wwPDB EM Validation Summary Report

Nov 24, 2024 – 12:25 AM JST

PDB ID	:	8XNY
EMDB ID	:	EMD-38519
Title	:	Respiratory complex Peripheral Arm of CI, open form B, focus-refined map of type II, Wild type mouse under Cold Acclimation
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-12-30
Resolution	:	4.10 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:

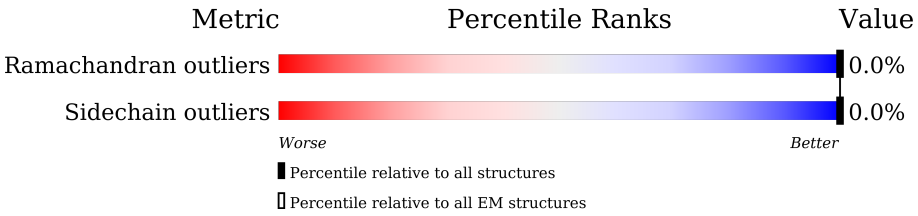
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	115	37% 78% 22%
2	B	224	11% 68% 31%
3	C	263	13% 75% 25%
4	D	463	13% 82% 17%
5	E	248	54% 85% 15%
6	F	464	54% 91% 8%
7	G	727	24% 93% 6%
8	H	318	33% 98%
9	I	212	10% 81% 19%

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Mol	Chain	Length	Quality of chain
10	P	377	42% 89% 10%
11	Q	175	33% 66% 34%
12	R	116	19% 39% 61%
13	S	99	23% 84% 16%
14	T	156	26% 48% 52%
15	V	116	10% 97%
16	W	131	28% 87% 13%
17	X	172	9% 83% 17%
18	Z	144	18% 95%
19	a	70	9% 96%
20	b	84	17% 95% 5%
21	q	145	66% 69% 31%
22	r	113	28% 42% 58%
23	s	104	22% 22% 78%

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 33176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	90	735	511	102	117	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	793	222	212	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1643	1061	279	300	3	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	D	383	3074	1962	529	560	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total 3288	C 2073	N 588	O 605	S 22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total 5287	C 3316	N 918	O 1012	S 41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	313	Total 2502	C 1683	N 379	O 418	S 22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total 1380	C 869	N 237	O 262	S 12	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	339	Total 2720	C 1759	N 476	O 478	S 7	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	116	Total 940	C 598	N 161	O 177	S 4	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	45	Total 336	C 209	N 60	O 64	S 3	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1164	736	209	209	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	138	Total	C	N	O	S	0	0
			1145	736	203	198	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	100	Total	C	N	O	S	0	0
			833	536	148	145	4		

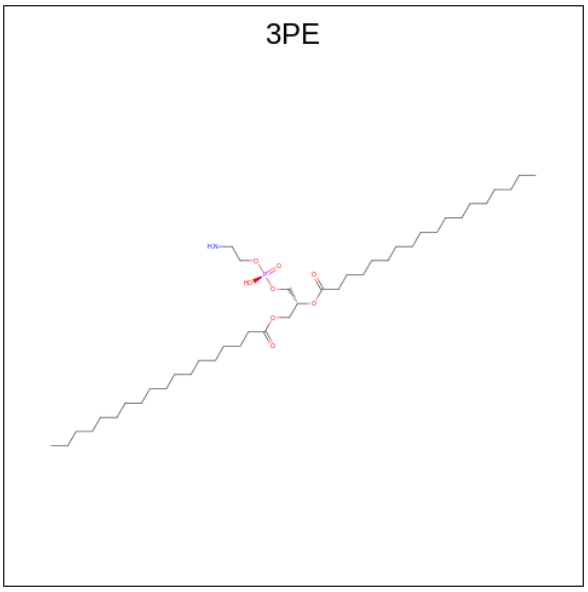
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	48	Total	C	N	O	S	0	0
			389	249	73	66	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

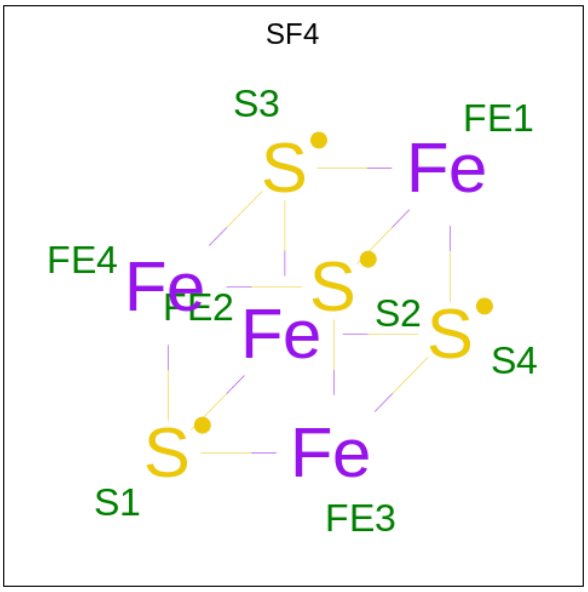
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	23	Total	C	N	O	0	0
			193	126	30	37		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	A	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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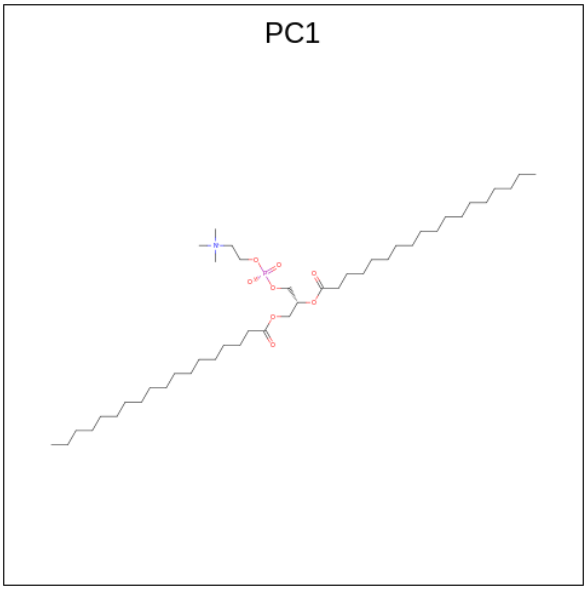
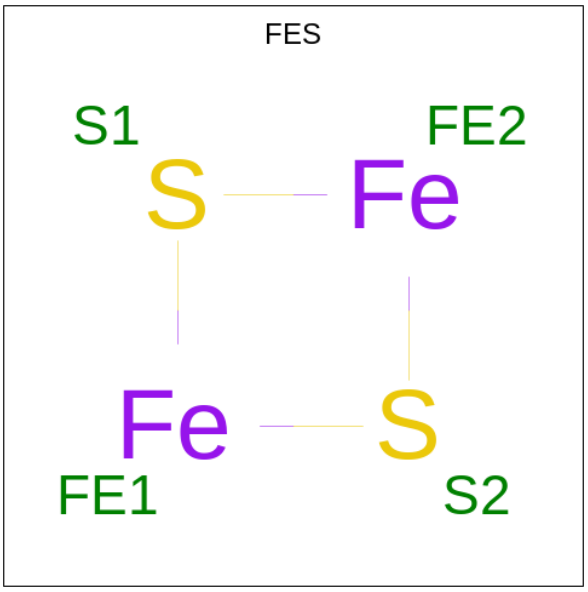
Mol	Chain	Residues	Atoms	AltConf
25	F	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



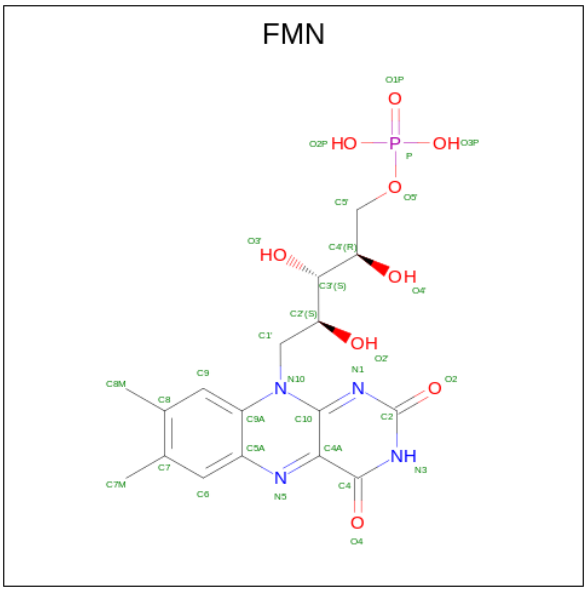
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C N O P 35 25 1 8 1	0
26	B	1	Total C N O P 43 33 1 8 1	0

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



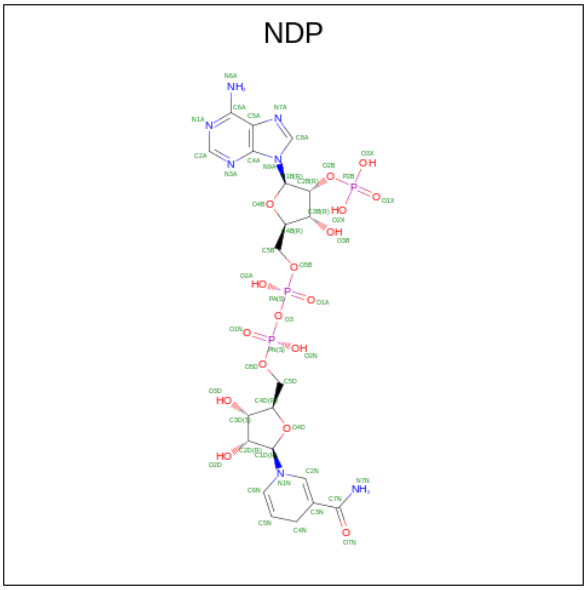
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 28 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

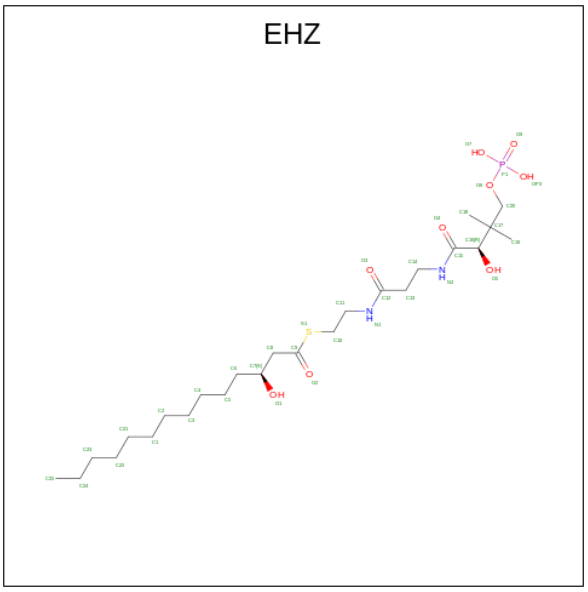


Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 30 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 31 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).

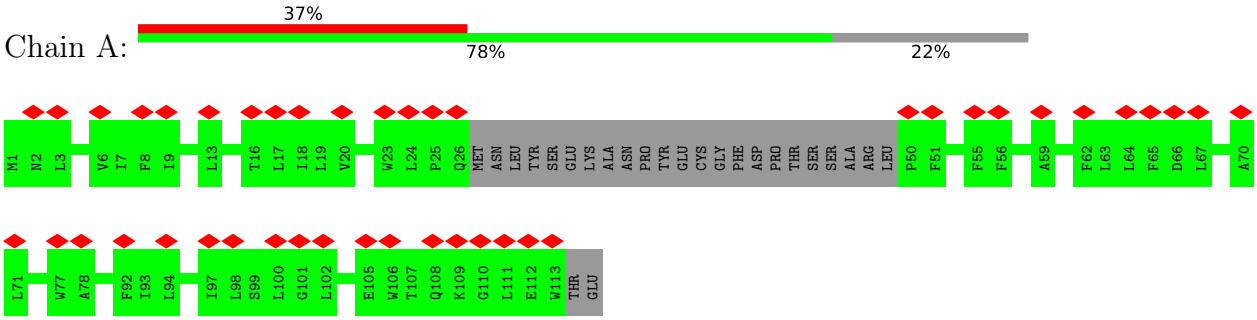


Mol	Chain	Residues	Atoms						AltConf
31	W	1	Total	C	N	O	P	S	0
			35	22	2	9	1	1	

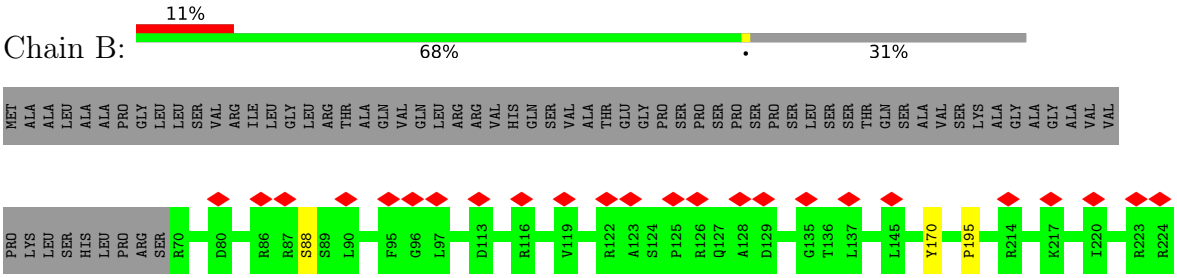
3 Residue-property plots (i)

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

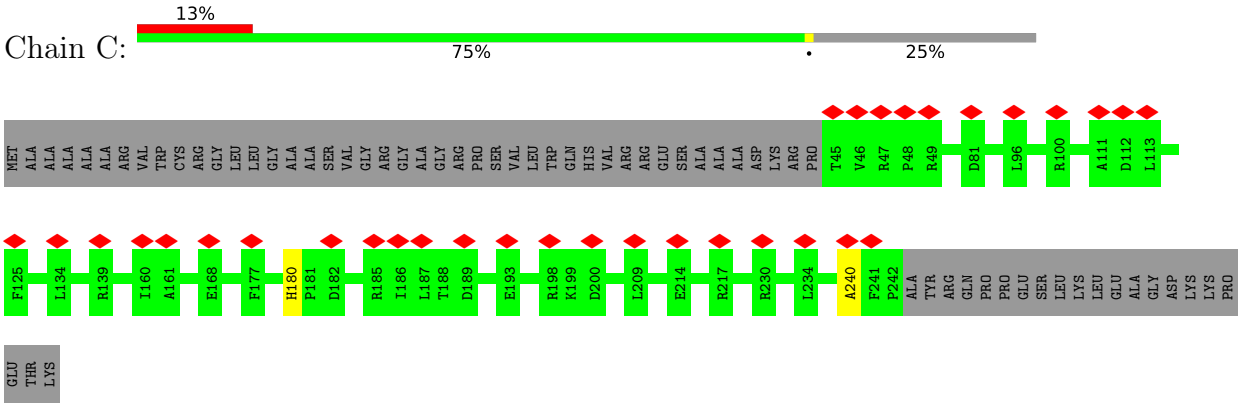
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

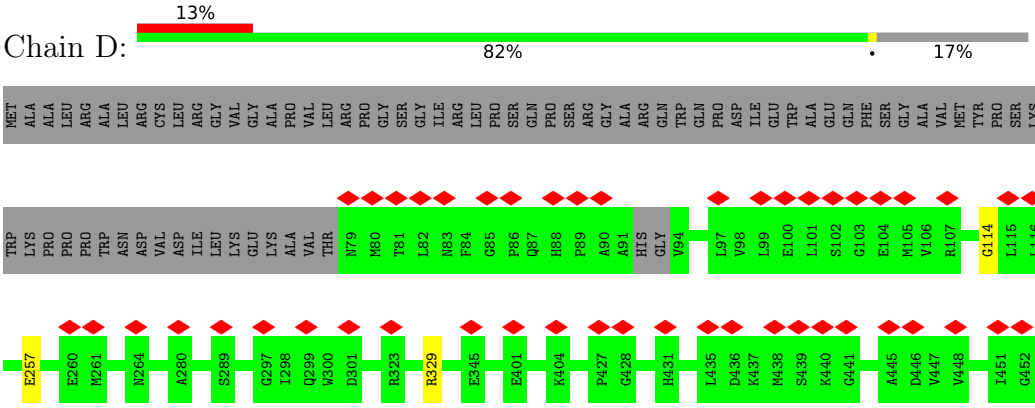


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



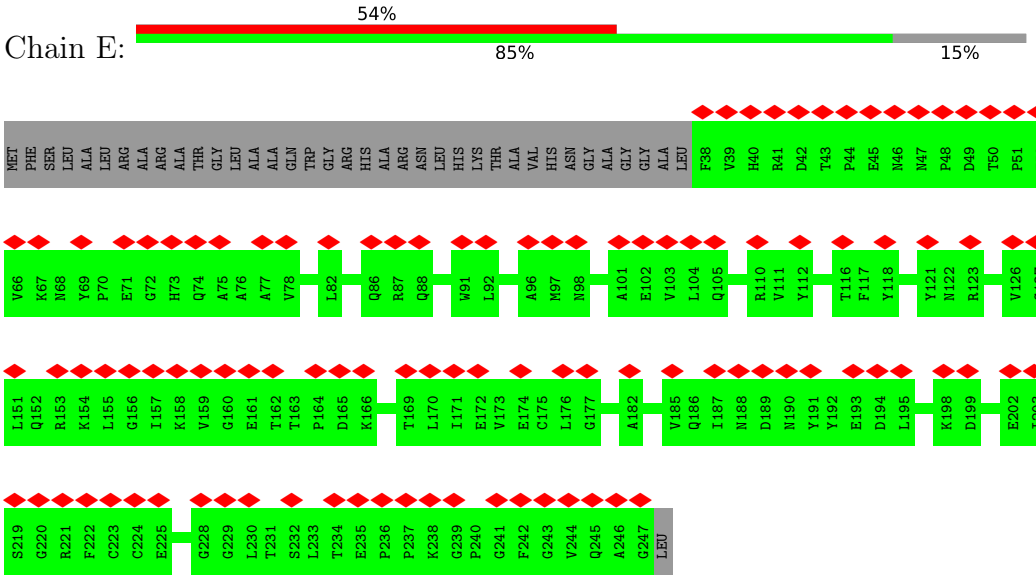
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:



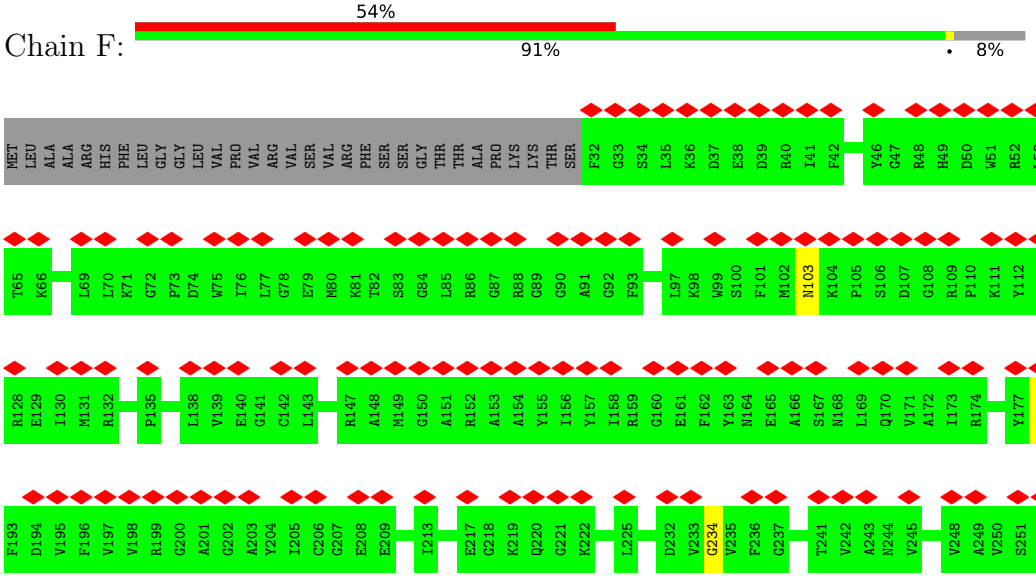
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

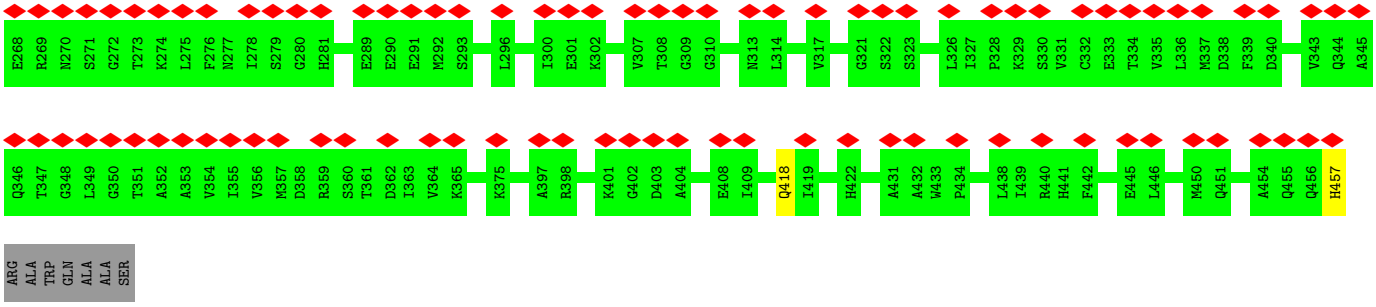
Chain E:



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

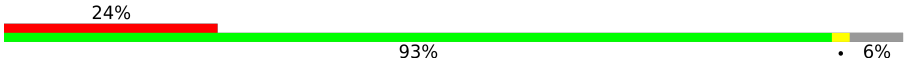
Chain F:

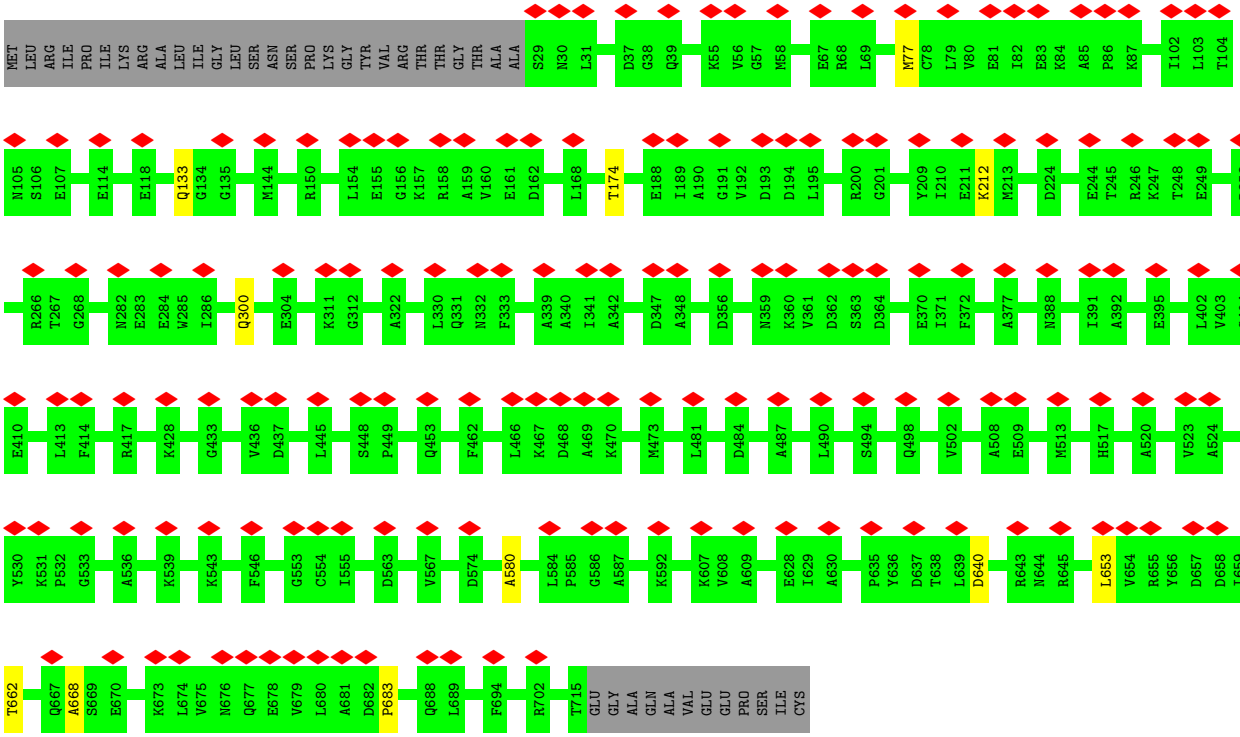




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

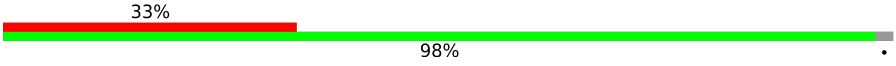
Chain G:

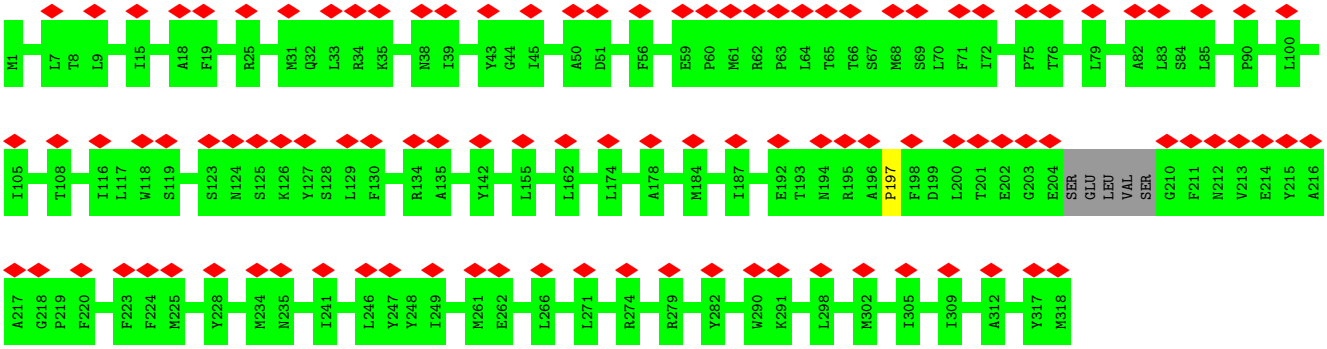




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

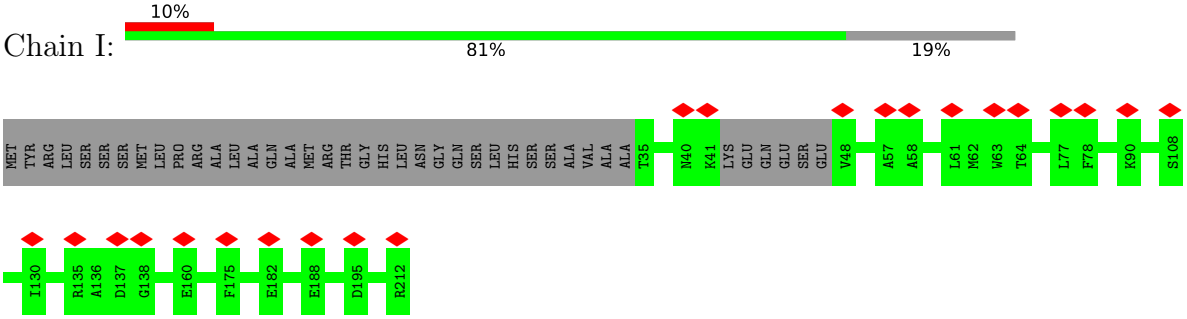
Chain H:





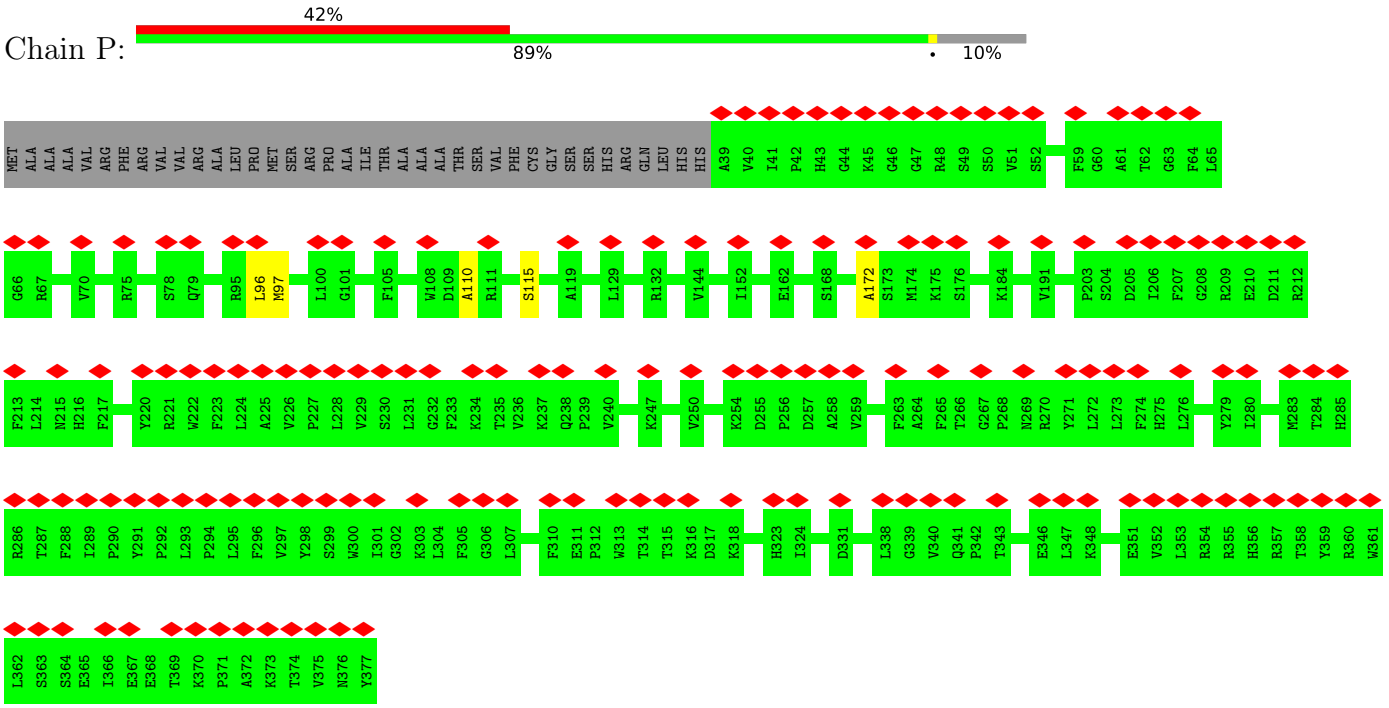
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



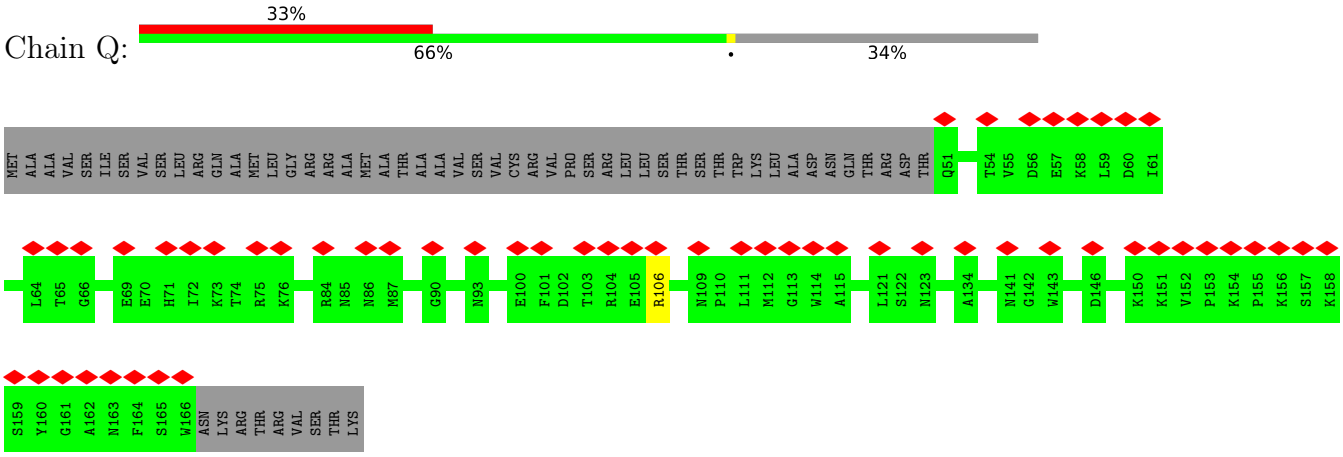
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



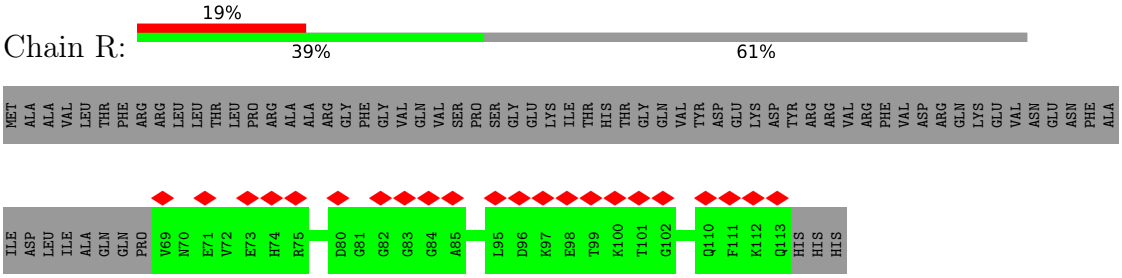
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



