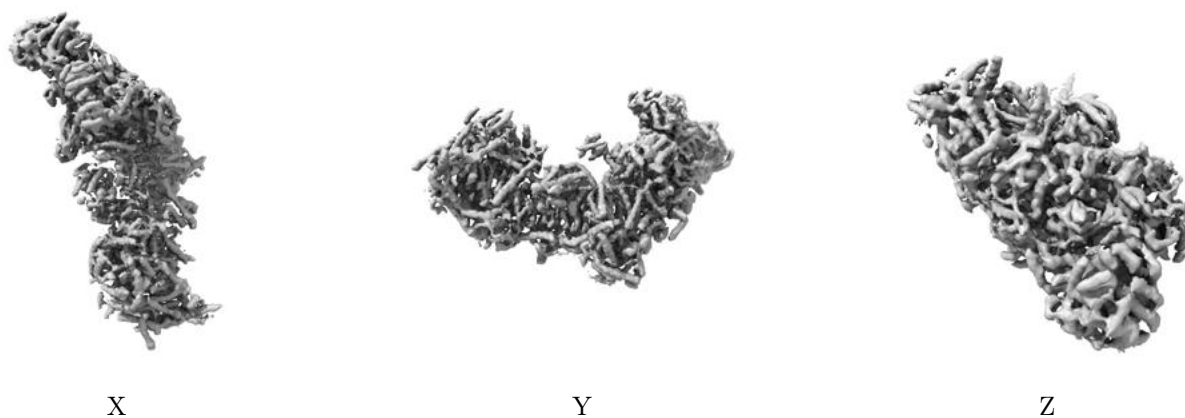
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

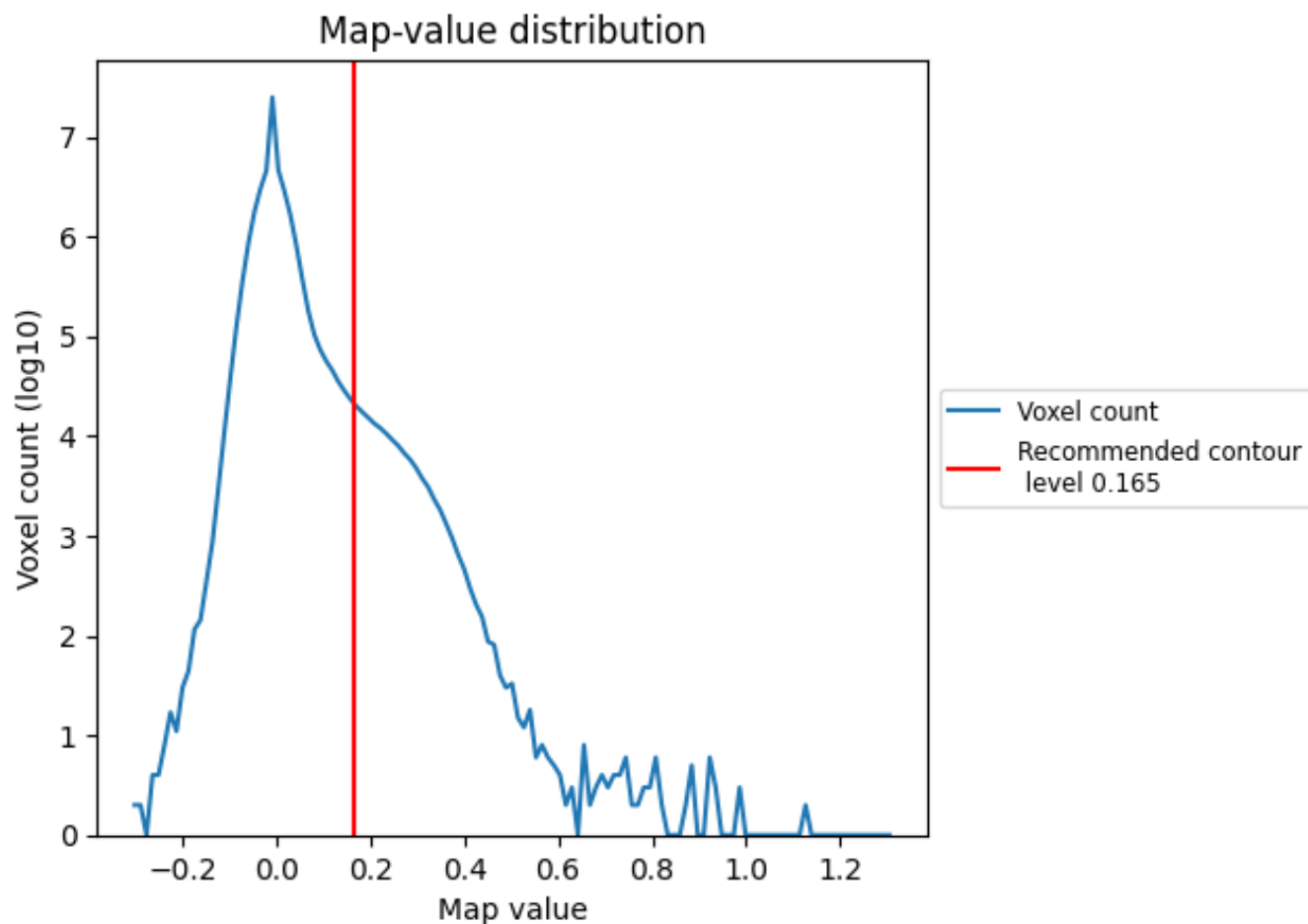
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

