



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:27 am BST

PDB ID : 3P4P
Title : Crystal structure of Menaquinol:fumarate oxidoreductase in complex with fumarate
Authors : Tomasiak, T.M.; Archuleta, T.L.; Andr ll, J.; Luna-Ch vez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on : 2010-10-06
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

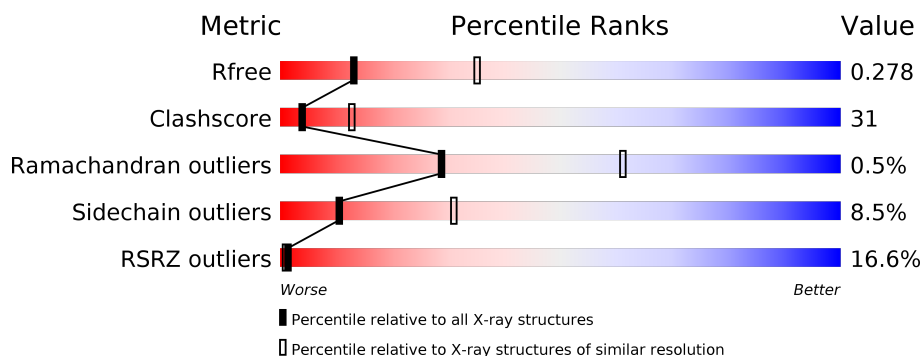
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	577	<div> <div>66%</div> <div>31%</div> <div>.</div> </div>
1	M	577	<div> <div>50%</div> <div>47%</div> <div>47%</div> <div>5%</div> </div>
2	B	243	<div> <div>2%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
2	N	243	<div> <div>20%</div> <div>44%</div> <div>47%</div> <div>9%</div> </div>
3	C	130	<div> <div>58%</div> <div>38%</div> <div>5%</div> </div>
3	O	130	<div> <div>4%</div> <div>58%</div> <div>38%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	119	
4	P	119	

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
5	FAD	M	601	-	-	X	-
7	FES	B	244	-	-	X	-
8	F3S	B	245	-	-	X	-
9	SF4	B	246	-	-	X	-
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16873 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			
1	M	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

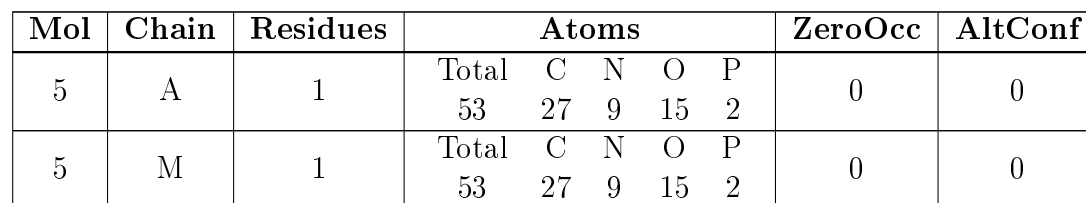
- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



- FUM
-
- The chemical structure of Fumaric acid (FUM) is shown. It consists of a central carbon-carbon double bond (C4=C5). Each carbon is part of a carboxylic acid group. Carbon C2 is double-bonded to an oxygen atom (O3) and single-bonded to a hydroxyl group (O1-H). Carbon C6 is double-bonded to an oxygen atom (O7) and single-bonded to a hydroxyl group (O8-H). The atoms are labeled with green text: O1, O3, C2, C4, C5, C6, O7, and O8. The hydroxyl groups are shown in red.

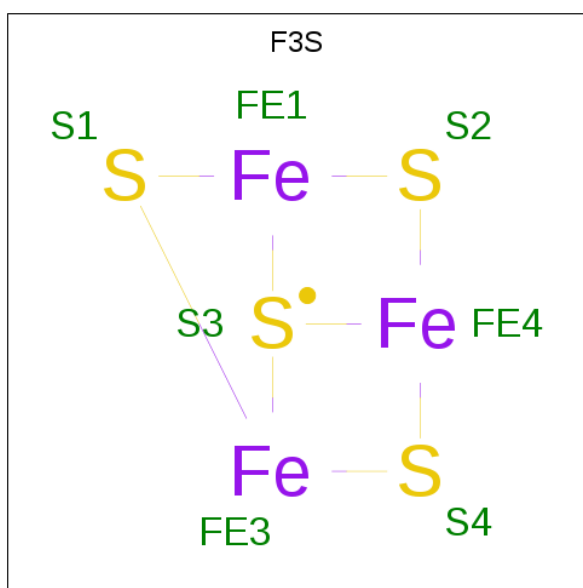
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	4	4		

