Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:39 am BST

PDB ID	:	6HL2
Title	:	wild-type NuoEF from Aquifex aeolicus - oxidized form
Authors	:	Gerhardt, S.; Friedrich, T.; Einsle, O.; Gnandt, E.; Schulte, M.; Fiegen, D.
Deposited on	:	2018-09-10
Resolution	:	1.95 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:

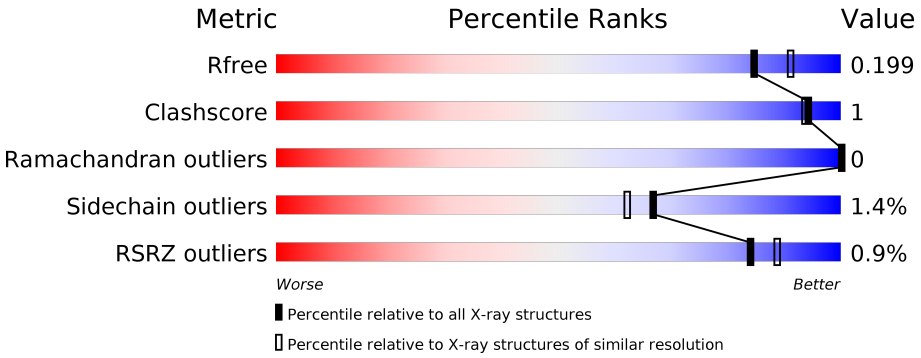
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

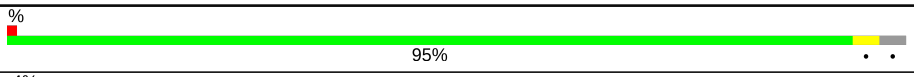
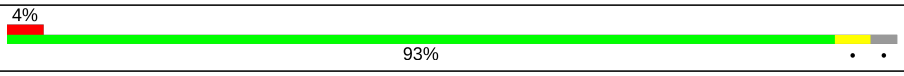
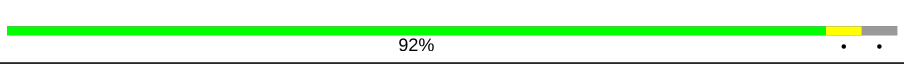
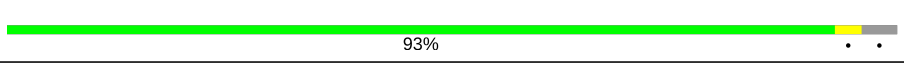
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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

There are 10 unique types of molecules in this entry. The entry contains 9945 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
1	A	156	Total	C	N	O	S	0	0	0
			1268	821	204	234	9			
1	C	155	Total	C	N	O	S	0	0	0
			1259	816	203	231	9			

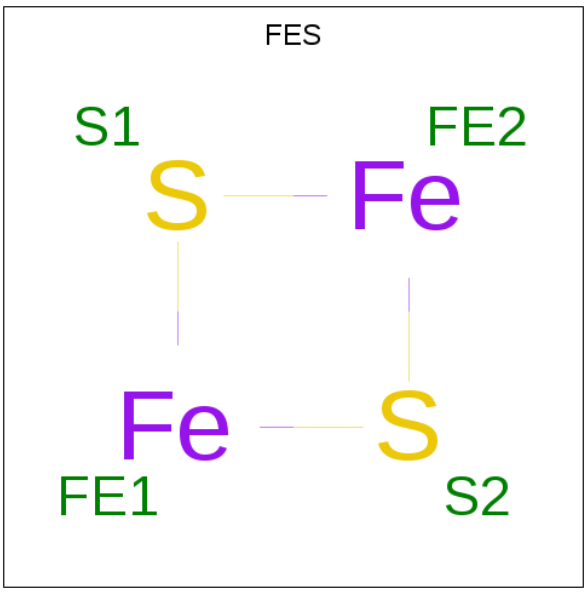
- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3273	2105	543	612	13			
2	D	417	Total	C	N	O	S	0	0	0
			3284	2111	547	613	13			

There are 16 discrepancies between the modelled and reference sequences:

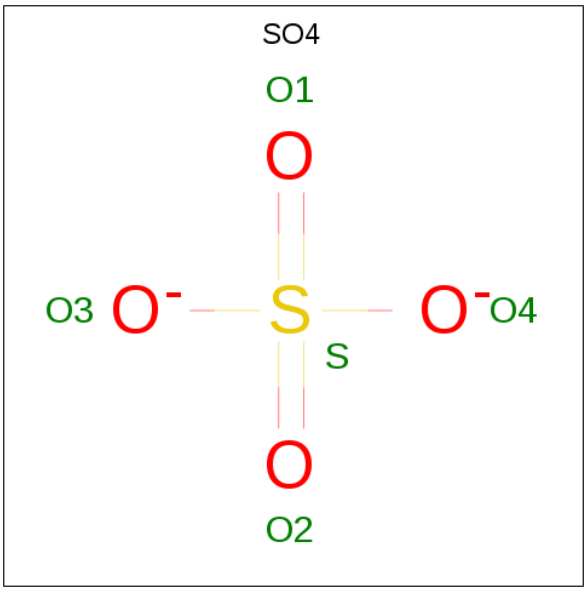
Chain	Residue	Modelled	Actual	Comment	Reference
B	427	ALA	-	expression tag	UNP O66841
B	428	GLY	-	expression tag	UNP O66841
B	429	HIS	-	expression tag	UNP O66841
B	430	HIS	-	expression tag	UNP O66841
B	431	HIS	-	expression tag	UNP O66841
B	432	HIS	-	expression tag	UNP O66841
B	433	HIS	-	expression tag	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: Fe_2S_2).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

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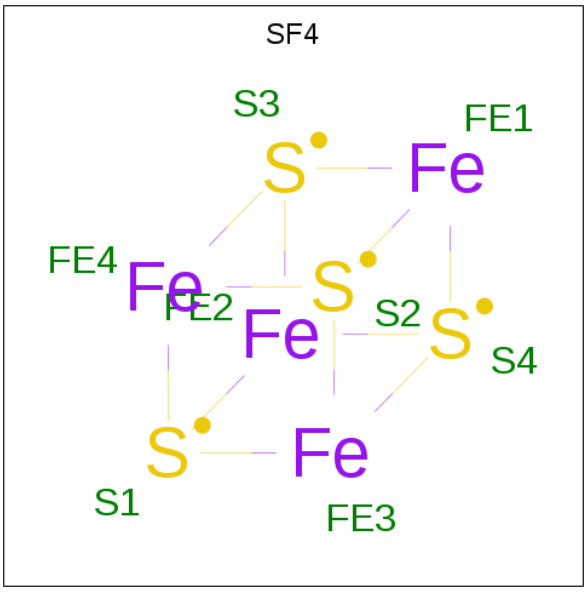
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

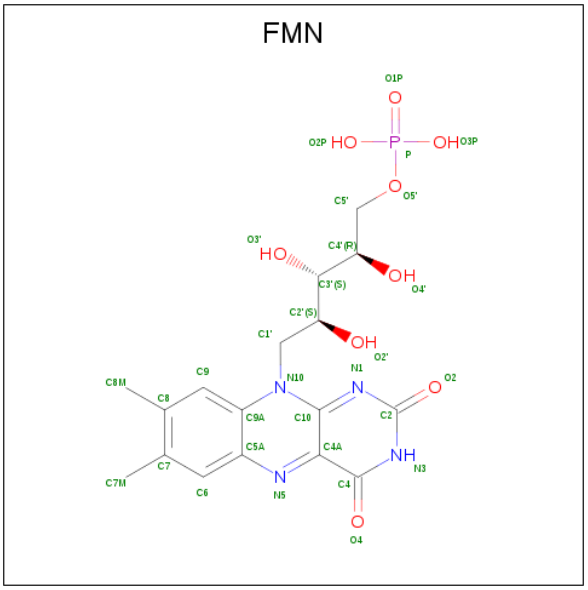
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Cl 3 3	0	0
5	A	1	Total Cl 1 1	0	0
5	D	2	Total Cl 2 2	0	0
5	C	2	Total Cl 2 2	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

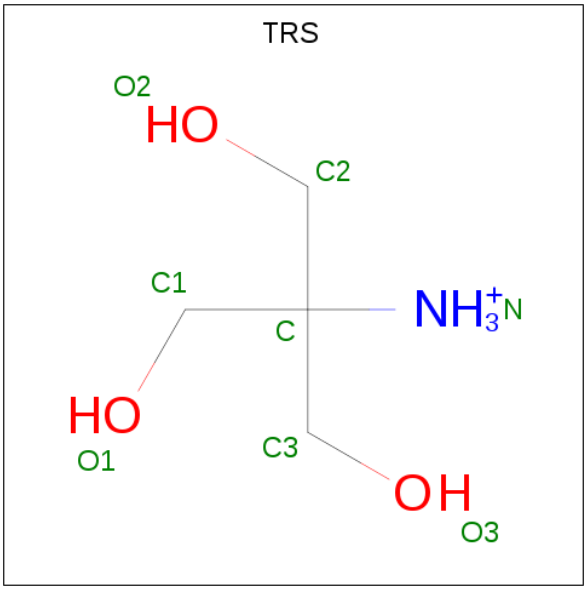


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 31 17 4 9 1	0	0
7	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 8 4 1 3	0	0
9	B	1	Total C N O 8 4 1 3	0	0
9	D	1	Total C N O 8 4 1 3	0	0
9	D	1	Total C N O 8 4 1 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	99	Total O 99 99	0	0
10	B	263	Total O 263 263	0	0

