Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 06:55 PM JST

PDB ID	:	8IBE
EMDB ID	:	EMD-35341
Title	:	Respiratory complex Peripheral Arm of CI, focus-refined map of type II, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

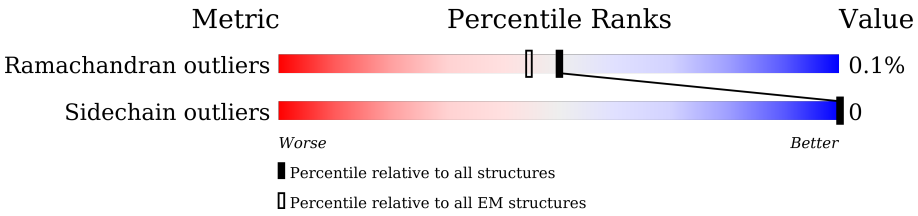
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



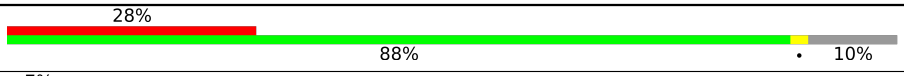
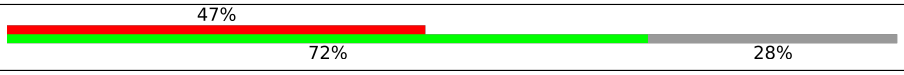
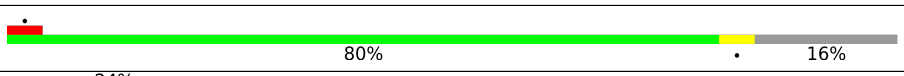
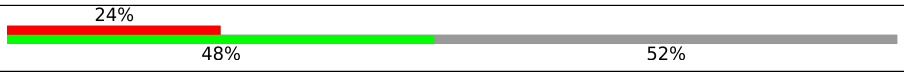
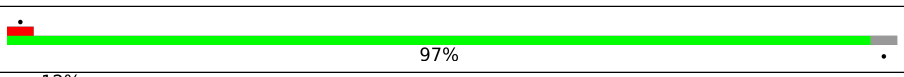
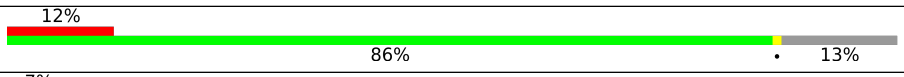
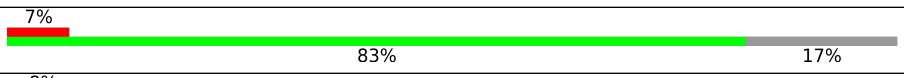
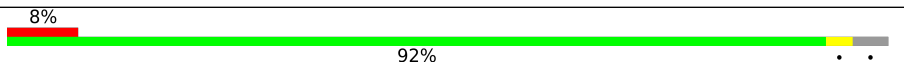
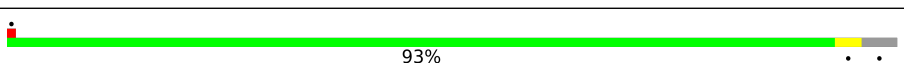
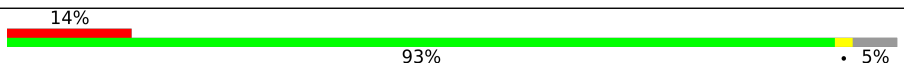
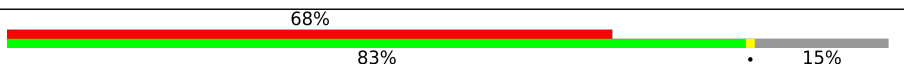
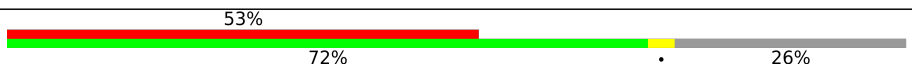
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	115	17%, 84%, 15%
2	B	224	65%, 31%
3	C	263	74%, 25%
4	D	463	81%, 17%
5	E	248	40%, 82%, 15%
6	F	464	36%, 89%, 8%
7	G	727	91%, 6%
8	H	318	6%, 98%
9	I	212	78%, 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	P	377	
11	Q	175	
12	R	116	
13	S	99	
14	T	156	
15	V	116	
16	W	131	
17	X	172	
18	Z	144	
19	a	70	
20	b	84	
21	q	145	
22	r	113	
23	s	104	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 34255 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	98	799	552	112	130	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1643	1061	279	300	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	385	3088	1970	533	562	23	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total 2532	C 1702	N 383	O 425	S 22	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	123	Total	C	N	O	S	0	0
			1025	658	181	182	4		

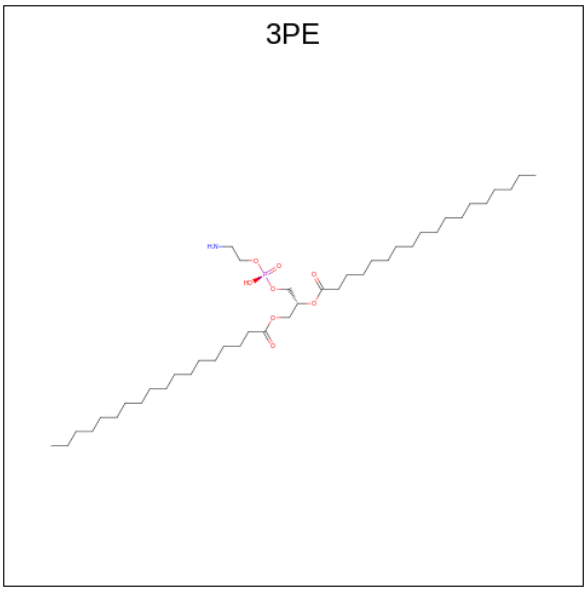
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	84	Total	C	N	O	S	0	0
			686	435	128	121	2		

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

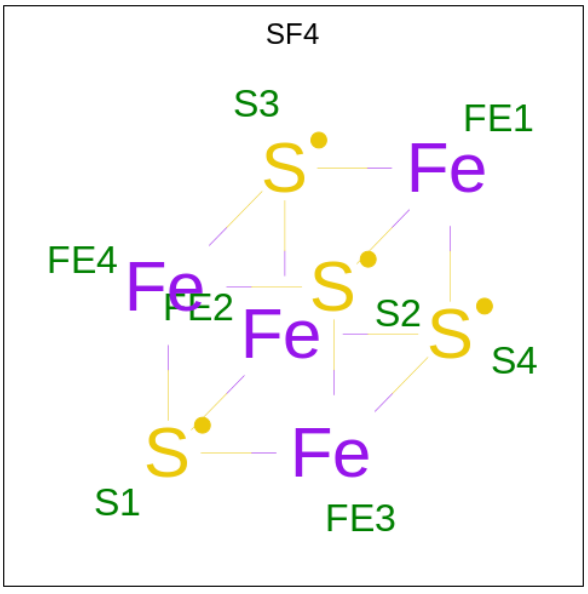
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	23	Total	C	N	O	0	0
			193	126	30	37		

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



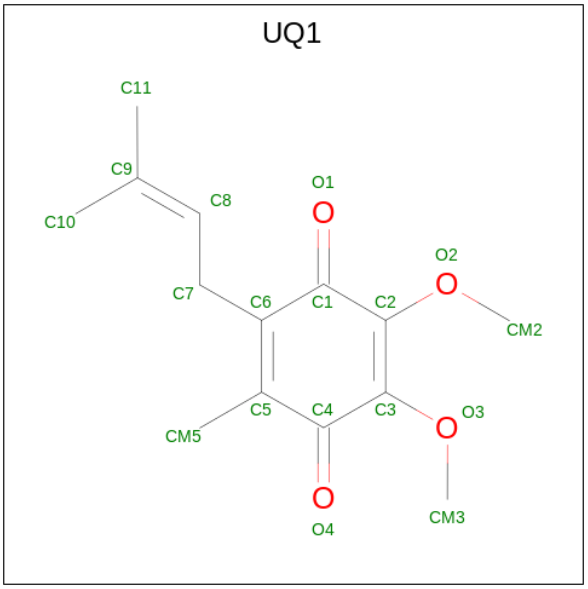
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
24	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
24	I	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



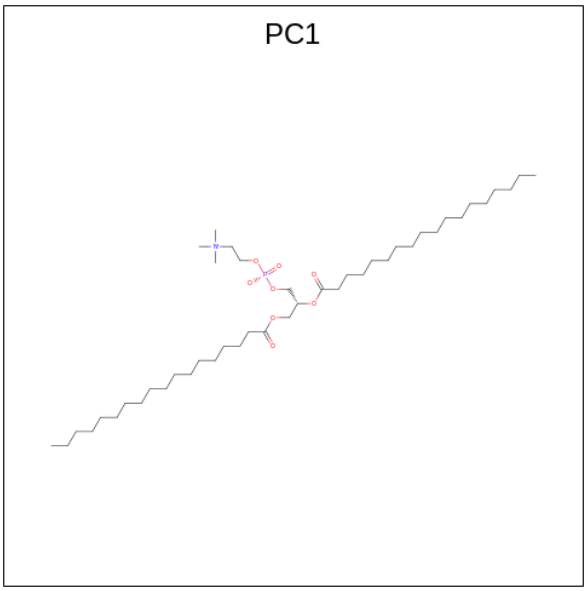
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total Fe S 8 4 4	0
25	F	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0

- Molecule 26 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



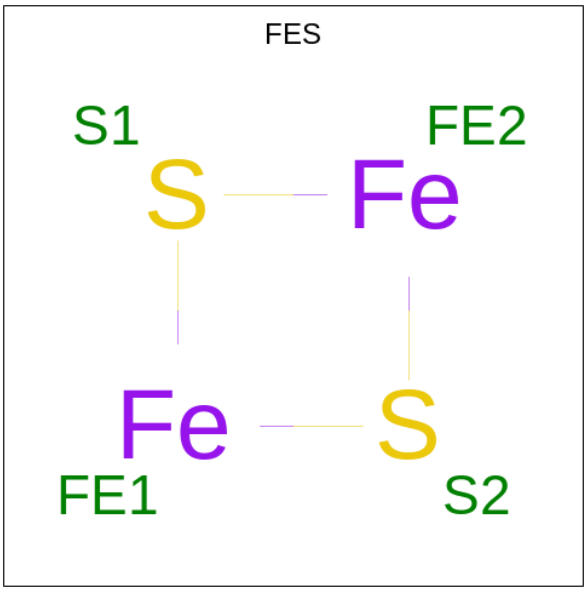
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O 18 14 4	0

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



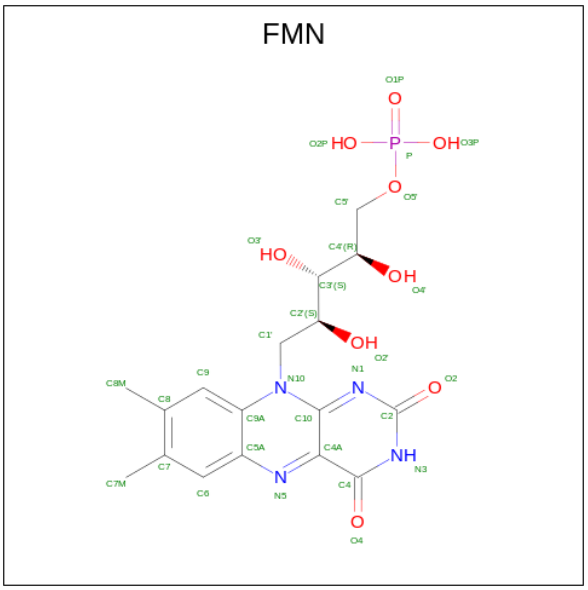
Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

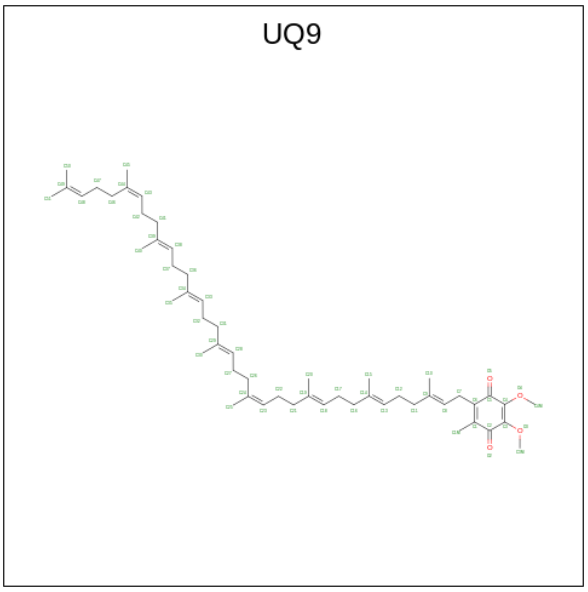
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 29 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



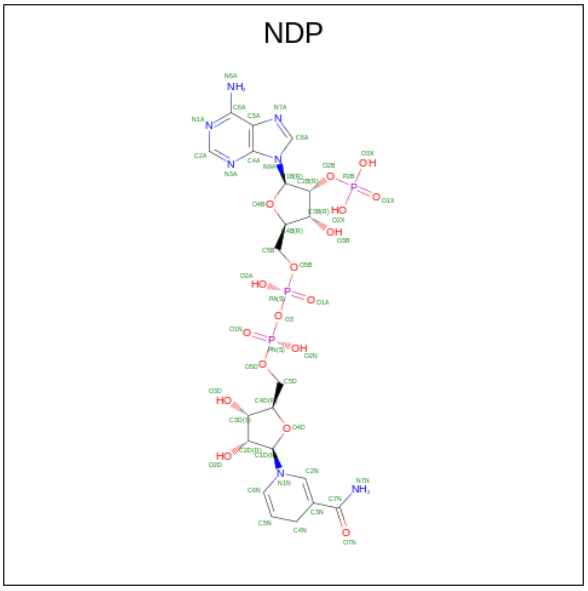
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 30 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 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).



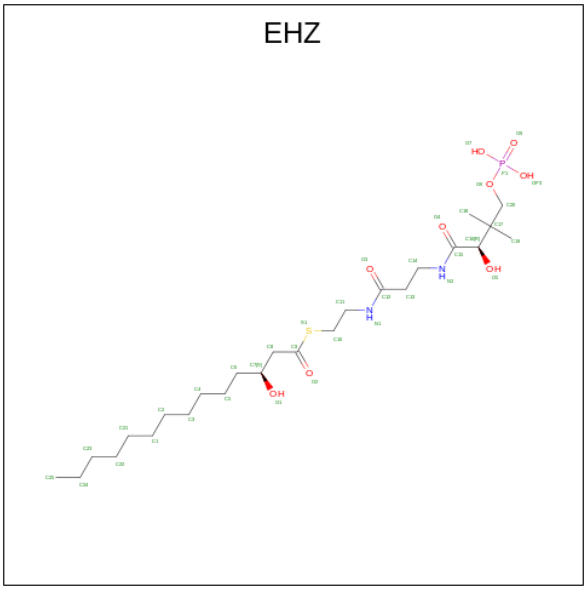
Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

Interest" by depositor).

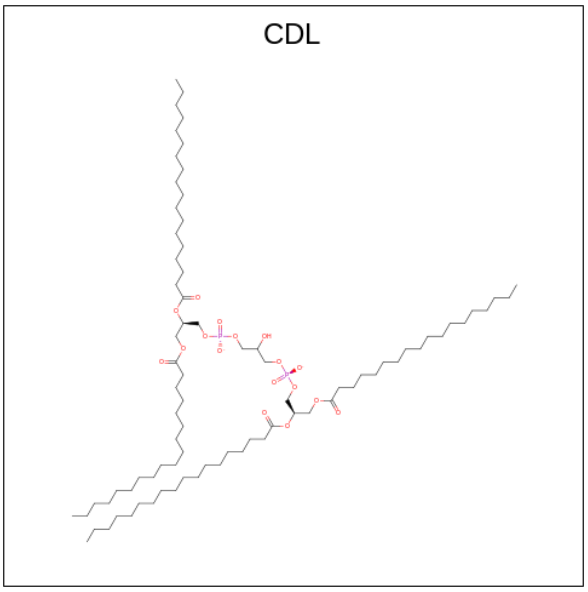
Mol	Chain	Residues	Atoms	AltConf
32	R	1	Total Zn 1 1	0

- Molecule 33 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

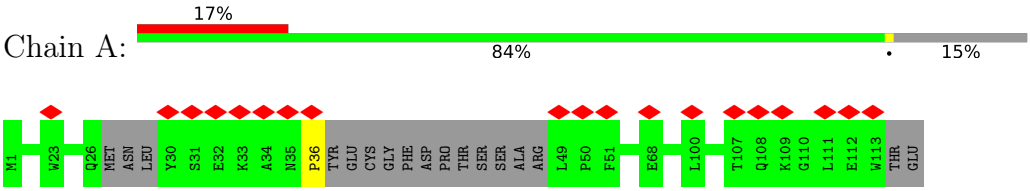


Mol	Chain	Residues	Atoms				AltConf
34	a	1	Total	C	O	P	0
			57	38	17	2	

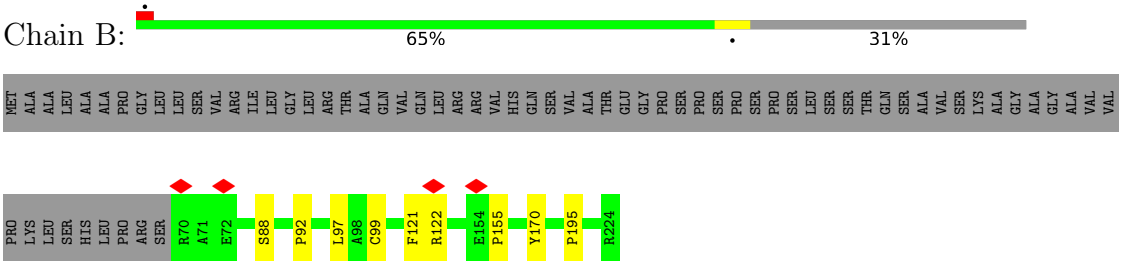
3 Residue-property plots (i)

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.