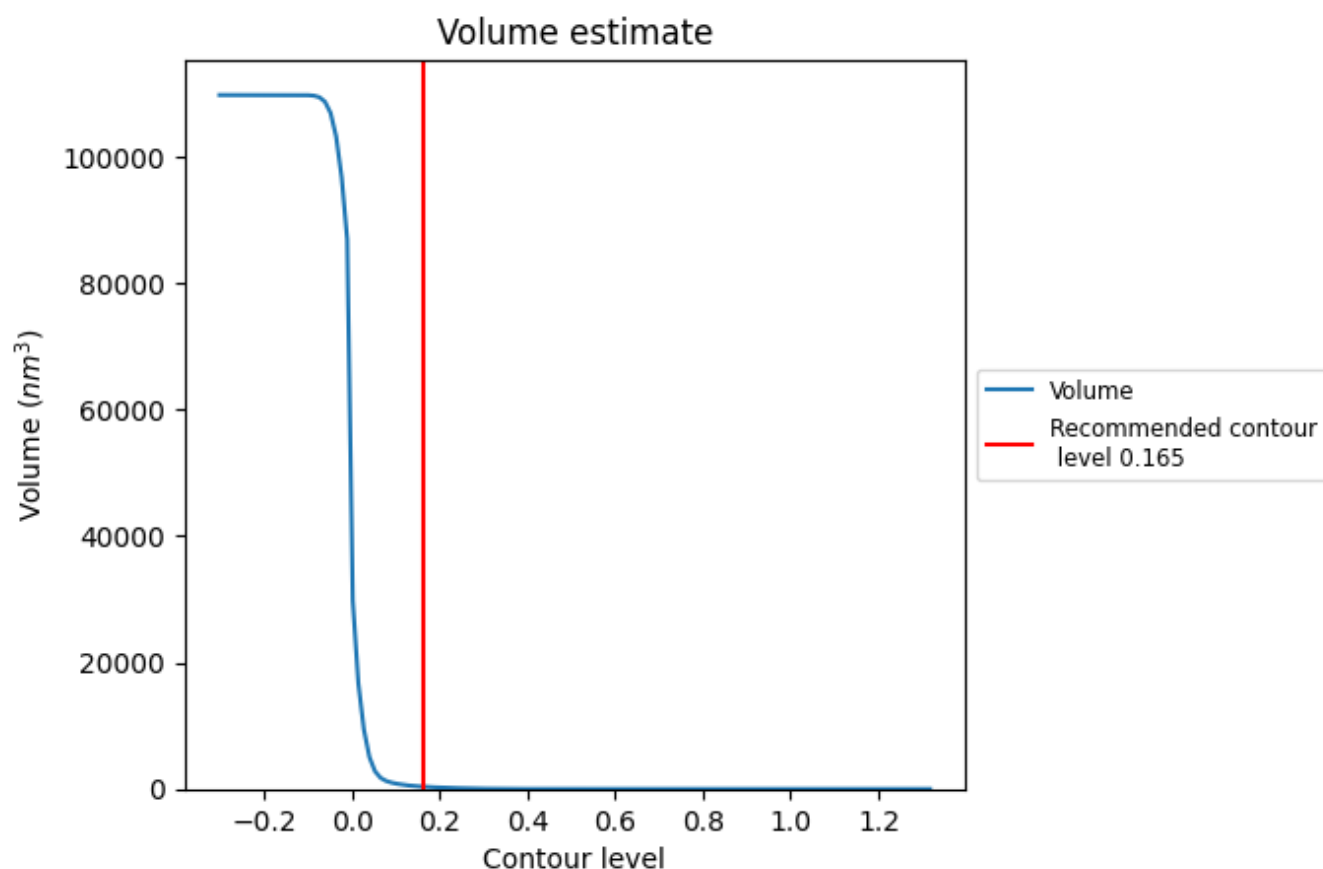
This section contains the results of statistical analysis of the map.

