wwPDB EM Validation Summary Report (i)

Nov 10, 2024 – 06:12 am GMT

PDB ID	:	6QC6
EMDB ID	:	EMD-4498
Title	:	Ovine respiratory complex I FRC open class 1
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-27
Resolution	:	4.10 Å(reported)
Based on initial model	:	5LNK

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

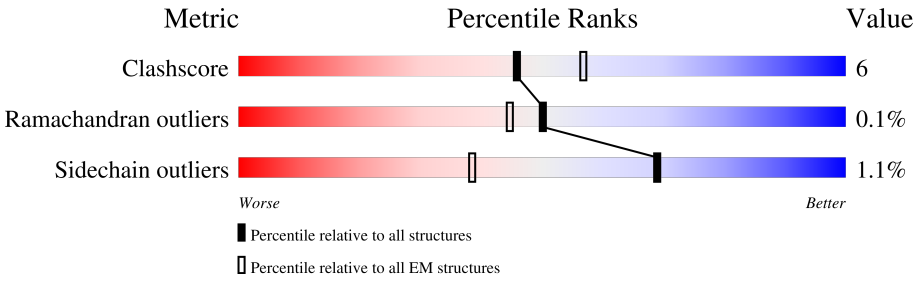
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	V1	445	16% 76% 21%
2	V2	217	18% 77% 19%
3	S1	704	17% 79% 18%
4	S2	430	21% 82% 16%
5	S3	228	13% 76% 15% 9%
6	S7	179	15% 66% 20% 13%
7	S8	176	12% 81% 18%
8	V3	75	11% 40% 11% 45%

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Mol	Chain	Length	Quality of chain
9	S6	96	25% 89% 9%
10	S4	133	19% 79% 16% 5%
11	A9	338	22% 65% 20% 15%
12	A2	98	22% 71% 12% 16%
13	A5	115	23% 83% 13%
14	A6	127	19% 78% 12% 10%
15	A7	112	32% 74% 9% 15%
16	AL	145	38% 83% 16%
17	AA	88	40% 80% 11% 9%
17	AB	88	39% 83% 16%
18	D3	115	35% 66% 12% 22%
19	D1	318	30% 73% 21% 5%
20	D6	175	58% 83% 14%
21	4L	98	50% 86% 13%
22	D5	606	37% 80% 20%
23	D4	459	27% 78% 21%
24	D2	347	27% 80% 20%
25	AK	140	65% 87% 12%
26	B5	143	21% 81% 15%
27	A8	171	24% 76% 23%
28	BJ	175	27% 83% 14%
29	AJ	320	29% 82% 17%
30	S5	105	25% 81% 13% 6%
31	A3	83	34% 76% 13% 11%
32	B3	97	36% 64% 9% 25%

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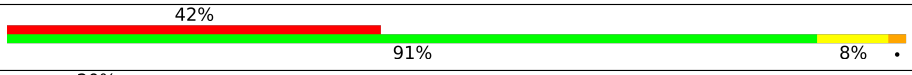
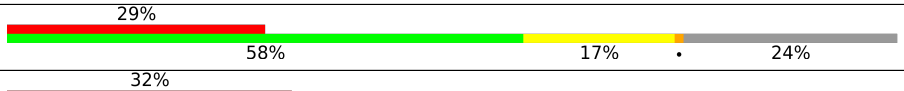
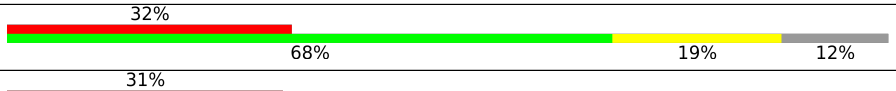
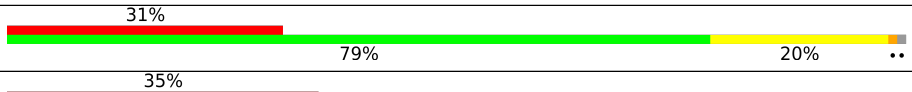
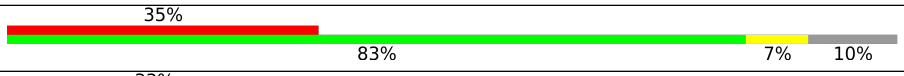
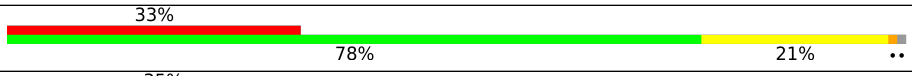
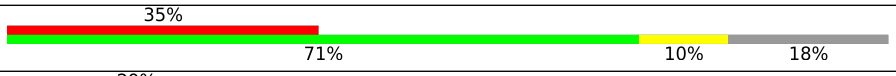
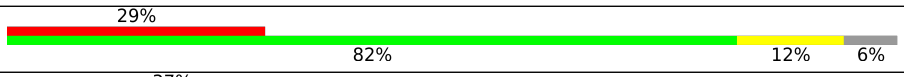
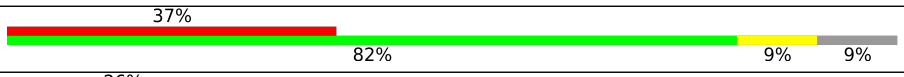
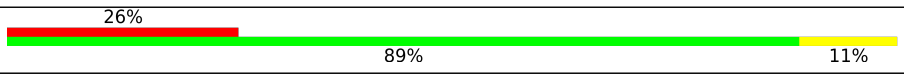
Mol	Chain	Length	Quality of chain
33	C2	120	
34	B4	128	
35	AM	143	
36	B6	127	
37	B7	136	
38	B9	178	
39	B2	72	
40	B8	158	
41	BK	125	
42	C1	49	
43	B1	57	
44	A1	70	

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 65344 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S2	424	3414	2180	584	625	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 NADH:ubiquinone oxidoreductase core subunit S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	287	Total	C	N	O	S	0	0
			2293	1464	419	405	5		

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

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

- Molecule 17 is a protein called Acyl carrier protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D1	303	Total	C	N	O	S	0	0
			2415	1633	368	395	19		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

unit 8.

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

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit B10.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

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

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

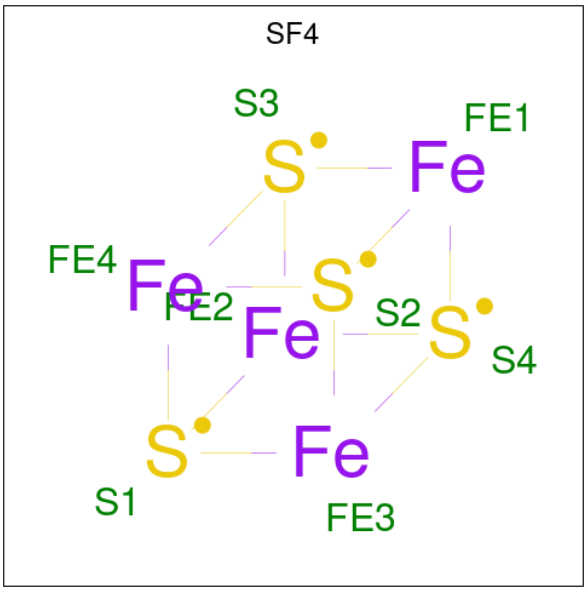
There are 3 discrepancies between the modelled and reference sequences:

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 NADH dehydrogenase 1 alpha subcomplex.

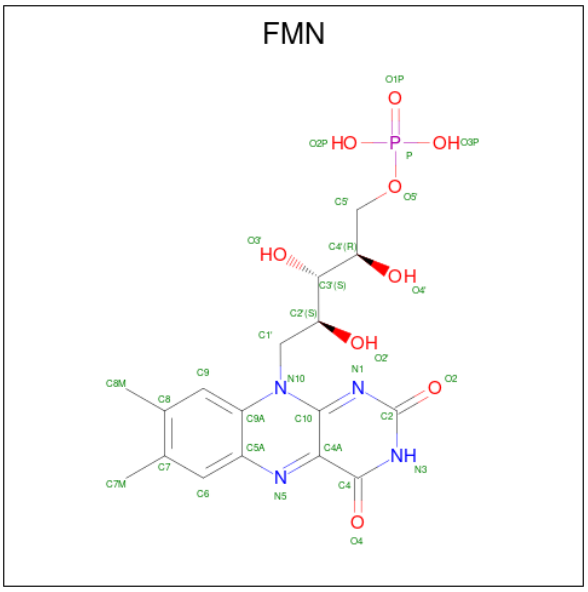
Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



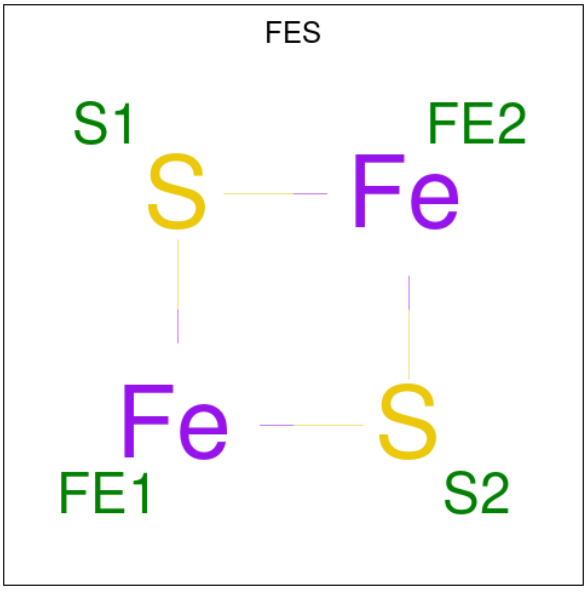
Mol	Chain	Residues	Atoms	AltConf
45	V1	1	Total Fe S 8 4 4	0
45	S1	1	Total Fe S 8 4 4	0
45	S1	1	Total Fe S 8 4 4	0
45	S7	1	Total Fe S 8 4 4	0
45	S8	1	Total Fe S 8 4 4	0
45	S8	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: 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 (three-letter code: FES) (formula: Fe_2S_2).

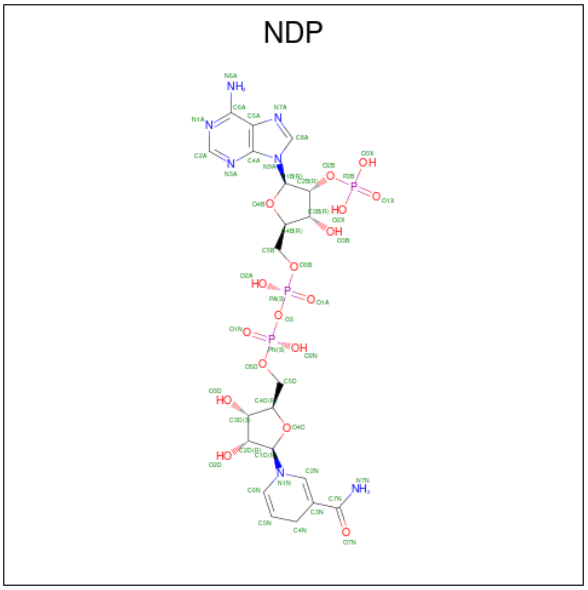


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

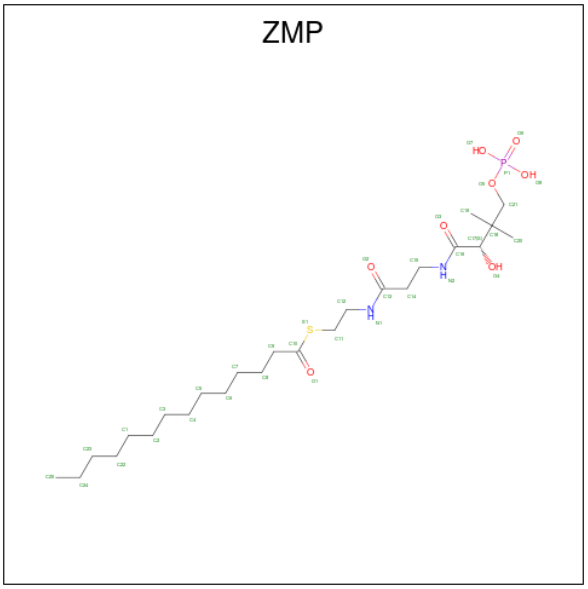
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	S6	1	1	1	0

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



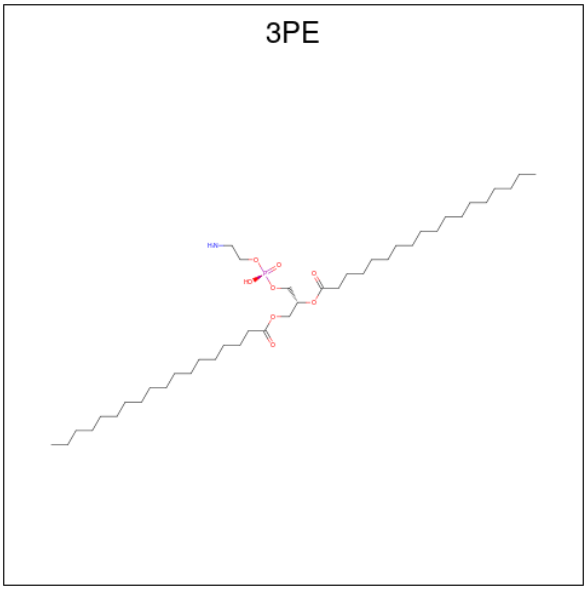
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	A9	1	48	21	7	17	3	0

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



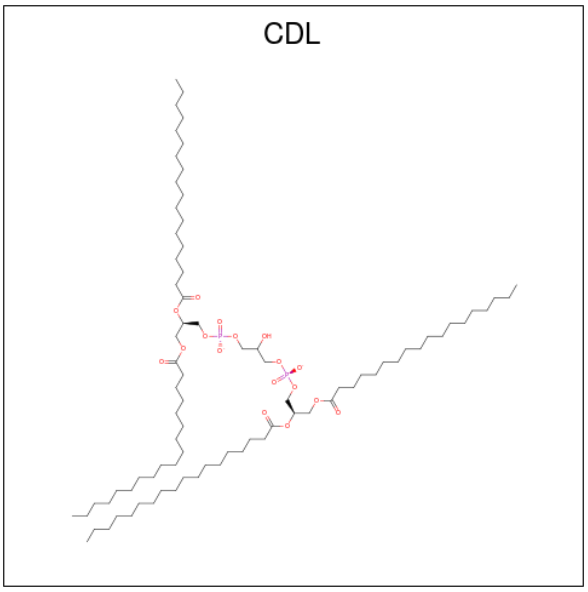
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

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



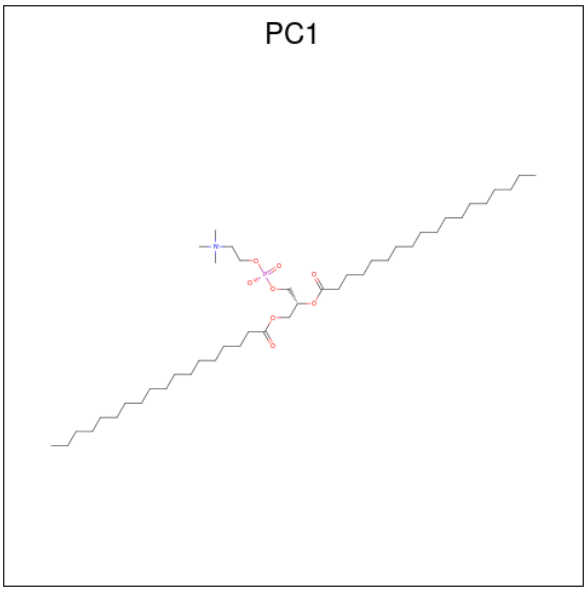
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			26	16	1	8	1	
51	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	B8	1	Total	C	N	O	P	0
			38	28	1	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
52	D5	1	Total	C	O	P	0
			60	41	17	2	

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



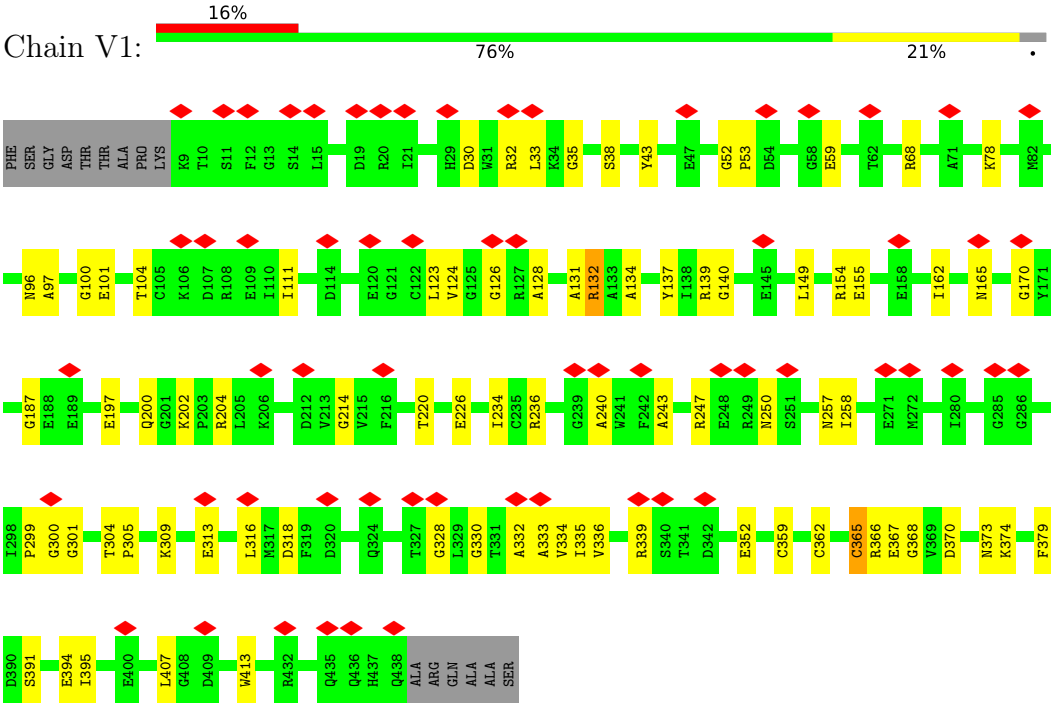
Mol	Chain	Residues	Atoms					AltConf
53	D4	1	Total	C	N	O	P	0
			28	18	1	8	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

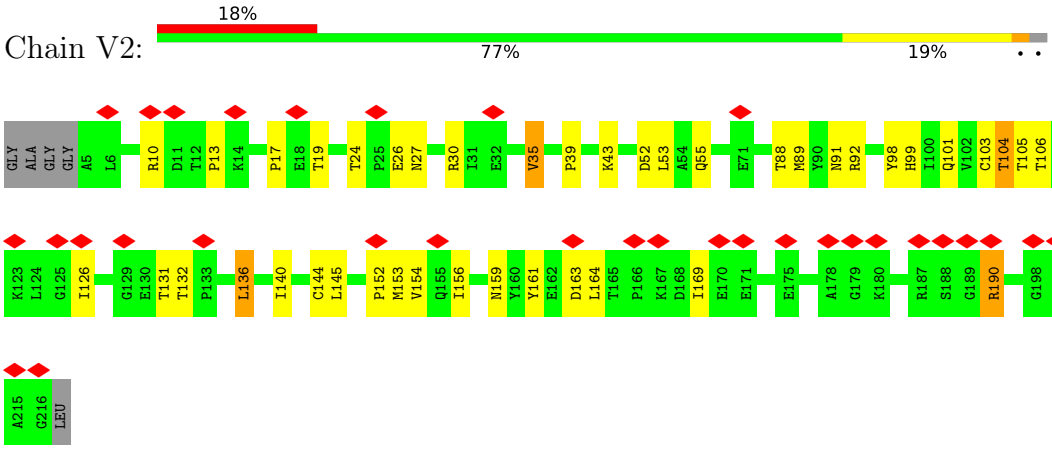
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



