



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 06:45 PM JST

PDB ID : 7EU3
EMDB ID : EMD-31307
Title : Chloroplast NDH complex
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2021-05-15
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

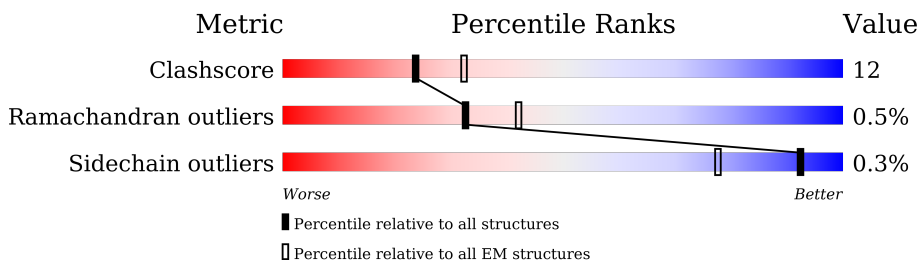
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	346	 10% 67% 23%
2	B	483	 77% 22%
3	C	117	 9% 77% 21%
4	D	499	 76% 24%
5	E	100	 77% 23%
6	F	777	 66% 20% 14%
7	G	176	 80% 20%
8	H	383	 39% 60% 40%

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Mol	Chain	Length	Quality of chain
9	I	165	30% 78% 22%
10	J	159	45% 63% 37%
11	K	245	25% 52% 27% 21%
12	L	192	23% 17% 18% 64%
13	M	213	19% 38% 15% 47%
14	N	233	17% 42% 20% 38%
15	T	61	93% 7%
16	1	154	69% 28% 2%
17	2	216	52% 8% 40%
18	3	227	46% 13% 41%
19	4	130	78% 22%
20	5	243	56% 14% 29%
21	6	469	51% 22% 27%
22	7	361	56% 30% 12%
23	8	119	71% 26% 3%
24	9	83	71% 28% 1%
25	0	155	85% 11% 4%

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 40775 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 NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	346	2608	1744	393	463	8	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	478	3646	2400	557	665	24	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	116	841	575	124	140	2	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	499	3874	2614	598	639	23	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	100	750	486	127	135	2	0	0

- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	671	5124	3425	796	882	21	0	0

- Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	176	1260	841	194	220	5	0	0

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	383	2991	1944	493	543	11	0	0

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	165	1229	772	214	231	12	0	0

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	159	1258	808	213	233	4	0	0

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	194	1474	932	250	282	10	0	0

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	69	572	399	89	81	3	0	0

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	112	876	558	150	162	6	0	0

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	145	1154	751	203	198	2	0	0

- Molecule 15 is a protein called Unidentified stromal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	T	61	305	183	61	61	0	0

- Molecule 16 is a protein called Photosynthetic NDH subunit of subcomplex L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	1	150	1185	752	206	227	0	0

- Molecule 17 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	2	129	915	580	156	175	4	0	0

- Molecule 18 is a protein called Photosynthetic NDH subunit of subcomplex L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	3	134	989	634	164	187	4	0	0

- Molecule 19 is a protein called Photosynthetic NDH subunit of subcomplex L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	4	130	878	553	153	163	9	0	0

- Molecule 20 is a protein called Photosynthetic NDH subunit of subcomplex L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	5	172	1289	812	229	241	7	0	0

- Molecule 21 is a protein called Photosynthetic NDH subunit of subcomplex B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	6	343	2541	1617	435	474	15	0	0

- Molecule 22 is a protein called Photosynthetic NDH subunit of subcomplex B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	7	317	2311	1444	409	448	10	0	0

- Molecule 23 is a protein called Photosynthetic NDH subunit of subcomplex B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	8	119	828	523	151	147	7	0	0

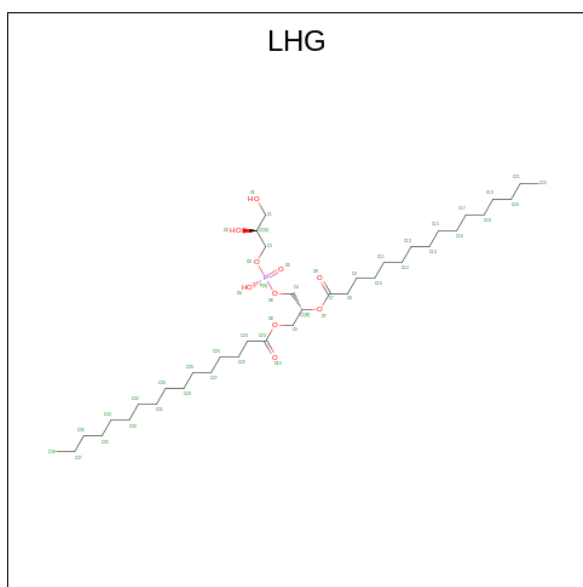
- Molecule 24 is a protein called Photosynthetic NDH subunit of subcomplex B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	9	82	617	395	101	118	3	0	0

- Molecule 25 is a protein called Photosynthetic NDH subunit of subcomplex B5.

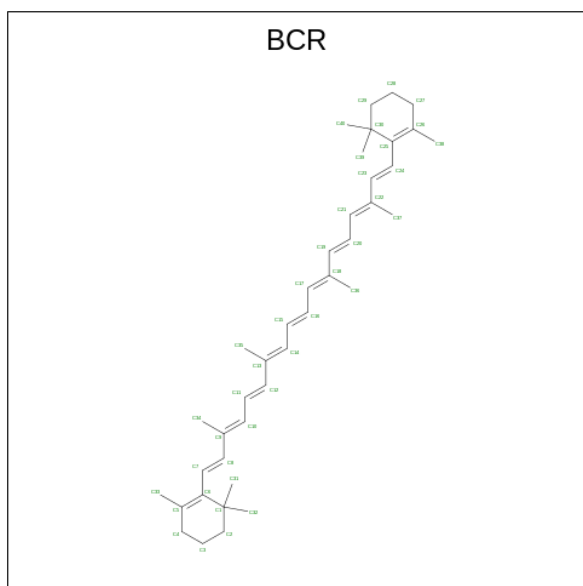
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	149	1089	704	175	204	6	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



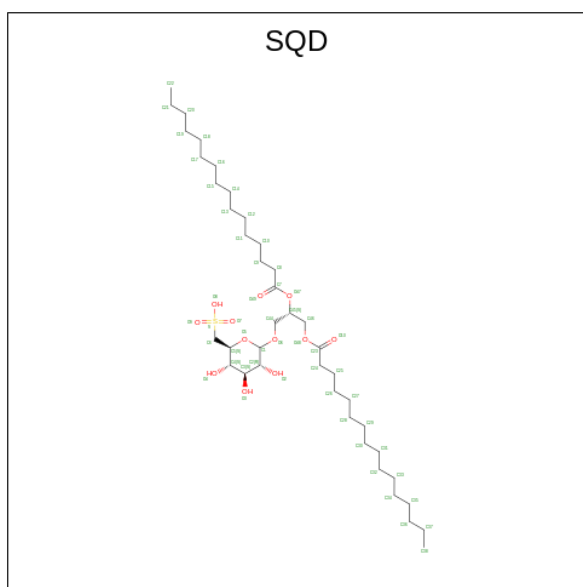
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	D	1	24	15	8	1	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



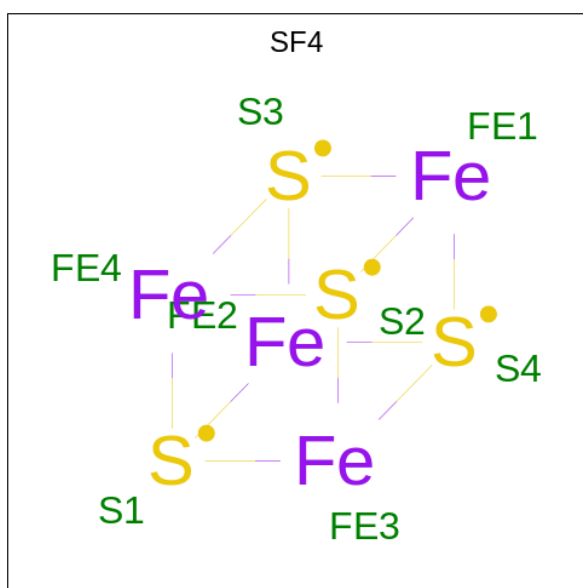
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	F	1	39	39	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms			AltConf	
28	F	1	Total	C	O	S	0
			100	74	24	2	
28	F	1	Total	C	O	S	0
			100	74	24	2	

