



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2023 – 10:36 pm BST

PDB ID : 8ACY
Title : X-ray structure of Na⁺-NQR from *Vibrio cholerae* at 3.5 Å resolution
Authors : Fritz, G.
Deposited on : 2022-07-07
Resolution : 3.50 Å (reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

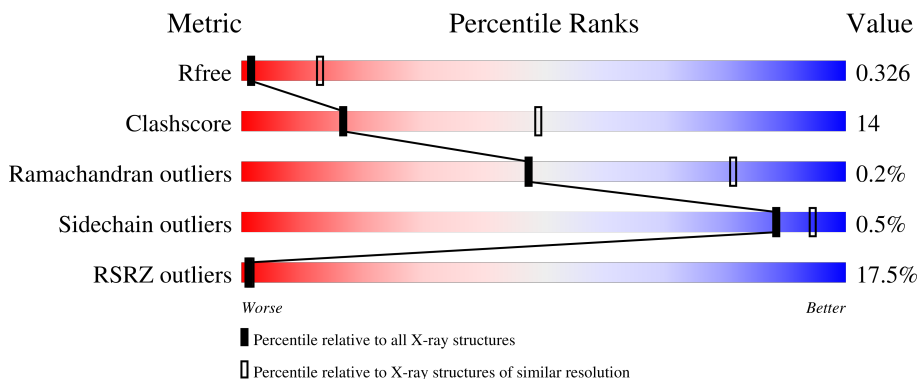
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	 11% 74% 13% 14%
2	B	415	 15% 74% 17% 8%
3	C	257	 33% 64% 32%
4	D	210	 8% 56% 40%
5	E	198	 12% 68% 28%

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Mol	Chain	Length	Quality of chain
6	F	408	

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
11	FES	F	1502	-	-	X	-
7	FMN	C	1000	-	-	-	X
8	RBF	B	502	-	-	-	X
9	LMT	B	504	-	-	-	X
9	LMT	D	301	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 28808 atoms, of which 14464 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Na(+)-translocating NADH-quinone reductase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	403	6191	1946	3121	521	588	15	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A655PZA5
A	-20	GLY	-	expression tag	UNP A0A655PZA5
A	-19	SER	-	expression tag	UNP A0A655PZA5
A	-18	SER	-	expression tag	UNP A0A655PZA5
A	-17	HIS	-	expression tag	UNP A0A655PZA5
A	-16	HIS	-	expression tag	UNP A0A655PZA5
A	-15	HIS	-	expression tag	UNP A0A655PZA5
A	-14	HIS	-	expression tag	UNP A0A655PZA5
A	-13	HIS	-	expression tag	UNP A0A655PZA5
A	-12	HIS	-	expression tag	UNP A0A655PZA5
A	-11	SER	-	expression tag	UNP A0A655PZA5
A	-10	SER	-	expression tag	UNP A0A655PZA5
A	-9	GLY	-	expression tag	UNP A0A655PZA5
A	-8	LEU	-	expression tag	UNP A0A655PZA5
A	-7	GLU	-	expression tag	UNP A0A655PZA5
A	-6	VAL	-	expression tag	UNP A0A655PZA5
A	-5	LEU	-	expression tag	UNP A0A655PZA5
A	-4	PHE	-	expression tag	UNP A0A655PZA5
A	-3	GLN	-	expression tag	UNP A0A655PZA5
A	-2	GLY	-	expression tag	UNP A0A655PZA5
A	-1	PRO	-	expression tag	UNP A0A655PZA5
A	0	HIS	-	expression tag	UNP A0A655PZA5

- Molecule 2 is a protein called Na(+)-translocating NADH-quinone reductase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	380	5818	1924	2907	475	490	22	0	0	0

- Molecule 3 is a protein called Na(+)-translocating NADH-quinone reductase subunit C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	248	3774	1192	1892	324	362	4	0	0	0

- Molecule 4 is a protein called Na(+)-translocating NADH-quinone reductase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	204	3208	1037	1646	247	268	10	0	0	0

- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	197	3078	1008	1574	229	257	10	0	0	0

- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

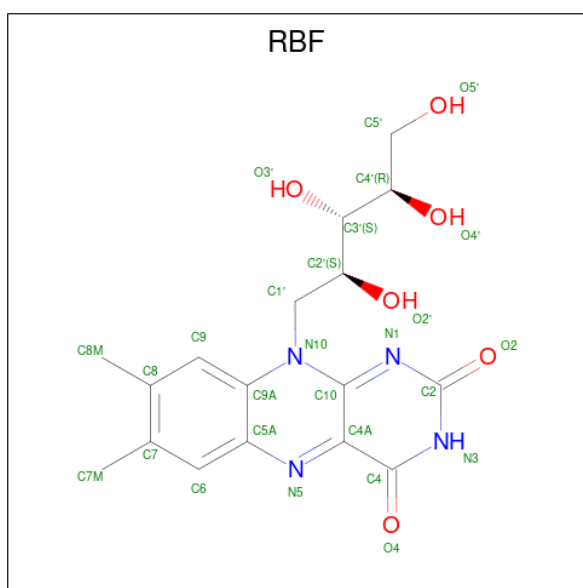
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	407	6259	2025	3098	518	594	24	0	0	0

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
7	B	1	49	17	19	4	8	1	0	0
7	C	1	49	17	19	4	8	1	0	0

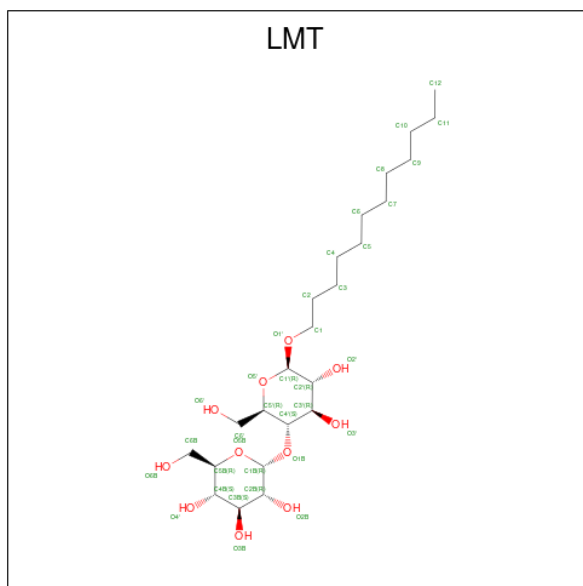
- Molecule 8 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	B	1	46	17	19	4	6	0	0

- Molecule 9 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:

C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			81	24	46	11		
9	B	1	Total	C	H	O	0	0
			81	24	46	11		
9	D	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

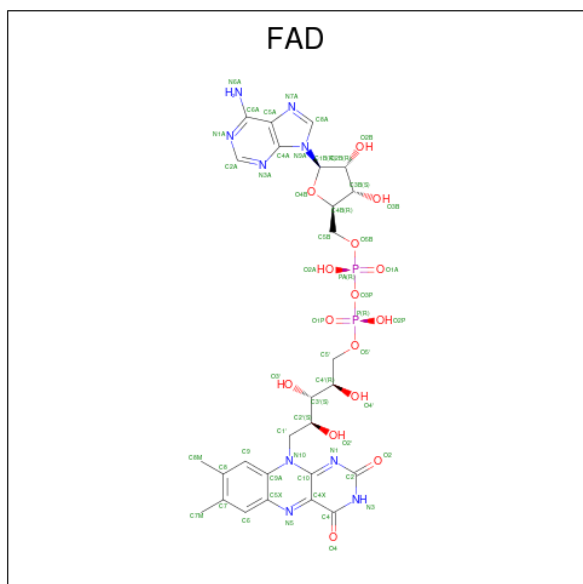
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Na	0	0
			1	1		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	Fe	S	0	0
			4	2	2		
11	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