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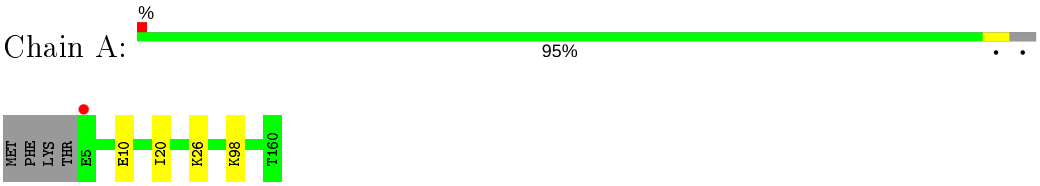
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	72	Total O 72 72	0	0
10	D	259	Total O 259 259	0	0

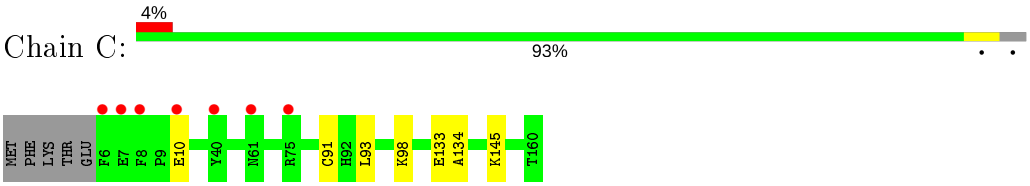
3 Residue-property plots (i)

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.

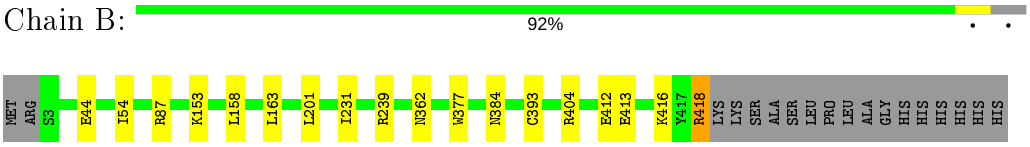
- Molecule 1: NADH-quinone oxidoreductase subunit E



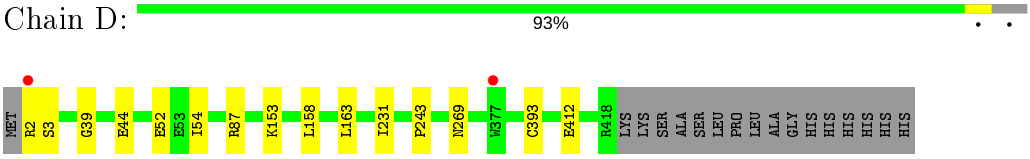
- Molecule 1: NADH-quinone oxidoreductase subunit E



- Molecule 2: NADH-quinone oxidoreductase subunit F



- Molecule 2: NADH-quinone oxidoreductase subunit F



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.19Å 116.44Å 189.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.48 – 1.95 73.48 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (73.48-1.95) 99.8 (73.48-1.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.170 , 0.195 0.173 , 0.199	Depositor DCC
R_{free} test set	5091 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9945	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.15 % 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 3.3155e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, SF4, FMN, SO4, TRS, 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	0.44	0/1297	0.61	0/1752
1	C	0.44	0/1288	0.61	0/1740
2	B	0.47	0/3354	0.56	0/4539
2	D	0.48	0/3365	0.56	0/4553
All	All	0.47	0/9304	0.58	0/12584

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

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	1268	0	1269	1	0
1	C	1259	0	1263	2	0
2	B	3273	0	3244	12	0
2	D	3284	0	3257	7	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	15	0	0	0	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	B	8	0	0	0	0
6	D	8	0	0	0	0
7	B	31	0	19	0	0
7	D	31	0	19	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	16	0	24	2	0
9	D	16	0	24	4	0
10	A	99	0	0	0	0
10	B	263	0	0	2	0
10	C	72	0	0	0	0
10	D	259	0	0	1	0
All	All	9945	0	9119	24	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 1.

