Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 04:23 PM JST

PDB ID	:	8IB5
EMDB ID	:	EMD-35332
Title	:	Respiratory complex Peripheral Arm of CI, focus-refined map of type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	3.30 Å(reported)

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

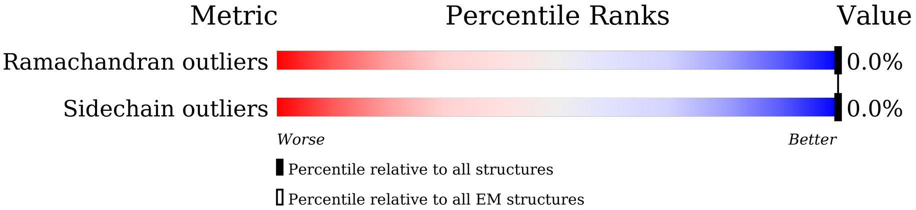
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

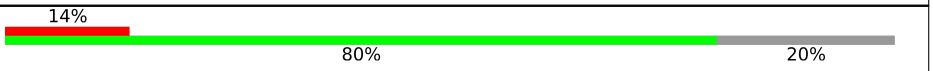
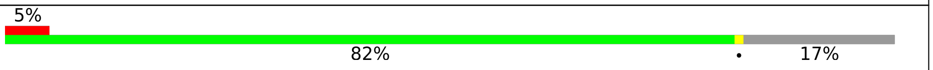
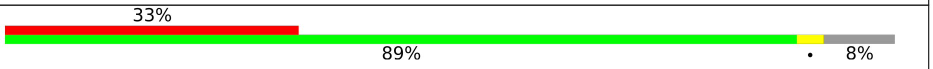
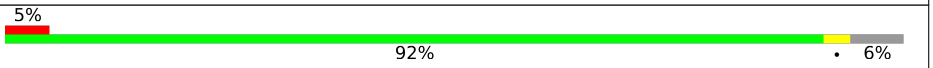
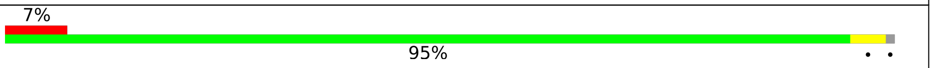
The reported resolution of this entry is 3.30 Å.

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	
2	B	224	
3	C	263	
4	D	463	
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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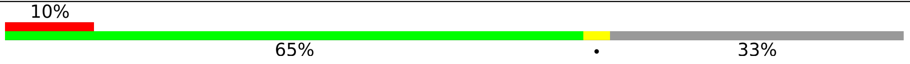
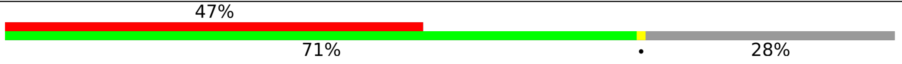
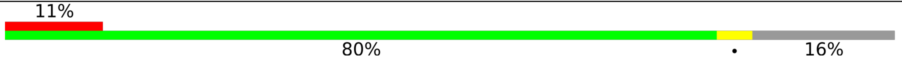
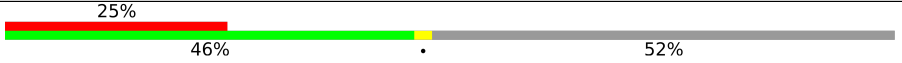
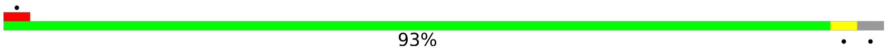
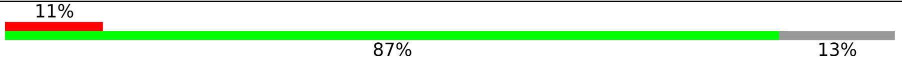
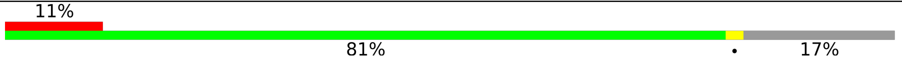
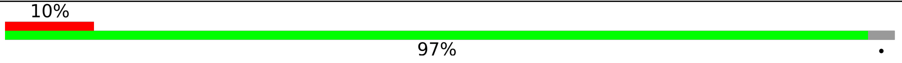
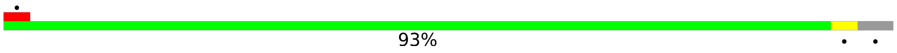
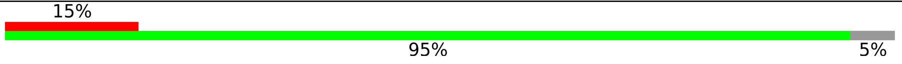
Mol	Chain	Length	Quality of chain
10	P	377	
11	Q	175	
12	R	116	
13	S	99	
14	T	156	
15	V	116	
16	W	131	
17	X	172	
18	Z	144	
19	a	70	
20	b	84	
21	q	145	
22	r	113	
23	s	104	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 33943 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	92	754	523	107	119	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1258	802	227	215	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	386	3095	1974	534	564	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
			Total	C	N	O	S		
6	F	426	3288	2073	588	605	22	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	314	2510	1687	380	421	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	174	1398	880	240	266	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	340	2730	1765	479	479	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	118	957	608	165	180	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	83	660	411	120	126	3	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	q	120	1004	645	178	177	4	0	0

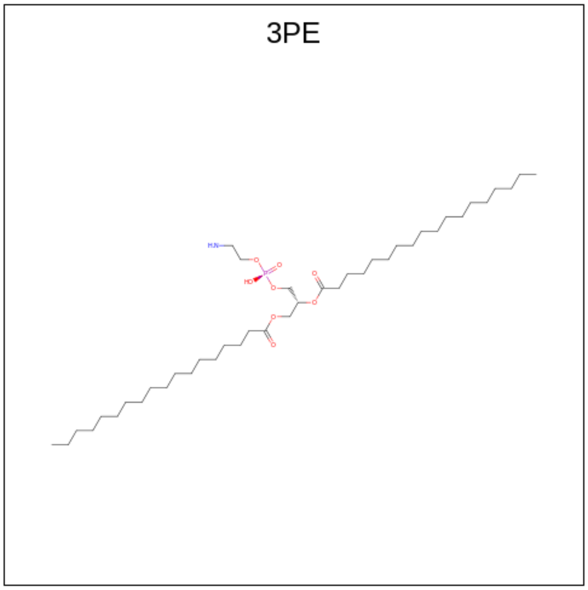
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	r	51	418	266	78	73	1	0	0

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

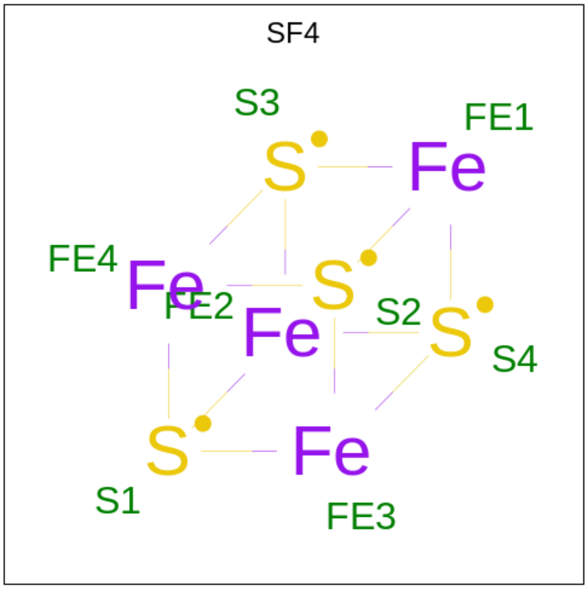
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	s	14	115	75	17	23	0	0

- 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).



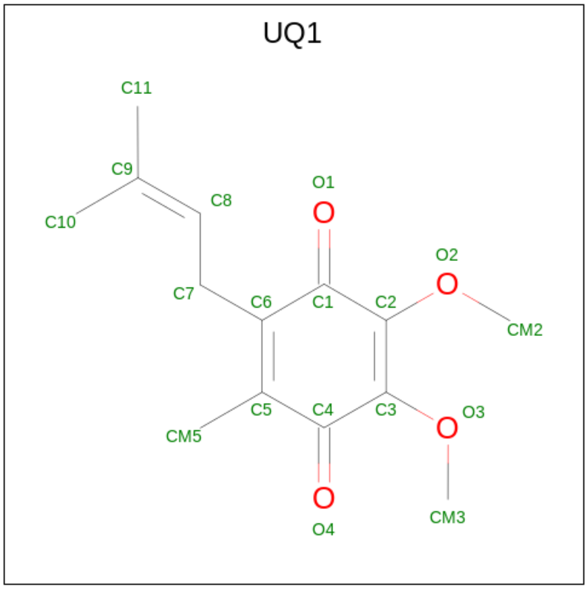
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C N O P 46 36 1 8 1	0
24	I	1	Total C N O P 51 41 1 8 1	0
24	b	1	Total C N O P 46 36 1 8 1	0

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



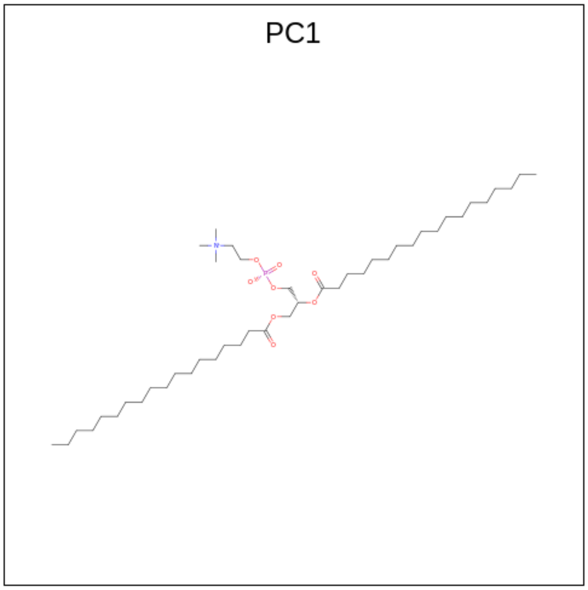
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total Fe S 8 4 4	0
25	F	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0

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



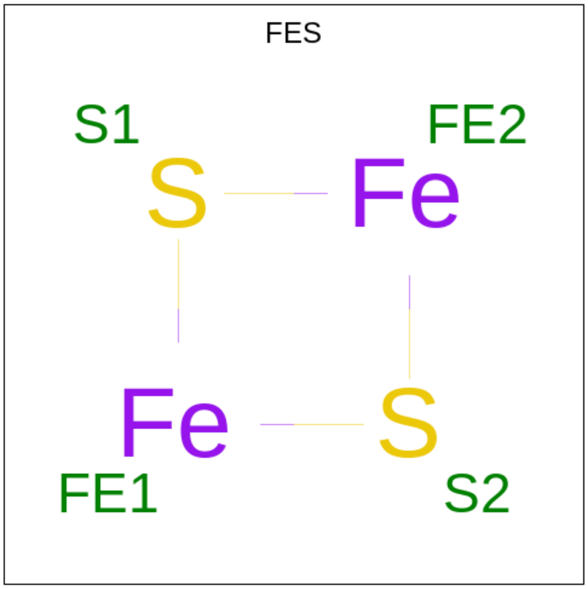
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O 18 14 4	0

- 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).



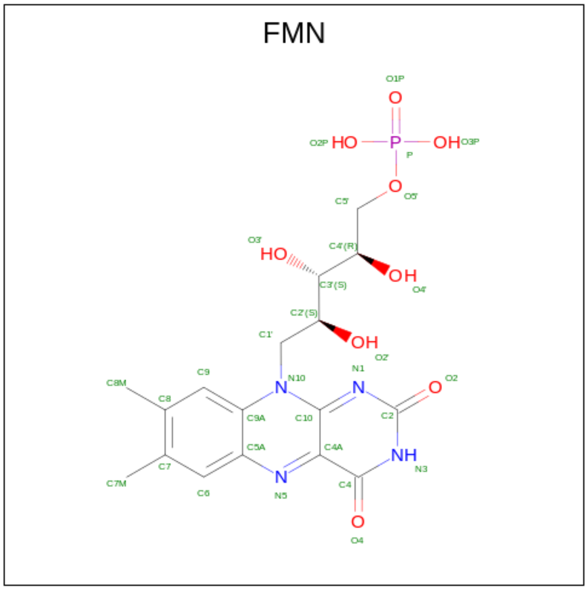
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C N O P 35 25 1 8 1	0
27	H	1	Total C N O P 42 32 1 8 1	0
27	I	1	Total C N O P 47 37 1 8 1	0

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



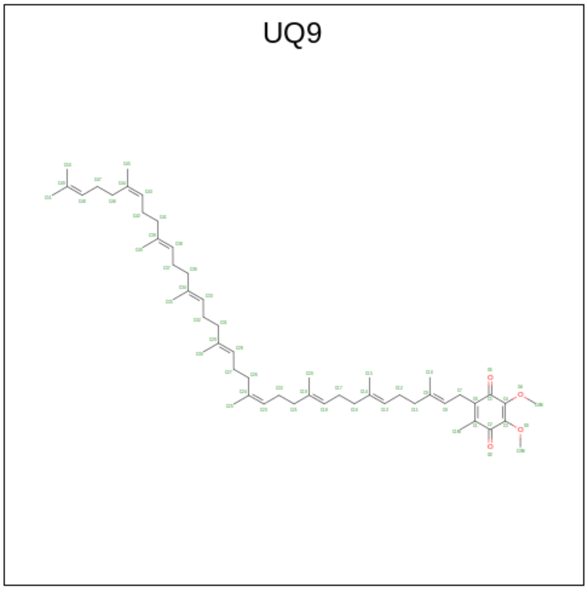
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	E	1	4	2	2	0
28	G	1	4	2	2	0

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



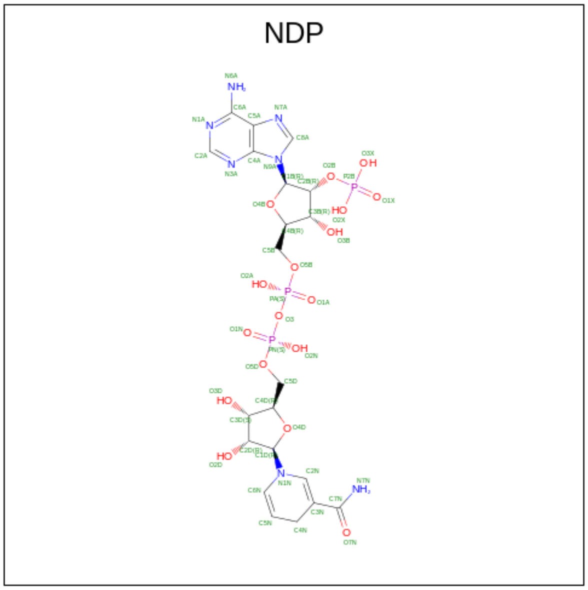
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	F	1	31	17	4	9	1	0

- 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
			Total	C	O	
30	H	1	35	31	4	0

- 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).



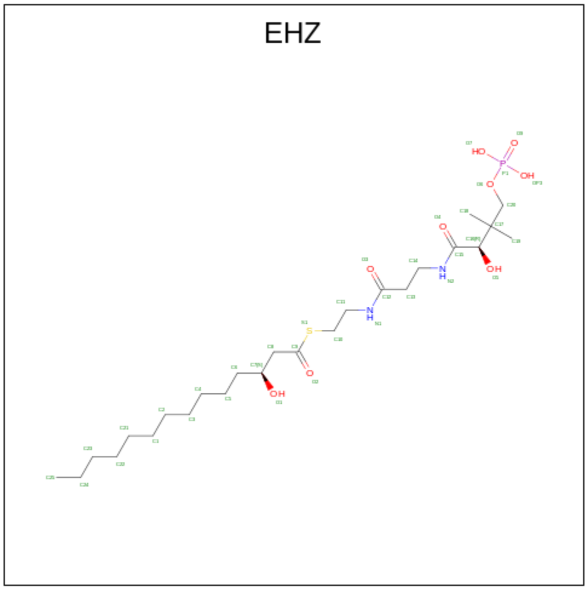
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	P	1	48	21	7	17	3	0

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

Interest" by depositor).

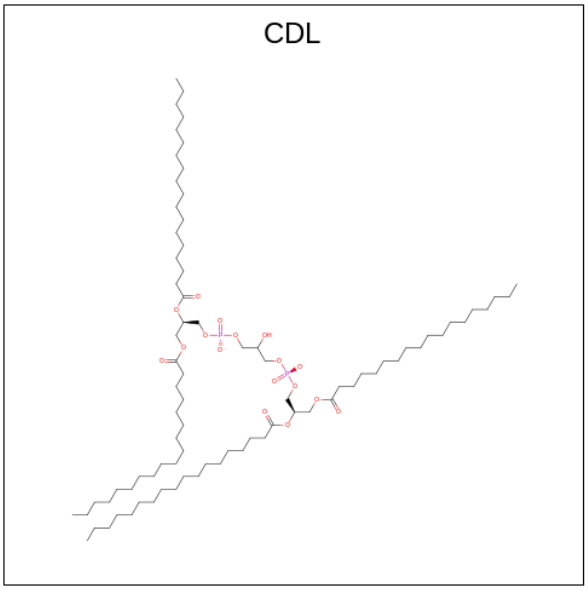
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
32	R	1	1	1	0

- 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
			Total	C	N	O	P	S	
33	W	1	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).

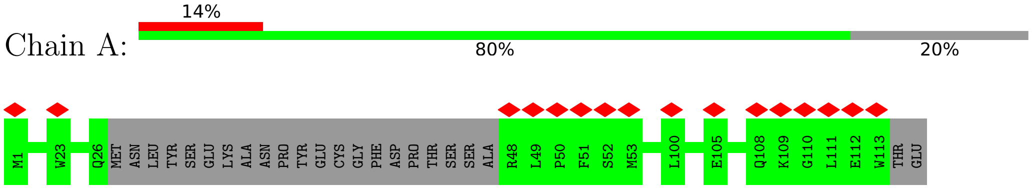


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	a	1	57	38	17	2	0

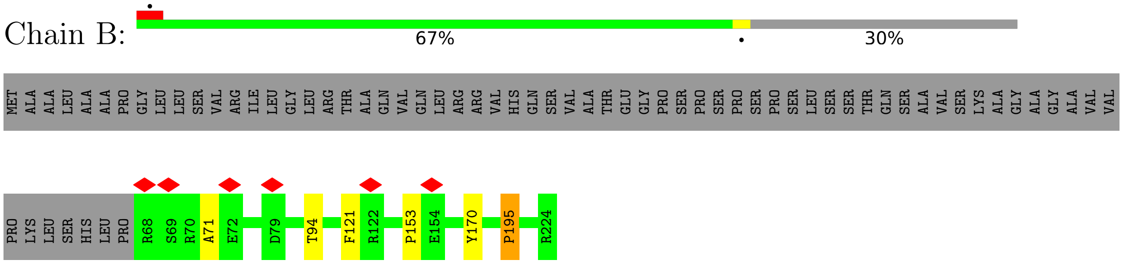
3 Residue-property plots ⓘ

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

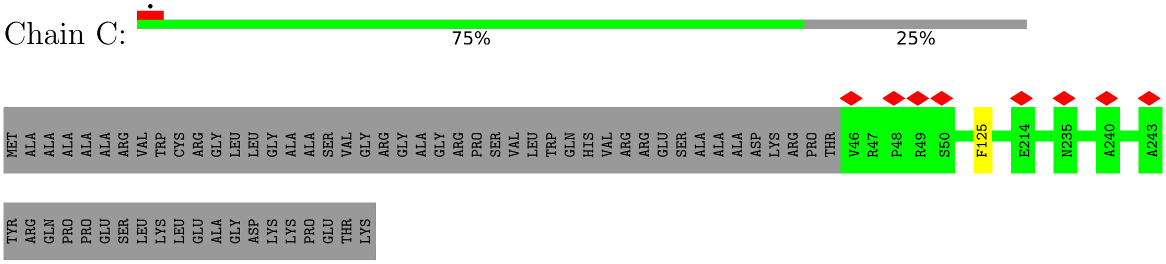
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



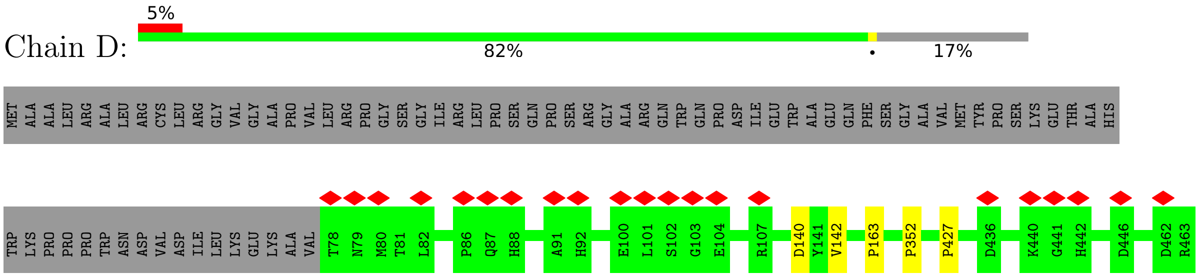
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

