wwPDB EM Validation Summary Report

Aug 6, 2026 – 08:02 PM JST

PDB ID	:	8XNN / pdb_00008xnn
EMDB ID	:	EMD-38508
Title	:	Respiratory complex Peripheral Arm of CI, open form A, focus-refined map of type I, Wild type mouse under thermoneutral temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-12-30
Resolution	:	3.60 Å(reported)

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

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

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

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

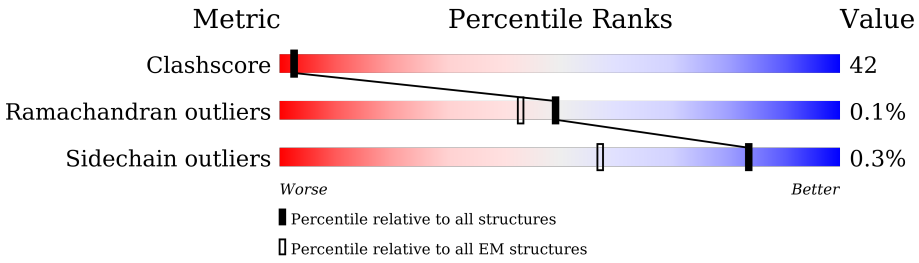
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

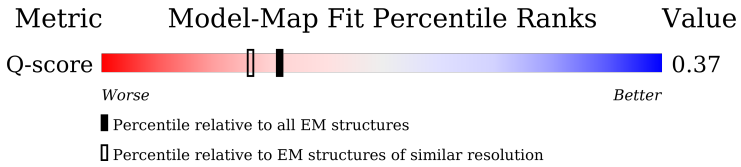
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	53% 32% 45% • 21%
2	B	224	11% 33% 31% 5% • 30%
3	C	263	6% 36% 37% • 25%
4	D	463	10% 33% 44% 5% 18%

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Mol	Chain	Length	Quality of chain
5	E	248	20% 31% 51% 15%
6	F	464	13% 32% 55% 5% 8%
7	G	727	8% 38% 50% 6% 6%
8	H	318	35% 33% 56% 8%
9	I	212	10% 36% 40% 8% 16%
10	P	377	36% 32% 55% 10%
11	Q	175	14% 36% 29% 33%
12	R	116	26% 31% 39% 28%
13	S	99	5% 26% 52% 6% 16%
14	T	156	26% 20% 27% 52%
15	V	116	15% 47% 44% 5%
16	W	131	18% 39% 44% 13%
17	X	172	37% 30% 50% 17%
18	Z	144	44% 44% 48%
19	a	70	24% 43% 53%
20	b	84	38% 30% 63% 6%
21	q	145	36% 45% 50%
22	r	113	43% 35% 47% 16%
23	s	104	11% 8% 13% 79%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	302	-	-	X	-
25	SF4	I	303	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	FES	E	301	-	-	X	-
26	FES	G	803	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 34420 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	91	743	517	103	118	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	157	1258	802	227	215	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	1641	1060	279	299	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	381	3056	1951	527	556	22	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	310	Total 2479	C 1667	N 376	O 414	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	178	Total 1431	C 898	N 245	O 276	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	118	Total 957	C 608	N 165	O 180	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	83	Total 660	C 411	N 120	O 126	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	139	Total	C	N	O	S	0	0
			1152	741	204	199	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	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

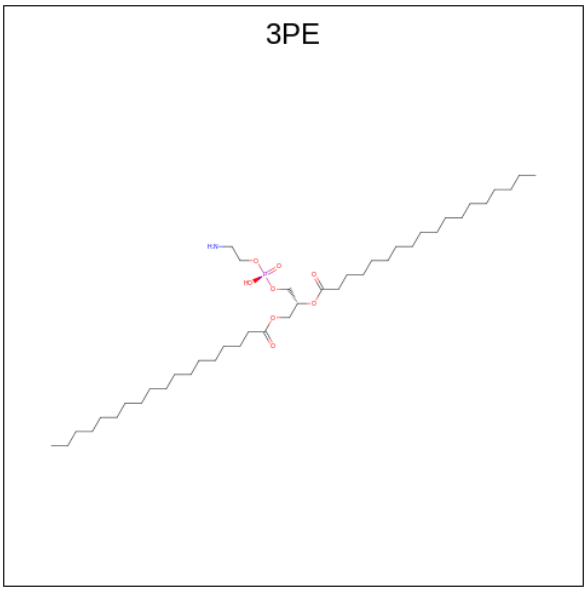
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

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

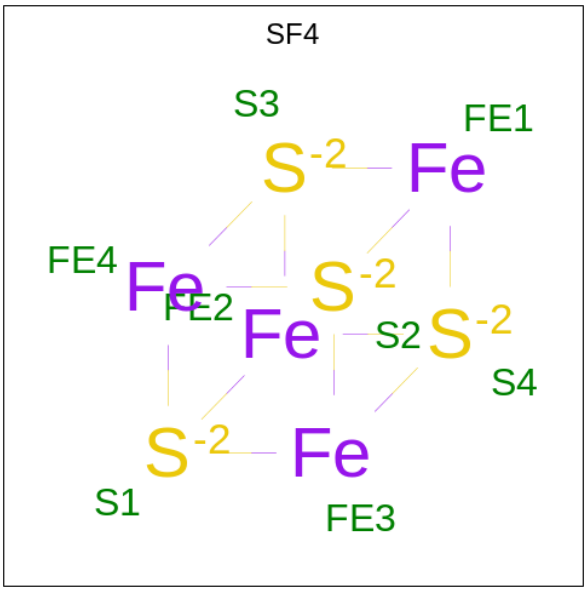
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	22	Total	C	N	O	0	0
			189	124	29	36		

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



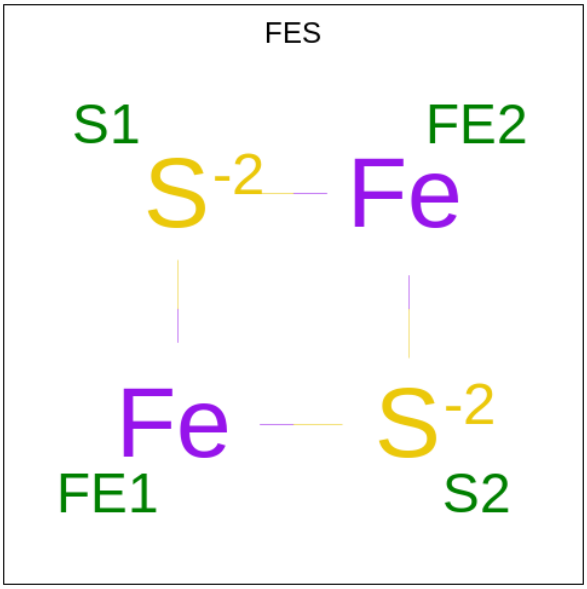
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



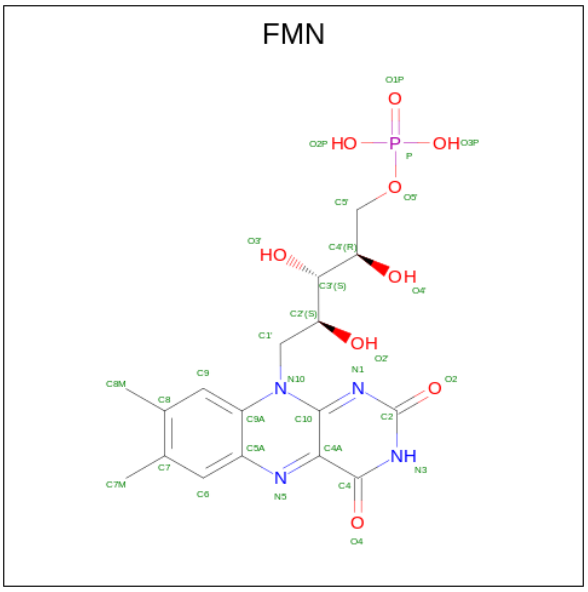
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total Fe S 8 4 4	0
25	F	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



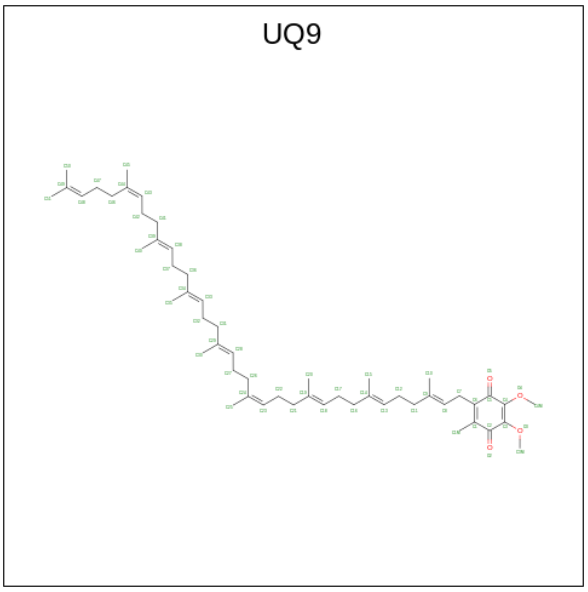
Mol	Chain	Residues	Atoms	AltConf
26	E	1	Total Fe S 4 2 2	0
26	G	1	Total Fe S 4 2 2	0

- Molecule 27 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



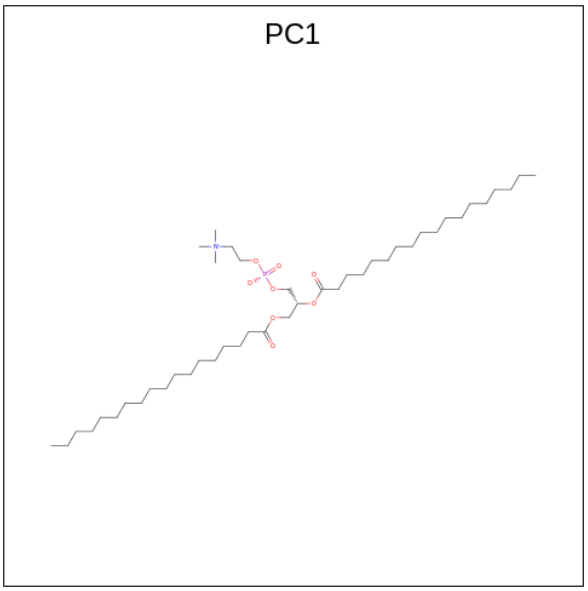
Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 28 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



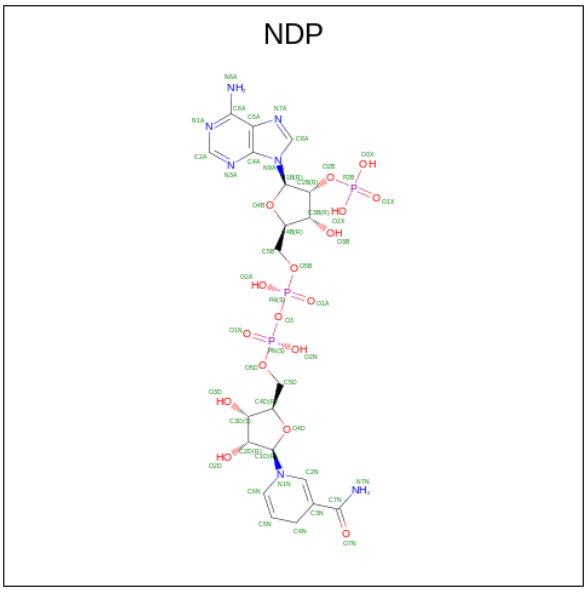
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			35	31	4	

- Molecule 29 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
29	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

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

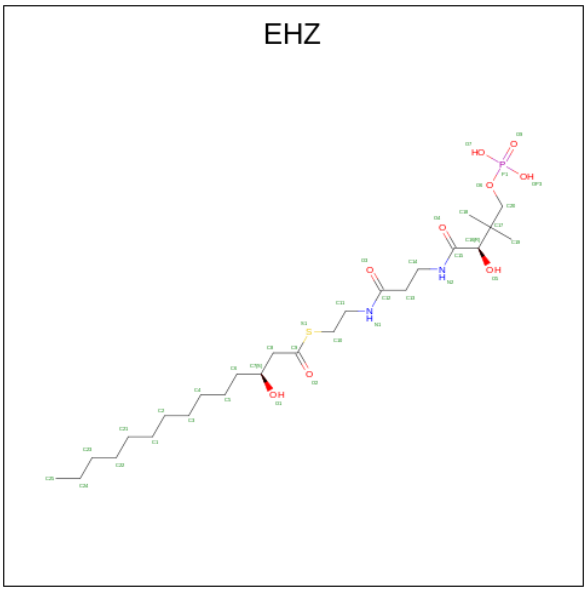


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

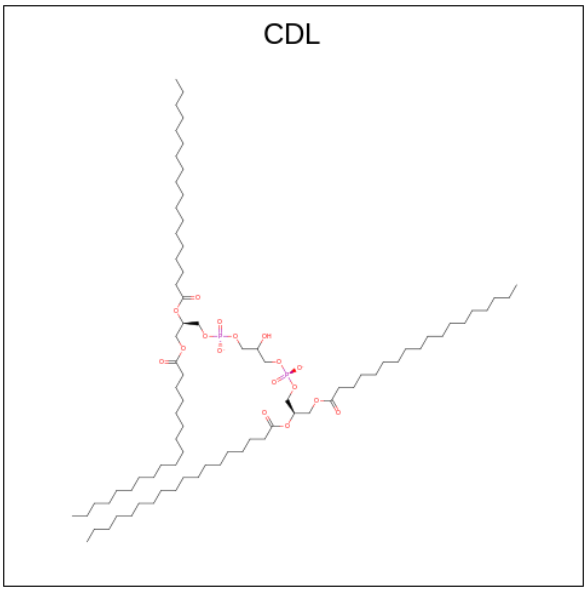
Mol	Chain	Residues	Atoms	AltConf
31	R	1	Total Zn 1 1	0

- Molecule 32 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
32	W	1	Total C N O P S 32 19 2 9 1 1	0

- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



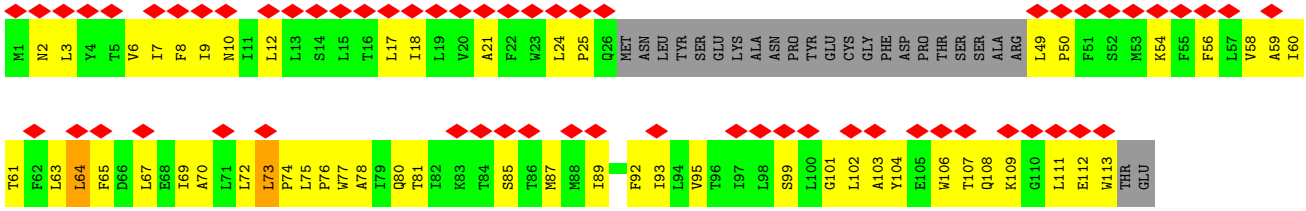
Mol	Chain	Residues	Atoms				AltConf
33	q	1	Total	C	O	P	0
			57	38	17	2	

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.

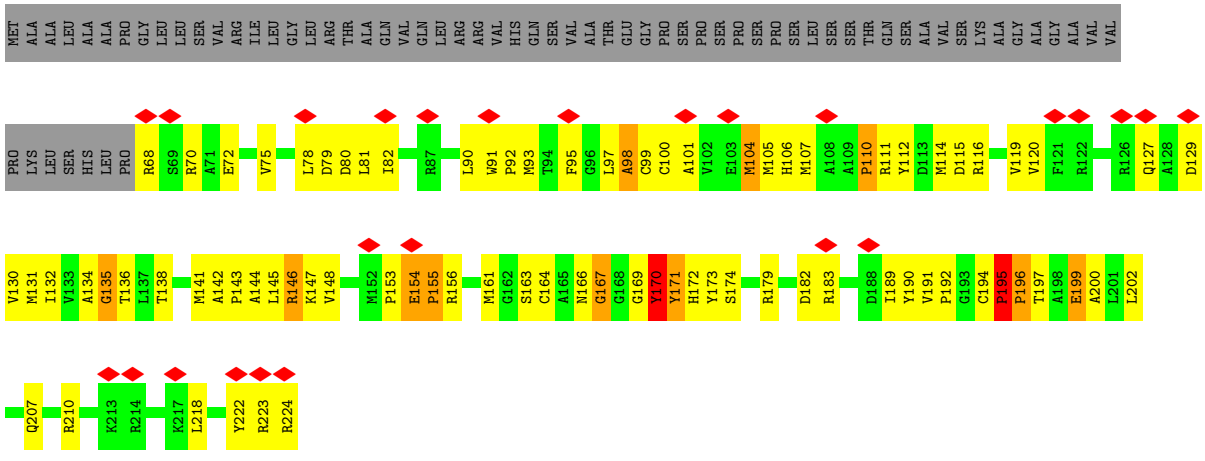
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



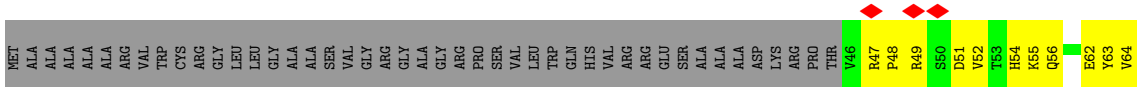
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

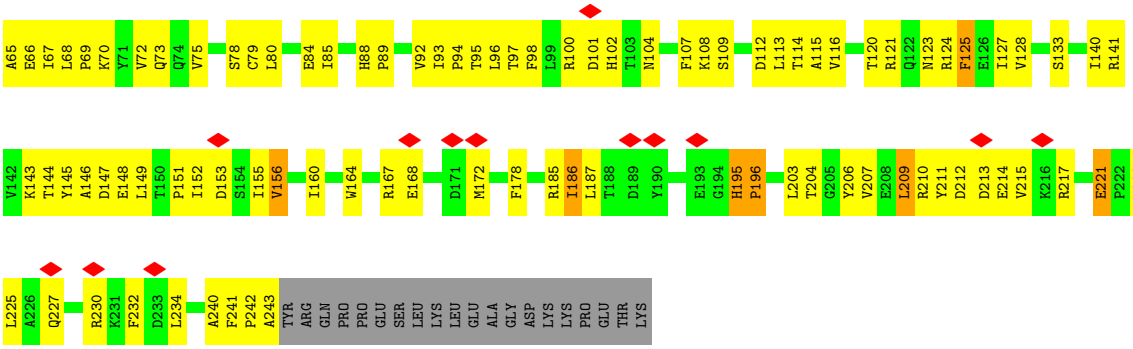
Chain B:



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

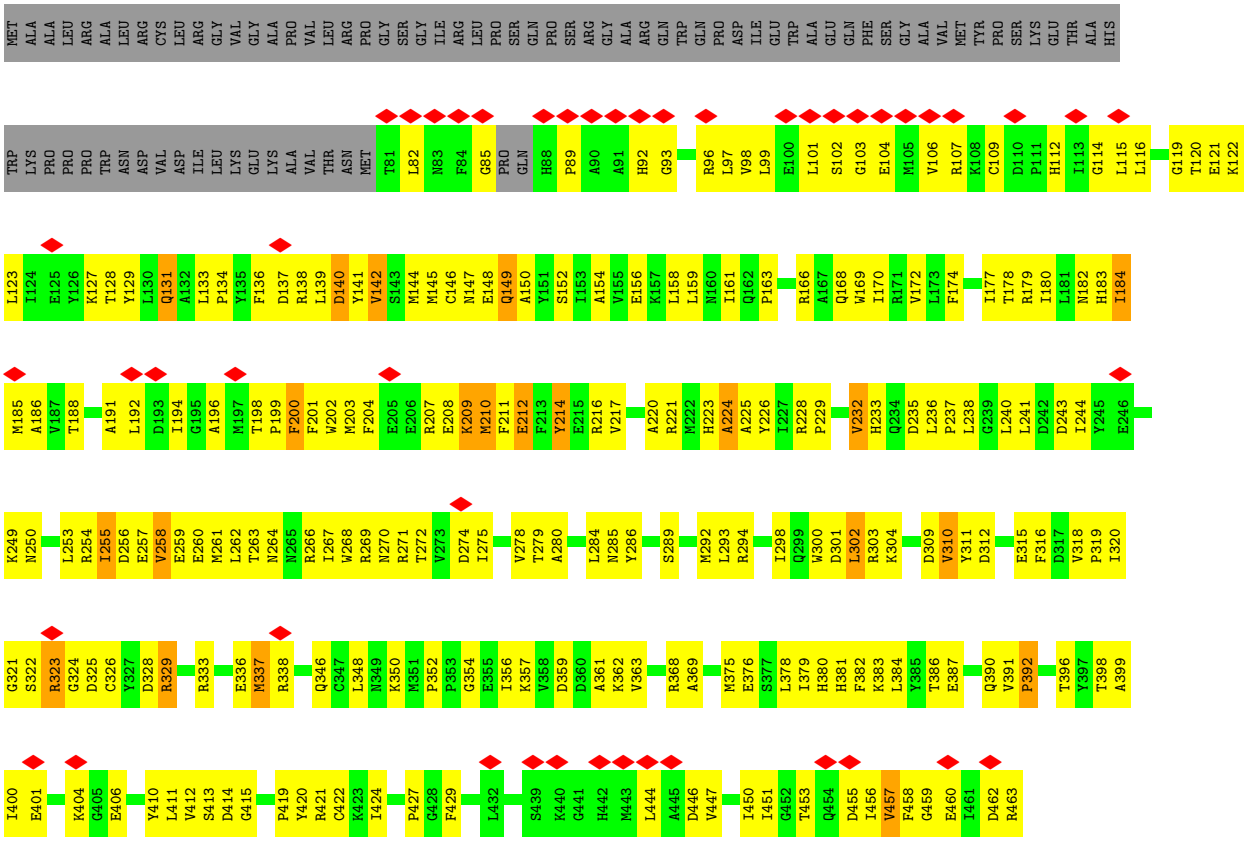
Chain C:





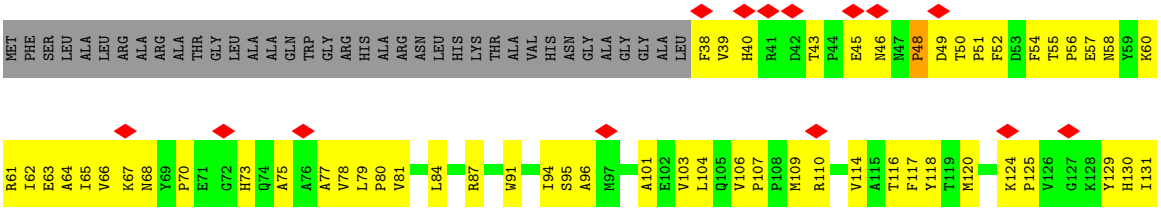
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

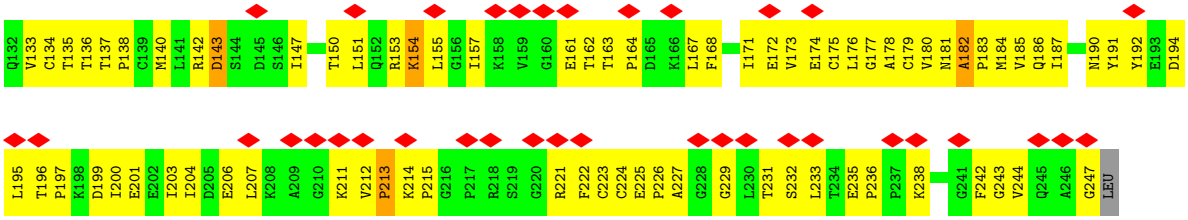
Chain D:



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

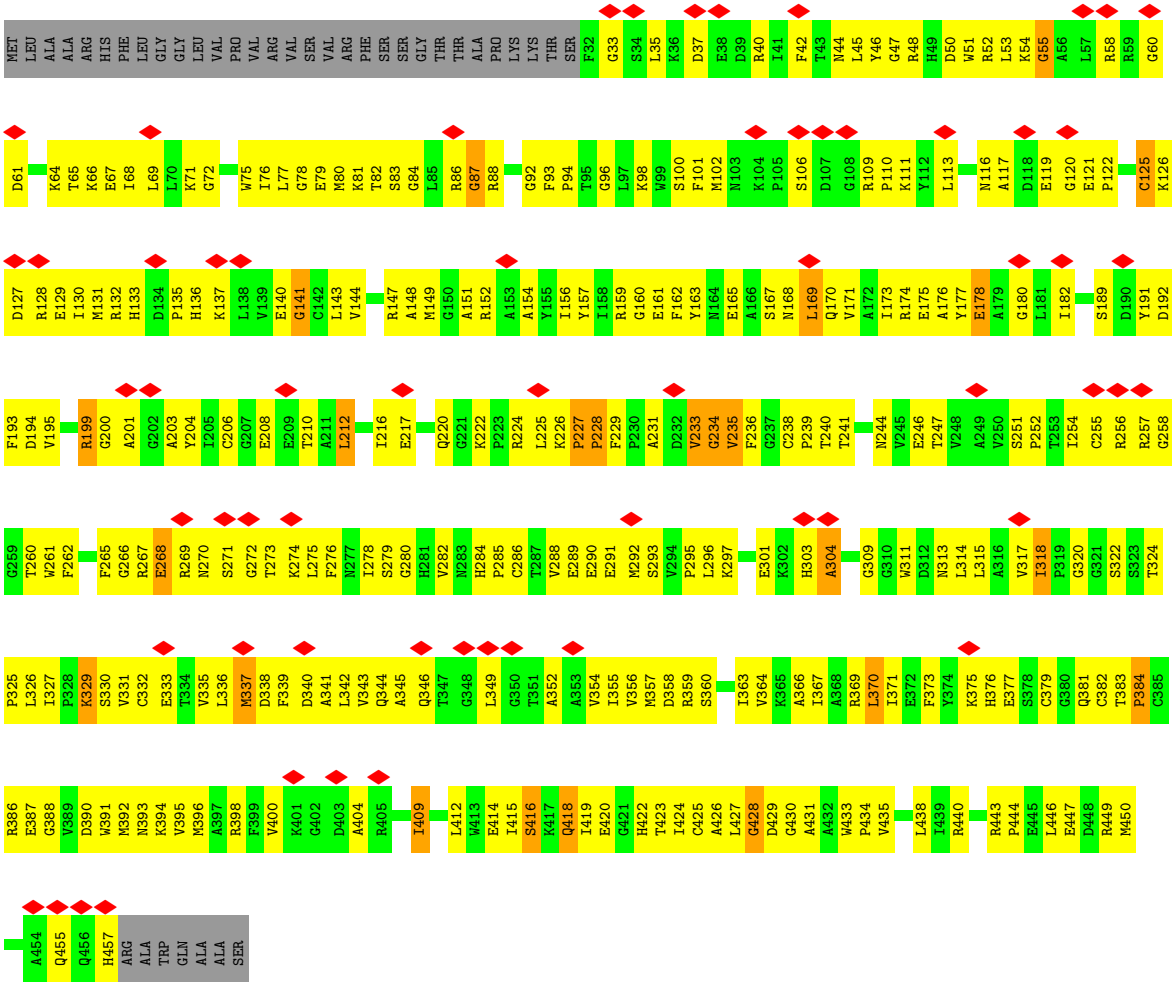
Chain E:





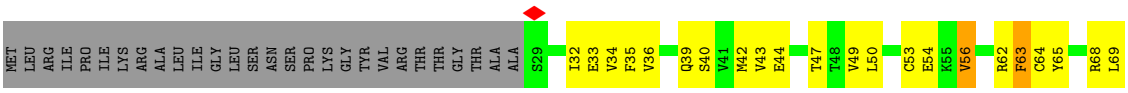
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

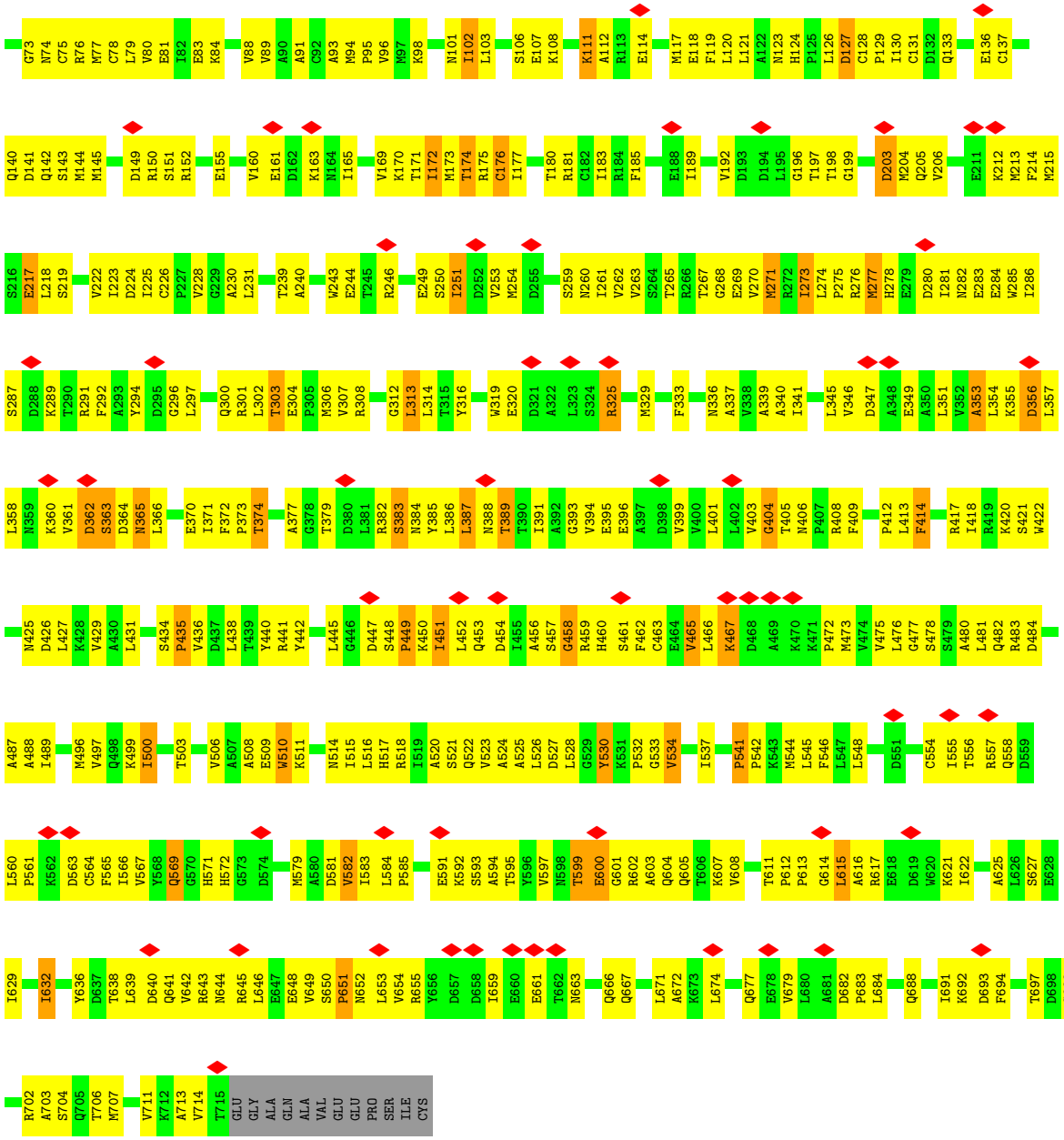
Chain F:



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

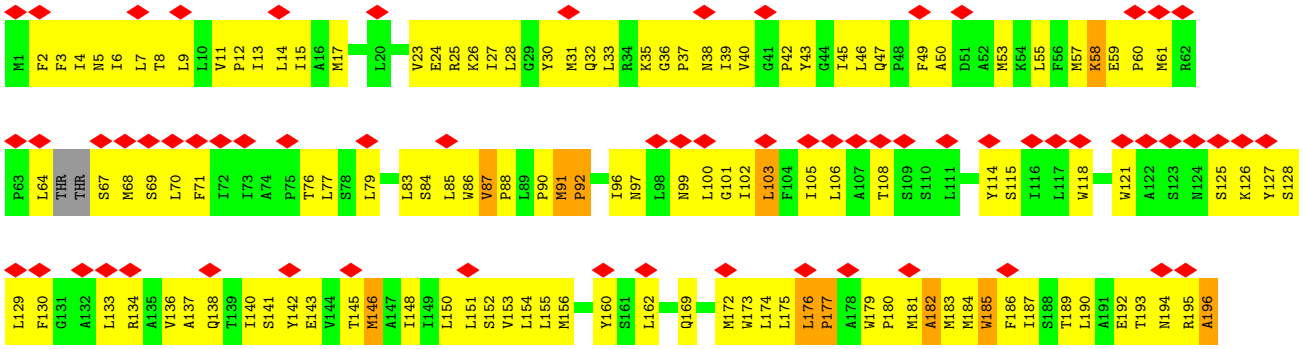
Chain G:

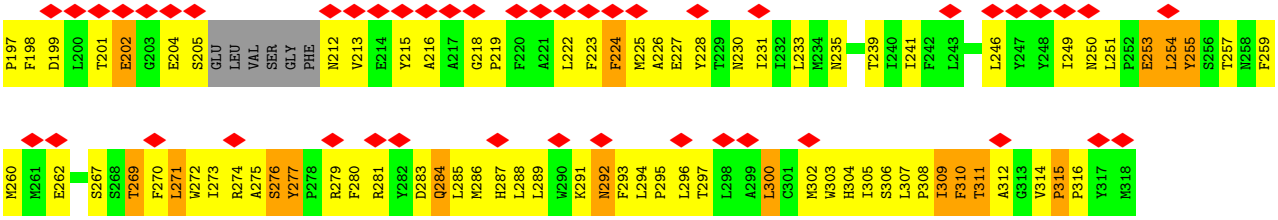




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

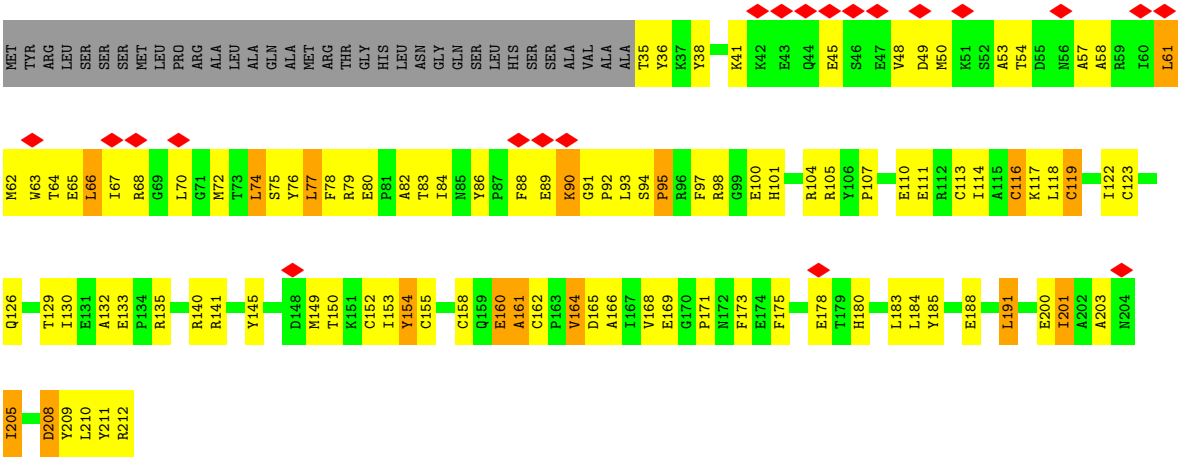
Chain H:





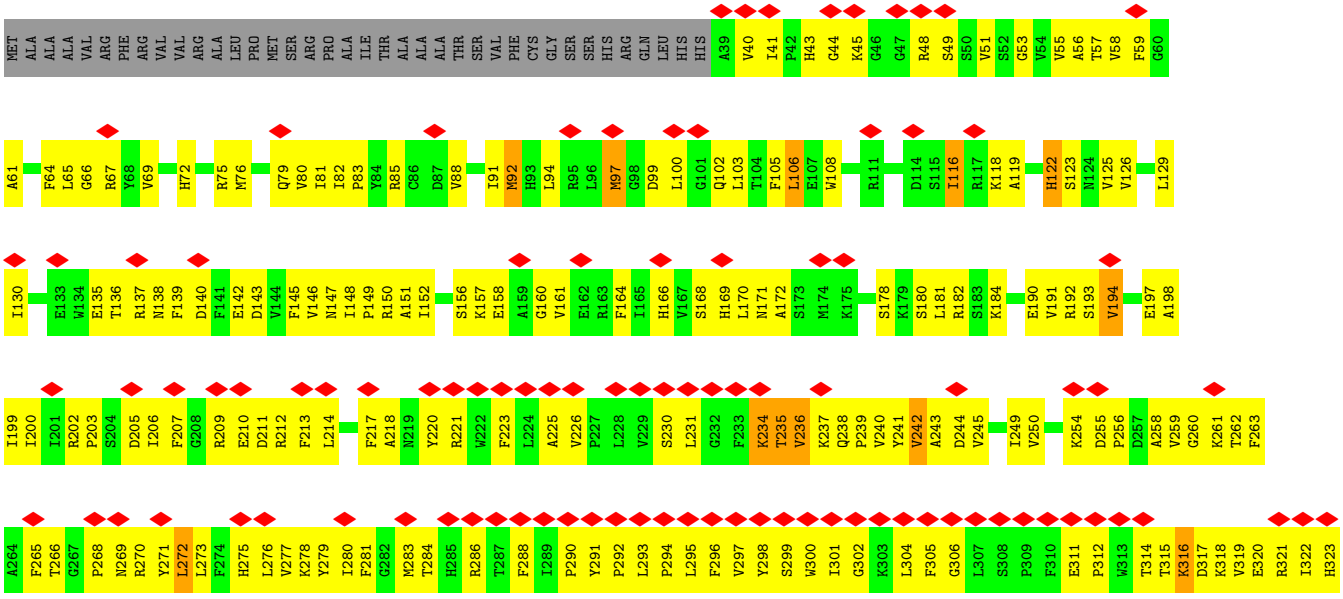
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