All (24) 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)
2:B:87:ARG:HH12	9:B:511:TRS:H31	1.43	0.83
2:B:87:ARG:NH1	9:B:511:TRS:H31	2.02	0.73
2:D:87:ARG:HH22	9:D:510:TRS:H32	1.54	0.73
2:D:243:PRO:HD3	2:D:269:ASN:HD22	1.61	0.65
2:D:87:ARG:HH12	9:D:510:TRS:H21	1.64	0.63
2:B:413:GLU:HG3	2:B:416:LYS:HE2	1.86	0.56
9:D:510:TRS:H12	10:D:676:HOH:O	2.05	0.56
2:B:384:ASN:HD22	2:B:404:ARG:HH21	1.57	0.53
2:B:413:GLU:O	2:B:416:LYS:HG2	2.13	0.48
2:B:54:ILE:HG23	2:B:231:ILE:HD11	1.96	0.47
2:D:39:GLY:HA2	9:D:509:TRS:H21	1.98	0.44
2:D:44:GLU:HG2	2:D:163:LEU:HD13	2.00	0.44
2:B:384:ASN:ND2	2:B:404:ARG:HE	2.16	0.44
2:B:362:ASN:HB2	10:B:675:HOH:O	2.18	0.43
2:D:153:LYS:HG3	2:D:158:LEU:HB2	2.01	0.42
2:B:153:LYS:HG3	2:B:158:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:HB3	1:C:145:LYS:HB2	2.01	0.42
2:B:44:GLU:HG2	2:B:163:LEU:HD13	2.02	0.42
1:C:91:CYS:HA	1:C:134:ALA:HB1	2.02	0.42
2:D:54:ILE:HG23	2:D:231:ILE:HD11	2.02	0.42
2:B:377:TRP:CZ2	2:B:418:ARG:HG2	2.54	0.42
7:D:502:FMN:H9	7:D:502:FMN:H1'1	1.86	0.42
2:B:201:LEU:HD12	10:B:628:HOH:O	2.20	0.41
1:A:20:ILE:HG23	1:A:26:LYS:HG2	2.02	0.41

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	154/160 (96%)	148 (96%)	6 (4%)	0	100	100
1	C	153/160 (96%)	147 (96%)	6 (4%)	0	100	100
2	B	414/434 (95%)	405 (98%)	9 (2%)	0	100	100
2	D	415/434 (96%)	404 (97%)	11 (3%)	0	100	100
All	All	1136/1188 (96%)	1104 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	142/146 (97%)	140 (99%)	2 (1%)	67	62
1	C	141/146 (97%)	138 (98%)	3 (2%)	53	46
2	B	342/357 (96%)	338 (99%)	4 (1%)	71	68
2	D	343/357 (96%)	338 (98%)	5 (2%)	65	60
All	All	968/1006 (96%)	954 (99%)	14 (1%)	67	62

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	98	LYS
2	B	239	ARG
2	B	393	CYS
2	B	412	GLU
2	B	418	ARG
1	C	10	GLU
1	C	93	LEU
1	C	98	LYS
2	D	2	ARG
2	D	3	SER
2	D	52	GLU
2	D	393	CYS
2	D	412	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	97	ASN
2	B	360	GLN
2	B	384	ASN
1	C	97	ASN
2	D	269	ASN
2	D	388	GLN

5.3.3 RNA

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 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	505	-	4,4,4	0.22	0	6,6,6	0.36	0
4	SO4	D	506	-	4,4,4	0.12	0	6,6,6	0.09	0
9	TRS	D	509	-	7,7,7	0.22	0	9,9,9	0.29	0
4	SO4	D	505	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	B	506	-	4,4,4	0.15	0	6,6,6	0.10	0
6	SF4	B	501	2	0,12,12	0.00	-	-		
7	FMN	D	502	-	31,33,33	1.64	5 (16%)	40,50,50	2.65	5 (12%)
9	TRS	D	510	-	7,7,7	0.15	0	9,9,9	0.23	0
6	SF4	D	501	2	0,12,12	0.00	-	-		
7	FMN	B	502	-	31,33,33	1.57	4 (12%)	40,50,50	2.66	6 (15%)
9	TRS	B	511	-	7,7,7	0.24	0	9,9,9	0.33	0
4	SO4	D	504	-	4,4,4	0.17	0	6,6,6	0.15	0
9	TRS	B	510	-	7,7,7	0.27	0	9,9,9	0.30	0
4	SO4	C	202	-	4,4,4	0.18	0	6,6,6	0.16	0
3	FES	C	201	1	0,4,4	0.00	-	-		
4	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	B	504	-	4,4,4	0.27	0	6,6,6	0.34	0
3	FES	A	201	1	0,4,4	0.00	-	-		