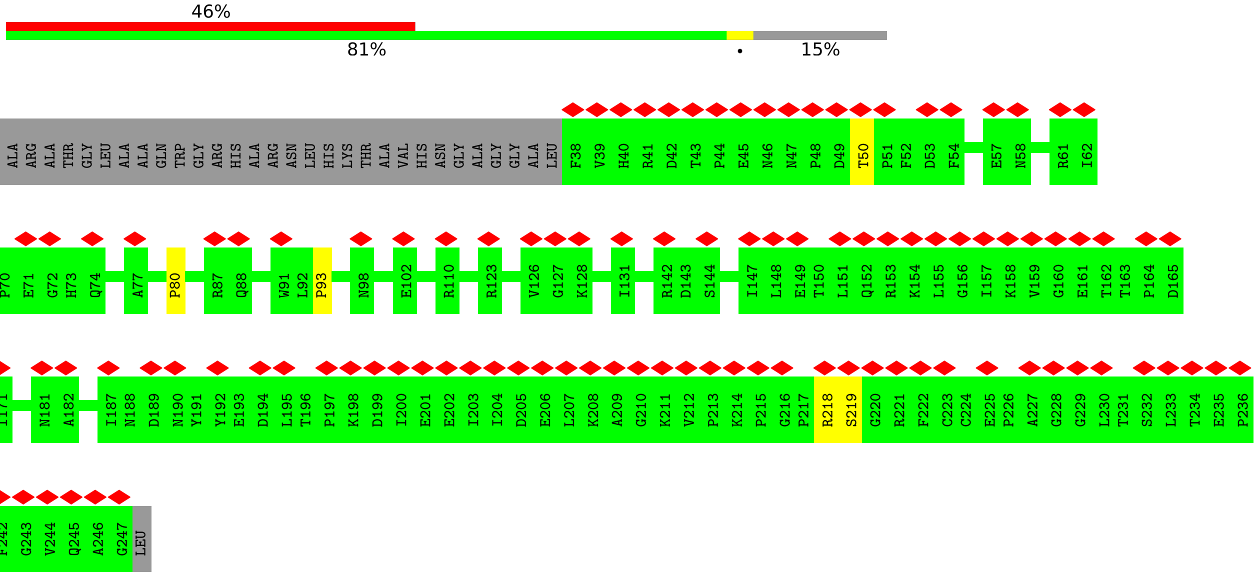


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



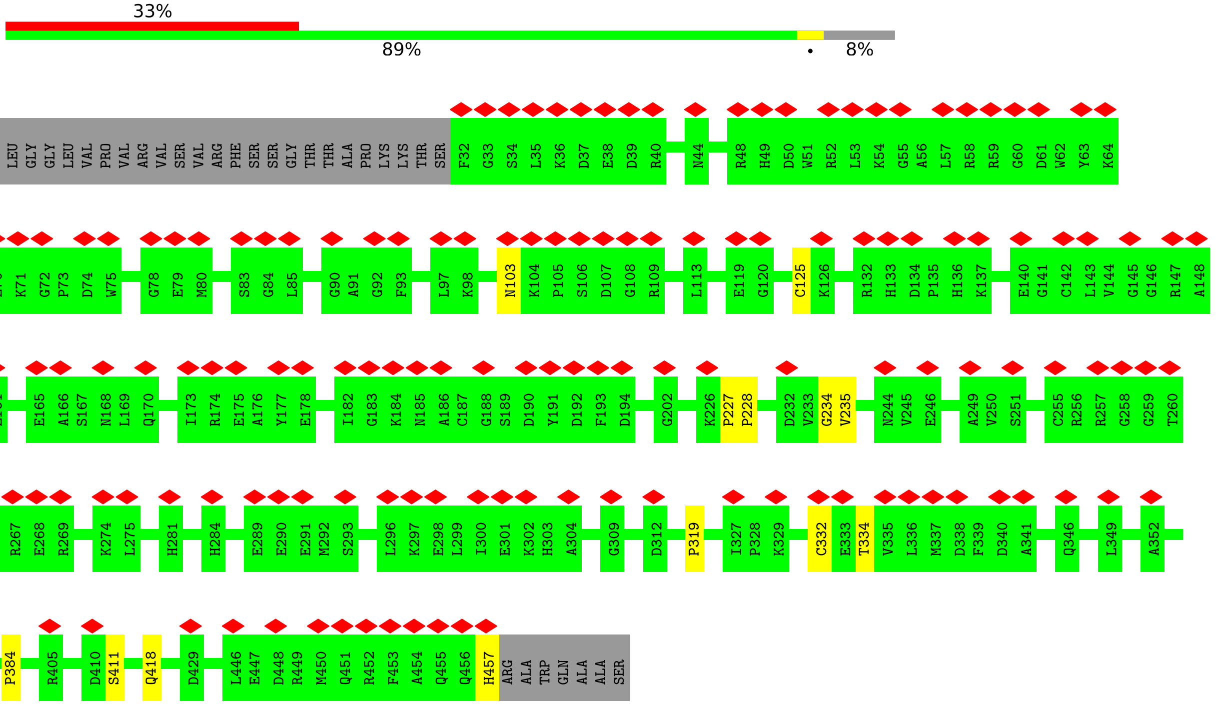
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



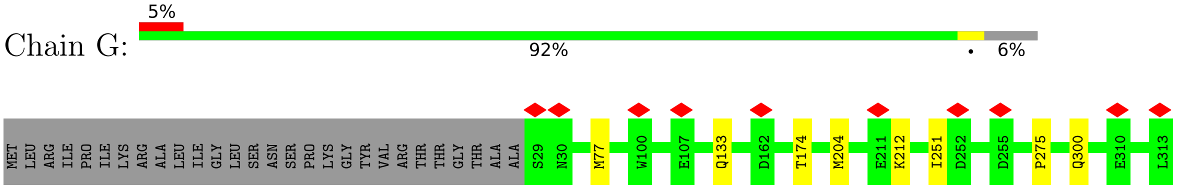
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

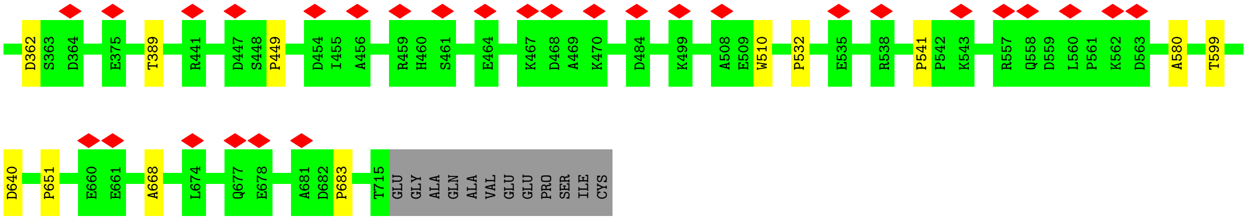
Chain F:



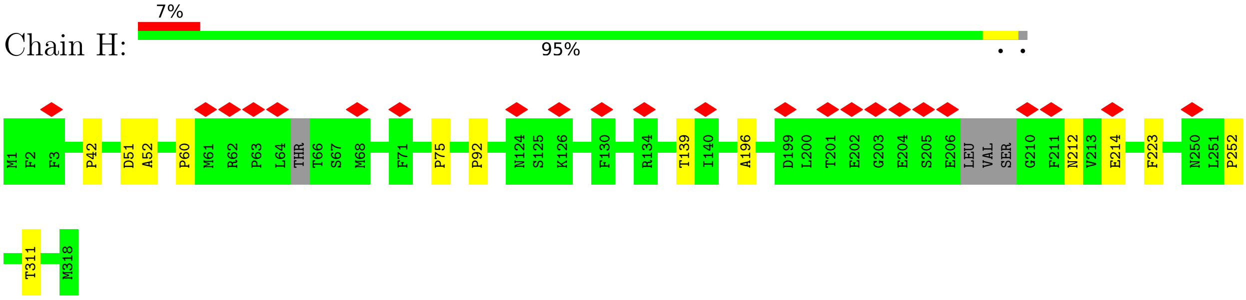
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

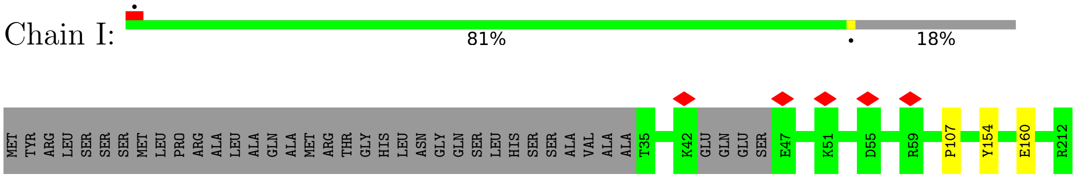




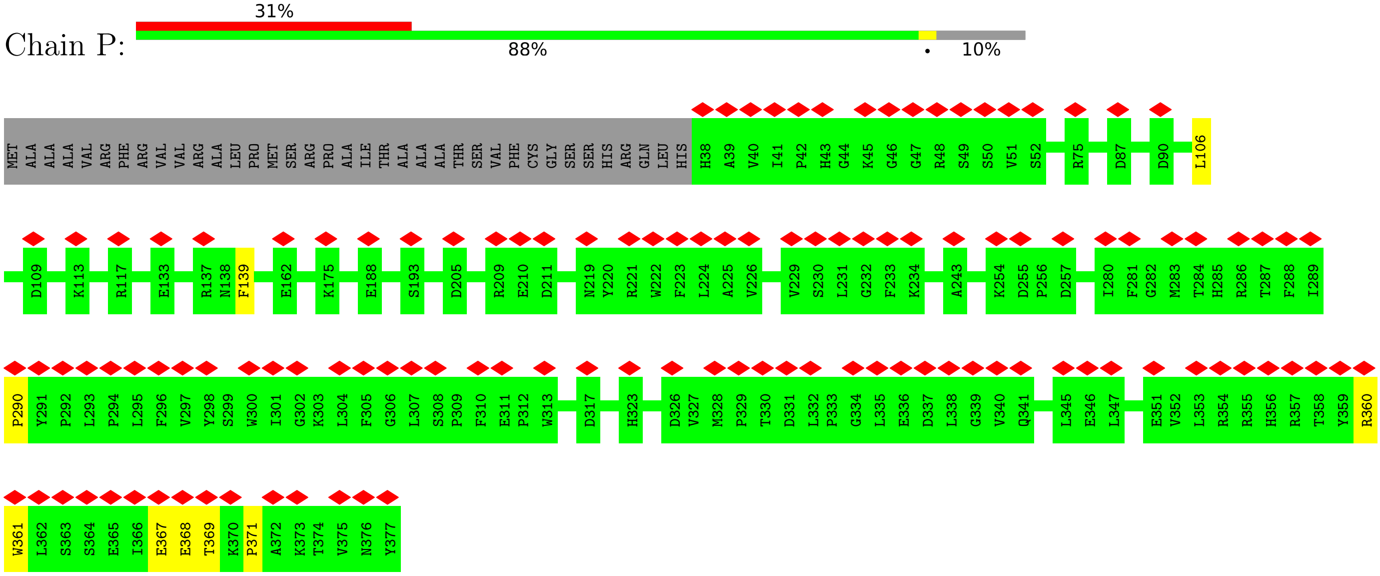
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



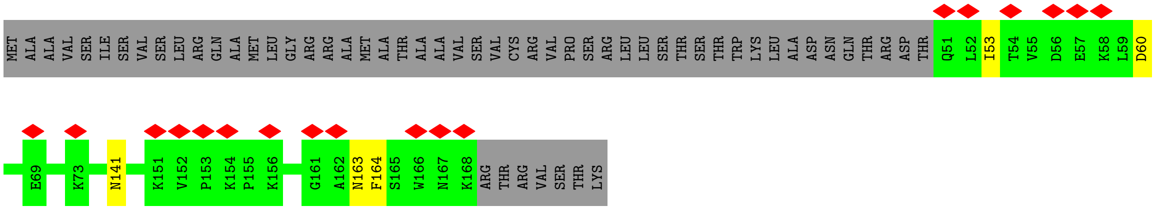
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



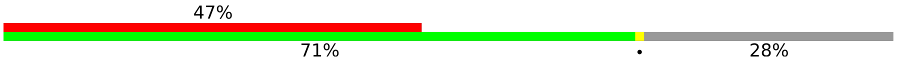
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

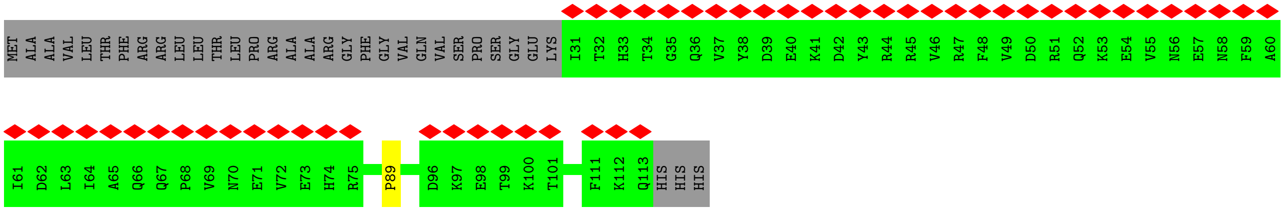


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



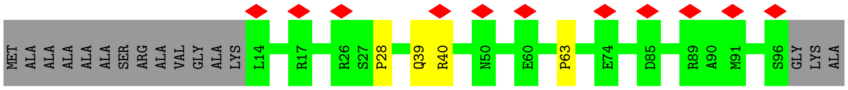
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:




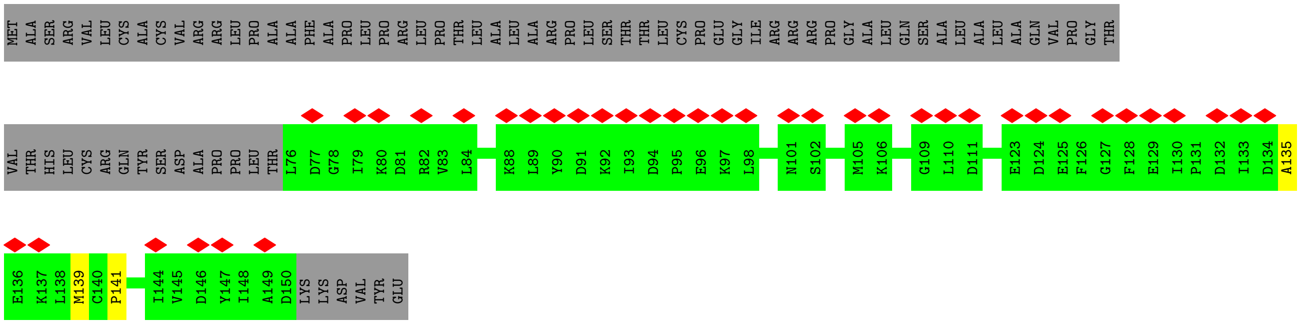
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:

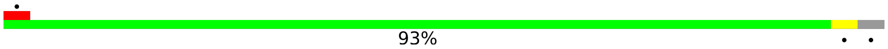



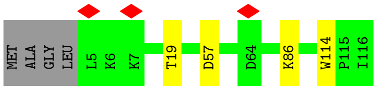
- Molecule 14: Acyl carrier protein, mitochondrial

Chain T:

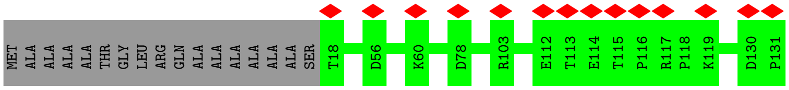
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:


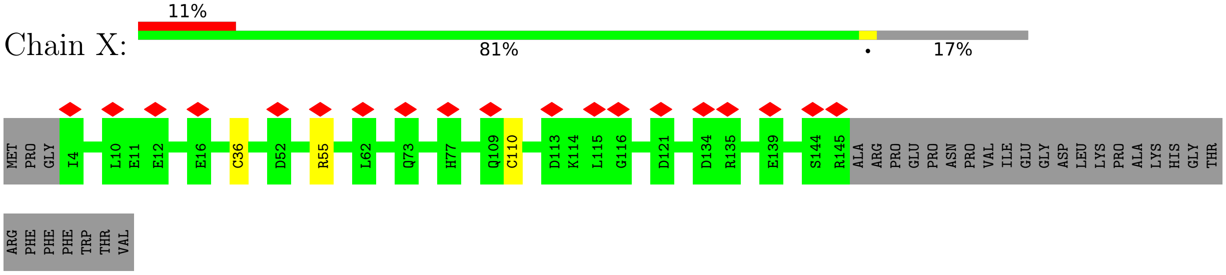


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

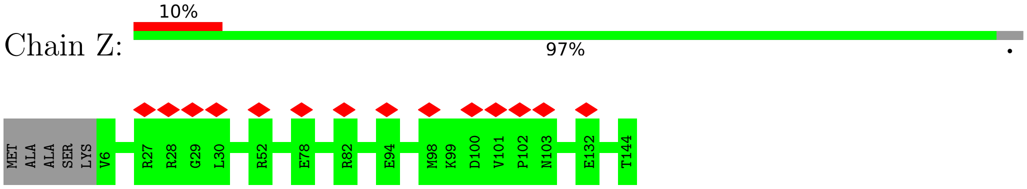
Chain W:

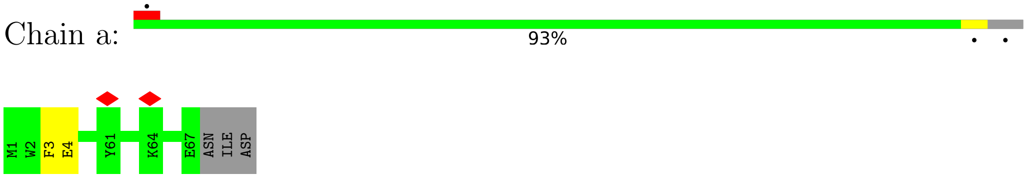
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



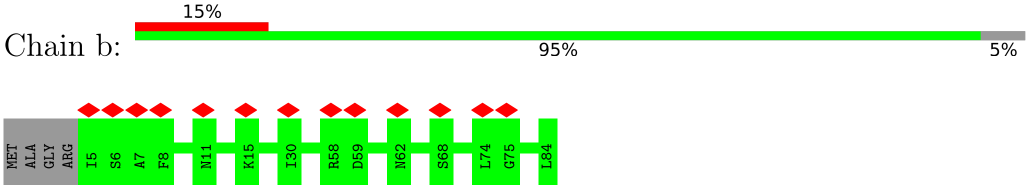
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



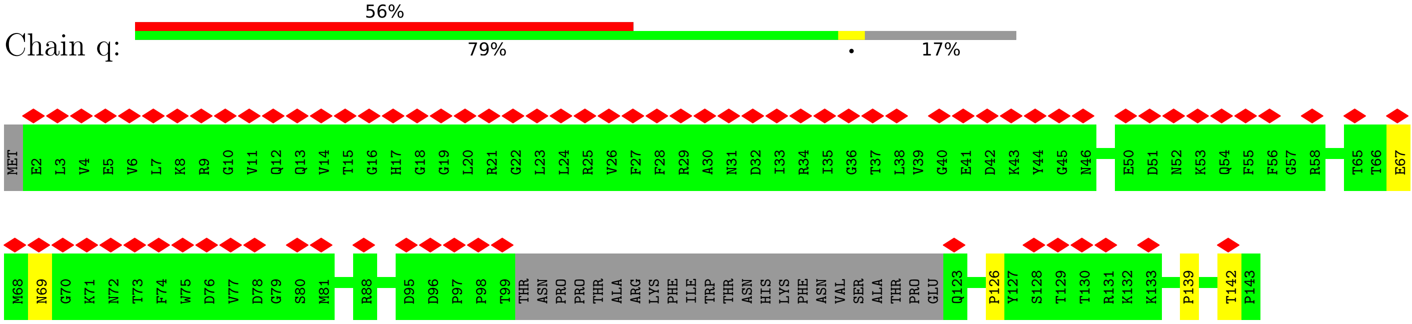
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