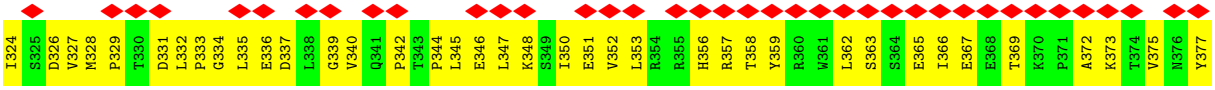
Chain I:



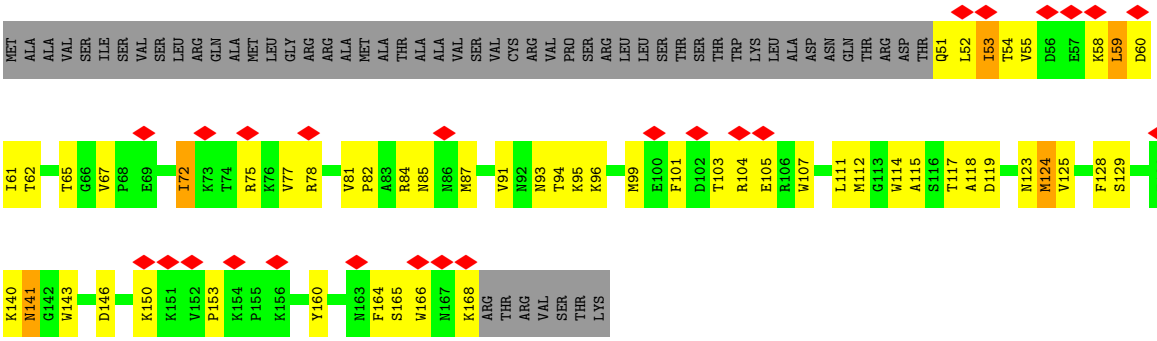
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

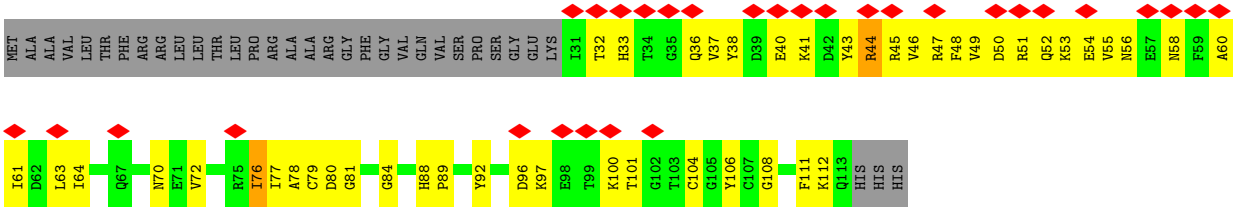




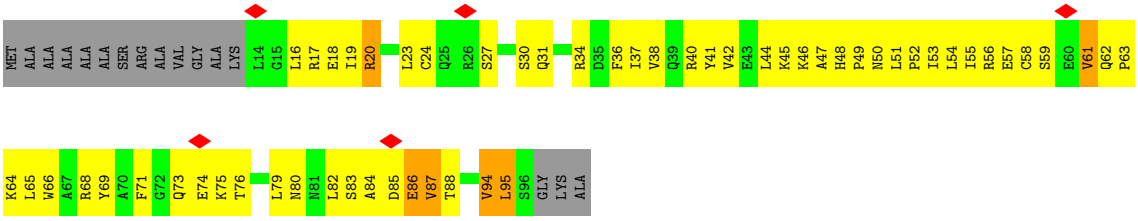
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



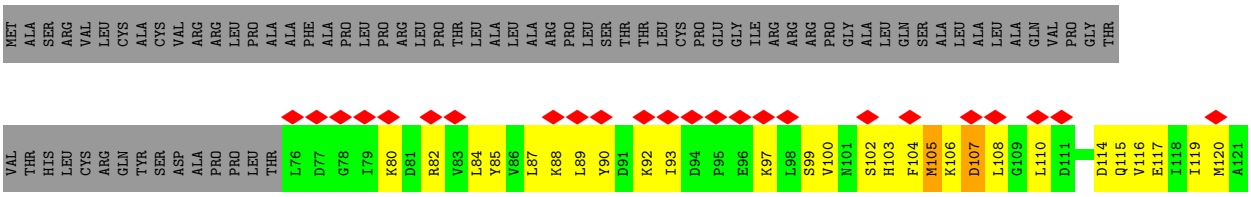
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

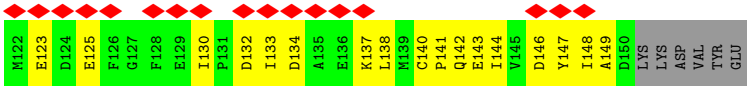


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

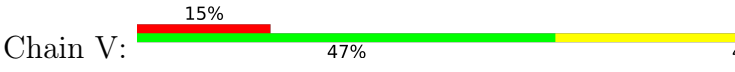


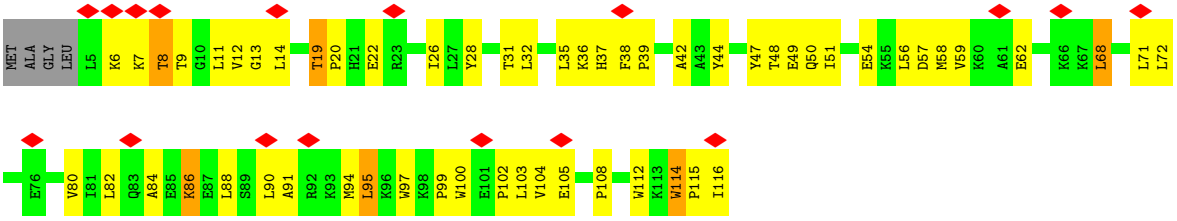
• Molecule 14: Acyl carrier protein, mitochondrial



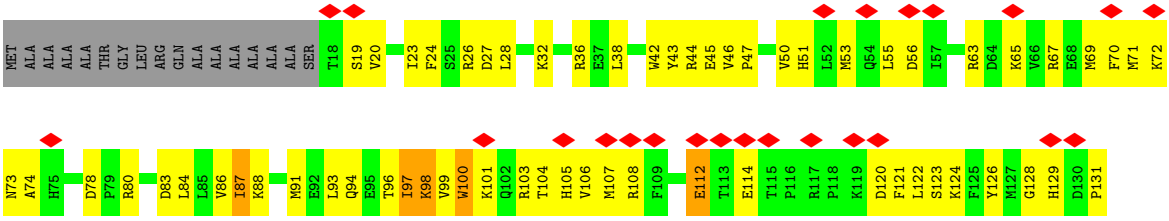


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

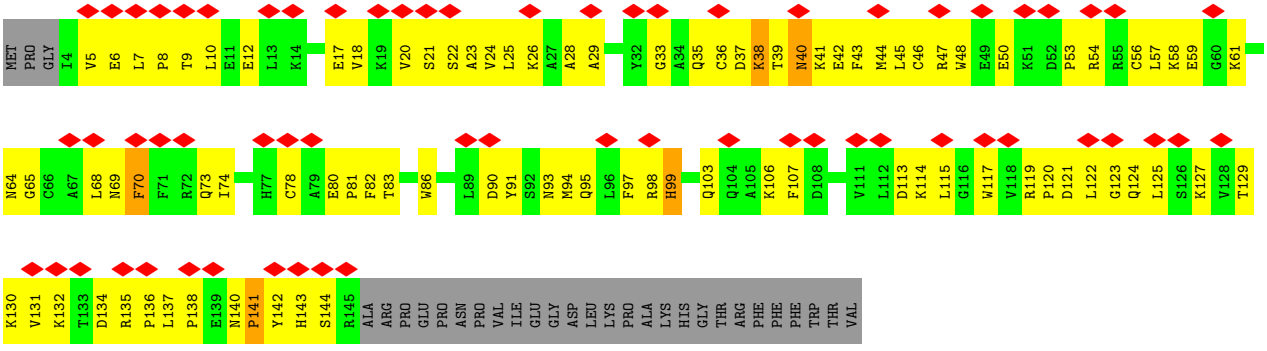




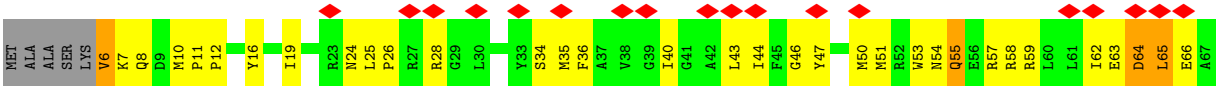
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

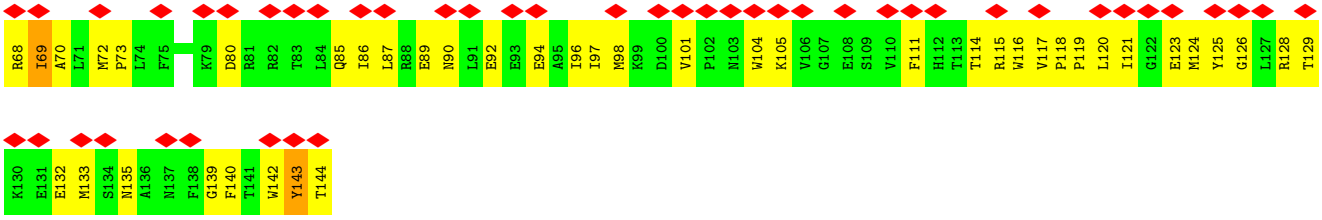


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



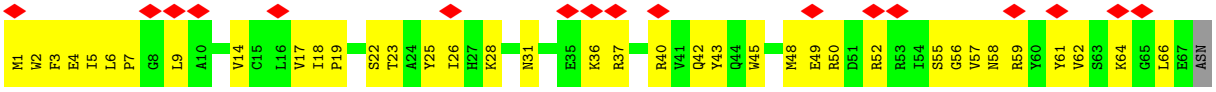
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13





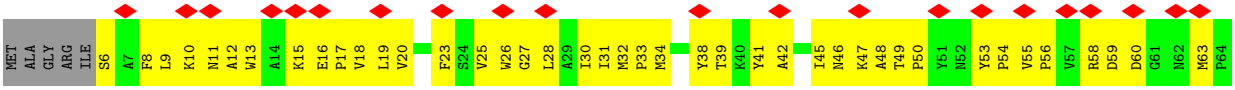
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



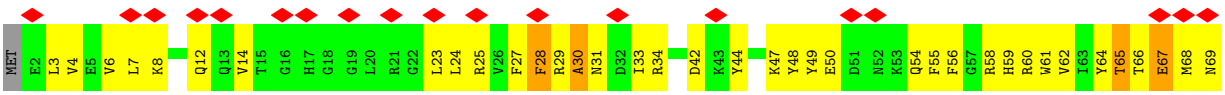
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

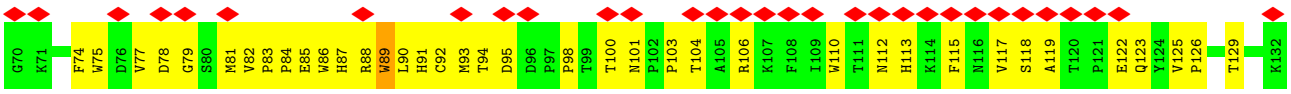
Chain b:



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

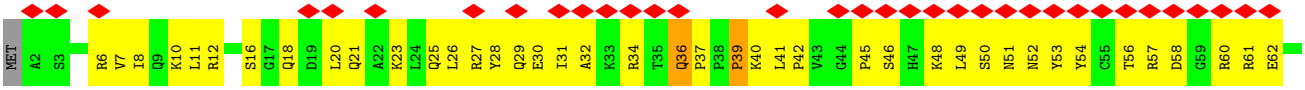
Chain q:

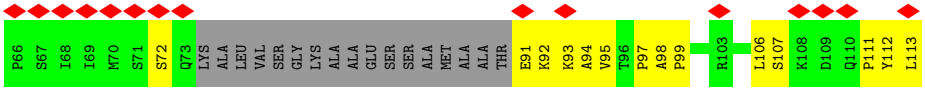




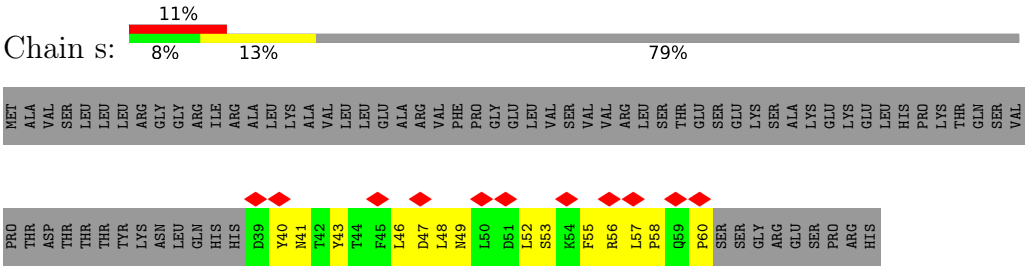
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

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	14488	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 ($e^-/Å^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.762	Depositor
Minimum map value	-0.854	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.55	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PC1, FMN, CDL, SF4, EHZ, NDP, UQ9, 3PE, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.81	0/763	1.16	7/1042 (0.7%)
2	B	0.93	1/1289 (0.1%)	1.46	20/1744 (1.1%)
3	C	0.88	0/1687	1.26	12/2297 (0.5%)
4	D	0.96	4/3128 (0.1%)	1.49	38/4228 (0.9%)
5	E	0.71	0/1675	1.07	10/2282 (0.4%)
6	F	0.89	5/3363 (0.1%)	1.37	47/4543 (1.0%)
7	G	0.90	8/5374 (0.1%)	1.55	96/7281 (1.3%)
8	H	0.94	2/2553 (0.1%)	1.41	39/3486 (1.1%)
9	I	0.89	0/1461	1.51	20/1974 (1.0%)
10	P	0.75	1/2793 (0.0%)	1.12	18/3787 (0.5%)
11	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
12	R	0.66	0/671	0.92	2/903 (0.2%)
13	S	0.87	1/678 (0.1%)	1.37	9/915 (1.0%)
14	T	0.61	0/613	0.91	2/826 (0.2%)
15	V	0.82	0/937	1.38	12/1270 (0.9%)
16	W	0.80	1/993 (0.1%)	1.05	7/1335 (0.5%)
17	X	0.71	0/1191	1.20	13/1605 (0.8%)
18	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
19	a	0.84	0/561	1.11	3/755 (0.4%)
20	b	0.70	0/643	1.01	3/884 (0.3%)
21	q	0.68	0/1234	1.13	10/1681 (0.6%)
22	r	0.61	0/782	1.04	6/1058 (0.6%)
23	s	0.44	0/194	0.69	0/264
All	All	0.84	25/34746 (0.1%)	1.32	395/47081 (0.8%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	234	GLY	CA-C	-10.39	1.40	1.52
6	F	227	PRO	N-CD	10.14	1.61	1.47
6	F	235	VAL	N-CA	-9.69	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	140	ASP	C-O	-7.92	1.14	1.24
11	Q	53	ILE	C-O	7.80	1.33	1.24

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	174	THR	N-CA-C	-17.51	89.01	114.39
7	G	632	ILE	N-CA-C	-13.65	88.01	107.80
7	G	251	ILE	N-CA-C	13.30	126.79	108.17
6	F	125	CYS	N-CA-C	-12.95	93.43	113.89
7	G	500	ILE	N-CA-C	-12.43	98.84	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	743	0	801	67	0
2	B	1258	0	1269	138	0
3	C	1641	0	1596	164	0
4	D	3056	0	3028	294	0
5	E	1635	0	1624	148	0
6	F	3288	0	3243	367	0
7	G	5287	0	5323	564	0
8	H	2479	0	2568	357	0
9	I	1431	0	1385	180	0
10	P	2720	0	2740	240	0
11	Q	957	0	949	73	0
12	R	660	0	639	62	0
13	S	667	0	683	68	0
14	T	604	0	596	66	0
15	V	915	0	954	97	0
16	W	970	0	991	88	0
17	X	1164	0	1154	109	0
18	Z	1152	0	1148	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	548	0	562	42	0
20	b	620	0	617	95	0
21	q	1192	0	1145	89	0
22	r	764	0	789	85	0
23	s	189	0	181	20	0
24	A	46	0	69	3	0
24	H	46	0	69	10	0
24	b	46	0	69	13	0
25	B	8	0	0	2	0
25	F	8	0	0	9	0
25	G	16	0	0	3	0
25	I	16	0	0	15	0
26	E	4	0	0	3	0
26	G	4	0	0	6	0
27	F	31	0	19	3	0
28	H	35	0	43	16	0
29	I	47	0	71	10	0
29	q	35	0	44	6	0
30	P	48	0	26	2	0
31	R	1	0	0	0	0
32	W	32	0	0	0	0
33	q	57	0	58	8	0
All	All	34420	0	34453	2921	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 42.