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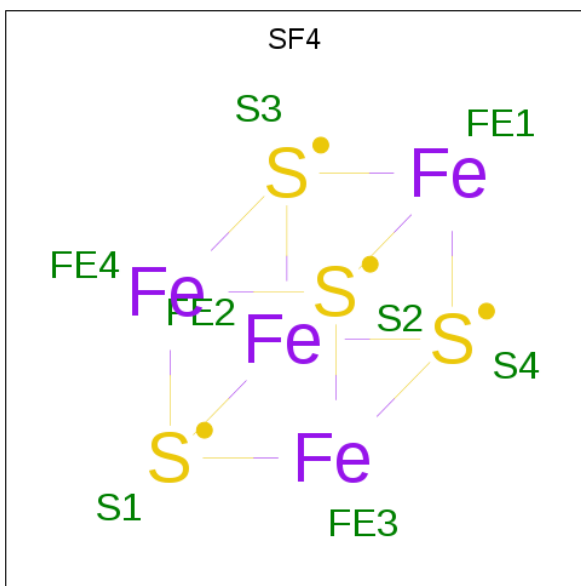
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

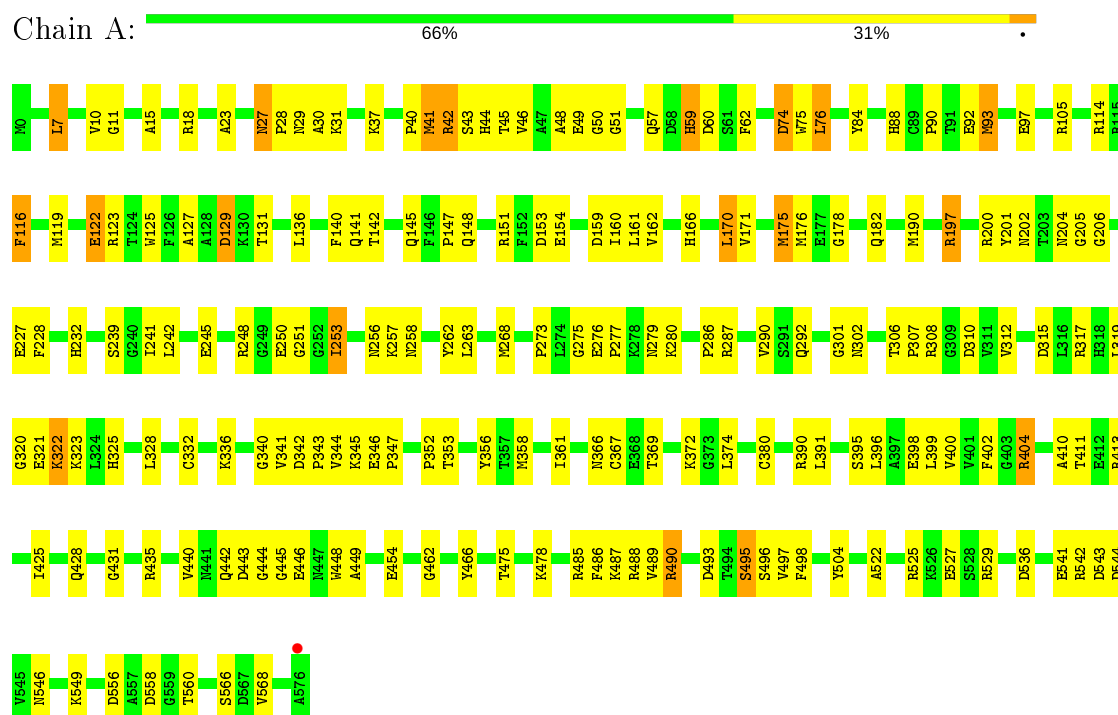
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	60	Total	O	0	0
			60	60		
10	B	10	Total	O	0	0
			10	10		
10	C	2	Total	O	0	0
			2	2		
10	D	4	Total	O	0	0
			4	4		
10	M	1	Total	O	0	0
			1	1		
10	N	2	Total	O	0	0
			2	2		

