



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 6, 2026 – 02:40 PM EDT

PDB ID : 4OMF / pdb\_00004omf  
Title : The F420-reducing [NiFe]-hydrogenase complex from Methanothermobacter marburgensis, the first X-ray structure of a group 3 family member  
Authors : Vitt, S.; Ma, K.; Warkentin, E.; Moll, J.; Pierik, A.; Shima, S.; Ermler, U.  
Deposited on : 2014-01-27  
Resolution : 1.71 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

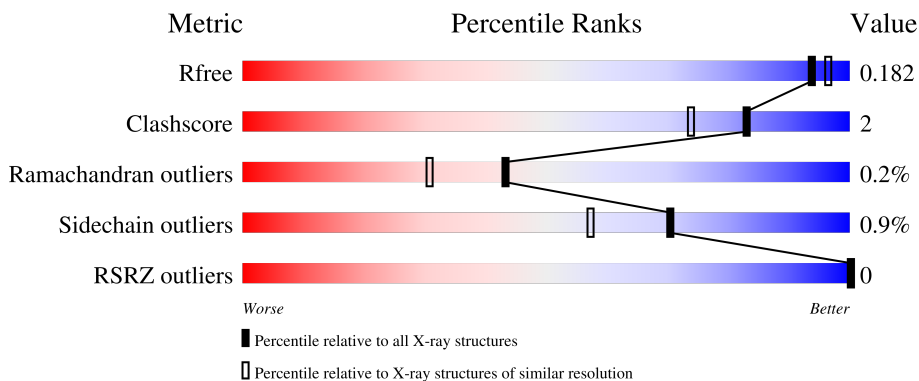
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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))
$R_{free}$	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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  $\geq 3$ , 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	G	275	 79% 5% 16%
2	A	405	 91% 5% 5%
3	B	281	 92% 8%

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
10	KEN	B	403	-	-	X	-
6	UNL	G	305	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7815 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 F420-reducing hydrogenase, subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	231	1784	1118	296	345	25	0	6	0

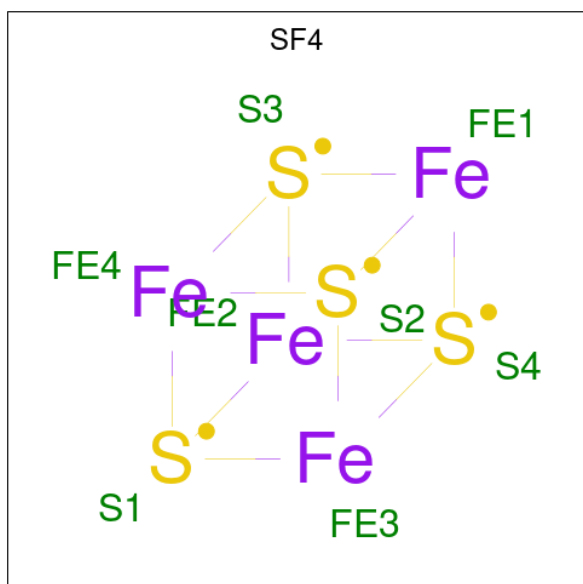
- Molecule 2 is a protein called F420-reducing hydrogenase, subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	385	2989	1880	532	560	17	0	1	0

- Molecule 3 is a protein called F420-reducing hydrogenase, subunit beta.

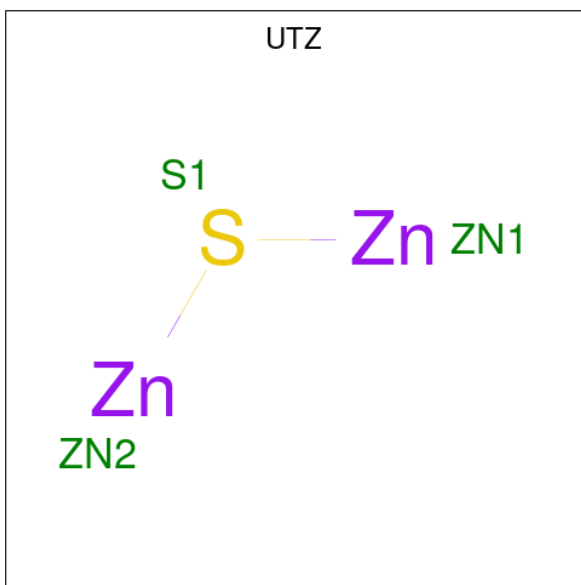
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	280	2167	1389	351	412	15	0	3	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 5 is zinciosulfanylzinc (CCD ID: UTZ) (formula:  $SZn_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	S	Zn	0	0
			3	1	2		