The worst 5 of 2921 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)
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.22
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.28	1.21
8:H:64:LEU:CD2	10:P:359:TYR:HB2	1.72	1.20
4:D:97:LEU:CD2	4:D:99:LEU:HD21	1.74	1.18
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.17

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	87/115 (76%)	83 (95%)	4 (5%)	0	100 100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	9 39
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100 100
4	D	377/463 (81%)	362 (96%)	15 (4%)	0	100 100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100 100
6	F	424/464 (91%)	407 (96%)	17 (4%)	0	100 100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100 100
8	H	304/318 (96%)	290 (95%)	13 (4%)	1 (0%)	36 65
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100 100
10	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36 65
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100 100
12	R	81/116 (70%)	78 (96%)	3 (4%)	0	100 100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100 100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100 100
15	V	110/116 (95%)	106 (96%)	4 (4%)	0	100 100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100 100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100 100
18	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100 100
19	a	65/70 (93%)	62 (95%)	3 (5%)	0	100 100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100 100
21	q	141/145 (97%)	135 (96%)	6 (4%)	0	100 100
22	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11 43
23	s	20/104 (19%)	20 (100%)	0	0	100 100
All	All	4193/5036 (83%)	3978 (95%)	210 (5%)	5 (0%)	49 79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
10	P	329	PRO
2	B	171	TYR
22	r	39	PRO
2	B	195	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	83/104 (80%)	83 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	328/395 (83%)	326 (99%)	2 (1%)	78	79
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	80
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	273/280 (98%)	273 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	P	296/325 (91%)	294 (99%)	2 (1%)	76	78
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
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	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	57/60 (95%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	b	70/73 (96%)	70 (100%)	0	100 100
21	q	129/131 (98%)	129 (100%)	0	100 100
22	r	85/96 (88%)	84 (99%)	1 (1%)	63 73
23	s	22/95 (23%)	22 (100%)	0	100 100
All	All	3685/4292 (86%)	3673 (100%)	12 (0%)	84 83

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

Mol	Chain	Res	Type
11	Q	96	LYS
12	R	76	ILE
22	r	92	LYS
13	S	68	ARG
5	E	124	LYS

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

Mol	Chain	Res	Type
10	P	43	HIS
13	S	25	GLN
10	P	102	GLN
10	P	323	HIS
16	W	94	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.23	7 (14%)
25	SF4	I	303	9	0,12,12	-	-	-		
30	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.67	11 (16%)
26	FES	E	301	5	0,4,4	-	-	-		
32	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	6 (16%)
29	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
24	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
24	3PE	H	402	-	45,45,50	0.95	2 (4%)	48,50,55	1.12	2 (4%)
25	SF4	B	301	2	0,12,12	-	-	-		
33	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
28	UQ9	H	401	-	35,35,58	0.80	2 (5%)	42,45,73	0.63	0
24	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
25	SF4	G	802	7	0,12,12	-	-	-		
26	FES	G	803	7	0,4,4	-	-	-		
25	SF4	I	302	9	0,12,12	-	-	-		
25	SF4	F	502	6	0,12,12	-	-	-		
29	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
25	SF4	G	801	7	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
27	FMN	F	501	-	-	0/18/18/18	0/3/3/3
25	SF4	I	303	9	-	-	0/6/5/5
30	NDP	P	401	-	-	2/34/77/77	0/5/5/5
25	SF4	F	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	FES	E	301	5	-	-	0/1/1/1
32	EHZ	W	201	-	-	12/39/39/45	-
29	PC1	q	202	-	-	14/38/38/57	-
24	3PE	A	401	-	-	18/49/49/54	-
24	3PE	H	402	-	-	13/49/49/54	-
25	SF4	B	301	2	-	-	0/6/5/5
28	UQ9	H	401	-	-	12/30/54/81	0/1/1/1
24	3PE	b	201	-	-	10/49/49/54	-
25	SF4	G	802	7	-	-	0/6/5/5
26	FES	G	803	7	-	-	0/1/1/1
25	SF4	I	302	9	-	-	0/6/5/5
33	CDL	q	201	-	-	15/67/67/110	-
29	PC1	I	301	-	-	10/50/50/57	-
25	SF4	G	801	7	-	-	0/6/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.19	1.45	1.33
32	W	201	EHZ	C12-N1	5.03	1.44	1.33
27	F	501	FMN	C9A-C5A	4.80	1.49	1.41
24	b	201	3PE	O31-C31	4.28	1.45	1.33
30	P	401	NDP	C5A-C4A	4.25	1.46	1.39

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	P	401	NDP	C5A-C4A-N3A	-6.14	118.74	126.75
32	W	201	EHZ	C8-C9-S1	6.06	121.13	113.63
30	P	401	NDP	N3A-C4A-N9A	4.75	134.91	127.08
24	A	401	3PE	O21-C21-C22	4.71	121.65	111.50
33	q	201	CDL	OA6-CA5-C11	4.38	120.94	111.50

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	O22-C21-O21-C2
24	H	402	3PE	C1-O11-P-O12
24	b	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
24	b	201	3PE	O22-C21-O21-C2
28	H	401	UQ9	C6-C7-C8-C9

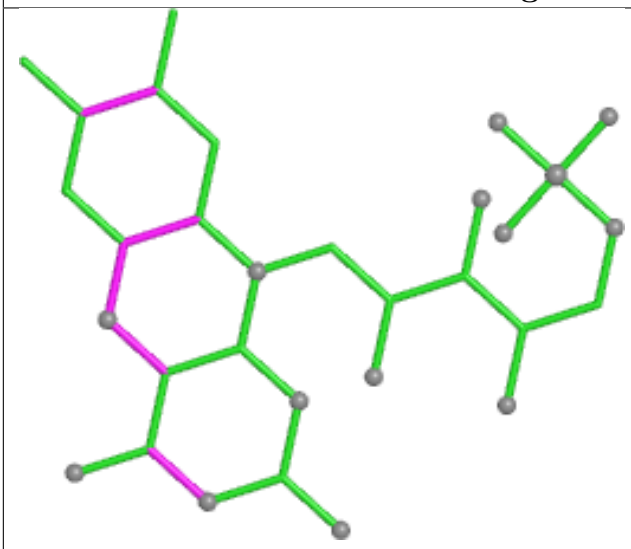
There are no ring outliers.

16 monomers are involved in 109 short contacts:

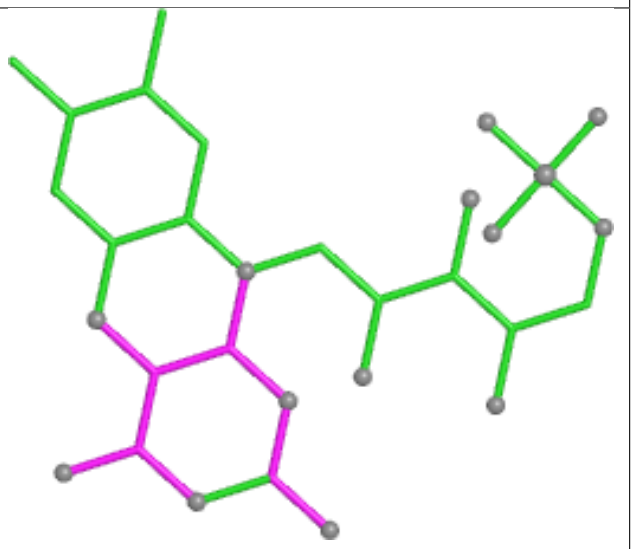
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	F	501	FMN	3	0
25	I	303	SF4	6	0
30	P	401	NDP	2	0
26	E	301	FES	3	0
29	q	202	PC1	6	0
24	A	401	3PE	3	0
24	H	402	3PE	10	0
25	B	301	SF4	2	0
33	q	201	CDL	8	0
28	H	401	UQ9	16	0
24	b	201	3PE	13	0
25	G	802	SF4	3	0
26	G	803	FES	6	0
25	I	302	SF4	9	0
25	F	502	SF4	9	0
29	I	301	PC1	10	0

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

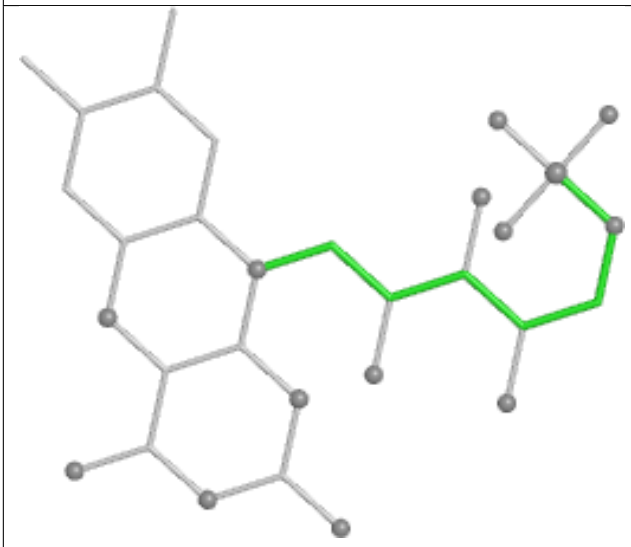
Ligand FMN F 501



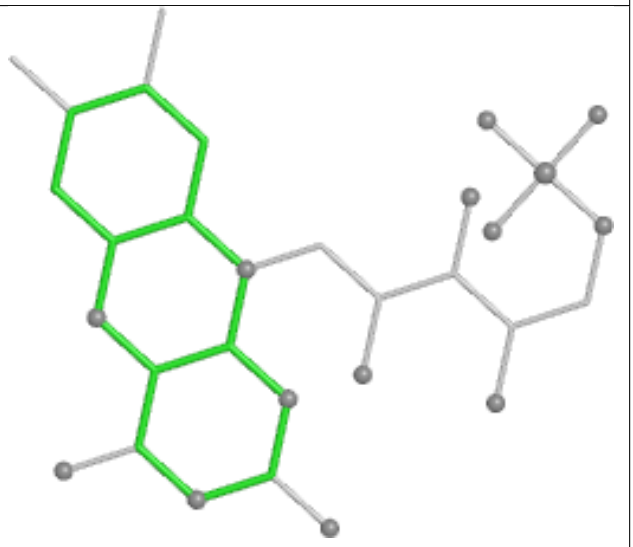
Bond lengths



Bond angles

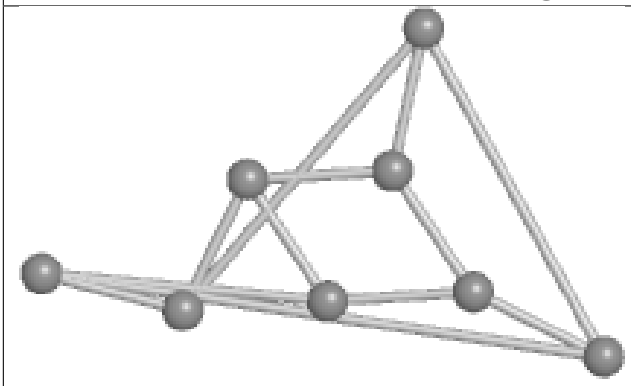


Torsions



Rings

Ligand SF4 I 303



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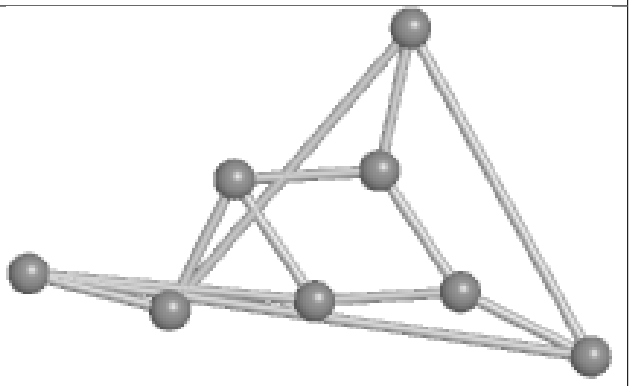

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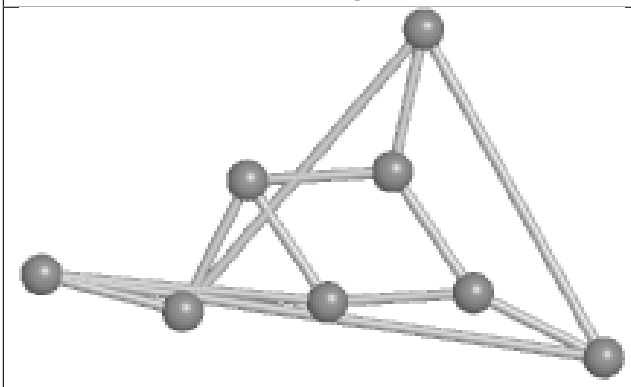

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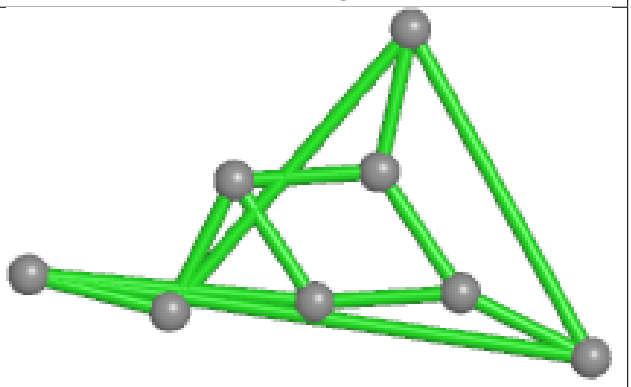
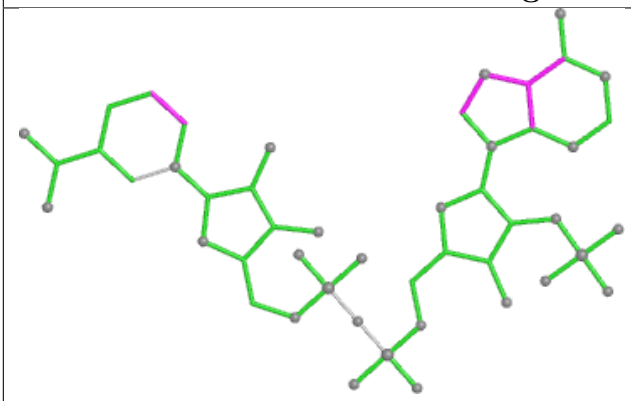
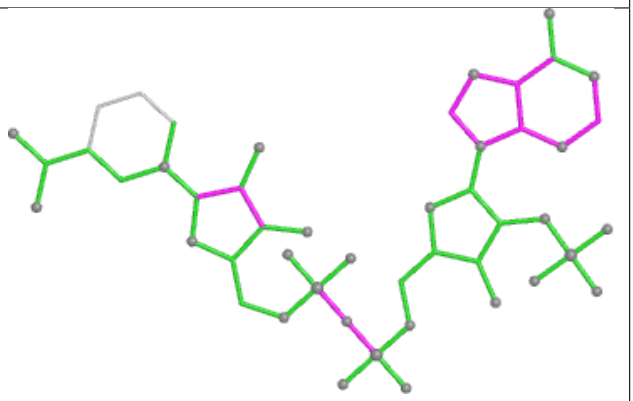


Rings

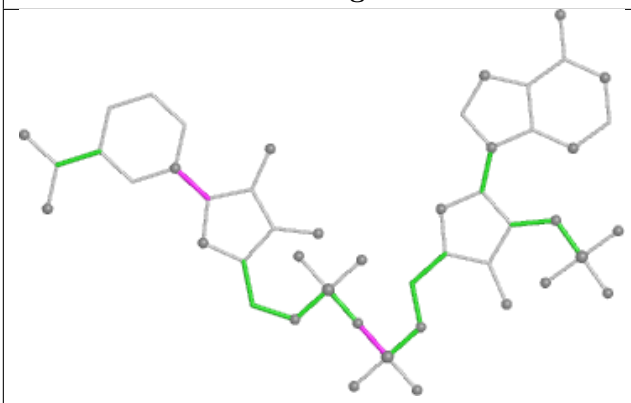
Ligand NDP P 401



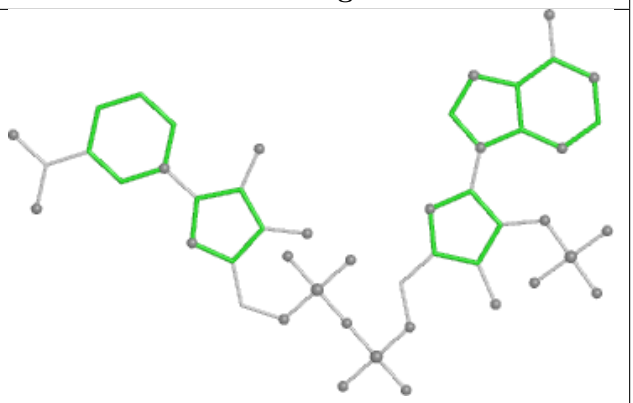
Bond lengths



Bond angles

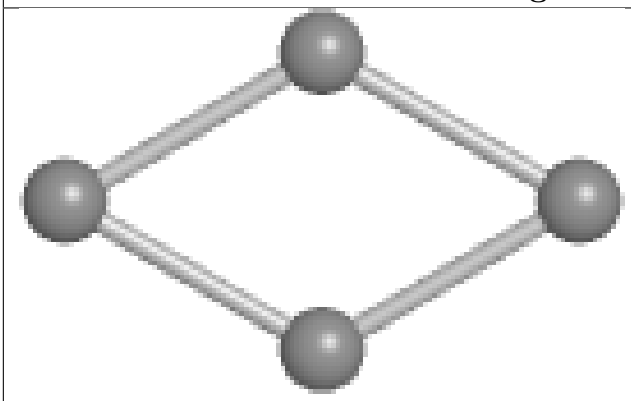


Torsions

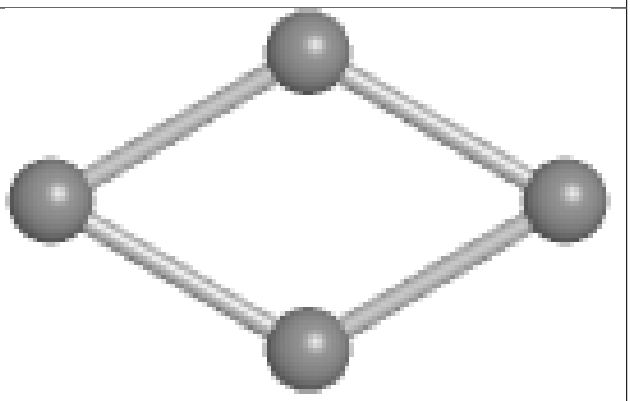


Rings

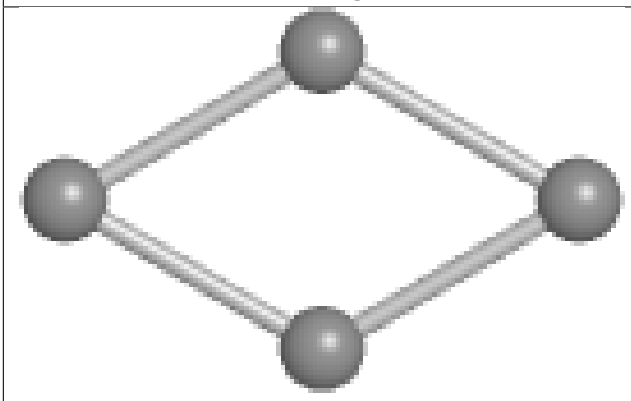
Ligand FES E 301



Bond lengths



Bond angles



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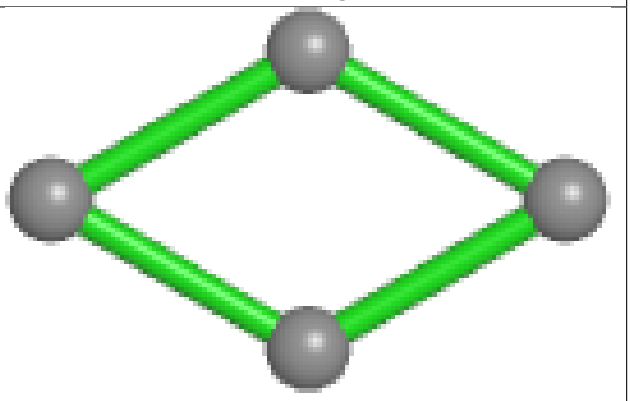
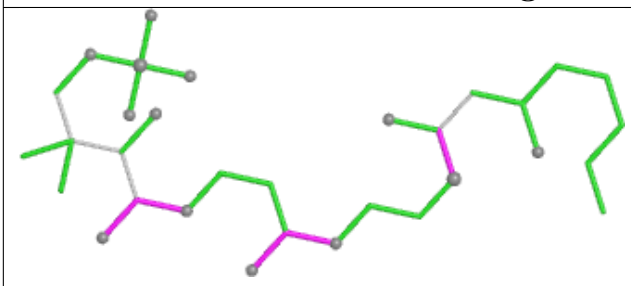
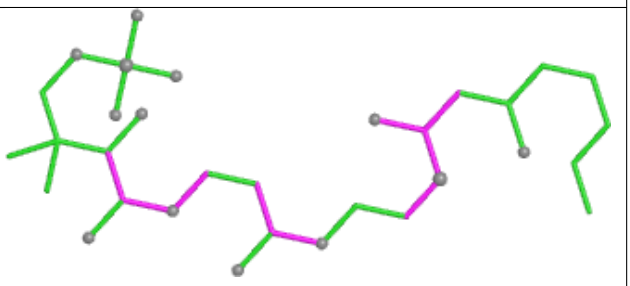


