wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 11:06 PM JST

PDB ID	:	7VBN
EMDB ID	:	EMD-31883
Title	:	Matrix arm of deactive state CI from DQ-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-31
Resolution	:	2.40 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

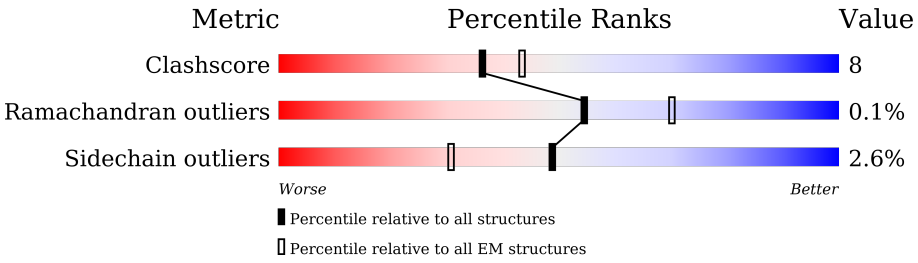
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	431	5% 77% 21%
2	B	176	81% 19%
3	C	156	80% 17%
4	E	115	82% 18%
5	F	86	8% 83% 17%
6	G	88	55% 70% 30%
7	H	112	86% 14%
8	I	112	21% 71% 14% 13%

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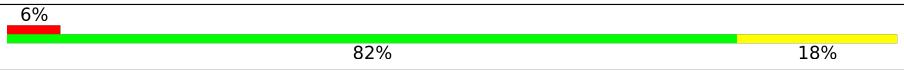
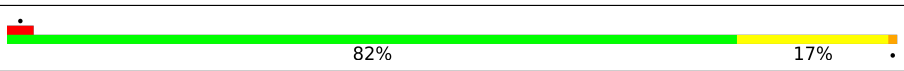
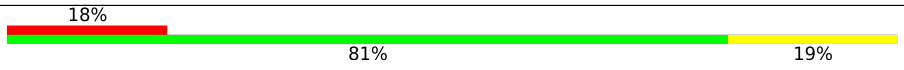
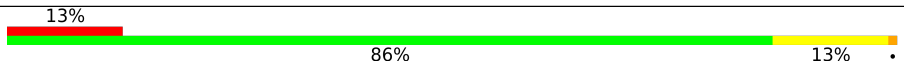
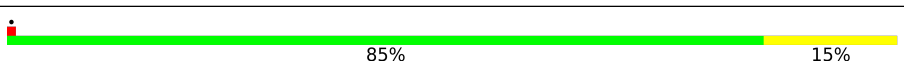
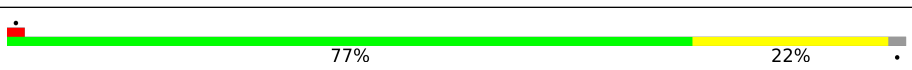
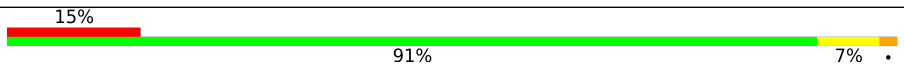
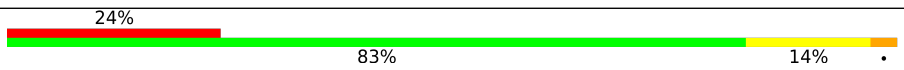
Mol	Chain	Length	Quality of chain
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	385	
17	T	96	
18	W	29	

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
19	SF4	A	501	-	-	X	-
19	SF4	C	301	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 29042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	691	434	129	126	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	331	Total	C	N	O	S	0	0
			2651	1719	466	458	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	379	Total	C	N	O	S	0	0
			3044	1945	522	554	23		

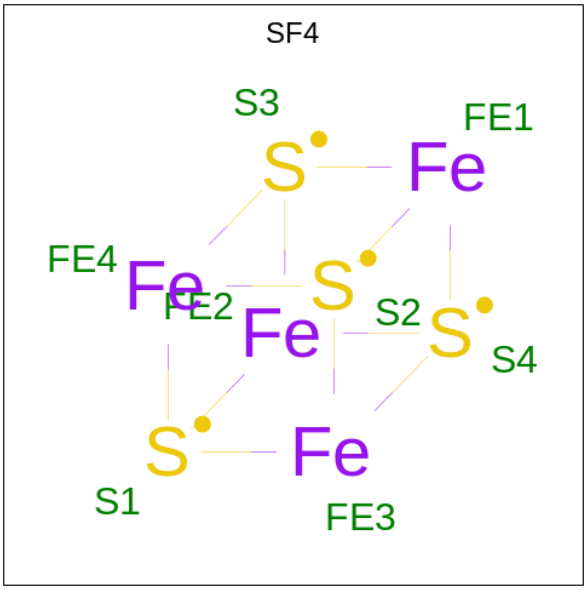
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

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

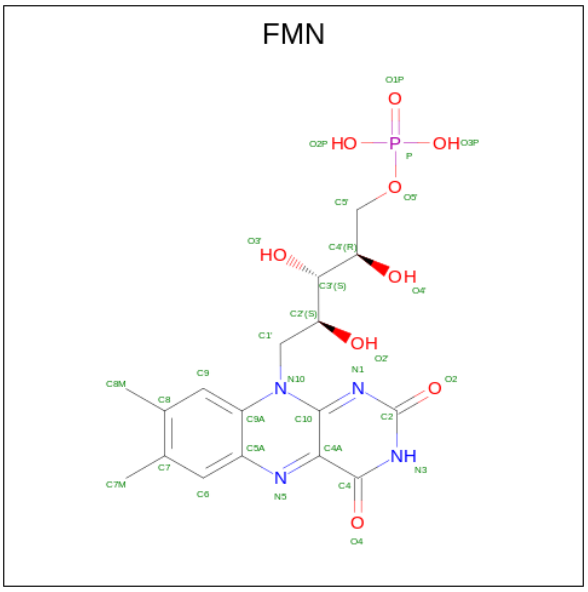
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			224	141	43	39	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



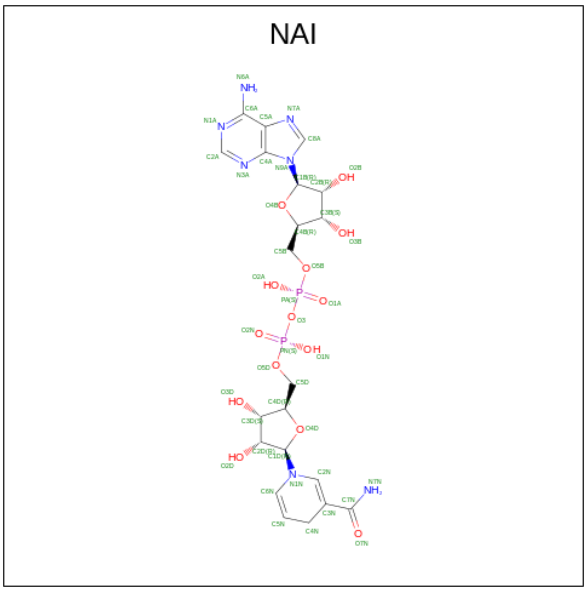
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	Fe	S		0
			8	4	4		
19	B	1	Total	Fe	S		0
			16	8	8		
19	B	1	Total	Fe	S		0
			16	8	8		
19	C	1	Total	Fe	S		0
			8	4	4		
19	M	1	Total	Fe	S		0
			16	8	8		
19	M	1	Total	Fe	S		0
			16	8	8		

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



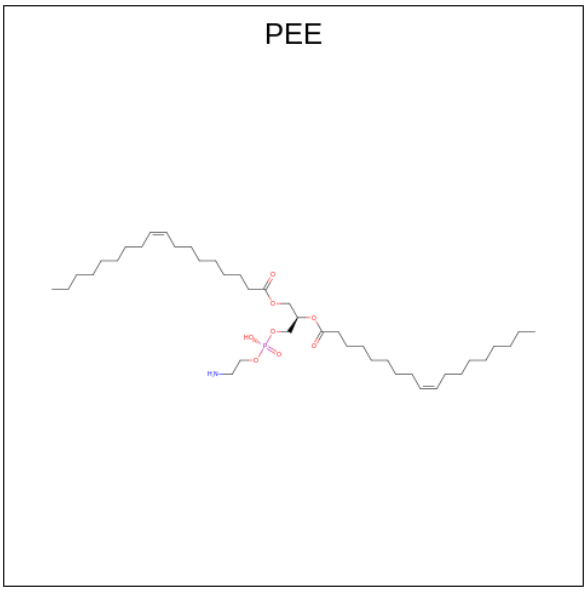
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



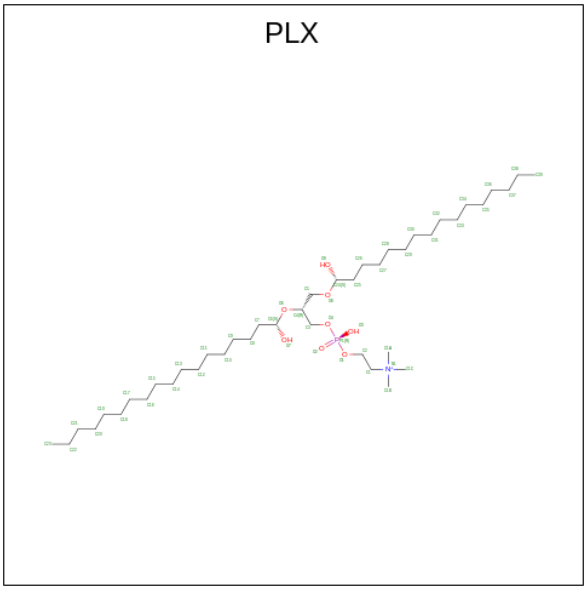
Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 22 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



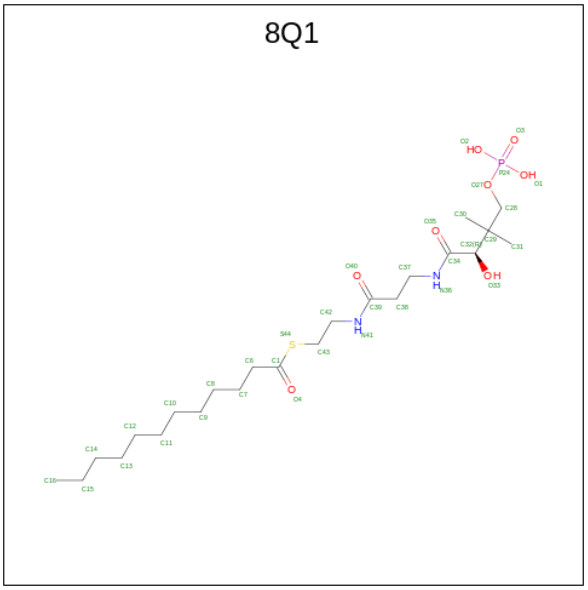
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 23 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



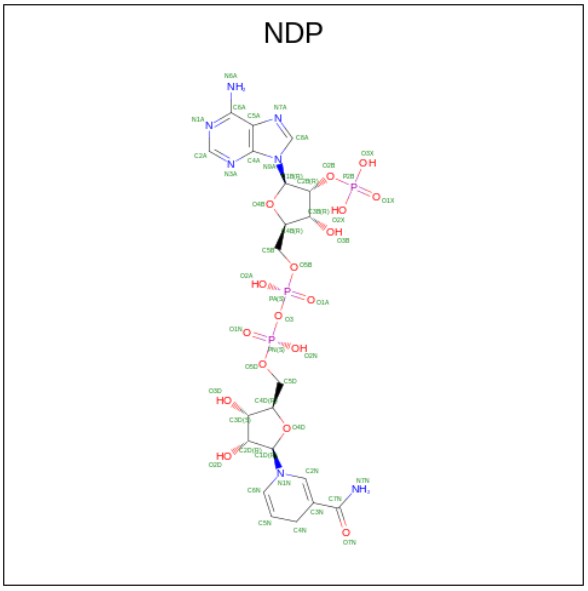
Mol	Chain	Residues	Atoms					AltConf
23	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 24 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



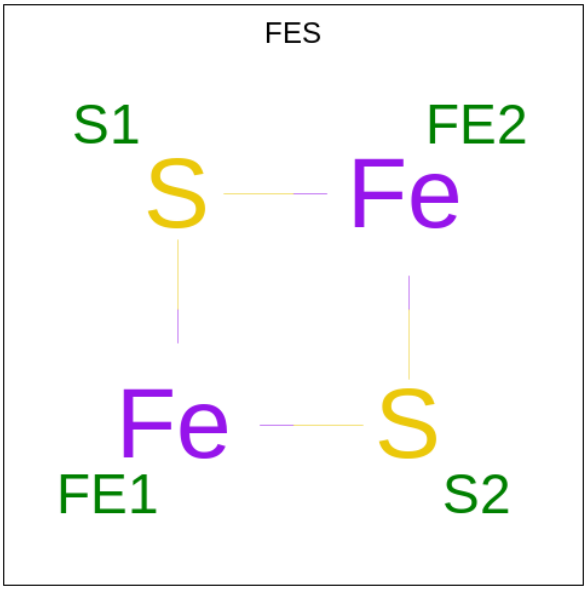
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
24	G	1	35	23	2	8	1	1	0

- Molecule 25 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
25	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