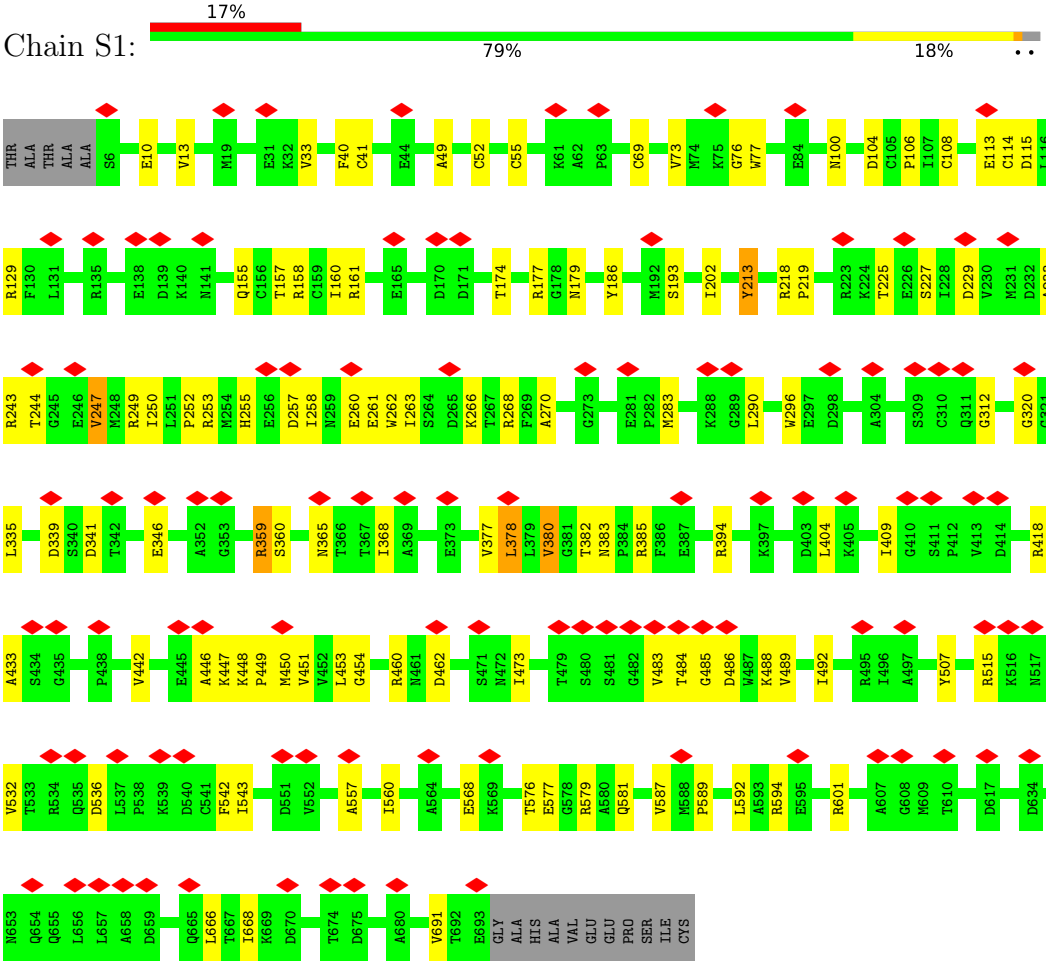
• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:



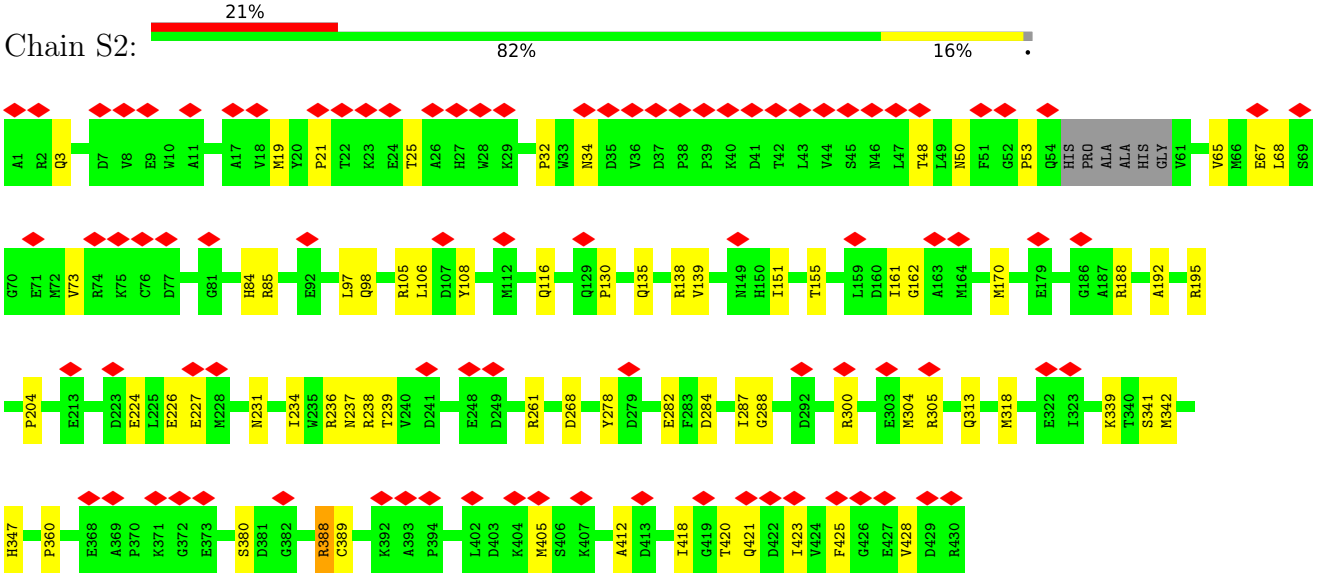
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1:



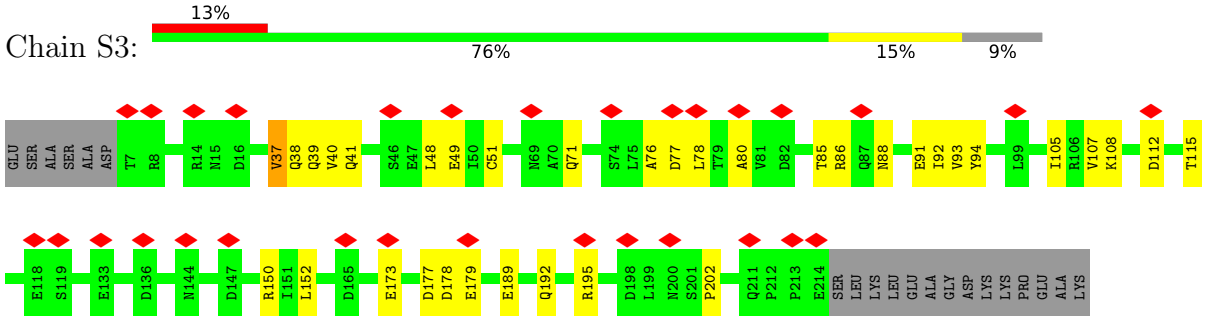
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2:



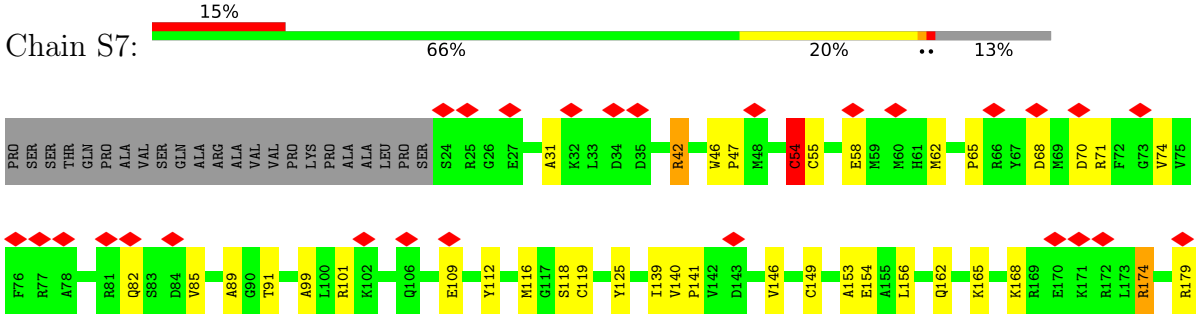
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



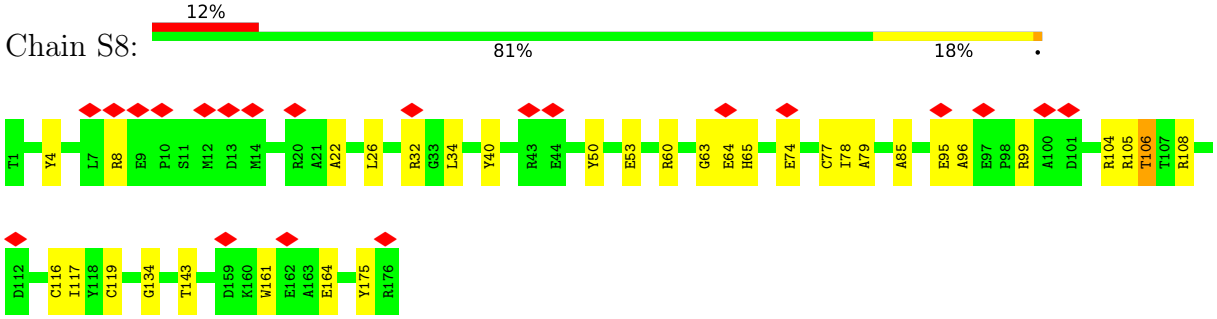
• Molecule 6: NADH:ubiquinone oxidoreductase core subunit S7

Chain S7:



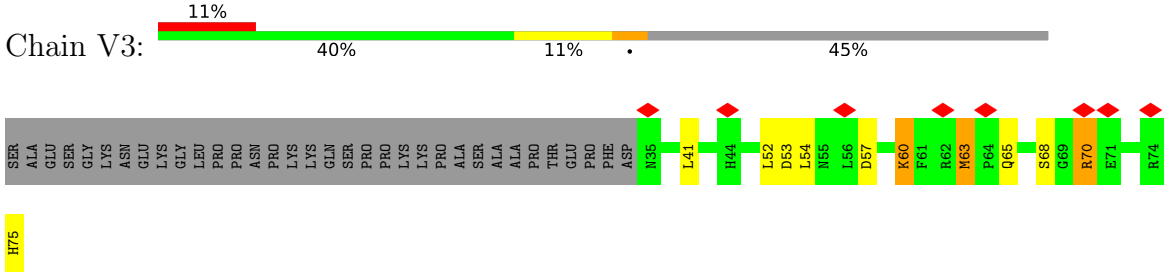
• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8:



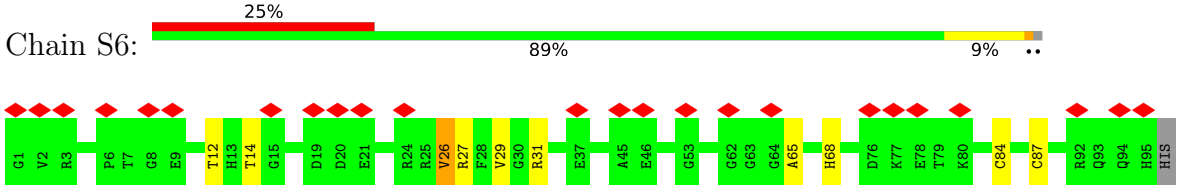
• Molecule 8: NADH:ubiquinone oxidoreductase subunit V3

Chain V3:



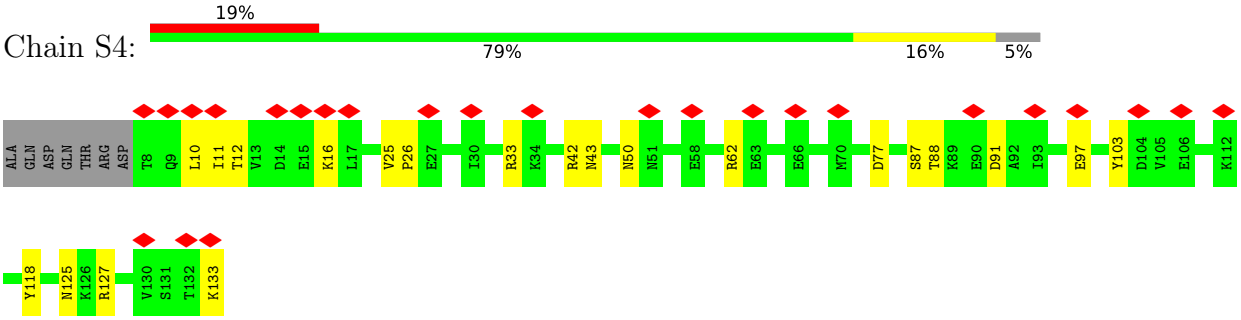
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:



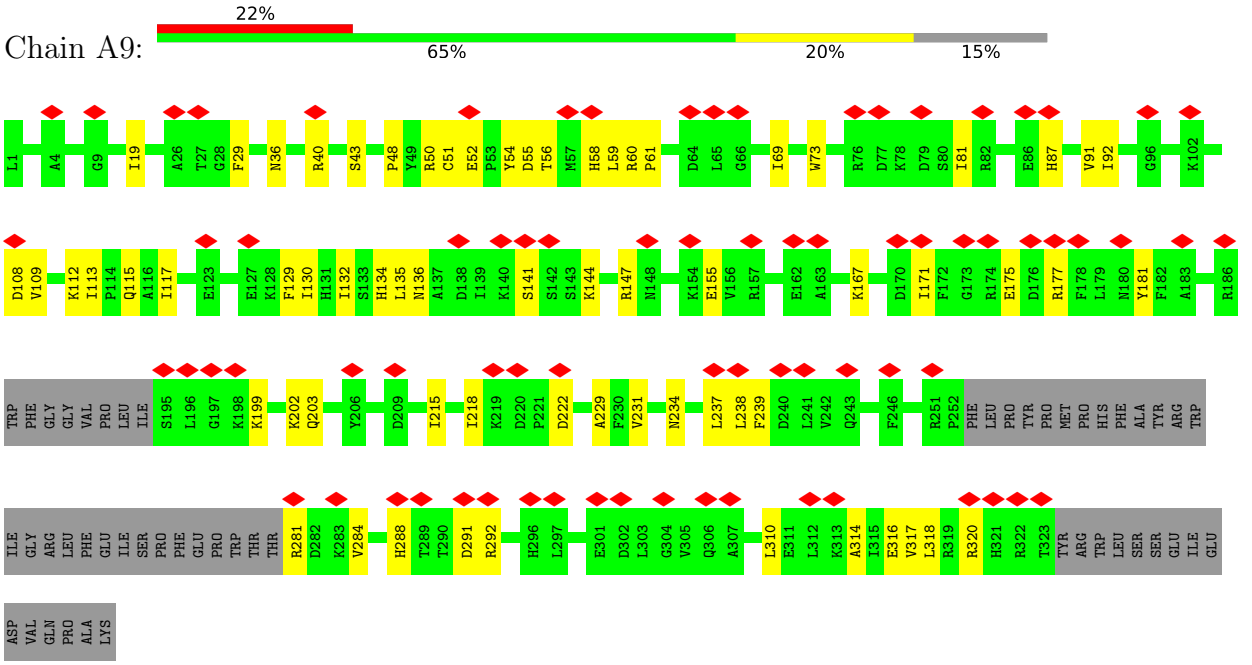
• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

Chain S4:



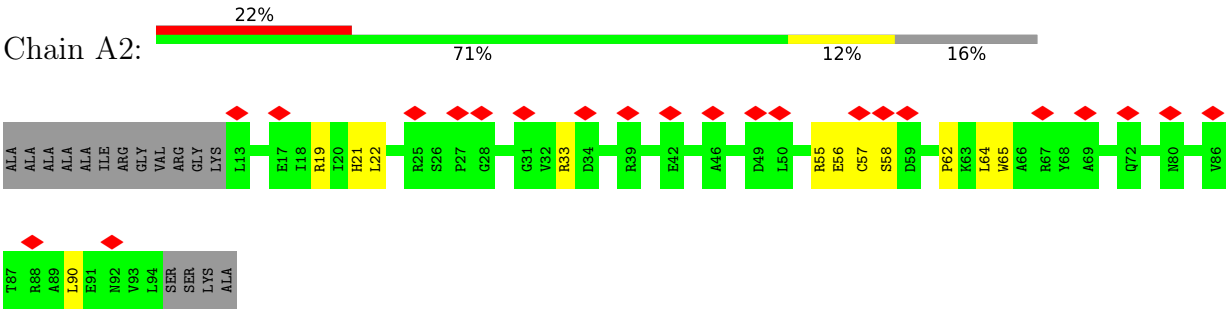
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

Chain A9:



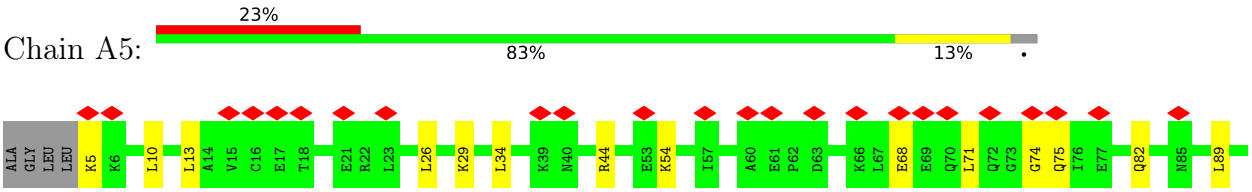
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

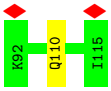
Chain A2:



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

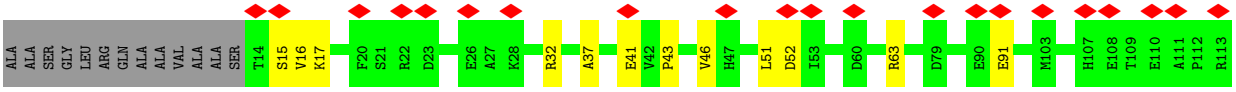
Chain A5:

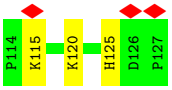




• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

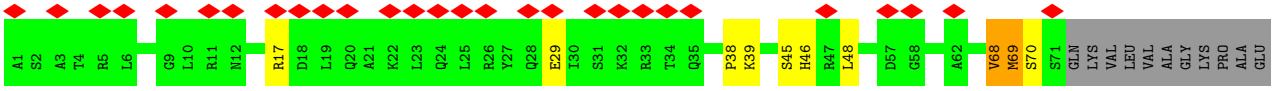
Chain A6:

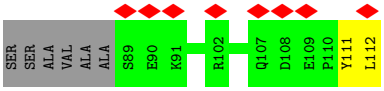




• Molecule 15: NADH:ubiquinone oxidoreductase subunit A7

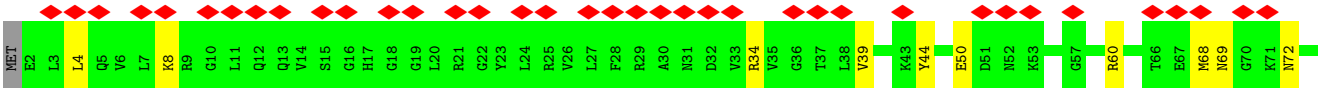
Chain A7:

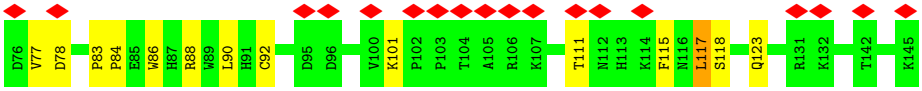




• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

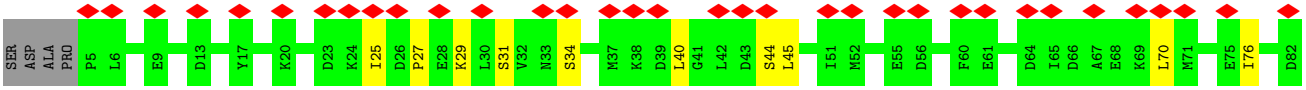
Chain AL:

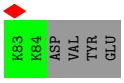




• Molecule 17: Acyl carrier protein

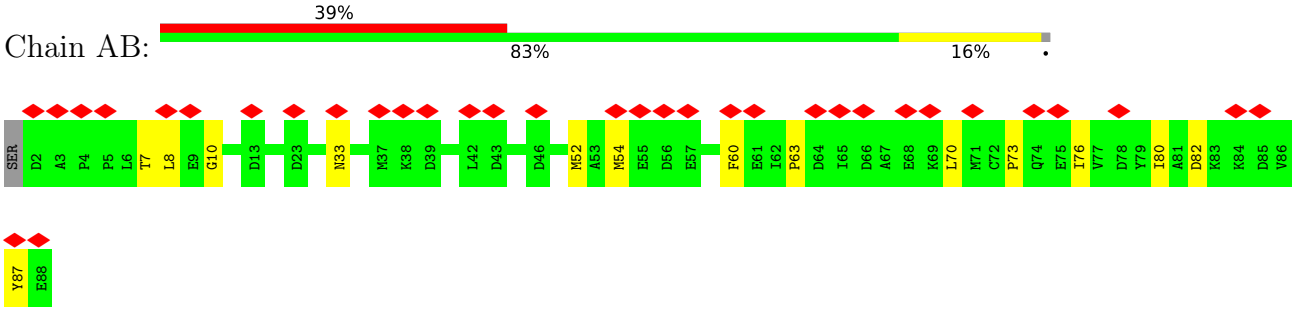
Chain AA:





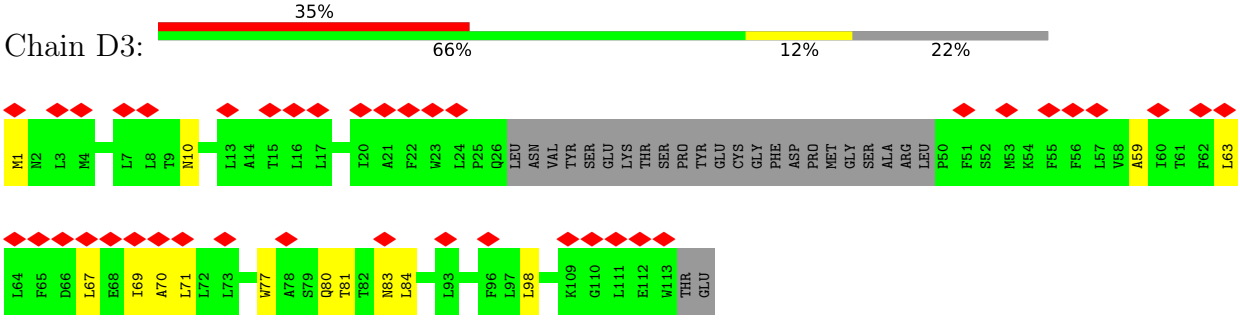
• Molecule 17: Acyl carrier protein

Chain AB:



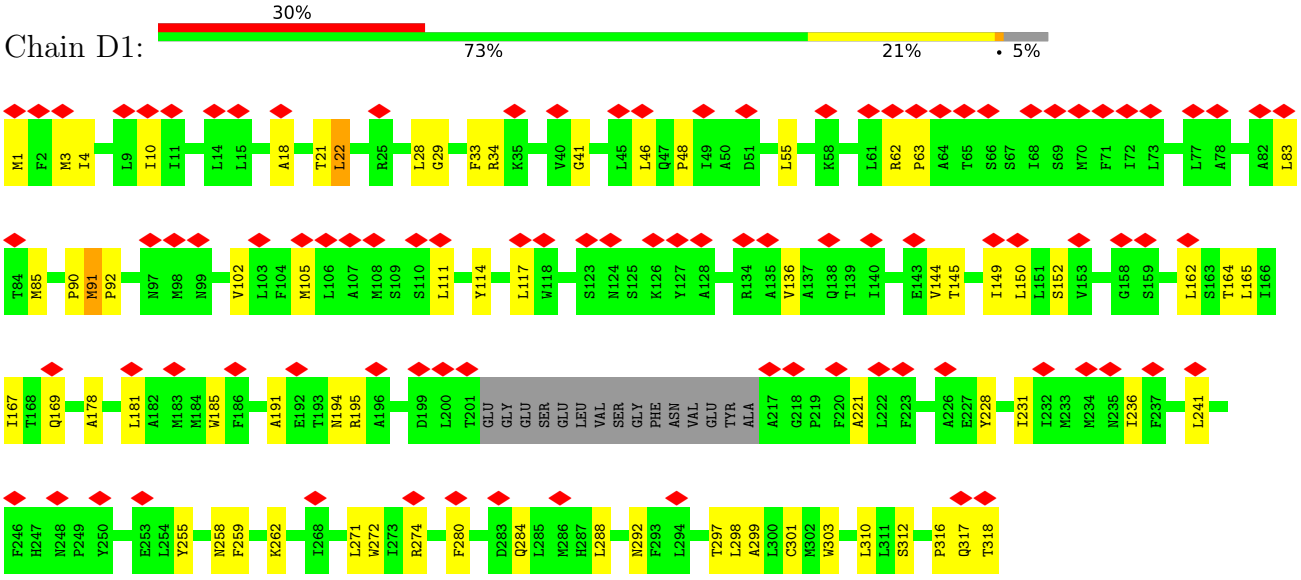
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain D3:



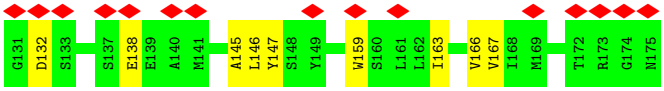
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain D1:



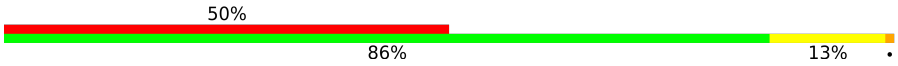
• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

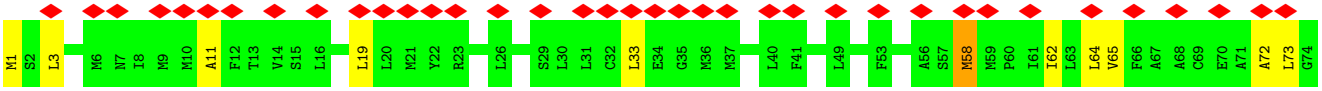
Chain D6:

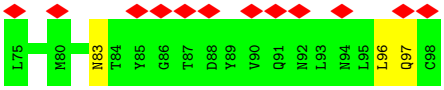


• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:

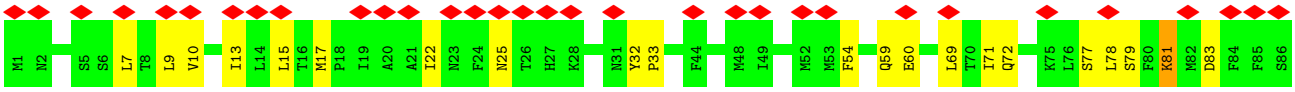


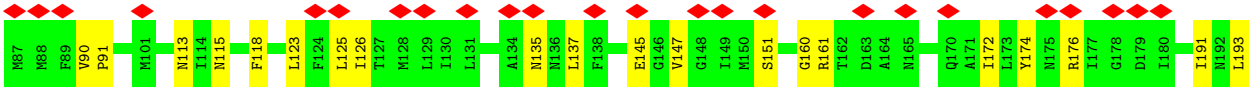


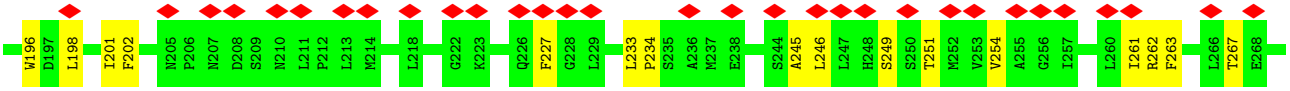


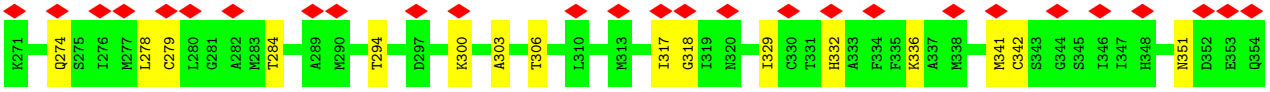
• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

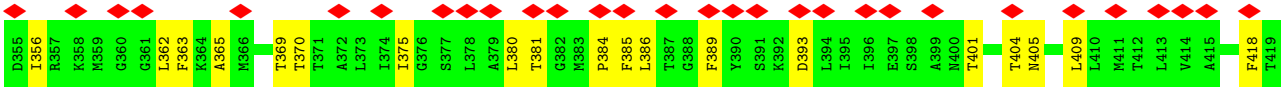
Chain D5:

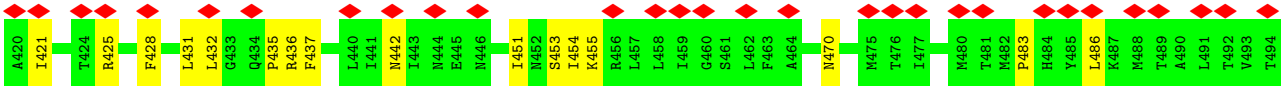


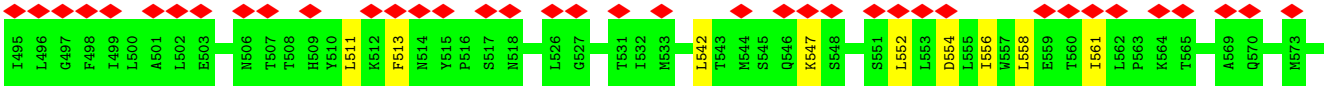


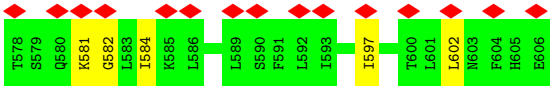






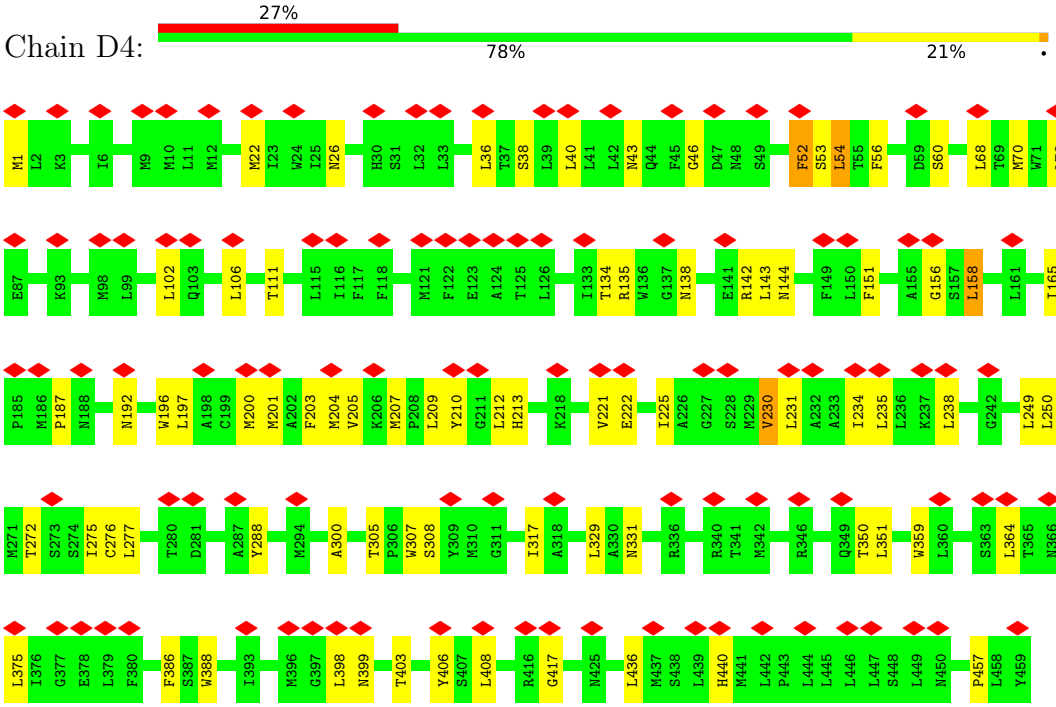






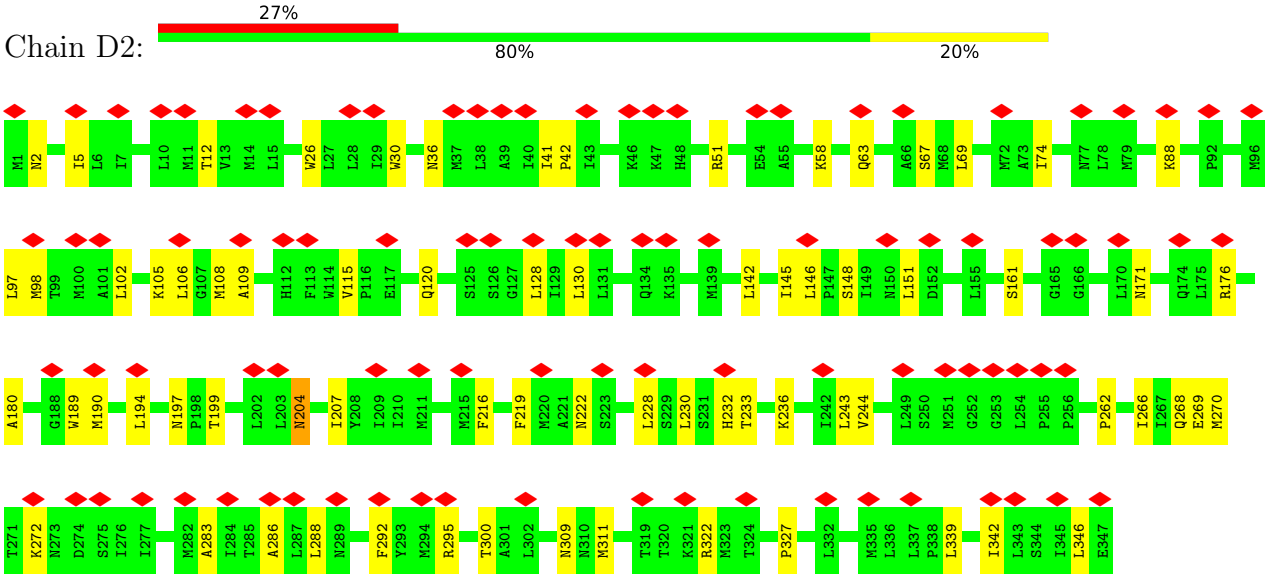
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



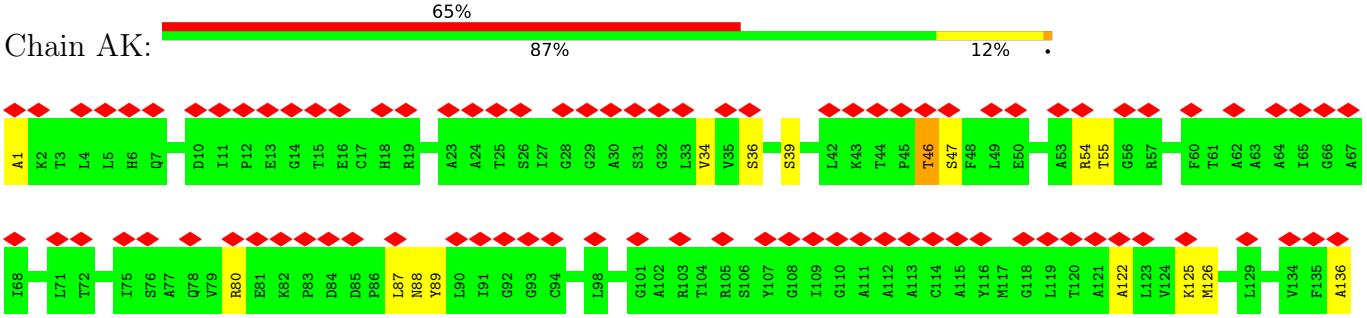
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain D2:



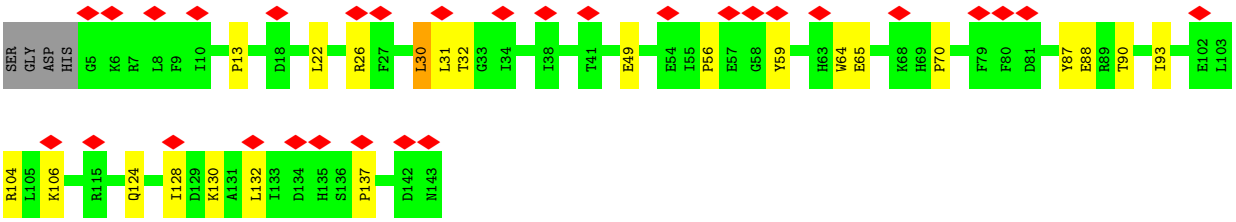
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AK:



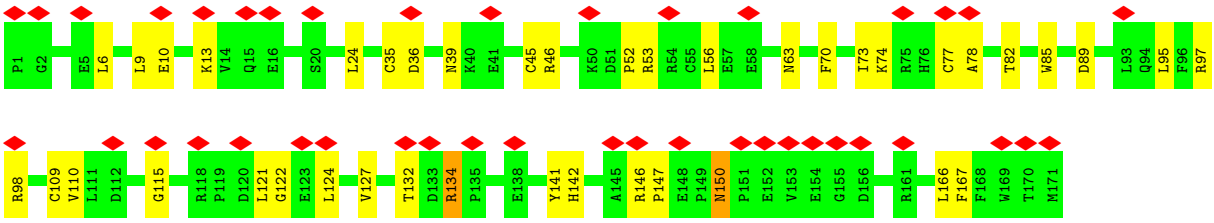
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5:



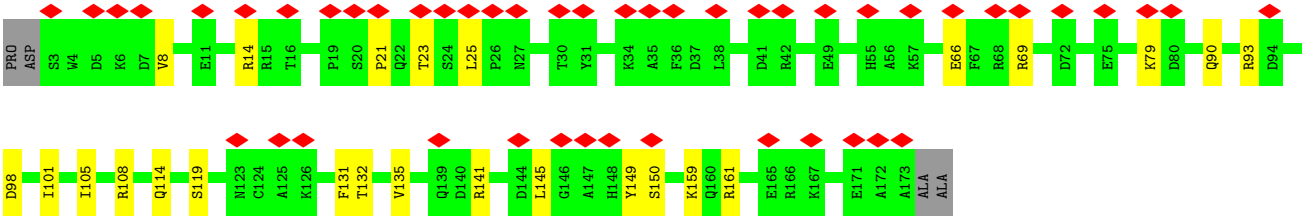
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:



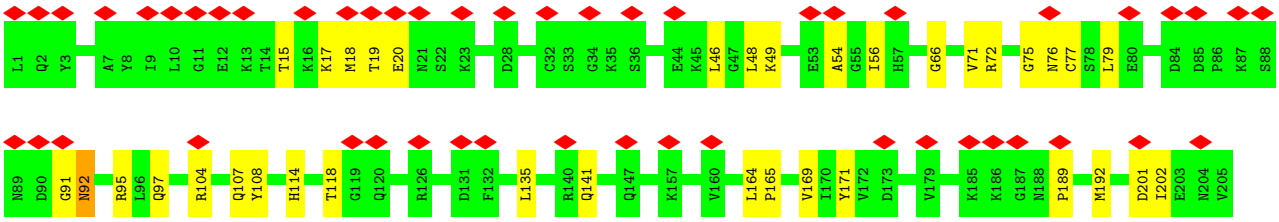
• Molecule 28: NADH:ubiquinone oxidoreductase subunit B10

