



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:27 am BST

PDB ID : 6QGR  
Title : The F420-reducing [NiFe] hydrogenase complex from *Methanosarcina barkeri* at the Nia-S state  
Authors : Ilina, Y.; Lorent, C.; Katz, S.; Jeoung, J.H.; Shima, S.; Horch, M.; Zebger, I.; Dobbek, H.  
Deposited on : 2019-01-12  
Resolution : 1.84 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](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 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

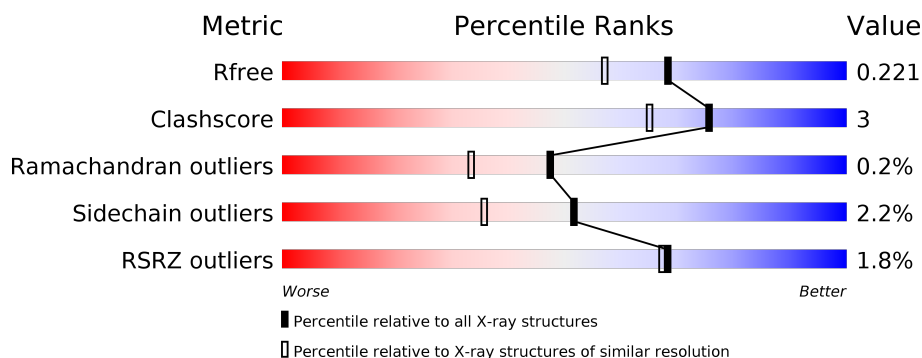
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	253	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	A	437	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
3	B	291	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

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
6	144	G	305	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 8521 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 Coenzyme F420 hydrogenase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	253	Total	C	N	O	S	0	1	0
			1927	1210	325	369	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	437	Total	C	N	O	S	0	4	0
			3430	2159	610	634	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	291	Total	C	N	O	S	0	4	0
			2295	1457	393	431	14			

There is a discrepancy between the modelled and reference sequences:

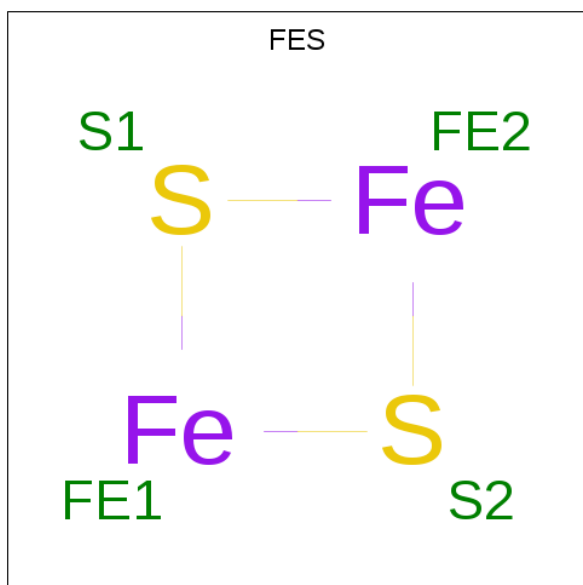
Chain	Residue	Modelled	Actual	Comment	Reference
B	265	GLN	GLU	conflict	UNP A0A0E3QWH3

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



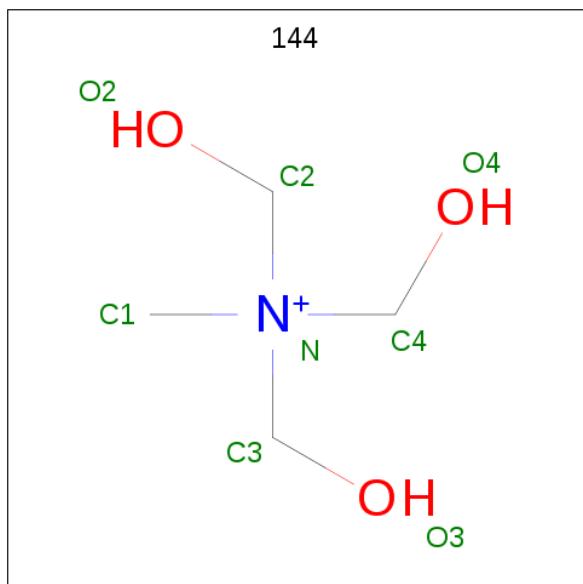
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