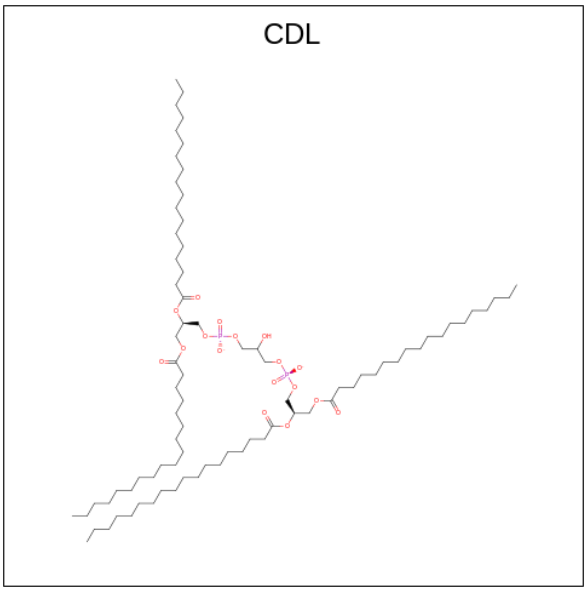


Mol	Chain	Residues	Atoms				AltConf
26	M	1	Total	Fe	S		0
			4	2	2		
26	O	1	Total	Fe	S		0
			4	2	2		

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	M	1	Total	Mg	0
			1	1	

- Molecule 28 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	N	1	Total	C	O	P	0
			51	32	17	2	

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
29	T	1	Total	Zn	0
			1	1	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	50	Total	O	0
			50	50	
30	B	77	Total	O	0
			77	77	
30	C	55	Total	O	0
			55	55	
30	E	2	Total	O	0
			2	2	
30	F	1	Total	O	0
			1	1	
30	H	4	Total	O	0
			4	4	
30	I	10	Total	O	0
			10	10	

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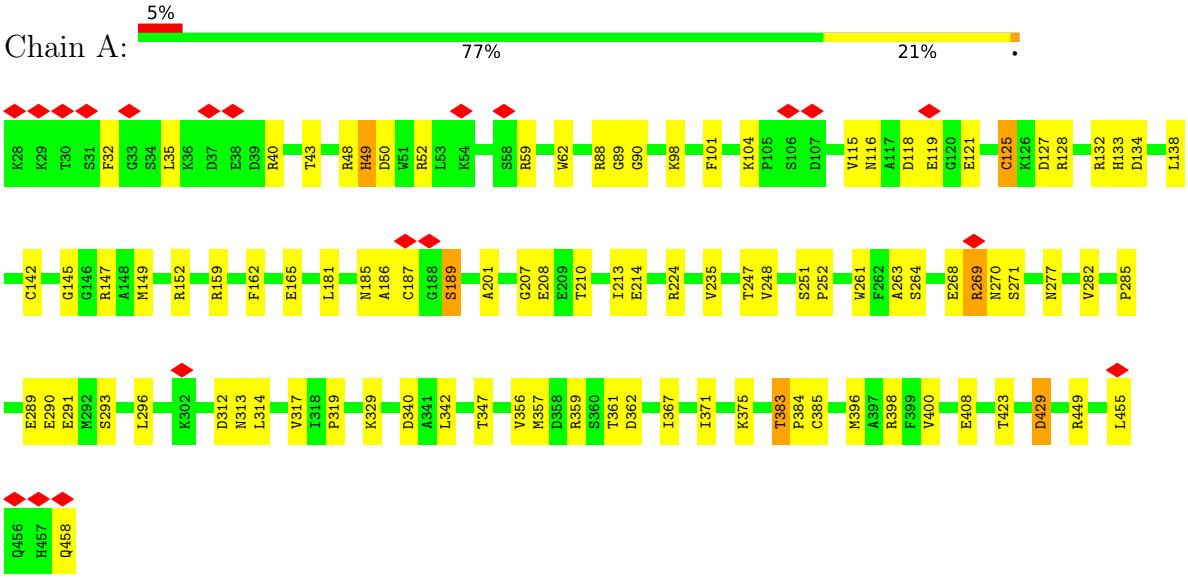
Mol	Chain	Residues	Atoms	AltConf
30	J	7	Total O 7 7	0
30	K	4	Total O 4 4	0
30	L	21	Total O 21 21	0
30	M	193	Total O 193 193	0
30	N	6	Total O 6 6	0
30	O	15	Total O 15 15	0
30	P	75	Total O 75 75	0
30	Q	181	Total O 181 181	0
30	T	10	Total O 10 10	0
30	W	2	Total O 2 2	0

3 Residue-property plots (i)

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

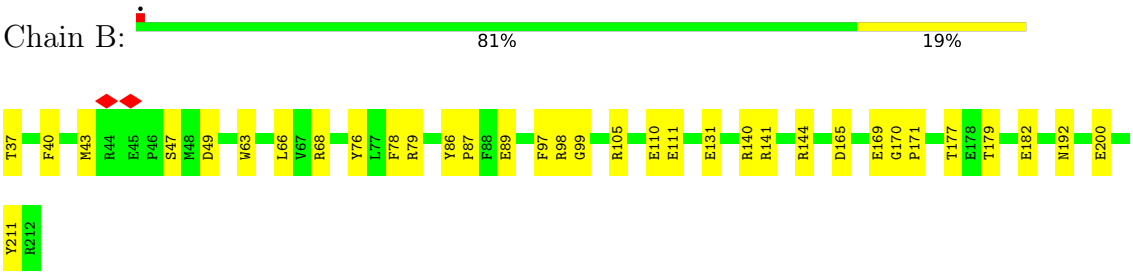
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A:



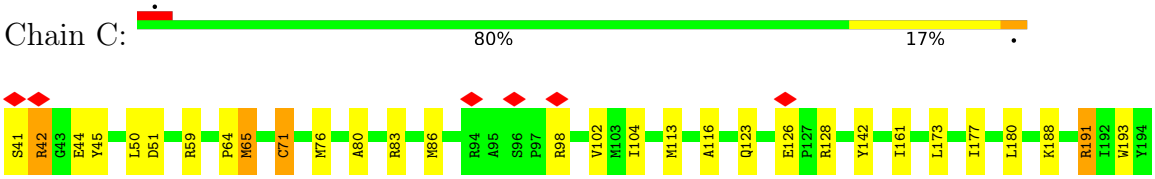
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B:



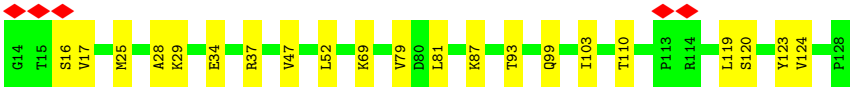
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:



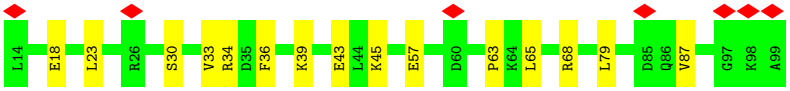
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



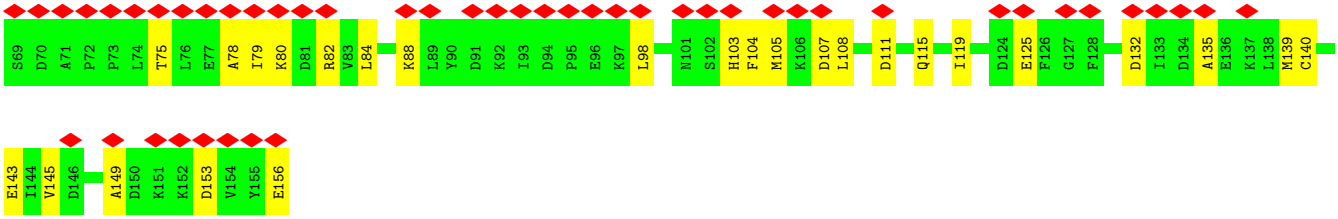
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



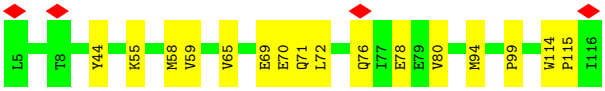
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G:



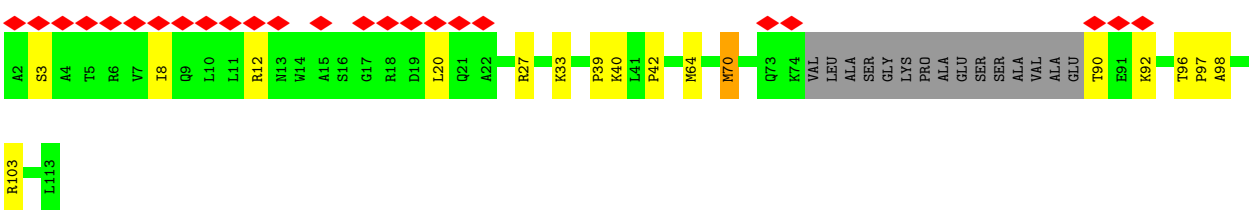
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:



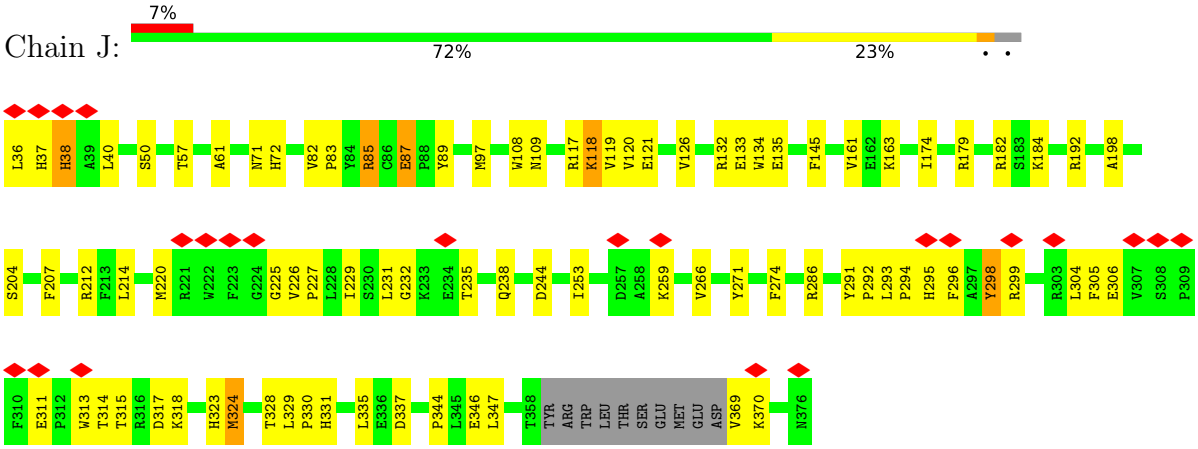
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:



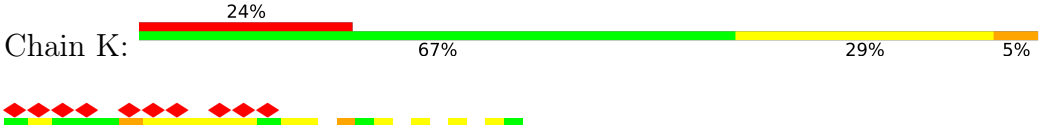
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

Chain J:



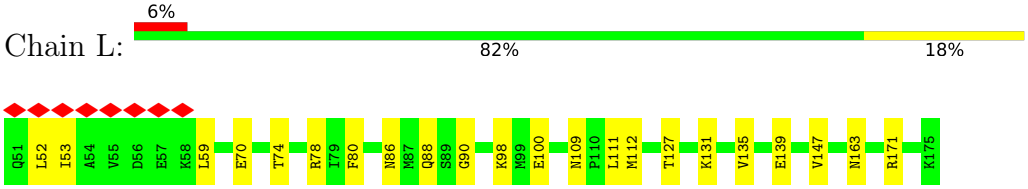
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



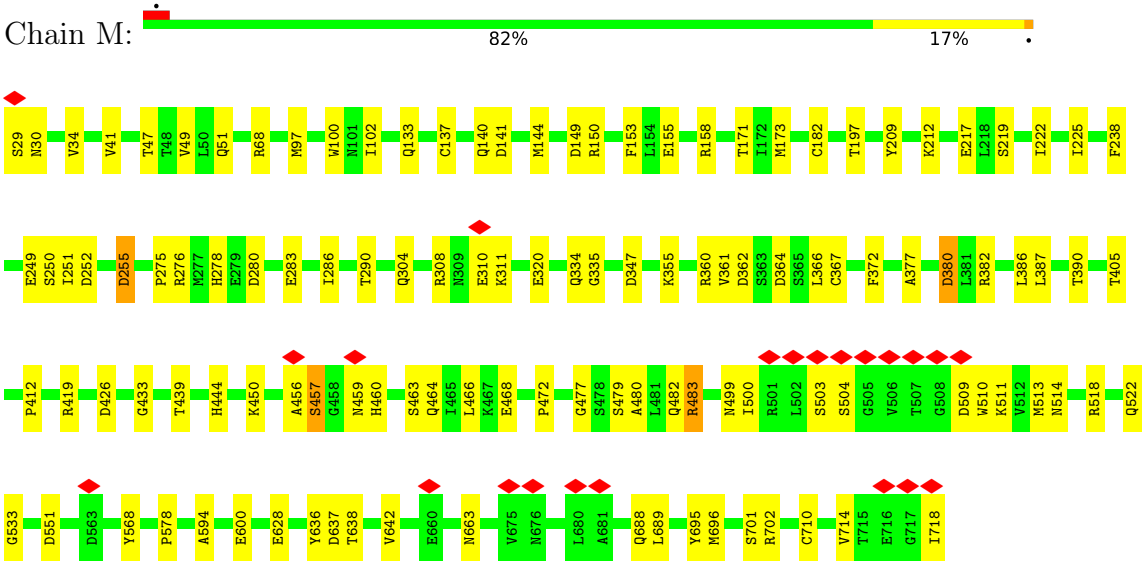
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



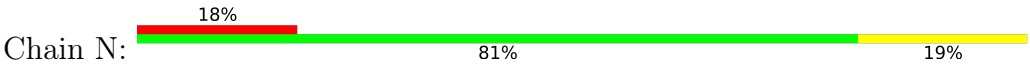
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