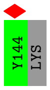


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

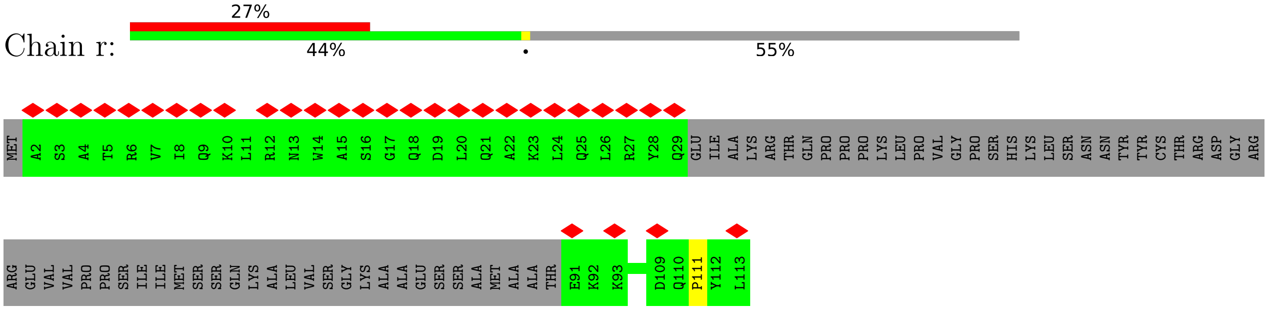


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

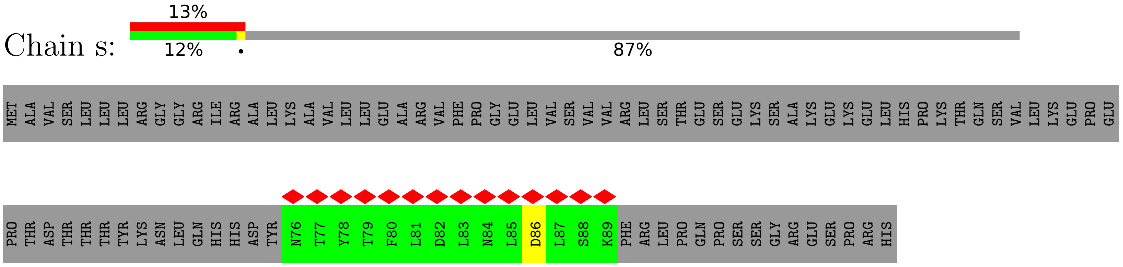




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	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 $(e^-/\text{Å}^2)$	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	6.168	Depositor
Minimum map value	-1.846	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.087	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: UQ9, CDL, FES, FMN, EHZ, NDP, SF4, 3PE, PC1, ZN, UQ1

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	0.54	0/774	0.79	0/1056
2	B	0.63	0/1289	0.94	5/1744 (0.3%)
3	C	0.55	0/1687	0.81	1/2297 (0.0%)
4	D	0.64	2/3169 (0.1%)	0.85	6/4286 (0.1%)
5	E	0.56	2/1675 (0.1%)	0.83	6/2282 (0.3%)
6	F	0.65	5/3363 (0.1%)	0.89	8/4543 (0.2%)
7	G	0.65	5/5374 (0.1%)	0.99	19/7281 (0.3%)
8	H	0.68	3/2585 (0.1%)	0.90	9/3529 (0.3%)
9	I	0.63	1/1427 (0.1%)	0.89	2/1927 (0.1%)
10	P	0.61	2/2804 (0.1%)	0.82	9/3802 (0.2%)
11	Q	0.58	1/980 (0.1%)	0.80	4/1324 (0.3%)
12	R	0.72	1/671 (0.1%)	0.74	1/903 (0.1%)
13	S	0.83	2/678 (0.3%)	1.08	5/915 (0.5%)
14	T	0.75	1/613 (0.2%)	0.90	4/826 (0.5%)
15	V	0.56	0/937	0.85	4/1270 (0.3%)
16	W	0.53	0/993	0.72	0/1335
17	X	0.54	0/1191	0.89	5/1605 (0.3%)
18	Z	0.50	0/1183	0.62	0/1597
19	a	0.54	0/561	0.86	2/755 (0.3%)
20	b	0.47	0/651	0.53	0/895
21	q	0.77	2/1037 (0.2%)	0.97	5/1408 (0.4%)
22	r	0.73	1/426 (0.2%)	0.98	1/573 (0.2%)
23	s	0.64	0/116	1.01	1/157 (0.6%)
All	All	0.63	28/34184 (0.1%)	0.88	97/46310 (0.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	89	PRO	N-CD	-15.12	1.26	1.47
21	q	139	PRO	N-CD	-13.51	1.28	1.47
10	P	371	PRO	N-CD	12.85	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	532	PRO	N-CD	-12.59	1.30	1.47
13	S	28	PRO	N-CD	-11.98	1.31	1.47
14	T	141	PRO	N-CD	11.68	1.64	1.47
8	H	42	PRO	N-CD	10.80	1.62	1.47
6	F	227	PRO	N-CD	9.98	1.61	1.47
10	P	290	PRO	N-CD	9.55	1.61	1.47
7	G	275	PRO	N-CD	-9.55	1.34	1.47
8	H	75	PRO	N-CD	9.20	1.60	1.47
6	F	319	PRO	N-CD	9.04	1.60	1.47
4	D	163	PRO	N-CD	-8.51	1.35	1.47
9	I	107	PRO	N-CD	8.48	1.59	1.47
4	D	352	PRO	N-CD	-7.97	1.36	1.47
13	S	63	PRO	N-CD	-7.96	1.36	1.47
22	r	111	PRO	N-CD	-7.51	1.37	1.47
7	G	541	PRO	N-CD	-6.82	1.38	1.47
6	F	234	GLY	CA-C	-6.76	1.41	1.51
7	G	449	PRO	N-CD	6.75	1.57	1.47
6	F	384	PRO	N-CD	-6.19	1.39	1.47
5	E	93	PRO	N-CD	-5.99	1.39	1.47
6	F	235	VAL	N-CA	-5.84	1.34	1.46
8	H	60	PRO	N-CD	5.70	1.55	1.47
5	E	80	PRO	N-CD	5.62	1.55	1.47
7	G	683	PRO	N-CD	-5.50	1.40	1.47
21	q	126	PRO	N-CD	5.32	1.55	1.47
11	Q	53	ILE	C-O	5.31	1.33	1.23

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	3	PHE	CB-CA-C	-10.42	89.56	110.40
21	q	139	PRO	CA-N-CD	9.58	125.12	111.70
4	D	142	VAL	N-CA-CB	9.50	132.39	111.50
5	E	219	SER	N-CA-CB	9.05	124.07	110.50
6	F	334	THR	N-CA-CB	8.92	127.25	110.30
7	G	532	PRO	CA-N-CD	8.53	123.64	111.70
7	G	174	THR	N-CA-C	-8.12	89.08	111.00
13	S	28	PRO	CA-N-CD	8.12	123.06	111.70
11	Q	60	ASP	N-CA-C	-7.67	90.30	111.00
6	F	411	SER	N-CA-CB	7.54	121.81	110.50
17	X	55	ARG	N-CA-CB	-7.42	97.24	110.60
7	G	204	MET	N-CA-C	-7.25	91.43	111.00
2	B	121	PHE	CB-CA-C	7.14	124.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	371	PRO	N-CA-CB	7.11	111.84	103.30
6	F	332	CYS	N-CA-C	7.07	130.09	111.00
17	X	55	ARG	N-CA-C	7.06	130.06	111.00
8	H	311	THR	N-CA-CB	6.95	123.50	110.30
10	P	369	THR	N-CA-CB	6.95	123.50	110.30
4	D	142	VAL	N-CA-C	-6.84	92.53	111.00
7	G	275	PRO	CA-N-CD	6.62	120.97	111.70
7	G	300	GLN	N-CA-CB	6.61	122.50	110.60
10	P	106	LEU	N-CA-C	6.59	128.79	111.00
17	X	36	CYS	CB-CA-C	-6.58	97.25	110.40
5	E	64	ALA	N-CA-CB	6.57	119.29	110.10
5	E	166	LYS	CB-CA-C	6.54	123.47	110.40
8	H	214	GLU	N-CA-CB	-6.51	98.89	110.60
6	F	125	CYS	N-CA-C	-6.50	93.46	111.00
10	P	360	ARG	N-CA-CB	-6.44	99.02	110.60
21	q	139	PRO	N-CA-CB	-6.39	95.57	102.60
8	H	52	ALA	N-CA-CB	6.38	119.03	110.10
4	D	427	PRO	N-CA-C	-6.34	95.62	112.10
9	I	154	TYR	N-CA-CB	-6.34	99.19	110.60
10	P	371	PRO	CA-N-CD	-6.33	102.64	111.50
8	H	196	ALA	N-CA-C	6.29	127.99	111.00
2	B	71	ALA	N-CA-CB	-6.25	101.34	110.10
23	s	86	ASP	N-CA-CB	6.24	121.84	110.60
10	P	139	PHE	N-CA-CB	6.17	121.72	110.60
4	D	140	ASP	CB-CA-C	-6.17	98.06	110.40
17	X	36	CYS	CA-CB-SG	6.14	125.06	114.00
14	T	141	PRO	N-CA-CB	6.13	110.66	103.30
14	T	141	PRO	CA-N-CD	-6.12	102.92	111.50
17	X	110	CYS	CA-CB-SG	6.11	125.00	114.00
7	G	212	LYS	N-CA-C	-6.06	94.63	111.00
7	G	133	GLN	N-CA-CB	6.05	121.48	110.60
21	q	69	ASN	N-CA-CB	5.99	121.39	110.60
7	G	389	THR	N-CA-CB	5.87	121.46	110.30
5	E	50	THR	N-CA-CB	5.87	121.45	110.30
7	G	251	ILE	N-CA-C	5.86	126.83	111.00
6	F	103	ASN	N-CA-CB	5.82	121.08	110.60
13	S	63	PRO	CA-N-CD	5.80	119.82	111.70
14	T	135	ALA	N-CA-CB	5.79	118.21	110.10
5	E	68	ASN	N-CA-CB	5.79	121.02	110.60
7	G	510	TRP	N-CA-CB	5.74	120.93	110.60
8	H	223	PHE	CB-CA-C	-5.68	99.05	110.40
11	Q	141	ASN	N-CA-CB	5.63	120.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	599	THR	N-CA-C	5.63	126.19	111.00
15	V	57	ASP	N-CA-CB	5.61	120.70	110.60
7	G	580	ALA	N-CA-CB	5.57	117.90	110.10
3	C	125	PHE	N-CA-CB	-5.55	100.61	110.60
11	Q	163	ASN	CB-CA-C	-5.55	99.30	110.40
8	H	252	PRO	CA-N-CD	5.52	119.43	111.70
8	H	212	ASN	N-CA-CB	5.50	120.50	110.60
15	V	19	THR	N-CA-CB	5.48	120.72	110.30
9	I	160	GLU	N-CA-CB	-5.46	100.77	110.60
7	G	389	THR	N-CA-C	-5.46	96.26	111.00
10	P	367	GLU	CB-CA-C	-5.45	99.51	110.40
22	r	111	PRO	CA-N-CD	5.42	119.29	111.70
7	G	651	PRO	CB-CA-C	-5.41	98.48	112.00
21	q	67	GLU	CB-CA-C	-5.40	99.60	110.40
2	B	195	PRO	N-CA-C	-5.39	98.10	112.10
6	F	457	HIS	N-CA-CB	-5.38	100.91	110.60
4	D	140	ASP	N-CA-C	-5.36	96.54	111.00
13	S	28	PRO	N-CA-CB	-5.35	96.71	102.60
13	S	39	GLN	N-CA-C	5.35	125.45	111.00
7	G	362	ASP	N-CA-C	5.35	125.44	111.00
15	V	114	TRP	N-CA-CB	5.35	120.22	110.60
8	H	139	THR	N-CA-CB	5.34	120.44	110.30
6	F	418	GLN	N-CA-CB	5.32	120.18	110.60
5	E	218	ARG	CB-CA-C	-5.31	99.78	110.40
13	S	40	ARG	N-CA-CB	-5.28	101.09	110.60
7	G	640	ASP	N-CA-CB	5.21	119.98	110.60
2	B	153	PRO	CB-CA-C	-5.21	98.98	112.00
8	H	51	ASP	CB-CA-C	-5.20	100.01	110.40
12	R	89	PRO	CA-N-CD	5.18	118.95	111.70
2	B	94	THR	CA-CB-CG2	-5.16	105.18	112.40
10	P	361	TRP	N-CA-CB	5.12	119.82	110.60
10	P	368	GLU	N-CA-CB	5.12	119.81	110.60
19	a	4	GLU	N-CA-C	5.11	124.81	111.00
11	Q	164	PHE	N-CA-CB	5.10	119.78	110.60
6	F	228	PRO	N-CA-C	-5.09	98.88	112.10
4	D	352	PRO	CA-N-CD	5.07	118.80	111.70
7	G	77	MET	N-CA-C	-5.07	97.31	111.00
7	G	668	ALA	N-CA-CB	5.05	117.17	110.10
21	q	142	THR	N-CA-CB	5.04	119.87	110.30
15	V	86	LYS	N-CA-CB	5.03	119.66	110.60
7	G	532	PRO	N-CA-CB	-5.01	97.08	102.60
14	T	139	MET	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	22	53
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	384/463 (83%)	357 (93%)	27 (7%)	0	100	100
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	37	66
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	317 (94%)	21 (6%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	77 (95%)	4 (5%)	0	100	100
13	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
20	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
21	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	12/104 (12%)	12 (100%)	0	0	100	100
All	All	4124/5036 (82%)	3873 (94%)	249 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	79	87
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	333/395 (84%)	333 (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	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	297 (100%)	0	100	100
11	Q	105/153 (69%)	105 (100%)	0	100	100
12	R	70/96 (73%)	70 (100%)	0	100	100
13	S	74/80 (92%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	69/135 (51%)	69 (100%)	0	100	100
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	120 (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	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	14/95 (15%)	14 (100%)	0	100	100
All	All	3622/4292 (84%)	3621 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
2	B	170	TYR

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

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	233	HIS

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Mol	Chain	Res	Type
4	D	265	ASN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	277	ASN
6	F	346	GLN
6	F	441	HIS
7	G	59	GLN
7	G	74	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	406	ASN
7	G	444	HIS
7	G	495	ASN
7	G	514	ASN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	169	GLN
8	H	171	HIS
8	H	292	ASN
10	P	71	ASN
10	P	79	GLN
10	P	169	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	341	GLN
11	Q	51	GLN
11	Q	88	GLN

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Mol	Chain	Res	Type
13	S	25	GLN
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
19	a	58	ASN
20	b	69	HIS
20	b	83	ASN
21	q	13	GLN
21	q	31	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN
23	s	84	ASN

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 ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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
34	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
25	SF4	F	502	6	0,12,12	-	-	-		
30	UQ9	H	401	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
25	SF4	I	304	9	0,12,12	-	-	-		
24	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
27	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
25	SF4	G	802	7	0,12,12	-	-	-		
27	PC1	H	402	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)
31	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.21	4 (7%)
27	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
25	SF4	G	801	7	0,12,12	-	-	-		
24	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
33	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
26	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
25	SF4	B	301	2	0,12,12	-	-	-		
25	SF4	I	303	9	0,12,12	-	-	-		
28	FES	G	803	7	0,4,4	-	-	-		
28	FES	E	301	5	0,4,4	-	-	-		
24	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
29	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)

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
34	CDL	a	101	-	-	14/67/67/110	-
25	SF4	F	502	6	-	-	0/6/5/5
30	UQ9	H	401	-	-	13/30/54/81	0/1/1/1
25	SF4	I	304	9	-	-	0/6/5/5
24	3PE	A	401	-	-	14/49/49/54	-
27	PC1	I	302	-	-	13/50/50/57	-
27	PC1	H	402	-	-	14/45/45/57	-
25	SF4	G	802	7	-	-	0/6/5/5
31	NDP	P	401	-	-	6/30/77/77	0/5/5/5
27	PC1	B	303	-	-	11/38/38/57	-
25	SF4	G	801	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	3PE	I	301	-	-	17/54/54/54	-
33	EHZ	W	201	-	-	22/39/39/45	-
26	UQ1	B	302	-	-	3/9/33/33	0/1/1/1
25	SF4	B	301	2	-	-	0/6/5/5
25	SF4	I	303	9	-	-	0/6/5/5
28	FES	G	803	7	-	-	0/1/1/1
28	FES	E	301	5	-	-	0/1/1/1
24	3PE	b	201	-	-	8/49/49/54	-
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	C15-N2	5.38	1.45	1.33
33	W	201	EHZ	C12-N1	5.11	1.45	1.33
29	F	501	FMN	C9A-C5A	4.79	1.49	1.41
27	H	402	PC1	O31-C31	4.24	1.45	1.33
34	a	101	CDL	OB8-CB7	4.20	1.45	1.33
27	B	303	PC1	O31-C31	4.17	1.45	1.33
27	I	302	PC1	O31-C31	4.17	1.45	1.33
34	a	101	CDL	OB6-CB5	4.14	1.46	1.34
24	b	201	3PE	O31-C31	4.14	1.45	1.33
34	a	101	CDL	OA8-CA7	4.11	1.45	1.33
24	A	401	3PE	O31-C31	4.10	1.45	1.33
27	H	402	PC1	O21-C21	4.10	1.45	1.34
27	I	302	PC1	O21-C21	4.09	1.45	1.34
24	I	301	3PE	O31-C31	4.08	1.45	1.33
34	a	101	CDL	OA6-CA5	4.05	1.45	1.34
27	B	303	PC1	O21-C21	4.04	1.45	1.34
24	b	201	3PE	O21-C21	4.01	1.45	1.34
24	I	301	3PE	O21-C21	3.97	1.45	1.34
24	A	401	3PE	O21-C21	3.96	1.45	1.34
31	P	401	NDP	C6N-C5N	3.26	1.39	1.33
29	F	501	FMN	C8-C7	3.15	1.48	1.40
26	B	302	UQ1	C3-C4	-2.96	1.40	1.48
29	F	501	FMN	C4-N3	-2.75	1.33	1.38
30	H	401	UQ9	C4-C5	-2.68	1.41	1.48
30	H	401	UQ9	C3-C2	-2.61	1.41	1.48
33	W	201	EHZ	P1-O7	2.55	1.64	1.54
33	W	201	EHZ	O4-C15	-2.48	1.18	1.23
29	F	501	FMN	C5A-N5	-2.41	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	W	201	EHZ	C9-S1	2.40	1.81	1.76
26	B	302	UQ1	C2-C1	-2.40	1.42	1.48
33	W	201	EHZ	O3-C12	-2.33	1.18	1.23
31	P	401	NDP	C5A-C4A	2.29	1.47	1.40
33	W	201	EHZ	P1-OP3	-2.22	1.46	1.54
29	F	501	FMN	C4A-N5	2.05	1.34	1.30

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
34	a	101	CDL	OA6-CA5-C11	4.33	120.84	111.50
27	I	302	PC1	O21-C21-C22	4.23	120.61	111.50
34	a	101	CDL	OB6-CB5-C51	4.07	120.28	111.50
27	H	402	PC1	O21-C21-C22	4.01	120.13	111.50
27	B	303	PC1	O21-C21-C22	3.81	119.71	111.50
24	A	401	3PE	O21-C21-C22	3.76	119.61	111.50
24	I	301	3PE	O21-C21-C22	3.68	119.43	111.50
31	P	401	NDP	PN-O3-PA	-3.56	120.62	132.83
24	b	201	3PE	O21-C21-C22	3.51	119.07	111.50
24	b	201	3PE	C2-O21-C21	-3.48	109.22	117.79
31	P	401	NDP	N3A-C2A-N1A	-3.14	123.78	128.68
33	W	201	EHZ	C13-C12-N1	3.10	121.64	116.42
33	W	201	EHZ	C14-C13-C12	-3.02	107.33	112.36
33	W	201	EHZ	OP3-P1-O9	-2.90	99.33	110.68
33	W	201	EHZ	C7-C8-C9	-2.89	107.30	113.89
27	I	302	PC1	C2-O21-C21	-2.83	110.83	117.79
27	B	303	PC1	O31-C31-C32	2.78	120.62	111.91
34	a	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
34	a	101	CDL	CA4-OA6-CA5	-2.74	111.06	117.79
31	P	401	NDP	C4A-C5A-N7A	-2.70	106.59	109.40
27	B	303	PC1	C2-O21-C21	-2.69	111.16	117.79
24	I	301	3PE	O31-C31-C32	2.67	120.28	111.91
29	F	501	FMN	C4A-C10-N1	-2.63	118.62	124.73
27	I	302	PC1	O31-C31-C32	2.59	120.04	111.91
24	A	401	3PE	O31-C31-C32	2.56	119.95	111.91
29	F	501	FMN	O4-C4-C4A	-2.53	119.90	126.60
24	b	201	3PE	O31-C31-C32	2.49	119.74	111.91
31	P	401	NDP	C3D-C2D-C1D	2.47	106.11	101.43
33	W	201	EHZ	C5-C6-C7	-2.39	107.98	114.85
34	a	101	CDL	OB8-CB7-C71	2.39	119.40	111.91
27	H	402	PC1	C2-O21-C21	-2.33	112.04	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	402	PC1	O31-C31-C32	2.33	119.23	111.91
33	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
34	a	101	CDL	CB4-OB6-CB5	-2.23	112.30	117.79
29	F	501	FMN	C4-C4A-N5	2.19	121.35	118.23
33	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
29	F	501	FMN	C4A-C10-N10	2.12	119.58	116.48
33	W	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
33	W	201	EHZ	O6-P1-O9	2.10	112.36	106.47
33	W	201	EHZ	O3-C12-N1	-2.07	119.11	123.01
29	F	501	FMN	O2-C2-N1	-2.06	118.41	121.83
29	F	501	FMN	C10-N1-C2	2.06	121.02	116.90
24	I	301	3PE	O31-C31-O32	-2.03	118.47	123.59
27	H	402	PC1	C11-C12-N	-2.01	109.05	115.78
24	I	301	3PE	C2-O21-C21	-2.01	112.85	117.79
29	F	501	FMN	C4A-C4-N3	2.00	118.28	113.19

There are no chirality outliers.