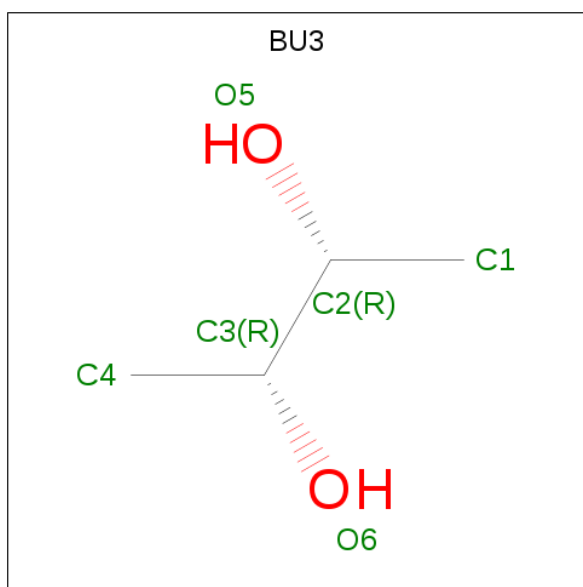
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	Fe	S	0	0
			3	1	2		

- Molecule 6 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula:  $C_4H_{12}NO_3$ ).



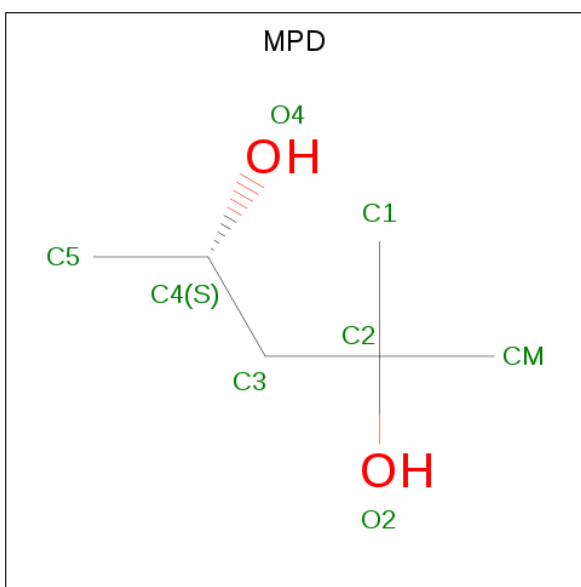
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula:  $C_4H_{10}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	A	1	Total	C	O	0	0
			6	4	2		
7	A	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			6	4	2		

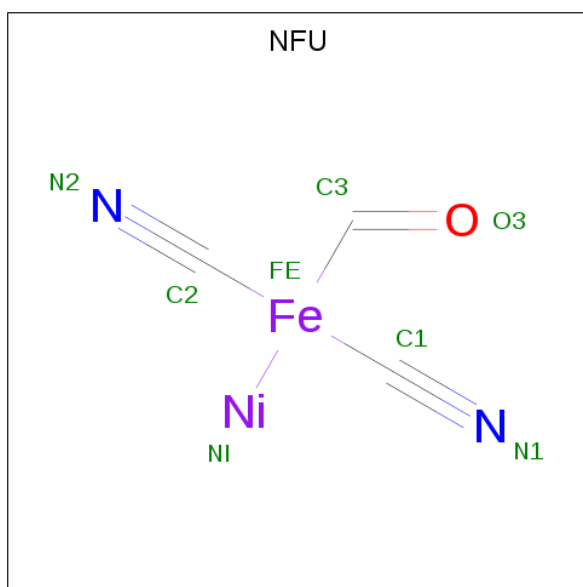
- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		
8	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (three-letter code: NFU) (formula: C<sub>3</sub>HFeN<sub>2</sub>NiO).





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

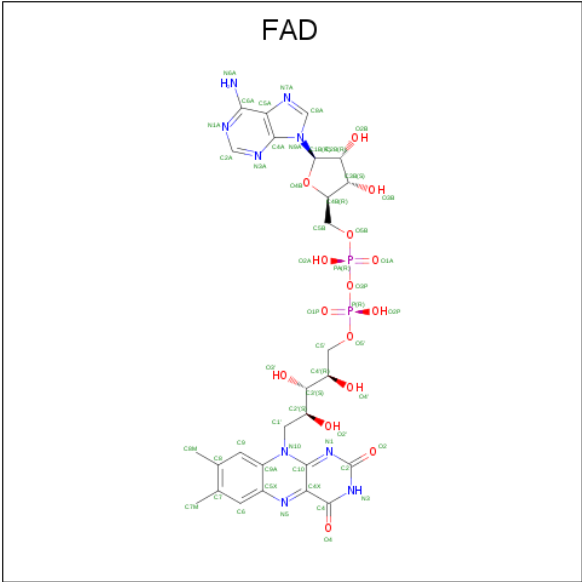
- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Mg	0	0
			1	1		