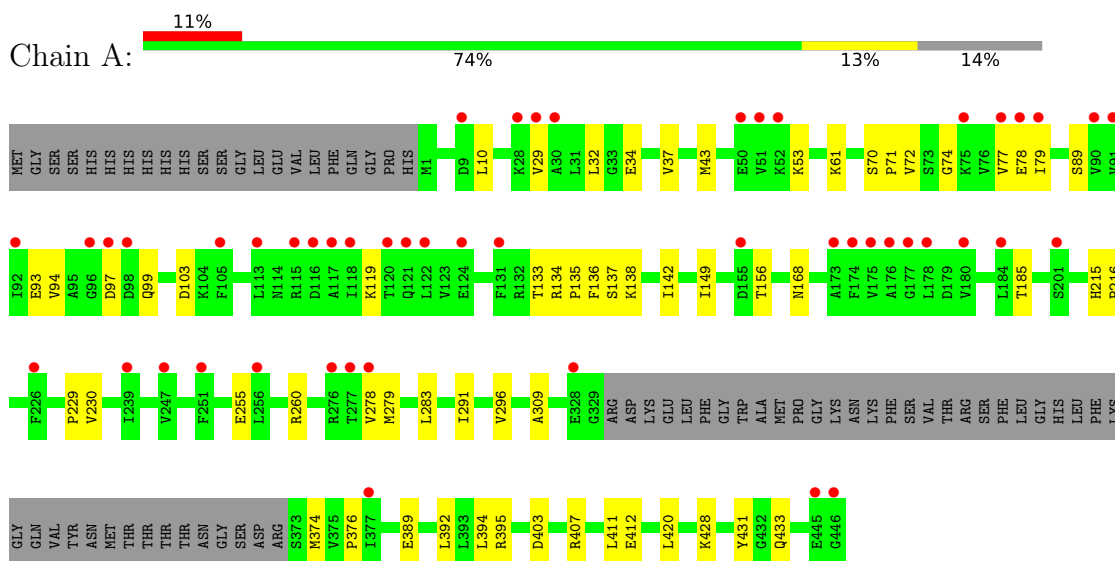


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
12	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

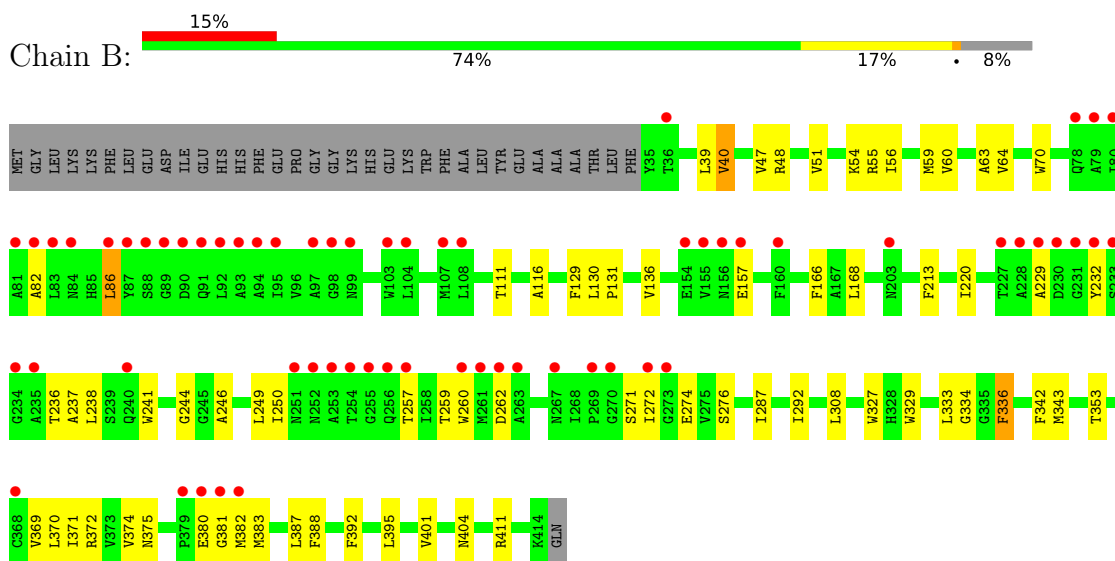
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

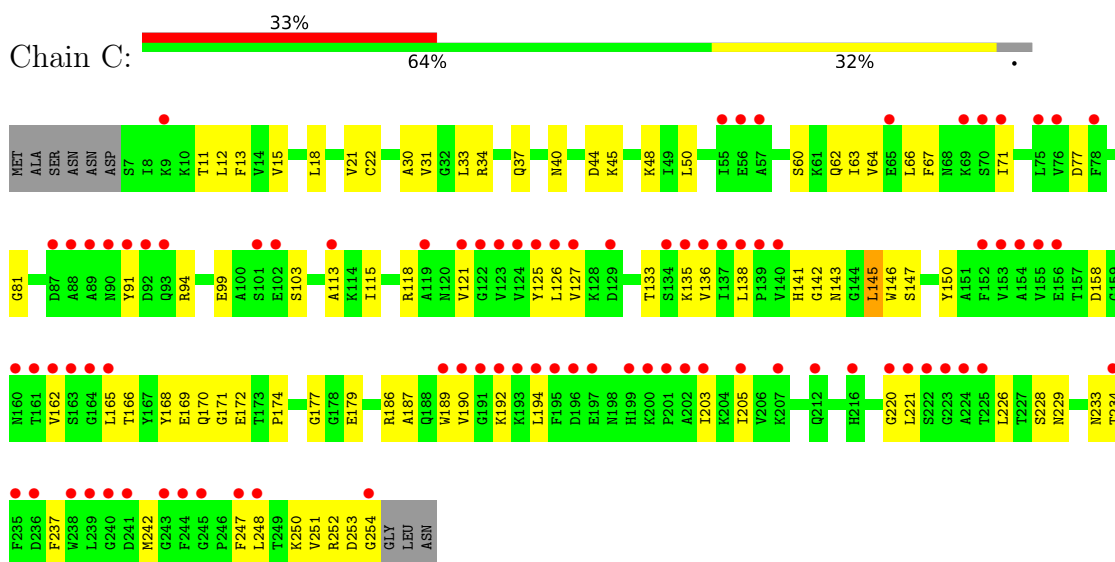
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



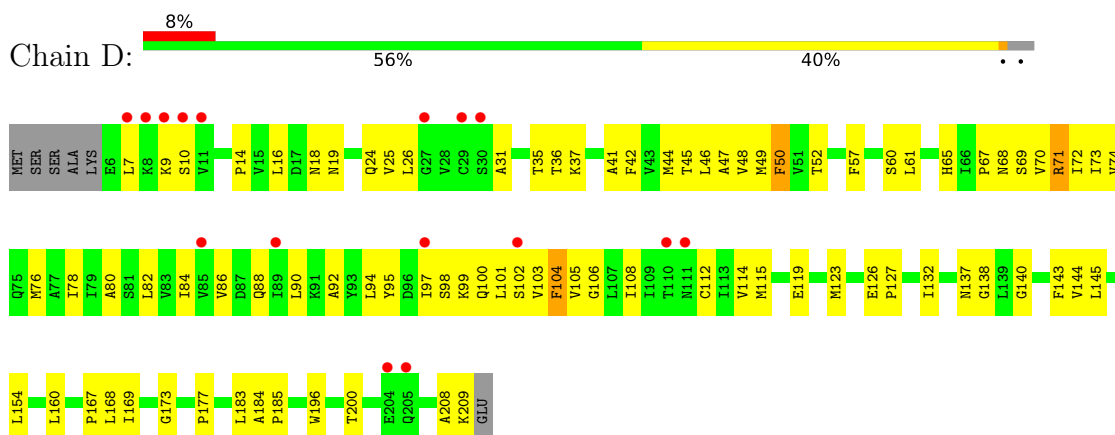
- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B