All (139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
24	I	301	3PE	C11-O13-P-O12
24	b	201	3PE	O22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
26	B	302	UQ1	C7-C8-C9-C11
27	B	303	PC1	C1-O11-P-O12
27	B	303	PC1	C1-O11-P-O14
27	B	303	PC1	C1-O11-P-O13
27	B	303	PC1	C22-C21-O21-C2
27	H	402	PC1	C11-O13-P-O12
27	H	402	PC1	C11-O13-P-O14
27	H	402	PC1	C1-O11-P-O12
27	H	402	PC1	C1-O11-P-O13
27	H	402	PC1	C12-C11-O13-P
27	I	302	PC1	C11-O13-P-O12
27	I	302	PC1	C11-O13-P-O14
27	I	302	PC1	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O12
29	F	501	FMN	N10-C1'-C2'-O2'
29	F	501	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
29	F	501	FMN	C5'-O5'-P-O3P
30	H	401	UQ9	C22-C23-C24-C26
30	H	401	UQ9	C22-C23-C24-C25
30	H	401	UQ9	C20-C19-C21-C22
30	H	401	UQ9	C7-C8-C9-C11
30	H	401	UQ9	C7-C8-C9-C10
31	P	401	NDP	C2N-C3N-C7N-N7N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C7-C8-C9-S1
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C11-C10-S1-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	a	101	CDL	CA3-OA5-PA1-OA2
34	a	101	CDL	CA3-OA5-PA1-OA3
34	a	101	CDL	CA3-OA5-PA1-OA4
27	I	302	PC1	O32-C31-O31-C3
27	I	302	PC1	C32-C31-O31-C3
27	H	402	PC1	O32-C31-O31-C3
27	B	303	PC1	O22-C21-O21-C2
27	H	402	PC1	C32-C31-O31-C3
30	H	401	UQ9	C18-C19-C21-C22
26	B	302	UQ1	C7-C8-C9-C10
30	H	401	UQ9	C25-C24-C26-C27
30	H	401	UQ9	C15-C14-C16-C17
30	H	401	UQ9	C23-C24-C26-C27
30	H	401	UQ9	C13-C14-C16-C17
24	A	401	3PE	C22-C21-O21-C2
27	H	402	PC1	C11-C12-N-C13
24	I	301	3PE	C32-C31-O31-C3
24	b	201	3PE	C32-C31-O31-C3
34	a	101	CDL	C12-C13-C14-C15
27	I	302	PC1	C11-C12-N-C15
24	I	301	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
30	H	401	UQ9	C19-C21-C22-C23
24	A	401	3PE	O22-C21-O21-C2
24	A	401	3PE	C11-O13-P-O11
24	I	301	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
24	I	301	3PE	C11-O13-P-O11
27	H	402	PC1	C11-O13-P-O11
27	I	302	PC1	C1-O11-P-O13
34	a	101	CDL	C31-CA7-OA8-CA6
27	H	402	PC1	C11-C12-N-C15
34	a	101	CDL	OA9-CA7-OA8-CA6
27	H	402	PC1	C11-C12-N-C14
27	I	302	PC1	C11-C12-N-C13
24	A	401	3PE	C31-C32-C33-C34
34	a	101	CDL	C51-CB5-OB6-CB4
34	a	101	CDL	OB7-CB5-OB6-CB4
27	I	302	PC1	C11-C12-N-C14
24	I	301	3PE	C22-C21-O21-C2
24	I	301	3PE	C24-C25-C26-C27
24	b	201	3PE	C2A-C2B-C2C-C2D
24	I	301	3PE	O22-C21-O21-C2
27	B	303	PC1	C2-C1-O11-P
27	B	303	PC1	C32-C33-C34-C35
33	W	201	EHZ	N2-C15-C16-C17
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
27	B	303	PC1	C32-C31-O31-C3
33	W	201	EHZ	O2-C9-S1-C10
24	A	401	3PE	C3-C2-O21-C21
31	P	401	NDP	C2B-O2B-P2B-O2X
27	B	303	PC1	O32-C31-O31-C3
24	A	401	3PE	C2E-C2F-C2G-C2H
24	A	401	3PE	C2-C1-O11-P
34	a	101	CDL	CA4-CA3-OA5-PA1
24	A	401	3PE	C11-O13-P-O14
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C1-O11-P-O14
24	I	301	3PE	C11-O13-P-O14
27	H	402	PC1	C1-O11-P-O14
24	A	401	3PE	O11-C1-C2-C3
24	A	401	3PE	O11-C1-C2-O21
27	B	303	PC1	O13-C11-C12-N
27	H	402	PC1	O13-C11-C12-N
24	I	301	3PE	O21-C2-C3-O31
33	W	201	EHZ	O4-C15-C16-O5
33	W	201	EHZ	C19-C17-C20-O6
24	b	201	3PE	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

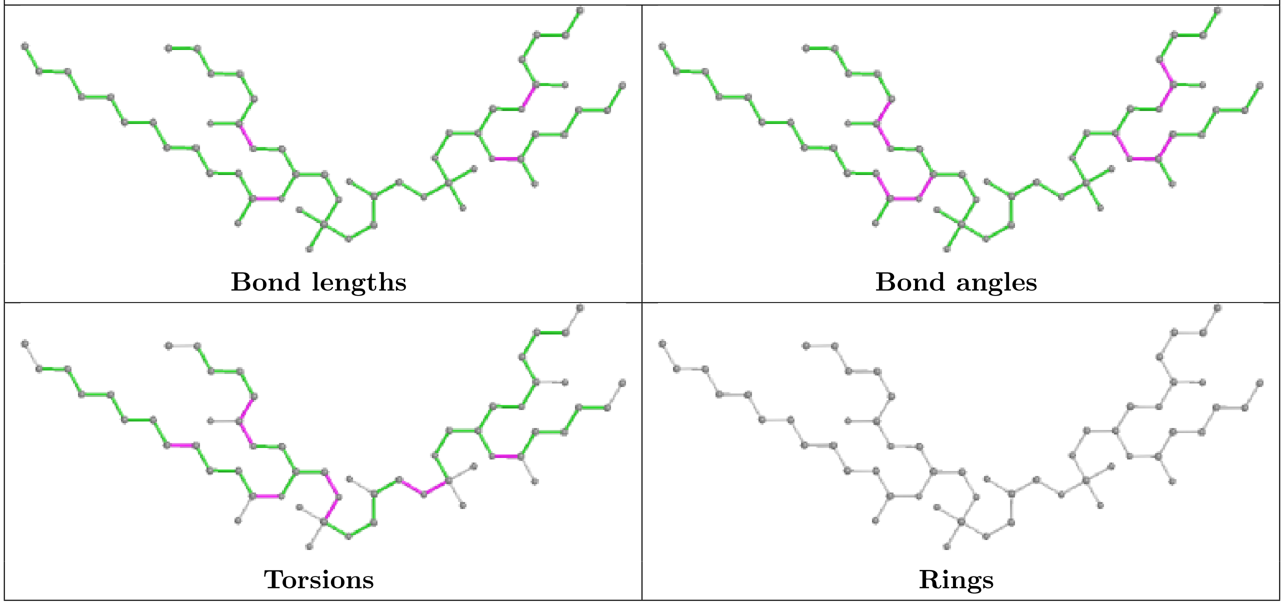
Mol	Chain	Res	Type	Atoms
34	a	101	CDL	CB2-OB2-PB2-OB5
33	W	201	EHZ	C2-C3-C4-C5
31	P	401	NDP	O4D-C1D-N1N-C6N
26	B	302	UQ1	C1-C2-O2-CM2
34	a	101	CDL	C1-CB2-OB2-PB2
27	B	303	PC1	C34-C35-C36-C37
31	P	401	NDP	C2D-C1D-N1N-C6N
24	I	301	3PE	C37-C38-C39-C3A
27	H	402	PC1	C34-C35-C36-C37
24	b	201	3PE	C24-C25-C26-C27
27	I	302	PC1	C2E-C2F-C2G-C2H
31	P	401	NDP	PN-O3-PA-O2A
30	H	401	UQ9	C12-C11-C9-C10
24	I	301	3PE	C35-C36-C37-C38
24	I	301	3PE	C33-C34-C35-C36
29	F	501	FMN	C5'-O5'-P-O2P
33	W	201	EHZ	N2-C15-C16-O5
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C8-C9-S1-C10
33	W	201	EHZ	C15-C16-C17-C18
31	P	401	NDP	C2B-O2B-P2B-O3X
33	W	201	EHZ	O5-C16-C17-C18
34	a	101	CDL	C32-C31-CA7-OA8
30	H	401	UQ9	C12-C11-C9-C8
24	I	301	3PE	C1-C2-C3-O31
24	A	401	3PE	O13-C11-C12-N
27	I	302	PC1	C12-C11-O13-P
33	W	201	EHZ	O4-C15-C16-C17
34	a	101	CDL	OA7-CA5-OA6-CA4
24	I	301	3PE	C2-C1-O11-P
34	a	101	CDL	C32-C31-CA7-OA9
24	b	201	3PE	C39-C3A-C3B-C3C
27	I	302	PC1	C2C-C2D-C2E-C2F

There are no ring outliers.

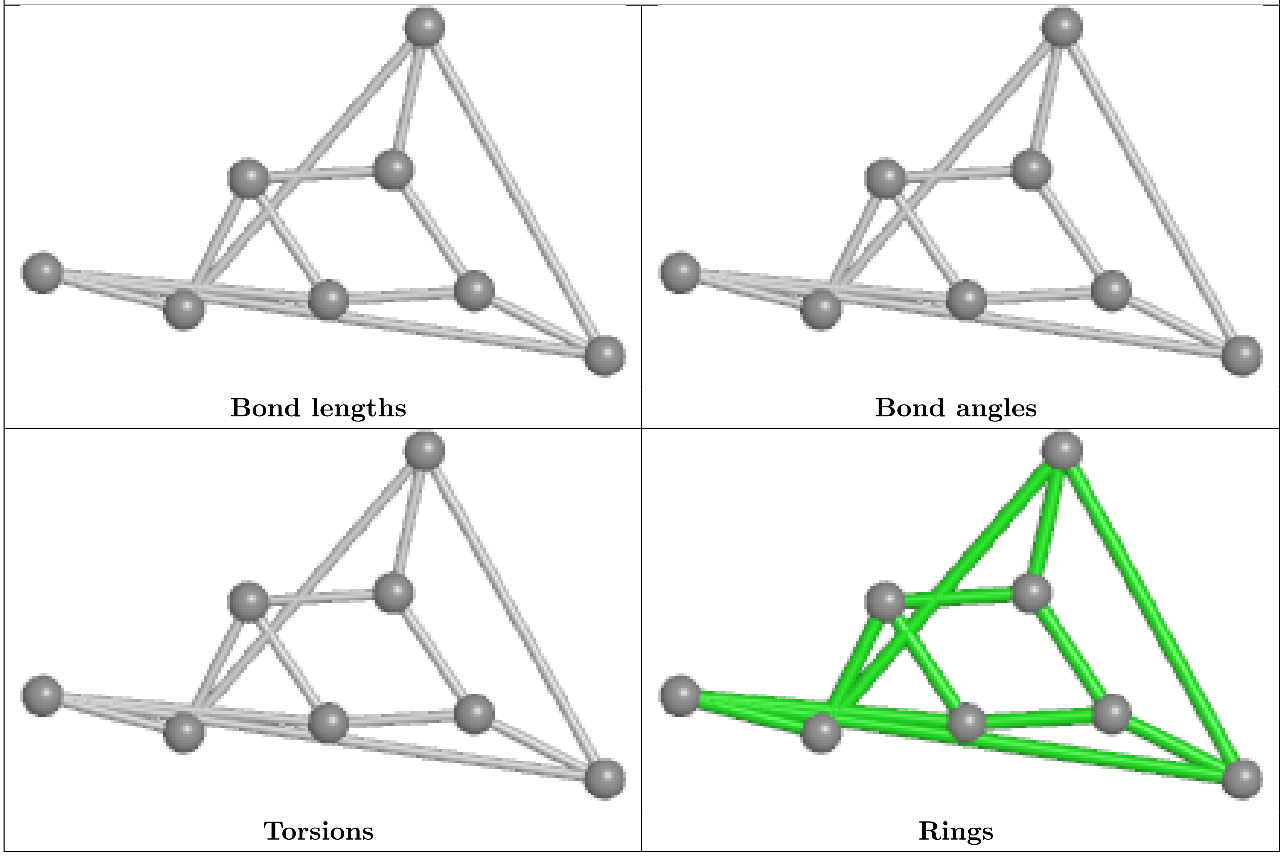
No monomer is involved in short contacts.

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.

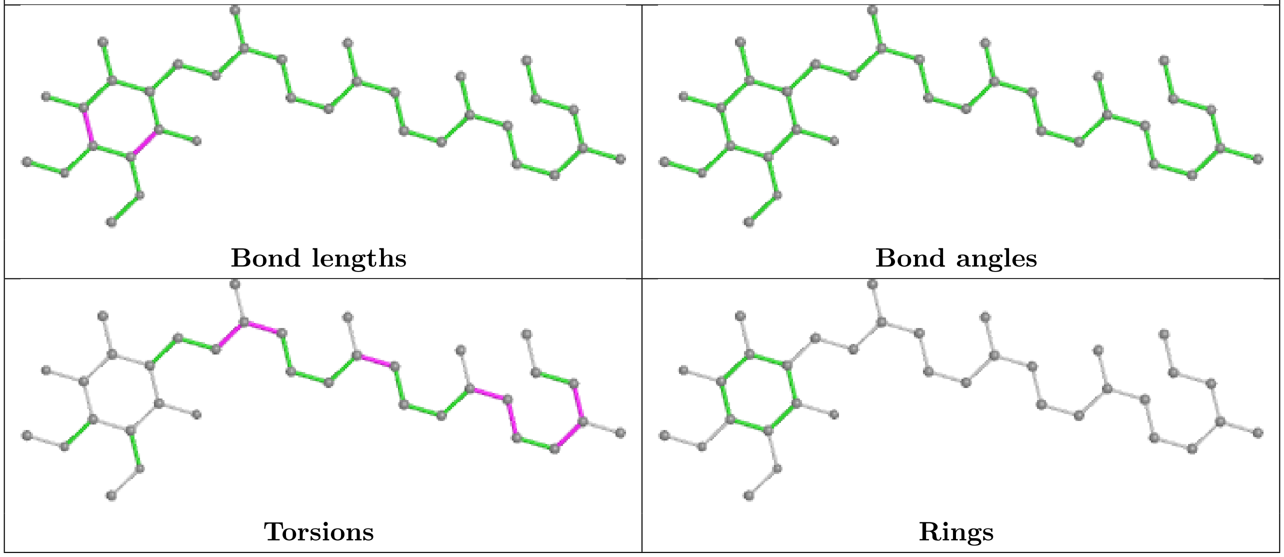
Ligand CDL a 101


Bond lengths **Bond angles**
Torsions **Rings**

Ligand SF4 F 502


Bond lengths **Bond angles**
Torsions **Rings**

Ligand UQ9 H 401



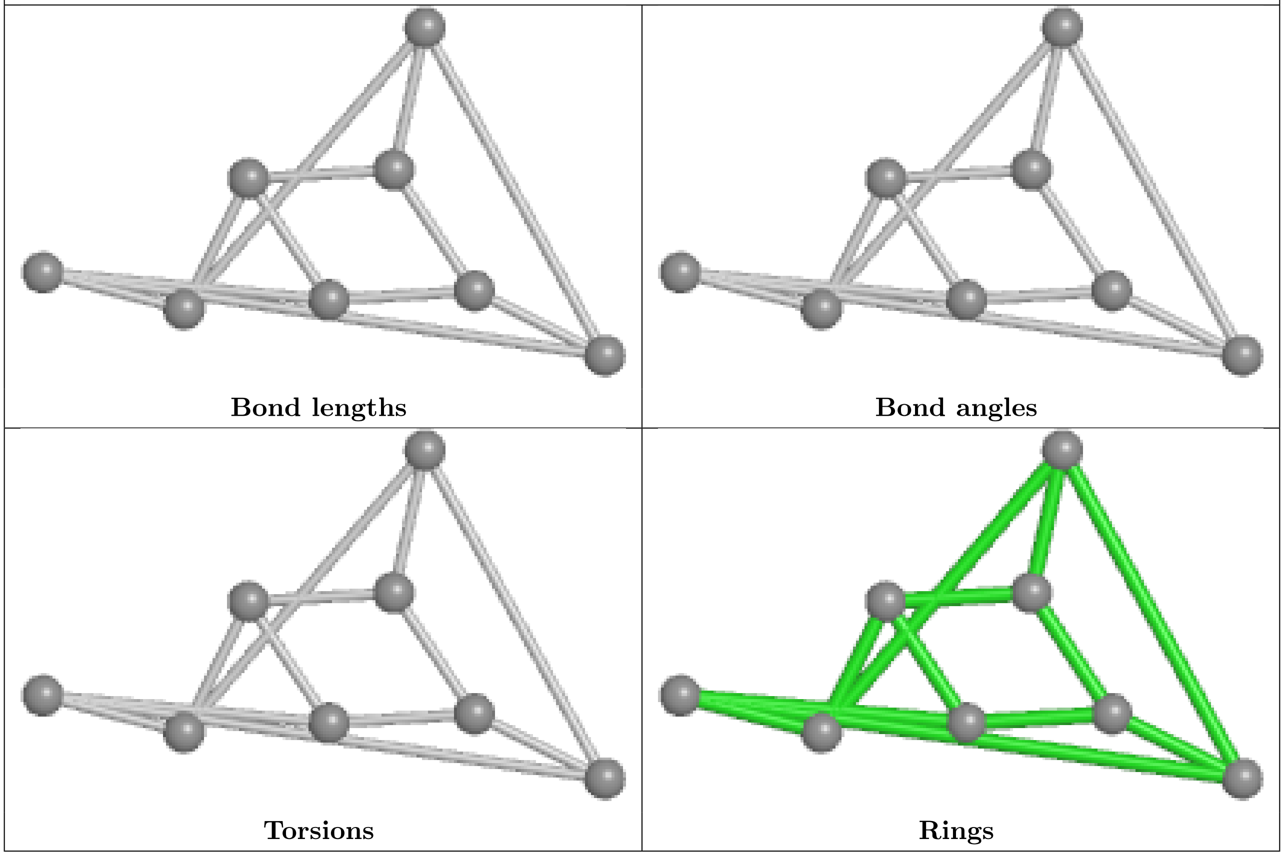
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 I 304



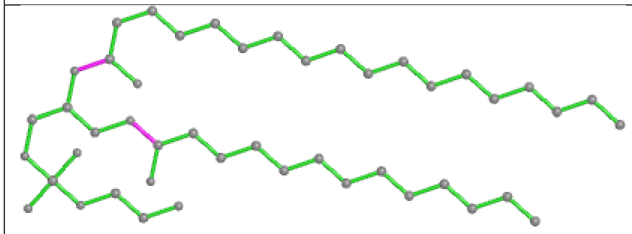
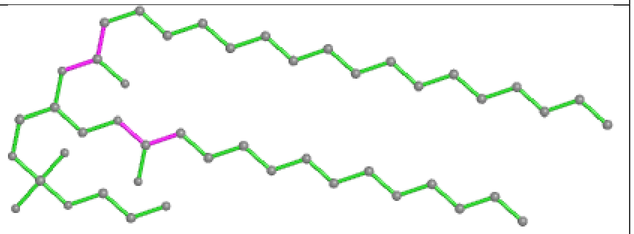
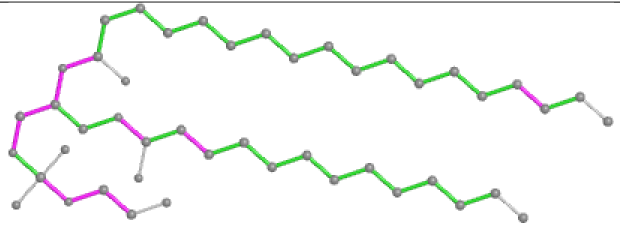
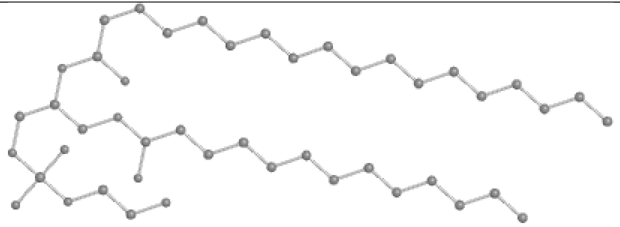
Bond lengths

