



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:05 pm BST

PDB ID : 6HLA
Title : wild-type NuoEF from Aquifex aeolicus - reduced form bound to NADH
Authors : Gerhardt, S.; Friedrich, T.; Einsle, O.; Gnannt, E.; Schulte, M.; Fiegen, D.
Deposited on : 2018-09-11
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

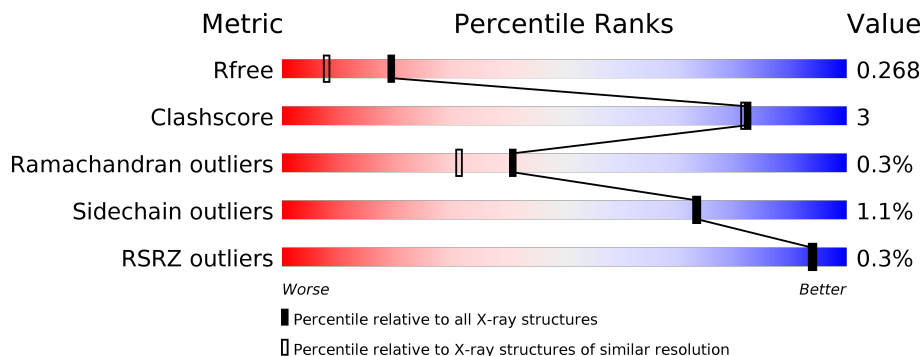
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	160	
1	C	160	
2	B	434	
2	D	434	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9973 atoms, of which 0 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 NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1259	816	203	231	9	0	0	0
1	C	155	1259	816	203	231	9	0	0	0

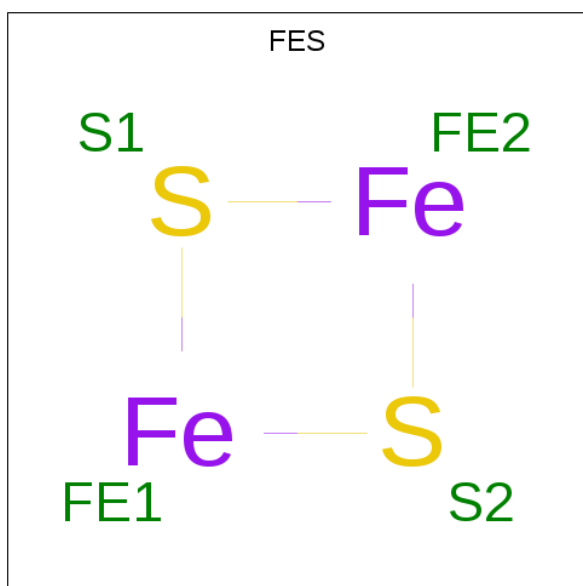
- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	417	3290	2115	547	615	13	0	1	0
2	D	418	3293	2117	549	614	13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

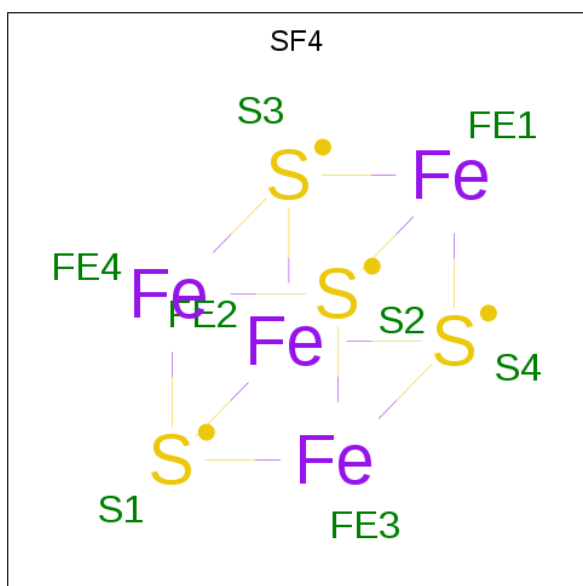
Chain	Residue	Modelled	Actual	Comment	Reference
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag	UNP O66841
B	434	HIS	-	expression tag	UNP O66841
D	427	ALA	-	expression tag	UNP O66841
D	428	GLY	-	expression tag	UNP O66841
D	429	HIS	-	expression tag	UNP O66841
D	430	HIS	-	expression tag	UNP O66841
D	431	HIS	-	expression tag	UNP O66841
D	432	HIS	-	expression tag	UNP O66841
D	433	HIS	-	expression tag	UNP O66841
D	434	HIS	-	expression tag	UNP O66841

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



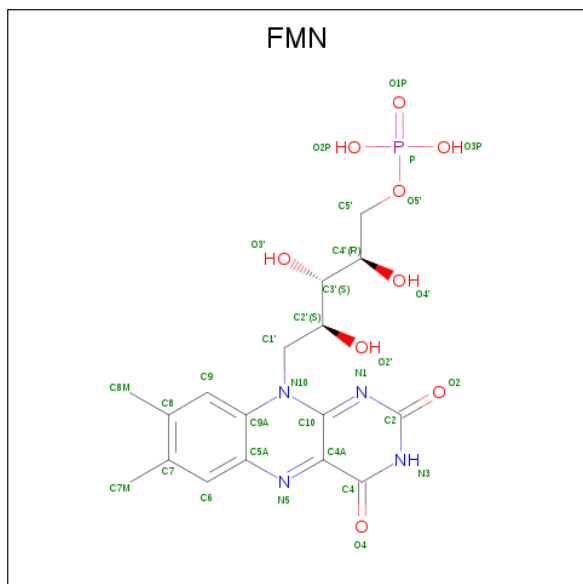
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		

