wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 09:32 am BST

PDB ID	:	7Z7S / pdb_00007z7s
EMDB ID	:	EMD-14536
Title	:	Complex I from E. coli, LMNG-purified, under Turnover at pH 6, Closed state
Authors	:	Kravchuk, V.; Kampjut, D.; Sazanov, L.
Deposited on	:	2022-03-16
Resolution	:	2.40 Å(reported)
Based on initial models	:	3RKO, 4HEA

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

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

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

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

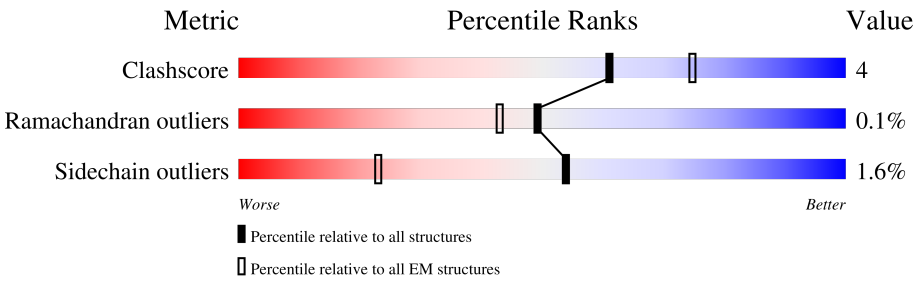
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

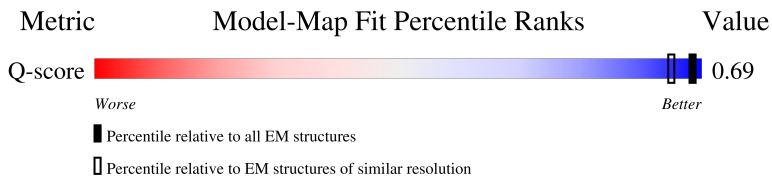
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	F	445	89% 10% •
2	E	166	86% 8% 6%
3	G	908	88% 11% •
4	C	596	89% 10% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	220	83% 14%
6	I	180	88% 12%
7	H	325	83% 15%
8	A	147	78% 10% 11%
9	L	613	85% 12%
10	M	509	86% 13%
11	N	485	83% 14%
12	K	100	87% 13%
13	J	184	73% 15% 12%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 39208 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-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	439	3407	2162	596	629	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase I subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	156	1220	768	215	229	8	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	905	7017	4388	1268	1324	37	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	589	4760	3049	828	859	24	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	213	1693	1070	295	312	16	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	180	1436	915	242	264	15	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	322	2534	1702	398	416	18	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	131	1037	688	177	167	5	0	0

- Molecule 9 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	598	4558	3036	726	764	32	0	0

- Molecule 10 is a protein called NADH dehydrogenase I subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	504	3953	2661	617	646	29	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	475	3601	2407	568	606	20	0	0

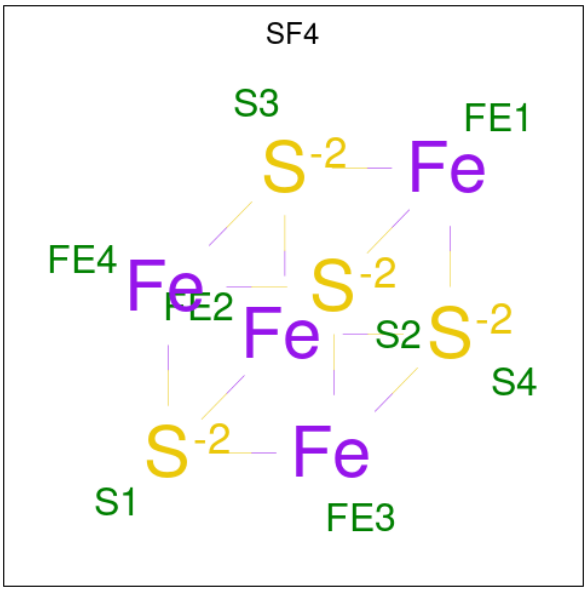
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	100	760	494	132	129	5	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit J.

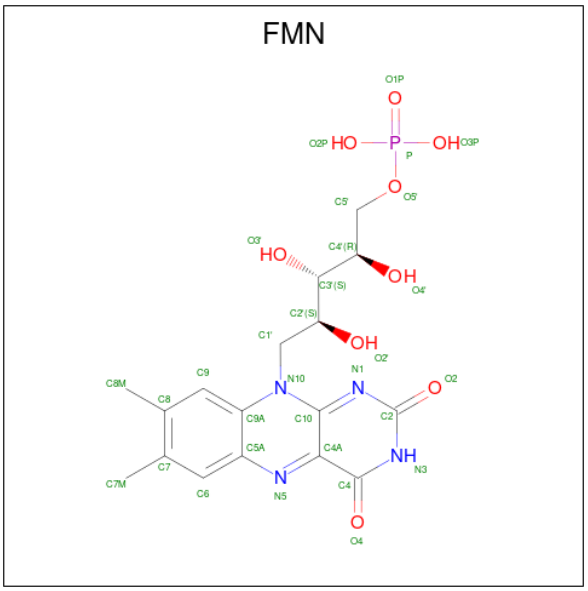
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	162	1226	824	188	207	7	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



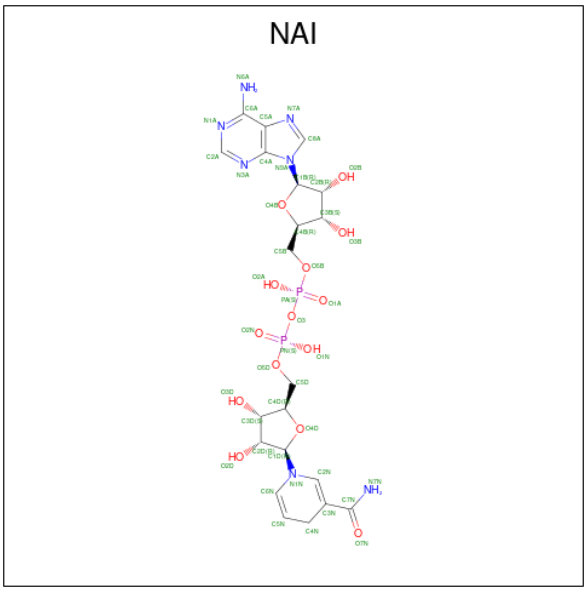
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
14	F	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	G	1	8	4	4	0
14	B	1	8	4	4	0
14	I	1	8	4	4	0
14	I	1	8	4	4	0

- Molecule 15 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



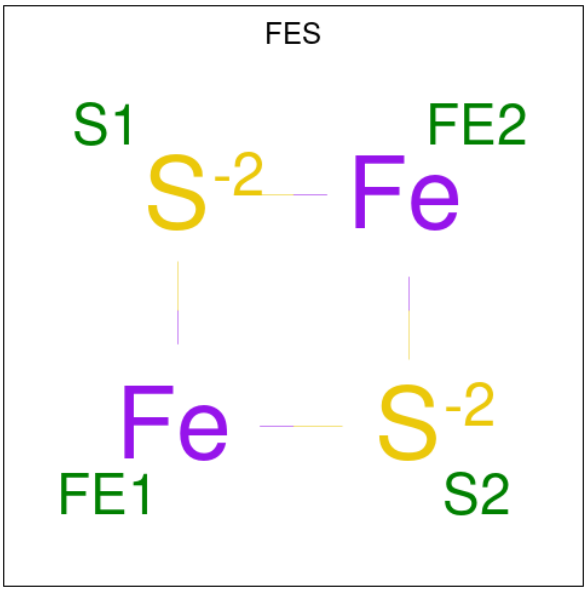
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	F	1	31	17	4	9	1	0

- Molecule 16 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

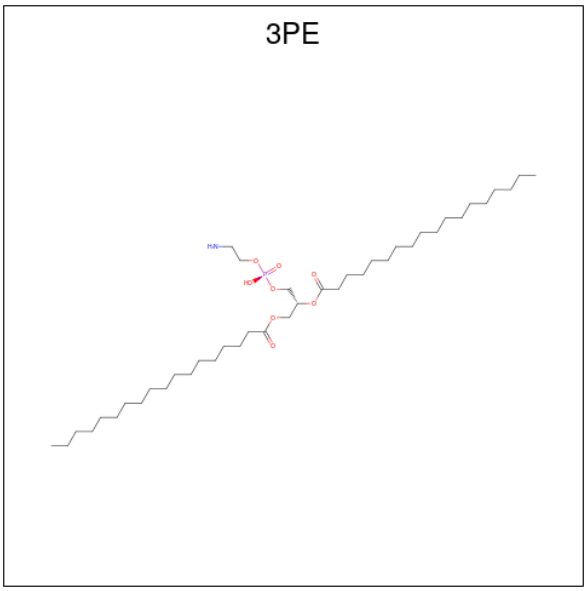


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	E	1	4	2	2	0
17	G	1	4	2	2	0

- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
18	G	1	1	1	0

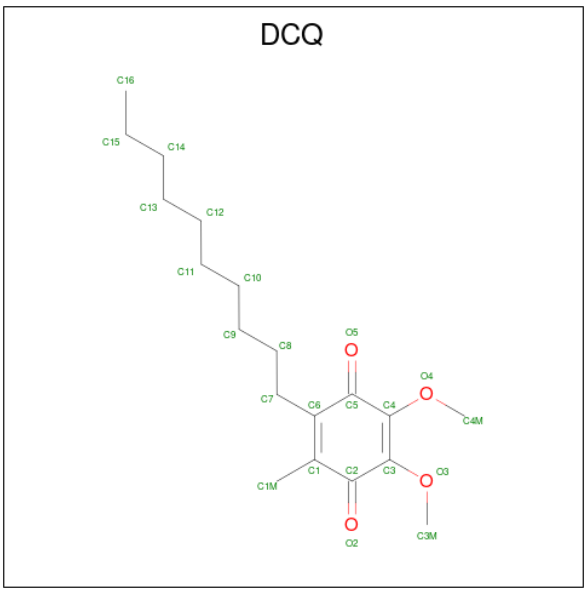
- Molecule 19 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	C	1	51	41	1	8	1	0
19	I	1	39	29	1	8	1	0
19	H	1	36	26	1	8	1	0
19	L	1	51	41	1	8	1	0
19	L	1	36	26	1	8	1	0
19	L	1	40	30	1	8	1	0
19	L	1	51	41	1	8	1	0
19	L	1	39	29	1	8	1	0
19	M	1	47	37	1	8	1	0
19	M	1	47	37	1	8	1	0
19	M	1	37	27	1	8	1	0
19	N	1	51	41	1	8	1	0
19	J	1	42	32	1	8	1	0

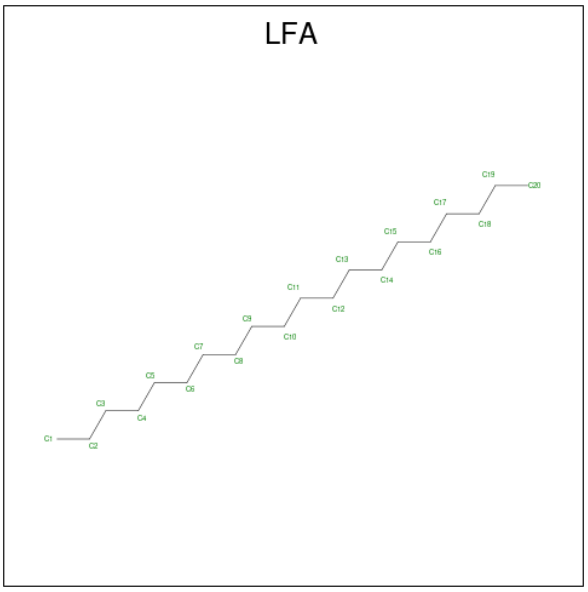
- Molecule 20 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID:

DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	C	1	23	19	4	0
			Total	C	O	
20	B	1	23	19	4	0

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	H	1	20	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	N	1	15	15	0
			Total	C	
21	N	1	14	14	0
			Total	C	
21	J	1	20	20	0

- Molecule 22 is water.

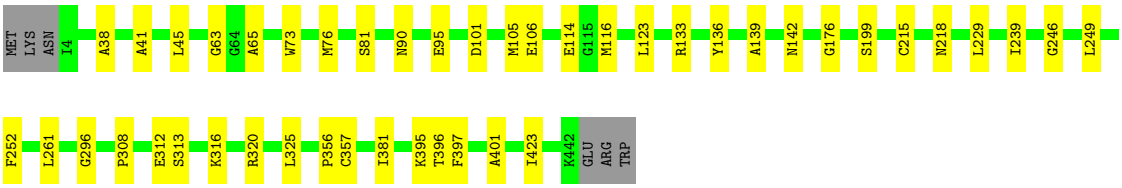
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
22	F	97	97	97	0
			Total	O	
22	E	26	26	26	0
			Total	O	
22	G	353	353	353	0
			Total	O	
22	C	206	206	206	0
			Total	O	
22	B	67	67	67	0
			Total	O	
22	I	95	95	95	0
			Total	O	
22	H	69	69	69	0
			Total	O	
22	A	38	38	38	0
			Total	O	
22	L	47	47	47	0
			Total	O	
22	M	85	85	85	0
			Total	O	
22	N	64	64	64	0
			Total	O	
22	K	17	17	17	0
			Total	O	
22	J	20	20	20	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.