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.

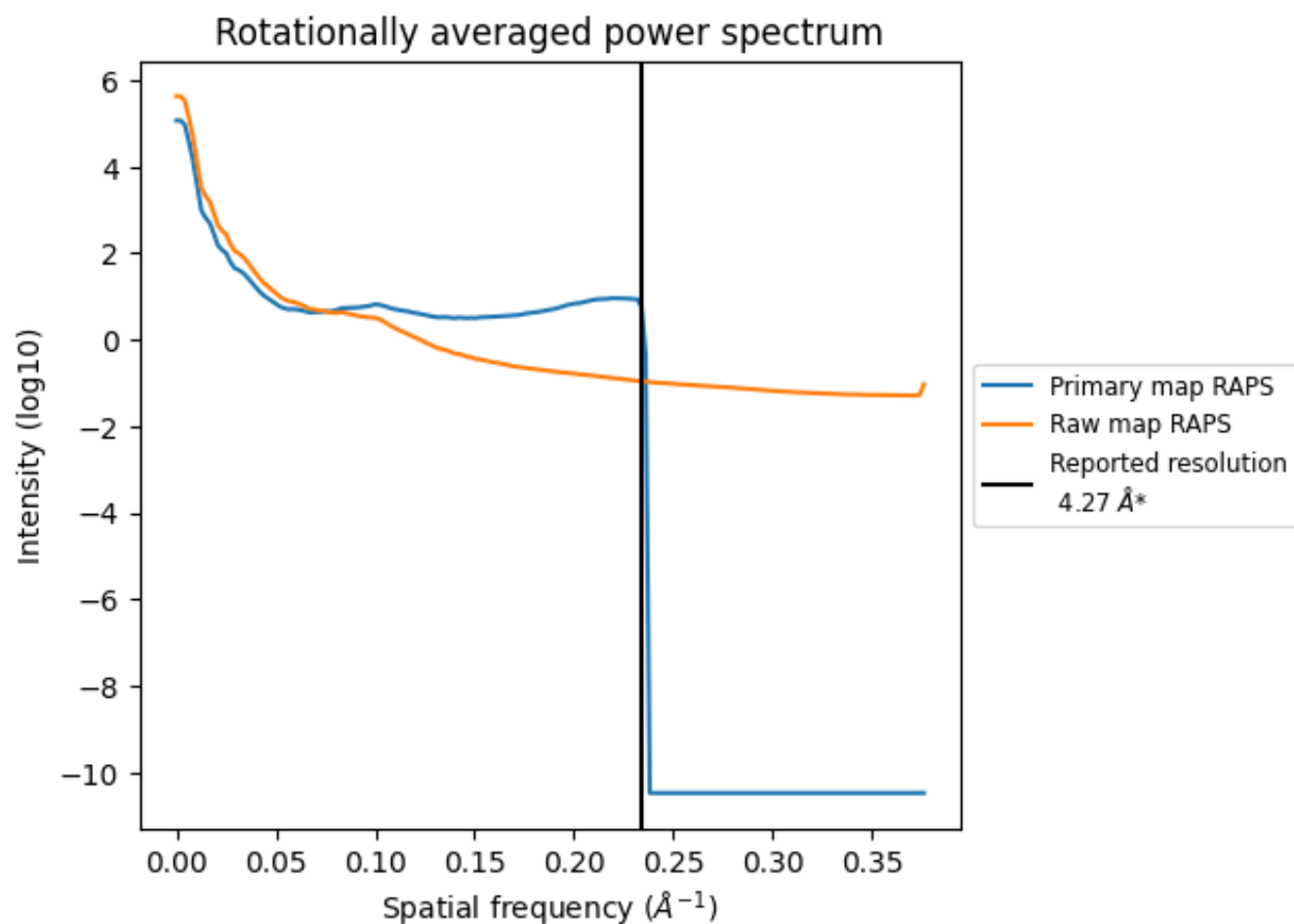
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm^3 ; this corresponds to an approximate mass of 316 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 ⓘ