- Molecule 29 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

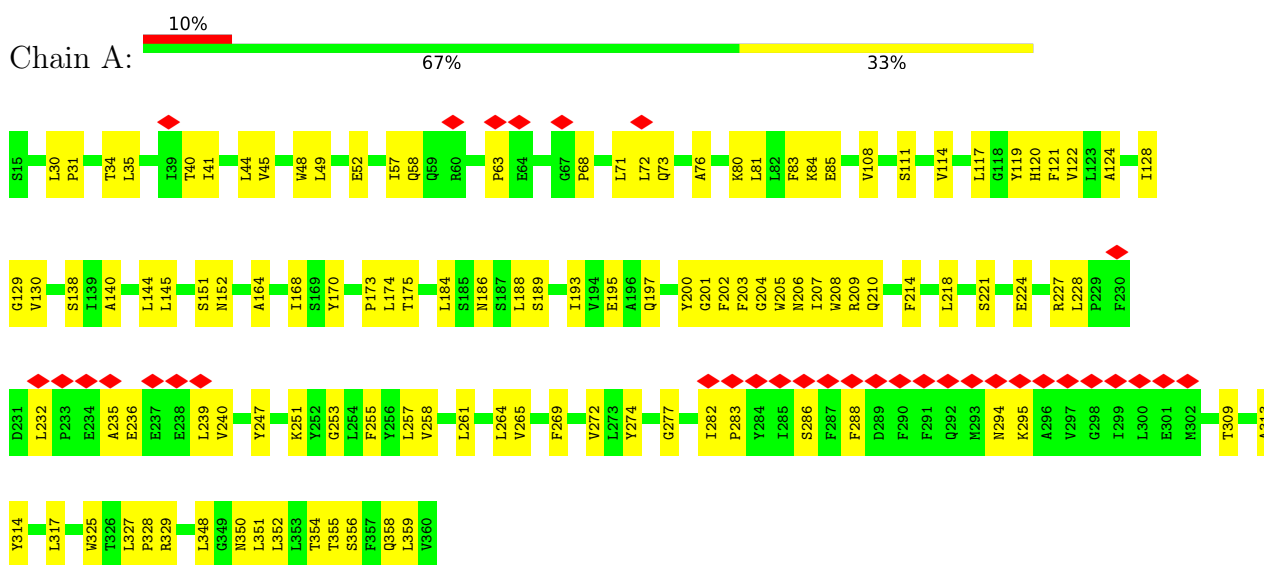


Mol	Chain	Residues	Atoms			AltConf	
29	8	1	Total	Fe	S		0
			8	4	4		

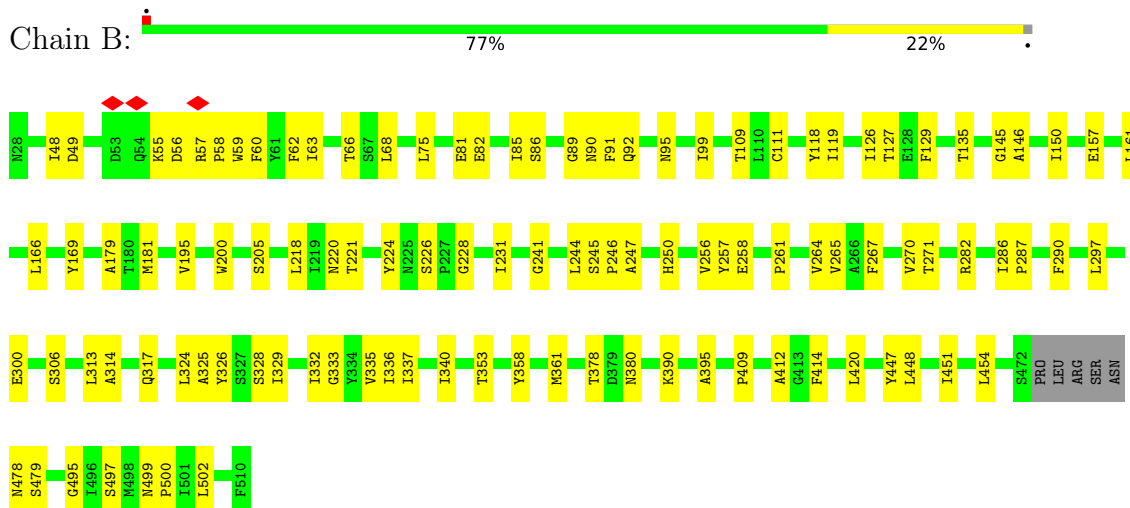
3 Residue-property plots

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.

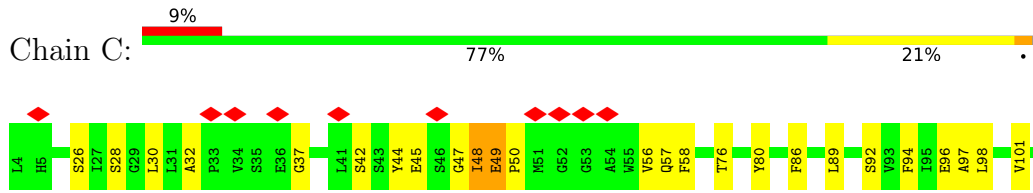
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



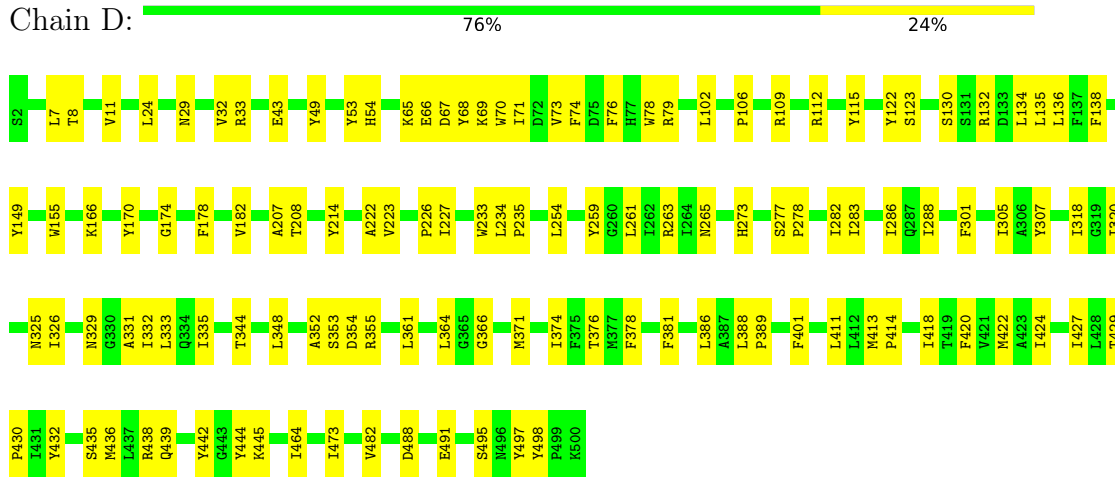
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic



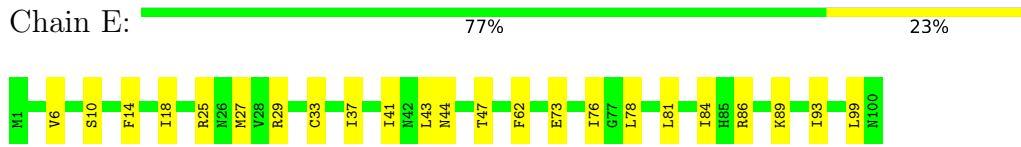
- Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



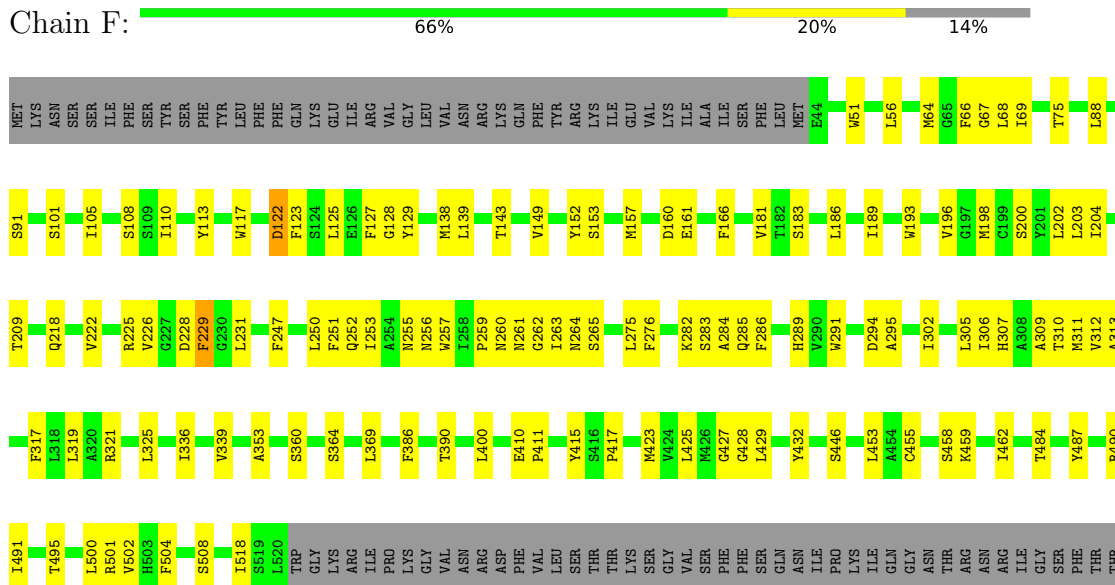
• Molecule 4: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic



• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic



• Molecule 6: NAD(P)H-quinone oxidoreductase subunit F

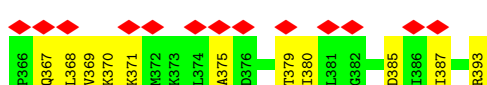
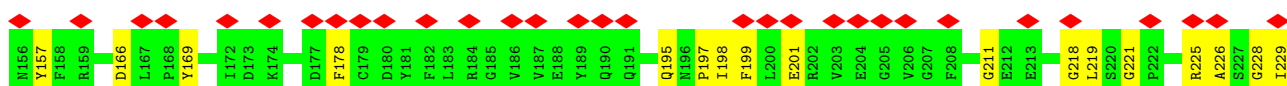
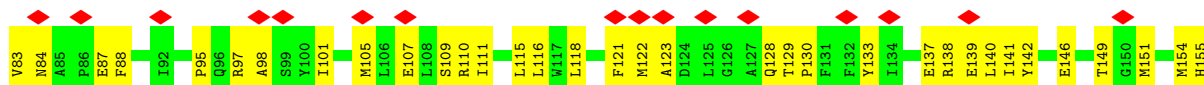
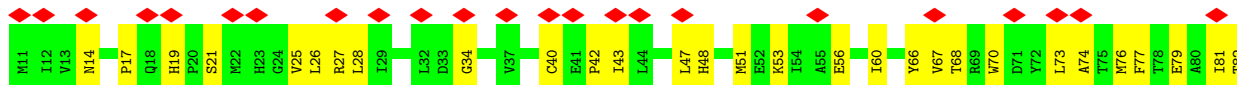




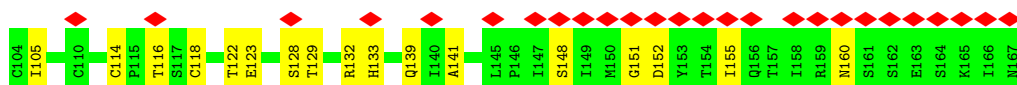
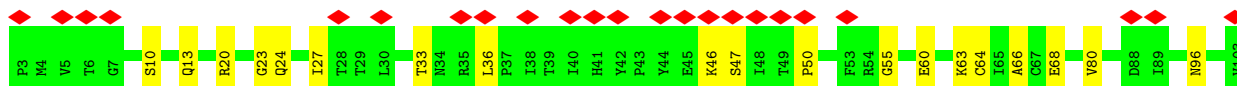
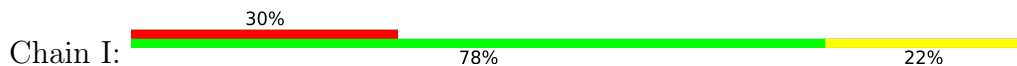
• Molecule 7: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic



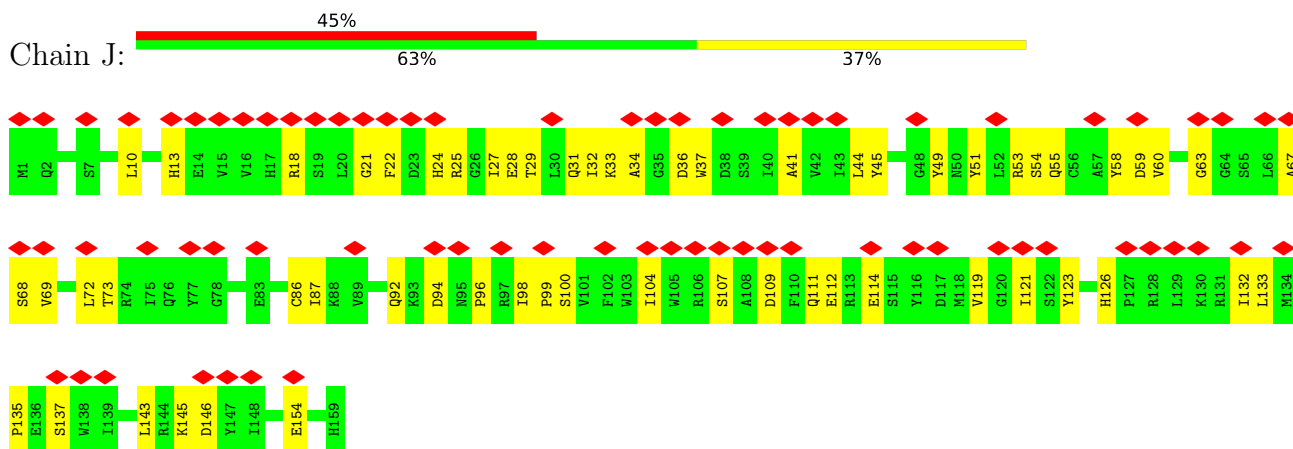
• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic