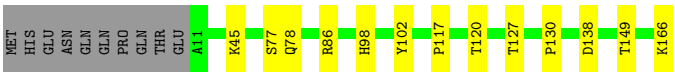
• Molecule 1: NADH-quinone oxidoreductase subunit F

Chain F:



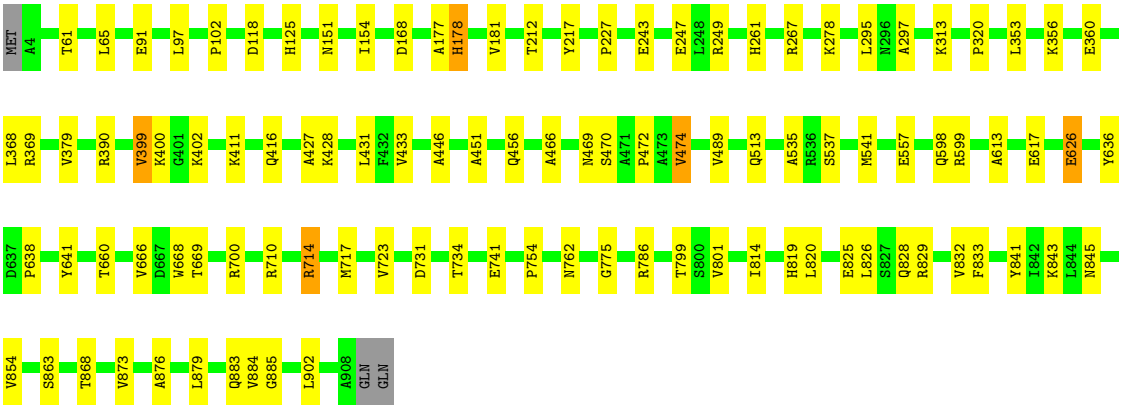
• Molecule 2: NADH dehydrogenase I subunit E

Chain E:



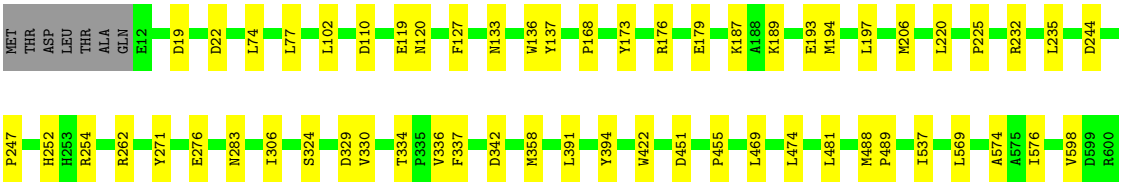
• Molecule 3: NADH-quinone oxidoreductase

Chain G:



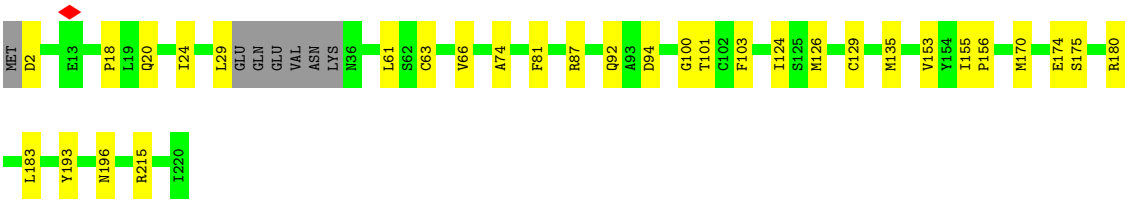
• Molecule 4: NADH-quinone oxidoreductase subunit C/D

Chain C:



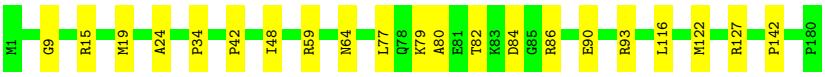
- Molecule 5: NADH-quinone oxidoreductase subunit B

Chain B:



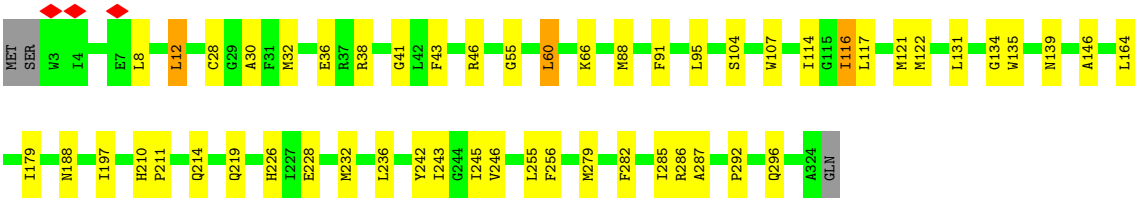
- Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:



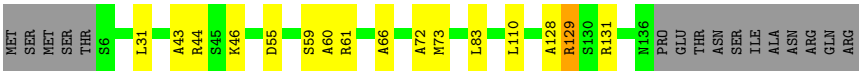
- Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



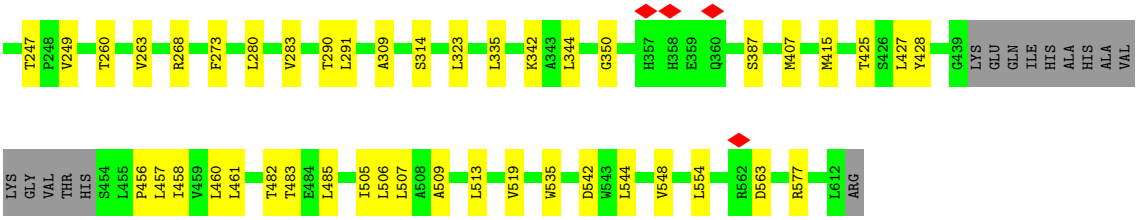
- Molecule 8: NADH-quinone oxidoreductase subunit A

Chain A:



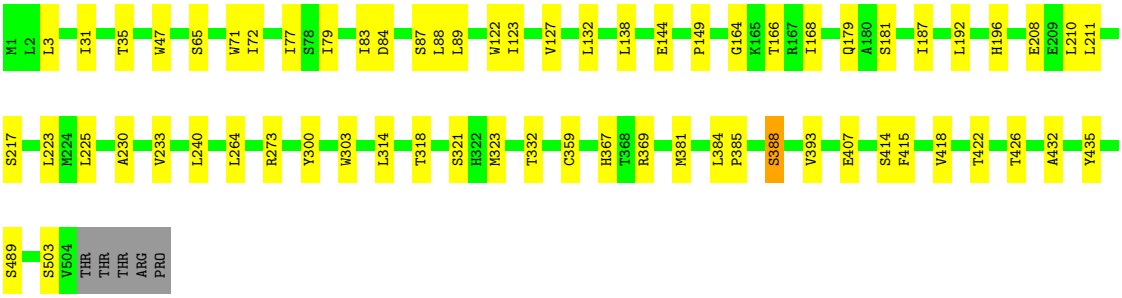
- Molecule 9: NADH dehydrogenase subunit L

Chain L:



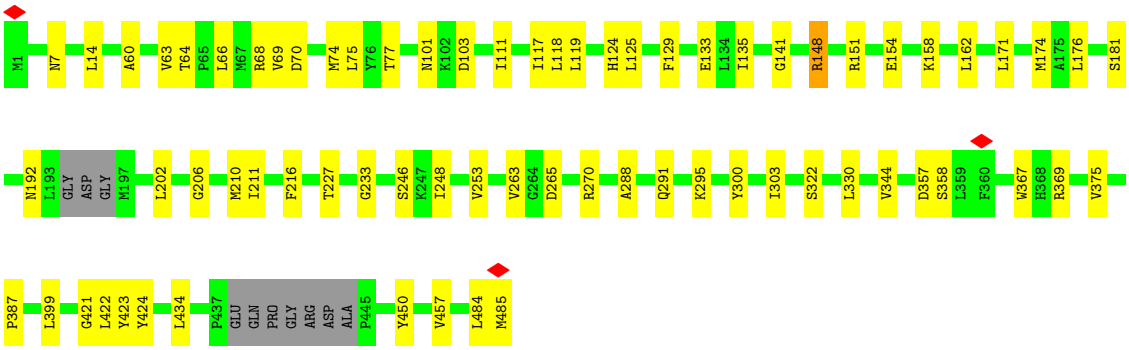
• Molecule 10: NADH dehydrogenase I subunit M

Chain M:



• Molecule 11: NADH-quinone oxidoreductase subunit N

Chain N:

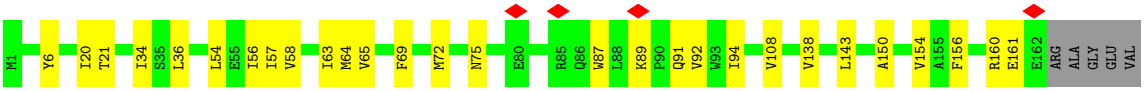


• Molecule 12: NADH-quinone oxidoreductase subunit K

Chain K:

• Molecule 13: NADH-quinone oxidoreductase subunit J

Chain J:



LEU
SER
ASN
ARG
LYS
ASP
ASP
SER
ALA
LYS
ARG
LYS
THR
GLU
GLU
HIS
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.661	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	153.5, 214.5, 235.0	wwPDB
Map dimensions	307, 429, 470	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	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: FES, SF4, LFA, FMN, CA, DCQ, NAI, 3PE

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	F	0.26	0/3486	0.42	0/4713
2	E	0.25	0/1248	0.41	0/1691
3	G	0.27	0/7168	0.41	0/9720
4	C	0.28	0/4891	0.44	0/6637
5	B	0.28	0/1730	0.44	0/2345
6	I	0.28	0/1470	0.45	0/1985
7	H	0.28	0/2610	0.48	1/3553 (0.0%)
8	A	0.27	0/1065	0.43	0/1443
9	L	0.24	0/4675	0.43	0/6372
10	M	0.27	0/4074	0.46	0/5546
11	N	0.26	0/3689	0.44	0/5033
12	K	0.27	0/769	0.44	1/1040 (0.1%)
13	J	0.23	0/1252	0.42	0/1708
All	All	0.27	0/38127	0.44	2/51786 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	95	VAL	CA-CB-CG1	5.41	119.60	110.40
7	H	232	MET	CB-CG-SD	5.12	128.06	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	177	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3407	0	3374	28	0
2	E	1220	0	1187	8	0
3	G	7017	0	6819	55	0
4	C	4760	0	4677	37	0
5	B	1693	0	1670	21	0
6	I	1436	0	1415	13	0
7	H	2534	0	2583	40	0
8	A	1037	0	1054	13	0
9	L	4558	0	4701	44	0
10	M	3953	0	4053	35	0
11	N	3601	0	3770	43	0
12	K	760	0	817	11	0
13	J	1226	0	1297	23	0
14	B	8	0	0	1	0
14	F	8	0	0	1	0
14	G	24	0	0	0	0
14	I	16	0	0	0	0
15	F	31	0	19	2	0
16	F	44	0	27	3	0
17	E	4	0	0	0	0
17	G	4	0	0	0	0
18	G	1	0	0	0	0
19	C	51	0	82	5	0
19	H	36	0	46	3	0
19	I	39	0	52	1	0
19	J	42	0	58	4	0
19	L	217	0	316	7	0
19	M	131	0	190	5	0
19	N	51	0	82	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	23	0	30	1	0
20	C	23	0	30	1	0
21	H	20	0	42	0	0
21	J	20	0	42	0	0
21	N	29	0	56	0	0
22	A	38	0	0	0	0
22	B	67	0	0	0	0
22	C	206	0	0	1	0
22	E	26	0	0	0	0
22	F	97	0	0	0	0
22	G	353	0	0	3	0
22	H	69	0	0	1	0
22	I	95	0	0	1	0
22	J	20	0	0	0	0
22	K	17	0	0	1	0
22	L	47	0	0	0	0
22	M	85	0	0	4	0
22	N	64	0	0	1	0
All	All	39208	0	38489	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 333 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HB2	16:F:503:NAI:H42N	1.62	0.80
11:N:248:ILE:HG12	11:N:330:LEU:HD22	1.74	0.69
9:L:223:LEU:HD13	9:L:283:VAL:HG22	1.75	0.69
10:M:359:CYS:SG	10:M:369:ARG:NH1	2.67	0.68
8:A:83:LEU:HD22	13:J:54:LEU:HD13	1.77	0.65

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	437/445 (98%)	426 (98%)	11 (2%)	0	100	100
2	E	154/166 (93%)	150 (97%)	4 (3%)	0	100	100
3	G	903/908 (99%)	879 (97%)	21 (2%)	3 (0%)	36	50
4	C	587/596 (98%)	576 (98%)	11 (2%)	0	100	100
5	B	209/220 (95%)	196 (94%)	13 (6%)	0	100	100
6	I	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
7	H	320/325 (98%)	308 (96%)	12 (4%)	0	100	100
8	A	129/147 (88%)	127 (98%)	2 (2%)	0	100	100
9	L	594/613 (97%)	583 (98%)	11 (2%)	0	100	100
10	M	502/509 (99%)	492 (98%)	10 (2%)	0	100	100
11	N	469/485 (97%)	462 (98%)	6 (1%)	1 (0%)	43	58
12	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
13	J	160/184 (87%)	158 (99%)	2 (1%)	0	100	100
All	All	4740/4878 (97%)	4629 (98%)	107 (2%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	178	HIS
3	G	261	HIS
3	G	669	THR
11	N	64	THR