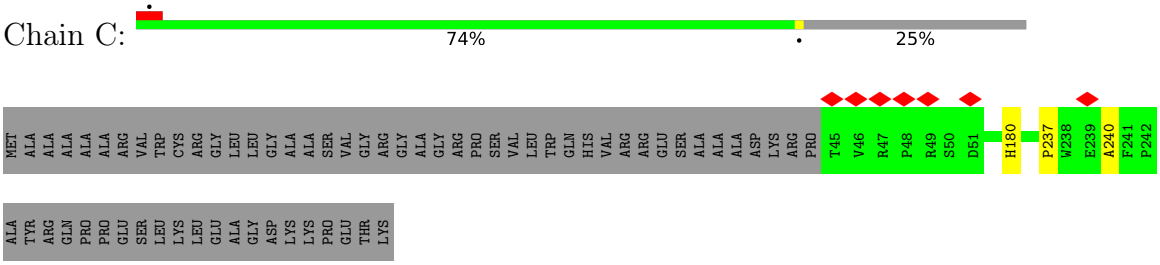
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



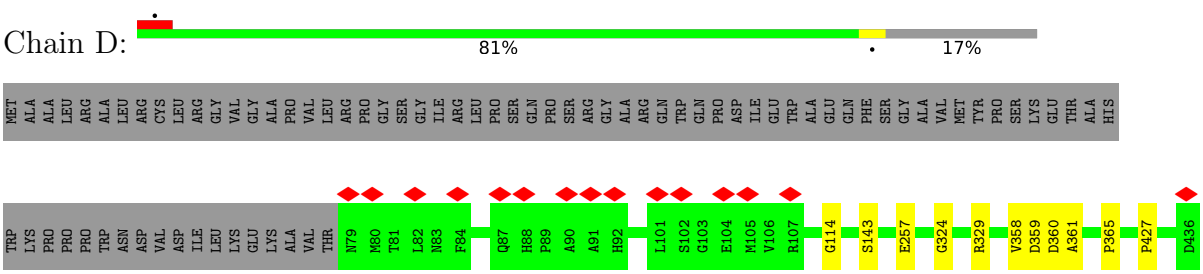
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

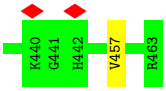


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



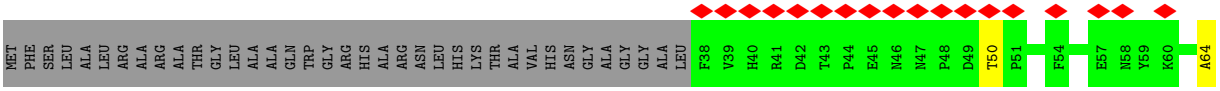
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

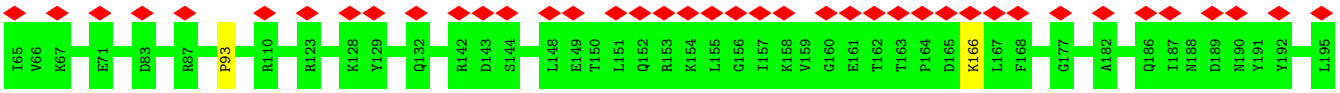


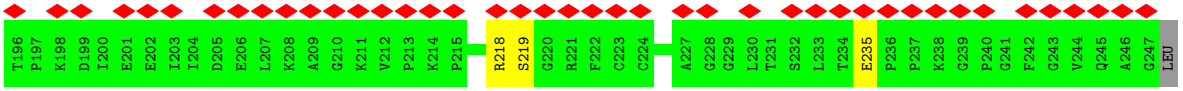


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

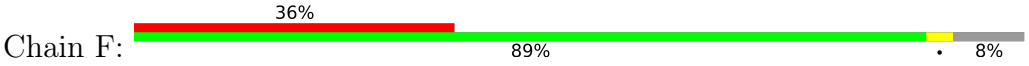


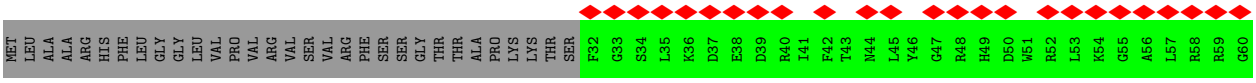


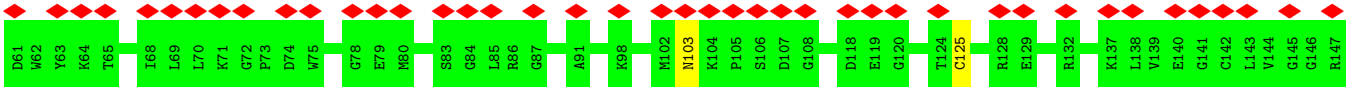


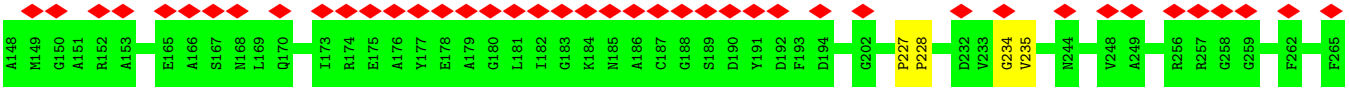
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

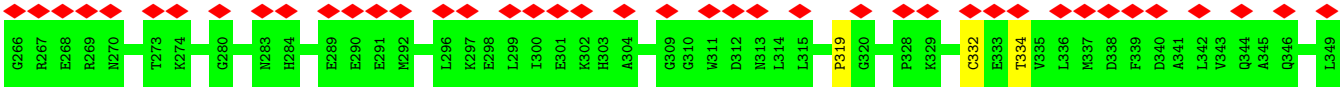
Chain F:





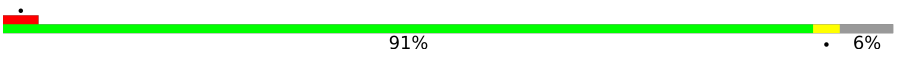


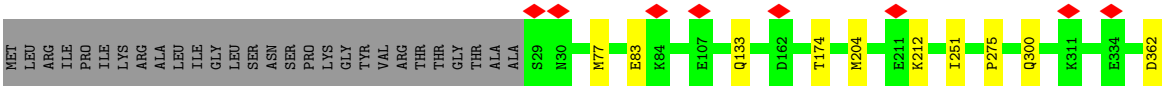


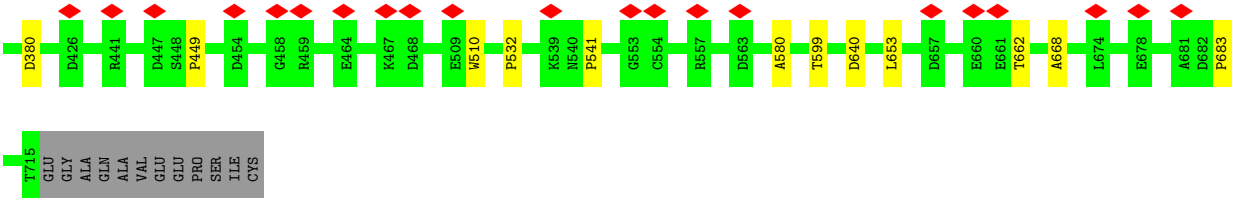


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

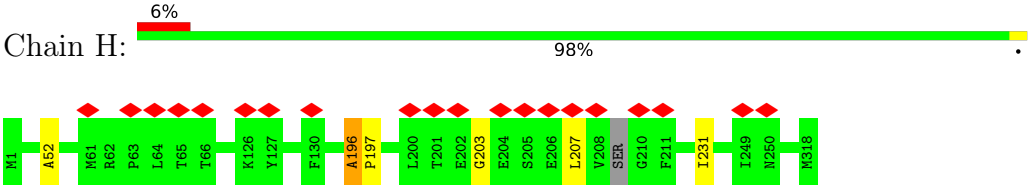
Chain G:



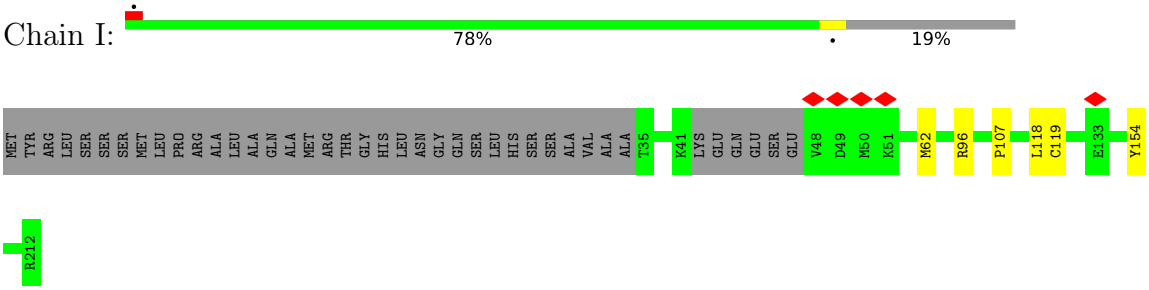




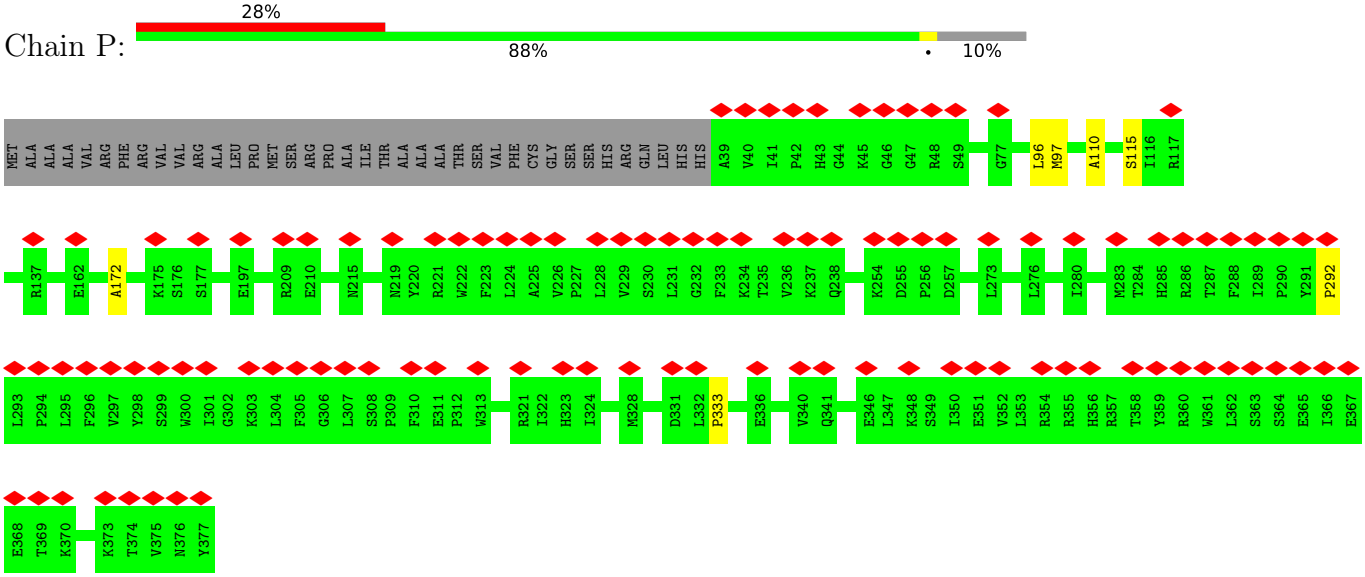
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



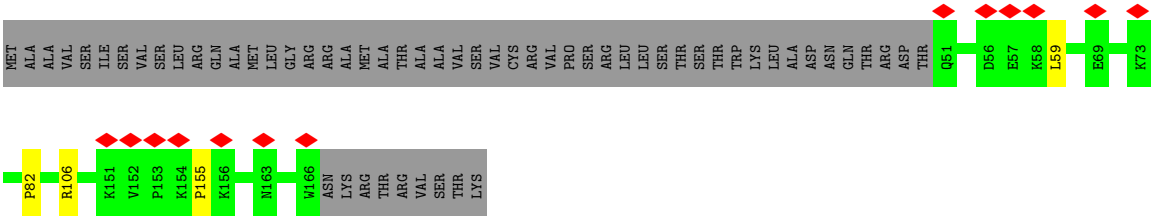
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



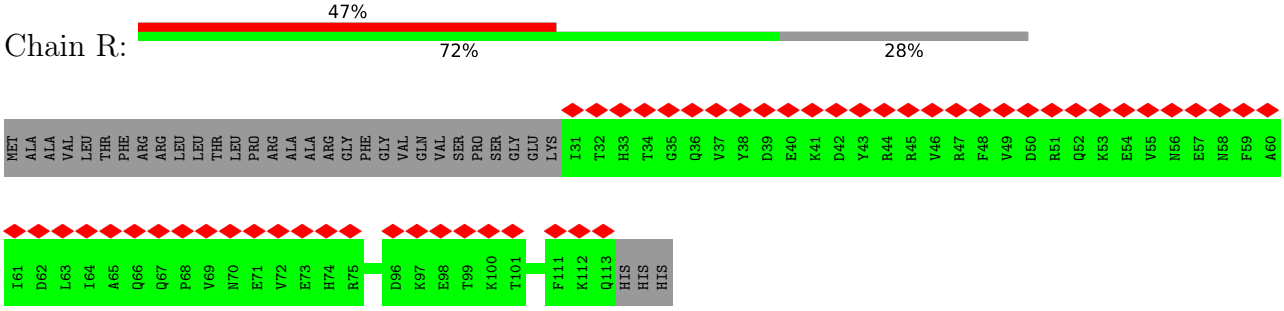
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



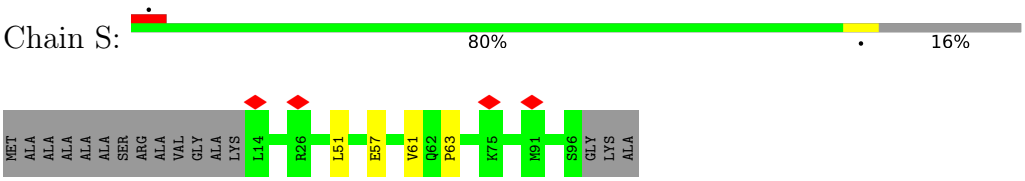
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



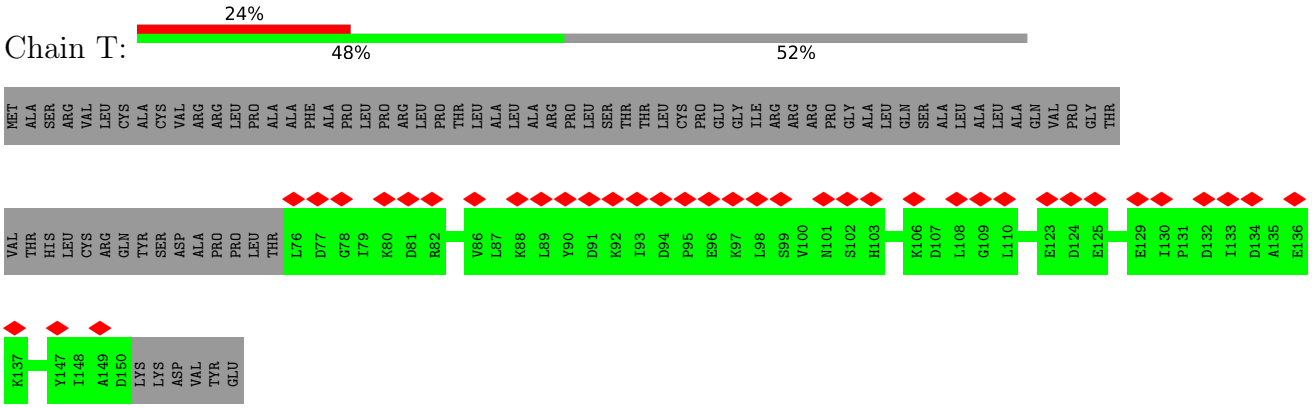
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



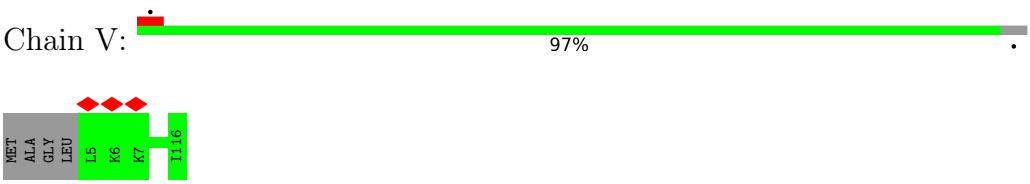
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



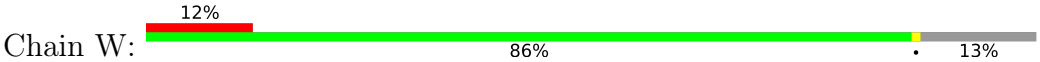
• Molecule 14: Acyl carrier protein, mitochondrial

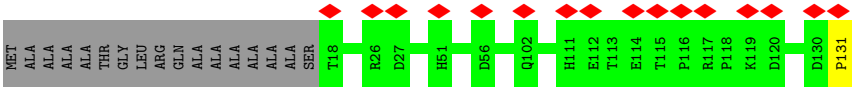


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

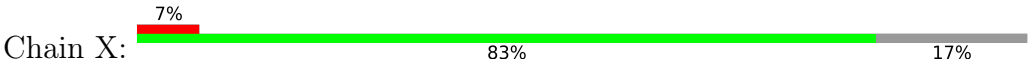


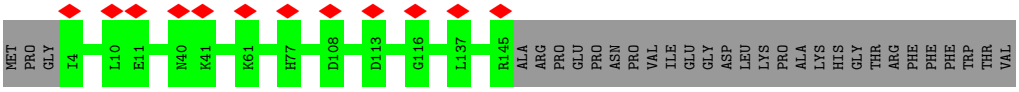
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



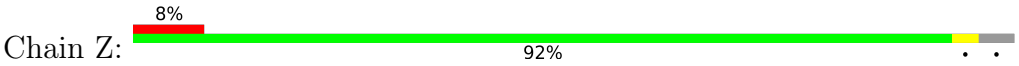


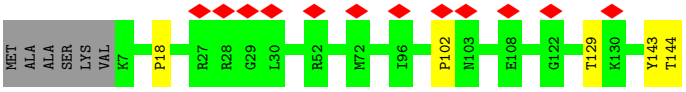
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



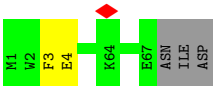


• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

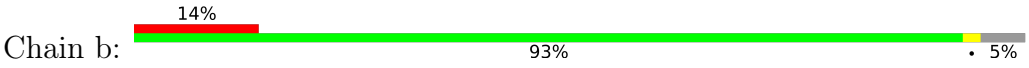


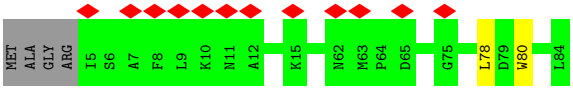


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

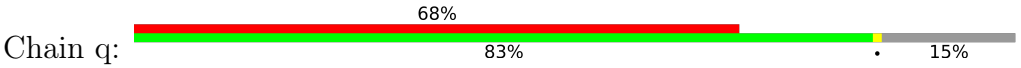


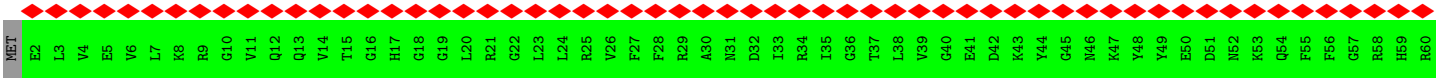
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

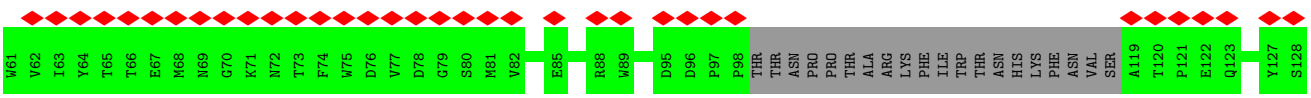


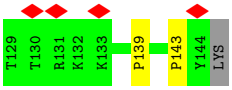


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



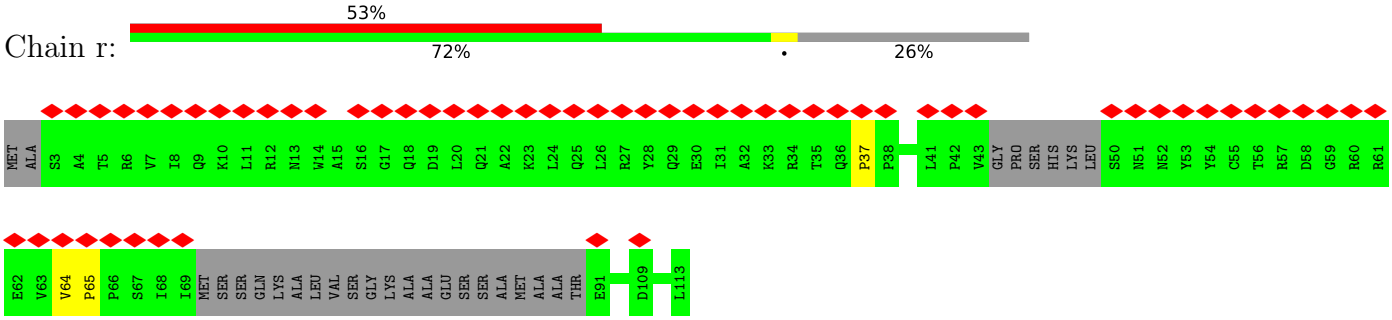






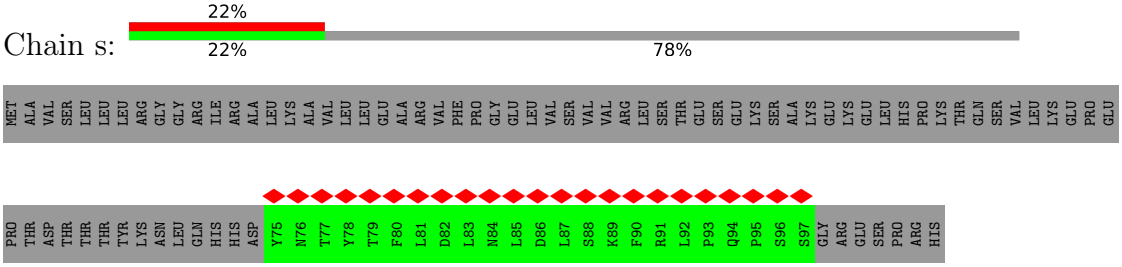
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



