wwPDB EM Validation Summary Report (i)

Sep 7, 2026 – 11:27 pm BST

PDB ID	:	6QA9 / pdb_00006qa9
EMDB ID	:	EMD-4482
Title	:	Isolated complex I class refinement from Ovine respiratory supercomplex I+III2
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-19
Resolution	:	4.10 Å(reported)
Based on initial model	:	1PPJ

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:

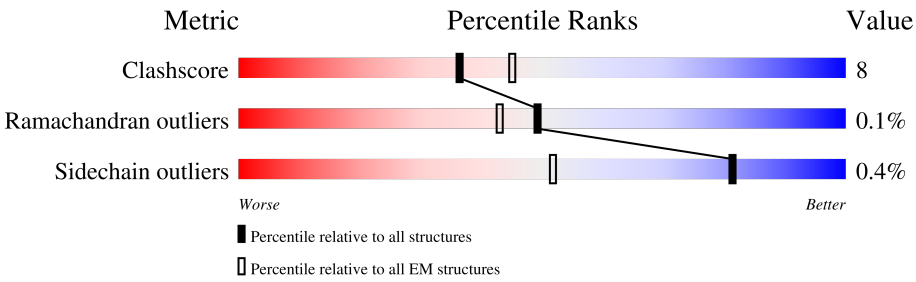
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

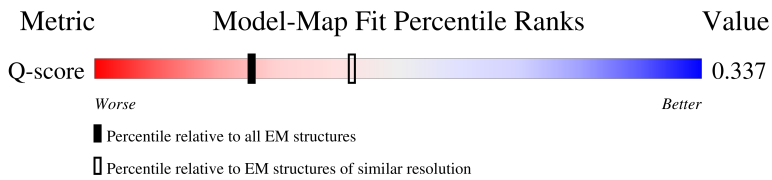
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	V1	445	18% 73% 23% • •
2	V2	217	24% 79% 18% •
3	S1	704	21% 75% 22% •
4	S2	430	25% 78% 21% •

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Mol	Chain	Length	Quality of chain
5	S3	228	17% 68% 22% 9%
6	S7	179	18% 69% 18% 13%
7	S8	176	19% 78% 21%
8	V3	75	15% 32% 20% 47%
9	S6	96	23% 77% 21%
10	S4	133	21% 78% 16% 5%
11	A9	338	33% 64% 22% 14%
12	A2	98	27% 66% 17% 16%
13	A5	115	30% 83% 12%
14	A6	127	28% 69% 21% 10%
15	A7	112	38% 63% 21% 16%
16	AL	145	57% 84% 12%
17	AA	88	64% 76% 15% 9%
17	AB	88	45% 82% 17%
18	D3	115	44% 77% 7% 16%
19	D1	318	31% 69% 24% 6%
20	D6	175	53% 77% 21%
21	4L	98	46% 80% 20%
22	D5	606	48% 74% 26%
23	D4	459	33% 76% 23%
24	D2	347	24% 79% 21%
25	AK	140	67% 86% 13%
26	B5	143	27% 84% 13%
27	A8	171	22% 80% 20%
28	BJ	175	31% 78% 19%

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Mol	Chain	Length	Quality of chain
29	AJ	320	33% 79% 21%
30	S5	105	24% 80% 13% 6%
31	A3	83	33% 67% 22% 11%
32	B3	97	48% 59% 15% 25%
33	C2	120	30% 84% 13%
34	B4	128	42% 86% 13%
35	AM	143	27% 79% 18%
36	B6	127	29% 57% 17% 24%
37	B7	136	39% 74% 13% 12%
38	B9	178	33% 76% 22%
39	B2	72	49% 69% 21% 10%
40	B8	158	43% 77% 23%
41	BK	125	36% 68% 14% 18%
42	C1	49	31% 86% 8% 6%
43	B1	57	44% 75% 14% 9%
44	A1	70	26% 86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	V1	500	-	-	X	-

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 65403 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	V1	430	3312	2086	593	613	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V2	212	1647	1052	277	308	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S2	427	3436	2194	589	628	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S3	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S7	156	1248	795	225	214	14	0	0

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	S8	176	1415	889	243	271	12	0	0

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V3	40	335	209	60	65	1	0	0

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S6	95	737	451	139	144	3	0	0

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S4	126	1025	646	182	194	3	0	0

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A9	290	2321	1483	423	410	5	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A2	82	665	419	124	120	2	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A5	111	902	583	151	166	2	0	0

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	A6	114	970	619	180	167	4	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	A7	94	752	470	143	136	3	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AL	143	1192	768	214	206	4	0	0

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AA	80	645	416	96	128	5	0	0
17	AB	87	702	451	103	143	5	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	D3	97	787	538	112	132	5	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	D1	299	2390	1618	364	389	19	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	D6	171	1308	878	187	230	13	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	4L	98	748	489	112	132	15	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	D5	606	4805	3187	746	828	44	0	0

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	D4	459	3646	2428	571	607	40	0	0

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	D2	347	2724	1808	416	460	40	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	AK	140	1025	654	175	190	6	0	0

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	B5	139	1156	761	194	199	2	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	A8	171	1404	889	253	252	10	0	0

- Molecule 28 is a protein called NDUFB10.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AJ	319	2583	1653	430	490	10	0	0

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	S5	99	822	520	154	142	6	0	0

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	A3	74	582	379	96	105	2	0	0

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	B3	73	578	378	100	98	2	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	C2	119	997	647	174	172	4	0	0

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	B4	128	1059	675	189	194	1	0	0

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AM	139	1143	733	200	201	9	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B6	96	815	536	139	139	1	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	B7	119	1026	641	196	181	8	0	0

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	B9	176	1515	970	278	261	6	0	0

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	B2	65	563	372	93	97	1	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	B8	157	1324	855	217	243	9	0	0

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

11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BK	102	853	547	141	161	4	0	0

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	C1	46	391	258	67	66	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	B1	52	449	296	79	74	0	0

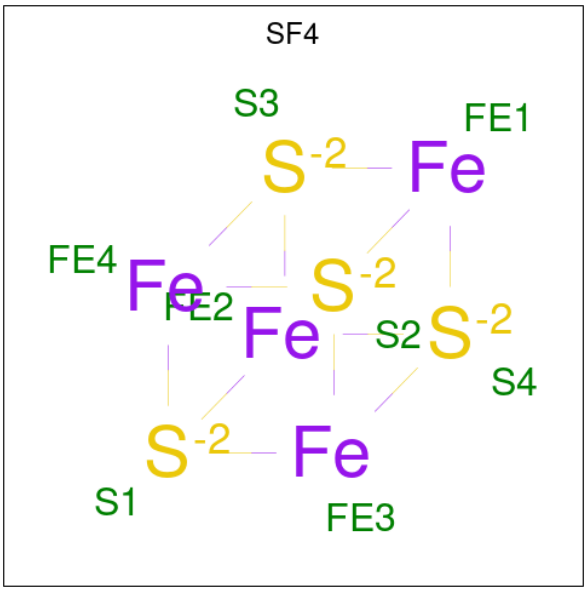
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NDUFA1.

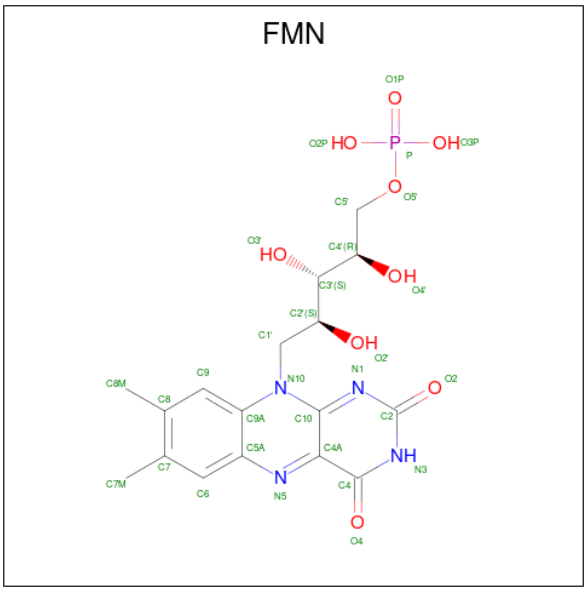
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	A1	70	577	369	106	97	5	0	0

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



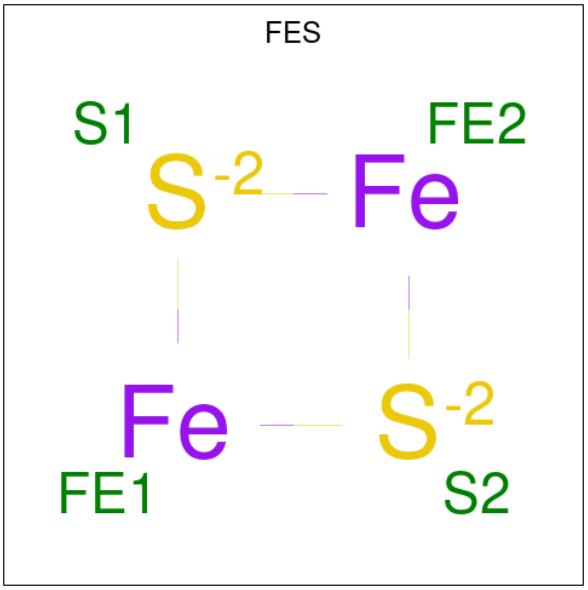
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	V1	1	8	4	4	0
45	S1	1	8	4	4	0
45	S1	1	8	4	4	0
45	S7	1	8	4	4	0
45	S8	1	8	4	4	0
45	S8	1	8	4	4	0

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



Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

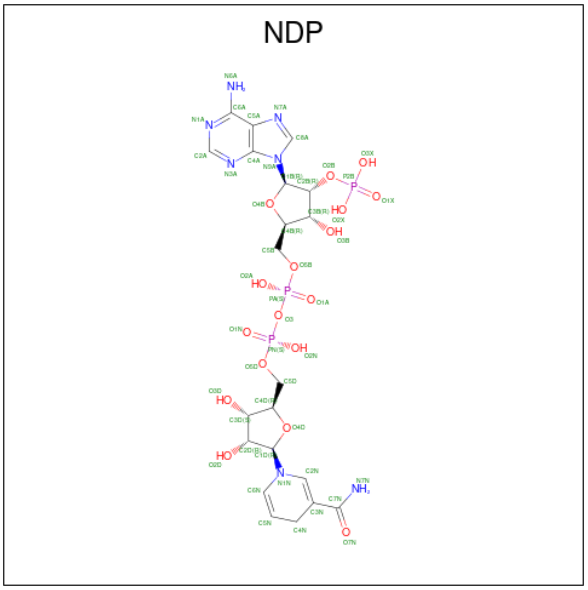


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

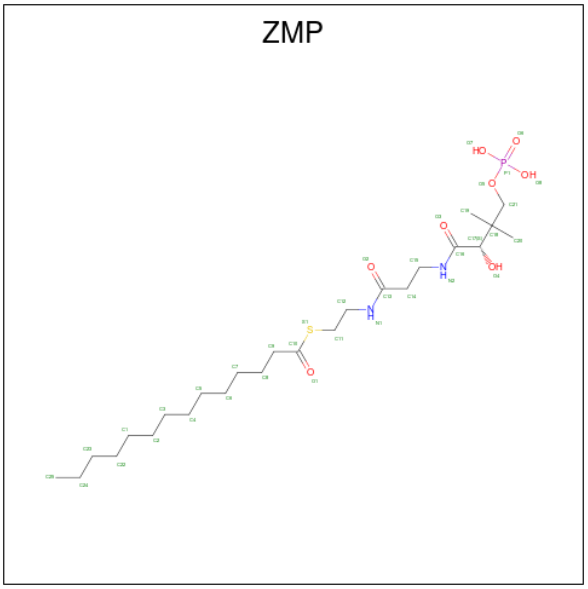
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	S6	1	1	1	0

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



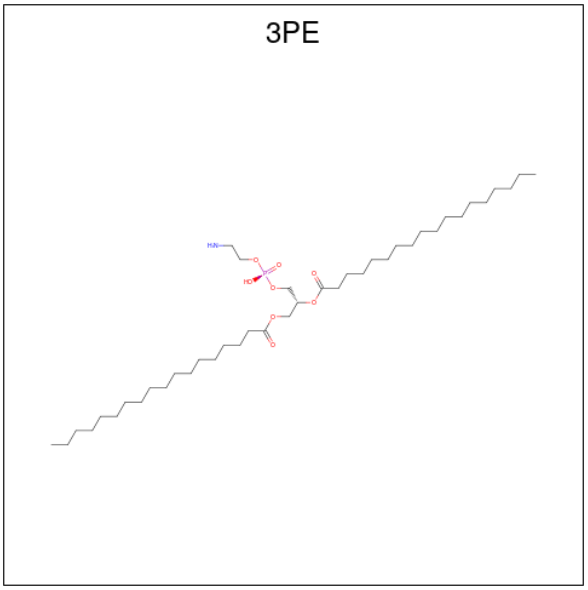
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	A9	1	48	21	7	17	3	0

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



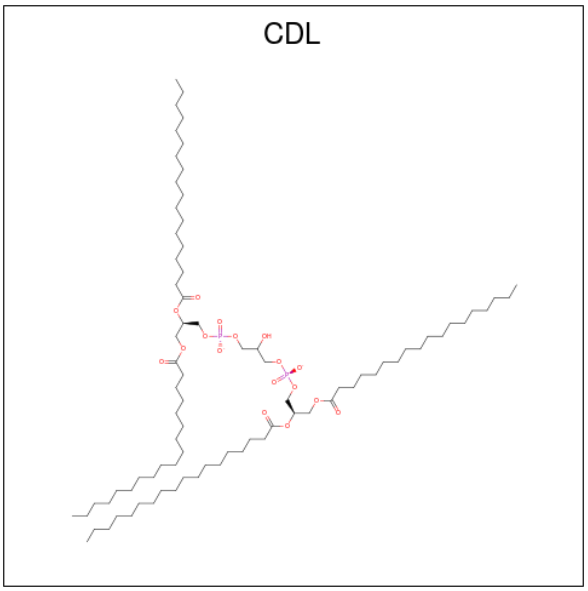
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	AA	1	34	23	2	7	1	1	0
50	B9	1	31	20	2	7	1	1	0

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



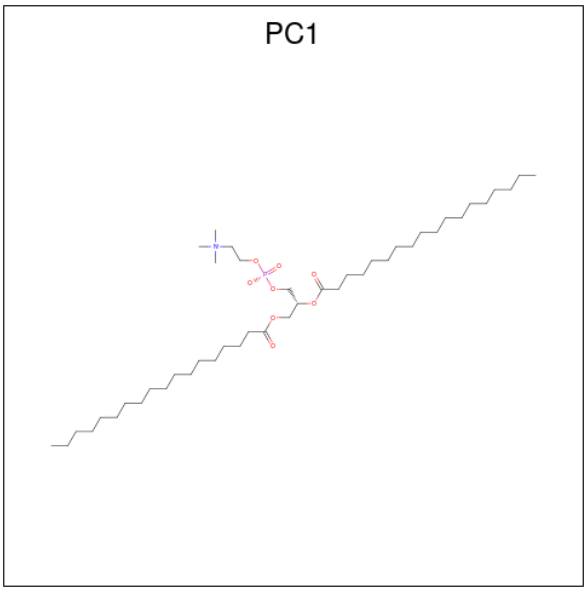
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	D1	1	19	9	1	8	1	0
51	D5	1	38	28	1	8	1	0
51	D4	1	40	30	1	8	1	0
51	A8	1	25	15	1	8	1	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	D5	1	36	17	17	2	0

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



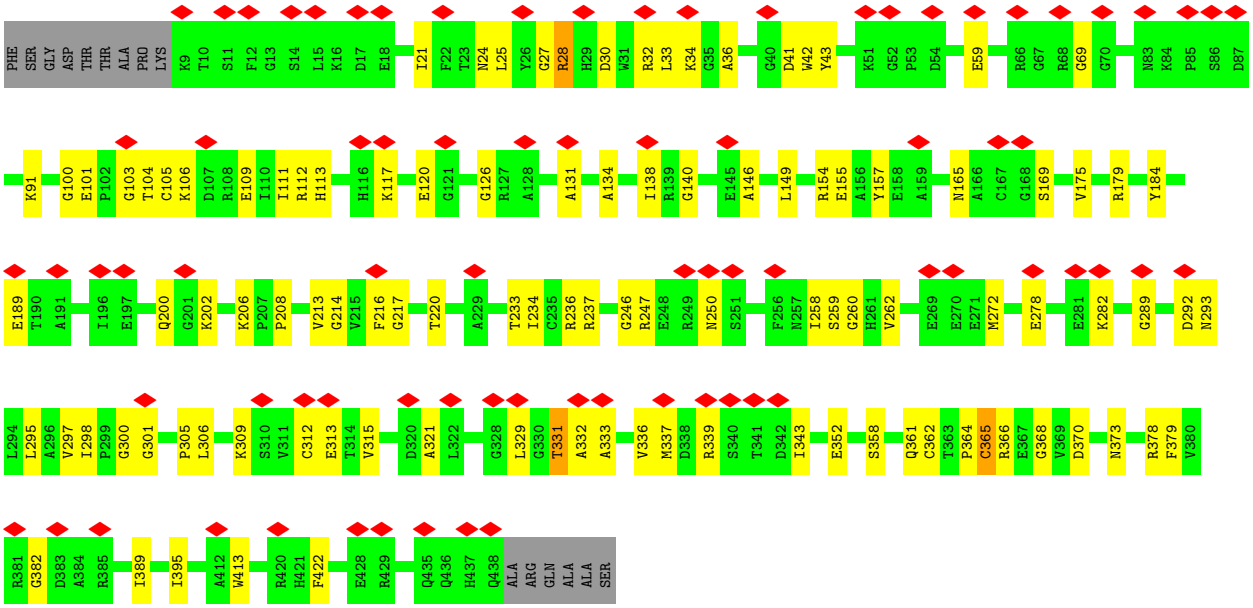
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	D4	1	28	18	1	8	1	0

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.