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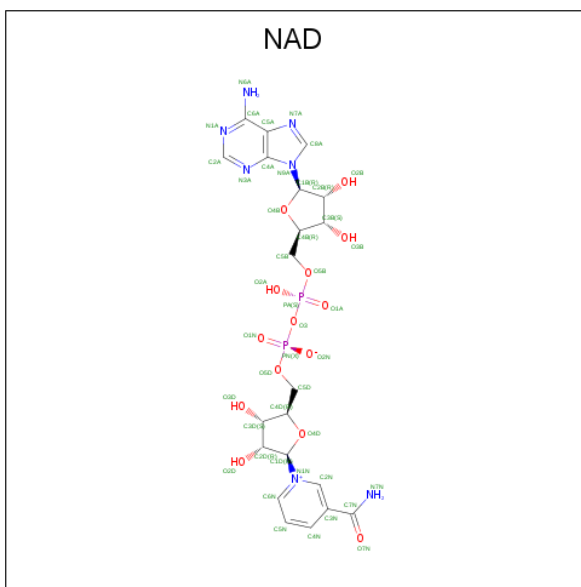
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

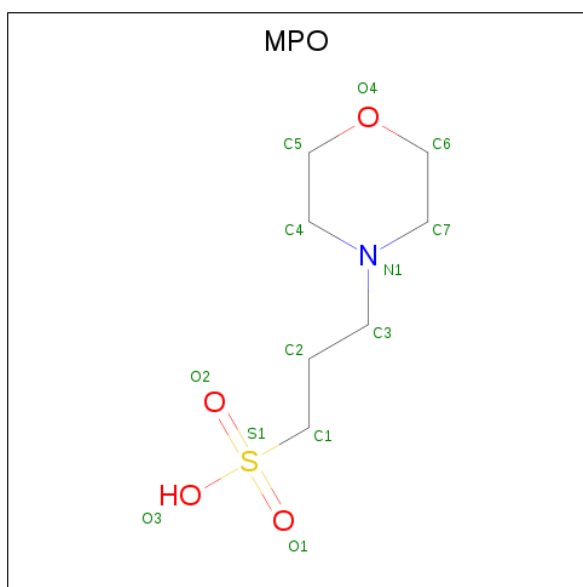


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
6	B	1	44	21	7	14	2	0	0
6	D	1	44	21	7	14	2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	B	1	1	1	0	0
7	D	1	1	1	0	0

- Molecule 8 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	B	1	13	7	1	4	1	0	0
8	D	1	13	7	1	4	1	0	0


- Molecule 9 is water.

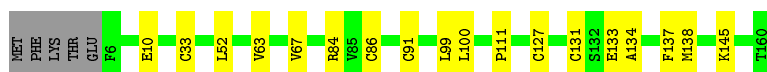
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	99	Total	O	0	0
			99	99		
9	B	278	Total	O	0	0
			278	278		
9	C	60	Total	O	0	0
			60	60		
9	D	233	Total	O	0	0
			233	233		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: NADH-quinone oxidoreductase subunit E

Chain A: 




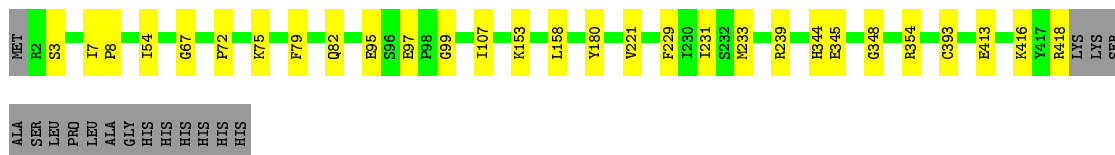
- Molecule 1: NADH-quinone oxidoreductase subunit E

Chain C: 




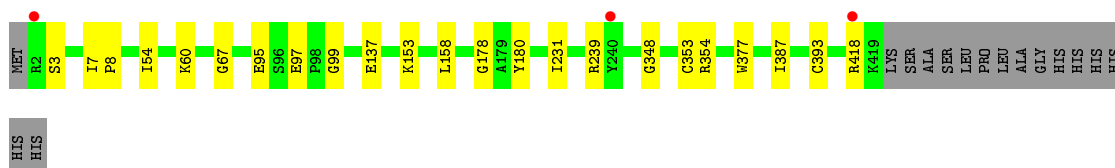
- Molecule 2: NADH-quinone oxidoreductase subunit F

Chain B: 



- Molecule 2: NADH-quinone oxidoreductase subunit F

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.64Å 116.43Å 189.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.20 – 1.90 99.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (99.20-1.90) 98.5 (99.20-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.90Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.240 0.236 , 0.268	Depositor DCC
R_{free} test set	5493 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6293e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAD, NA, SF4, FMN, FES, MPO

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	0.46	0/1288	0.66	0/1740
1	C	0.45	0/1288	0.65	0/1740
2	B	0.48	0/3374	0.61	0/4565
2	D	0.48	0/3374	0.62	0/4564
All	All	0.47	0/9324	0.63	0/12609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1259	0	1263	10	0
1	C	1259	0	1263	12	0
2	B	3290	0	3263	15	0
2	D	3293	0	3270	14	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	B	8	0	0	0	0
4	D	8	0	0	0	0
5	B	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	31	0	19	1	0
6	B	44	0	26	4	0
6	D	44	0	26	4	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	13	0	14	0	0
8	D	13	0	14	0	0
9	A	99	0	0	0	0
9	B	278	0	0	0	0
9	C	60	0	0	0	0
9	D	233	0	0	1	0
All	All	9973	0	9177	47	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 3.