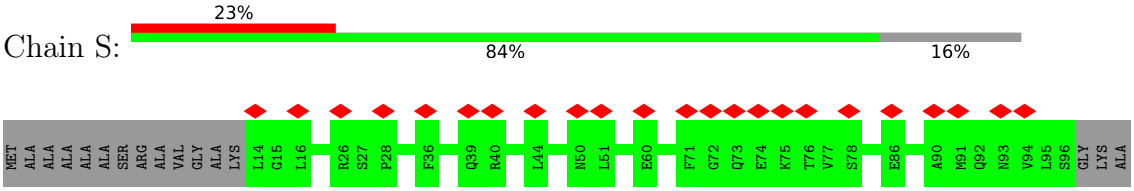
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



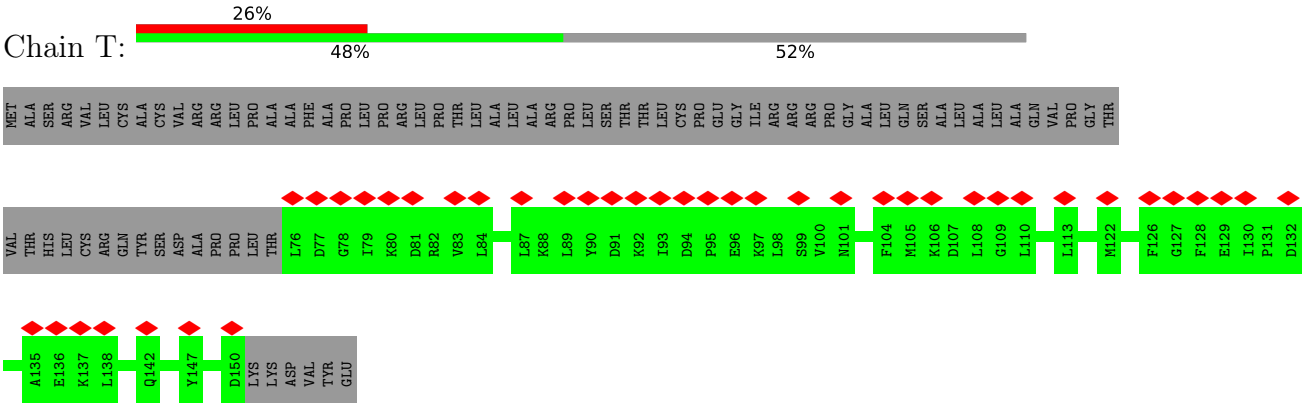
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



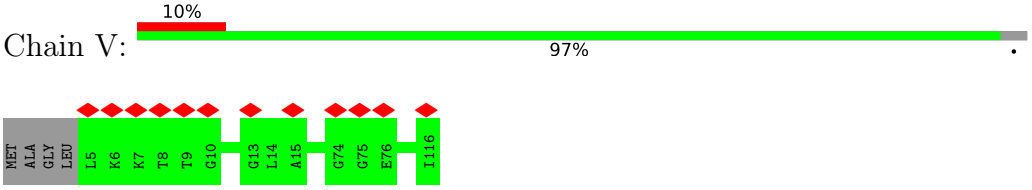
• Molecule 14: Acyl carrier protein, mitochondrial

Chain T:



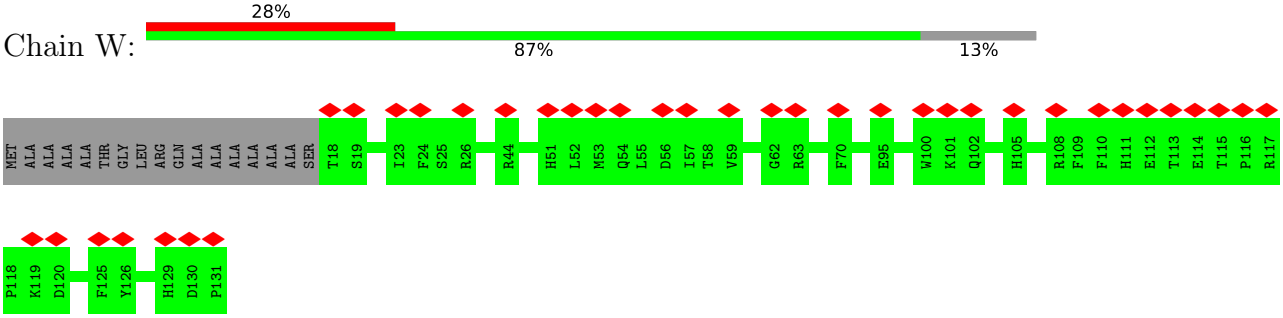
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



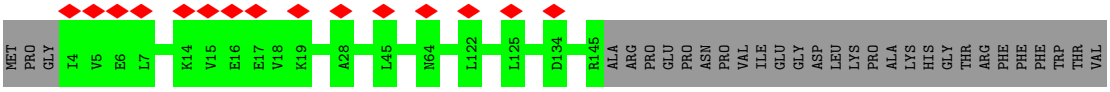
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



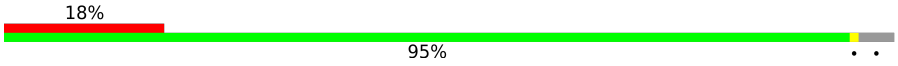
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

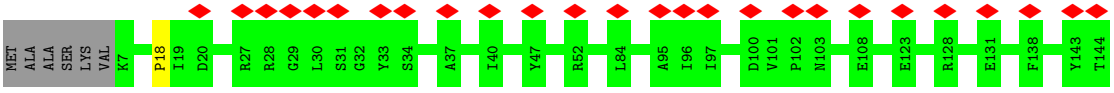
Chain X:



• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

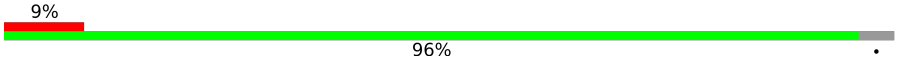
Chain Z:

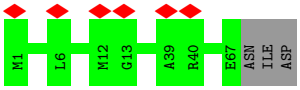




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

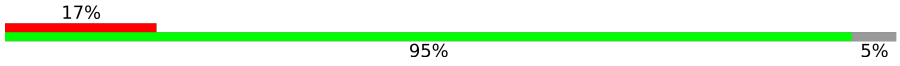
Chain a:

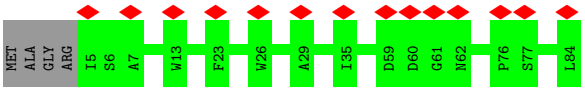




• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

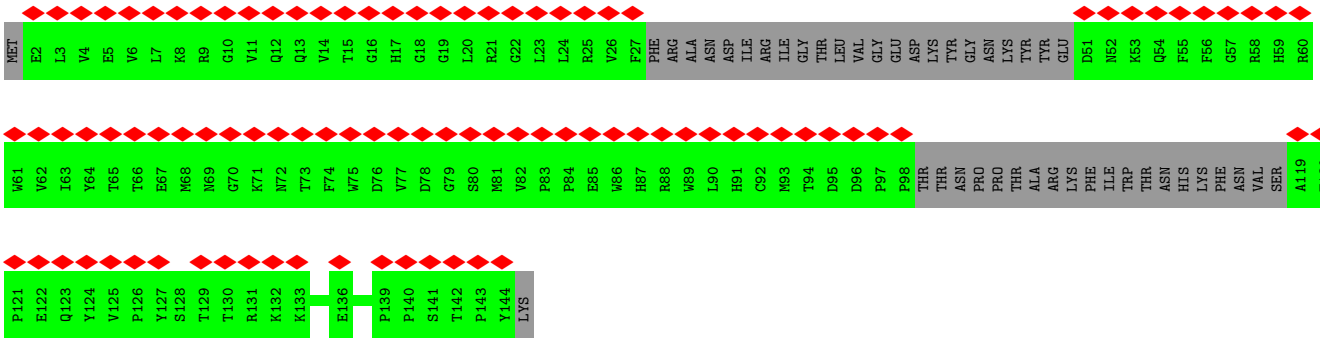
Chain b:





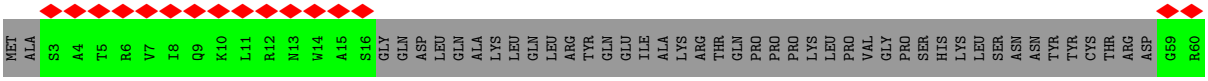
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

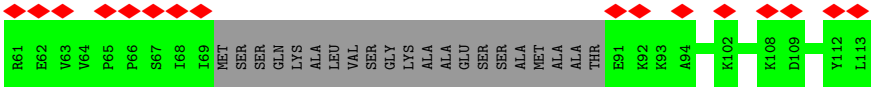
Chain q:



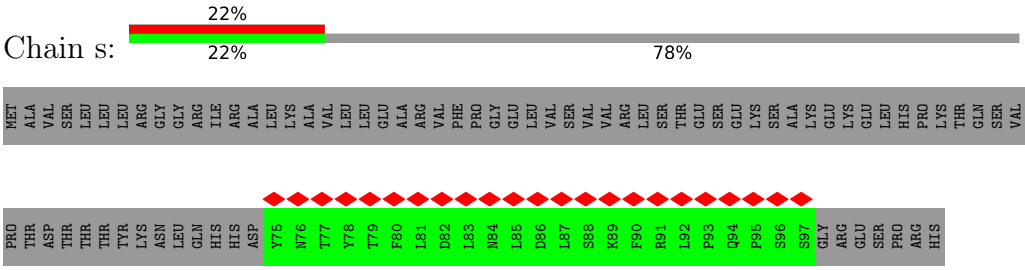
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:





• Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.750	Depositor
Minimum map value	-0.668	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.53	0/755	0.71	0/1030
2	B	0.66	0/1272	0.87	1/1722 (0.1%)
3	C	0.64	0/1689	0.87	2/2300 (0.1%)
4	D	0.63	0/3146	0.87	5/4253 (0.1%)
5	E	0.48	0/1675	0.63	0/2282
6	F	0.57	0/3363	0.84	6/4543 (0.1%)
7	G	0.60	1/5374 (0.0%)	0.92	10/7281 (0.1%)
8	H	0.58	0/2578	0.72	1/3522 (0.0%)
9	I	0.55	0/1409	0.83	0/1904
10	P	0.50	0/2793	0.74	5/3787 (0.1%)
11	Q	0.60	1/963 (0.1%)	0.78	0/1302
12	R	0.51	0/341	0.74	0/457
13	S	0.51	0/678	0.69	0/915
14	T	0.48	0/613	0.62	0/826
15	V	0.54	0/937	0.71	0/1270
16	W	0.52	0/993	0.58	0/1335
17	X	0.48	0/1191	0.67	0/1605
18	Z	0.45	0/1176	0.69	0/1587
19	a	0.59	0/561	0.78	0/755
20	b	0.51	0/651	0.58	0/895
21	q	0.50	0/862	0.78	0/1173
22	r	0.57	0/397	0.86	0/535
23	s	0.59	0/198	0.70	0/269
All	All	0.56	2/33615 (0.0%)	0.79	30/45548 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	106	ARG	C-O	5.78	1.34	1.23
7	G	683	PRO	N-CD	-5.41	1.40	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	174	THR	N-CA-C	-8.13	89.06	111.00
7	G	300	GLN	N-CA-CB	6.60	122.48	110.60
6	F	125	CYS	N-CA-C	-6.49	93.47	111.00
6	F	234	GLY	N-CA-C	6.18	128.55	113.10
7	G	212	LYS	N-CA-C	-6.09	94.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	86/115 (75%)	83 (96%)	3 (4%)	0	100	100
2	B	153/224 (68%)	143 (94%)	9 (6%)	1 (1%)	19	56
3	C	196/263 (74%)	188 (96%)	8 (4%)	0	100	100
4	D	379/463 (82%)	359 (95%)	20 (5%)	0	100	100
5	E	208/248 (84%)	192 (92%)	16 (8%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	637 (93%)	48 (7%)	0	100	100
8	H	309/318 (97%)	278 (90%)	31 (10%)	0	100	100
9	I	168/212 (79%)	155 (92%)	13 (8%)	0	100	100
10	P	337/377 (89%)	311 (92%)	26 (8%)	0	100	100
11	Q	114/175 (65%)	102 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R	43/116 (37%)	40 (93%)	3 (7%)	0	100	100
13	S	81/99 (82%)	72 (89%)	9 (11%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
16	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
17	X	140/172 (81%)	124 (89%)	16 (11%)	0	100	100
18	Z	136/144 (94%)	127 (93%)	8 (6%)	1 (1%)	19	56
19	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
20	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
21	q	94/145 (65%)	86 (92%)	8 (8%)	0	100	100
22	r	42/113 (37%)	42 (100%)	0	0	100	100
23	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
All	All	4054/5036 (80%)	3765 (93%)	287 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	195	PRO
18	Z	18	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/104 (79%)	82 (100%)	0	100	100
2	B	131/185 (71%)	130 (99%)	1 (1%)	79	84
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	331/395 (84%)	331 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	341/370 (92%)	341 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	579/610 (95%)	579 (100%)	0	100	100
8	H	275/280 (98%)	275 (100%)	0	100	100
9	I	146/178 (82%)	146 (100%)	0	100	100
10	P	296/325 (91%)	296 (100%)	0	100	100
11	Q	103/153 (67%)	103 (100%)	0	100	100
12	R	35/96 (36%)	35 (100%)	0	100	100
13	S	74/80 (92%)	74 (100%)	0	100	100
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	119/123 (97%)	119 (100%)	0	100	100
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	91/131 (70%)	91 (100%)	0	100	100
22	r	43/96 (45%)	43 (100%)	0	100	100
23	s	23/95 (24%)	23 (100%)	0	100	100
All	All	3566/4292 (83%)	3565 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
15	V	110	ASN
16	W	61	GLN
17	X	99	HIS
7	G	74	ASN
7	G	59	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
28	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.19	6 (12%)
24	3PE	A	202	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	2 (4%)
31	EHZ	W	201	-	30,34,37	1.80	7 (23%)	40,44,47	1.41	5 (12%)
25	SF4	G	802	-	0,12,12	-	-	-		
27	FES	E	301	5	0,4,4	-	-	-		
24	3PE	A	201	-	41,41,50	1.00	2 (4%)	44,46,55	1.09	2 (4%)
26	PC1	B	303	-	42,42,53	1.04	2 (4%)	48,50,61	1.01	3 (6%)
29	NDP	P	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.20	4 (7%)
27	FES	G	803	7	0,4,4	-	-	-		
25	SF4	I	301	9	0,12,12	-	-	-		
25	SF4	G	801	7	0,12,12	-	-	-		
25	SF4	B	301	2	0,12,12	-	-	-		
25	SF4	F	502	6	0,12,12	-	-	-		
25	SF4	I	302	9	0,12,12	-	-	-		
26	PC1	B	302	-	34,34,53	1.14	2 (5%)	40,42,61	1.12	3 (7%)

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	FMN	F	501	-	-	4/18/18/18	0/3/3/3
24	3PE	A	202	-	-	13/51/51/54	-
31	EHZ	W	201	-	-	26/42/42/45	-
25	SF4	G	802	-	-	-	0/6/5/5
27	FES	E	301	5	-	-	0/1/1/1
24	3PE	A	201	-	-	12/45/45/54	-
26	PC1	B	303	-	-	14/46/46/57	-
29	NDP	P	401	-	-	6/30/77/77	0/5/5/5
27	FES	G	803	7	-	-	0/1/1/1
25	SF4	I	301	9	-	-	0/6/5/5
25	SF4	G	801	7	-	-	0/6/5/5
25	SF4	B	301	2	-	-	0/6/5/5
25	SF4	F	502	6	-	-	0/6/5/5
25	SF4	I	302	9	-	-	0/6/5/5
26	PC1	B	302	-	-	13/38/38/57	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	W	201	EHZ	C15-N2	5.44	1.45	1.33
31	W	201	EHZ	C12-N1	5.23	1.45	1.33
28	F	501	FMN	C9A-C5A	4.77	1.49	1.41
24	A	201	3PE	O31-C31	4.26	1.45	1.33
26	B	302	PC1	O31-C31	4.19	1.45	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	W	201	EHZ	C8-C9-S1	4.96	119.77	113.63
29	P	401	NDP	PN-O3-PA	-4.03	119.00	132.83
24	A	202	3PE	O21-C21-C22	4.02	120.17	111.50
26	B	303	PC1	O21-C21-C22	3.98	120.07	111.50
24	A	201	3PE	O21-C21-C22	3.89	119.89	111.50

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

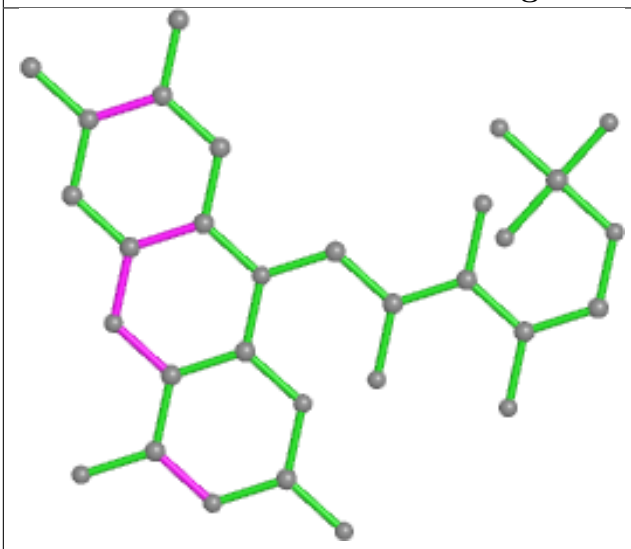
Mol	Chain	Res	Type	Atoms
24	A	201	3PE	C1-O11-P-O14
24	A	201	3PE	C11-O13-P-O11
24	A	201	3PE	C11-O13-P-O14
24	A	201	3PE	C22-C21-O21-C2
24	A	202	3PE	C1-O11-P-O14

There are no ring outliers.