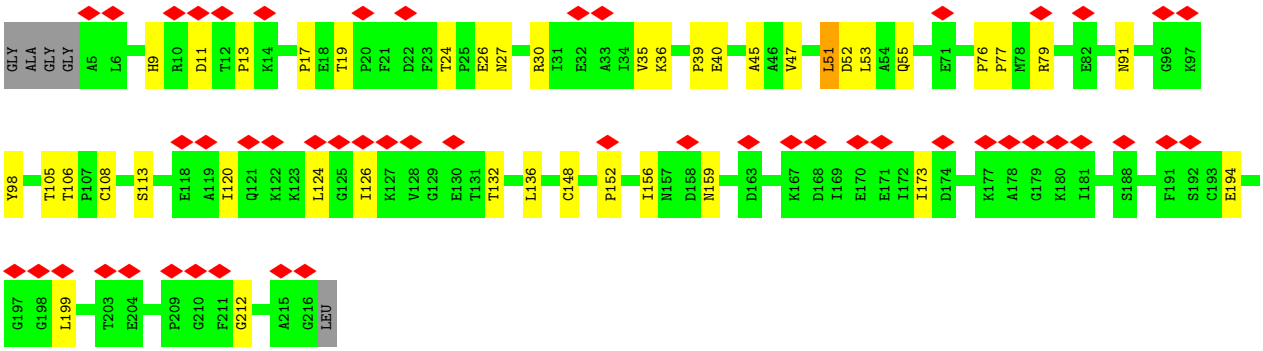
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



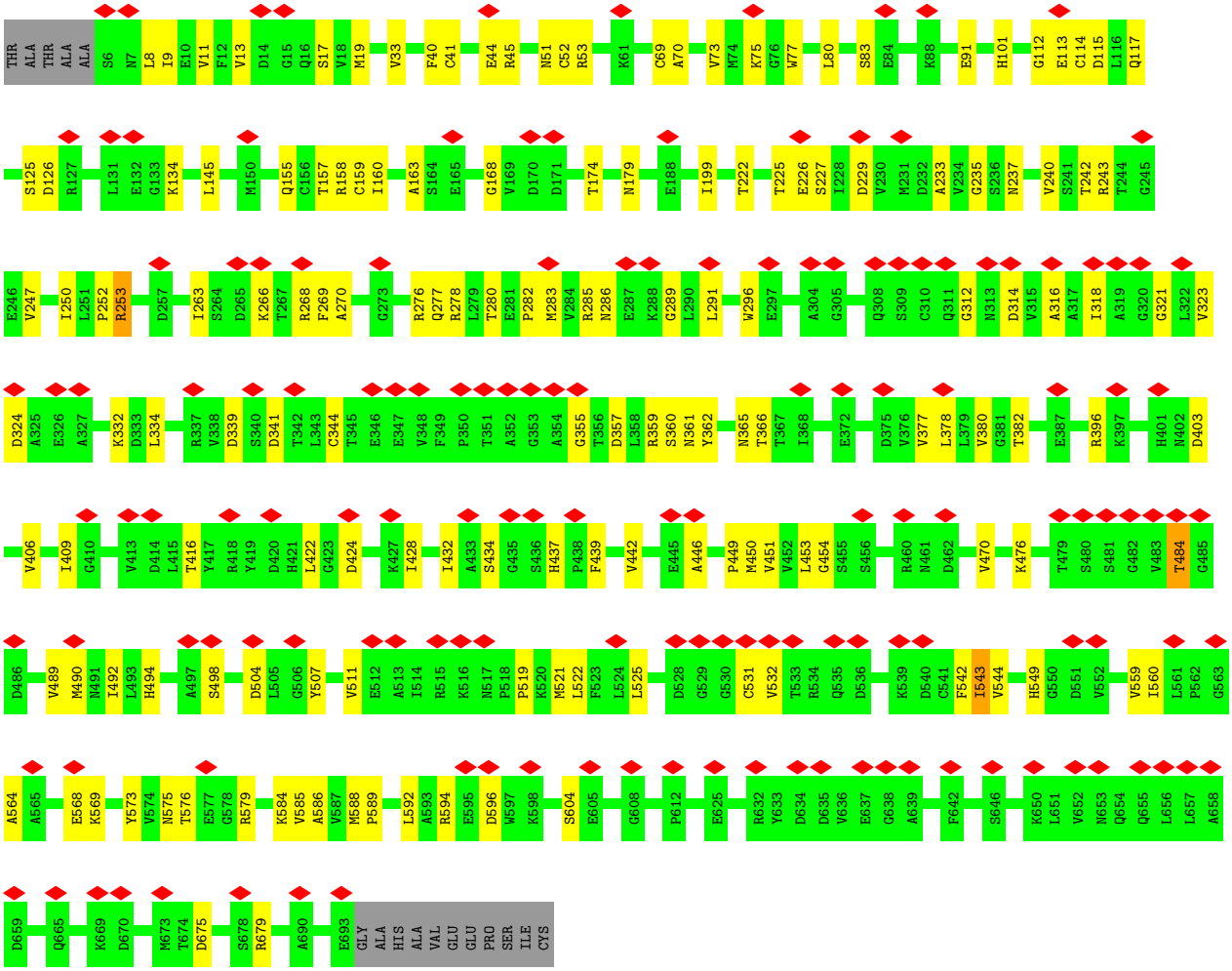
• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:



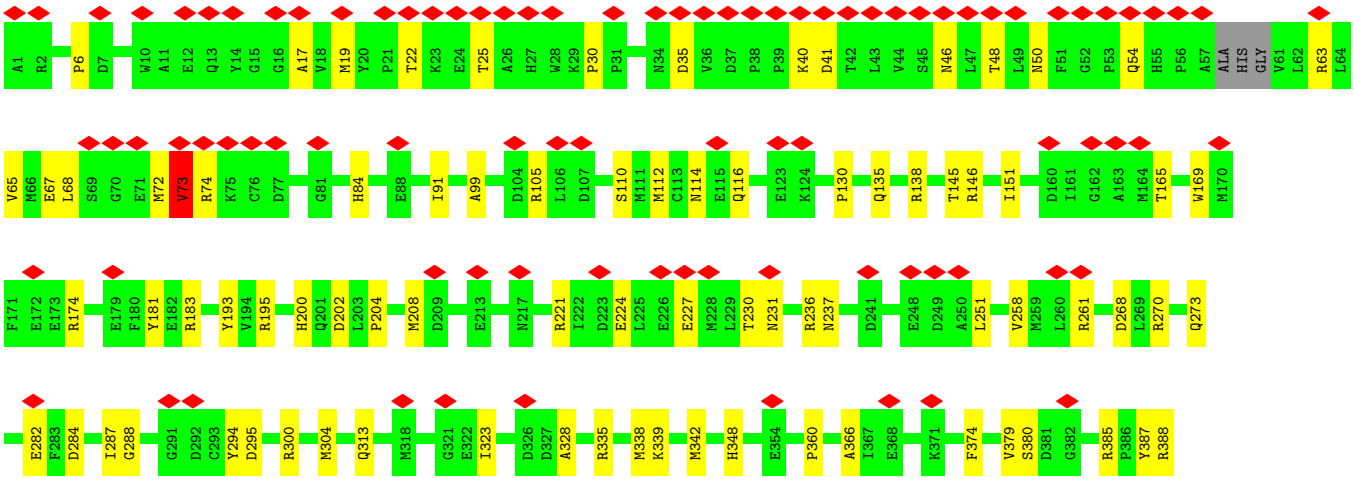
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1:



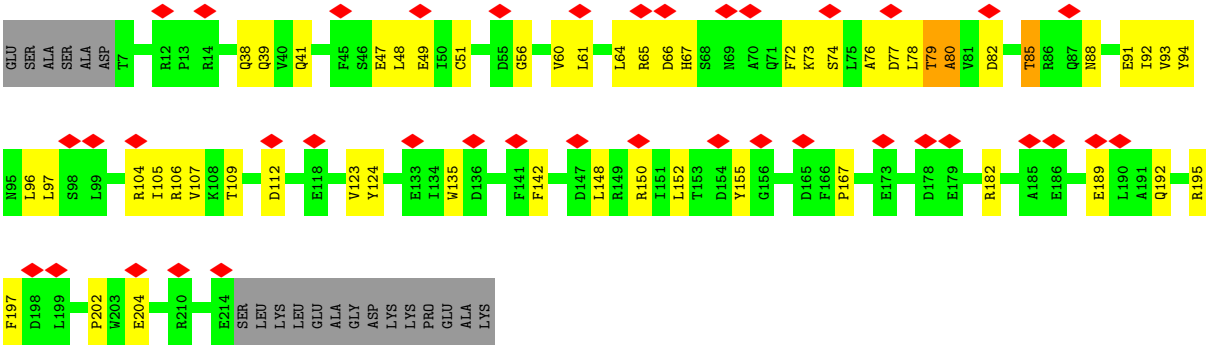
- Molecule 4: NDUFS2

Chain S2:



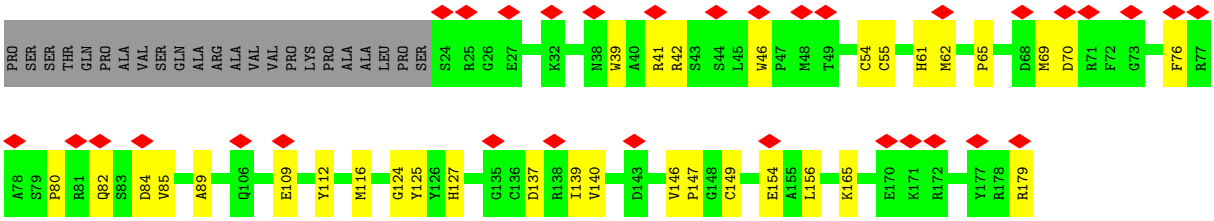
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



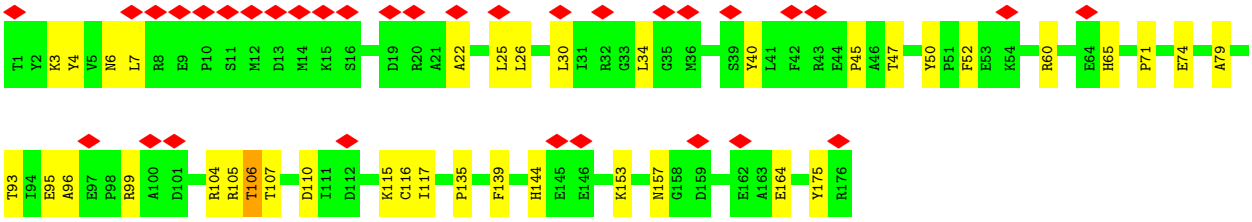
- Molecule 6: NDUFS7

Chain S7:



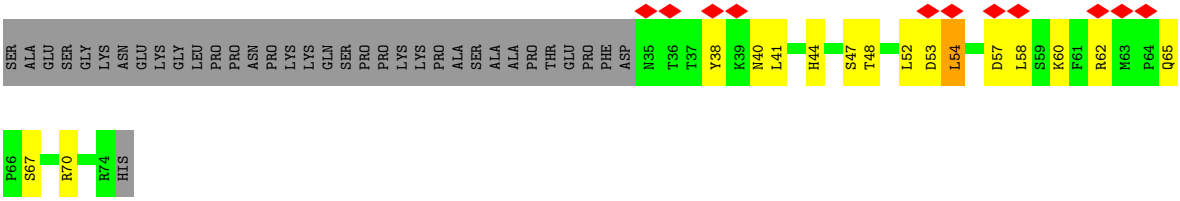
- Molecule 7: NDUFS8

Chain S8:



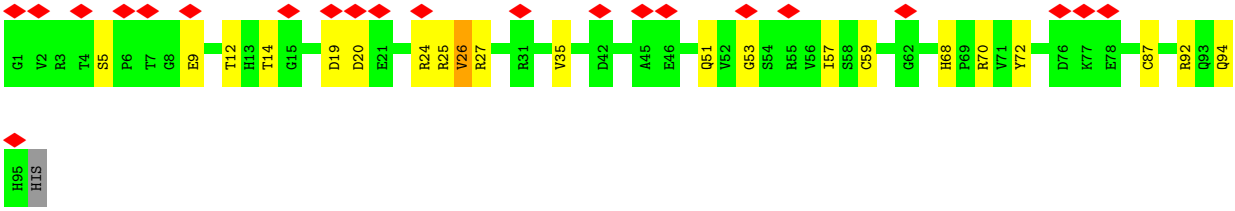
- Molecule 8: NDUFV3

Chain V3:



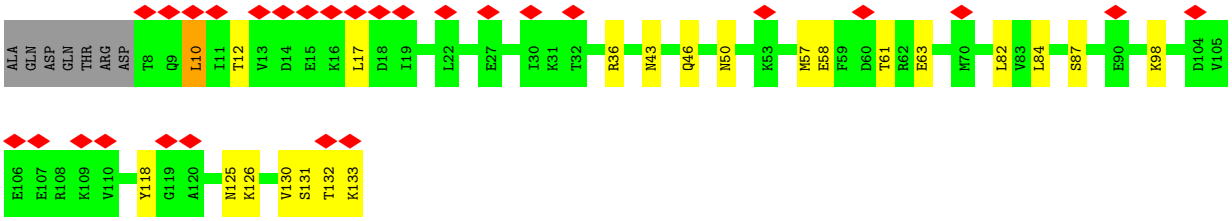
• Molecule 9: NDUFS6

Chain S6:



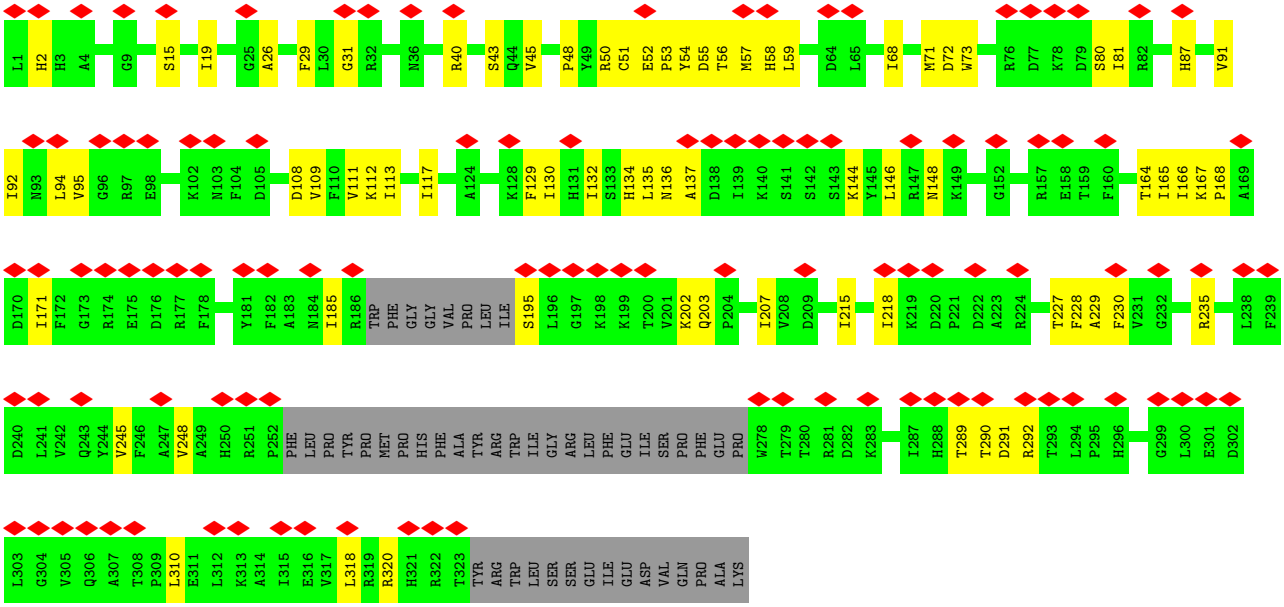
• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

Chain S4:



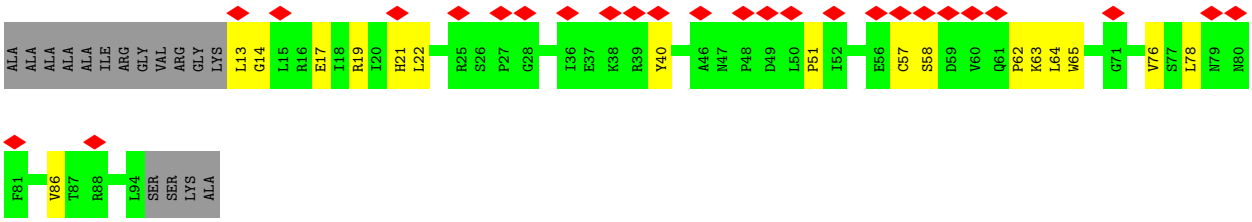
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

Chain A9:



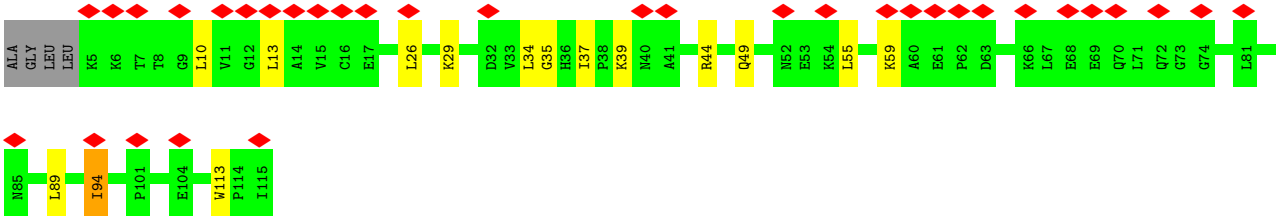
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



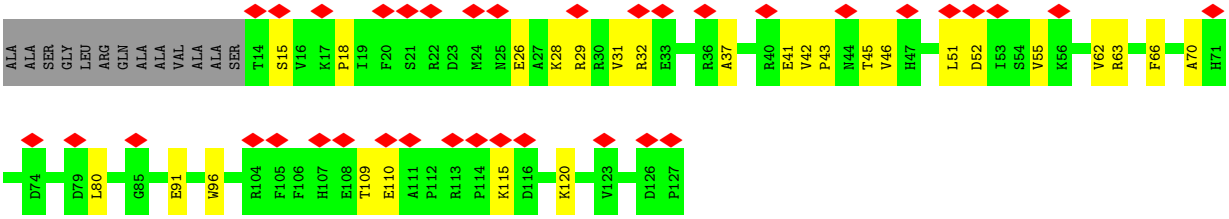
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:



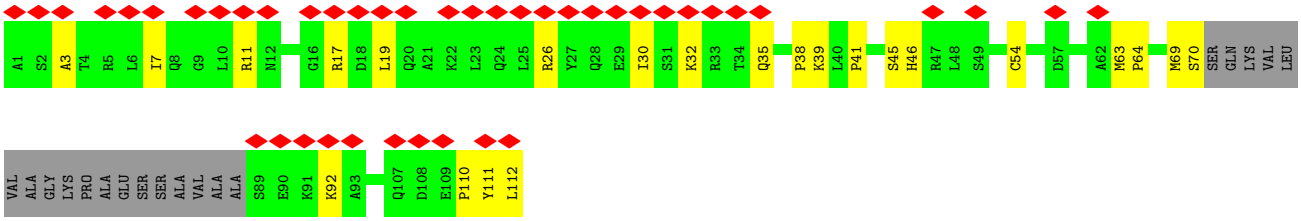
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



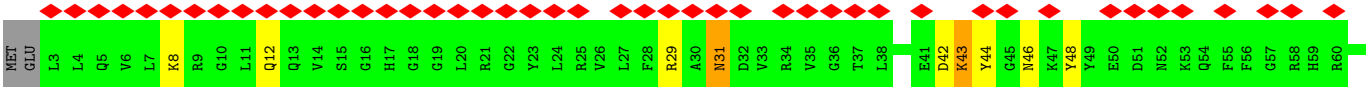
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

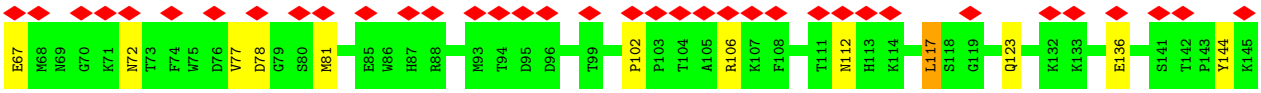
Chain A7:



• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

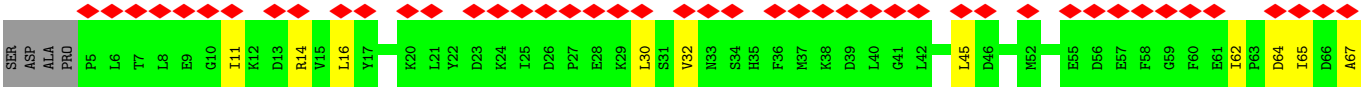
Chain AL:

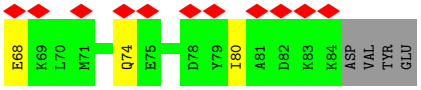




• Molecule 17: Acyl carrier protein

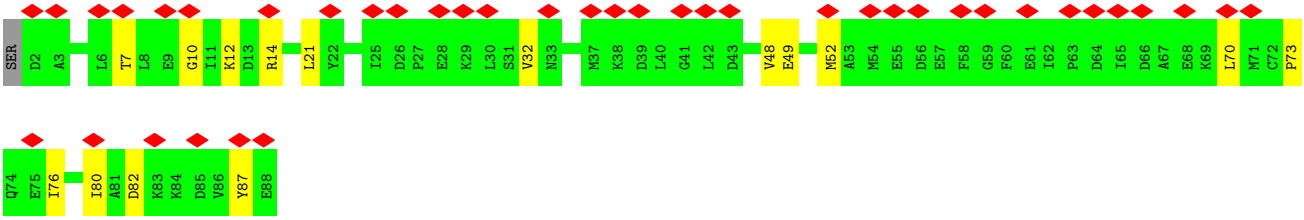
Chain AA:





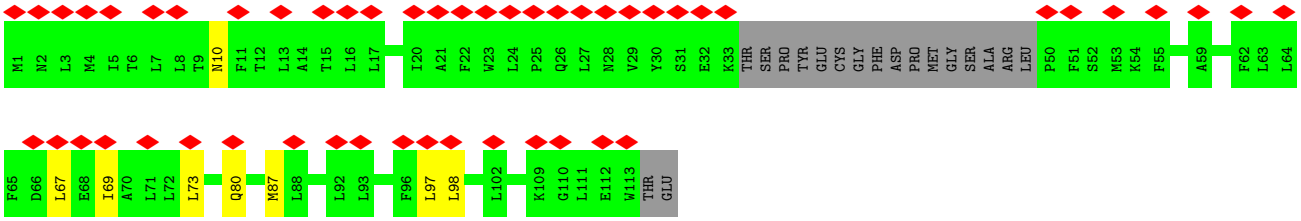
• Molecule 17: Acyl carrier protein

Chain AB:



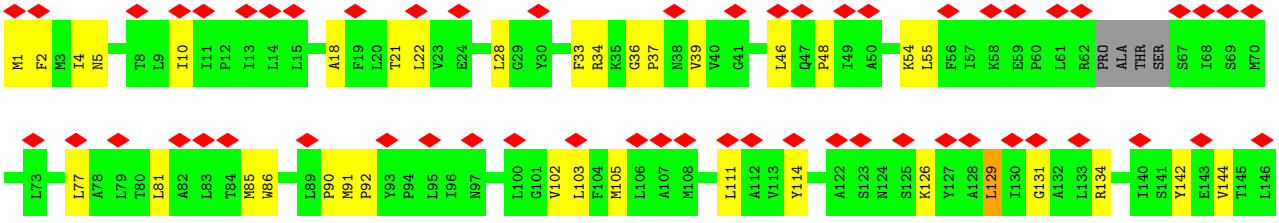
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

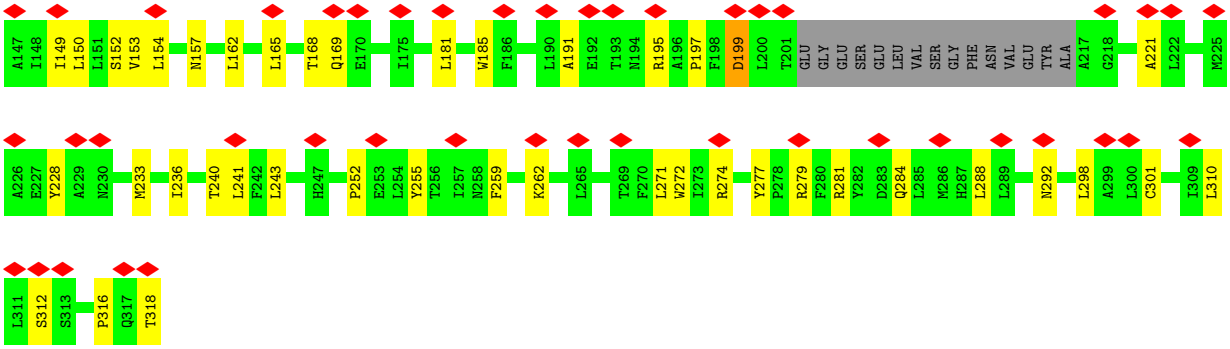
Chain D3:



• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

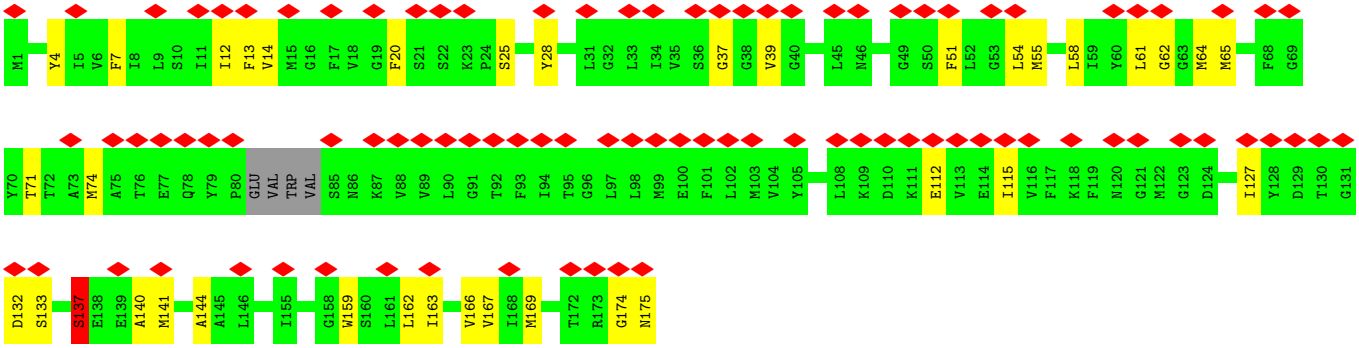
Chain D1:





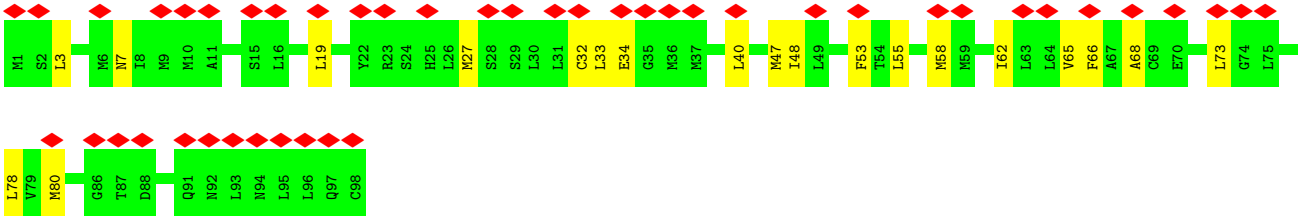
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6:



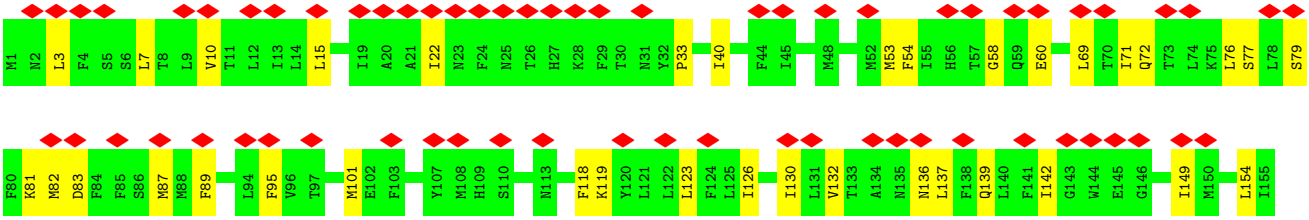
- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

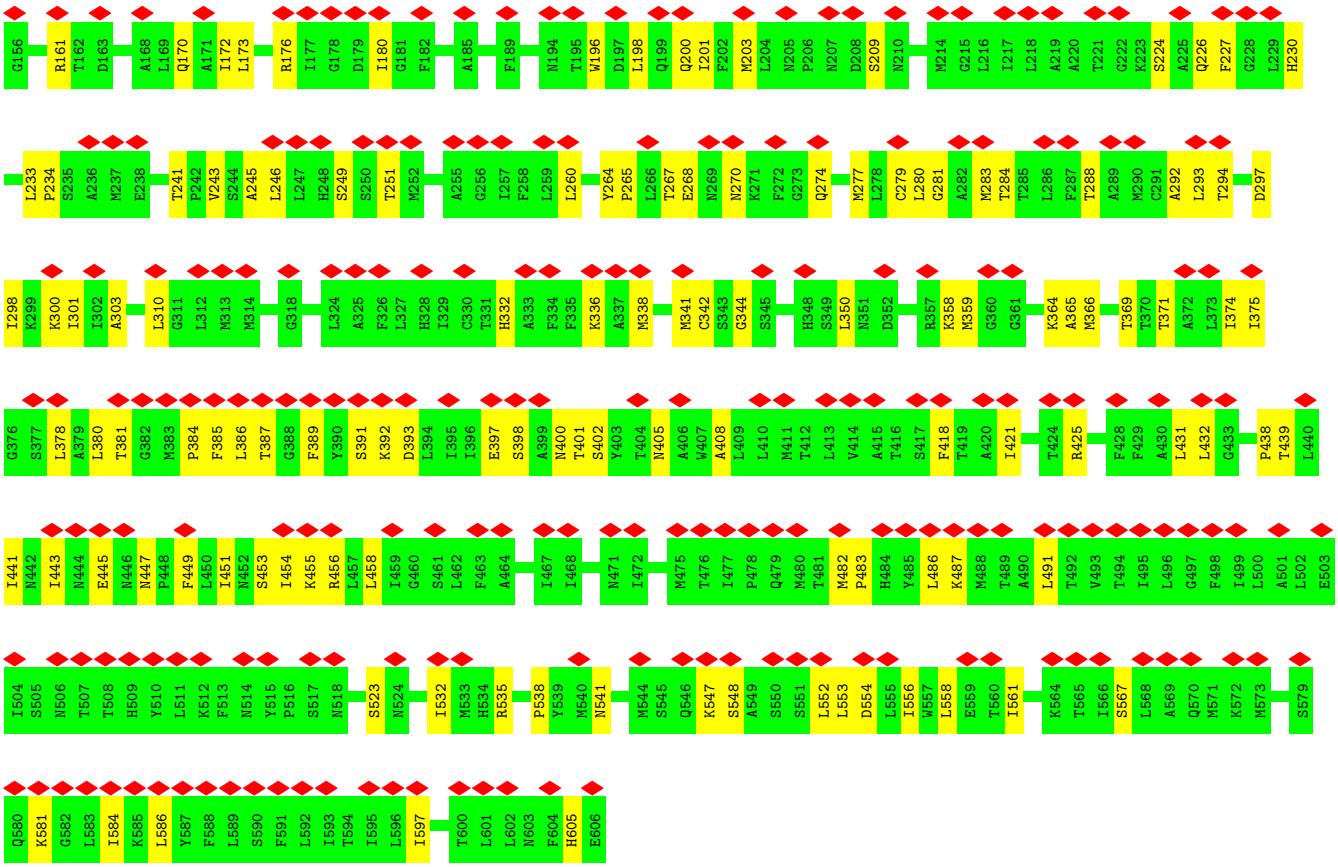
Chain 4L:



- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

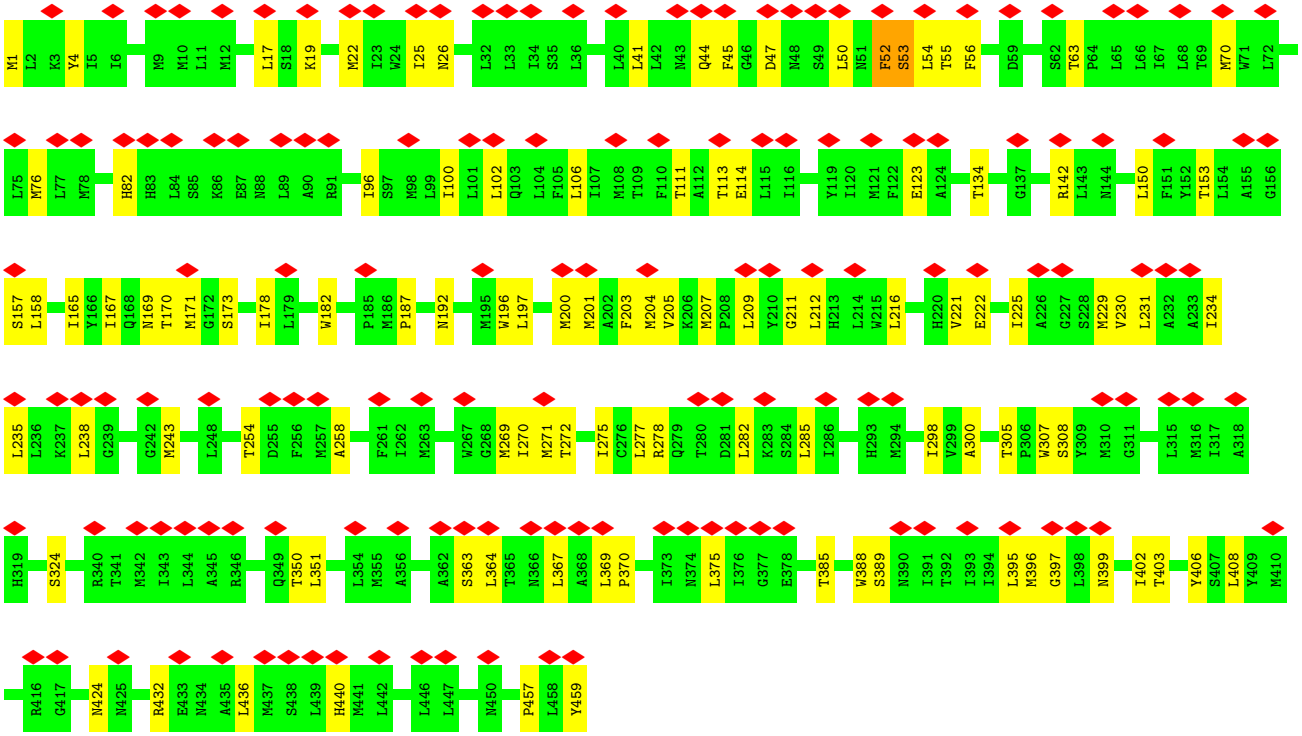
Chain D5:





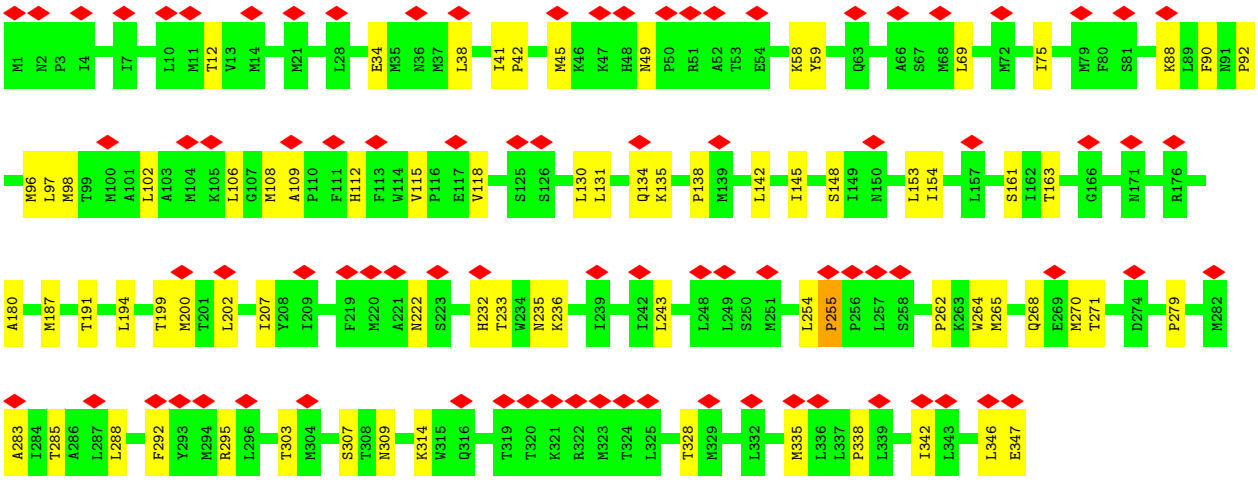
- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain D2: 24% 79% 21%

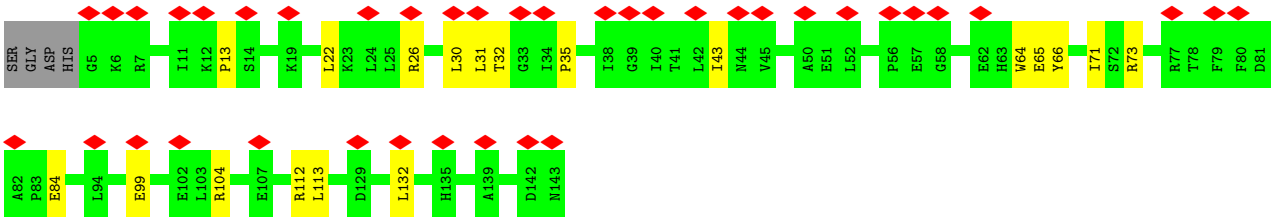


• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AK: 67% 86% 13%

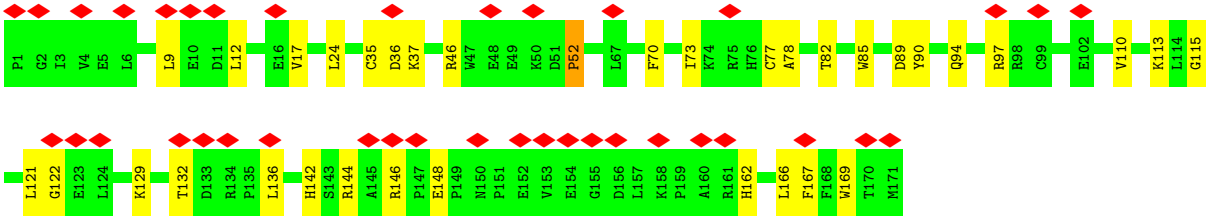
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5: 27% 84% 13%



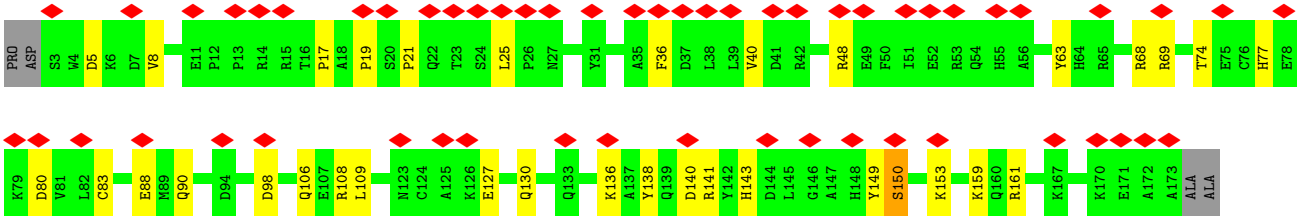
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8: 22% 80% 20%



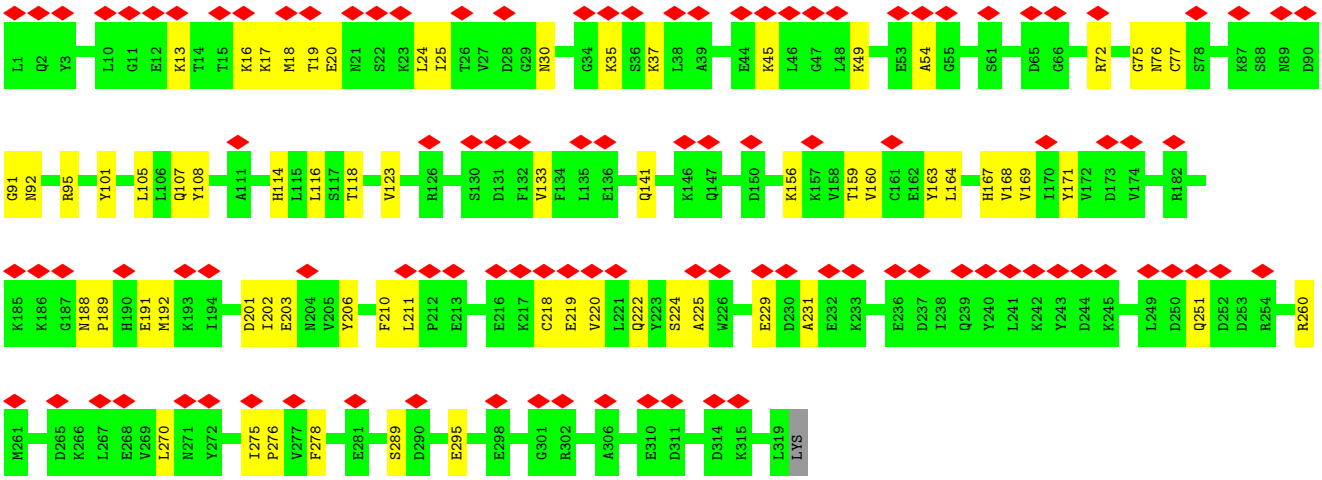
• Molecule 28: NDUFB10

Chain BJ:



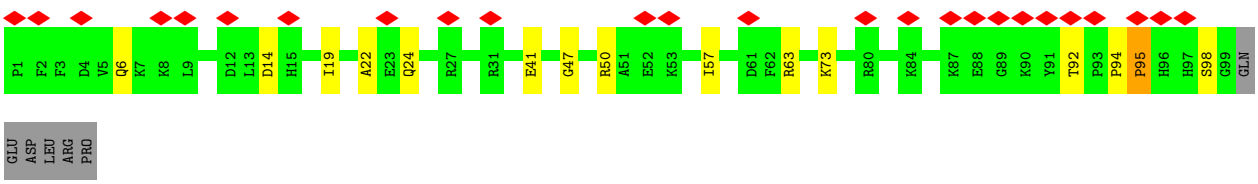
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:



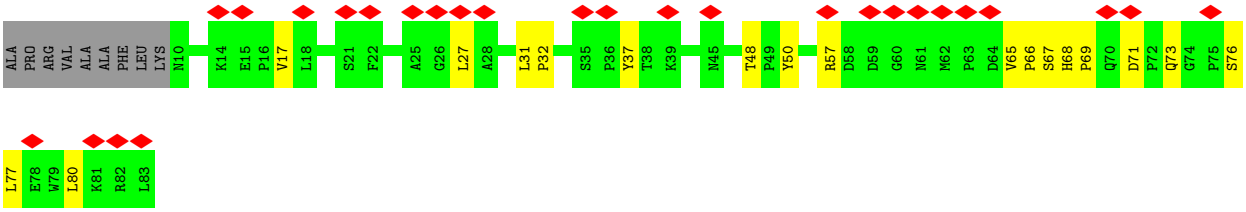
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain S5:



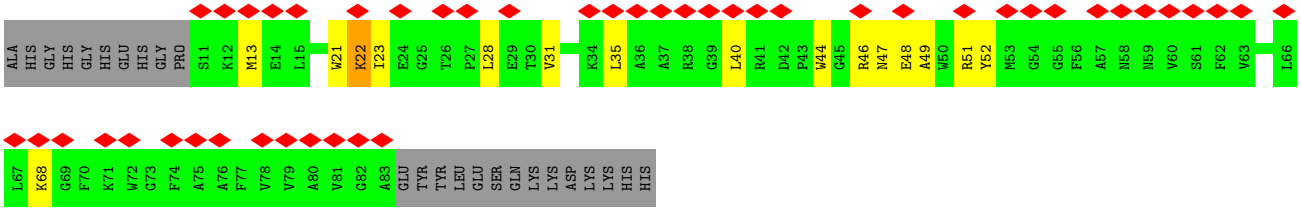
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain A3:



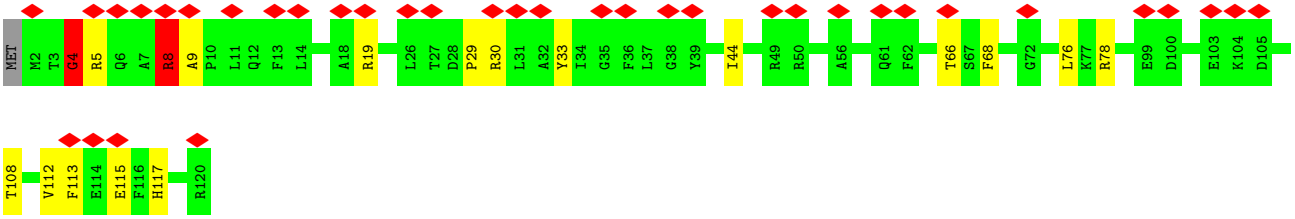
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain B3:



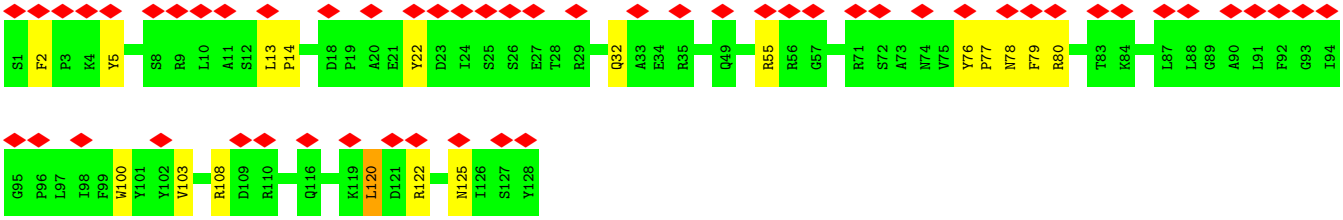
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:



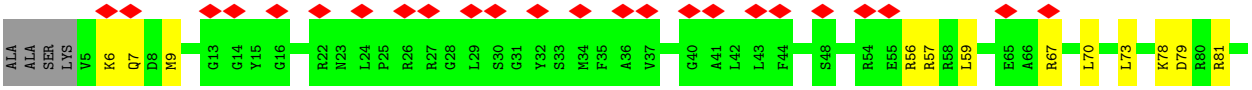
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



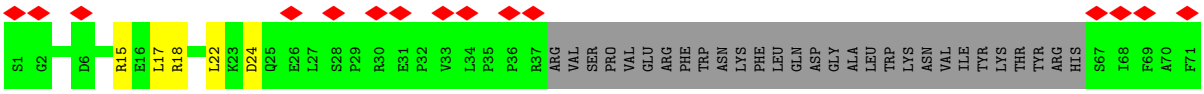
- Molecule 35: NDUFA13

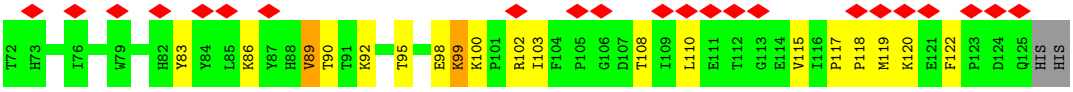
Chain AM:



• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

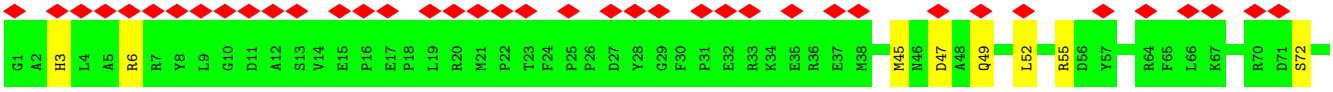
Chain B6:

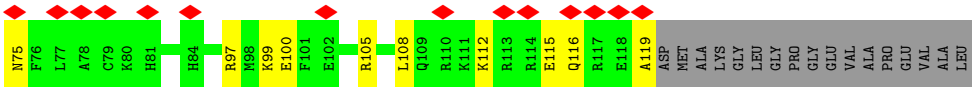




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

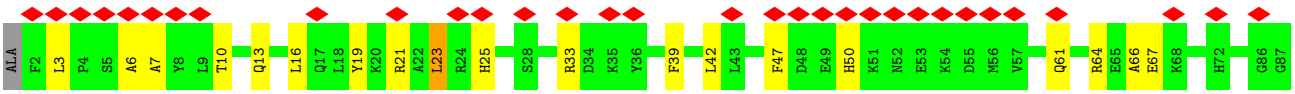
Chain B7:

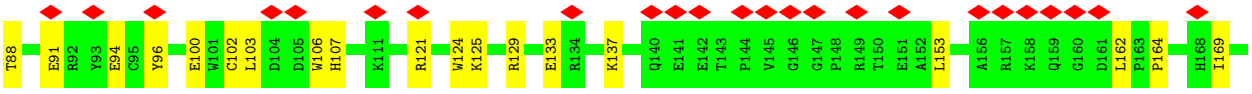


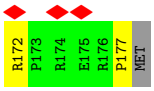


• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:

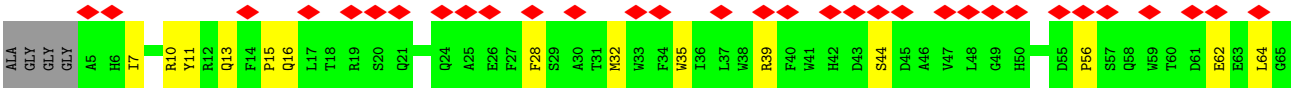


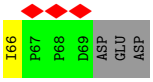




• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

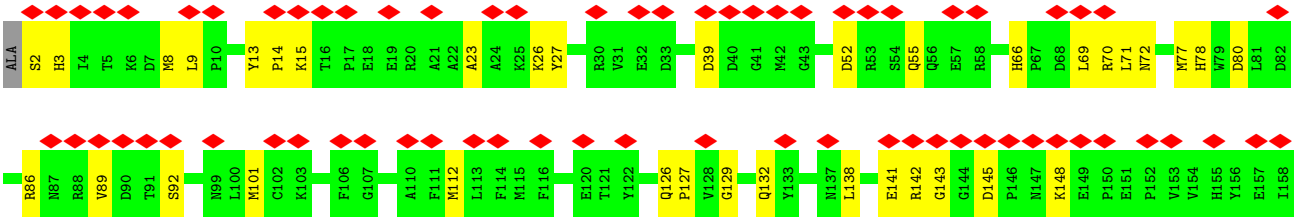
Chain B2:





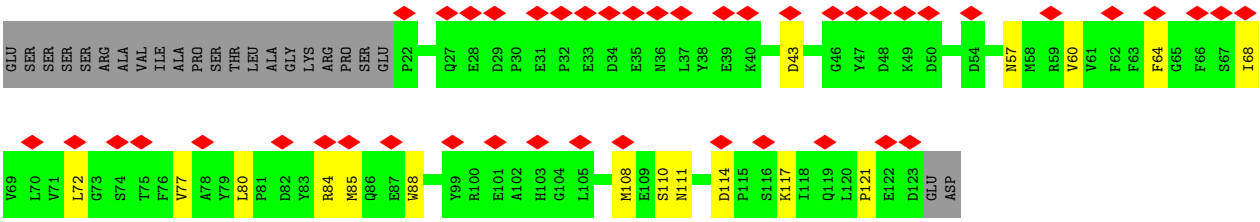
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



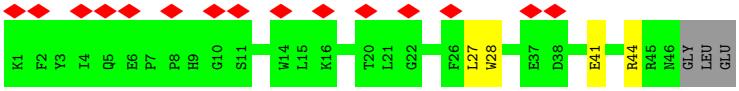
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BK:



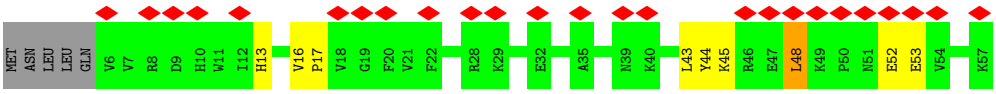
• Molecule 42: NDUFC1

Chain C1:



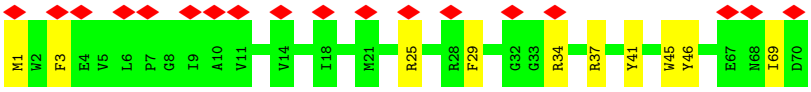
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:



• Molecule 44: NDUFA1

Chain A1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.169	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	V1	0.30	0/3386	0.63	0/4575
2	V2	0.31	0/1687	0.78	1/2295 (0.0%)
3	S1	0.31	0/5362	0.64	0/7266
4	S2	0.35	0/3526	0.65	4/4778 (0.1%)
5	S3	0.31	0/1776	0.66	0/2417
6	S7	0.36	0/1279	0.67	0/1728
7	S8	0.37	0/1446	0.65	0/1956
8	V3	0.28	0/344	0.69	0/465
9	S6	0.27	0/749	0.56	0/1009
10	S4	0.28	0/1048	0.62	2/1415 (0.1%)
11	A9	0.27	0/2373	0.65	1/3207 (0.0%)
12	A2	0.24	0/676	0.62	0/911
13	A5	0.27	0/922	0.66	0/1249
14	A6	0.26	0/994	0.62	2/1336 (0.1%)
15	A7	0.27	0/770	0.63	0/1040
16	AL	0.26	0/1233	0.62	0/1676
17	AA	0.23	0/655	0.63	0/881
17	AB	0.24	0/714	0.58	0/963
18	D3	0.29	0/807	0.61	0/1103
19	D1	0.35	0/2460	0.74	2/3361 (0.1%)
20	D6	0.28	0/1339	0.69	0/1810
21	4L	0.30	0/758	0.67	0/1024
22	D5	0.31	0/4933	0.71	1/6710 (0.0%)
23	D4	0.35	0/3740	0.74	0/5095
24	D2	0.36	0/2788	0.69	2/3795 (0.1%)
25	AK	0.24	0/1046	0.71	4/1419 (0.3%)
26	B5	0.27	0/1189	0.56	0/1607
27	A8	0.29	0/1441	0.72	2/1942 (0.1%)
28	BJ	0.28	0/1475	0.66	3/1989 (0.2%)
29	AJ	0.28	0/2644	0.69	5/3579 (0.1%)
30	S5	0.29	0/843	0.64	0/1128
31	A3	0.26	0/602	0.65	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	B3	0.28	0/595	0.76	0/803
33	C2	0.28	0/1028	0.70	4/1388 (0.3%)
34	B4	0.24	0/1085	0.61	0/1467
35	AM	0.30	0/1172	0.65	0/1579
36	B6	0.29	0/841	0.77	2/1144 (0.2%)
37	B7	0.27	0/1051	0.68	0/1408
38	B9	0.26	0/1568	0.62	0/2123
39	B2	0.30	0/590	0.73	2/810 (0.2%)
40	B8	0.29	0/1379	0.77	4/1884 (0.2%)
41	BK	0.27	0/880	0.64	0/1196
42	C1	0.24	0/404	0.60	0/548
43	B1	0.24	0/462	0.59	0/624
44	A1	0.29	0/592	0.67	0/795
All	All	0.30	0/66652	0.67	41/90326 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V1	0	2
2	V2	0	3
3	S1	0	5
4	S2	0	1
5	S3	0	3
7	S8	0	1
11	A9	0	1
13	A5	0	1
15	A7	0	1
16	AL	0	3
19	D1	0	1
20	D6	0	2
22	D5	0	3
23	D4	0	3
25	AK	0	1
27	A8	0	1
28	BJ	0	1
29	AJ	0	1
30	S5	0	1
32	B3	0	1
33	C2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	B4	0	1
36	B6	0	3
39	B2	0	1
40	B8	0	1
43	B1	0	1
All	All	0	45

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V2	36	LYS	N-CA-C	-8.28	104.04	114.56
28	BJ	21	PRO	CA-C-N	7.87	135.86	121.70
28	BJ	21	PRO	C-N-CA	7.87	135.86	121.70
29	AJ	229	GLU	CA-C-N	7.72	135.60	121.70
29	AJ	229	GLU	C-N-CA	7.72	135.60	121.70

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	13	PRO	Peptide
2	V2	194	GLU	Peptide
2	V2	35	VAL	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	V1	3312	0	3268	70	0
2	V2	1647	0	1660	28	0
3	S1	5275	0	5304	106	0
4	S2	3436	0	3379	60	0
5	S3	1726	0	1676	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S7	1248	0	1256	27	0
7	S8	1415	0	1374	33	0
8	V3	335	0	316	13	0
9	S6	737	0	710	12	0
10	S4	1025	0	1023	21	0
11	A9	2321	0	2350	48	0
12	A2	665	0	678	10	0
13	A5	902	0	936	12	0
14	A6	970	0	980	25	0
15	A7	752	0	766	19	0
16	AL	1192	0	1164	14	0
17	AA	645	0	649	7	0
17	AB	702	0	692	13	0
18	D3	787	0	832	7	0
19	D1	2390	0	2517	54	0
20	D6	1308	0	1329	27	0
21	4L	748	0	794	18	0
22	D5	4805	0	4950	114	0
23	D4	3646	0	3850	73	0
24	D2	2724	0	2930	57	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	15	0
27	A8	1404	0	1384	30	0
28	BJ	1441	0	1417	26	0
29	AJ	2583	0	2547	38	0
30	S5	822	0	820	13	0
31	A3	582	0	583	16	0
32	B3	578	0	570	15	0
33	C2	997	0	983	17	0
34	B4	1059	0	1062	13	0
35	AM	1143	0	1137	22	0
36	B6	815	0	837	17	0
37	B7	1026	0	995	15	0
38	B9	1515	0	1469	28	0
39	B2	563	0	509	10	0
40	B8	1324	0	1219	25	0
41	BK	853	0	800	15	0
42	C1	391	0	391	5	0
43	B1	449	0	453	9	0
44	A1	577	0	570	10	0
45	S1	16	0	0	1	0
45	S7	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	S8	16	0	0	0	0
45	V1	8	0	0	2	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	5	0
50	AA	34	0	40	7	0
50	B9	31	0	34	3	0
51	A8	25	0	24	1	0
51	D1	19	0	12	0	0
51	D4	40	0	54	2	0
51	D5	38	0	50	4	0
52	D5	36	0	16	2	0
53	D4	28	0	30	0	0
All	All	65403	0	65644	1011	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 8.