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	F	353/359 (98%)	350 (99%)	3 (1%)	73	86
2	E	129/139 (93%)	128 (99%)	1 (1%)	73	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	730/736 (99%)	718 (98%)	12 (2%)	55	76
4	C	509/515 (99%)	504 (99%)	5 (1%)	68	84
5	B	185/192 (96%)	182 (98%)	3 (2%)	55	76
6	I	154/154 (100%)	151 (98%)	3 (2%)	50	71
7	H	266/269 (99%)	263 (99%)	3 (1%)	65	82
8	A	104/119 (87%)	102 (98%)	2 (2%)	50	71
9	L	471/485 (97%)	461 (98%)	10 (2%)	47	69
10	M	413/418 (99%)	403 (98%)	10 (2%)	43	65
11	N	378/385 (98%)	369 (98%)	9 (2%)	43	65
12	K	79/79 (100%)	78 (99%)	1 (1%)	61	80
13	J	128/146 (88%)	126 (98%)	2 (2%)	55	76
All	All	3899/3996 (98%)	3835 (98%)	64 (2%)	54	76

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	N	246	SER
11	N	322	SER
6	I	64	ASN
5	B	175	SER
11	N	358	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
11	N	291	GLN
11	N	305	HIS
4	C	212	ASN
3	G	806	GLN
12	K	27	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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\#\|Z\| > 2$
14	SF4	G	1002	3	0,12,12	-	-	-		
19	3PE	M	1003	-	36,36,50	0.35	0	39,41,55	0.34	0
21	LFA	N	502	-	13,13,19	0.13	0	12,12,18	0.12	0
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	F	501	1	0,12,12	-	-	-		
19	3PE	M	1001	-	46,46,50	0.31	0	49,51,55	0.34	0
19	3PE	L	803	-	39,39,50	0.34	0	42,44,55	0.34	0
19	3PE	H	602	-	35,35,50	0.37	0	38,40,55	0.41	0
19	3PE	L	805	-	38,38,50	0.34	0	41,43,55	0.35	0
14	SF4	B	301	5	0,12,12	-	-	-		
19	3PE	C	701	-	50,50,50	0.30	0	53,55,55	0.33	0
19	3PE	I	203	-	38,38,50	0.35	0	41,43,55	0.30	0
19	3PE	L	804	-	50,50,50	0.30	0	53,55,55	0.31	0
17	FES	G	1004	3	0,4,4	-	-	-		
20	DCQ	C	702	-	23,23,23	0.25	0	26,29,29	0.37	0
21	LFA	H	601	-	19,19,19	0.11	0	18,18,18	0.12	0
17	FES	E	201	2	0,4,4	-	-	-		
15	FMN	F	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.34	9 (18%)
14	SF4	I	201	6	0,12,12	-	-	-		
19	3PE	N	503	-	50,50,50	0.29	0	53,55,55	0.36	0
19	3PE	L	801	-	50,50,50	0.30	0	53,55,55	0.28	0
21	LFA	J	901	-	19,19,19	0.12	0	18,18,18	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	3PE	J	902	-	41,41,50	0.33	0	44,46,55	0.33	0
19	3PE	L	802	-	35,35,50	0.36	0	38,40,55	0.36	0
20	DCQ	B	302	-	23,23,23	0.25	0	26,29,29	0.43	0
16	NAI	F	503	-	45,48,48	0.32	0	60,73,73	0.35	0
21	LFA	N	501	-	14,14,19	0.16	0	13,13,18	0.11	0
14	SF4	G	1003	3	0,12,12	-	-	-		
19	3PE	M	1002	-	46,46,50	0.30	0	49,51,55	0.29	0
14	SF4	G	1001	3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	G	1002	3	-	-	0/6/5/5
19	3PE	M	1003	-	-	4/40/40/54	-
21	LFA	N	502	-	-	0/11/11/17	-
14	SF4	I	202	6	-	-	0/6/5/5
14	SF4	F	501	1	-	-	0/6/5/5
19	3PE	M	1001	-	-	5/50/50/54	-
19	3PE	L	803	-	-	11/43/43/54	-
19	3PE	H	602	-	-	3/39/39/54	-
19	3PE	L	805	-	-	13/42/42/54	-
14	SF4	B	301	5	-	-	0/6/5/5
19	3PE	C	701	-	-	8/54/54/54	-
19	3PE	I	203	-	-	3/42/42/54	-
19	3PE	L	804	-	-	11/54/54/54	-
17	FES	G	1004	3	-	-	0/1/1/1
20	DCQ	C	702	-	-	5/14/38/38	0/1/1/1
21	LFA	H	601	-	-	1/17/17/17	-
17	FES	E	201	2	-	-	0/1/1/1
15	FMN	F	502	-	-	8/18/18/18	0/3/3/3
19	3PE	N	503	-	-	14/54/54/54	-
14	SF4	I	201	6	-	-	0/6/5/5
19	3PE	L	801	-	-	8/54/54/54	-
21	LFA	J	901	-	-	0/17/17/17	-
19	3PE	J	902	-	-	14/45/45/54	-
19	3PE	L	802	-	-	8/39/39/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DCQ	B	302	-	-	4/14/38/38	0/1/1/1
16	NAI	F	503	-	-	4/29/72/72	0/5/5/5
21	LFA	N	501	-	-	0/12/12/17	-
14	SF4	G	1003	3	-	-	0/6/5/5
19	3PE	M	1002	-	-	8/50/50/54	-
14	SF4	G	1001	3	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	FMN	C4A-N5	3.59	1.37	1.30
15	F	502	FMN	C10-N1	2.00	1.37	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	502	FMN	C4-N3-C2	-3.28	119.58	125.64
15	F	502	FMN	C4A-C10-N10	2.90	120.72	116.48
15	F	502	FMN	C4A-C4-N3	2.80	120.29	113.19
15	F	502	FMN	C10-C4A-N5	-2.44	119.67	124.86
15	F	502	FMN	C4A-C10-N1	-2.39	119.18	124.73

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	502	FMN	C5'-O5'-P-O2P
15	F	502	FMN	C5'-O5'-P-O3P
16	F	503	NAI	C5B-O5B-PA-O1A
19	C	701	3PE	C11-O13-P-O14
19	H	602	3PE	O13-C11-C12-N

There are no ring outliers.

18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	1003	3PE	1	0
14	F	501	SF4	1	0
19	M	1001	3PE	3	0
19	L	803	3PE	1	0

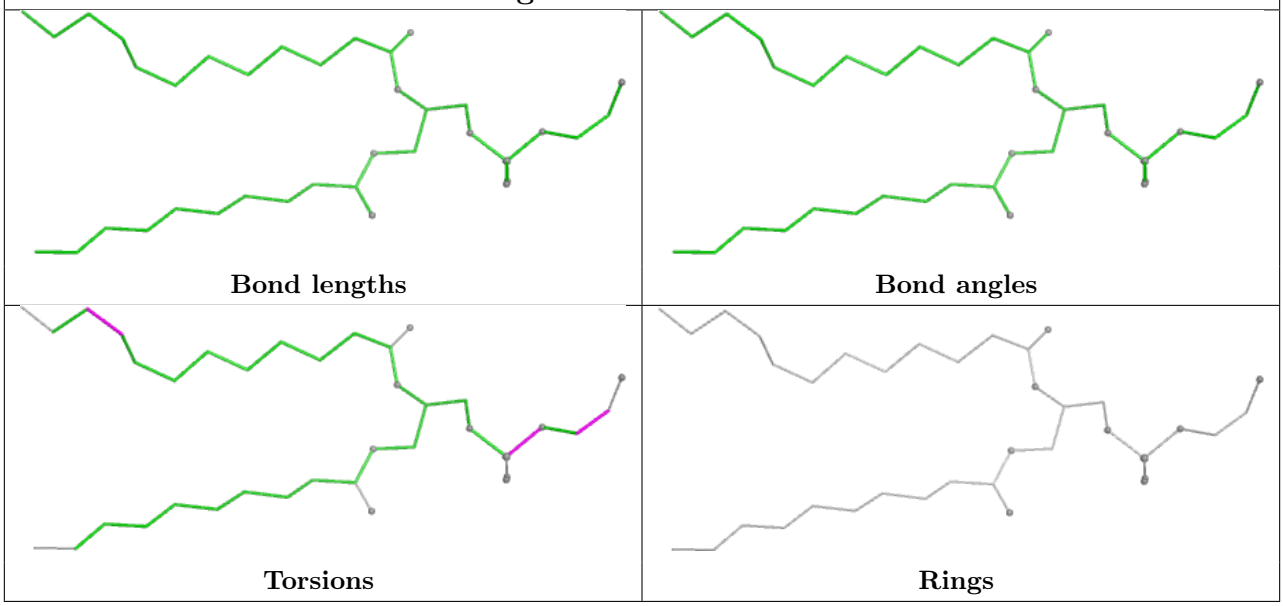
Continued on next page...

Continued from previous page...

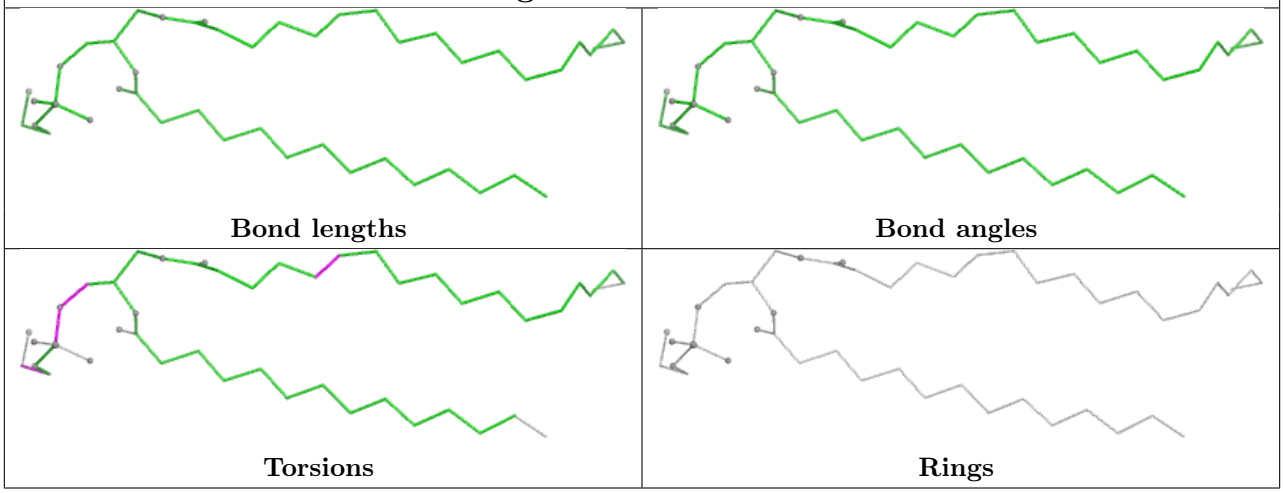
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	602	3PE	3	0
14	B	301	SF4	1	0
19	C	701	3PE	5	0
19	I	203	3PE	1	0
19	L	804	3PE	3	0
20	C	702	DCQ	1	0
15	F	502	FMN	2	0
19	N	503	3PE	1	0
19	L	801	3PE	2	0
19	J	902	3PE	4	0
19	L	802	3PE	2	0
20	B	302	DCQ	1	0
16	F	503	NAI	3	0
19	M	1002	3PE	1	0