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

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.925	Depositor
Minimum map value	-2.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.086	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: FMN, SF4, 3PE, ZN, NDP, CDL, PC1, UQ1, UQ9, EHZ, 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	0.67	1/820 (0.1%)	0.77	2/1118 (0.2%)
2	B	0.82	4/1272 (0.3%)	1.04	10/1722 (0.6%)
3	C	0.66	0/1689	0.90	3/2300 (0.1%)
4	D	0.68	1/3162 (0.0%)	0.93	11/4276 (0.3%)
5	E	0.53	1/1675 (0.1%)	0.81	6/2282 (0.3%)
6	F	0.65	5/3363 (0.1%)	0.90	8/4543 (0.2%)
7	G	0.66	5/5374 (0.1%)	0.99	20/7281 (0.3%)
8	H	0.56	0/2608	0.79	8/3563 (0.2%)
9	I	0.65	2/1409 (0.1%)	0.92	5/1904 (0.3%)
10	P	0.55	2/2793 (0.1%)	0.76	6/3787 (0.2%)
11	Q	0.66	3/963 (0.3%)	0.87	2/1302 (0.2%)
12	R	0.45	0/671	0.70	0/903
13	S	0.58	1/678 (0.1%)	0.91	4/915 (0.4%)
14	T	0.47	0/613	0.62	0/826
15	V	0.54	0/937	0.71	0/1270
16	W	0.65	1/993 (0.1%)	0.66	2/1335 (0.1%)
17	X	0.47	0/1191	0.66	0/1605
18	Z	0.58	1/1176 (0.1%)	0.82	5/1587 (0.3%)
19	a	0.58	0/561	0.95	2/755 (0.3%)
20	b	0.52	0/651	0.69	2/895 (0.2%)
21	q	0.65	2/1059 (0.2%)	0.82	3/1439 (0.2%)
22	r	0.67	2/701 (0.3%)	0.95	1/948 (0.1%)
23	s	0.81	0/198	1.04	0/269
All	All	0.62	31/34557 (0.1%)	0.87	100/46825 (0.2%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	532	PRO	N-CD	-12.70	1.30	1.47
16	W	131	PRO	N-CD	-12.46	1.30	1.47
1	A	36	PRO	N-CD	-11.16	1.32	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	q	143	PRO	N-CD	-10.60	1.33	1.47
10	P	333	PRO	N-CD	-10.22	1.33	1.47
6	F	227	PRO	N-CD	10.06	1.61	1.47
4	D	365	PRO	N-CD	-9.68	1.34	1.47
7	G	275	PRO	N-CD	-9.47	1.34	1.47
2	B	92	PRO	N-CD	9.34	1.60	1.47
6	F	319	PRO	N-CD	8.96	1.60	1.47
18	Z	102	PRO	N-CD	-8.83	1.35	1.47
9	I	107	PRO	N-CD	8.53	1.59	1.47
21	q	139	PRO	N-CD	-8.02	1.36	1.47
22	r	65	PRO	N-CD	7.10	1.57	1.47
7	G	541	PRO	N-CD	-6.89	1.38	1.47
7	G	449	PRO	N-CD	6.78	1.57	1.47
6	F	234	GLY	CA-C	-6.76	1.41	1.51
11	Q	155	PRO	N-CD	-6.40	1.38	1.47
9	I	154	TYR	C-O	6.25	1.35	1.23
6	F	384	PRO	N-CD	-6.21	1.39	1.47
2	B	121	PHE	C-O	-6.21	1.11	1.23
10	P	292	PRO	N-CD	-6.20	1.39	1.47
5	E	93	PRO	N-CD	-6.03	1.39	1.47
6	F	235	VAL	N-CA	-5.88	1.34	1.46
2	B	122	ARG	CA-CB	-5.73	1.41	1.53
11	Q	106	ARG	C-O	5.72	1.34	1.23
13	S	63	PRO	N-CD	-5.71	1.39	1.47
11	Q	82	PRO	N-CD	-5.65	1.40	1.47
2	B	170	TYR	CB-CG	-5.54	1.43	1.51
7	G	683	PRO	N-CD	-5.46	1.40	1.47
22	r	37	PRO	N-CD	5.34	1.55	1.47

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	122	ARG	N-CA-CB	-13.93	85.52	110.60
19	a	3	PHE	CB-CA-C	-10.35	89.71	110.40
2	B	121	PHE	N-CA-C	-9.17	86.23	111.00
5	E	219	SER	N-CA-CB	9.03	124.04	110.50
6	F	334	THR	N-CA-CB	8.96	127.31	110.30
8	H	197	PRO	N-CA-CB	8.69	113.73	103.30
4	D	360	ASP	N-CA-C	-8.62	87.74	111.00
7	G	532	PRO	CA-N-CD	8.56	123.69	111.70
16	W	131	PRO	CA-N-CD	8.54	123.65	111.70
18	Z	102	PRO	N-CA-CB	-8.41	93.20	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	196	ALA	N-CA-C	8.14	132.97	111.00
7	G	174	THR	N-CA-C	-8.12	89.07	111.00
18	Z	144	THR	N-CA-CB	-8.03	95.05	110.30
4	D	359	ASP	CB-CA-C	-7.85	94.71	110.40
2	B	170	TYR	N-CA-C	-7.80	89.93	111.00
1	A	36	PRO	CA-N-CD	7.73	122.52	111.70
2	B	122	ARG	CB-CA-C	7.57	125.53	110.40
6	F	411	SER	N-CA-CB	7.53	121.79	110.50
1	A	36	PRO	N-CA-CB	-7.52	94.28	103.30
8	H	231	ILE	N-CA-C	-7.42	90.97	111.00
13	S	51	LEU	N-CA-C	-7.38	91.07	111.00
8	H	52	ALA	N-CA-CB	7.36	120.40	110.10
7	G	204	MET	N-CA-C	-7.26	91.41	111.00
2	B	99	CYS	N-CA-C	-7.24	91.45	111.00
6	F	332	CYS	N-CA-C	7.08	130.11	111.00
8	H	231	ILE	N-CA-CB	7.01	126.93	110.80
10	P	333	PRO	CA-N-CD	6.99	121.49	111.70
9	I	62	MET	N-CA-C	-6.99	92.12	111.00
18	Z	102	PRO	N-CA-C	6.94	130.15	112.10
18	Z	143	TYR	N-CA-C	6.84	129.48	111.00
7	G	380	ASP	N-CA-C	6.79	129.32	111.00
22	r	64	VAL	N-CA-CB	-6.76	96.63	111.50
4	D	365	PRO	CA-N-CD	6.71	121.09	111.70
7	G	275	PRO	CA-N-CD	6.66	121.02	111.70
7	G	300	GLN	N-CA-CB	6.59	122.46	110.60
21	q	143	PRO	CA-N-CD	6.58	120.91	111.70
5	E	64	ALA	N-CA-CB	6.57	119.30	110.10
5	E	166	LYS	CB-CA-C	6.56	123.52	110.40
16	W	131	PRO	N-CA-CB	-6.54	95.40	102.60
6	F	125	CYS	N-CA-C	-6.51	93.43	111.00
5	E	235	GLU	N-CA-CB	6.46	122.23	110.60
20	b	78	LEU	CB-CA-C	-6.40	98.04	110.20
4	D	427	PRO	N-CA-C	-6.38	95.52	112.10
8	H	203	GLY	N-CA-C	-6.35	97.22	113.10
8	H	196	ALA	C-N-CD	6.34	141.72	128.40
2	B	155	PRO	N-CA-C	-6.32	95.68	112.10
7	G	212	LYS	N-CA-C	-6.09	94.56	111.00
7	G	83	GLU	N-CA-C	6.09	127.43	111.00
7	G	133	GLN	N-CA-CB	6.04	121.48	110.60
8	H	207	LEU	N-CA-C	-6.02	94.75	111.00
10	P	110	ALA	N-CA-CB	-6.00	101.70	110.10
10	P	97	MET	N-CA-CB	5.95	121.32	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	50	THR	N-CA-CB	5.88	121.47	110.30
9	I	119	CYS	N-CA-C	5.88	126.86	111.00
7	G	251	ILE	N-CA-C	5.85	126.79	111.00
9	I	118	LEU	N-CA-C	5.84	126.77	111.00
4	D	358	VAL	N-CA-C	-5.83	95.26	111.00
4	D	361	ALA	N-CA-CB	-5.81	101.97	110.10
10	P	172	ALA	N-CA-CB	5.79	118.21	110.10
6	F	103	ASN	N-CA-CB	5.79	121.03	110.60
4	D	329	ARG	CB-CA-C	5.77	121.95	110.40
21	q	143	PRO	N-CA-CB	-5.76	96.26	102.60
7	G	510	TRP	N-CA-CB	5.72	120.90	110.60
3	C	180	HIS	N-CA-C	-5.64	95.76	111.00
4	D	143	SER	CB-CA-C	5.63	120.80	110.10
11	Q	59	LEU	N-CA-CB	-5.63	99.13	110.40
7	G	599	THR	N-CA-C	5.61	126.14	111.00
7	G	580	ALA	N-CA-CB	5.59	117.93	110.10
3	C	240	ALA	N-CA-CB	-5.57	102.30	110.10
13	S	57	GLU	N-CA-C	5.56	126.02	111.00
18	Z	102	PRO	CA-N-CD	5.54	119.46	111.70
13	S	61	VAL	N-CA-C	-5.54	96.04	111.00
10	P	96	LEU	CB-CA-C	-5.53	99.70	110.20
7	G	653	LEU	N-CA-CB	5.52	121.45	110.40
9	I	119	CYS	N-CA-CB	-5.50	100.70	110.60
4	D	257	GLU	N-CA-CB	5.49	120.48	110.60
4	D	114	GLY	N-CA-C	-5.43	99.53	113.10
7	G	662	THR	N-CA-C	-5.39	96.45	111.00
21	q	139	PRO	CA-N-CD	5.38	119.23	111.70
6	F	457	HIS	N-CA-CB	-5.36	100.95	110.60
7	G	362	ASP	N-CA-C	5.34	125.41	111.00
6	F	418	GLN	N-CA-CB	5.30	120.14	110.60
2	B	121	PHE	CA-C-O	-5.26	109.04	120.10
5	E	218	ARG	CB-CA-C	-5.26	99.87	110.40
13	S	61	VAL	N-CA-CB	5.25	123.05	111.50
11	Q	155	PRO	N-CA-CB	-5.24	96.83	102.60
7	G	640	ASP	N-CA-CB	5.24	120.03	110.60
4	D	457	VAL	N-CA-C	-5.22	96.90	111.00
2	B	122	ARG	N-CA-C	5.17	124.96	111.00
19	a	4	GLU	N-CA-C	5.11	124.79	111.00
6	F	228	PRO	N-CA-C	-5.10	98.85	112.10
2	B	88	SER	N-CA-CB	5.09	118.14	110.50
7	G	77	MET	N-CA-C	-5.08	97.29	111.00
2	B	97	LEU	CA-CB-CG	5.07	126.96	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	80	TRP	N-CA-CB	5.06	119.72	110.60
3	C	237	PRO	N-CD-CG	-5.05	95.62	103.20
10	P	115	SER	N-CA-C	-5.04	97.38	111.00
9	I	96	ARG	NE-CZ-NH1	-5.03	117.78	120.30
7	G	668	ALA	N-CA-CB	5.03	117.14	110.10
7	G	532	PRO	N-CA-CB	-5.00	97.10	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
2	B	153/224 (68%)	141 (92%)	11 (7%)	1 (1%)	19	50
3	C	196/263 (74%)	189 (96%)	7 (4%)	0	100	100
4	D	383/463 (83%)	360 (94%)	22 (6%)	1 (0%)	37	66
5	E	208/248 (84%)	194 (93%)	14 (7%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	635 (93%)	50 (7%)	0	100	100
8	H	313/318 (98%)	281 (90%)	31 (10%)	1 (0%)	37	66
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	P	337/377 (89%)	309 (92%)	28 (8%)	0	100	100
11	Q	114/175 (65%)	100 (88%)	14 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	R	81/116 (70%)	72 (89%)	9 (11%)	0	100 100
13	S	81/99 (82%)	74 (91%)	7 (9%)	0	100 100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100 100
15	V	110/116 (95%)	99 (90%)	11 (10%)	0	100 100
16	W	112/131 (86%)	103 (92%)	9 (8%)	0	100 100
17	X	140/172 (81%)	125 (89%)	15 (11%)	0	100 100
18	Z	136/144 (94%)	129 (95%)	5 (4%)	2 (2%)	8 33
19	a	65/70 (93%)	59 (91%)	6 (9%)	0	100 100
20	b	78/84 (93%)	69 (88%)	9 (12%)	0	100 100
21	q	119/145 (82%)	110 (92%)	9 (8%)	0	100 100
22	r	78/113 (69%)	75 (96%)	3 (4%)	0	100 100
23	s	21/104 (20%)	20 (95%)	1 (5%)	0	100 100
All	All	4167/5036 (83%)	3858 (93%)	304 (7%)	5 (0%)	50 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	324	GLY
8	H	196	ALA
18	Z	129	THR
2	B	195	PRO
18	Z	18	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	89/104 (86%)	89 (100%)	0	100 100
2	B	131/185 (71%)	131 (100%)	0	100 100
3	C	181/227 (80%)	181 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	332/395 (84%)	332 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	579 (100%)	0	100	100
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	146/178 (82%)	146 (100%)	0	100	100
10	P	296/325 (91%)	296 (100%)	0	100	100
11	Q	103/153 (67%)	103 (100%)	0	100	100
12	R	70/96 (73%)	70 (100%)	0	100	100
13	S	74/80 (92%)	74 (100%)	0	100	100
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	119/123 (97%)	119 (100%)	0	100	100
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100
21	q	110/131 (84%)	110 (100%)	0	100	100
22	r	76/96 (79%)	76 (100%)	0	100	100
23	s	23/95 (24%)	23 (100%)	0	100	100
All	All	3665/4292 (85%)	3665 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	209	GLN
3	C	88	HIS
3	C	102	HIS
3	C	130	ASN
3	C	195	HIS
4	D	79	ASN
4	D	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	117	HIS
4	D	147	ASN
4	D	149	GLN
4	D	168	GLN
4	D	182	ASN
4	D	234	GLN
4	D	270	ASN
4	D	285	ASN
4	D	313	GLN
4	D	381	HIS
5	E	152	GLN
5	E	245	GLN
6	F	277	ASN
6	F	346	GLN
6	F	441	HIS
7	G	51	GLN
7	G	59	GLN
7	G	74	ASN
7	G	140	GLN
7	G	205	GLN
7	G	384	ASN
7	G	388	ASN
7	G	444	HIS
7	G	495	ASN
7	G	514	ASN
7	G	571	HIS
7	G	572	HIS
7	G	605	GLN
7	G	667	GLN
8	H	124	ASN
8	H	171	HIS
8	H	235	ASN
8	H	284	GLN
8	H	287	HIS
8	H	292	ASN
9	I	172	ASN
9	I	180	HIS
10	P	79	GLN
10	P	102	GLN
10	P	128	ASN
10	P	166	HIS
10	P	251	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	P	285	HIS
11	Q	86	ASN
11	Q	88	GLN
13	S	22	HIS
13	S	25	GLN
13	S	48	HIS
13	S	81	ASN
13	S	92	GLN
15	V	50	GLN
15	V	110	ASN
16	W	54	GLN
16	W	61	GLN
16	W	102	GLN
16	W	105	HIS
16	W	129	HIS
17	X	64	ASN
17	X	99	HIS
18	Z	8	GLN
18	Z	24	ASN
18	Z	90	ASN
20	b	46	ASN
21	q	17	HIS
21	q	91	HIS
22	r	18	GLN
22	r	21	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
31	NDP	P	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.20	4 (7%)
27	PC1	B	304	-	42,42,53	1.04	2 (4%)	48,50,61	1.01	3 (6%)
26	UQ1	B	302	-	18,18,18	1.96	2 (11%)	22,25,25	1.25	4 (18%)
27	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.11	3 (7%)
24	3PE	I	301	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	2 (3%)
25	SF4	B	301	2	0,12,12	-	-	-		
25	SF4	G	802	-	0,12,12	-	-	-		
24	3PE	H	401	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	3 (6%)
25	SF4	F	502	6	0,12,12	-	-	-		
30	UQ9	H	400	-	35,35,58	0.80	2 (5%)	42,45,73	0.47	0
25	SF4	G	801	7	0,12,12	-	-	-		
34	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.20	6 (9%)
28	FES	G	803	7	0,4,4	-	-	-		
25	SF4	I	302	9	0,12,12	-	-	-		
25	SF4	I	303	9	0,12,12	-	-	-		
28	FES	E	301	5	0,4,4	-	-	-		
24	3PE	A	201	-	41,41,50	1.01	2 (4%)	44,46,55	1.09	2 (4%)
29	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.19	6 (12%)
33	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)

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
31	NDP	P	401	-	-	6/30/77/77	0/5/5/5
27	PC1	B	304	-	-	14/46/46/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
27	PC1	B	303	-	-	13/38/38/57	-
24	3PE	I	301	-	-	17/54/54/54	-
25	SF4	B	301	2	-	-	0/6/5/5
25	SF4	G	802	-	-	-	0/6/5/5
24	3PE	H	401	-	-	13/51/51/54	-
25	SF4	F	502	6	-	-	0/6/5/5
30	UQ9	H	400	-	-	16/30/54/81	0/1/1/1
25	SF4	G	801	7	-	-	0/6/5/5
34	CDL	a	101	-	-	18/67/67/110	-
28	FES	G	803	7	-	-	0/1/1/1
25	SF4	I	302	9	-	-	0/6/5/5
25	SF4	I	303	9	-	-	0/6/5/5
28	FES	E	301	5	-	-	0/1/1/1
24	3PE	A	201	-	-	12/45/45/54	-
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3
33	EHZ	W	201	-	-	12/39/39/45	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	302	UQ1	C6-C5	7.34	1.48	1.35
33	W	201	EHZ	C15-N2	5.16	1.44	1.33
33	W	201	EHZ	C12-N1	5.03	1.44	1.33
29	F	501	FMN	C9A-C5A	4.84	1.49	1.41
34	a	101	CDL	OA8-CA7	4.31	1.45	1.33
24	A	201	3PE	O31-C31	4.28	1.45	1.33
27	B	303	PC1	O31-C31	4.20	1.45	1.33
27	B	304	PC1	O31-C31	4.16	1.45	1.33
34	a	101	CDL	OB8-CB7	4.16	1.45	1.33
27	B	304	PC1	O21-C21	4.16	1.46	1.34
24	I	301	3PE	O31-C31	4.15	1.45	1.33
24	H	401	3PE	O31-C31	4.12	1.45	1.33
24	I	301	3PE	O21-C21	4.08	1.45	1.34
24	H	401	3PE	O21-C21	4.06	1.45	1.34
24	A	201	3PE	O21-C21	4.06	1.45	1.34
34	a	101	CDL	OA6-CA5	4.04	1.45	1.34
27	B	303	PC1	O21-C21	3.94	1.45	1.34
34	a	101	CDL	OB6-CB5	3.93	1.45	1.34
31	P	401	NDP	C6N-C5N	3.25	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	501	FMN	C8-C7	3.11	1.48	1.40
26	B	302	UQ1	C3-C2	3.09	1.48	1.36
29	F	501	FMN	C4-N3	-2.76	1.33	1.38
30	H	400	UQ9	C3-C2	-2.66	1.41	1.48
30	H	400	UQ9	C4-C5	-2.53	1.41	1.48
33	W	201	EHZ	O4-C15	-2.44	1.18	1.23
29	F	501	FMN	C5A-N5	-2.38	1.34	1.39
33	W	201	EHZ	O3-C12	-2.37	1.18	1.23
33	W	201	EHZ	C9-S1	2.23	1.81	1.76
31	P	401	NDP	C5A-C4A	2.19	1.46	1.40
29	F	501	FMN	C4A-N5	2.06	1.34	1.30

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	W	201	EHZ	C8-C9-S1	6.03	121.09	113.63
34	a	101	CDL	OA6-CA5-C11	4.21	120.58	111.50
24	I	301	3PE	O21-C21-C22	4.10	120.34	111.50
24	H	401	3PE	O21-C21-C22	4.05	120.22	111.50
31	P	401	NDP	PN-O3-PA	-4.05	118.94	132.83
27	B	304	PC1	O21-C21-C22	3.96	120.03	111.50
24	A	201	3PE	O21-C21-C22	3.92	119.96	111.50
27	B	303	PC1	O21-C21-C22	3.67	119.42	111.50
34	a	101	CDL	OB6-CB5-C51	3.53	119.11	111.50
31	P	401	NDP	N3A-C2A-N1A	-3.24	123.61	128.68
24	H	401	3PE	O31-C31-C32	2.88	120.94	111.91
26	B	302	UQ1	CM5-C5-C6	-2.82	119.80	124.40
27	B	303	PC1	O31-C31-C32	2.81	120.73	111.91
34	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
24	A	201	3PE	O31-C31-C32	2.65	120.23	111.91
27	B	303	PC1	C2-O21-C21	-2.64	111.29	117.79
33	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
24	I	301	3PE	O31-C31-C32	2.50	119.76	111.91
29	F	501	FMN	C4A-C10-N1	-2.50	118.92	124.73
29	F	501	FMN	O4-C4-C4A	-2.48	120.02	126.60
31	P	401	NDP	C4A-C5A-N7A	-2.48	106.81	109.40
33	W	201	EHZ	C13-C12-N1	2.48	120.59	116.42
34	a	101	CDL	OB8-CB7-C71	2.45	119.60	111.91
33	W	201	EHZ	C14-N2-C15	-2.44	118.24	122.59
26	B	302	UQ1	C11-C9-C10	2.41	119.92	114.60
27	B	304	PC1	O31-C31-C32	2.36	119.33	111.91
33	W	201	EHZ	O2-C9-S1	-2.34	119.58	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	501	FMN	C4-C4A-N5	2.31	121.53	118.23
34	a	101	CDL	CB4-OB6-CB5	-2.16	112.47	117.79
27	B	304	PC1	C2-O21-C21	-2.13	112.53	117.79
26	B	302	UQ1	C7-C8-C9	-2.13	120.60	127.26
34	a	101	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
31	P	401	NDP	C3D-C2D-C1D	2.09	105.39	101.43
29	F	501	FMN	C4A-C10-N10	2.04	119.46	116.48
26	B	302	UQ1	C8-C7-C6	-2.03	106.57	112.05
29	F	501	FMN	C4A-C4-N3	2.03	118.34	113.19
29	F	501	FMN	C10-N1-C2	2.02	120.94	116.90
24	H	401	3PE	O21-C21-O22	-2.00	118.86	123.70

