



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:59 pm BST

PDB ID : 6ZK9 / pdb_00006zk9
EMDB ID : EMD-11241
Title : Peripheral domain of open complex I during turnover
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.30 Å (reported)
Based on initial model : 5LNK

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.dev117
Mogul : 1.8.4, 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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

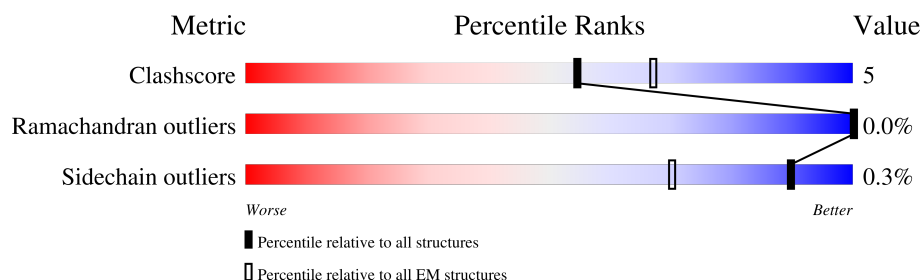
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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






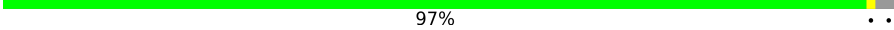


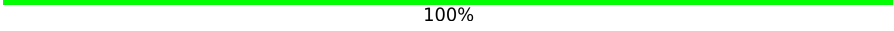


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	464	80% 13% 7%
2	2	246	75% 11% 13%
3	3	727	81% 13% 5%
4	4	463	66% 16% 18%
5	5	266	65% 13% 22%
6	6	223	62% 7% 30%
7	9	217	71% 11% 19%
8	a	109	40% 60%
9	b	124	77% 23%

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Mol	Chain	Length	Quality of chain
10	c	170	 74%26%
11	d	380	 78%22%
12	e	99	 87%13%
13	f	116	 97%..
14	g	140	 81%19%
15	h	114	 83%.16%
16	i	145	 100%
17	j	157	 52%48%
18	q	144	 22%78%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	6	201	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 29587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	380	Total	C	N	O	S	0	0
			3047	1943	523	557	24		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 9 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 13 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called Mitochondrial complex I, B16.6 subunit.

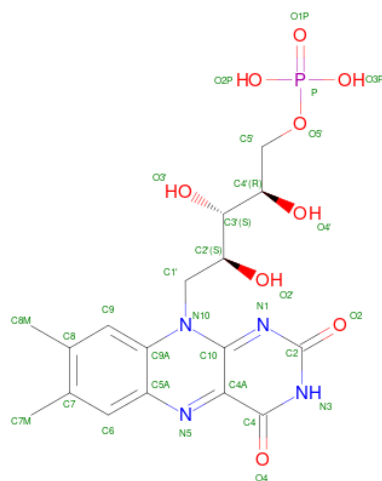
Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	31	Total	C	N	O	S	0	0
			245	157	44	42	2		

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



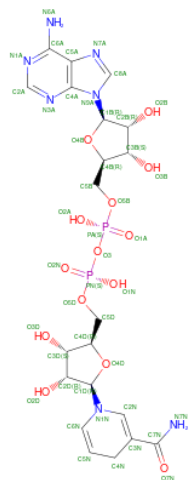
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	Fe	S	0
			8	4	4	
19	3	1	Total	Fe	S	0
			8	4	4	
19	3	1	Total	Fe	S	0
			8	4	4	
19	6	1	Total	Fe	S	0
			8	4	4	
19	9	1	Total	Fe	S	0
			8	4	4	
19	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



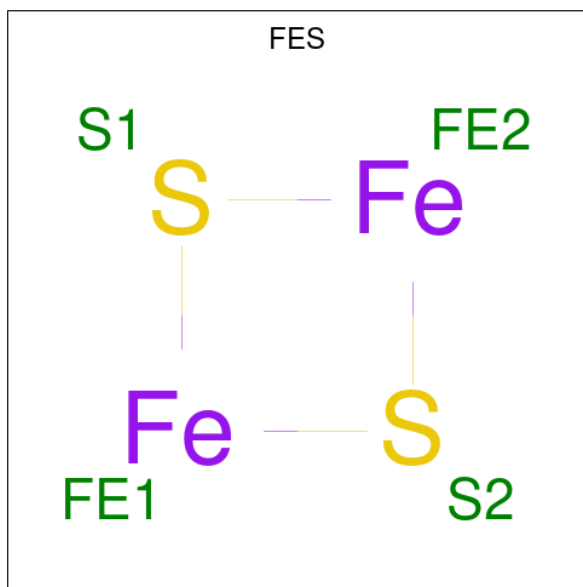
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).



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

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

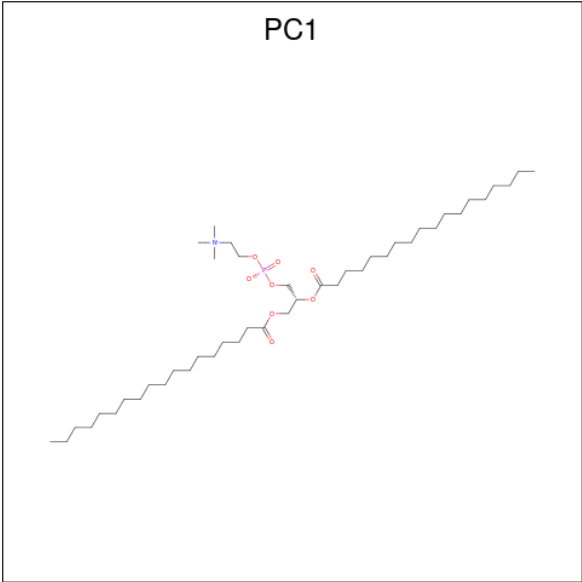


Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	Fe	S	0
			4	2	2	
22	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

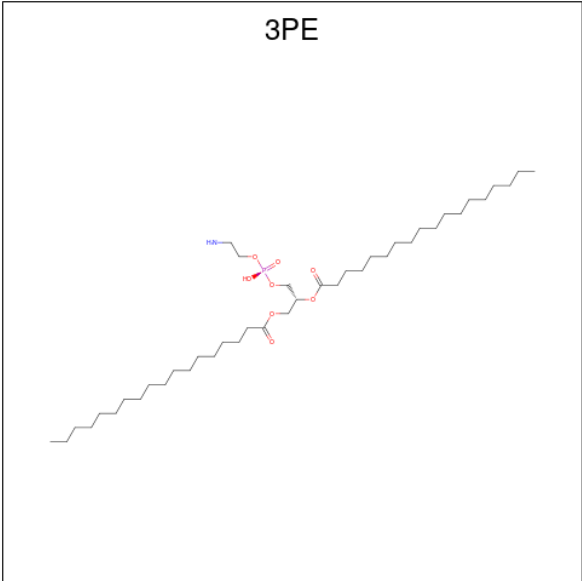
Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	K	0
			1	1	

- Molecule 24 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	9	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	N	O	P	0
			51	41	1	8	1	

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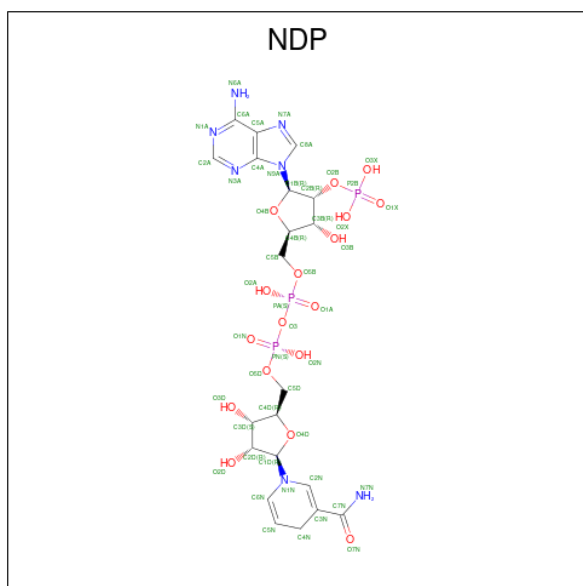
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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