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

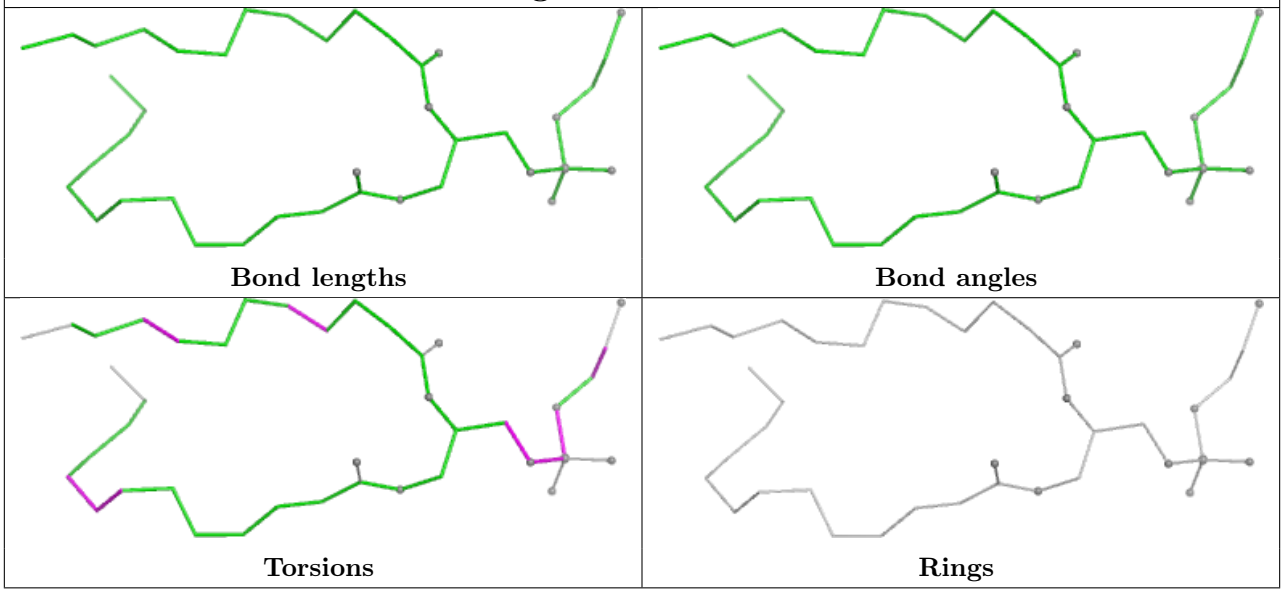
Ligand 3PE M 1003



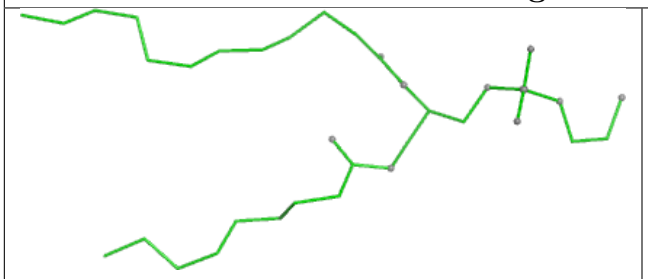
Ligand 3PE M 1001



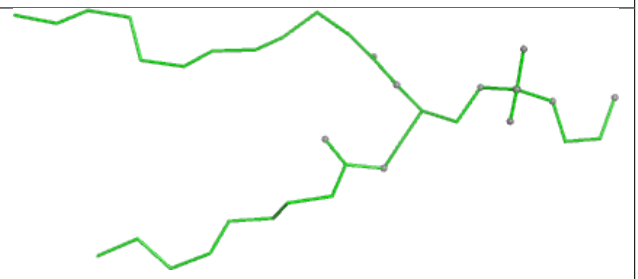
Ligand 3PE L 803



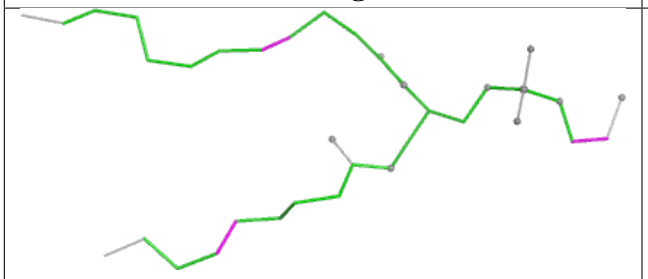
Ligand 3PE H 602



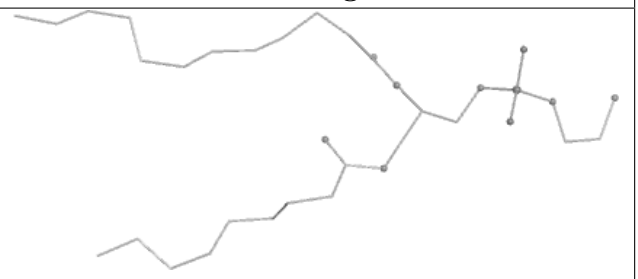
Bond lengths



Bond angles

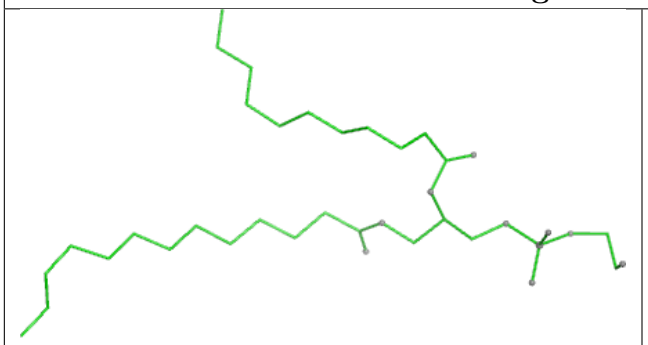


Torsions

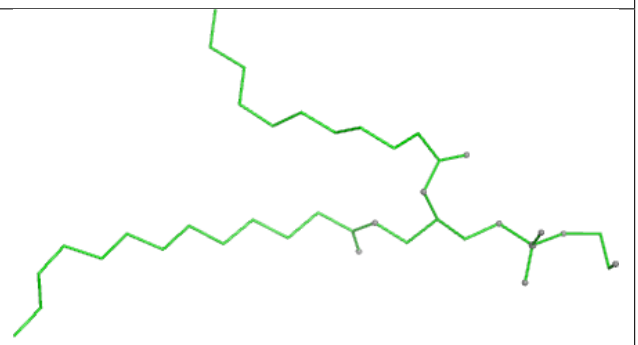


Rings

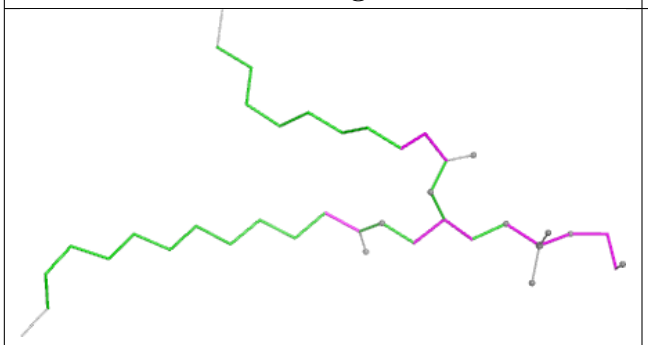
Ligand 3PE L 805



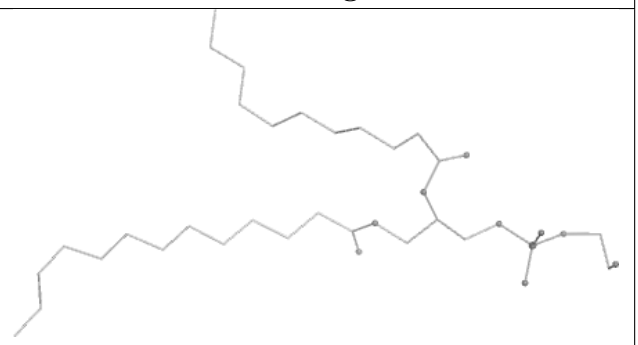
Bond lengths



Bond angles

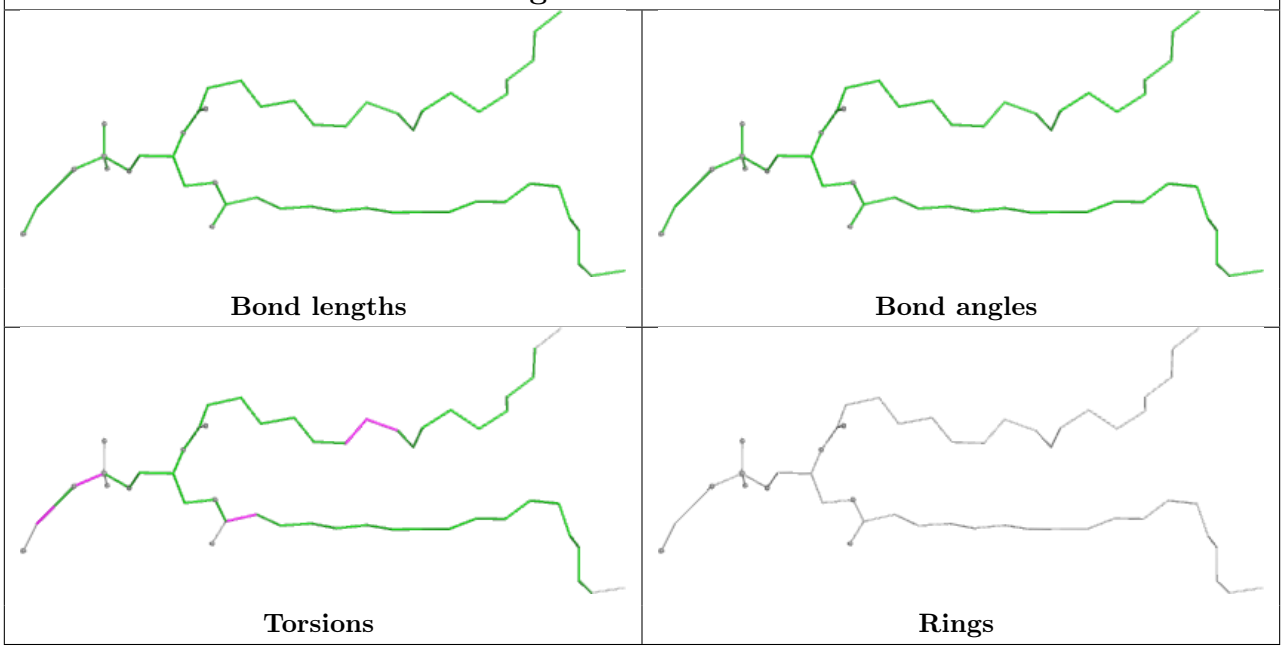


