



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 10:31 AM JST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

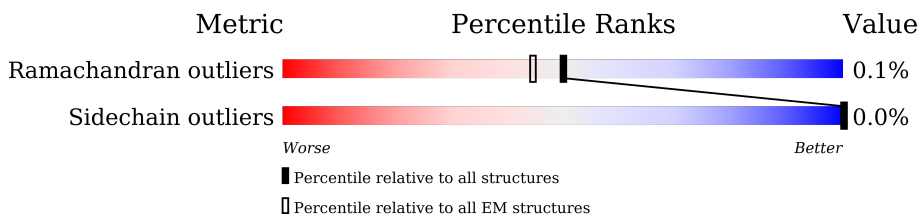
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.60 Å.

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



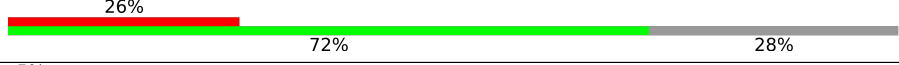

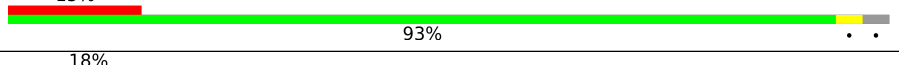
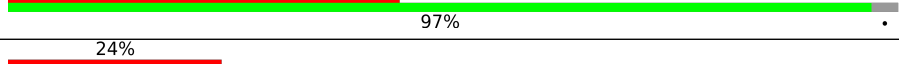
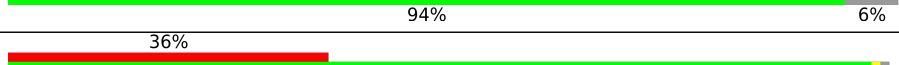
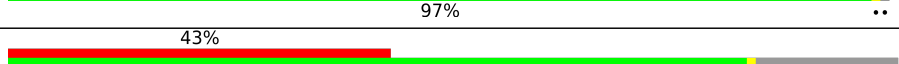
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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 33 unique types of molecules in this entry. The entry contains 34420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	91	743	517	103	118	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	381	3056	1951	527	556	22	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			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	310	2479	1667	376	414	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	178	1431	898	245	276	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	339	2720	1759	476	478	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
			Total	C	N	O	S		
13	S	83	667	419	126	119	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

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

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

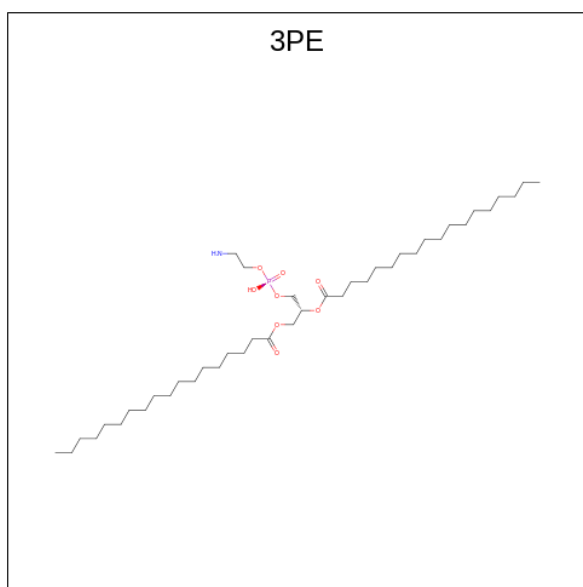
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

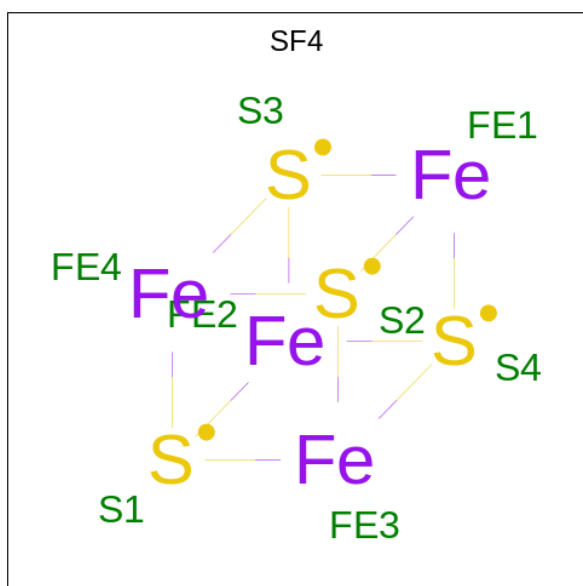
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



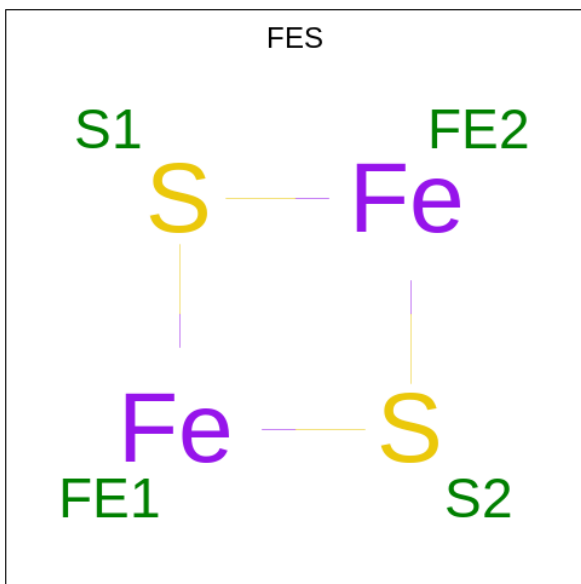
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	A	1	46	36	1	8	1	0
24	H	1	46	36	1	8	1	0
24	b	1	46	36	1	8	1	0

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



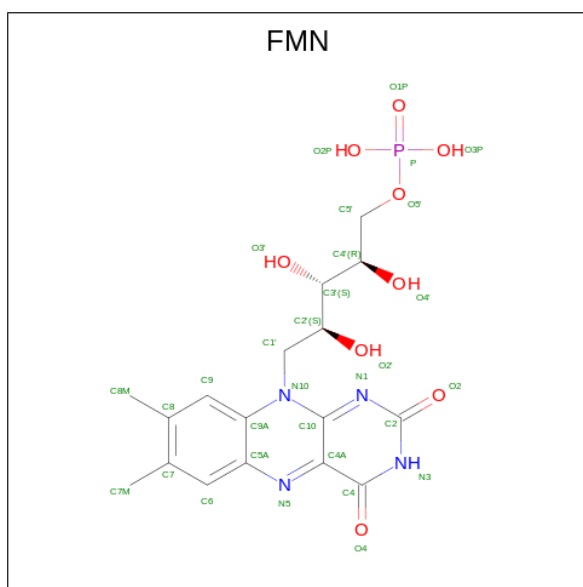
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	
25	F	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	G	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	
25	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



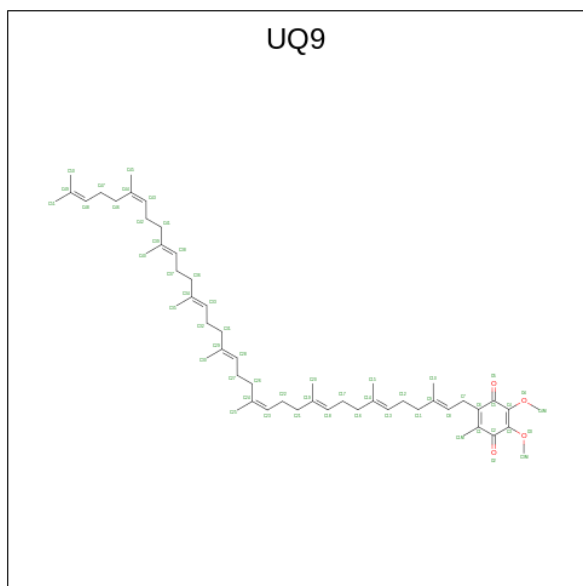
Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	Fe	S	0
			4	2	2	
26	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



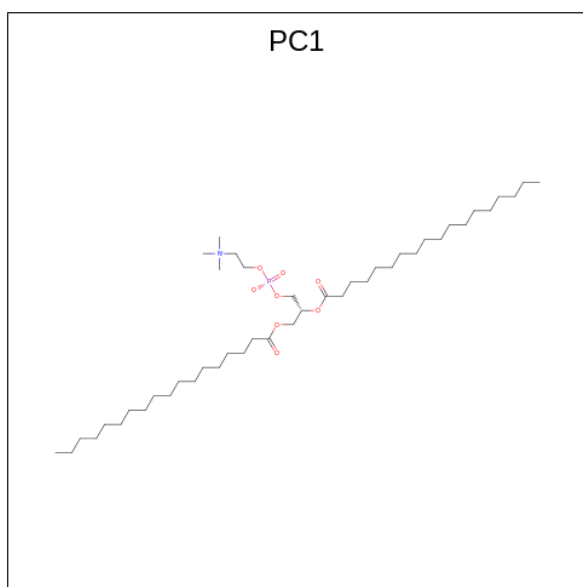
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	F	1	31	17	4	9	1	0

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



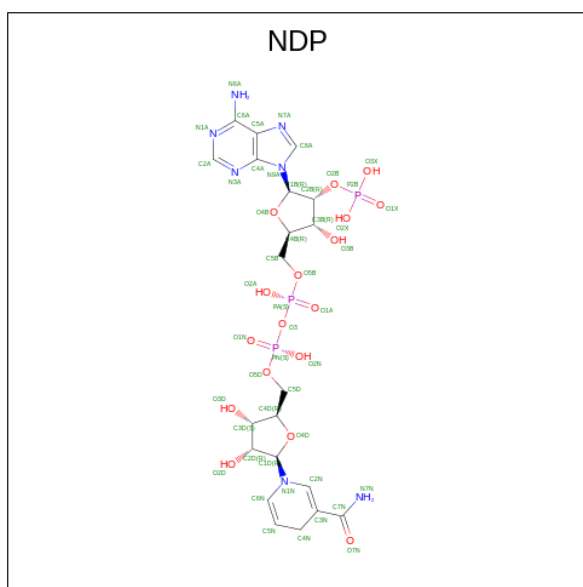
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	H	1	35	31	4	0

- Molecule 29 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
			Total	C	N	O	P	
29	I	1	47	37	1	8	1	0
29	q	1	35	25	1	8	1	0

- Molecule 30 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).

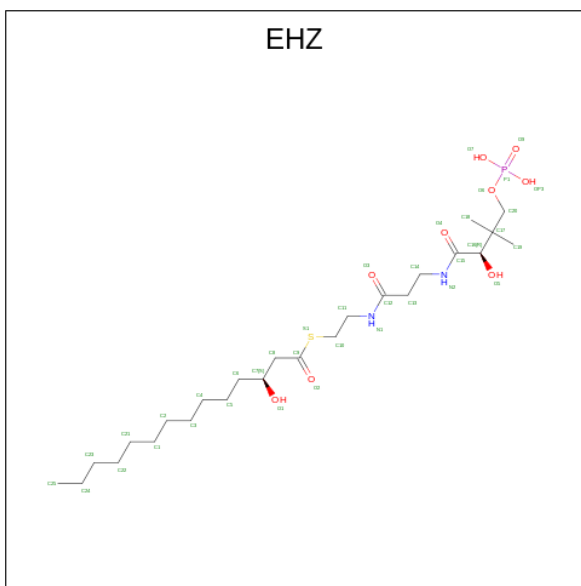


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
30	P	1	48	21	7	17	3	0

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

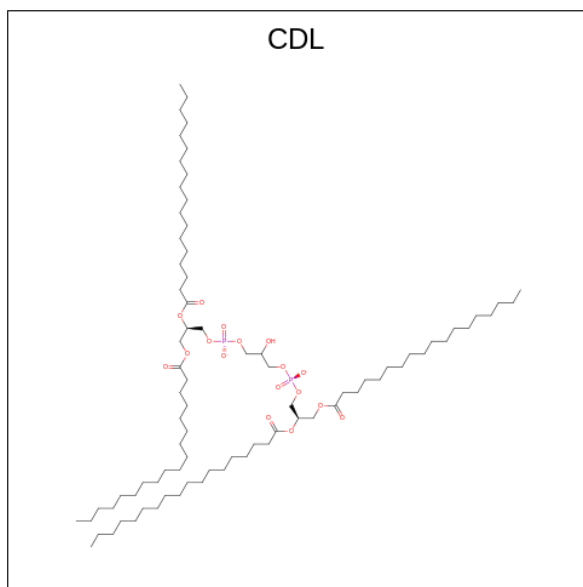
Mol	Chain	Residues	Atoms	AltConf
31	R	1	Total Zn 1 1	0

- Molecule 32 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

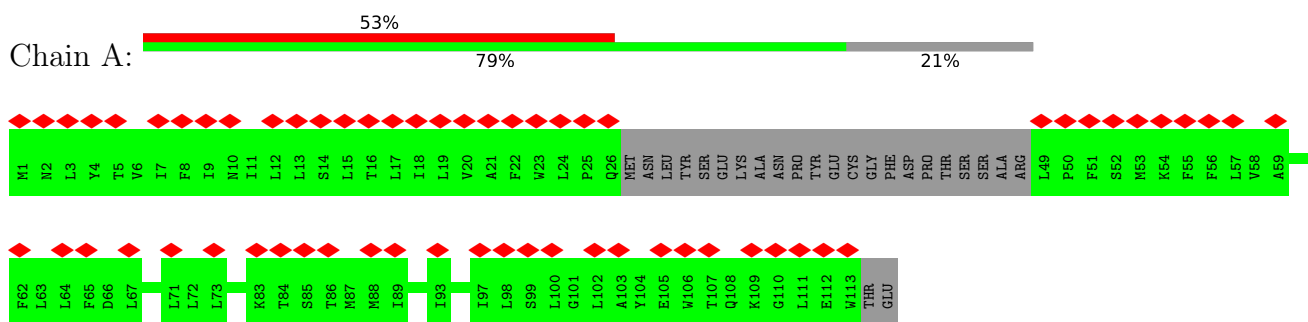


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	q	1	57	38	17	2	0

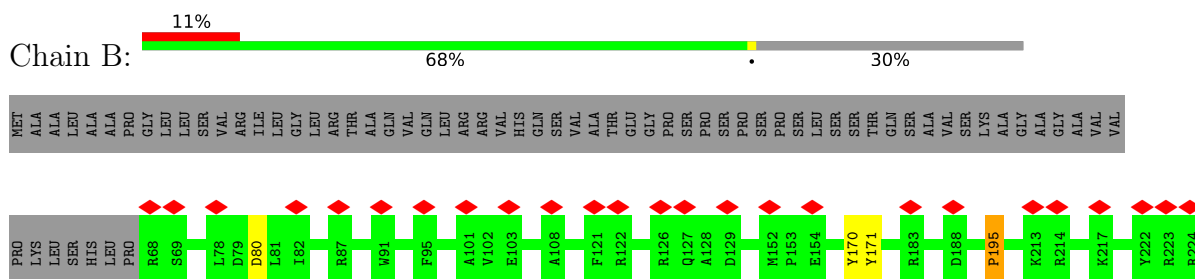
3 Residue-property plots [i](#)

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

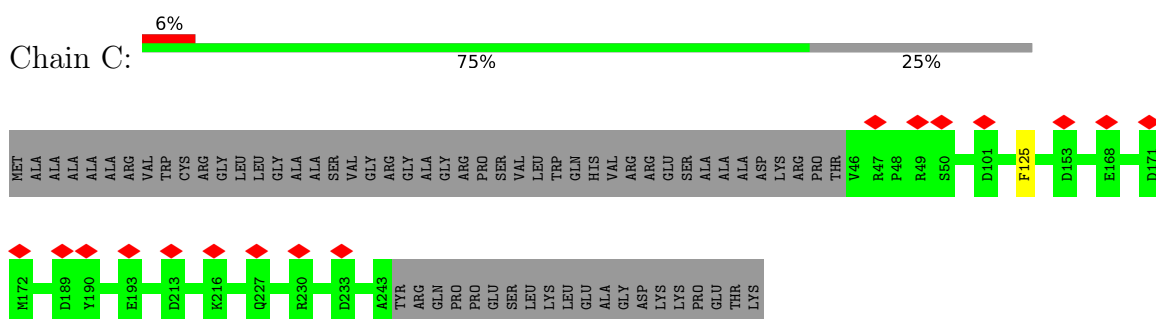
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



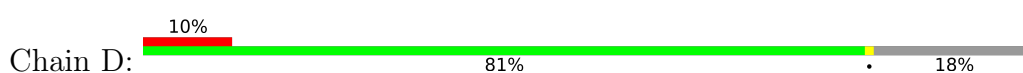
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