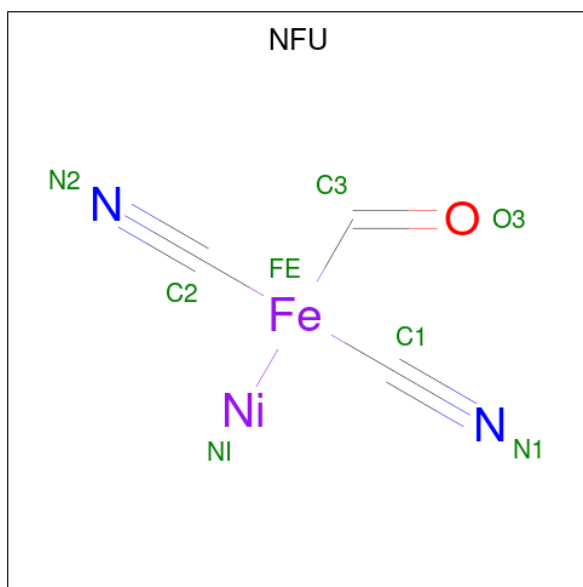
- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	S	0	0
			5	4	1		
6	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Mg 3 3	0	0
7	B	1	Total Mg 1 1	0	0

- Molecule 8 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C<sub>3</sub>HFeN<sub>2</sub>NiO).

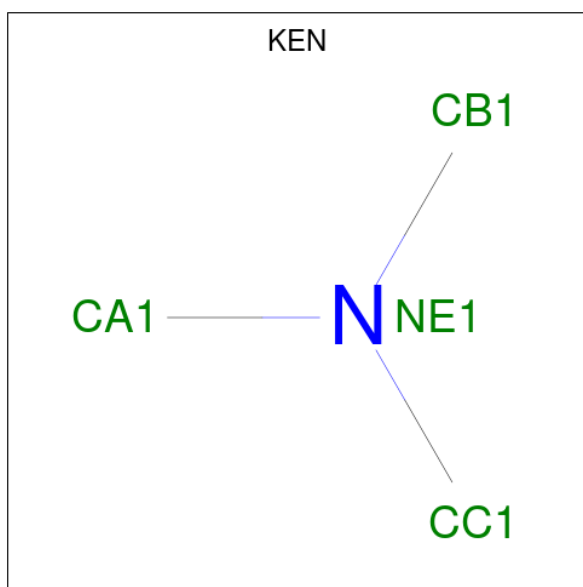


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C Fe N Ni O 8 3 1 2 1 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

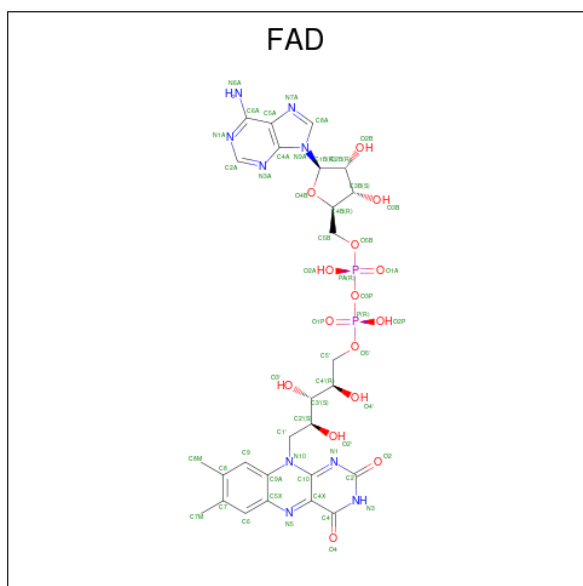
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0

- Molecule 10 is N,N-dimethylmethanamine (CCD ID: KEN) (formula: C<sub>3</sub>H<sub>9</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
10	B	1	4	3	1	0	0

- Molecule 11 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	B	1	53	27	9	15	2	0	0

- Molecule 12 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	G	198	Total 198	O 198	0	0
12	A	368	Total 368	O 368	0	0
12	B	195	Total 195	O 195	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	233.16Å 233.16Å 233.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.71 19.99 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.99-1.71) 99.8 (19.99-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.150 , 0.181 0.151 , 0.182	Depositor DCC
$R_{free}$ test set	5932 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.109 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: UNL, CL, FAD, KEN, UTZ, NFU, MG, SF4

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	G	0.62	0/1835	0.79	0/2488
2	A	0.65	1/3055 (0.0%)	0.85	0/4144
3	B	0.54	0/2212	0.74	0/2982
All	All	0.61	1/7102 (0.0%)	0.80	0/9614