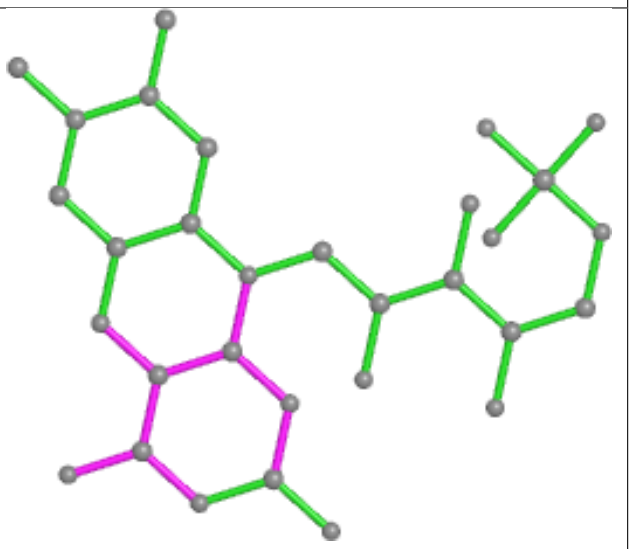
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

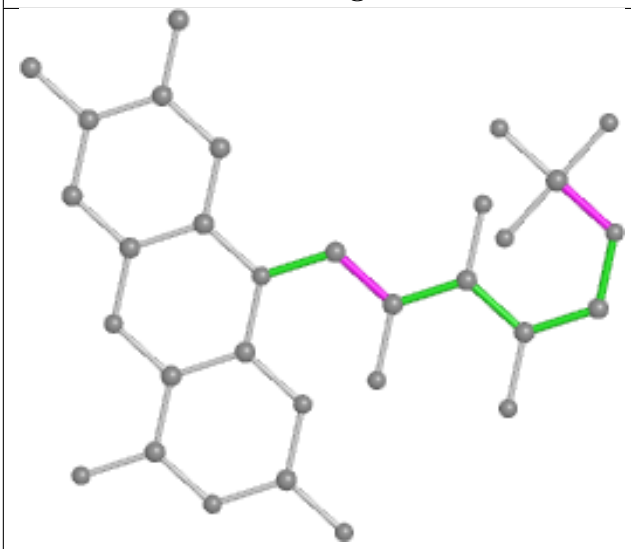
Ligand FMN F 501



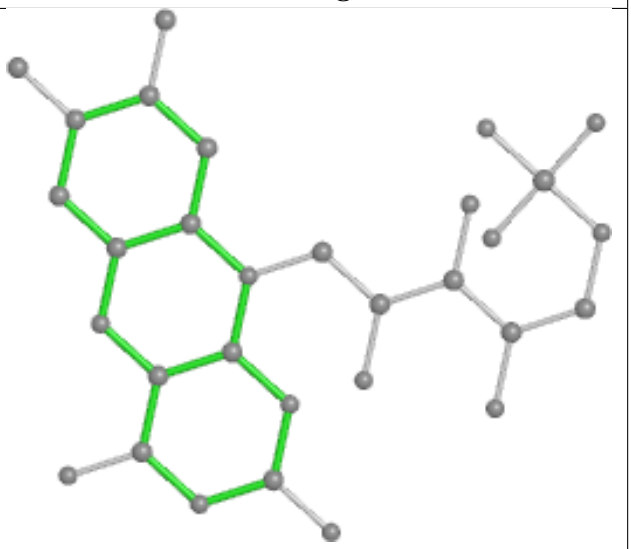
Bond lengths



Bond angles

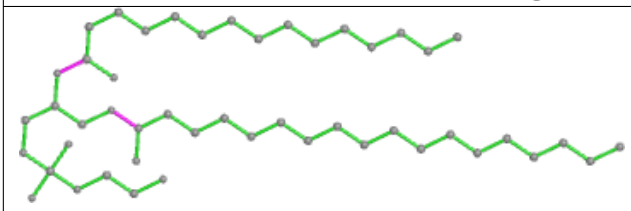


Torsions

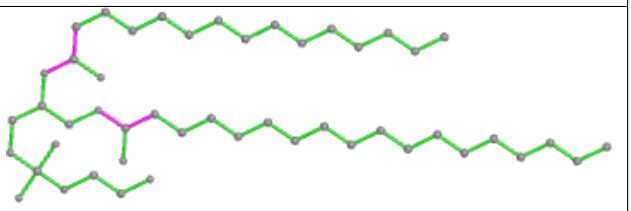


Rings

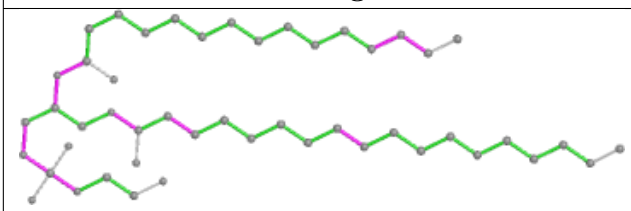
Ligand 3PE A 202



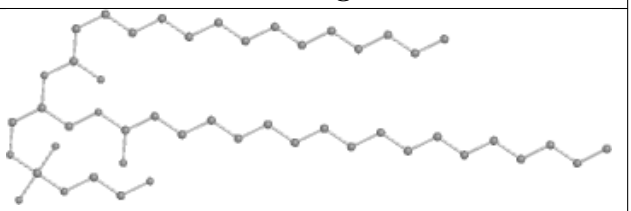
Bond lengths



Bond angles

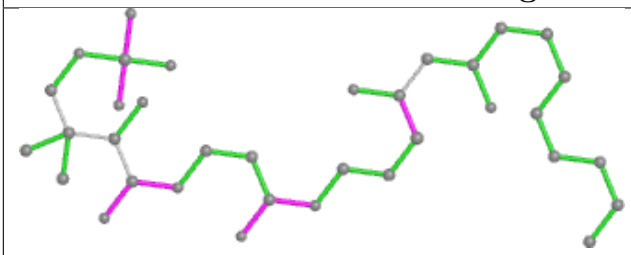


Torsions

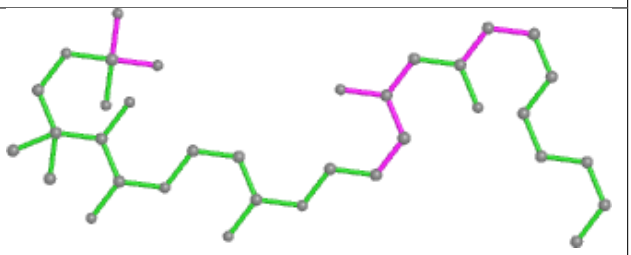


Rings

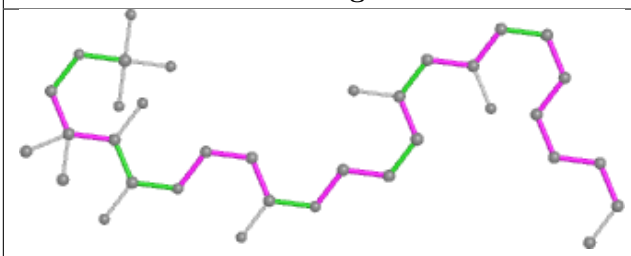
Ligand EHZ W 201



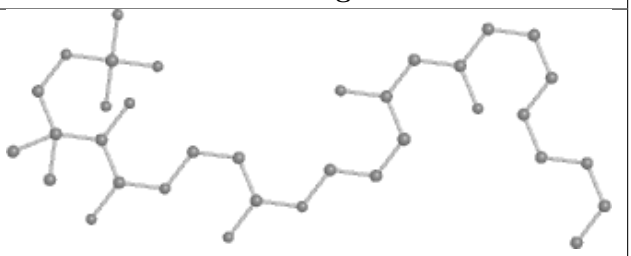
Bond lengths



Bond angles

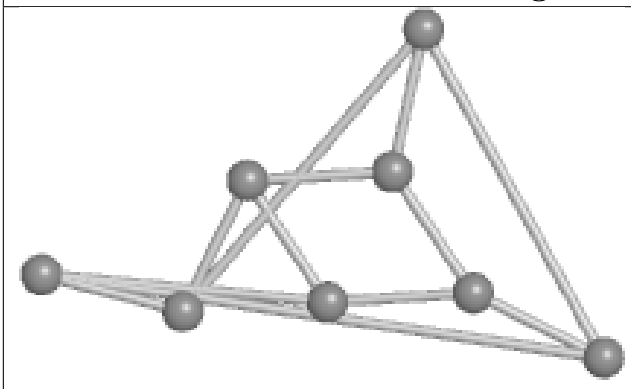


Torsions

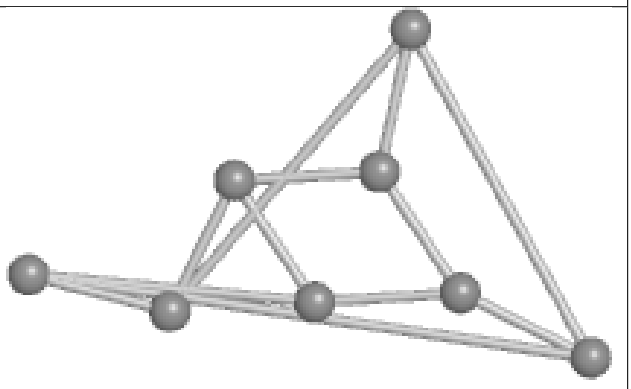


Rings

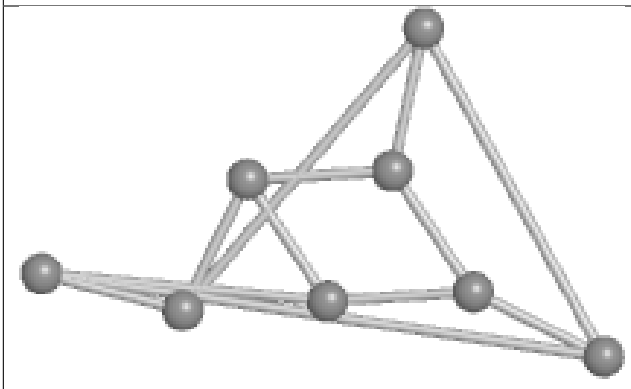
Ligand SF4 G 802



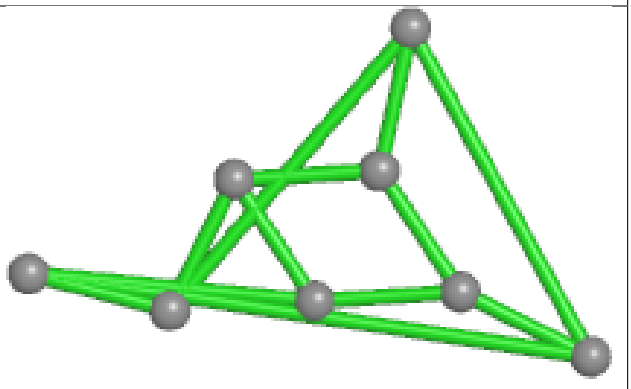
Bond lengths



Bond angles

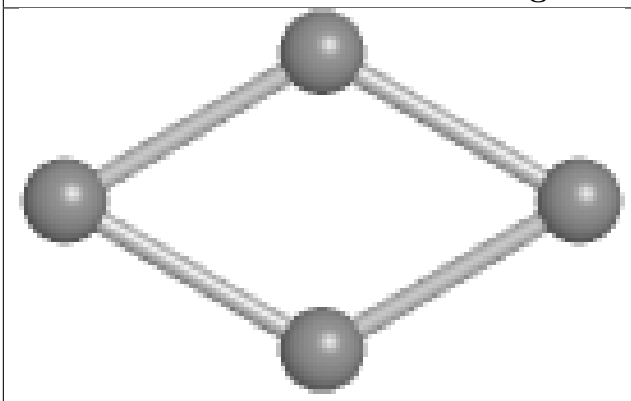


Torsions

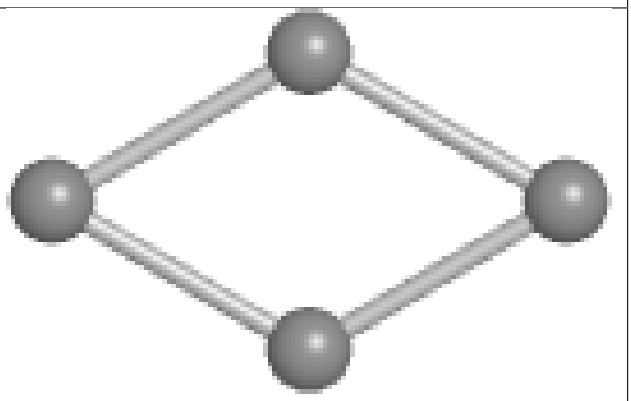


Rings

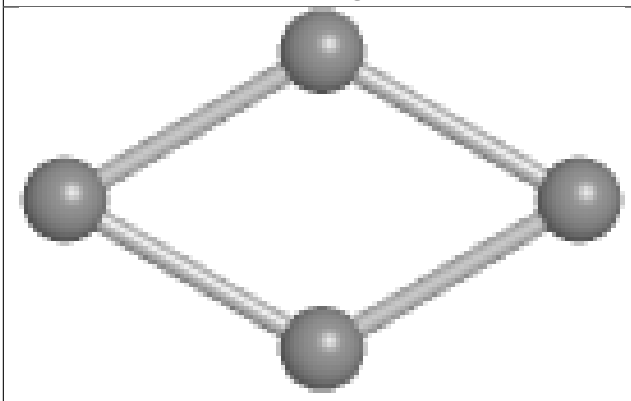
Ligand FES E 301



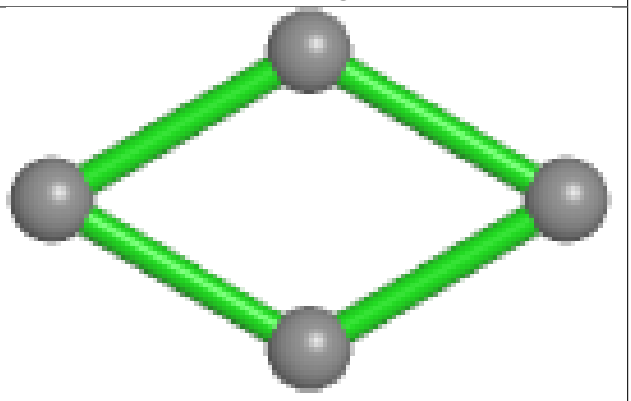
Bond lengths



Bond angles

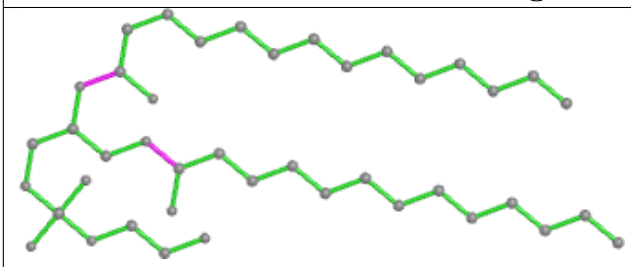


Torsions

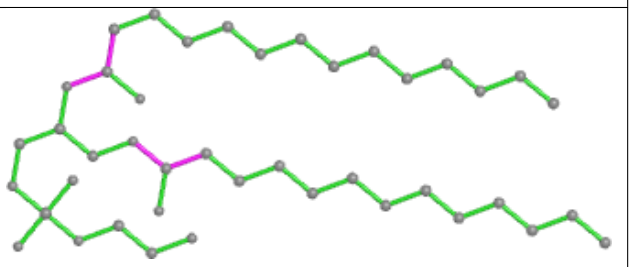


Rings

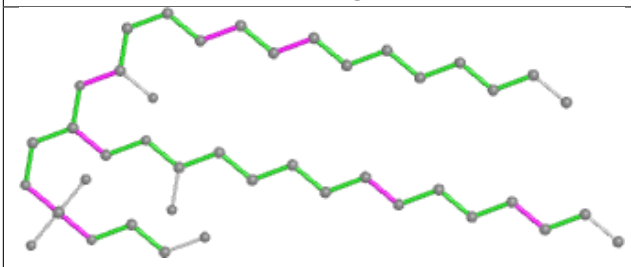