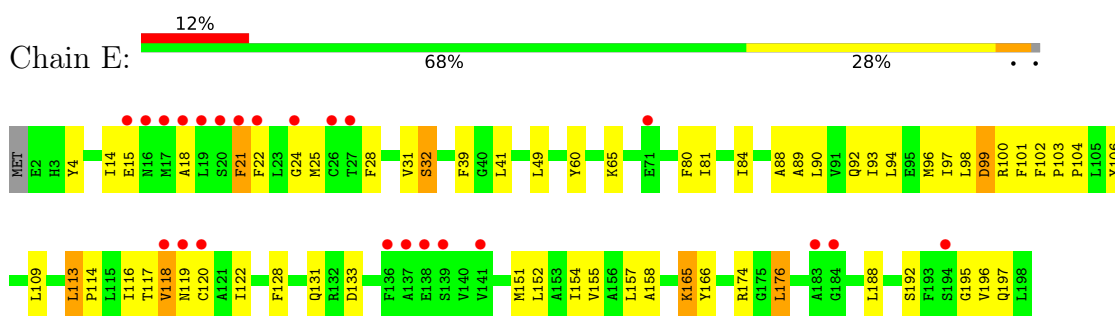
- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C



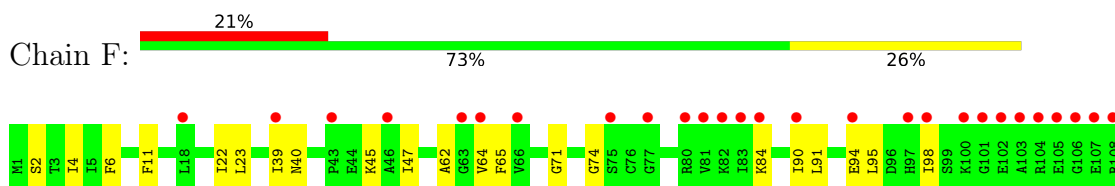
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

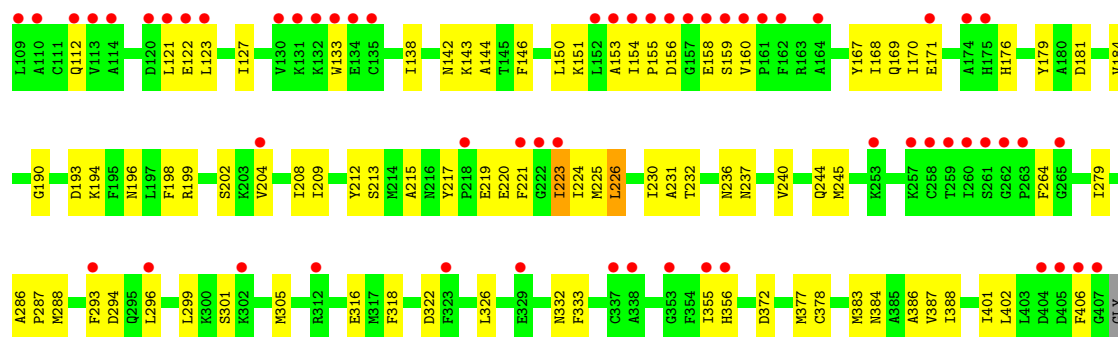


• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



• Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.27Å 143.32Å 104.37Å 90.00° 110.98° 90.00°	Depositor
Resolution (Å)	48.73 – 3.50 48.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.73-3.50) 99.6 (48.73-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.266 , 0.290 0.264 , 0.326	Depositor DCC
R_{free} test set	1647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	165.3	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28808	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NA, LMT, FAD, RBF, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/3124	0.67	0/4236
2	B	0.33	0/2998	0.69	6/4083 (0.1%)
3	C	0.36	0/1914	0.76	4/2583 (0.2%)
4	D	0.37	0/1594	0.90	6/2164 (0.3%)
5	E	0.42	0/1537	0.94	8/2084 (0.4%)
6	F	0.36	0/3239	0.71	3/4384 (0.1%)
All	All	0.35	0/14406	0.76	27/19534 (0.1%)

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
4	D	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	113	LEU	CB-CG-CD1	-6.92	99.24	111.00
3	C	145	LEU	CB-CG-CD2	6.67	122.34	111.00
2	B	388	PHE	CB-CG-CD1	-6.50	116.25	120.80
6	F	223	ILE	CG1-CB-CG2	-6.48	97.15	111.40
5	E	21	PHE	CB-CG-CD2	-6.27	116.41	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	208	ALA	Peptide
5	E	32	SER	Mainchain

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	A	3070	3121	3123	43	2
2	B	2911	2907	2907	63	0
3	C	1882	1892	1892	70	0
4	D	1562	1646	1648	88	0
5	E	1504	1574	1574	98	0
6	F	3161	3098	3098	91	2
7	B	30	19	19	4	0
7	C	30	19	19	2	0
8	B	27	19	20	4	0
9	B	70	92	84	8	0
9	D	35	46	43	1	0
10	B	1	0	0	0	0
11	E	4	0	0	0	0
11	F	4	0	0	2	0
12	F	53	31	31	3	0
All	All	14344	14464	14458	406	2

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 14.

The worst 5 of 406 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)
5:E:98:LEU:HD12	5:E:113:LEU:HD11	1.12	1.07
5:E:98:LEU:HD12	5:E:113:LEU:CD1	1.93	0.98
6:F:388:ILE:HD13	6:F:401:ILE:HD13	1.47	0.97
5:E:28:PHE:O	5:E:32:SER:OG	1.80	0.96
5:E:98:LEU:CD1	5:E:113:LEU:HD11	1.99	0.93

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASN:O	6:F:199:ARG:NH1[2_444]	1.90	0.30
1:A:168:ASN:O	6:F:199:ARG:HH11[2_444]	1.49	0.11

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 X-ray entries followed by that with respect to entries of similar resolution.

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	399/468 (85%)	393 (98%)	6 (2%)	0	100	100
2	B	378/415 (91%)	370 (98%)	7 (2%)	1 (0%)	41	75
3	C	246/257 (96%)	245 (100%)	1 (0%)	0	100	100
4	D	202/210 (96%)	198 (98%)	4 (2%)	0	100	100
5	E	195/198 (98%)	187 (96%)	6 (3%)	2 (1%)	15	54
6	F	405/408 (99%)	399 (98%)	6 (2%)	0	100	100
All	All	1825/1956 (93%)	1792 (98%)	30 (2%)	3 (0%)	47	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	99	ASP
5	E	118	VAL
2	B	40	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	339/395 (86%)	337 (99%)	2 (1%)	86	94
2	B	292/320 (91%)	292 (100%)	0	100	100
3	C	198/205 (97%)	197 (100%)	1 (0%)	88	94
4	D	171/176 (97%)	170 (99%)	1 (1%)	86	94
5	E	164/165 (99%)	163 (99%)	1 (1%)	86	94
6	F	337/337 (100%)	334 (99%)	3 (1%)	78	90
All	All	1501/1598 (94%)	1493 (100%)	8 (0%)	88	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	322	ASP
6	F	181	ASP
5	E	133	ASP
4	D	71	ARG
6	F	171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	229	ASN
5	E	197	GLN
6	F	356	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
7	FMN	B	501	2	29,32,33	1.18	2 (6%)	40,47,50	1.60	8 (20%)
9	LMT	B	503	-	36,36,36	1.20	5 (13%)	47,47,47	1.11	3 (6%)
8	RBF	B	502	-	29,29,29	0.60	0	41,43,43	0.72	2 (4%)
11	FES	E	1001	4,5	0,4,4	-	-	-	-	-
7	FMN	C	1000	3	29,32,33	1.17	2 (6%)	40,47,50	1.49	10 (25%)
9	LMT	B	504	-	36,36,36	1.26	5 (13%)	47,47,47	1.20	2 (4%)
12	FAD	F	1501	-	53,58,58	0.48	0	68,89,89	0.53	1 (1%)
11	FES	F	1502	6	0,4,4	-	-	-	-	-
9	LMT	D	301	-	36,36,36	1.24	5 (13%)	47,47,47	1.02	1 (2%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
9	LMT	B	503	-	-	6/21/61/61	0/2/2/2
8	RBF	B	502	-	-	2/14/14/14	0/3/3/3
11	FES	E	1001	4,5	-	-	0/1/1/1
7	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
9	LMT	B	504	-	-	11/21/61/61	0/2/2/2
12	FAD	F	1501	-	-	5/30/50/50	0/6/6/6
11	FES	F	1502	6	-	-	0/1/1/1
9	LMT	D	301	-	-	9/21/61/61	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	FMN	C4A-N5	4.00	1.38	1.30
7	C	1000	FMN	C4A-N5	3.78	1.38	1.30
9	D	301	LMT	O3'-C3'	-3.26	1.35	1.43
9	D	301	LMT	O2'-C2'	-3.22	1.35	1.43
9	B	504	LMT	O2'-C2'	-3.14	1.35	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	LMT	O5'-C1'-O1'	-4.45	99.45	109.97
7	B	501	FMN	C4'-C3'-C2'	-3.87	105.32	113.36
7	C	1000	FMN	C4-N3-C2	-3.54	119.11	125.64
7	B	501	FMN	C4-N3-C2	-3.44	119.29	125.64
9	B	503	LMT	C3'-C4'-C5'	-3.38	103.17	110.93