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
9	TRS	D	509	-	-	3/9/9/9	-
6	SF4	B	501	2	-	-	0/6/5/5
7	FMN	D	502	-	-	4/18/18/18	0/3/3/3
9	TRS	D	510	-	-	1/9/9/9	-
9	TRS	B	510	-	-	0/9/9/9	-
7	FMN	B	502	-	-	4/18/18/18	0/3/3/3
9	TRS	B	511	-	-	3/9/9/9	-
6	SF4	D	501	2	-	-	0/6/5/5
3	FES	C	201	1	-	-	0/1/1/1
3	FES	A	201	1	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	502	FMN	C4A-C10	6.45	1.45	1.38
7	B	502	FMN	C4A-C10	6.08	1.44	1.38
7	B	502	FMN	C4-N3	3.50	1.39	1.33
7	D	502	FMN	C4-N3	3.48	1.39	1.33
7	B	502	FMN	C9A-N10	3.18	1.42	1.38
7	D	502	FMN	C9A-N10	2.91	1.42	1.38
7	B	502	FMN	C4-C4A	2.44	1.45	1.41
7	D	502	FMN	C4-C4A	2.33	1.45	1.41
7	D	502	FMN	C5A-N5	2.31	1.39	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	502	FMN	C4-N3-C2	12.78	125.93	115.14
7	D	502	FMN	C4-N3-C2	12.73	125.89	115.14
7	D	502	FMN	C4A-C4-N3	-6.91	113.98	123.43
7	B	502	FMN	C4A-C4-N3	-6.83	114.09	123.43
7	B	502	FMN	C10-C4A-N5	4.73	124.53	121.26
7	D	502	FMN	C10-C4A-N5	4.63	124.46	121.26
7	B	502	FMN	C4-C4A-C10	-4.29	117.11	119.95
7	D	502	FMN	C4-C4A-C10	-4.07	117.26	119.95
7	B	502	FMN	C4A-C10-N10	-3.35	116.86	120.30
7	D	502	FMN	C4A-C10-N10	-3.32	116.89	120.30
7	B	502	FMN	C1'-N10-C10	2.10	120.29	118.41

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	511	TRS	C1-C-C2-O2
7	D	502	FMN	C4'-C5'-O5'-P
7	B	502	FMN	C4'-C5'-O5'-P
9	D	509	TRS	C2-C-C1-O1
9	D	509	TRS	C3-C-C1-O1
9	B	511	TRS	C3-C-C2-O2
9	B	511	TRS	N-C-C2-O2
7	B	502	FMN	N10-C1'-C2'-C3'
7	D	502	FMN	N10-C1'-C2'-C3'
7	B	502	FMN	O2'-C2'-C3'-C4'
7	D	502	FMN	O2'-C2'-C3'-C4'
9	D	510	TRS	C1-C-C3-O3
9	D	509	TRS	N-C-C1-O1
7	B	502	FMN	N10-C1'-C2'-O2'
7	D	502	FMN	N10-C1'-C2'-O2'

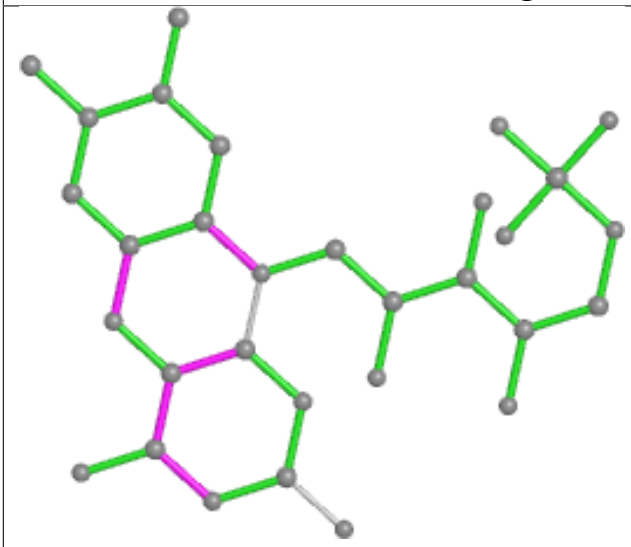
There are no ring outliers.