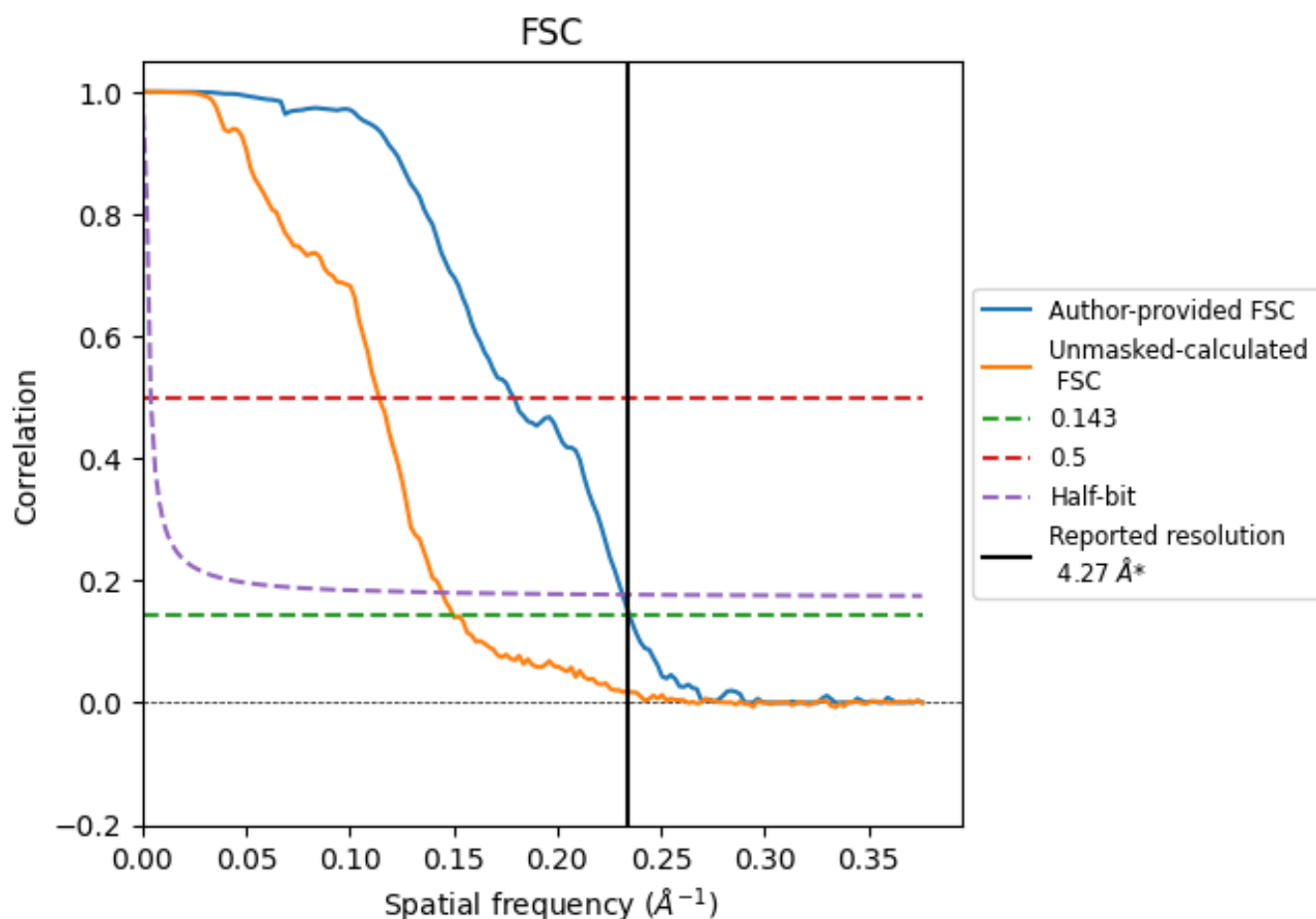


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

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 0.234 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

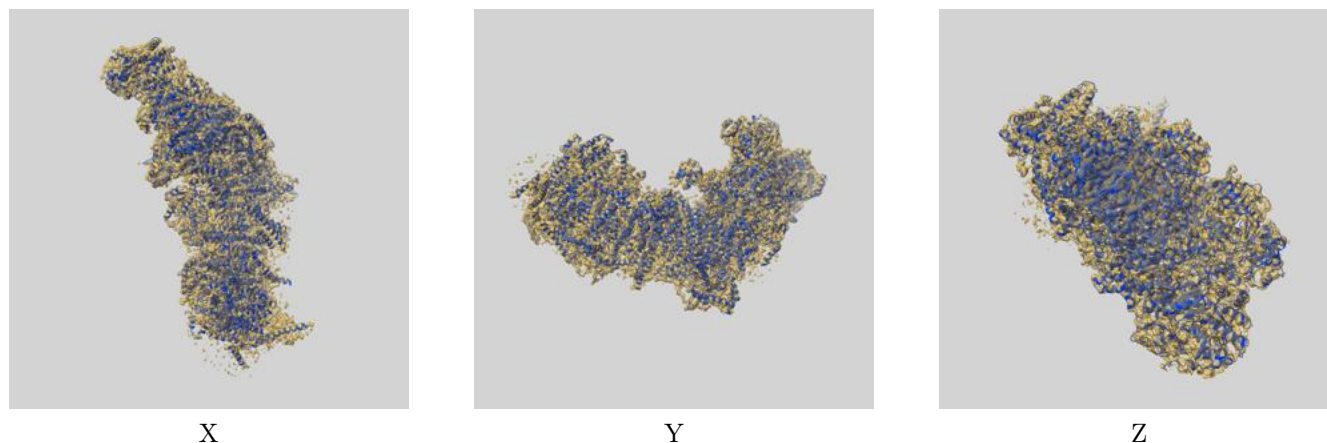
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.27	-	-
Author-provided FSC curve	4.26	5.59	4.32
Unmasked-calculated*	6.68	8.76	6.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.68 differs from the reported value 4.27 by more than 10 %