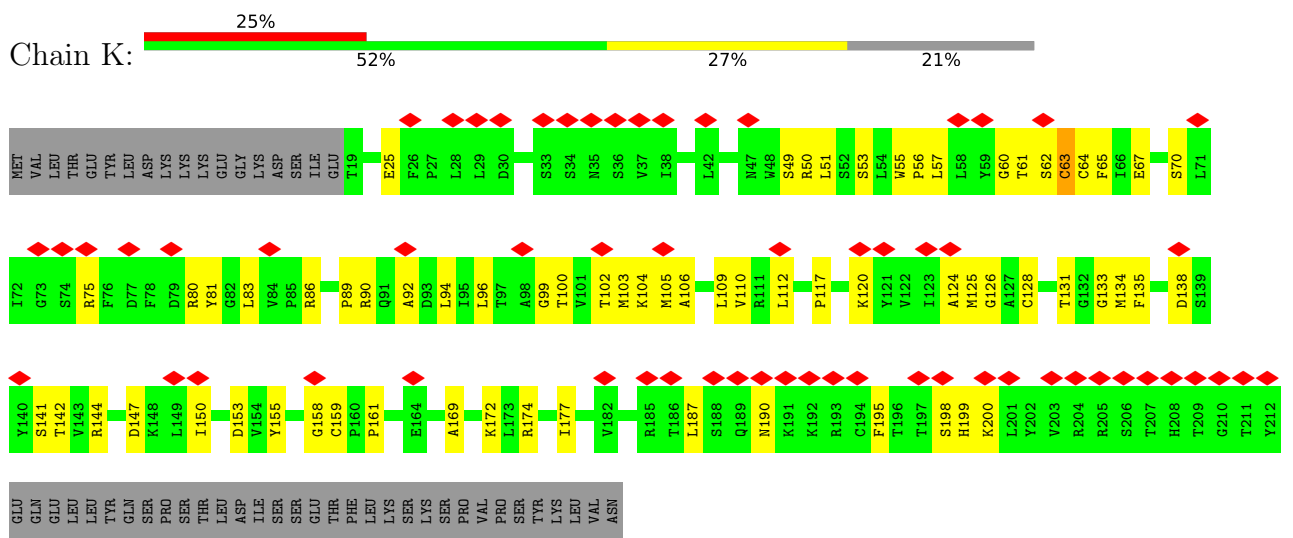
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic



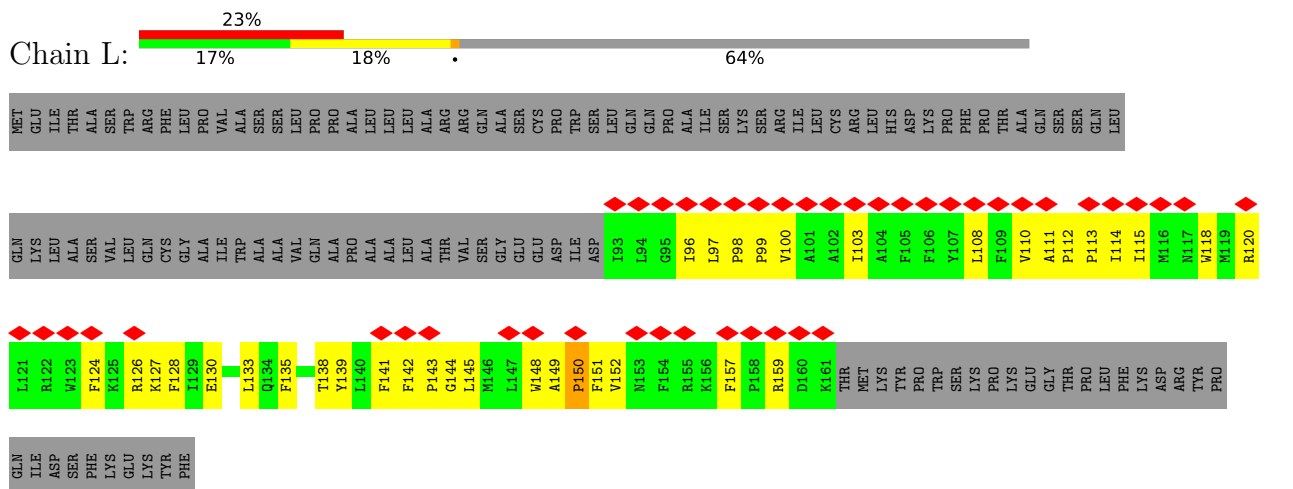
- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J



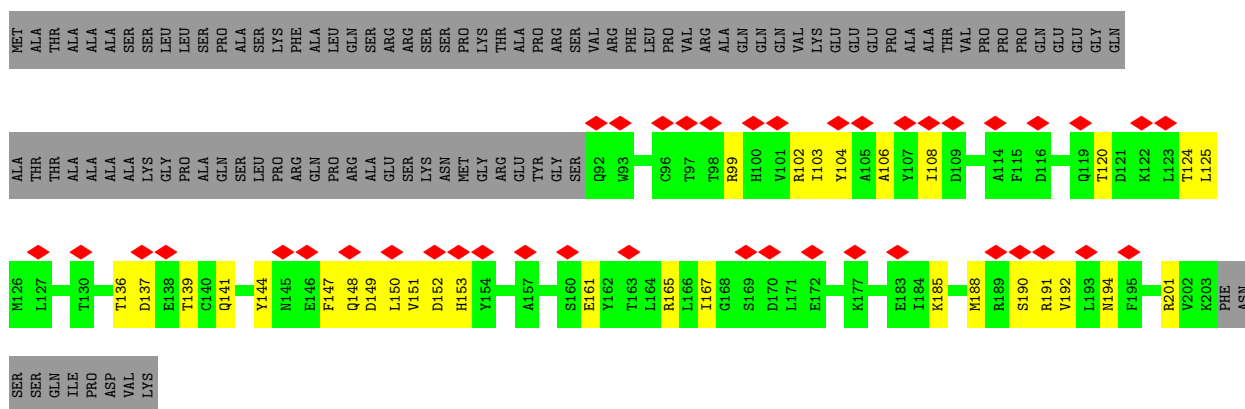
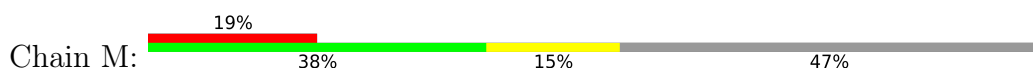
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic



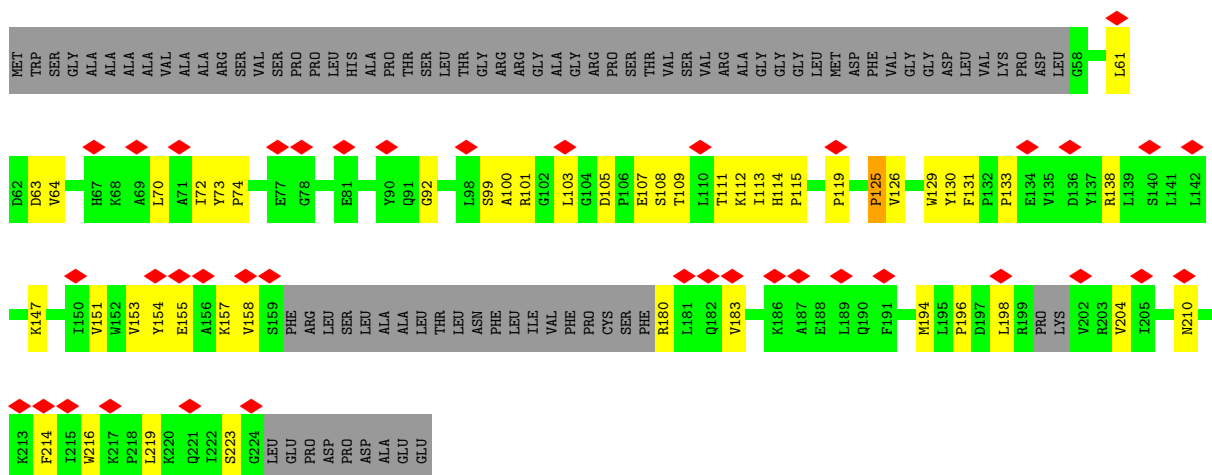
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



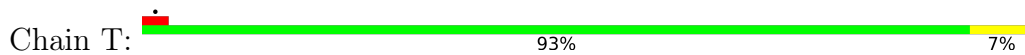
- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



● Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



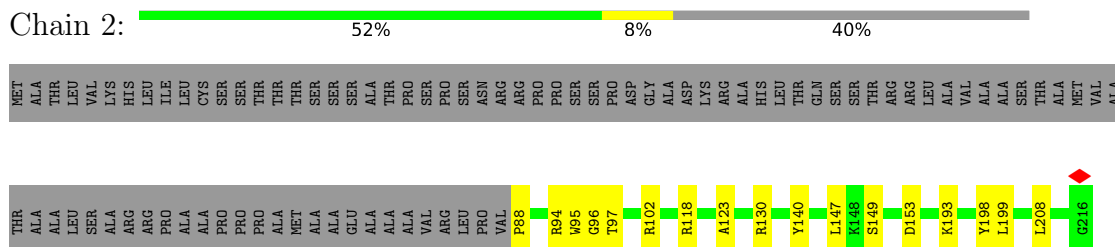
● Molecule 15: Unidentified stromal protein



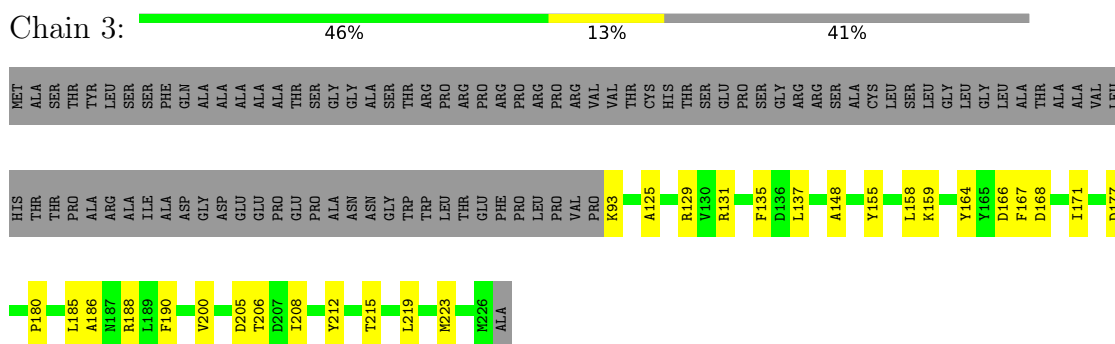
● Molecule 16: Photosynthetic NDH subunit of subcomplex L1