Torsions

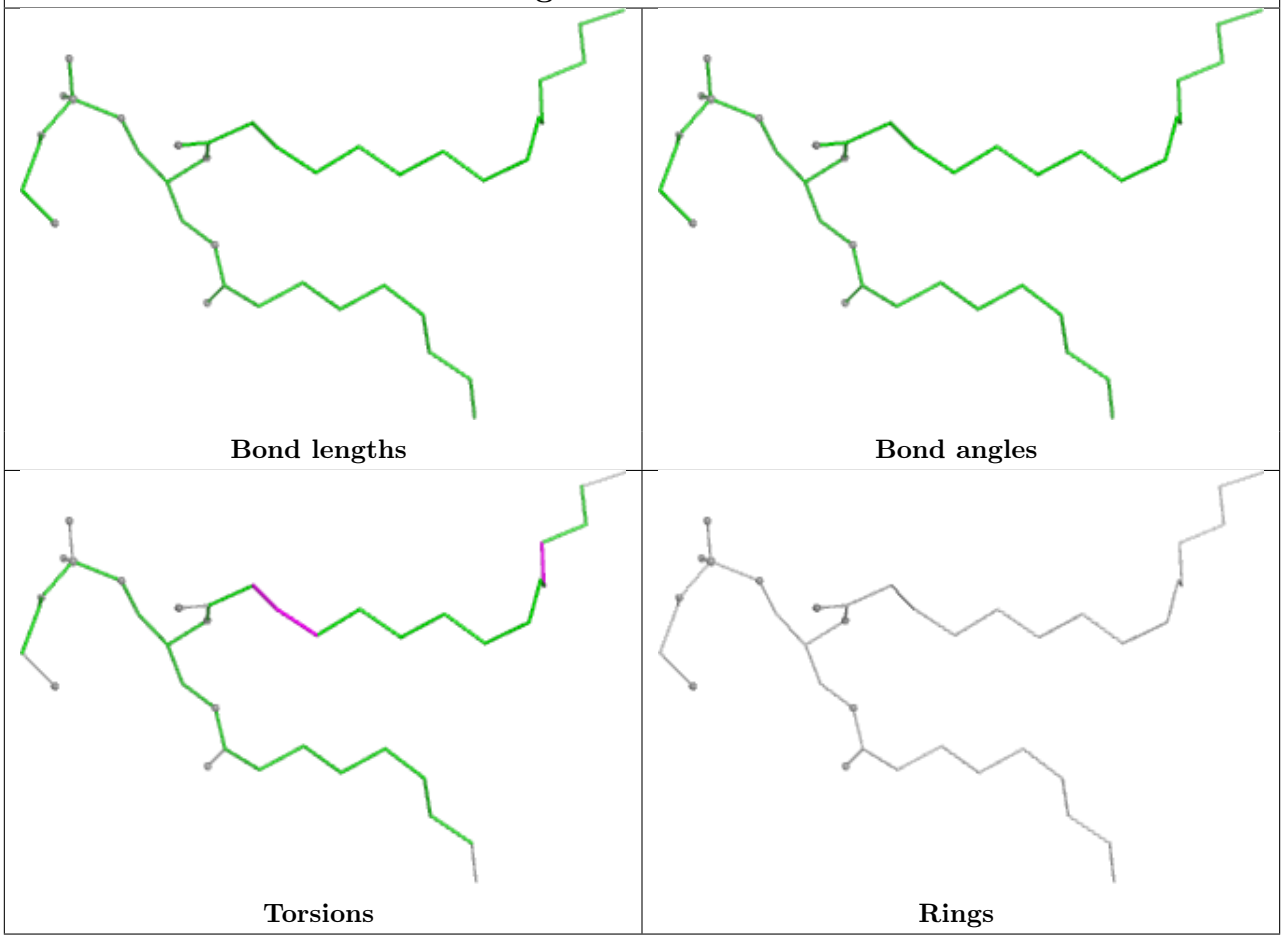


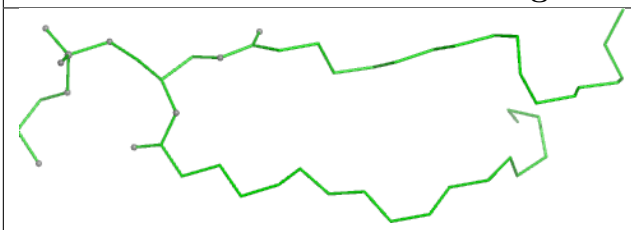
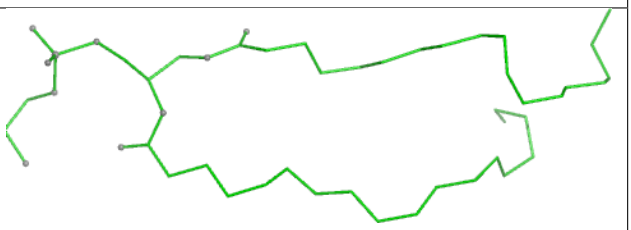
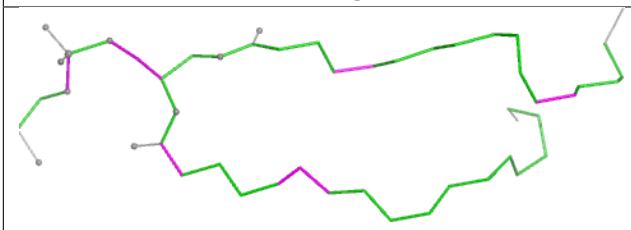
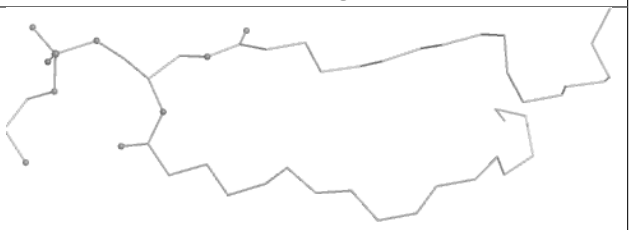
Rings

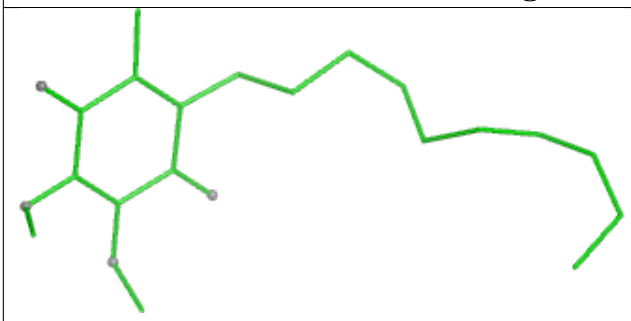
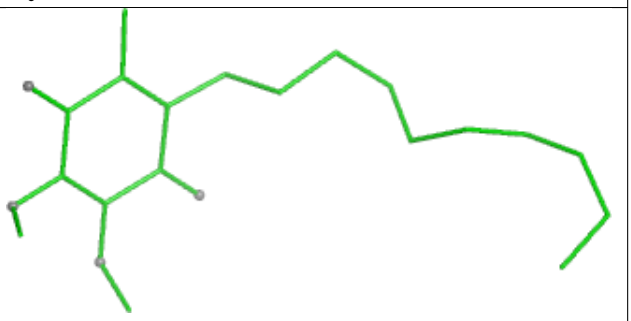
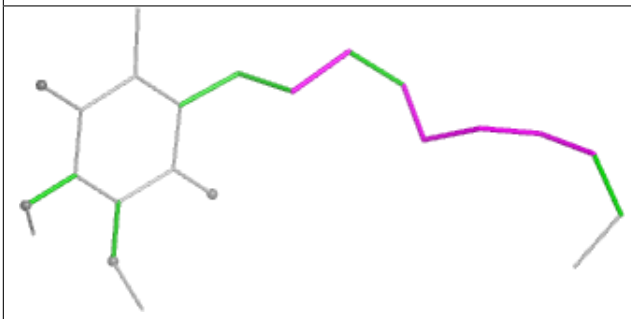
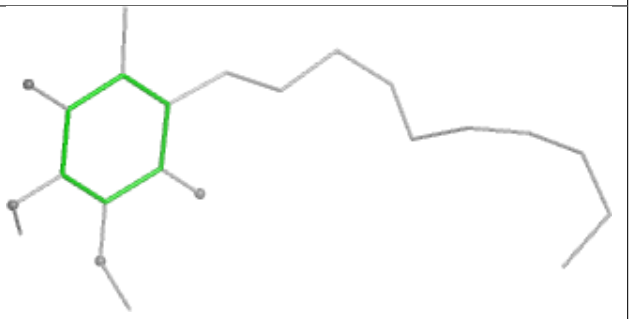
Ligand 3PE C 701



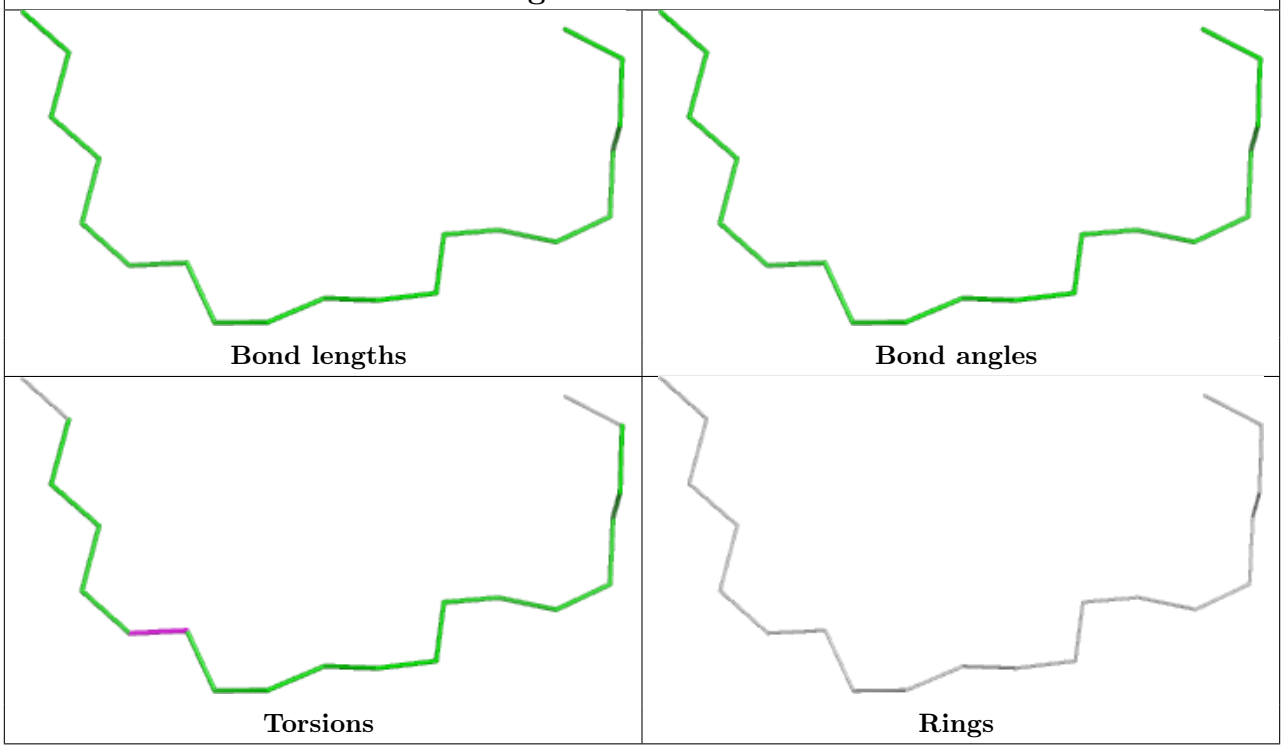
Ligand 3PE I 203



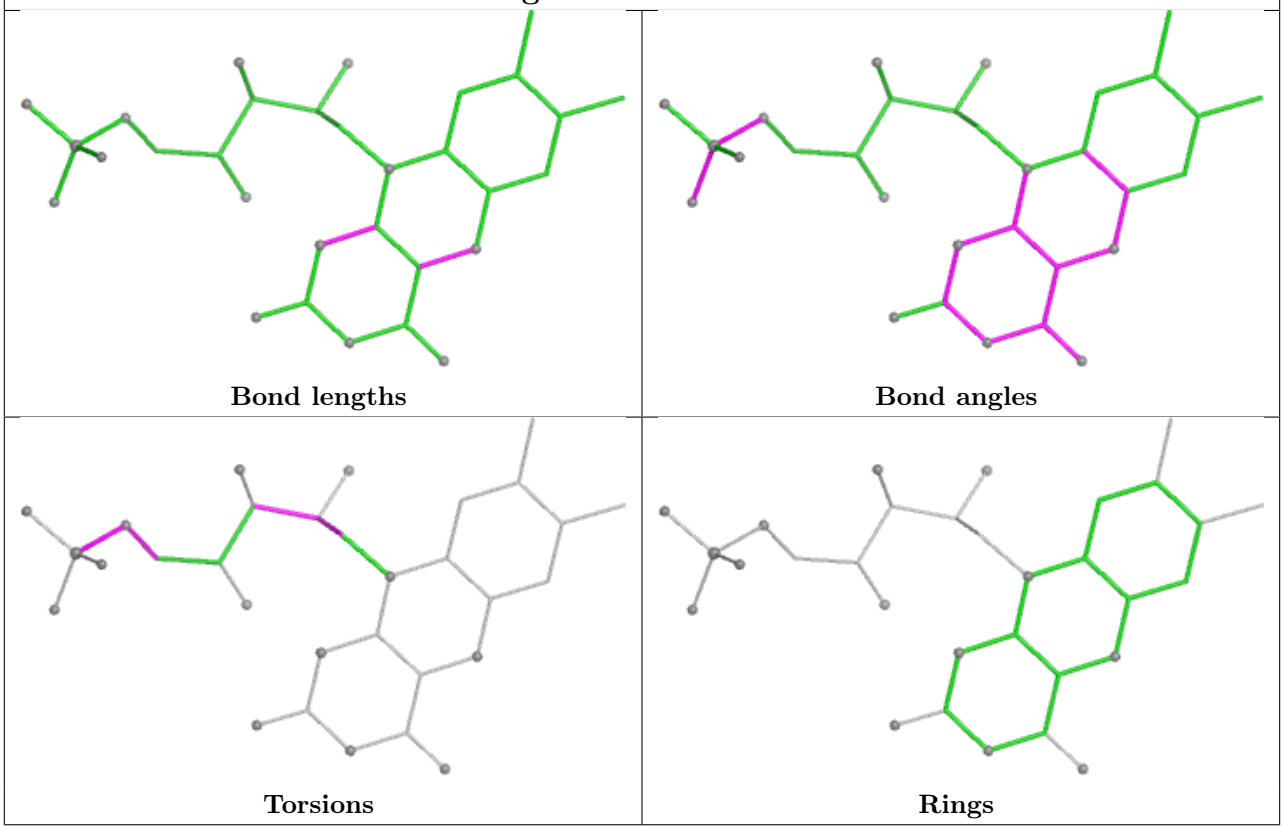
Ligand 3PE L 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DCQ C 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