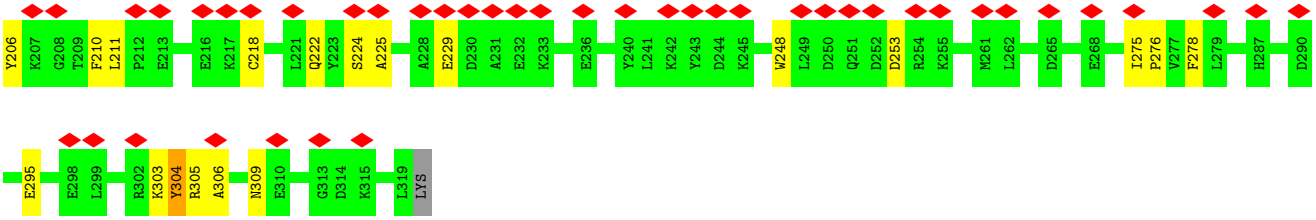
Chain BJ:



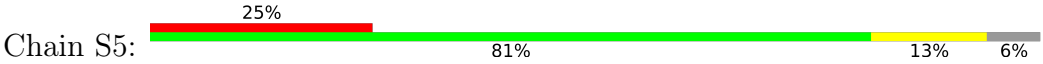
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

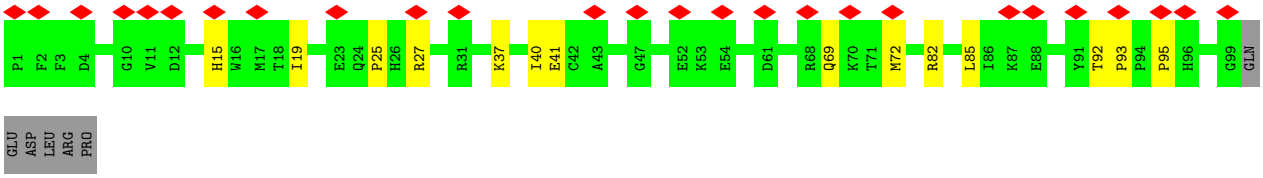
Chain AJ:



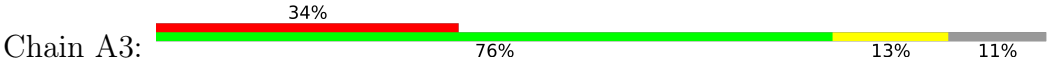


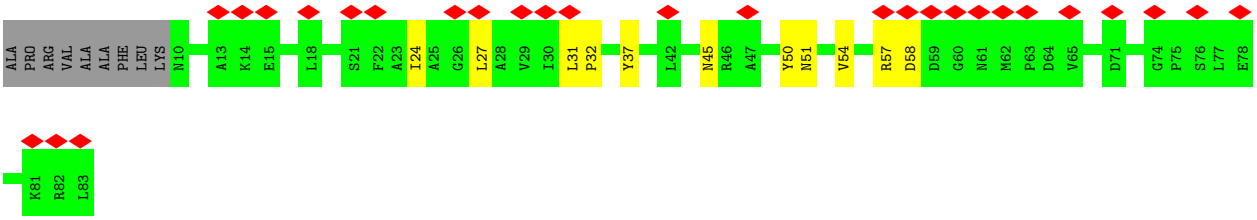
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



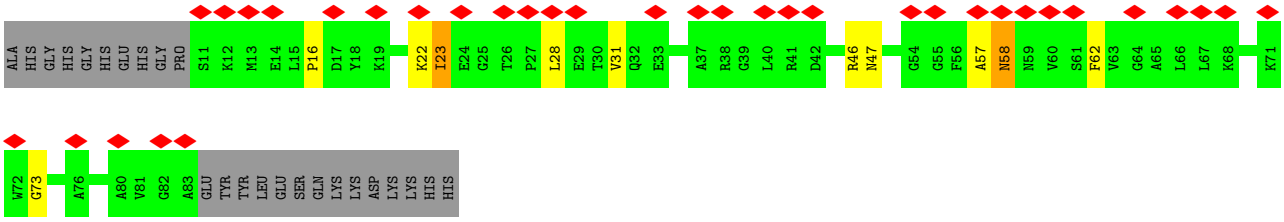


• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

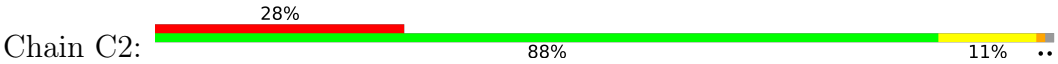


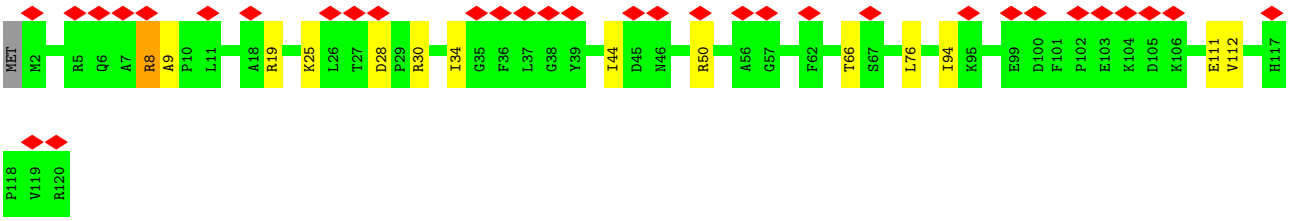


• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



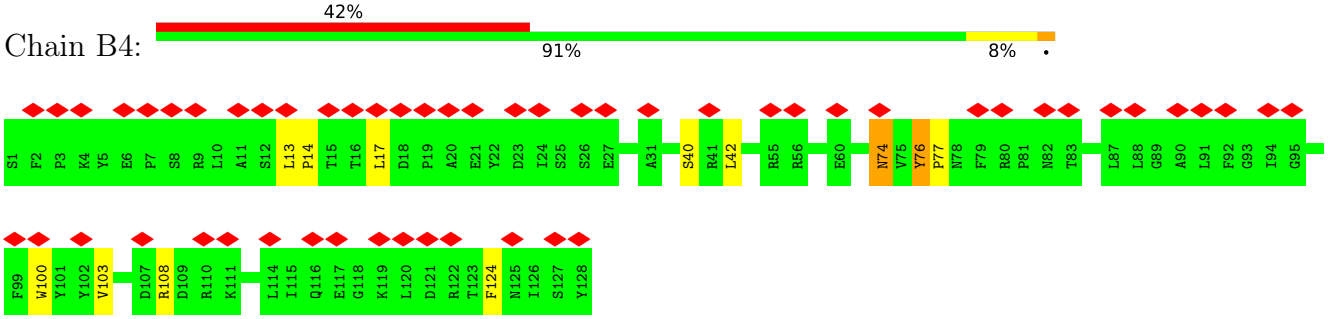
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2





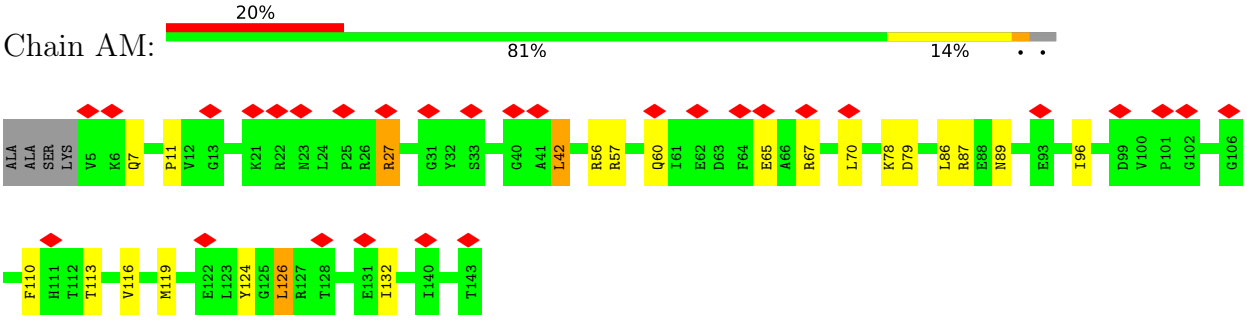
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



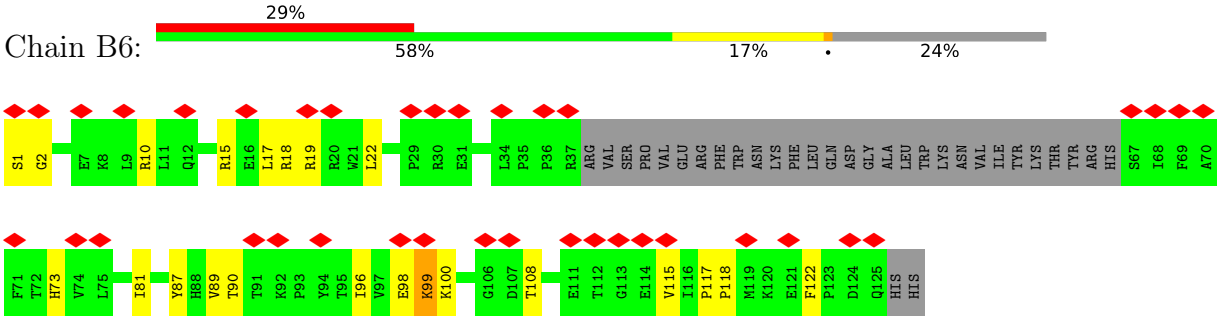
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AM:



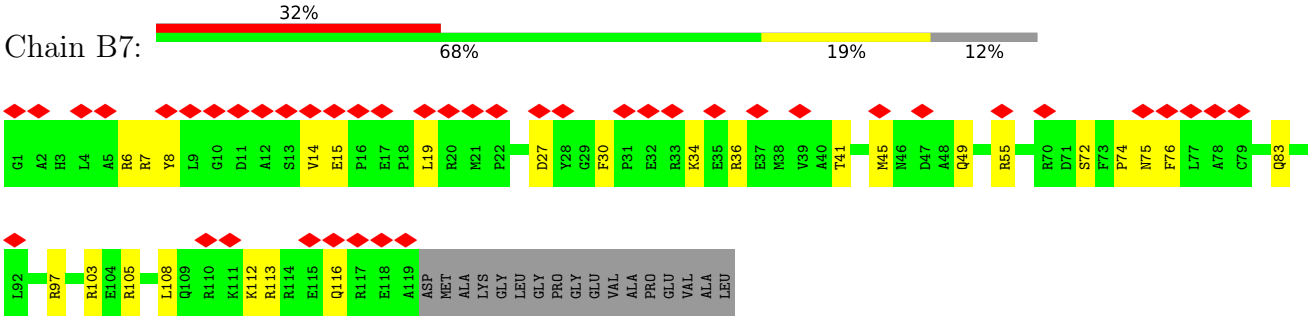
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



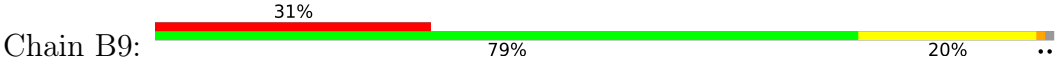
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

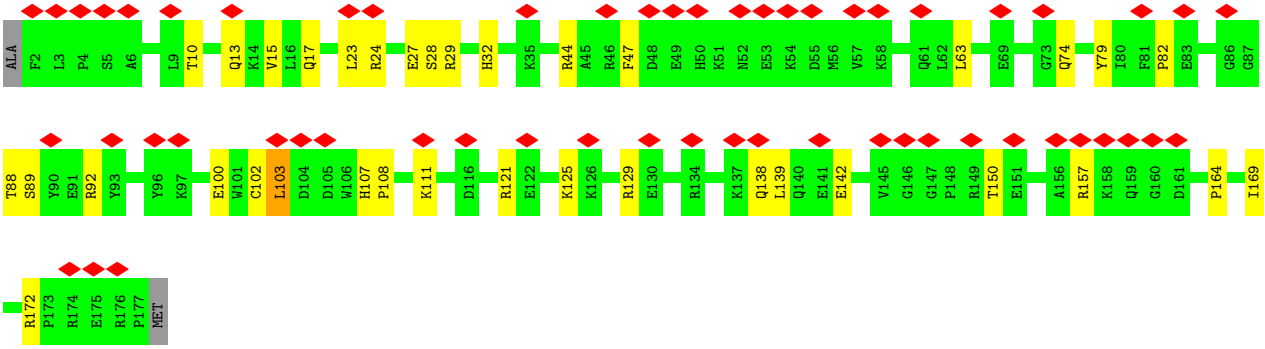
Chain B7:



• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

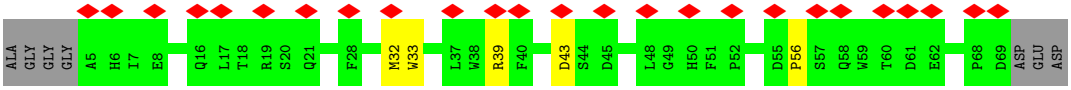
Chain B9:





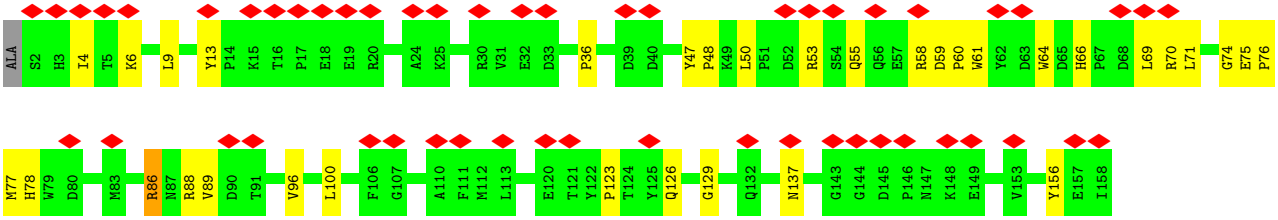
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:



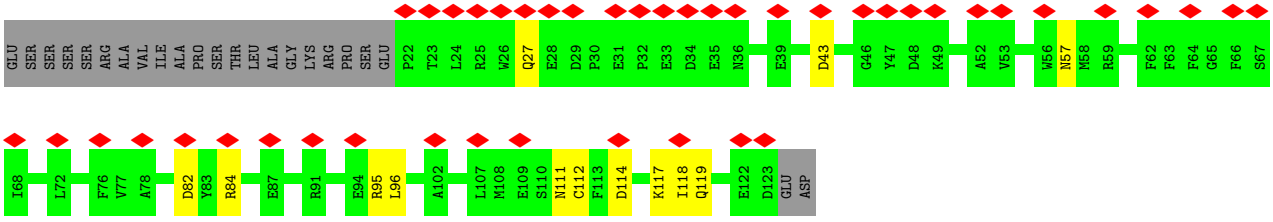
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



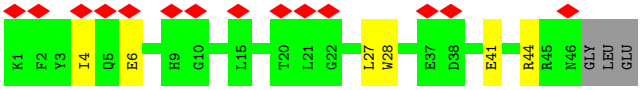
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BK:



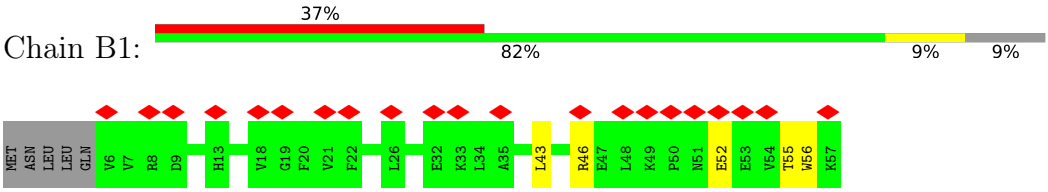
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain C1:



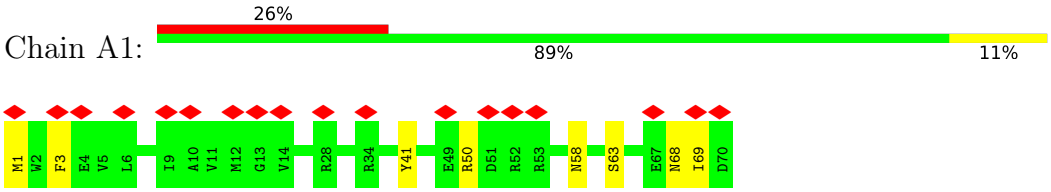
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:



• Molecule 44: NADH dehydrogenase 1 alpha subcomplex

Chain A1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26978	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)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.343	Depositor
Minimum map value	-0.394	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	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: CDL, 3PE, ZN, NDP, FMN, PC1, ZMP, SF4, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	V1	0.33	0/3386	0.61	1/4575 (0.0%)
2	V2	0.34	0/1687	0.70	2/2295 (0.1%)
3	S1	0.32	0/5362	0.62	2/7266 (0.0%)
4	S2	0.35	0/3502	0.60	1/4744 (0.0%)
5	S3	0.34	0/1776	0.63	1/2417 (0.0%)
6	S7	0.35	0/1278	0.57	0/1728
7	S8	0.40	1/1445 (0.1%)	0.61	0/1956
8	V3	0.29	0/355	0.67	1/480 (0.2%)
9	S6	0.32	0/749	0.56	0/1009
10	S4	0.30	0/1047	0.58	0/1415
11	A9	0.31	0/2343	0.63	1/3164 (0.0%)
12	A2	0.29	0/676	0.58	0/911
13	A5	0.31	0/921	0.64	1/1249 (0.1%)
14	A6	0.30	0/993	0.53	0/1336
15	A7	0.30	0/775	0.64	0/1048
16	AL	0.31	0/1242	0.61	0/1688
17	AA	0.27	0/655	0.61	0/881
17	AB	0.32	0/714	0.60	0/963
18	D3	0.32	0/747	0.66	0/1022
19	D1	0.37	0/2487	0.69	3/3401 (0.1%)
20	D6	0.34	0/1339	0.64	1/1810 (0.1%)
21	4L	0.33	0/758	0.73	1/1024 (0.1%)
22	D5	0.34	0/4933	0.70	4/6710 (0.1%)
23	D4	0.35	0/3740	0.69	4/5095 (0.1%)
24	D2	0.35	0/2788	0.65	2/3795 (0.1%)
25	AK	0.31	0/1046	0.66	1/1419 (0.1%)
26	B5	0.31	0/1189	0.57	1/1607 (0.1%)
27	A8	0.32	0/1441	0.65	1/1942 (0.1%)
28	BJ	0.31	0/1475	0.58	2/1989 (0.1%)
29	AJ	0.33	0/2644	0.62	3/3579 (0.1%)
30	S5	0.32	0/843	0.60	0/1128
31	A3	0.31	0/602	0.67	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	B3	0.31	0/595	0.66	0/803
33	C2	0.33	0/1028	0.61	0/1388
34	B4	0.30	0/1085	0.62	1/1467 (0.1%)
35	AM	0.31	0/1172	0.59	2/1579 (0.1%)
36	B6	0.32	0/841	0.68	0/1144
37	B7	0.32	0/1051	0.63	2/1408 (0.1%)
38	B9	0.32	0/1568	0.61	1/2123 (0.0%)
39	B2	0.30	0/590	0.60	0/810
40	B8	0.32	0/1379	0.66	2/1884 (0.1%)
41	BK	0.31	0/880	0.61	0/1196
42	C1	0.28	0/404	0.53	0/548
43	B1	0.29	0/462	0.62	0/624
44	A1	0.31	0/592	0.61	0/795
All	All	0.33	1/66585 (0.0%)	0.63	41/90243 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V2	0	4
3	S1	0	4
4	S2	0	4
5	S3	0	1
7	S8	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	1
22	D5	0	1
23	D4	0	2
25	AK	0	1
27	A8	0	1
28	BJ	0	2
29	AJ	0	1
30	S5	0	1
32	B3	0	4
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	44