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

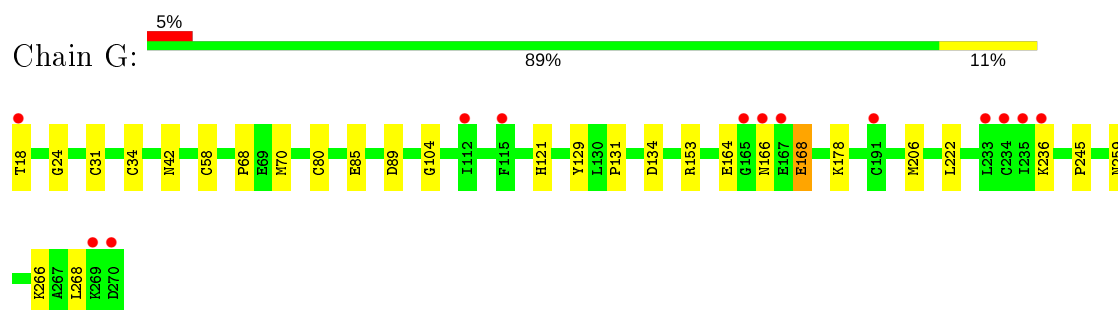
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	132	Total	O	0	5
			137	137		
13	A	339	Total	O	0	7
			346	346		
13	B	174	Total	O	0	4
			178	178		

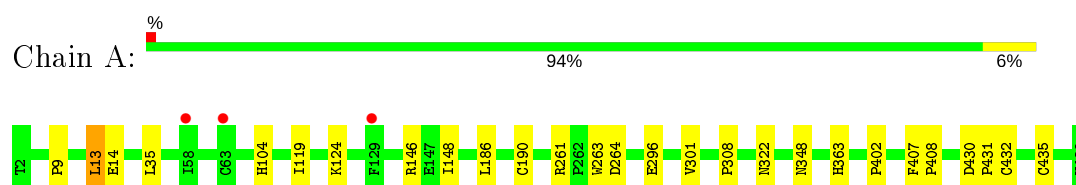
### 3 Residue-property plots [i](#)

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.

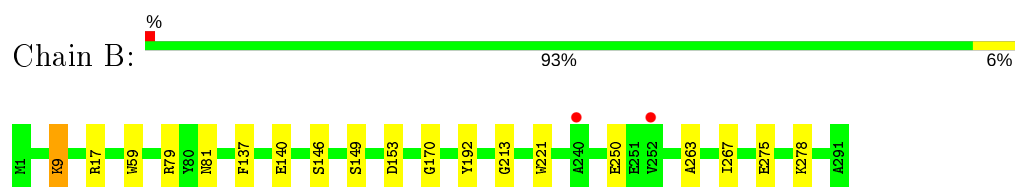
- Molecule 1: Coenzyme F420 hydrogenase subunit gamma



- Molecule 2: Coenzyme F420 hydrogenase subunit alpha



- Molecule 3: Coenzyme F420 hydrogenase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.83Å 235.83Å 235.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 1.84 48.14 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.14-1.84) 100.0 (48.14-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.175 , 0.221 0.175 , 0.221	Depositor DCC
$R_{free}$ test set	1073 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8521	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: MG, BU3, SF4, 144, NFU, FE, MPD, FAD, 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	G	0.70	0/1959	0.70	0/2647
2	A	0.74	2/3511 (0.1%)	0.70	0/4770
3	B	0.64	0/2342	0.67	0/3160
All	All	0.70	2/7812 (0.0%)	0.69	0/10577

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	435	CYS	CB-SG	-5.18	1.73	1.81
2	A	296	GLU	CB-CG	5.12	1.61	1.52