The worst 5 of 1011 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)
5:S3:38:GLN:O	15:A7:70:SER:HA	1.62	0.98
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.62	0.97
5:S3:38:GLN:HA	15:A7:70:SER:O	1.78	0.82
3:S1:266:LYS:O	3:S1:270:ALA:HB2	1.79	0.81
37:B7:108:LEU:O	37:B7:112:LYS:HB2	1.80	0.81

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	V1	428/445 (96%)	380 (89%)	48 (11%)	0	100	100
2	V2	210/217 (97%)	166 (79%)	44 (21%)	0	100	100
3	S1	686/704 (97%)	619 (90%)	66 (10%)	1 (0%)	48	81
4	S2	423/430 (98%)	373 (88%)	50 (12%)	0	100	100
5	S3	206/228 (90%)	174 (84%)	32 (16%)	0	100	100
6	S7	154/179 (86%)	135 (88%)	19 (12%)	0	100	100
7	S8	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
8	V3	38/75 (51%)	29 (76%)	9 (24%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	105 (85%)	19 (15%)	0	100	100
11	A9	284/338 (84%)	253 (89%)	31 (11%)	0	100	100
12	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
13	A5	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
14	A6	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
15	A7	90/112 (80%)	80 (89%)	10 (11%)	0	100	100
16	AL	141/145 (97%)	112 (79%)	29 (21%)	0	100	100
17	AA	78/88 (89%)	66 (85%)	12 (15%)	0	100	100
17	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100	100
18	D3	93/115 (81%)	84 (90%)	9 (10%)	0	100	100
19	D1	293/318 (92%)	264 (90%)	29 (10%)	0	100	100
20	D6	167/175 (95%)	141 (84%)	25 (15%)	1 (1%)	21	58
21	4L	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	46
22	D5	604/606 (100%)	537 (89%)	67 (11%)	0	100	100
23	D4	457/459 (100%)	418 (92%)	38 (8%)	1 (0%)	43	76
24	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
25	AK	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
26	B5	137/143 (96%)	125 (91%)	12 (9%)	0	100	100
27	A8	169/171 (99%)	139 (82%)	30 (18%)	0	100	100
28	BJ	169/175 (97%)	153 (90%)	16 (10%)	0	100	100
29	AJ	317/320 (99%)	279 (88%)	38 (12%)	0	100	100
30	S5	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
31	A3	72/83 (87%)	63 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B3	71/97 (73%)	60 (84%)	11 (16%)	0	100	100
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100	100
34	B4	126/128 (98%)	108 (86%)	18 (14%)	0	100	100
35	AM	137/143 (96%)	122 (89%)	15 (11%)	0	100	100
36	B6	92/127 (72%)	80 (87%)	12 (13%)	0	100	100
37	B7	117/136 (86%)	97 (83%)	20 (17%)	0	100	100
38	B9	174/178 (98%)	142 (82%)	32 (18%)	0	100	100
39	B2	63/72 (88%)	55 (87%)	8 (13%)	0	100	100
40	B8	155/158 (98%)	127 (82%)	27 (17%)	1 (1%)	21	58
41	BK	100/125 (80%)	88 (88%)	12 (12%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
44	A1	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	7983/8509 (94%)	7022 (88%)	956 (12%)	5 (0%)	49	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	D4	53	SER
20	D6	137	SER
21	4L	3	LEU
3	S1	359	ARG
40	B8	143	GLY

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	V1	344/354 (97%)	343 (100%)	1 (0%)	86	85
2	V2	182/183 (100%)	181 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S1	578/588 (98%)	576 (100%)	2 (0%)	86	85
4	S2	370/371 (100%)	367 (99%)	3 (1%)	73	77
5	S3	189/204 (93%)	188 (100%)	1 (0%)	81	82
6	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
7	S8	151/151 (100%)	151 (100%)	0	100	100
8	V3	39/68 (57%)	38 (97%)	1 (3%)	40	61
9	S6	79/80 (99%)	78 (99%)	1 (1%)	61	72
10	S4	113/119 (95%)	113 (100%)	0	100	100
11	A9	249/292 (85%)	249 (100%)	0	100	100
12	A2	73/81 (90%)	73 (100%)	0	100	100
13	A5	99/101 (98%)	98 (99%)	1 (1%)	68	76
14	A6	107/113 (95%)	107 (100%)	0	100	100
15	A7	82/94 (87%)	82 (100%)	0	100	100
16	AL	129/131 (98%)	128 (99%)	1 (1%)	73	77
17	AA	74/81 (91%)	73 (99%)	1 (1%)	59	71
17	AB	80/81 (99%)	79 (99%)	1 (1%)	61	72
18	D3	88/103 (85%)	87 (99%)	1 (1%)	65	74
19	D1	263/278 (95%)	261 (99%)	2 (1%)	73	77
20	D6	140/144 (97%)	138 (99%)	2 (1%)	59	71
21	4L	87/87 (100%)	87 (100%)	0	100	100
22	D5	539/539 (100%)	538 (100%)	1 (0%)	87	87
23	D4	412/412 (100%)	409 (99%)	3 (1%)	76	79
24	D2	315/315 (100%)	315 (100%)	0	100	100
25	AK	101/101 (100%)	101 (100%)	0	100	100
26	B5	122/125 (98%)	122 (100%)	0	100	100
27	A8	154/154 (100%)	154 (100%)	0	100	100
28	BJ	155/157 (99%)	155 (100%)	0	100	100
29	AJ	283/284 (100%)	283 (100%)	0	100	100
30	S5	88/94 (94%)	87 (99%)	1 (1%)	65	74
31	A3	65/71 (92%)	65 (100%)	0	100	100
32	B3	55/75 (73%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	C2	106/107 (99%)	106 (100%)	0	100	100
34	B4	114/114 (100%)	113 (99%)	1 (1%)	70	76
35	AM	119/121 (98%)	119 (100%)	0	100	100
36	B6	92/121 (76%)	90 (98%)	2 (2%)	45	64
37	B7	108/119 (91%)	108 (100%)	0	100	100
38	B9	159/160 (99%)	158 (99%)	1 (1%)	78	80
39	B2	59/62 (95%)	59 (100%)	0	100	100
40	B8	142/142 (100%)	141 (99%)	1 (1%)	76	79
41	BK	93/112 (83%)	93 (100%)	0	100	100
42	C1	42/44 (96%)	42 (100%)	0	100	100
43	B1	48/53 (91%)	47 (98%)	1 (2%)	47	65
44	A1	59/59 (100%)	59 (100%)	0	100	100
All	All	7078/7395 (96%)	7047 (100%)	31 (0%)	81	83

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	D3	73	LEU
36	B6	90	THR
20	D6	12	ILE
40	B8	9	LEU
30	S5	95	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
34	B4	47	GLN
36	B6	13	GLN
40	B8	66	HIS
16	AL	72	ASN
16	AL	31	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
51	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.32	0
46	FMN	V1	501	-	33,33,33	0.34	0	48,50,50	0.40	0
50	ZMP	AA	101	17	27,33,36	0.71	1 (3%)	32,40,45	0.95	1 (3%)
53	PC1	D4	502	-	27,27,53	0.39	0	33,35,61	0.39	0
45	SF4	S8	201	7	0,12,12	-	-	-		
47	FES	V2	300	2	0,4,4	-	-	-		
50	ZMP	B9	201	17	24,30,36	0.68	0	29,37,45	1.01	2 (6%)
45	SF4	V1	500	1	0,12,12	-	-	-		
51	3PE	A8	301	-	24,24,50	0.43	0	27,29,55	0.36	0
45	SF4	S8	202	7	0,12,12	-	-	-		
45	SF4	S7	300	6	0,12,12	-	-	-		
45	SF4	S1	801	3	0,12,12	-	-	-		
49	NDP	A9	401	-	49,52,52	0.44	0	66,80,80	0.44	0
45	SF4	S1	802	3	0,12,12	-	-	-		
51	3PE	D1	501	-	18,18,50	0.42	0	21,23,55	0.43	0
47	FES	S1	803	3	0,4,4	-	-	-		
51	3PE	D5	902	-	37,37,50	0.36	0	40,42,55	0.34	0
52	CDL	D5	901	-	35,35,99	0.43	0	41,47,111	0.73	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	D4	501	-	-	7/43/43/54	-
46	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
50	ZMP	AA	101	17	-	14/38/40/43	-
53	PC1	D4	502	-	-	8/31/31/57	-
45	SF4	S8	201	7	-	-	0/6/5/5
47	FES	V2	300	2	-	-	0/1/1/1
50	ZMP	B9	201	17	-	11/35/37/43	-
51	3PE	A8	301	-	-	5/28/28/54	-
45	SF4	V1	500	1	-	-	0/6/5/5
49	NDP	A9	401	-	-	14/34/77/77	0/5/5/5
45	SF4	S1	801	3	-	-	0/6/5/5
45	SF4	S7	300	6	-	-	0/6/5/5
45	SF4	S8	202	7	-	-	0/6/5/5
45	SF4	S1	802	3	-	-	0/6/5/5
51	3PE	D1	501	-	-	11/20/20/54	-
47	FES	S1	803	3	-	-	0/1/1/1
51	3PE	D5	902	-	-	9/41/41/54	-
52	CDL	D5	901	-	-	16/42/42/110	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AA	101	ZMP	C9-C10	2.45	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	D5	901	CDL	CB4-OB6-CB5	2.84	123.19	117.90
50	B9	201	ZMP	O1-C10-C9	-2.42	121.13	123.99
50	B9	201	ZMP	C11-C12-N1	-2.34	107.50	112.42
50	AA	101	ZMP	O1-C10-C9	-2.30	121.28	123.99
52	D5	901	CDL	OB6-CB4-CB3	2.09	115.96	108.40

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	N10-C1'-C2'-O2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C1'-C2'-C3'-O3'
46	V1	501	FMN	C1'-C2'-C3'-C4'
46	V1	501	FMN	C5'-O5'-P-O1P
46	V1	501	FMN	C5'-O5'-P-O2P

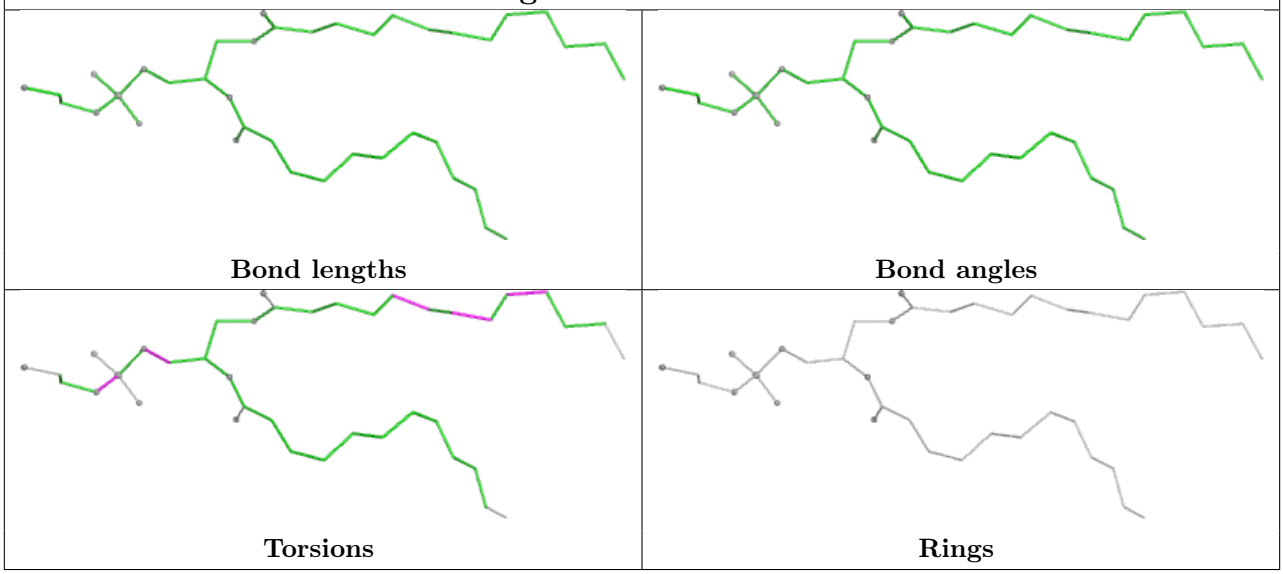
There are no ring outliers.

10 monomers are involved in 28 short contacts:

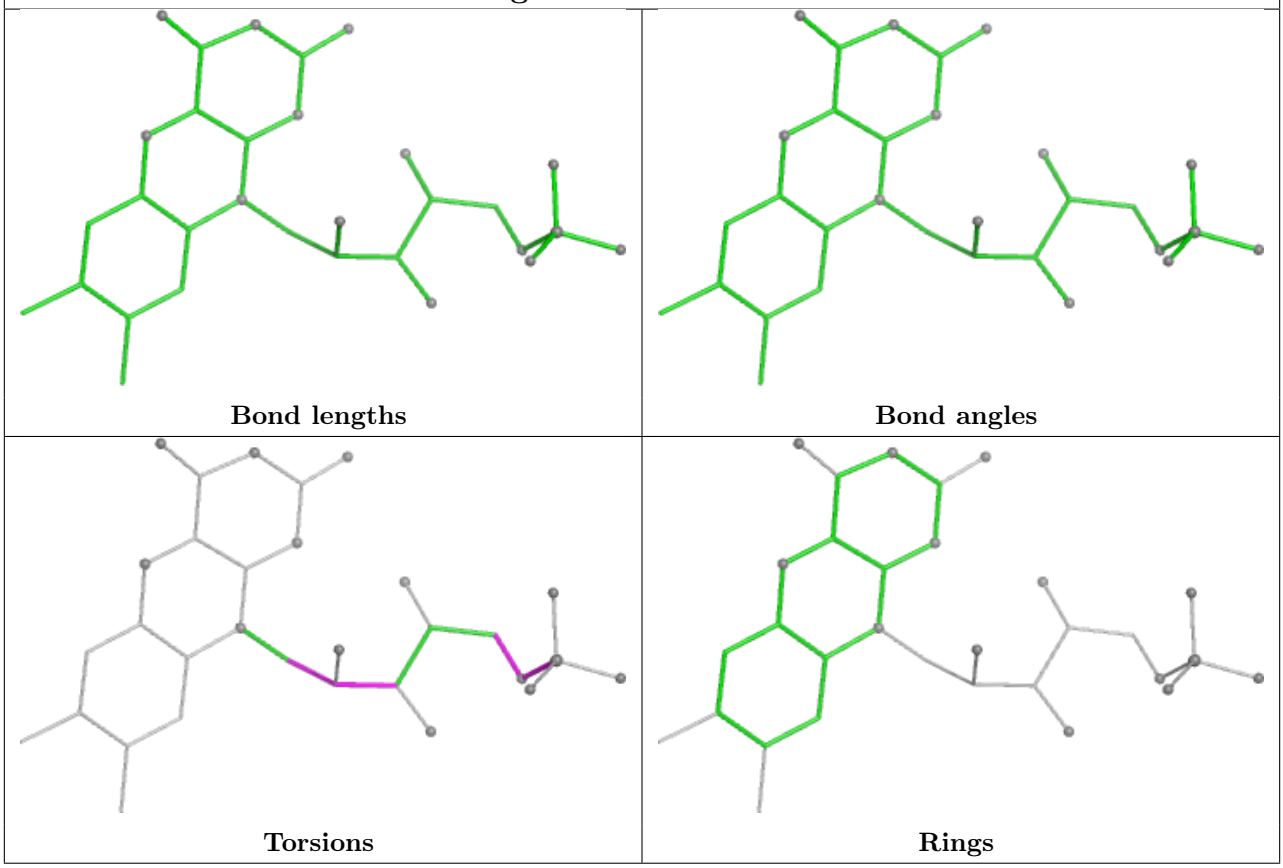
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	D4	501	3PE	2	0
46	V1	501	FMN	1	0
50	AA	101	ZMP	7	0
50	B9	201	ZMP	3	0
45	V1	500	SF4	2	0
51	A8	301	3PE	1	0
45	S1	801	SF4	1	0
49	A9	401	NDP	5	0
51	D5	902	3PE	4	0
52	D5	901	CDL	2	0

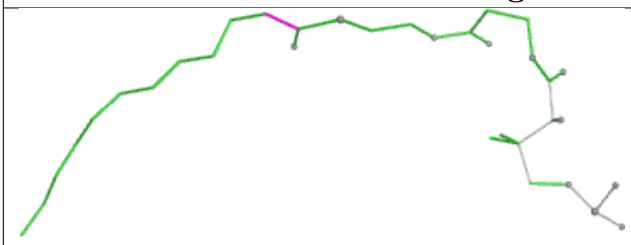
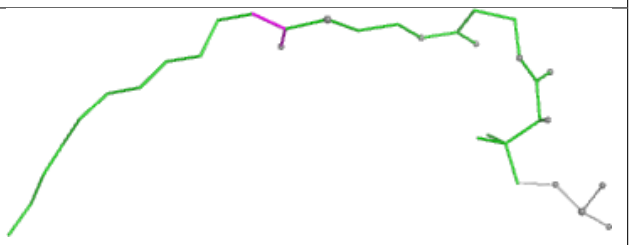
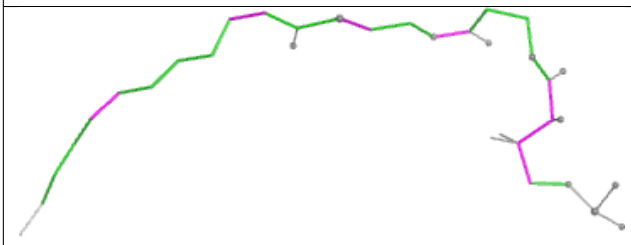
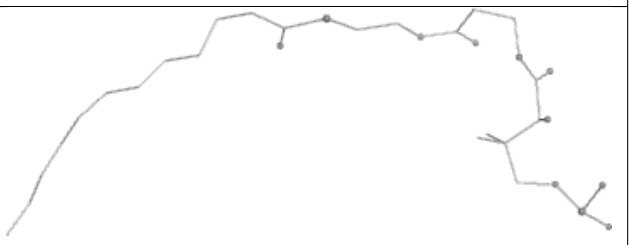
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

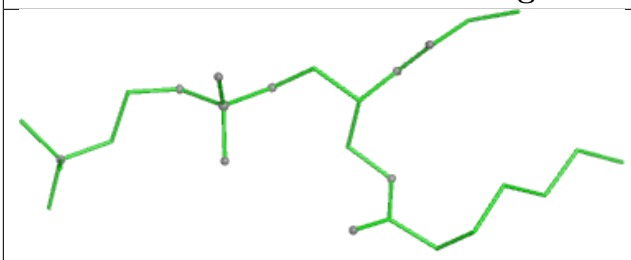
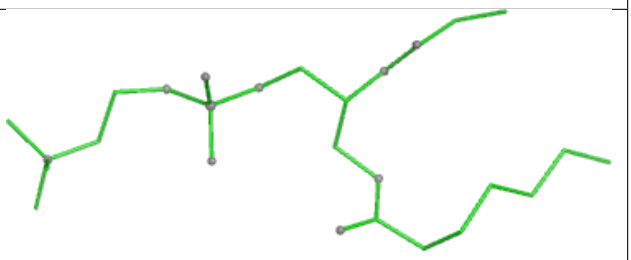
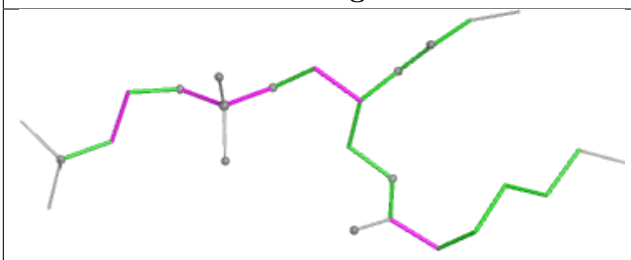
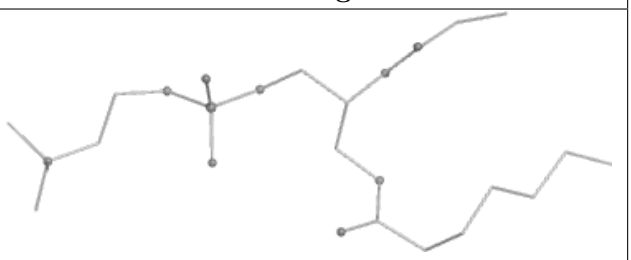
Ligand 3PE D4 501