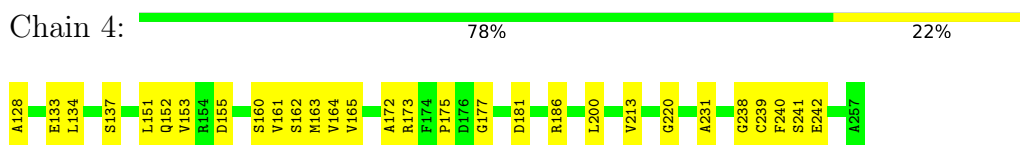
- Molecule 17: Photosynthetic NDH subunit of subcomplex L2



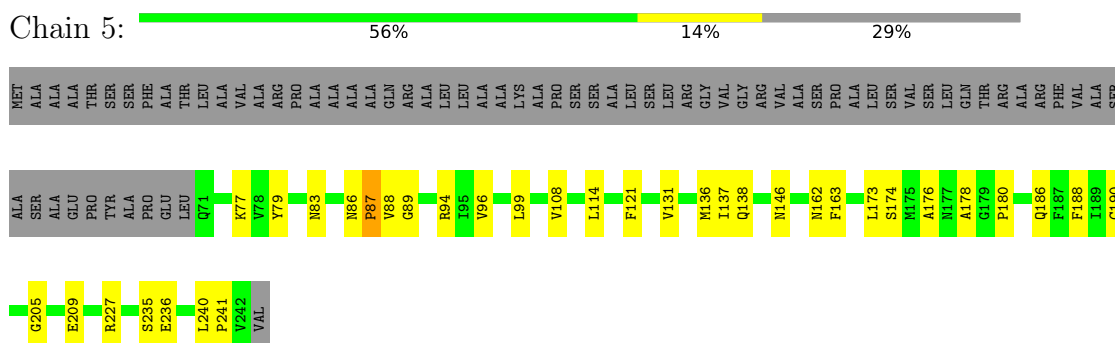
- Molecule 18: Photosynthetic NDH subunit of subcomplex L3



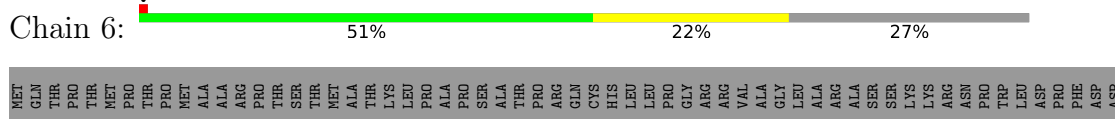
- Molecule 19: Photosynthetic NDH subunit of subcomplex L4

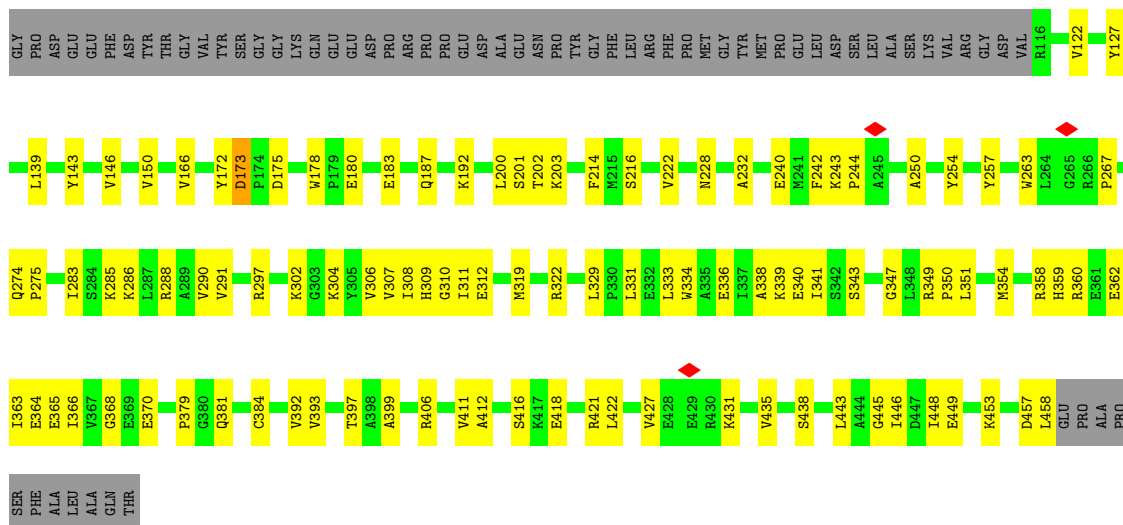


- Molecule 20: Photosynthetic NDH subunit of subcomplex L5

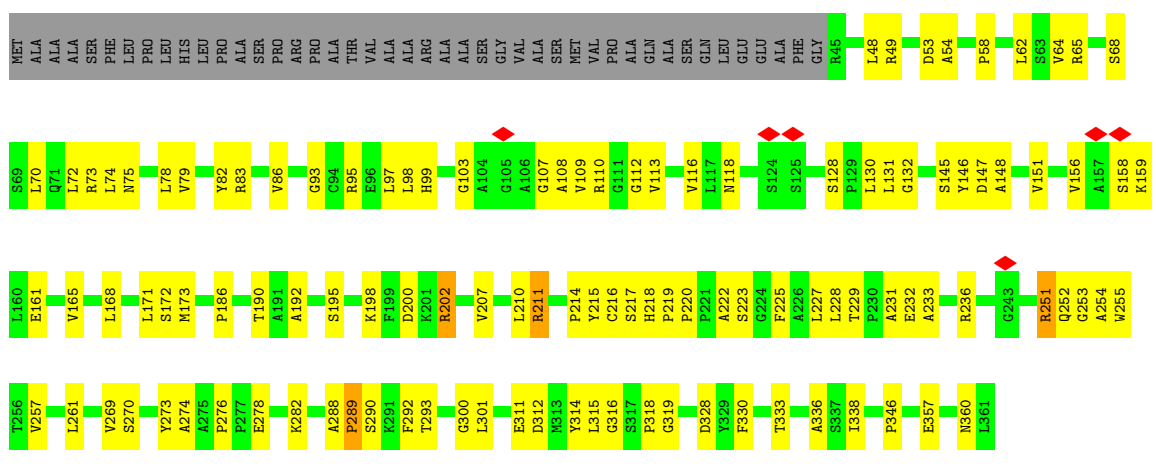


- Molecule 21: Photosynthetic NDH subunit of subcomplex B1

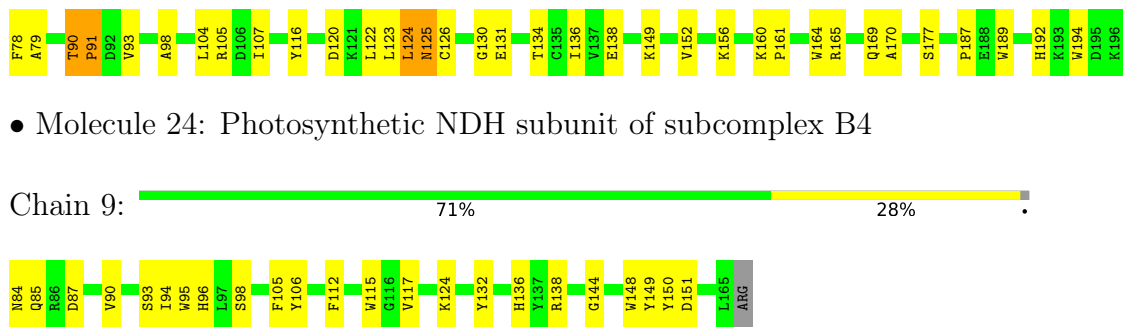




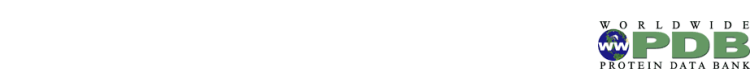
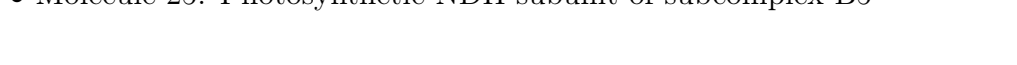
• Molecule 22: Photosynthetic NDH subunit of subcomplex B2



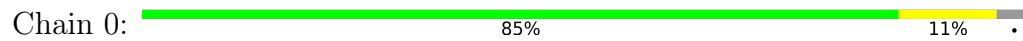
• Molecule 23: Photosynthetic NDH subunit of subcomplex B3



• Molecule 24: Photosynthetic NDH subunit of subcomplex B4



• Molecule 25: Photosynthetic NDH subunit of subcomplex B5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.925	Depositor
Minimum map value	-17.534	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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: SF4, BCR, SQD, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/2670	0.45	0/3644
2	B	0.27	0/3730	0.44	0/5082
3	C	0.30	0/865	0.50	0/1188
4	D	0.28	0/3987	0.47	1/5427 (0.0%)
5	E	0.26	0/759	0.41	0/1028
6	F	0.27	0/5270	0.45	0/7186
7	G	0.27	0/1288	0.45	0/1765
8	H	0.25	0/3070	0.46	0/4173
9	I	0.26	0/1254	0.52	0/1702
10	J	0.23	0/1297	0.45	0/1771
11	K	0.25	0/1505	0.47	0/2048
12	L	0.27	0/597	0.46	0/816
13	M	0.23	0/896	0.47	0/1218
14	N	0.29	0/1189	0.54	1/1617 (0.1%)
16	1	0.28	0/1213	0.55	0/1651
17	2	0.25	0/935	0.43	0/1276
18	3	0.26	0/1006	0.43	0/1365
19	4	0.26	0/894	0.54	0/1216
20	5	0.26	0/1314	0.47	0/1771
21	6	0.28	0/2589	0.50	0/3513
22	7	0.28	0/2358	0.57	0/3200
23	8	0.30	0/844	0.60	0/1145
24	9	0.27	0/636	0.48	0/868
25	0	0.27	0/1122	0.54	0/1536
All	All	0.27	0/41288	0.48	2/56206 (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
4	D	0	1
6	F	0	2
9	I	0	1
14	N	0	1
16	1	0	1
17	2	0	1
20	5	0	1
21	6	0	4
22	7	0	1
23	8	0	2
25	0	0	3
All	All	0	18

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	157	LYS	N-CA-C	7.50	131.24	111.00
4	D	497	TYR	C-N-CA	-5.08	108.99	121.70

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	495	SER	Peptide
6	F	122	ASP	Peptide
6	F	261	ASN	Peptide
9	I	122	THR	Mainchain
14	N	125	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2608	0	2609	82	0
2	B	3646	0	3652	78	0
3	C	841	0	761	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3874	0	3923	84	0
5	E	750	0	760	20	0
6	F	5124	0	4962	121	0
7	G	1260	0	1197	28	0
8	H	2991	0	2849	133	0
9	I	1229	0	1109	26	0
10	J	1258	0	1151	49	0
11	K	1474	0	1442	54	0
12	L	572	0	559	26	0
13	M	876	0	801	27	0
14	N	1154	0	1117	29	0
15	T	305	0	69	3	0
16	1	1185	0	1086	29	0
17	2	915	0	764	13	0
18	3	989	0	927	19	0
19	4	878	0	823	19	0
20	5	1289	0	1247	21	0
21	6	2541	0	2461	65	0
22	7	2311	0	2232	85	0
23	8	828	0	742	26	0
24	9	617	0	520	15	0
25	0	1089	0	901	12	0
26	D	24	0	19	1	0
27	F	39	0	53	6	0
28	F	100	0	137	5	0
29	8	8	0	0	1	0
All	All	40775	0	38873	967	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 12.