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	LMT	C2'-C1'-O1'-C1
9	B	503	LMT	O5'-C1'-O1'-C1
9	B	504	LMT	C2B-C1B-O1B-C4'
12	F	1501	FAD	N10-C1'-C2'-O2'
9	B	503	LMT	C3'-C4'-O1B-C1B

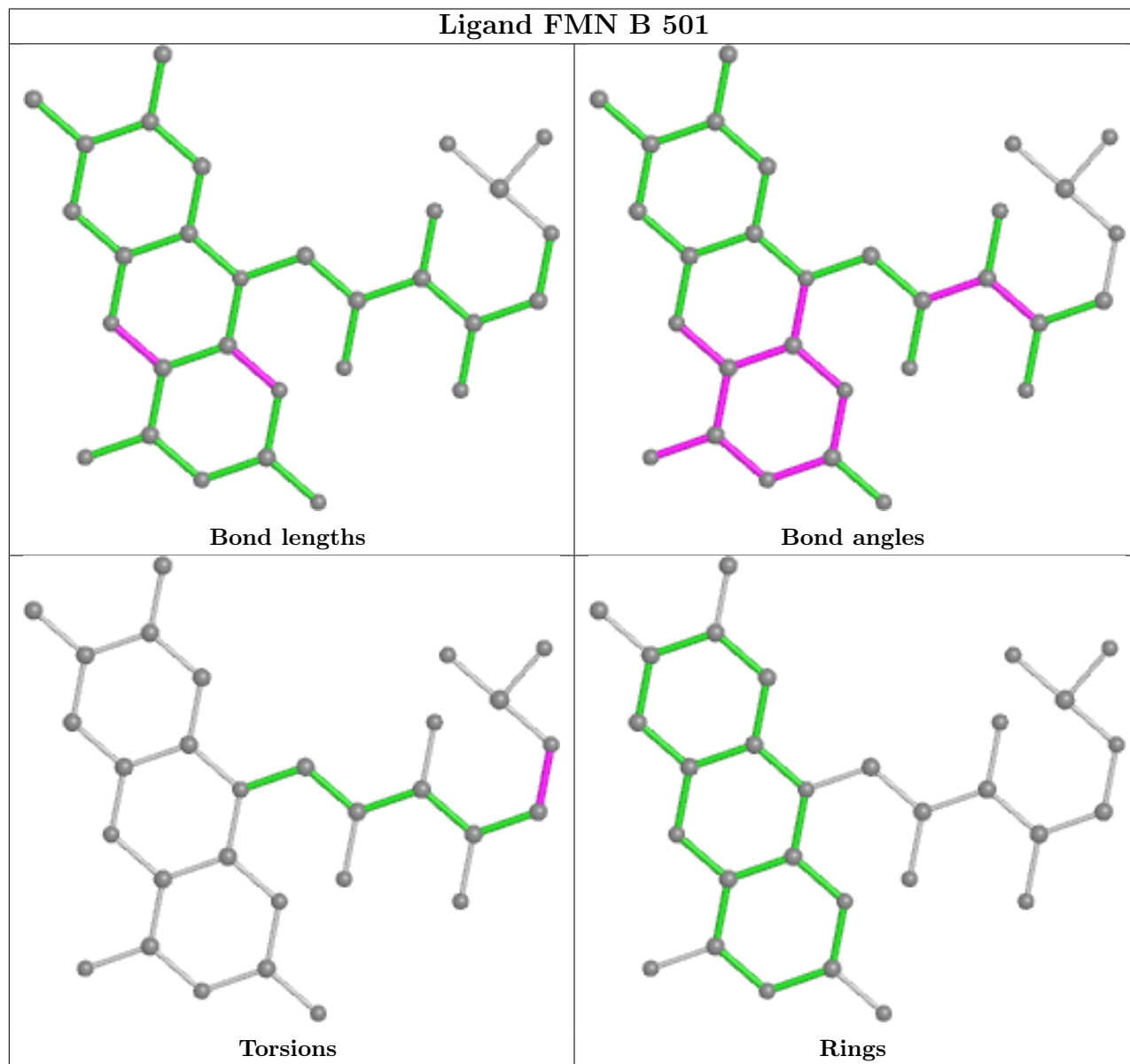
There are no ring outliers.

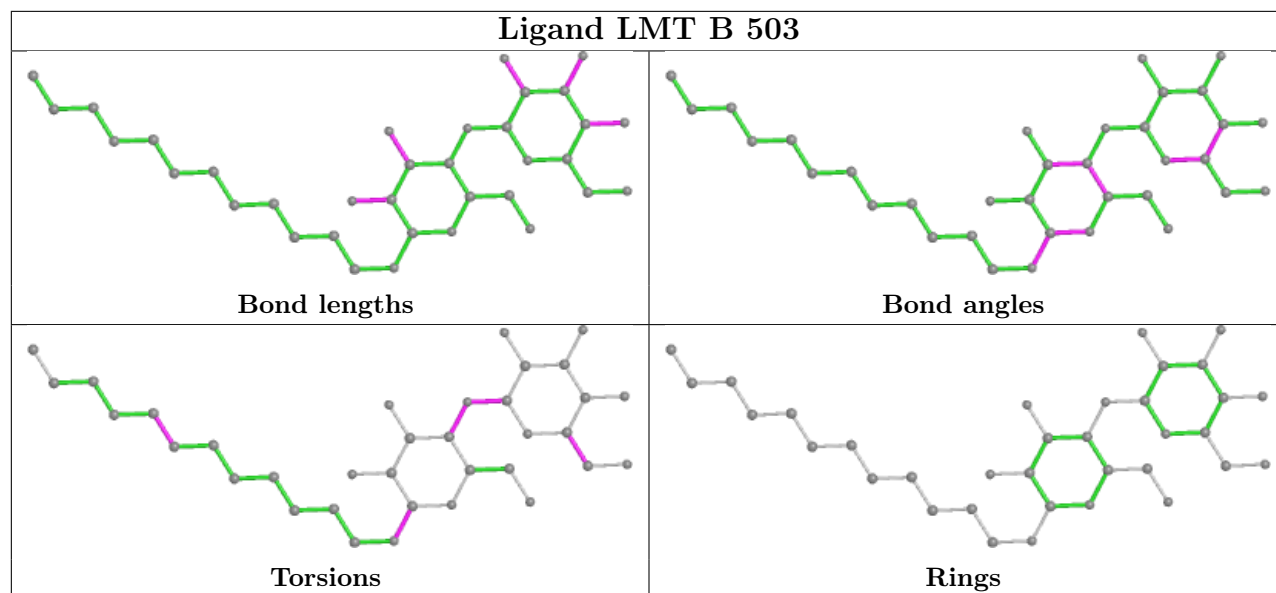
8 monomers are involved in 24 short contacts:

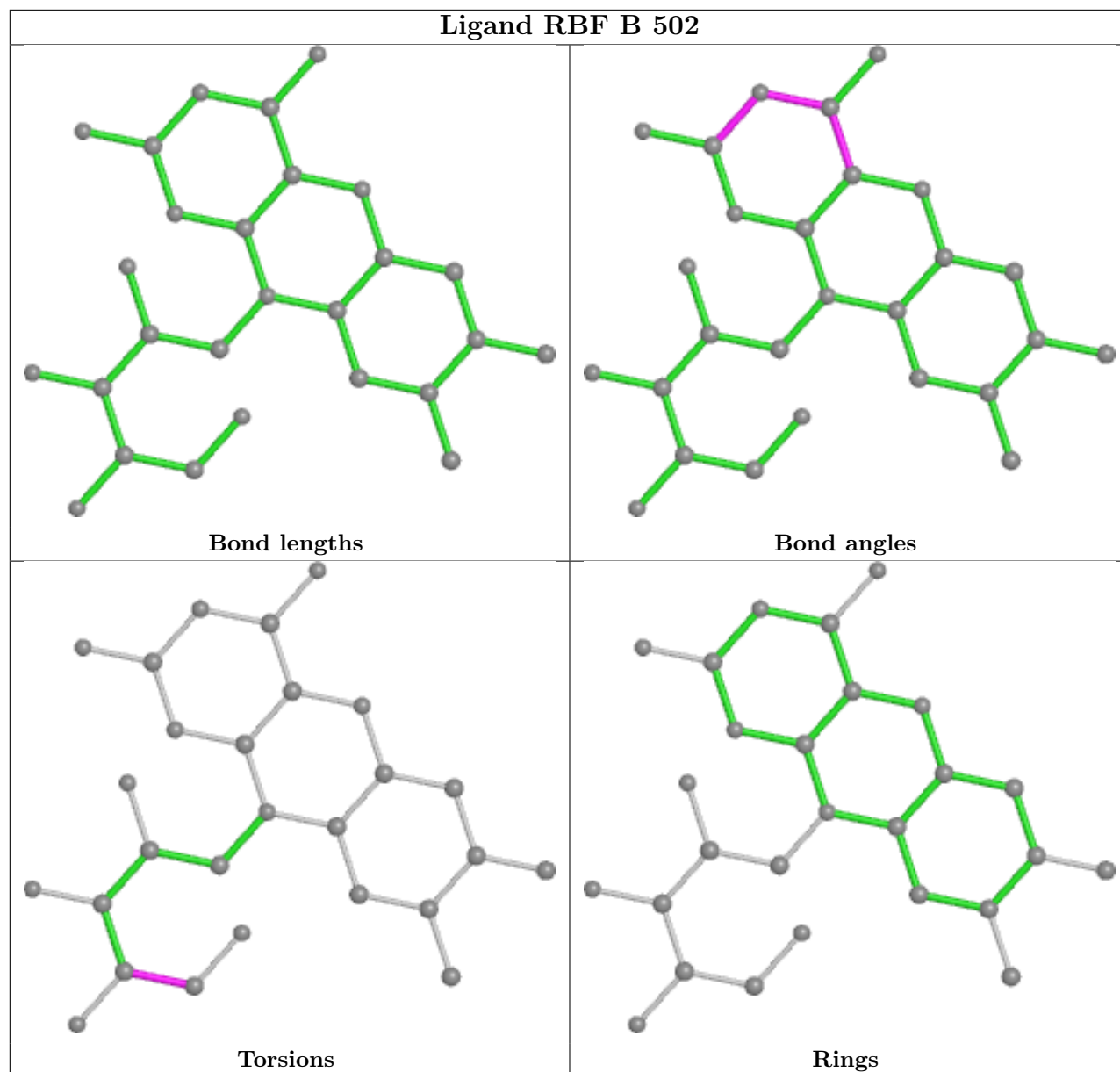
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	FMN	4	0
9	B	503	LMT	4	0
8	B	502	RBF	4	0
7	C	1000	FMN	2	0
9	B	504	LMT	4	0
12	F	1501	FAD	3	0
11	F	1502	FES	2	0
9	D	301	LMT	1	0

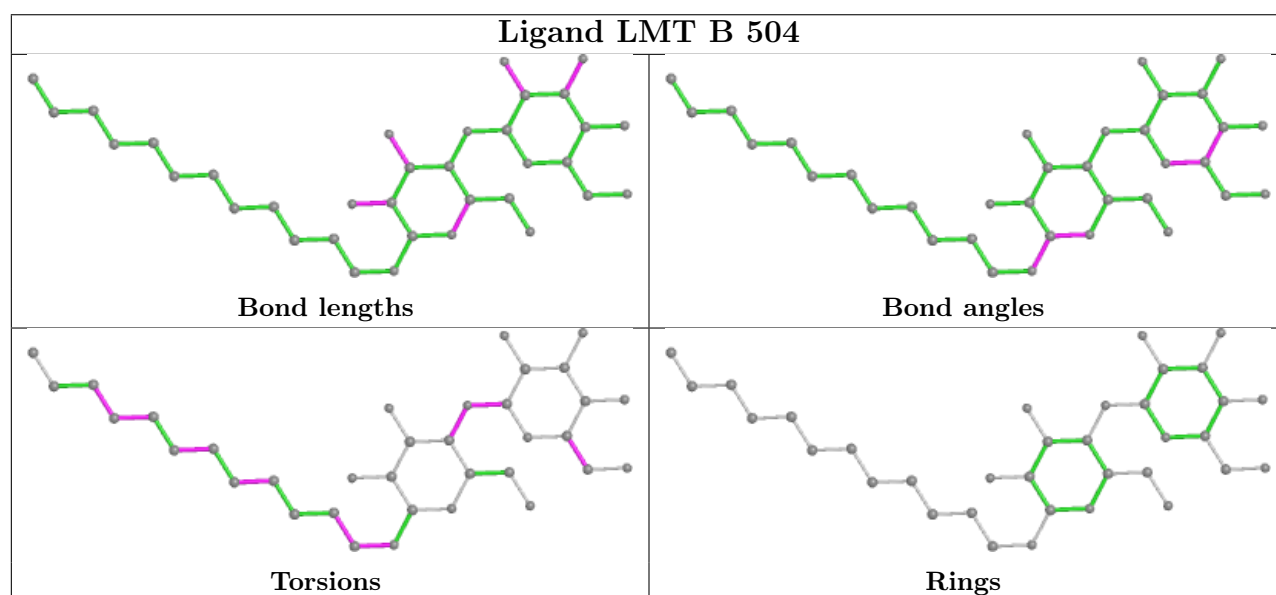
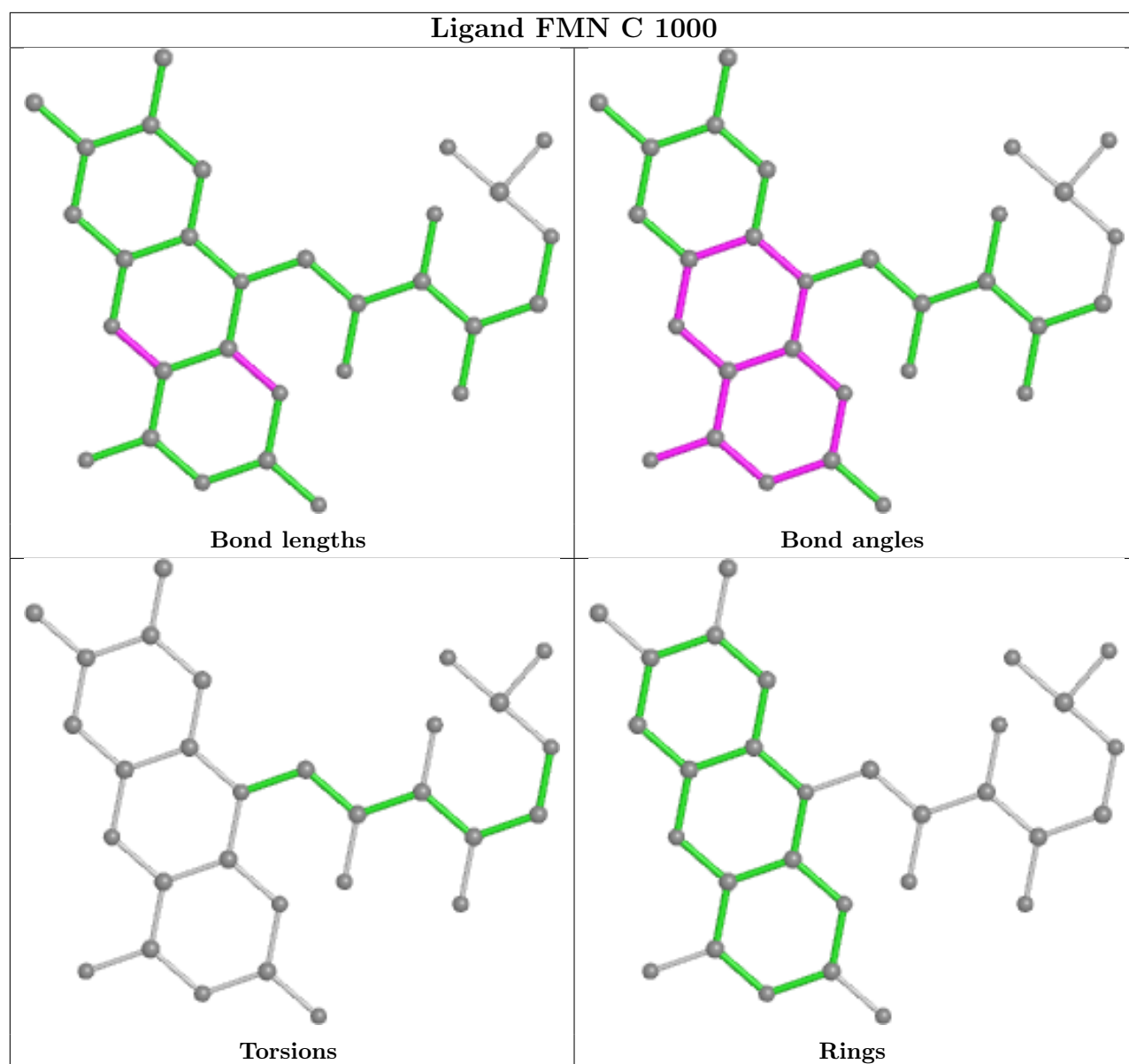
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