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	1927	0	1912	16	0
2	A	3430	0	3399	16	0
3	B	2295	0	2328	11	0
4	B	8	0	0	0	0
4	G	24	0	0	0	0
5	G	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	12	1	0
6	G	8	0	11	8	0
7	A	12	0	20	0	0
7	B	24	0	40	2	0
7	G	18	0	30	2	0
8	A	32	0	56	1	0
8	G	8	0	14	0	0
9	A	8	0	0	1	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
12	B	53	0	31	0	0
13	A	346	0	0	2	0
13	B	178	0	0	1	0
13	G	137	0	0	4	0
All	All	8521	0	7853	49	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 (49) 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)
6:G:305:144:C2	6:G:305:144:N	1.73	1.50
6:G:305:144:C2	6:G:305:144:C1	2.58	0.81
1:G:222:LEU:H	7:G:307:BU3:H13	1.51	0.75
6:G:305:144:C3	6:G:305:144:C2	2.67	0.72
1:G:89:ASP:OD1	6:G:305:144:H13	1.90	0.72
3:B:263:ALA:O	3:B:267:ILE:HG12	1.92	0.70
6:G:305:144:C4	6:G:305:144:C2	2.70	0.69
1:G:222:LEU:H	7:G:307:BU3:C1	2.10	0.65
3:B:17:ARG:HD3	3:B:221:TRP:CE2	2.34	0.62
2:A:148:ILE:HG23	2:A:186:LEU:HB3	1.82	0.62
2:A:348[B]:ASN:ND2	13:A:603:HOH:O	2.34	0.59
2:A:301:VAL:HG13	2:A:408:PRO:HG3	1.85	0.58
1:G:42:ASN:ND2	13:G:401:HOH:O	2.32	0.57
1:G:85:GLU:OE2	6:G:305:144:H12	2.05	0.56
3:B:250:GLU:H	3:B:250:GLU:CD	2.10	0.55
3:B:137:PHE:CD2	3:B:213:GLY:HA3	2.44	0.53
3:B:146:SER:HB3	3:B:192:TYR:HB3	1.91	0.53
1:G:178:LYS:HG2	13:G:466:HOH:O	2.09	0.52
1:G:80:CYS:HB2	1:G:129:TYR:CE2	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:GLU:HB3	2:A:432:CYS:HA	1.94	0.50
1:G:153:ARG:HD3	13:G:409:HOH:O	2.12	0.49
2:A:13:LEU:HD12	2:A:13:LEU:C	2.34	0.48
3:B:170:GLY:H	7:B:305:BU3:H42	1.79	0.48
1:G:166:ASN:OD1	1:G:168:GLU:HB3	2.15	0.46
1:G:266:LYS:HE2	1:G:266:LYS:HB3	1.71	0.46
2:A:430:ASP:N	2:A:431:PRO:HD3	2.31	0.45
2:A:363:HIS:HE1	13:A:893:HOH:O	1.99	0.45
2:A:13:LEU:CD1	2:A:13:LEU:C	2.85	0.45
2:A:148:ILE:HG21	2:A:190:CYS:HB2	1.99	0.45
2:A:13:LEU:O	2:A:13:LEU:HD12	2.17	0.44
8:A:506:MPD:H52	8:A:506:MPD:HM1	1.99	0.44
2:A:322:ASN:OD1	6:A:505:144:H11	2.17	0.44
1:G:34:CYS:SG	1:G:104:GLY:HA3	2.59	0.43
2:A:119:ILE:HD12	2:A:124:LYS:HD3	2.01	0.42
2:A:402:PRO:HG2	9:A:501:NFU:C2	2.49	0.42
3:B:9:LYS:HE2	3:B:9:LYS:HB2	1.73	0.42
1:G:131:PRO:HD2	1:G:134:ASP:OD2	2.19	0.42
1:G:24:GLY:HA3	1:G:70:MET:SD	2.58	0.42
2:A:146:ARG:CZ	2:A:146:ARG:HB3	2.48	0.42
3:B:149:SER:O	3:B:153:ASP:HB2	2.18	0.42
6:G:305:144:H11	13:G:523:HOH:O	2.18	0.42
3:B:59:TRP:CZ2	7:B:306:BU3:H3	2.55	0.42
1:G:18:THR:HB	1:G:164:GLU:OE1	2.20	0.41
3:B:17:ARG:HD3	3:B:221:TRP:CZ2	2.55	0.41
1:G:153:ARG:HD2	1:G:268:LEU:HD11	2.02	0.41
3:B:278:LYS:HG2	13:B:507:HOH:O	2.21	0.41
2:A:308:PRO:HB3	2:A:408:PRO:HG2	2.03	0.40
1:G:236:LYS:HB3	1:G:236:LYS:HE3	1.91	0.40
6:G:305:144:H41	2:A:9:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	252/253 (100%)	239 (95%)	12 (5%)	1 (0%)	34	20
2	A	438/437 (100%)	431 (98%)	6 (1%)	1 (0%)	47	33
3	B	293/291 (101%)	285 (97%)	8 (3%)	0	100	100
All	All	983/981 (100%)	955 (97%)	26 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	58	CYS
2	A	263	TRP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	216/215 (100%)	209 (97%)	7 (3%)	39	21
2	A	371/367 (101%)	365 (98%)	6 (2%)	62	49
3	B	250/246 (102%)	245 (98%)	5 (2%)	55	40
All	All	837/828 (101%)	819 (98%)	18 (2%)	52	36