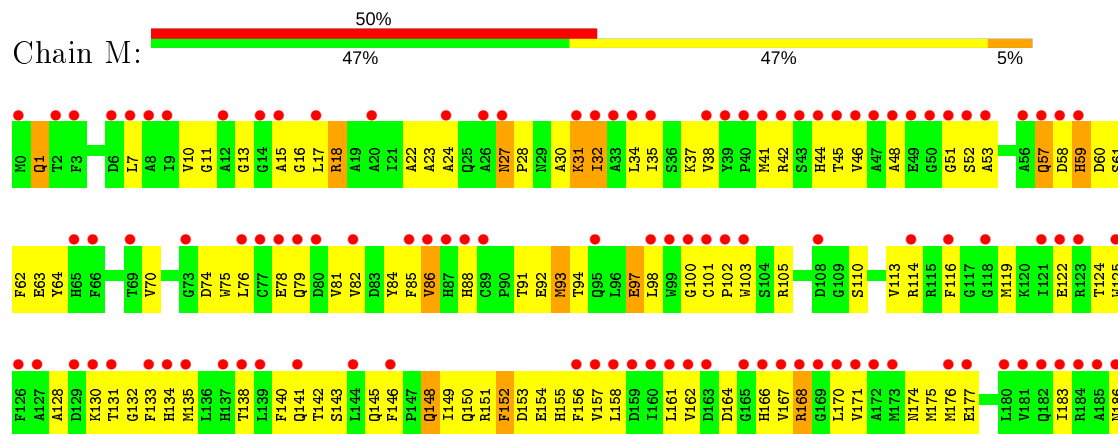
3 Residue-property plots

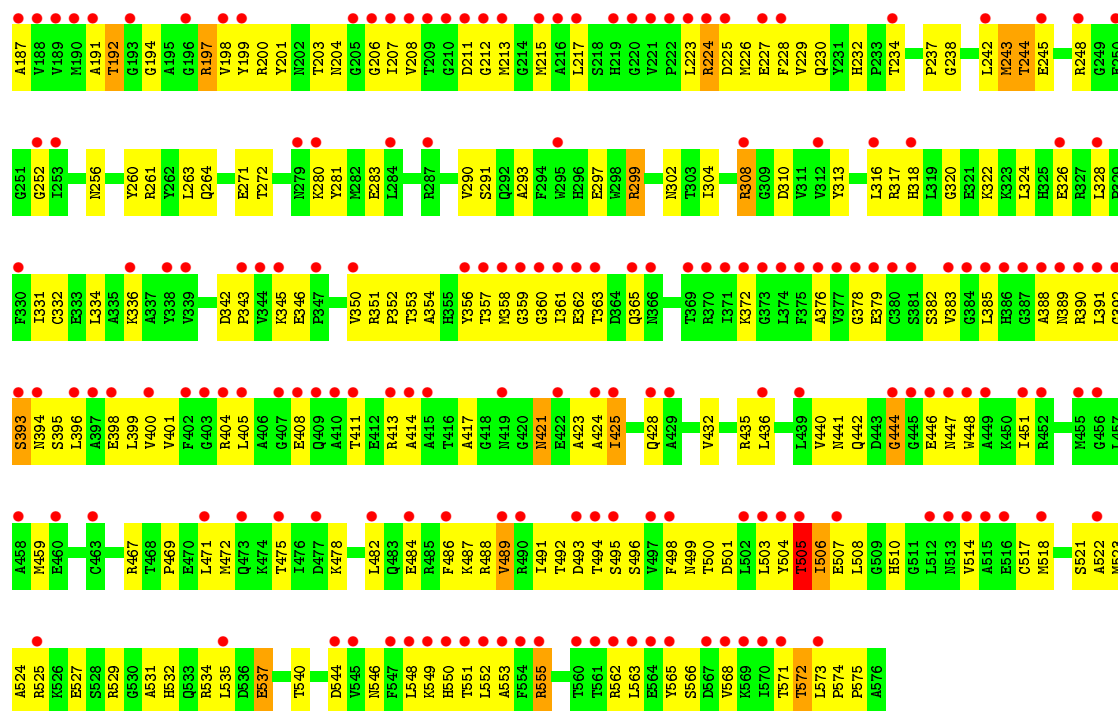
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Fumarate reductase flavoprotein subunit

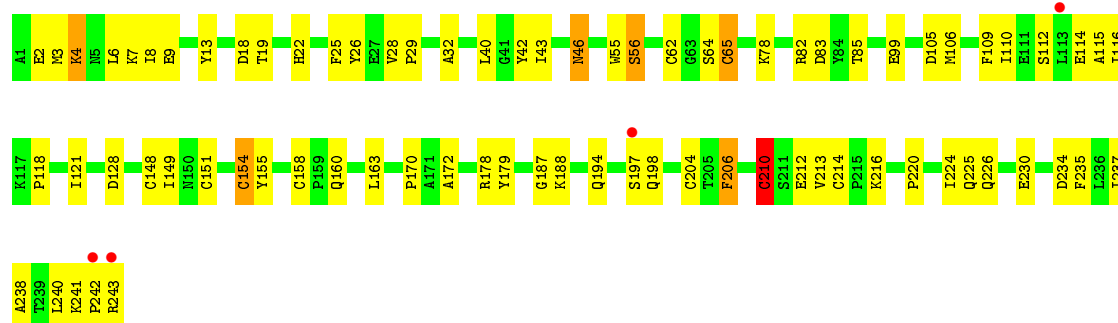


- Molecule 1: Fumarate reductase flavoprotein subunit

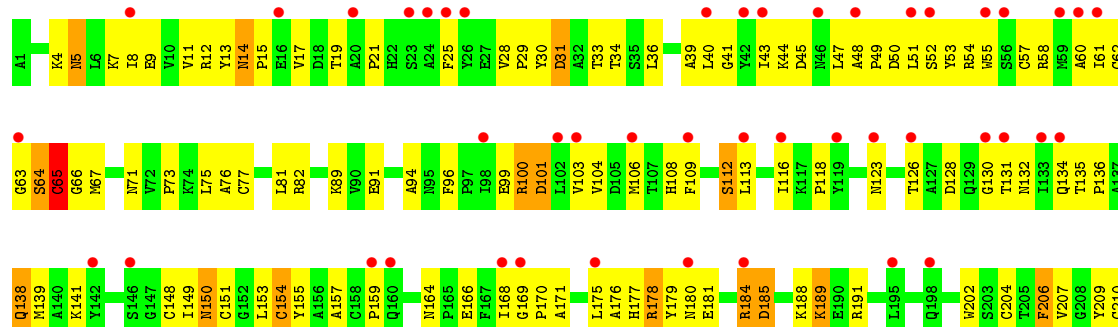
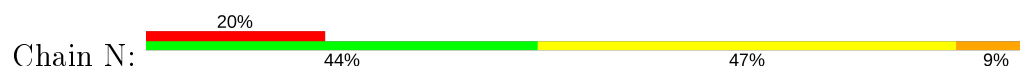