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	201	3PE	C1-O11-P-O14
24	A	201	3PE	C11-O13-P-O11
24	A	201	3PE	C11-O13-P-O14
24	A	201	3PE	C22-C21-O21-C2
24	H	401	3PE	C1-O11-P-O14
24	H	401	3PE	C11-O13-P-O14
24	H	401	3PE	O22-C21-O21-C2
24	H	401	3PE	C22-C21-O21-C2
24	I	301	3PE	C1-O11-P-O14
24	I	301	3PE	C11-O13-P-O12
27	B	303	PC1	C11-O13-P-O14
27	B	303	PC1	C22-C21-O21-C2
27	B	304	PC1	C1-O11-P-O14
27	B	304	PC1	C22-C21-O21-C2
29	F	501	FMN	C5'-O5'-P-O2P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	400	UQ9	C22-C23-C24-C26
30	H	400	UQ9	C22-C23-C24-C25
30	H	400	UQ9	C20-C19-C21-C22
30	H	400	UQ9	C18-C19-C21-C22
30	H	400	UQ9	C15-C14-C16-C17
30	H	400	UQ9	C13-C14-C16-C17
30	H	400	UQ9	C12-C13-C14-C16
30	H	400	UQ9	C12-C13-C14-C15
30	H	400	UQ9	C11-C12-C13-C14
31	P	401	NDP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	O2-C9-S1-C10
33	W	201	EHZ	C8-C9-S1-C10
34	a	101	CDL	CA2-OA2-PA1-OA4
34	a	101	CDL	OA7-CA5-OA6-CA4
34	a	101	CDL	C11-CA5-OA6-CA4
34	a	101	CDL	CB2-OB2-PB2-OB3
27	B	304	PC1	O32-C31-O31-C3
24	A	201	3PE	O22-C21-O21-C2
27	B	303	PC1	O22-C21-O21-C2
27	B	304	PC1	O22-C21-O21-C2
27	B	304	PC1	C32-C31-O31-C3
24	I	301	3PE	C32-C31-O31-C3
24	H	401	3PE	O32-C31-O31-C3
24	I	301	3PE	O32-C31-O31-C3
24	H	401	3PE	C32-C31-O31-C3
34	a	101	CDL	C31-CA7-OA8-CA6
24	I	301	3PE	C22-C21-O21-C2
34	a	101	CDL	OA9-CA7-OA8-CA6
30	H	400	UQ9	C9-C11-C12-C13
30	H	400	UQ9	C17-C18-C19-C20
24	I	301	3PE	O22-C21-O21-C2
30	H	400	UQ9	C17-C18-C19-C21
27	B	303	PC1	C11-C12-N-C13
30	H	400	UQ9	C19-C21-C22-C23
24	I	301	3PE	C1-O11-P-O13
24	I	301	3PE	C11-O13-P-O11
27	B	303	PC1	C11-O13-P-O11
27	B	303	PC1	C1-O11-P-O13
34	a	101	CDL	CA2-OA2-PA1-OA5
27	B	303	PC1	C11-C12-N-C14
24	I	301	3PE	C32-C33-C34-C35
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C19-C17-C20-O6
27	B	303	PC1	C11-C12-N-C15
34	a	101	CDL	C13-C14-C15-C16
27	B	304	PC1	C1-O11-P-O13
34	a	101	CDL	C14-C15-C16-C17
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	H	401	3PE	C3-C2-O21-C21
24	H	401	3PE	C2-C1-O11-P
29	F	501	FMN	C5'-O5'-P-O1P
24	I	301	3PE	C3B-C3C-C3D-C3E
33	W	201	EHZ	C5-C6-C7-C8
30	H	400	UQ9	C14-C16-C17-C18
27	B	303	PC1	C2-C1-O11-P
24	A	201	3PE	C1-C2-C3-O31
24	H	401	3PE	C2B-C2C-C2D-C2E
27	B	304	PC1	C38-C39-C3A-C3B
24	H	401	3PE	C2C-C2D-C2E-C2F
31	P	401	NDP	C2B-O2B-P2B-O1X
27	B	303	PC1	C31-C32-C33-C34
31	P	401	NDP	PN-O3-PA-O2A
31	P	401	NDP	O4D-C1D-N1N-C6N
34	a	101	CDL	CB4-CB3-OB5-PB2
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C11-O13-P-O14
27	B	303	PC1	C11-O13-P-O12
27	B	303	PC1	C1-O11-P-O14
27	B	304	PC1	C1-O11-P-O12
29	F	501	FMN	N10-C1'-C2'-O2'
33	W	201	EHZ	C2-C3-C4-C5
27	B	304	PC1	C11-C12-N-C14
30	H	400	UQ9	C12-C11-C9-C10
33	W	201	EHZ	O4-C15-C16-O5
24	A	201	3PE	O21-C2-C3-O31
24	A	201	3PE	C1-O11-P-O13
24	H	401	3PE	C11-O13-P-O11
34	a	101	CDL	CB3-OB5-PB2-OB2
34	a	101	CDL	C71-CB7-OB8-CB6
30	H	400	UQ9	C12-C11-C9-C8
27	B	304	PC1	C2-C1-O11-P
24	H	401	3PE	C31-C32-C33-C34
24	A	201	3PE	C23-C24-C25-C26
24	I	301	3PE	O11-C1-C2-C3
34	a	101	CDL	OB9-CB7-OB8-CB6
31	P	401	NDP	PN-O3-PA-O1A
34	a	101	CDL	C15-C16-C17-C18
24	A	201	3PE	C39-C3A-C3B-C3C
27	B	304	PC1	C11-C12-N-C13
24	A	201	3PE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

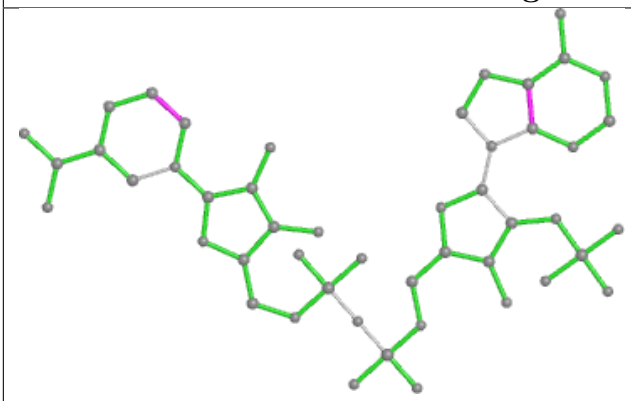
Mol	Chain	Res	Type	Atoms
24	I	301	3PE	C31-C32-C33-C34
27	B	304	PC1	C3A-C3B-C3C-C3D
27	B	304	PC1	C11-C12-N-C15
31	P	401	NDP	C5D-O5D-PN-O3
24	H	401	3PE	C37-C38-C39-C3A
34	a	101	CDL	C18-C19-C20-C21
34	a	101	CDL	CB3-OB5-PB2-OB3
24	A	201	3PE	C25-C26-C27-C28
24	I	301	3PE	C12-C11-O13-P
27	B	303	PC1	C33-C34-C35-C36
34	a	101	CDL	C12-C11-CA5-OA7
27	B	304	PC1	C3F-C3G-C3H-C3I
24	I	301	3PE	O31-C31-C32-C33
34	a	101	CDL	C12-C11-CA5-OA6
24	I	301	3PE	O32-C31-C32-C33

There are no ring outliers.

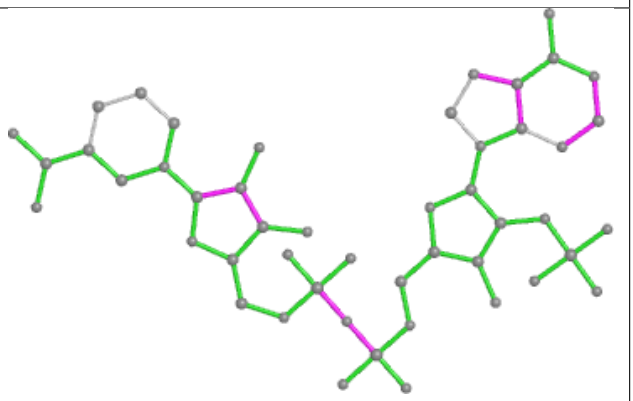
No monomer is involved in short contacts.