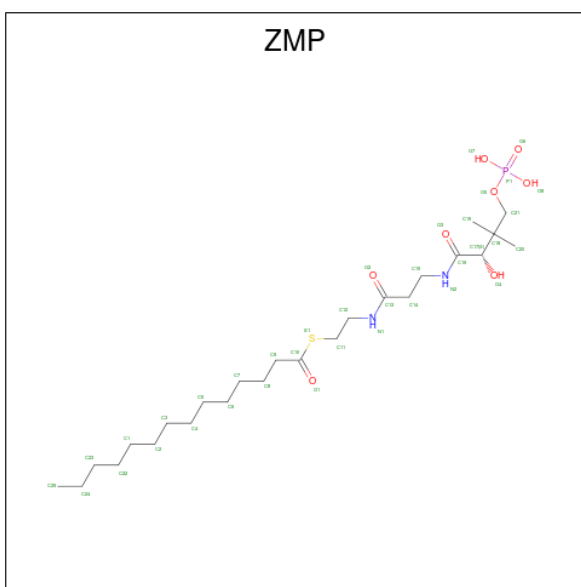
Mol	Chain	Residues	Atoms		AltConf
26	b	1	Total	Zn	0
			1	1	

- Molecule 27 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



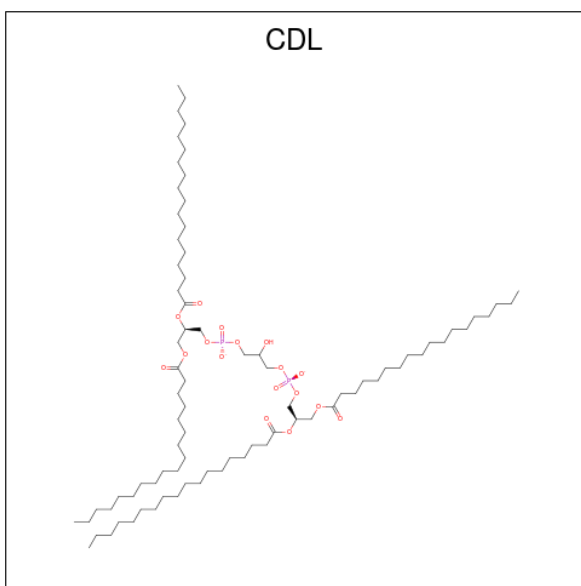
Mol	Chain	Residues	Atoms					AltConf
27	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 28 is S-[2-(N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
28	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
29	h	1	Total	C	O	P	
			58	39	17	2	0

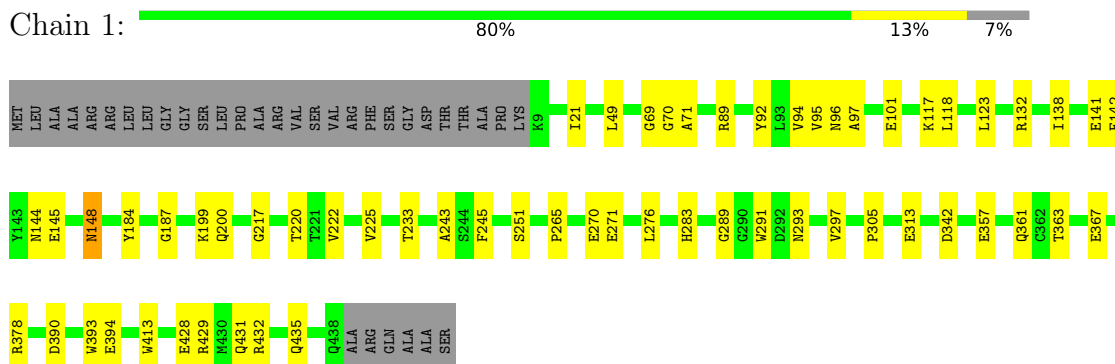
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	1	123	Total 123	O 123	0
30	2	44	Total 44	O 44	0
30	3	285	Total 285	O 285	0
30	4	200	Total 200	O 200	0
30	5	129	Total 129	O 129	0
30	6	81	Total 81	O 81	0
30	9	110	Total 110	O 110	0
30	a	6	Total 6	O 6	0
30	b	67	Total 67	O 67	0
30	c	109	Total 109	O 109	0
30	d	79	Total 79	O 79	0
30	e	7	Total 7	O 7	0
30	f	39	Total 39	O 39	0
30	g	38	Total 38	O 38	0
30	h	71	Total 71	O 71	0
30	i	83	Total 83	O 83	0
30	q	1	Total 1	O 1	0

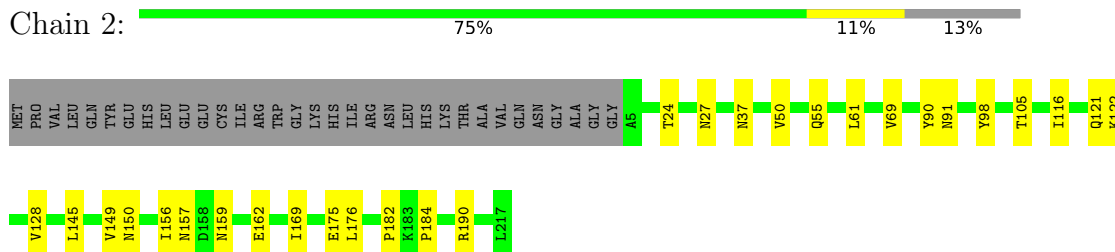
3 Residue-property plots [i](#)

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

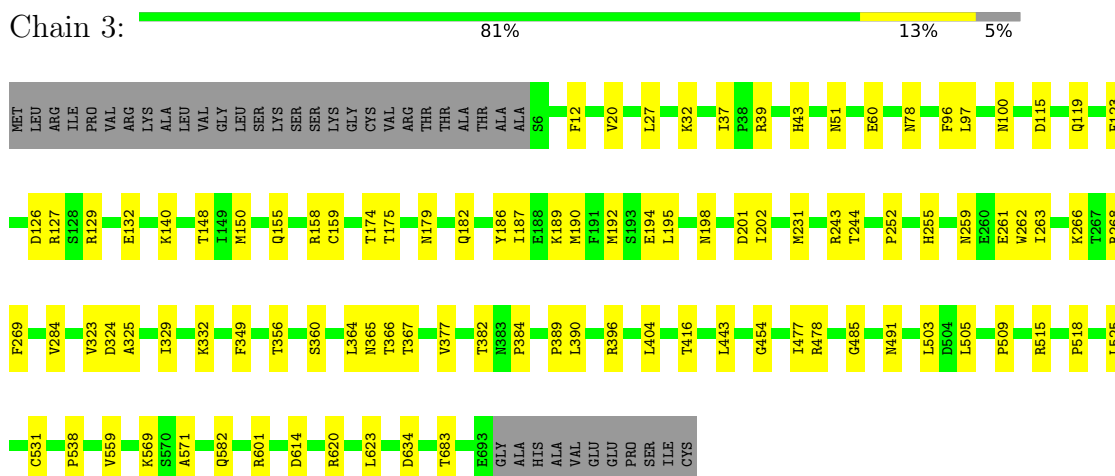
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