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S8	119	CYS	CB-SG	-5.48	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S3	37	VAL	C-N-CA	10.35	147.57	121.70
22	D5	69	LEU	CA-CB-CG	7.42	132.37	115.30
13	A5	89	LEU	CA-CB-CG	7.13	131.69	115.30
37	B7	19	LEU	CA-CB-CG	6.66	130.61	115.30
22	D5	78	LEU	CA-CB-CG	6.58	130.44	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S1	213	TYR	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	152	PRO	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	3266	59	0
2	V2	1647	0	1657	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S1	5275	0	5300	84	0
4	S2	3414	0	3360	46	0
5	S3	1726	0	1675	30	0
6	S7	1247	0	1256	29	0
7	S8	1414	0	1371	22	0
8	V3	345	0	323	9	0
9	S6	737	0	710	7	0
10	S4	1024	0	1023	17	0
11	A9	2293	0	2326	43	0
12	A2	665	0	678	6	0
13	A5	901	0	936	9	0
14	A6	969	0	980	12	0
15	A7	757	0	771	10	0
16	AL	1201	0	1170	14	0
17	AA	645	0	649	6	0
17	AB	702	0	692	10	0
18	D3	728	0	773	14	0
19	D1	2415	0	2542	42	0
20	D6	1308	0	1329	20	0
21	4L	748	0	794	12	0
22	D5	4805	0	4950	82	0
23	D4	3646	0	3850	60	0
24	D2	2724	0	2930	49	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	17	0
27	A8	1404	0	1384	28	0
28	BJ	1441	0	1417	17	0
29	AJ	2583	0	2547	33	0
30	S5	822	0	820	13	0
31	A3	582	0	583	12	0
32	B3	578	0	570	4	0
33	C2	997	0	983	13	0
34	B4	1059	0	1062	8	0
35	AM	1143	0	1137	18	0
36	B6	815	0	837	18	0
37	B7	1026	0	995	14	0
38	B9	1515	0	1469	24	0
39	B2	563	0	509	3	0
40	B8	1324	0	1219	20	0
41	BK	853	0	800	12	0
42	C1	391	0	391	5	0
43	B1	449	0	453	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	A1	577	0	570	4	0
45	S1	16	0	0	1	0
45	S7	8	0	0	1	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	2	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	2	0
50	AA	34	0	40	0	0
50	AB	31	0	34	1	0
51	B8	38	0	50	1	0
51	D1	26	0	26	0	0
51	D4	40	0	54	2	0
52	D5	60	0	64	3	0
53	D4	28	0	30	0	0
All	All	65344	0	65610	791	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 791 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:S3:80:ALA:HA	5:S3:91:GLU:O	1.12	1.27
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.51	1.08
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.08	1.01
5:S3:38:GLN:HA	15:A7:70:SER:O	1.69	0.92
23:D4:52:PHE:O	23:D4:56:PHE:HB2	1.74	0.88

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%)	385 (90%)	43 (10%)	0	100	100
2	V2	210/217 (97%)	173 (82%)	37 (18%)	0	100	100
3	S1	686/704 (97%)	620 (90%)	65 (10%)	1 (0%)	48	82
4	S2	420/430 (98%)	379 (90%)	41 (10%)	0	100	100
5	S3	206/228 (90%)	182 (88%)	24 (12%)	0	100	100
6	S7	154/179 (86%)	139 (90%)	14 (9%)	1 (1%)	22	59
7	S8	174/176 (99%)	159 (91%)	15 (9%)	0	100	100
8	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
9	S6	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
10	S4	124/133 (93%)	116 (94%)	8 (6%)	0	100	100
11	A9	281/338 (83%)	249 (89%)	32 (11%)	0	100	100
12	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
13	A5	109/115 (95%)	97 (89%)	12 (11%)	0	100	100
14	A6	112/127 (88%)	103 (92%)	9 (8%)	0	100	100
15	A7	91/112 (81%)	75 (82%)	15 (16%)	1 (1%)	12	46
16	AL	142/145 (98%)	122 (86%)	20 (14%)	0	100	100
17	AA	78/88 (89%)	68 (87%)	10 (13%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	82 (95%)	4 (5%)	0	100	100
19	D1	299/318 (94%)	276 (92%)	23 (8%)	0	100	100
20	D6	167/175 (95%)	146 (87%)	20 (12%)	1 (1%)	22	59
21	4L	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	D5	604/606 (100%)	543 (90%)	61 (10%)	0	100	100
23	D4	457/459 (100%)	422 (92%)	34 (7%)	1 (0%)	44	77
24	D2	345/347 (99%)	324 (94%)	21 (6%)	0	100	100
25	AK	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
26	B5	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
27	A8	169/171 (99%)	146 (86%)	23 (14%)	0	100	100
28	BJ	169/175 (97%)	157 (93%)	12 (7%)	0	100	100
29	AJ	317/320 (99%)	283 (89%)	34 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	S5	97/105 (92%)	81 (84%)	16 (16%)	0	100 100
31	A3	72/83 (87%)	59 (82%)	13 (18%)	0	100 100
32	B3	71/97 (73%)	56 (79%)	14 (20%)	1 (1%)	9 40
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100 100
34	B4	126/128 (98%)	112 (89%)	14 (11%)	0	100 100
35	AM	137/143 (96%)	127 (93%)	10 (7%)	0	100 100
36	B6	92/127 (72%)	85 (92%)	7 (8%)	0	100 100
37	B7	117/136 (86%)	99 (85%)	18 (15%)	0	100 100
38	B9	174/178 (98%)	154 (88%)	20 (12%)	0	100 100
39	B2	63/72 (88%)	58 (92%)	5 (8%)	0	100 100
40	B8	155/158 (98%)	125 (81%)	30 (19%)	0	100 100
41	BK	100/125 (80%)	89 (89%)	11 (11%)	0	100 100
42	C1	44/49 (90%)	39 (89%)	5 (11%)	0	100 100
43	B1	50/57 (88%)	44 (88%)	6 (12%)	0	100 100
44	A1	68/70 (97%)	66 (97%)	2 (3%)	0	100 100
All	All	7979/8509 (94%)	7152 (90%)	821 (10%)	6 (0%)	50 82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	359	ARG
23	D4	54	LEU
6	S7	54	CYS
20	D6	138	GLU
15	A7	69	MET

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%)	341 (99%)	3 (1%)	75 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	V2	182/183 (100%)	180 (99%)	2 (1%)	70 80
3	S1	578/588 (98%)	576 (100%)	2 (0%)	91 92
4	S2	368/371 (99%)	365 (99%)	3 (1%)	79 84
5	S3	189/204 (93%)	189 (100%)	0	100 100
6	S7	132/150 (88%)	129 (98%)	3 (2%)	45 64
7	S8	151/151 (100%)	150 (99%)	1 (1%)	81 86
8	V3	40/68 (59%)	37 (92%)	3 (8%)	11 33
9	S6	79/80 (99%)	77 (98%)	2 (2%)	42 62
10	S4	113/119 (95%)	112 (99%)	1 (1%)	75 83
11	A9	246/292 (84%)	242 (98%)	4 (2%)	58 74
12	A2	73/81 (90%)	72 (99%)	1 (1%)	62 76
13	A5	99/101 (98%)	99 (100%)	0	100 100
14	A6	107/113 (95%)	107 (100%)	0	100 100
15	A7	83/94 (88%)	83 (100%)	0	100 100
16	AL	130/131 (99%)	126 (97%)	4 (3%)	35 56
17	AA	74/81 (91%)	74 (100%)	0	100 100
17	AB	80/81 (99%)	78 (98%)	2 (2%)	42 62
18	D3	81/103 (79%)	80 (99%)	1 (1%)	67 79
19	D1	266/278 (96%)	263 (99%)	3 (1%)	70 80
20	D6	140/144 (97%)	138 (99%)	2 (1%)	62 76
21	4L	87/87 (100%)	85 (98%)	2 (2%)	45 64
22	D5	539/539 (100%)	535 (99%)	4 (1%)	81 86
23	D4	412/412 (100%)	407 (99%)	5 (1%)	67 79
24	D2	315/315 (100%)	311 (99%)	4 (1%)	65 77
25	AK	101/101 (100%)	100 (99%)	1 (1%)	73 81
26	B5	122/125 (98%)	121 (99%)	1 (1%)	79 84
27	A8	154/154 (100%)	150 (97%)	4 (3%)	41 61
28	BJ	155/157 (99%)	155 (100%)	0	100 100
29	AJ	283/284 (100%)	282 (100%)	1 (0%)	89 91
30	S5	88/94 (94%)	88 (100%)	0	100 100
31	A3	65/71 (92%)	65 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	B3	55/75 (73%)	53 (96%)	2 (4%)	30 53
33	C2	106/107 (99%)	106 (100%)	0	100 100
34	B4	114/114 (100%)	113 (99%)	1 (1%)	75 83
35	AM	119/121 (98%)	115 (97%)	4 (3%)	32 54
36	B6	92/121 (76%)	91 (99%)	1 (1%)	70 80
37	B7	108/119 (91%)	104 (96%)	4 (4%)	29 52
38	B9	159/160 (99%)	157 (99%)	2 (1%)	65 77
39	B2	59/62 (95%)	59 (100%)	0	100 100
40	B8	142/142 (100%)	139 (98%)	3 (2%)	48 66
41	BK	93/112 (83%)	91 (98%)	2 (2%)	47 65
42	C1	42/44 (96%)	42 (100%)	0	100 100
43	B1	48/53 (91%)	48 (100%)	0	100 100
44	A1	59/59 (100%)	56 (95%)	3 (5%)	20 43
All	All	7072/7395 (96%)	6991 (99%)	81 (1%)	69 80

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	A8	150	ASN
38	B9	44	ARG
32	B3	47	ASN
35	AM	89	ASN
40	B8	137	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
26	B5	143	ASN
29	AJ	204	ASN
17	AB	47	GLN
28	BJ	122	GLN
31	A3	51	ASN

5.3.3 RNA

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	SF4	S1	801	3	0,12,12	-	-	-		
51	3PE	B8	201	-	37,37,50	0.35	0	40,42,55	0.34	0
53	PC1	D4	502	-	27,27,53	0.39	0	33,35,61	0.38	0
50	ZMP	AB	101	17	24,30,36	0.82	1 (4%)	29,37,45	0.95	1 (3%)
51	3PE	D1	501	-	25,25,50	0.39	0	28,30,55	0.37	0
52	CDL	D5	901	-	59,59,99	0.39	0	65,71,111	0.54	1 (1%)
45	SF4	S8	201	7	0,12,12	-	-	-		
49	NDP	A9	401	-	45,52,52	0.58	0	53,80,80	0.64	1 (1%)
47	FES	S1	803	3	0,4,4	-	-	-		
45	SF4	V1	500	1	0,12,12	-	-	-		
45	SF4	S8	202	7	0,12,12	-	-	-		
45	SF4	S1	802	3	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.28	0	48,50,50	0.45	0
47	FES	V2	300	2	0,4,4	-	-	-		
50	ZMP	AA	101	17	27,33,36	0.70	1 (3%)	32,40,45	1.09	3 (9%)
51	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.32	0
45	SF4	S7	300	6	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
45	SF4	S1	801	3	-	-	0/6/5/5
51	3PE	B8	201	-	-	11/41/41/54	-
53	PC1	D4	502	-	-	14/31/31/57	-
50	ZMP	AB	101	17	-	8/35/37/43	-
51	3PE	D1	501	-	-	4/28/28/54	-
52	CDL	D5	901	-	-	18/70/70/110	-
49	NDP	A9	401	-	-	14/30/77/77	0/5/5/5
45	SF4	S8	201	7	-	-	0/6/5/5
51	3PE	D4	501	-	-	7/43/43/54	-
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
45	SF4	V1	500	1	-	-	0/6/5/5
50	ZMP	AA	101	17	-	6/38/40/43	-
45	SF4	S1	802	3	-	-	0/6/5/5
45	SF4	S8	202	7	-	-	0/6/5/5
47	FES	V2	300	2	-	-	0/1/1/1
47	FES	S1	803	3	-	-	0/1/1/1
45	SF4	S7	300	6	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.85	1.53	1.50
50	AA	101	ZMP	C9-C10	2.37	1.53	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	AB	101	ZMP	O1-C10-C9	-2.59	120.93	123.99
50	AA	101	ZMP	C11-C12-N1	-2.42	107.33	112.42
50	AA	101	ZMP	O1-C10-C9	-2.38	121.18	123.99
52	D5	901	CDL	CB4-OB6-CB5	2.34	123.55	117.79
49	A9	401	NDP	C5A-C6A-N6A	2.33	123.89	120.35

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	O3'-C3'-C4'-O4'

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

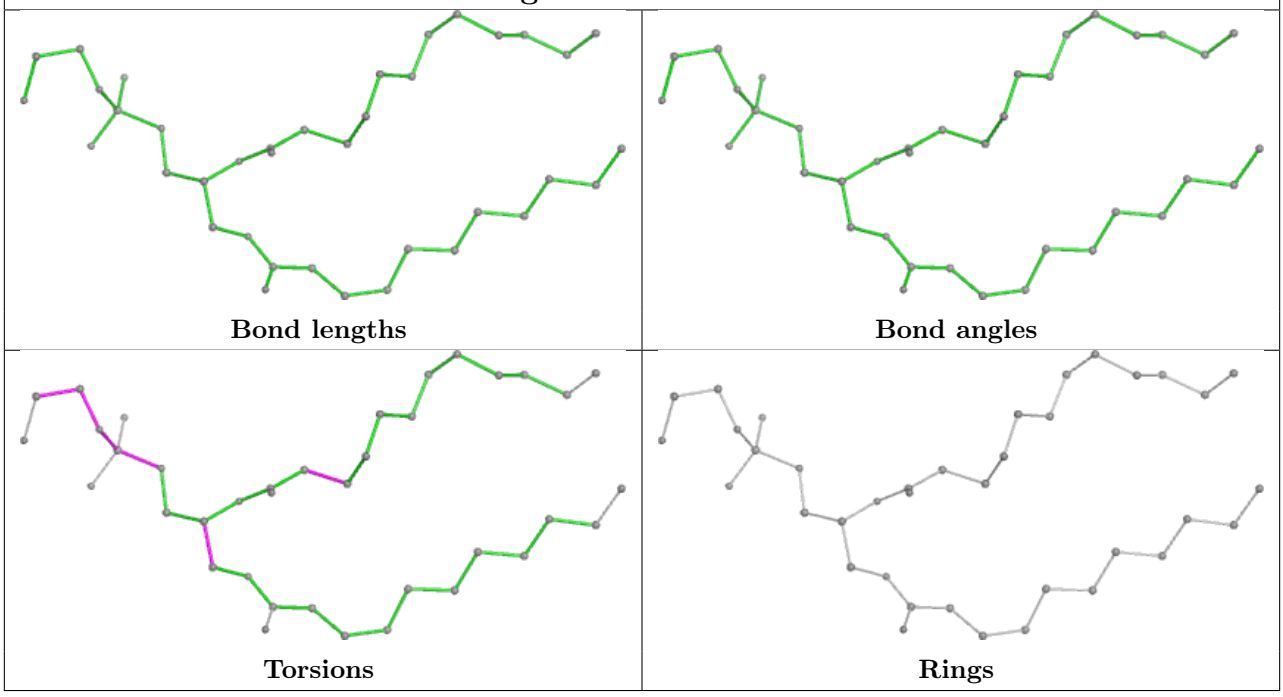
There are no ring outliers.

9 monomers are involved in 14 short contacts:

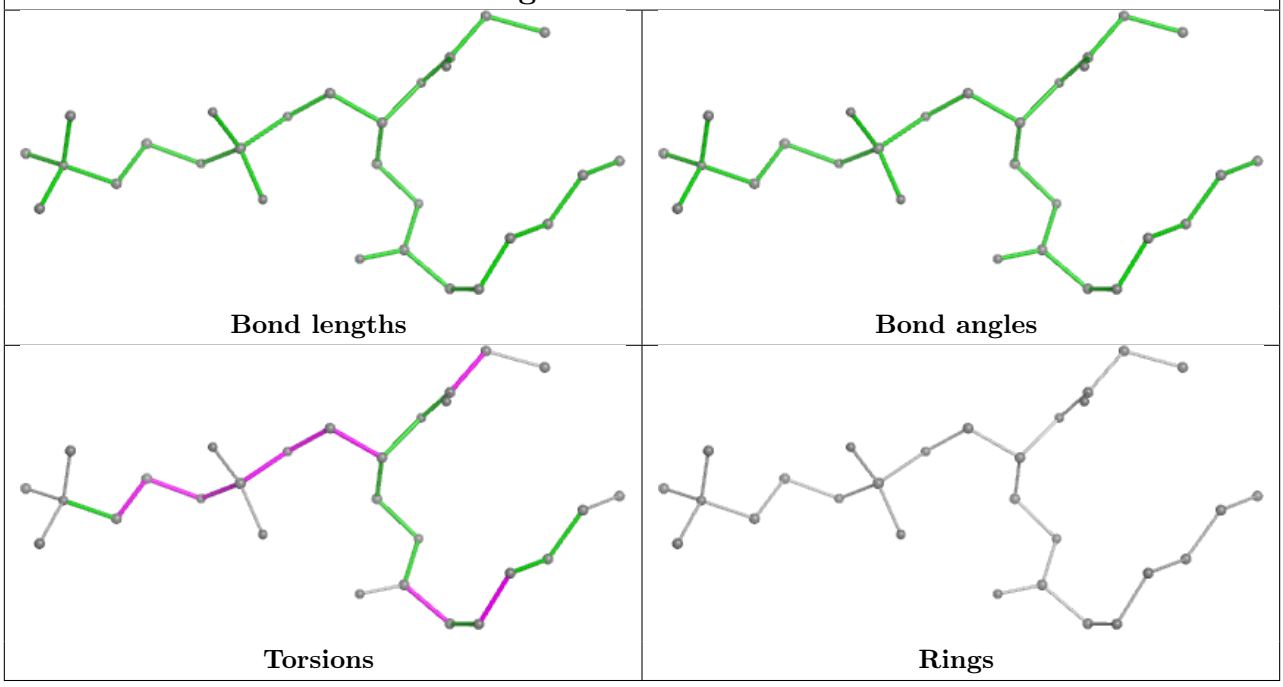
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	S1	801	SF4	1	0
51	B8	201	3PE	1	0
50	AB	101	ZMP	1	0
52	D5	901	CDL	3	0
49	A9	401	NDP	2	0
45	V1	500	SF4	1	0
46	V1	501	FMN	2	0
51	D4	501	3PE	2	0
45	S7	300	SF4	1	0

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.