• Molecule 2: Fumarate reductase iron-sulfur protein



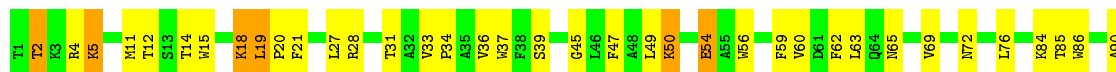
• Molecule 2: Fumarate reductase iron-sulfur protein





• Molecule 3: Fumarate reductase subunit C

Chain C: 58% 38% 5%



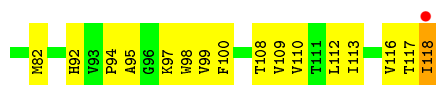
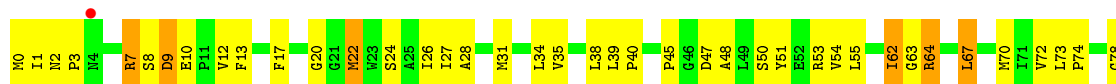
• Molecule 3: Fumarate reductase subunit C

Chain O: 4% 58% 38% 0%



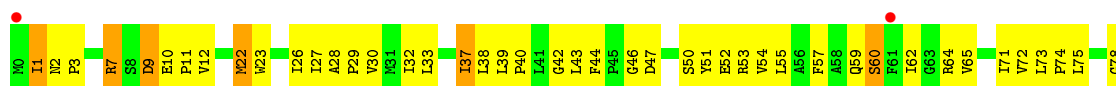
• Molecule 4: Fumarate reductase subunit D

Chain D: 2% 53% 41% 6%



• Molecule 4: Fumarate reductase subunit D

Chain P: 3% 49% 45% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 137.63Å 270.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.80 90.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.80) 94.9 (90.74-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.272 0.258 , 0.278	Depositor DCC
R_{free} test set	1408 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16873	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, FUM, FES, FAD

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	0.77	0/4541	0.83	3/6139 (0.0%)
1	M	0.53	1/4541 (0.0%)	0.64	2/6139 (0.0%)
2	B	0.76	1/1931 (0.1%)	0.84	3/2617 (0.1%)
2	N	0.58	3/1931 (0.2%)	0.73	3/2617 (0.1%)
3	C	0.60	0/1094	0.70	2/1496 (0.1%)
3	O	0.57	0/1094	0.65	0/1496
4	D	0.60	0/956	0.72	0/1303
4	P	0.55	0/956	0.68	0/1303
All	All	0.65	5/17044 (0.0%)	0.74	13/23110 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	CYS	C-N	10.72	1.58	1.34
2	N	77	CYS	C-N	8.04	1.52	1.34
2	N	65	CYS	CB-SG	7.05	1.94	1.82
1	M	505	THR	C-N	6.89	1.49	1.34
2	N	77	CYS	CB-SG	5.33	1.91	1.82

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	CYS	O-C-N	10.16	138.96	122.70
2	B	210	CYS	CA-C-N	-8.65	98.16	117.20
2	N	65	CYS	N-CA-CB	-7.65	96.83	110.60
2	B	210	CYS	C-N-CA	-7.21	103.66	121.70
3	C	28	ARG	NE-CZ-NH1	6.72	123.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	64	SER	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4449	0	4335	169	0
1	M	4449	0	4335	401	0
2	B	1888	0	1844	91	0
2	N	1888	0	1839	199	0
3	C	1058	0	1108	63	0
3	O	1058	0	1108	74	0
4	D	926	0	971	79	0
4	P	926	0	970	68	0
5	A	53	0	30	14	0
5	M	53	0	30	25	0
6	A	8	0	2	1	0
7	B	4	0	0	3	0
7	N	4	0	0	1	0
8	B	7	0	0	4	0
8	N	7	0	0	1	0
9	B	8	0	0	12	0
9	N	8	0	0	6	0
10	A	60	0	0	2	0
10	B	10	0	0	0	0
10	C	2	0	0	0	0
10	D	4	0	0	0	0
10	M	1	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	2	0	0	0	0
All	All	16873	0	16572	1016	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 31.