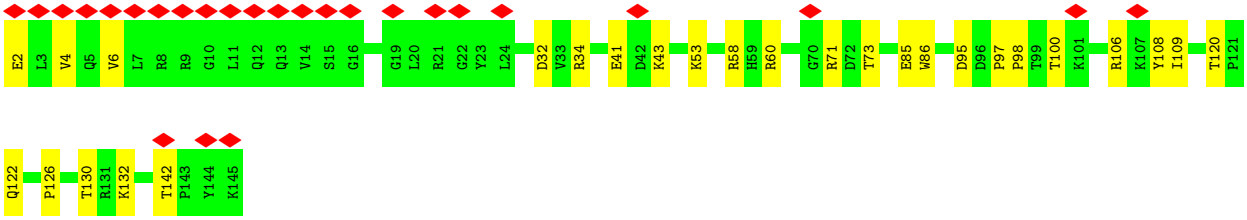
Chain M:



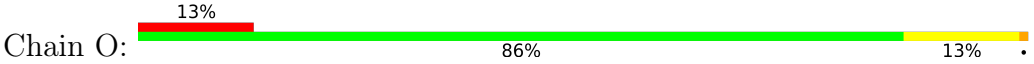
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

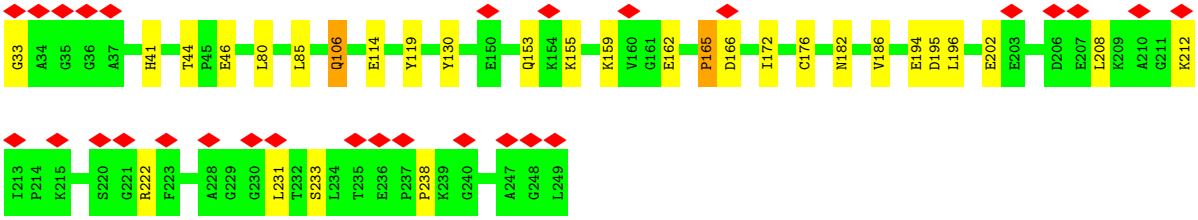
Chain N:



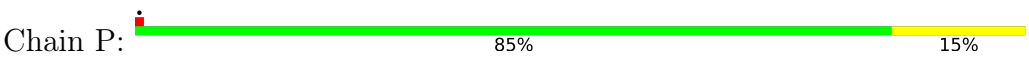


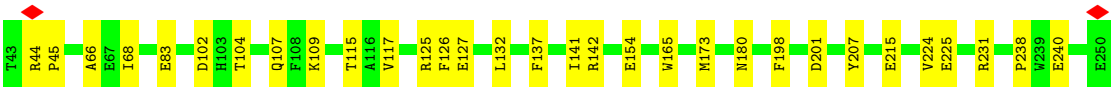
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



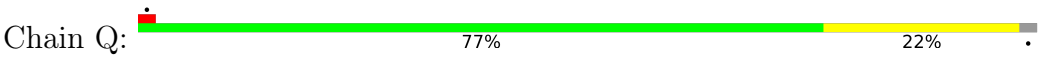


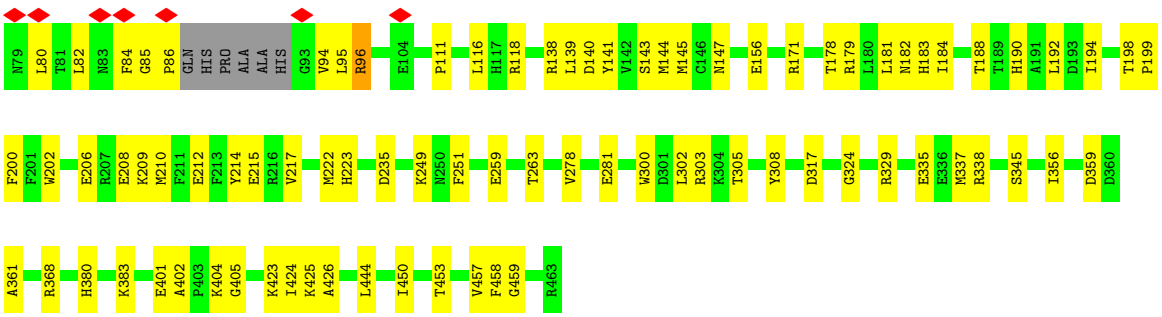
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



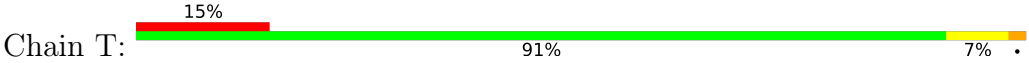


• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



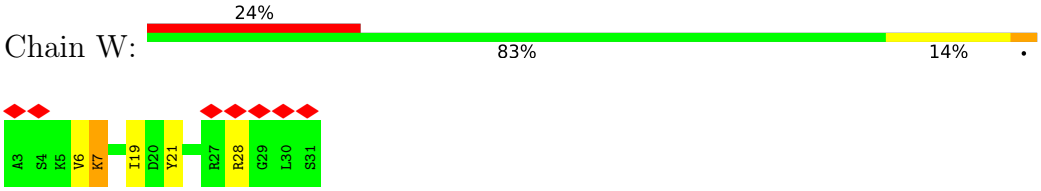


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	387112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	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: 2MR, NAI, 8Q1, NDP, FMN, FES, PEE, MG, SF4, ZN, CDL, PLX

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	0.26	0/3393	0.49	0/4584
2	B	0.26	0/1443	0.50	0/1952
3	C	0.26	0/1279	0.54	0/1730
4	E	0.25	0/995	0.52	0/1340
5	F	0.27	0/702	0.54	0/945
6	G	0.26	0/705	0.49	0/956
7	H	0.24	0/929	0.43	0/1258
8	I	0.25	0/798	0.55	0/1079
9	J	0.25	0/2724	0.49	0/3691
10	K	0.24	0/365	0.48	0/493
11	L	0.25	0/1039	0.51	0/1403
12	M	0.25	0/5384	0.50	0/7295
13	N	0.25	0/1245	0.51	0/1694
14	O	0.30	1/1711 (0.1%)	0.55	3/2328 (0.1%)
15	P	0.27	0/1789	0.52	0/2436
16	Q	0.27	0/3101	0.52	0/4189
17	T	0.25	0/755	0.52	0/1018
18	W	0.27	0/230	0.52	0/309
All	All	0.26	1/28587 (0.0%)	0.51	3/38700 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	165	PRO	CG-CD	-5.46	1.32	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	165	PRO	N-CD-CG	-9.27	89.30	103.20
14	O	165	PRO	CA-CB-CG	-7.11	90.50	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	165	PRO	N-CA-CB	-5.58	96.46	102.60

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	3318	0	3280	63	0
2	B	1412	0	1363	25	0
3	C	1248	0	1254	32	0
4	E	971	0	975	12	0
5	F	691	0	704	11	0
6	G	693	0	671	16	0
7	H	910	0	950	9	0
8	I	780	0	808	14	0
9	J	2651	0	2681	78	0
10	K	355	0	329	10	0
11	L	1016	0	1016	15	0
12	M	5296	0	5326	74	0
13	N	1204	0	1162	19	0
14	O	1671	0	1673	22	0
15	P	1738	0	1693	23	0
16	Q	3044	0	3018	81	0
17	T	741	0	702	6	0
18	W	224	0	230	5	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	2	0
19	M	16	0	0	0	0
20	A	31	0	19	2	0
21	A	44	0	27	5	0
22	C	47	0	71	20	0
23	C	52	0	88	10	0
24	G	35	0	0	0	0
25	J	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	M	4	0	0	0	0
26	O	4	0	0	0	0
27	M	1	0	0	0	0
28	N	51	0	46	6	0
29	T	1	0	0	0	0
30	A	50	0	0	0	0
30	B	77	0	0	1	0
30	C	55	0	0	3	0
30	E	2	0	0	1	0
30	F	1	0	0	0	0
30	H	4	0	0	0	0
30	I	10	0	0	0	0
30	J	7	0	0	1	0
30	K	4	0	0	0	0
30	L	21	0	0	0	0
30	M	193	0	0	3	0
30	N	6	0	0	0	0
30	O	15	0	0	0	0
30	P	75	0	0	3	0
30	Q	181	0	0	10	0
30	T	10	0	0	0	0
30	W	2	0	0	0	0
All	All	29042	0	28112	472	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 472 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LEU:CD1	22:C:302:PEE:H25	1.19	1.57
3:C:50:LEU:HD13	22:C:302:PEE:C17	1.52	1.37
3:C:50:LEU:CD1	22:C:302:PEE:C17	1.99	1.36
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.21
3:C:50:LEU:HD11	22:C:302:PEE:H25	1.28	1.12

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	429/431 (100%)	417 (97%)	11 (3%)	1 (0%)	47 62
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100 100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100 100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100 100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100 100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100 100
7	H	110/112 (98%)	104 (94%)	6 (6%)	0	100 100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100 100
9	J	327/341 (96%)	315 (96%)	10 (3%)	2 (1%)	25 36
10	K	40/42 (95%)	39 (98%)	1 (2%)	0	100 100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100 100
12	M	688/690 (100%)	669 (97%)	18 (3%)	1 (0%)	51 68
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100 100
14	O	215/217 (99%)	208 (97%)	7 (3%)	0	100 100
15	P	206/208 (99%)	195 (95%)	11 (5%)	0	100 100
16	Q	374/385 (97%)	366 (98%)	8 (2%)	0	100 100
17	T	94/96 (98%)	92 (98%)	2 (2%)	0	100 100
18	W	27/29 (93%)	25 (93%)	2 (7%)	0	100 100
All	All	3479/3553 (98%)	3366 (97%)	109 (3%)	4 (0%)	54 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
9	J	38	HIS
9	J	227	PRO
12	M	283	GLU

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	345/345 (100%)	335 (97%)	10 (3%)	42	62
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	84
3	C	132/132 (100%)	125 (95%)	7 (5%)	22	37
4	E	107/107 (100%)	103 (96%)	4 (4%)	34	53
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	73 (96%)	3 (4%)	32	50
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	83 (95%)	4 (5%)	27	43
9	J	285/295 (97%)	274 (96%)	11 (4%)	32	50
10	K	41/41 (100%)	37 (90%)	4 (10%)	8	11
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	90
12	M	580/580 (100%)	566 (98%)	14 (2%)	49	68
13	N	130/130 (100%)	127 (98%)	3 (2%)	50	70
14	O	183/183 (100%)	178 (97%)	5 (3%)	44	65
15	P	190/190 (100%)	188 (99%)	2 (1%)	73	87
16	Q	327/331 (99%)	323 (99%)	4 (1%)	71	85
17	T	79/79 (100%)	76 (96%)	3 (4%)	33	51
18	W	24/24 (100%)	23 (96%)	1 (4%)	30	47
All	All	3025/3054 (99%)	2947 (97%)	78 (3%)	49	66

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	M	636	TYR
16	Q	183	HIS
12	M	688	GLN
14	O	165	PRO
17	T	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	J	323	HIS
15	P	82	ASN
16	Q	182	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.01	1 (10%)	5,13,15	6.09	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.69	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.46	130.90	119.48
16	Q	118	2MR	CD-NE-CZ	3.99	130.87	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.36	131.29	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
19	SF4	C	301	16,3	0,12,12	-	-	-		
19	SF4	A	501	1	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		
26	FES	M	803	12	0,4,4	-	-	-		
23	PLX	C	303	-	51,51,51	1.15	5 (9%)	55,59,59	0.62	1 (1%)
21	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.30	7 (14%)
25	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.14	3 (5%)
26	FES	O	301	14	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	8Q1	G	201	-	31,34,34	2.04	6 (19%)	40,43,43	1.77	10 (25%)
19	SF4	B	301	2	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.23	8 (16%)
28	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.26	5 (8%)
22	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)
19	SF4	M	801	12	0,12,12	-	-	-		
19	SF4	M	802	12	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
19	SF4	C	301	16,3	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
26	FES	M	803	12	-	-	0/1/1/1
23	PLX	C	303	-	-	28/55/55/55	-
21	NAI	A	503	-	-	7/25/72/72	0/5/5/5
25	NDP	J	401	-	-	6/30/77/77	0/5/5/5
26	FES	O	301	14	-	-	0/1/1/1
24	8Q1	G	201	-	-	12/41/41/41	-
19	SF4	B	301	2	-	-	0/6/5/5
20	FMN	A	502	-	-	10/18/18/18	0/3/3/3
28	CDL	N	201	-	-	22/61/61/110	-
22	PEE	C	302	-	-	31/50/50/54	-
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	503	NAI	O4B-C1B	16.29	1.63	1.41
21	A	503	NAI	C2B-C1B	-15.29	1.30	1.53
21	A	503	NAI	C3D-C4D	-10.32	1.26	1.53
21	A	503	NAI	O4B-C4B	-8.19	1.26	1.45
21	A	503	NAI	C2D-C1D	-7.59	1.29	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	201	8Q1	C6-C1-S44	5.28	119.61	113.46
21	A	503	NAI	N3A-C2A-N1A	-4.30	121.96	128.68
28	N	201	CDL	OB6-CB5-C51	4.01	120.15	111.50
28	N	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
22	C	302	PEE	O2-C10-C11	3.94	120.00	111.50

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	N10-C1'-C2'-O2'
20	A	502	FMN	N10-C1'-C2'-C3'
20	A	502	FMN	C1'-C2'-C3'-O3'
20	A	502	FMN	C1'-C2'-C3'-C4'
20	A	502	FMN	C3'-C4'-C5'-O5'

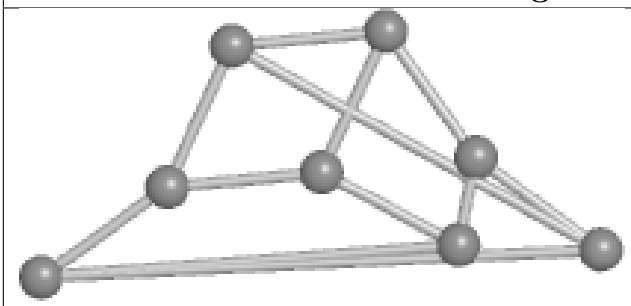
There are no ring outliers.