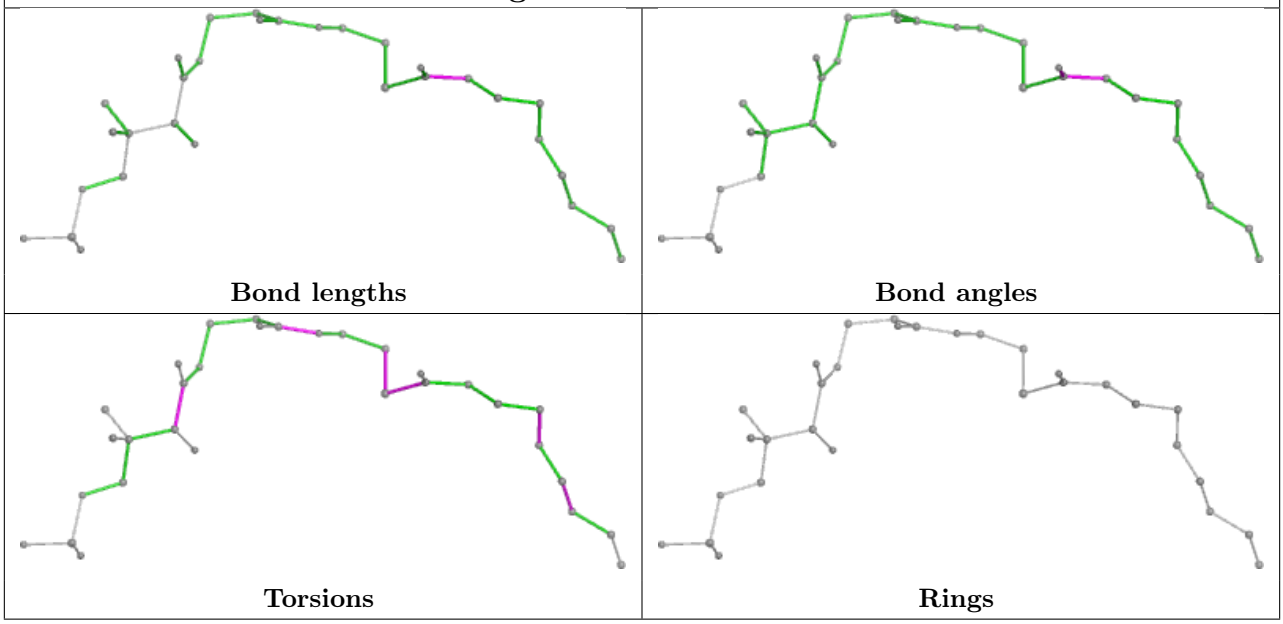
Ligand 3PE B8 201



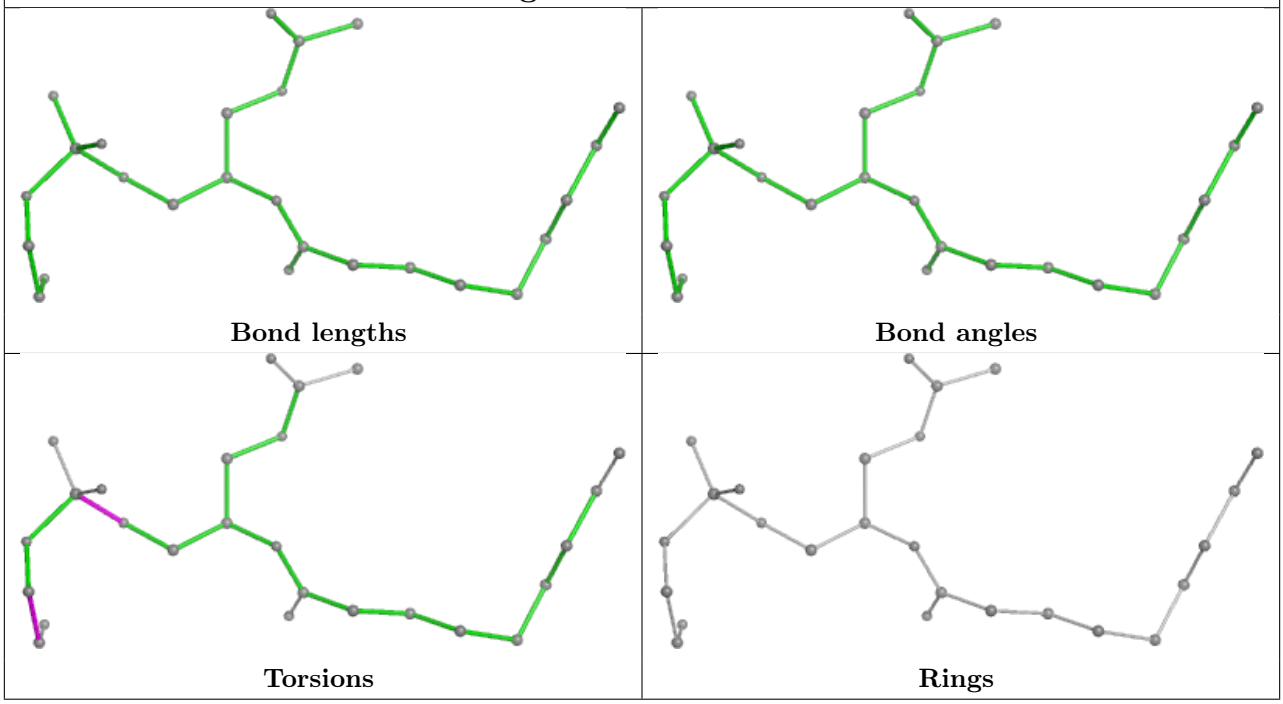
Ligand PC1 D4 502



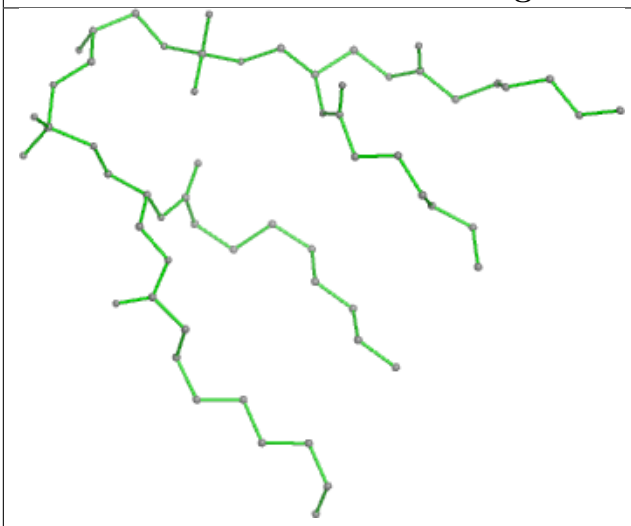
Ligand ZMP AB 101



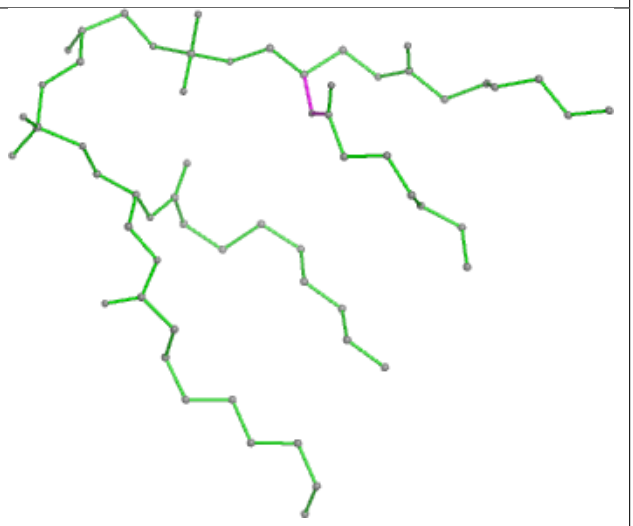
Ligand 3PE D1 501



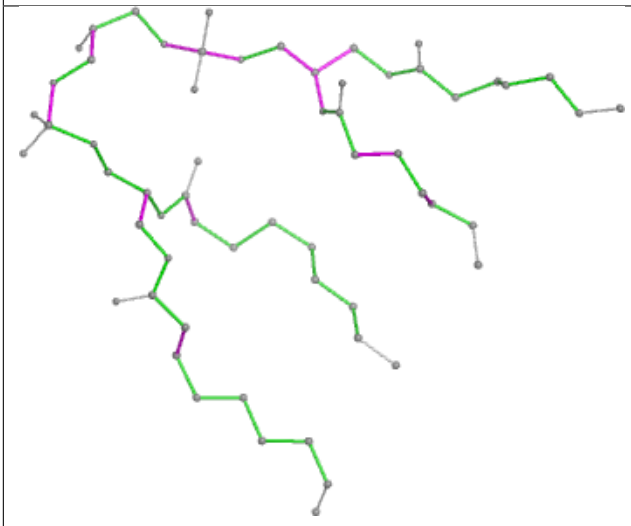
Ligand CDL D5 901



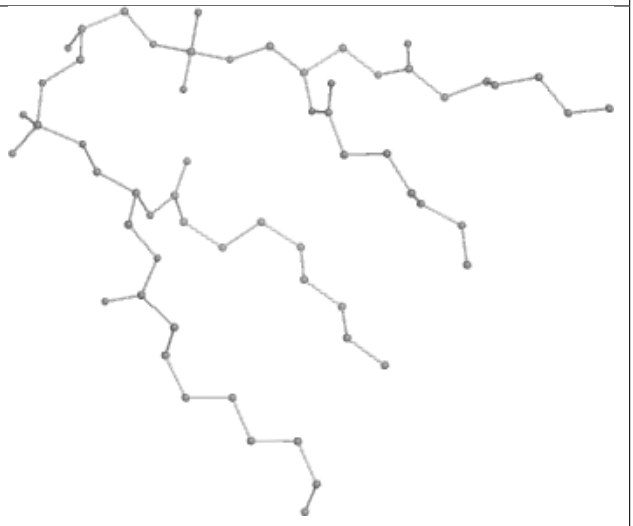
Bond lengths



Bond angles

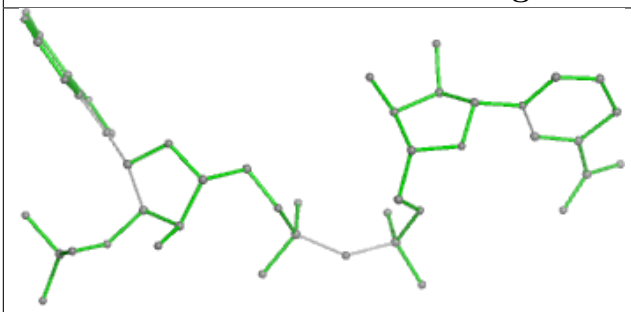


Torsions

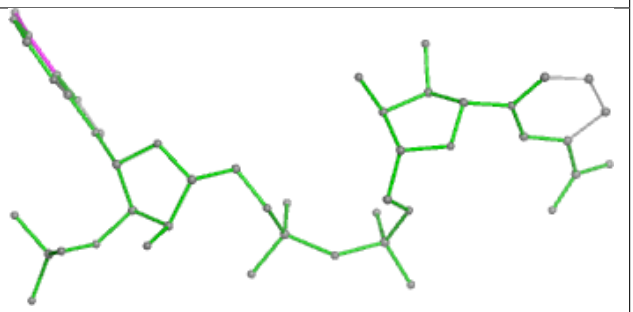


Rings

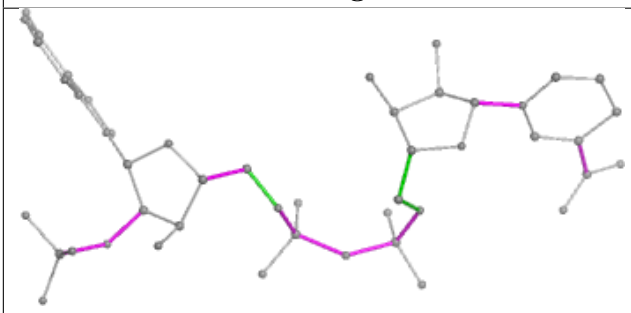
Ligand NDP A9 401



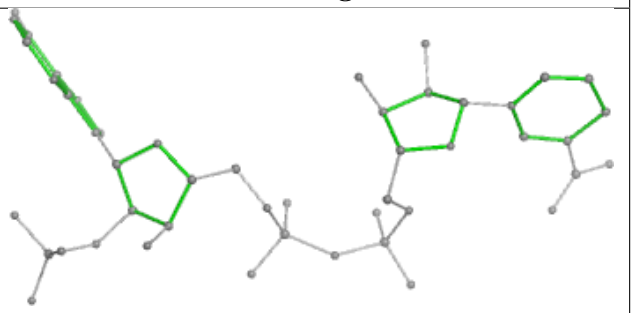
Bond lengths



Bond angles

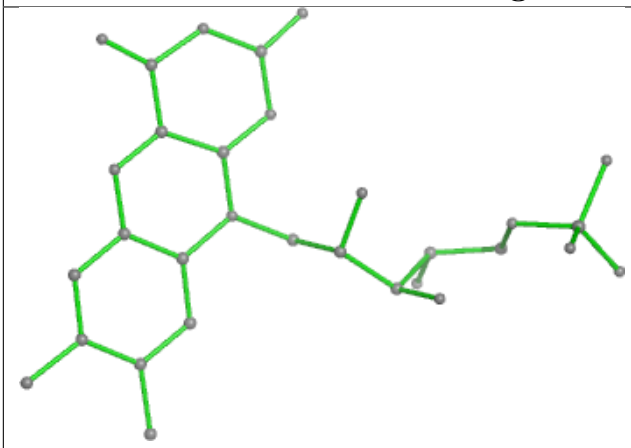


Torsions

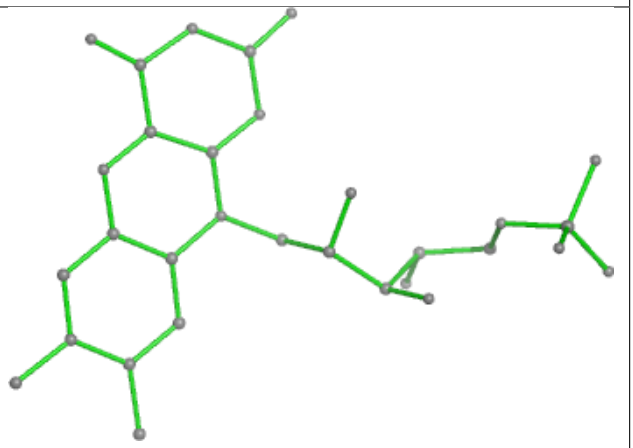


Rings

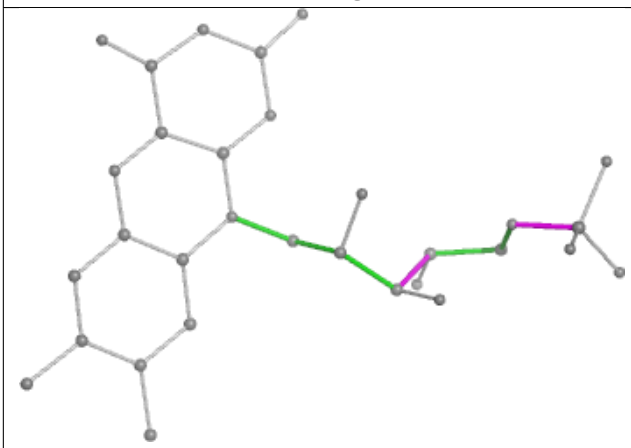
Ligand FMN V1 501



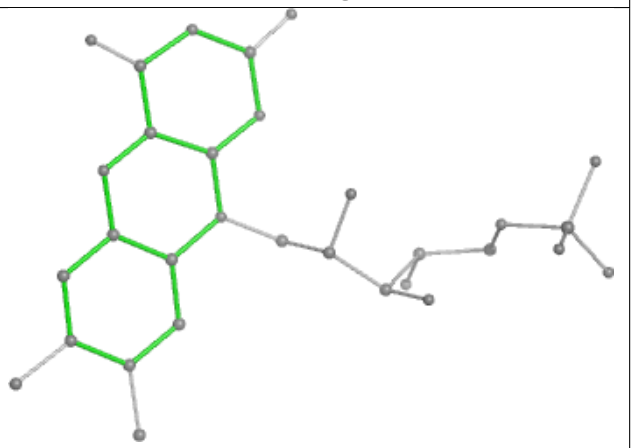
Bond lengths



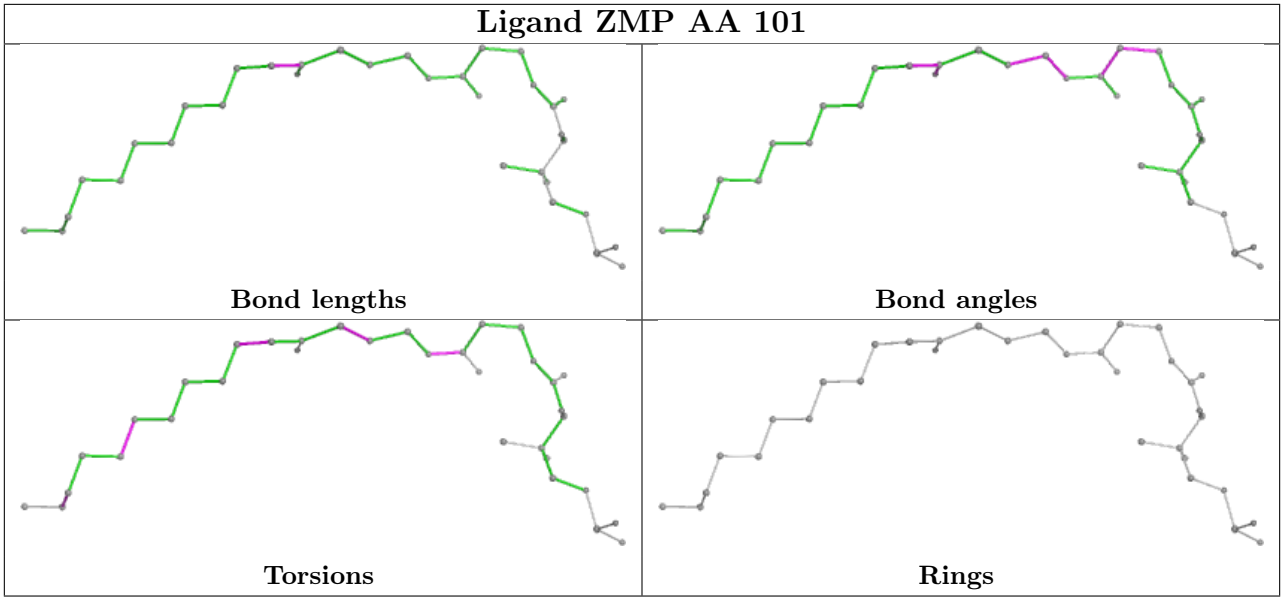
Bond angles

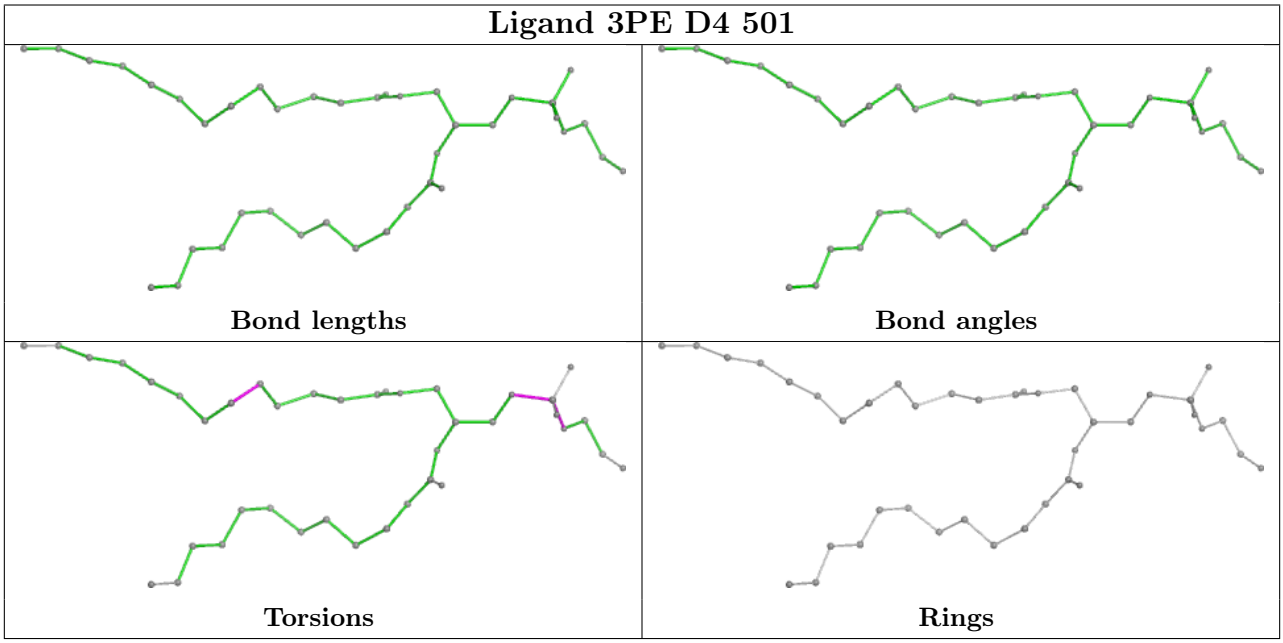


Torsions



Rings





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.

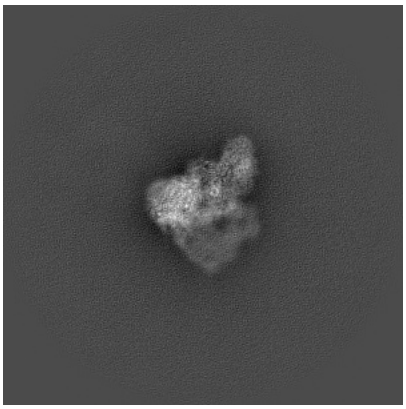
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4498. These allow visual inspection of the internal detail of the map and identification of artifacts.