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	31	CYS
1	G	68	PRO
1	G	121	HIS
1	G	168	GLU
1	G	206	MET
1	G	245	PRO
1	G	259	ASN
2	A	13	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	35	LEU
2	A	104	HIS
2	A	261	ARG
2	A	264	ASP
2	A	407	PHE
3	B	9	LYS
3	B	79	ARG
3	B	81	ASN
3	B	140	GLU
3	B	275	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z  > 2$
8	MPD	A	504	-	7,7,7	0.54	0	9,10,10	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	144	A	505	-	1,7,7	7.45	1 (100%)	3,9,9	0.08	0
7	BU3	B	301	-	4,5,5	0.90	0	6,6,6	0.54	0
7	BU3	G	309	-	4,5,5	0.95	0	6,6,6	0.34	0
4	SF4	G	303	1	0,12,12	0.00	-	-		
4	SF4	B	303	3	0,12,12	0.00	-	-		
7	BU3	B	306	-	4,5,5	0.75	0	6,6,6	0.65	0
6	144	G	305	-	1,7,7	0.88	0	3,9,9	0.13	0
7	BU3	B	304	-	4,5,5	0.60	0	6,6,6	0.74	0
8	MPD	A	506	-	7,7,7	0.57	0	9,10,10	0.76	0
5	FES	G	304	1	0,2,4	0.00	-	-		
7	BU3	G	307	-	4,5,5	0.80	0	6,6,6	0.59	0
7	BU3	A	508	-	4,5,5	0.69	0	6,6,6	0.39	0
8	MPD	G	308	-	7,7,7	0.33	0	9,10,10	0.80	0
8	MPD	A	507	-	7,7,7	0.37	0	9,10,10	0.40	0
8	MPD	A	509	-	7,7,7	0.52	0	9,10,10	0.76	0
12	FAD	B	302	-	51,58,58	4.14	24 (47%)	60,89,89	3.04	21 (35%)
7	BU3	A	510	-	4,5,5	0.78	0	6,6,6	0.44	0
9	NFU	A	501	2	2,7,7	1.77	1 (50%)	-		
7	BU3	B	305	-	4,5,5	0.74	0	6,6,6	0.70	0
4	SF4	G	301	1	0,12,12	0.00	-	-		
7	BU3	G	306	-	4,5,5	0.58	0	6,6,6	0.85	0
4	SF4	G	302	1	0,12,12	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
8	MPD	A	504	-	-	1/5/5/5	-
12	FAD	B	302	-	-	2/30/50/50	0/6/6/6
6	144	A	505	-	-	0/0/9/9	-
4	SF4	B	303	3	-	-	0/6/5/5
7	BU3	B	301	-	-	4/4/4/4	-
7	BU3	G	309	-	-	4/4/4/4	-
4	SF4	G	303	1	-	-	0/6/5/5
8	MPD	A	506	-	-	2/5/5/5	-
4	SF4	G	301	1	-	-	0/6/5/5
7	BU3	G	307	-	-	4/4/4/4	-
7	BU3	B	304	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BU3	A	510	-	-	4/4/4/4	-
6	144	G	305	-	-	0/0/9/9	-
8	MPD	G	308	-	-	0/5/5/5	-
8	MPD	A	507	-	-	2/5/5/5	-
7	BU3	B	306	-	-	4/4/4/4	-
8	MPD	A	509	-	-	2/5/5/5	-
7	BU3	A	508	-	-	4/4/4/4	-
7	BU3	G	306	-	-	0/4/4/4	-
4	SF4	G	302	1	-	-	0/6/5/5
7	BU3	B	305	-	-	0/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	302	FAD	O4B-C1B	12.45	1.58	1.41
12	B	302	FAD	C4X-N5	11.92	1.50	1.33
12	B	302	FAD	C10-N1	10.90	1.47	1.33
6	A	505	144	C1-N	-7.45	1.19	1.50
12	B	302	FAD	C2B-C1B	-7.26	1.42	1.53
12	B	302	FAD	C4A-N3A	7.15	1.45	1.35
12	B	302	FAD	C5X-N5	5.89	1.45	1.35
12	B	302	FAD	C2-N1	5.53	1.49	1.38
12	B	302	FAD	C9A-N10	5.45	1.45	1.38
12	B	302	FAD	C8A-N7A	4.98	1.43	1.34
12	B	302	FAD	C1'-N10	4.85	1.53	1.48
12	B	302	FAD	C4-N3	4.64	1.41	1.33
12	B	302	FAD	C4-C4X	4.58	1.49	1.41
12	B	302	FAD	C6-C7	4.22	1.48	1.37
12	B	302	FAD	C2-N3	4.22	1.46	1.38
12	B	302	FAD	C7M-C7	4.10	1.59	1.51
12	B	302	FAD	C4X-C10	3.95	1.42	1.38
12	B	302	FAD	O4B-C4B	-3.94	1.36	1.45
12	B	302	FAD	C2A-N1A	3.41	1.40	1.33
12	B	302	FAD	C9-C9A	3.11	1.46	1.40
12	B	302	FAD	C2A-N3A	3.04	1.37	1.32
12	B	302	FAD	C6A-N6A	2.76	1.44	1.34
12	B	302	FAD	C8-C7	2.49	1.47	1.40
12	B	302	FAD	O2'-C2'	2.46	1.48	1.43
9	A	501	NFU	C1-N1	2.33	1.18	1.13
12	B	302	FAD	O4-C4	-2.06	1.19	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	302	FAD	C1'-N10-C9A	9.82	126.02	118.29
12	B	302	FAD	C4-N3-C2	9.49	123.15	115.14
12	B	302	FAD	C7M-C7-C8	7.16	135.42	120.74
12	B	302	FAD	C7M-C7-C6	-6.76	104.18	120.34
12	B	302	FAD	C5A-C6A-N6A	6.66	130.48	120.35
12	B	302	FAD	C5X-C9A-N10	5.84	121.95	117.72
12	B	302	FAD	N3A-C2A-N1A	-5.82	119.59	128.68
12	B	302	FAD	N6A-C6A-N1A	-5.50	107.16	118.57
12	B	302	FAD	C9A-N10-C10	-4.06	116.59	121.91
12	B	302	FAD	C3B-C2B-C1B	3.62	106.43	100.98
12	B	302	FAD	O4B-C1B-C2B	-3.03	102.50	106.93
12	B	302	FAD	O2P-P-O5'	2.95	121.44	107.75
12	B	302	FAD	C7-C6-C5X	-2.93	117.07	121.22
12	B	302	FAD	C8M-C8-C7	-2.84	114.92	120.74
12	B	302	FAD	C4X-N5-C5X	-2.52	114.25	116.77
12	B	302	FAD	C4'-C3'-C2'	-2.35	108.48	113.36
12	B	302	FAD	C4X-C4-N3	-2.33	120.24	123.43
12	B	302	FAD	O4B-C4B-C3B	2.33	109.72	105.11
12	B	302	FAD	C6-C5X-N5	-2.24	116.58	119.05
12	B	302	FAD	C4-C4X-C10	-2.07	118.58	119.95
12	B	302	FAD	C10-C4X-N5	2.06	122.68	121.26