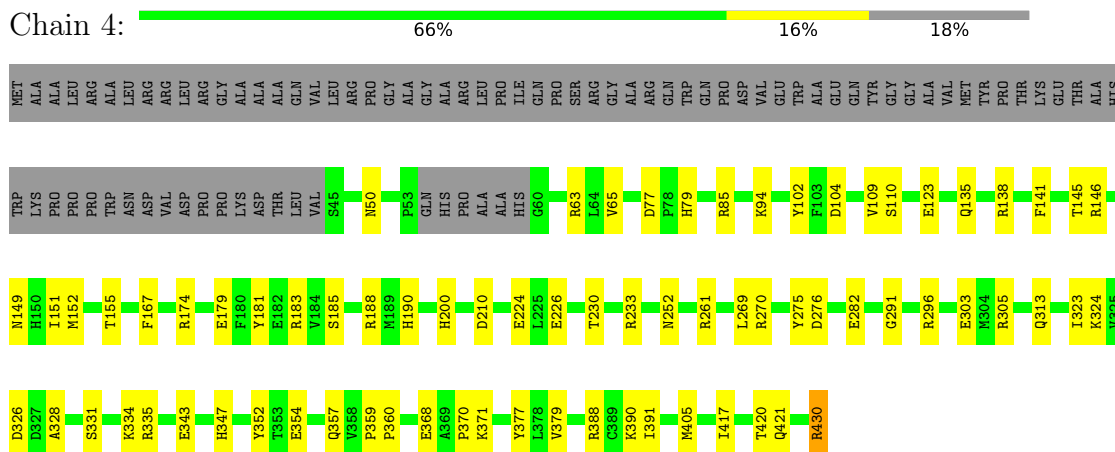
- Molecule 2: Mitochondrial complex I, 24 kDa subunit



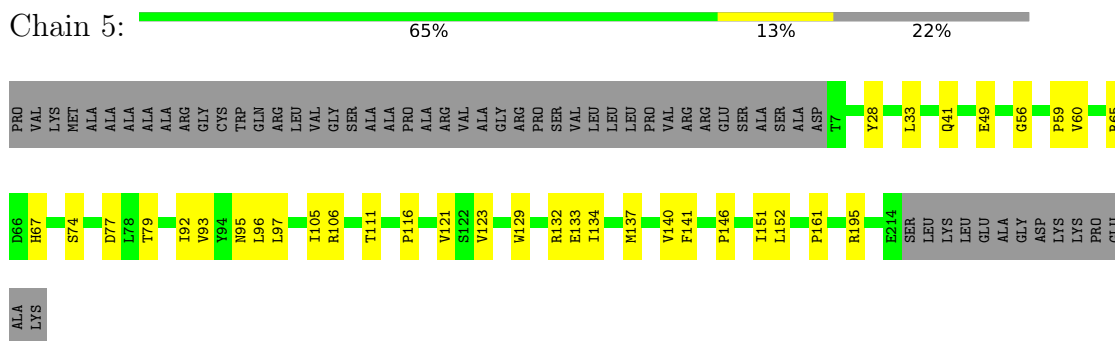
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1



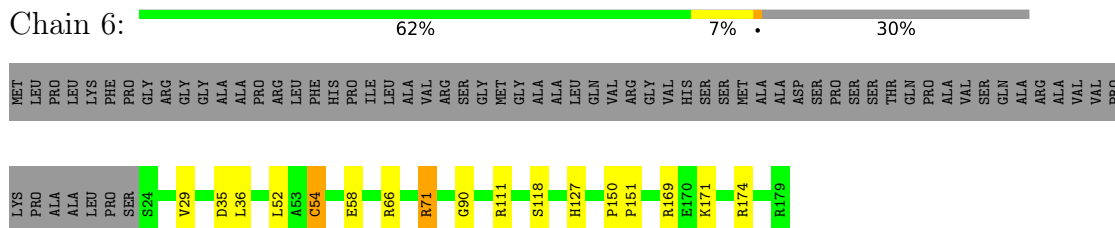
- Molecule 4: Mitochondrial complex I, 49 kDa subunit



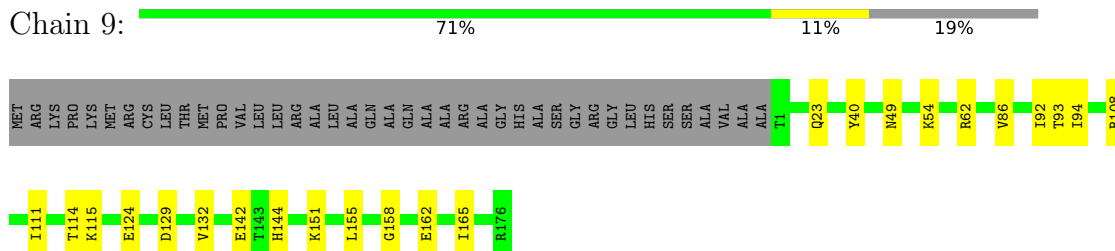
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



- Molecule 6: Mitochondrial complex I, PSST subunit

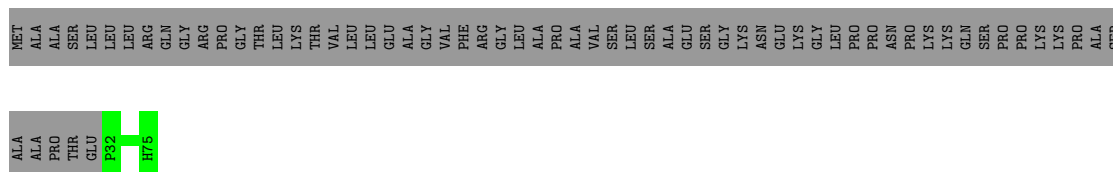


- Molecule 7: Mitochondrial complex I, TYKY subunit




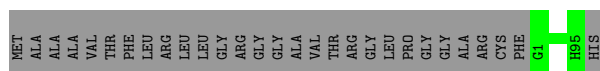
- Molecule 8: Mitochondrial complex I, 10 kDa subunit

Chain a:  40% 60%



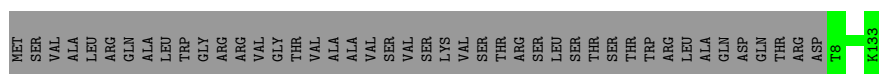
- Molecule 9: Mitochondrial complex I, 13 kDa subunit

Chain b:  77% 23%




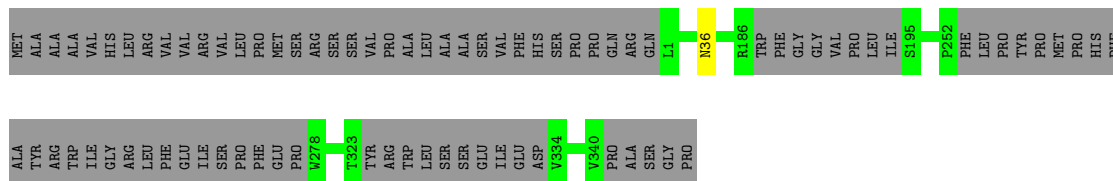
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  74% 26%



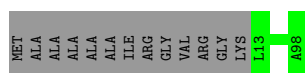
- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

Chain d:  78% 22%



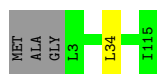
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:  87% 13%




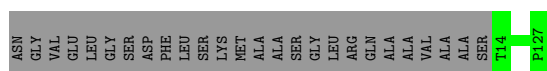
- Molecule 13: Mitochondrial complex I, B13 subunit

Chain f:  97% ..



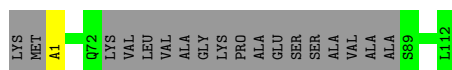
- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain g:  81% 19%



- Molecule 15: Mitochondrial complex I, B14.5a subunit

Chain h: 83% 16%



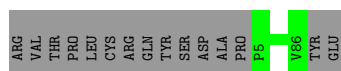
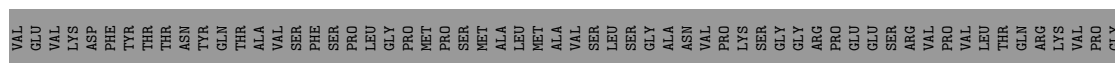
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i: 100%

There are no outlier residues recorded for this chain.