8 monomers are involved in 43 short contacts:

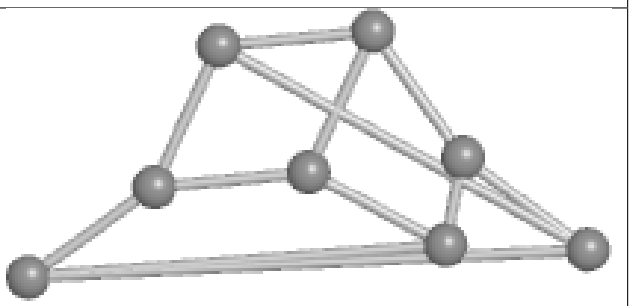
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	301	SF4	2	0
19	A	501	SF4	2	0
23	C	303	PLX	10	0
21	A	503	NAI	5	0
25	J	401	NDP	2	0
20	A	502	FMN	2	0
28	N	201	CDL	6	0
22	C	302	PEE	20	0

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.

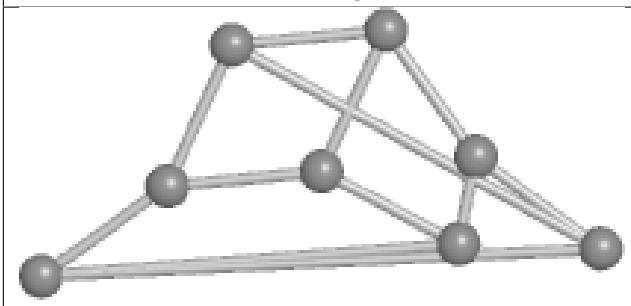
Ligand SF4 C 301



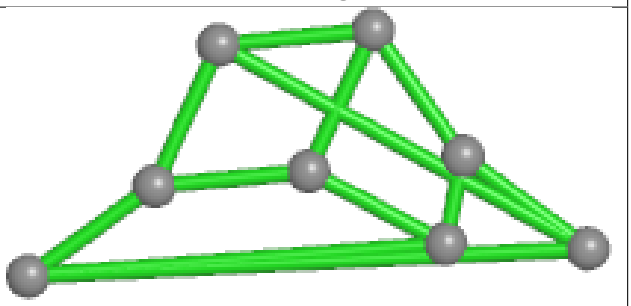
Bond lengths



Bond angles

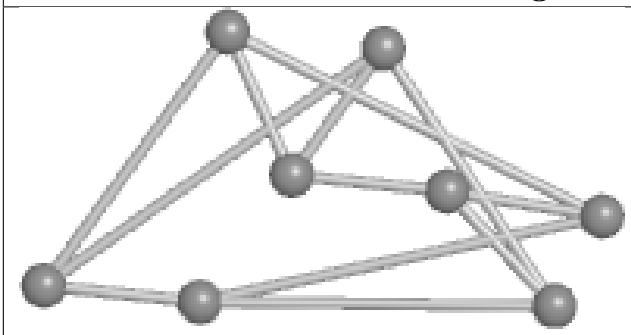


Torsions



Rings

Ligand SF4 A 501



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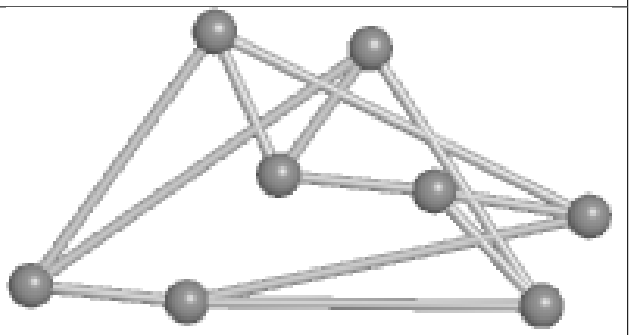

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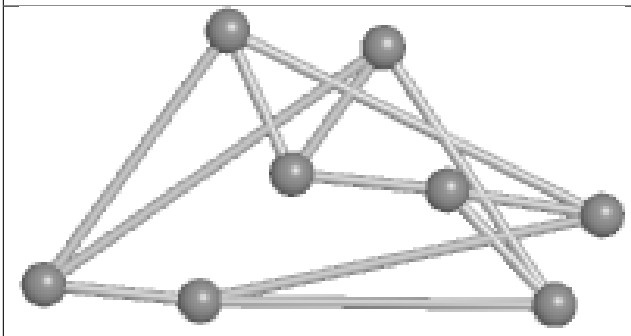

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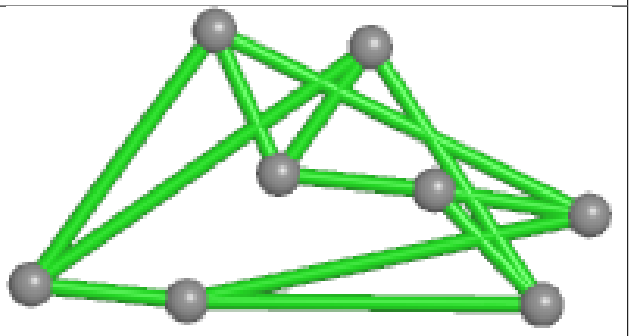
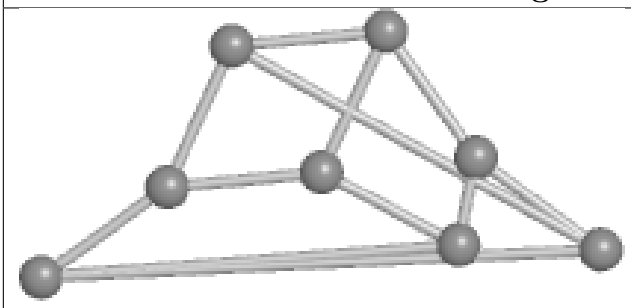


Rings

Ligand SF4 B 302



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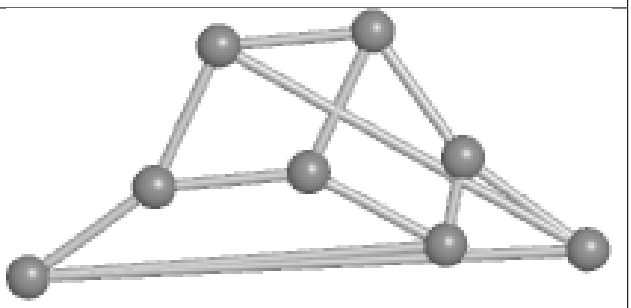
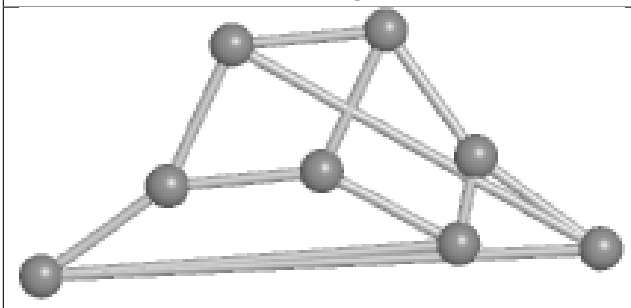


Bond angles



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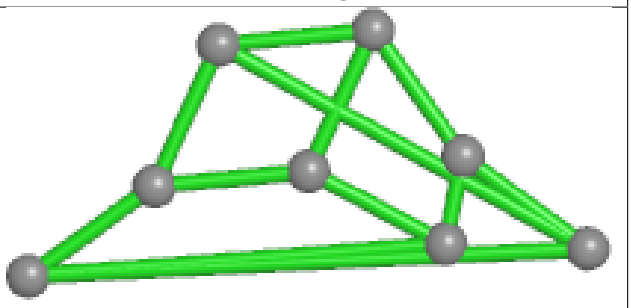
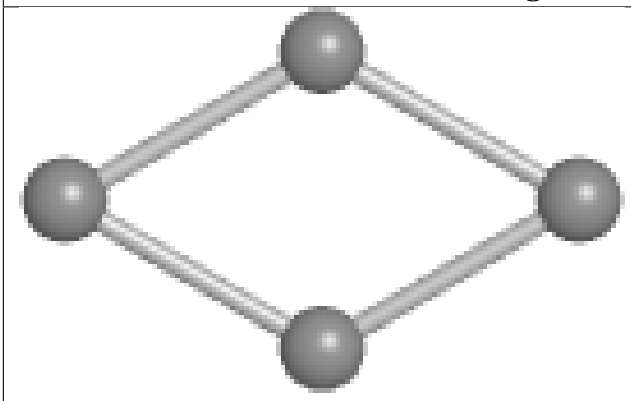


Rings

Ligand FES M 803



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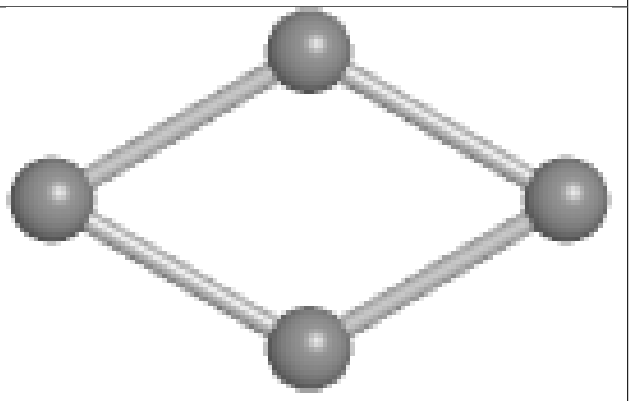

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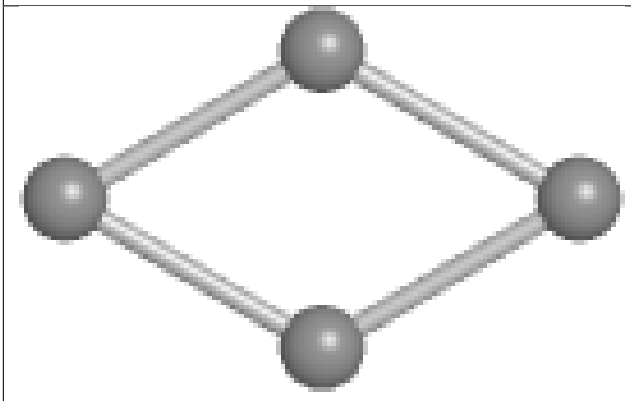

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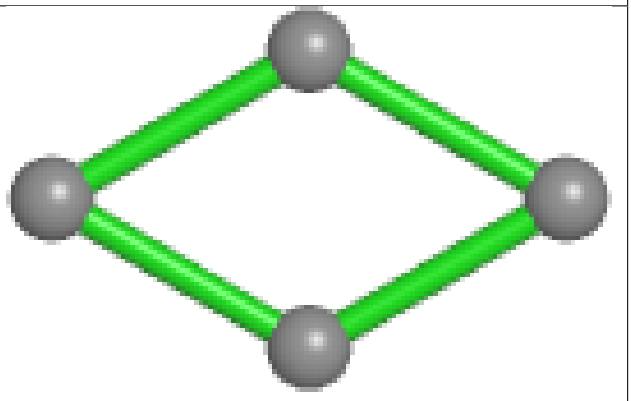
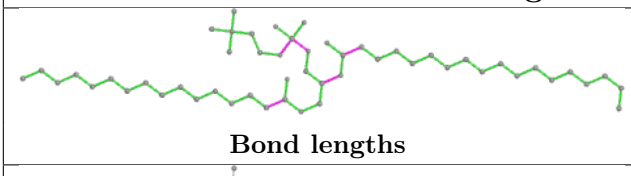


Rings

Ligand PLX C 303



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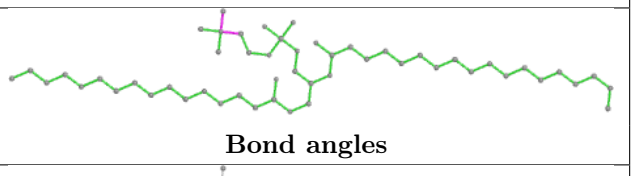

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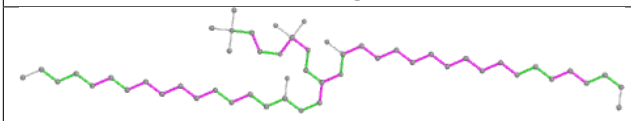

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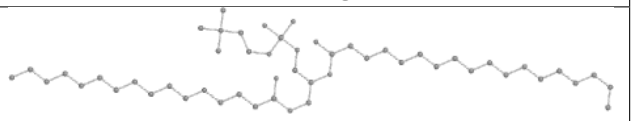
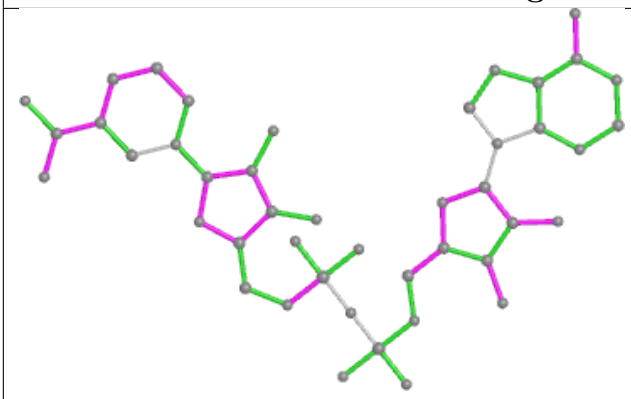


Rings

Ligand NAI A 503



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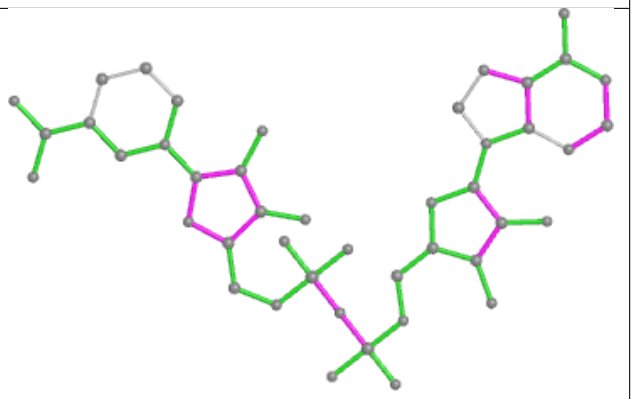