All (47) 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:C:133:GLU:HG3	2:D:8:PRO:HB2	1.67	0.75
1:A:133:GLU:HG3	2:B:8:PRO:HB2	1.77	0.67
2:B:67:GLY:O	6:B:503:NAD:H2N	1.97	0.64
2:D:67:GLY:O	6:D:503:NAD:H2N	1.99	0.62
1:A:133:GLU:HB3	1:A:145:LYS:HB2	1.86	0.58
2:B:72:PRO:HB2	2:B:75:LYS:HG3	1.86	0.57
1:C:133:GLU:HB3	1:C:145:LYS:HB2	1.87	0.56
2:B:97:GLU:HB2	6:B:503:NAD:C4N	2.37	0.55
1:C:131:CYS:SG	2:D:99:GLY:HA2	2.47	0.54
2:D:54:ILE:HG23	2:D:231:ILE:HD11	1.89	0.54
2:D:60:LYS:O	2:D:239:ARG:HD2	2.09	0.53
2:B:153:LYS:HG2	2:B:158:LEU:HB2	1.93	0.51
2:D:153:LYS:HG2	2:D:158:LEU:HB2	1.93	0.51
2:B:54:ILE:HG23	2:B:231:ILE:HD11	1.92	0.49
1:C:91:CYS:HA	1:C:134:ALA:HB1	1.95	0.49
2:B:79:PHE:O	2:B:82:GLN:HG2	2.12	0.49
2:D:348:GLY:HA2	2:D:354:ARG:HB2	1.94	0.48
1:A:33:CYS:HB3	1:A:52:LEU:HD11	1.97	0.47
2:B:348:GLY:HA2	2:B:354:ARG:HB2	1.96	0.46
1:C:33:CYS:HB3	1:C:52:LEU:HD11	1.97	0.46
2:D:97:GLU:HB2	6:D:503:NAD:C4N	2.45	0.46
1:A:91:CYS:HA	1:A:134:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD21	1:C:137:PHE:HB3	1.97	0.46
2:B:180:TYR:CE1	6:B:503:NAD:H5N	2.51	0.46
2:D:353:CYS:HA	2:D:387:ILE:HG23	1.99	0.45
1:A:99:LEU:HD21	1:A:137:PHE:HB3	1.99	0.44
1:A:86:CYS:SG	1:A:127:CYS:HA	2.59	0.43
1:A:131:CYS:SG	2:B:99:GLY:HA2	2.57	0.43
1:A:100:LEU:HD22	1:A:111:PRO:HG3	2.01	0.43
1:C:84:ARG:HB2	1:C:138:MET:HB2	2.00	0.43
1:A:84:ARG:HB2	1:A:138:MET:HB2	2.00	0.43
1:C:63:VAL:O	1:C:67:VAL:HG23	2.19	0.42
2:D:180:TYR:CZ	6:D:503:NAD:H5N	2.55	0.42
2:D:377:TRP:CZ2	2:D:418:ARG:HA	2.55	0.42
1:A:63:VAL:O	1:A:67:VAL:HG23	2.20	0.42
2:B:180:TYR:CZ	6:B:503:NAD:H5N	2.55	0.41
1:C:100:LEU:HD22	1:C:111:PRO:HG3	2.02	0.41
1:C:25:LYS:HE3	9:D:795:HOH:O	2.21	0.41
2:B:413:GLU:O	2:B:416:LYS:HG2	2.20	0.41
2:B:344:HIS:HD2	2:B:345:GLU:OE2	2.04	0.41
2:D:137:GLU:OE2	2:D:178:GLY:HA2	2.21	0.41
1:C:131:CYS:SG	2:D:99:GLY:CA	3.09	0.41
1:C:103:LEU:HG	1:C:152:LEU:HD21	2.02	0.41
5:D:502:FMN:H9	5:D:502:FMN:H1'1	1.92	0.41
2:D:180:TYR:CE1	6:D:503:NAD:H5N	2.56	0.40
2:B:107:ILE:HD11	2:B:221:VAL:HG21	2.02	0.40
2:B:229:PHE:O	2:B:233:MET:HG2	2.21	0.40

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 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	153/160 (96%)	144 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	153/160 (96%)	145 (95%)	7 (5%)	1 (1%)	22	12
2	B	416/434 (96%)	406 (98%)	9 (2%)	1 (0%)	47	38
2	D	416/434 (96%)	403 (97%)	12 (3%)	1 (0%)	47	38
All	All	1138/1188 (96%)	1098 (96%)	37 (3%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	95	GLU
2	D	95	GLU
1	C	95	GLY

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	141/146 (97%)	140 (99%)	1 (1%)	84	84
1	C	141/146 (97%)	139 (99%)	2 (1%)	67	65
2	B	344/357 (96%)	339 (98%)	5 (2%)	65	62
2	D	344/357 (96%)	341 (99%)	3 (1%)	78	79
All	All	970/1006 (96%)	959 (99%)	11 (1%)	73	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
2	B	3	SER
2	B	7	ILE
2	B	239	ARG
2	B	393	CYS
2	B	418	ARG
1	C	43	TYR
1	C	76	GLU