Bond angles

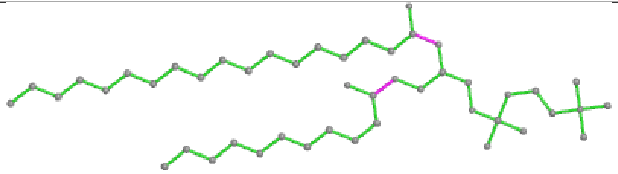
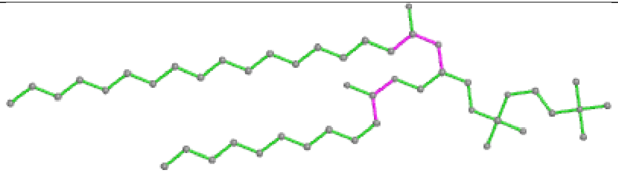
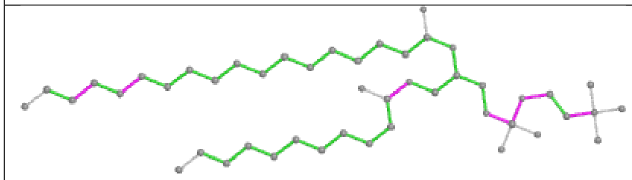
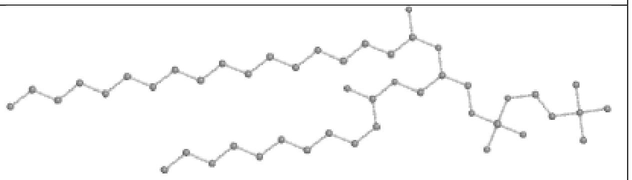
Torsions

Rings

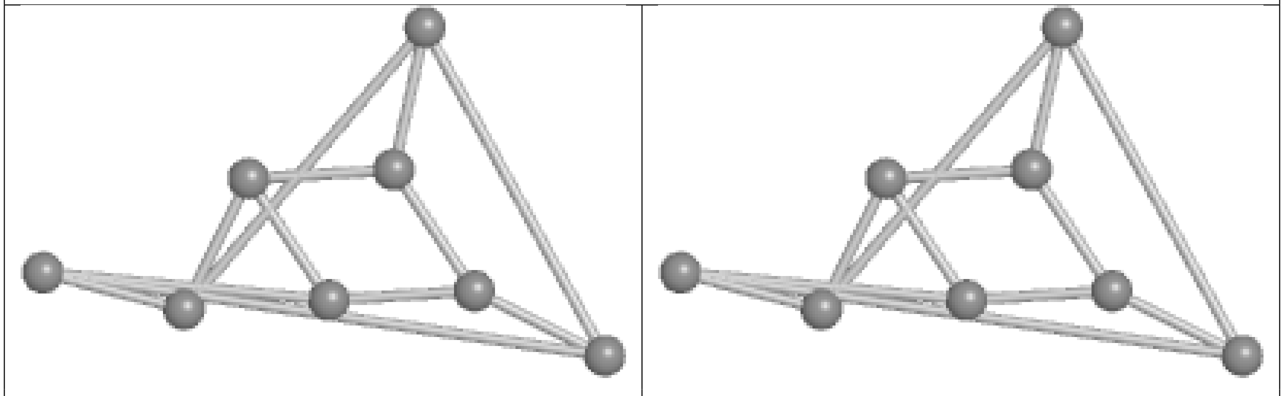
Ligand 3PE A 401

 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 I 302

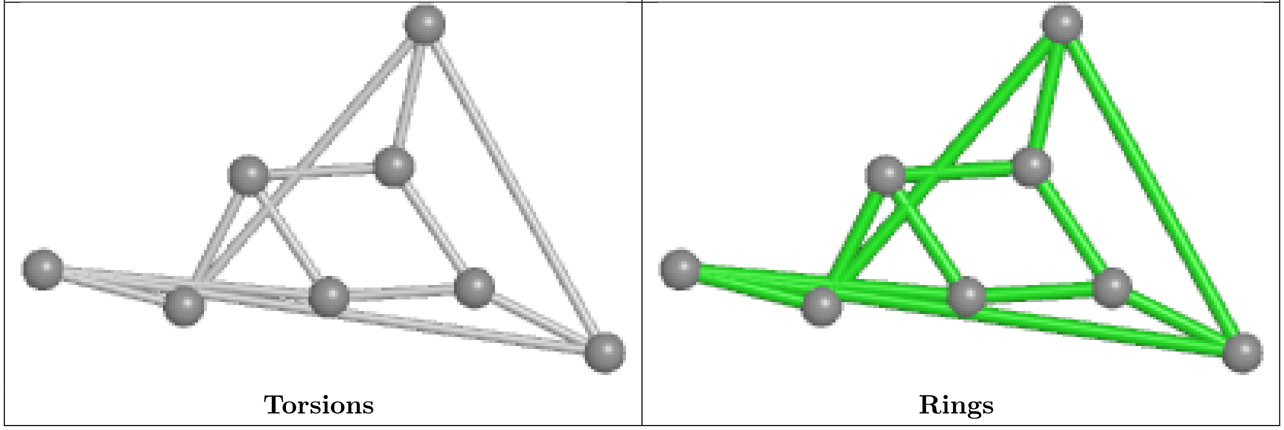
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 G 802



Bond lengths

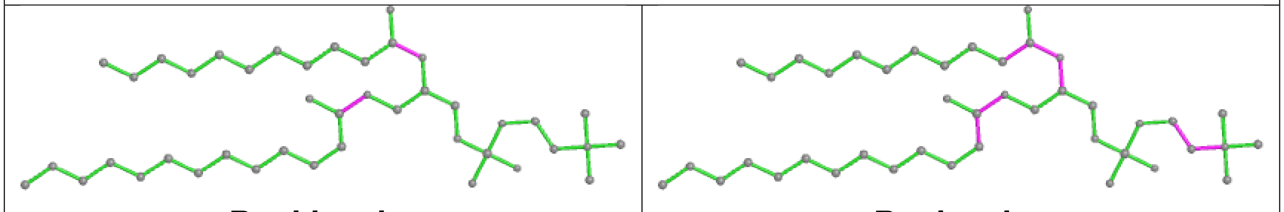
Bond angles



Torsions

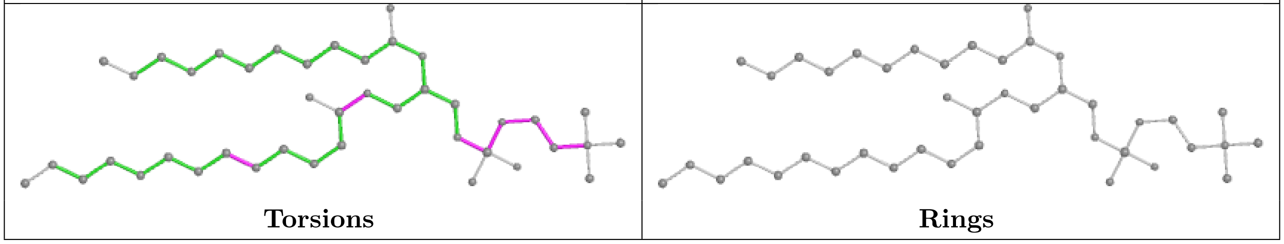
Rings

Ligand PC1 H 402



Bond lengths

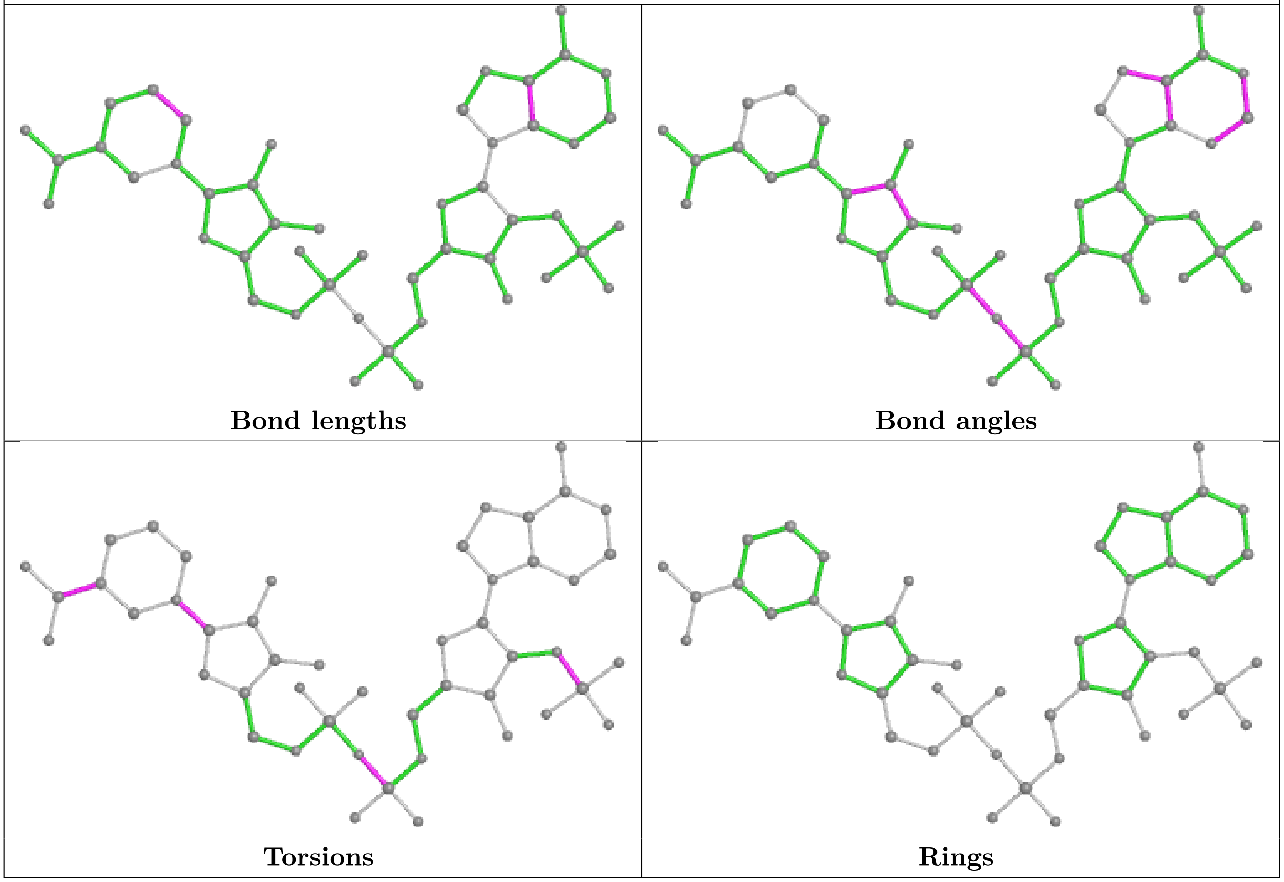
Bond angles



Torsions

Rings

Ligand NDP P 401



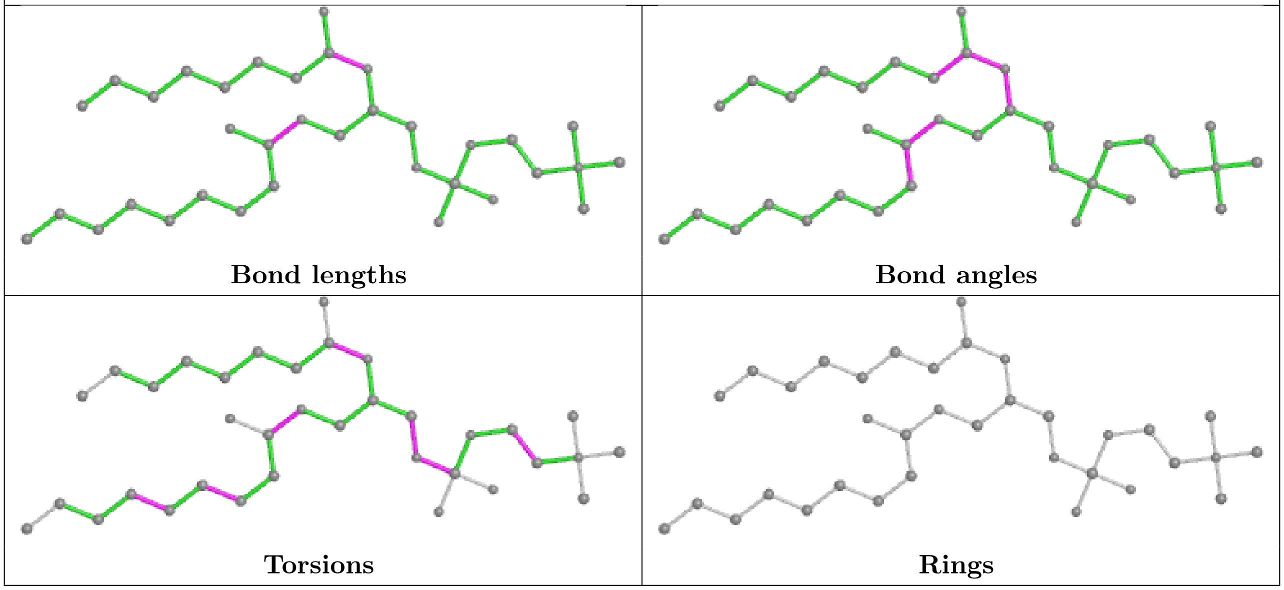
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 303



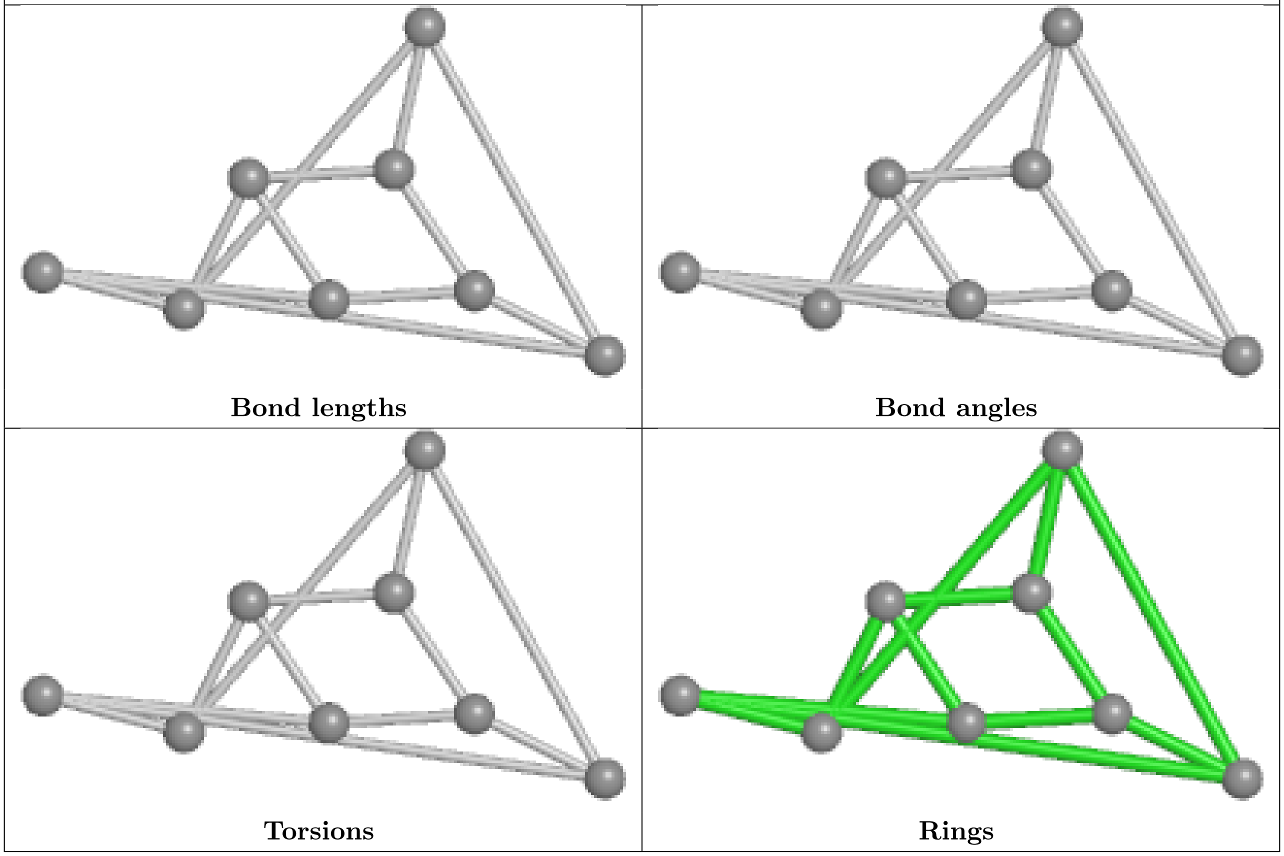
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 G 801



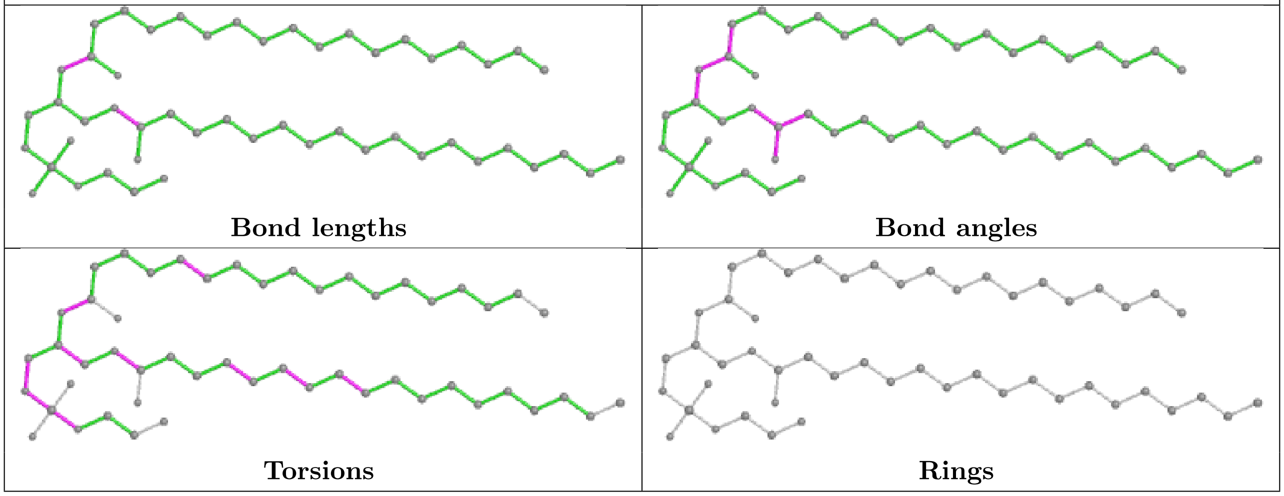
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE I 301