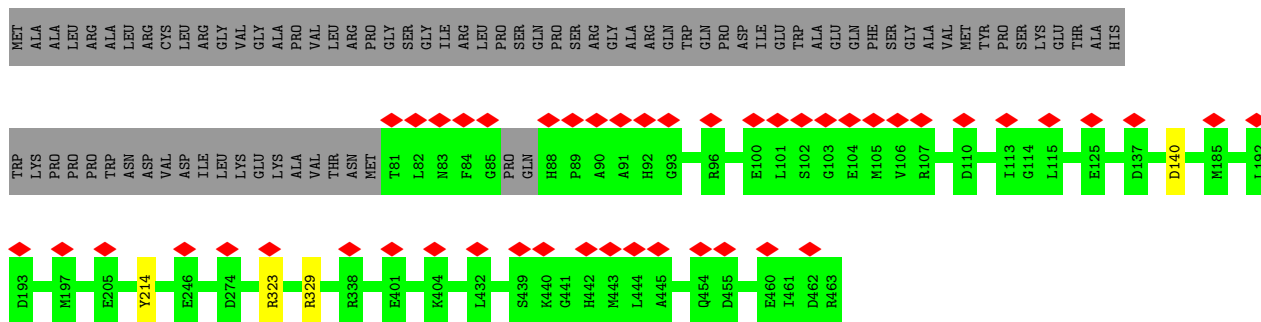


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

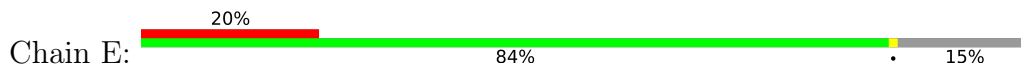


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

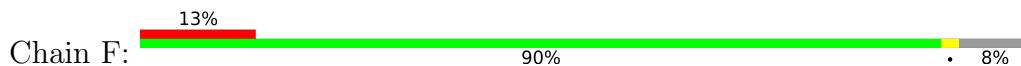




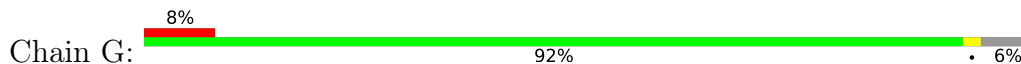
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



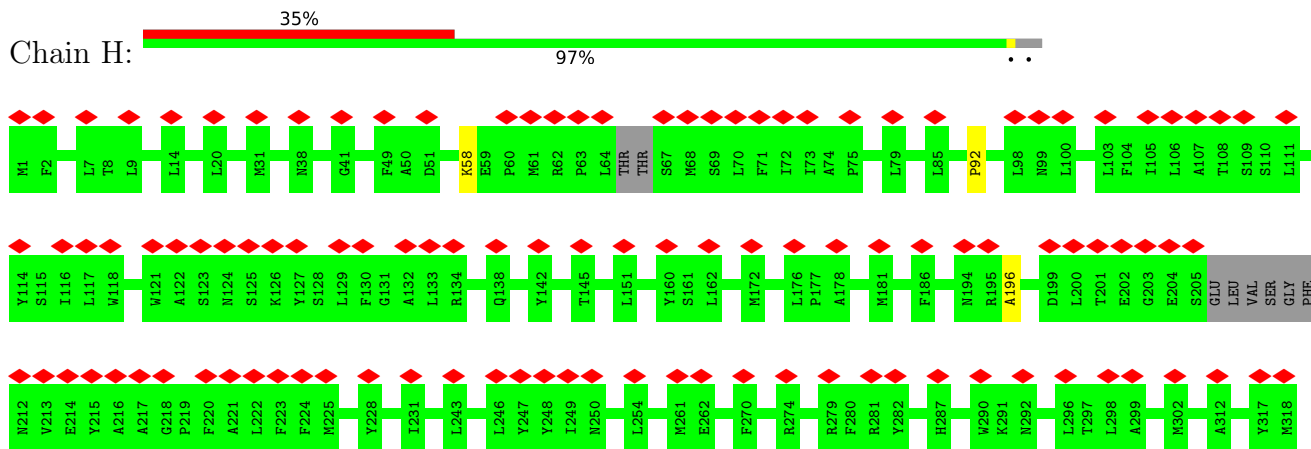
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



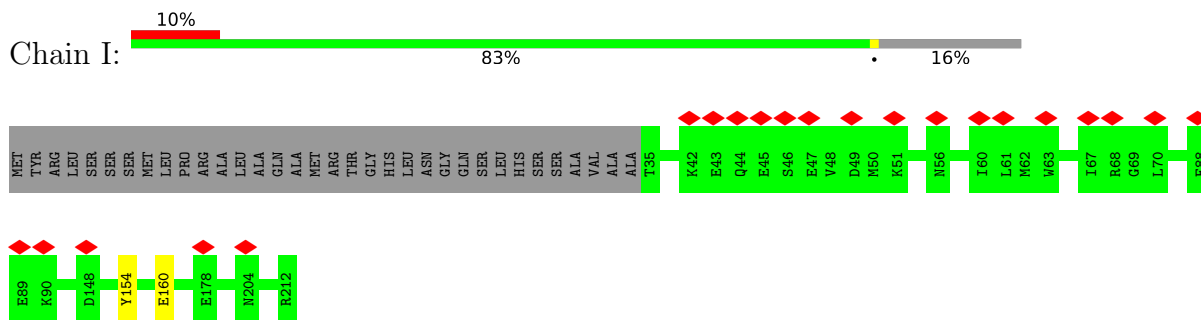
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



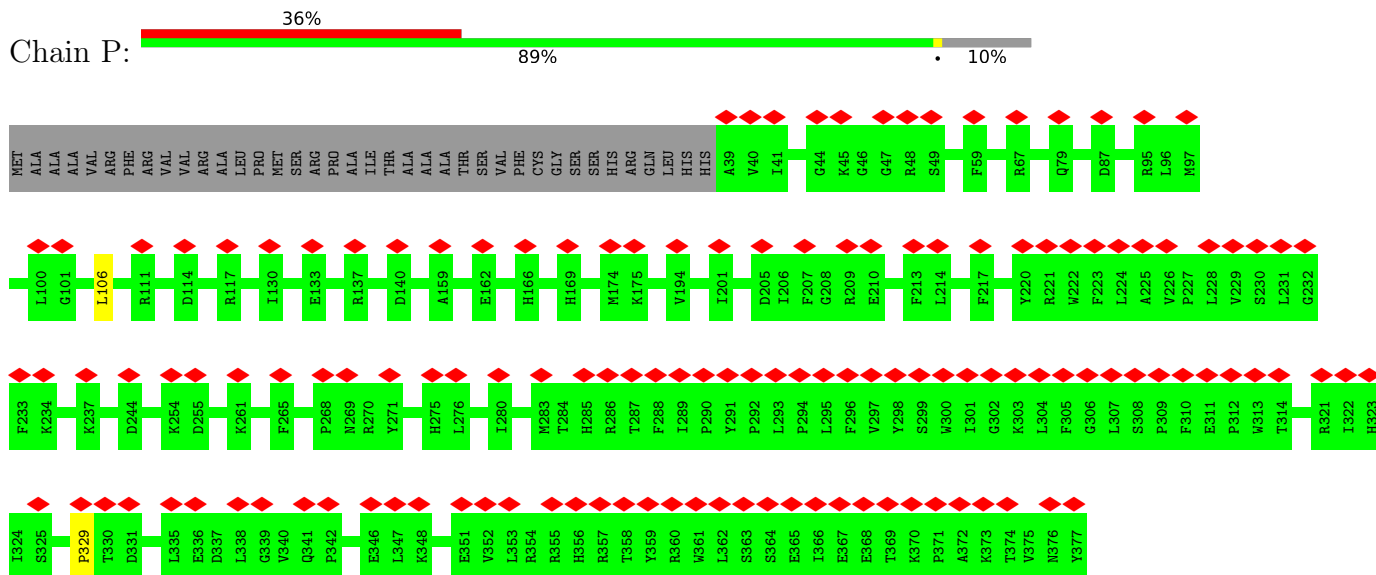
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

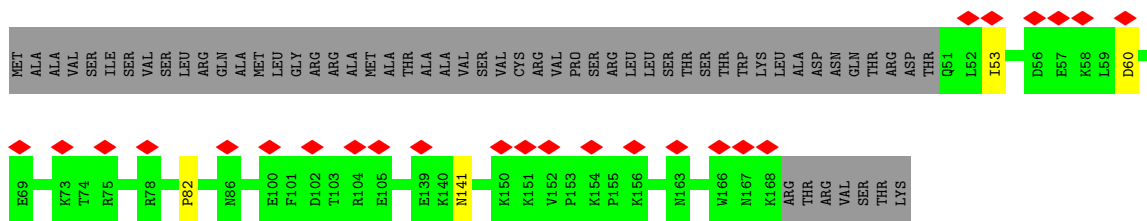


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

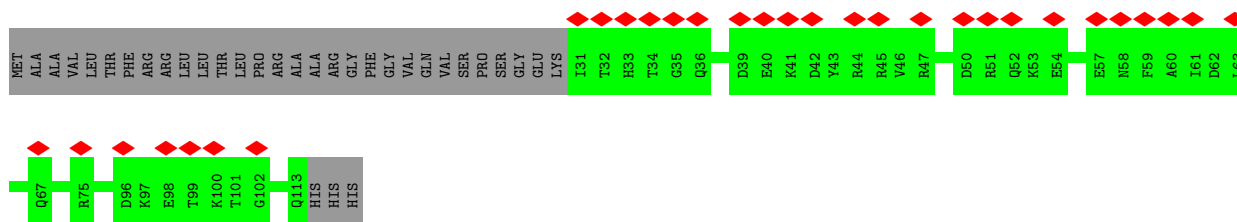
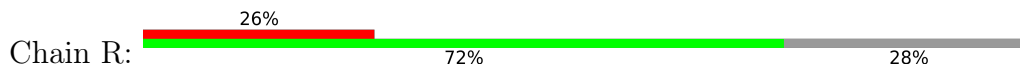


• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

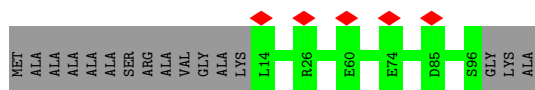
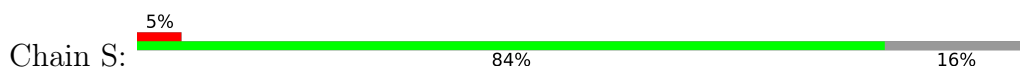




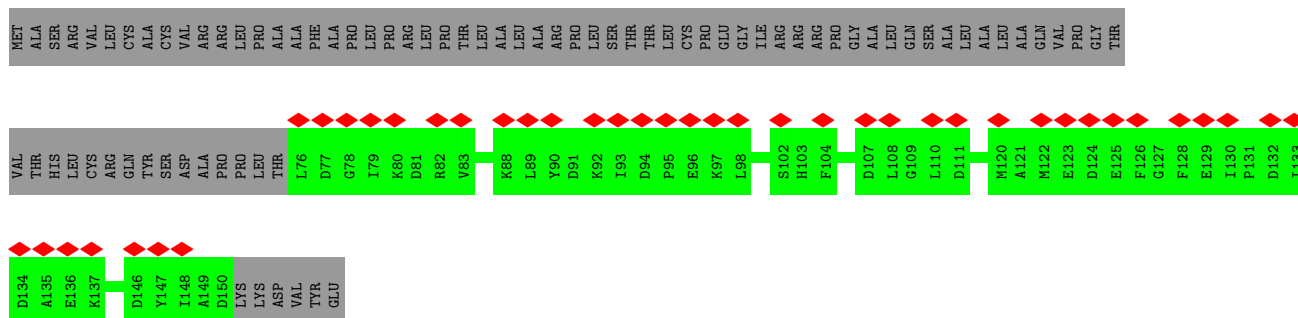
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



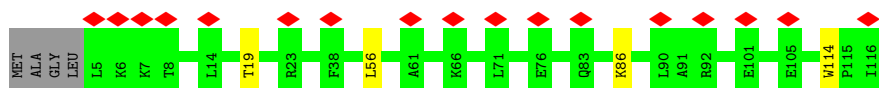
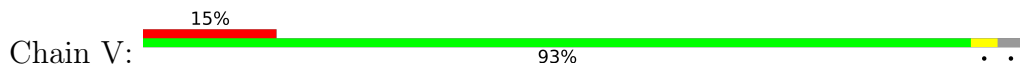
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



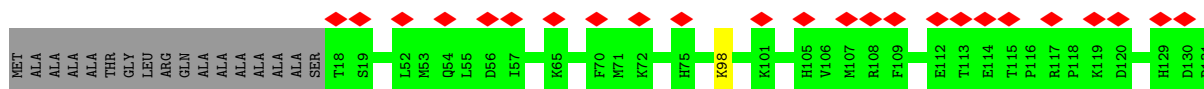
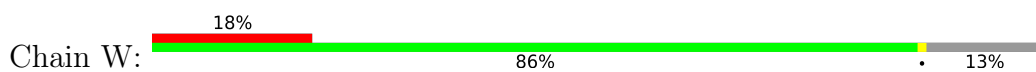
- Molecule 14: Acyl carrier protein, mitochondrial



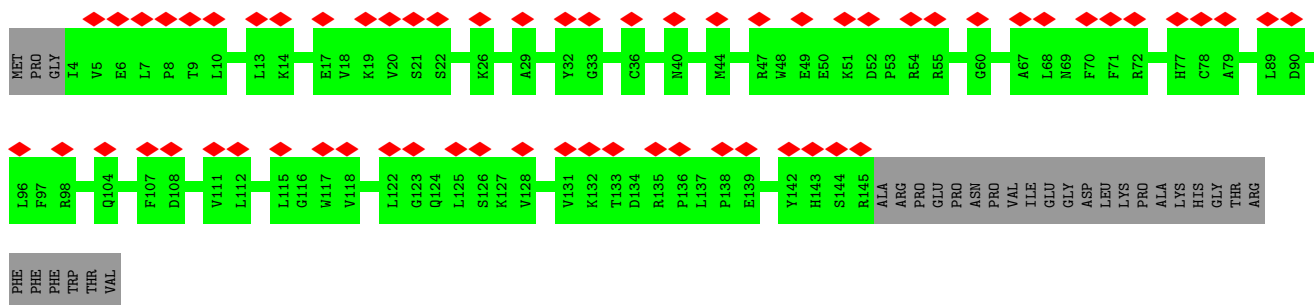
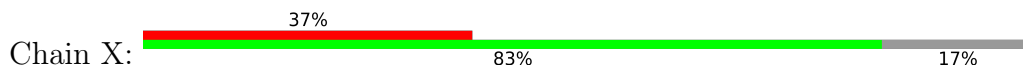
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



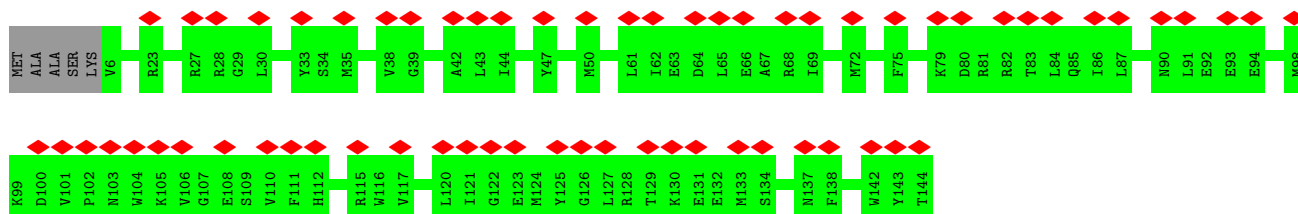
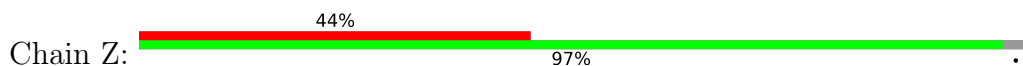
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



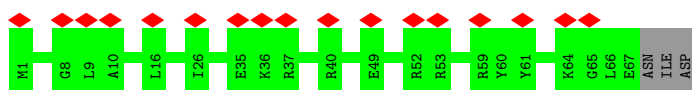
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



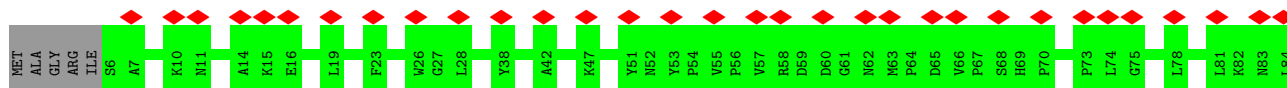
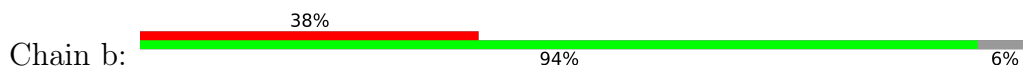
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