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	504	MPD	C2-C3-C4-C5
7	B	301	BU3	O5-C2-C3-O6
7	B	301	BU3	C1-C2-C3-O6
7	B	301	BU3	O5-C2-C3-C4
7	B	301	BU3	C1-C2-C3-C4
7	G	309	BU3	O5-C2-C3-O6
7	G	309	BU3	C1-C2-C3-O6
7	B	306	BU3	O5-C2-C3-O6
7	B	306	BU3	C1-C2-C3-C4
7	B	304	BU3	O5-C2-C3-O6
7	B	304	BU3	C1-C2-C3-C4
8	A	506	MPD	C2-C3-C4-O4
8	A	506	MPD	C2-C3-C4-C5
7	G	307	BU3	O5-C2-C3-O6
7	G	307	BU3	C1-C2-C3-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	G	307	BU3	O5-C2-C3-C4
7	G	307	BU3	C1-C2-C3-C4
7	A	508	BU3	O5-C2-C3-O6
7	A	508	BU3	C1-C2-C3-C4
8	A	507	MPD	C2-C3-C4-O4
7	A	510	BU3	O5-C2-C3-O6
7	G	309	BU3	O5-C2-C3-C4
7	B	306	BU3	C1-C2-C3-O6
7	B	306	BU3	O5-C2-C3-C4
7	B	304	BU3	C1-C2-C3-O6
7	B	304	BU3	O5-C2-C3-C4
7	A	508	BU3	C1-C2-C3-O6
7	A	508	BU3	O5-C2-C3-C4
7	A	510	BU3	C1-C2-C3-O6
7	A	510	BU3	O5-C2-C3-C4
12	B	302	FAD	PA-O3P-P-O2P
8	A	509	MPD	C2-C3-C4-C5
7	G	309	BU3	C1-C2-C3-C4
7	A	510	BU3	C1-C2-C3-C4
12	B	302	FAD	O4B-C4B-C5B-O5B
8	A	507	MPD	O2-C2-C3-C4
8	A	509	MPD	C2-C3-C4-O4