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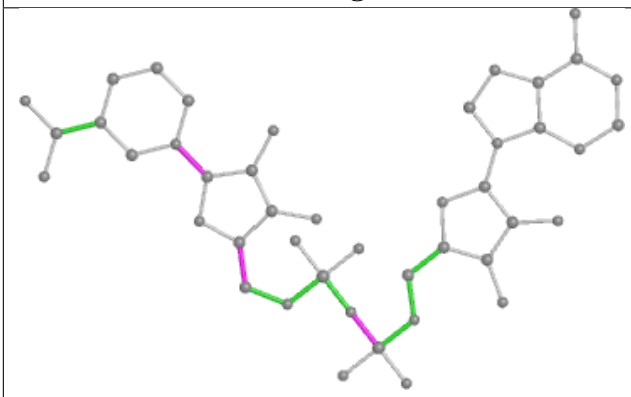

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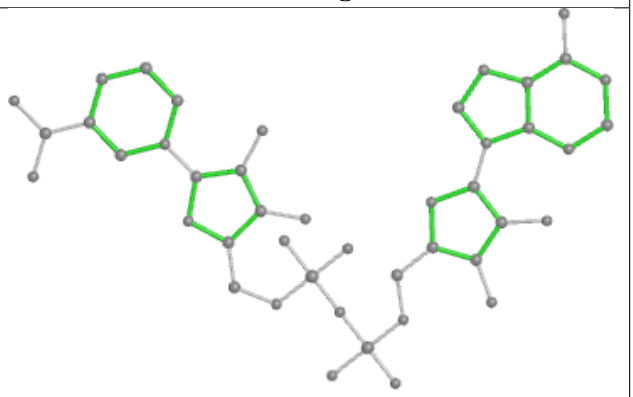
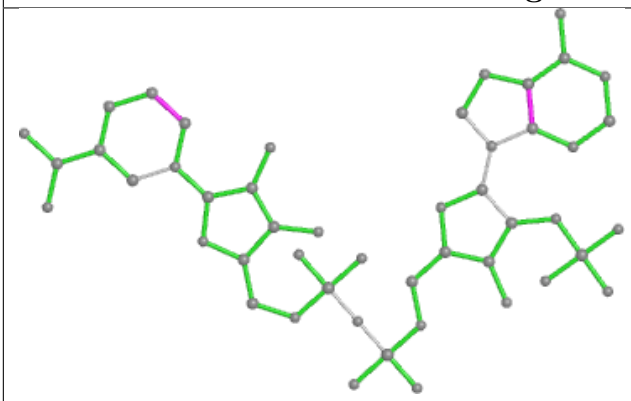


Rings

Ligand NDP J 401



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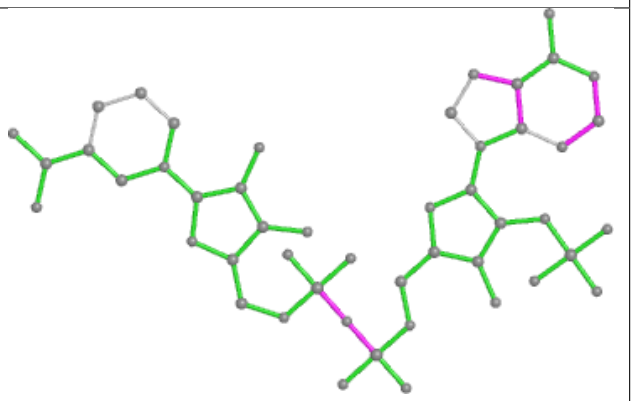

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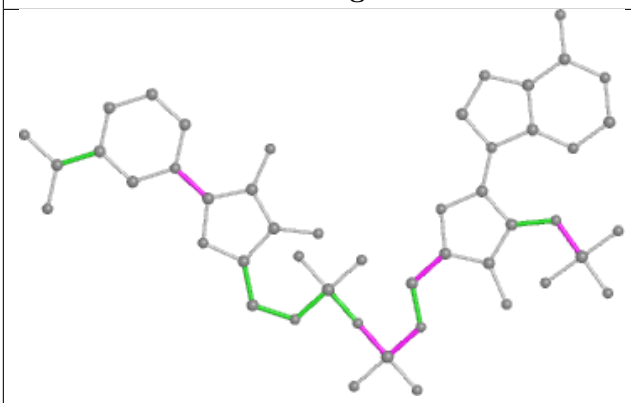

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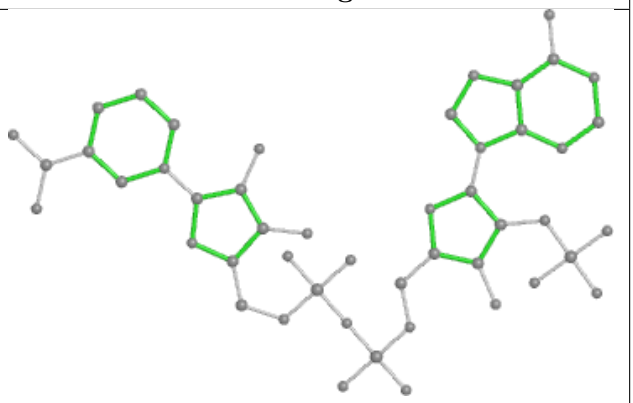
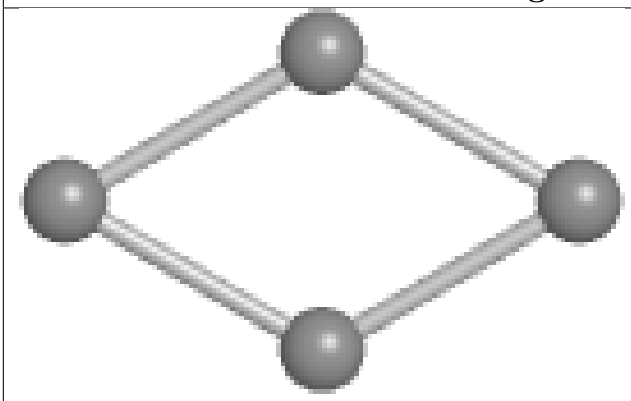


Rings

Ligand FES O 301



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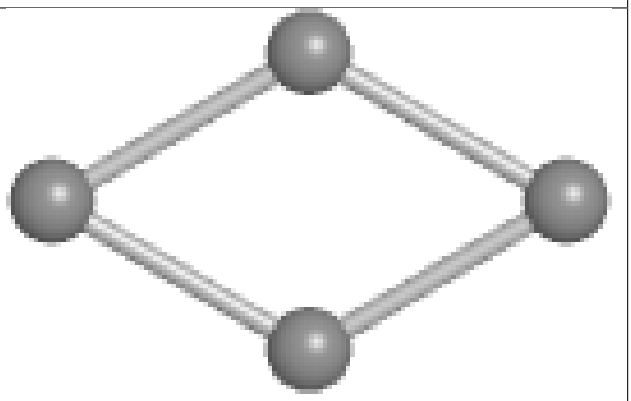

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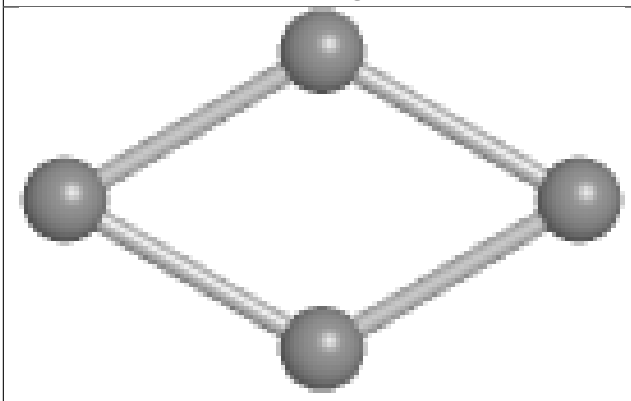

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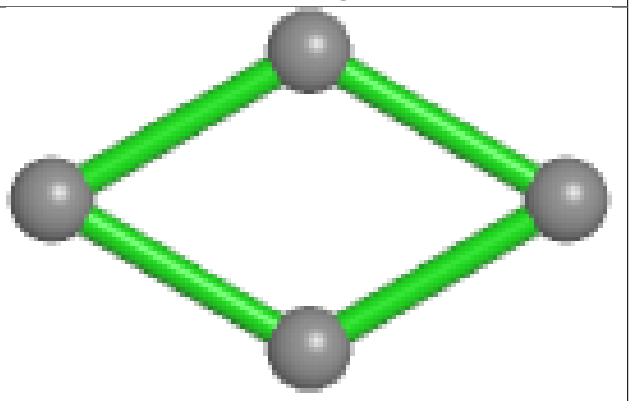
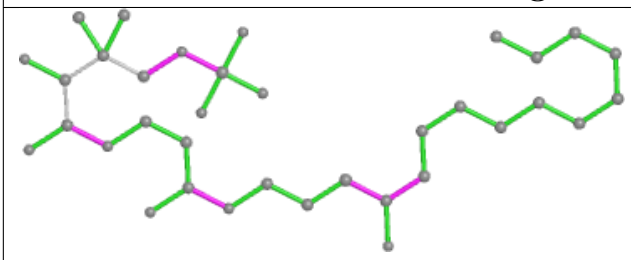


Rings

Ligand 8Q1 G 201



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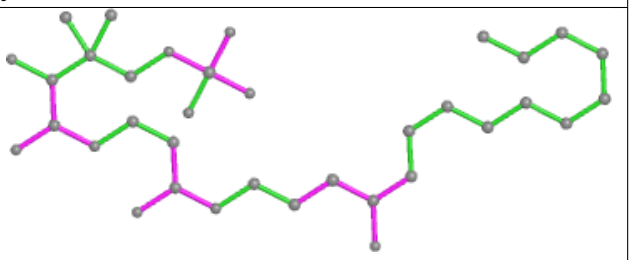

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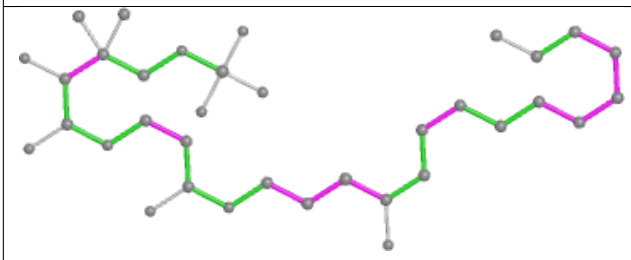

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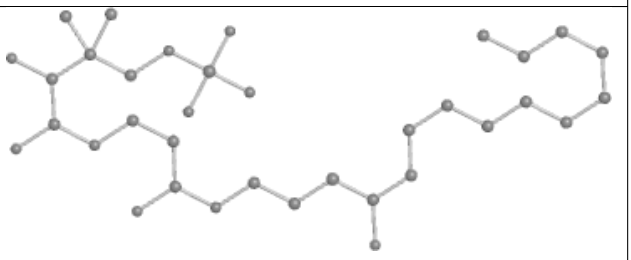
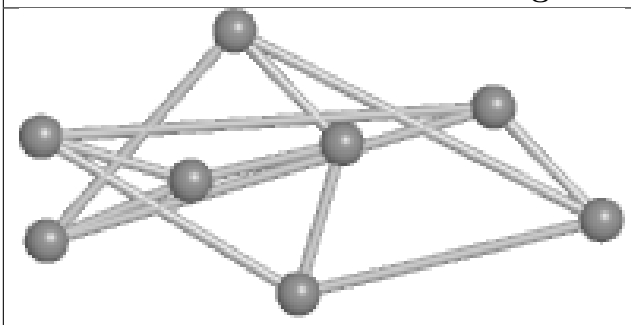


Rings

Ligand SF4 B 301



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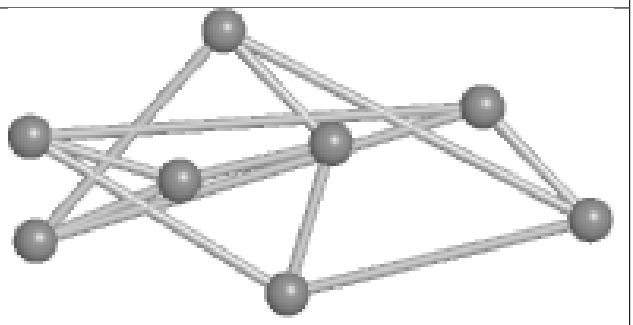

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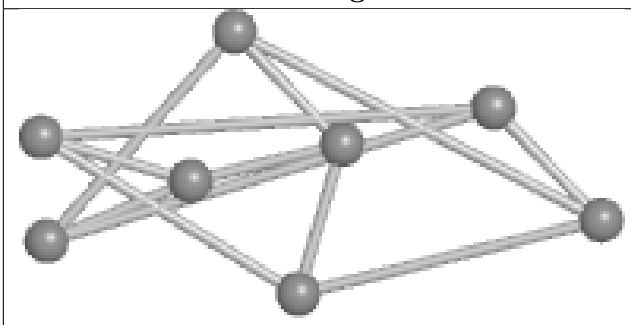