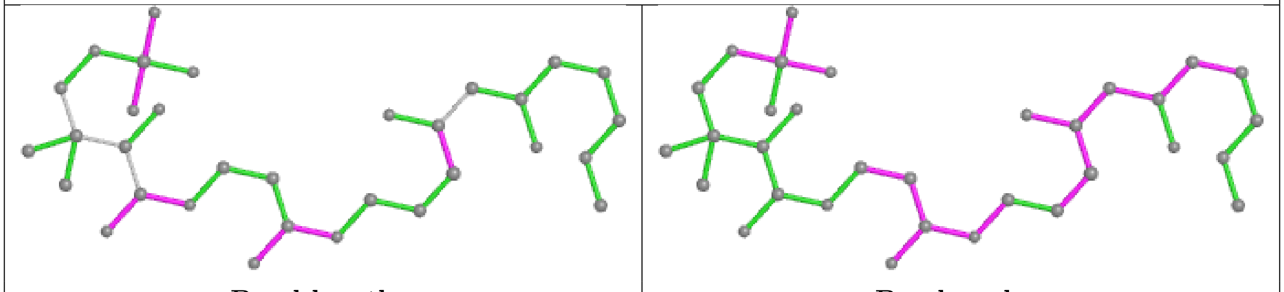
Bond lengths

Bond angles

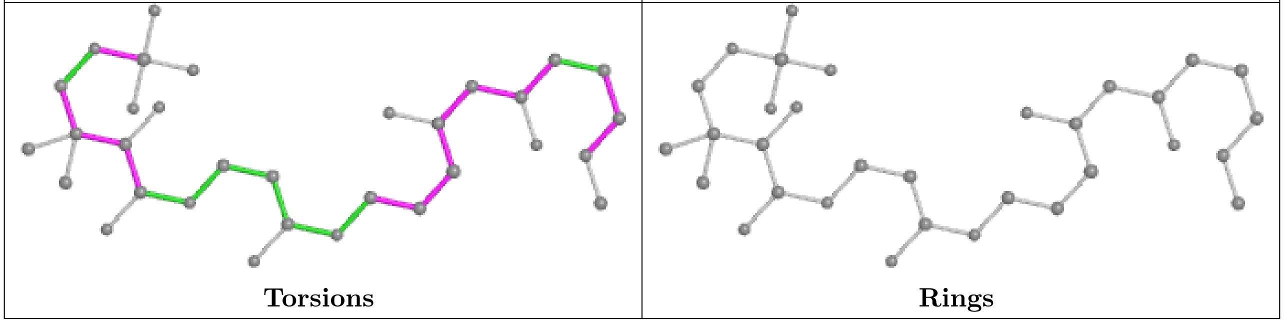
Torsions

Rings

Ligand EHZ W 201

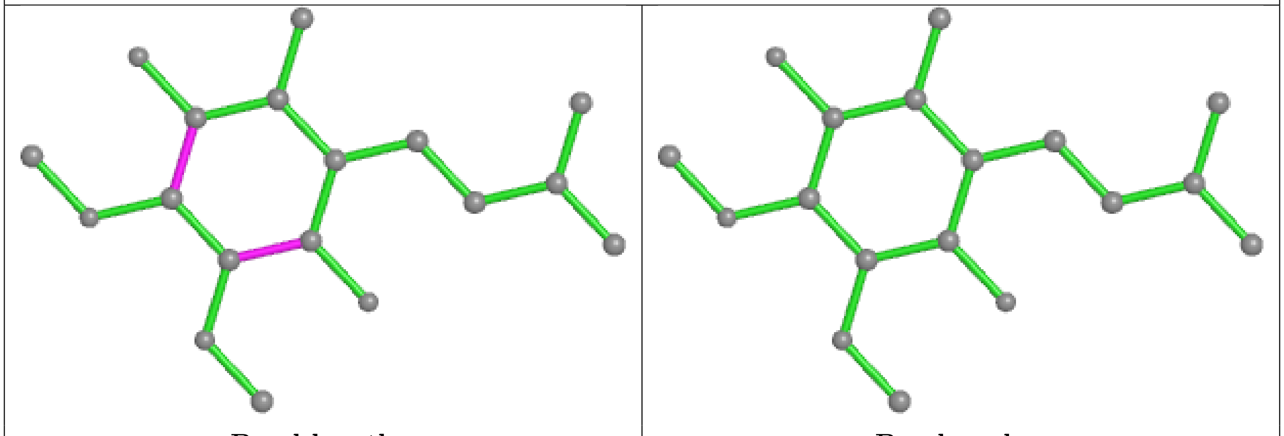


Bond lengths **Bond angles**

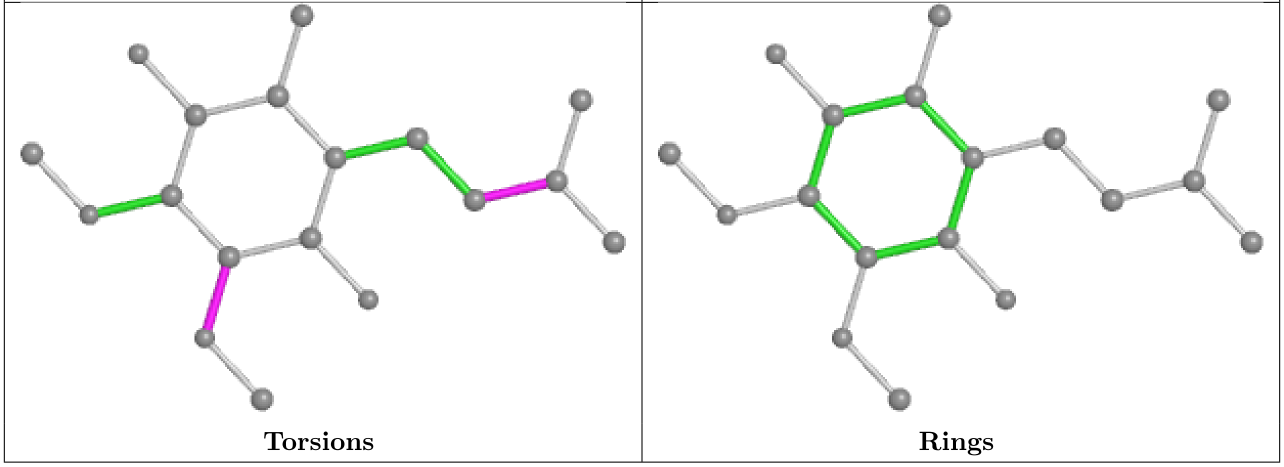


Torsions **Rings**

Ligand UQ1 B 302

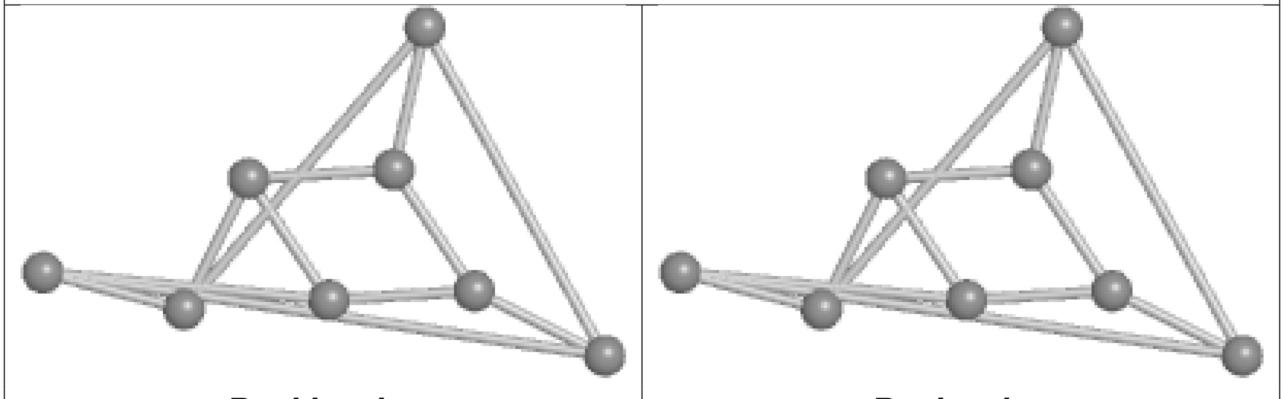


Bond lengths **Bond angles**

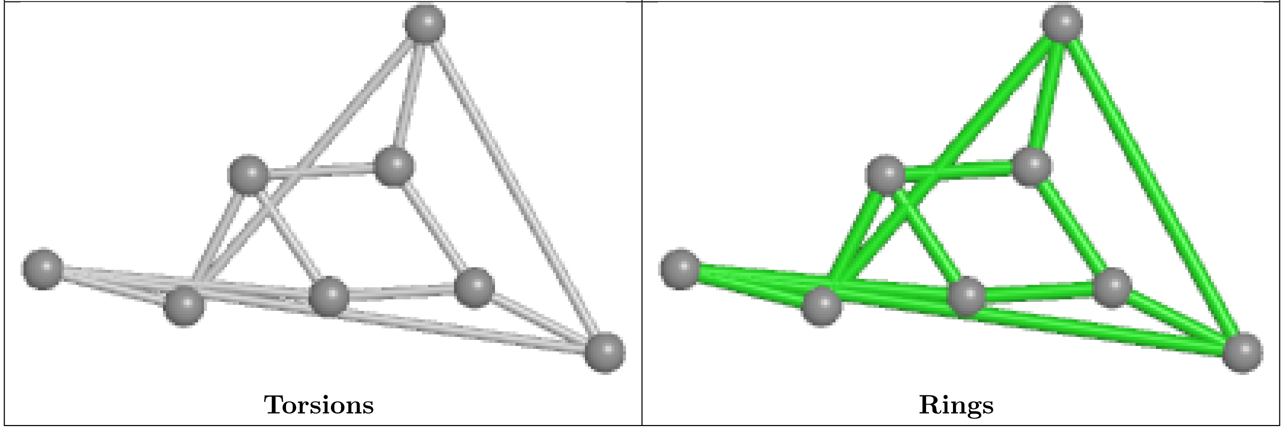


Torsions **Rings**

Ligand SF4 B 301

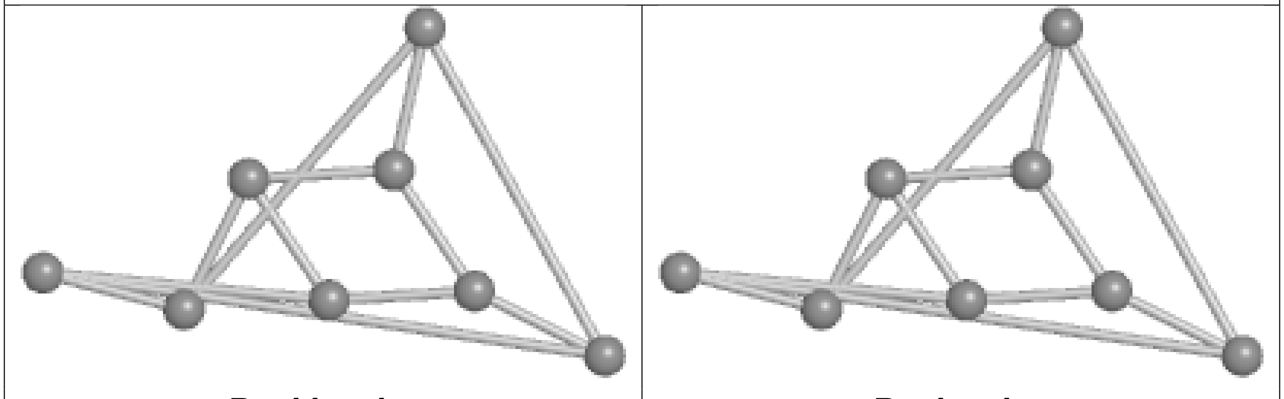


Bond lengths **Bond angles**

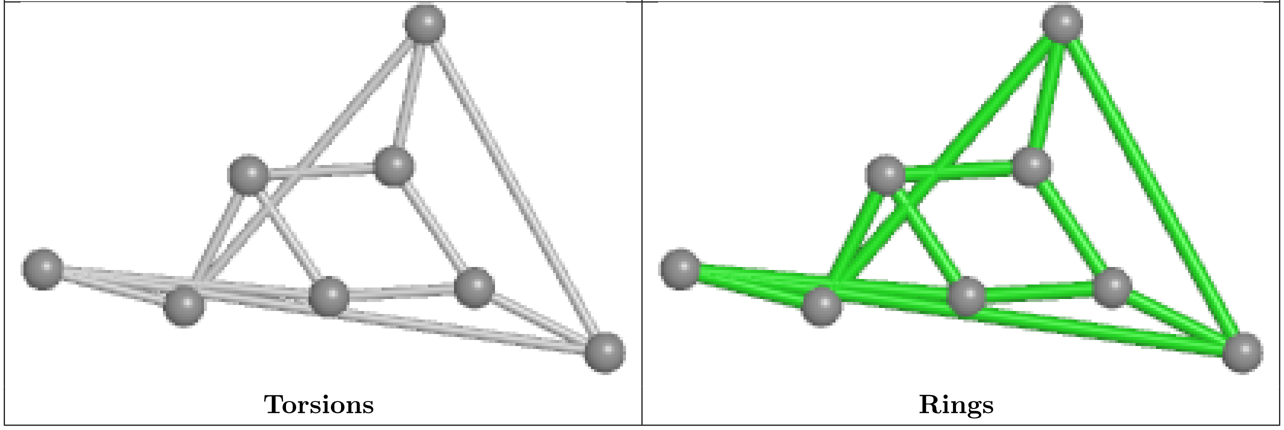


Torsions **Rings**

Ligand SF4 I 303

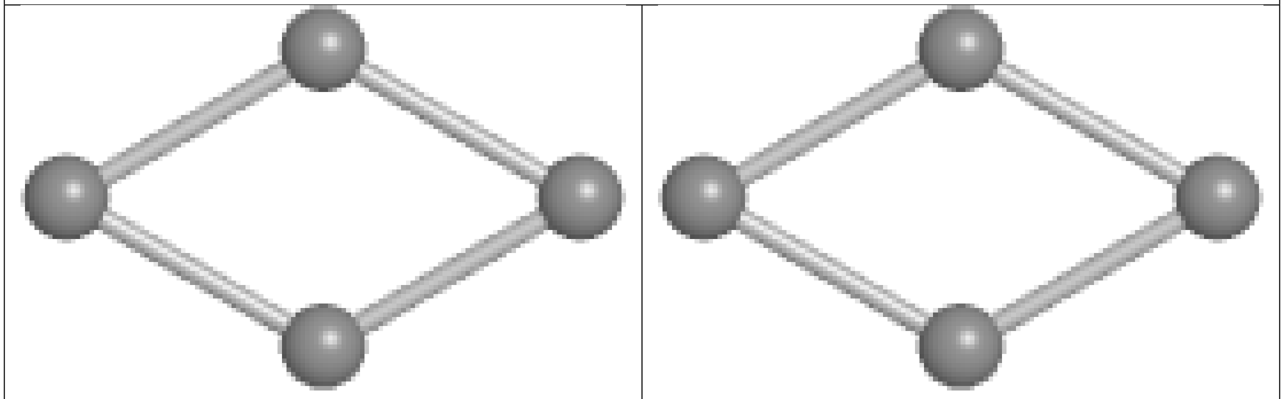


Bond lengths **Bond angles**



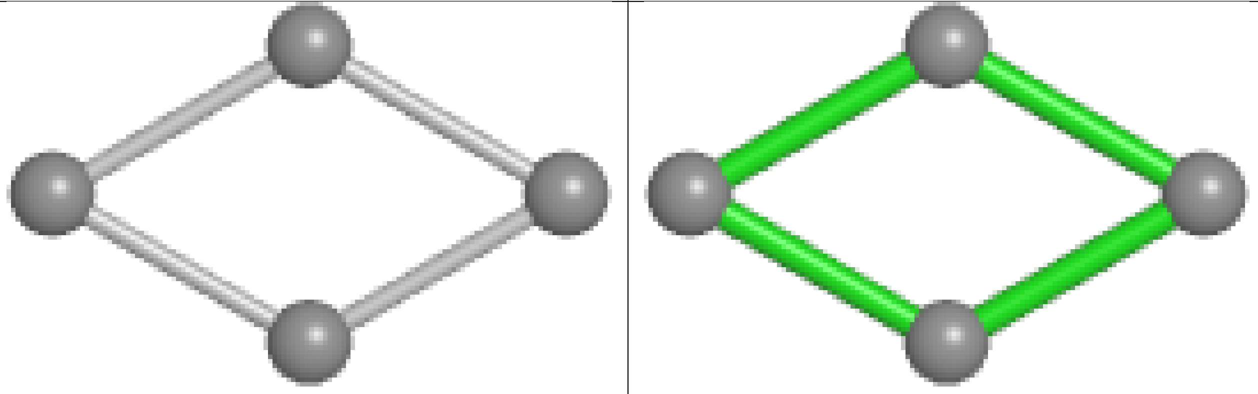
Torsions **Rings**

Ligand FES G 803



Bond lengths

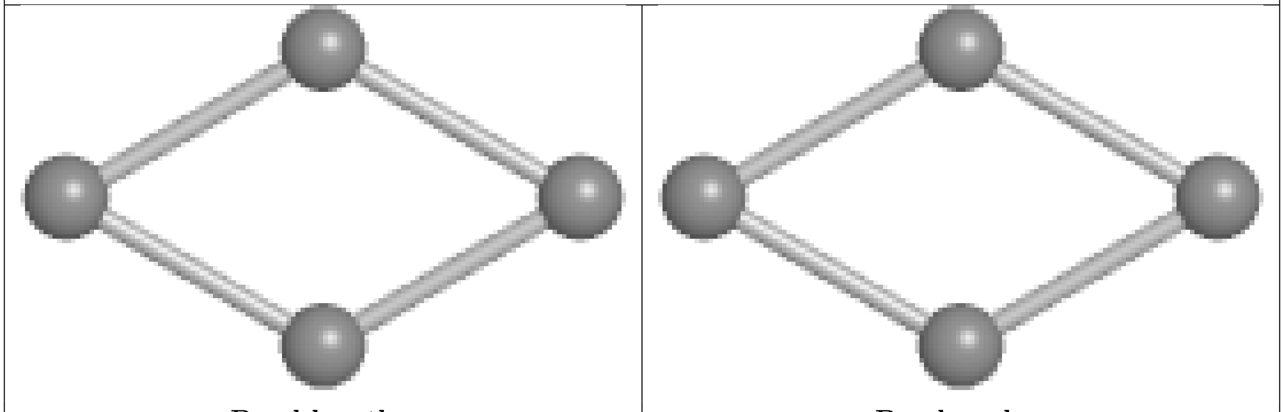
Bond angles



Torsions

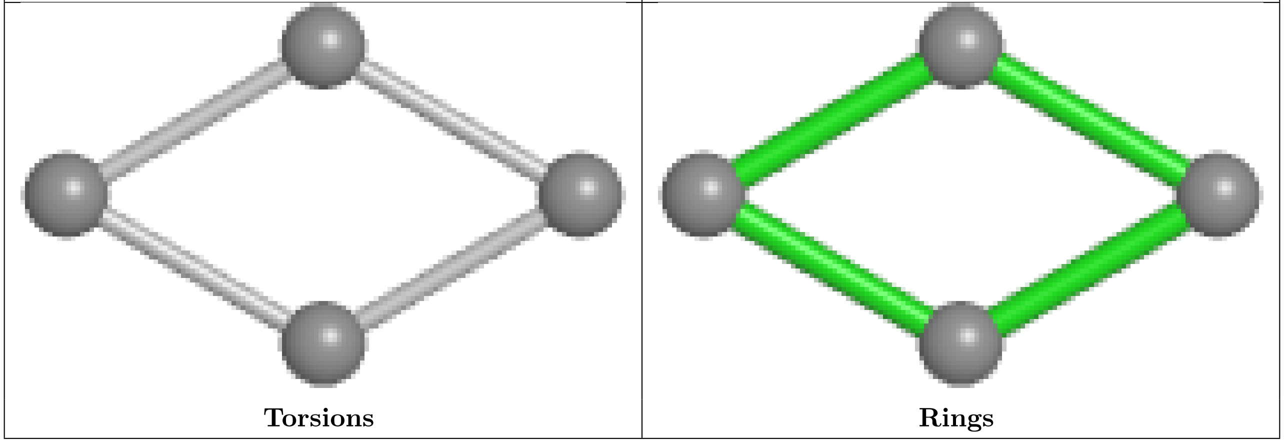
Rings

Ligand FES E 301



Bond lengths

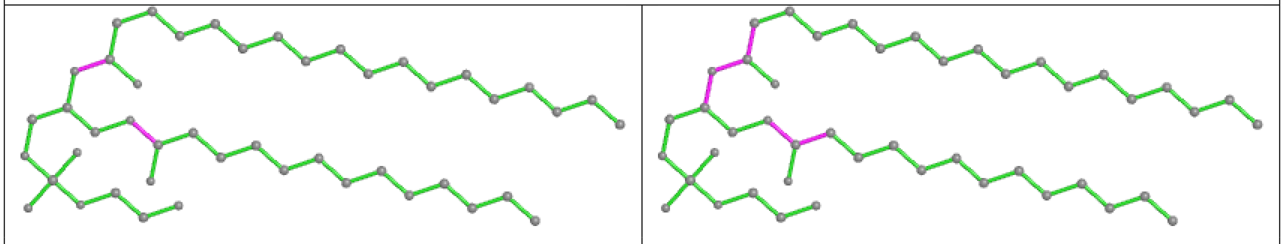
Bond angles



Torsions

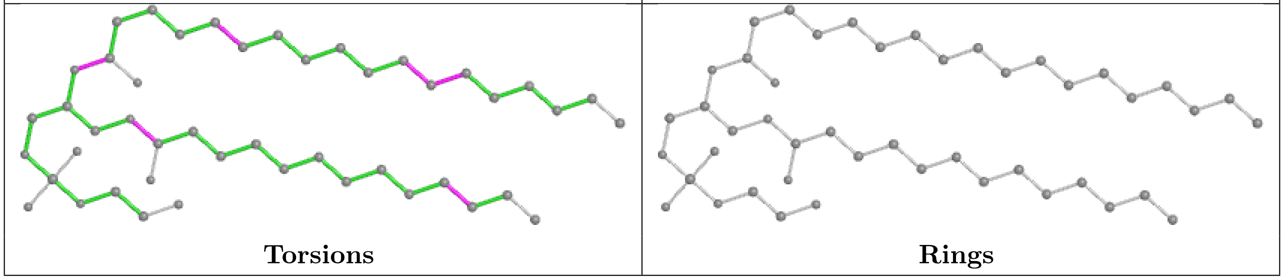
Rings

Ligand 3PE b 201



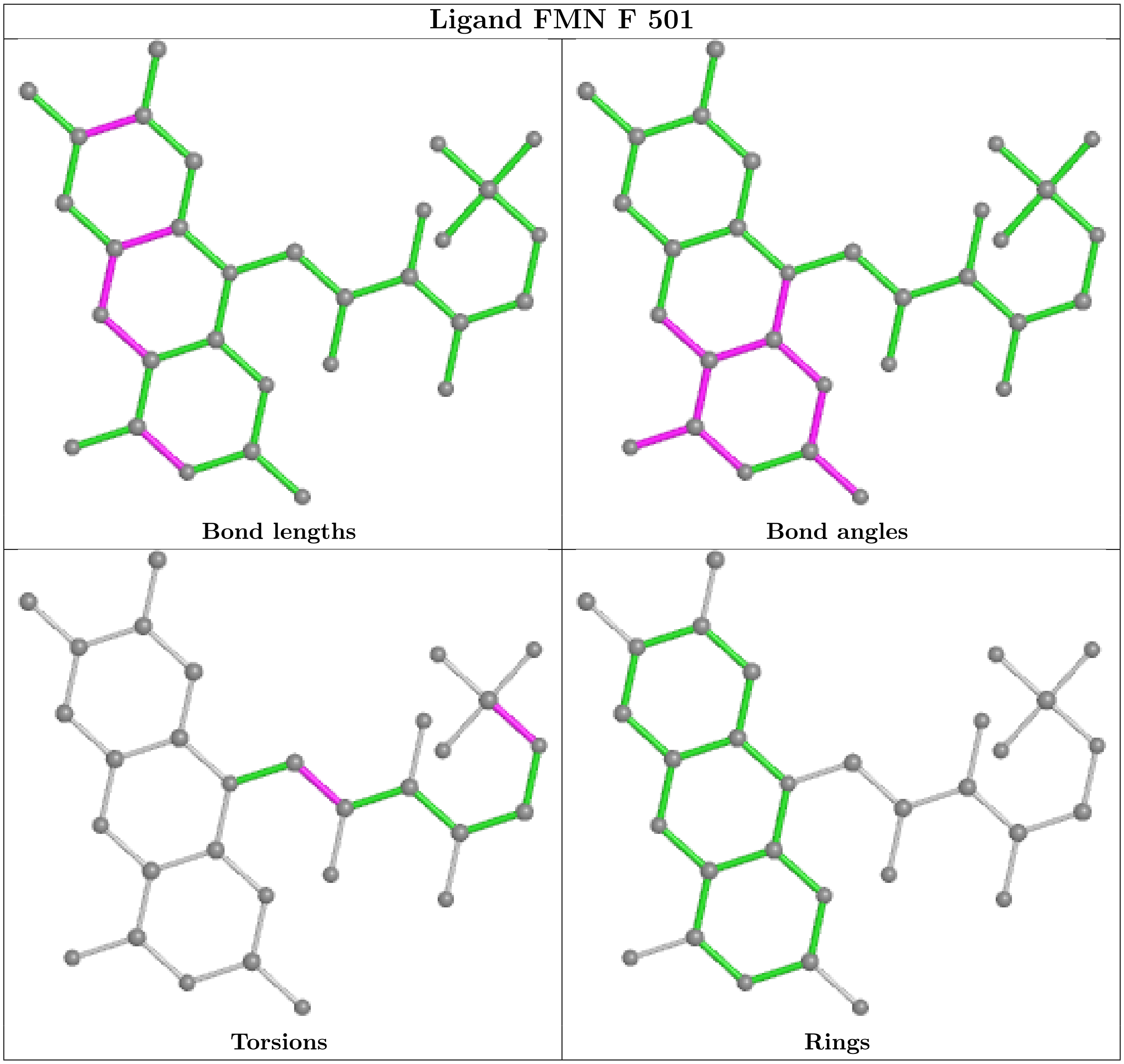
Bond lengths

Bond angles



Torsions

Rings


Ligand FMN F 501

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.