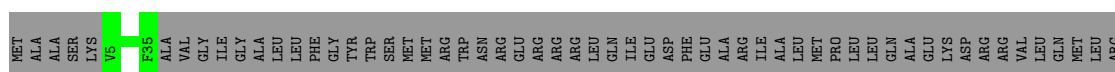
- Molecule 17: Acyl carrier protein

Chain j: 52% 48%



- Molecule 18: Mitochondrial complex I, B16.6 subunit

Chain q: 22% 78%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315484	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 ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, FMN, SF4, ZN, NAI, CDL, AYA, FES, PC1, NDP, ZMP, K, 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	1	0.39	0/3386	0.57	0/4575
2	2	0.36	0/1695	0.56	0/2306
3	3	0.40	1/5362 (0.0%)	0.57	0/7266
4	4	0.42	0/3103	0.58	0/4190
5	5	0.39	0/1776	0.55	0/2417
6	6	0.45	0/1278	0.55	0/1728
7	9	0.44	0/1445	0.59	0/1956
8	a	0.31	0/383	0.47	0/518
9	b	0.36	0/749	0.51	0/1009
10	c	0.34	0/1047	0.52	0/1415
11	d	0.34	0/2424	0.53	0/3276
12	e	0.31	0/702	0.51	0/945
13	f	0.32	0/937	0.52	1/1271 (0.1%)
14	g	0.35	0/993	0.53	0/1336
15	h	0.37	0/779	0.54	0/1053
16	i	0.38	0/1250	0.50	0/1698
17	j	0.30	0/670	0.50	0/902
18	q	0.36	0/252	0.52	0/338
All	All	0.38	1/28231 (0.0%)	0.55	1/38199 (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	3	0	2
4	4	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	159	CYS	CB-SG	-7.68	1.69	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	f	34	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	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	1	3312	0	3269	42	0
2	2	1655	0	1668	16	0
3	3	5275	0	5300	59	0
4	4	3047	0	3021	50	0
5	5	1726	0	1676	20	0
6	6	1247	0	1259	16	0
7	9	1414	0	1371	17	0
8	a	371	0	344	0	0
9	b	737	0	710	0	0
10	c	1024	0	1023	0	0
11	d	2372	0	2407	0	0
12	e	691	0	706	0	0
13	f	917	0	958	0	0
14	g	969	0	980	0	0
15	h	769	0	780	0	0
16	i	1209	0	1182	0	0
17	j	660	0	663	0	0
18	q	245	0	244	0	0
19	1	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	3	16	0	0	0	0
19	6	8	0	0	3	0
19	9	16	0	0	0	0
20	1	31	0	19	1	0
21	1	44	0	27	4	0
22	2	4	0	0	1	0
22	3	4	0	0	0	0
23	3	1	0	0	0	0
24	6	46	0	69	0	0
24	9	54	0	88	1	0
25	6	51	0	82	3	0
25	i	51	0	82	0	0
26	b	1	0	0	0	0
27	d	48	0	26	0	0
28	g	34	0	40	0	0
29	h	58	0	60	0	0
30	1	123	0	0	3	0
30	2	44	0	0	1	0
30	3	285	0	0	4	0
30	4	200	0	0	5	0
30	5	129	0	0	1	0
30	6	81	0	0	2	0
30	9	110	0	0	1	0
30	a	6	0	0	0	0
30	b	67	0	0	0	0
30	c	109	0	0	0	0
30	d	79	0	0	0	0
30	e	7	0	0	0	0
30	f	39	0	0	0	0
30	g	38	0	0	0	0
30	h	71	0	0	0	0
30	i	83	0	0	0	0
30	q	1	0	0	0	0
All	All	29587	0	28054	198	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 5.

The worst 5 of 198 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)
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.33	0.76
1:1:101:GLU:HB2	21:1:503:NAI:H42N	1.76	0.68
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.61	0.66
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.80	0.62
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.81	0.62

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	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
2	2	211/246 (86%)	196 (93%)	15 (7%)	0	100	100
3	3	686/727 (94%)	664 (97%)	21 (3%)	1 (0%)	48	60
4	4	375/463 (81%)	365 (97%)	10 (3%)	0	100	100
5	5	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
6	6	154/223 (69%)	149 (97%)	5 (3%)	0	100	100
7	9	174/217 (80%)	168 (97%)	6 (3%)	0	100	100
8	a	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
9	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
10	c	124/170 (73%)	122 (98%)	2 (2%)	0	100	100
11	d	289/380 (76%)	285 (99%)	4 (1%)	0	100	100
12	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
13	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
14	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
15	h	92/114 (81%)	88 (96%)	4 (4%)	0	100	100
16	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	j	80/157 (51%)	76 (95%)	4 (5%)	0	100	100
18	q	29/144 (20%)	27 (93%)	2 (7%)	0	100	100
All	All	3433/4304 (80%)	3323 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	367	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	343 (100%)	1 (0%)	91	96
2	2	183/210 (87%)	182 (100%)	1 (0%)	86	93
3	3	578/608 (95%)	576 (100%)	2 (0%)	91	96
4	4	328/391 (84%)	326 (99%)	2 (1%)	84	92
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	129 (98%)	3 (2%)	45	63
7	9	151/179 (84%)	151 (100%)	0	100	100
8	a	43/93 (46%)	43 (100%)	0	100	100
9	b	79/97 (81%)	79 (100%)	0	100	100
10	c	113/150 (75%)	113 (100%)	0	100	100
11	d	255/326 (78%)	254 (100%)	1 (0%)	89	95
12	e	76/82 (93%)	76 (100%)	0	100	100
13	f	101/102 (99%)	101 (100%)	0	100	100
14	g	107/124 (86%)	107 (100%)	0	100	100
15	h	84/96 (88%)	84 (100%)	0	100	100
16	i	131/131 (100%)	131 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	j	76/141 (54%)	76 (100%)	0	100	100
18	q	26/122 (21%)	26 (100%)	0	100	100
All	All	2996/3631 (82%)	2986 (100%)	10 (0%)	90	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	71	ARG
6	6	111	ARG
11	d	36	ASN
3	3	179	ASN
4	4	252	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	4	252	ASN
13	f	49	GLN
14	g	125	HIS
4	4	50	ASN
1	1	373	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2MR	4	85	4	10,12,13	2.31	3 (30%)	5,13,15	2.19	2 (40%)
15	AYA	h	1	15	6,7,8	1.25	1 (16%)	5,8,10	1.01	0

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
4	2MR	4	85	4	-	1/10/13/15	-
15	AYA	h	1	15	-	0/4/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.70	1.43	1.33
4	4	85	2MR	CZ-NE	4.43	1.43	1.34
15	h	1	AYA	CA-N	-2.52	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.20	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	85	2MR	NE-CZ-NH2	-3.91	115.90	119.48
4	4	85	2MR	CD-NE-CZ	-2.43	118.86	123.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	85	2MR	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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
20	FMN	1	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.35	7 (14%)
27	NDP	d	401	-	45,52,52	0.58	0	53,80,80	0.54	1 (1%)
19	SF4	1	501	1	0,12,12	-	-	-	-	-
28	ZMP	g	201	-	27,33,36	0.66	0	32,40,45	1.28	3 (9%)
19	SF4	9	403	7	0,12,12	-	-	-	-	-
22	FES	3	803	3	0,4,4	-	-	-	-	-
19	SF4	3	802	3	0,12,12	-	-	-	-	-
24	PC1	6	202	-	45,45,53	0.31	0	51,53,61	0.32	0
25	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.30	0
22	FES	2	300	2	0,4,4	-	-	-	-	-
24	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.53	0
25	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.29	0
19	SF4	3	801	3	0,12,12	-	-	-	-	-
19	SF4	9	402	7	0,12,12	-	-	-	-	-
29	CDL	h	201	-	57,57,99	0.36	0	63,69,111	0.30	0
19	SF4	6	201	6	0,12,12	-	-	-	-	-
21	NAI	1	503	-	42,48,48	0.58	0	47,73,73	1.96	4 (8%)