The worst 5 of 1016 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:A:44:HIS:NE2	5:A:601:FAD:C8M	1.77	1.45
1:A:44:HIS:CE1	5:A:601:FAD:HM82	1.53	1.44
1:M:44:HIS:NE2	5:M:601:FAD:HM82	1.41	1.34
2:N:31:ASP:OD2	2:N:33:THR:N	1.57	1.33
1:M:168:ARG:HD2	10:M:577:HOH:O	1.19	1.27

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	575/577 (100%)	551 (96%)	23 (4%)	1 (0%)	47	78
1	M	575/577 (100%)	546 (95%)	24 (4%)	5 (1%)	17	46
2	B	241/243 (99%)	225 (93%)	15 (6%)	1 (0%)	34	66
2	N	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	19	49
3	C	128/130 (98%)	124 (97%)	3 (2%)	1 (1%)	19	49
3	O	128/130 (98%)	118 (92%)	10 (8%)	0	100	100
4	D	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
4	P	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	46
All	All	2122/2138 (99%)	2008 (95%)	103 (5%)	11 (0%)	29	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	65	CYS
1	M	1	GLN
1	M	244	THR
4	P	46	GLY
1	M	128	ALA

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	A	460/460 (100%)	430 (94%)	30 (6%)	17	44
1	M	460/460 (100%)	417 (91%)	43 (9%)	9	26
2	B	205/205 (100%)	193 (94%)	12 (6%)	19	49
2	N	205/205 (100%)	180 (88%)	25 (12%)	5	15
3	C	111/111 (100%)	99 (89%)	12 (11%)	6	19
3	O	111/111 (100%)	104 (94%)	7 (6%)	18	46
4	D	97/97 (100%)	87 (90%)	10 (10%)	7	21
4	P	97/97 (100%)	88 (91%)	9 (9%)	9	26
All	All	1746/1746 (100%)	1598 (92%)	148 (8%)	10	31

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	31	LYS
1	M	224	ARG
3	O	40	ILE
1	M	41	MET
1	M	143	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	92	HIS
1	M	134	HIS
2	N	132	ASN
1	M	27	ASN
1	M	59	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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	F3S	B	245	2	0,9,9	0.00	-	-		
9	SF4	N	246	2	0,12,12	0.00	-	-		
7	FES	B	244	2	0,4,4	0.00	-	-		
5	FAD	M	601	-	51,58,58	2.08	9 (17%)	60,89,89	1.96	14 (23%)
8	F3S	N	245	2	0,9,9	0.00	-	-		
6	FUM	A	577	-	1,7,7	4.15	1 (100%)	2,8,8	3.82	1 (50%)
7	FES	N	244	2	0,4,4	0.00	-	-		
5	FAD	A	601	-	51,58,58	2.19	8 (15%)	60,89,89	2.07	17 (28%)
9	SF4	B	246	-	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	F3S	B	245	2	-	-	0/3/3/3
9	SF4	N	246	2	-	-	0/6/5/5
7	FES	B	244	2	-	-	0/1/1/1
5	FAD	M	601	-	-	7/30/50/50	0/6/6/6
8	F3S	N	245	2	-	-	0/3/3/3
6	FUM	A	577	-	-	0/0/5/5	-
7	FES	N	244	2	-	-	0/1/1/1
5	FAD	A	601	-	-	9/30/50/50	0/6/6/6
9	SF4	B	246	-	-	-	0/6/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	O2B-C2B	-10.06	1.19	1.43
5	M	601	FAD	O2B-C2B	-9.28	1.21	1.43
5	A	601	FAD	C2B-C1B	6.44	1.63	1.53
5	M	601	FAD	C2B-C1B	5.33	1.61	1.53
5	A	601	FAD	C9A-N10	4.76	1.45	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C4X-N5-C5X	7.09	123.85	116.77
5	M	601	FAD	C4-N3-C2	5.82	120.06	115.14
5	M	601	FAD	C4X-N5-C5X	5.82	122.58	116.77
5	A	601	FAD	C4-N3-C2	5.43	119.72	115.14
6	A	577	FUM	C6-C5-C4	-5.30	112.36	123.69