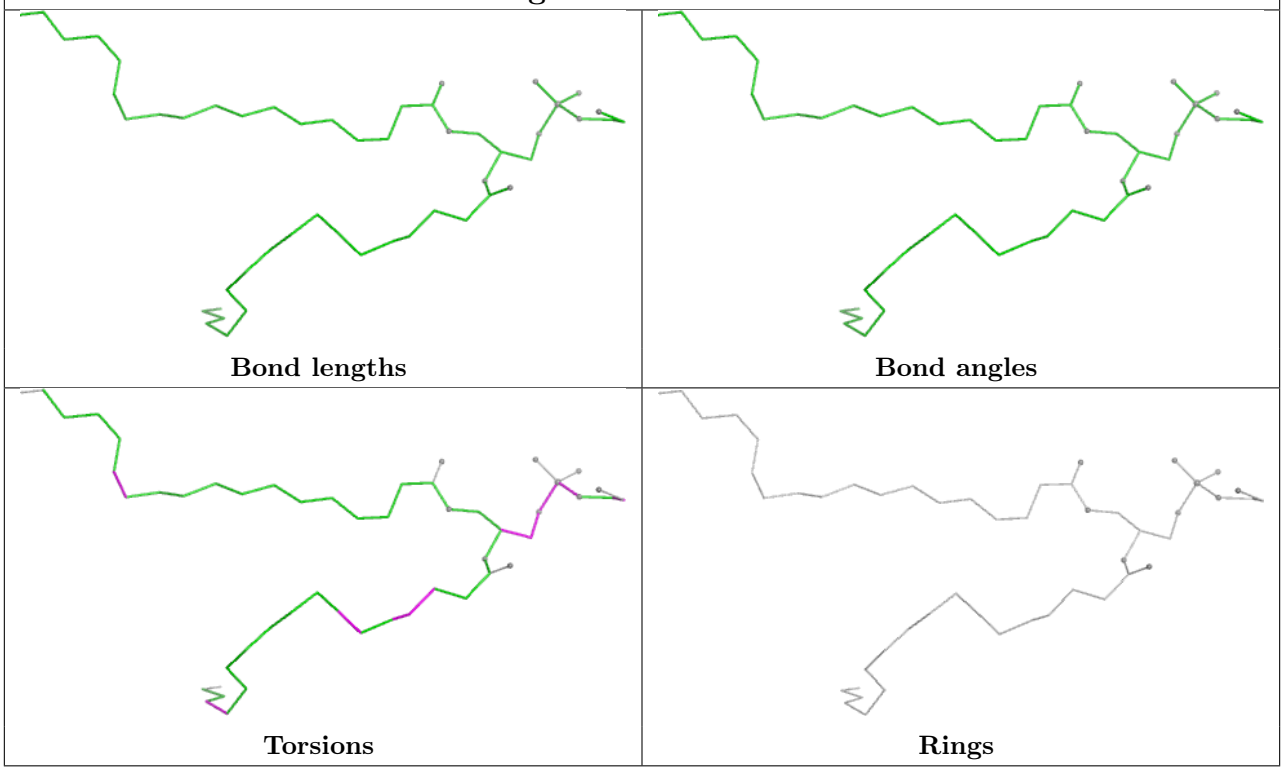
Ligand LFA H 601



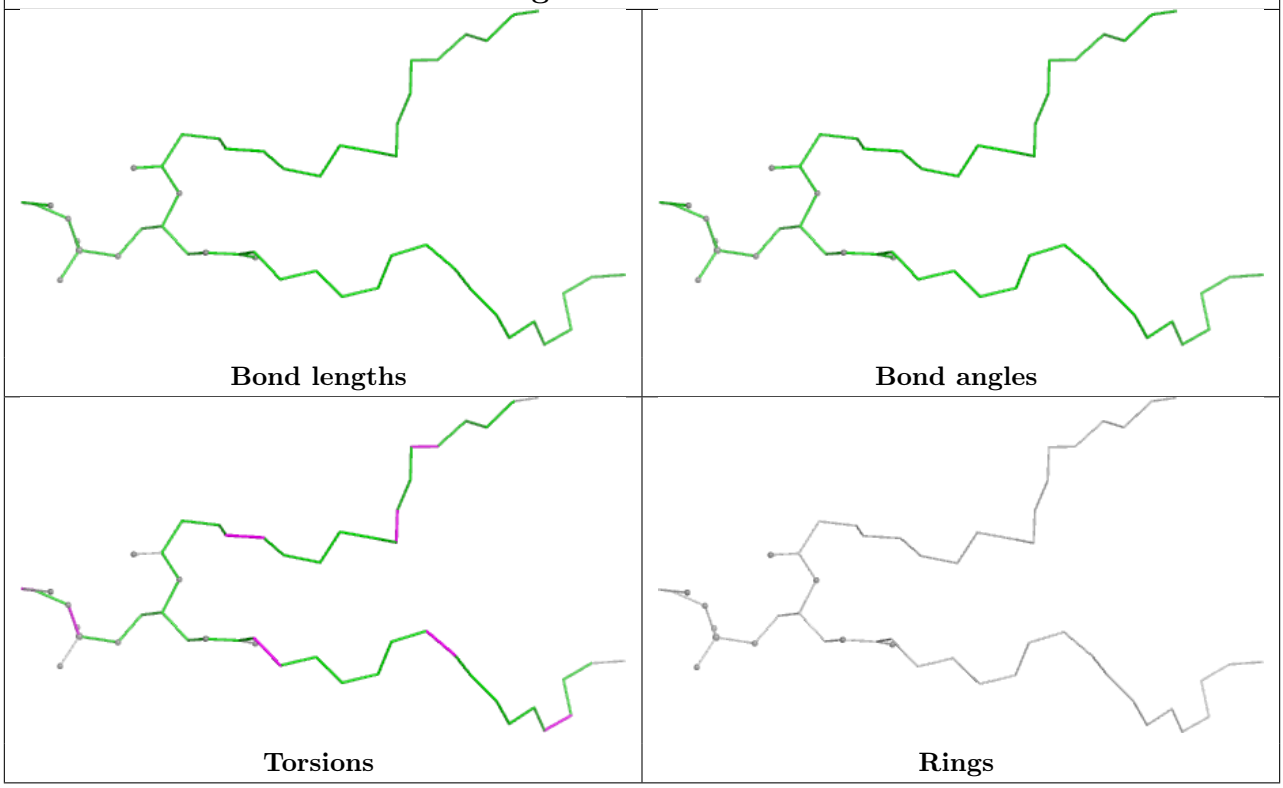
Ligand FMN F 502



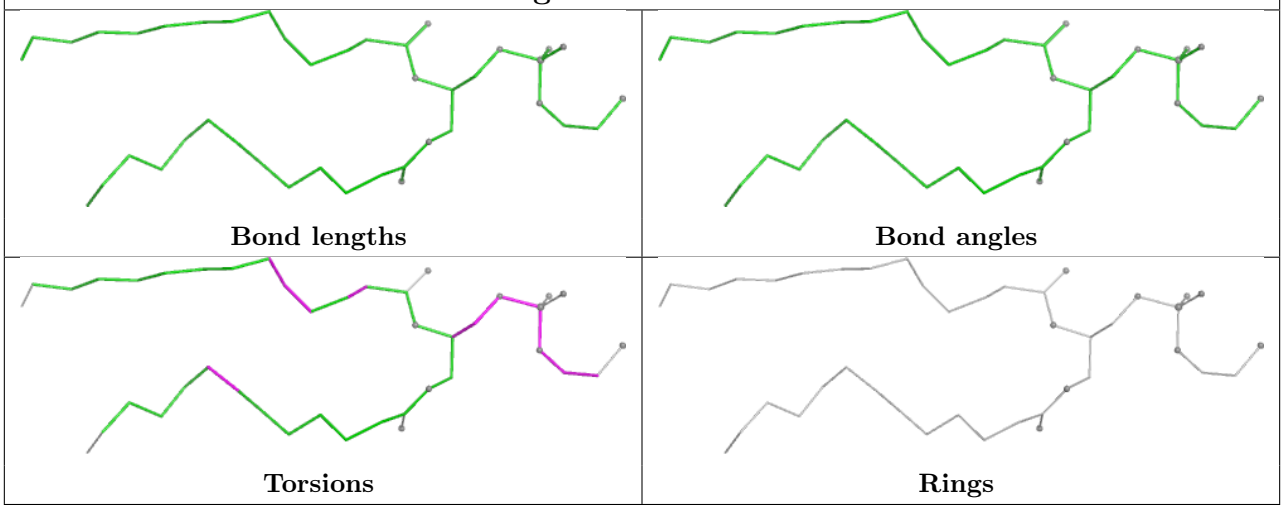
Ligand 3PE N 503



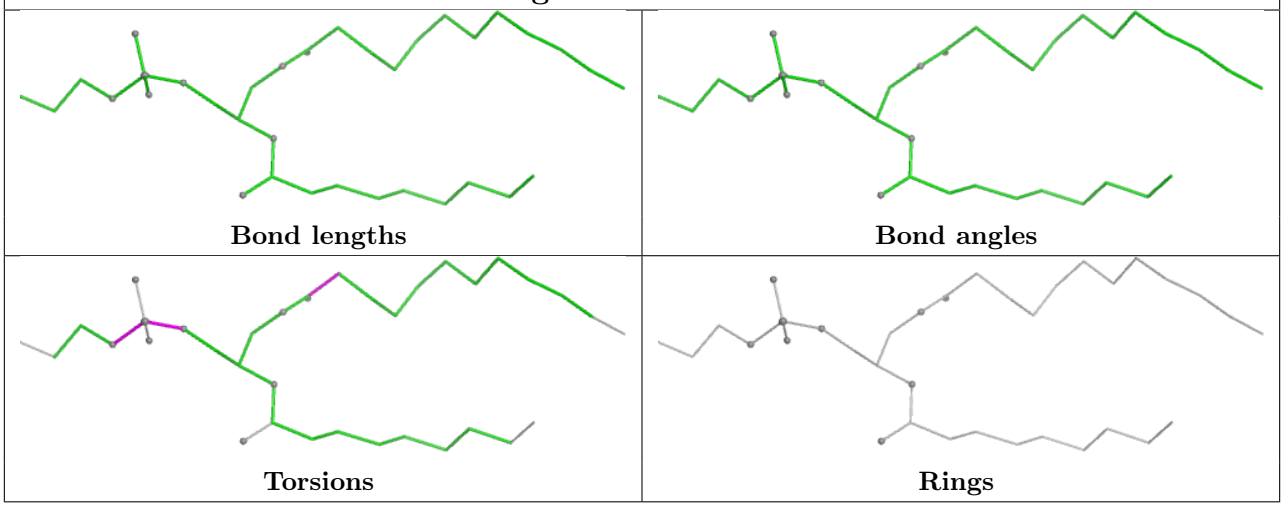
Ligand 3PE L 801



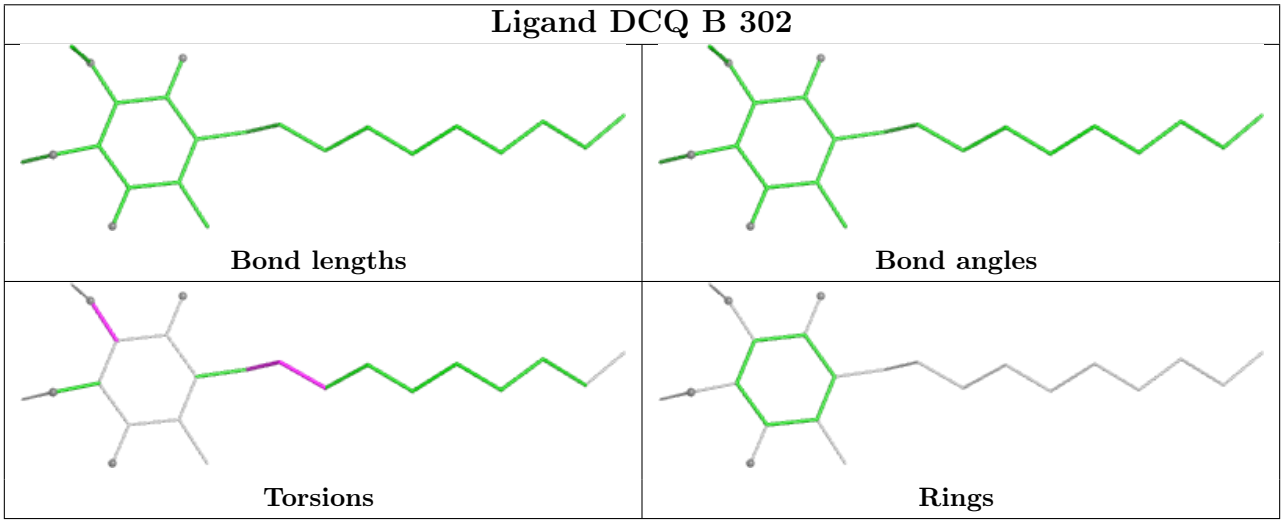
Ligand 3PE J 902

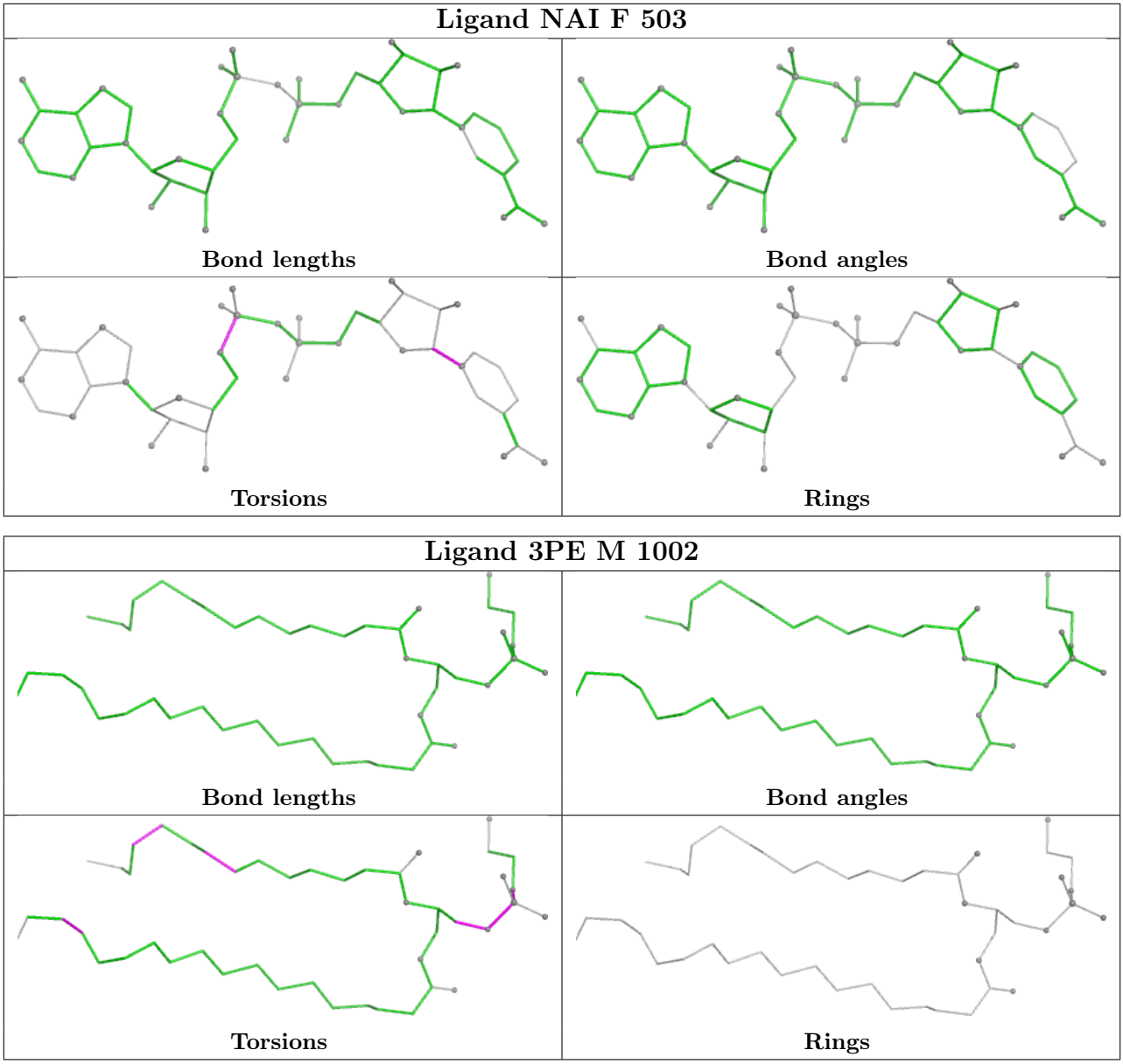


Ligand 3PE L 802



Ligand DCQ B 302





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.

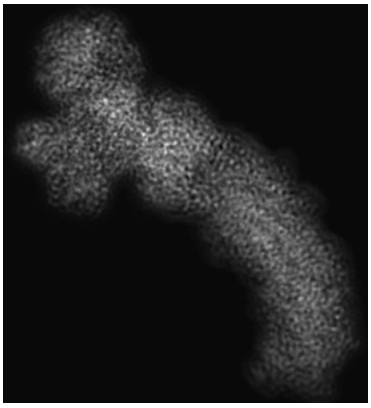
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14536. These allow visual inspection of the internal detail of the map and identification of artifacts.

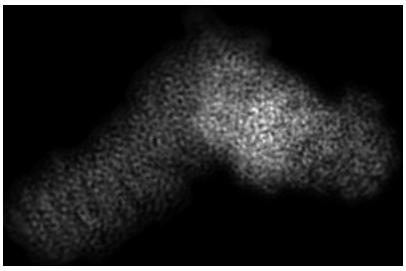
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

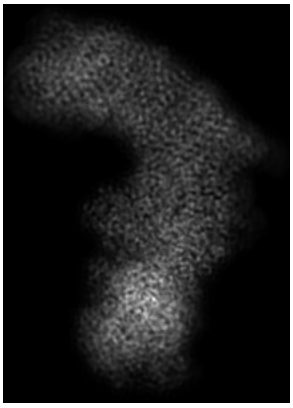
6.1.1 Primary map



X



Y



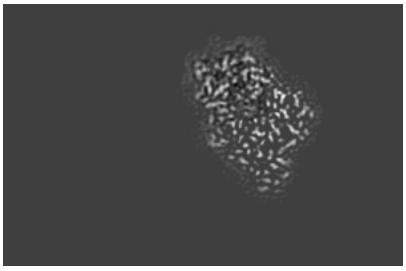
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 153