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
20	FMN	1	502	-	-	10/18/18/18	0/3/3/3
27	NDP	d	401	-	-	4/30/77/77	0/5/5/5
19	SF4	1	501	1	-	-	0/6/5/5
28	ZMP	g	201	-	-	4/38/40/43	-
24	PC1	6	202	-	-	8/49/49/57	-
19	SF4	9	403	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	6	203	-	-	12/54/54/54	-
19	SF4	3	802	3	-	-	0/6/5/5
22	FES	3	803	3	-	-	0/1/1/1
25	3PE	i	201	-	-	7/54/54/54	-
24	PC1	9	401	-	-	10/57/57/57	-
29	CDL	h	201	-	-	19/68/68/110	-
19	SF4	3	801	3	-	-	0/6/5/5
19	SF4	9	402	7	-	-	0/6/5/5
22	FES	2	300	2	-	-	0/1/1/1
19	SF4	6	201	6	-	-	0/6/5/5
21	NAI	1	503	-	-	7/25/72/72	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	502	FMN	C4A-N5	3.22	1.37	1.30
20	1	502	FMN	C10-N1	2.12	1.37	1.33
20	1	502	FMN	C4A-C10	-2.03	1.38	1.44

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	503	NAI	O5B-PA-O1A	-9.94	70.25	109.07
21	1	503	NAI	O2A-PA-O1A	-7.76	73.86	112.24
20	1	502	FMN	C4-N3-C2	-3.65	118.89	125.64
28	g	201	ZMP	C14-C15-N2	-3.14	105.55	111.90
28	g	201	ZMP	C15-C14-C13	-3.02	107.33	112.36

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

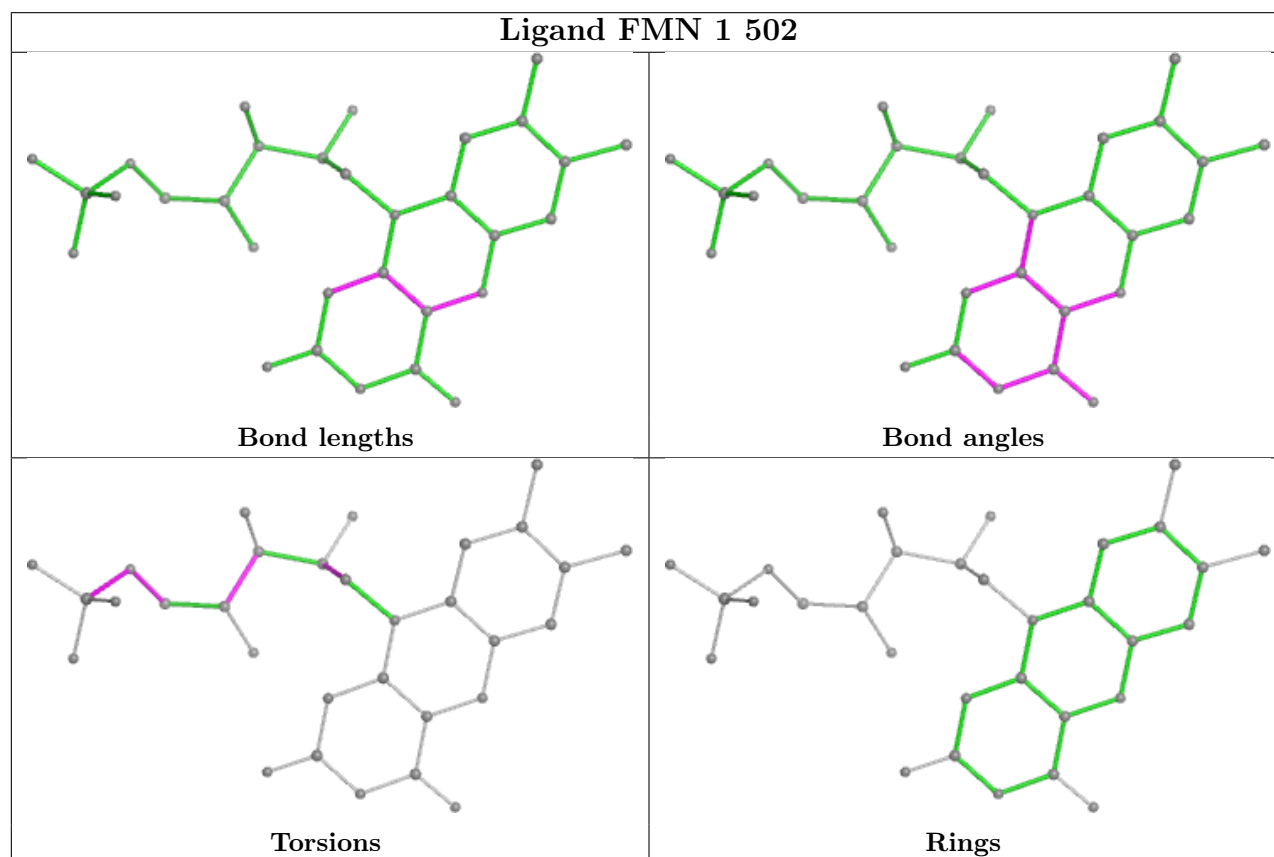
Mol	Chain	Res	Type	Atoms
20	1	502	FMN	C5'-O5'-P-O2P
20	1	502	FMN	C5'-O5'-P-O3P
21	1	503	NAI	C5D-O5D-PN-O3
24	6	202	PC1	C11-O13-P-O12
24	6	202	PC1	C11-O13-P-O14