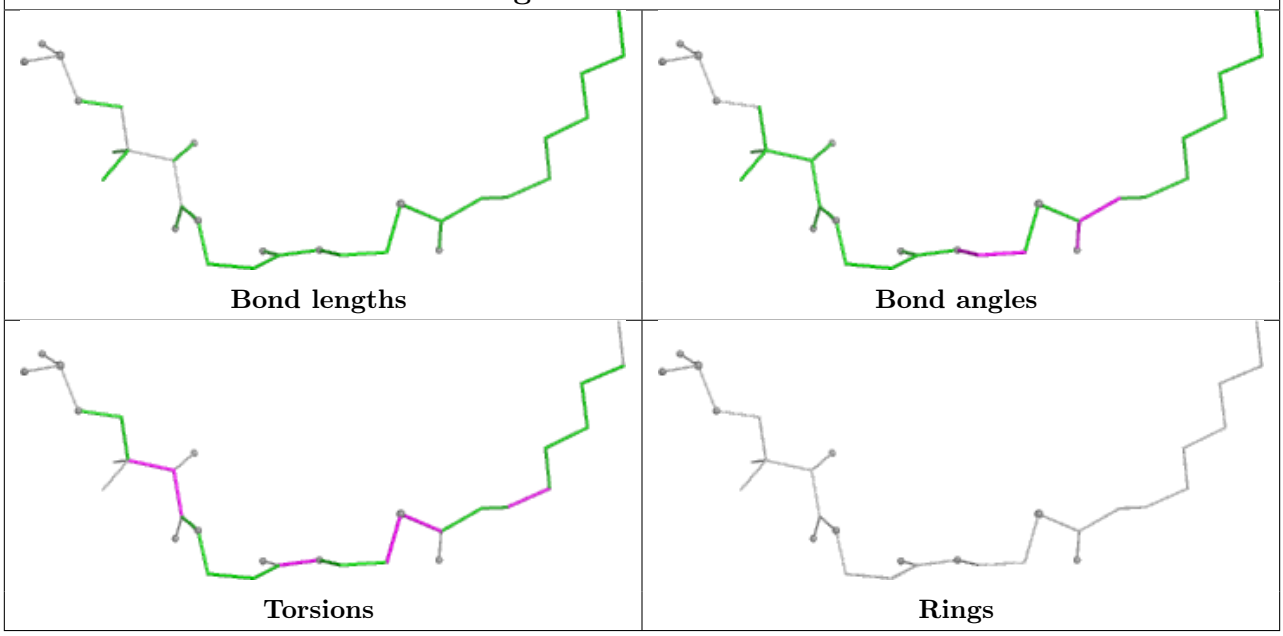
Ligand FMN V1 501



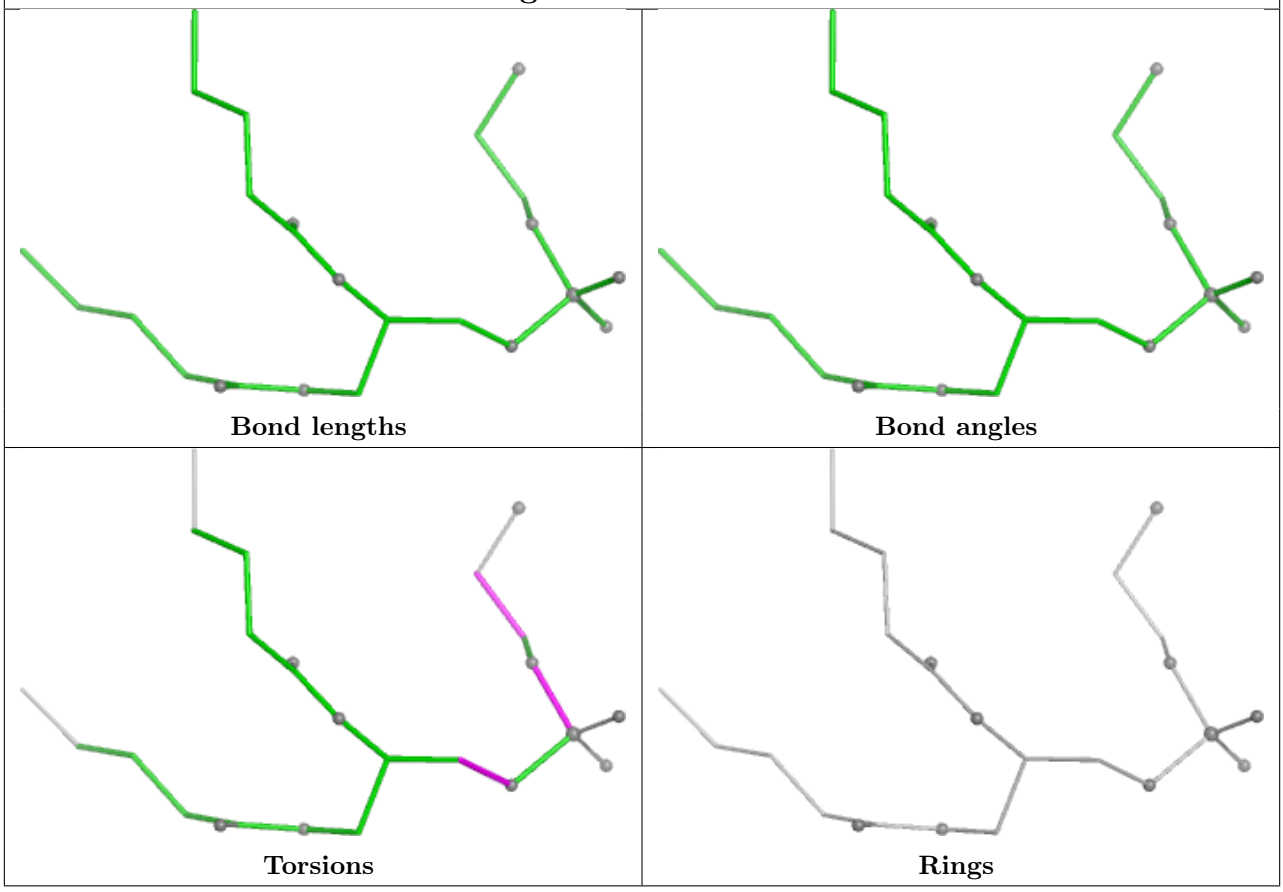
Ligand ZMP AA 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 D4 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

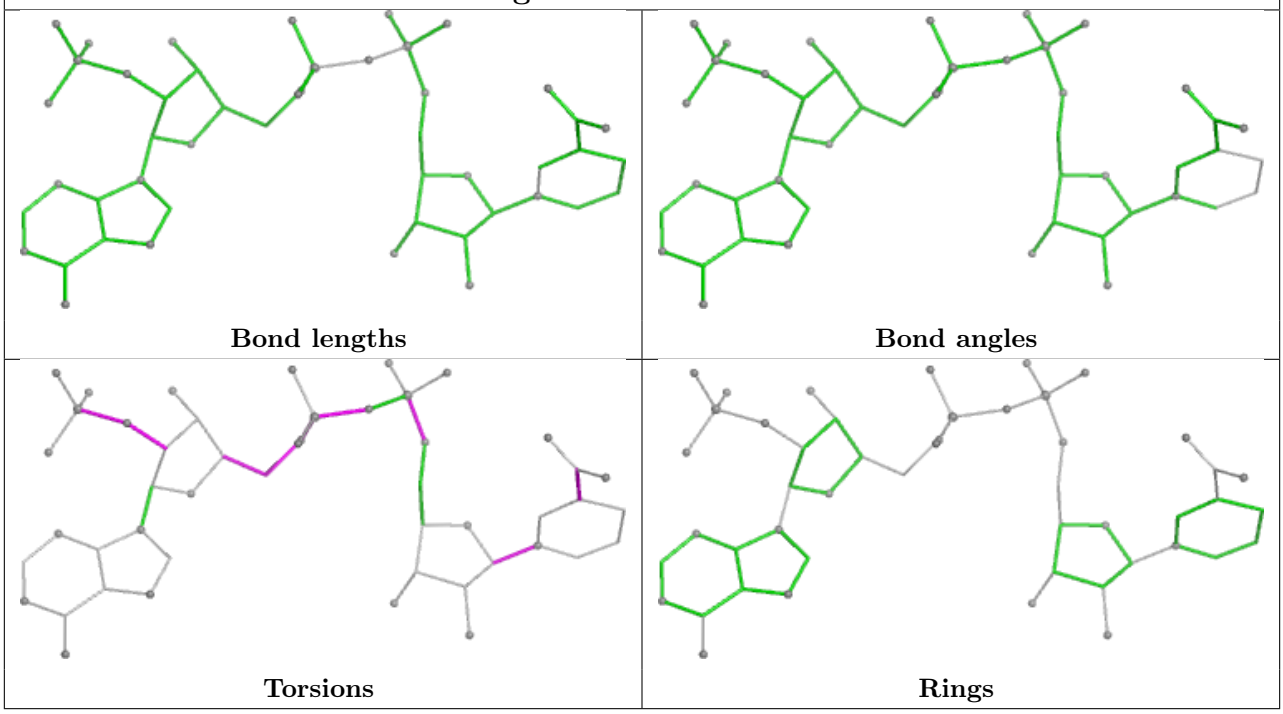
Ligand ZMP B9 201



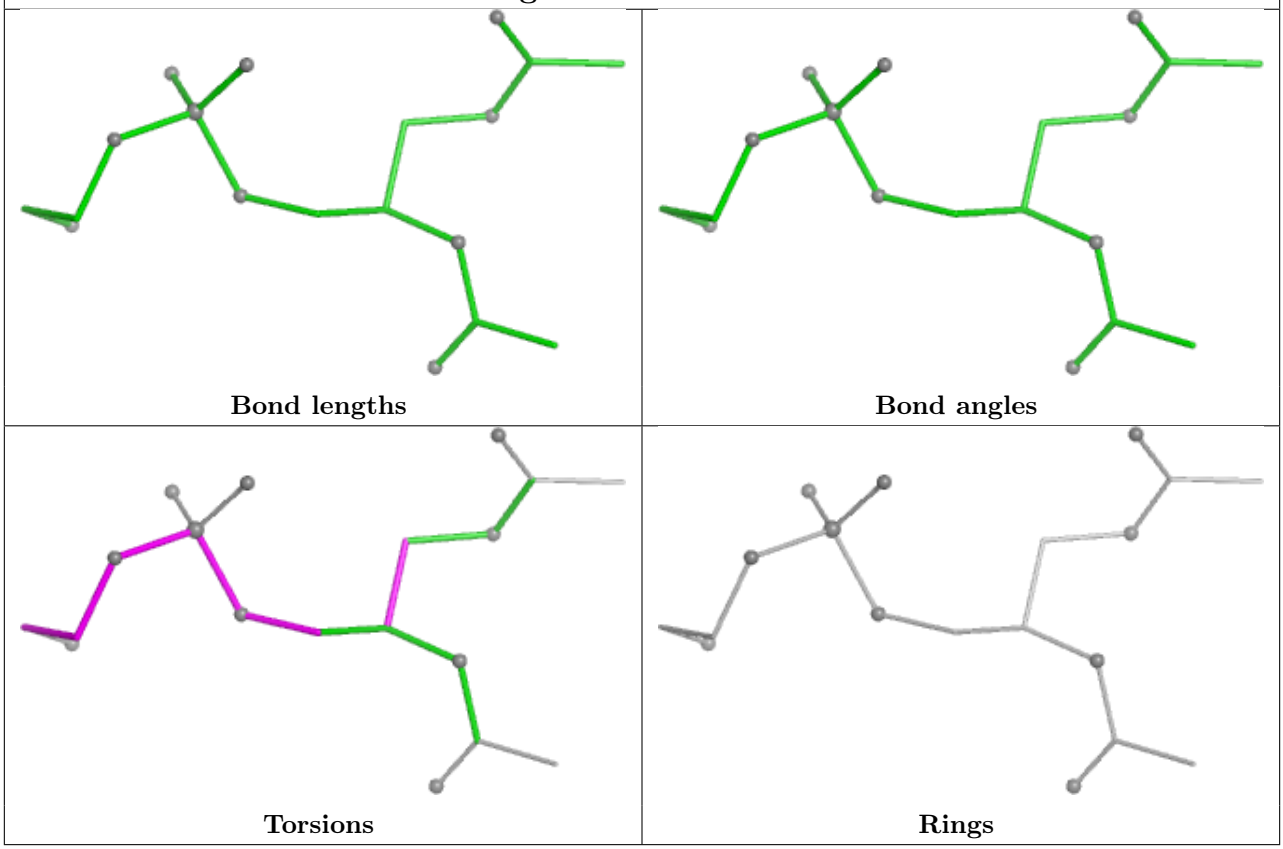
Ligand 3PE A8 301



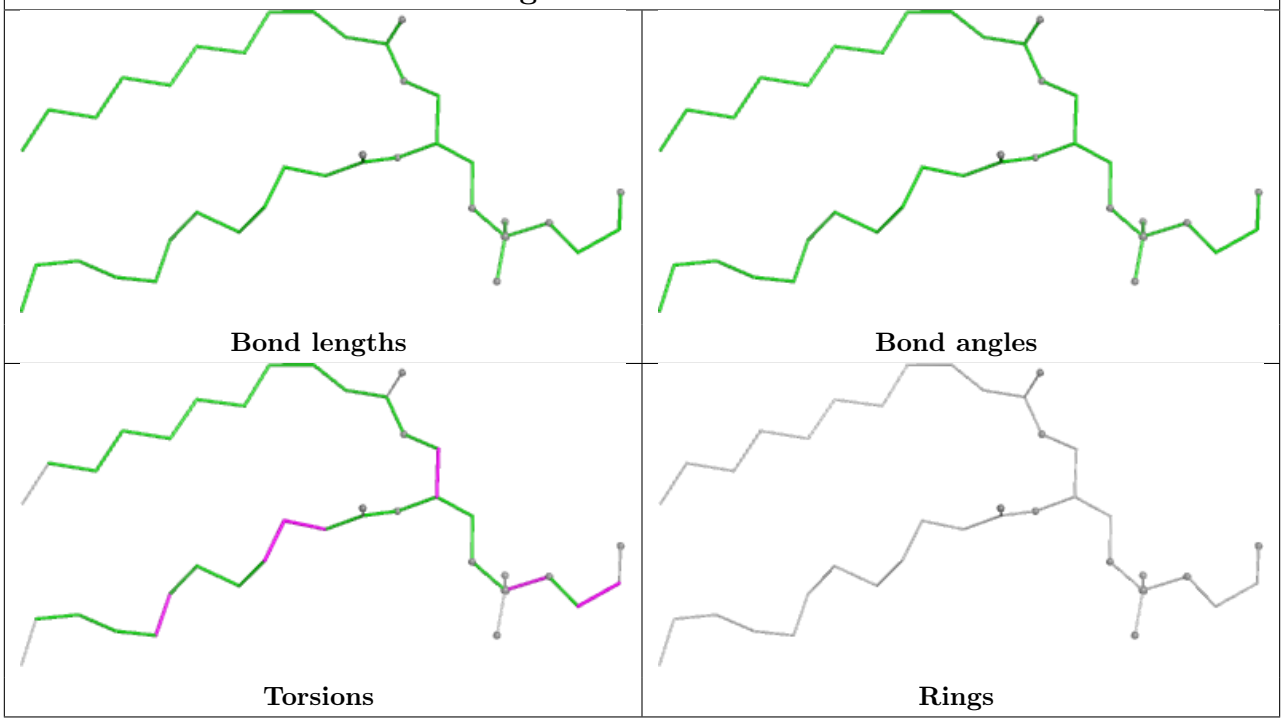
Ligand NDP A9 401



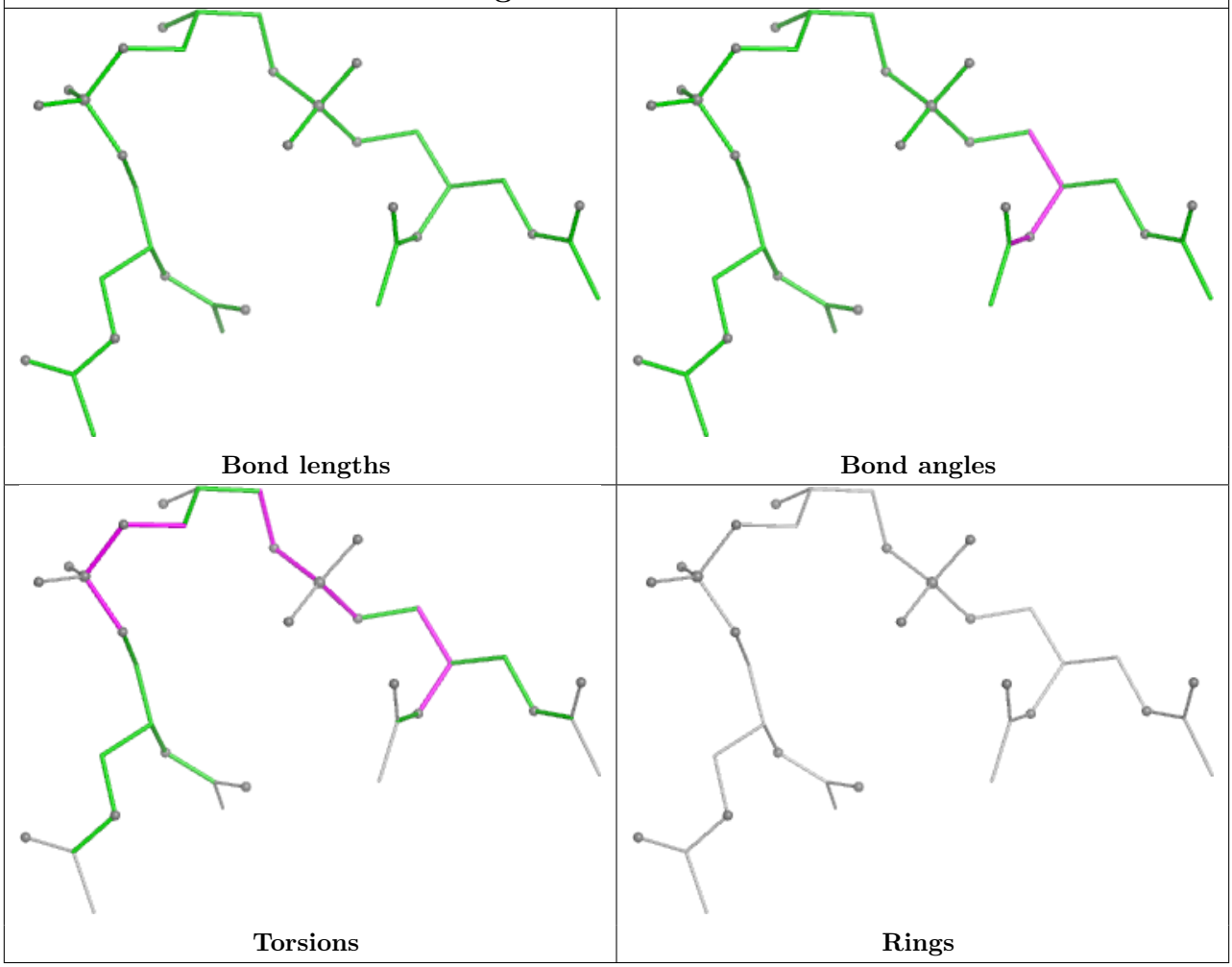
Ligand 3PE D1 501



Ligand 3PE D5 902



Ligand CDL D5 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

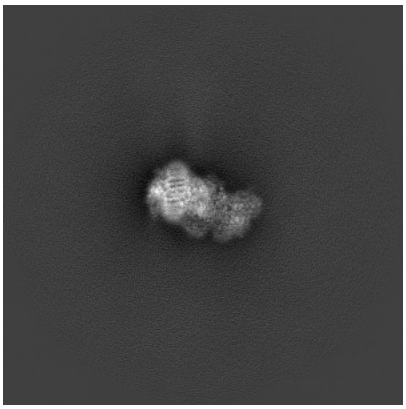
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4482. These allow visual inspection of the internal detail of the map and identification of artifacts.