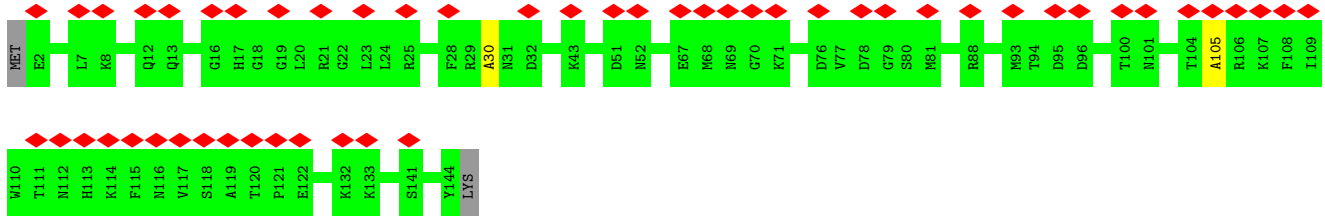


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

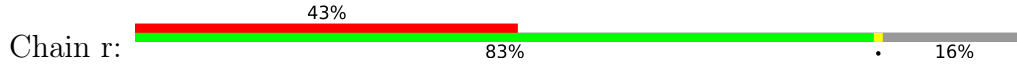


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

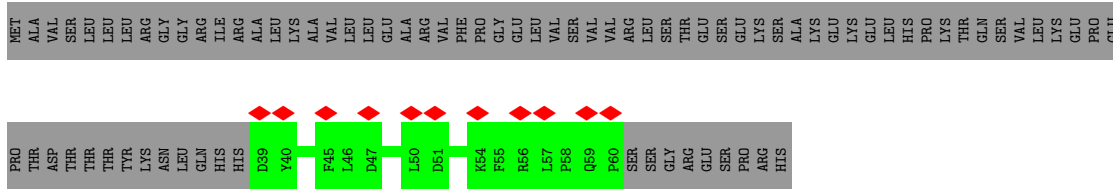




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- 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	14488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.762	Depositor
Minimum map value	-0.854	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: CDL, NDP, 3PE, UQ9, FES, FMN, SF4, EHZ, PC1, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/763	0.68	0/1042
2	B	0.61	0/1289	0.83	2/1744 (0.1%)
3	C	0.55	0/1687	0.78	1/2297 (0.0%)
4	D	0.63	0/3128	0.91	4/4228 (0.1%)
5	E	0.45	0/1675	0.62	2/2282 (0.1%)
6	F	0.60	4/3363 (0.1%)	0.79	4/4543 (0.1%)
7	G	0.61	3/5374 (0.1%)	0.96	16/7281 (0.2%)
8	H	0.61	1/2553 (0.0%)	0.79	1/3486 (0.0%)
9	I	0.58	0/1461	0.88	2/1974 (0.1%)
10	P	0.50	0/2793	0.67	1/3787 (0.0%)
11	Q	0.60	2/980 (0.2%)	0.79	2/1324 (0.2%)
12	R	0.47	0/671	0.58	0/903
13	S	0.56	0/678	0.81	0/915
14	T	0.39	0/613	0.62	0/826
15	V	0.54	0/937	0.81	4/1270 (0.3%)
16	W	0.50	0/993	0.62	1/1335 (0.1%)
17	X	0.47	0/1191	0.70	0/1605
18	Z	0.45	0/1183	0.64	0/1597
19	a	0.55	0/561	0.61	0/755
20	b	0.45	0/643	0.56	0/884
21	q	0.47	0/1234	0.73	2/1681 (0.1%)
22	r	0.40	0/782	0.59	0/1058
23	s	0.32	0/194	0.57	0/264
All	All	0.55	10/34746 (0.0%)	0.79	42/47081 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	227	PRO	N-CD	10.07	1.61	1.47
6	F	234	GLY	CA-C	-6.88	1.40	1.51
7	G	541	PRO	N-CD	-6.83	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	449	PRO	N-CD	6.62	1.57	1.47
6	F	384	PRO	N-CD	-6.21	1.39	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	632	ILE	N-CA-C	-8.52	88.01	111.00
16	W	98	LYS	N-CA-C	-8.15	89.00	111.00
7	G	174	THR	N-CA-C	-8.15	89.01	111.00
11	Q	60	ASP	N-CA-C	-7.64	90.37	111.00
7	G	204	MET	N-CA-C	-7.24	91.45	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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	10	41
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	377/463 (81%)	362 (96%)	15 (4%)	0	100	100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	407 (96%)	17 (4%)	0	100	100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	304/318 (96%)	290 (95%)	13 (4%)	1 (0%)	37	67
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	37	67
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
15	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
16	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
19	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
20	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
21	q	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	12	45
23	s	20/104 (19%)	20 (100%)	0	0	100	100
All	All	4193/5036 (83%)	3978 (95%)	210 (5%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
10	P	329	PRO
2	B	171	TYR
22	r	39	PRO
2	B	195	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/104 (80%)	83 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	79	88
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	328/395 (83%)	328 (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	273/280 (98%)	273 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	P	296/325 (91%)	296 (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
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	70/73 (96%)	70 (100%)	0	100	100
21	q	129/131 (98%)	129 (100%)	0	100	100
22	r	85/96 (88%)	85 (100%)	0	100	100
23	s	22/95 (23%)	22 (100%)	0	100	100
All	All	3685/4292 (86%)	3684 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
2	B	170	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
10	P	251	ASN

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Mol	Chain	Res	Type
17	X	69	ASN
10	P	275	HIS
13	S	25	GLN
19	a	31	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
25	SF4	G	801	7	0,12,12	-	-	-	-	-
26	FES	E	301	5	0,4,4	-	-	-	-	-
32	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	6 (16%)
24	3PE	H	402	-	45,45,50	0.95	2 (4%)	48,50,55	1.12	2 (4%)
29	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
24	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
25	SF4	F	502	6	0,12,12	-	-	-	-	-
25	SF4	I	302	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.23	7 (14%)
28	UQ9	H	401	-	35,35,58	0.80	2 (5%)	42,45,73	0.63	0
25	SF4	G	802	7	0,12,12	-	-	-	-	-
29	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
25	SF4	I	303	9	0,12,12	-	-	-	-	-
25	SF4	B	301	2	0,12,12	-	-	-	-	-
33	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
26	FES	G	803	7	0,4,4	-	-	-	-	-
30	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.19	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	3PE	b	201	-	-	10/49/49/54	-
25	SF4	G	801	7	-	-	0/6/5/5
26	FES	E	301	5	-	-	0/1/1/1
32	EHZ	W	201	-	-	12/39/39/45	-
24	3PE	H	402	-	-	13/49/49/54	-
24	3PE	A	401	-	-	18/49/49/54	-
25	SF4	F	502	6	-	-	0/6/5/5
28	UQ9	H	401	-	-	12/30/54/81	0/1/1/1
27	FMN	F	501	-	-	0/18/18/18	0/3/3/3
25	SF4	I	302	9	-	-	0/6/5/5
26	FES	G	803	7	-	-	0/1/1/1
29	PC1	I	301	-	-	10/50/50/57	-
25	SF4	G	802	7	-	-	0/6/5/5
25	SF4	I	303	9	-	-	0/6/5/5
25	SF4	B	301	2	-	-	0/6/5/5
33	CDL	q	201	-	-	15/67/67/110	-
29	PC1	q	202	-	-	14/38/38/57	-
30	NDP	P	401	-	-	2/30/77/77	0/5/5/5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C12-N1	5.03	1.44	1.33
27	F	501	FMN	C9A-C5A	4.80	1.49	1.41
24	b	201	3PE	O31-C31	4.28	1.45	1.33
33	q	201	CDL	OB8-CB7	4.16	1.45	1.33

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C8-C9-S1	6.06	121.13	113.63
24	A	401	3PE	O21-C21-C22	4.71	121.65	111.50
33	q	201	CDL	OA6-CA5-C11	4.38	120.94	111.50
24	H	402	3PE	O21-C21-C22	4.37	120.91	111.50
29	I	301	PC1	O21-C21-C22	4.33	120.84	111.50

There are no chirality outliers.

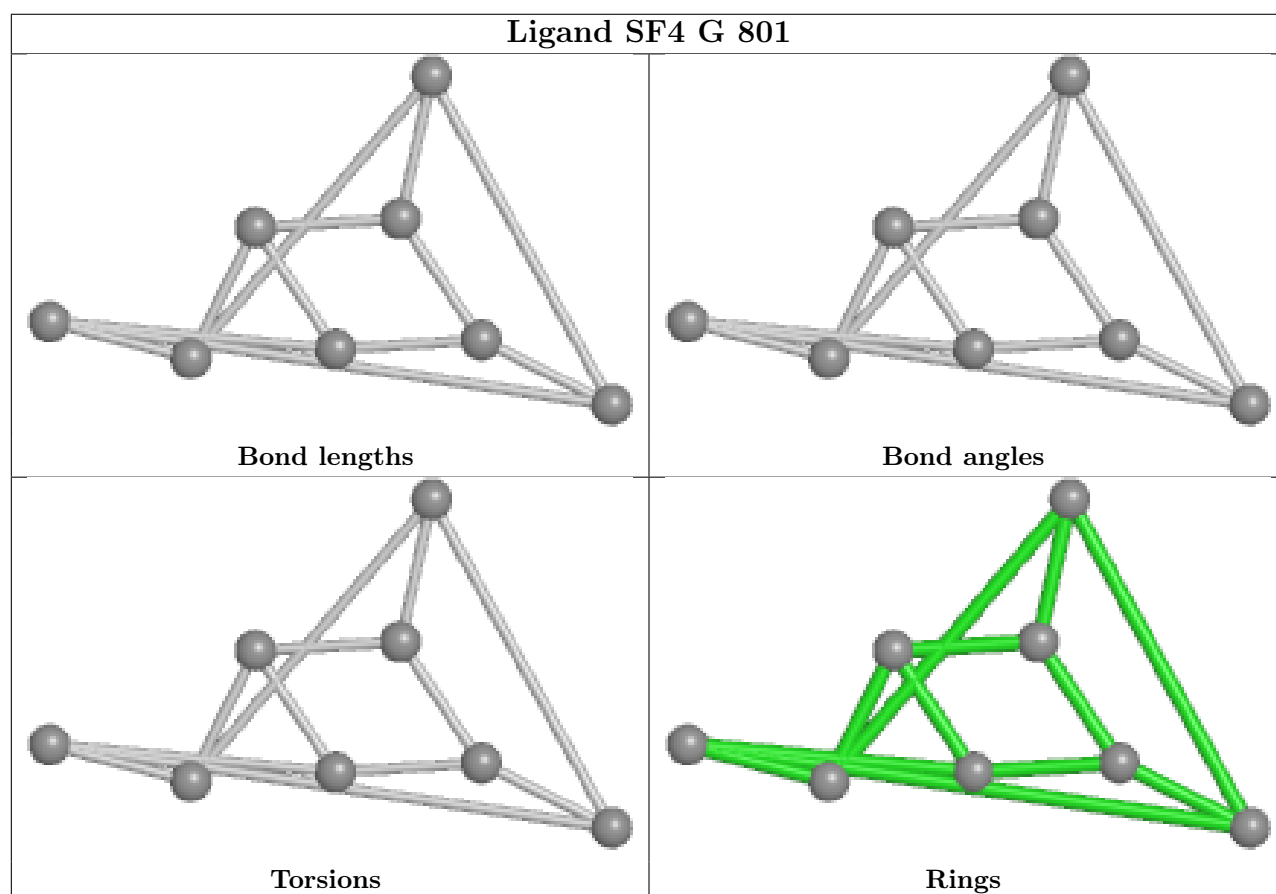
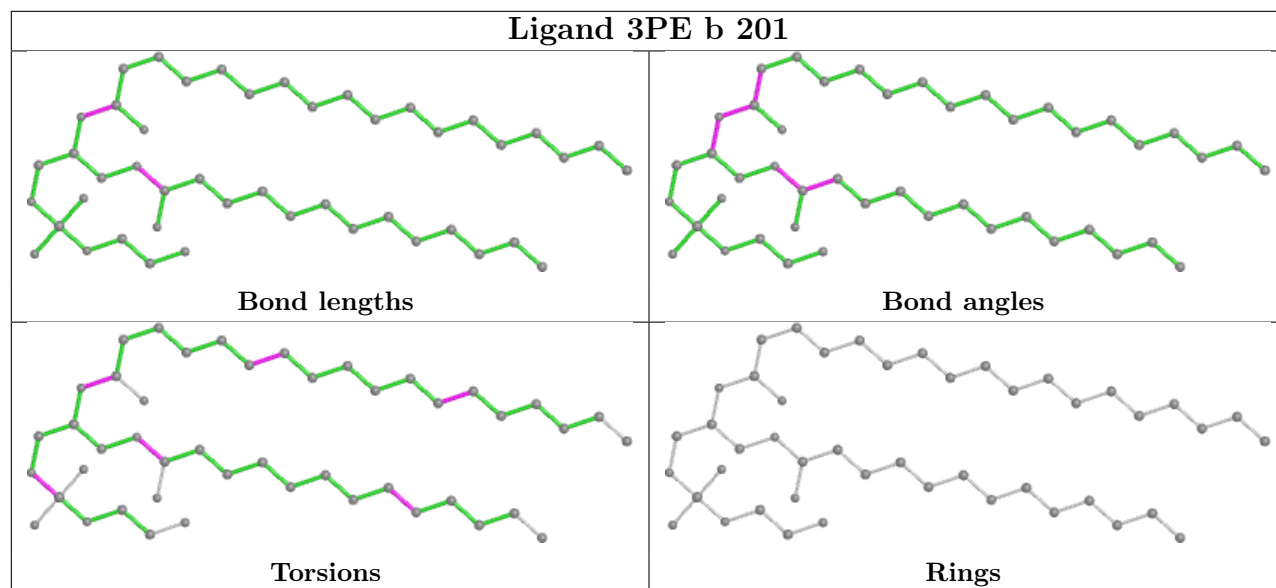
5 of 106 torsion outliers are listed below:

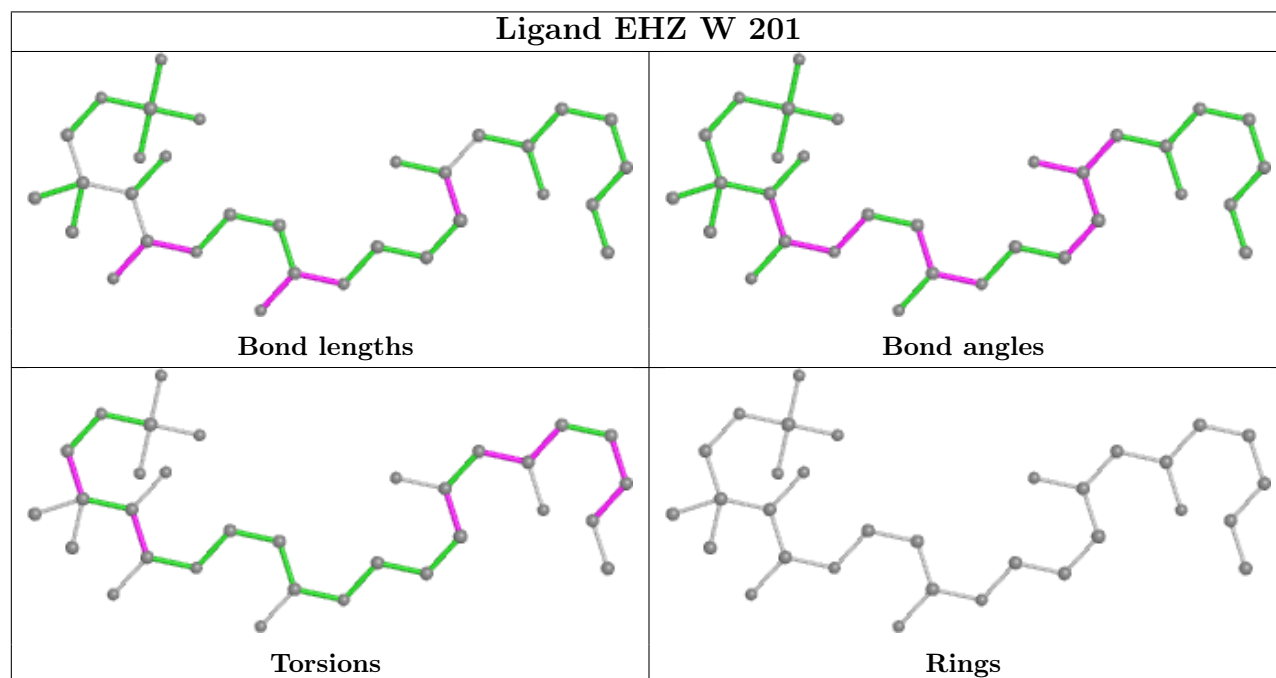
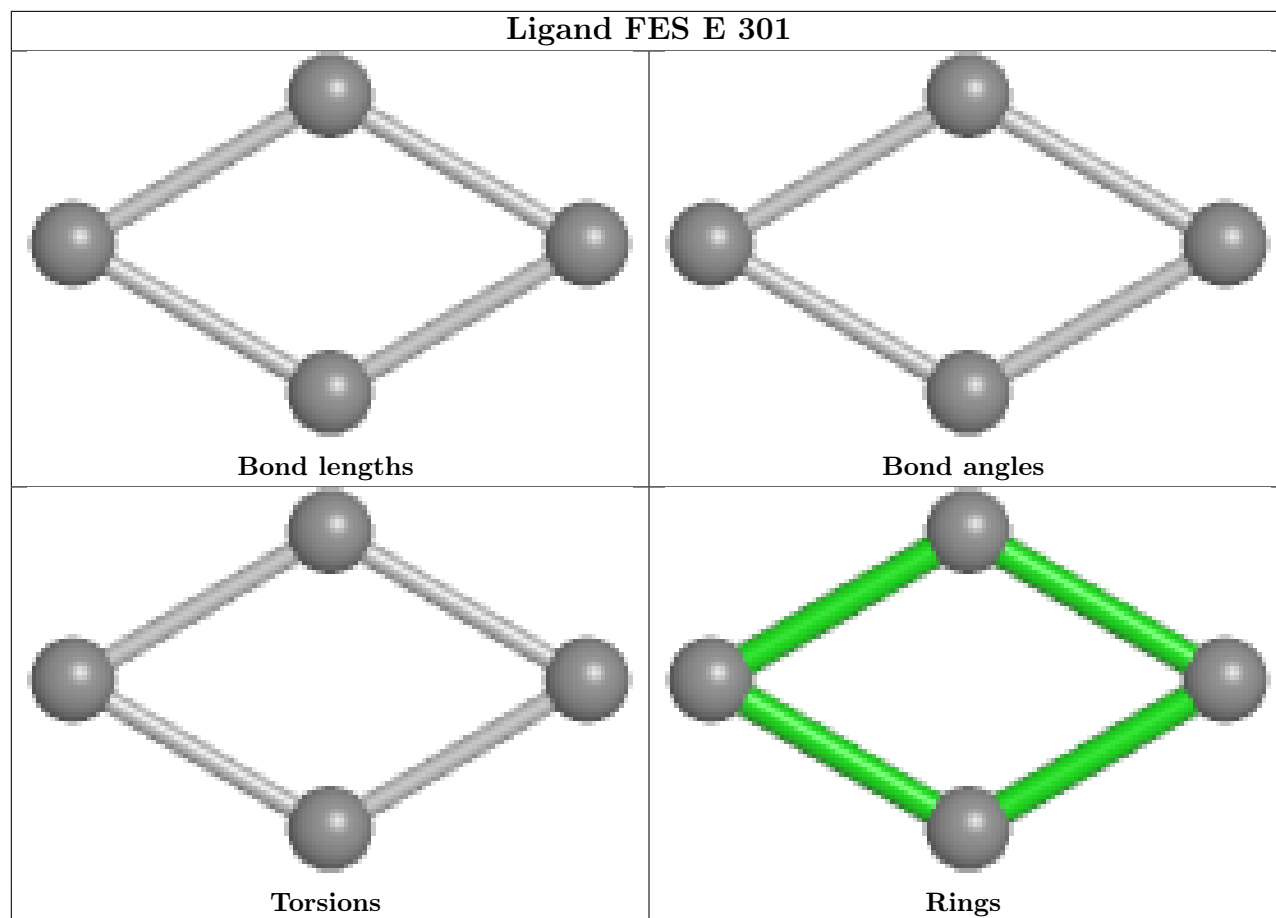
Mol	Chain	Res	Type	Atoms
24	A	401	3PE	O22-C21-O21-C2
24	H	402	3PE	C1-O11-P-O12
24	b	201	3PE	C1-O11-P-O14
24	b	201	3PE	O22-C21-O21-C2
28	H	401	UQ9	C6-C7-C8-C9

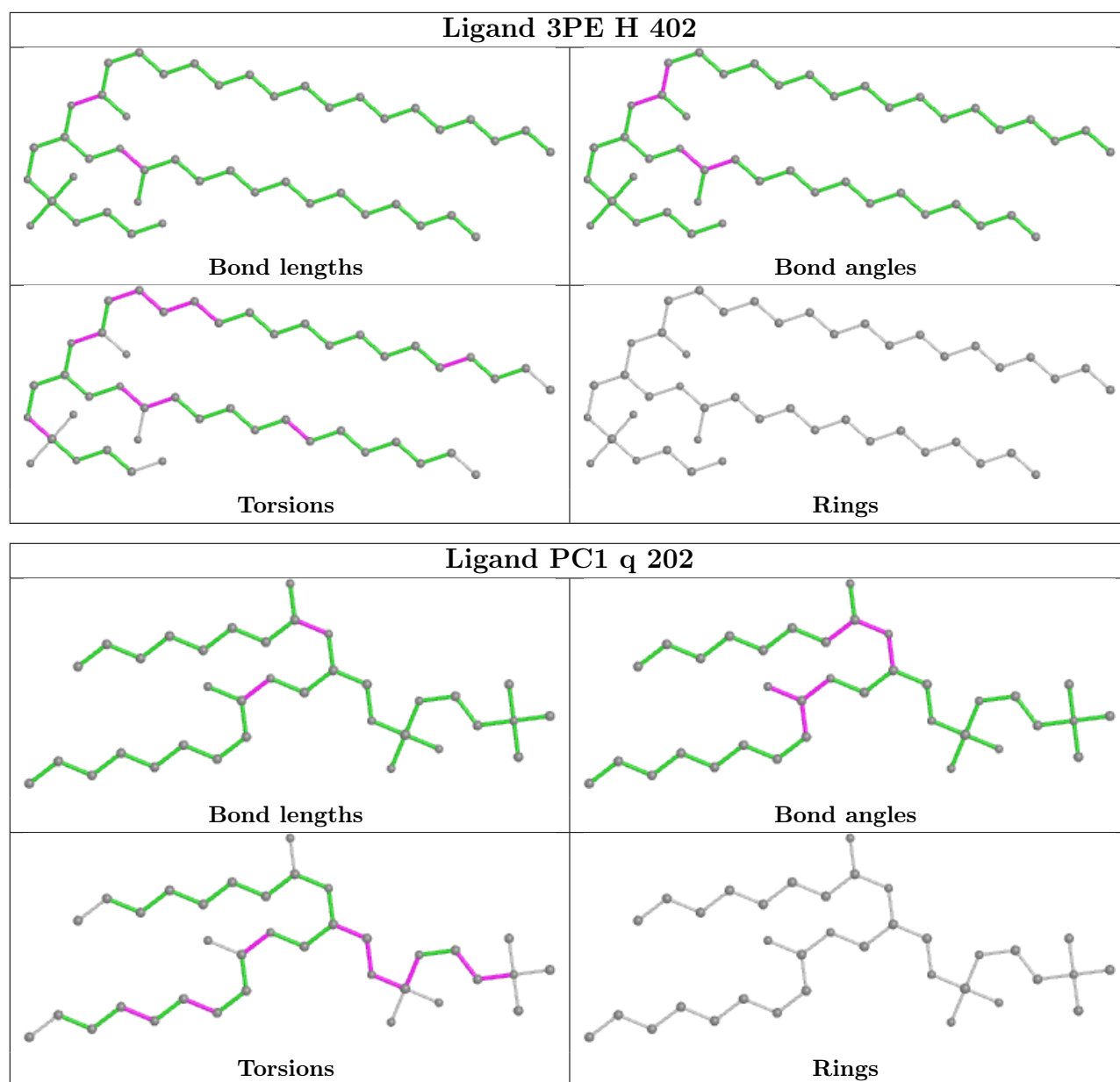
There are no ring outliers.

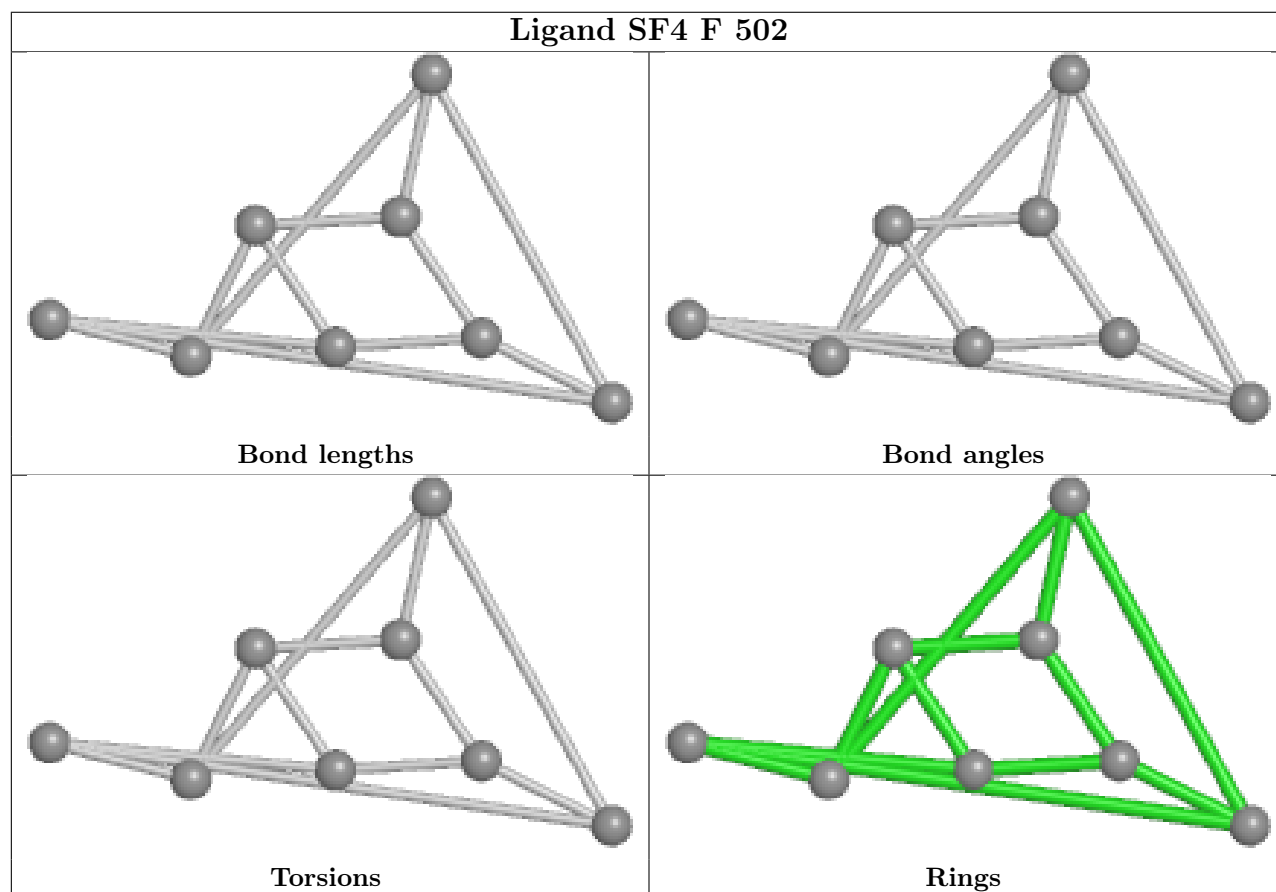
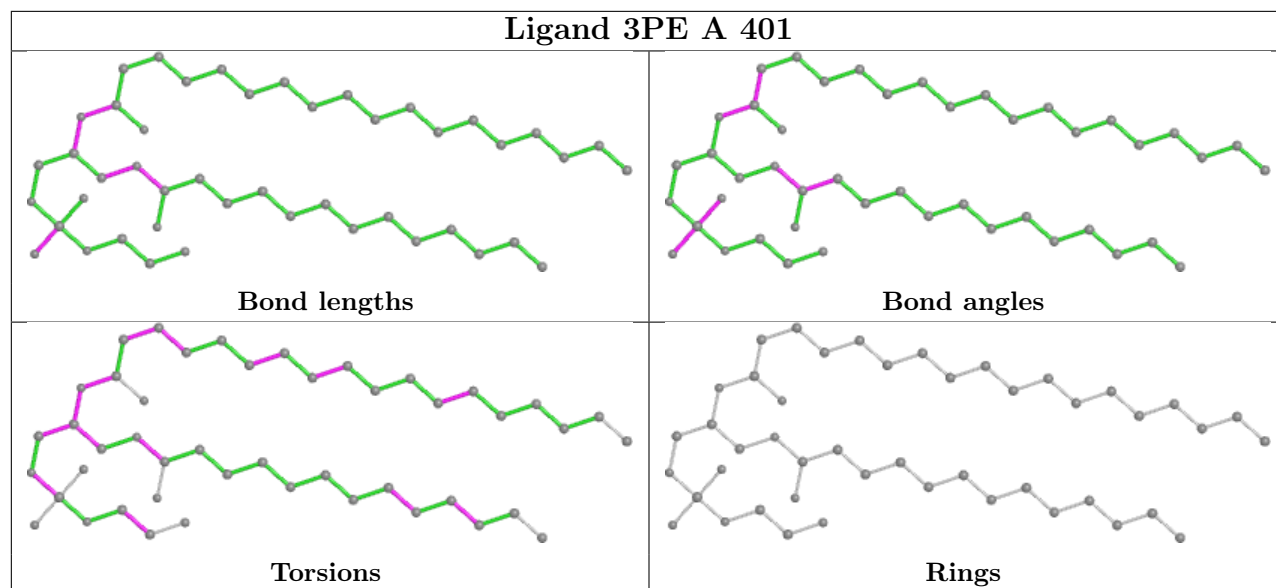
No monomer is involved in short contacts.

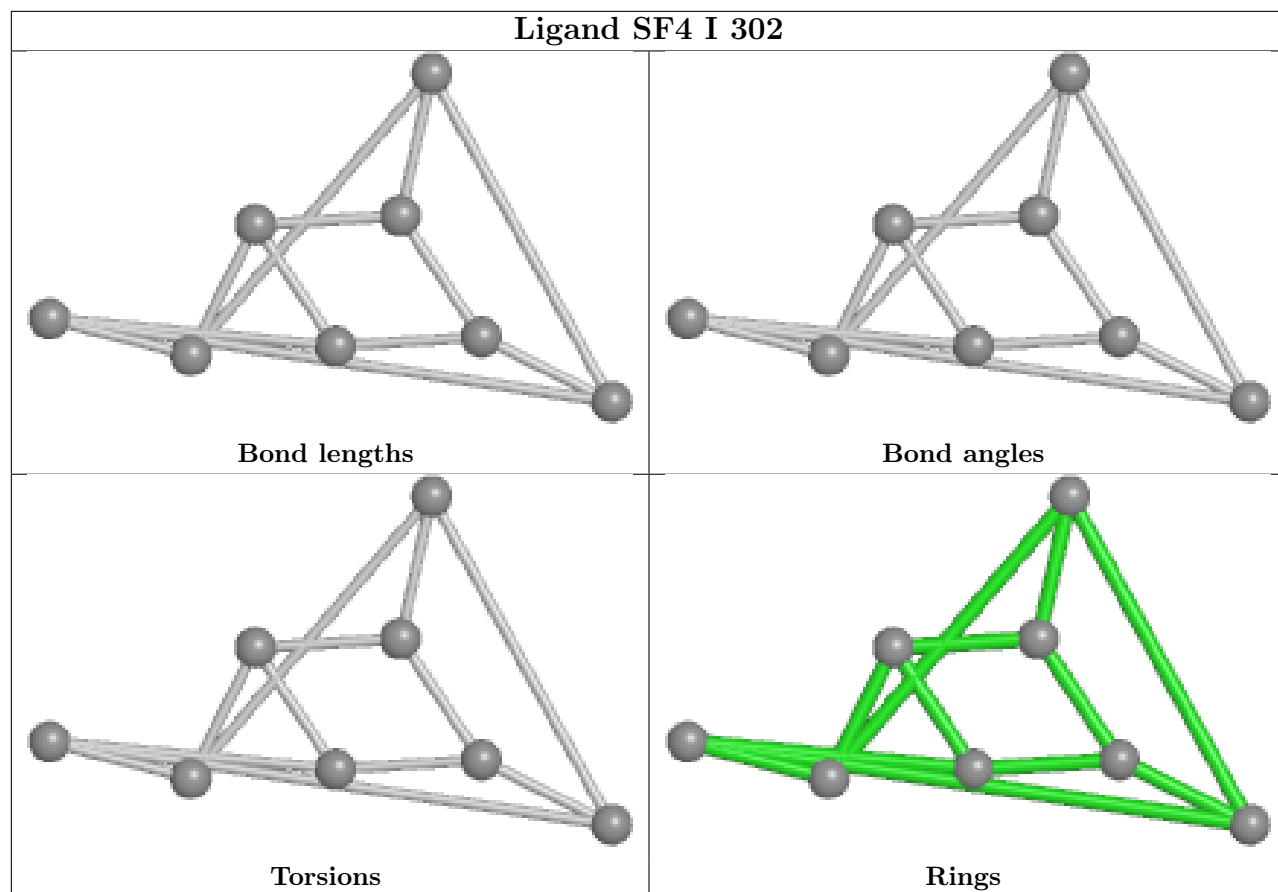
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