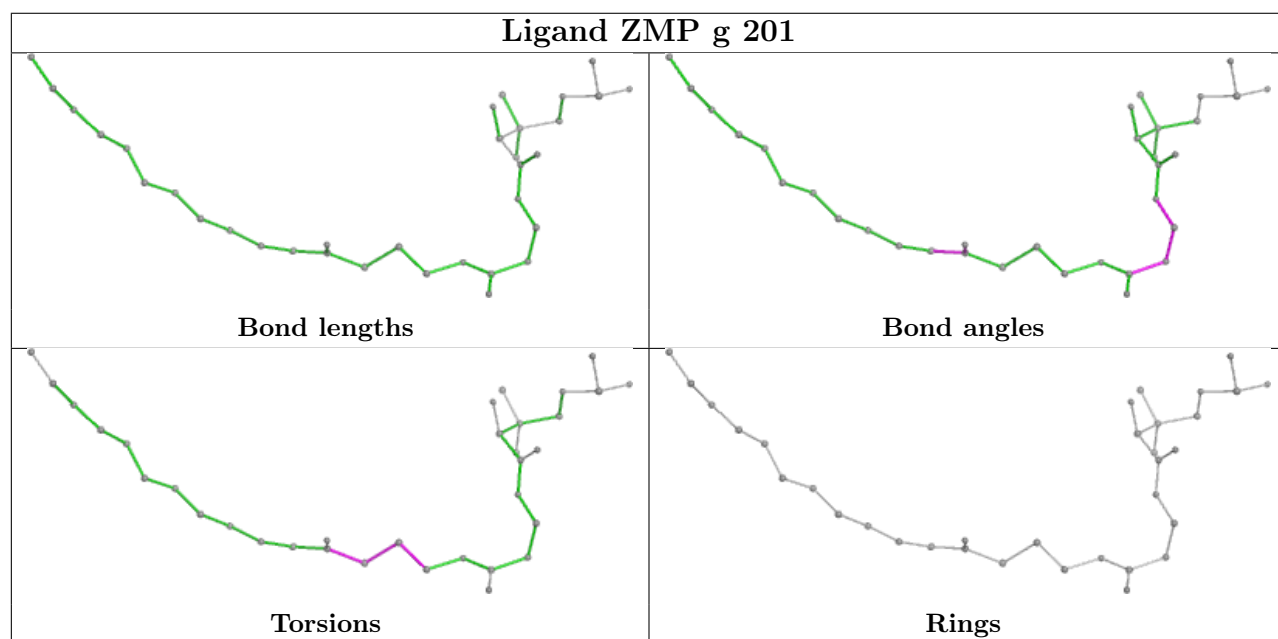
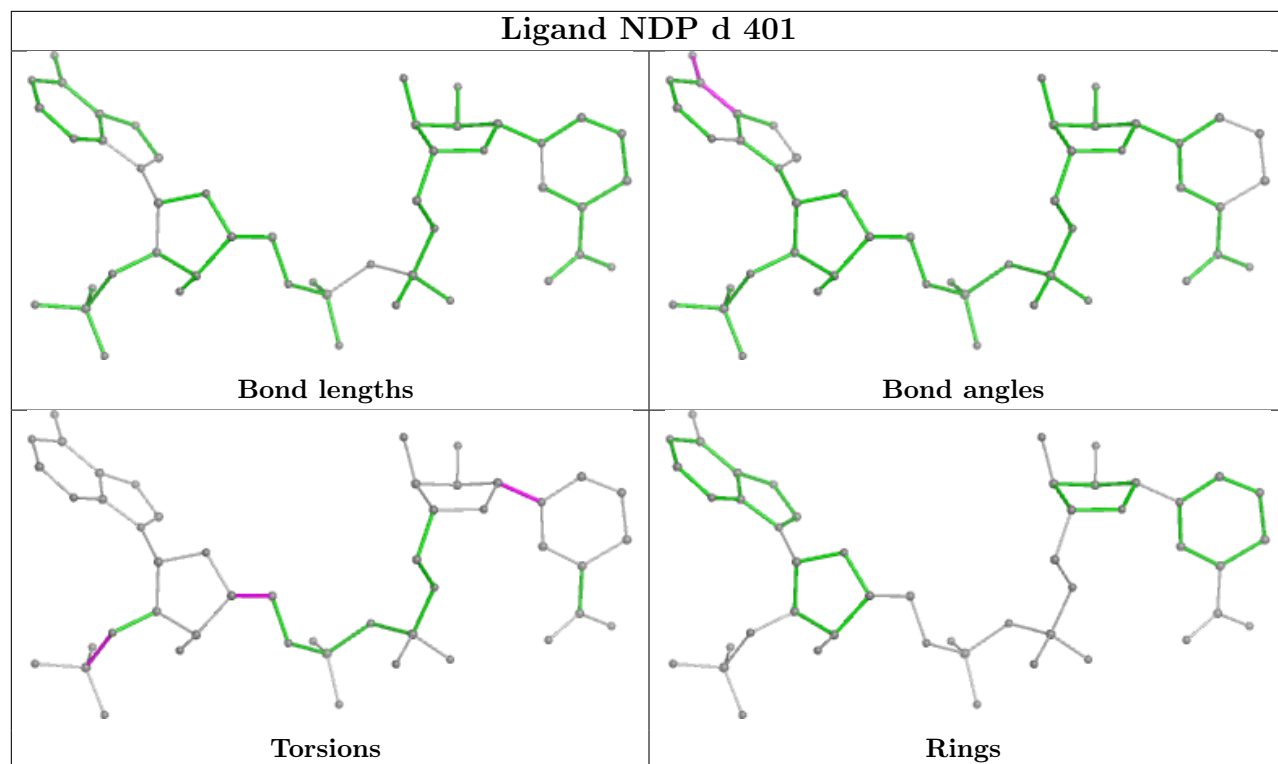
There are no ring outliers.

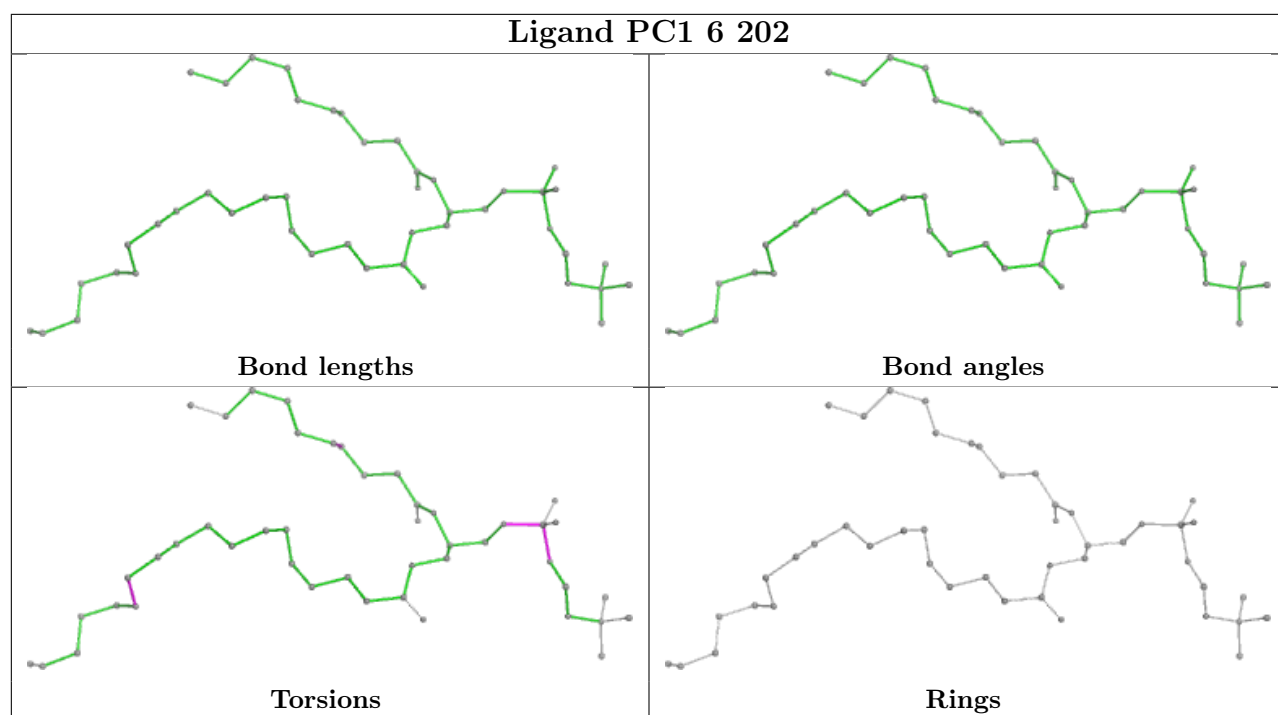
7 monomers are involved in 14 short contacts:

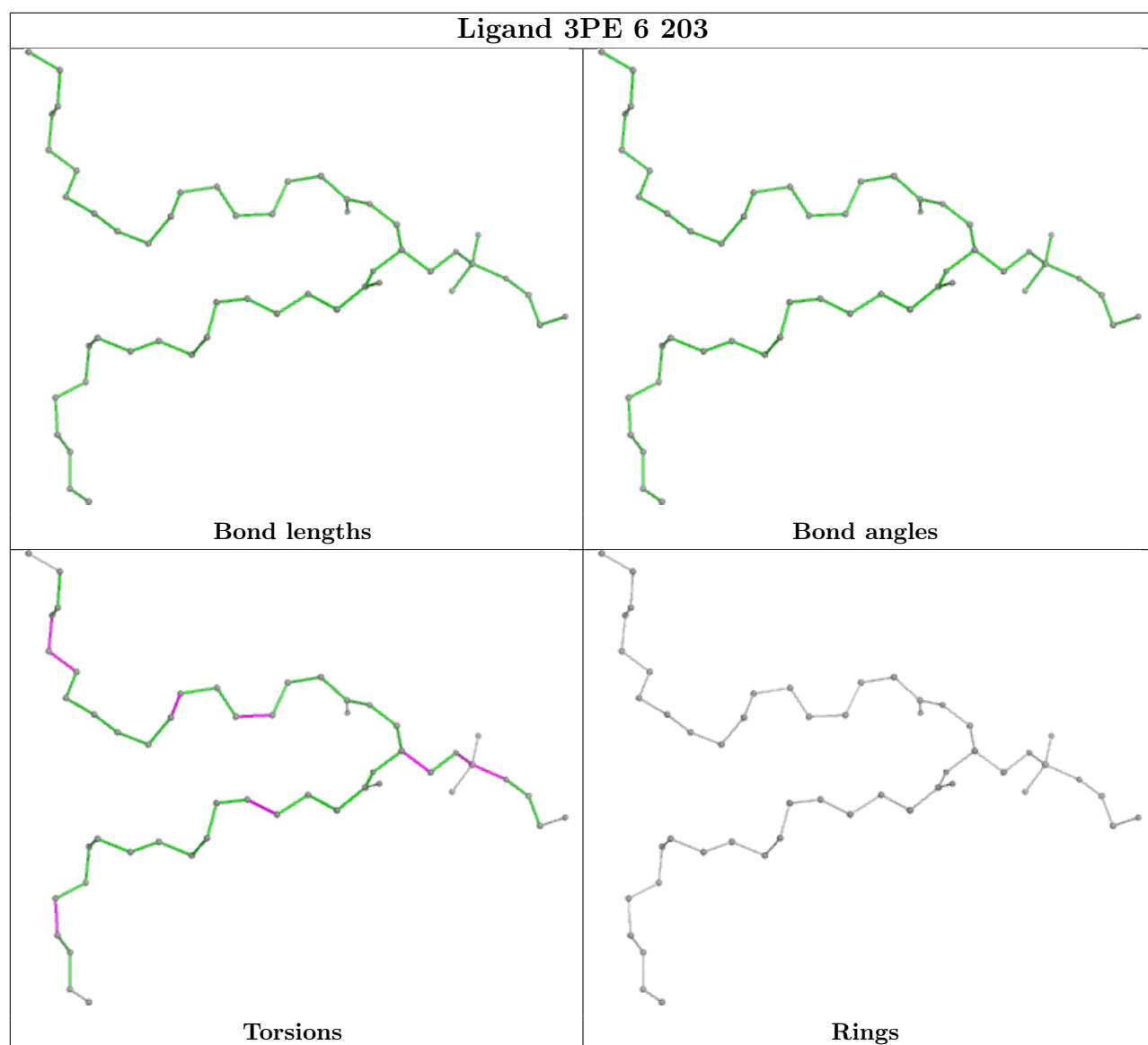
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	502	FMN	1	0
19	1	501	SF4	1	0
25	6	203	3PE	3	0
22	2	300	FES	1	0
24	9	401	PC1	1	0
19	6	201	SF4	3	0
21	1	503	NAI	4	0

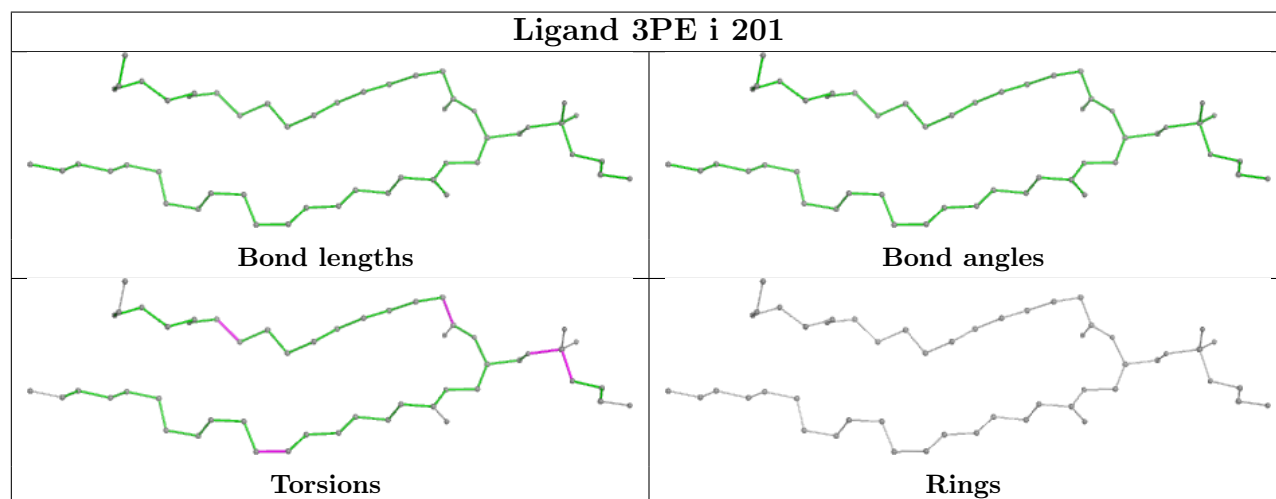
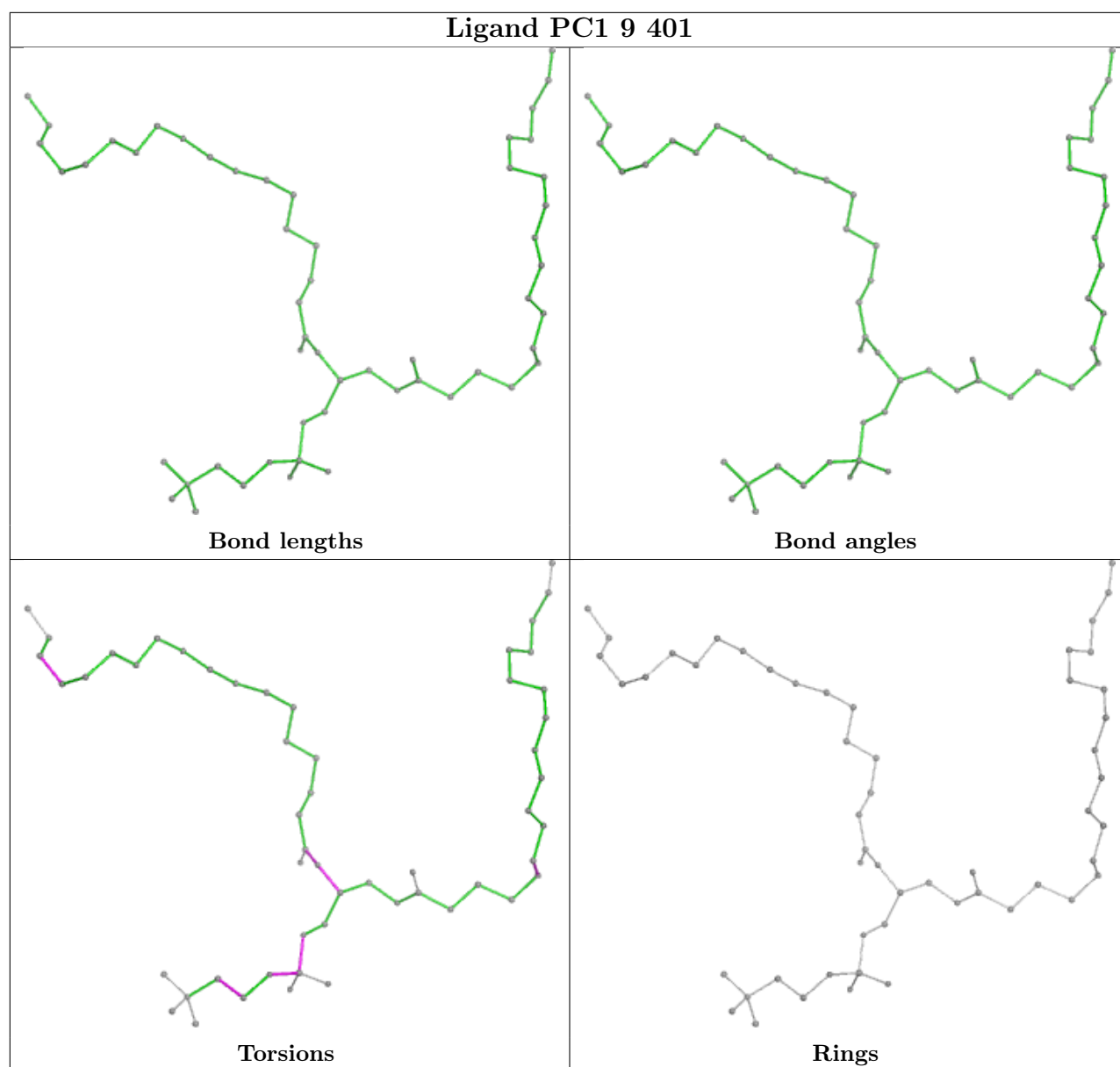
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