The worst 5 of 967 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)
3:C:47:GLY:HA3	8:H:14:ASN:ND2	1.45	1.30
3:C:47:GLY:CA	8:H:14:ASN:HD21	1.48	1.26
3:C:47:GLY:HA3	8:H:14:ASN:HD21	1.02	1.00
23:8:123:LEU:O	23:8:124:LEU:O	1.82	0.96
3:C:47:GLY:N	8:H:14:ASN:HD21	1.67	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	41	74
2	B	474/483 (98%)	424 (90%)	50 (10%)	0	100	100
3	C	114/117 (97%)	96 (84%)	15 (13%)	3 (3%)	5	34
4	D	497/499 (100%)	450 (90%)	46 (9%)	1 (0%)	47	78
5	E	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
6	F	665/777 (86%)	598 (90%)	65 (10%)	2 (0%)	41	74
7	G	174/176 (99%)	148 (85%)	26 (15%)	0	100	100
8	H	381/383 (100%)	339 (89%)	42 (11%)	0	100	100
9	I	163/165 (99%)	123 (76%)	40 (24%)	0	100	100
10	J	157/159 (99%)	141 (90%)	16 (10%)	0	100	100
11	K	192/245 (78%)	174 (91%)	17 (9%)	1 (0%)	29	66
12	L	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	10	44
13	M	110/213 (52%)	92 (84%)	18 (16%)	0	100	100
14	N	139/233 (60%)	116 (84%)	20 (14%)	3 (2%)	6	37
16	1	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	22	59
17	2	127/216 (59%)	106 (84%)	21 (16%)	0	100	100
18	3	132/227 (58%)	116 (88%)	16 (12%)	0	100	100
19	4	128/130 (98%)	102 (80%)	26 (20%)	0	100	100
20	5	170/243 (70%)	156 (92%)	13 (8%)	1 (1%)	25	62
21	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	25	62
22	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	41	74
23	8	117/119 (98%)	79 (68%)	33 (28%)	5 (4%)	2	24
24	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	12	47
25	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	22	59
All	All	5280/6245 (84%)	4465 (85%)	791 (15%)	24 (0%)	32	66

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
3	C	49	GLU
21	6	275	PRO
23	8	124	LEU
3	C	48	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/301 (90%)	270 (100%)	1 (0%)	91	95
2	B	397/419 (95%)	396 (100%)	1 (0%)	92	96
3	C	71/100 (71%)	71 (100%)	0	100	100
4	D	399/427 (93%)	399 (100%)	0	100	100
5	E	78/88 (89%)	77 (99%)	1 (1%)	69	83
6	F	513/674 (76%)	511 (100%)	2 (0%)	91	95
7	G	119/154 (77%)	119 (100%)	0	100	100
8	H	298/336 (89%)	298 (100%)	0	100	100
9	I	123/155 (79%)	123 (100%)	0	100	100
10	J	126/141 (89%)	126 (100%)	0	100	100
11	K	162/226 (72%)	161 (99%)	1 (1%)	86	93
12	L	55/167 (33%)	54 (98%)	1 (2%)	59	77
13	M	86/184 (47%)	86 (100%)	0	100	100
14	N	115/192 (60%)	115 (100%)	0	100	100
16	1	116/132 (88%)	116 (100%)	0	100	100
17	2	74/181 (41%)	74 (100%)	0	100	100
18	3	92/183 (50%)	92 (100%)	0	100	100
19	4	80/102 (78%)	80 (100%)	0	100	100
20	5	135/191 (71%)	135 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	6	250/389 (64%)	250 (100%)	0	100	100
22	7	233/279 (84%)	230 (99%)	3 (1%)	69	83
23	8	69/102 (68%)	69 (100%)	0	100	100
24	9	55/70 (79%)	53 (96%)	2 (4%)	35	63
25	0	93/137 (68%)	93 (100%)	0	100	100
All	All	4010/5330 (75%)	3998 (100%)	12 (0%)	92	96

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

Mol	Chain	Res	Type
22	7	202	ARG
22	7	211	ARG
24	9	138	ARG
22	7	251	ARG
6	F	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	13	HIS
23	8	184	GLN
13	M	194	ASN
22	7	252	GLN
13	M	145	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 monosaccharides in this entry.

5.6 Ligand geometry

5 ligands are modelled in this entry.

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
28	SQD	F	802	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	4 (6%)
28	SQD	F	803	-	45,46,54	1.28	4 (8%)	54,57,65	1.15	7 (12%)
26	LHG	D	601	-	23,23,48	1.32	2 (8%)	26,28,54	1.32	3 (11%)
27	BCR	F	801	-	40,40,41	0.77	0	54,54,56	2.99	21 (38%)
29	SF4	8	201	23	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
28	SQD	F	802	-	-	9/49/69/69	0/1/1/1
28	SQD	F	803	-	-	9/41/61/69	0/1/1/1
26	LHG	D	601	-	-	3/27/27/53	-
27	BCR	F	801	-	-	10/27/61/63	0/2/2/2
29	SF4	8	201	23	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	802	SQD	O8-S	4.60	1.63	1.47
28	F	803	SQD	O8-S	4.59	1.63	1.47
28	F	803	SQD	O47-C7	4.28	1.46	1.34
28	F	802	SQD	O48-C23	4.24	1.45	1.33
28	F	803	SQD	O48-C23	4.24	1.45	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	801	BCR	C11-C10-C9	-10.58	112.21	127.31
27	F	801	BCR	C7-C8-C9	-8.72	113.06	126.23
27	F	801	BCR	C24-C23-C22	-5.98	117.20	126.23
27	F	801	BCR	C13-C12-C11	-5.67	112.19	124.81
27	F	801	BCR	C15-C16-C17	-5.01	113.22	123.47

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

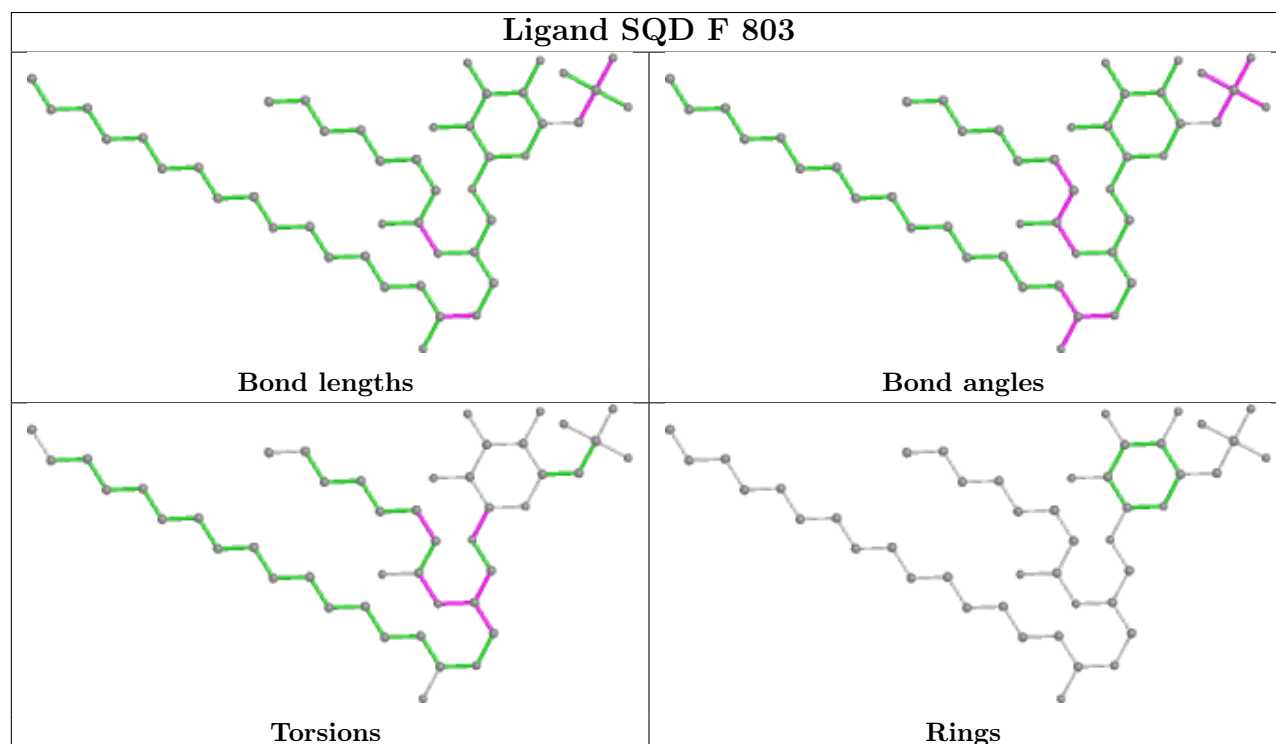
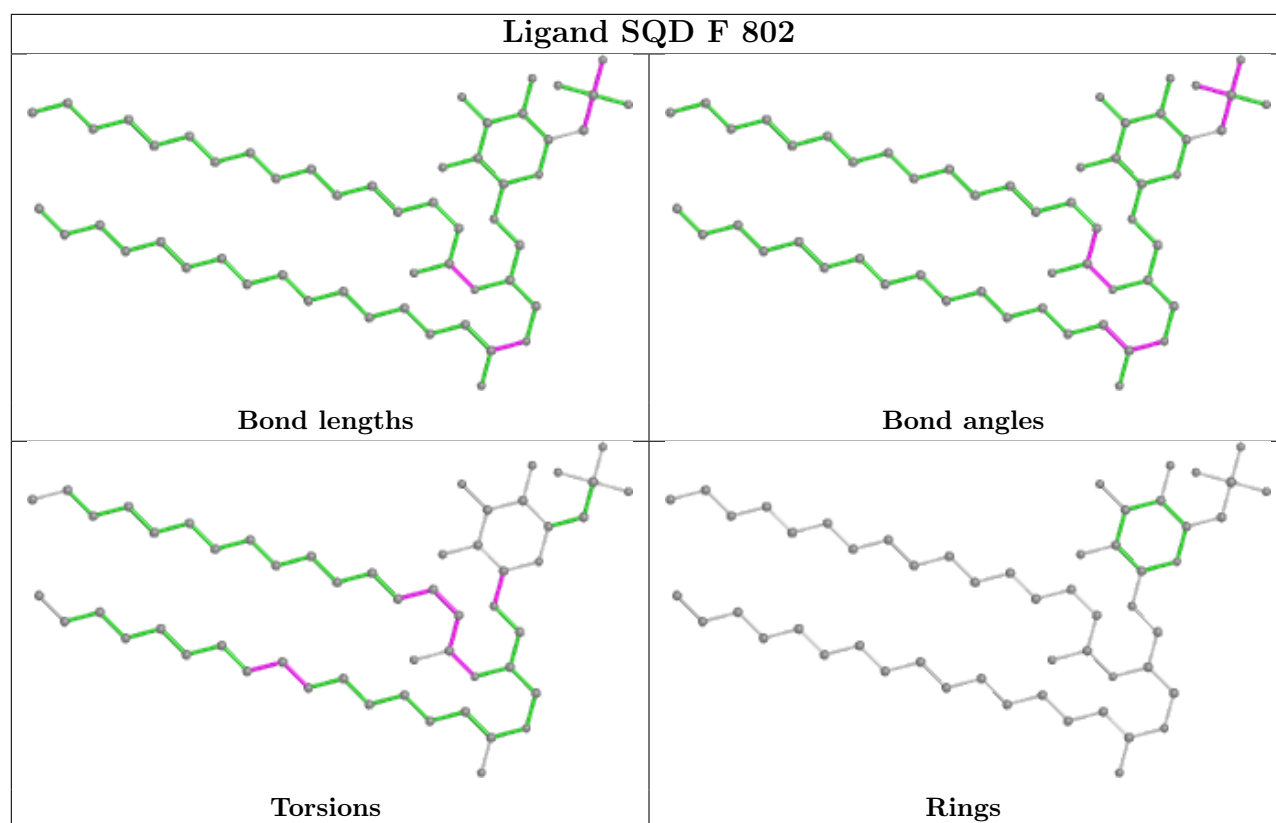
Mol	Chain	Res	Type	Atoms
27	F	801	BCR	C37-C22-C23-C24
28	F	802	SQD	O5-C1-O6-C44
28	F	803	SQD	C2-C1-O6-C44
28	F	803	SQD	O5-C1-O6-C44
27	F	801	BCR	C21-C22-C23-C24