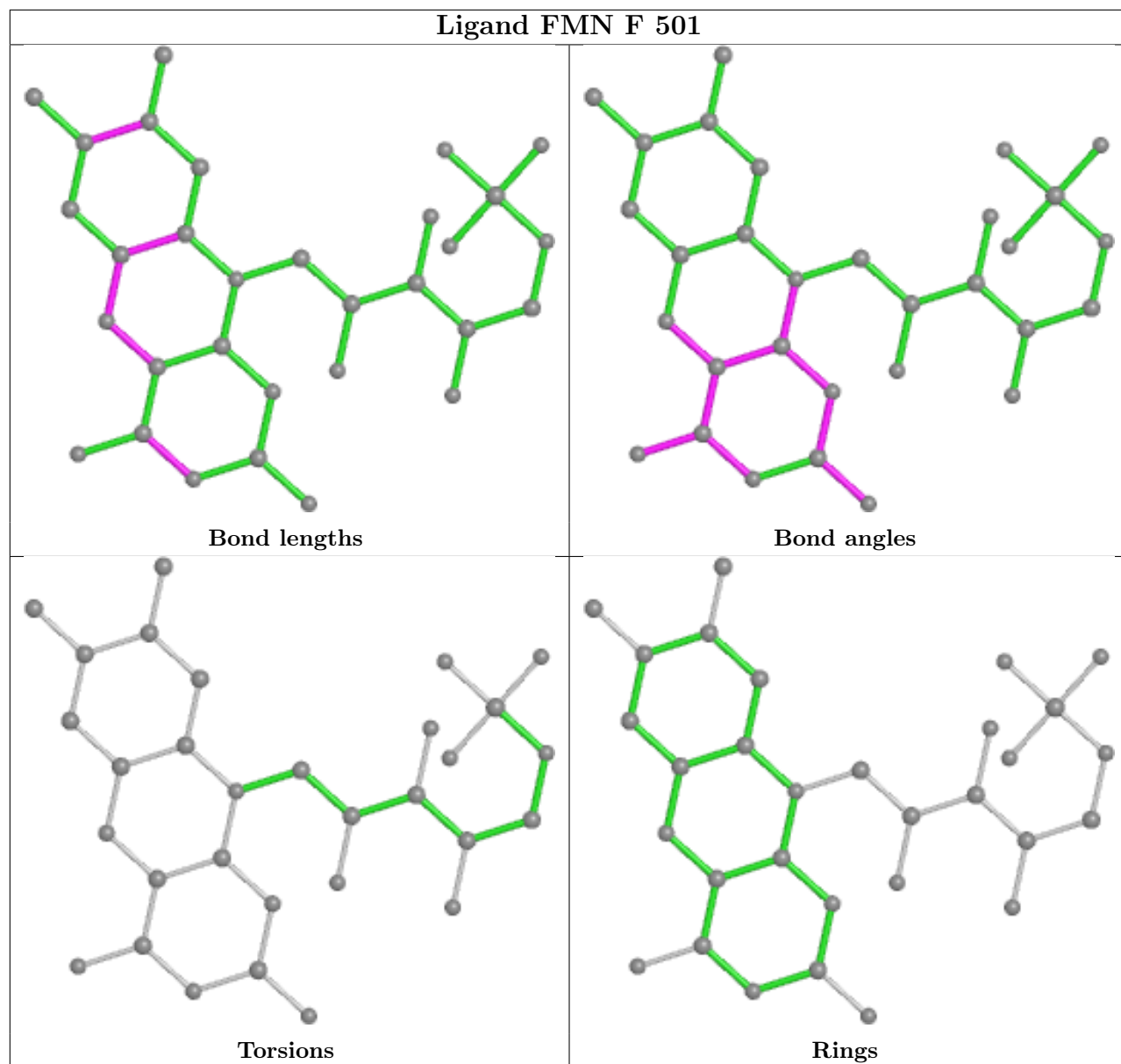


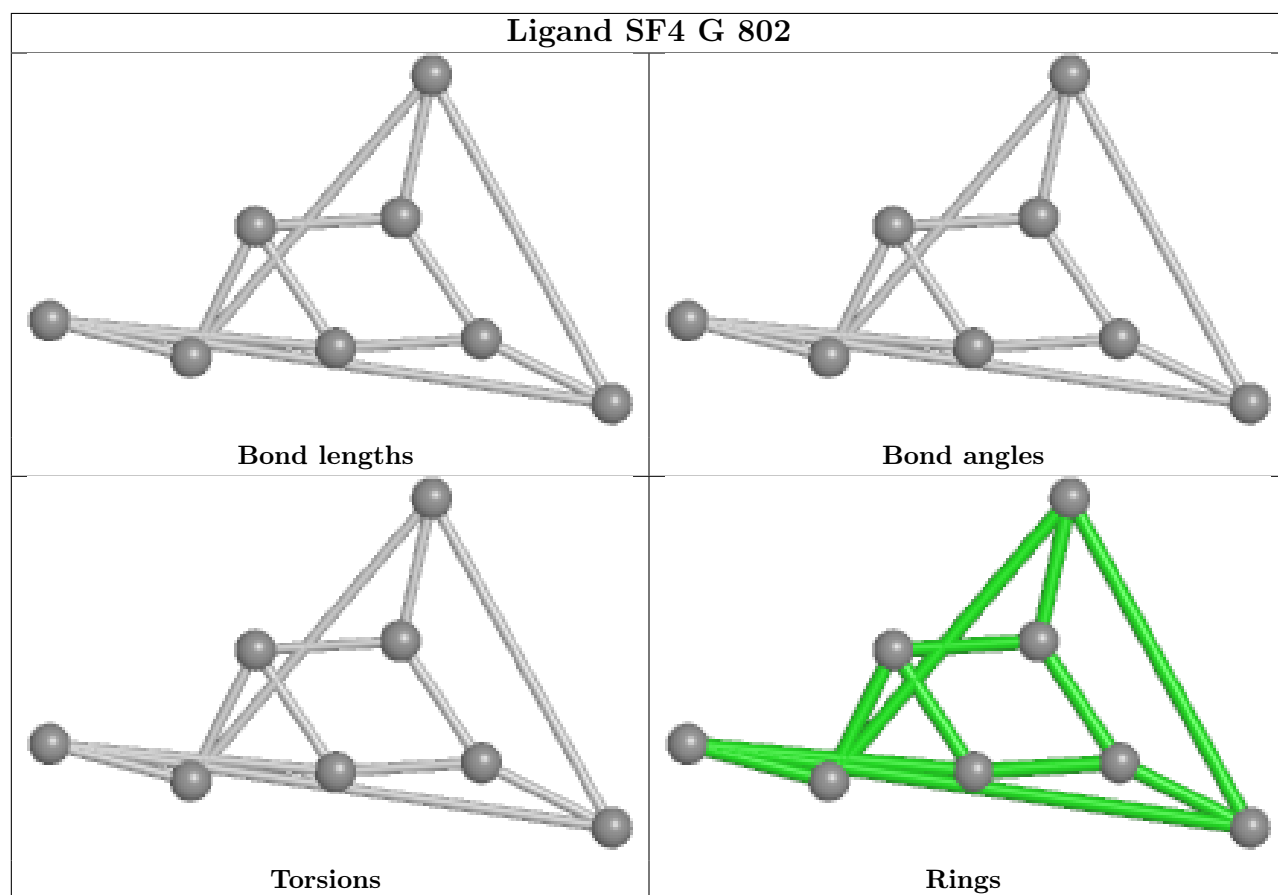
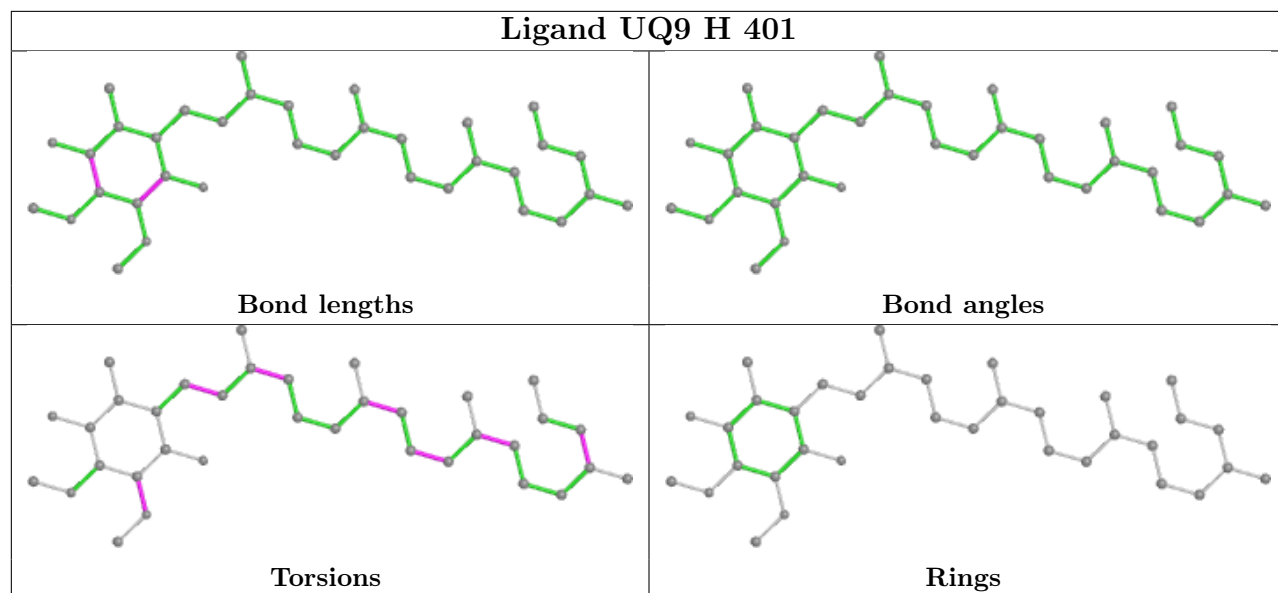


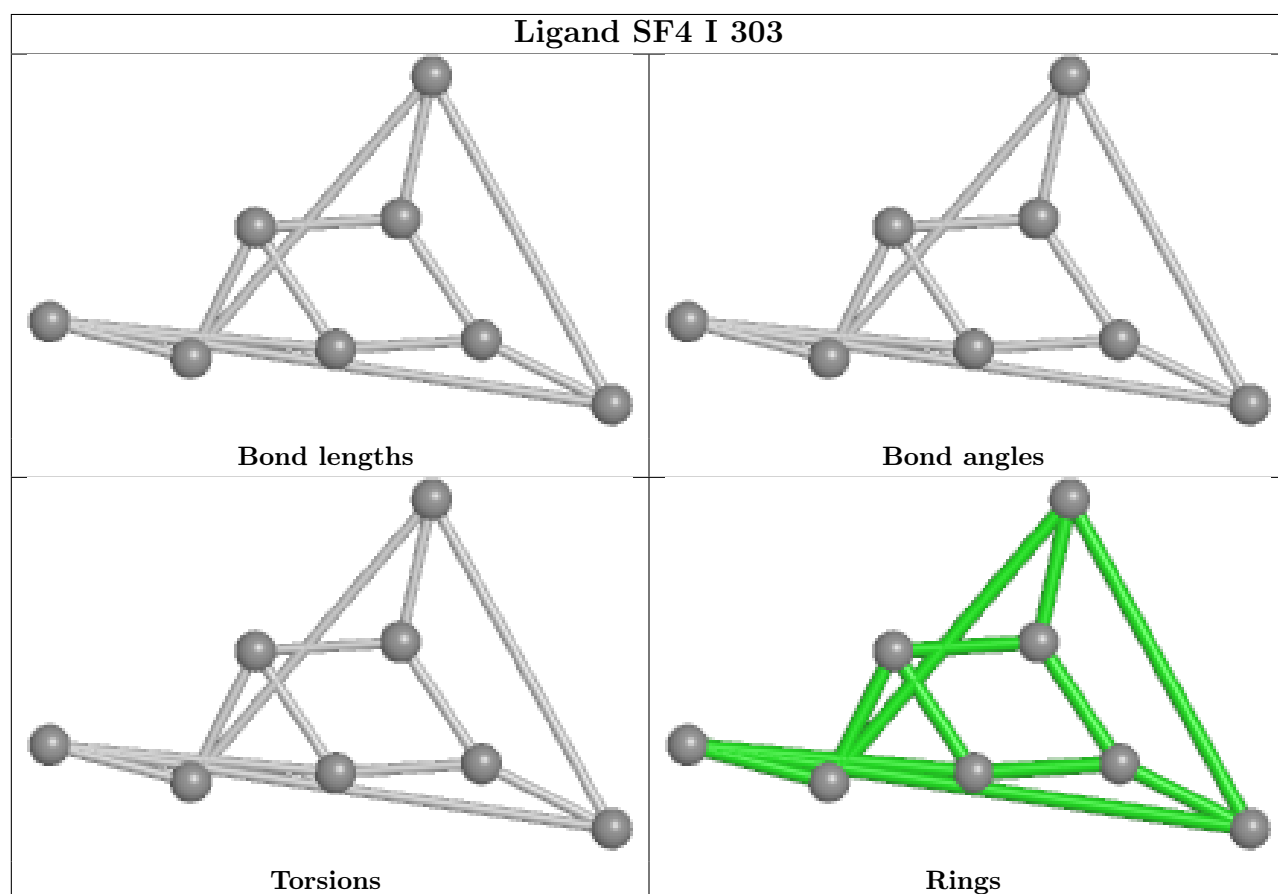
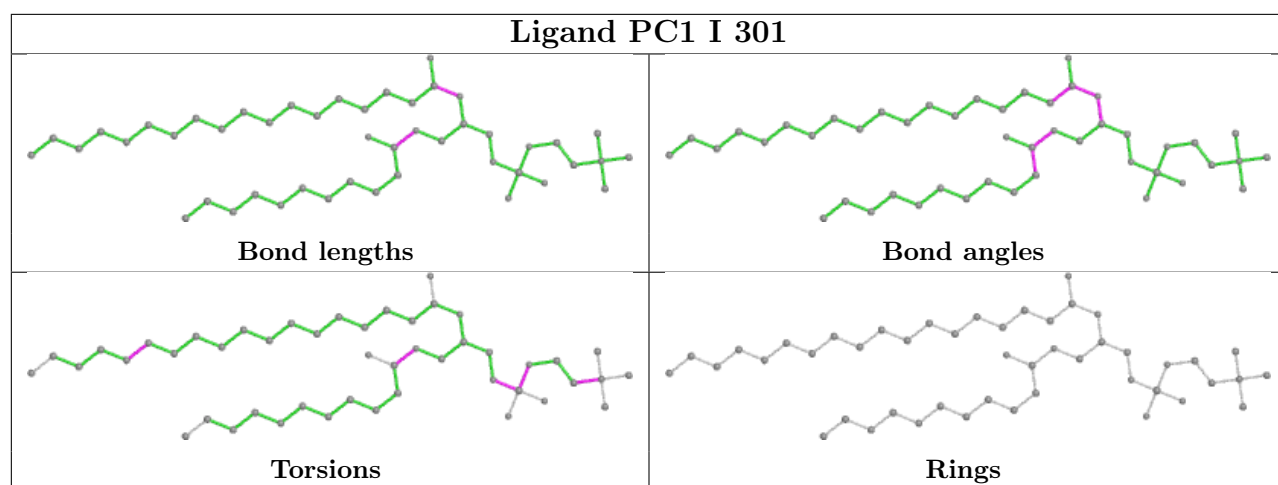