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

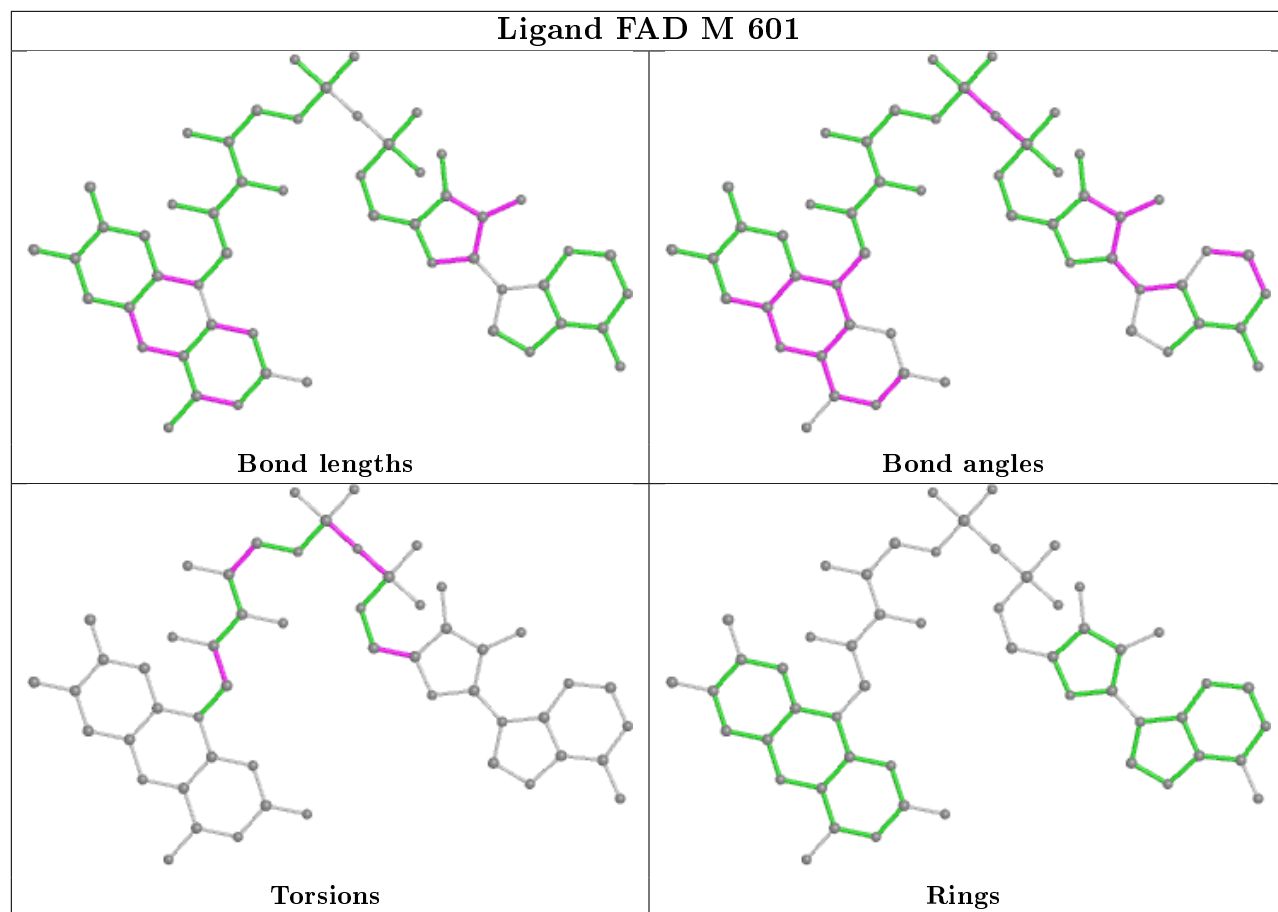
Mol	Chain	Res	Type	Atoms
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	P-O3P-PA-O1A
5	M	601	FAD	PA-O3P-P-O5'

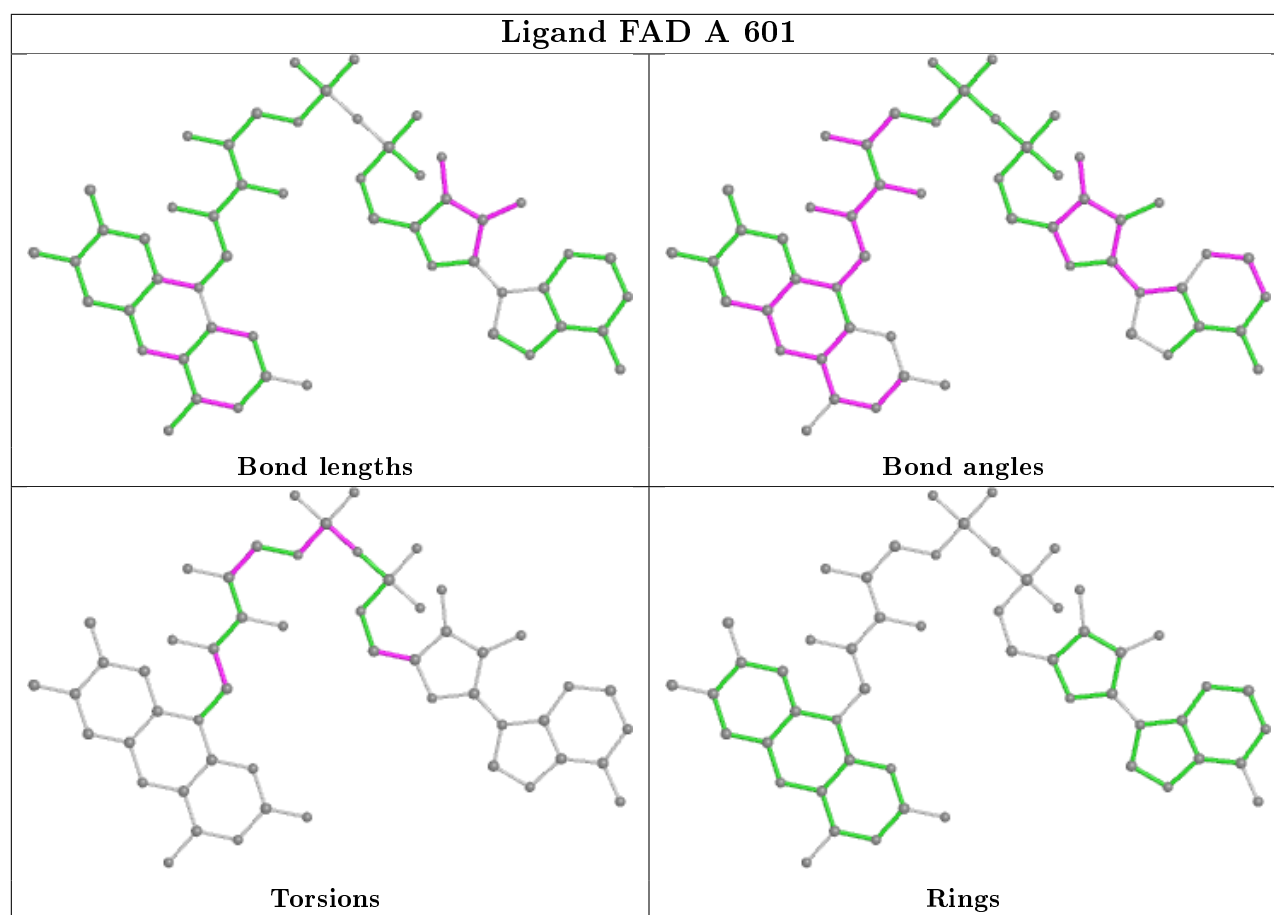
There are no ring outliers.