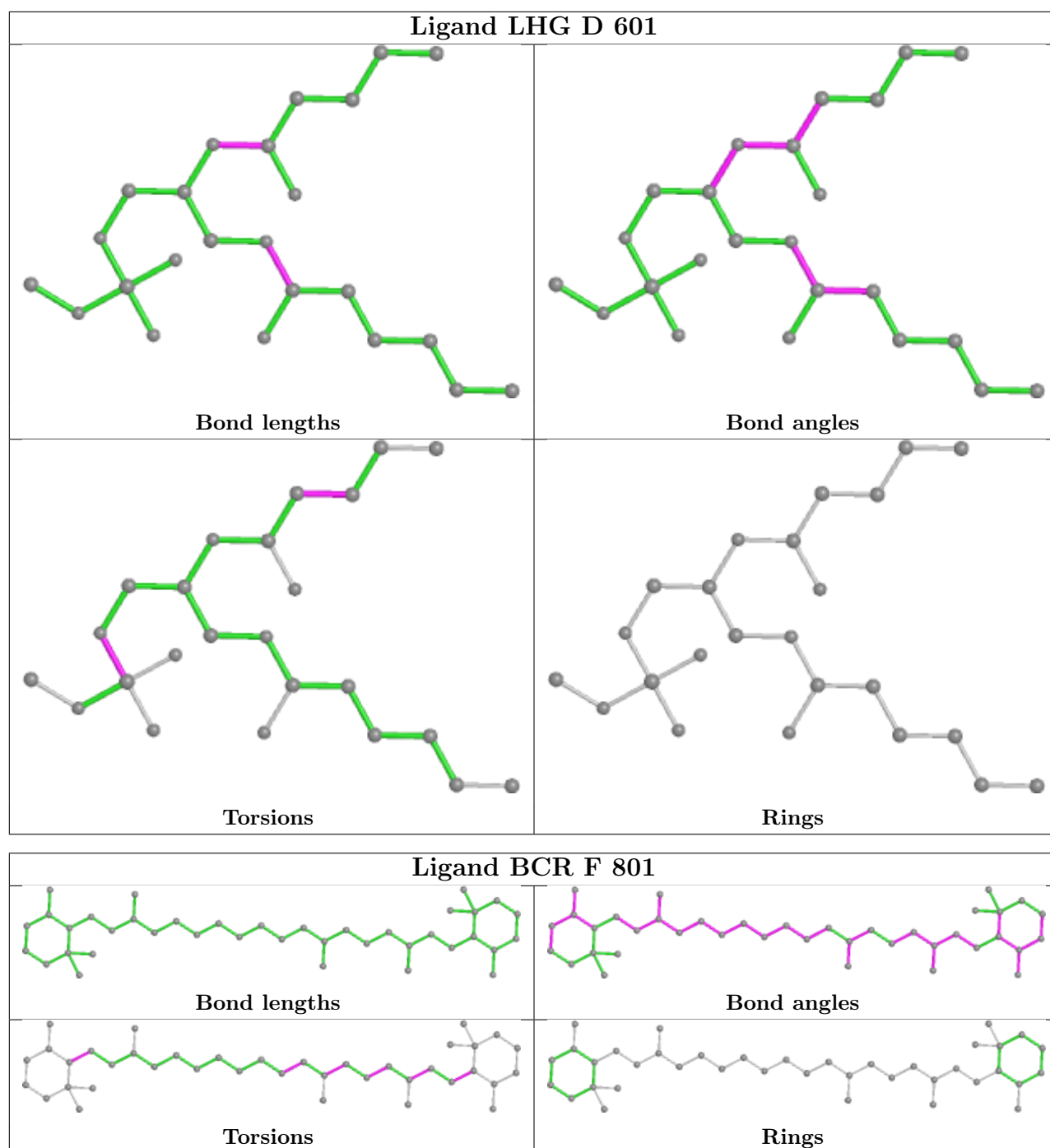
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	802	SQD	1	0
28	F	803	SQD	4	0
26	D	601	LHG	1	0
27	F	801	BCR	6	0
29	8	201	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

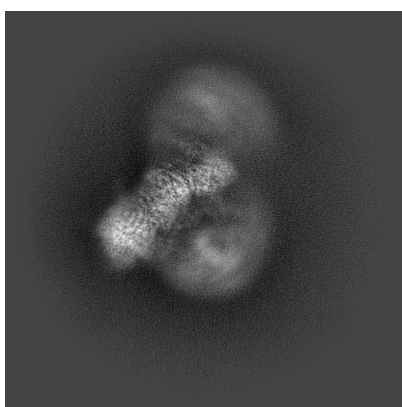
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31307. These allow visual inspection of the internal detail of the map and identification of artifacts.

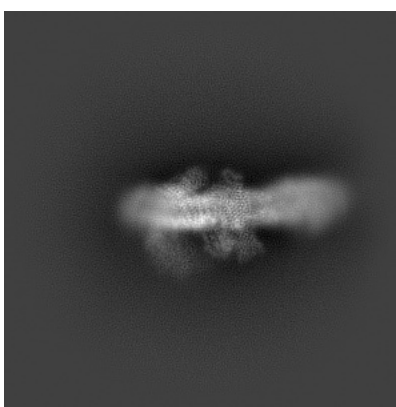
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

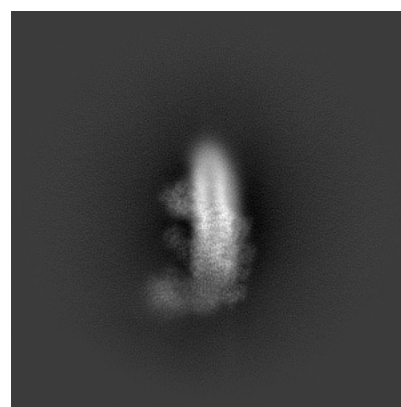
6.1.1 Primary map



X



Y

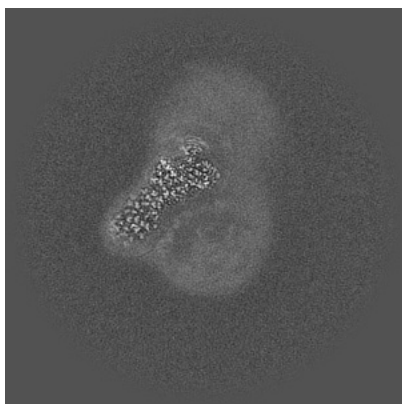


Z

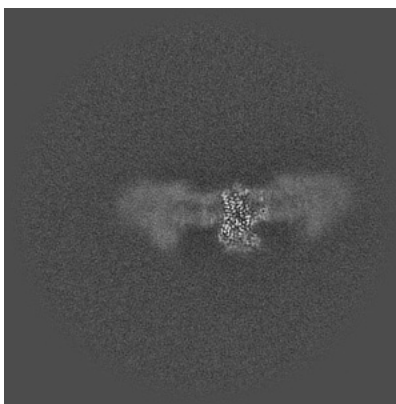
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

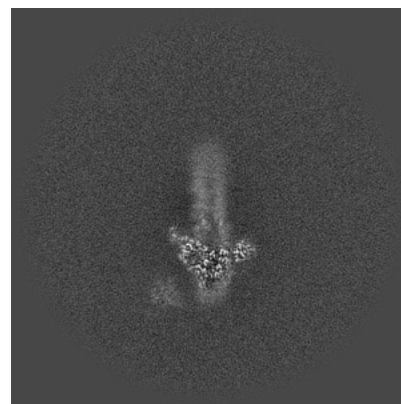
6.2.1 Primary map



X Index: 220



Y Index: 220

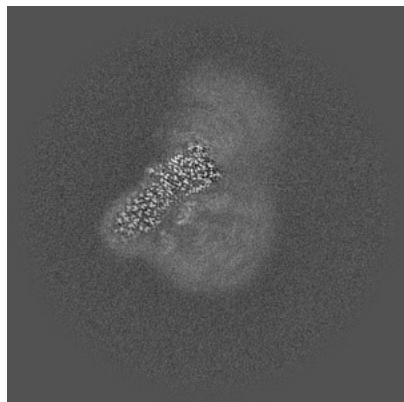


Z Index: 220

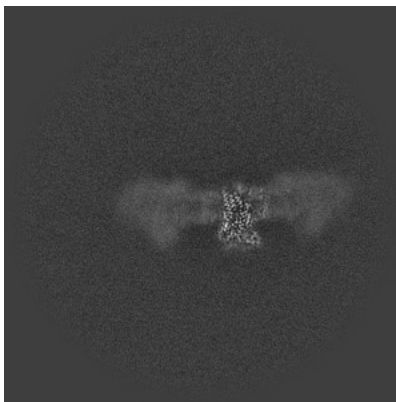
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