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	68	ILE	CA-CB	6.95	1.58	1.54

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	G	1784	0	1760	13	0
2	A	2989	0	2981	8	0
3	B	2167	0	2215	13	1
4	B	8	0	0	0	0
4	G	24	0	0	0	0
5	G	3	0	0	0	0
6	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	5	0	0	5	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
8	A	8	0	0	0	0
9	A	1	0	0	0	0
10	B	4	0	9	4	0
11	B	53	0	28	0	0
12	A	368	0	0	4	2
12	B	195	0	0	3	1
12	G	198	0	0	0	0
All	All	7815	0	6993	34	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 2.

The worst 5 of 34 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)
3:B:110:ARG:HH22	10:B:403:KEN:HC1B	1.29	0.98
1:G:114[B]:HIS:NE2	6:G:305:UNL:S	2.39	0.95
1:G:111:HIS:ND1	6:G:305:UNL:S	2.42	0.92
1:G:114[B]:HIS:NE2	6:G:305:UNL:C1	2.35	0.90
3:B:204:ASP:OD2	10:B:403:KEN:HC1A	1.86	0.76

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:813:HOH:O	12:B:677:HOH:O[9_555]	2.06	0.14
3:B:174:ASP:OD2	12:A:878:HOH:O[5_555]	2.09	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	G	235/275 (86%)	228 (97%)	7 (3%)	0	100	100
2	A	384/405 (95%)	378 (98%)	5 (1%)	1 (0%)	36	24
3	B	281/281 (100%)	273 (97%)	7 (2%)	1 (0%)	30	16
All	All	900/961 (94%)	879 (98%)	19 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	215	ILE
3	B	153	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	G	201/232 (87%)	201 (100%)	0	100	100
2	A	322/341 (94%)	319 (99%)	3 (1%)	70	57
3	B	232/230 (101%)	228 (98%)	4 (2%)	53	31
All	All	755/803 (94%)	748 (99%)	7 (1%)	70	57

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	136	GLU
3	B	228	SER
3	B	248	LYS
3	B	245	GLU
2	A	368	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	16	HIS
3	B	105	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are unknown and 5 are monoatomic - leaving 8 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	SF4	B	401	-	0,12,12	-	-	-		
11	FAD	B	405	-	58,58,58	2.31	12 (20%)	85,89,89	1.75	20 (23%)
4	SF4	G	301	-	0,12,12	-	-	-		
4	SF4	G	302	-	0,12,12	-	-	-		
5	UTZ	G	304	-	0,2,2	-	-	-		
8	NFU	A	502	-	2,7,7	1.84	1 (50%)	-		
4	SF4	G	303	-	0,12,12	-	-	-		
10	KEN	B	403	-	3,3,3	1.91	1 (33%)	3,3,3	0.34	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	SF4	B	401	-	-	-	0/6/5/5
11	FAD	B	405	-	-	4/34/50/50	0/6/6/6
4	SF4	G	301	-	-	-	0/6/5/5
4	SF4	G	302	-	-	-	0/6/5/5
4	SF4	G	303	-	-	-	0/6/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	405	FAD	C2'-C3'	-10.36	1.35	1.53
11	B	405	FAD	C4X-N5	8.47	1.49	1.30
11	B	405	FAD	C5A-C4A	4.28	1.46	1.39
11	B	405	FAD	C5X-N5	4.28	1.47	1.39
11	B	405	FAD	O2'-C2'	-3.60	1.35	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	405	FAD	C5A-C4A-N3A	-4.61	120.37	126.72
11	B	405	FAD	N3A-C4A-N9A	4.22	134.35	127.17
11	B	405	FAD	C4A-N9A-C8A	4.13	110.08	105.74
11	B	405	FAD	O2'-C2'-C3'	3.53	117.52	109.25
11	B	405	FAD	C5X-N5-C4X	-3.49	112.44	118.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