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

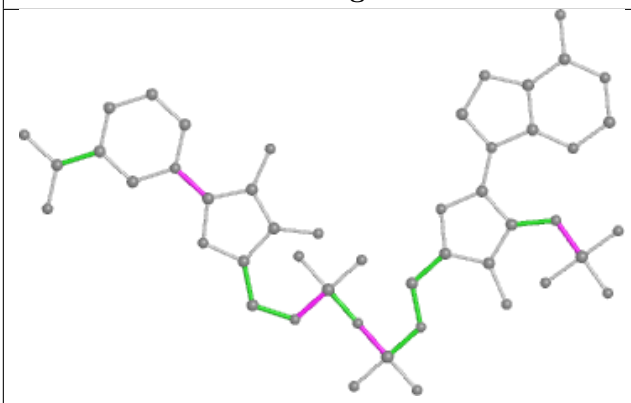
Ligand NDP P 401



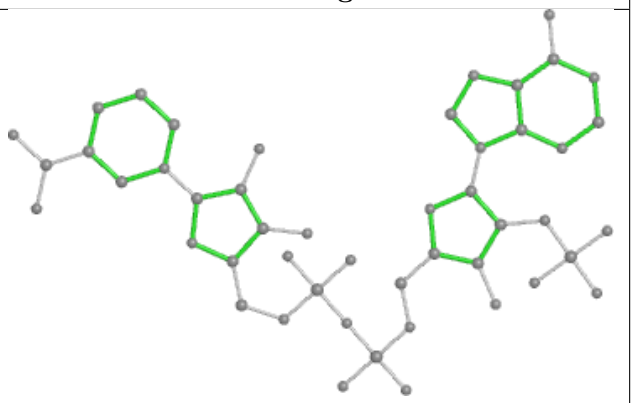
Bond lengths



Bond angles

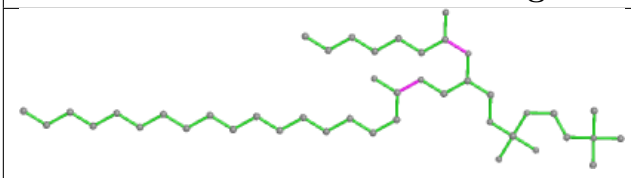


Torsions

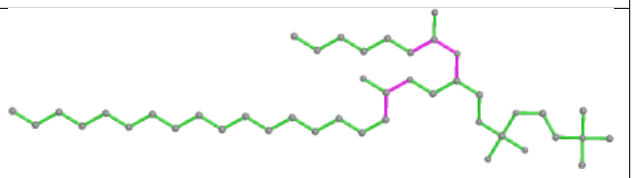


Rings

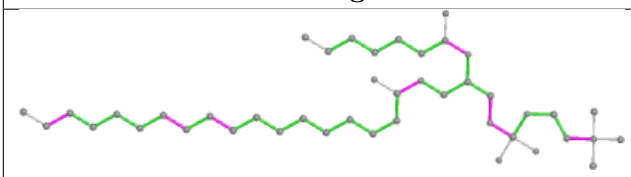
Ligand PC1 B 304



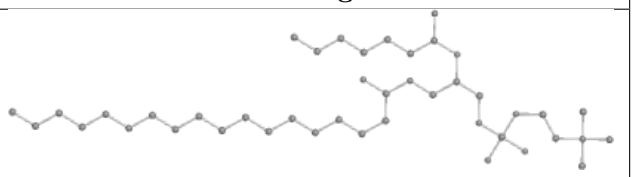
Bond lengths



Bond angles

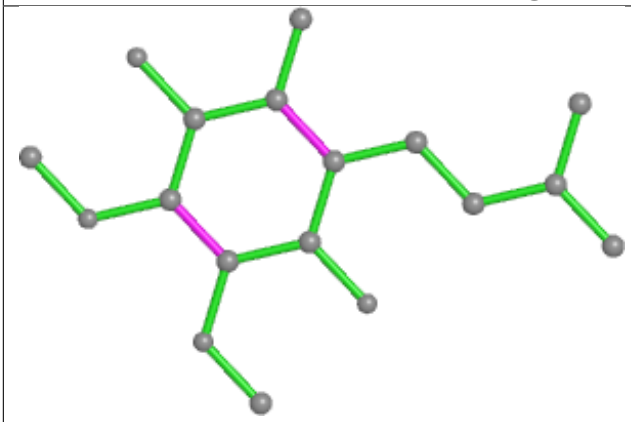


Torsions

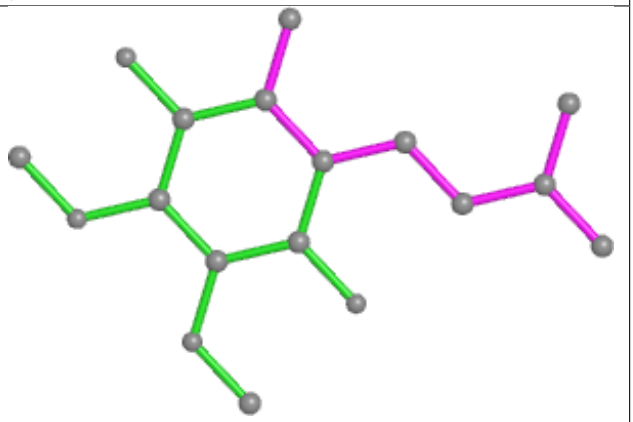


Rings

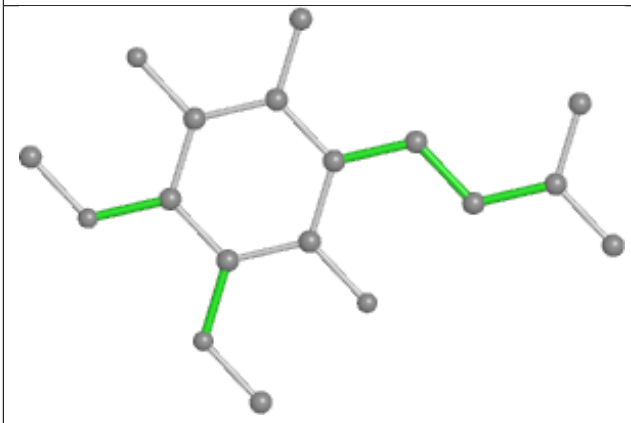
Ligand UQ1 B 302



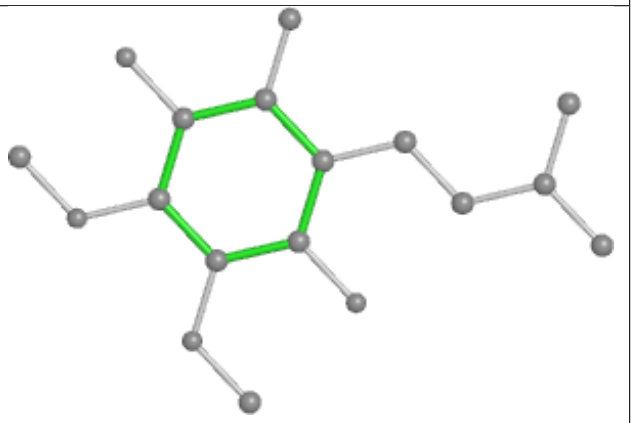
Bond lengths



Bond angles

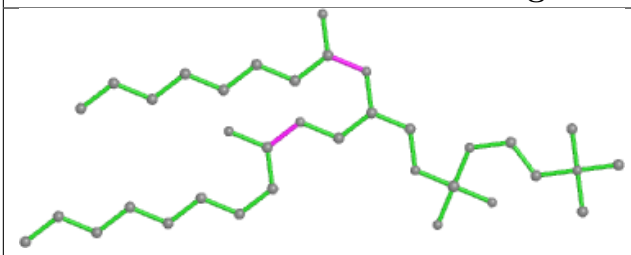


Torsions

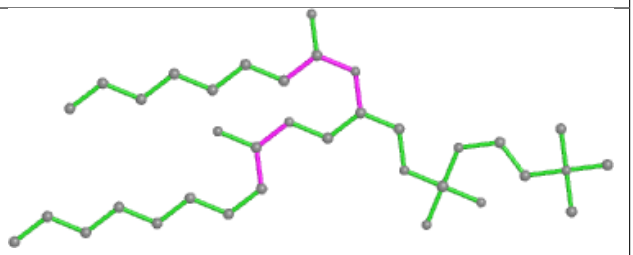


Rings

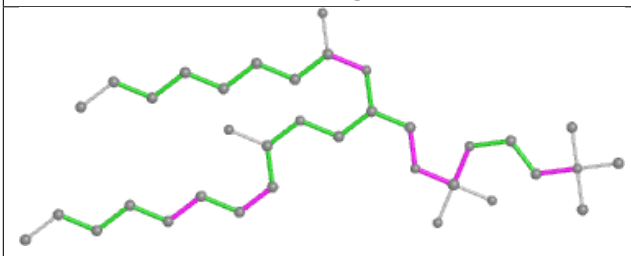
Ligand PC1 B 303



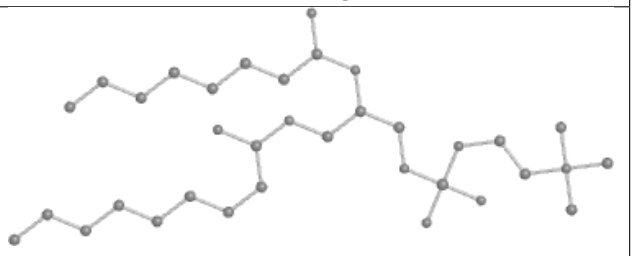
Bond lengths



Bond angles

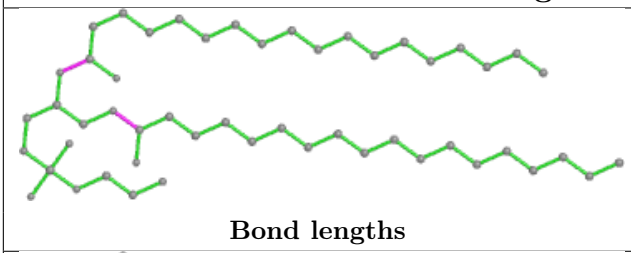


Torsions

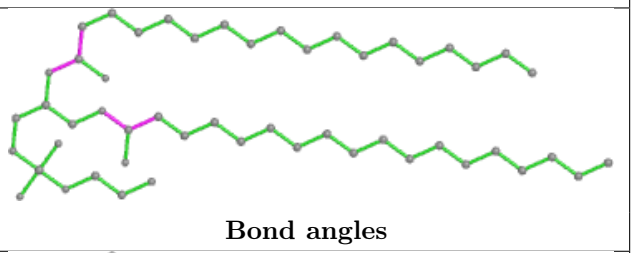


Rings

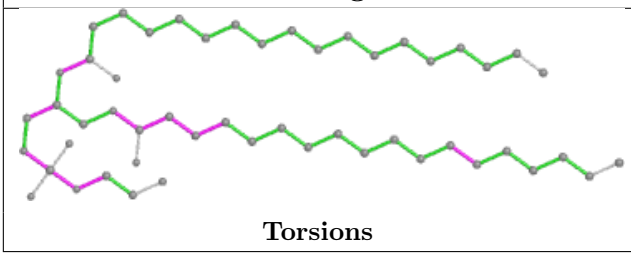
Ligand 3PE I 301



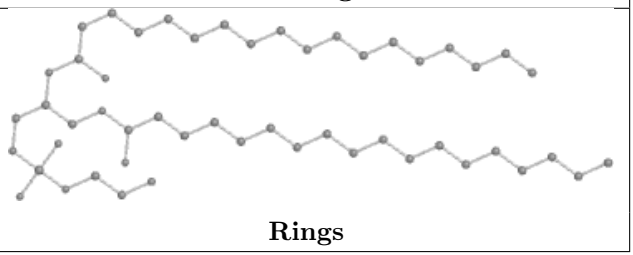
Bond lengths



Bond angles

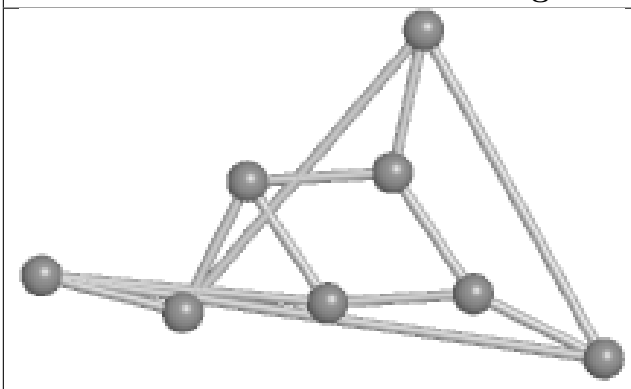


Torsions

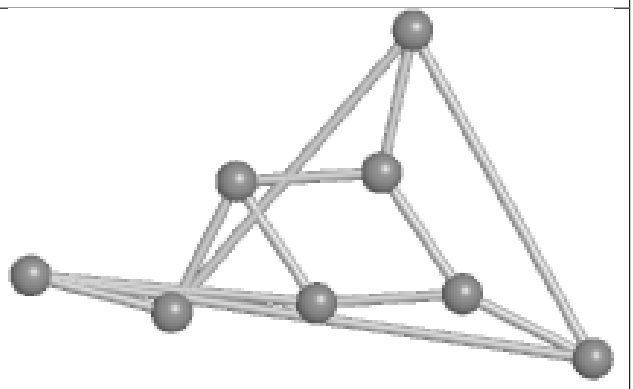


Rings

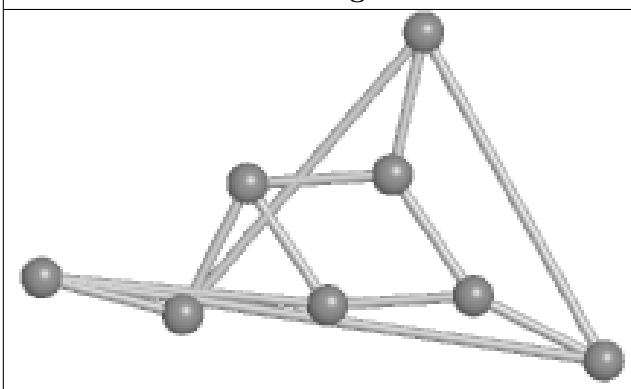
Ligand SF4 B 301



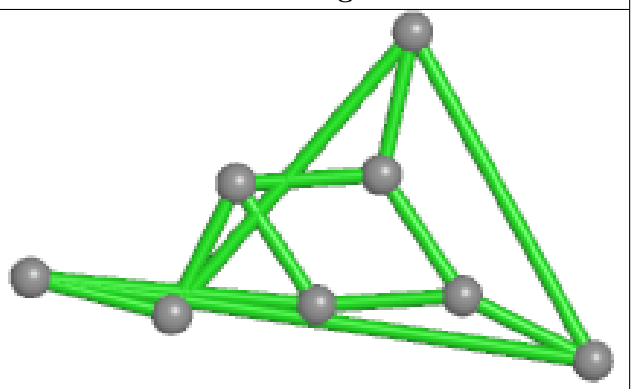
Bond lengths



Bond angles

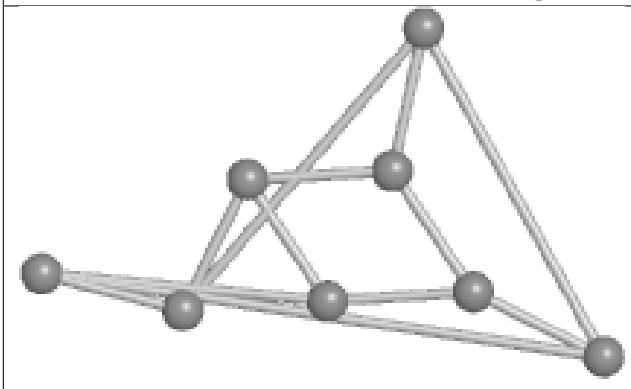


Torsions

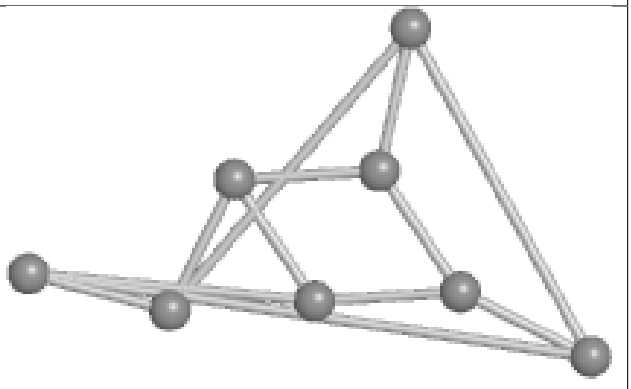


Rings

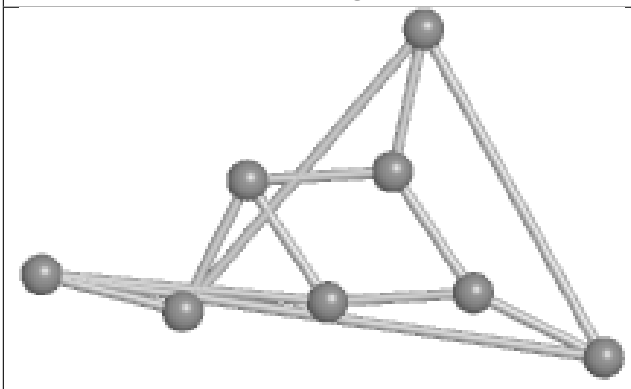
Ligand SF4 G 802



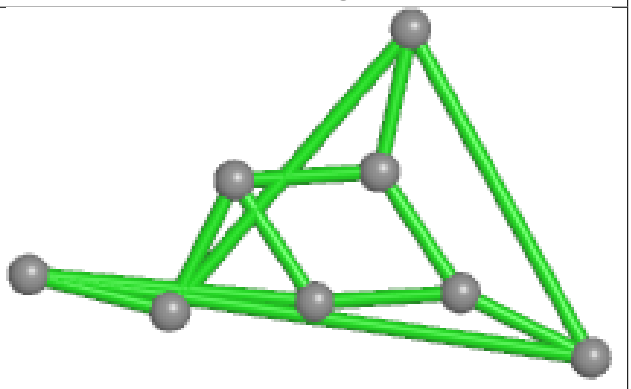
Bond lengths



Bond angles

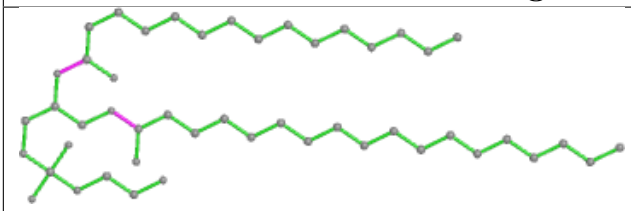


Torsions

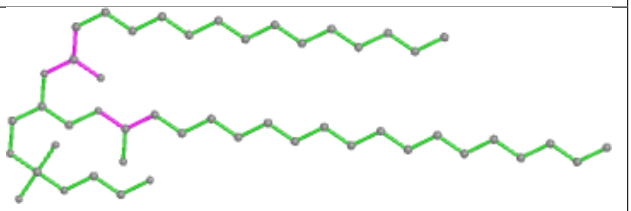


Rings

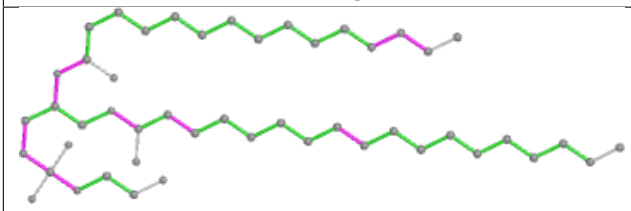
Ligand 3PE H 401



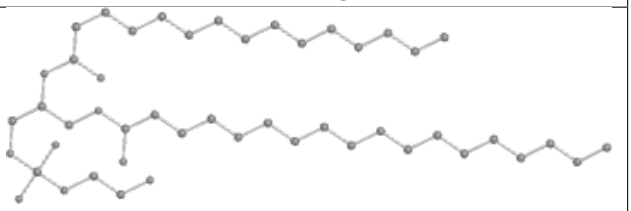
Bond lengths



Bond angles

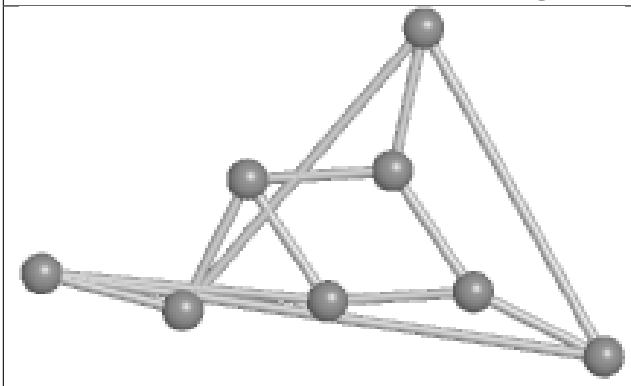


Torsions

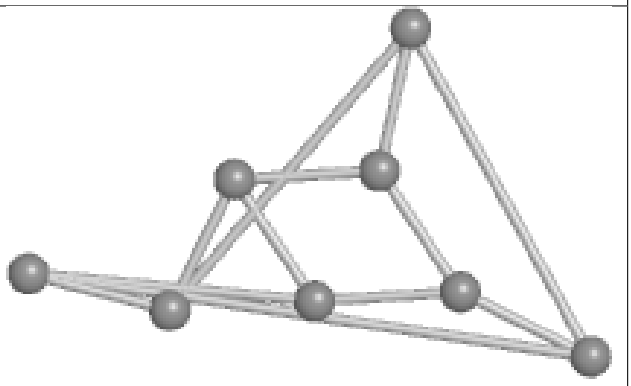


Rings

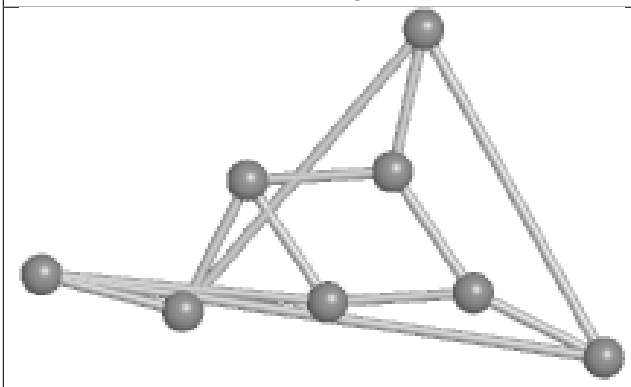
Ligand SF4 F 502



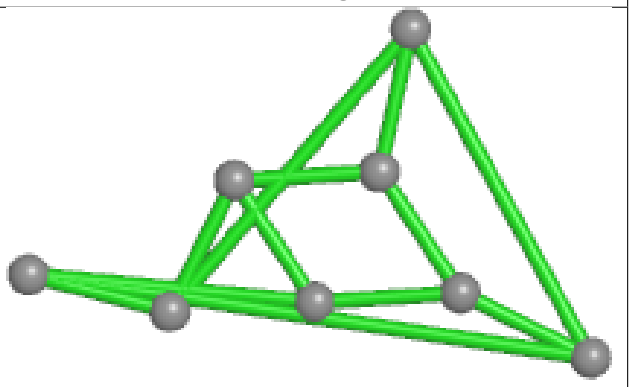
Bond lengths



Bond angles

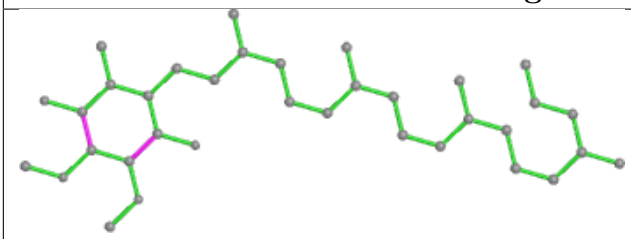


Torsions

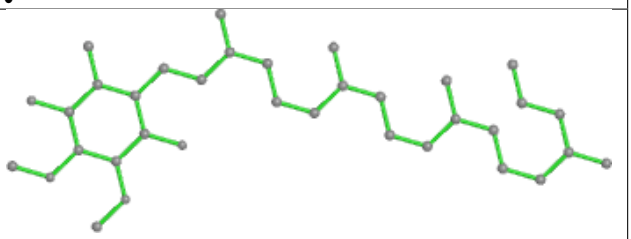


Rings

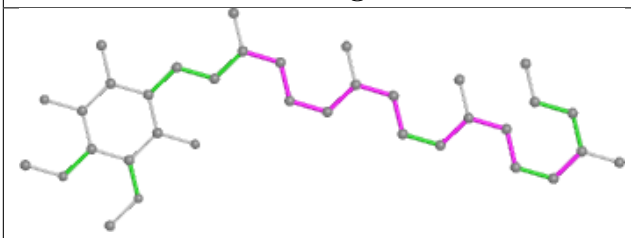
Ligand UQ9 H 400



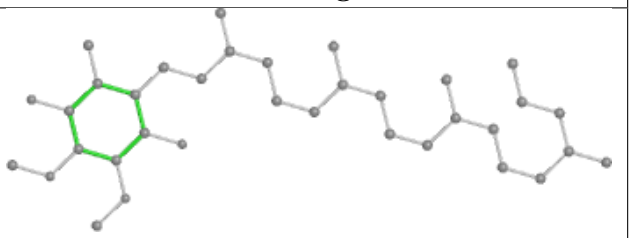
Bond lengths



Bond angles