9 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	245	F3S	4	0
9	N	246	SF4	6	0
7	B	244	FES	3	0
5	M	601	FAD	25	0
8	N	245	F3S	1	0
6	A	577	FUM	1	0
7	N	244	FES	1	0
5	A	601	FAD	14	0
9	B	246	SF4	12	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, 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	577/577 (100%)	0.47	1 (0%) 95 94	38, 56, 93, 138	0
1	M	577/577 (100%)	2.35	290 (50%) 0 0	68, 160, 235, 266	0
2	B	243/243 (100%)	0.71	4 (1%) 72 66	39, 71, 104, 151	0
2	N	243/243 (100%)	1.35	49 (20%) 1 0	64, 131, 202, 235	0
3	C	130/130 (100%)	0.22	0 100 100	51, 74, 110, 136	0
3	O	130/130 (100%)	0.44	5 (3%) 40 30	60, 93, 154, 215	0
4	D	119/119 (100%)	0.34	2 (1%) 70 63	55, 76, 107, 144	0
4	P	119/119 (100%)	0.46	3 (2%) 57 47	64, 86, 144, 224	0
All	All	2138/2138 (100%)	1.08	354 (16%) 1 1	38, 88, 208, 266	0

The worst 5 of 354 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	407	GLY	15.2
1	M	219	HIS	10.7
1	M	167	VAL	10.3
1	M	386	HIS	10.2
1	M	411	THR	10.2

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 ⓘ

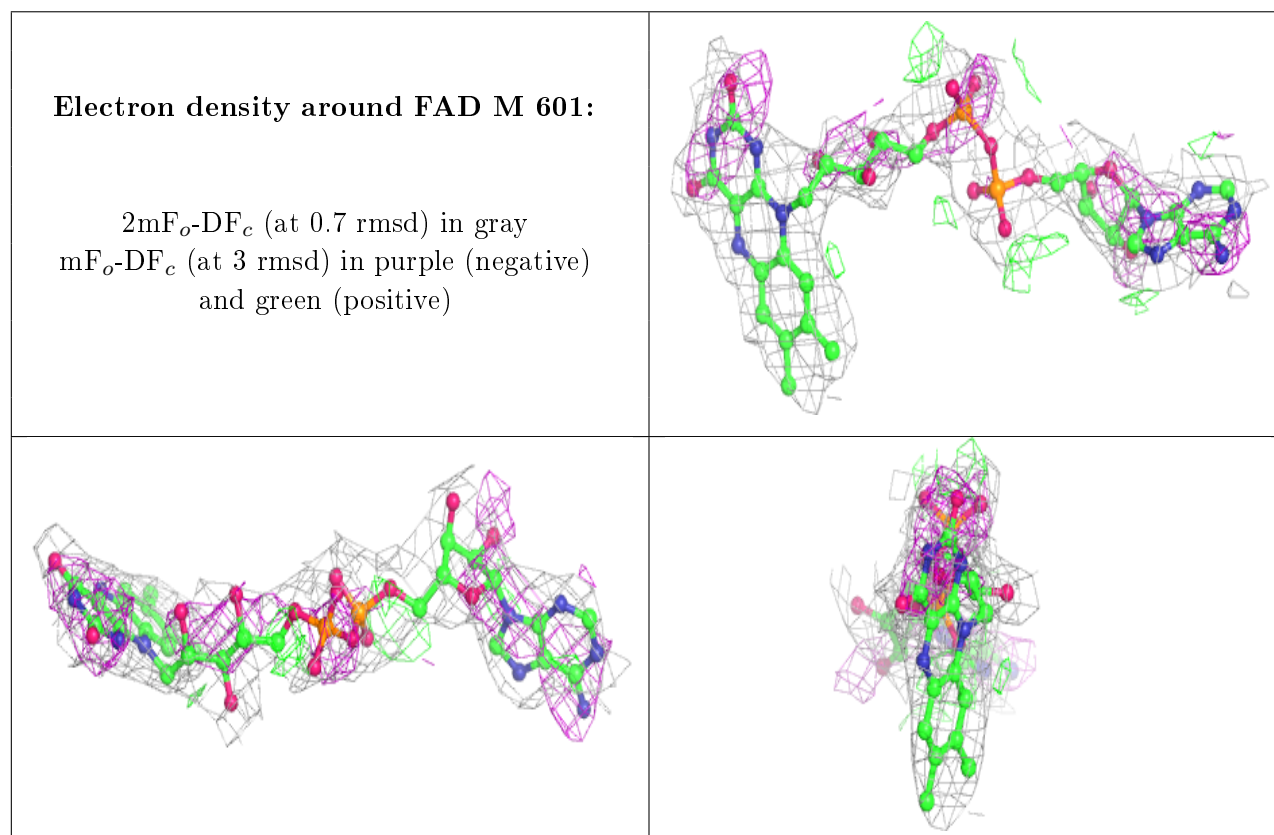
There are no carbohydrates in this entry.