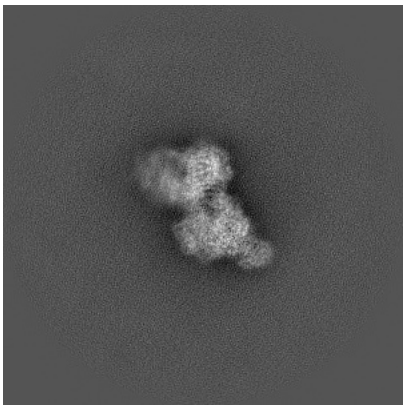
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

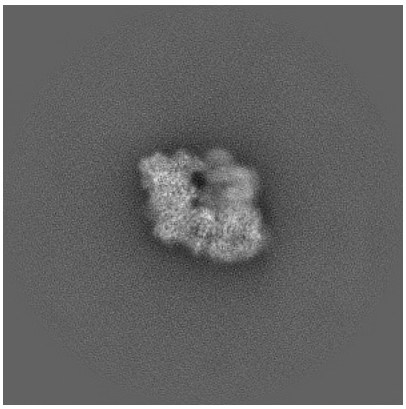
6.1.1 Primary map



X

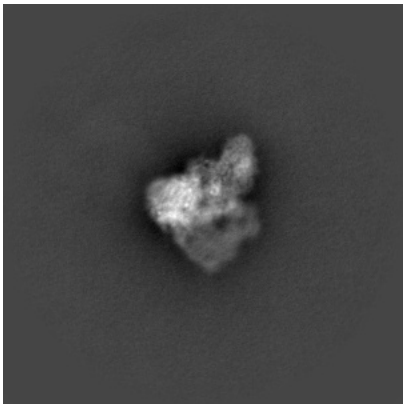


Y

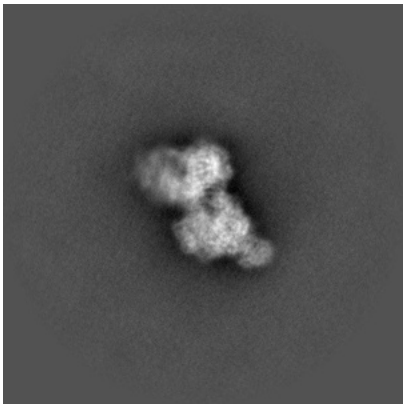


Z

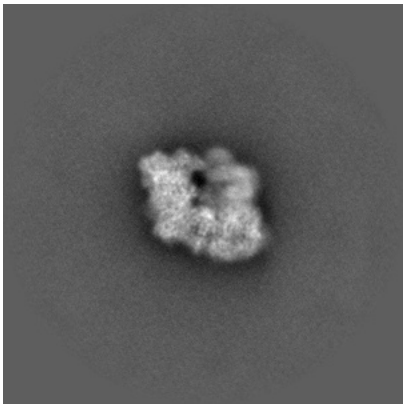
6.1.2 Raw map



X



Y

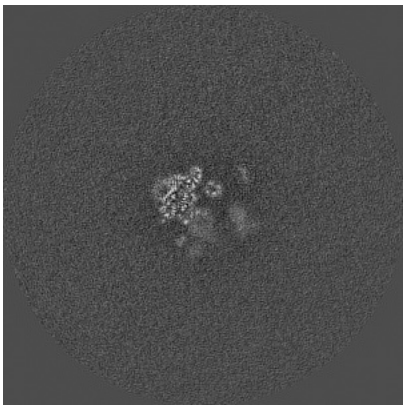


Z

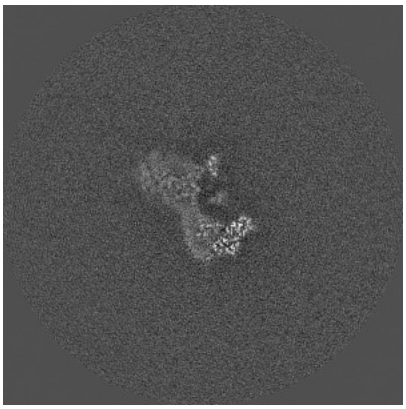
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256



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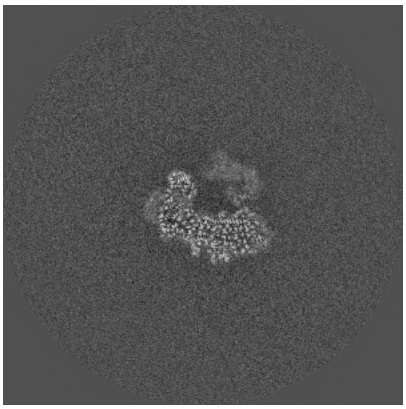

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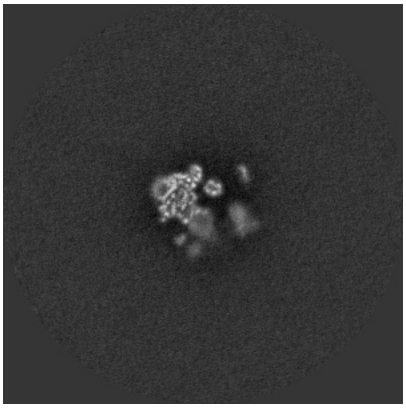
6.2.2 Raw map



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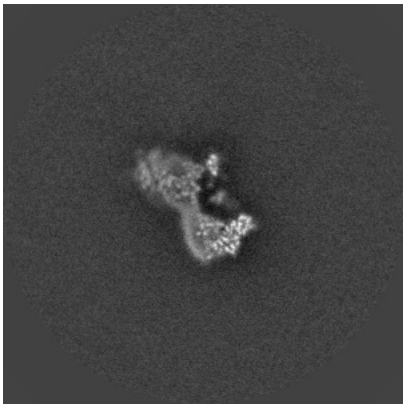

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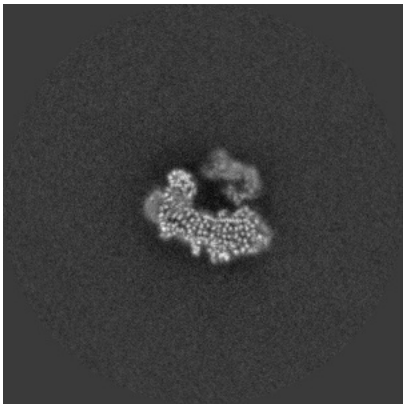
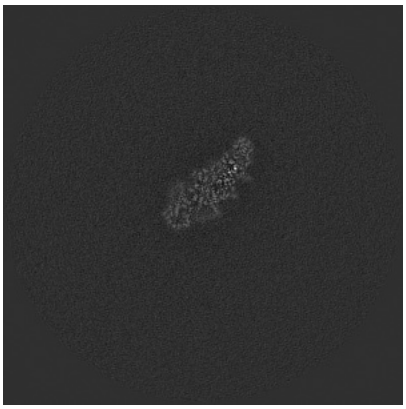


Z Index: 256

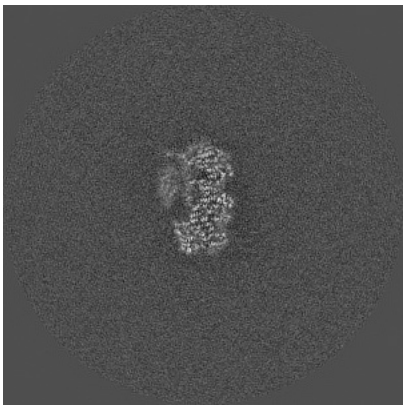
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

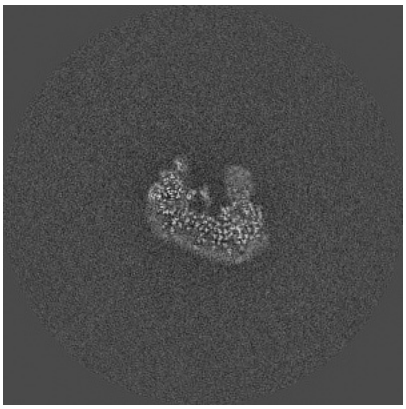
6.3.1 Primary map



X Index: 207

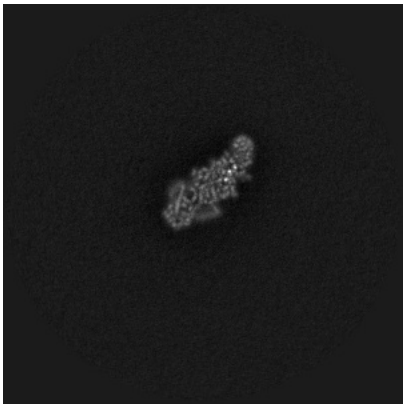


Y Index: 228

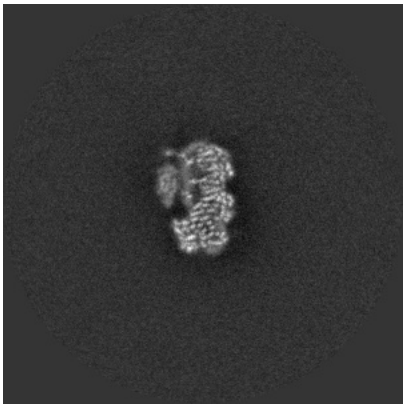


Z Index: 269

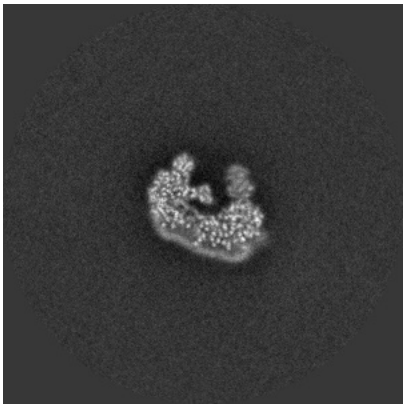
6.3.2 Raw map



X Index: 206



Y Index: 229

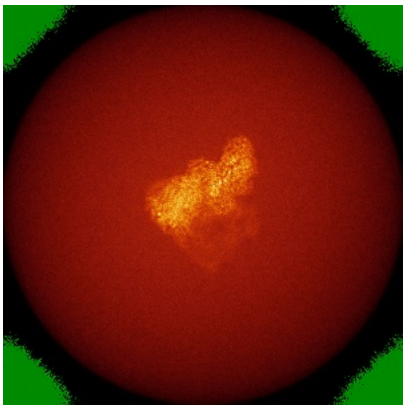


Z Index: 273

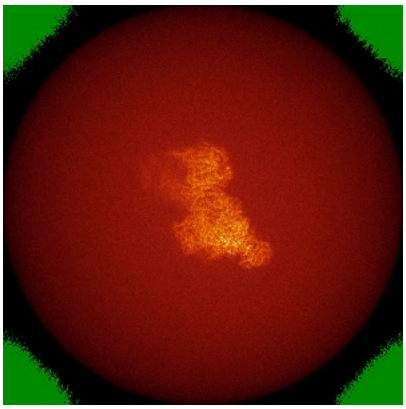
The images above show the largest variance slices of the map in three orthogonal directions.

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

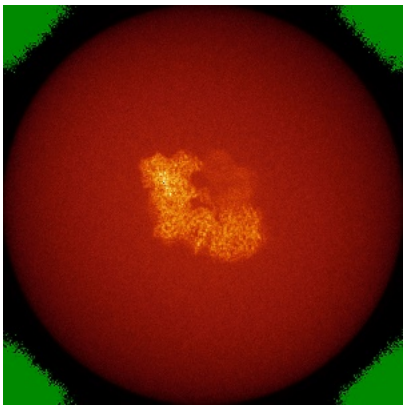
6.4.1 Primary map



X

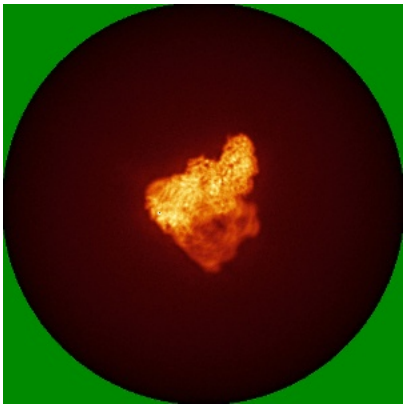


Y

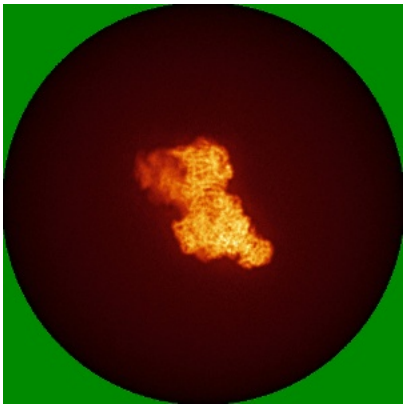


Z

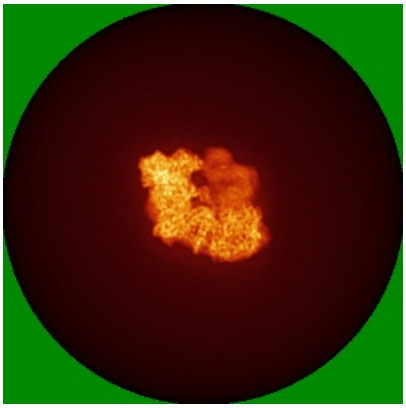
6.4.2 Raw map



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 0.15. 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.

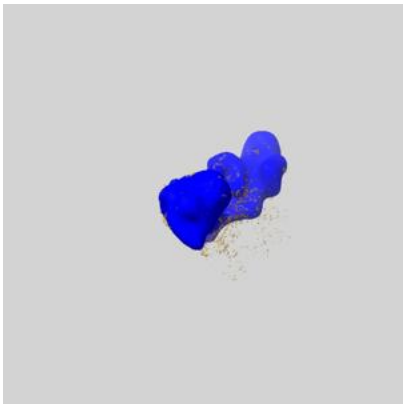
6.6 Mask visualisation (i)

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

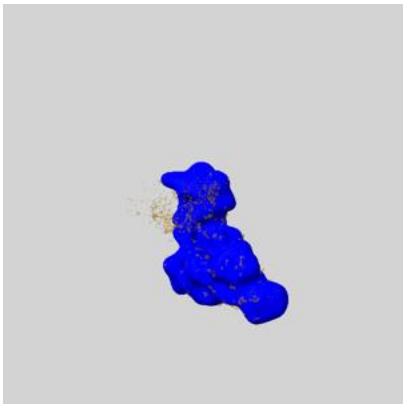
A mask typically either:

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

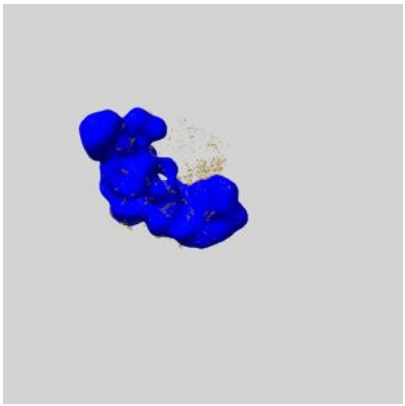
6.6.1 emd_4498_msk_1.map (i)



X



Y

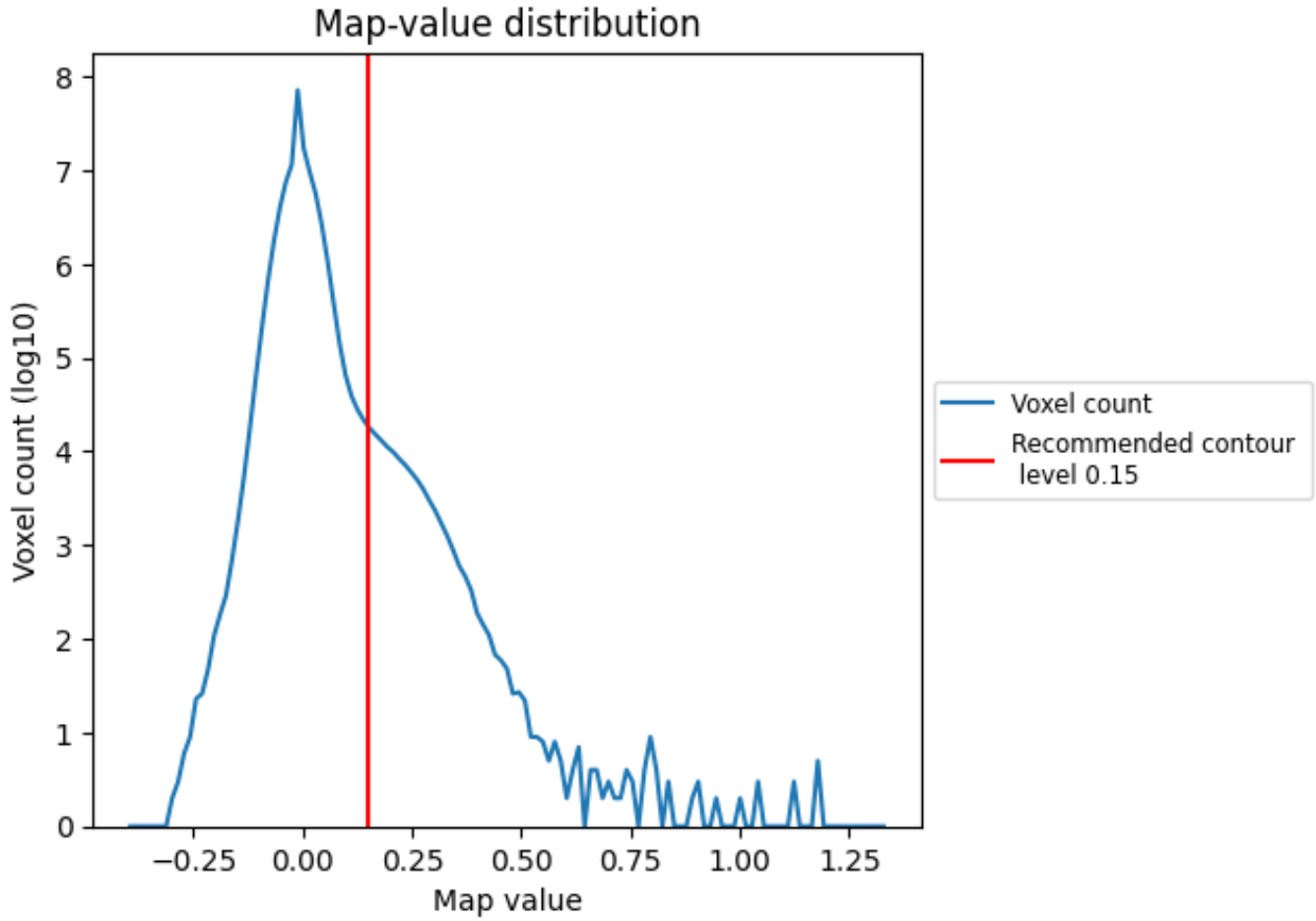


Z

7 Map analysis

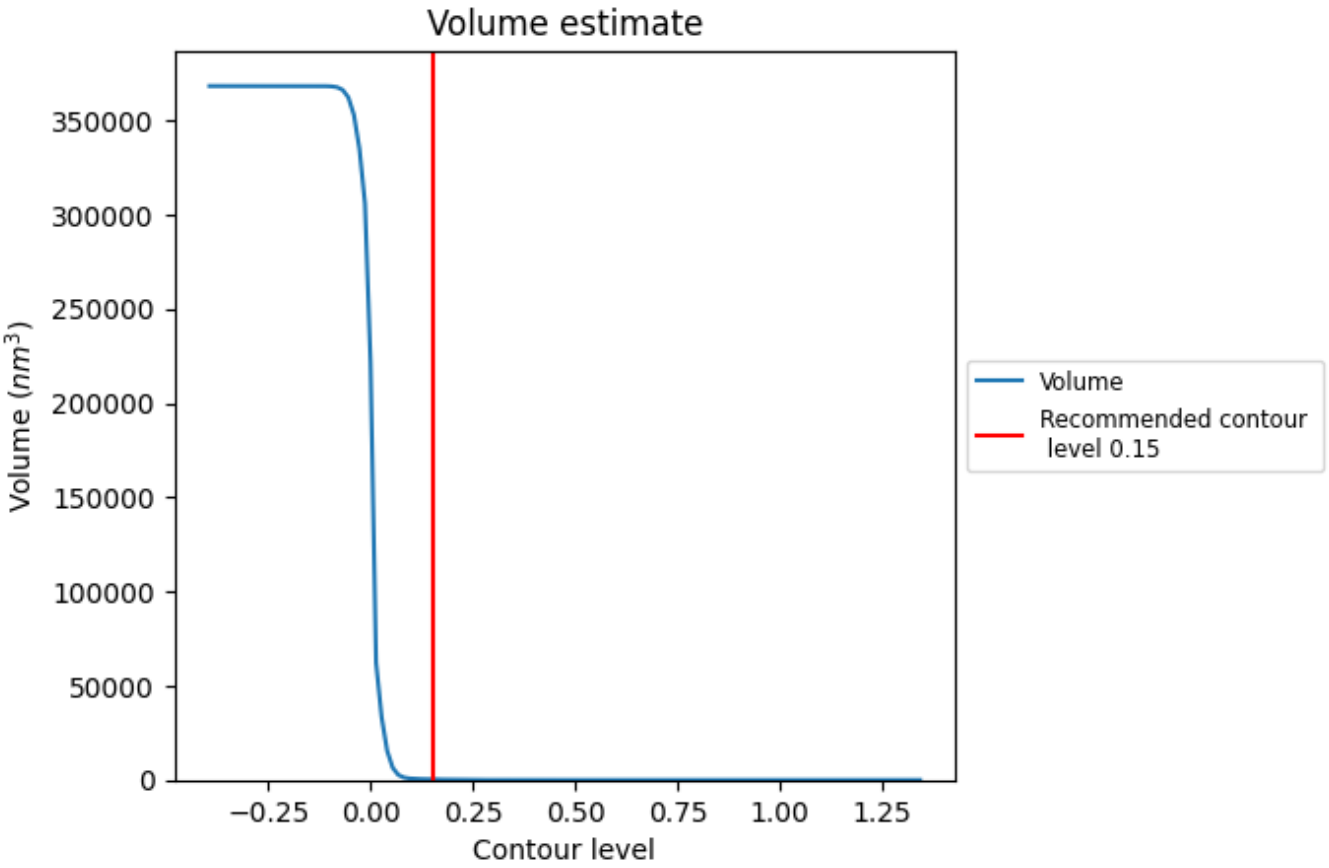
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