4 monomers are involved in 7 short contacts:

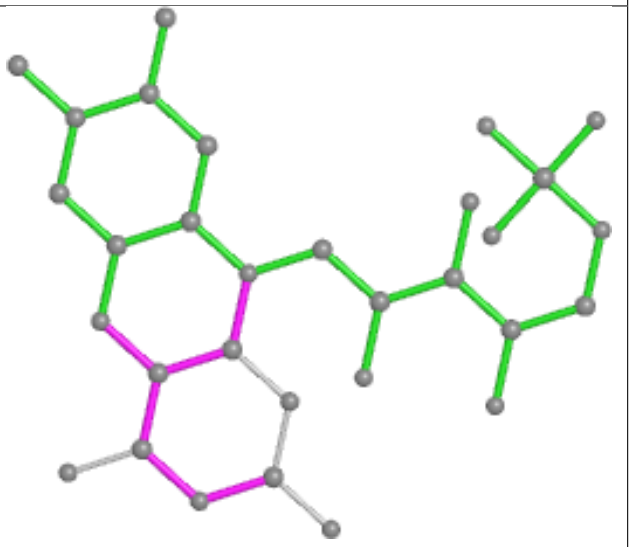
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	509	TRS	1	0
7	D	502	FMN	1	0
9	D	510	TRS	3	0
9	B	511	TRS	2	0