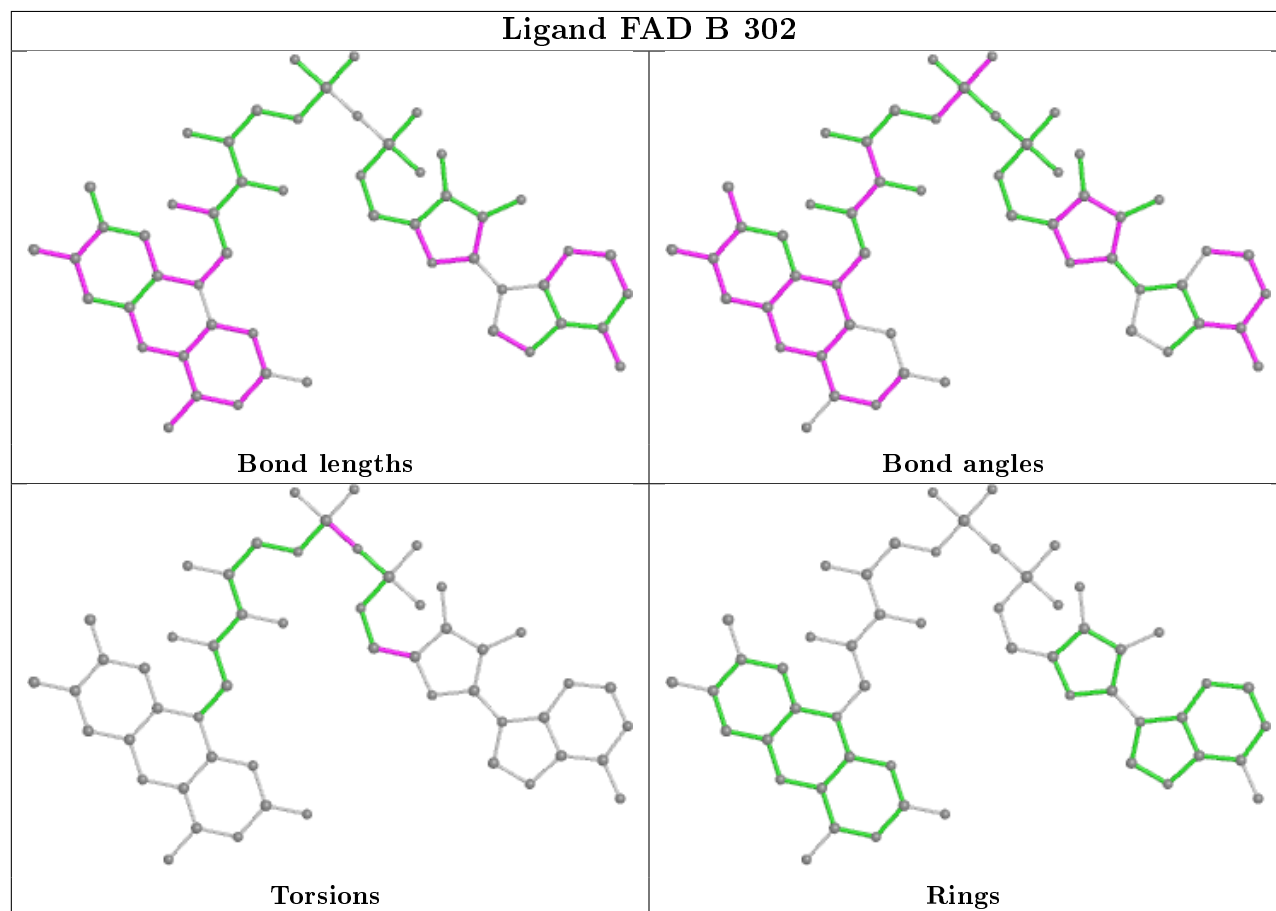
There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	505	144	1	0
7	B	306	BU3	1	0
6	G	305	144	8	0
8	A	506	MPD	1	0
7	G	307	BU3	2	0
9	A	501	NFU	1	0
7	B	305	BU3	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 [i](#)