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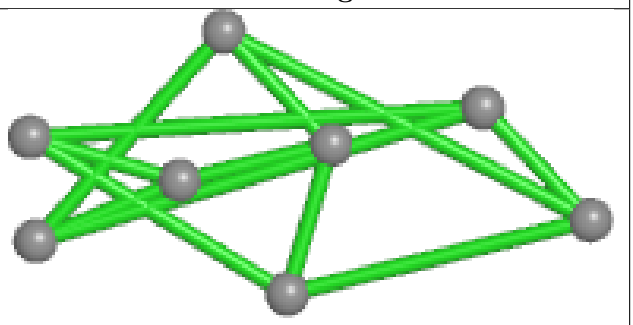
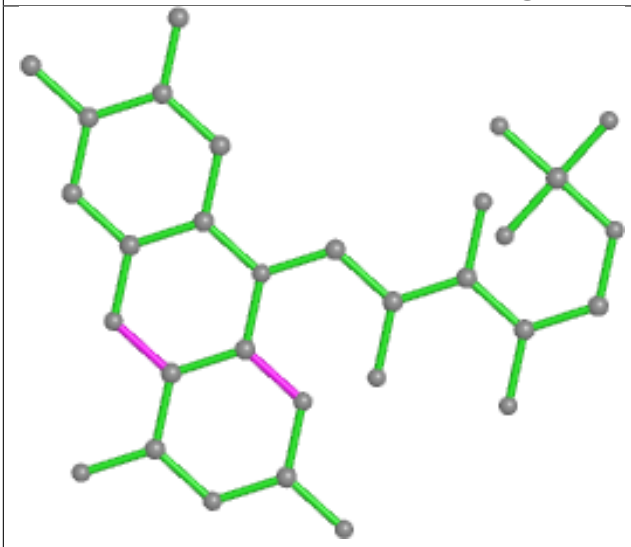


Rings

Ligand FMN A 502



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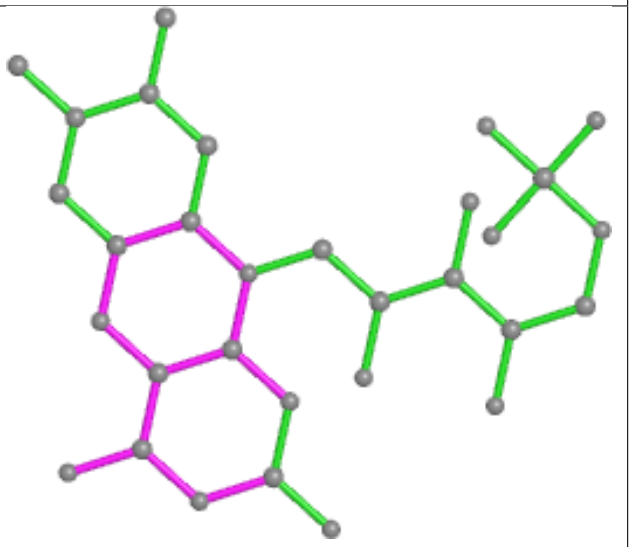

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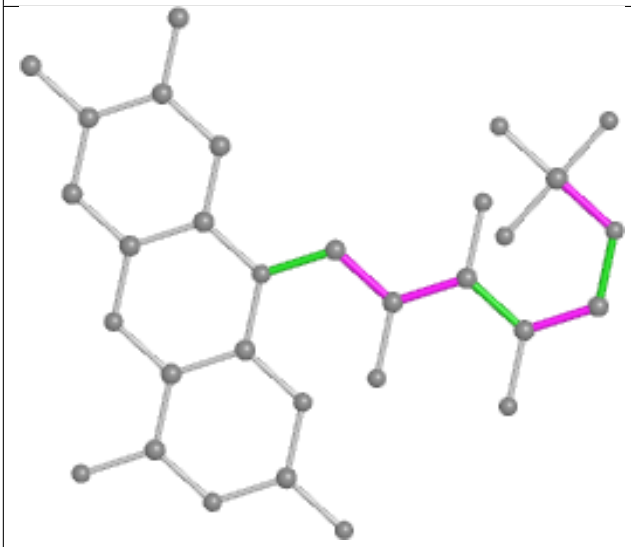

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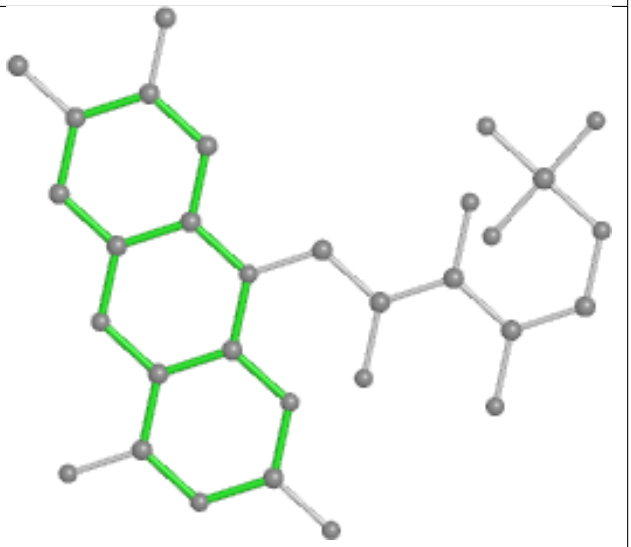
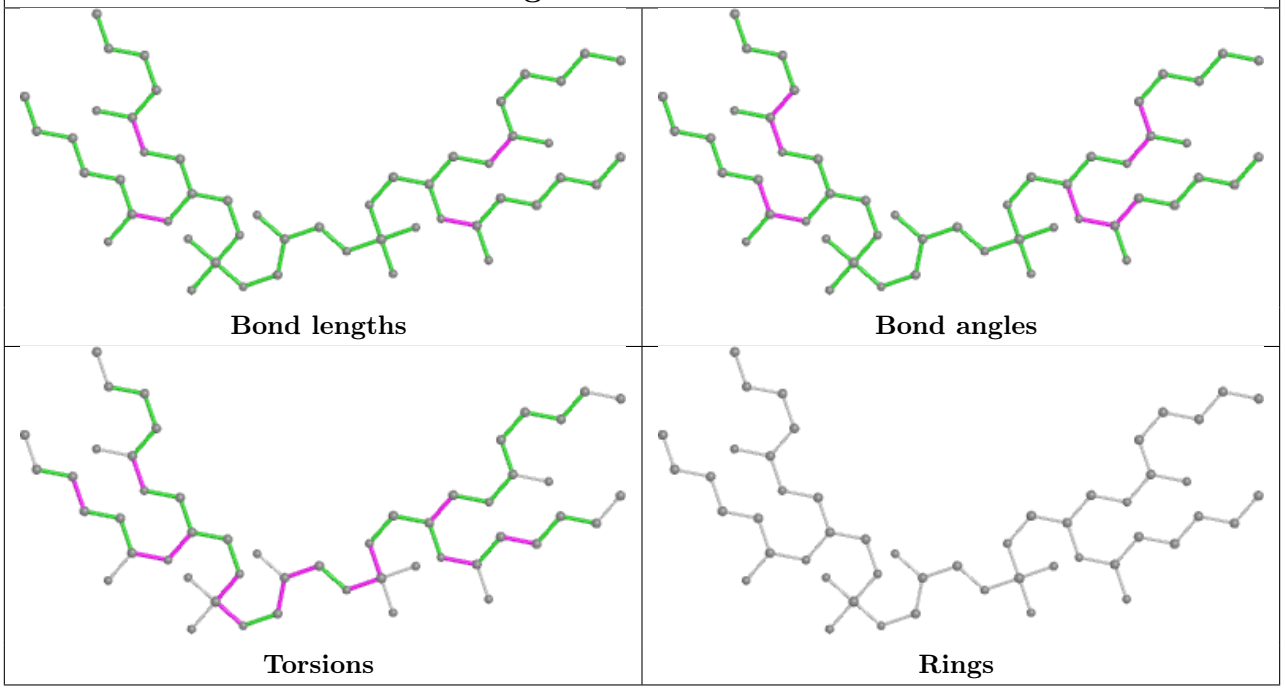
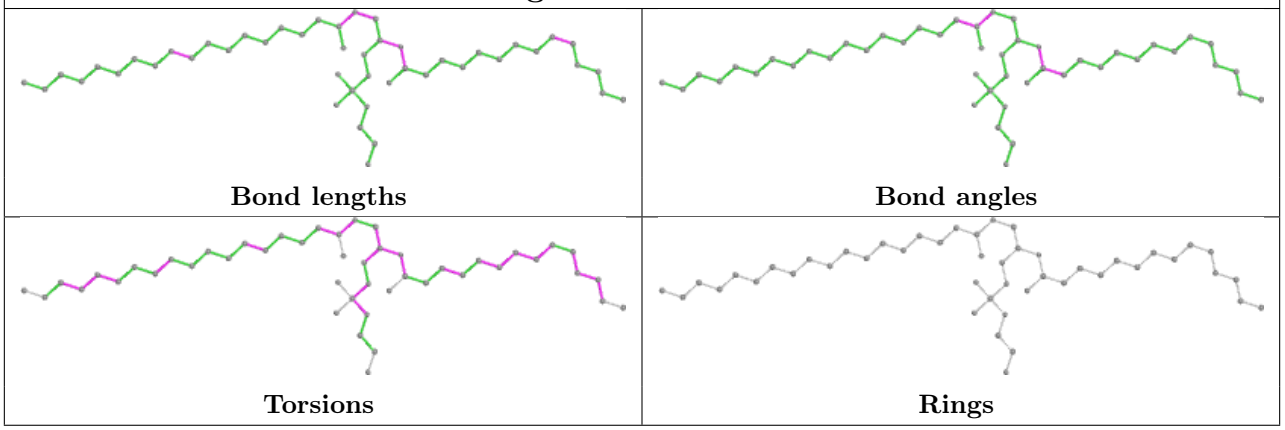


Rings

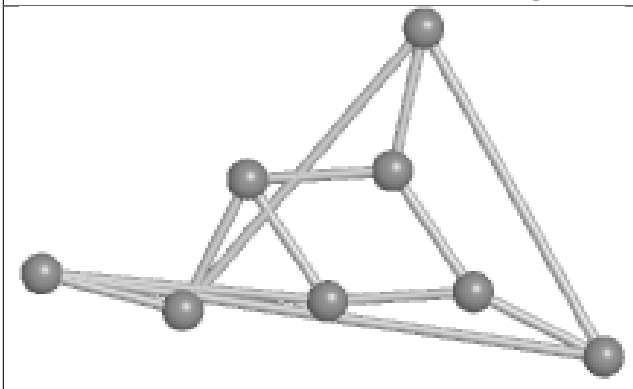
Ligand CDL N 201



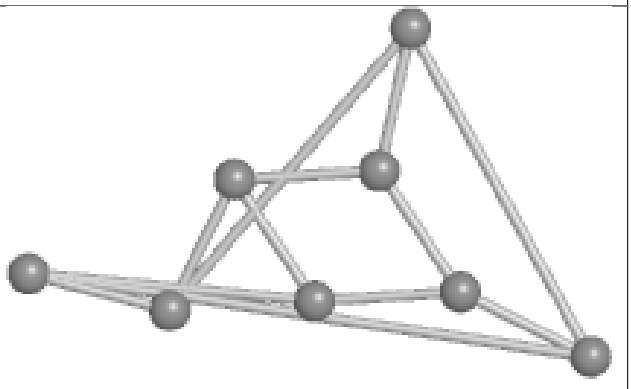
Ligand PEE C 302



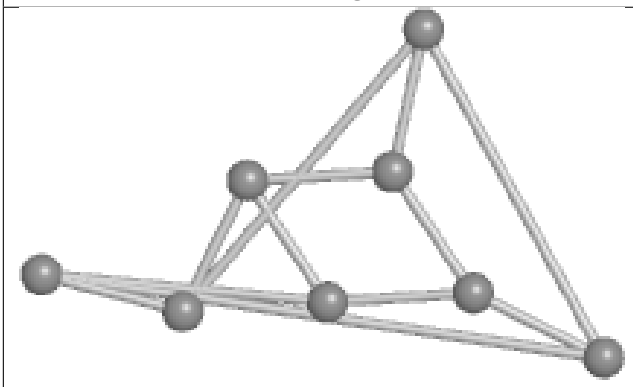
Ligand SF4 M 801



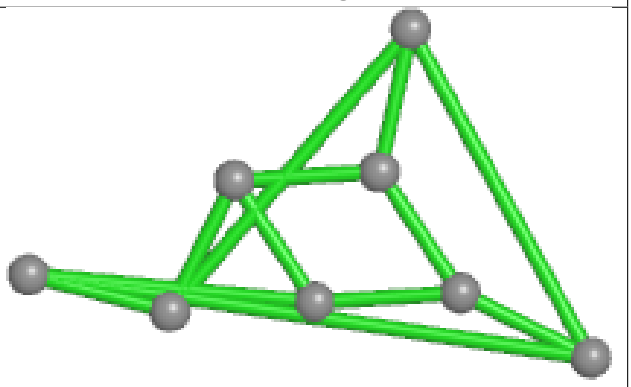
Bond lengths



Bond angles

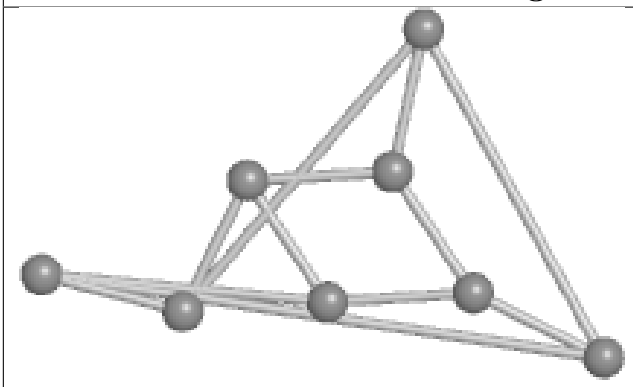


Torsions



Rings

Ligand SF4 M 802



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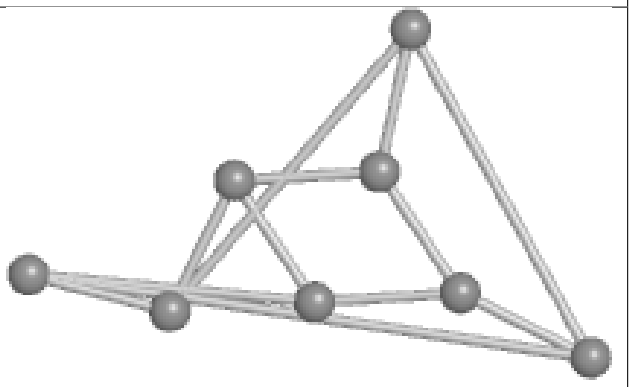
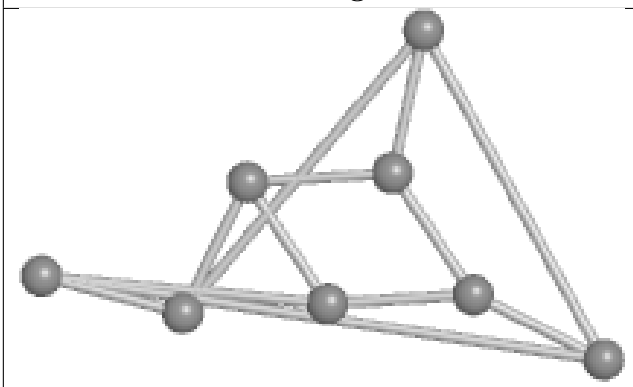
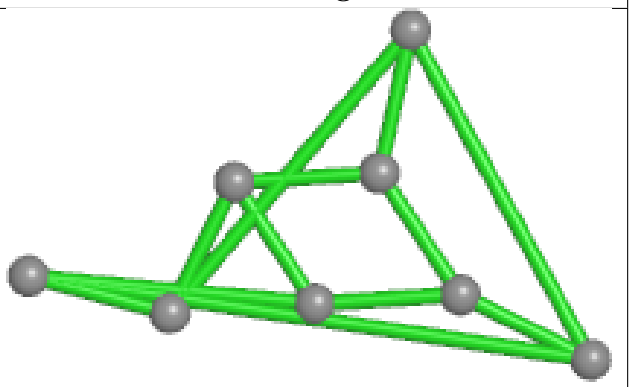