Ligand 3PE A 201



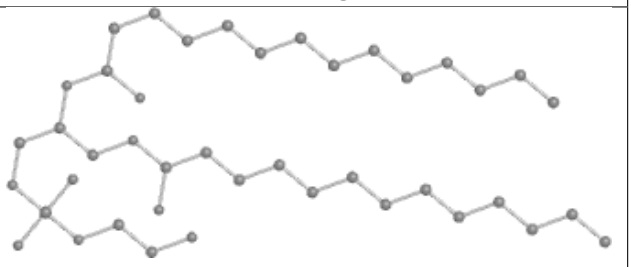
Bond lengths



Bond angles

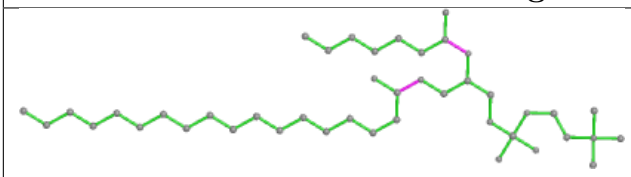


Torsions

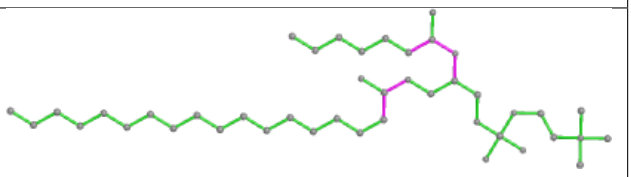


Rings

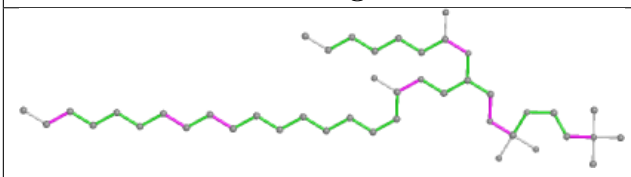
Ligand PC1 B 303



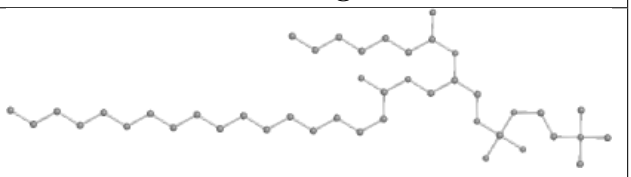
Bond lengths



Bond angles

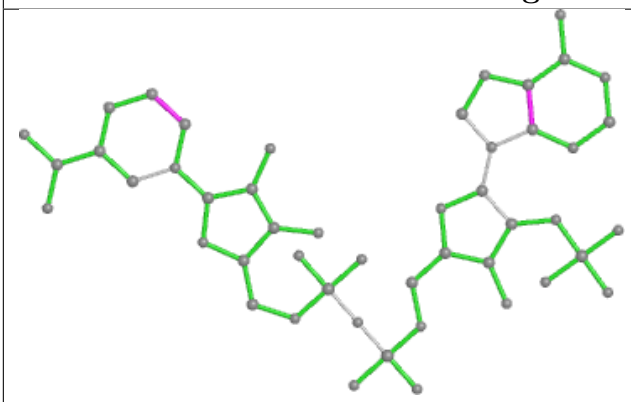


Torsions

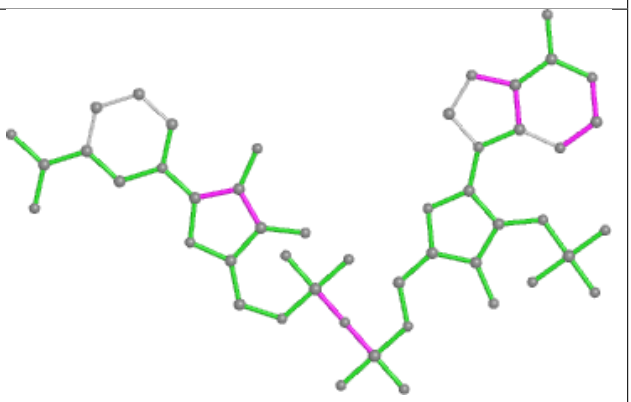


Rings

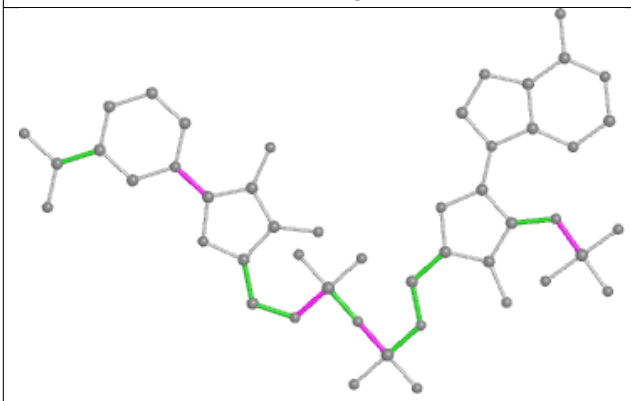
Ligand NDP P 401



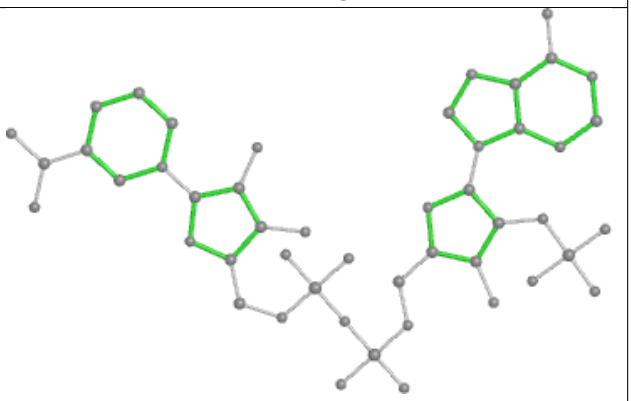
Bond lengths



Bond angles

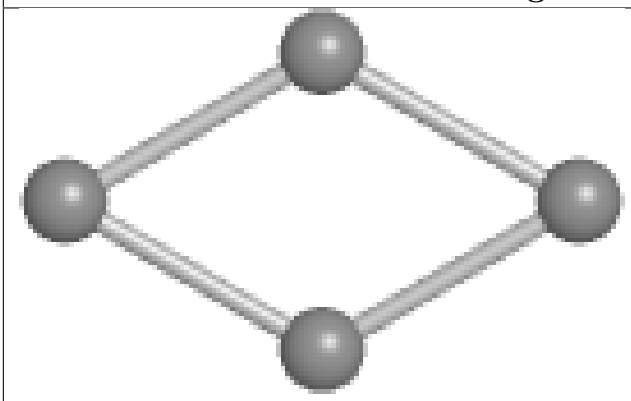


Torsions

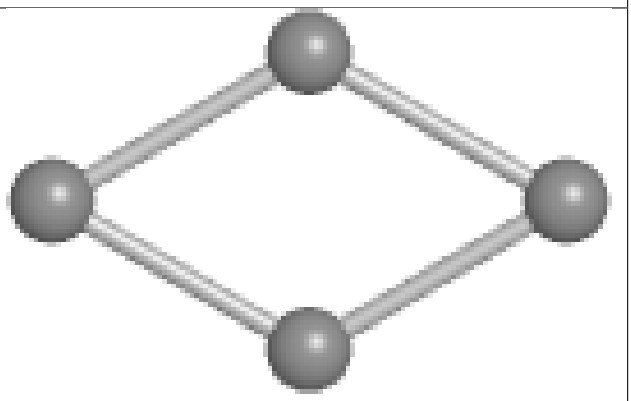


Rings

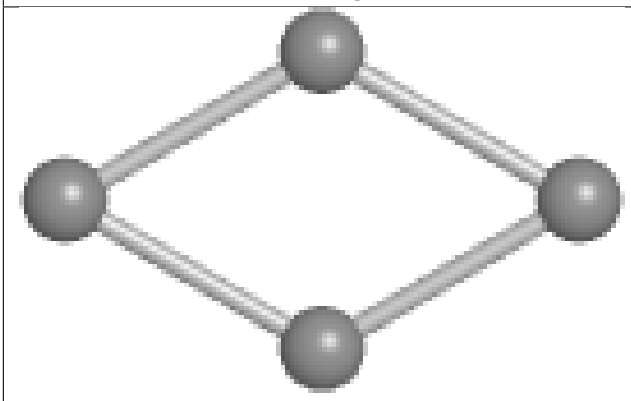
Ligand FES G 803



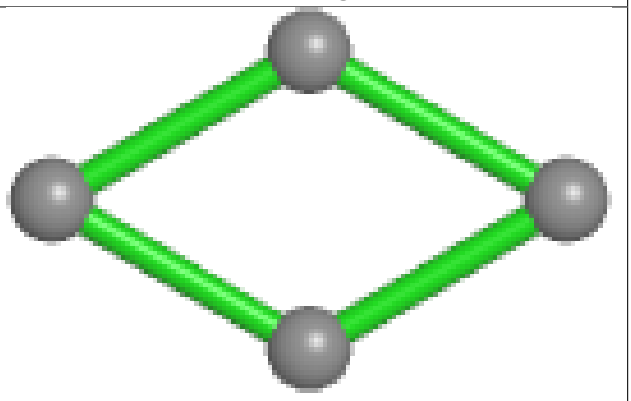
Bond lengths



Bond angles

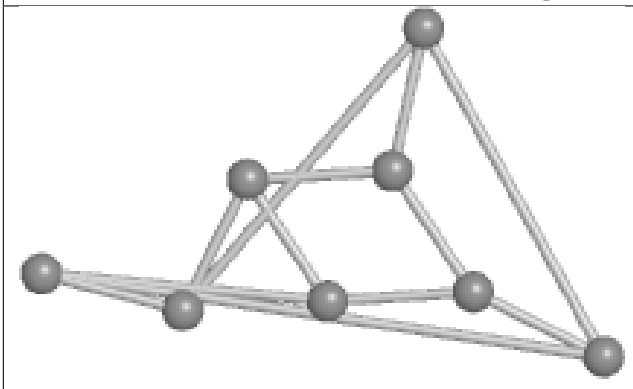


Torsions

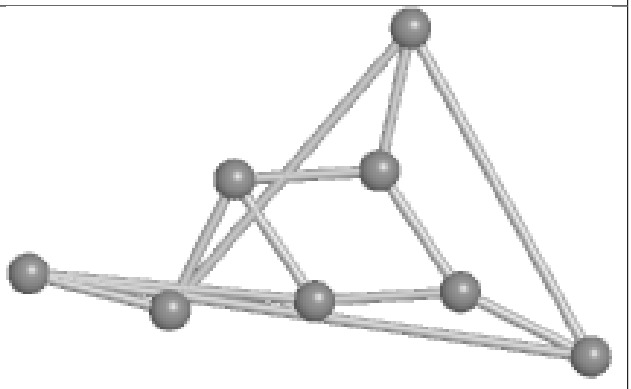


Rings

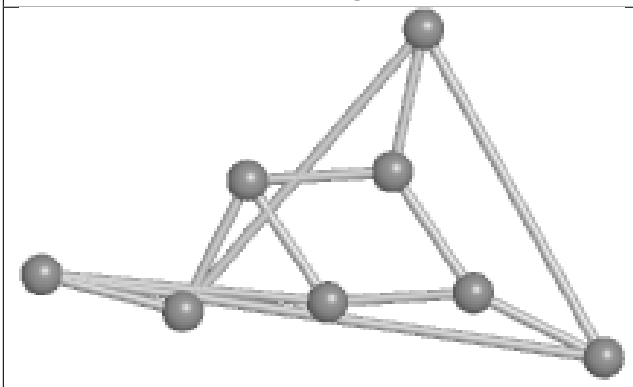
Ligand SF4 I 301



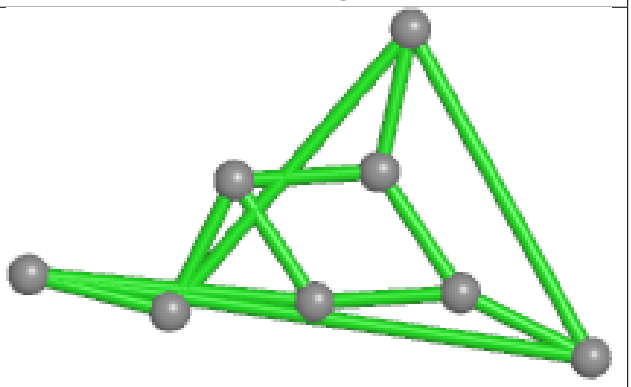
Bond lengths



Bond angles

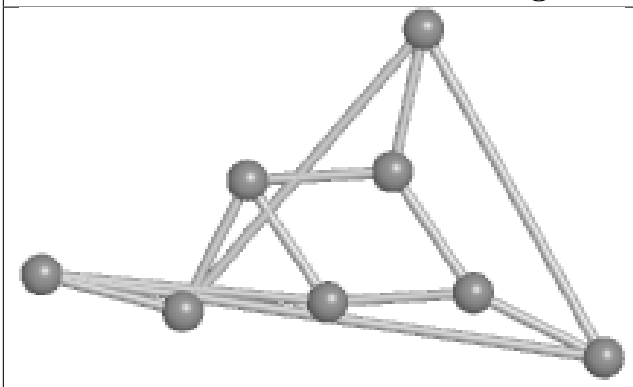


Torsions

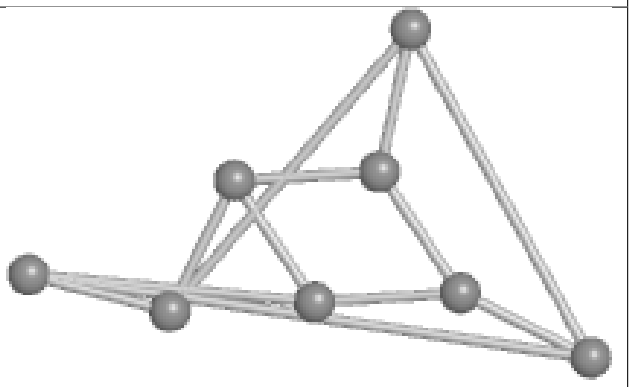


Rings

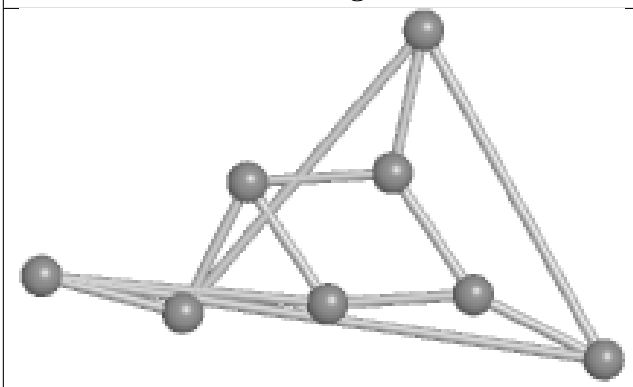
Ligand SF4 G 801



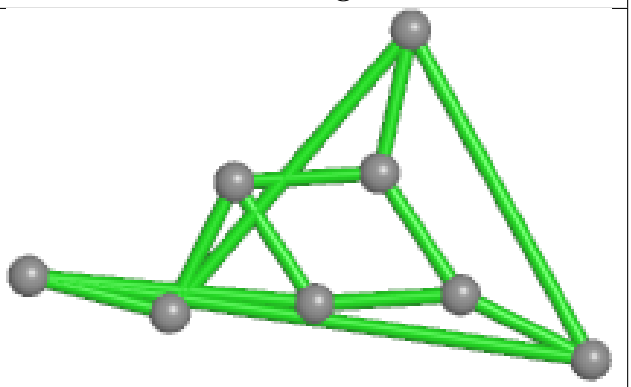
Bond lengths



Bond angles

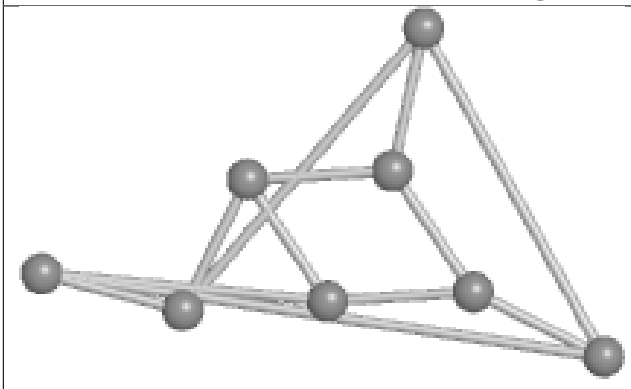