Rings

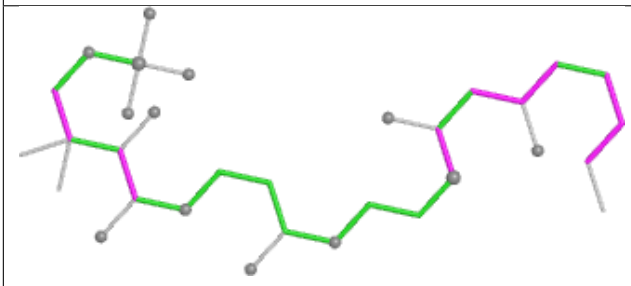
Ligand EHZ W 201



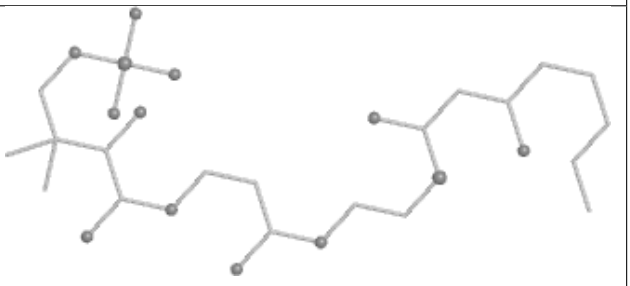
Bond lengths



Bond angles



Torsions



Rings

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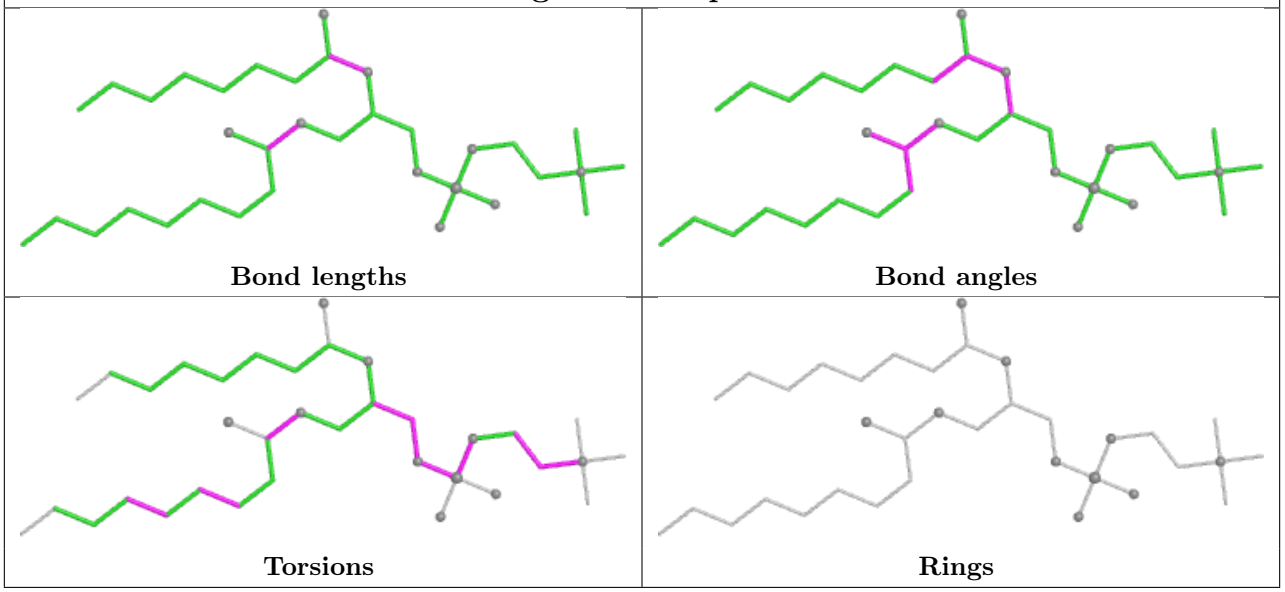
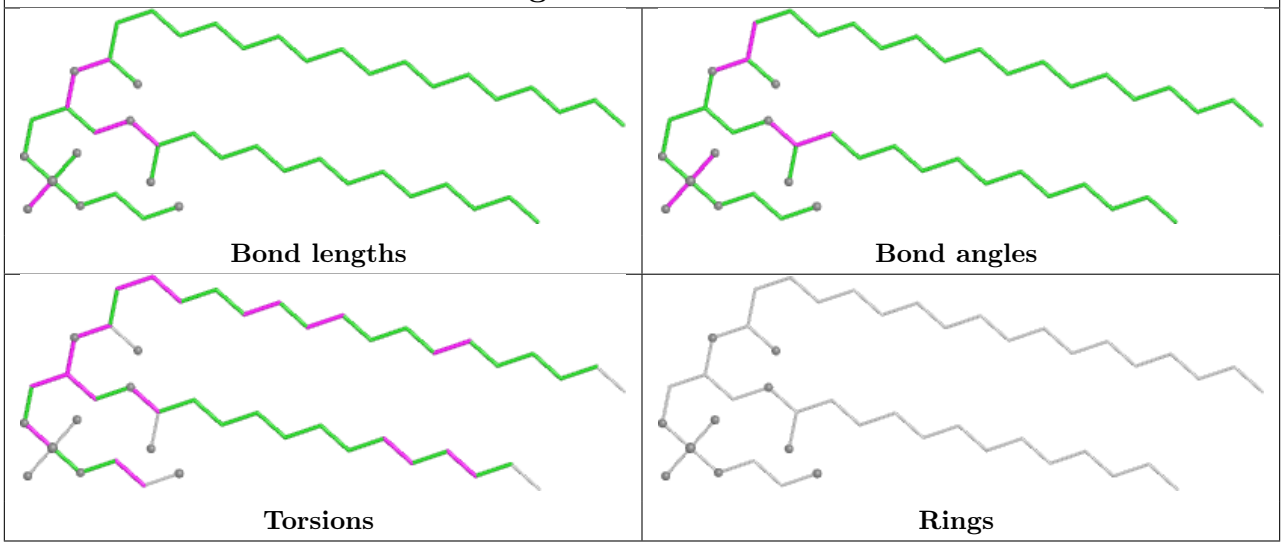
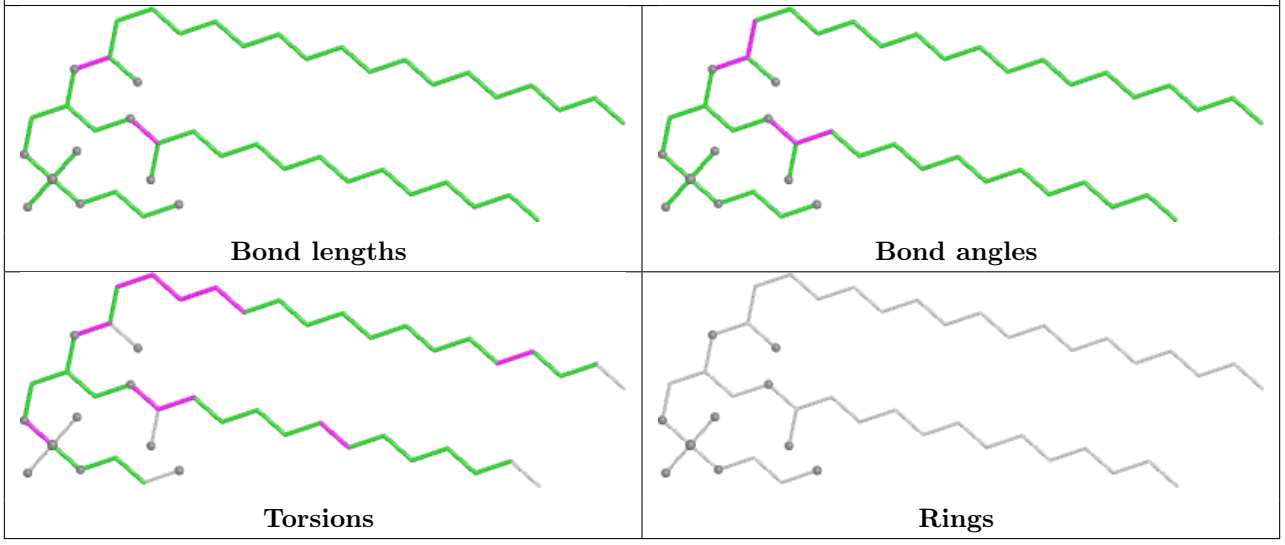


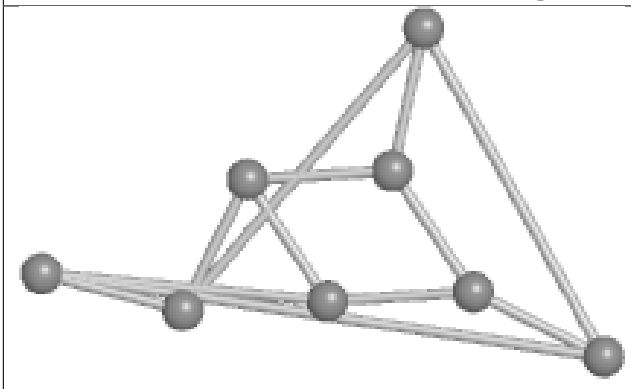
Ligand 3PE A 401



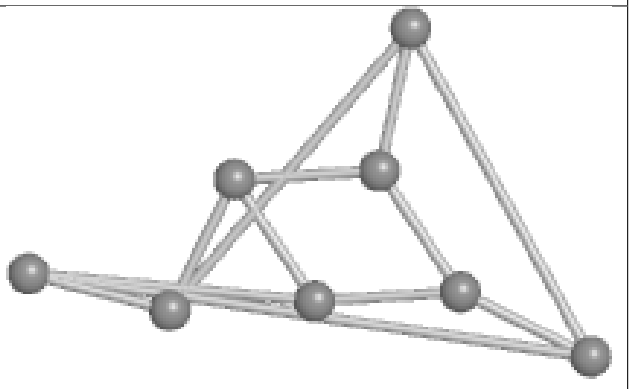
Ligand 3PE H 402



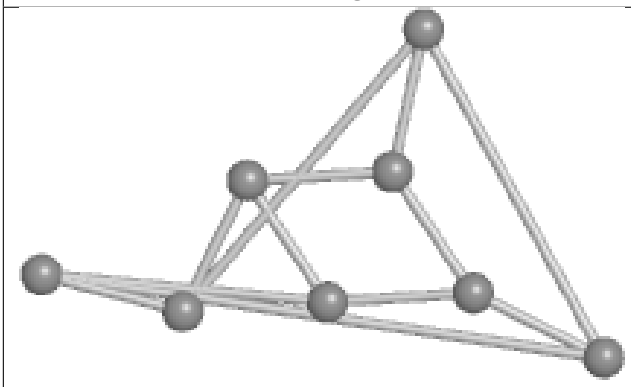
Ligand SF4 B 301



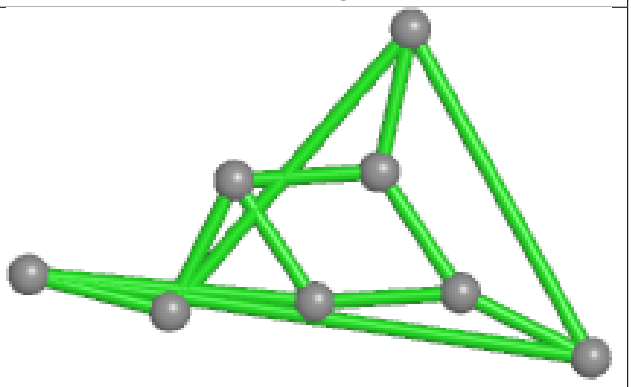
Bond lengths



Bond angles

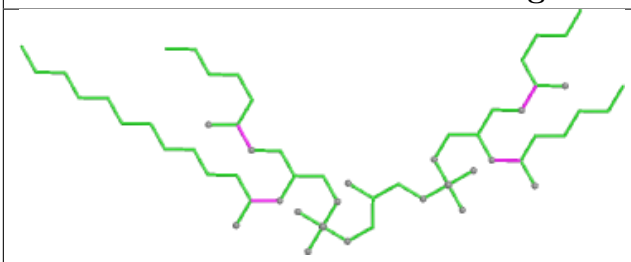


Torsions



Rings

Ligand CDL q 201



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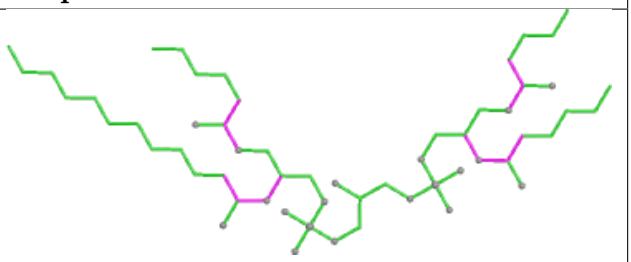
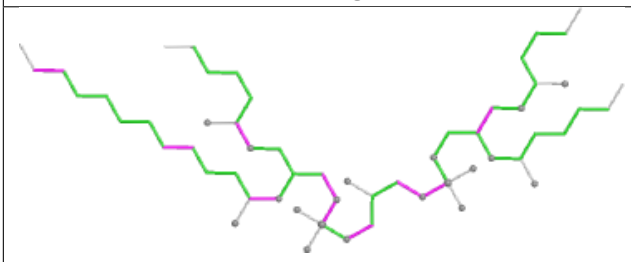
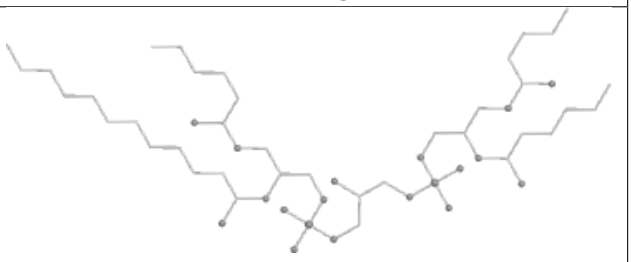