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<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	253/253 (100%)	0.20	13 (5%) 28 25	30, 38, 58, 97	2 (0%)
2	A	437/437 (100%)	-0.23	3 (0%) 87 87	26, 34, 48, 65	4 (0%)
3	B	291/291 (100%)	-0.25	2 (0%) 87 87	32, 42, 60, 78	4 (1%)
All	All	981/981 (100%)	-0.12	18 (1%) 68 67	26, 37, 56, 97	10 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	18	THR	4.4
1	G	270	ASP	3.6
1	G	166	ASN	3.2
1	G	235	ILE	3.2
1	G	167	GLU	3.0
2	A	129	PHE	3.0
1	G	269	LYS	2.6
1	G	234	CYS	2.6
1	G	112	ILE	2.5
2	A	58	ILE	2.4
1	G	165	GLY	2.2
1	G	236	LYS	2.2
3	B	252	VAL	2.2
1	G	115	PHE	2.1
3	B	240	ALA	2.1
2	A	63	CYS	2.1
1	G	233	LEU	2.1
1	G	191	CYS	2.0

### 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 ⓘ

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.

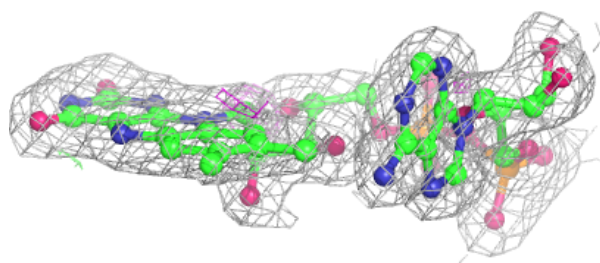
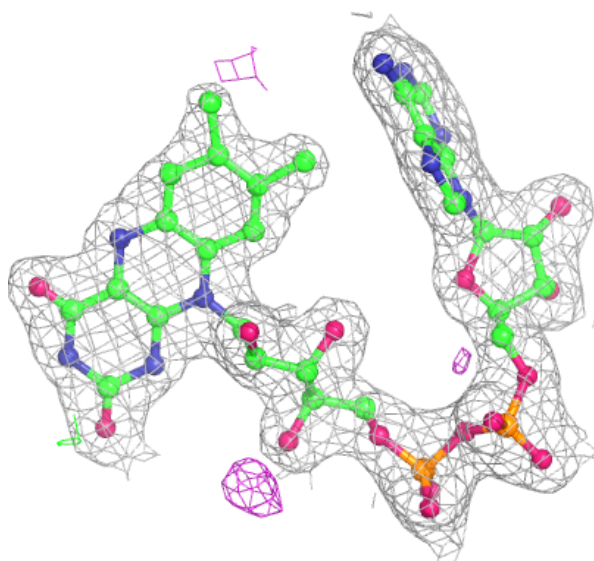
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MPD	A	507	8/8	0.70	0.34	49,66,73,74	8
7	BU3	G	307	6/6	0.75	0.25	37,56,62,67	0
8	MPD	A	506	8/8	0.78	0.35	45,58,62,63	8
7	BU3	B	305	6/6	0.79	0.21	53,58,66,70	0
8	MPD	A	509	8/8	0.81	0.24	53,60,63,64	0
7	BU3	A	508	6/6	0.81	0.41	54,64,67,81	0
7	BU3	G	309	6/6	0.85	0.18	44,57,60,61	0
7	BU3	G	306	6/6	0.85	0.19	47,54,58,64	0
7	BU3	B	306	6/6	0.86	0.16	52,65,69,69	0
8	MPD	A	504	8/8	0.86	0.17	45,59,65,68	0
6	144	A	505	8/8	0.90	0.39	38,38,39,41	8
7	BU3	B	304	6/6	0.91	0.10	47,59,62,67	0
8	MPD	G	308	8/8	0.93	0.18	45,53,56,57	8
7	BU3	A	510	6/6	0.94	0.29	53,56,60,68	6
7	BU3	B	301	6/6	0.95	0.08	50,54,61,71	6
6	144	G	305	8/8	0.96	0.07	34,42,49,50	0
12	FAD	B	302	53/53	0.98	0.08	30,37,42,44	0
11	MG	A	503	1/1	0.98	0.13	34,34,34,34	1
4	SF4	B	303	8/8	0.99	0.04	37,38,40,40	0
4	SF4	G	303	8/8	0.99	0.06	34,35,36,39	0
4	SF4	G	301	8/8	0.99	0.09	32,34,35,36	0
5	FES	G	304	3/4	0.99	0.12	35,35,36,37	2
4	SF4	G	302	8/8	0.99	0.09	32,33,34,34	0
10	FE	A	502	1/1	1.00	0.07	33,33,33,33	0
9	NFU	A	501	8/8	1.00	0.11	28,32,34,37	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 FAD B 302:**

$2mF_o-DF_c$  (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.