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Mol	Chain	Res	Type
2	D	3	SER
2	D	7	ILE
2	D	393	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	344	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
3	FES	C	200	1	0,4,4	0.00	-	-		
8	MPO	B	505	-	13,13,13	1.38	1 (7%)	17,17,17	0.47	0
5	FMN	B	502	-	31,33,33	1.76	5 (16%)	40,50,50	2.68	6 (15%)
3	FES	A	200	1	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMN	D	502	-	31,33,33	1.69	5 (16%)	40,50,50	2.68	6 (15%)
6	NAD	D	503	-	42,48,48	0.58	0	50,73,73	0.74	2 (4%)
6	NAD	B	503	-	42,48,48	0.62	0	50,73,73	0.78	2 (4%)
4	SF4	B	501	2	0,12,12	0.00	-	-	-	-
4	SF4	D	501	2	0,12,12	0.00	-	-	-	-
8	MPO	D	505	-	13,13,13	1.08	1 (7%)	17,17,17	0.44	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
3	FES	C	200	1	-	-	0/1/1/1
8	MPO	B	505	-	-	2/7/15/15	0/1/1/1
5	FMN	B	502	-	-	3/18/18/18	0/3/3/3
3	FES	A	200	1	-	-	0/1/1/1
5	FMN	D	502	-	-	3/18/18/18	0/3/3/3
6	NAD	D	503	-	-	2/26/62/62	0/5/5/5
6	NAD	B	503	-	-	3/26/62/62	0/5/5/5
4	SF4	B	501	2	-	-	0/6/5/5
4	SF4	D	501	2	-	-	0/6/5/5
8	MPO	D	505	-	-	0/7/15/15	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	FMN	C4A-C10	6.78	1.45	1.38
5	D	502	FMN	C4A-C10	6.08	1.44	1.38
8	B	505	MPO	C1-S1	-4.89	1.70	1.77
8	D	505	MPO	C1-S1	-3.81	1.72	1.77
5	D	502	FMN	C4-N3	3.66	1.39	1.33
5	D	502	FMN	C4-C4A	3.49	1.47	1.41
5	B	502	FMN	C9A-N10	3.48	1.43	1.38
5	B	502	FMN	C4-N3	3.44	1.39	1.33
5	B	502	FMN	C4-C4A	3.31	1.47	1.41
5	D	502	FMN	C9A-N10	2.84	1.42	1.38
5	D	502	FMN	C5A-N5	2.81	1.40	1.35
5	B	502	FMN	C5A-N5	2.54	1.39	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	FMN	C4-N3-C2	12.76	125.91	115.14
5	D	502	FMN	C4-N3-C2	12.67	125.83	115.14
5	B	502	FMN	C4A-C4-N3	-6.94	113.93	123.43
5	D	502	FMN	C4A-C4-N3	-6.92	113.97	123.43
5	B	502	FMN	C10-C4A-N5	4.65	124.47	121.26
5	D	502	FMN	C10-C4A-N5	4.64	124.47	121.26
5	B	502	FMN	C4-C4A-C10	-4.29	117.11	119.95
5	D	502	FMN	C4-C4A-C10	-4.24	117.14	119.95
5	B	502	FMN	C4A-C10-N10	-3.45	116.76	120.30
5	D	502	FMN	C4A-C10-N10	-3.41	116.79	120.30
5	D	502	FMN	C1'-N10-C9A	2.87	120.55	118.29
6	B	503	NAD	C2N-N1N-C1D	-2.46	113.66	119.14
5	B	502	FMN	C1'-N10-C9A	2.32	120.12	118.29
6	D	503	NAD	C5A-C6A-N6A	2.27	123.80	120.35
6	B	503	NAD	C5A-C6A-N6A	2.18	123.66	120.35
6	D	503	NAD	PN-O3-PA	2.17	140.26	132.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	503	NAD	C5B-O5B-PA-O1A
6	D	503	NAD	O4D-C1D-N1N-C6N
6	B	503	NAD	O4D-C1D-N1N-C6N
8	B	505	MPO	C2-C3-N1-C7
8	B	505	MPO	C2-C3-N1-C4
5	D	502	FMN	O2'-C2'-C3'-C4'
5	B	502	FMN	O2'-C2'-C3'-C4'
5	B	502	FMN	C4'-C5'-O5'-P
5	D	502	FMN	C4'-C5'-O5'-P
6	B	503	NAD	PN-O3-PA-O5B
5	D	502	FMN	O2'-C2'-C3'-O3'
5	B	502	FMN	O2'-C2'-C3'-O3'
6	B	503	NAD	C5B-O5B-PA-O1A

There are no ring outliers.

3 monomers are involved in 9 short contacts:

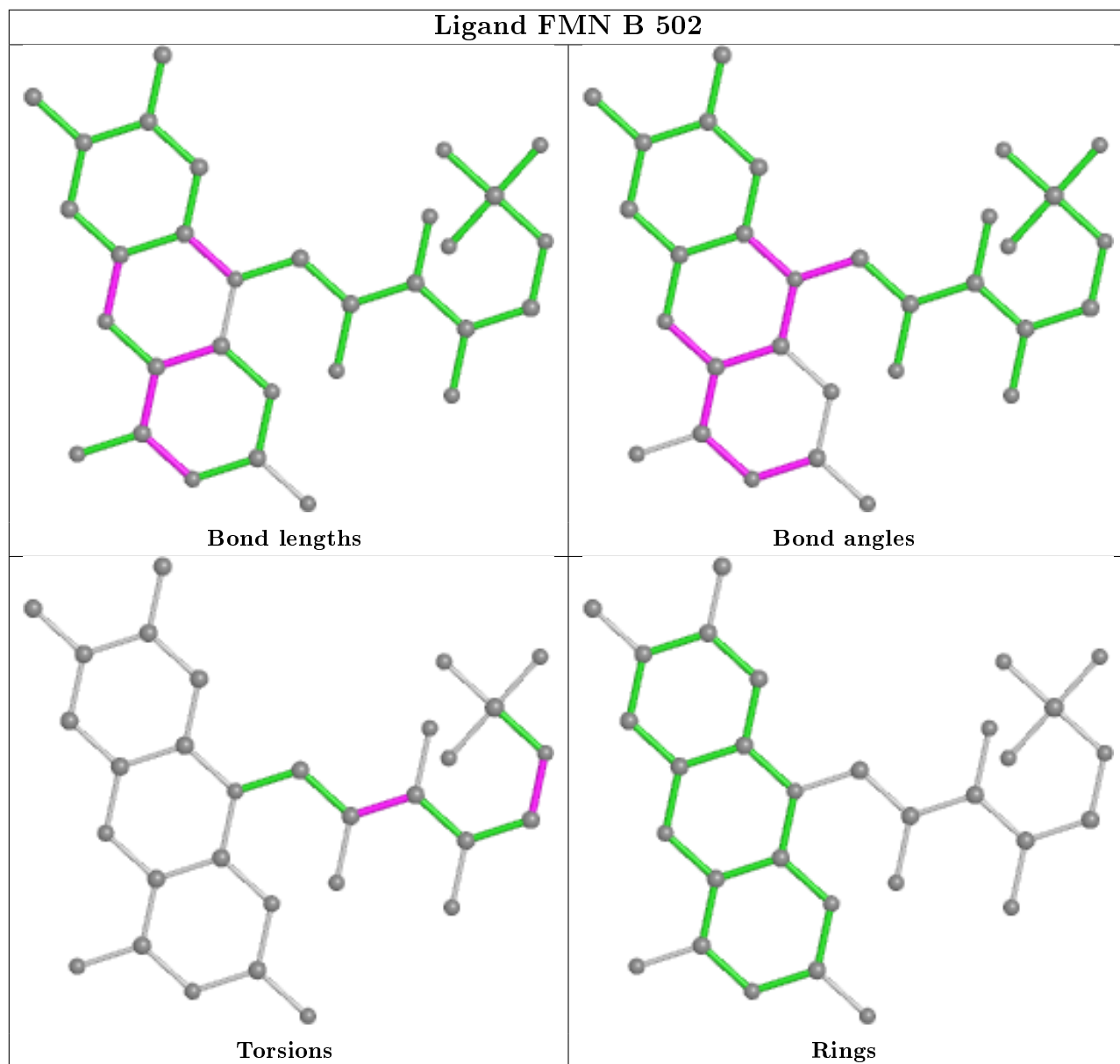
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	FMN	1	0