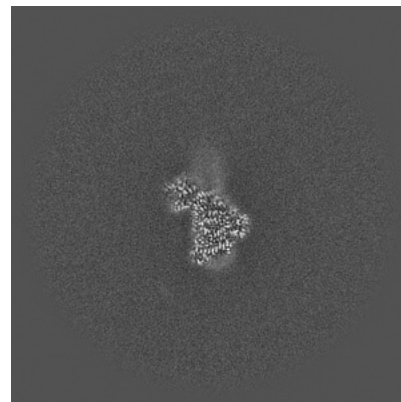
6.3.1 Primary map



X Index: 213



Y Index: 221



Z Index: 255

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

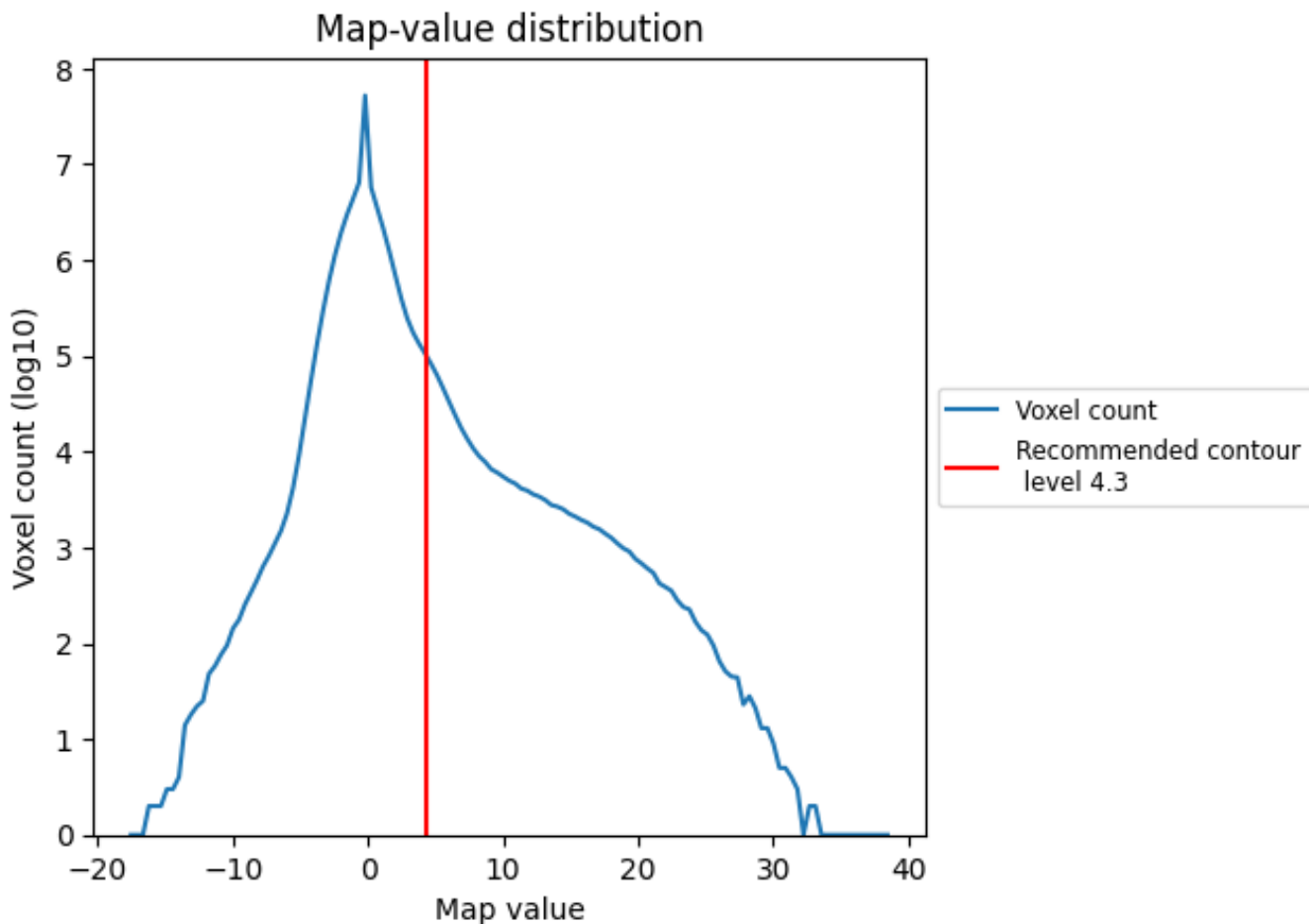
6.5 Mask visualisation

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

7 Map analysis [i](#)

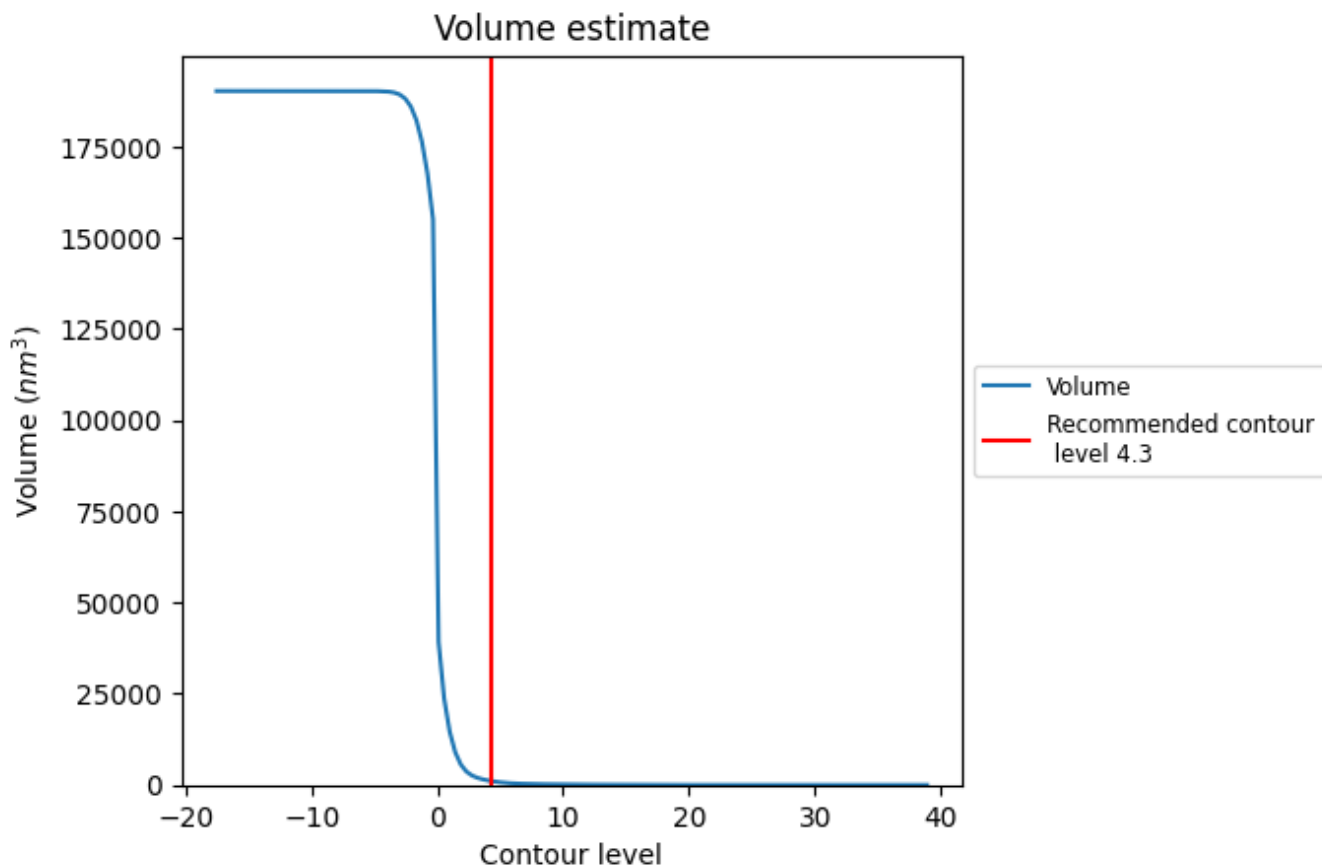
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

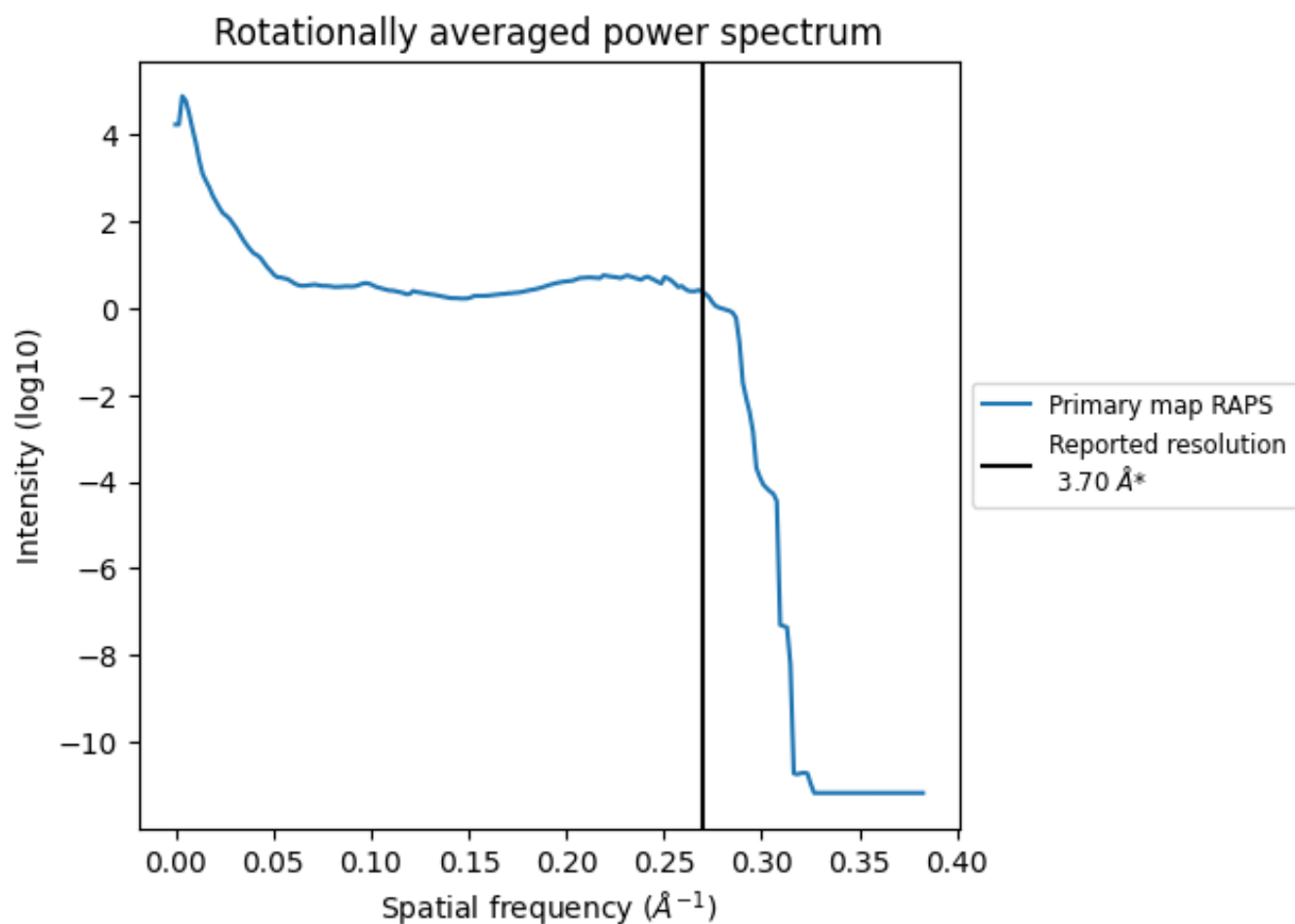
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1068 nm³; this corresponds to an approximate mass of 965 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 0.270\AA^{-1}