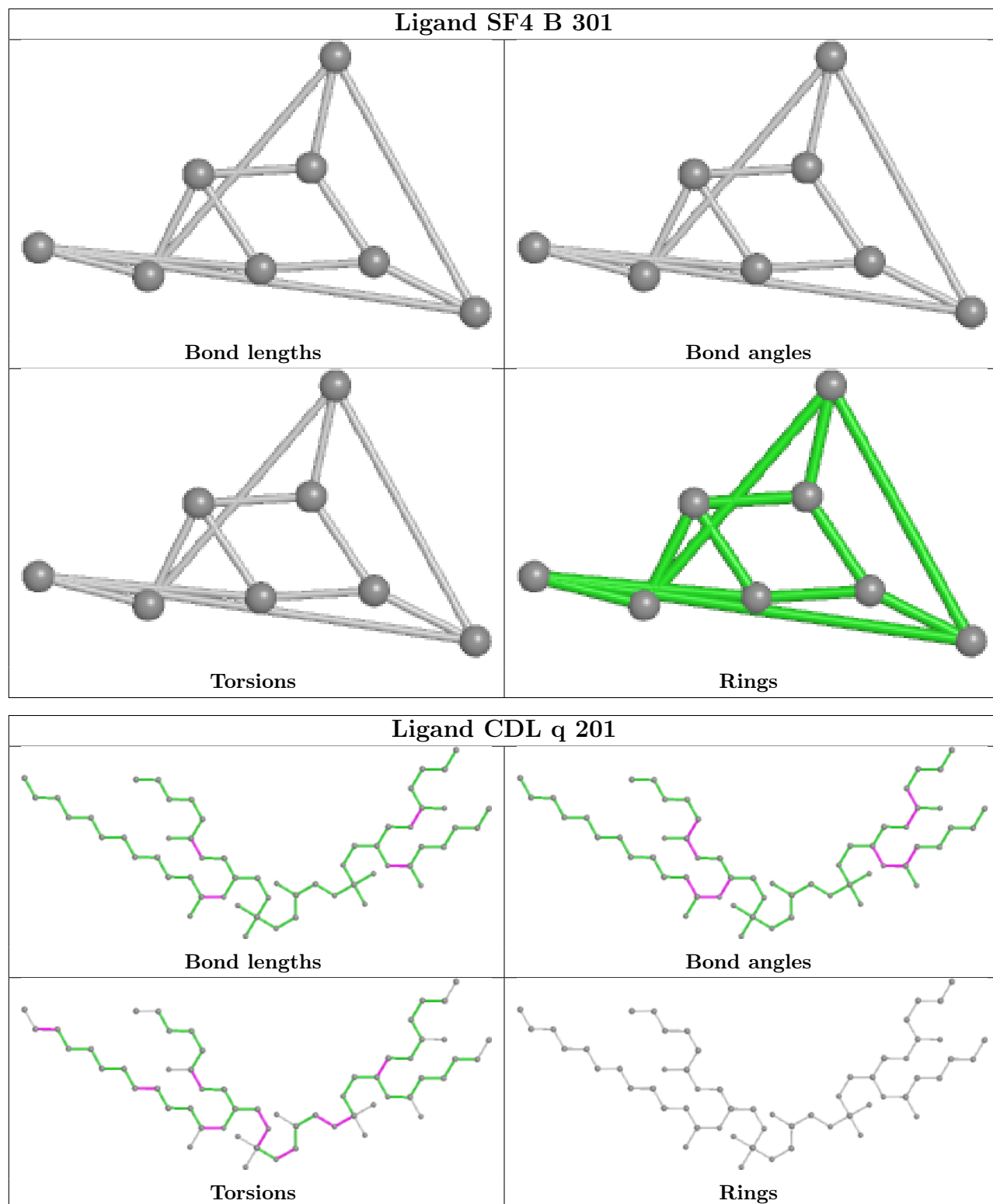


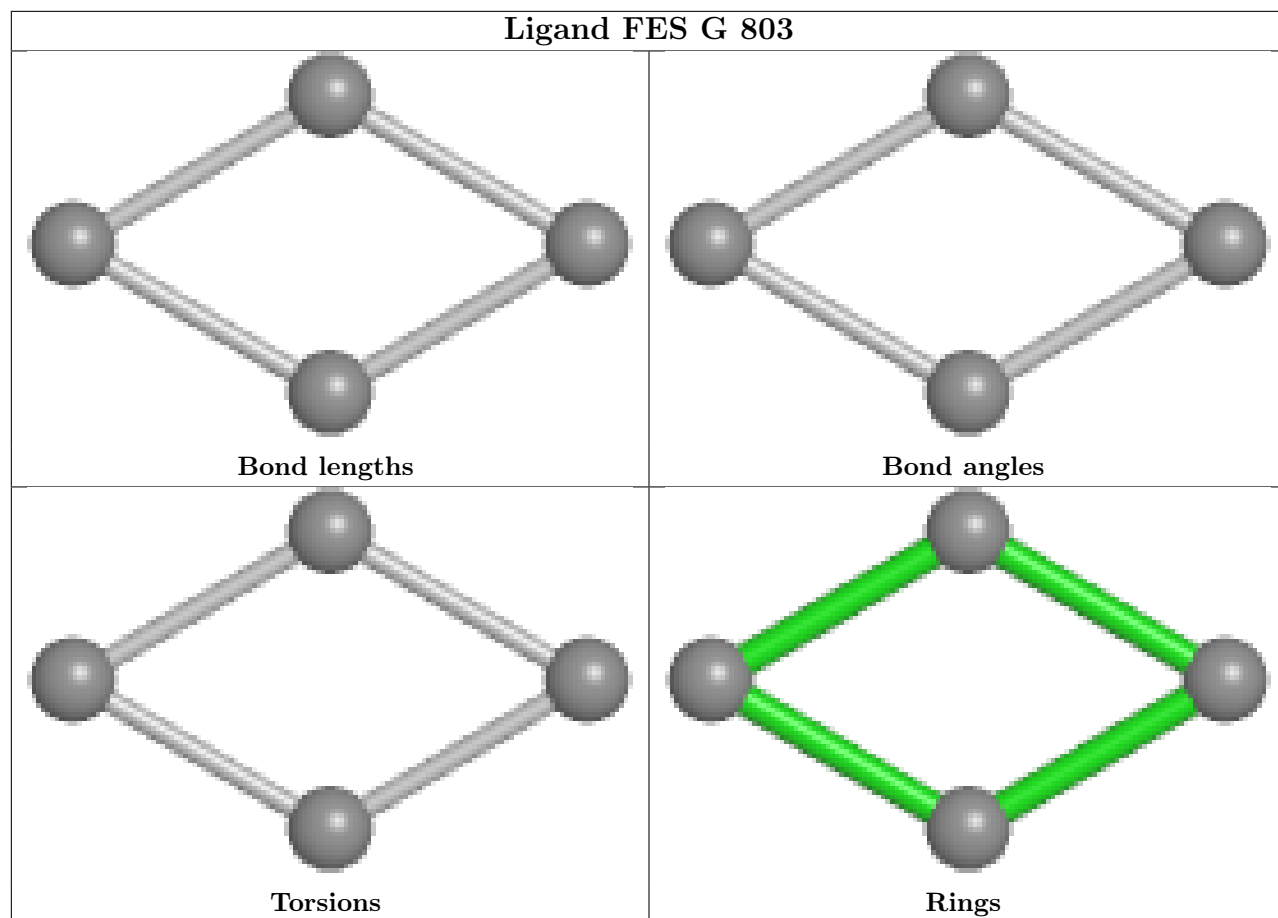


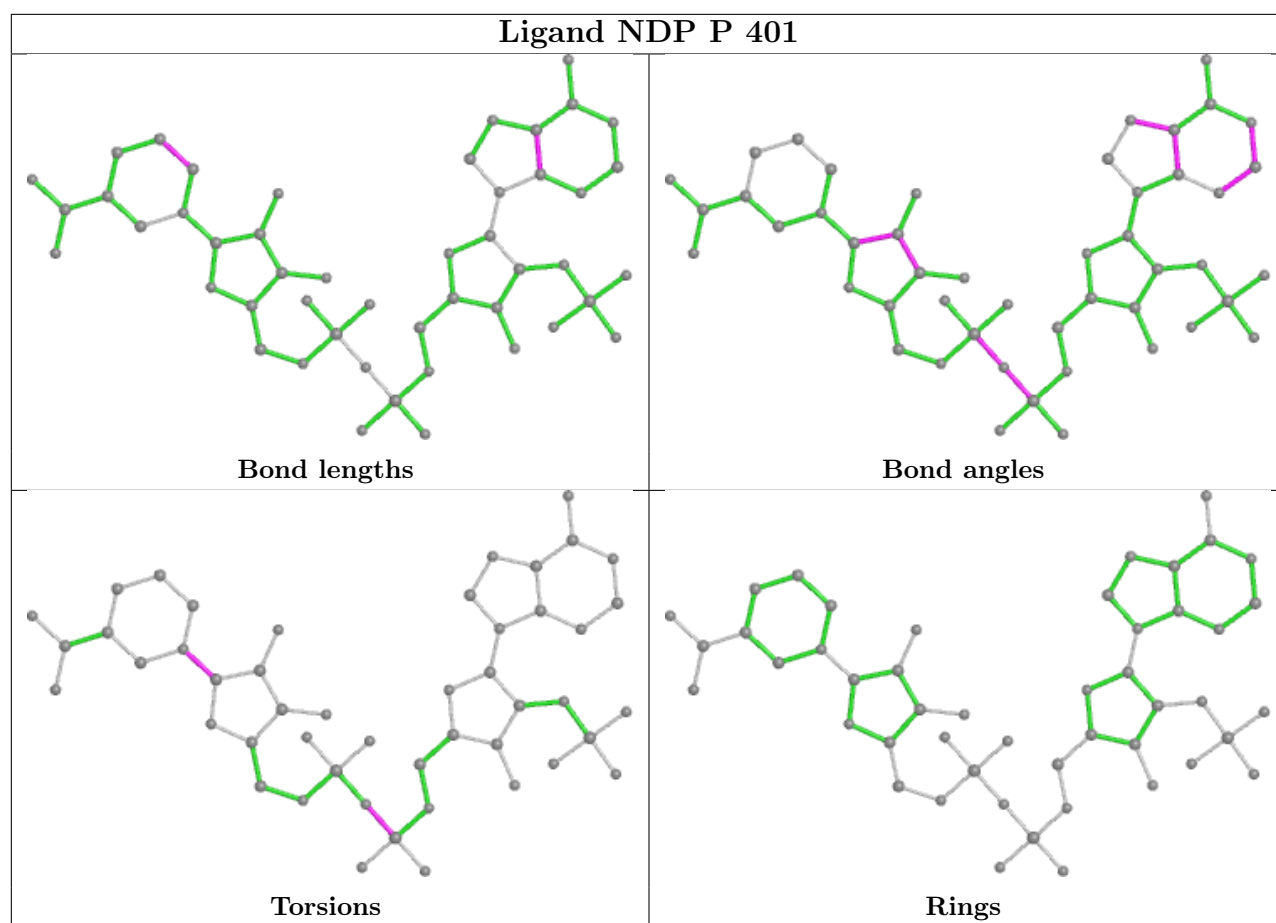












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

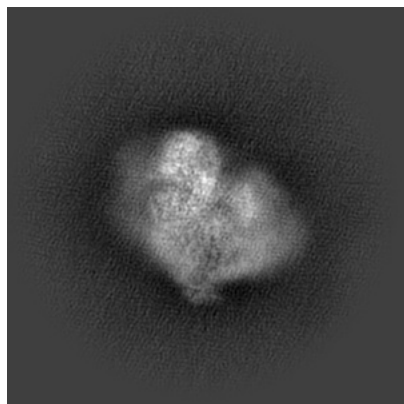
6 Map visualisation [i](#)

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

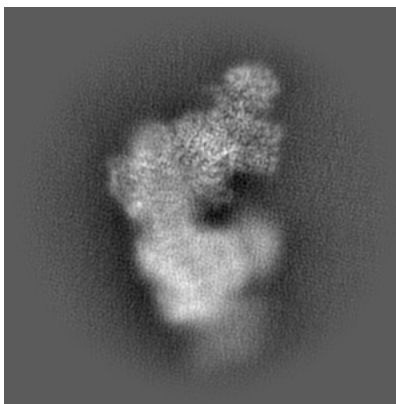
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

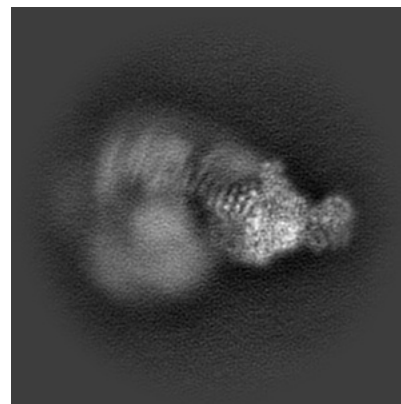
6.1.1 Primary map



X

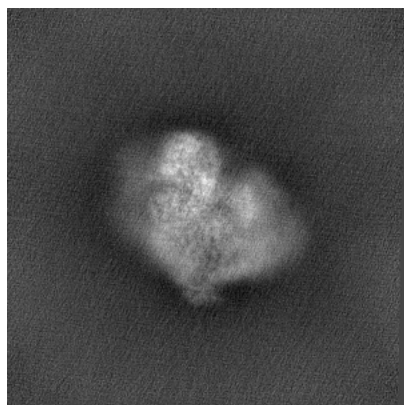


Y

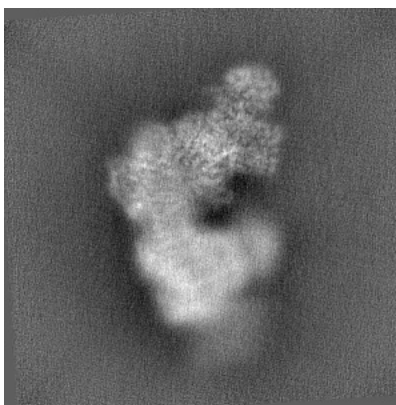


Z

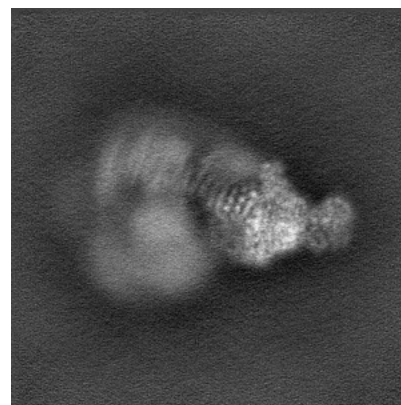
6.1.2 Raw map



X



Y

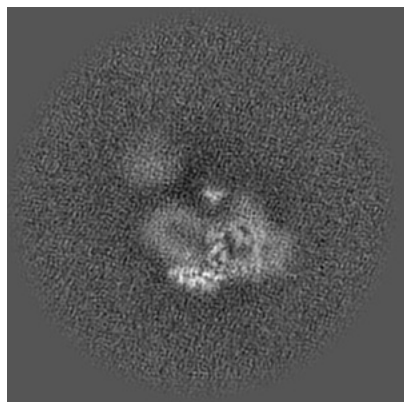


Z

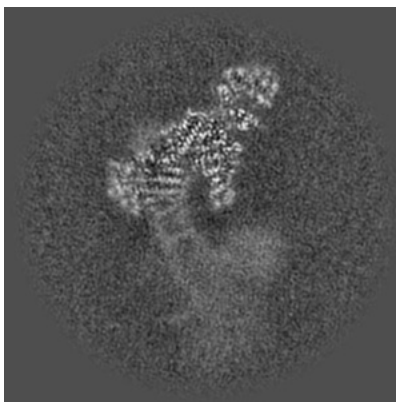
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

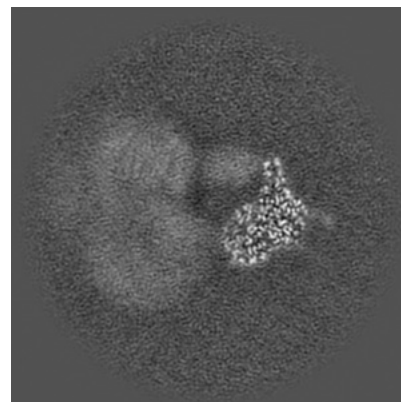
6.2.1 Primary map



X Index: 192



Y Index: 192

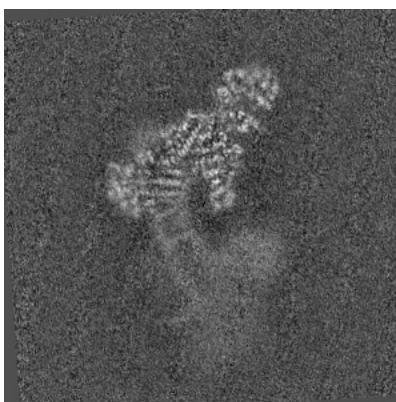


Z Index: 192

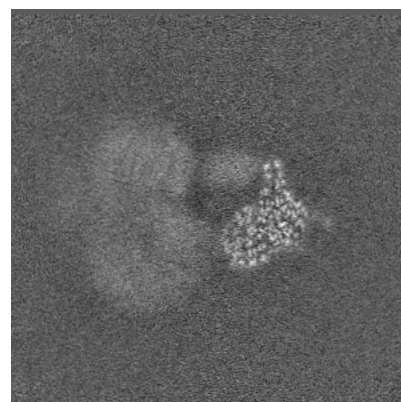
6.2.2 Raw map



X Index: 192



Y Index: 192

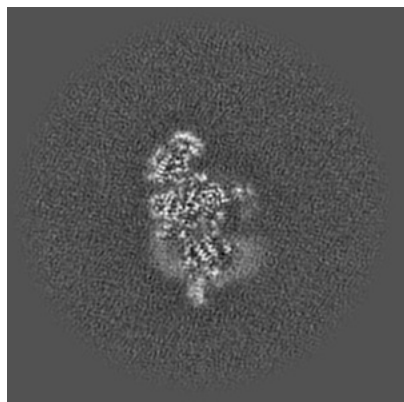


Z Index: 192

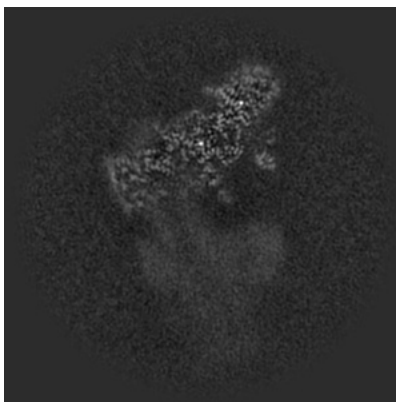
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