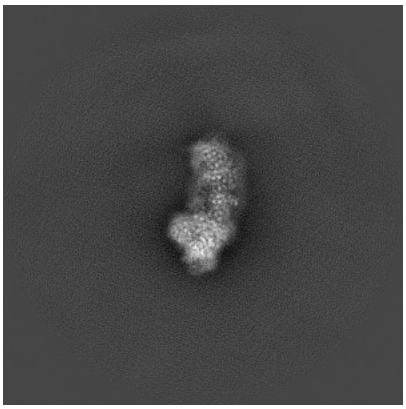
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

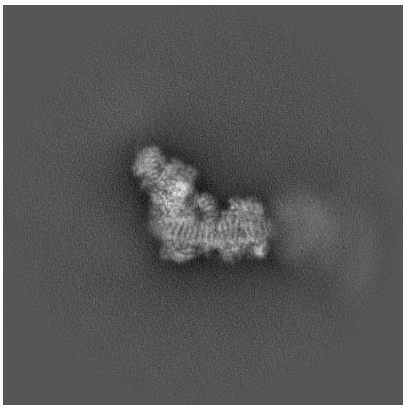
6.1.1 Primary map



X

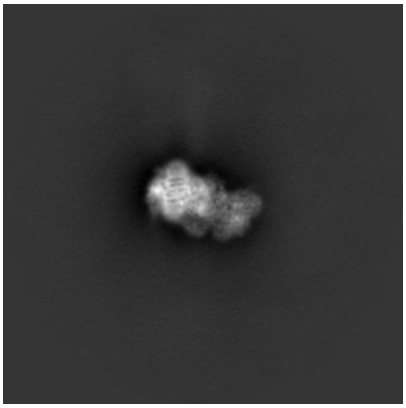


Y

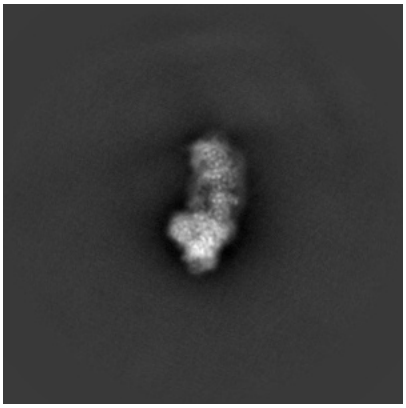


Z

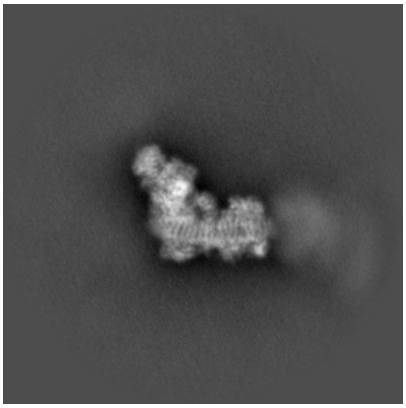
6.1.2 Raw map



X



Y

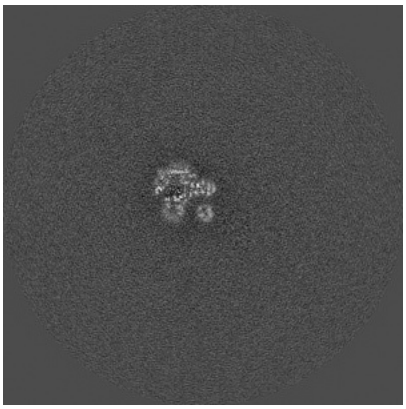


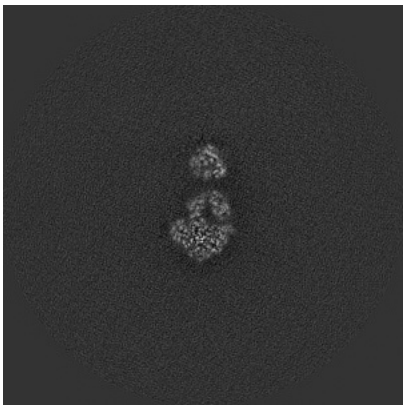
Z

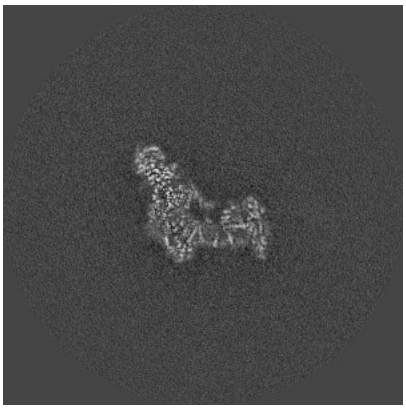
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

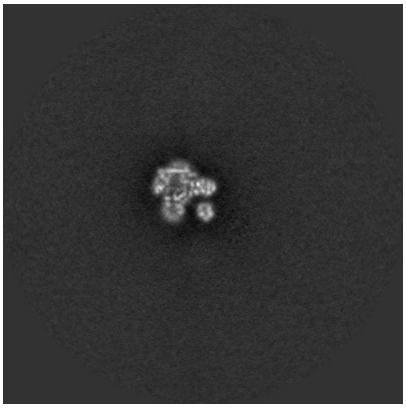
6.2.1 Primary map

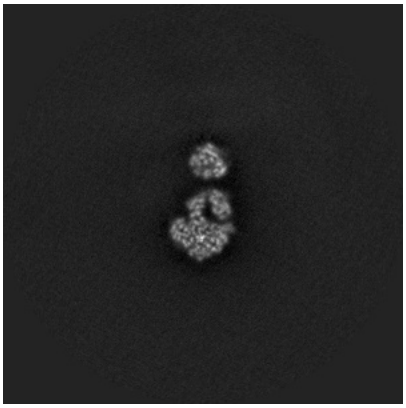

X Index: 256

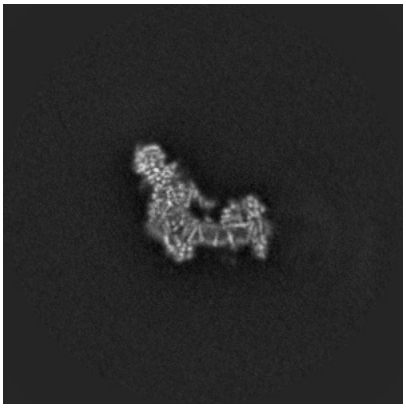

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

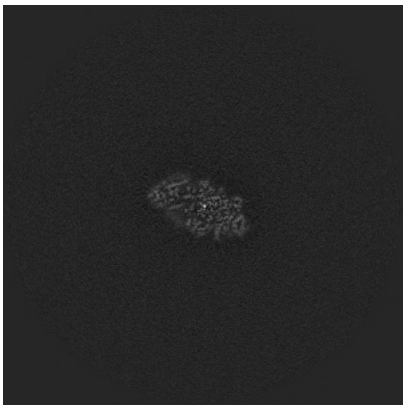

Y Index: 256

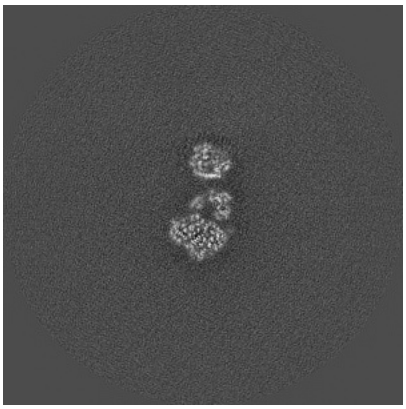

Z Index: 256

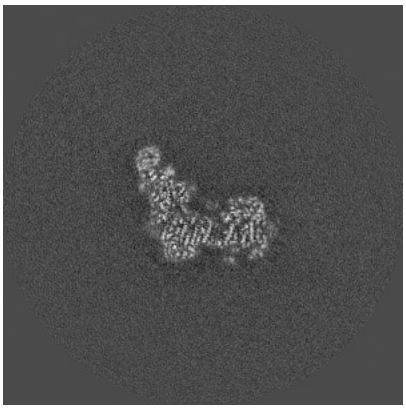
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

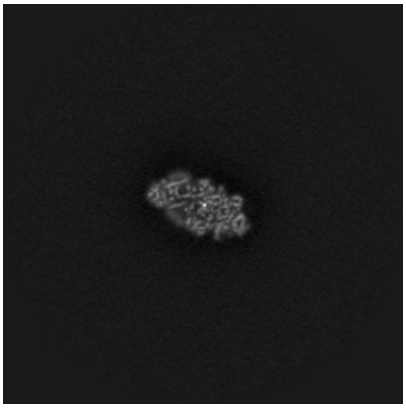
6.3.1 Primary map

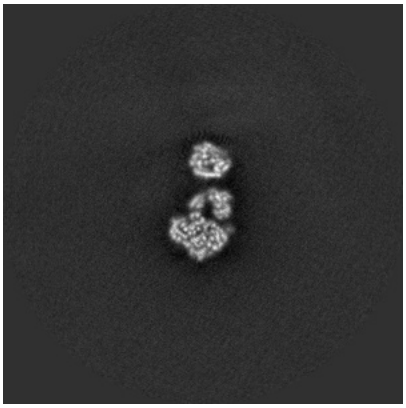

X Index: 212

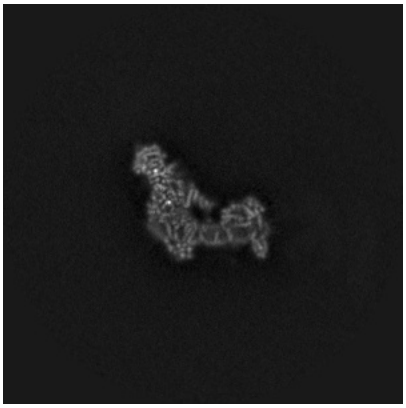

Y Index: 252


Z Index: 263

6.3.2 Raw map


X Index: 212

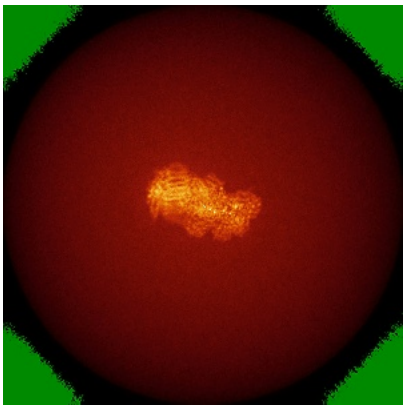

Y Index: 253

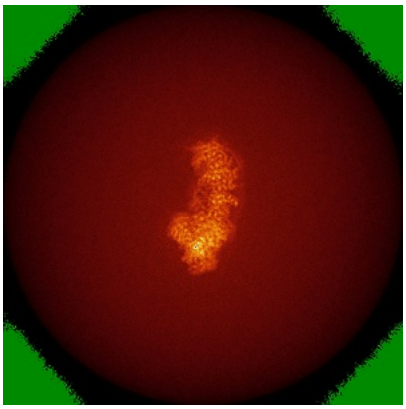

Z Index: 254

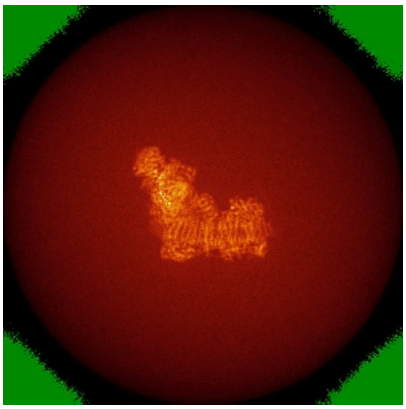
The images above show the largest variance slices of the map in three orthogonal directions.

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

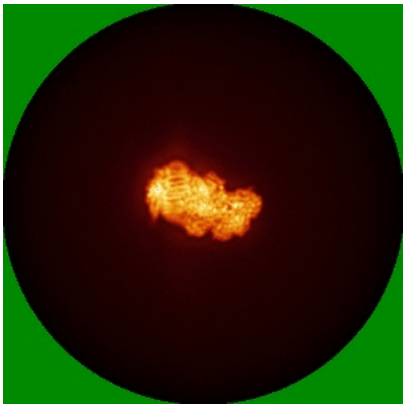
6.4.1 Primary map

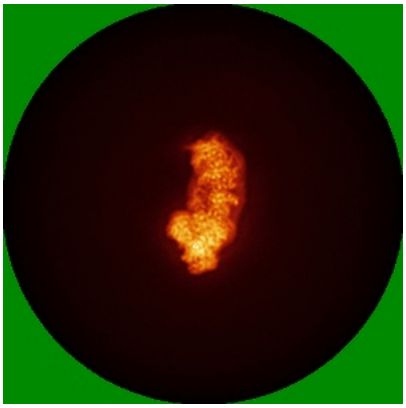

X

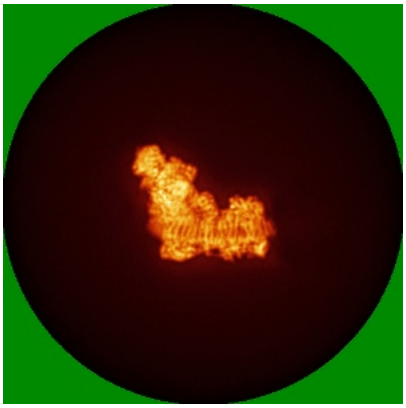

Y


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

X Y Z

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

6.5.2 Raw map

X Y Z

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.

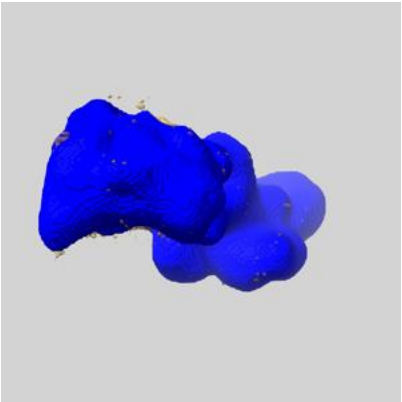
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

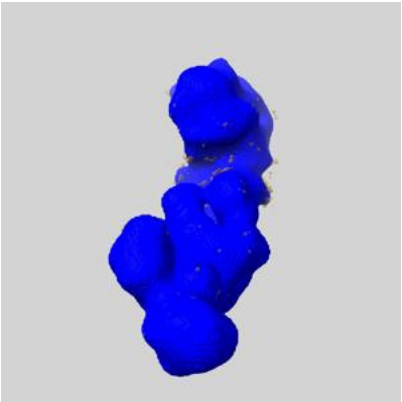
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

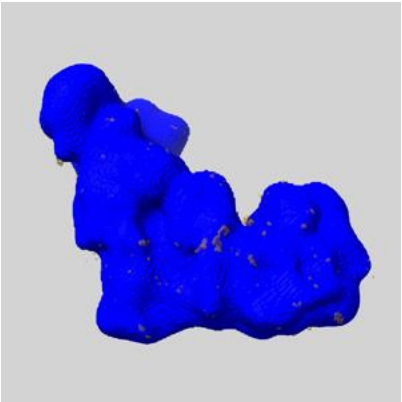
6.6.1 emd_4482_msk_1.map (i)



X



Y

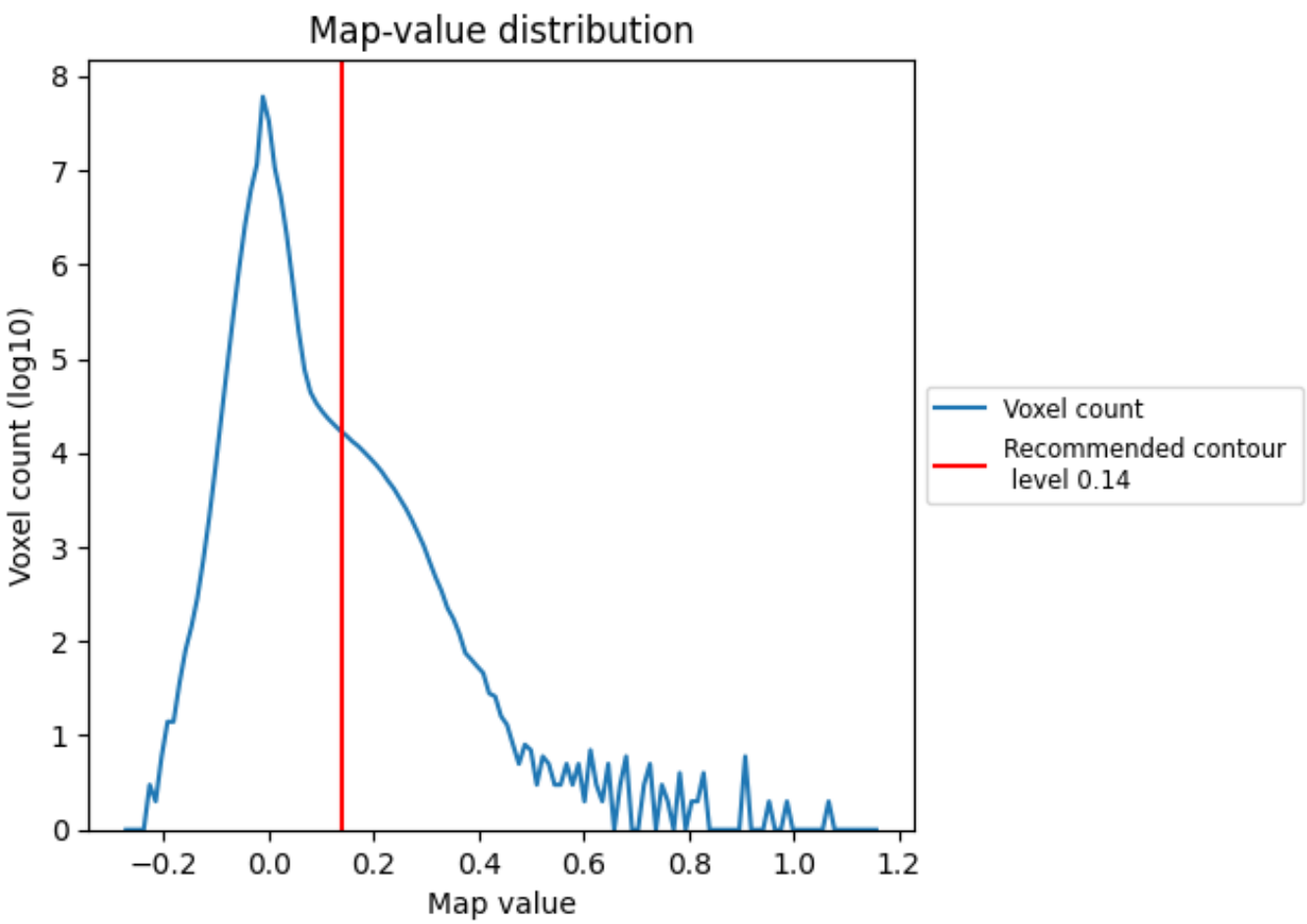


Z

7 Map analysis (i)

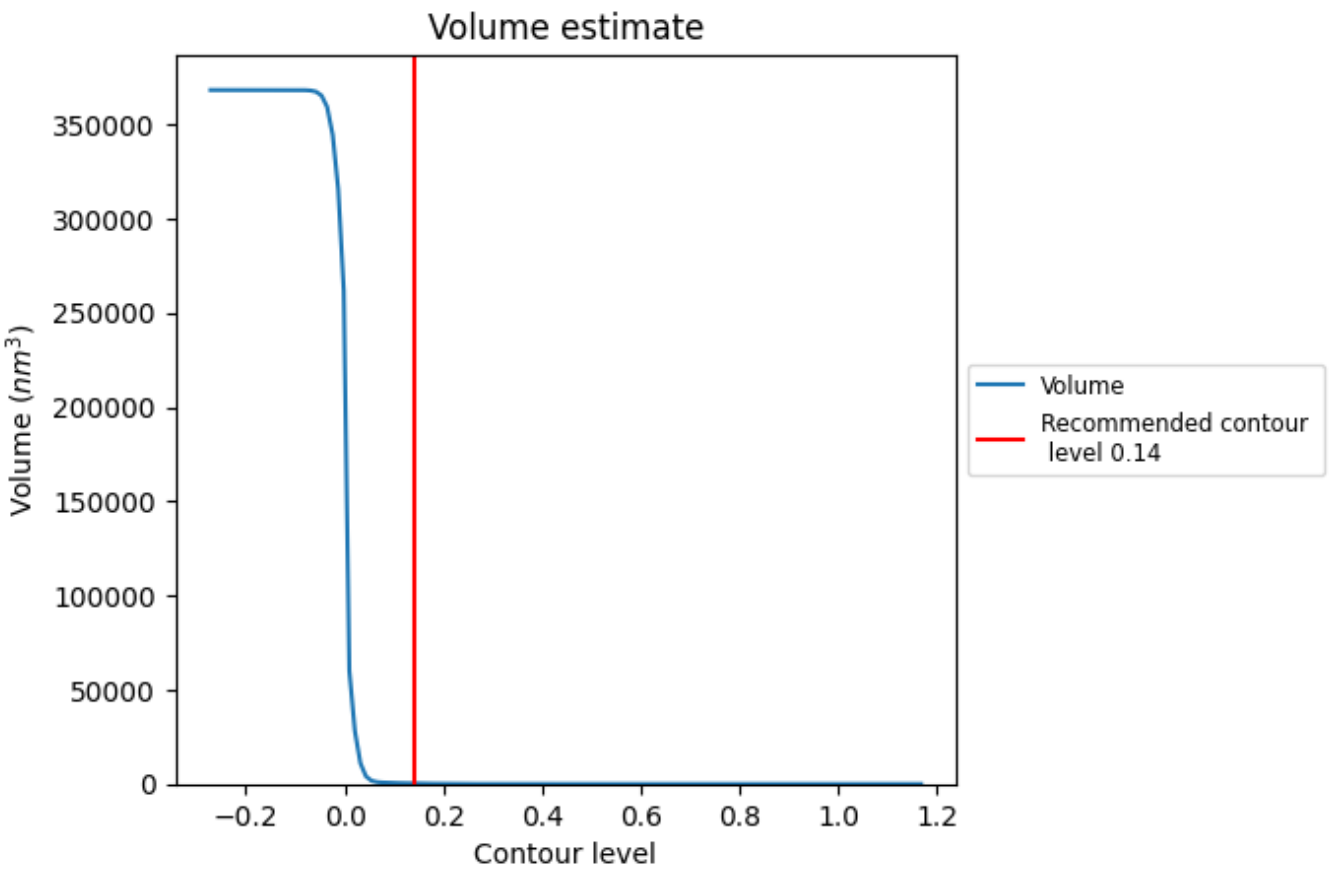
This section contains the results of statistical analysis of the map.

