



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2017 – 03:21 PM EST

PDB ID : 5MRL
Title : Crystal structure of human monoamine oxidase B (MAO B) in complex with N(Furan2ylmethyl)Nmethylprop2yn1amine (F2MPA)
Authors : Binda, C.; De Deurwaerdere, P.; Corne, R.; Leone, C.; Valeri, A.; Valoti, M.; Ramsay, R.R.; Fall, Y.; Marco-Contelles, J.
Deposited on : 2016-12-23
Resolution : 2.42 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	F2M	A	601	-	-	-	X
3	F2M	B	601	-	-	-	X

2 Entry composition [i](#)

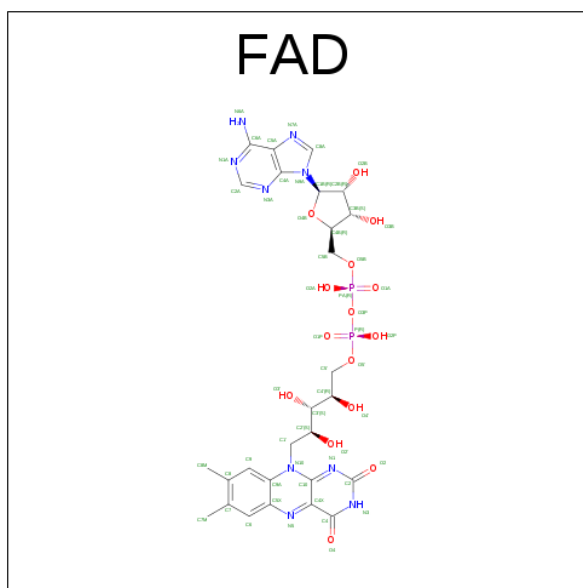
There are 4 unique types of molecules in this entry. The entry contains 8310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amine oxidase [flavin-containing] B.

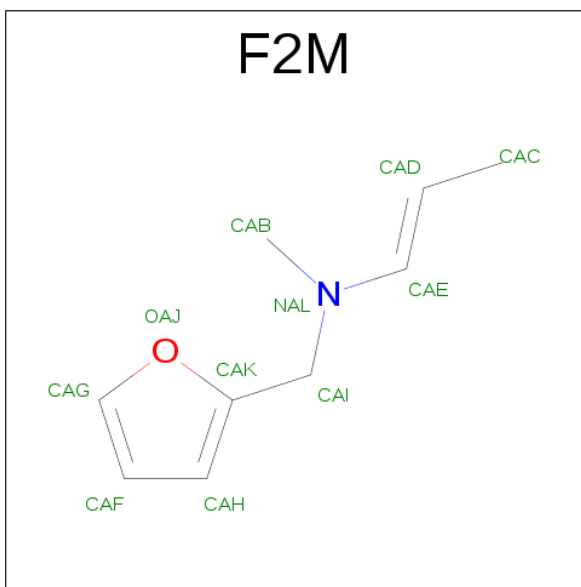
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3974	2541	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ({E})- {N}-(furan-2-ylmethyl)- {N}-methyl-prop-1-en-1-amine (three-letter code: F2M) (formula: $C_9H_{13}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	9	1	1		
3	B	1	Total	C	N	O	0	0
			11	9	1	1		

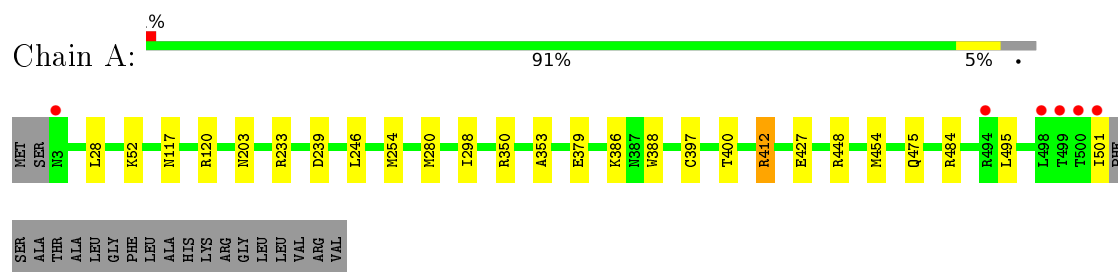
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	158	Total	O	0	0
			158	158		