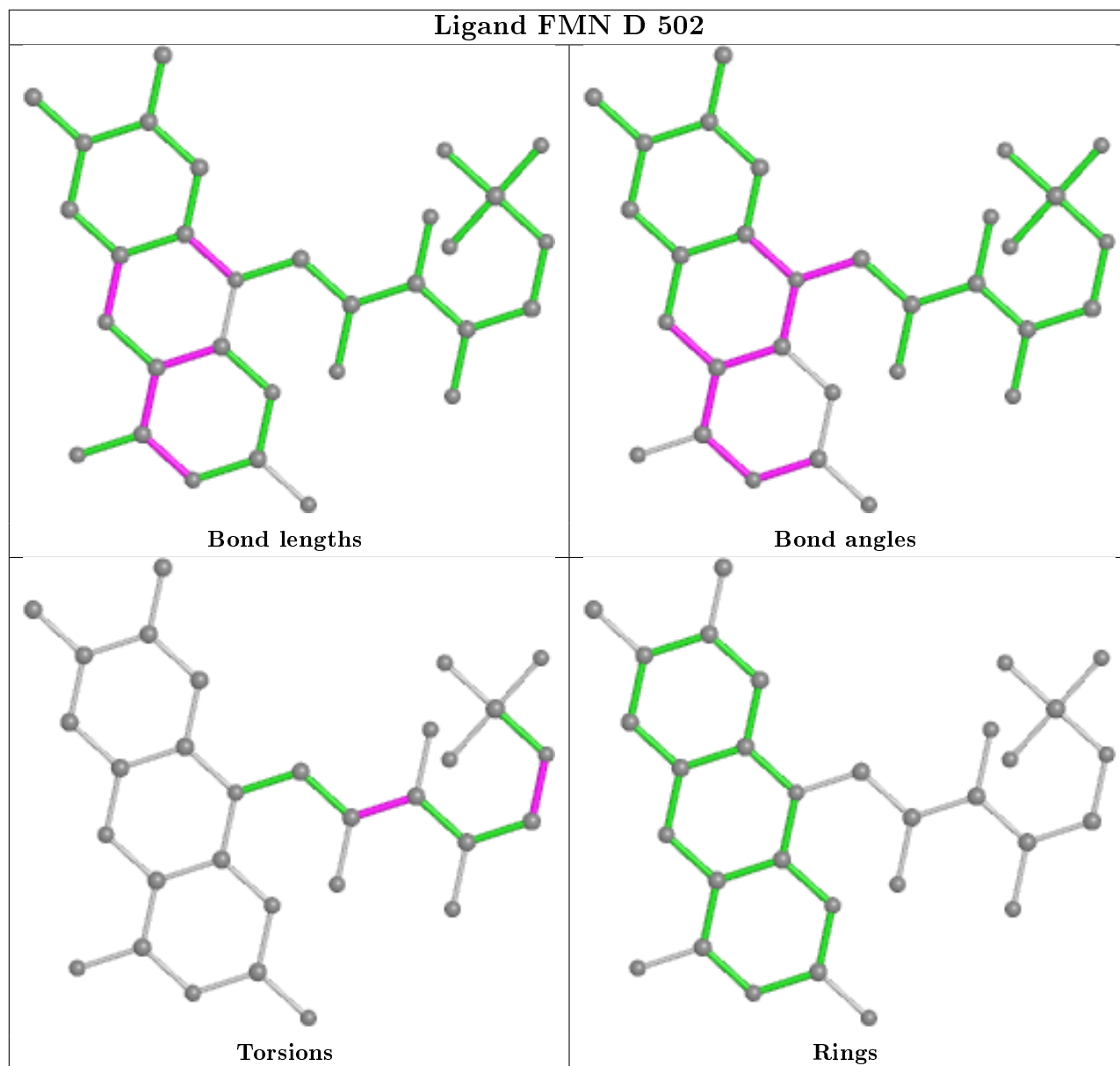
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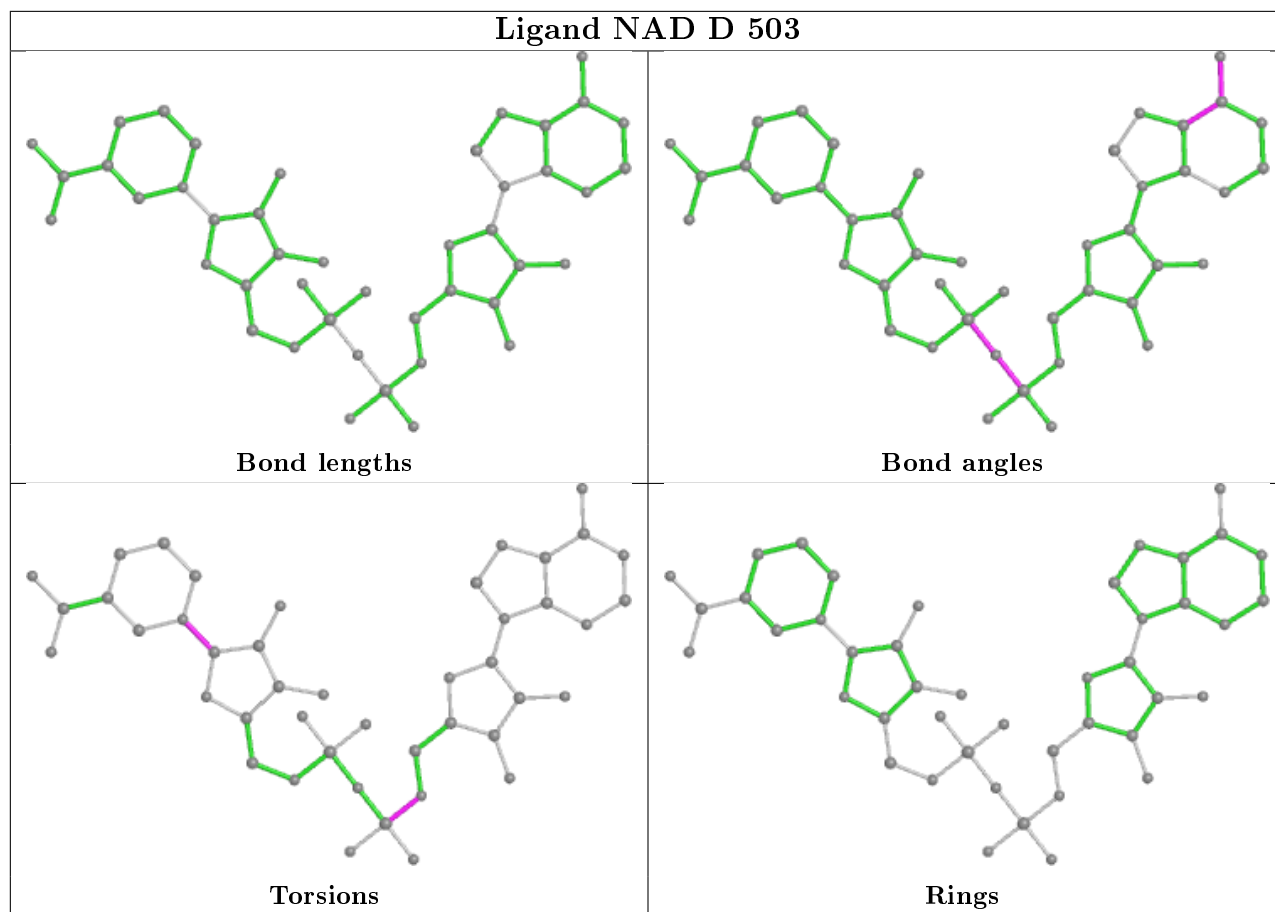