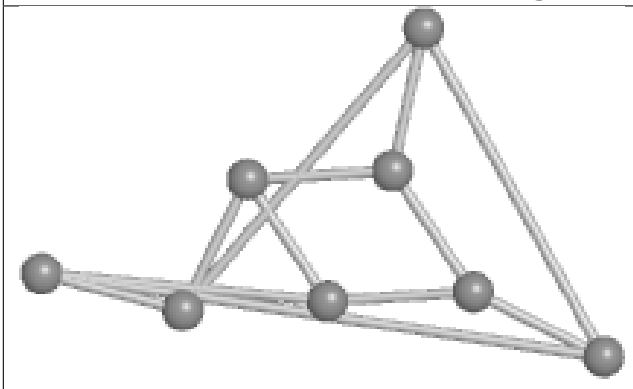


Torsions

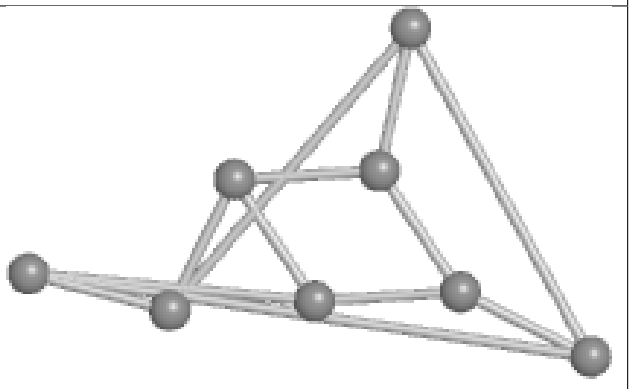


Rings

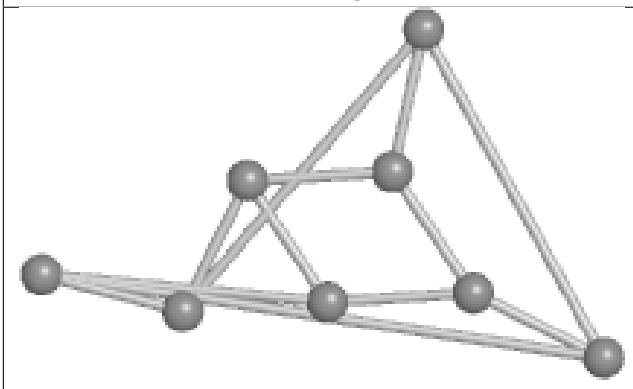
Ligand SF4 G 801



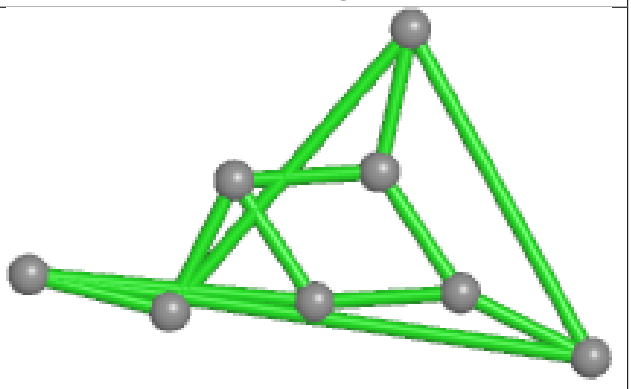
Bond lengths



Bond angles

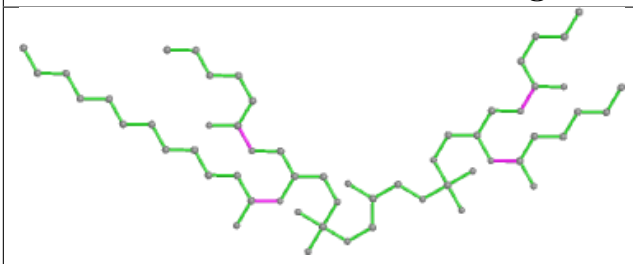


Torsions

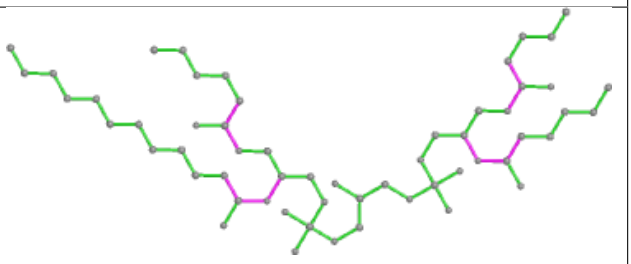


Rings

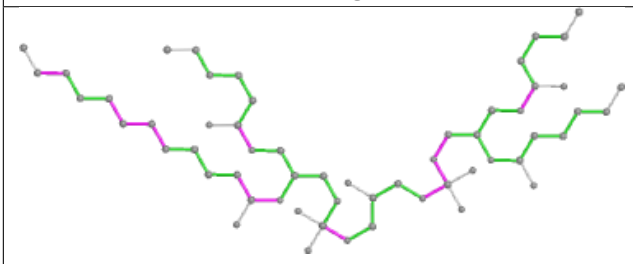
Ligand CDL a 101



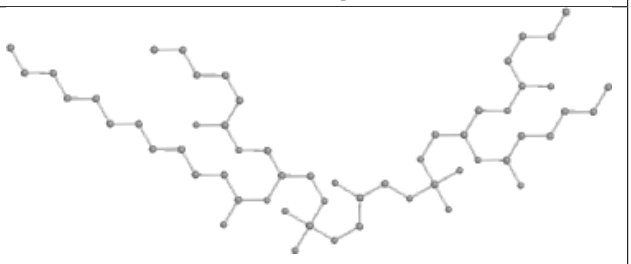
Bond lengths



Bond angles

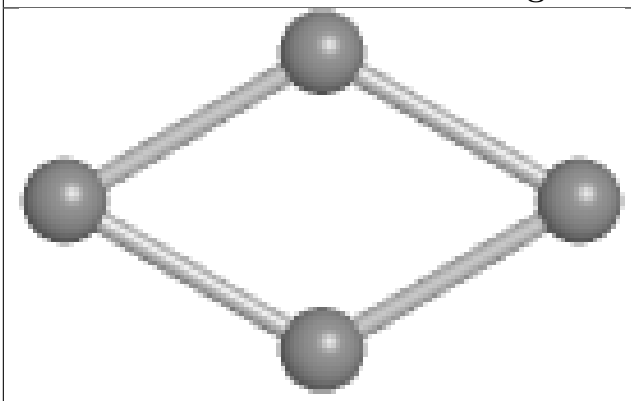


Torsions

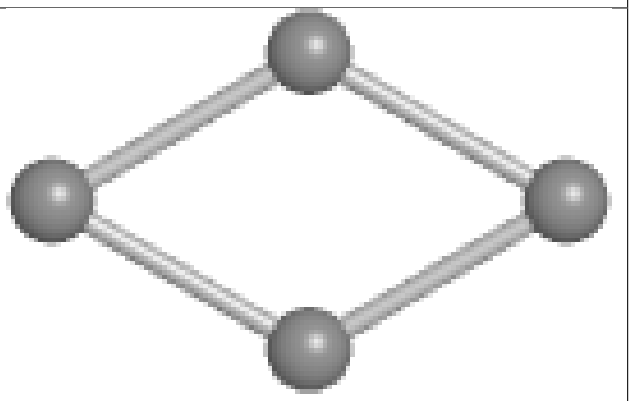


Rings

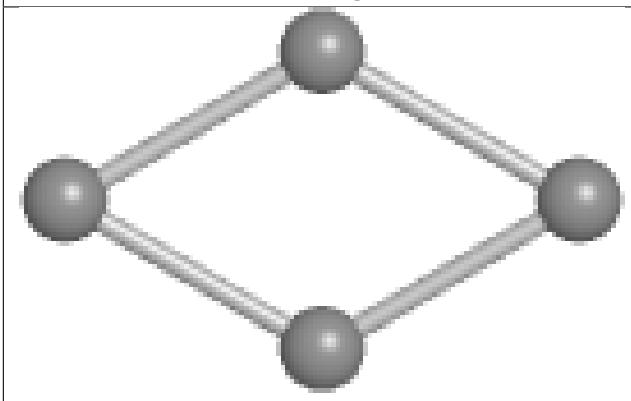
Ligand FES G 803



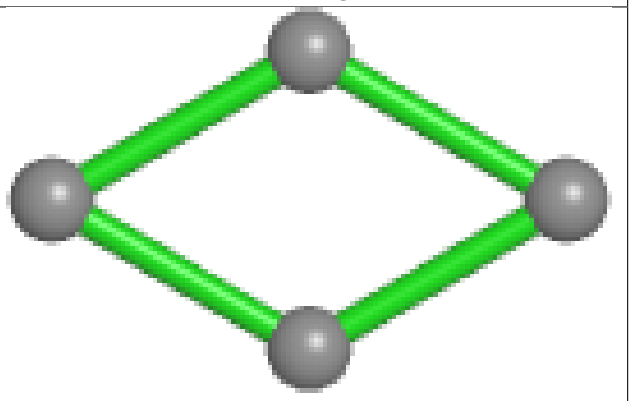
Bond lengths



Bond angles

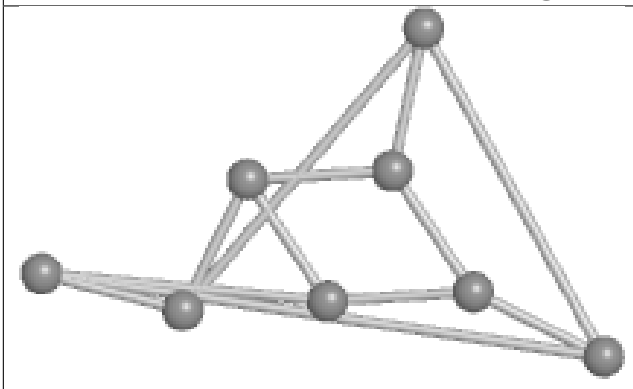


Torsions

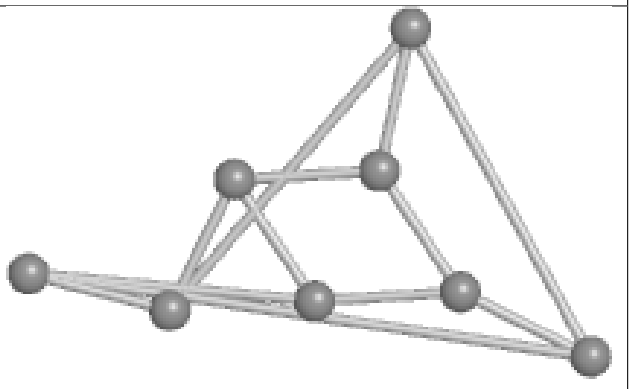


Rings

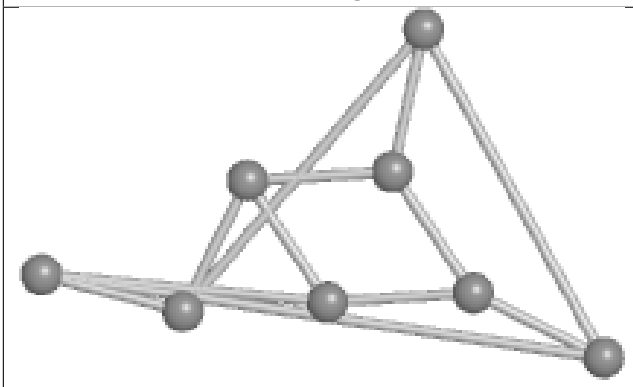
Ligand SF4 I 302



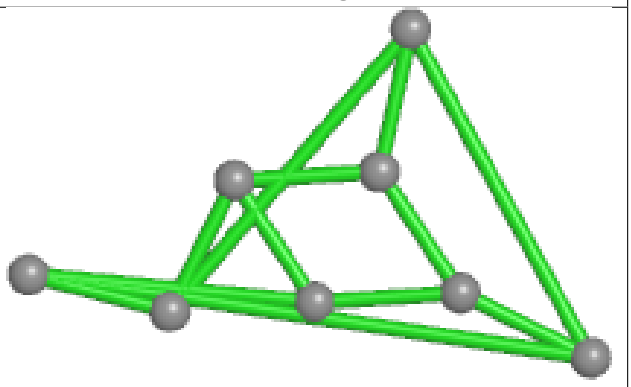
Bond lengths



Bond angles

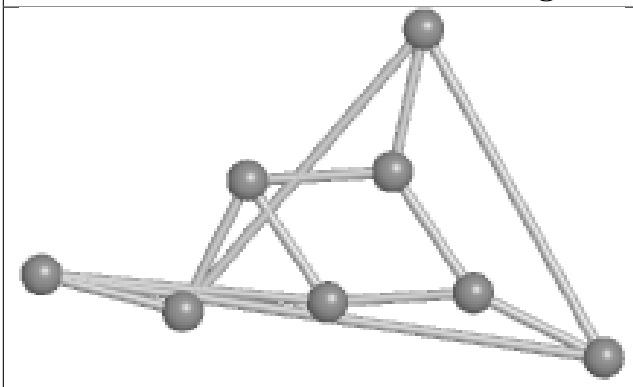


Torsions

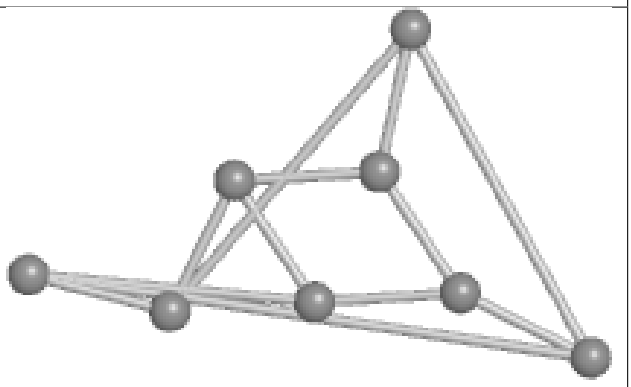


Rings

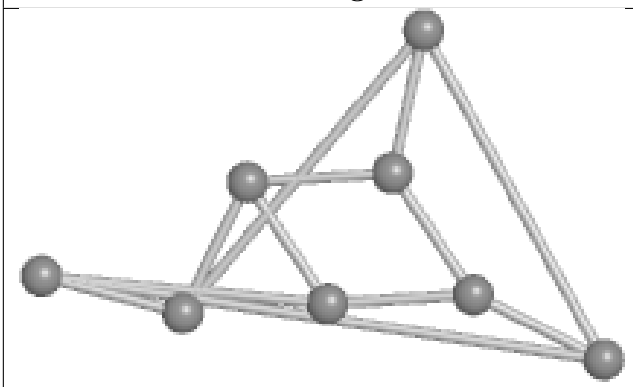
Ligand SF4 I 303



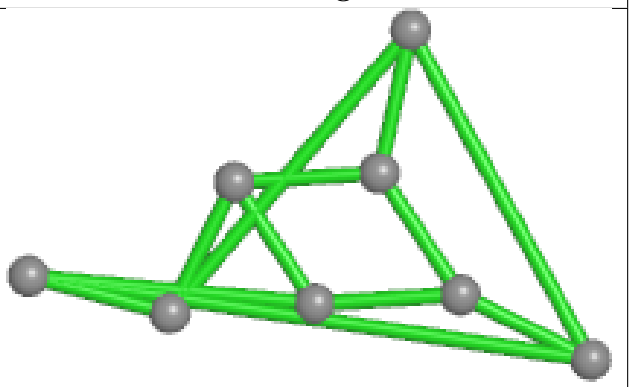
Bond lengths



Bond angles

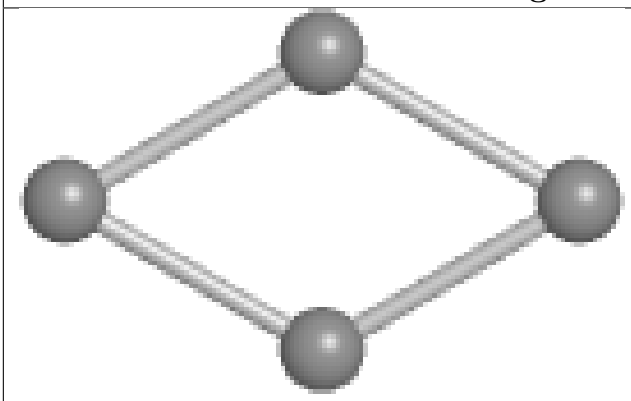


Torsions

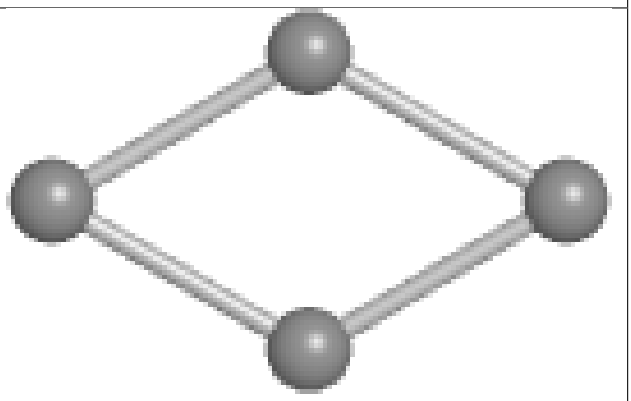


Rings

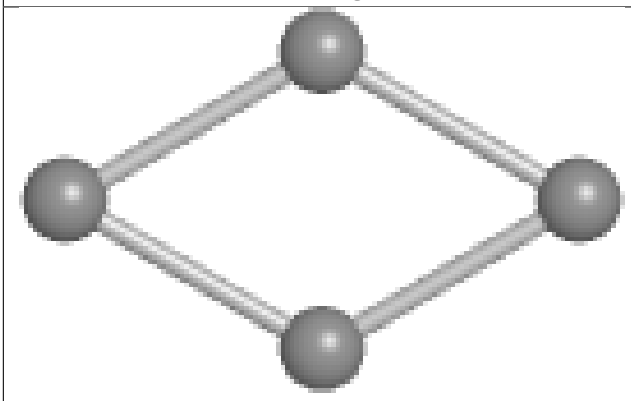
Ligand FES E 301



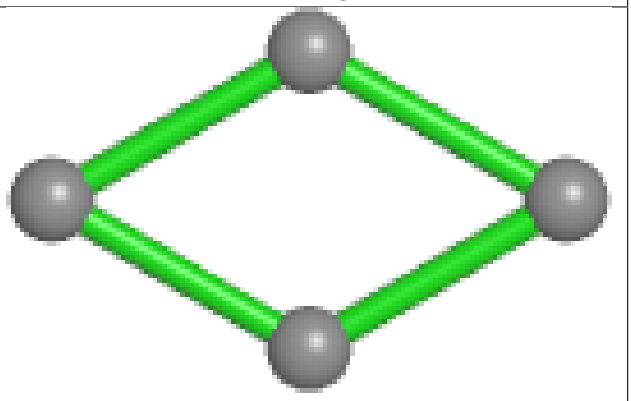
Bond lengths



Bond angles

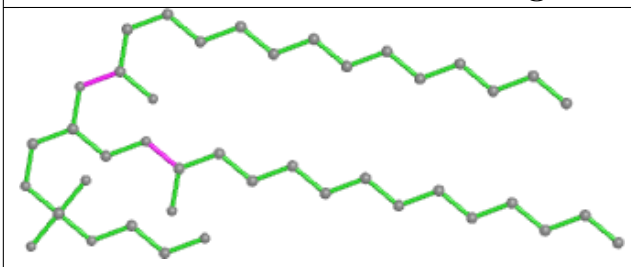


Torsions

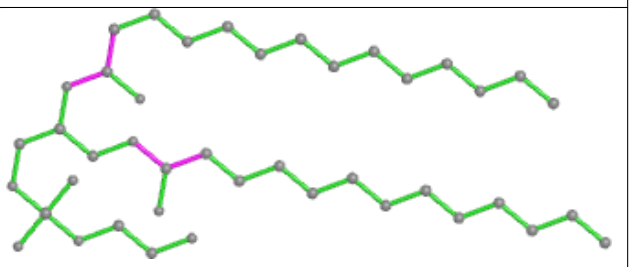


Rings

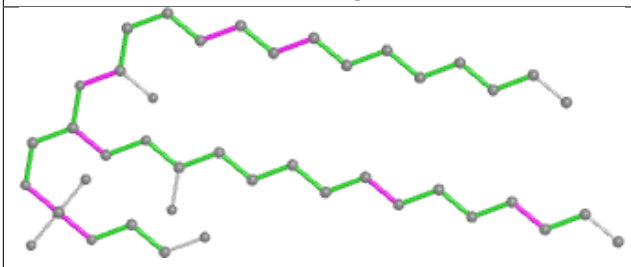
Ligand 3PE A 201



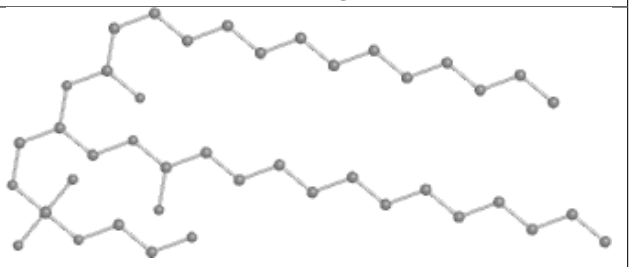
Bond lengths



Bond angles

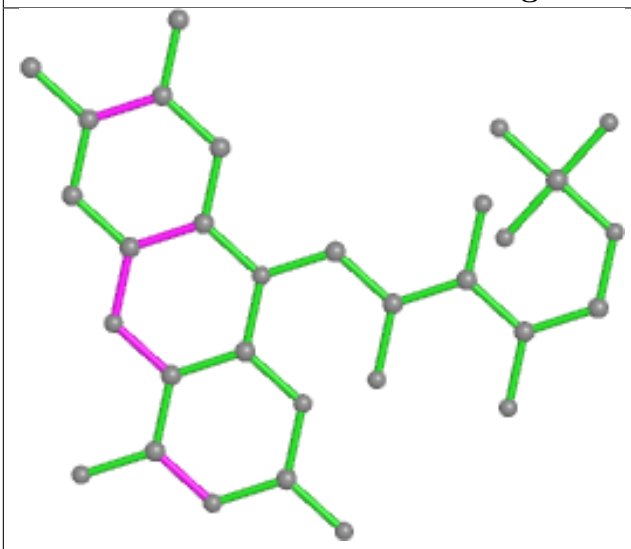


Torsions

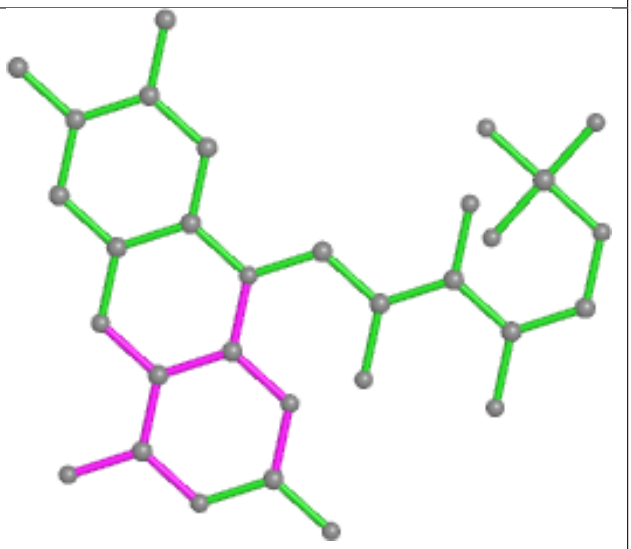


Rings

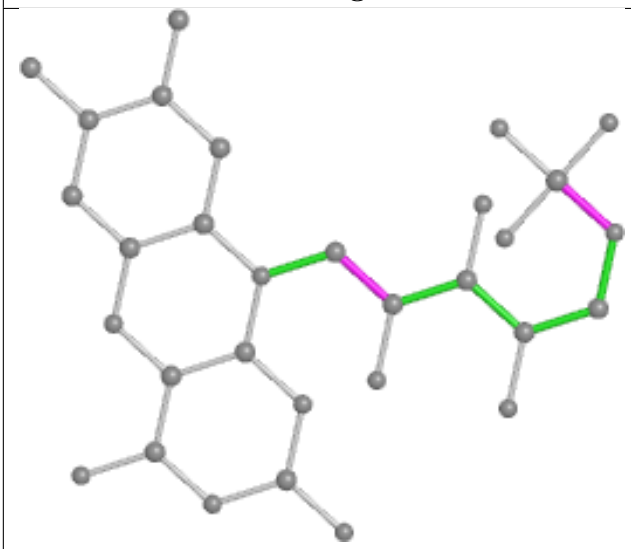
Ligand FMN F 501



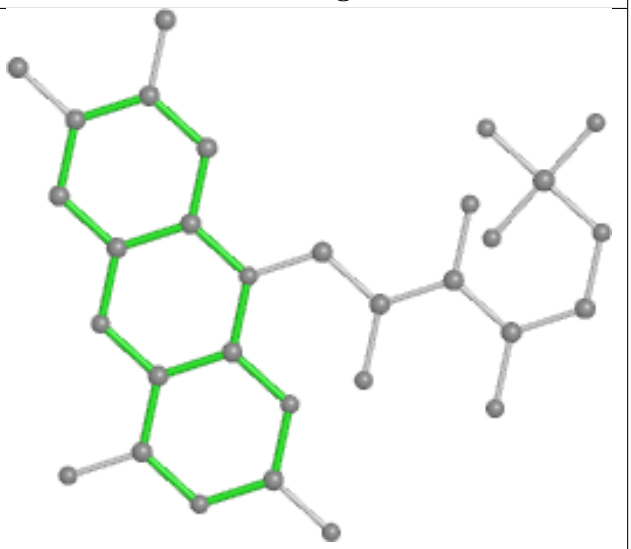
Bond lengths



Bond angles

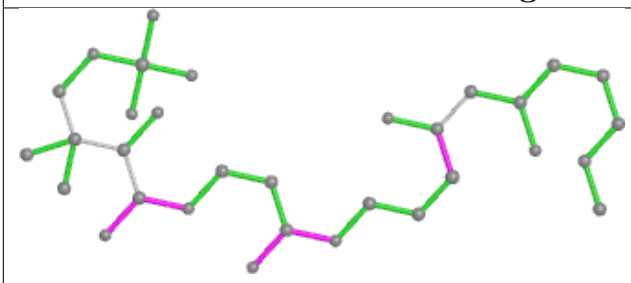


Torsions

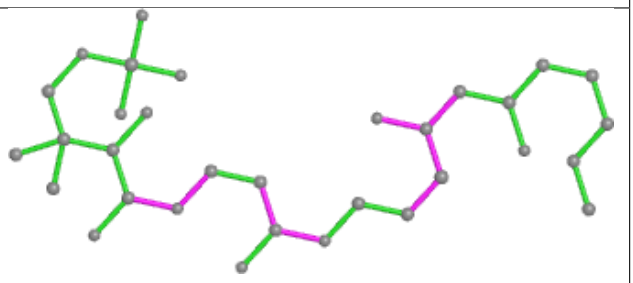


Rings

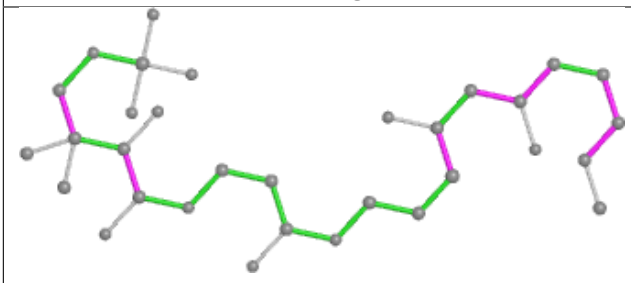
Ligand EHZ W 201



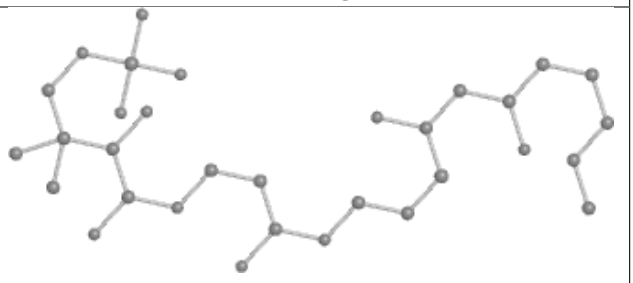
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

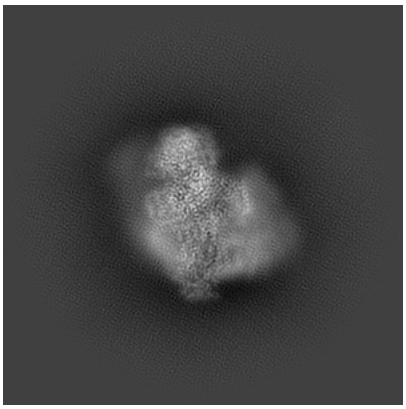
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35341. These allow visual inspection of the internal detail of the map and identification of artifacts.