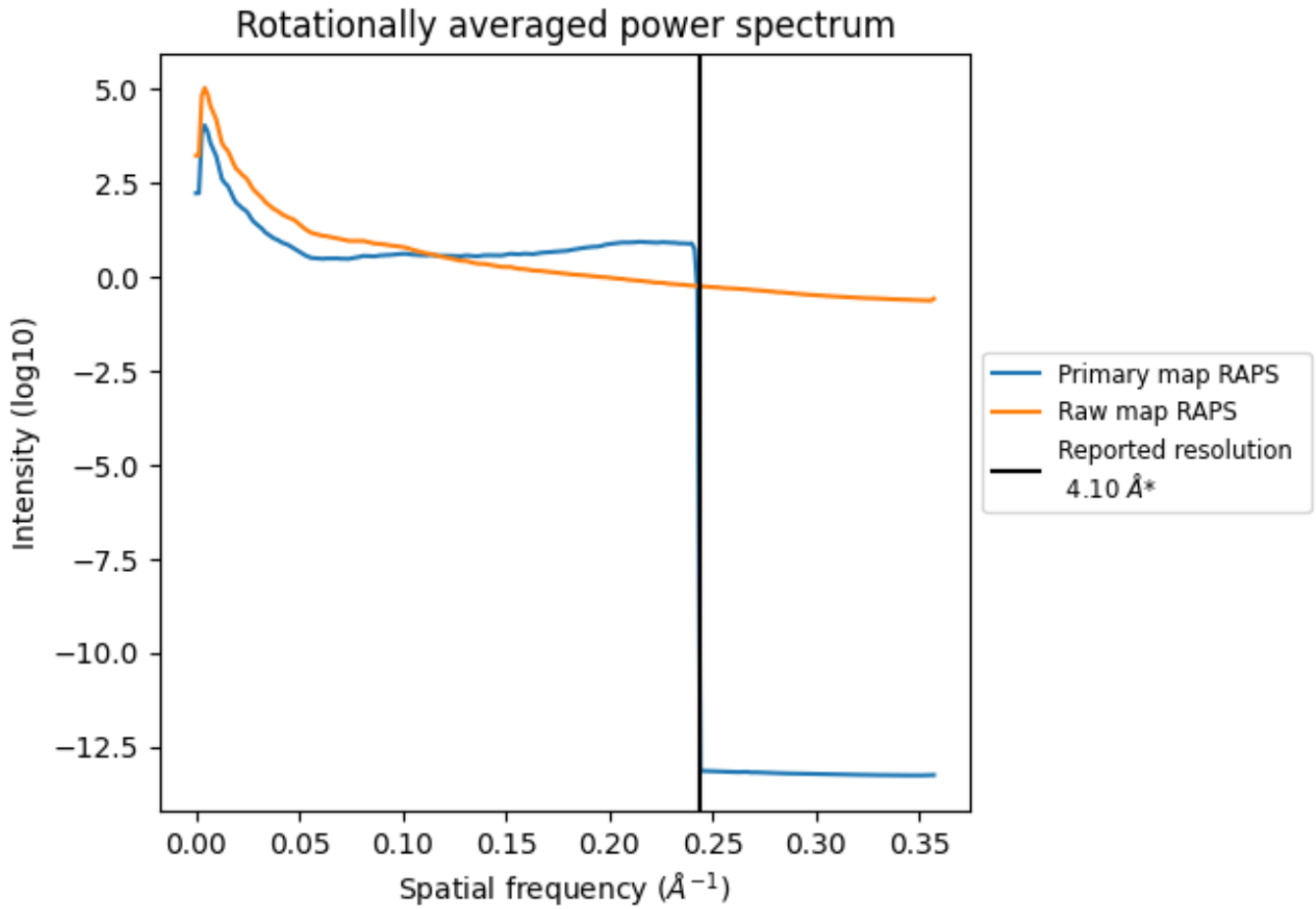
7.2 Volume estimate (i)



The volume at the recommended contour level is 311 nm^3; this corresponds to an approximate mass of 281 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)

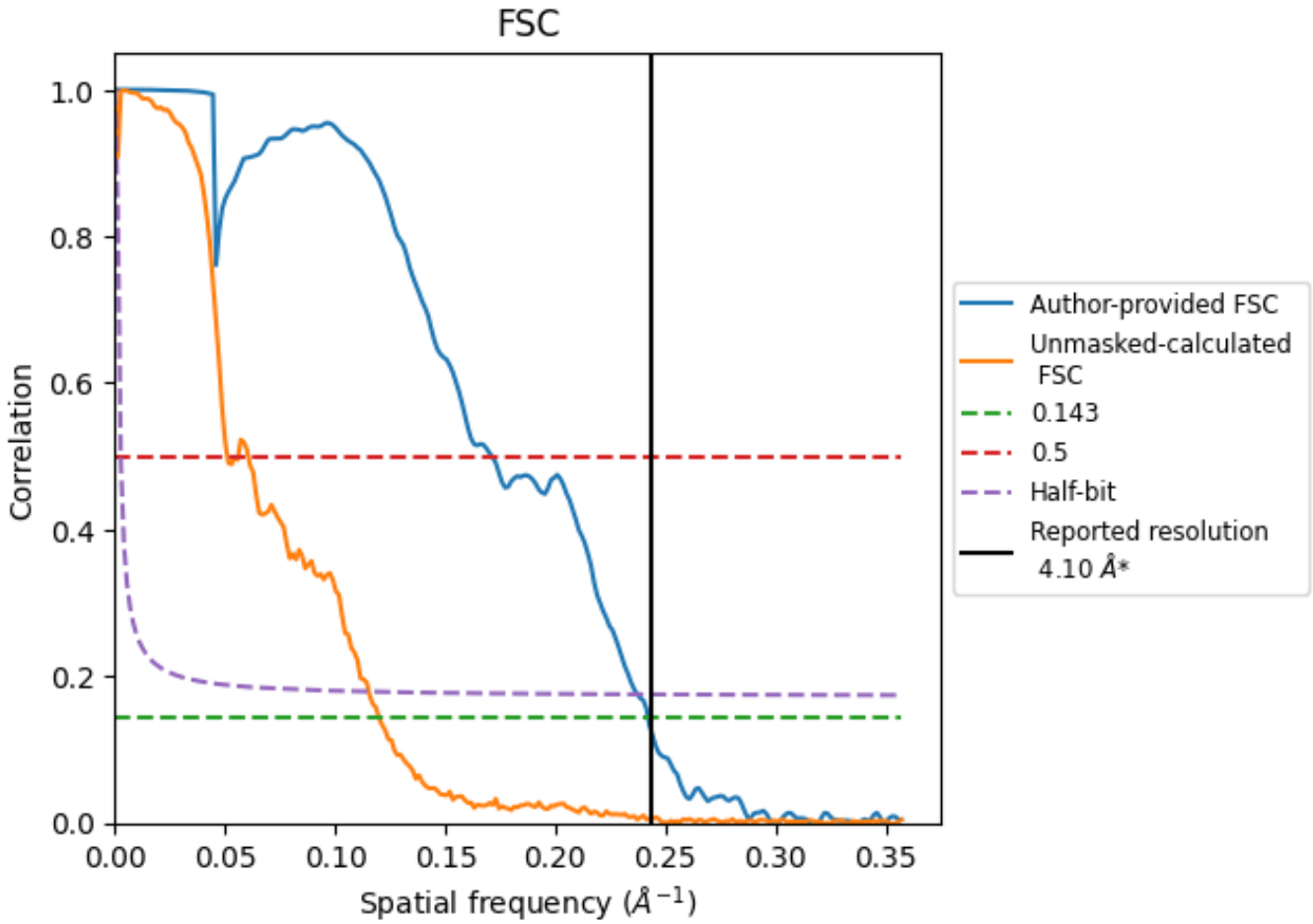


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

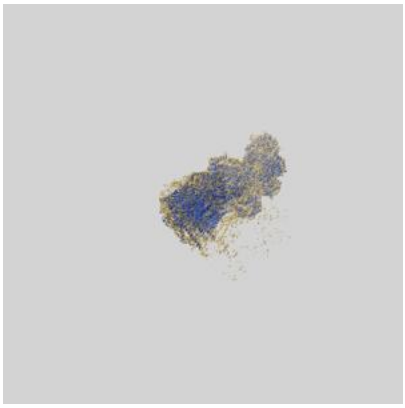
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.13	5.84	4.22
Unmasked-calculated*	8.34	19.53	8.67

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

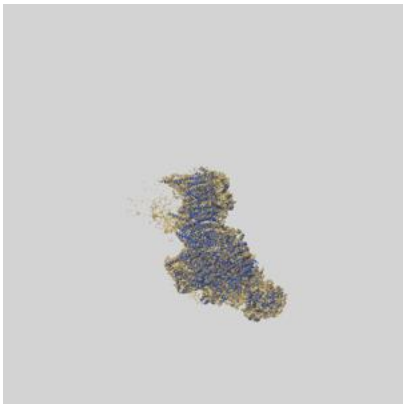
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4498 and PDB model 6QC6. Per-residue inclusion information can be found in section 3 on page 17.

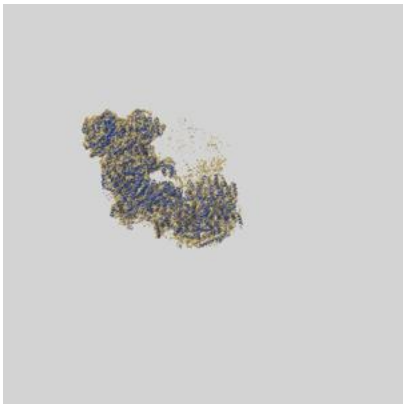
9.1 Map-model overlay



X



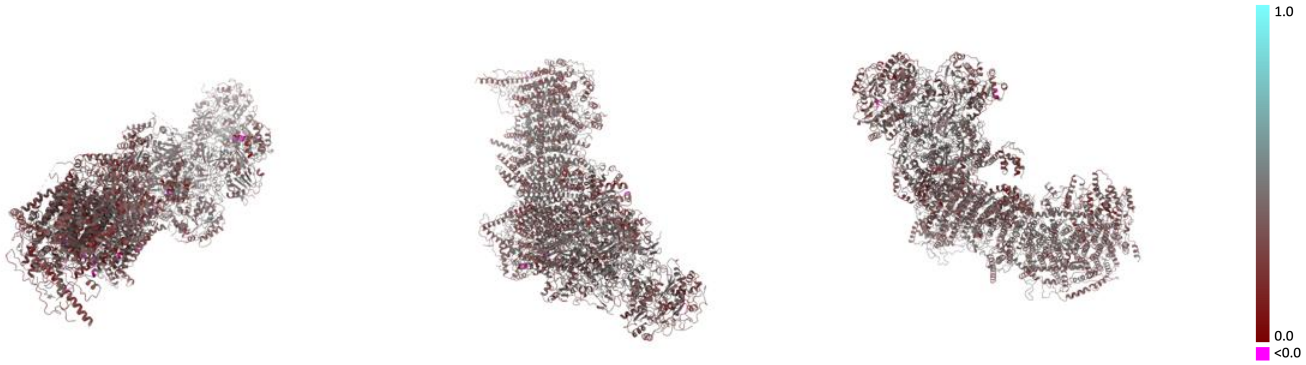
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

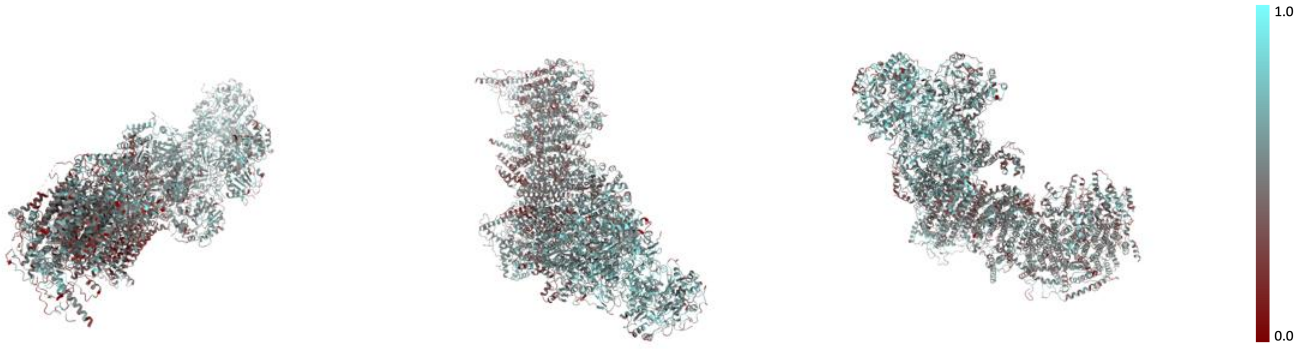
9.2 Q-score mapped to coordinate model (i)



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.

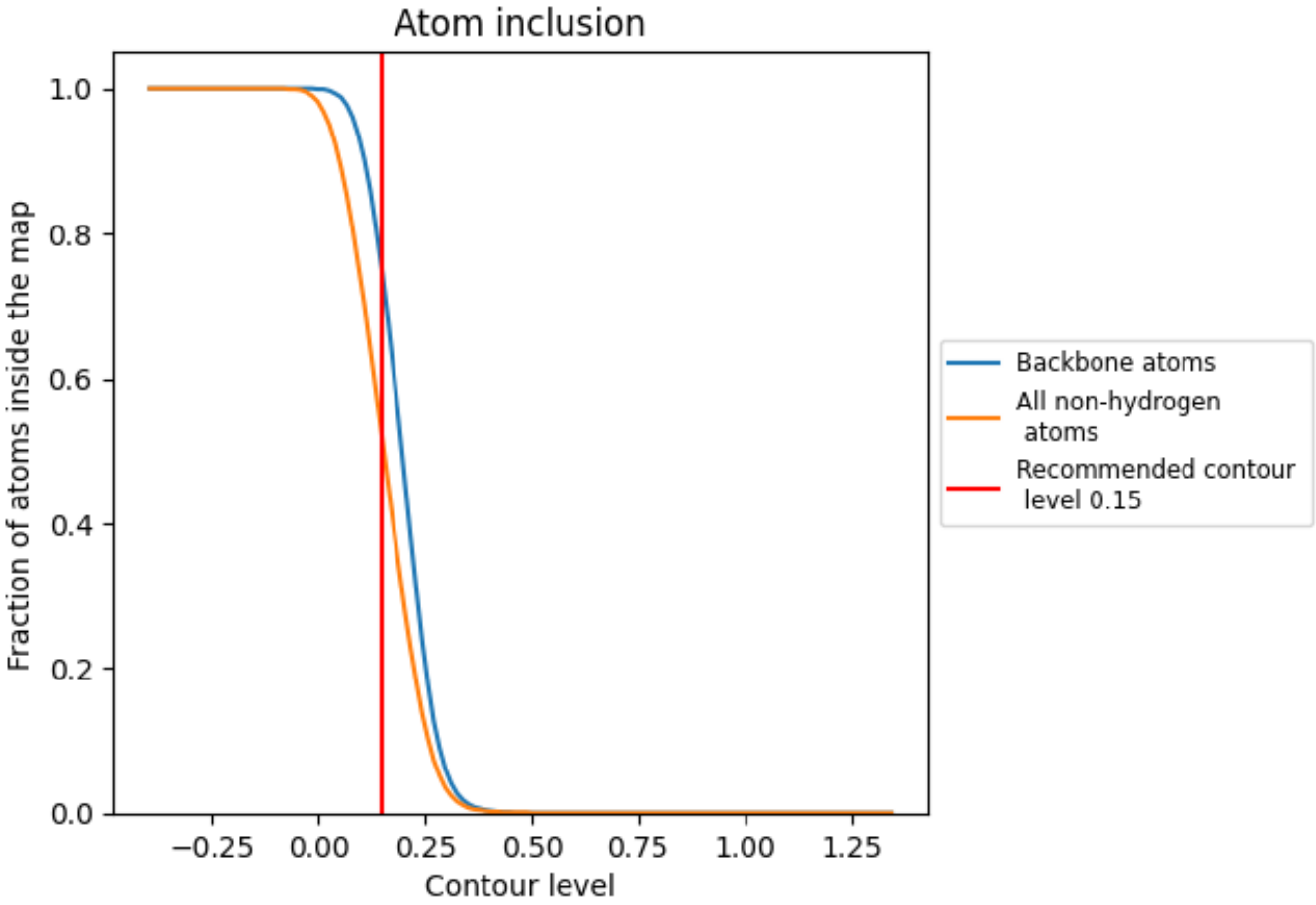
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5130	0.3620
4L	0.4300	0.3560
A1	0.5430	0.3540
A2	0.5490	0.3280
A3	0.5230	0.3750
A5	0.5650	0.3640
A6	0.5360	0.3820
A7	0.4710	0.3660
A8	0.5420	0.3510
A9	0.5290	0.3660
AA	0.4330	0.3060
AB	0.4370	0.3220
AJ	0.4940	0.3560
AK	0.3480	0.3320
AL	0.4830	0.3690
AM	0.5390	0.3480
B1	0.4360	0.3480
B2	0.4400	0.3020
B3	0.4150	0.3350
B4	0.4570	0.3470
B5	0.5260	0.3650
B6	0.4570	0.3320
B7	0.4560	0.2950
B8	0.4560	0.3490
B9	0.5180	0.3340
BJ	0.5220	0.3430
BK	0.4390	0.3520
C1	0.4790	0.3450
C2	0.4970	0.3830
D1	0.4810	0.3630
D2	0.4920	0.3770
D3	0.4360	0.3480
D4	0.4860	0.3800
D5	0.4510	0.3480
D6	0.3630	0.3400

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Chain	Atom inclusion	Q-score
S1	0.5870	0.3840
S2	0.5530	0.3810
S3	0.5990	0.4040
S4	0.5520	0.4020
S5	0.5280	0.3610
S6	0.5780	0.3930
S7	0.5960	0.3930
S8	0.6320	0.3950
V1	0.5950	0.3530
V2	0.5830	0.3570
V3	0.5590	0.3500