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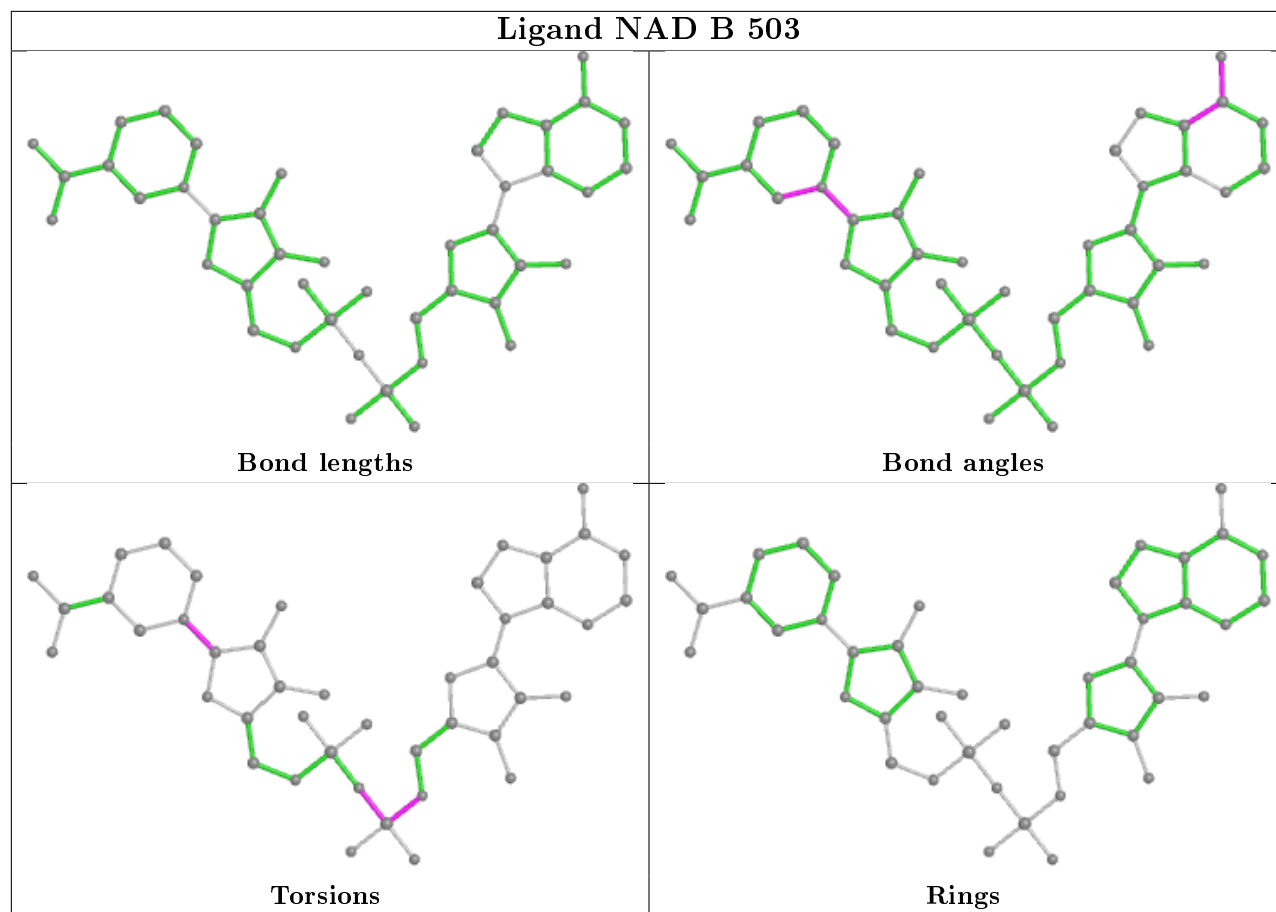
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	503	NAD	4	0
6	B	503	NAD	4	0