Torsions

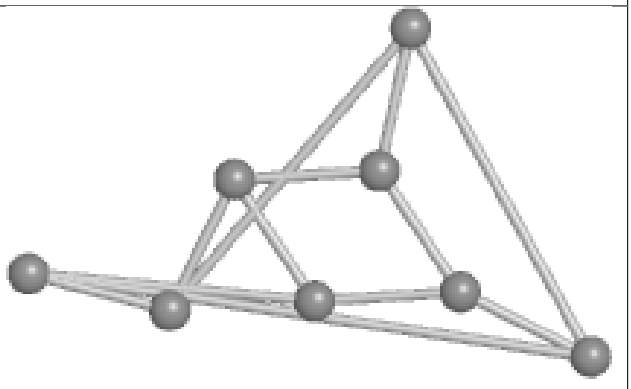


Rings

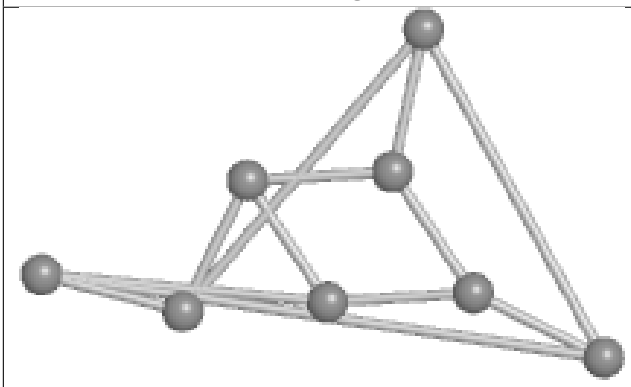
Ligand SF4 B 301



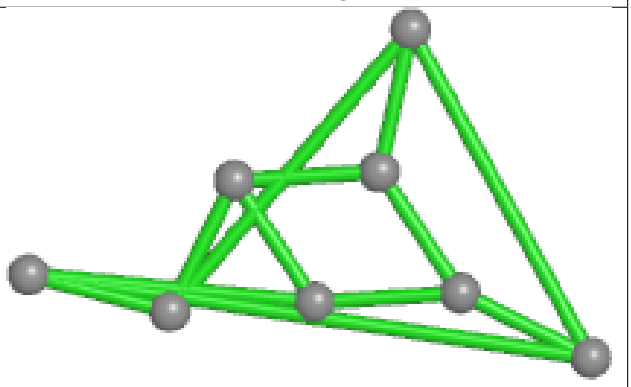
Bond lengths



Bond angles

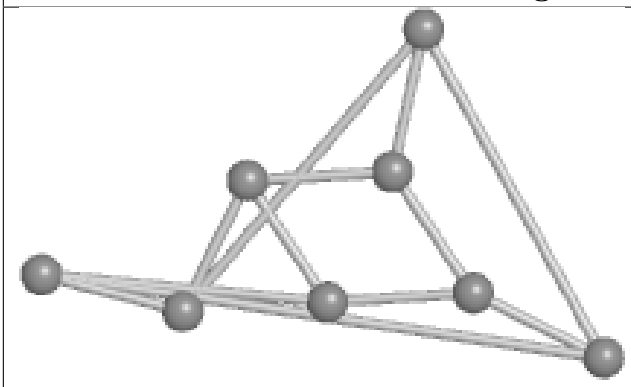


Torsions

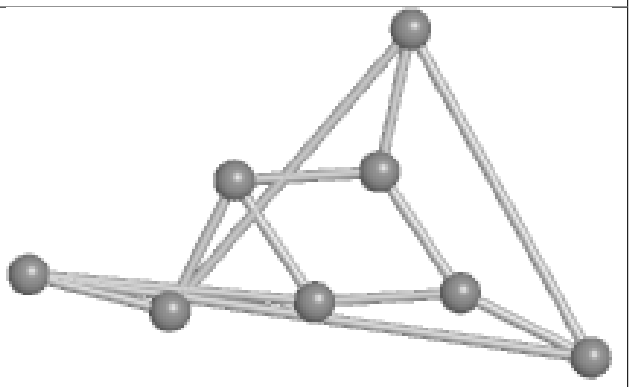


Rings

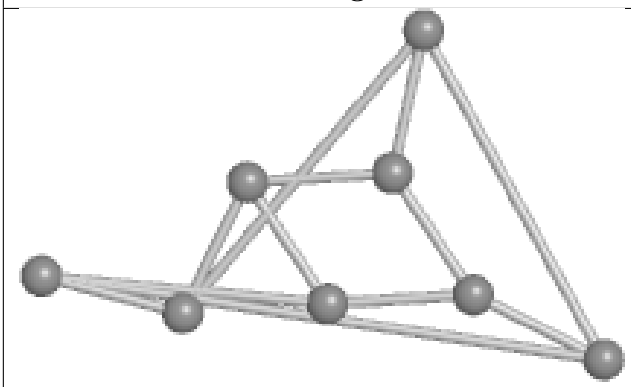
Ligand SF4 F 502



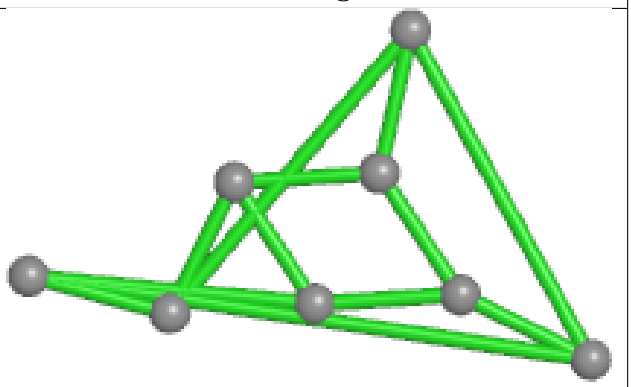
Bond lengths



Bond angles

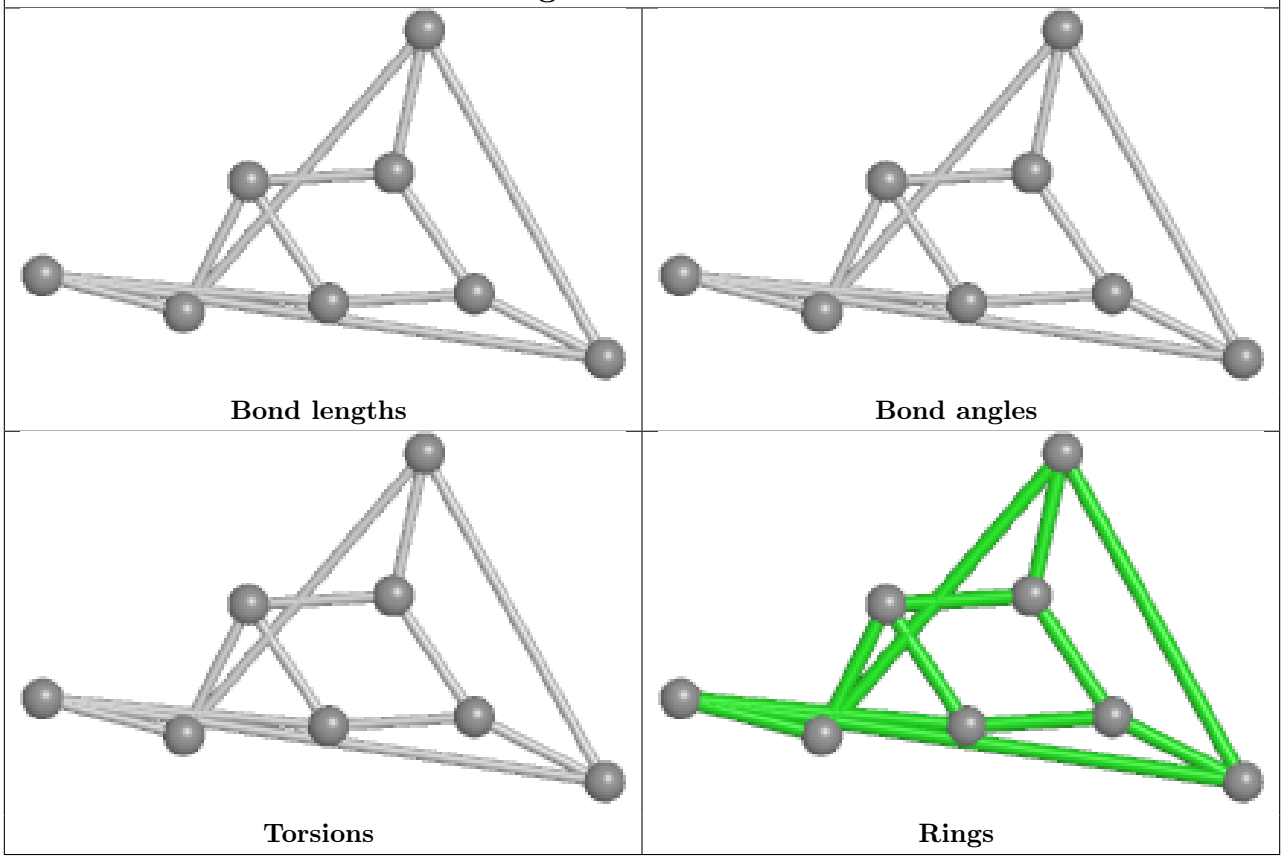


Torsions

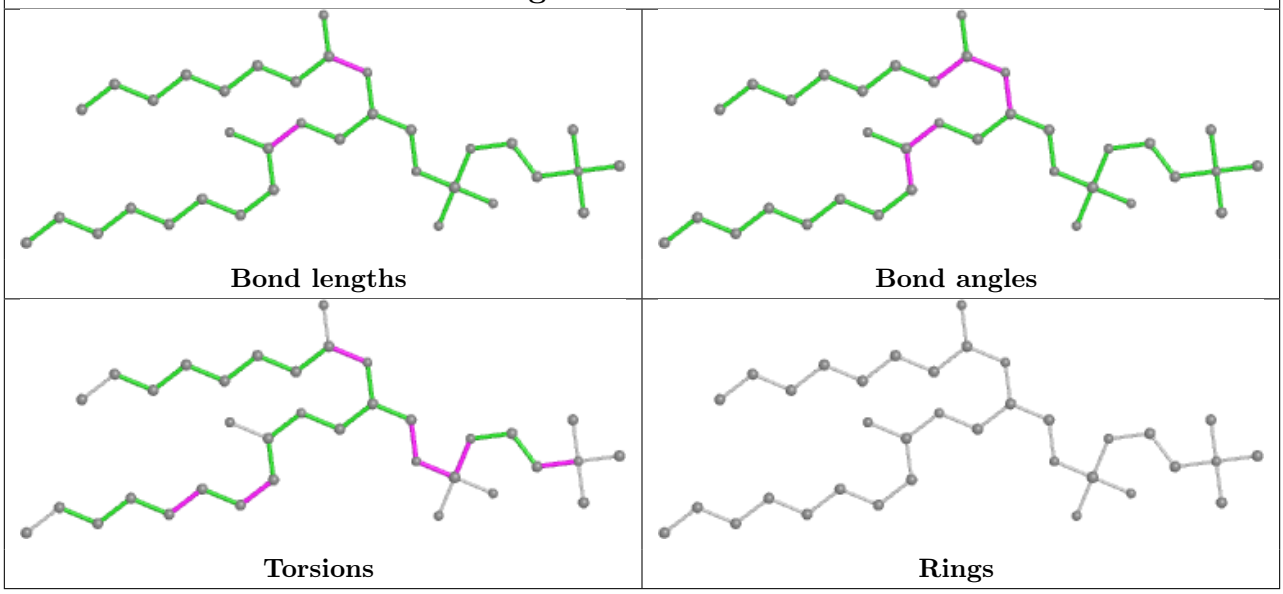


Rings

Ligand SF4 I 302



Ligand PC1 B 302



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.

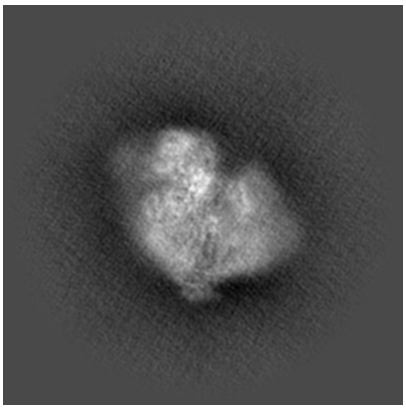
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38519. These allow visual inspection of the internal detail of the map and identification of artifacts.

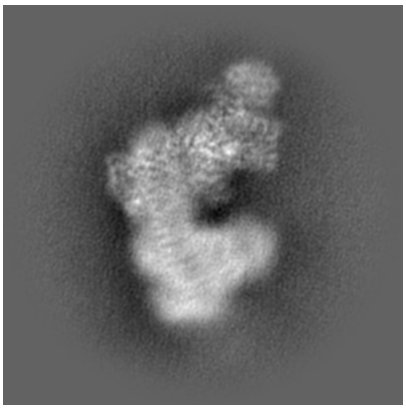
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

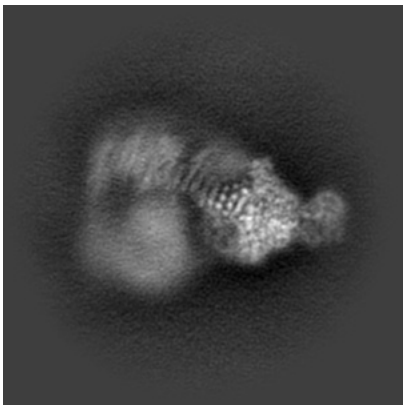
6.1.1 Primary map



X

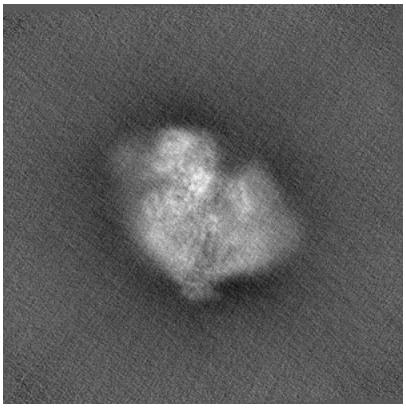


Y

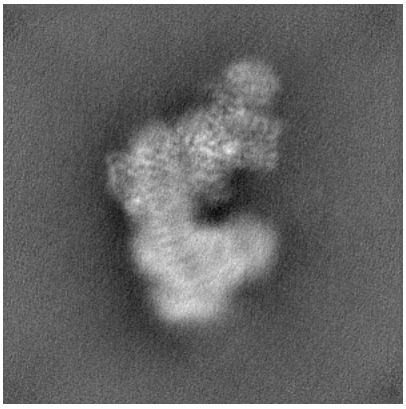


Z

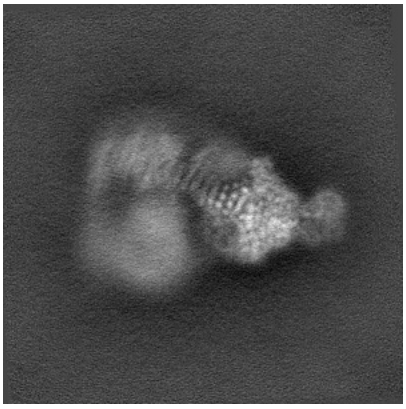
6.1.2 Raw map



X



Y

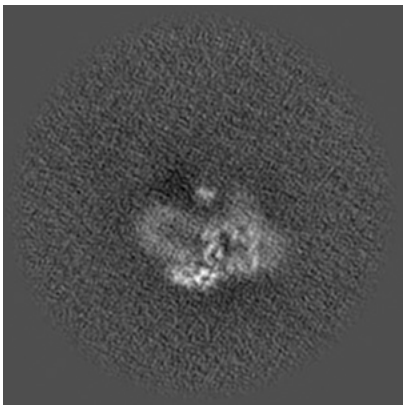


Z

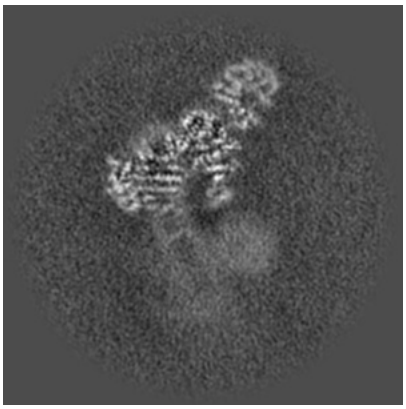
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