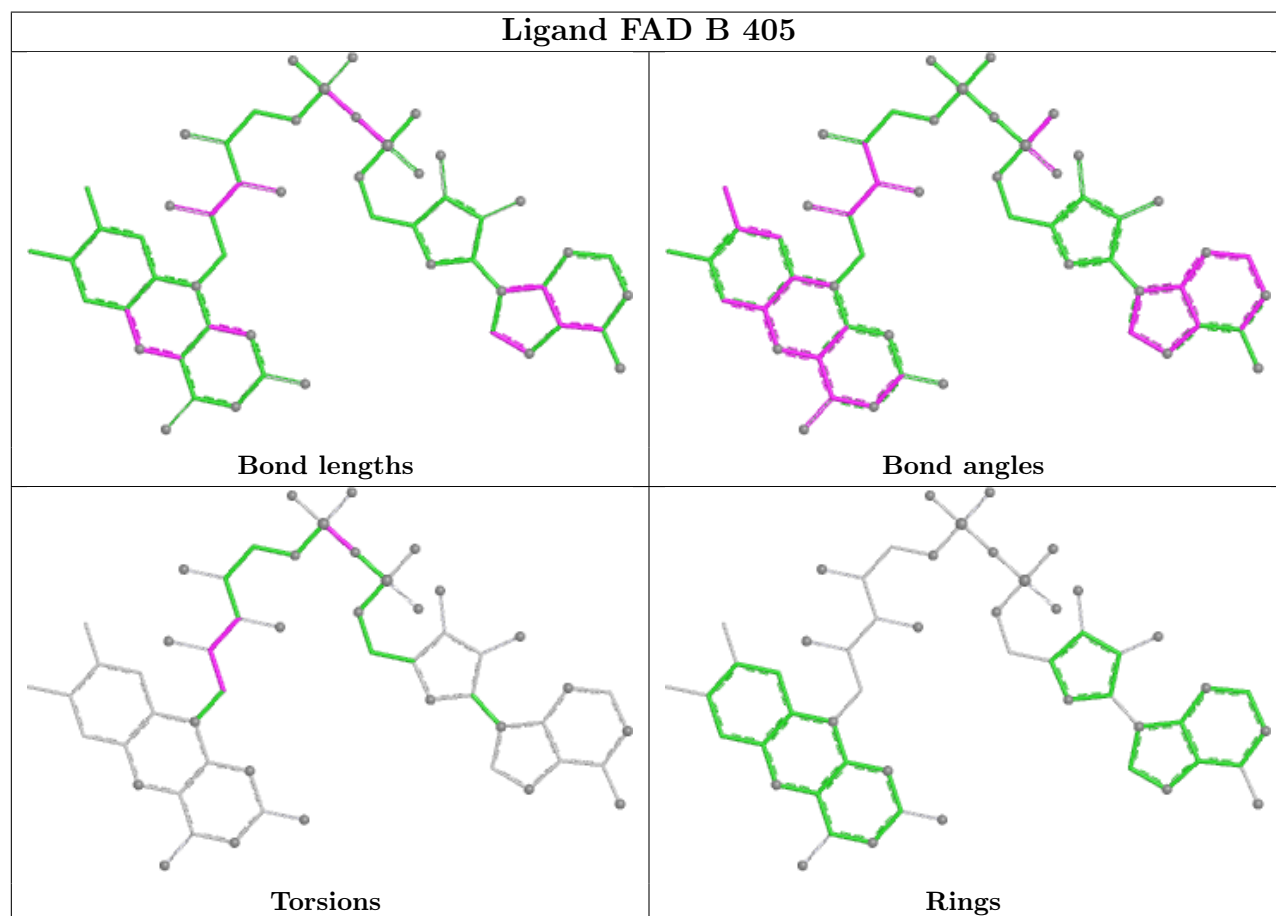
Mol	Chain	Res	Type	Atoms
11	B	405	FAD	N10-C1'-C2'-O2'
11	B	405	FAD	PA-O3P-P-O2P
11	B	405	FAD	O2'-C2'-C3'-C4'
11	B	405	FAD	PA-O3P-P-O1P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	403	KEN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	231/275 (84%)	-1.56	0 100 100	12, 19, 34, 56	6 (2%)
2	A	385/405 (95%)	-1.59	0 100 100	13, 17, 30, 43	1 (0%)
3	B	280/281 (99%)	-1.52	0 100 100	11, 24, 40, 57	3 (1%)
All	All	896/961 (93%)	-1.56	0 100 100	11, 20, 36, 57	10 (1%)

There are no RSRZ outliers to report.

### 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 oligosaccharides 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<sup>th</sup> 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.