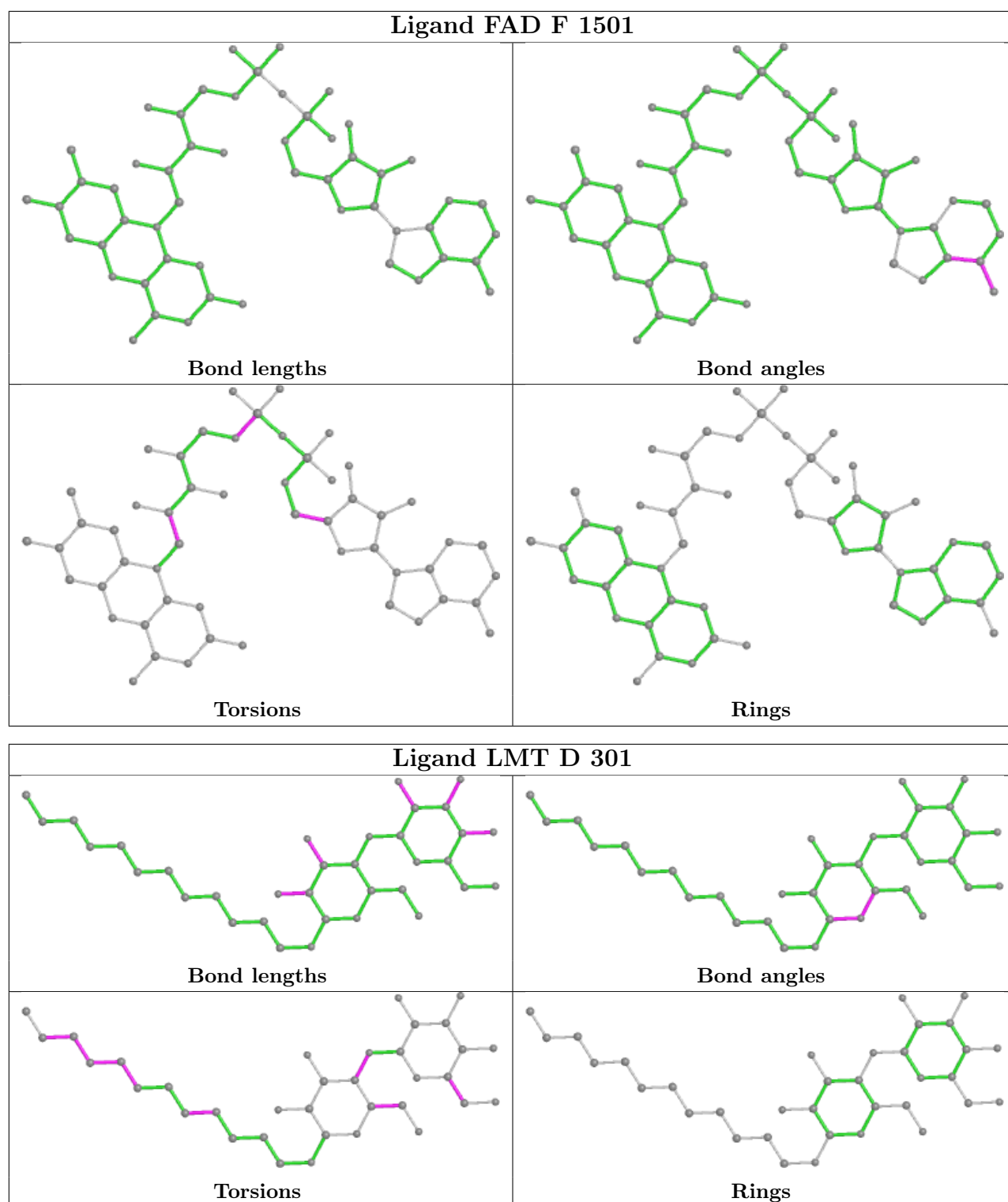
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	403/468 (86%)	0.60	50 (12%) 4 5	129, 156, 190, 258	0
2	B	380/415 (91%)	0.80	62 (16%) 1 2	122, 163, 208, 245	0
3	C	248/257 (96%)	1.79	85 (34%) 0 0	163, 201, 233, 258	0
4	D	204/210 (97%)	0.39	16 (7%) 13 13	124, 161, 199, 226	0
5	E	197/198 (99%)	0.65	23 (11%) 4 5	115, 150, 199, 221	0
6	F	407/408 (99%)	1.04	86 (21%) 1 1	145, 201, 259, 292	0
All	All	1839/1956 (94%)	0.88	322 (17%) 1 1	115, 171, 232, 292	0

The worst 5 of 322 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	244	PHE	12.4
3	C	137	ILE	10.3
3	C	91	TYR	10.1
3	C	122	GLY	9.3
2	B	227	THR	8.9