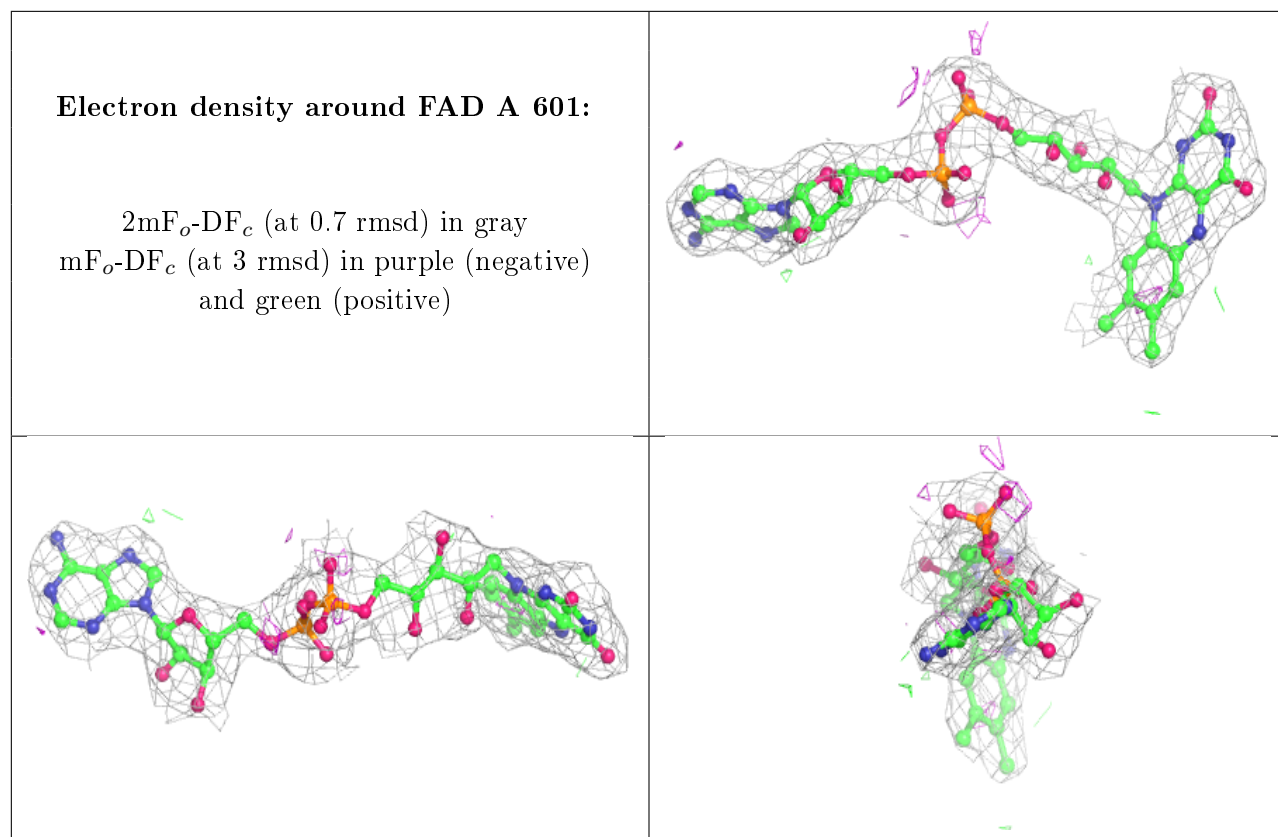
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FAD	M	601	53/53	0.87	0.29	49,74,85,86	0
6	FUM	A	577	8/8	0.89	0.38	66,67,70,103	0
9	SF4	B	246	8/8	0.92	0.27	86,104,134,134	0
7	FES	B	244	4/4	0.94	0.31	98,107,110,114	0
7	FES	N	244	4/4	0.96	0.22	76,90,94,104	0
8	F3S	N	245	7/7	0.96	0.20	86,90,101,134	0
9	SF4	N	246	8/8	0.97	0.19	103,112,131,134	0
5	FAD	A	601	53/53	0.98	0.25	34,41,78,78	0
8	F3S	B	245	7/7	0.98	0.20	60,64,70,93	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.