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 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	155/160 (96%)	0.13	0 100 100	12, 32, 54, 70	0
1	C	155/160 (96%)	0.24	1 (0%) 89 90	18, 39, 63, 89	0
2	B	417/434 (96%)	0.02	0 100 100	9, 22, 42, 79	0
2	D	418/434 (96%)	0.07	3 (0%) 87 88	9, 25, 48, 101	0
All	All	1145/1188 (96%)	0.08	4 (0%) 94 94	9, 26, 52, 101	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	ARG	2.6
2	D	418	ARG	2.5
1	C	160	THR	2.2
2	D	240	TYR	2.2

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](#)

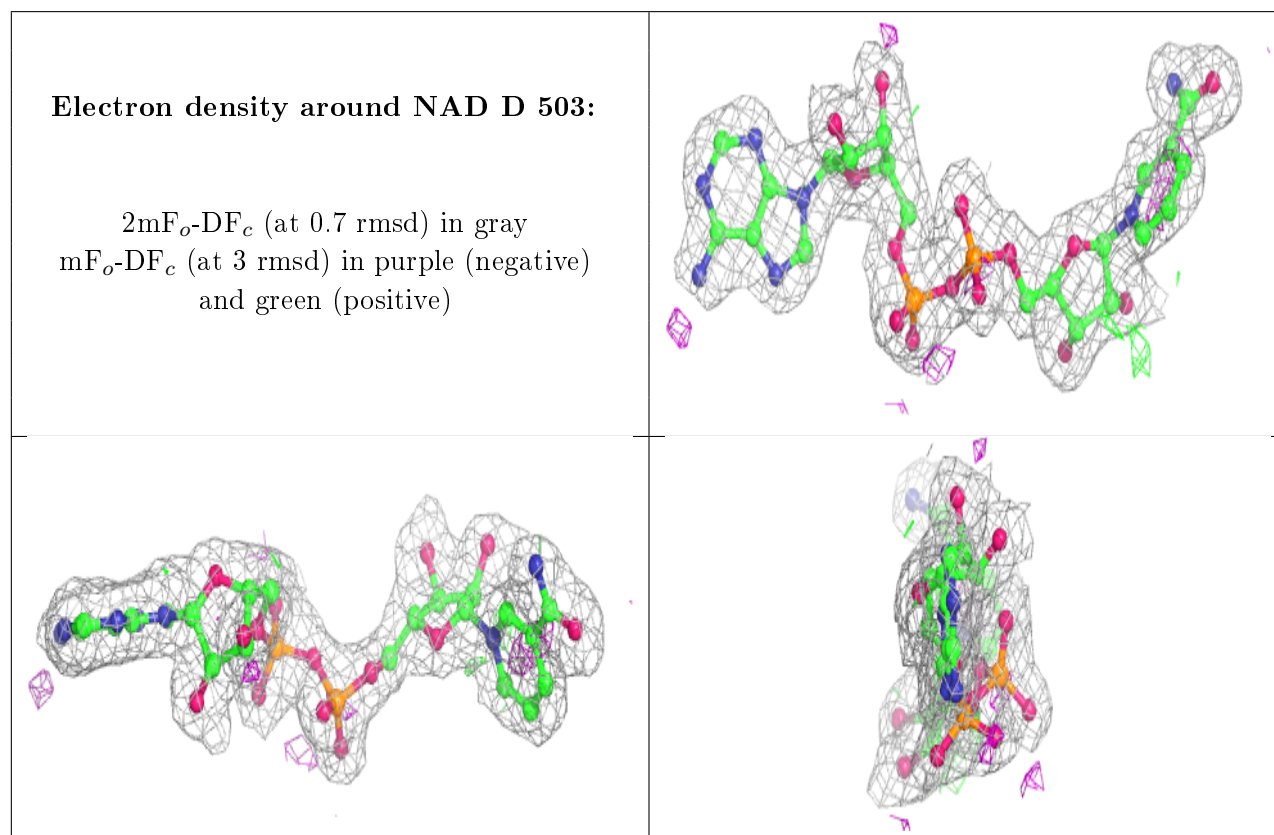
There are no carbohydrates in this entry.

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.

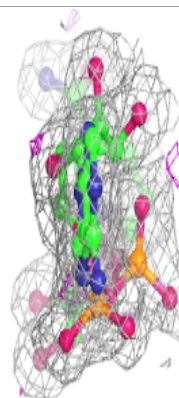
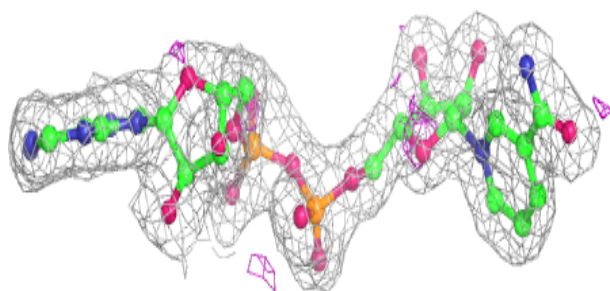
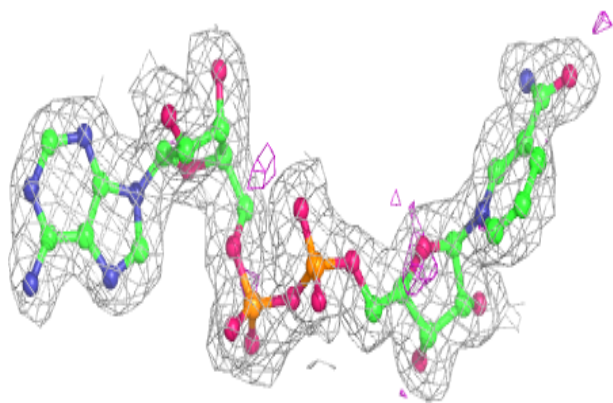
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MPO	B	505	13/13	0.69	0.25	65,68,82,82	0
8	MPO	D	505	13/13	0.82	0.20	39,44,70,72	0
7	NA	D	504	1/1	0.94	0.09	31,31,31,31	0
6	NAD	D	503	44/44	0.95	0.12	13,25,33,37	0
7	NA	B	504	1/1	0.96	0.11	30,30,30,30	0
6	NAD	B	503	44/44	0.97	0.10	10,18,23,25	0
5	FMN	D	502	31/31	0.97	0.10	10,17,22,22	0
5	FMN	B	502	31/31	0.97	0.10	7,12,17,21	0
4	SF4	B	501	8/8	0.99	0.06	18,19,20,24	0
4	SF4	D	501	8/8	0.99	0.08	21,23,27,28	0
3	FES	A	200	4/4	0.99	0.07	19,19,20,23	0
3	FES	C	200	4/4	0.99	0.06	18,19,21,24	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.