9 Map-model fit [i](#)

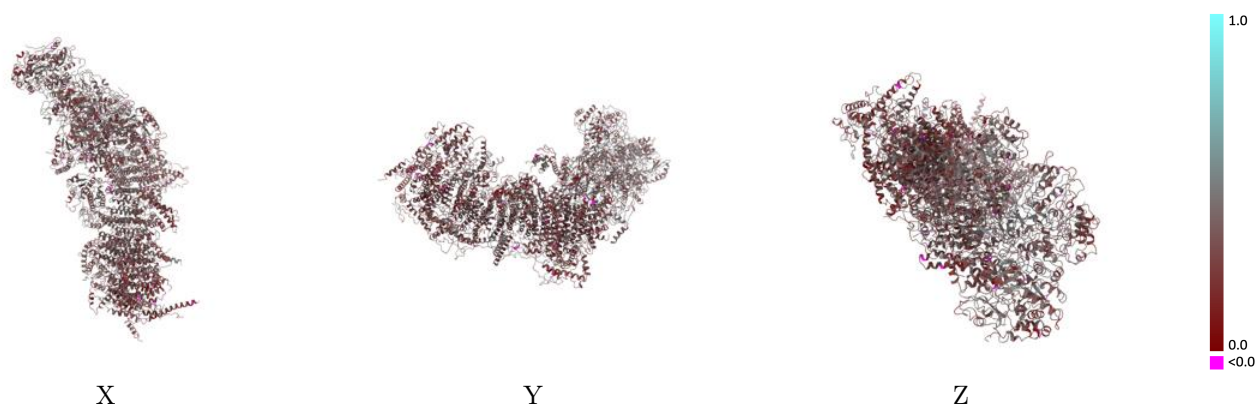
This section contains information regarding the fit between EMDB map EMD-4040 and PDB model 5LDW. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



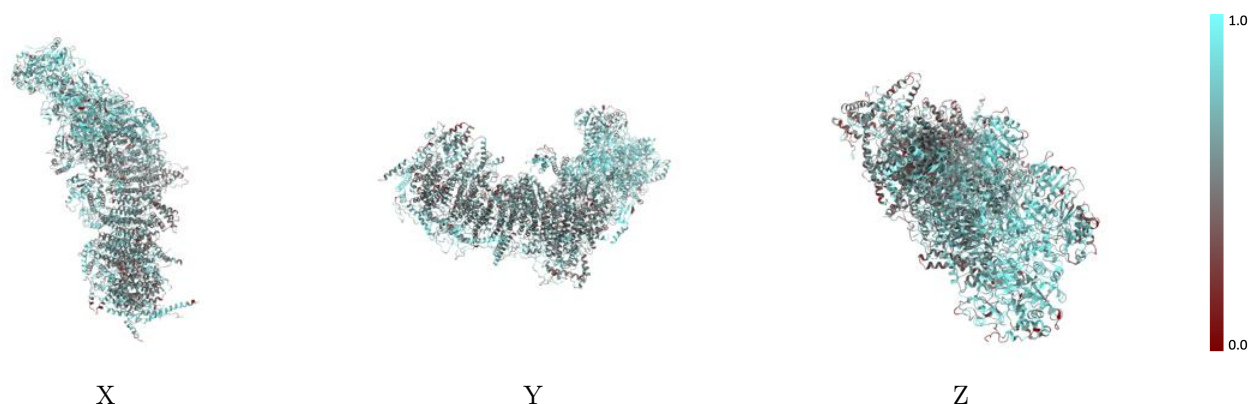
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