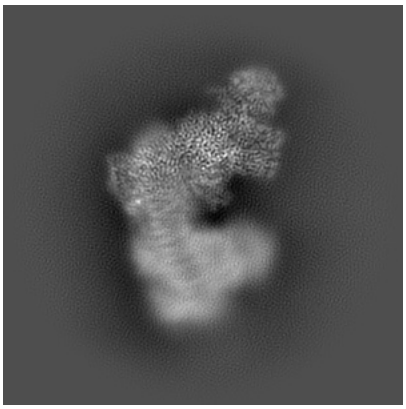
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

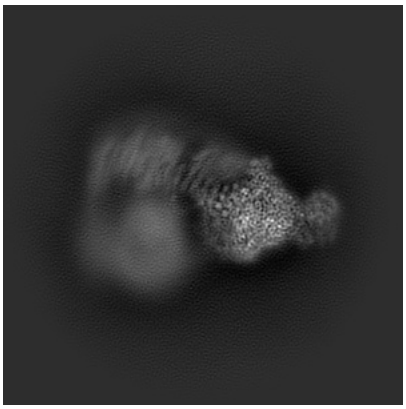
6.1.1 Primary map



X

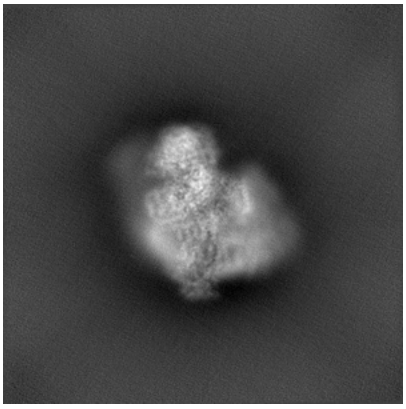


Y

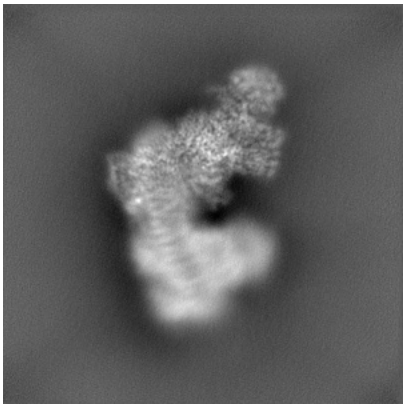


Z

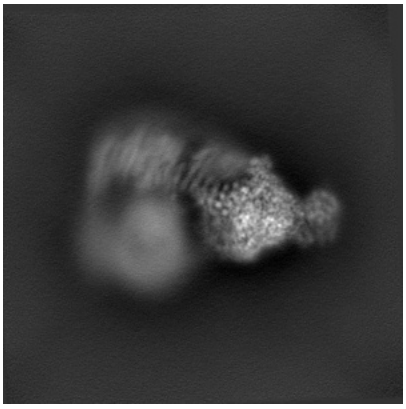
6.1.2 Raw map



X



Y

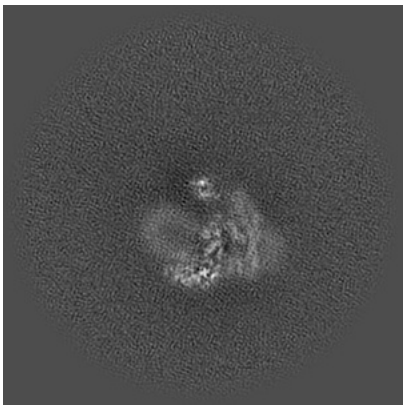


Z

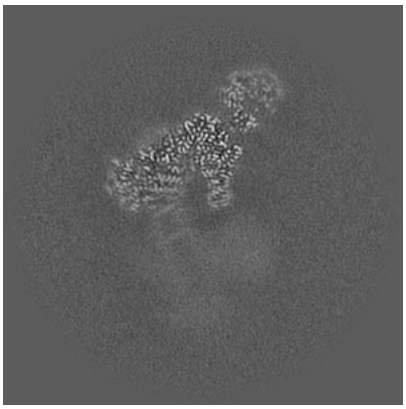
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

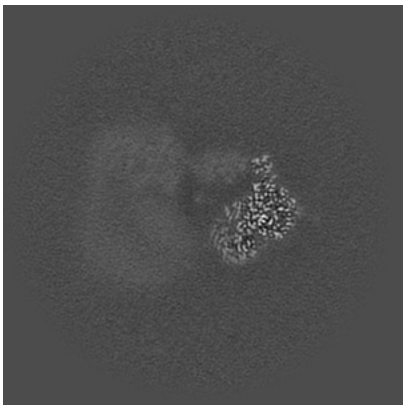
6.2.1 Primary map



X Index: 192

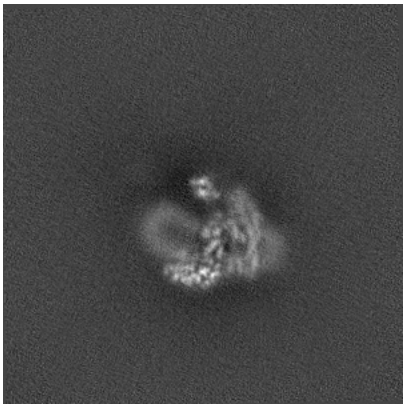


Y Index: 192

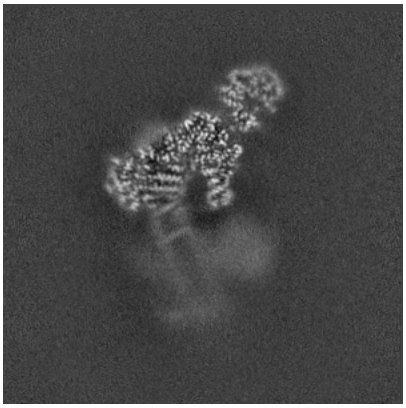


Z Index: 192

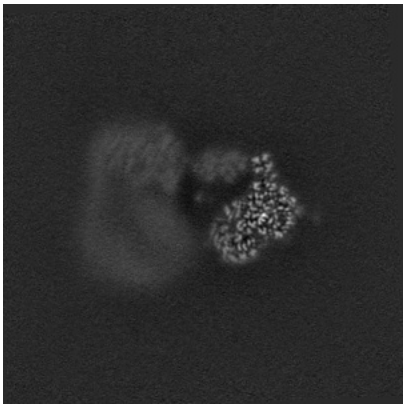
6.2.2 Raw map



X Index: 192



Y Index: 192

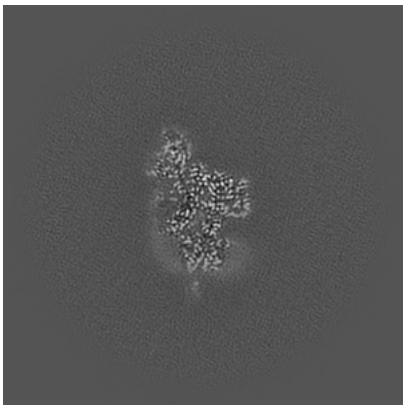


Z Index: 192

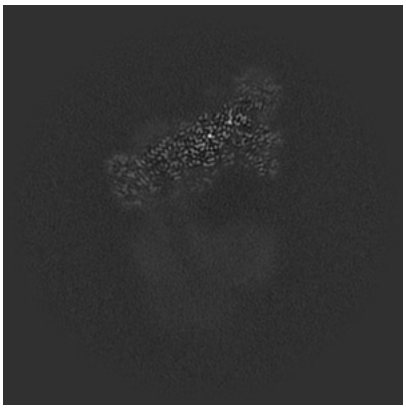
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

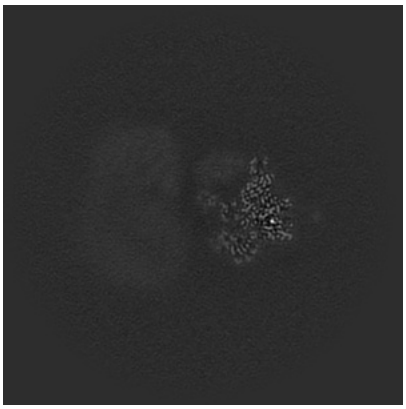
6.3.1 Primary map



X Index: 243

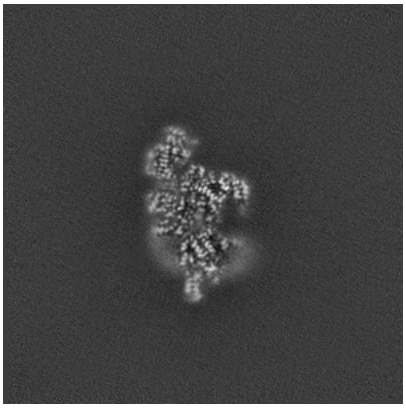


Y Index: 176

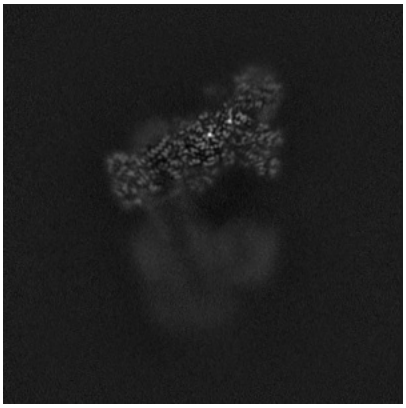


Z Index: 198

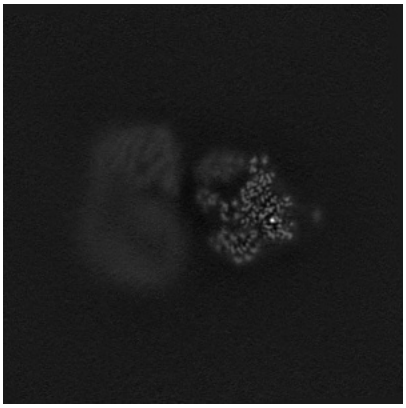
6.3.2 Raw map



X Index: 238



Y Index: 176

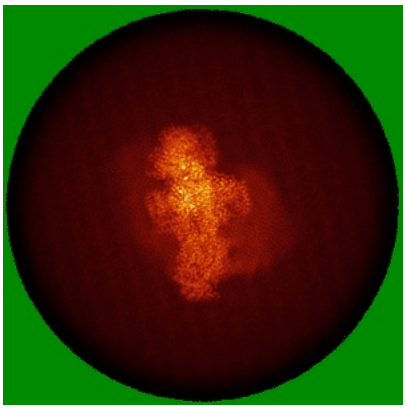


Z Index: 198

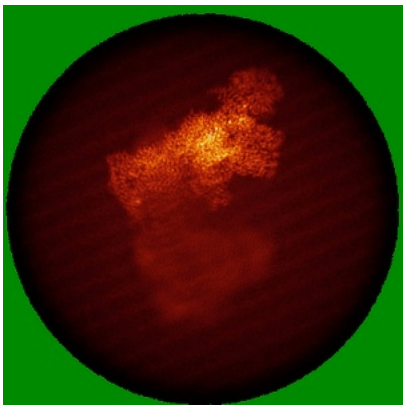
The images above show the largest variance slices of the map in three orthogonal directions.

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

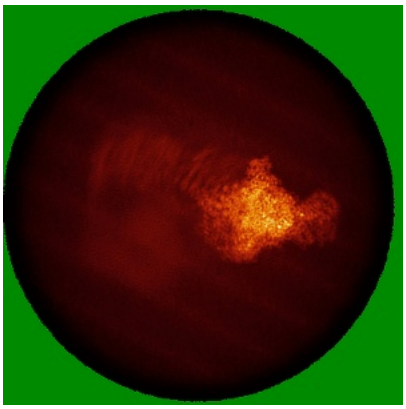
6.4.1 Primary map



X

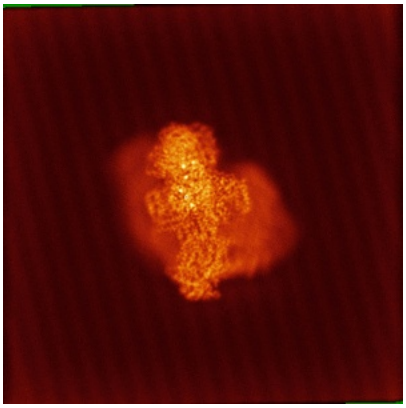


Y

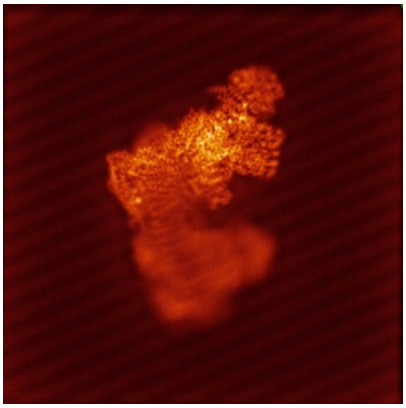


Z

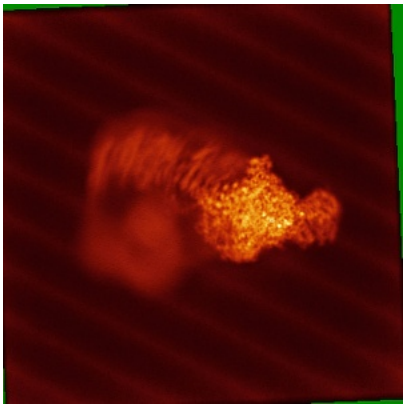
6.4.2 Raw map



X



Y

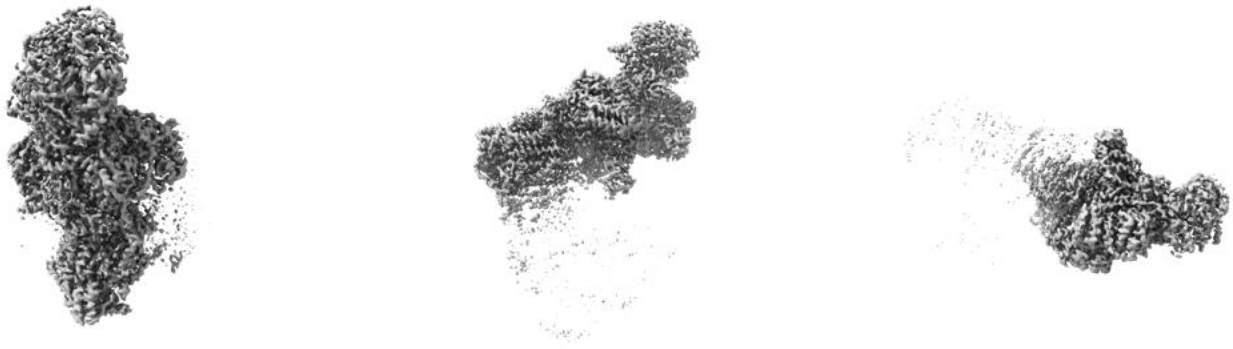


Z

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.

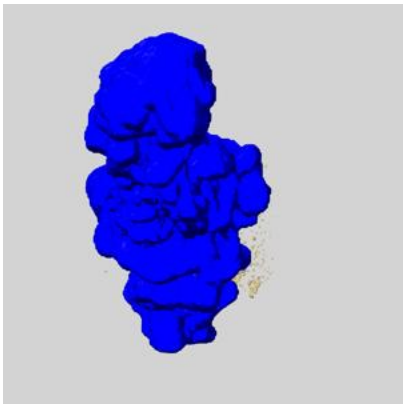
6.6 Mask visualisation

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

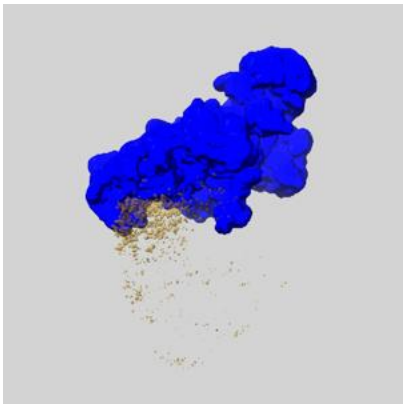
A mask typically either:

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

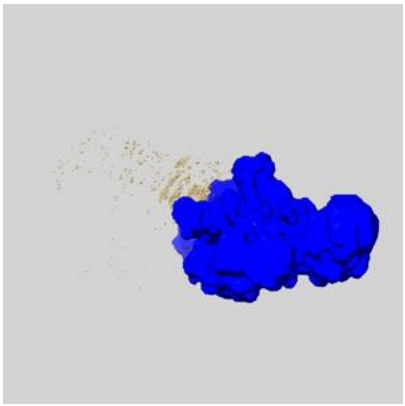
6.6.1 emd_35341_msk_1.map



X



Y

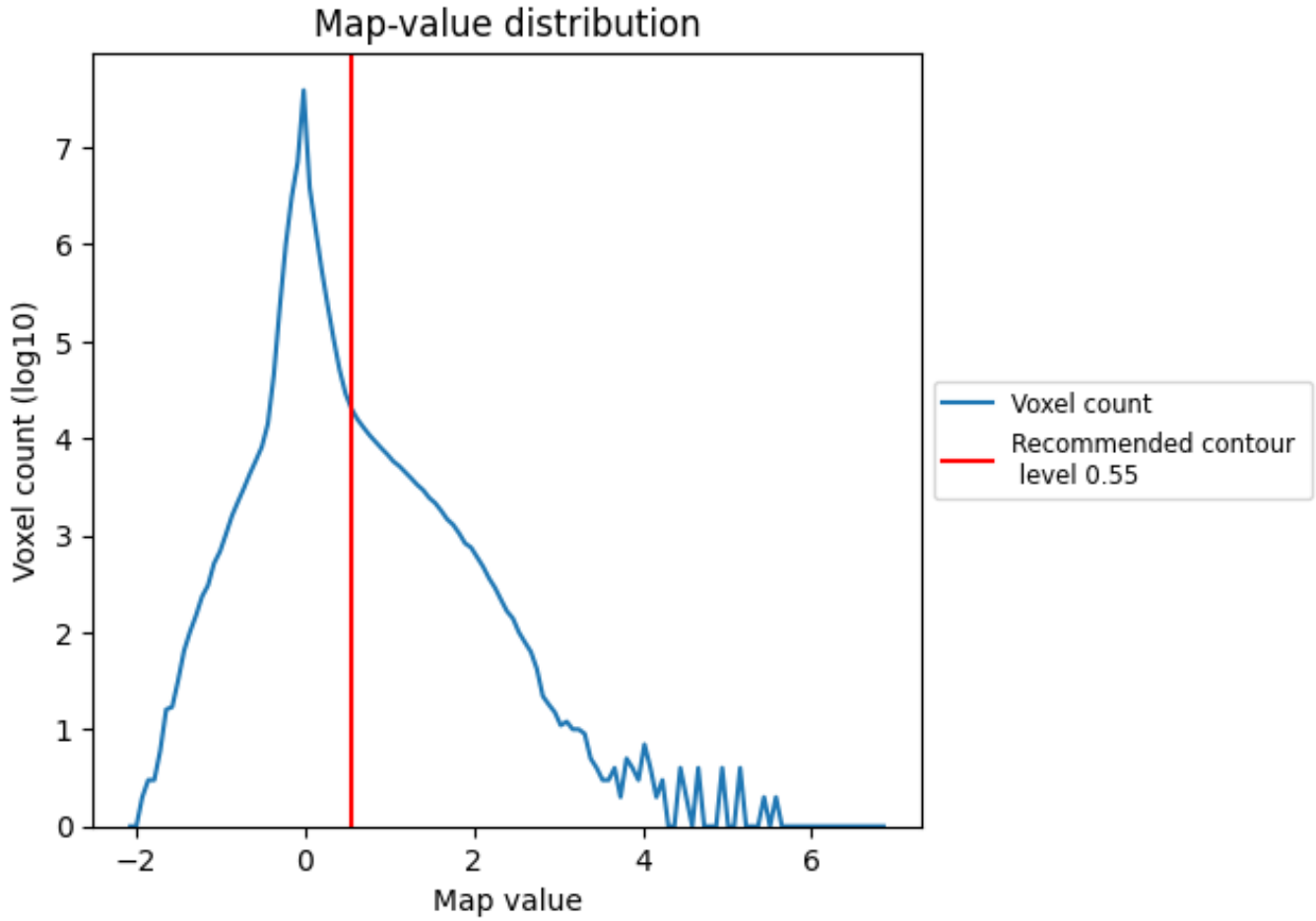


Z

7 Map analysis

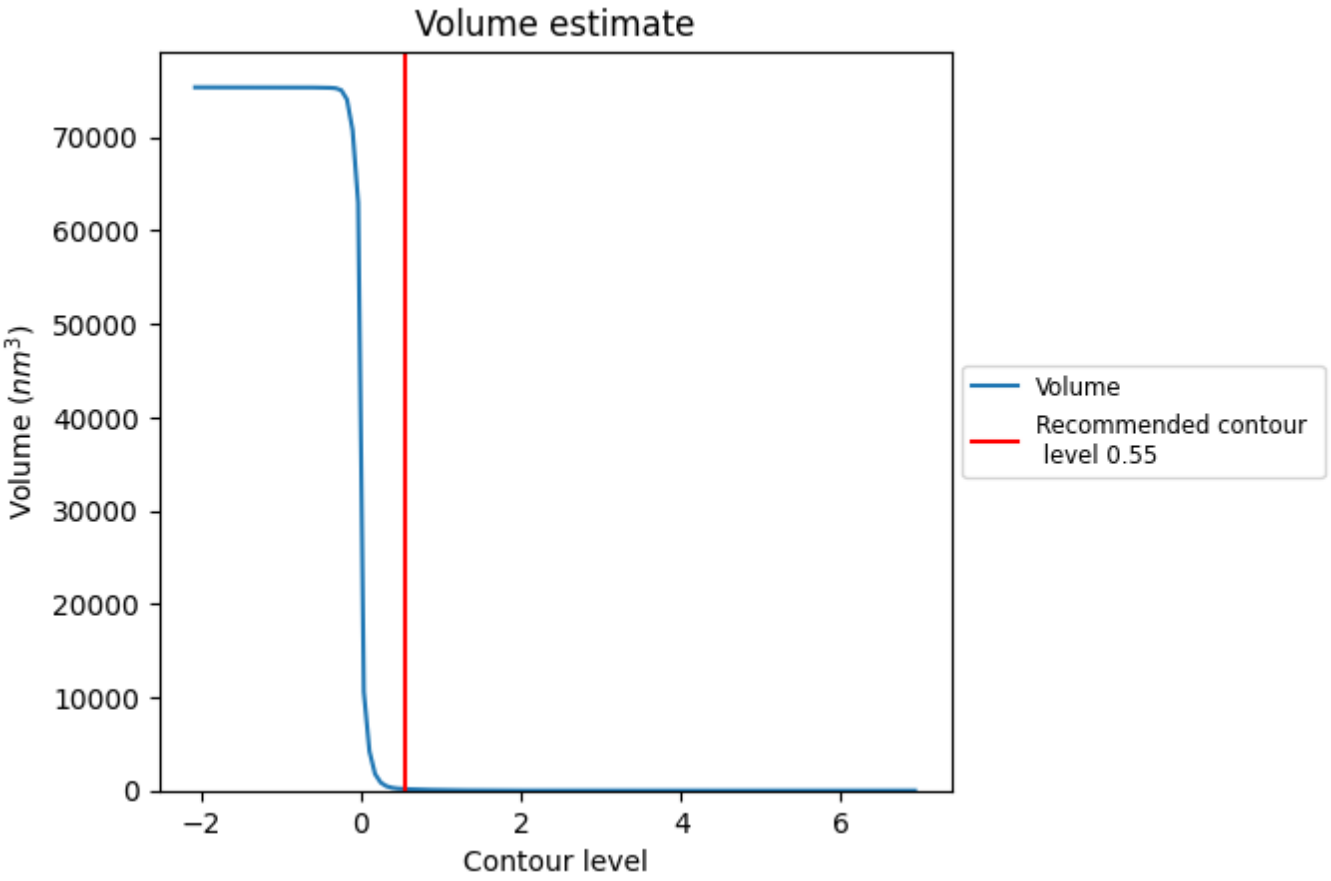
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

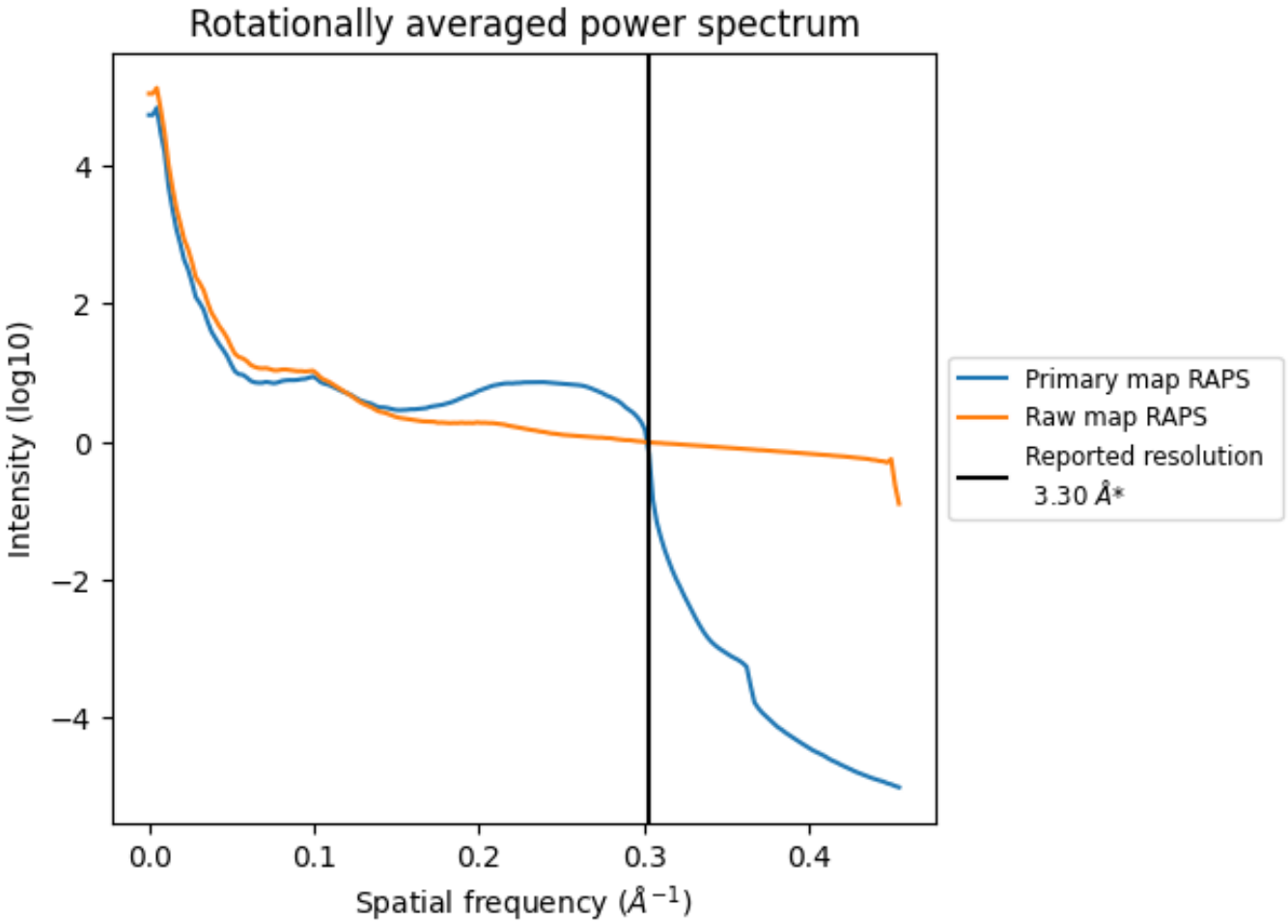
7.2 Volume estimate



The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 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)

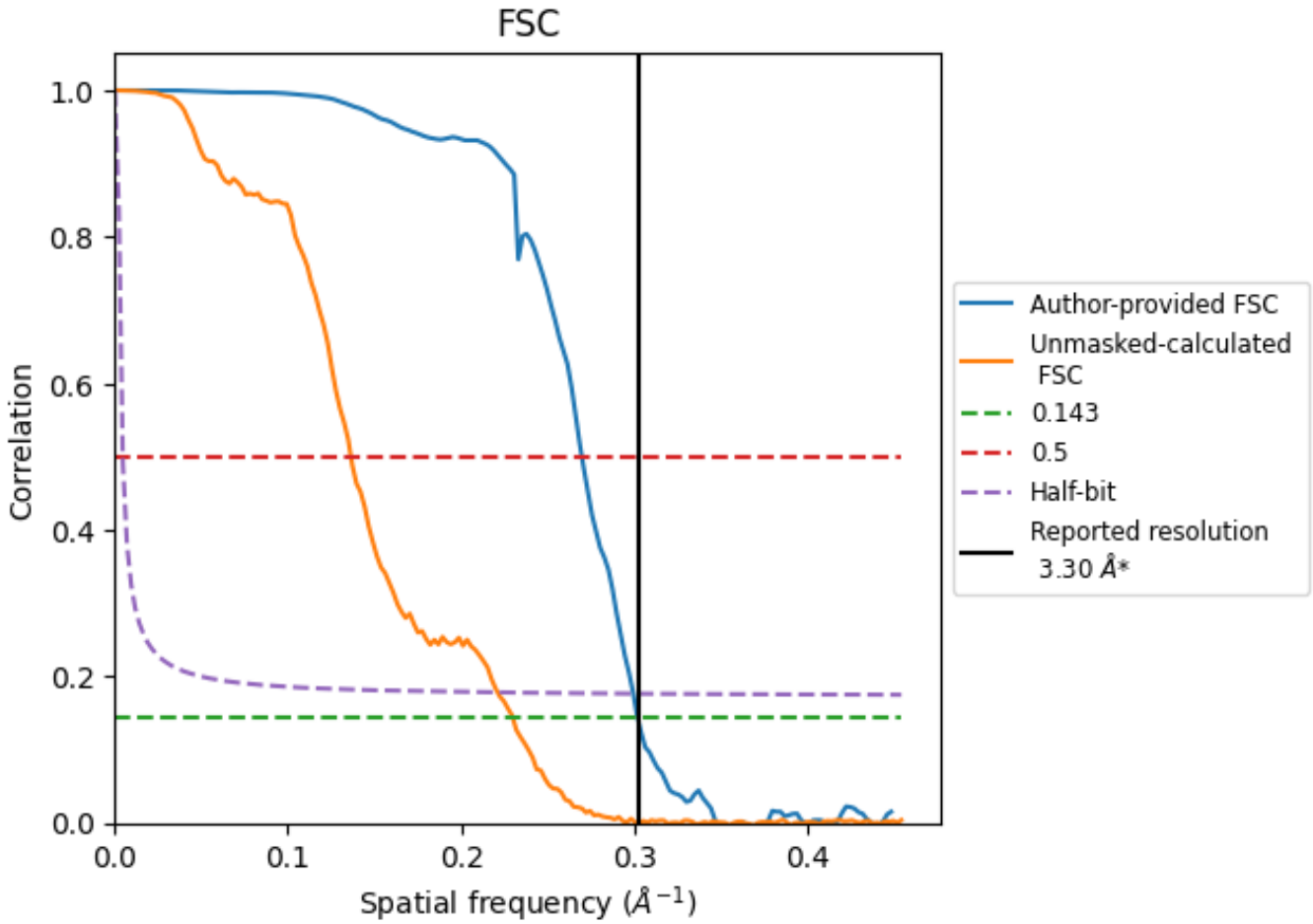


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

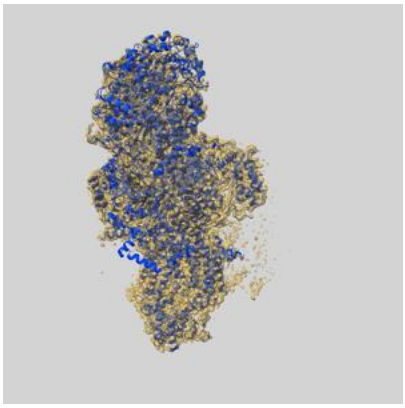
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.71	3.34
Unmasked-calculated*	4.35	7.33	4.52

*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 4.35 differs from the reported value 3.3 by more than 10 %

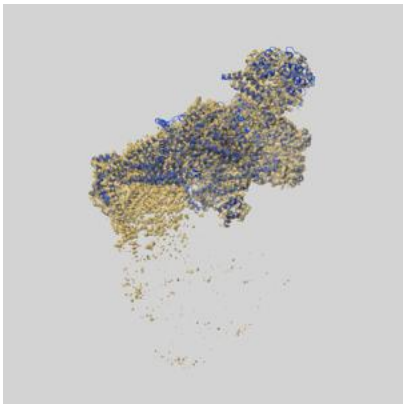
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35341 and PDB model 8IBE. Per-residue inclusion information can be found in section 3 on page 15.

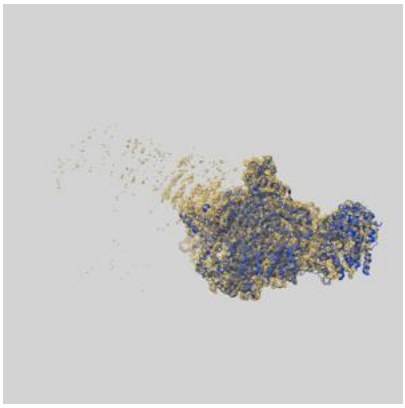
9.1 Map-model overlay



X



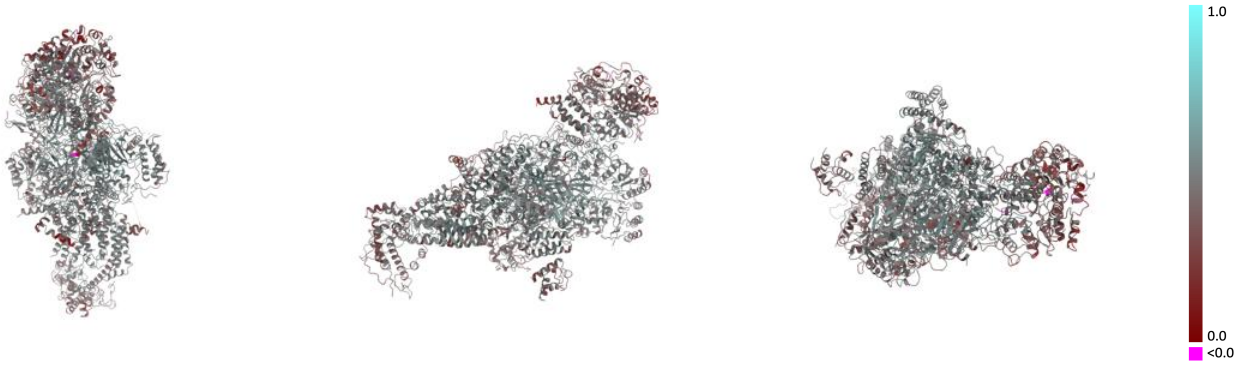
Y



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.

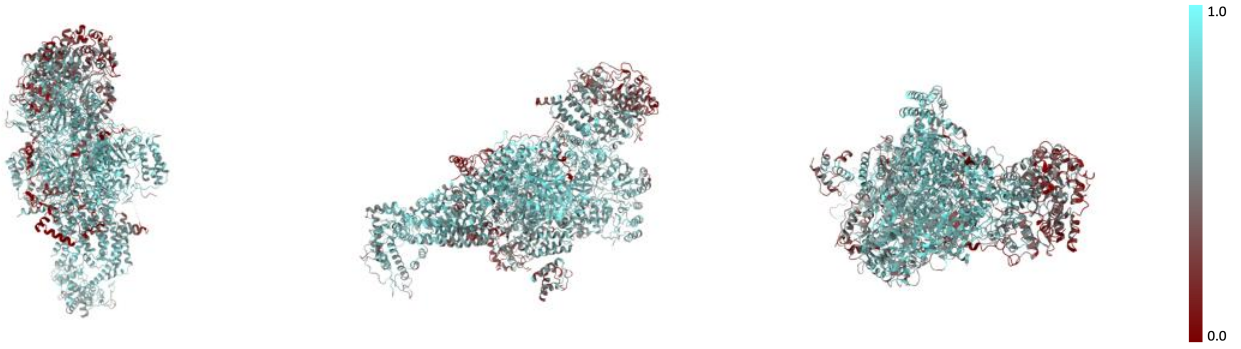
9.2 Q-score mapped to coordinate model



X Y Z

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

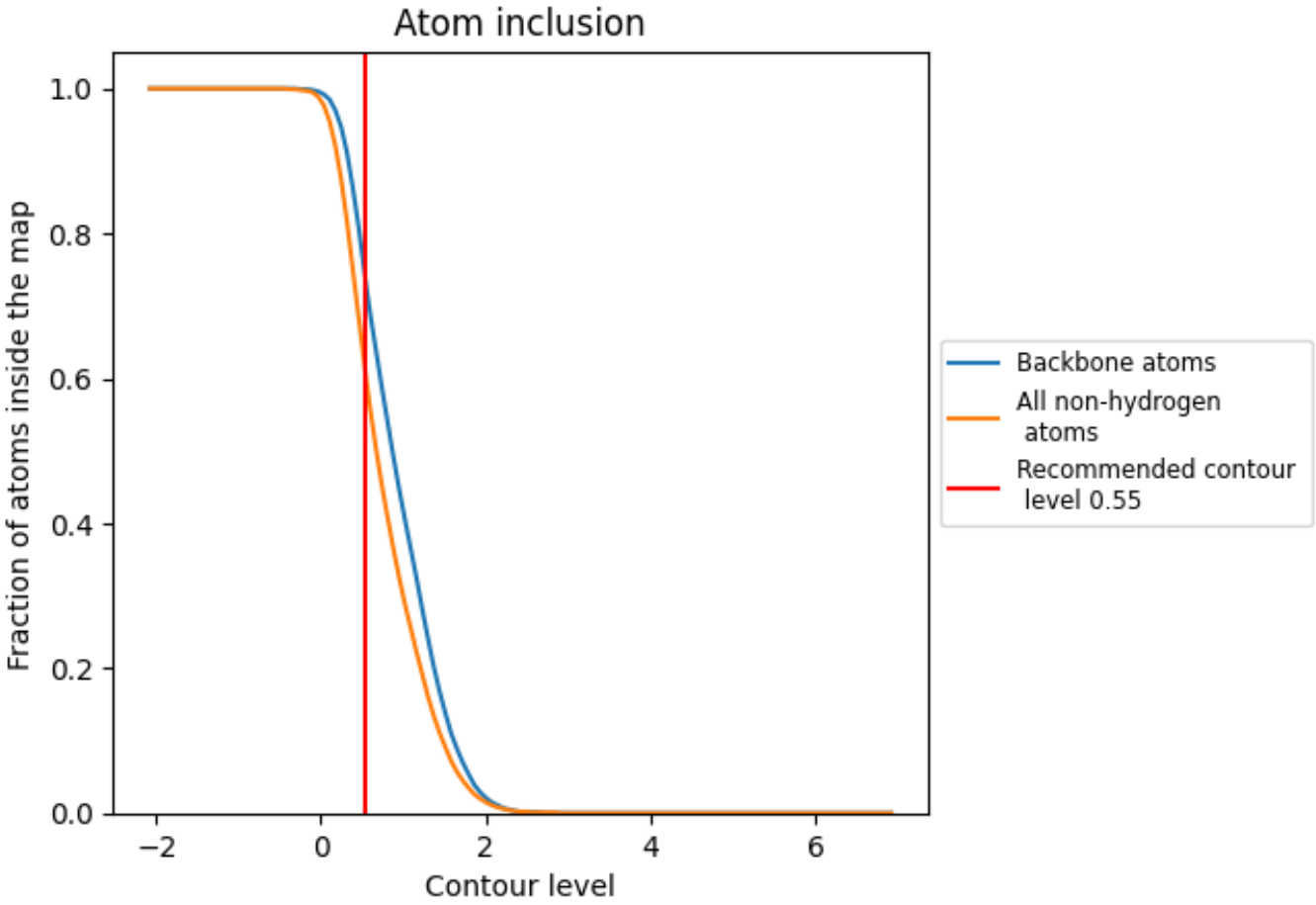
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 60% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.4580
A	0.5020	0.4600
B	0.7080	0.5020
C	0.7680	0.5310
D	0.7670	0.5210
E	0.3900	0.3770
F	0.4690	0.3940
G	0.7010	0.4790
H	0.6690	0.4920
I	0.7660	0.5030
P	0.5050	0.4330
Q	0.6390	0.5060
R	0.2780	0.4370
S	0.6670	0.4530
T	0.4210	0.3820
V	0.7140	0.4910
W	0.6230	0.4830
X	0.6170	0.3960
Z	0.6390	0.4370
a	0.6650	0.4730
b	0.6070	0.4310
q	0.1920	0.3940
r	0.2230	0.3600
s	0.0740	0.2940