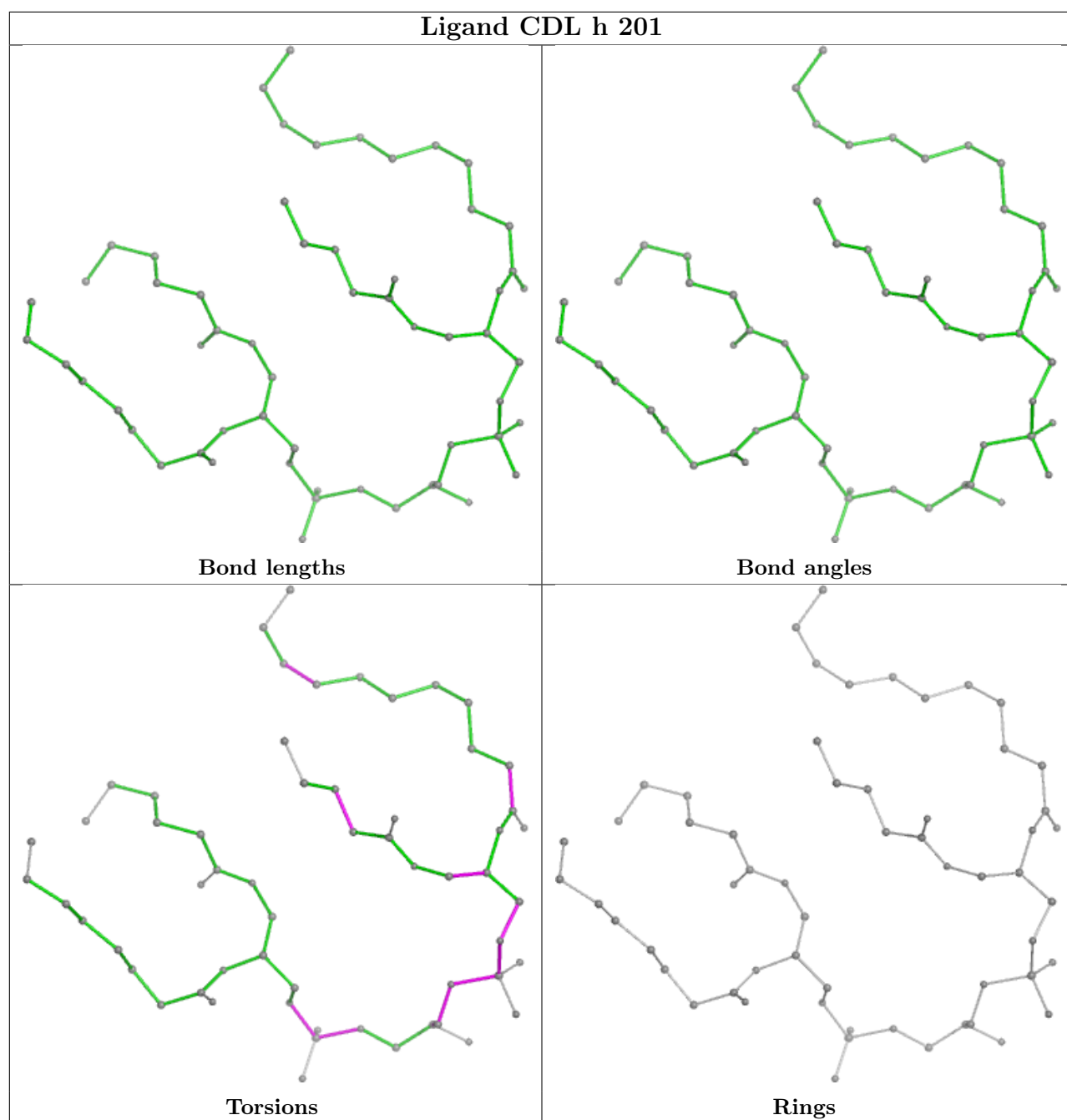


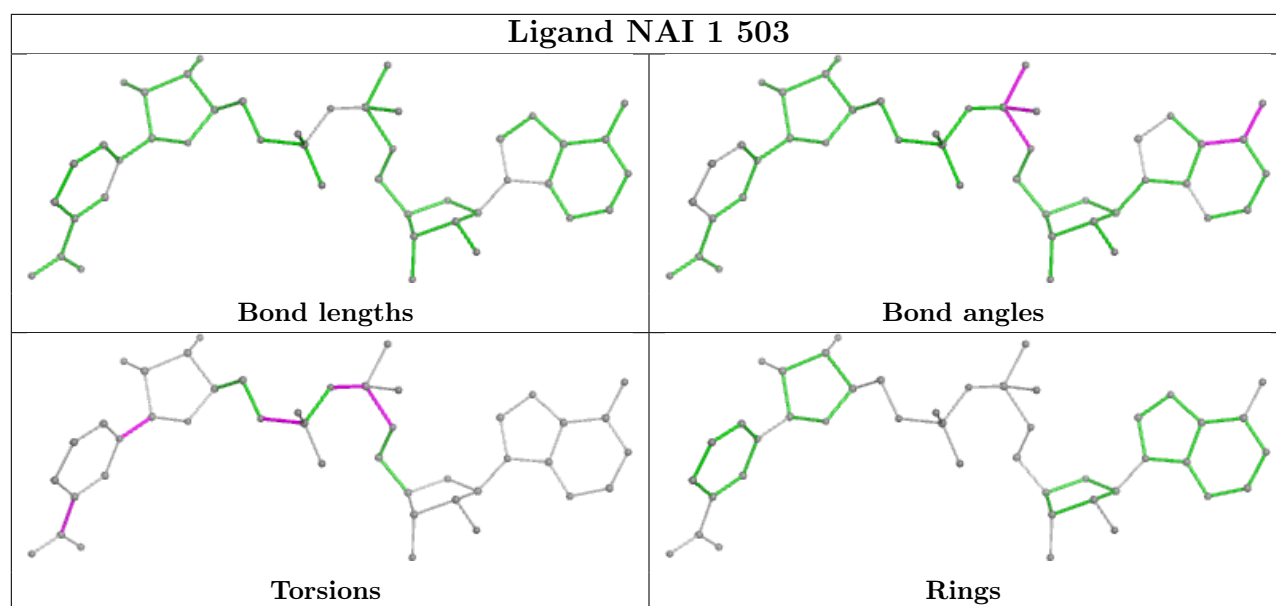












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-11241. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.