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

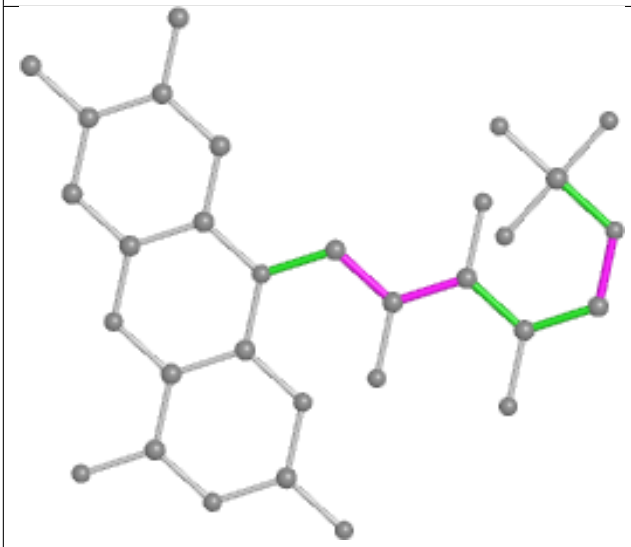
Ligand FMN D 502



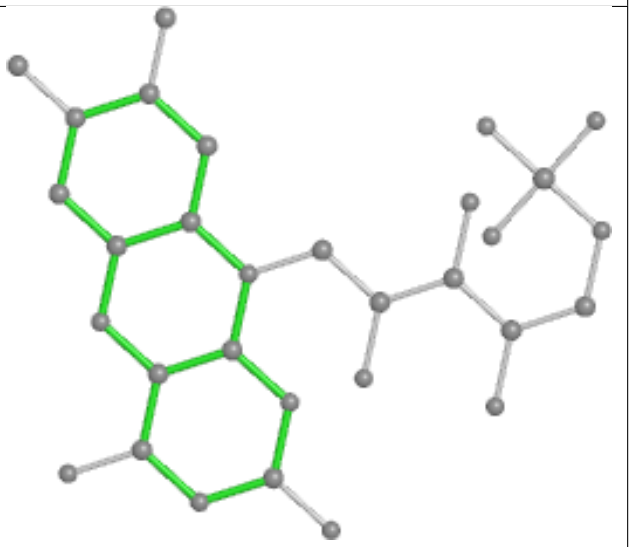
Bond lengths



Bond angles

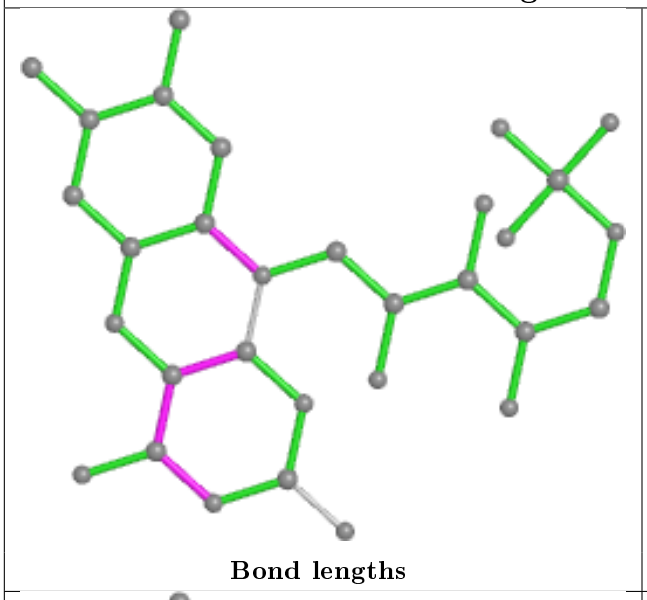


Torsions

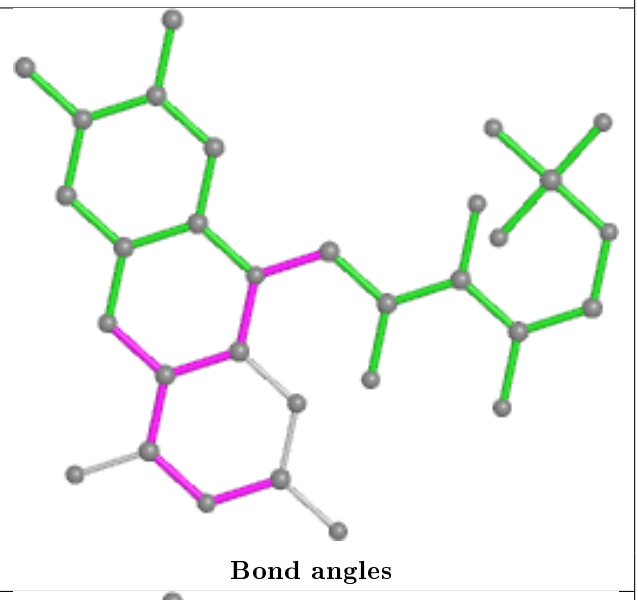


Rings

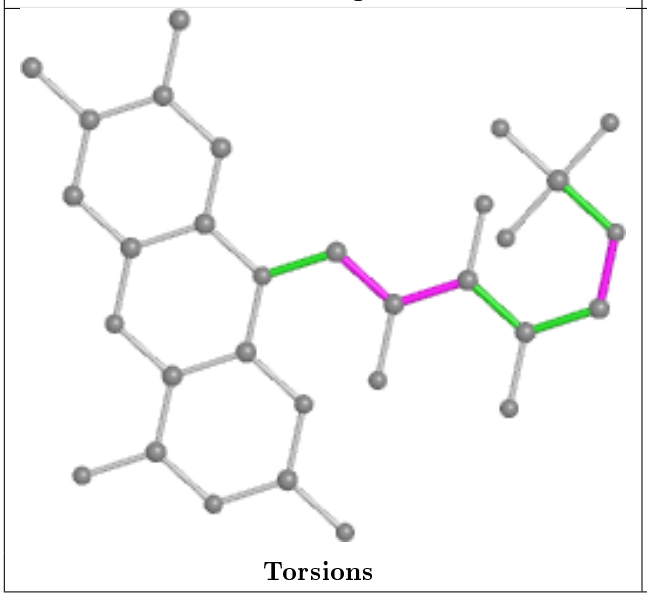
Ligand FMN B 502



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	156/160 (97%)	-0.14	1 (0%) 89 93	18, 34, 60, 91	0
1	C	155/160 (96%)	0.38	7 (4%) 33 43	20, 39, 62, 82	0
2	B	416/434 (95%)	-0.25	0 100 100	16, 27, 46, 81	0
2	D	417/434 (96%)	-0.25	2 (0%) 91 94	17, 28, 50, 93	0
All	All	1144/1188 (96%)	-0.15	10 (0%) 84 89	16, 29, 54, 93	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	PHE	5.2
1	C	40	TYR	3.1
1	A	5	GLU	2.9
1	C	7	GLU	2.8
2	D	2	ARG	2.7
1	C	75	ARG	2.7
1	C	10	GLU	2.7
1	C	8	PHE	2.4
2	D	377	TRP	2.2
1	C	61	ASN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

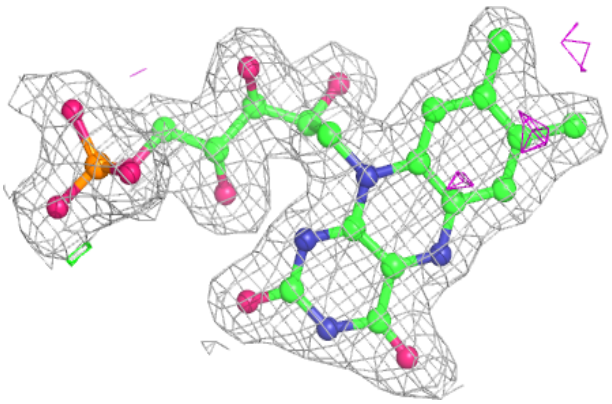
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