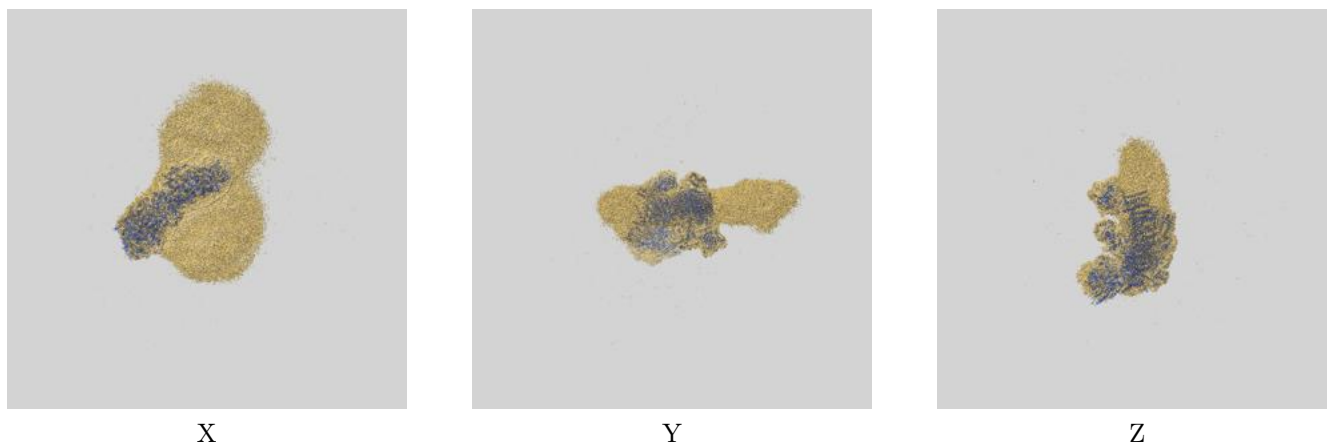
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

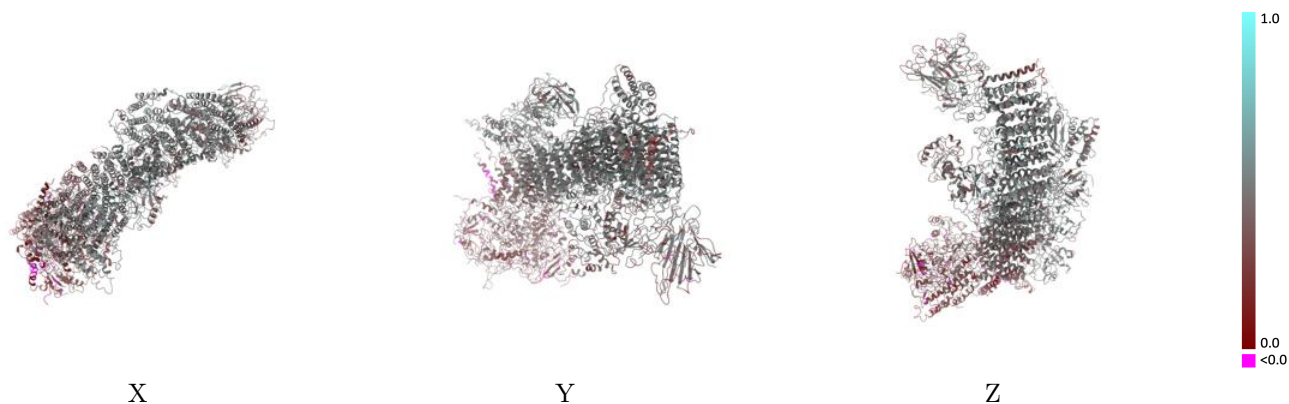
This section contains information regarding the fit between EMDB map EMD-31307 and PDB model 7EU3. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



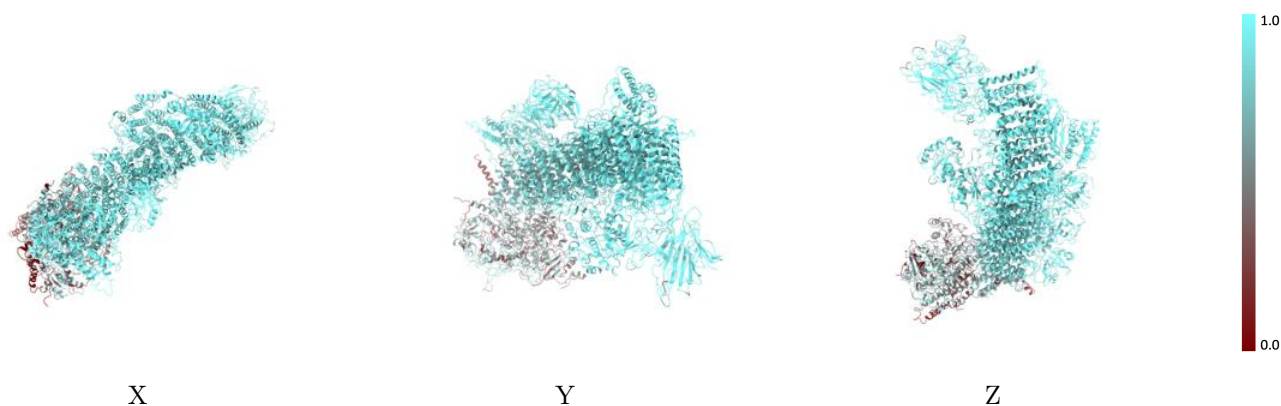
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



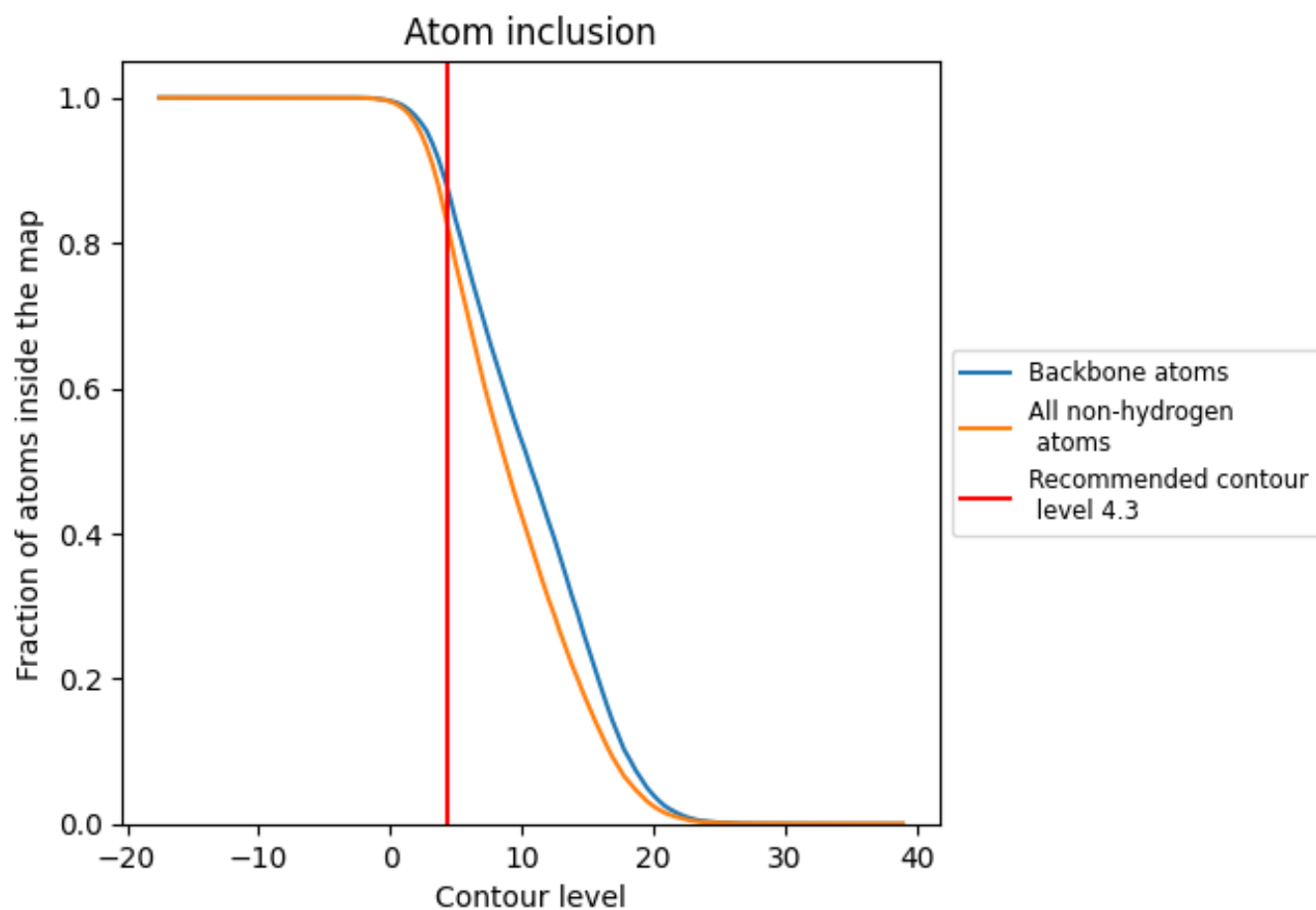
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.3).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8276	 0.4020
0	 0.9487	 0.4610
1	 0.9557	 0.4310
2	 0.9720	 0.4580
3	 0.9743	 0.4660
4	 0.9688	 0.4720
5	 0.9566	 0.4750
6	 0.9334	 0.4230
7	 0.9133	 0.4070
8	 0.9440	 0.4470
9	 0.9536	 0.4480
A	 0.7935	 0.3470
B	 0.9258	 0.4570
C	 0.8424	 0.3870
D	 0.9517	 0.4890
E	 0.9216	 0.4800
F	 0.9390	 0.4660
G	 0.9008	 0.4400
H	 0.4876	 0.2680
I	 0.5674	 0.2970
J	 0.4789	 0.2510
K	 0.5465	 0.2970
L	 0.3136	 0.0790
M	 0.4847	 0.2800
N	 0.5941	 0.2650
T	 0.9246	 0.4040