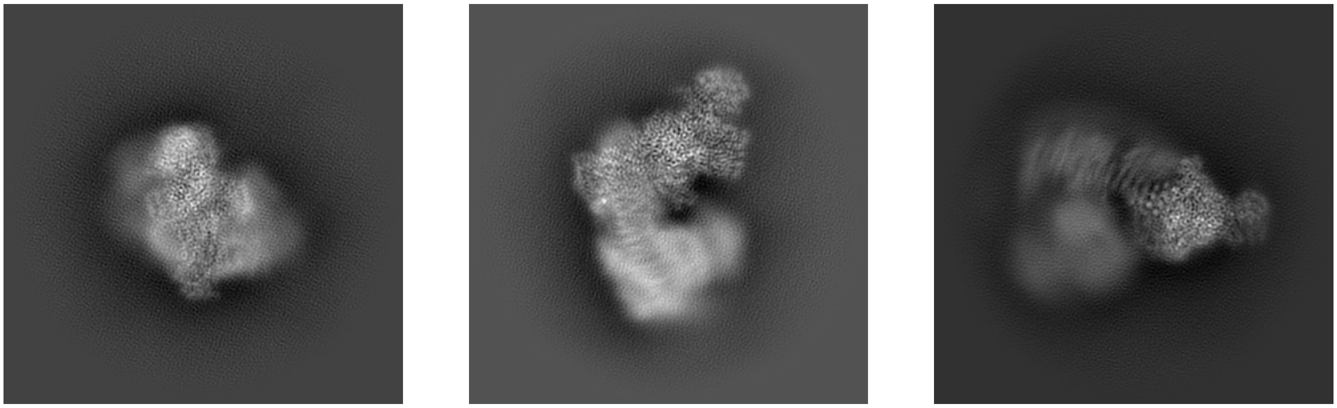
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-35332. 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.

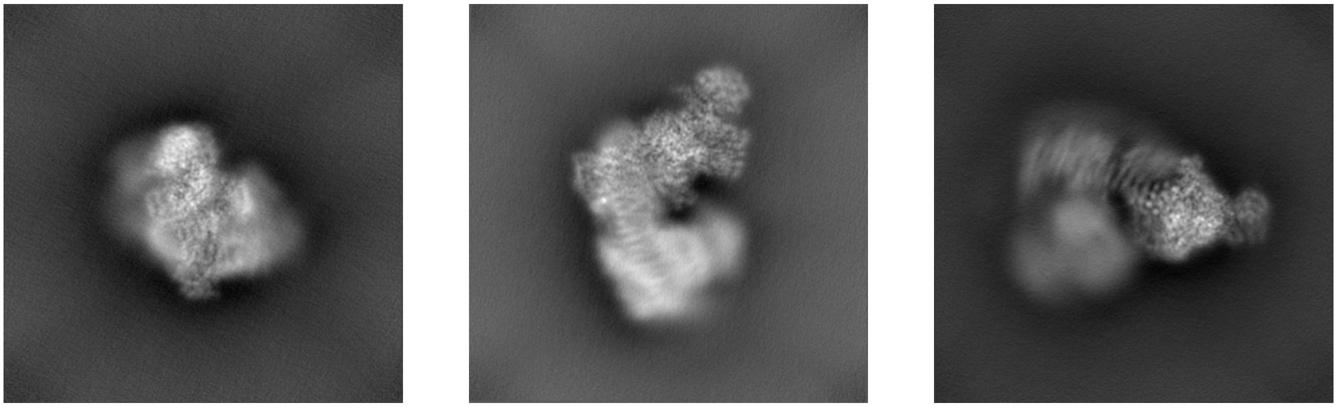
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

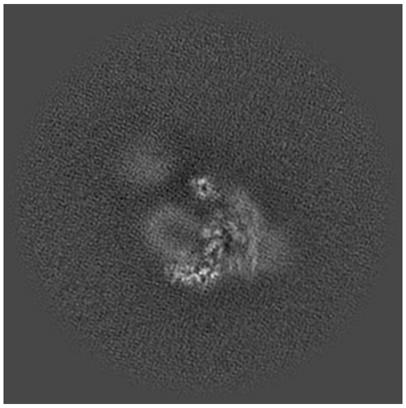


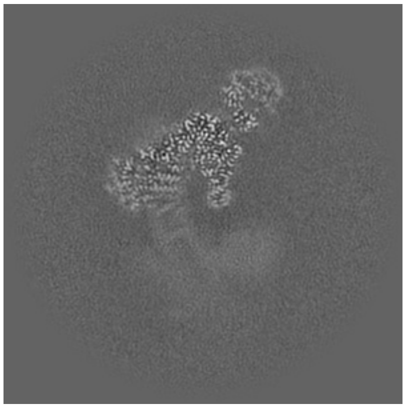
X Y Z

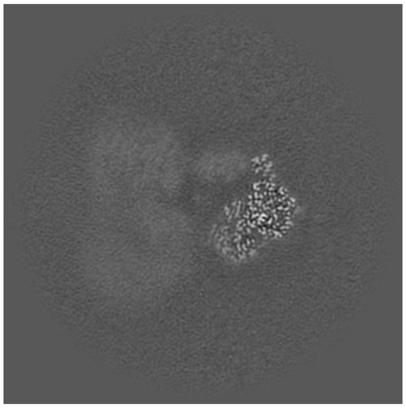
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

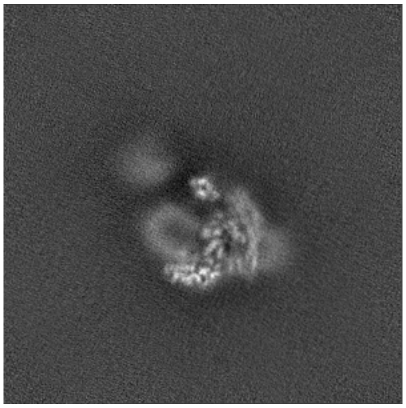
6.2.1 Primary map

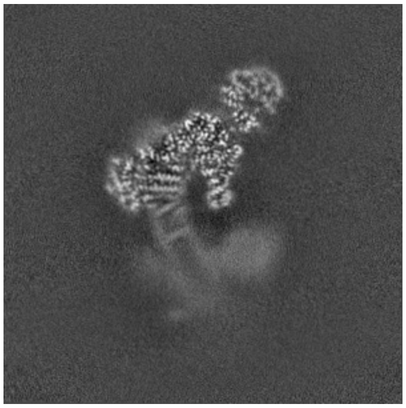

X Index: 192

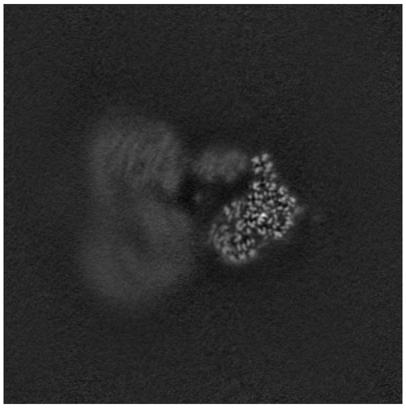

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

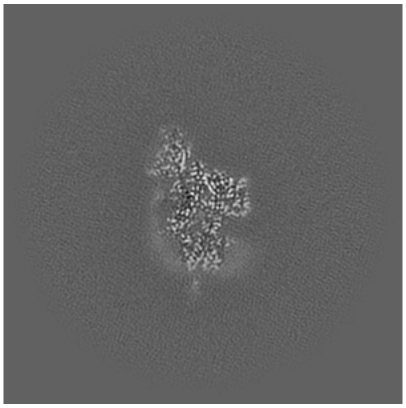

Y Index: 192


Z Index: 192

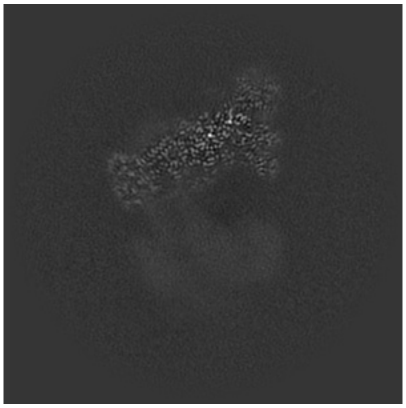
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

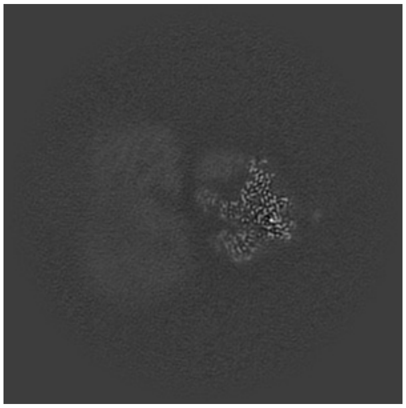
6.3.1 Primary map



X Index: 243

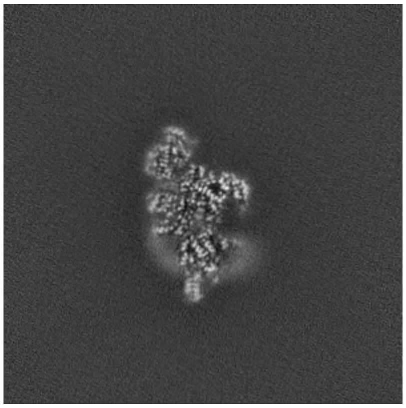


Y Index: 176

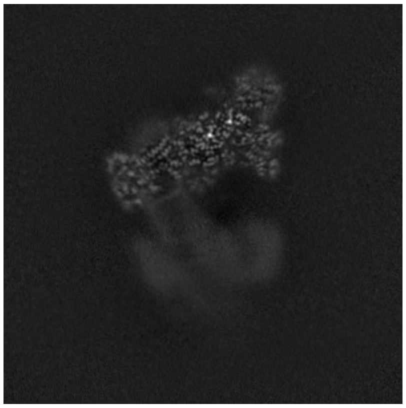


Z Index: 199

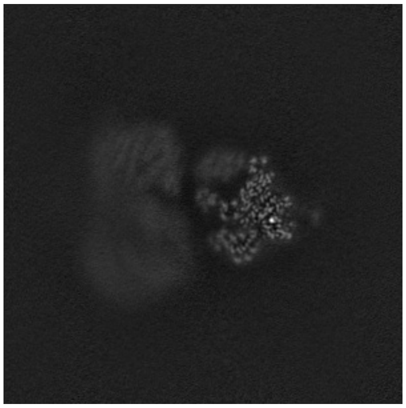
6.3.2 Raw map



X Index: 238



Y Index: 176

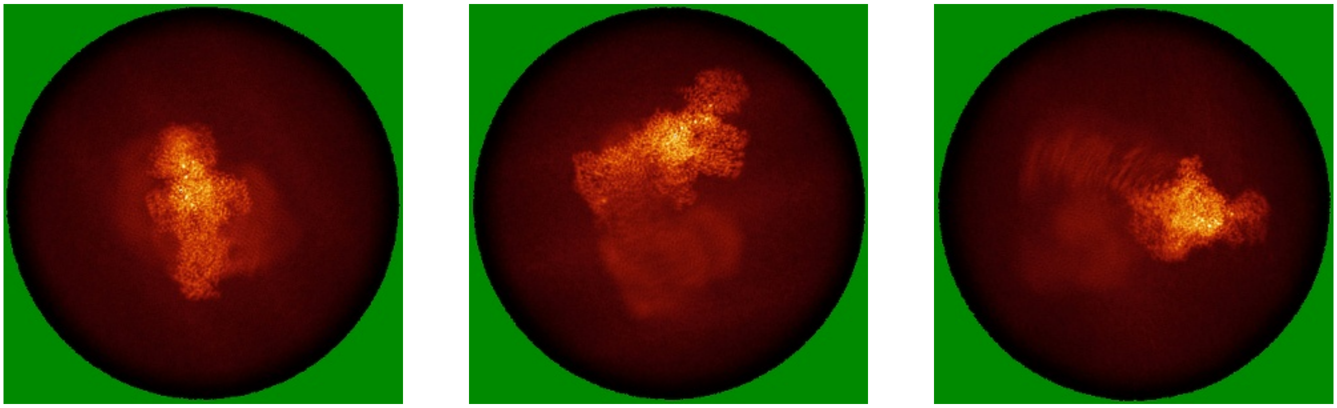


Z Index: 198

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

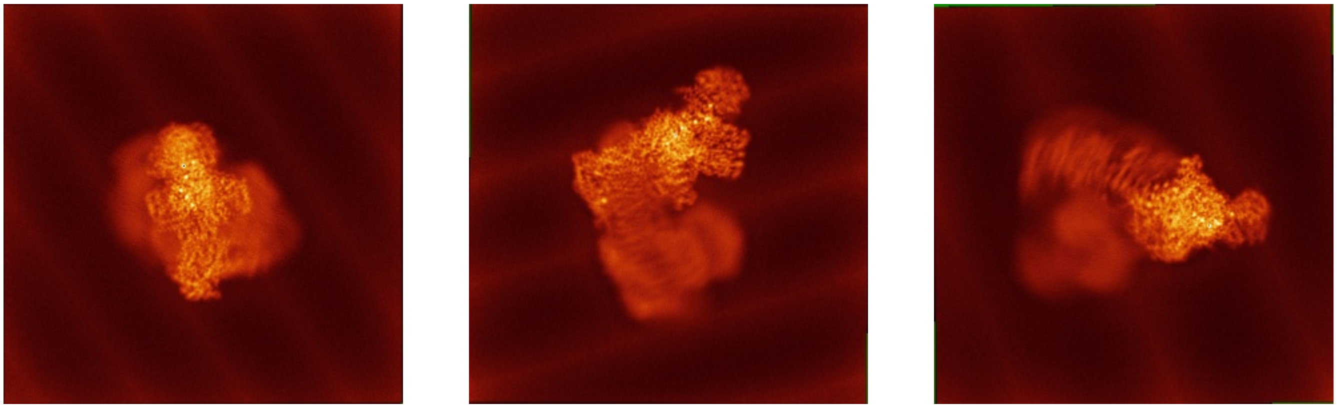
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

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 ⓘ

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.

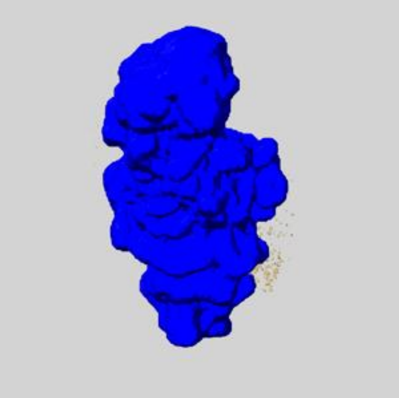
6.6 Mask visualisation ⓘ

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

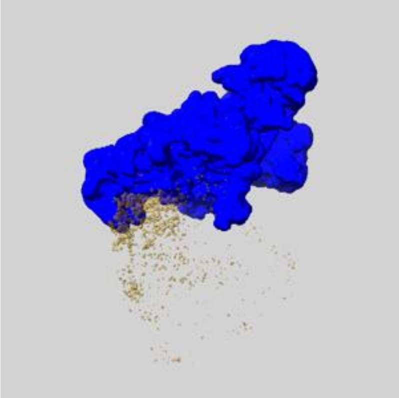
A mask typically either:

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

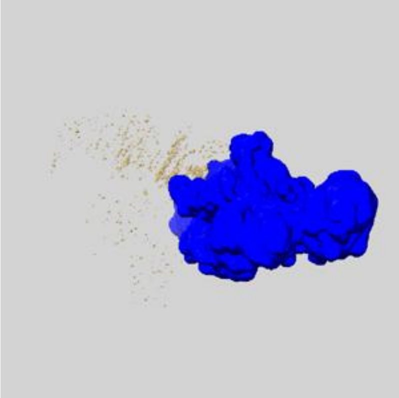
6.6.1 emd_35332_msk_1.map ⓘ



X



Y

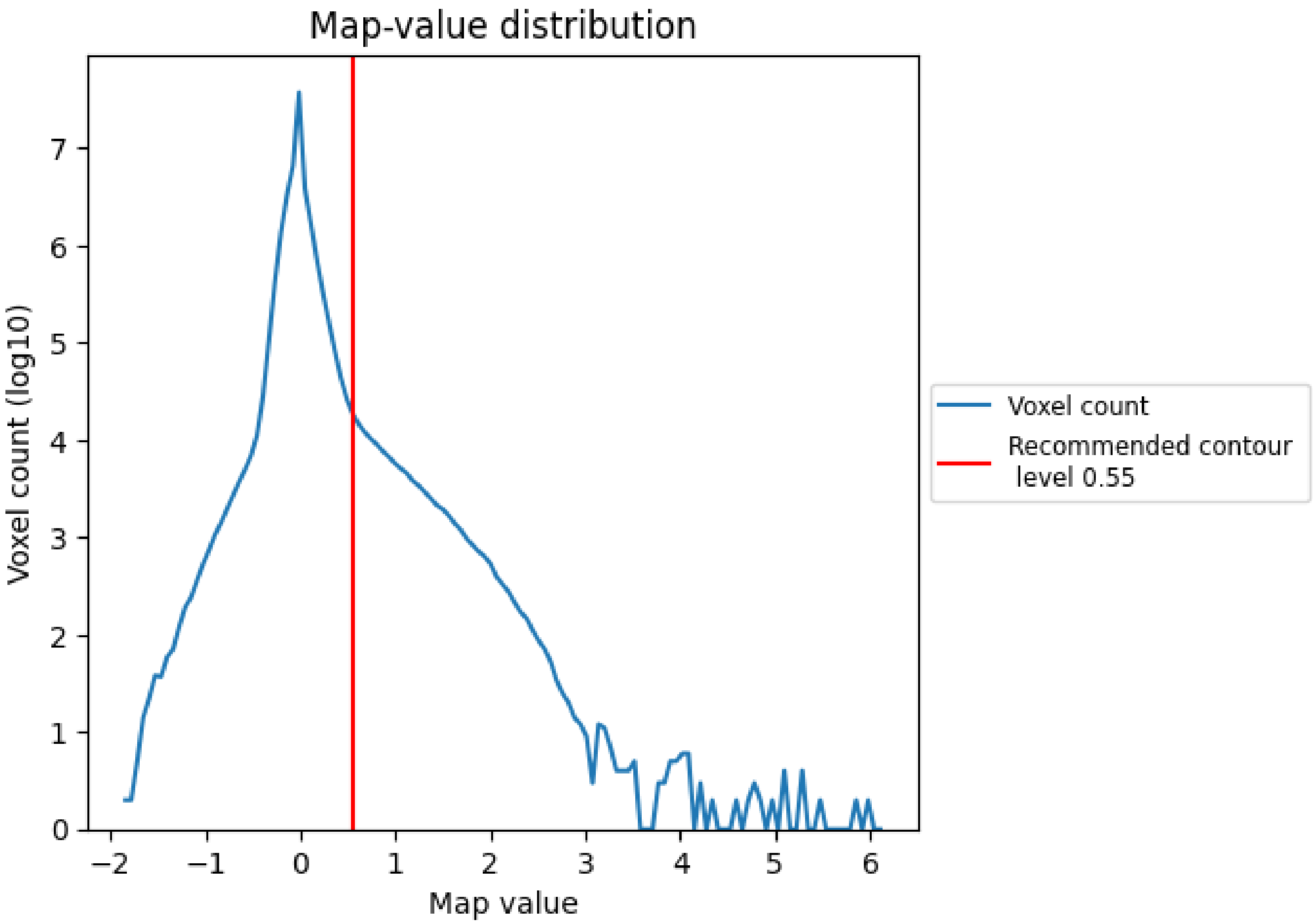


Z

7 Map analysis ⓘ

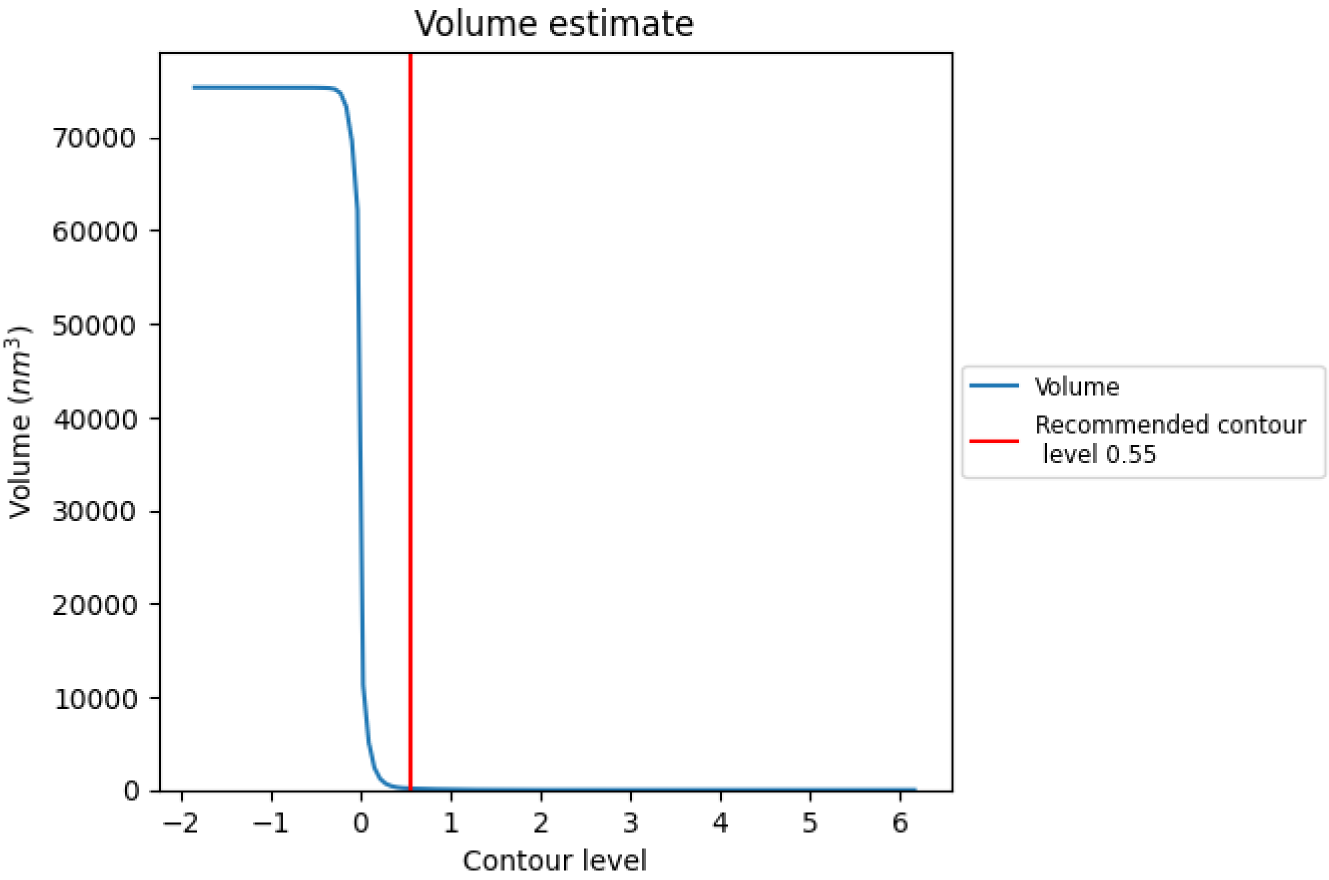
This section contains the results of statistical analysis of the map.

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.

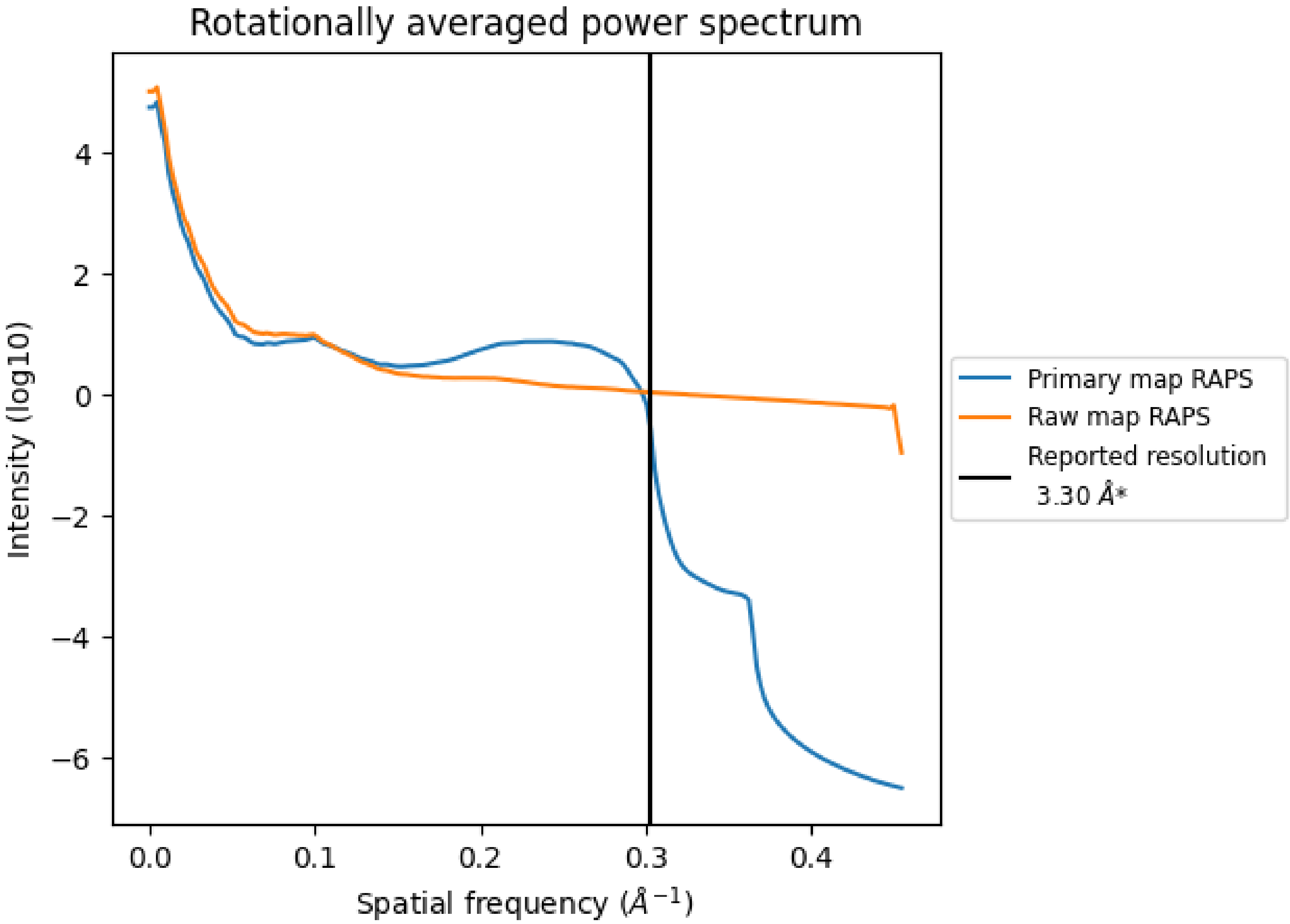
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 148 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 ⓘ

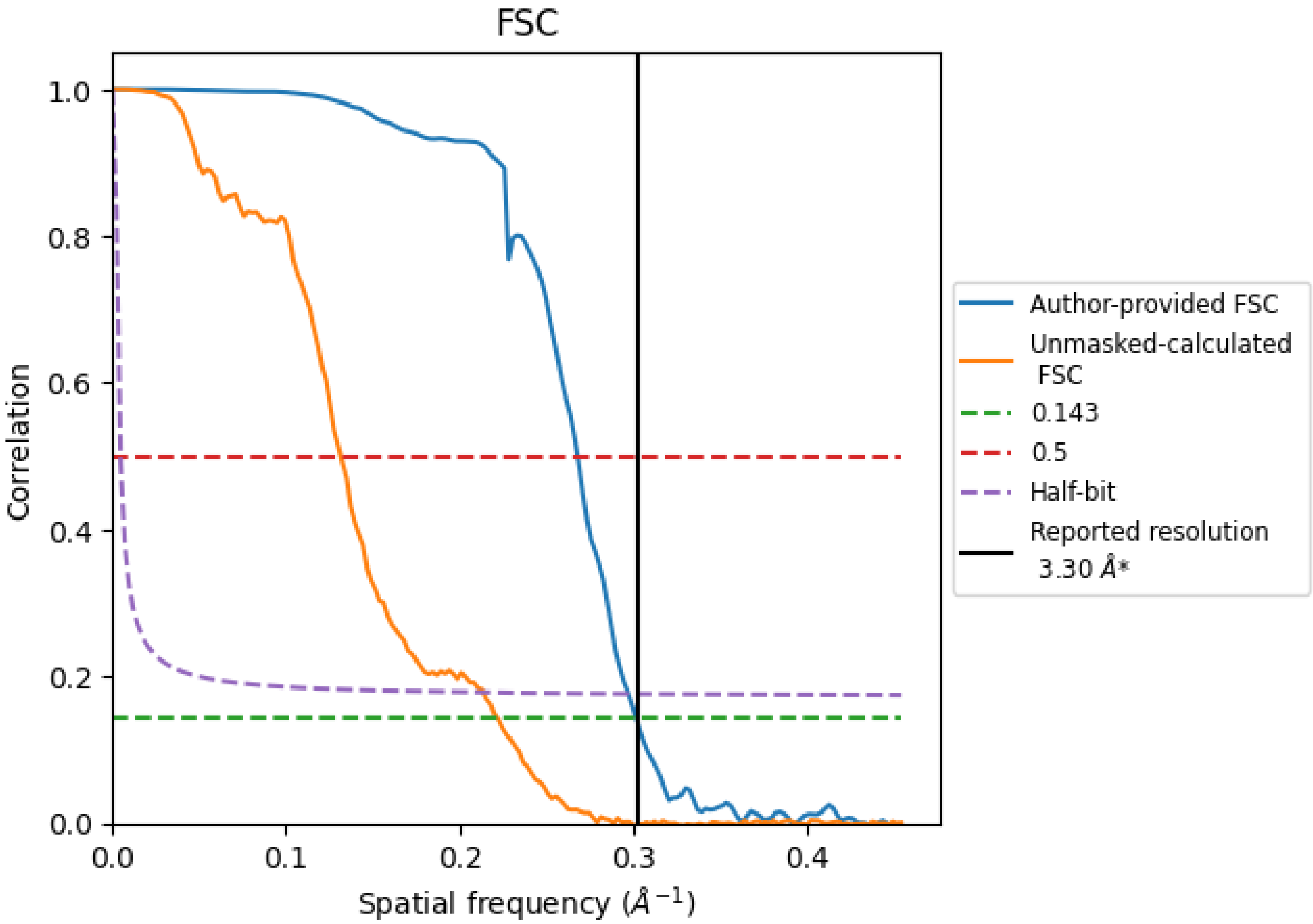


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 ⓘ

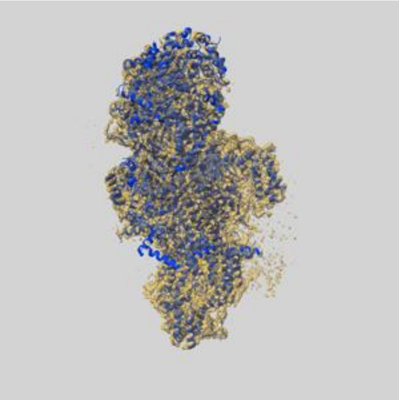
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.73	3.36
Unmasked-calculated*	4.50	7.60	4.68

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

9 Map-model fit ⓘ

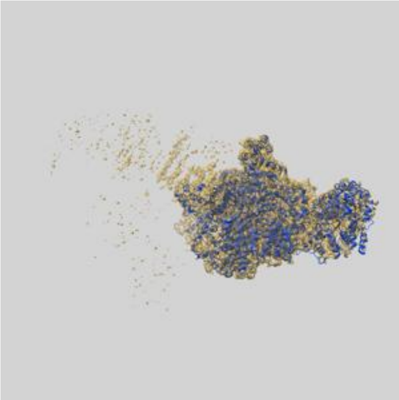
This section contains information regarding the fit between EMDB map EMD-35332 and PDB model 8IB5. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay ⓘ



X

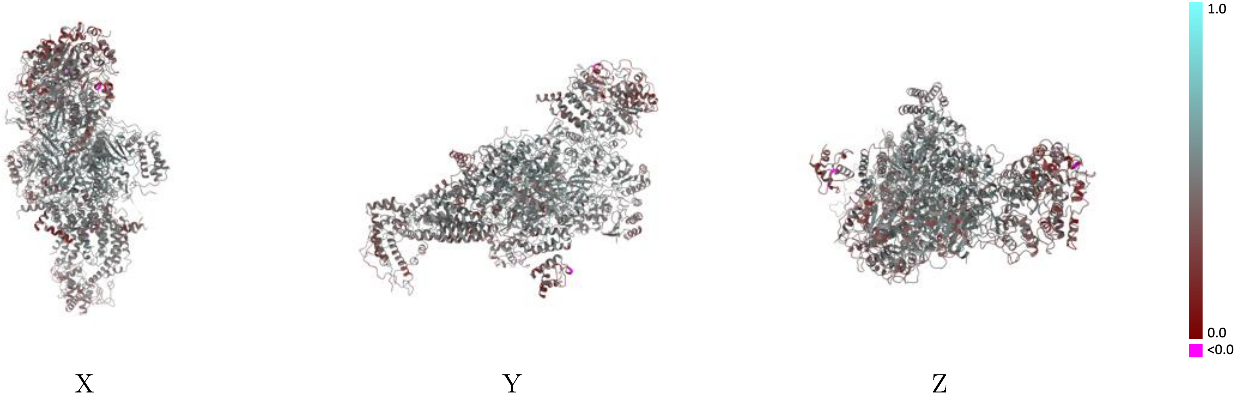
Y



Z

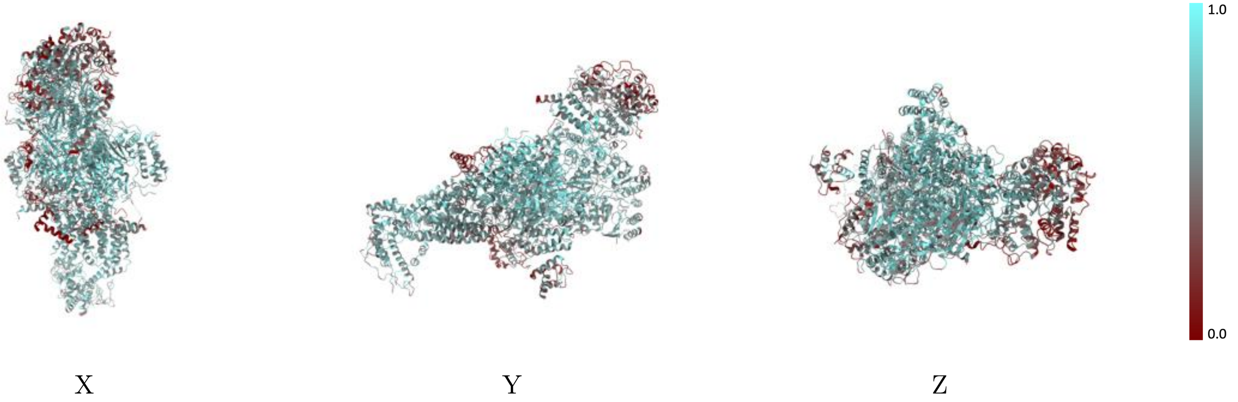
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



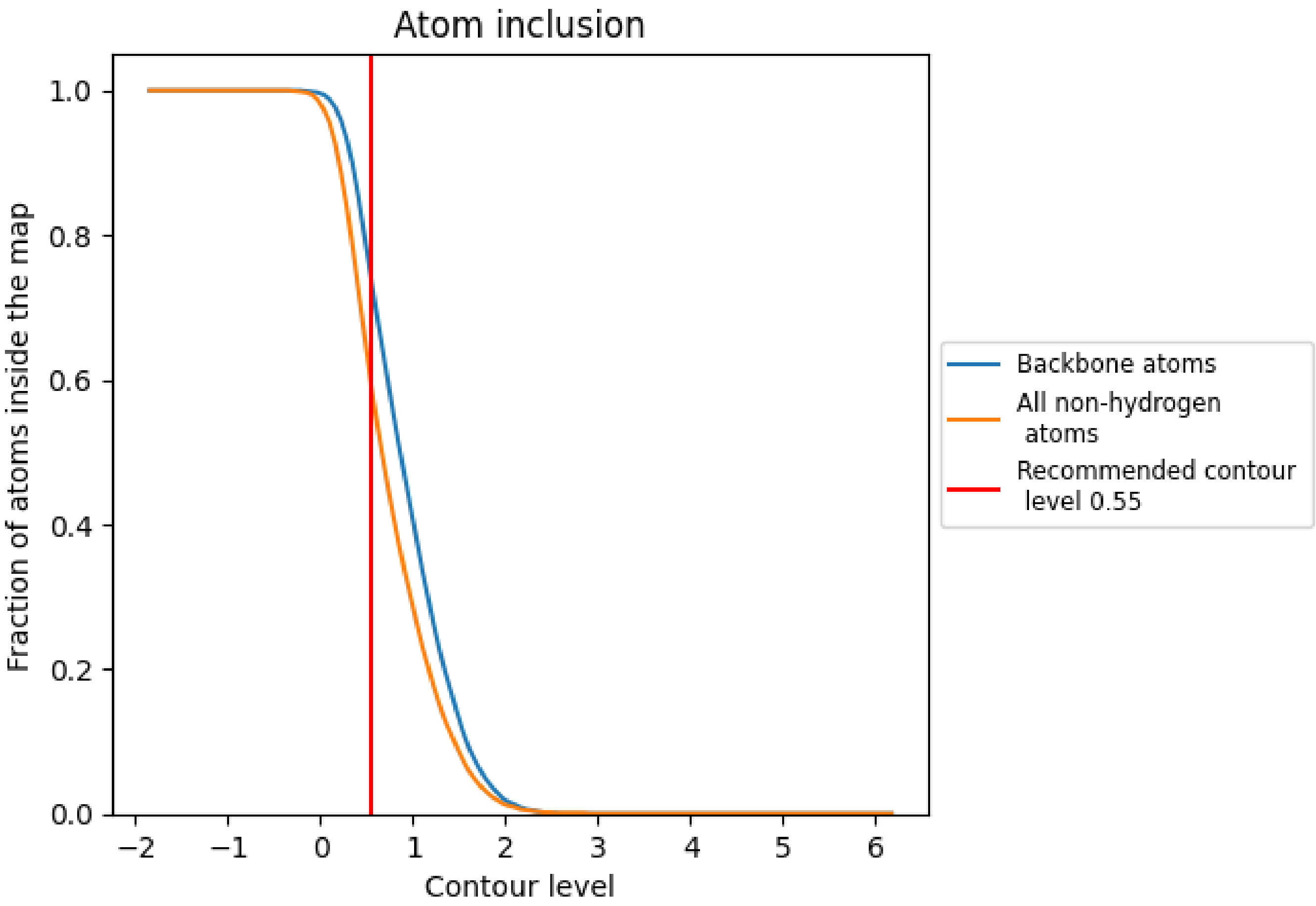
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 ⓘ



At the recommended contour level, 74% of all backbone atoms, 59% 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	0.5900	0.4470
A	0.5110	0.4430
B	0.7060	0.5030
C	0.7550	0.5190
D	0.7540	0.5140
E	0.3690	0.3900
F	0.4820	0.3970
G	0.6830	0.4660
H	0.6260	0.4750
I	0.7400	0.5030
P	0.4820	0.4230
Q	0.6150	0.4940
R	0.2630	0.3910
S	0.5990	0.3990
T	0.4110	0.2890
V	0.6620	0.4510
W	0.6020	0.4650
X	0.6160	0.3900
Z	0.6250	0.4130
a	0.6430	0.4470
b	0.5260	0.4310
q	0.2690	0.3810
r	0.3250	0.3660
s	0.0790	0.2480