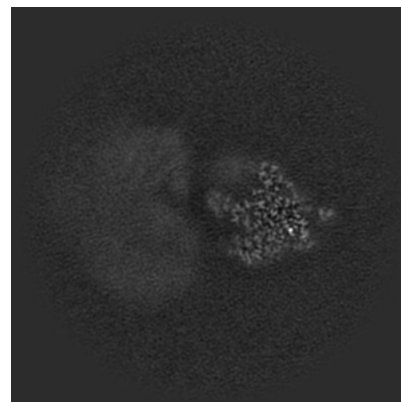
6.3.1 Primary map



X Index: 238

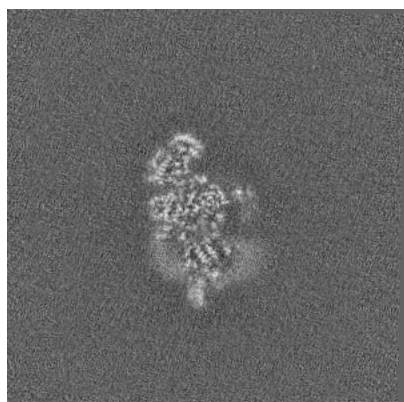


Y Index: 180

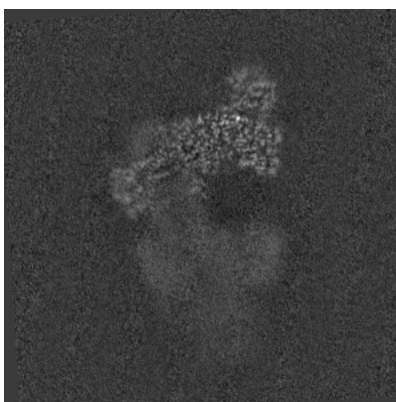


Z Index: 202

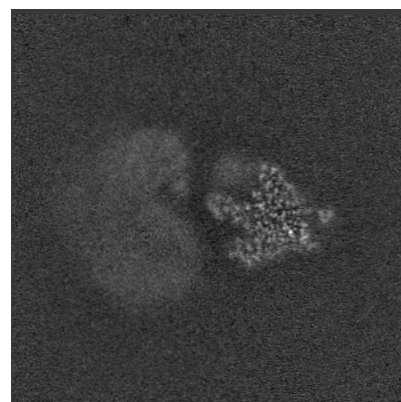
6.3.2 Raw map



X Index: 238



Y Index: 172

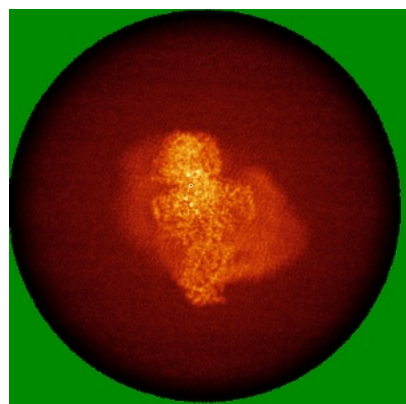


Z Index: 203

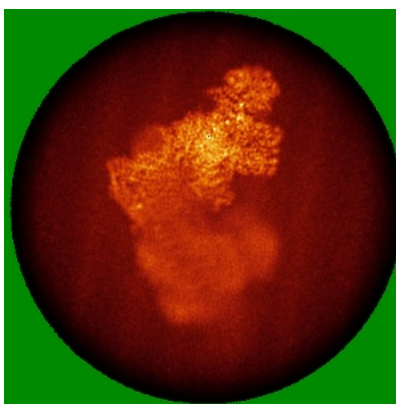
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

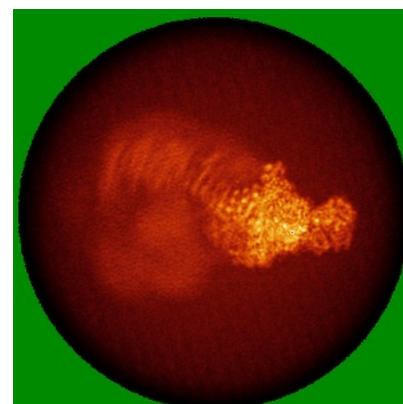
6.4.1 Primary map



X

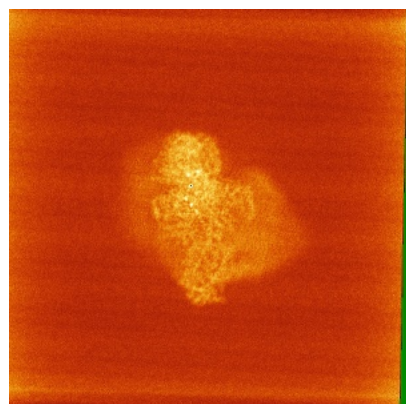


Y

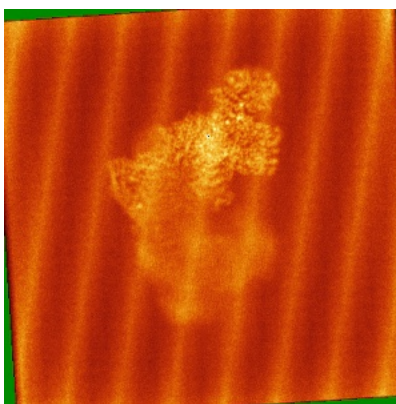


Z

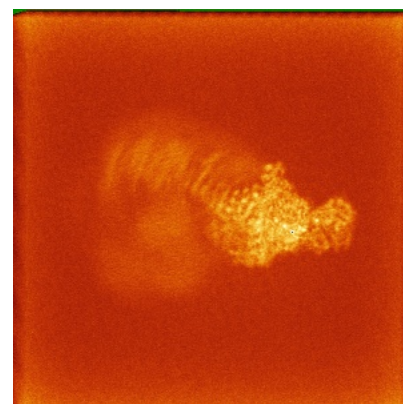
6.4.2 Raw map



X



Y

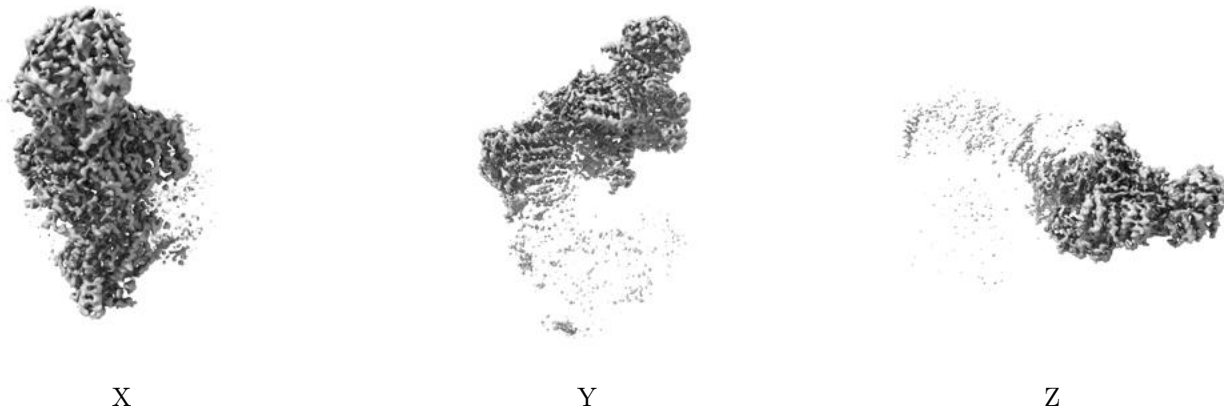


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

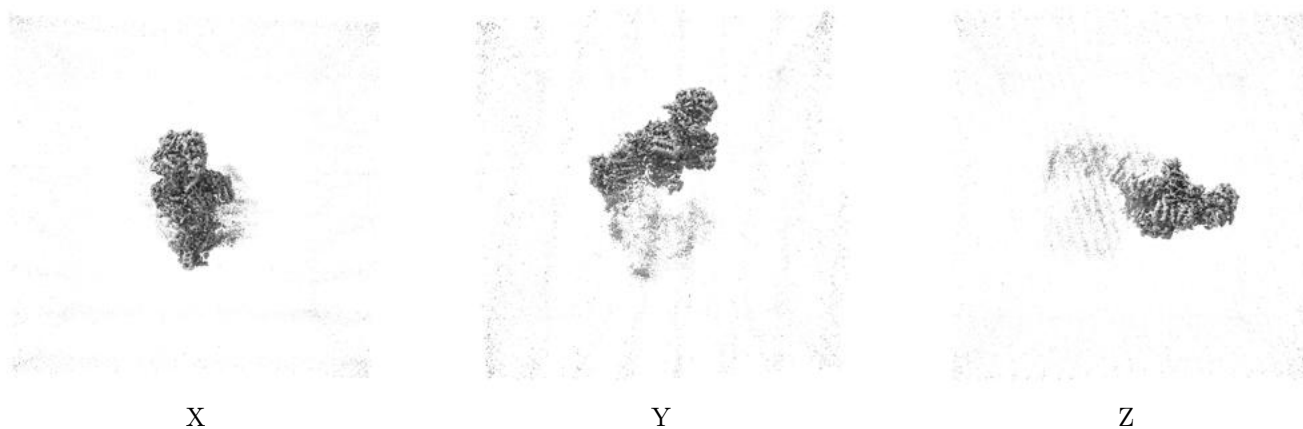
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

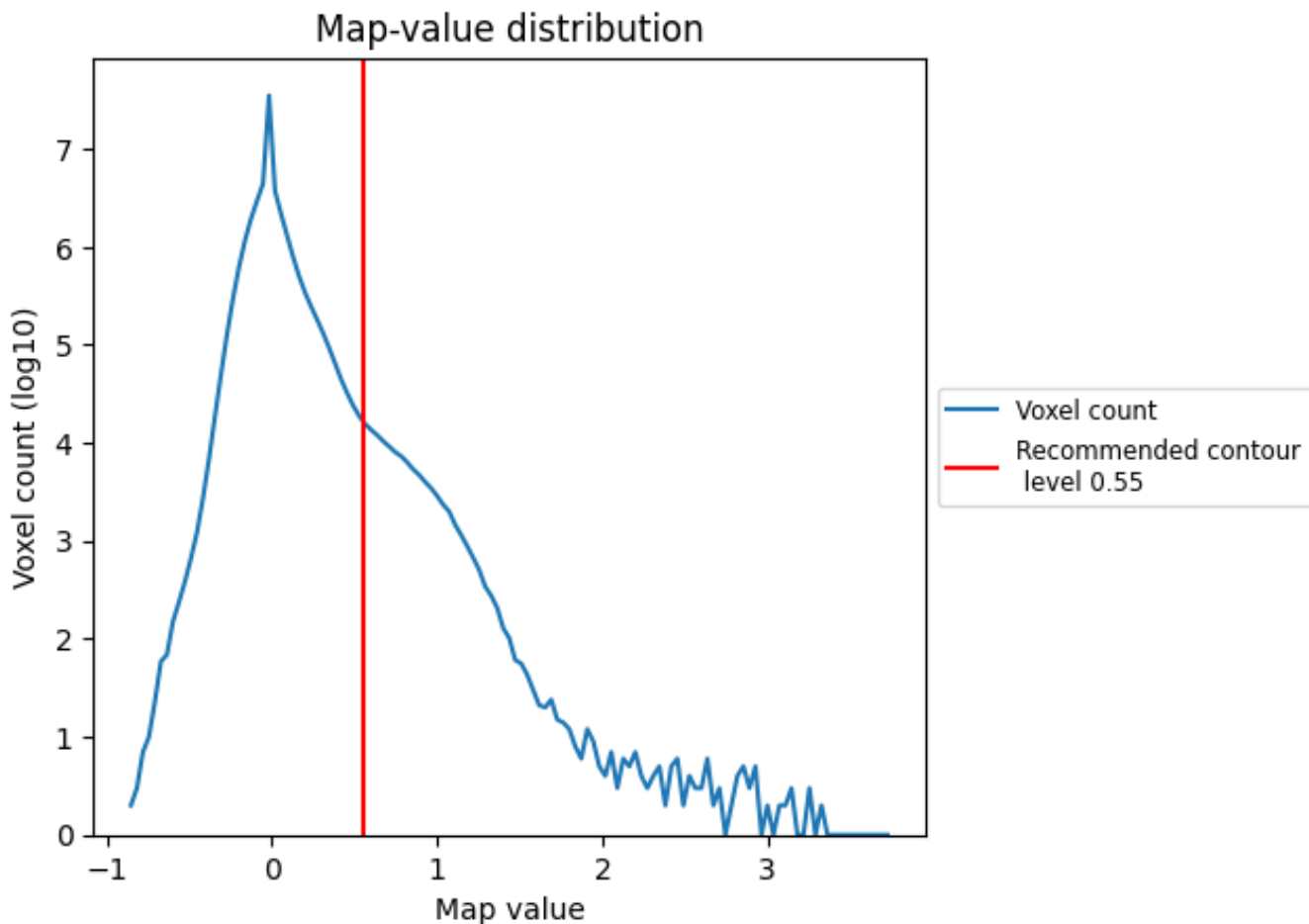
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

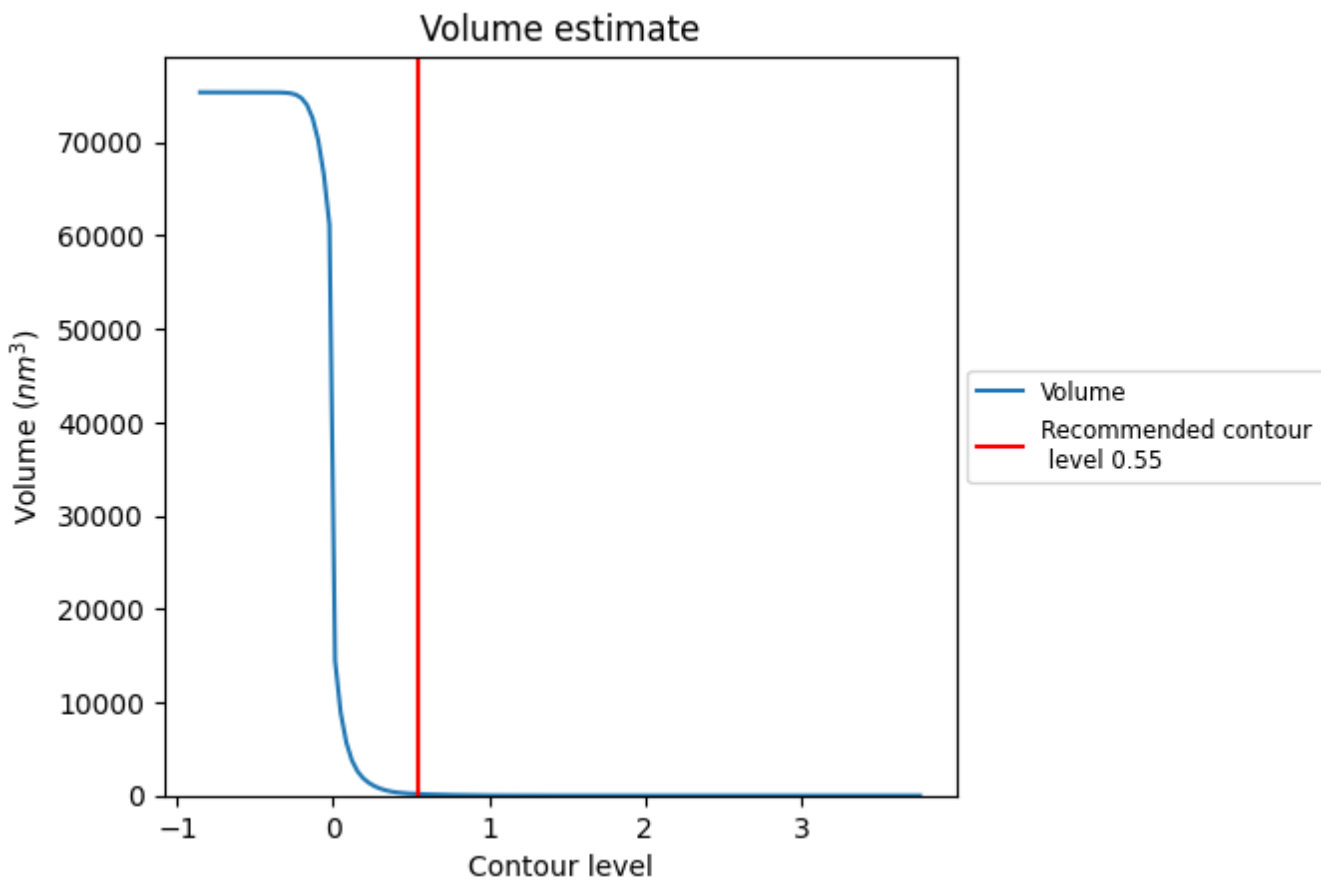
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