Bond angles

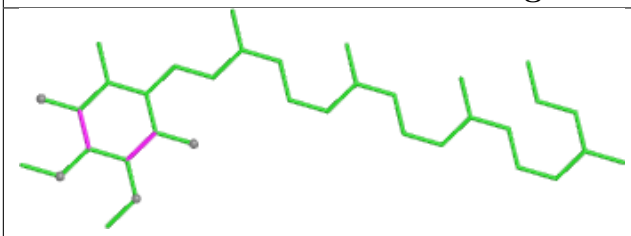


Torsions

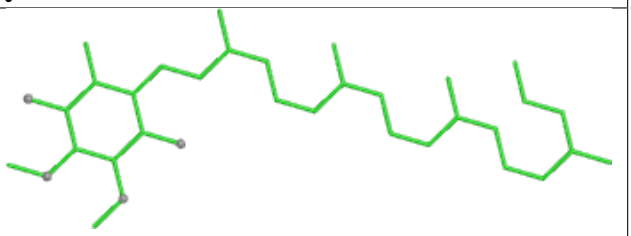


Rings

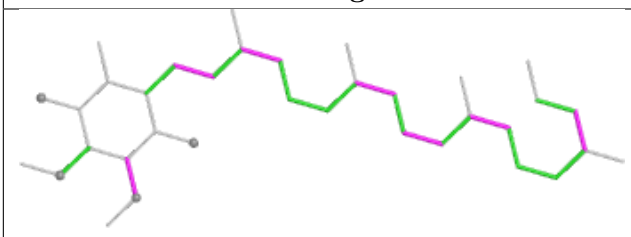
Ligand UQ9 H 401



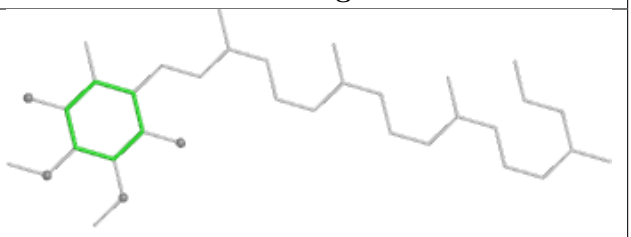
Bond lengths



Bond angles

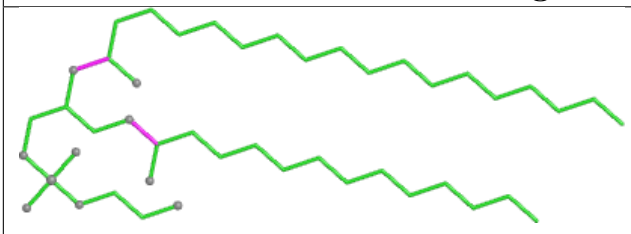


Torsions

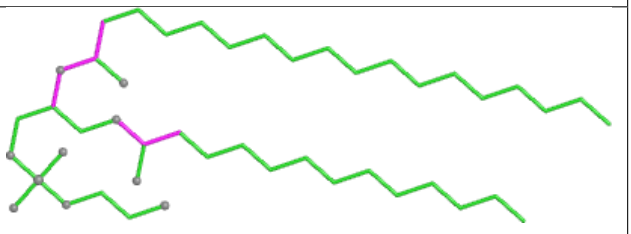


Rings

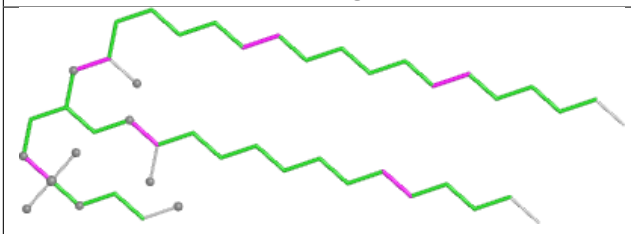
Ligand 3PE b 201



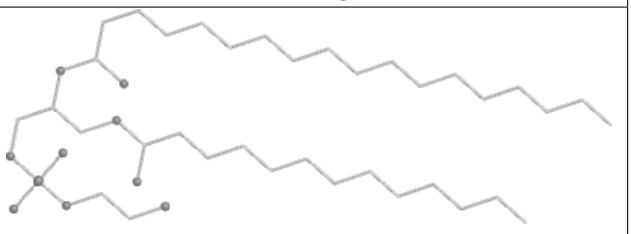
Bond lengths



Bond angles

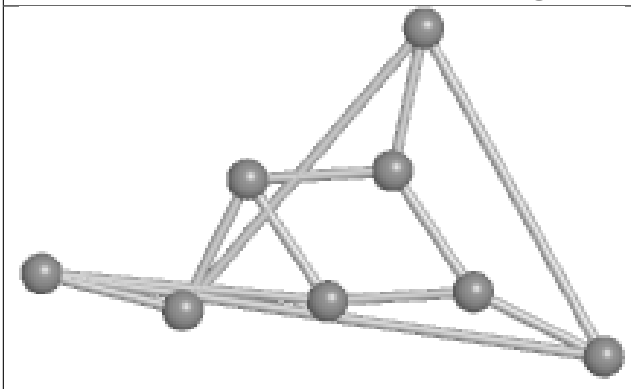


Torsions

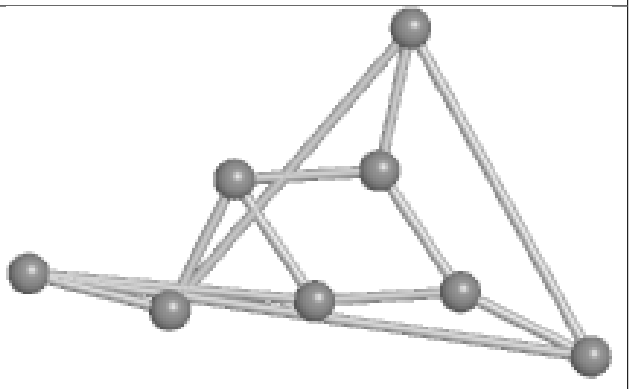


Rings

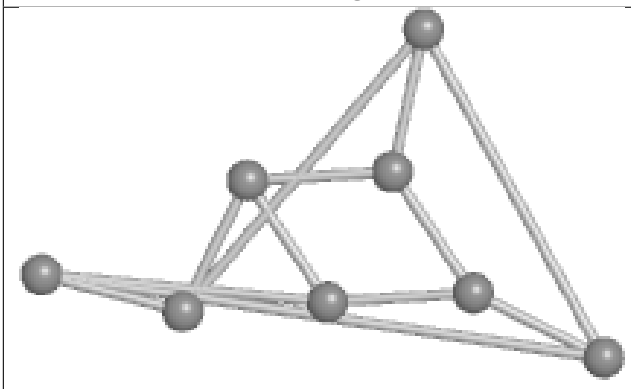
Ligand SF4 G 802



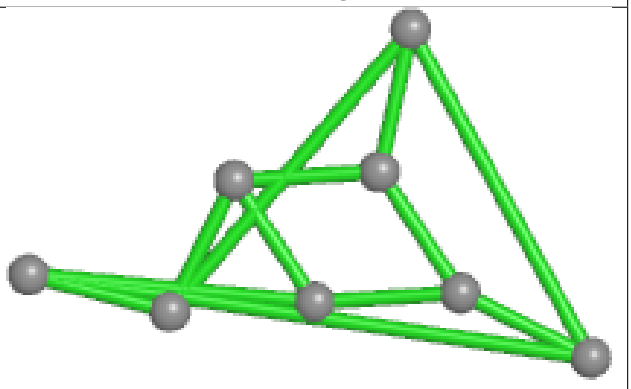
Bond lengths



Bond angles

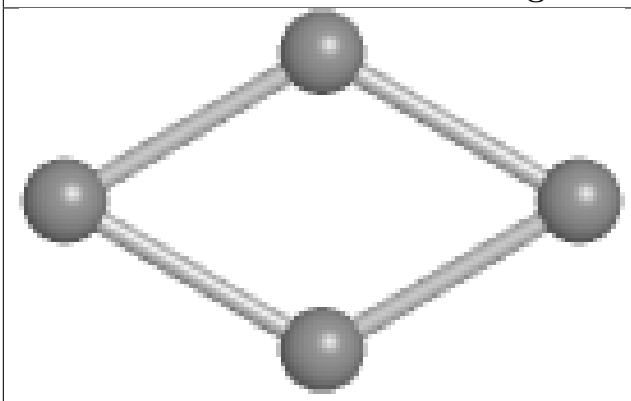


Torsions

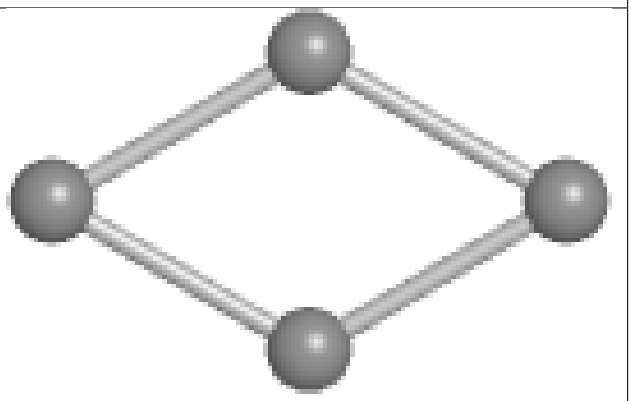


Rings

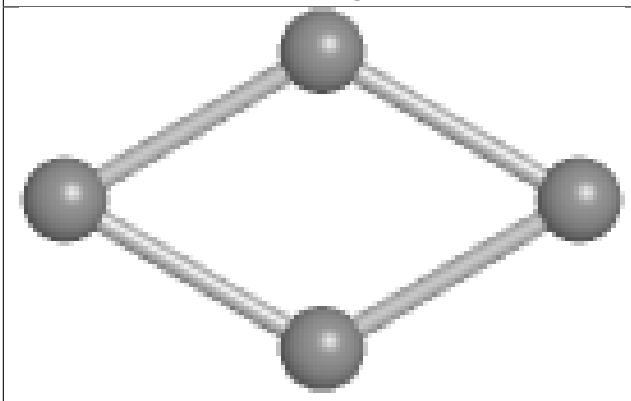
Ligand FES G 803



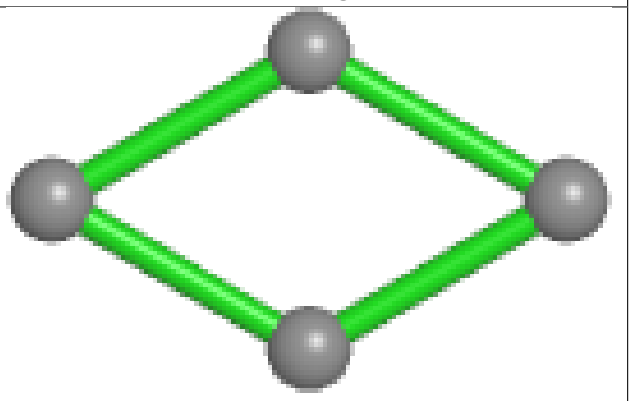
Bond lengths



Bond angles

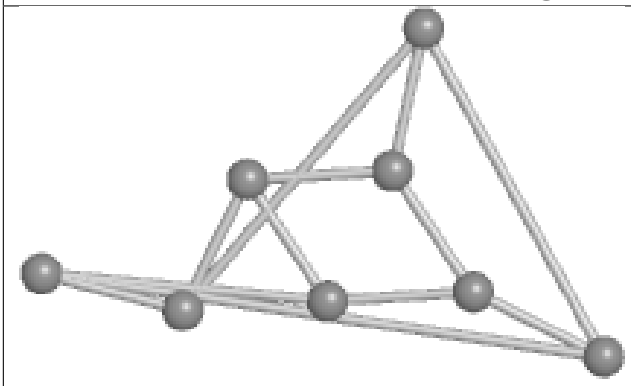


Torsions

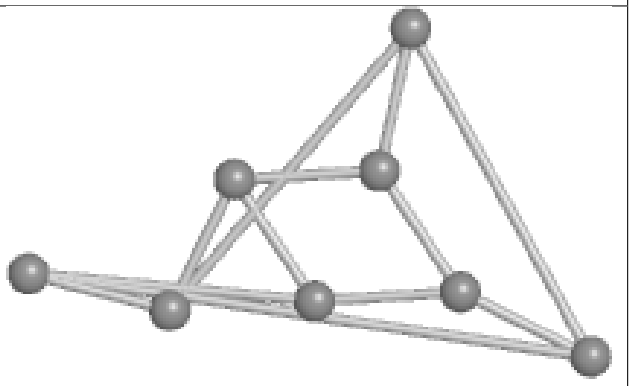


Rings

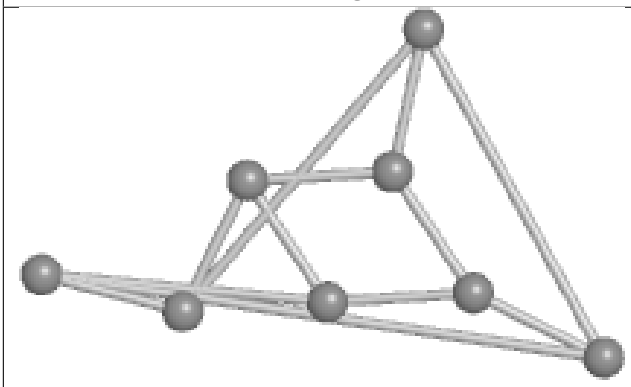
Ligand SF4 I 302



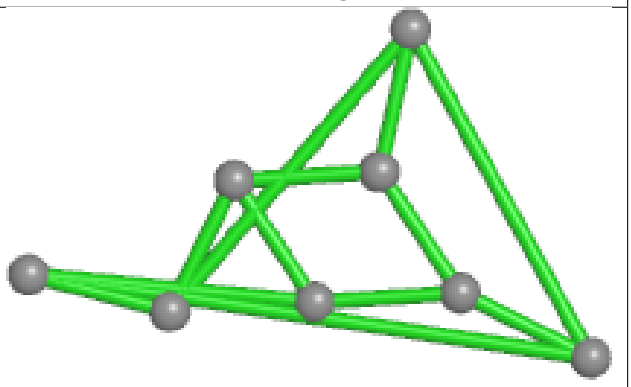
Bond lengths



Bond angles

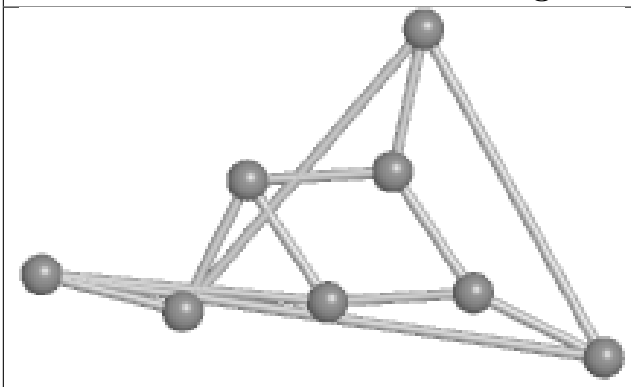


Torsions

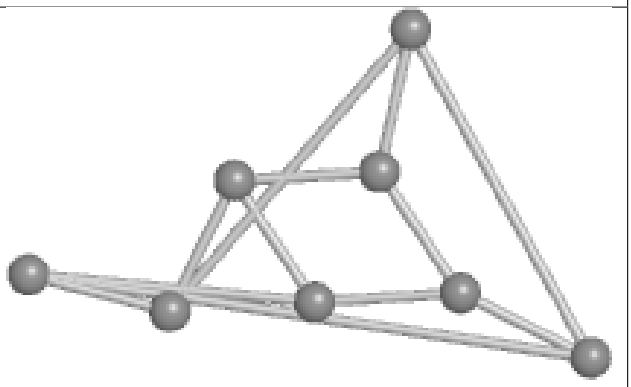


Rings

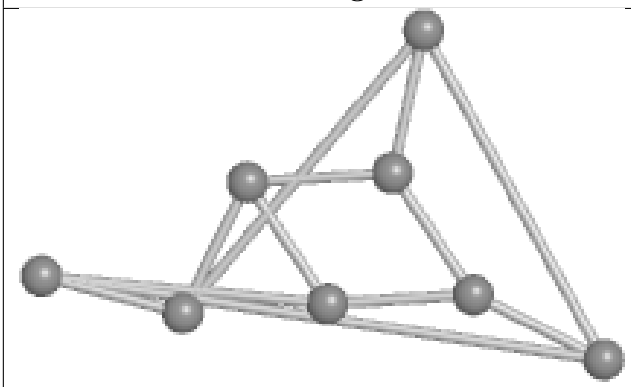
Ligand SF4 F 502



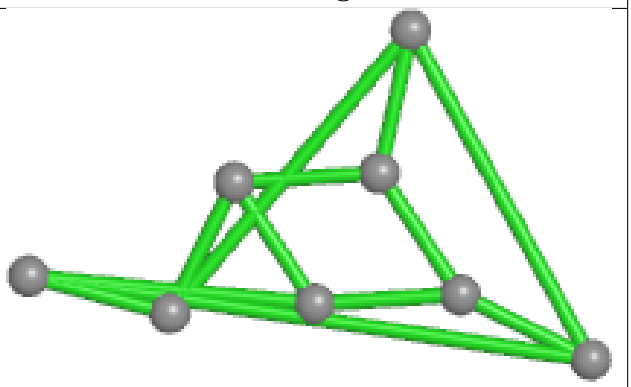
Bond lengths



Bond angles



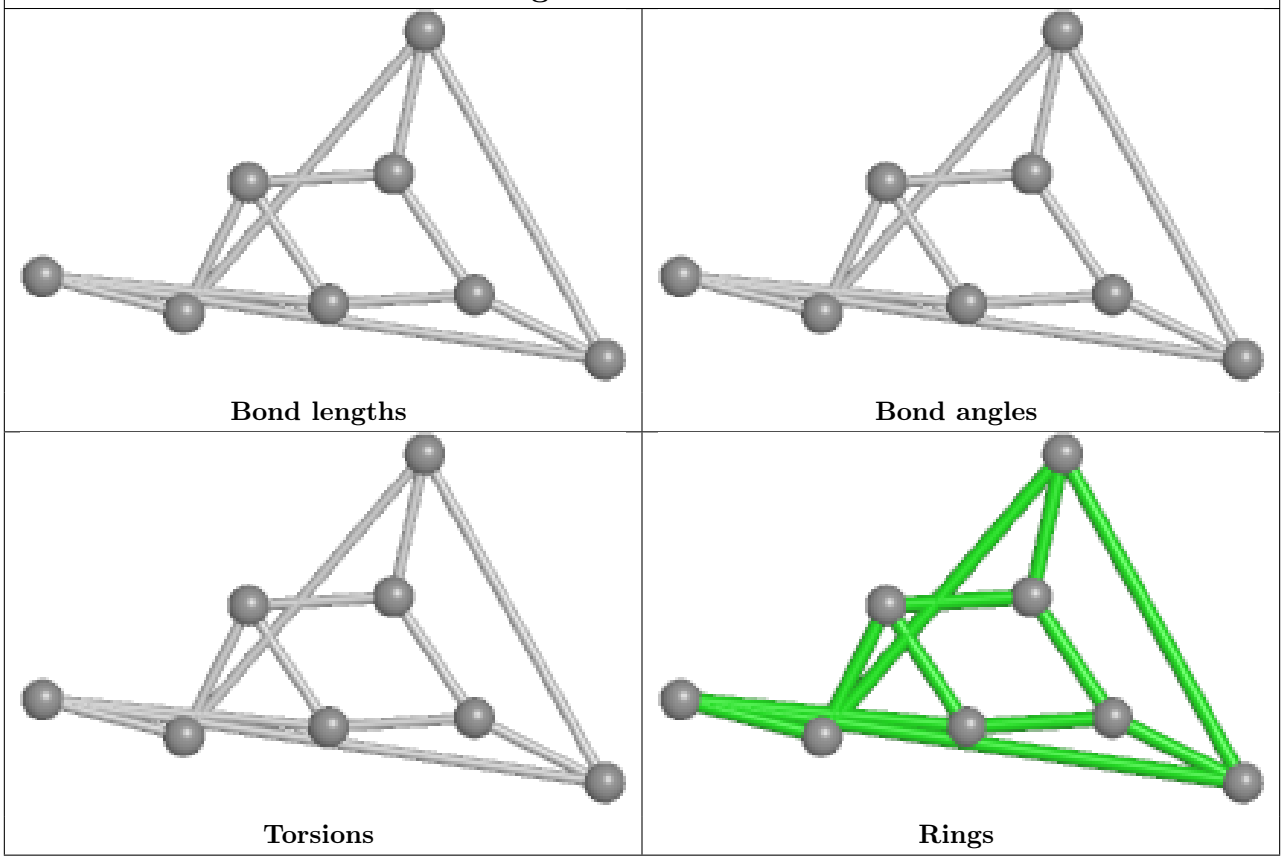
Torsions



Rings

Ligand PC1 I 301

Ligand SF4 G 801



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.

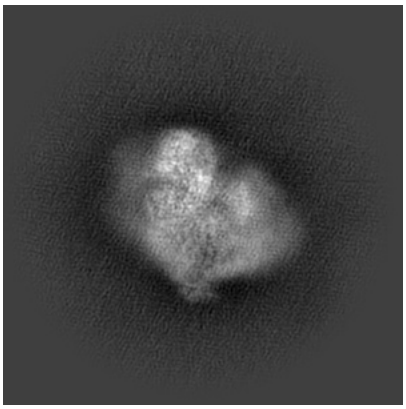
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38508. These allow visual inspection of the internal detail of the map and identification of artifacts.