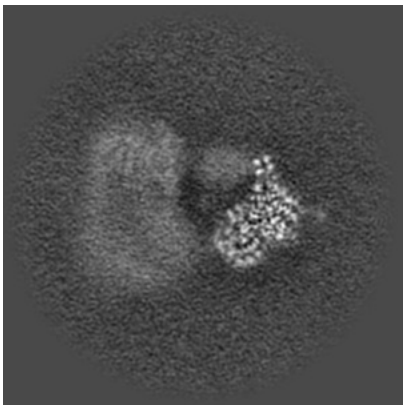
6.2.1 Primary map



X Index: 192

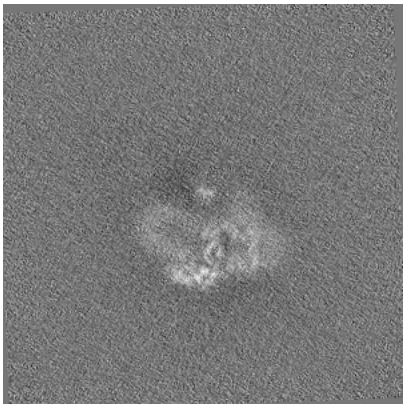


Y Index: 192

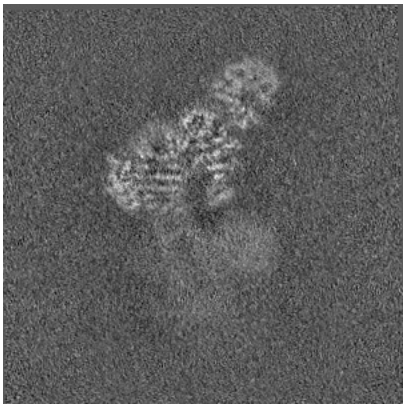


Z Index: 192

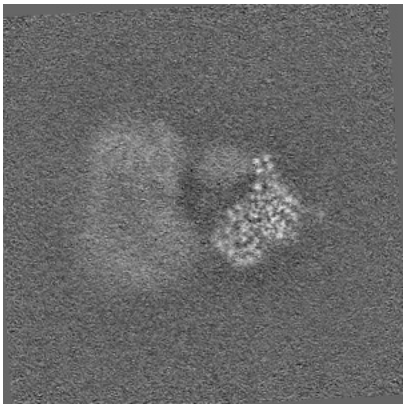
6.2.2 Raw map



X Index: 192



Y Index: 192

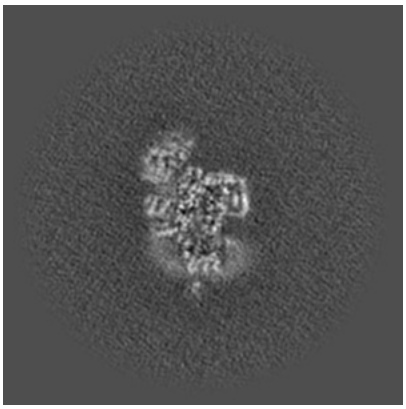


Z Index: 192

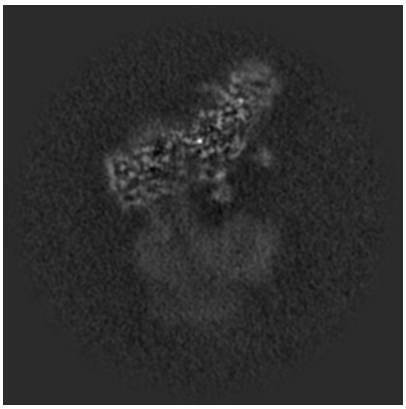
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

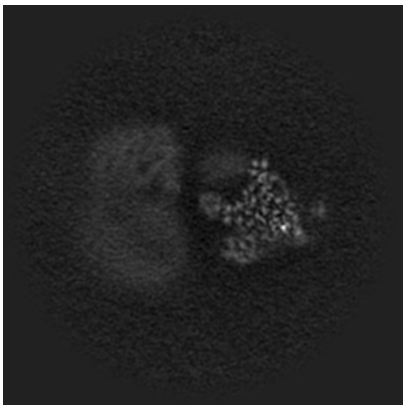
6.3.1 Primary map



X Index: 243

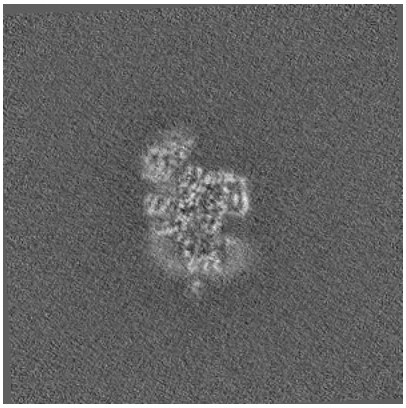


Y Index: 181

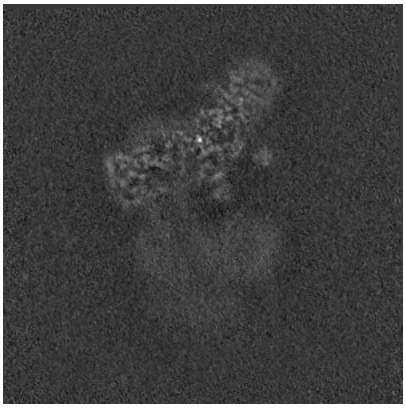


Z Index: 201

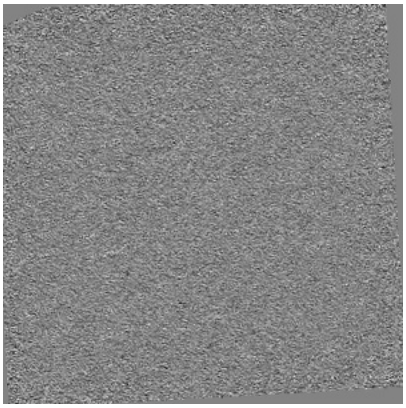
6.3.2 Raw map



X Index: 243



Y Index: 180

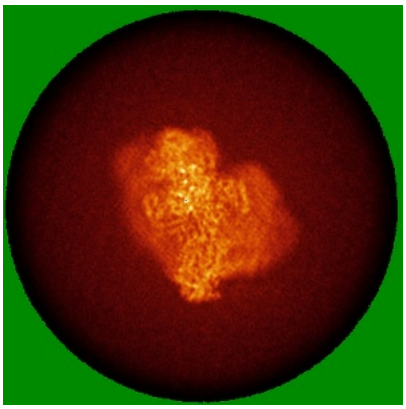


Z Index: 8

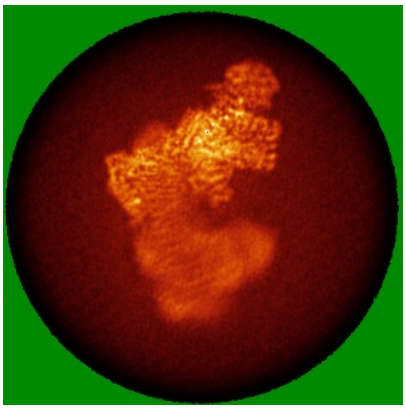
The images above show the largest variance slices of the map in three orthogonal directions.

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

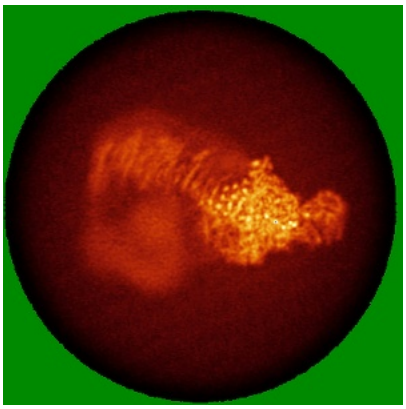
6.4.1 Primary map



X

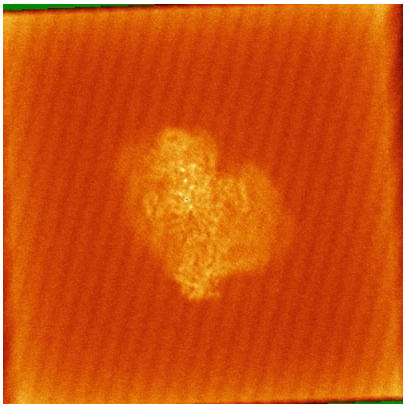


Y

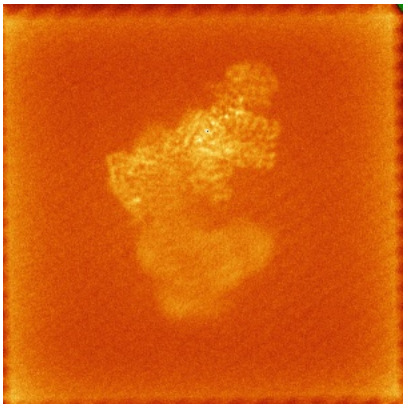


Z

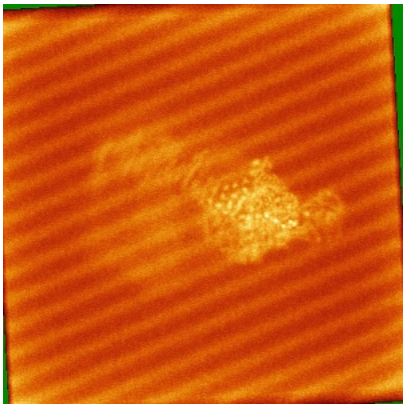
6.4.2 Raw map



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 0.4. 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.

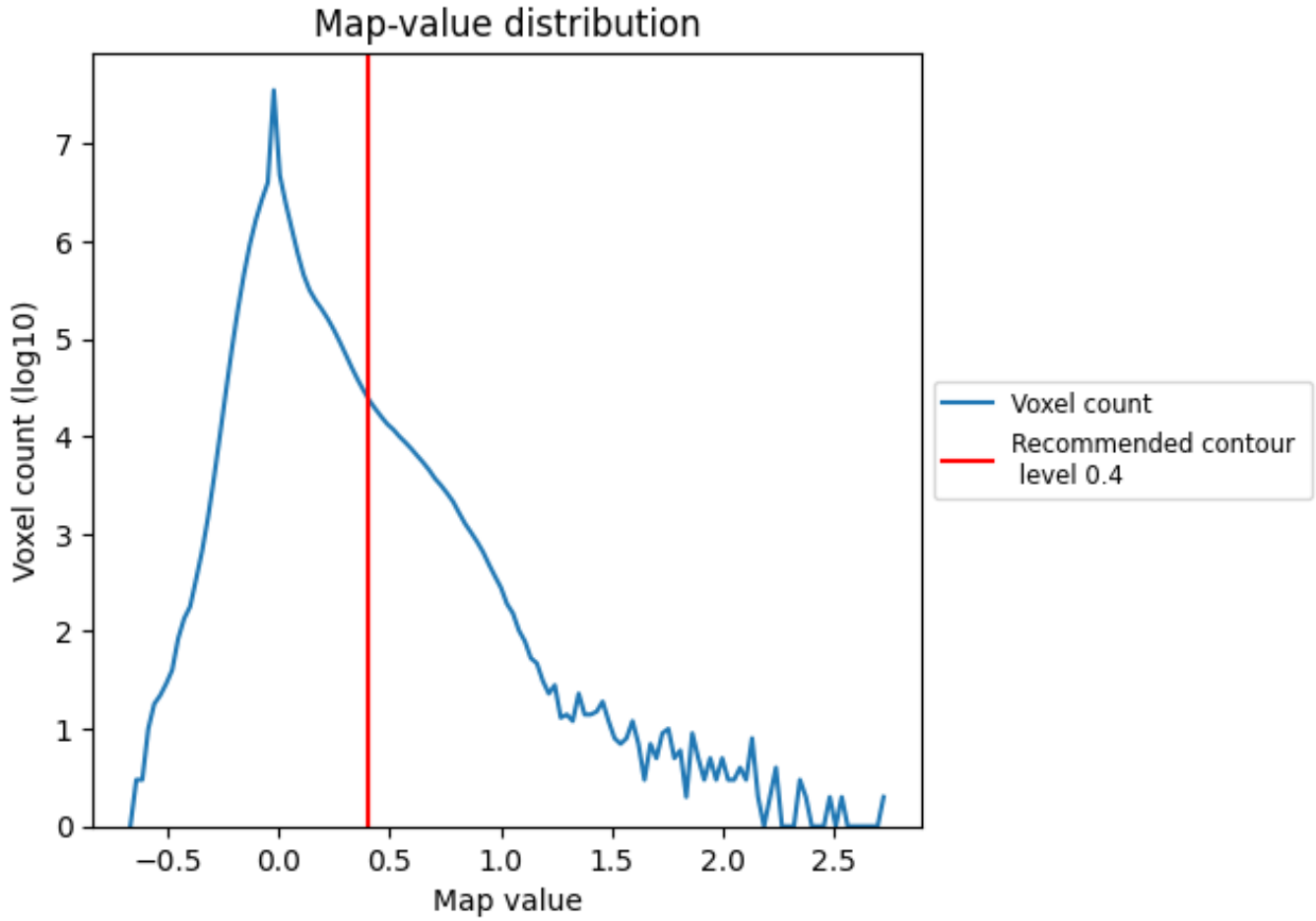
6.6 Mask visualisation (i)

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

7 Map analysis

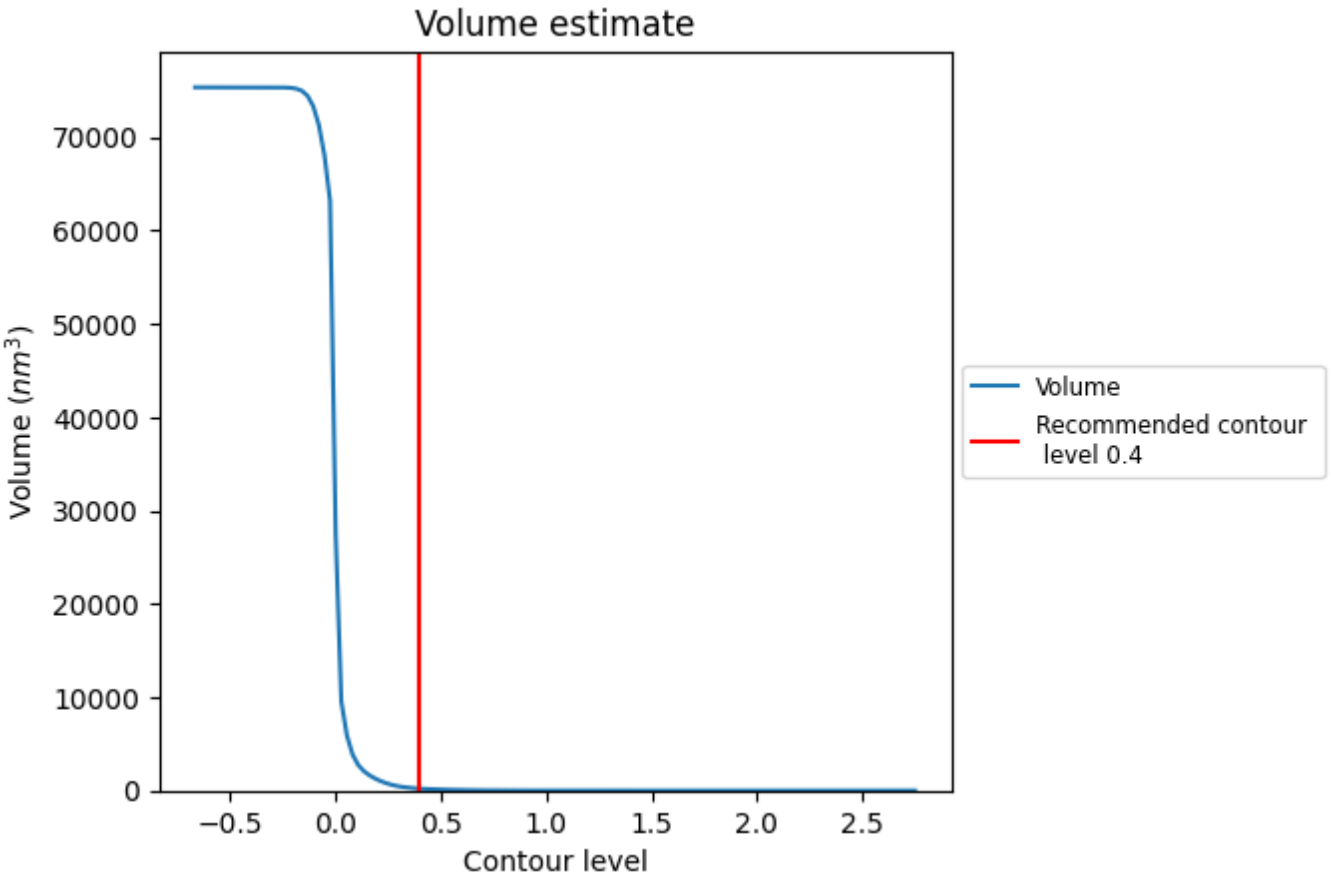
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