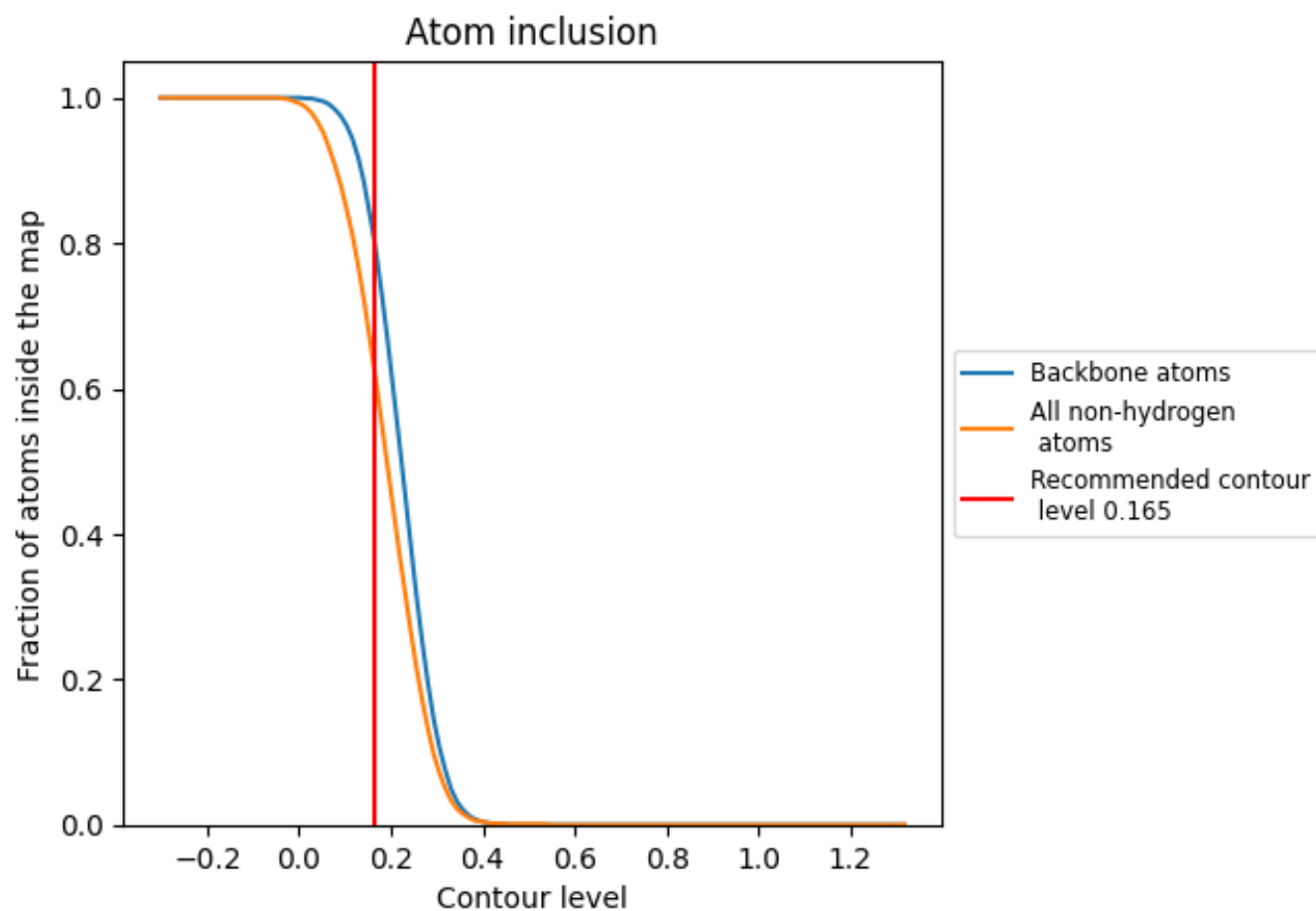
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 62% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.3300
A	 0.5400	 0.2900
B	 0.6410	 0.3420
C	 0.6010	 0.3160
D	 0.6190	 0.3470
E	 0.7640	 0.3750
F	 0.6610	 0.3360
G	 0.7140	 0.3740
H	 0.5640	 0.3150
I	 0.6230	 0.3300
J	 0.5170	 0.2900
K	 0.5850	 0.3250
L	 0.5420	 0.2910
M	 0.5760	 0.3210
N	 0.6030	 0.3350
O	 0.6910	 0.3540
P	 0.7290	 0.3720
Q	 0.8140	 0.4160
R	 0.7340	 0.4020
S	 0.6740	 0.3420
T	 0.5850	 0.3390
U	 0.6900	 0.3650
V	 0.5600	 0.2950
W	 0.5860	 0.3080
X	 0.5350	 0.2950
Y	 0.4730	 0.2670
Z	 0.5840	 0.2960
a	 0.5610	 0.2770
b	 0.5490	 0.3150
c	 0.6250	 0.3190
d	 0.6460	 0.3470
e	 0.6200	 0.3430
f	 0.5580	 0.3040
g	 0.5590	 0.3000
h	 0.7020	 0.3540



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6250	 0.3320
j	 0.7150	 0.3300
k	 0.5700	 0.3250
l	 0.7090	 0.3500
m	 0.5890	 0.3150
n	 0.6000	 0.3190
o	 0.7400	 0.2540
p	 0.6690	 0.3340
q	 0.7770	 0.3930
r	 0.7260	 0.3590
s	 0.8110	 0.4110