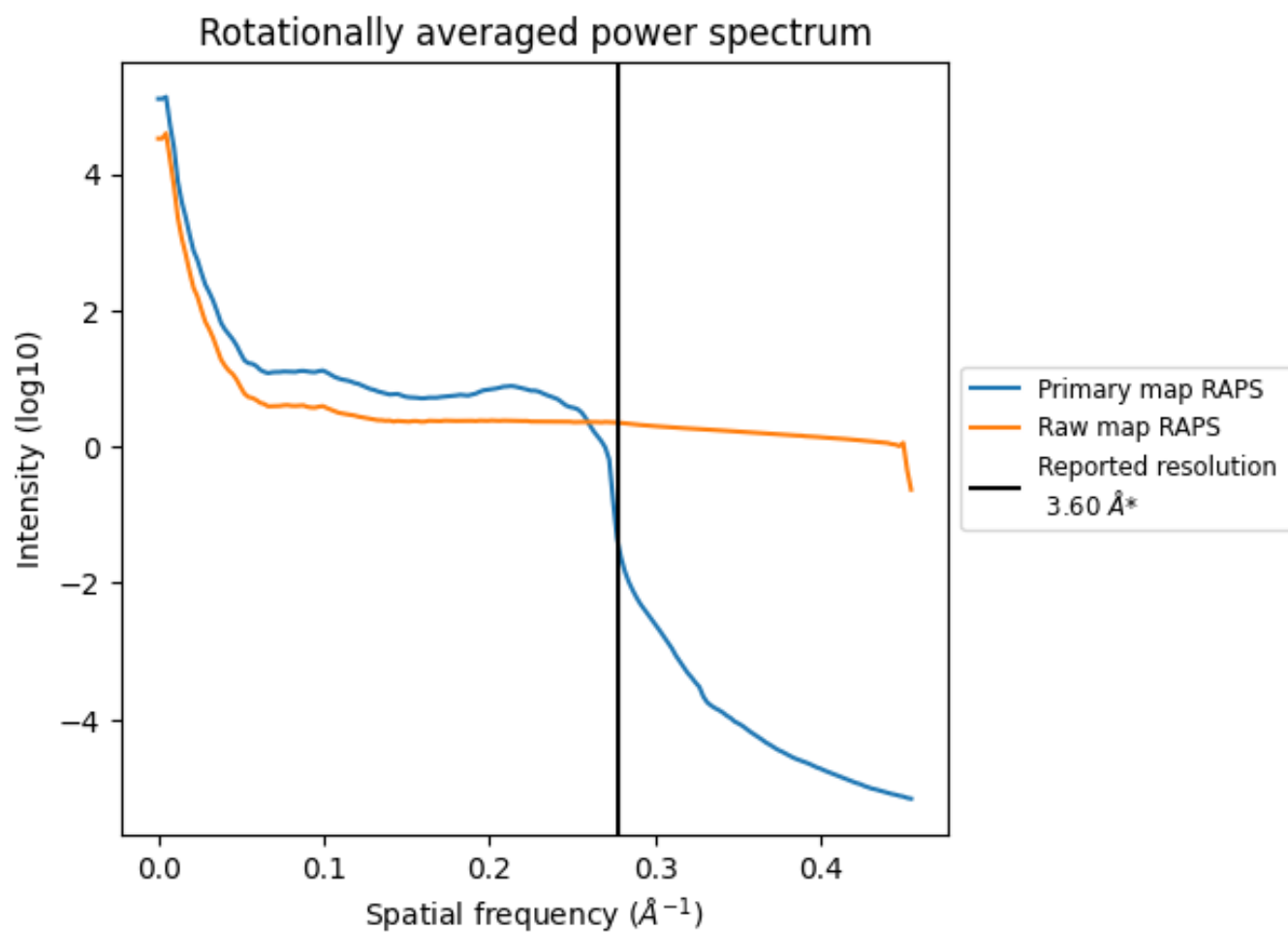
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; this corresponds to an approximate mass of 145 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

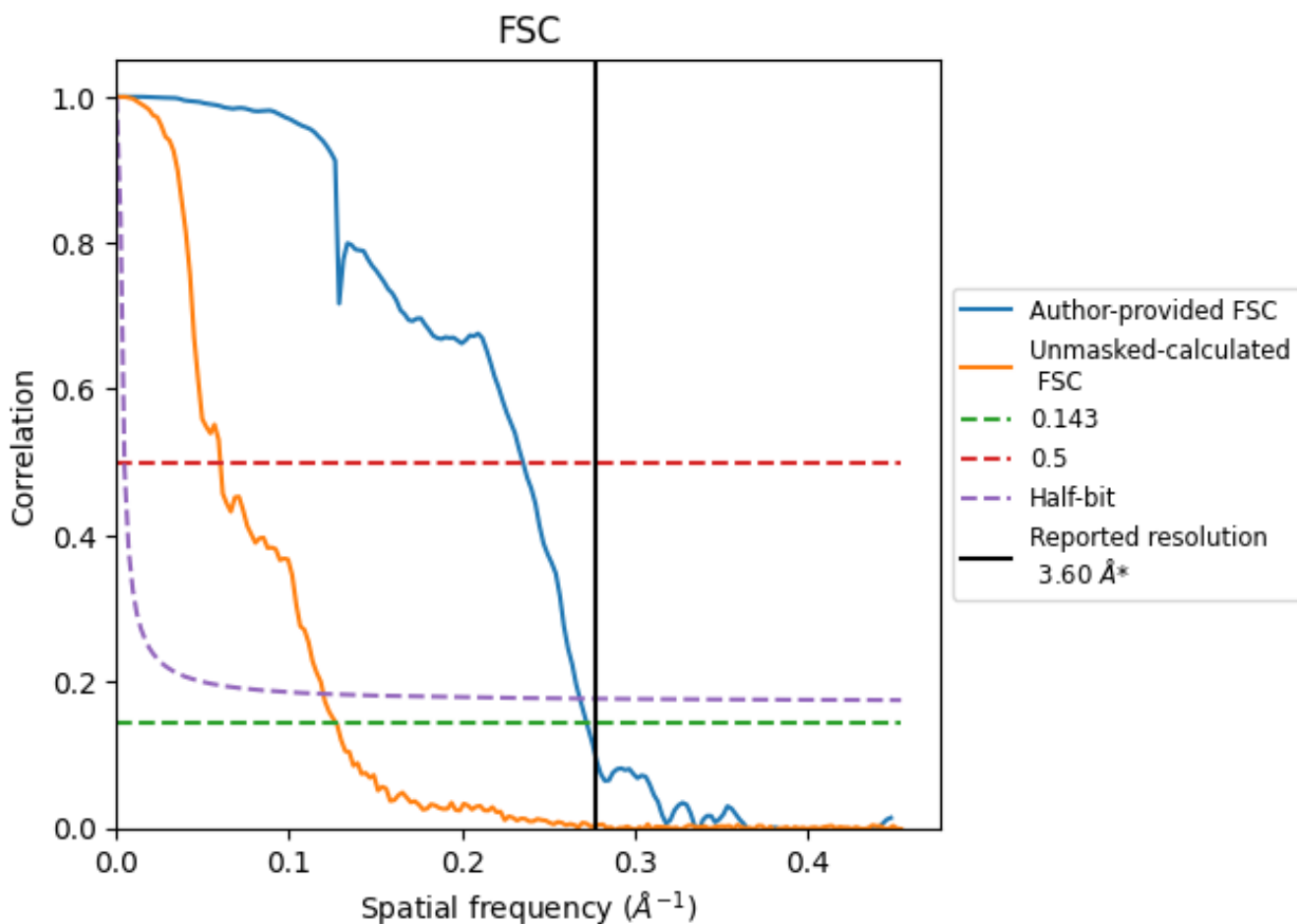


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



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

8.2 Resolution estimates [i](#)

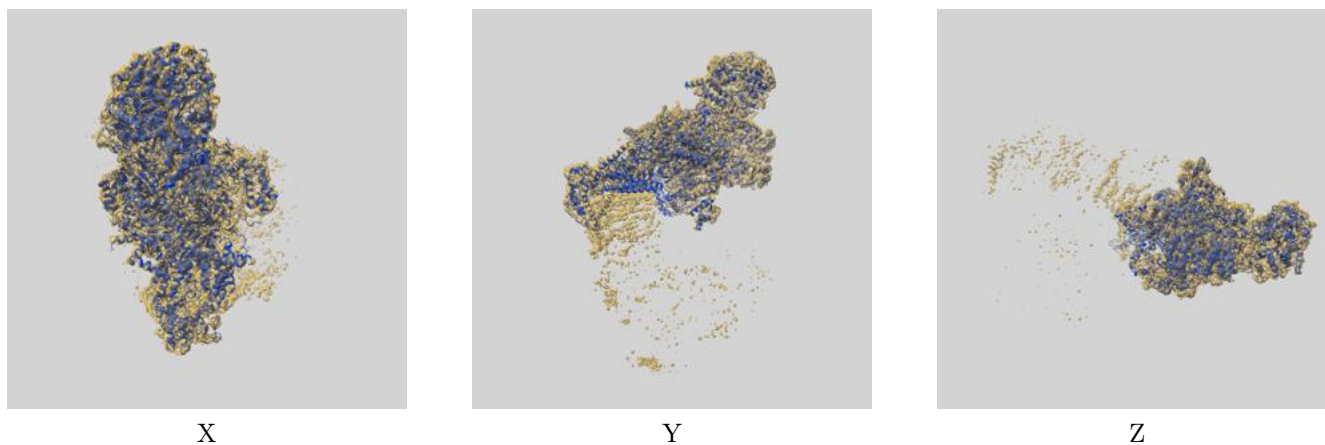
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.67	4.25	3.72
Unmasked-calculated*	7.86	16.61	8.34

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

9 Map-model fit [i](#)

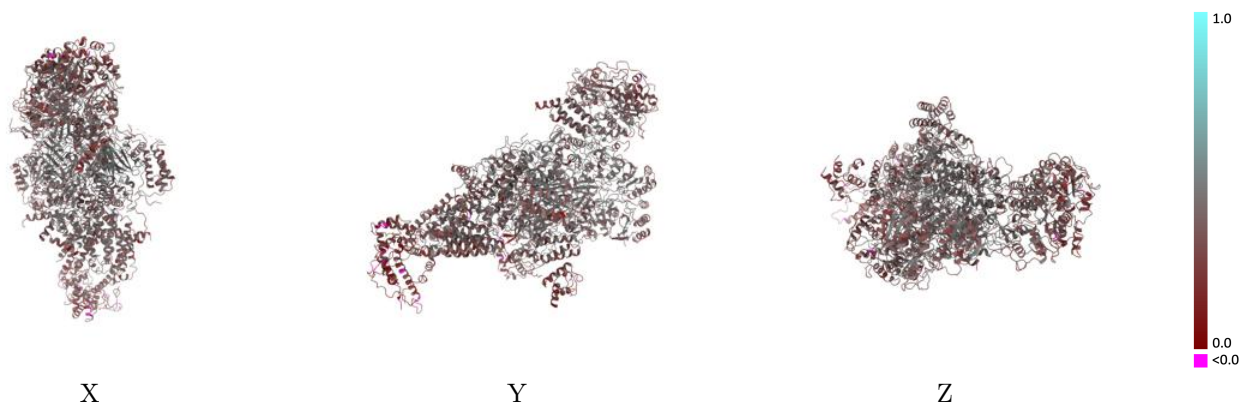
This section contains information regarding the fit between EMDB map EMD-38508 and PDB model 8XNN. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



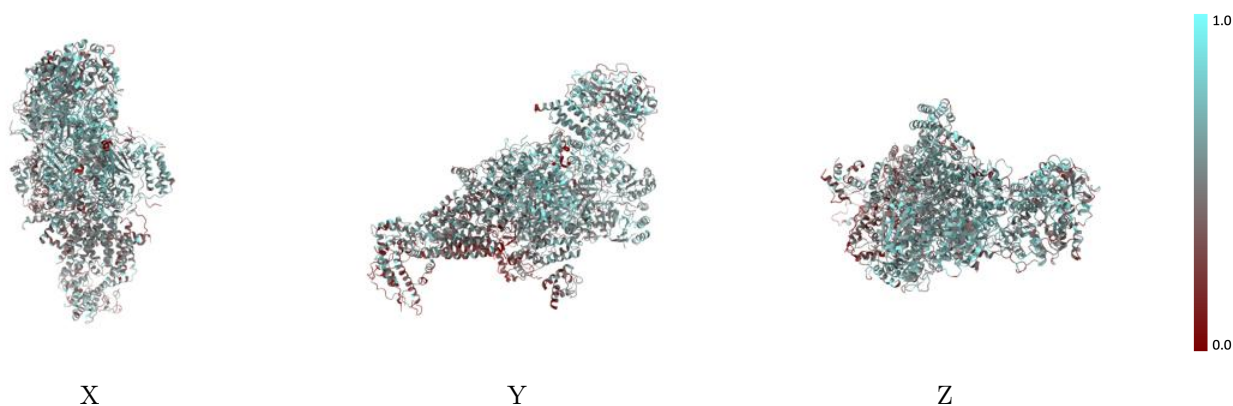
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



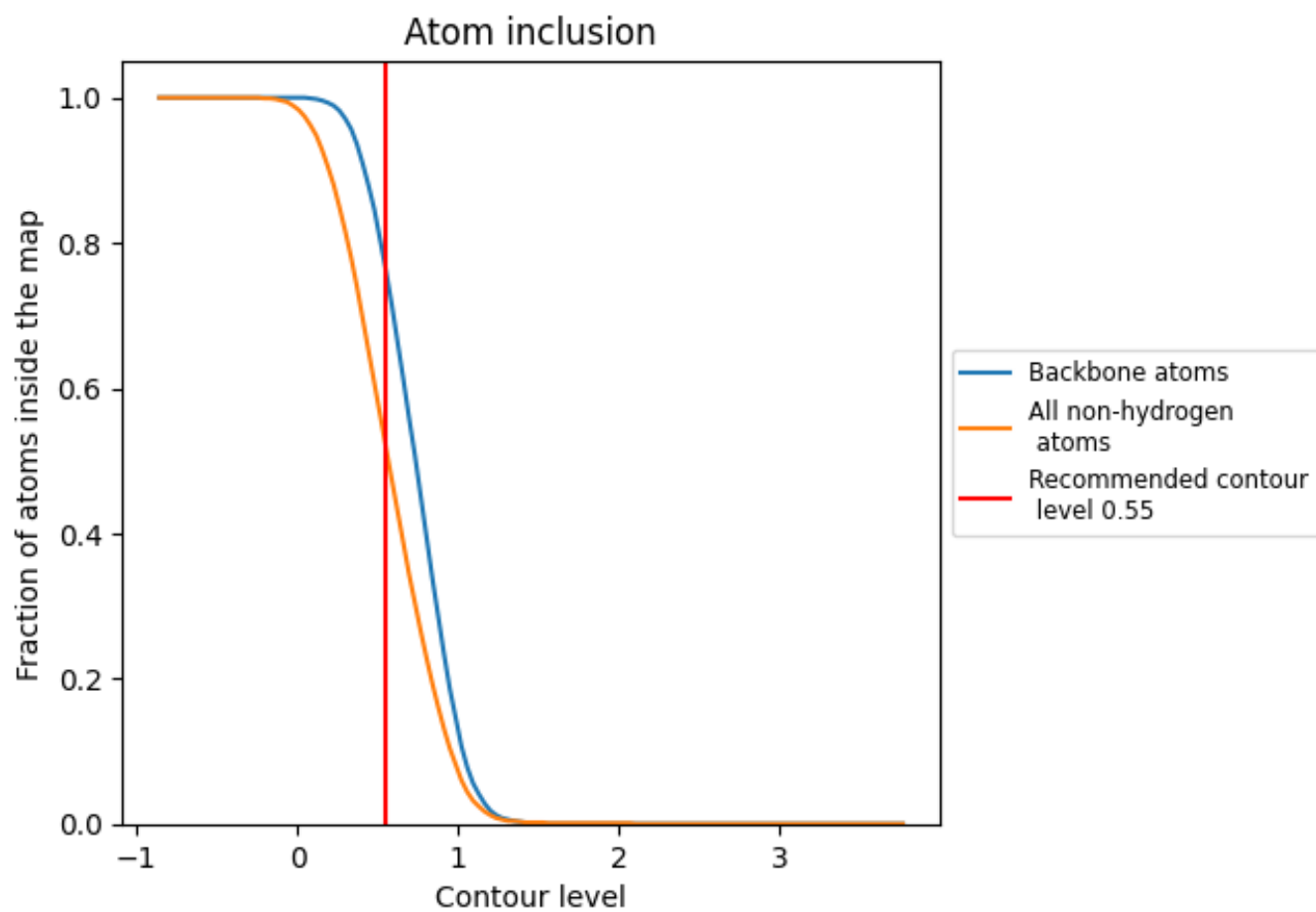
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

9.5 Map-model fit summary

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

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