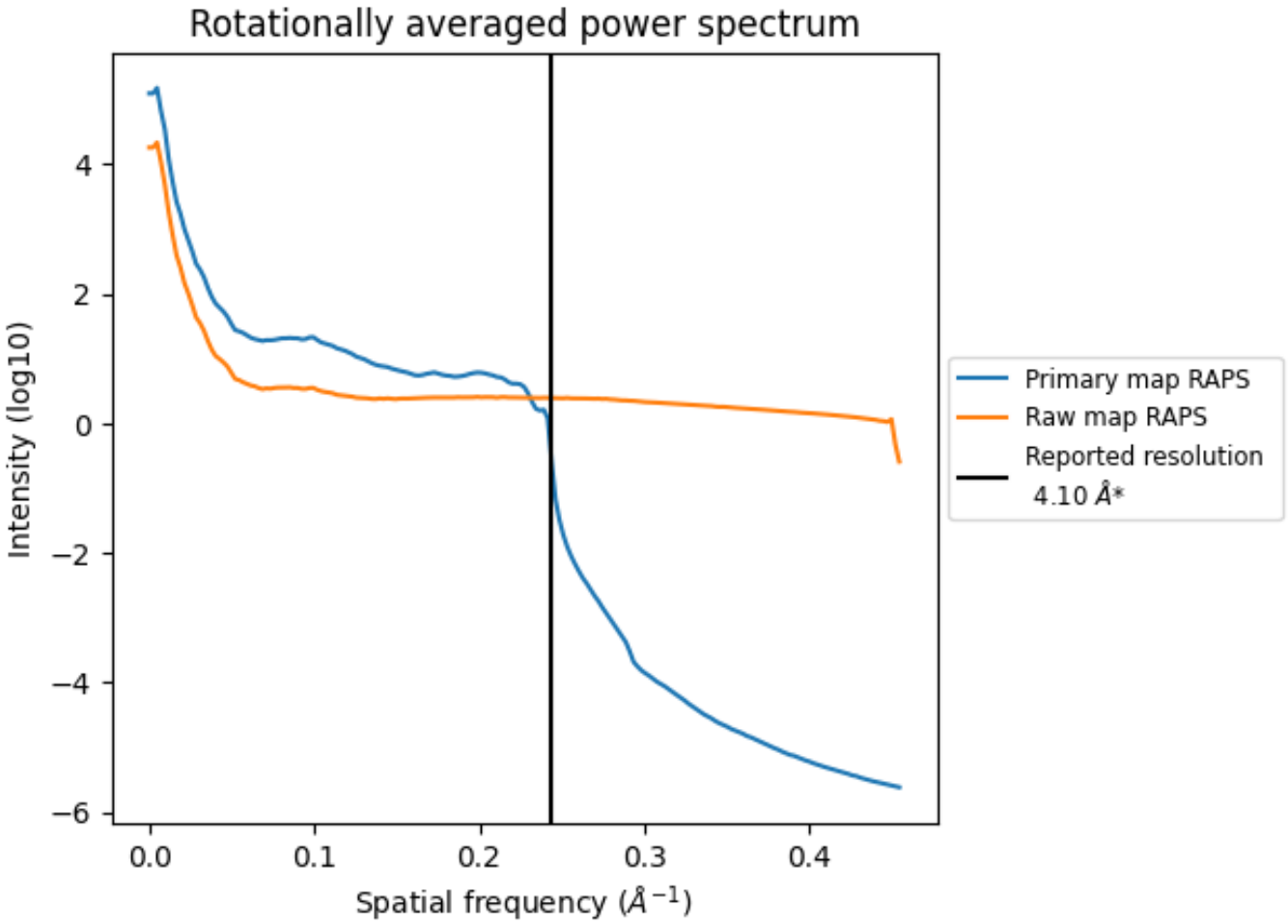
7.2 Volume estimate (i)



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 185 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)

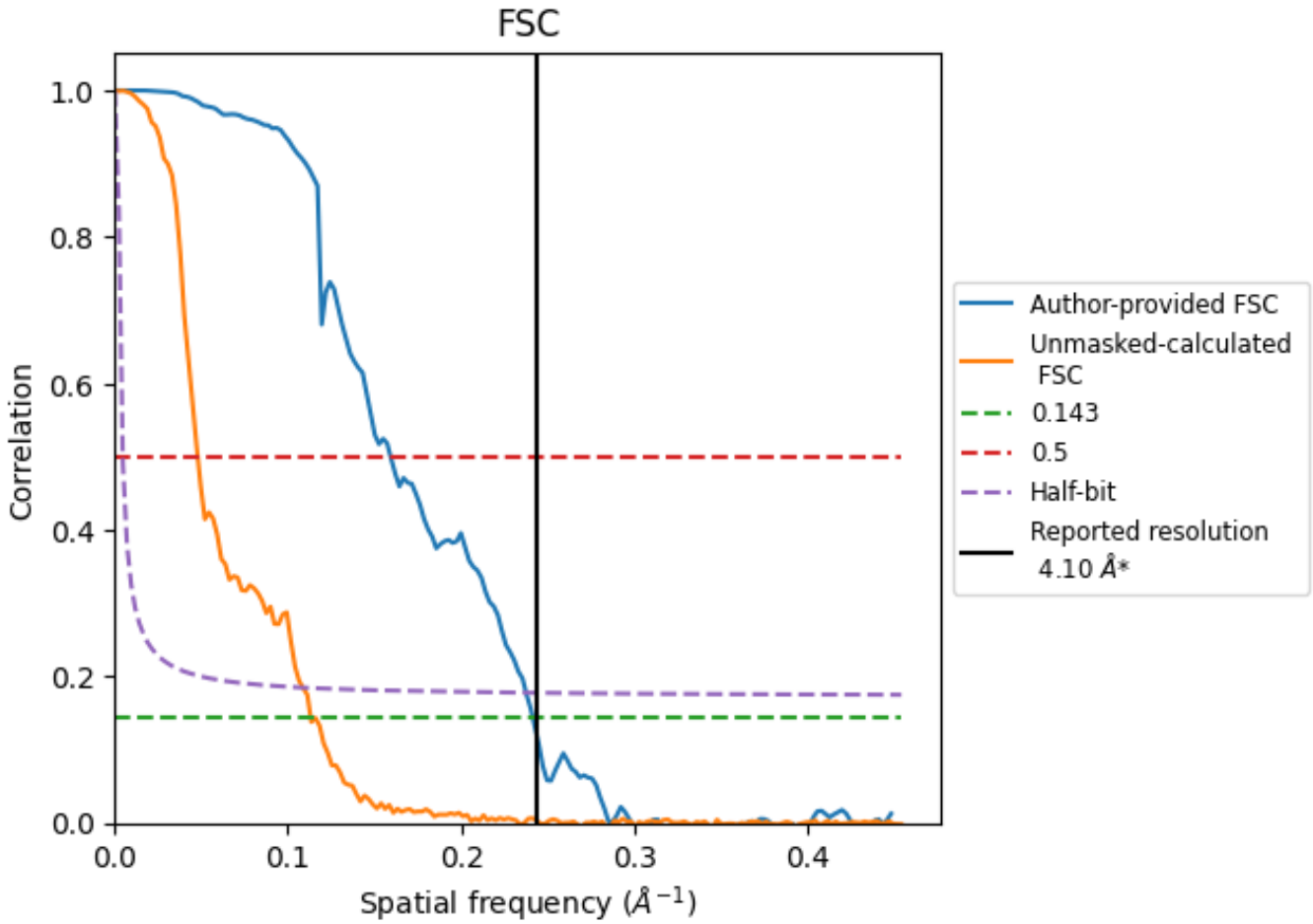


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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)

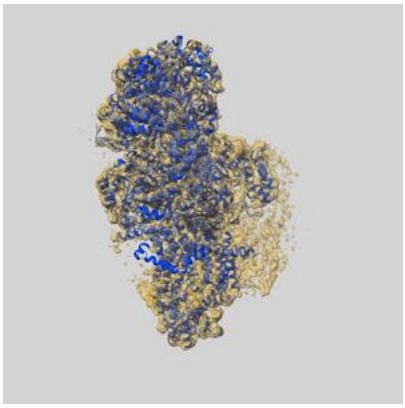
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	6.27	4.21
Unmasked-calculated*	8.83	20.83	9.20

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

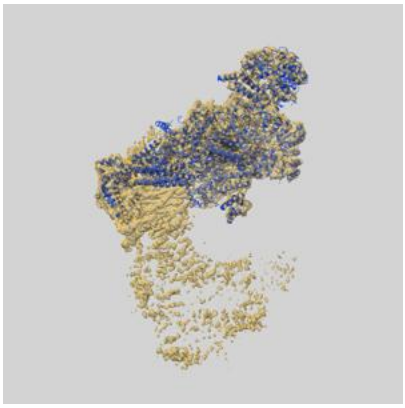
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38519 and PDB model 8XNY. Per-residue inclusion information can be found in section 3 on page 13.

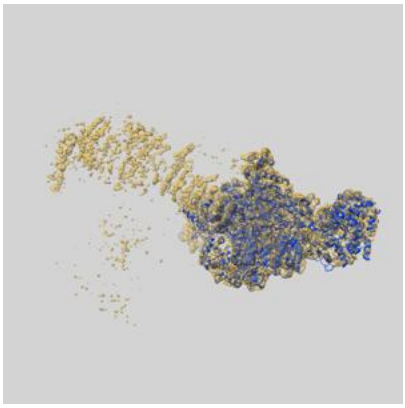
9.1 Map-model overlay



X



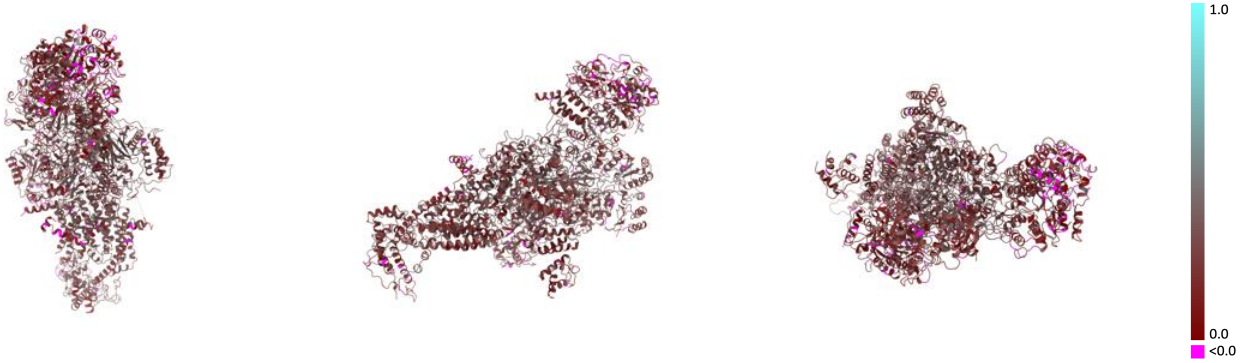
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

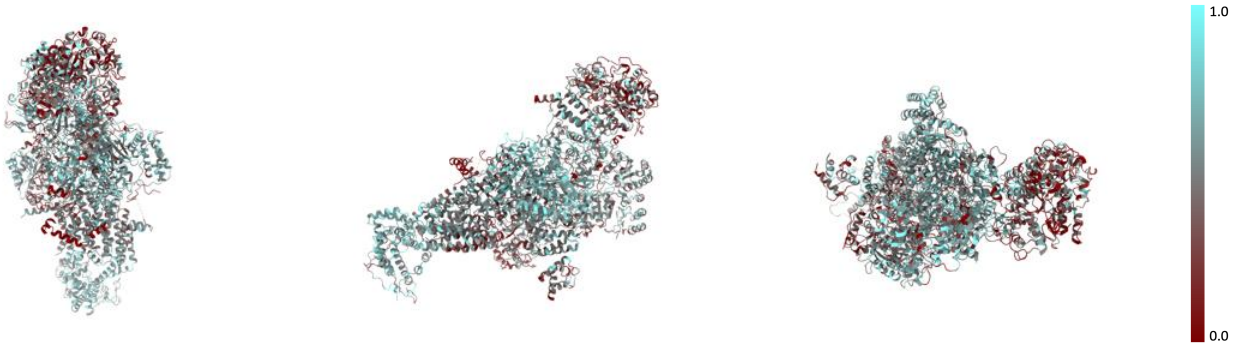
9.2 Q-score mapped to coordinate model



X Y Z

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

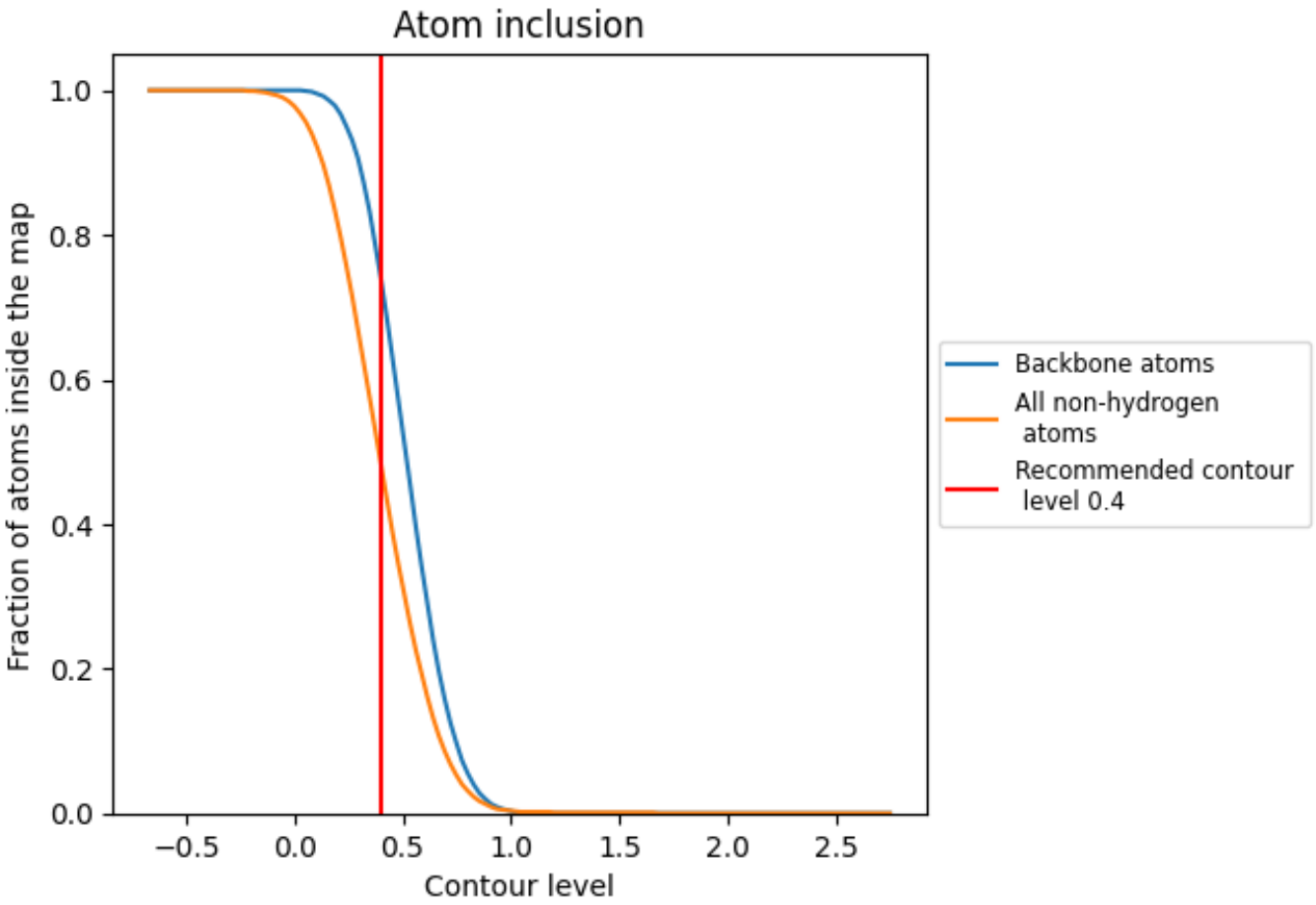
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 48% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4820	0.2450
A	0.3630	0.2210
B	0.5590	0.2940
C	0.5910	0.3080
D	0.5910	0.3020
E	0.3210	0.1930
F	0.3500	0.1810
G	0.5460	0.2600
H	0.4800	0.2740
I	0.6310	0.2890
P	0.4020	0.1960
Q	0.3810	0.2930
R	0.4260	0.2160
S	0.5650	0.2230
T	0.3920	0.2070
V	0.5900	0.2510
W	0.4590	0.2440
X	0.6260	0.2440
Z	0.5940	0.2360
a	0.6160	0.2710
b	0.5750	0.2560
q	0.0480	0.1580
r	0.2500	0.1960
s	0.0370	0.1360