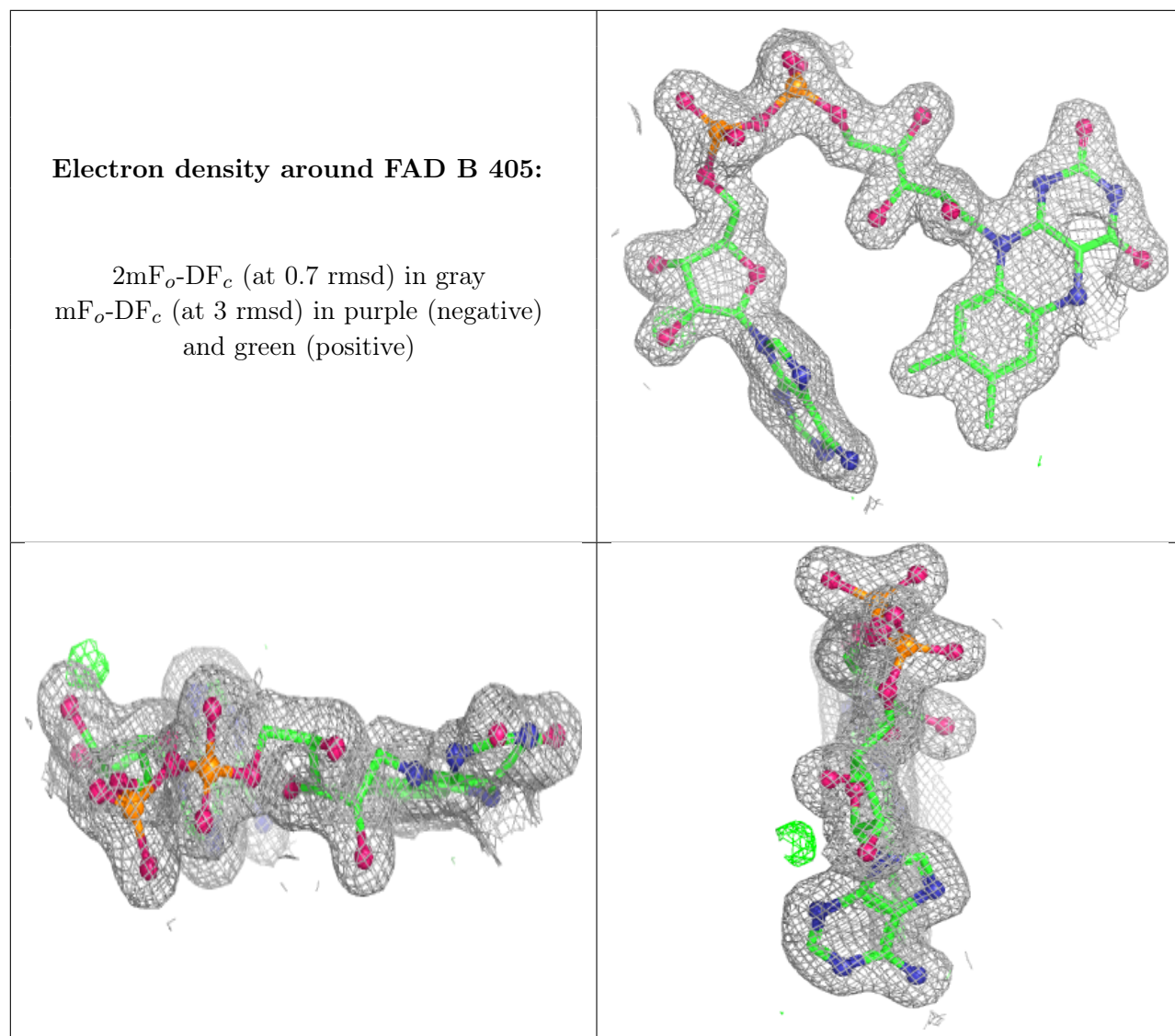
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	UNL	G	305	5/-	0.99	0.06	25,51,54,54	0
10	KEN	B	403	4/4	0.99	0.08	30,39,43,45	0
4	SF4	G	303	8/8	1.00	0.01	15,16,17,17	0
4	SF4	B	401	8/8	1.00	0.01	17,18,19,19	0
5	UTZ	G	304	3/3	1.00	0.05	53,53,54,60	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SF4	G	301	8/8	1.00	0.01	15,16,16,17	0
6	UNL	B	404	4/-	1.00	0.02	21,21,22,22	0
7	MG	A	501	1/1	1.00	0.04	20,20,20,20	0
7	MG	A	503	1/1	1.00	0.01	12,12,12,12	0
7	MG	A	504	1/1	1.00	0.03	36,36,36,36	0
7	MG	B	402	1/1	1.00	0.05	37,37,37,37	0
8	NFU	A	502	8/8	1.00	0.01	12,14,15,19	0
9	CL	A	505	1/1	1.00	0.01	20,20,20,20	0
4	SF4	G	302	8/8	1.00	0.01	13,15,16,16	0
11	FAD	B	405	53/53	1.00	0.01	17,20,24,29	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.