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.

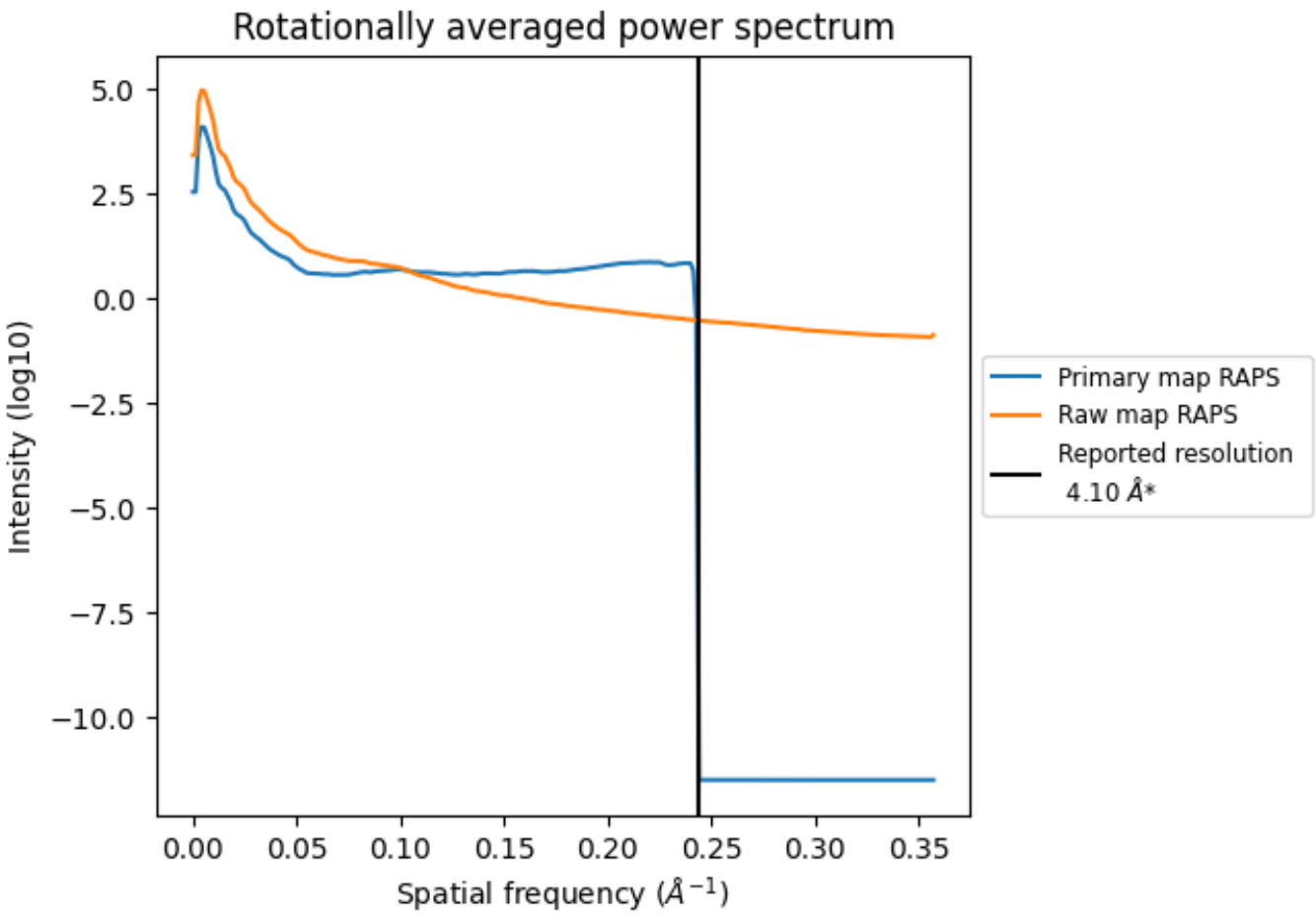
7.2 Volume estimate (i)



The volume at the recommended contour level is 294 nm^3; this corresponds to an approximate mass of 266 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)

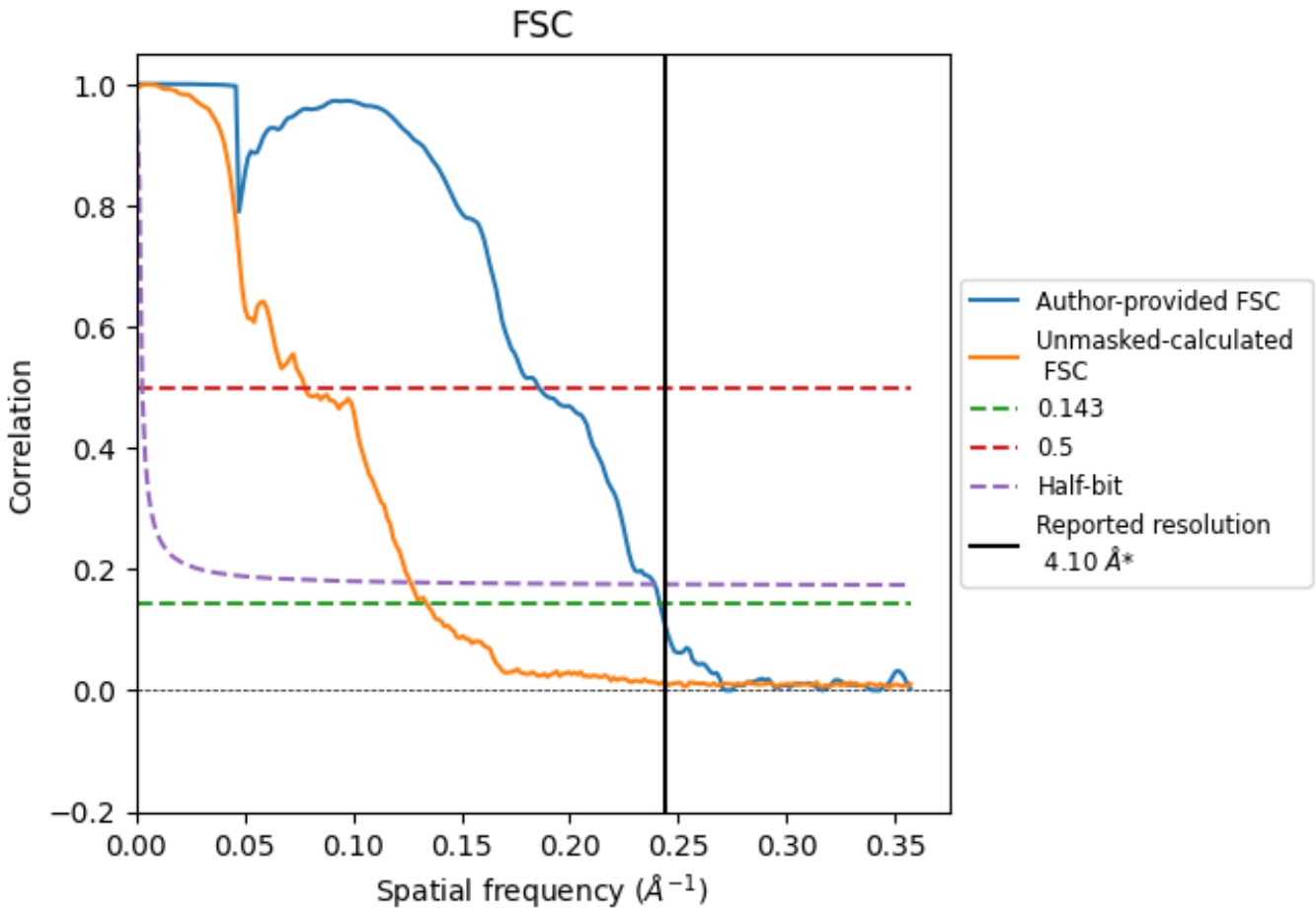


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

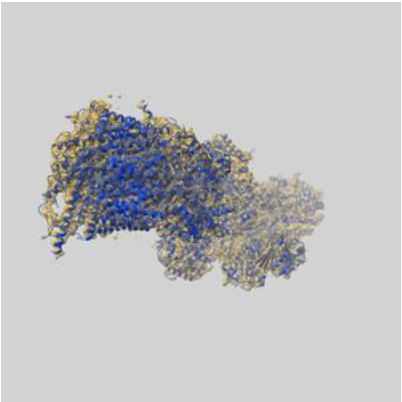
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	5.39	4.18
Unmasked-calculated*	7.47	12.85	7.91

*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 7.47 differs from the reported value 4.1 by more than 10 %

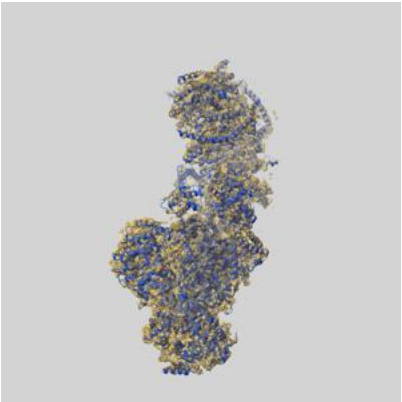
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4482 and PDB model 6QA9. Per-residue inclusion information can be found in section 3 on page 17.

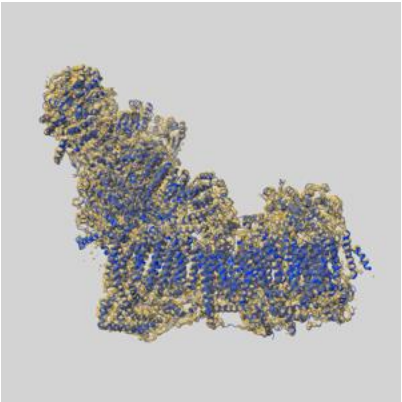
9.1 Map-model overlay (i)



X



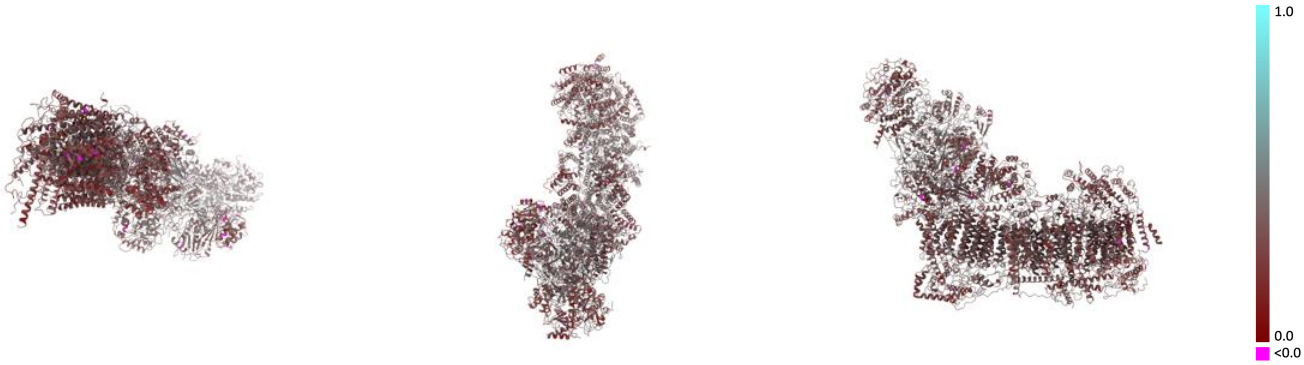
Y



Z

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

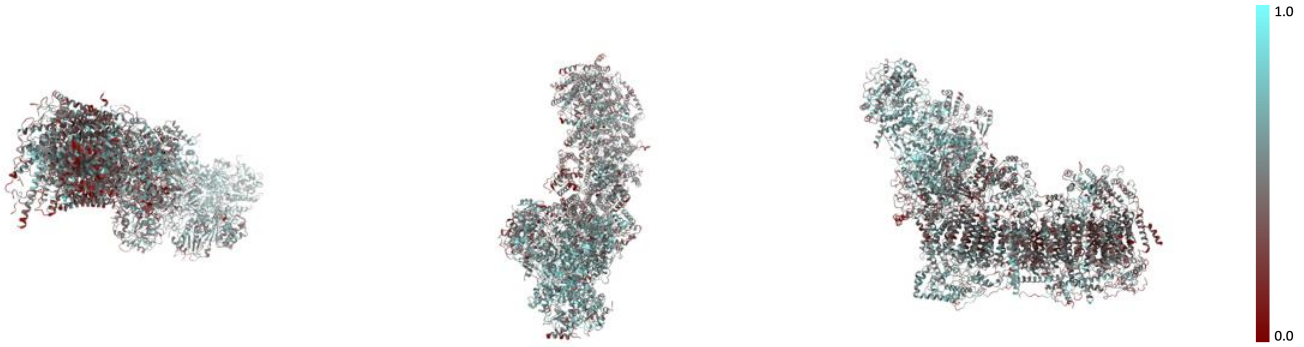
9.2 Q-score mapped to coordinate model (i)



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.

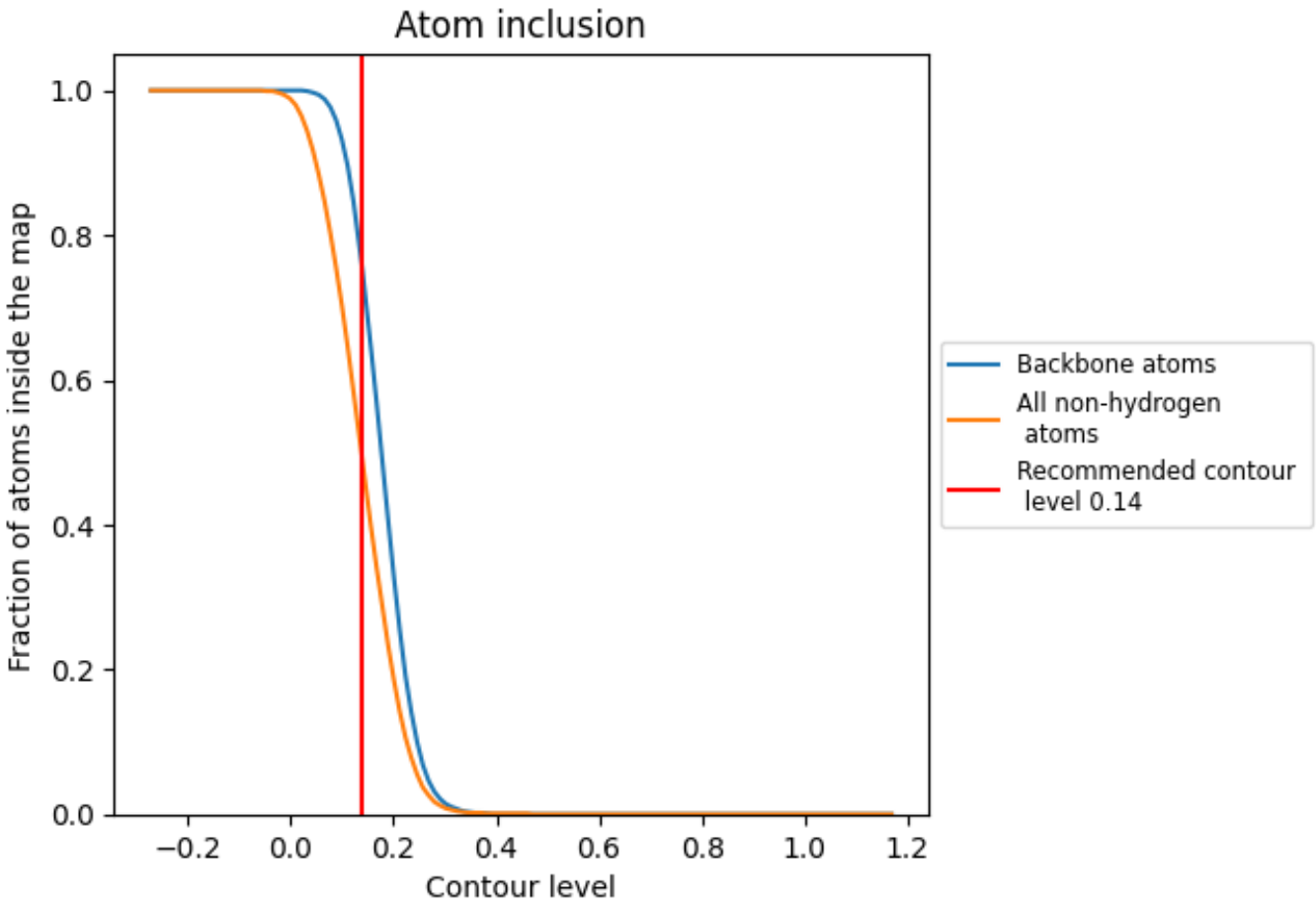
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.4870	0.3370
4L	0.4330	0.3330
A1	0.5540	0.3400
A2	0.4890	0.2930
A3	0.4980	0.3470
A5	0.5120	0.3270
A6	0.4690	0.3290
A7	0.4300	0.3650
A8	0.5420	0.3340
A9	0.4630	0.3220
AA	0.2730	0.2560
AB	0.4250	0.2950
AJ	0.4670	0.3350
AK	0.3350	0.3040
AL	0.3600	0.3630
AM	0.5170	0.3260
B1	0.3900	0.3110
B2	0.3850	0.2960
B3	0.3470	0.2840
B4	0.4470	0.3120
B5	0.5190	0.3560
B6	0.4250	0.3000
B7	0.4240	0.2790
B8	0.4490	0.3290
B9	0.4920	0.3100
BJ	0.5000	0.3190
BK	0.4130	0.3130
C1	0.4710	0.3390
C2	0.4860	0.3340
D1	0.4880	0.3460
D2	0.5070	0.3630
D3	0.3850	0.3360
D4	0.4720	0.3590
D5	0.4170	0.3160
D6	0.3840	0.3110

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Chain	Atom inclusion	Q-score
S1	0.5570	0.3520
S2	0.5260	0.3680
S3	0.5750	0.3850
S4	0.5300	0.3790
S5	0.5270	0.3420
S6	0.5560	0.3780
S7	0.5630	0.3860
S8	0.6080	0.3900
V1	0.5730	0.3220
V2	0.5440	0.3160
V3	0.5640	0.3150