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

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

6.3 Carbohydrates [i](#)

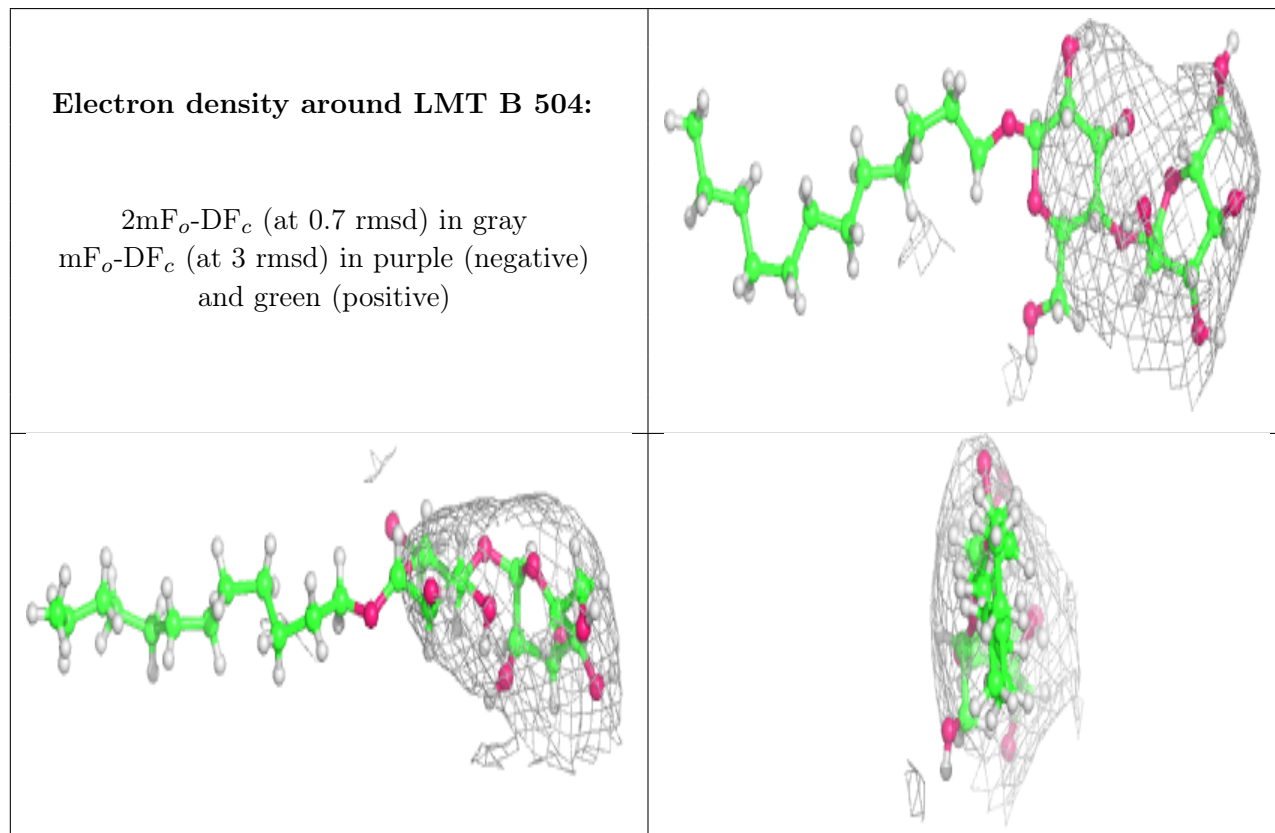
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

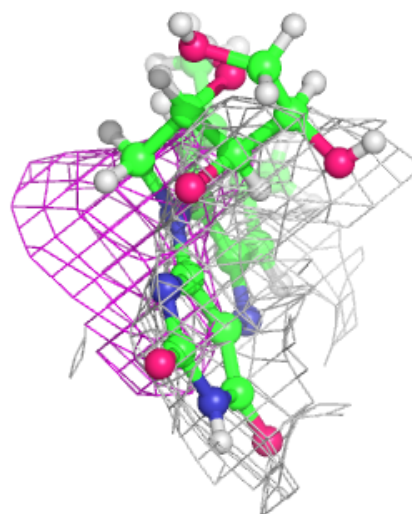
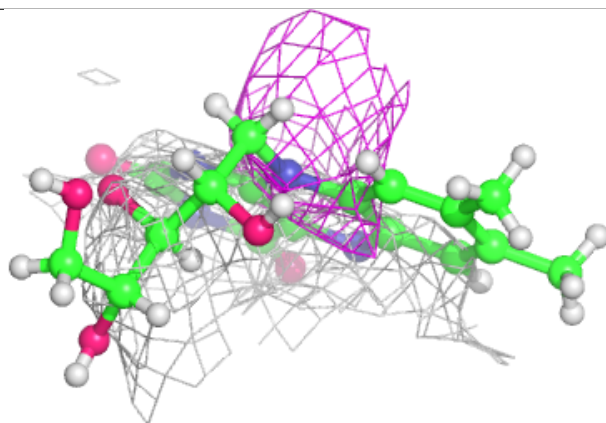
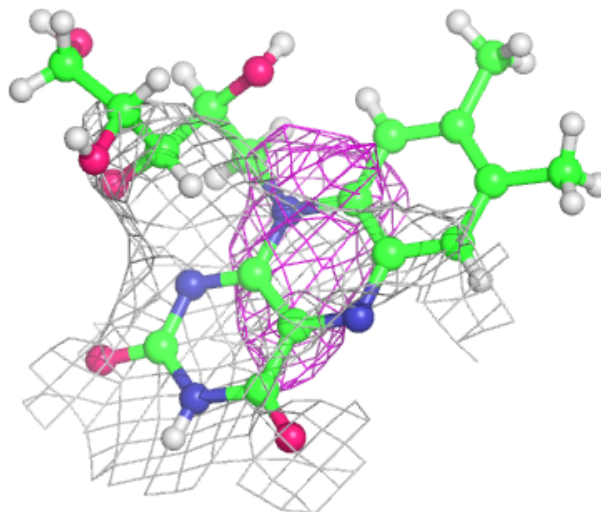
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LMT	B	504	35/35	0.64	0.56	149,185,216,236	0
8	RBF	B	502	27/27	0.68	0.74	159,191,246,264	0
7	FMN	C	1000	30/31	0.72	0.64	160,182,213,220	0
9	LMT	D	301	35/35	0.77	0.41	165,205,238,246	0
7	FMN	B	501	30/31	0.81	0.46	145,170,204,209	0
9	LMT	B	503	35/35	0.84	0.48	130,169,236,250	0
12	FAD	F	1501	53/53	0.85	0.25	196,220,264,284	0
11	FES	F	1502	4/4	0.89	0.10	260,274,274,275	0
10	NA	B	505	1/1	0.95	0.83	138,138,138,138	0
11	FES	E	1001	4/4	0.98	0.47	143,144,146,147	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



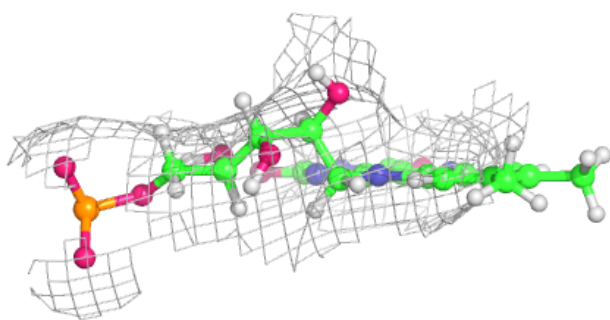
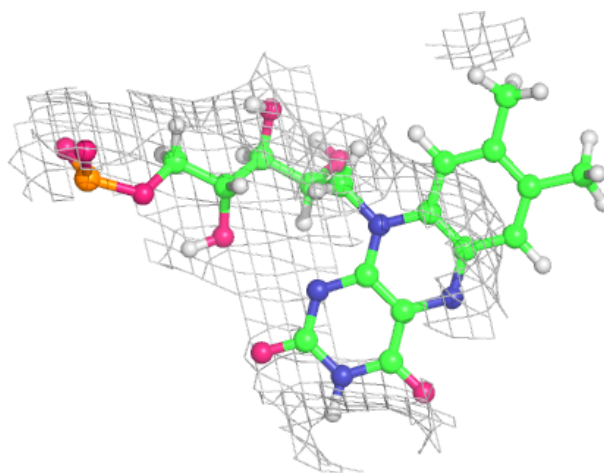
Electron density around RBF B 502:

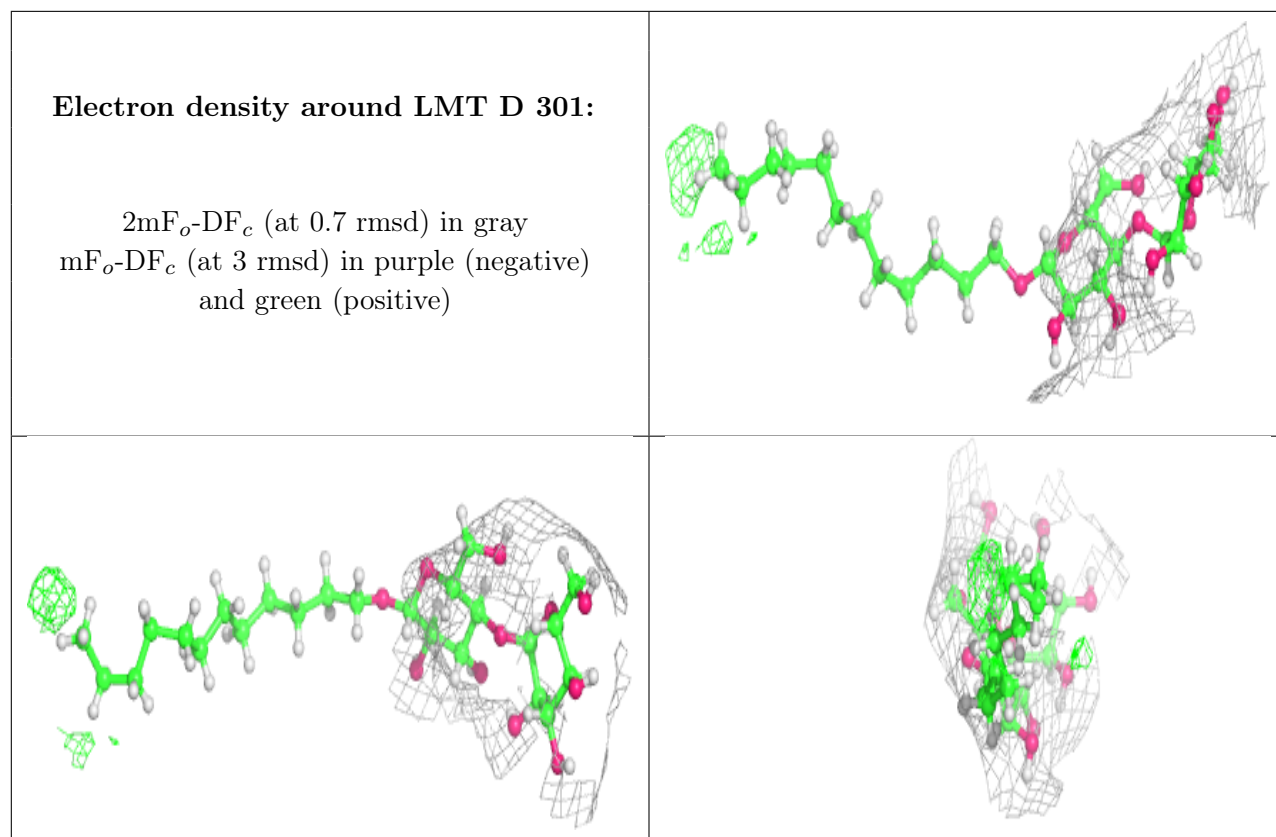
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN C 1000:

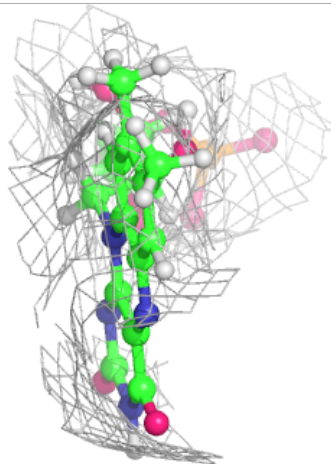
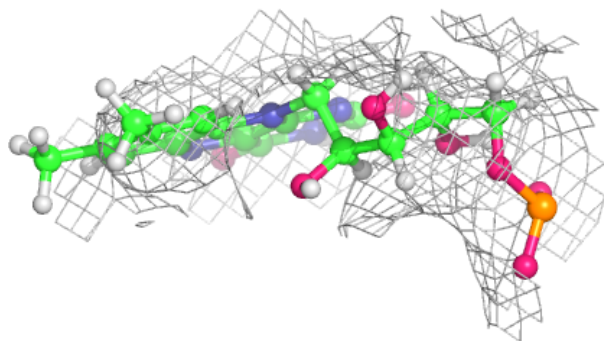
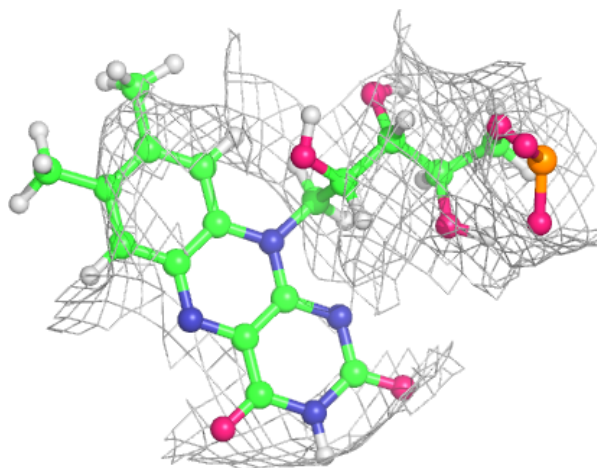
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





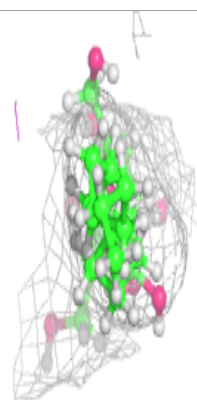
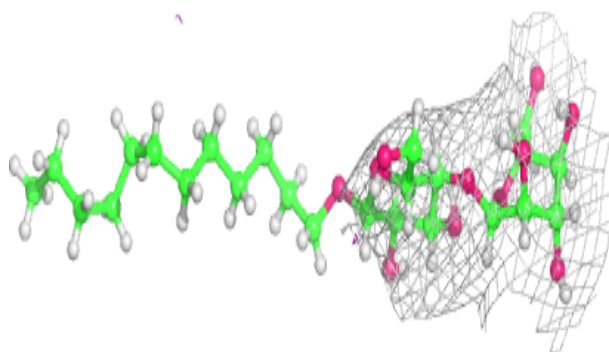
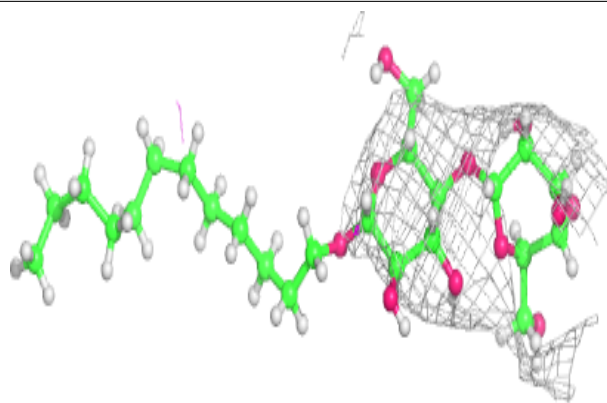
Electron density around FMN B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

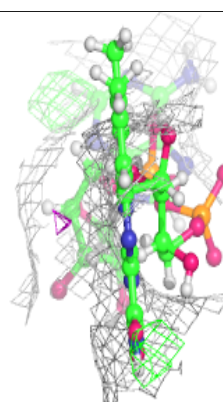
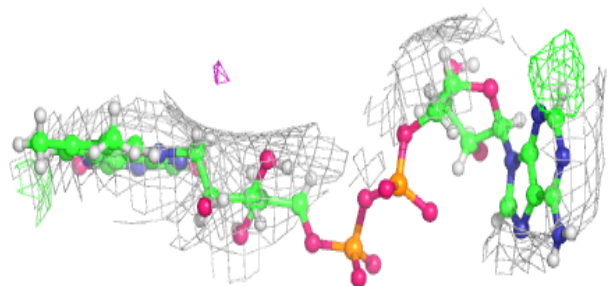
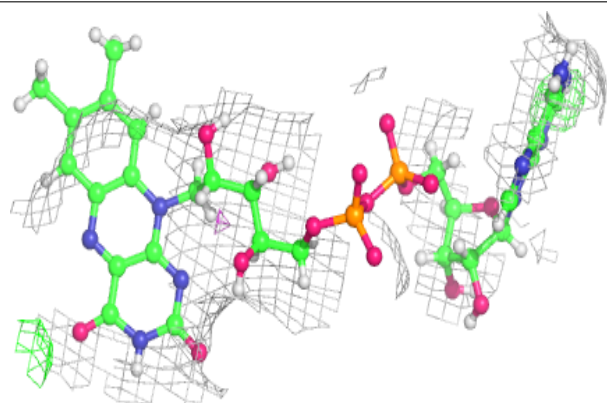


Electron density around LMT B 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD F 1501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.