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

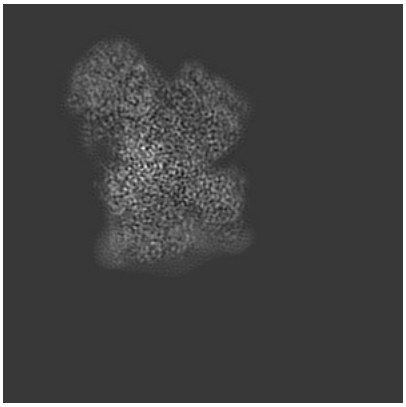
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31883. These allow visual inspection of the internal detail of the map and identification of artifacts.

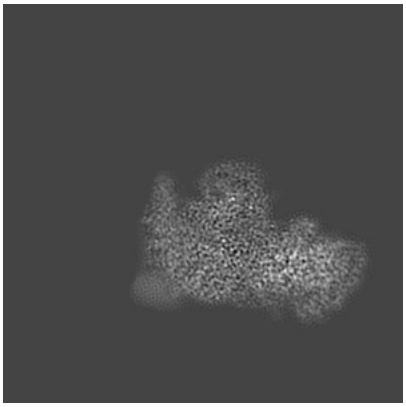
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

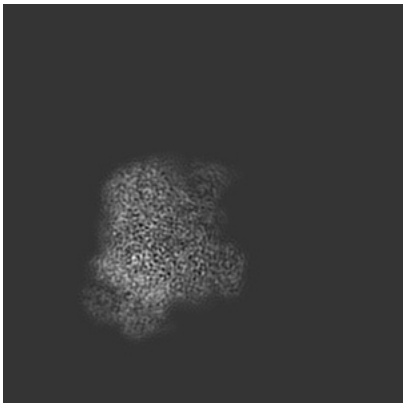
6.1.1 Primary map



X



Y



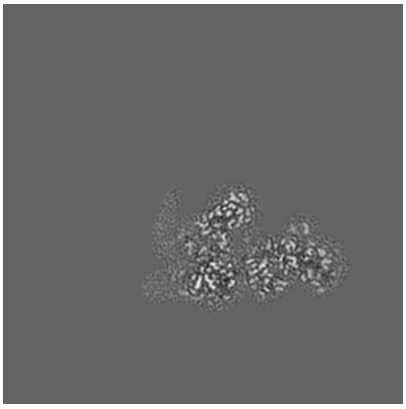
Z

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

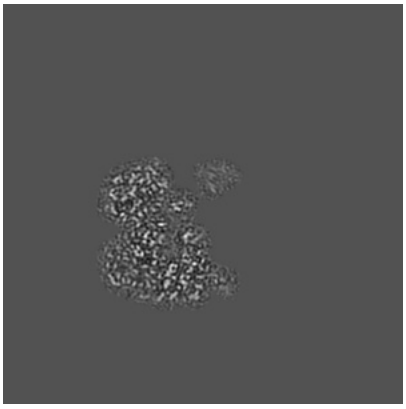
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

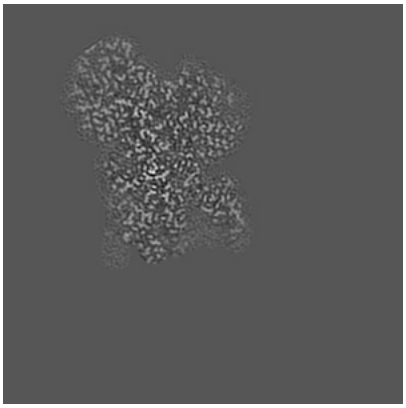


Z Index: 256

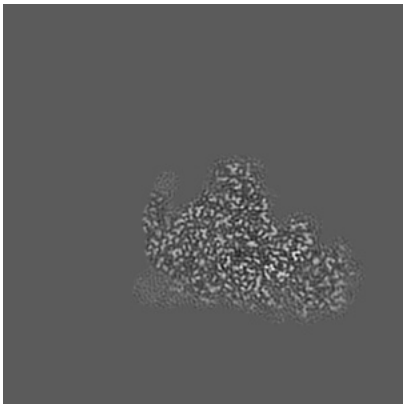
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 184



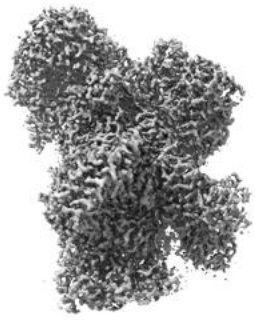
Y Index: 176

Z Index: 290

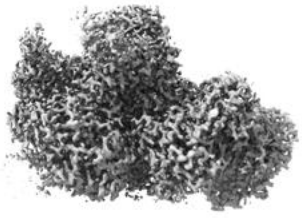
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

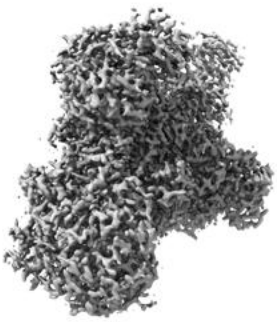
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

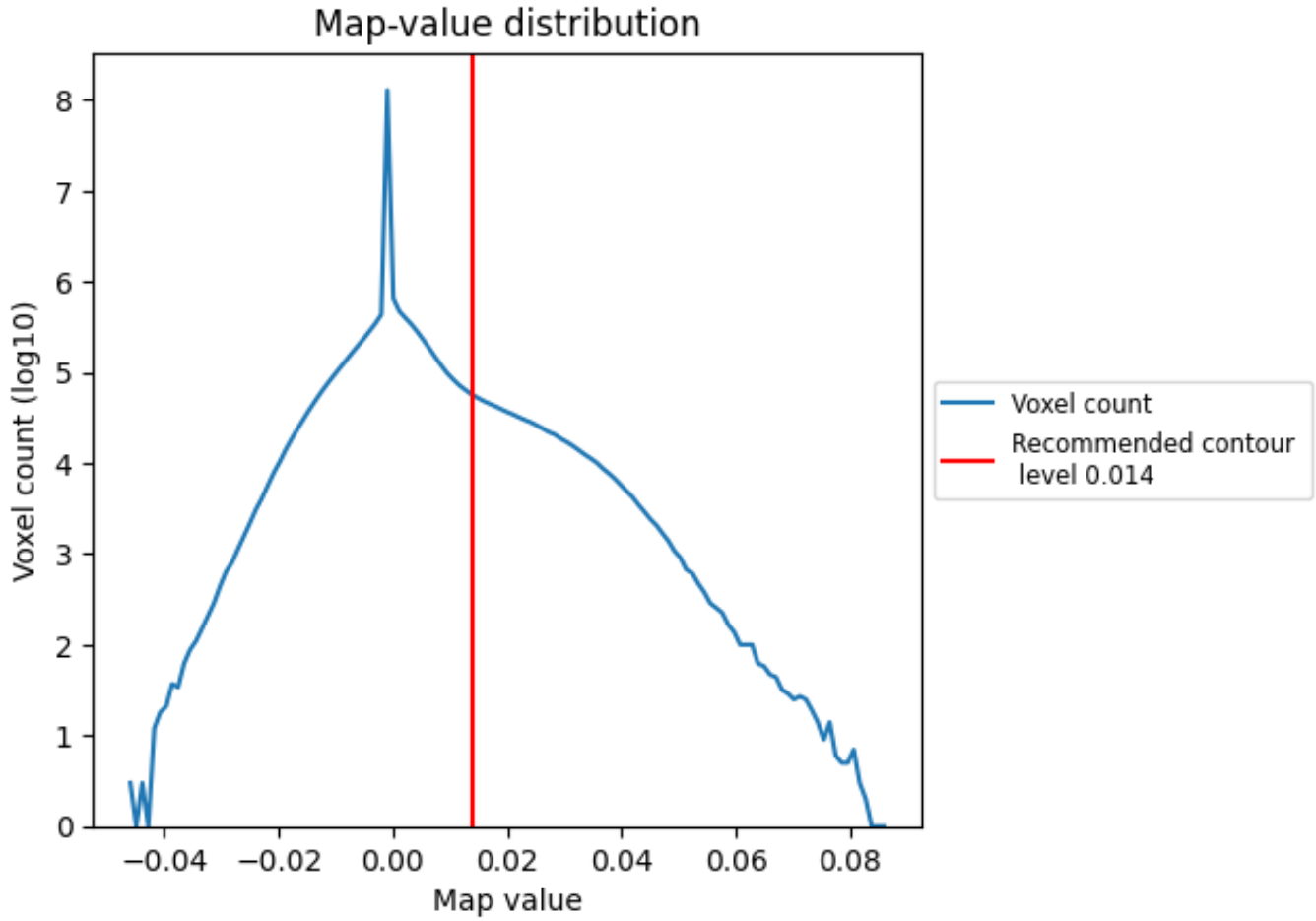
6.5 Mask visualisation (i)

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

7 Map analysis

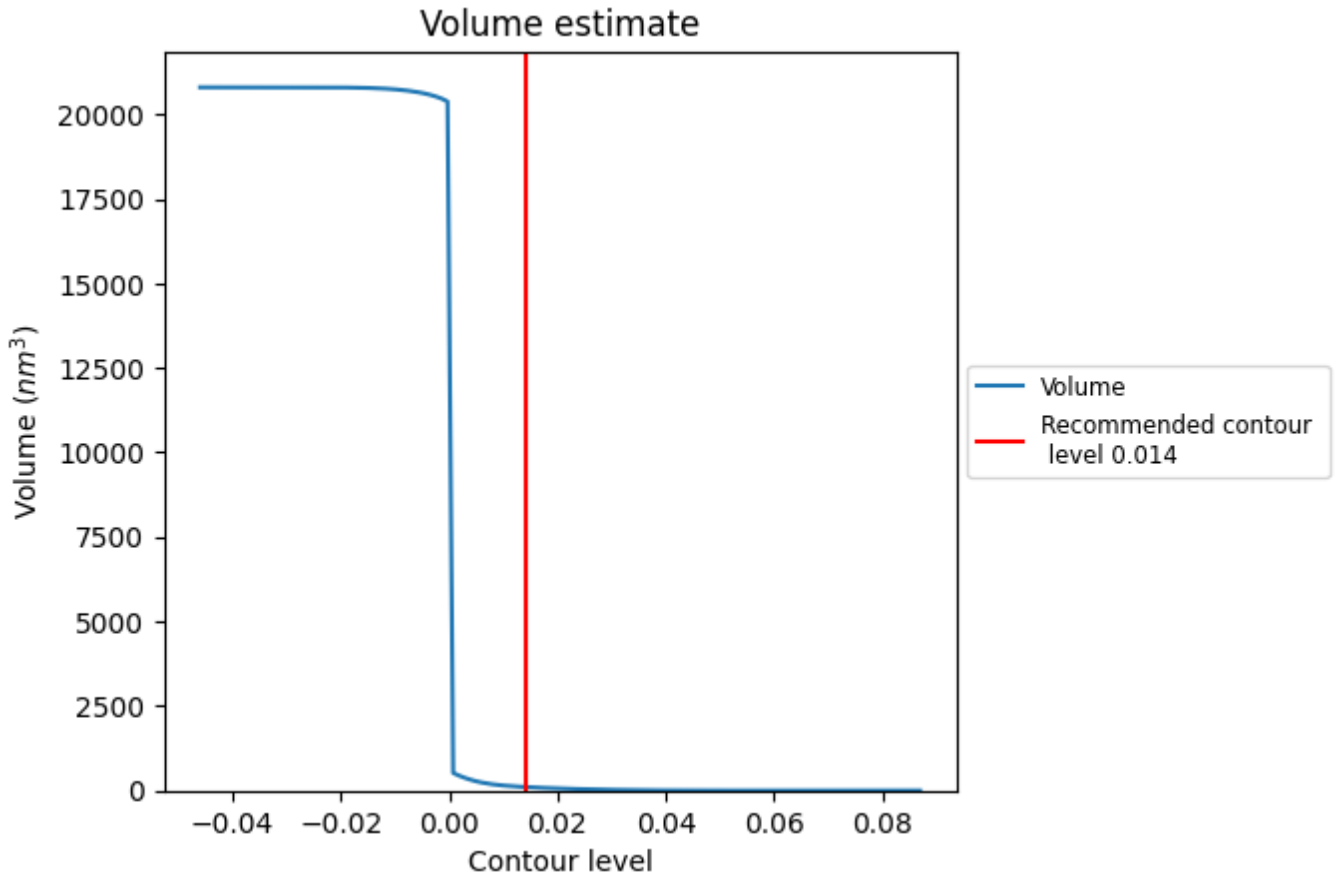
This section contains the results of statistical analysis of the map.