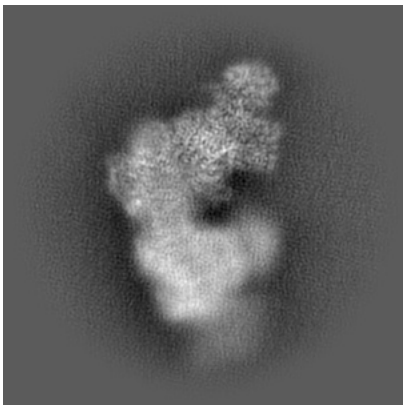
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

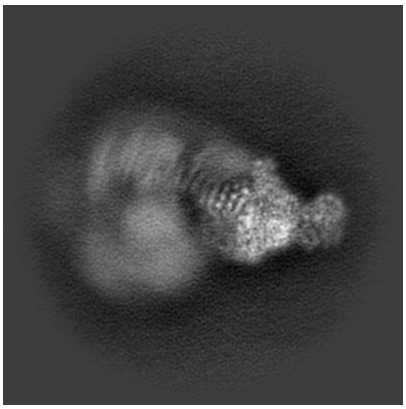
6.1.1 Primary map



X

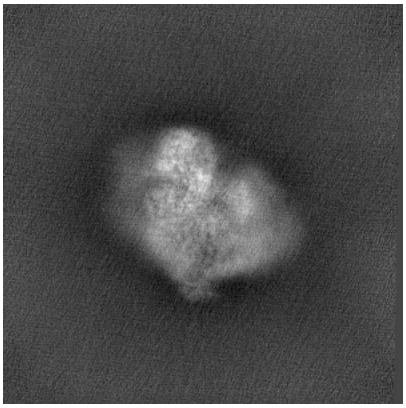


Y

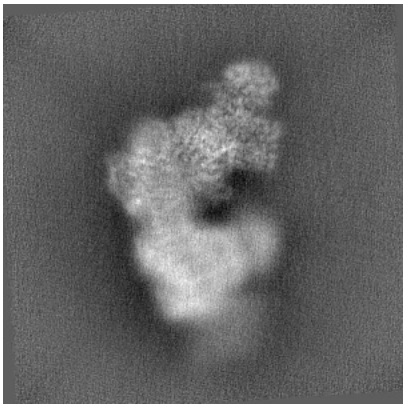


Z

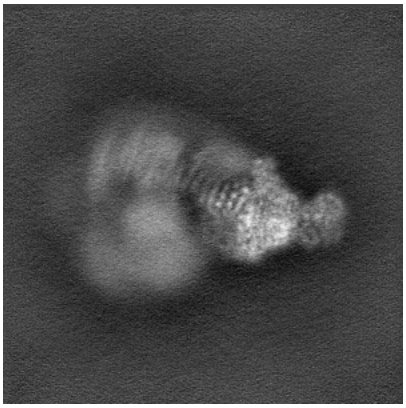
6.1.2 Raw map



X



Y

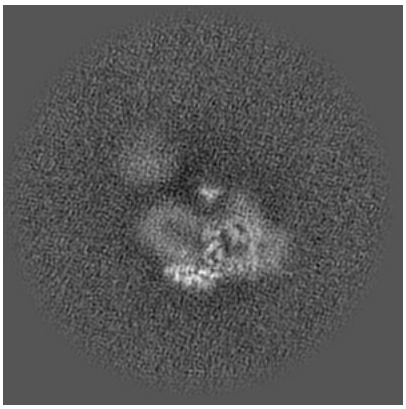


Z

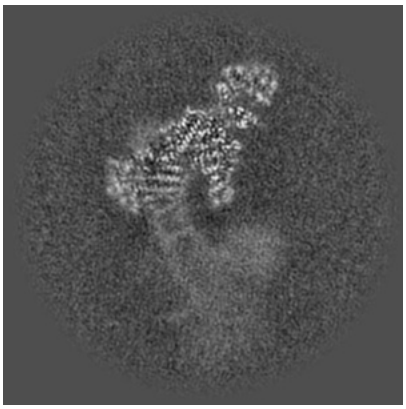
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

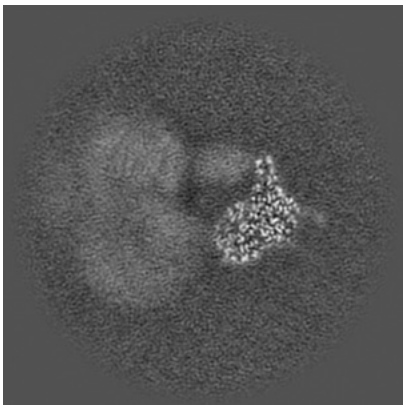
6.2.1 Primary map



X Index: 192

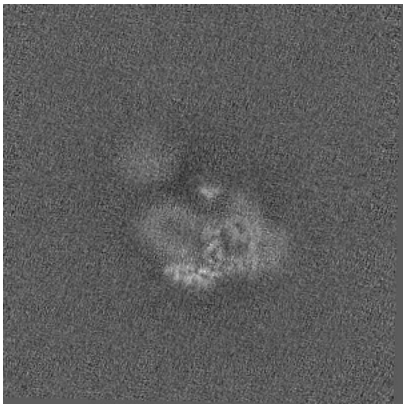


Y Index: 192

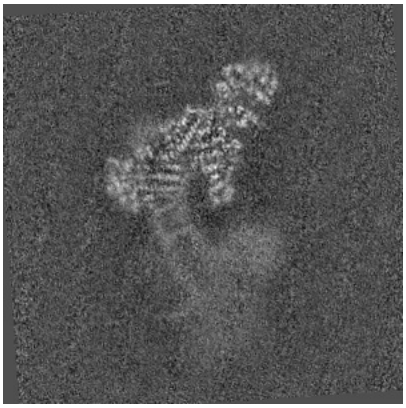


Z Index: 192

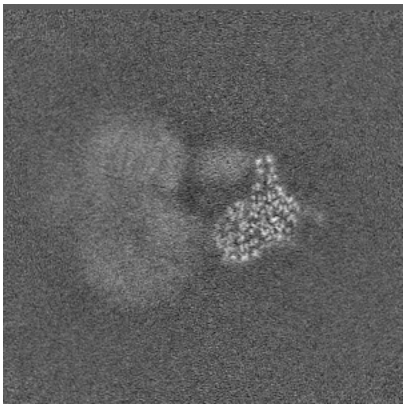
6.2.2 Raw map



X Index: 192



Y Index: 192

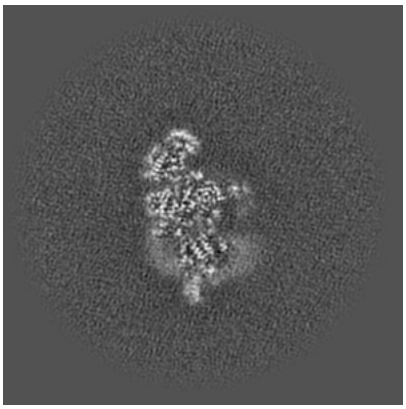


Z Index: 192

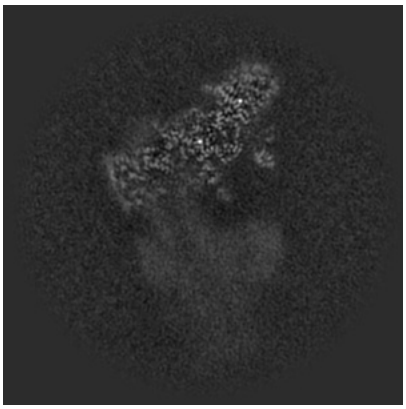
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

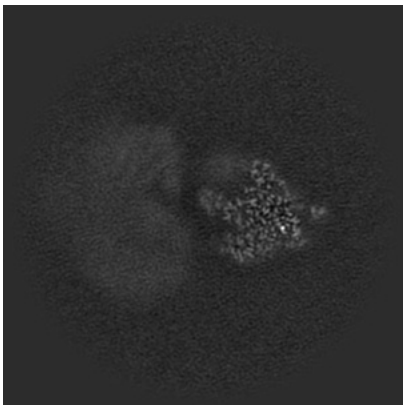
6.3.1 Primary map



X Index: 238

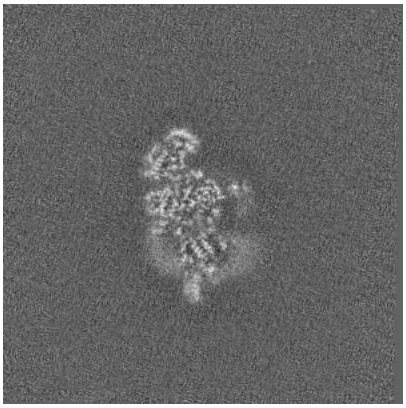


Y Index: 180

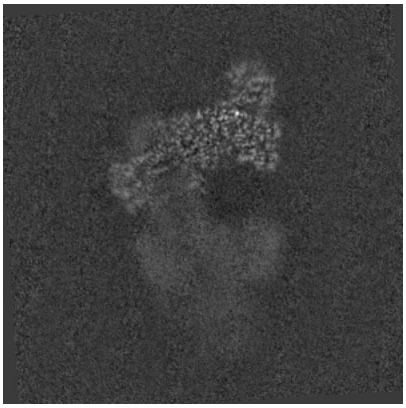


Z Index: 202

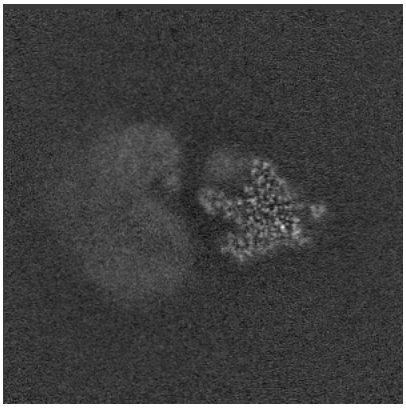
6.3.2 Raw map



X Index: 238



Y Index: 172

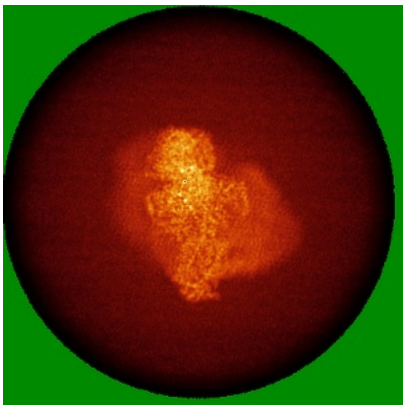


Z Index: 203

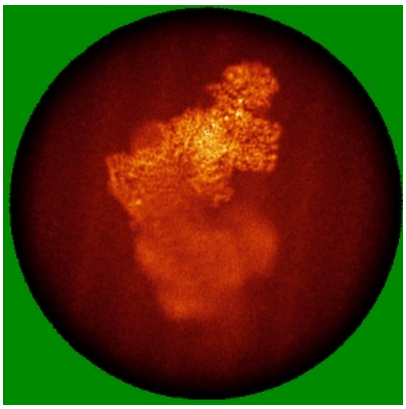
The images above show the largest variance slices of the map in three orthogonal directions.

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

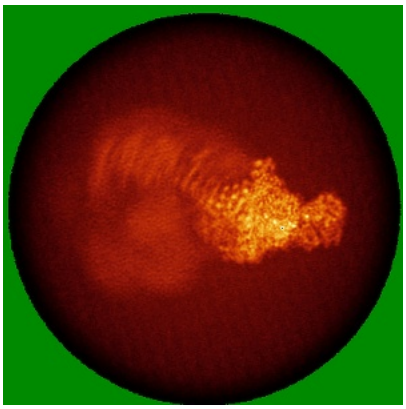
6.4.1 Primary map



X

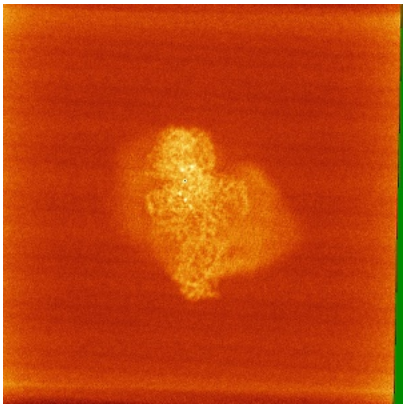


Y

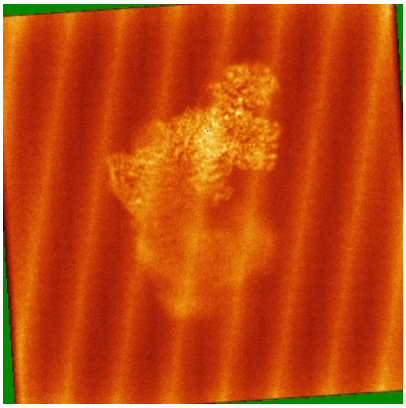


Z

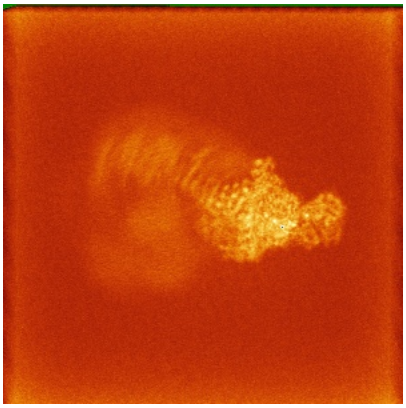
6.4.2 Raw map



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.

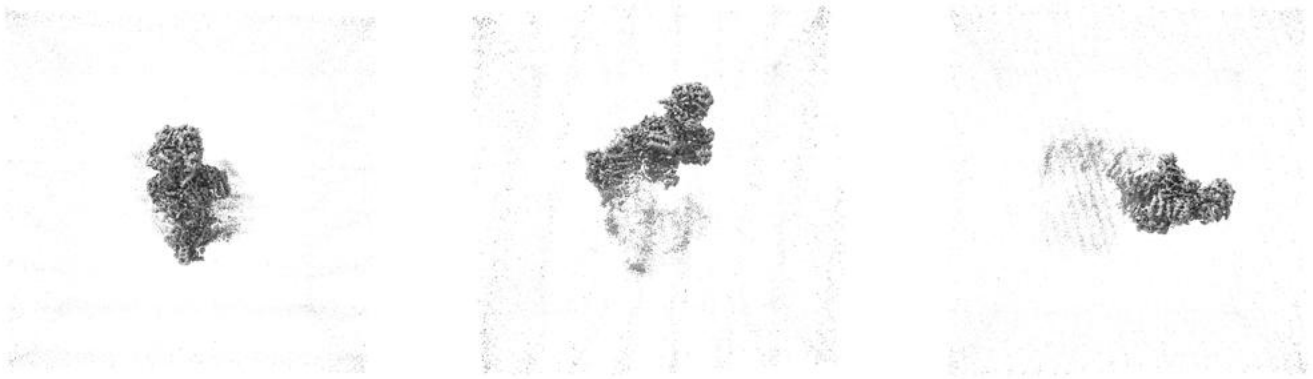
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

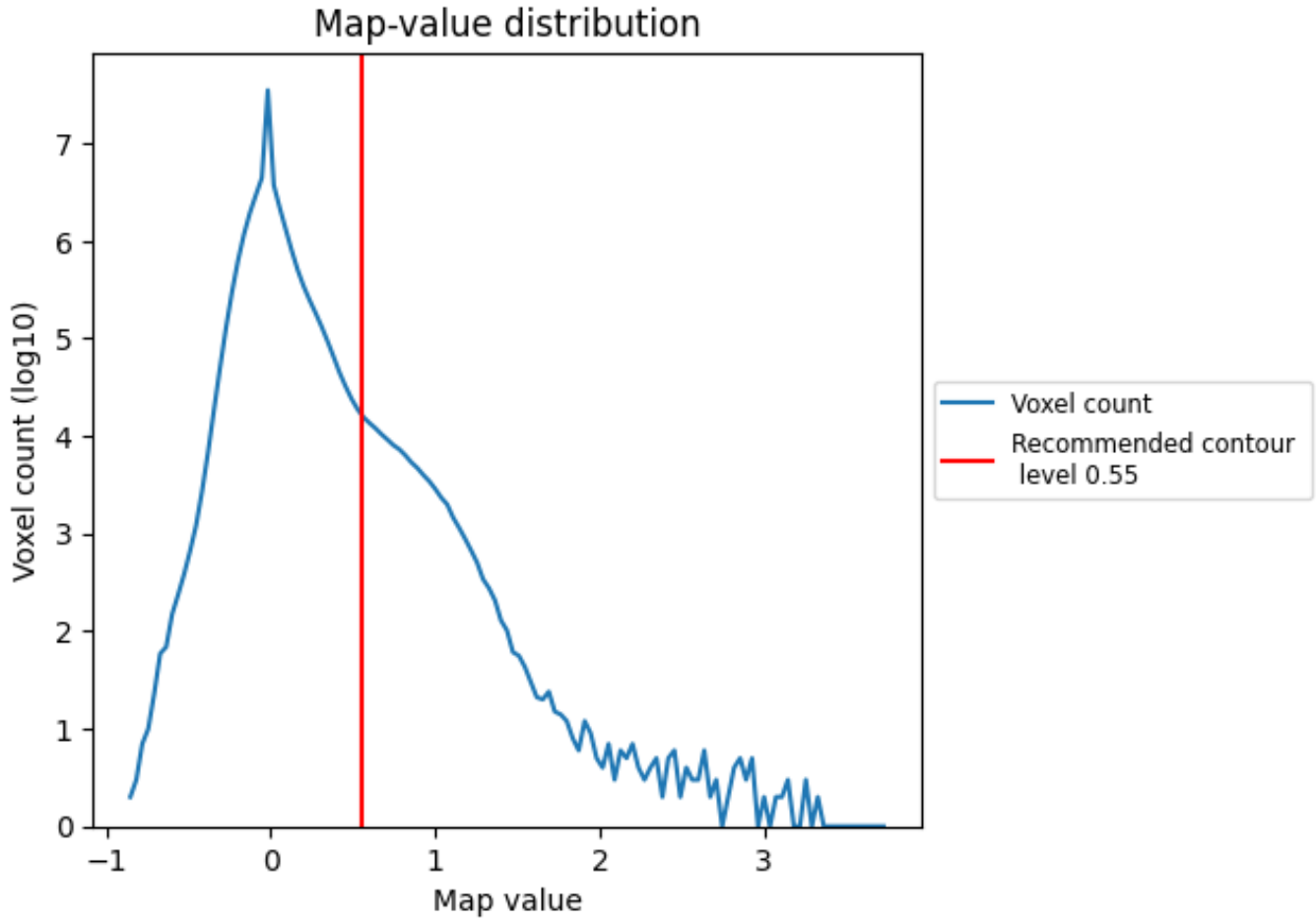
6.6 Mask visualisation (i)

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

7 Map analysis

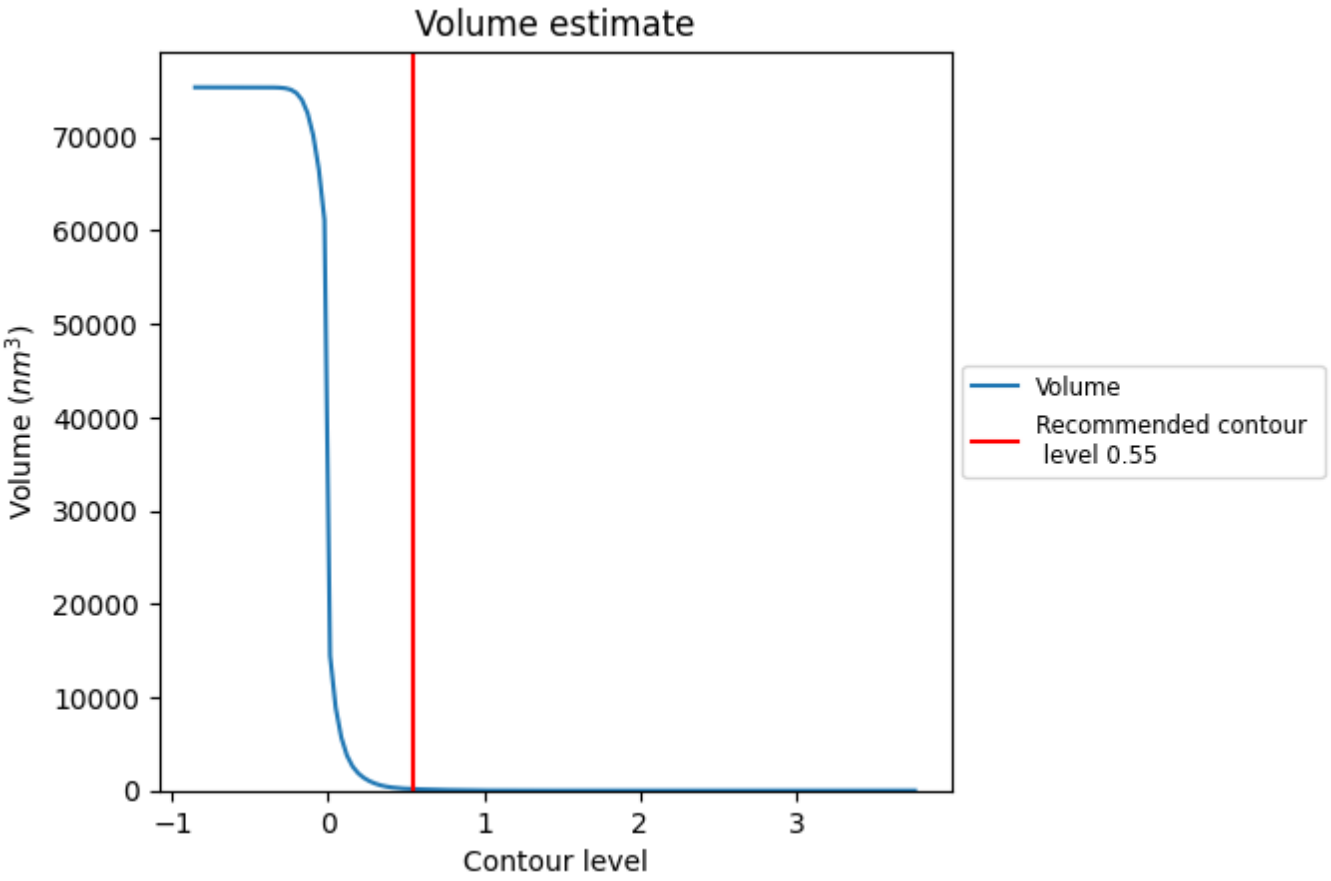
This section contains the results of statistical analysis of the map.