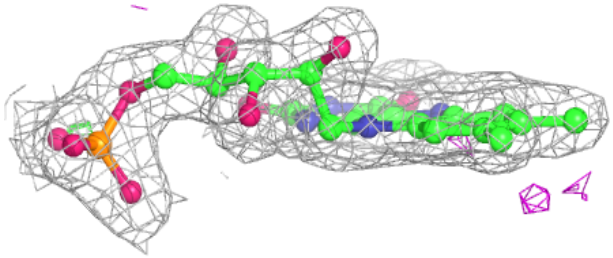
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	TRS	B	510	8/8	0.69	0.28	60,61,61,62	0
9	TRS	B	511	8/8	0.72	0.27	53,59,61,62	0
5	CL	D	508	1/1	0.83	0.18	72,72,72,72	0
9	TRS	D	509	8/8	0.83	0.23	48,50,52,53	0
5	CL	A	203	1/1	0.84	0.12	71,71,71,71	0
4	SO4	C	202	5/5	0.86	0.16	85,85,86,86	0
9	TRS	D	510	8/8	0.89	0.28	61,66,70,74	0
4	SO4	D	506	5/5	0.89	0.16	95,95,96,96	0
5	CL	B	509	1/1	0.90	0.11	64,64,64,64	0
5	CL	C	204	1/1	0.90	0.07	70,70,70,70	0
4	SO4	A	202	5/5	0.90	0.13	89,89,90,90	0
5	CL	B	508	1/1	0.91	0.14	69,69,69,69	0
4	SO4	D	505	5/5	0.91	0.28	55,57,57,58	5
4	SO4	B	505	5/5	0.95	0.12	39,42,45,51	0
5	CL	C	203	1/1	0.95	0.07	63,63,63,63	0
5	CL	D	507	1/1	0.96	0.05	50,50,50,50	0
4	SO4	D	504	5/5	0.97	0.10	56,58,59,60	0
5	CL	B	507	1/1	0.98	0.14	54,54,54,54	0
4	SO4	B	506	5/5	0.98	0.10	67,68,69,71	0
7	FMN	B	502	31/31	0.98	0.09	17,20,23,23	0
8	NA	B	503	1/1	0.98	0.09	34,34,34,34	0
4	SO4	B	504	5/5	0.98	0.09	37,38,40,43	0
8	NA	D	503	1/1	0.98	0.10	36,36,36,36	0
3	FES	A	201	4/4	0.99	0.09	17,19,21,23	0
7	FMN	D	502	31/31	0.99	0.08	17,20,22,23	0
3	FES	C	201	4/4	0.99	0.06	21,22,25,26	0
6	SF4	B	501	8/8	0.99	0.06	19,23,25,25	0
6	SF4	D	501	8/8	0.99	0.05	20,22,25,25	0

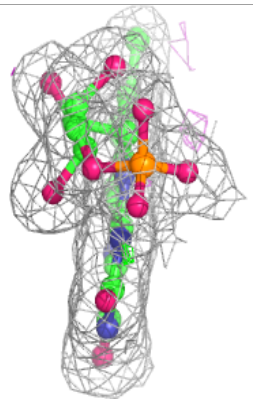
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN 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)

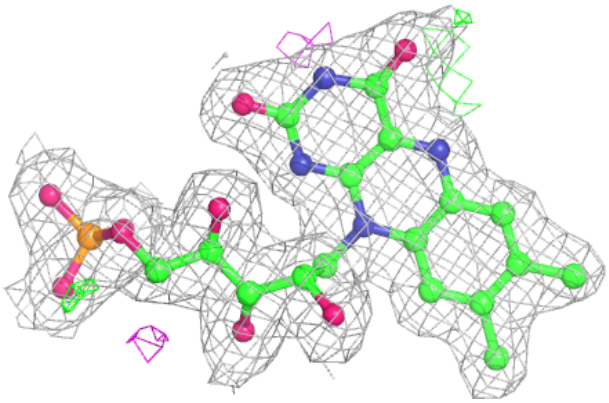


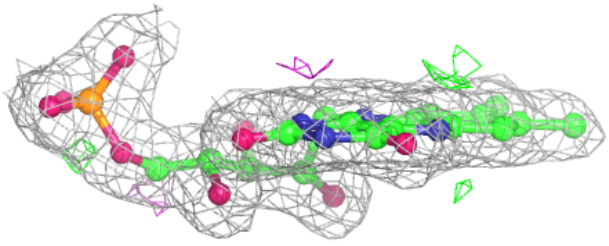


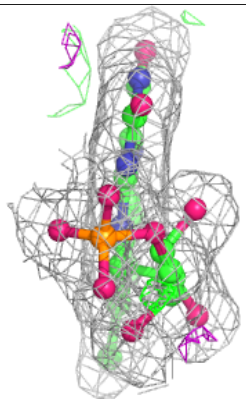


Electron density around FMN D 502:

$2mF_o$-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.