Y Index: 214

Z Index: 235

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: 160

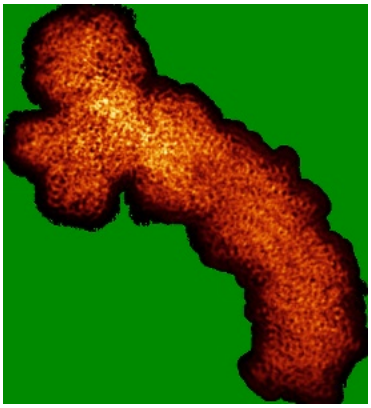
Y Index: 110

Z Index: 305

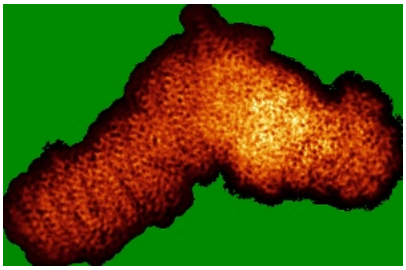
The images above show the largest variance slices of the map in three orthogonal directions.

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

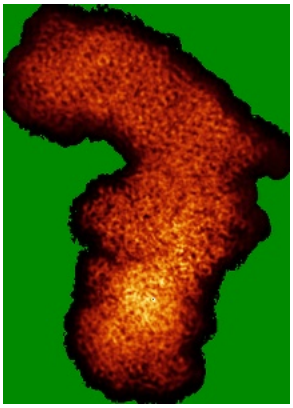
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

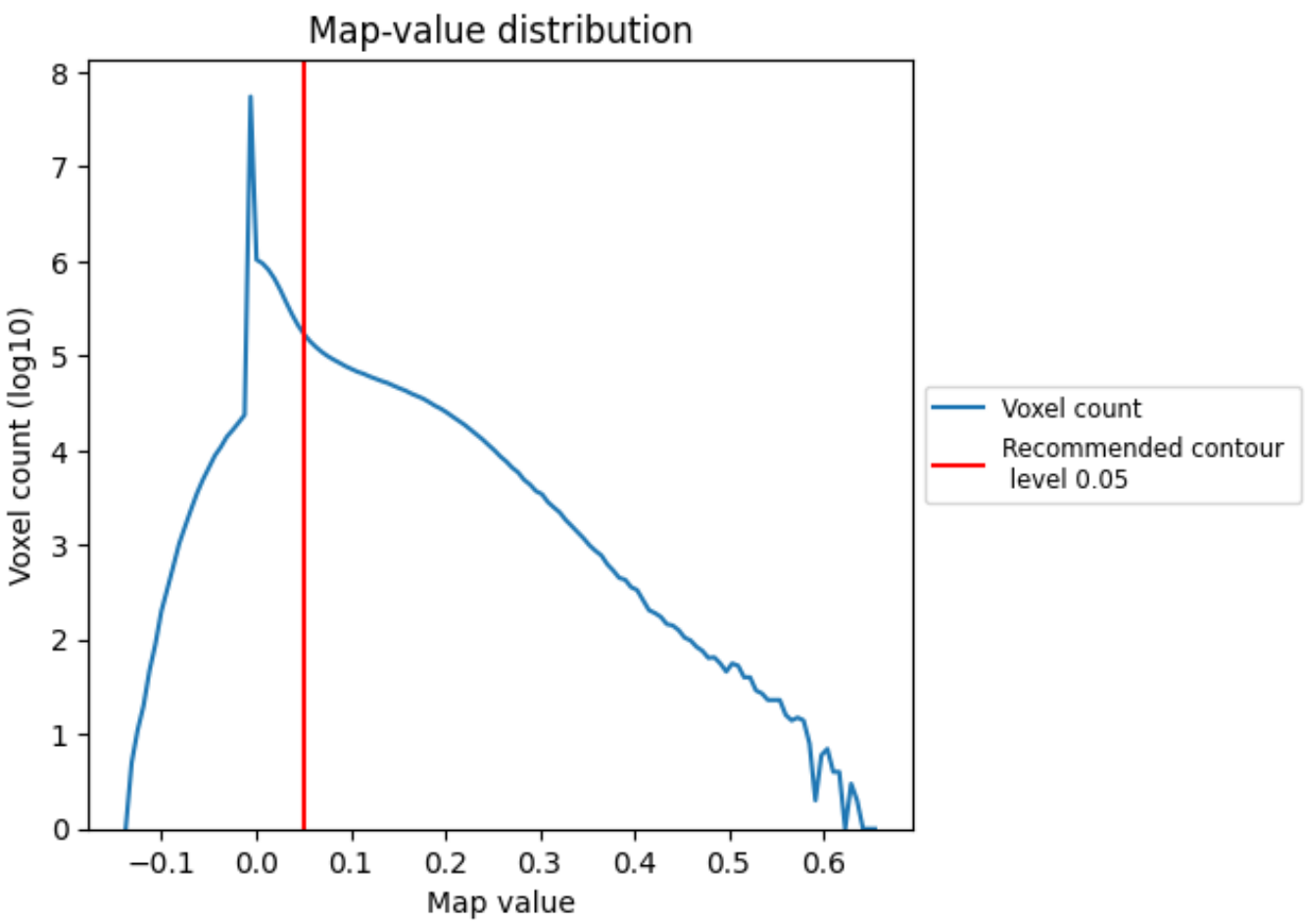
6.6 Mask visualisation (i)

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

7 Map analysis (i)

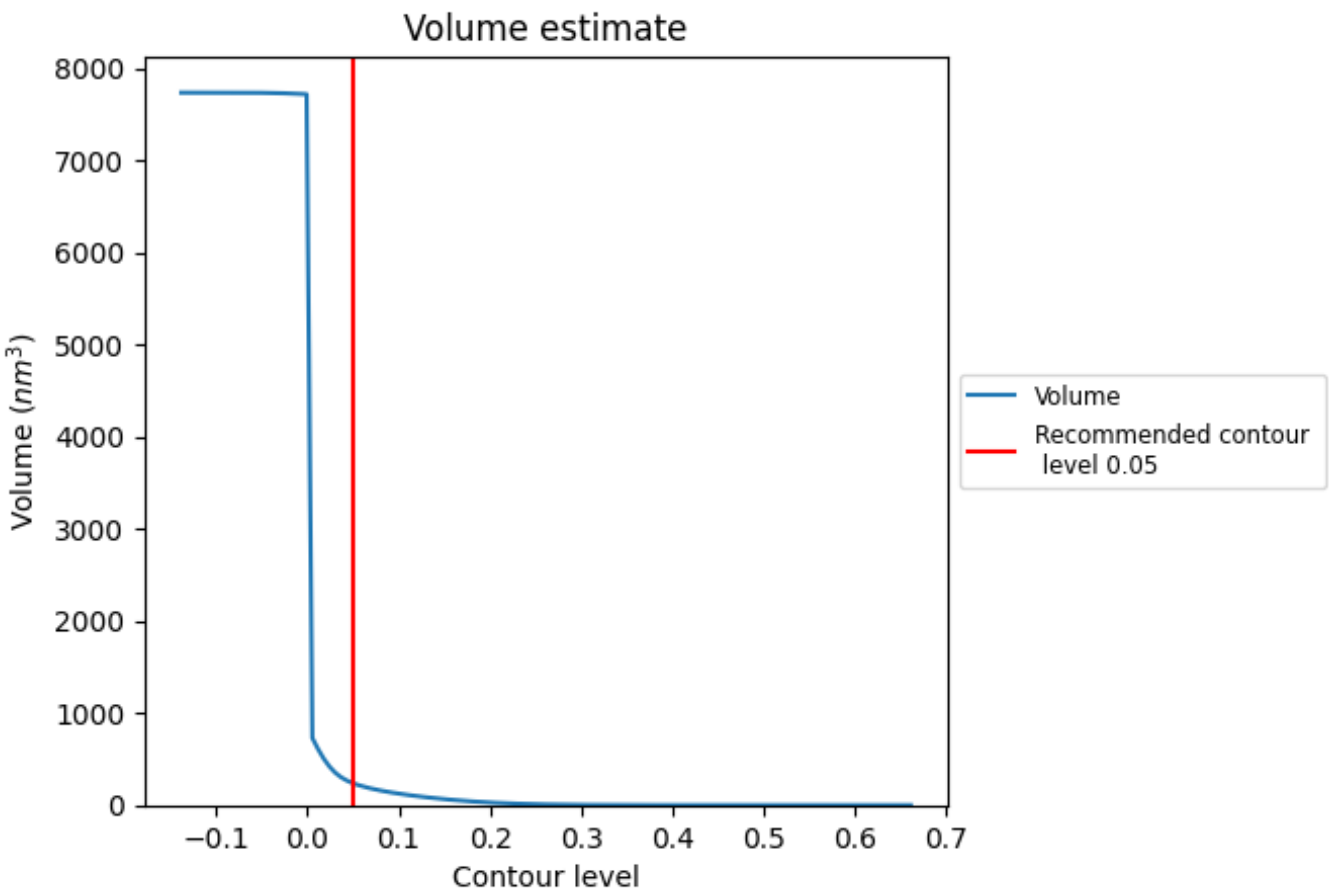
This section contains the results of statistical analysis of the map.

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 239 nm^3; this corresponds to an approximate mass of 216 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.