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.

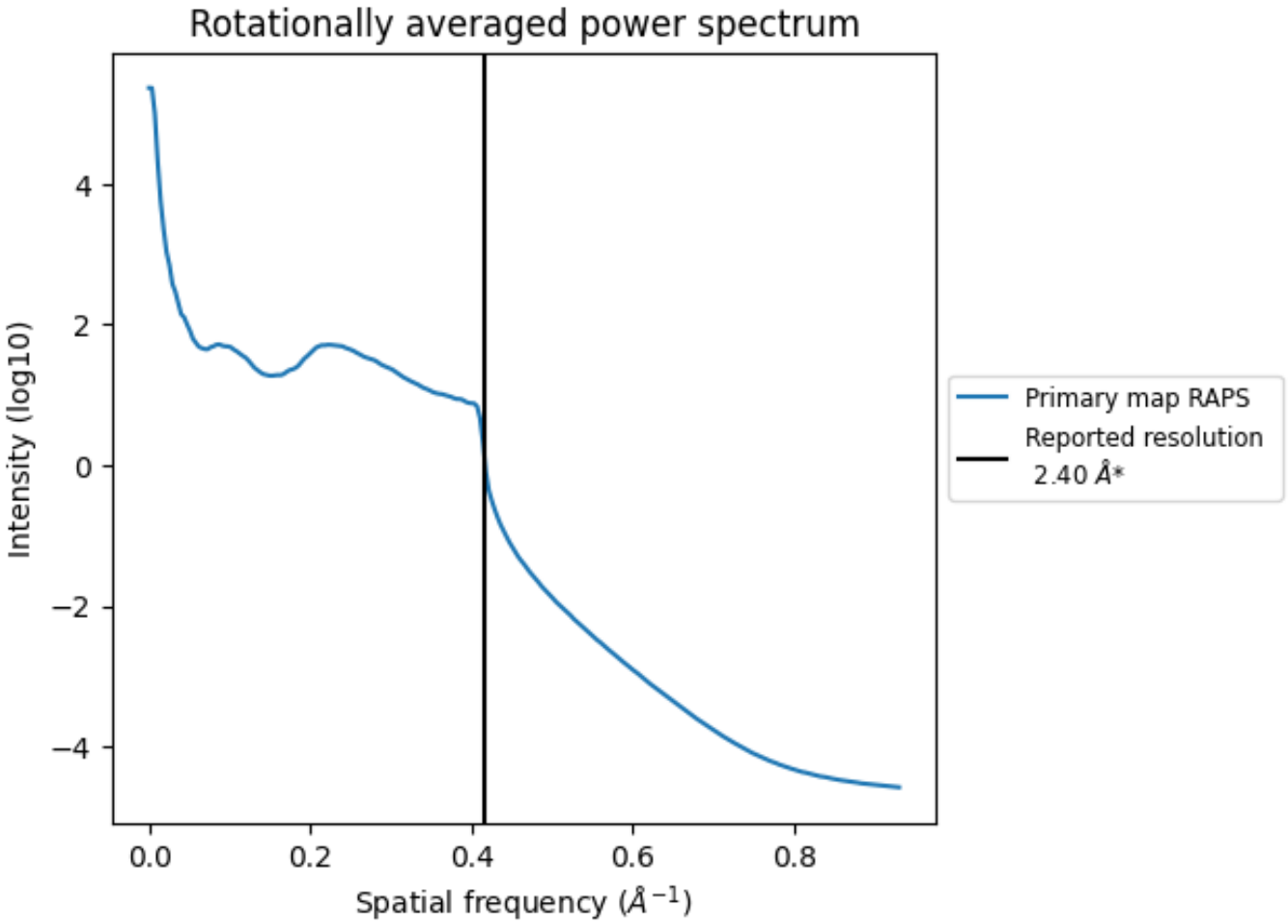
7.2 Volume estimate (i)



The volume at the recommended contour level is 105 nm^3; this corresponds to an approximate mass of 95 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 0.417 $Å^{-1}$

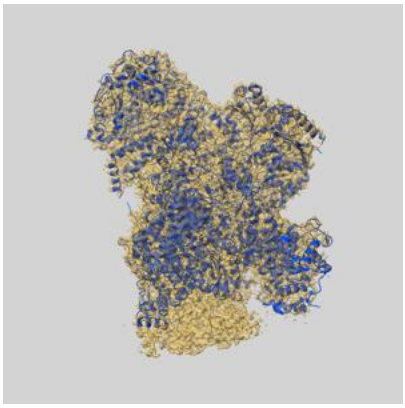
8 Fourier-Shell correlation (i)

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

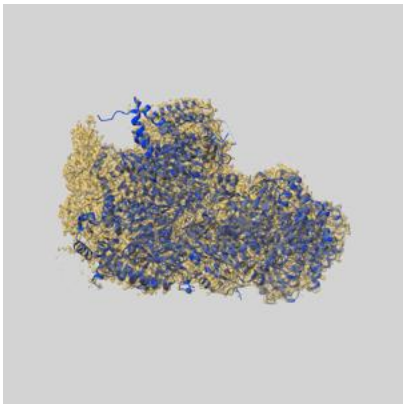
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31883 and PDB model 7VBN. Per-residue inclusion information can be found in section 3 on page 14.

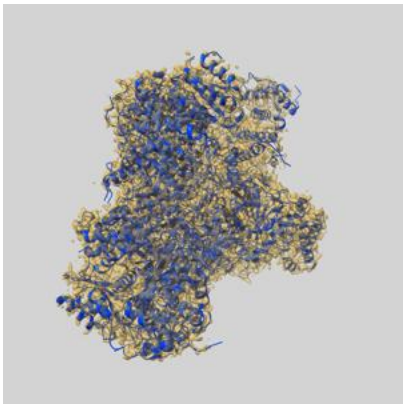
9.1 Map-model overlay



X



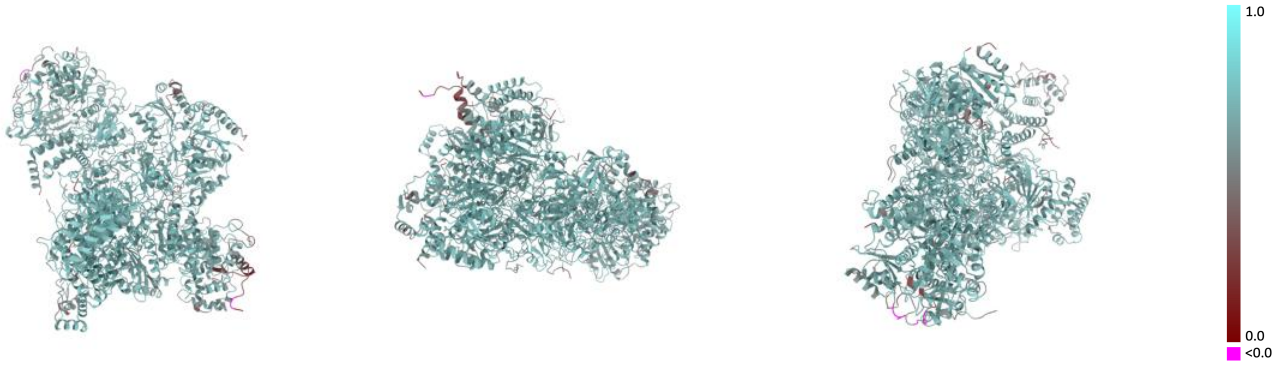
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

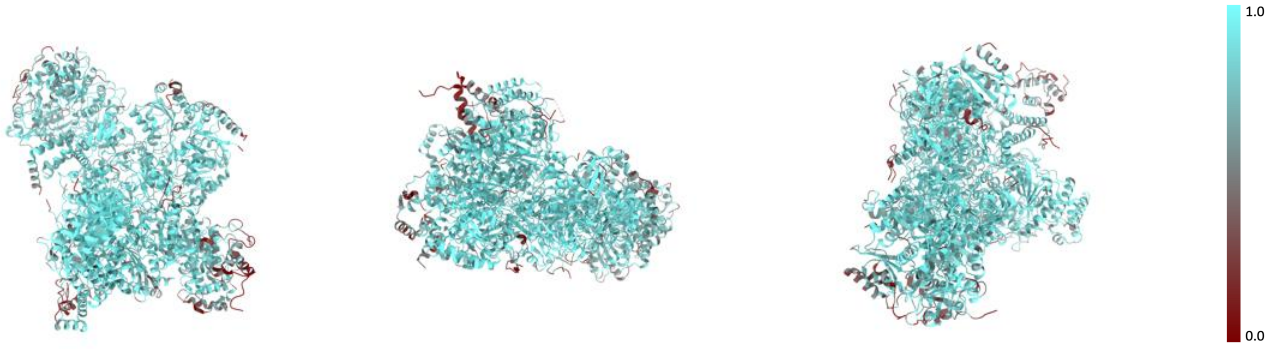
9.2 Q-score mapped to coordinate model (i)



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.

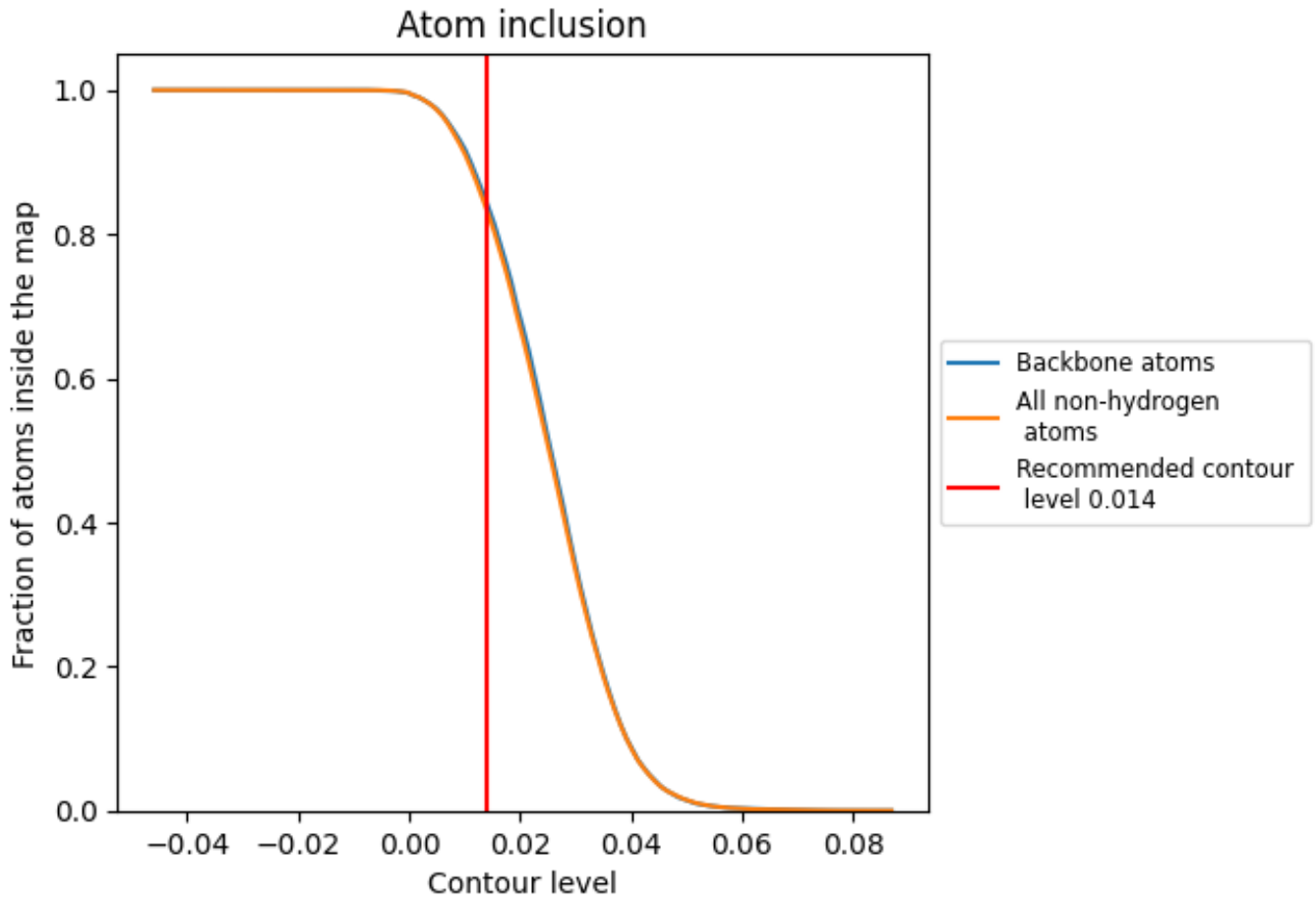
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8337	0.6650
A	0.8278	0.6600
B	0.9294	0.7020
C	0.8607	0.6740
E	0.8482	0.6730
F	0.7649	0.6300
G	0.4294	0.5020
H	0.8514	0.6590
I	0.6918	0.6270
J	0.8162	0.6580
K	0.6570	0.5810
L	0.8753	0.6840
M	0.8944	0.6840
N	0.6743	0.6360
O	0.7412	0.6290
P	0.9497	0.7050
Q	0.9384	0.7010
T	0.7590	0.6540
W	0.6852	0.6120