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.

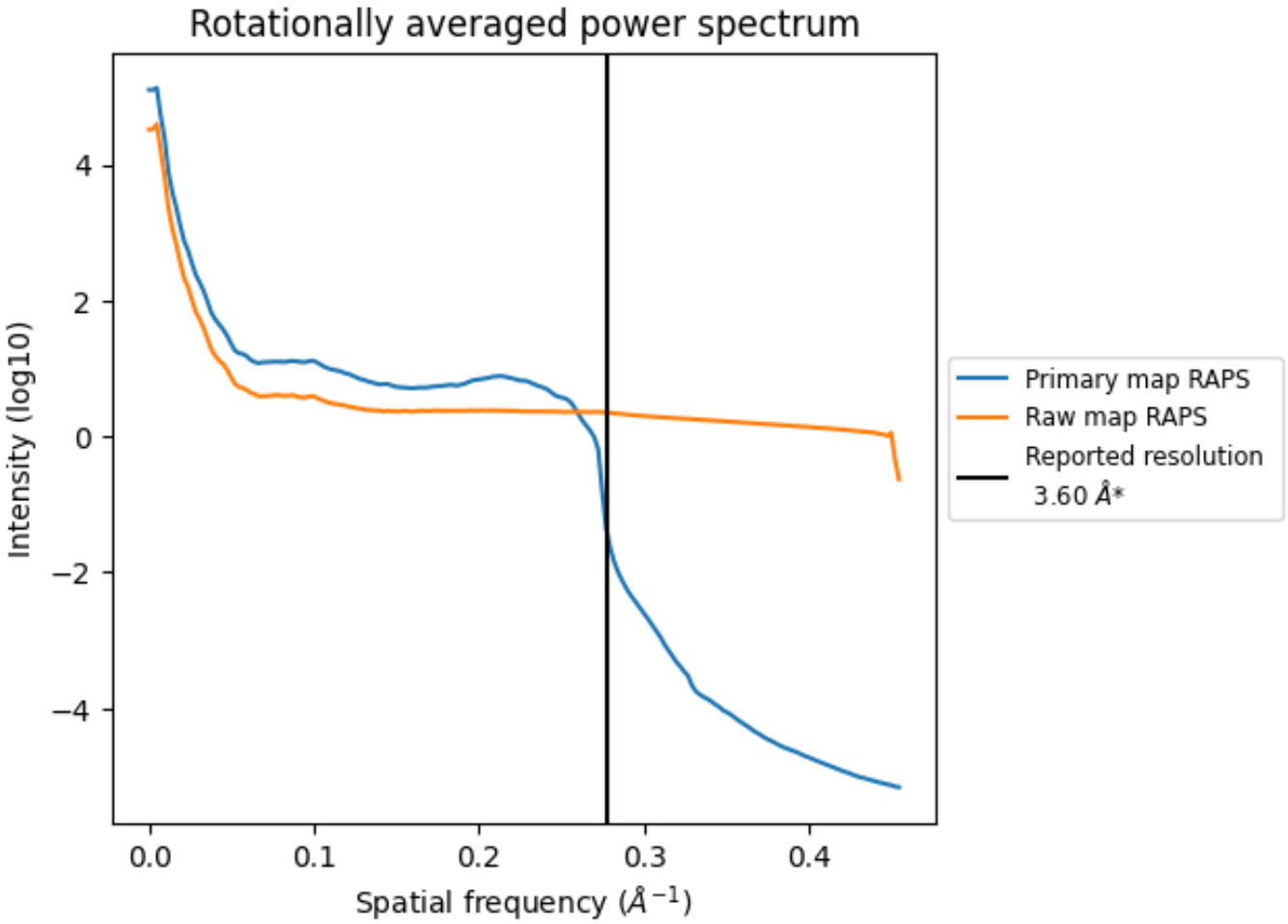
7.2 Volume estimate (i)



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 145 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)

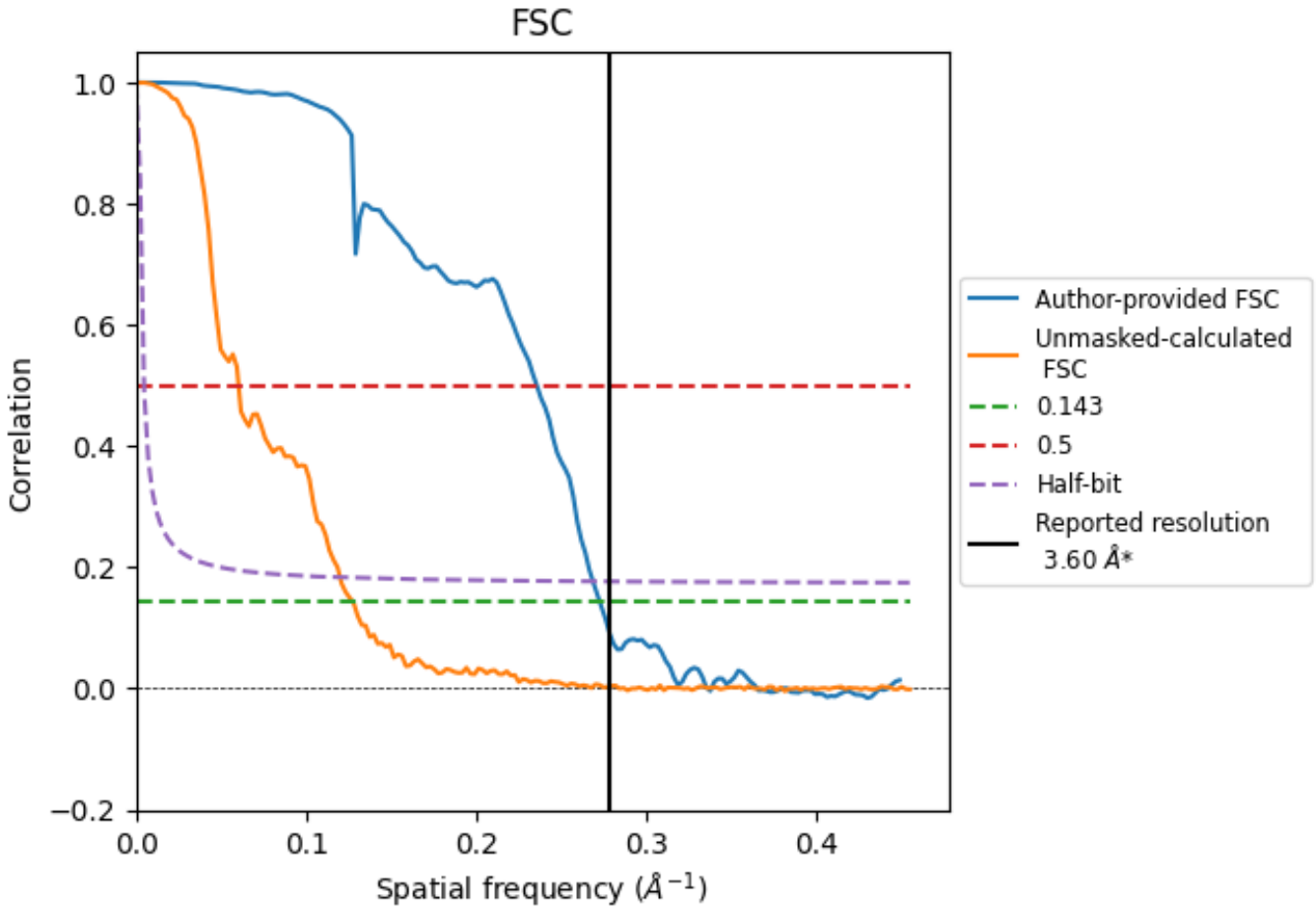


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

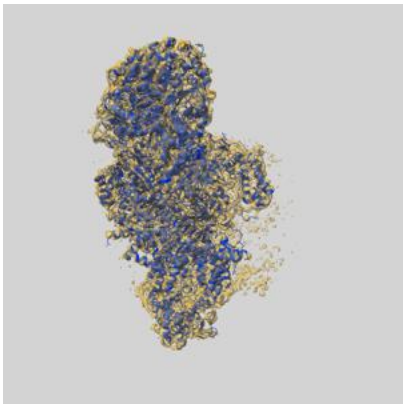
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.67	4.25	3.72
Unmasked-calculated*	7.86	16.61	8.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.86 differs from the reported value 3.6 by more than 10 %

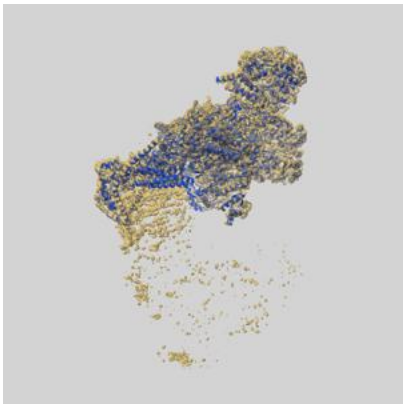
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38508 and PDB model 8XNN. Per-residue inclusion information can be found in section 3 on page 15.

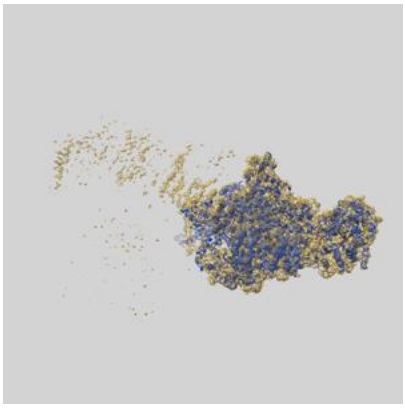
9.1 Map-model overlay



X



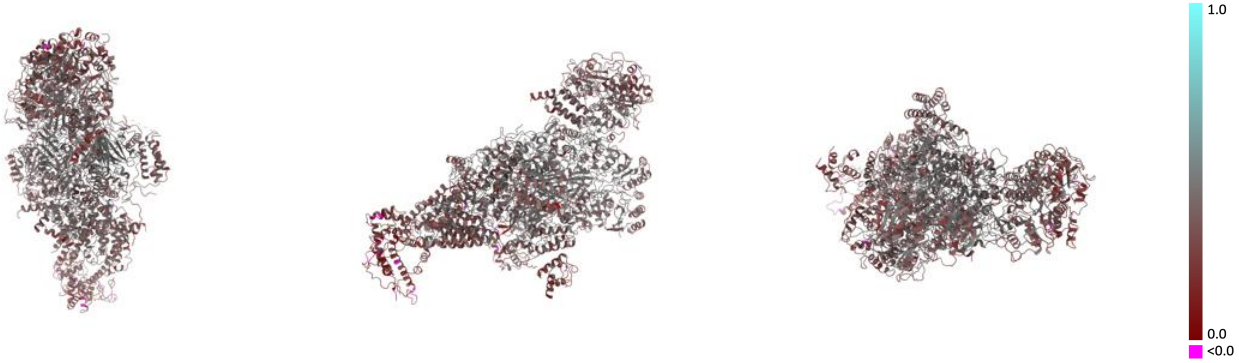
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

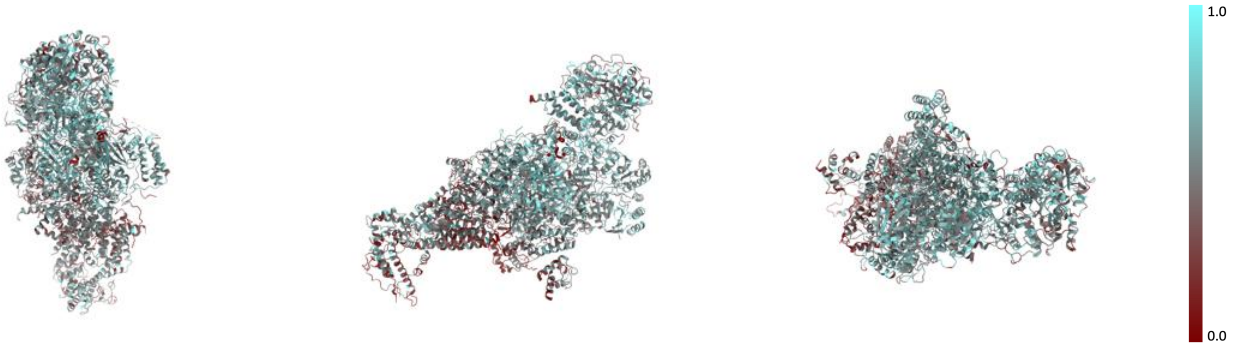
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

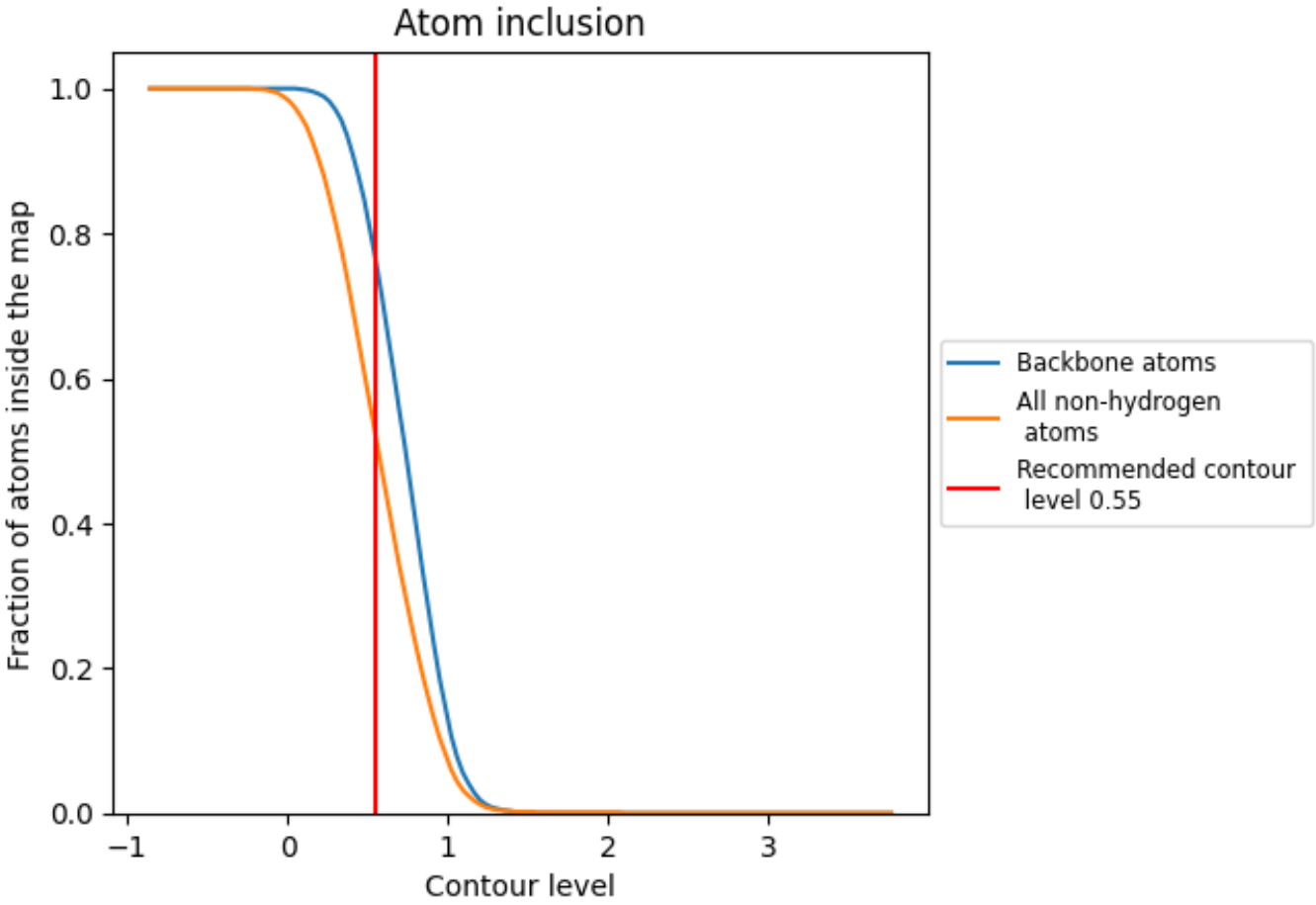
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5220	0.3700
A	0.2710	0.3220
B	0.5740	0.4130
C	0.6190	0.4350
D	0.5940	0.4220
E	0.5220	0.3380
F	0.5770	0.3540
G	0.6160	0.4070
H	0.4340	0.3840
I	0.5980	0.4160
P	0.4250	0.3350
Q	0.5130	0.4100
R	0.4840	0.3850
S	0.6220	0.3700
T	0.3820	0.2760
V	0.5870	0.3570
W	0.4980	0.3720
X	0.4300	0.2200
Z	0.4340	0.2810
a	0.5010	0.3100
b	0.3890	0.2730
q	0.4560	0.3860
r	0.3760	0.3730
s	0.3460	0.2780