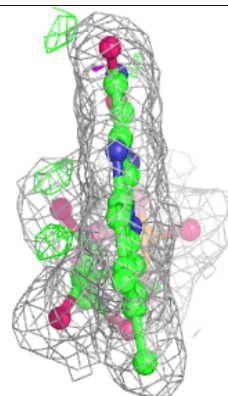
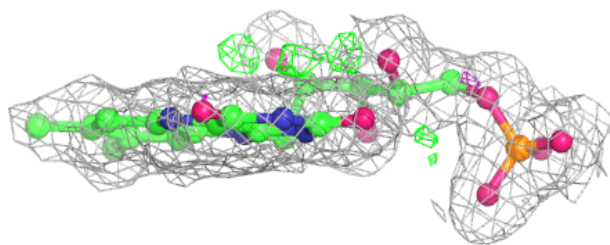
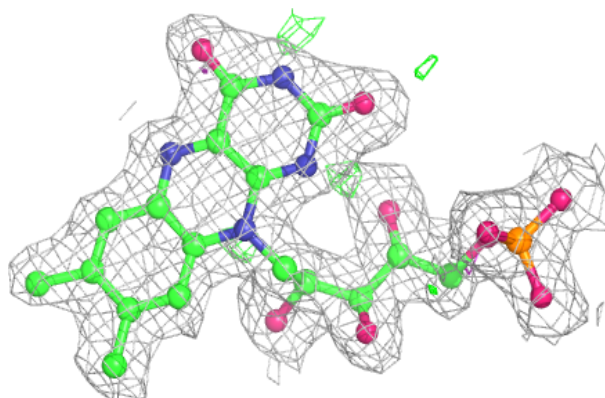


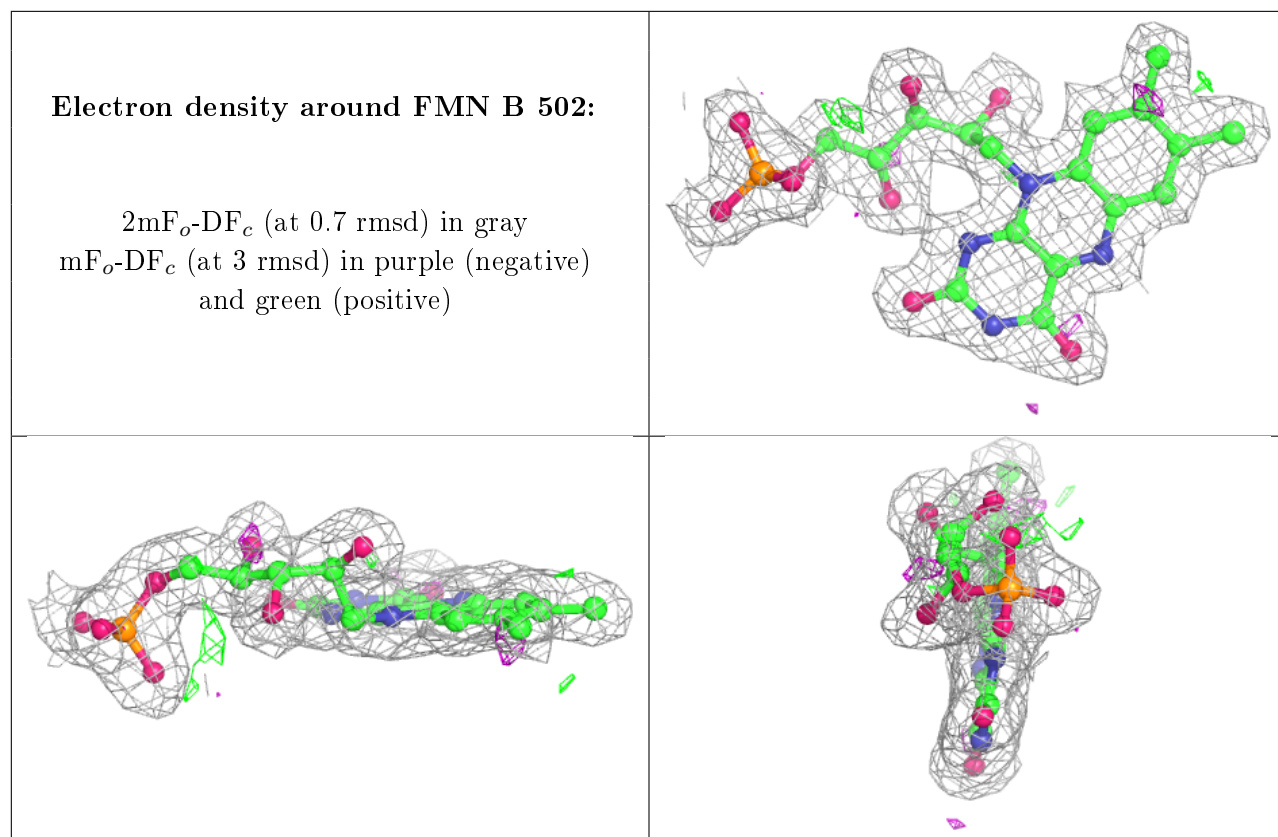
Electron density around NAD B 503:

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

**Electron density around FMN D 502:**

$2mF_o-DF_c$ (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.