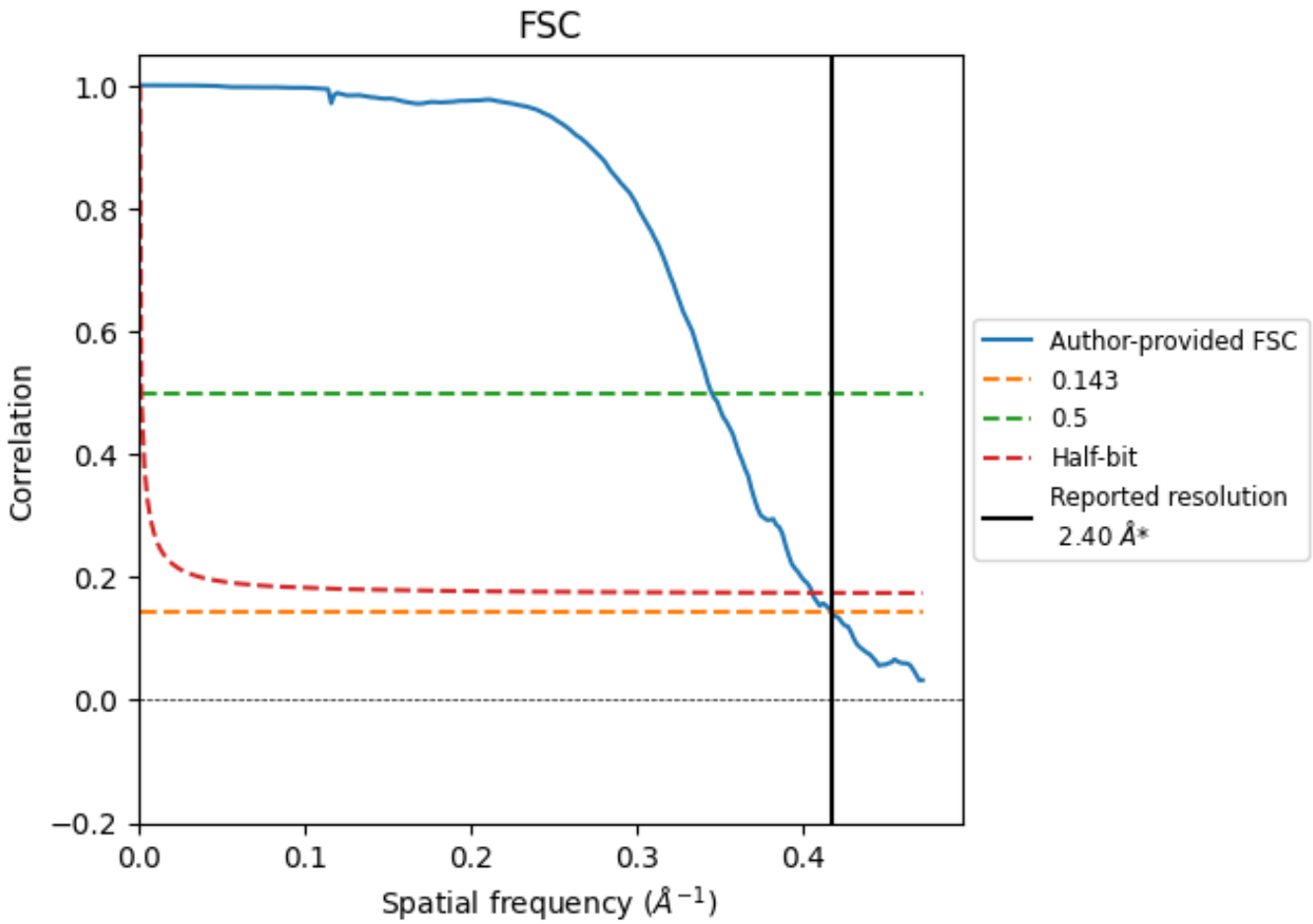
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

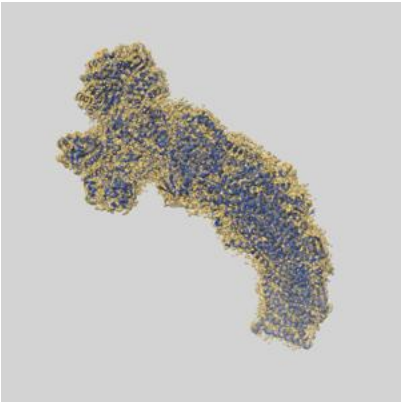
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.90	2.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

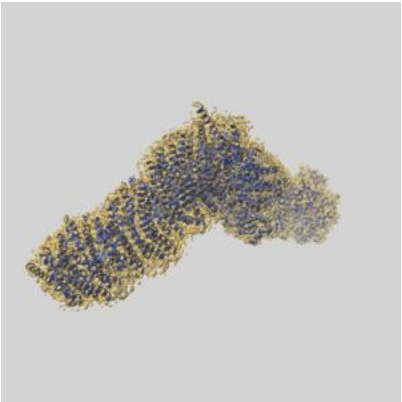
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14536 and PDB model 7Z7S. Per-residue inclusion information can be found in section 3 on page 12.

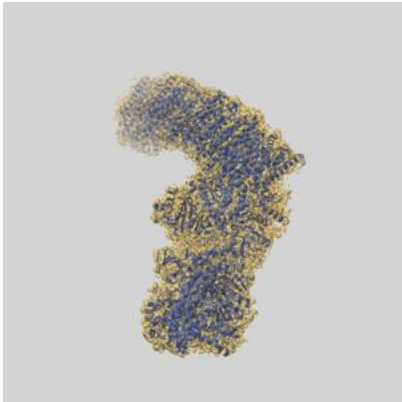
9.1 Map-model overlay (i)



X



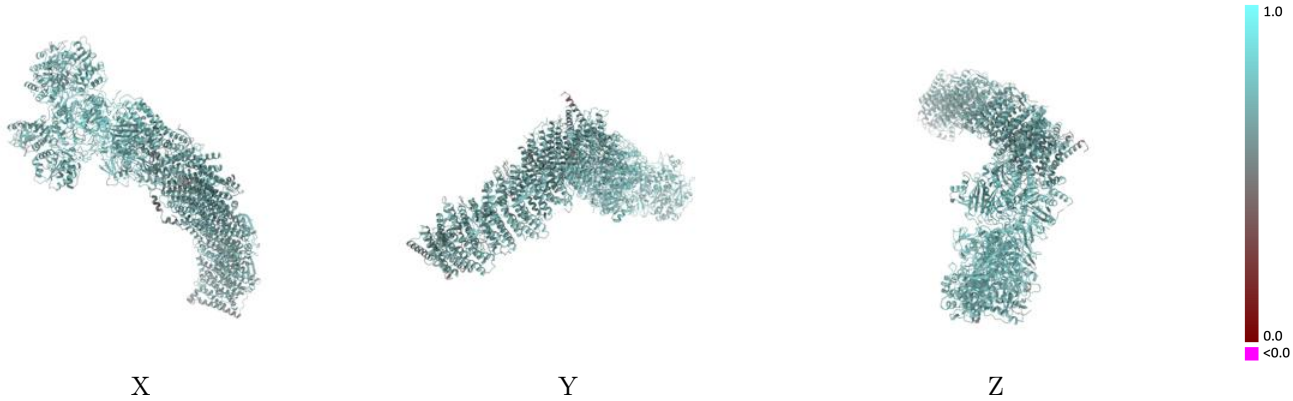
Y



Z

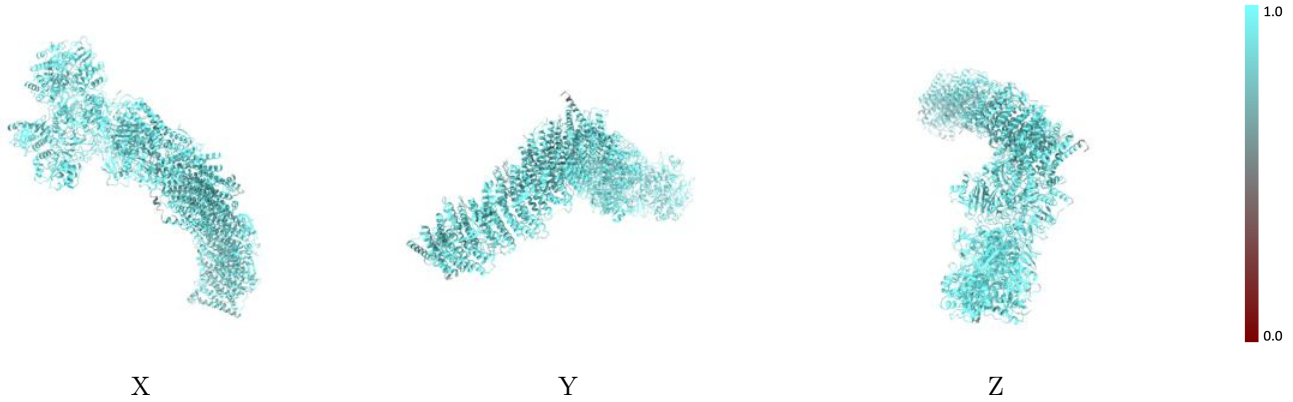
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



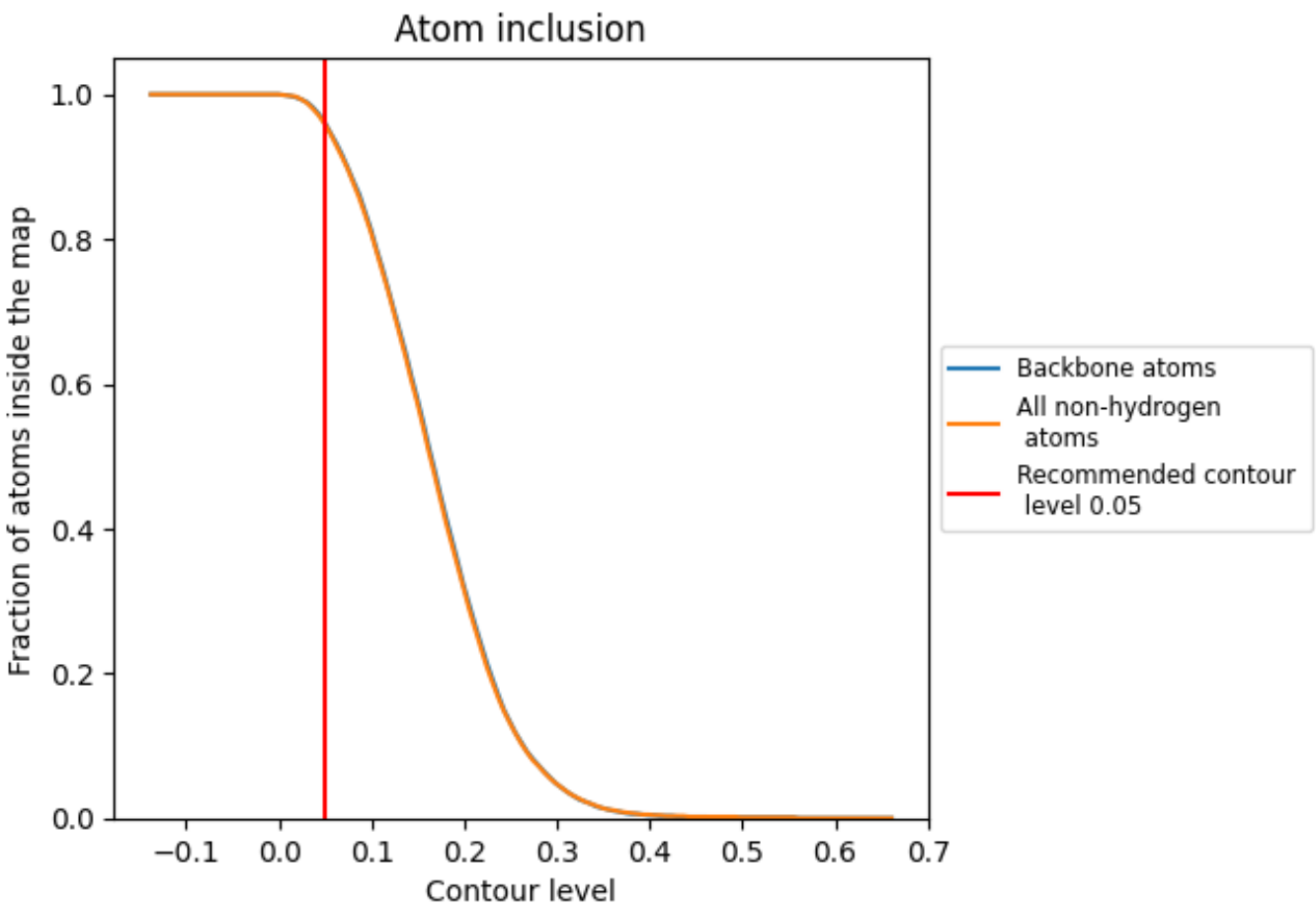
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.6900
A	0.9700	0.6740
B	0.9670	0.7120
C	0.9770	0.7270
E	0.9560	0.6890
F	0.9680	0.6980
G	0.9750	0.7190
H	0.9580	0.6650
I	0.9730	0.7330
J	0.9170	0.6480
K	0.9690	0.6860
L	0.9150	0.6320
M	0.9520	0.6690
N	0.9630	0.6820