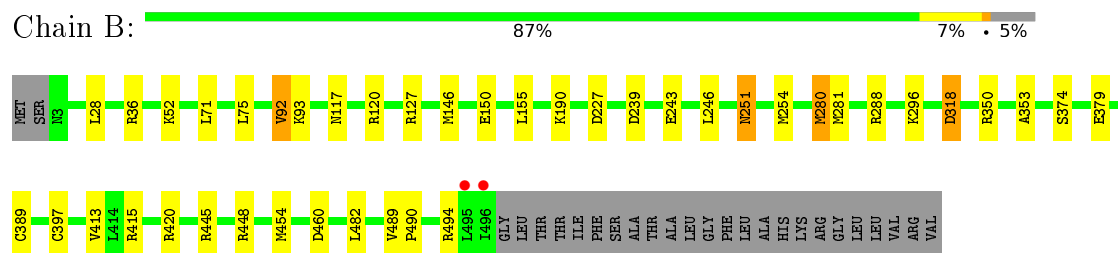
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Amine oxidase [flavin-containing] B



- Molecule 1: Amine oxidase [flavin-containing] B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.85Å 223.24Å 86.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.00 – 2.42 43.12 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.0 (113.00-2.42) 98.0 (43.12-2.42)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.168 , 0.234 0.175 , 0.241	Depositor DCC
R_{free} test set	1251 reflections (2.67%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8310	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: FAD, F2M

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	0/4071	0.87	5/5526 (0.1%)
1	B	0.82	1/4037 (0.0%)	0.92	13/5479 (0.2%)
All	All	0.79	1/8108 (0.0%)	0.89	18/11005 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	GLU	CD-OE2	5.33	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ASP	CB-CG-OD1	7.98	125.48	118.30
1	B	318	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	233	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	288	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	233	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	445	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	448	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	146	MET	CB-CA-C	-5.75	98.91	110.40
1	B	318	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	36	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	239	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	280	MET	CG-SD-CE	-5.40	91.56	100.20
1	B	415	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	412	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	227	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	415	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	448	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	127	ARG	NE-CZ-NH1	5.18	122.89	120.30

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	3974	0	3976	15	0
1	B	3940	0	3937	17	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
3	A	11	0	0	0	0
3	B	11	0	0	0	0
4	A	110	0	0	2	0
4	B	158	0	0	3	1
All	All	8310	0	7971	27	1

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.

All (27) 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:B:494:ARG:NH2	4:B:701:HOH:O	2.01	0.92
1:A:280:MET:HE1	1:B:353:ALA:HB1	1.70	0.73
1:A:353:ALA:HB1	1:B:280:MET:HE1	1.75	0.67
1:A:353:ALA:CB	1:B:280:MET:HE1	2.24	0.67
1:A:280:MET:HE1	1:B:353:ALA:CB	2.28	0.62
1:A:386:LYS:HD3	1:A:388:TRP:CE2	2.43	0.53
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.91	0.52
1:B:246:LEU:HB3	1:B:254:MET:HE1	1.91	0.52
1:A:280:MET:HG3	1:B:389:CYS:HB2	1.92	0.50
1:A:203:ASN:ND2	1:A:475:GLN:HB2	2.26	0.50
1:A:246:LEU:HB3	1:A:254:MET:HE1	1.92	0.50
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.60	0.49
1:B:92:VAL:HB	1:B:318:ASP:OD2	2.12	0.49
1:B:281:MET:HB3	1:B:413:VAL:HG11	1.96	0.47
1:A:386:LYS:HE3	4:A:750:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD11	1:B:454:MET:HE1	2.01	0.42
1:A:400:THR:HB	1:A:427:GLU:HG2	2.02	0.42
1:B:246:LEU:HD22	1:B:254:MET:HE2	2.02	0.42
1:B:71:LEU:O	1:B:75:LEU:HG	2.20	0.41
1:A:484:ARG:NH1	4:A:708:HOH:O	2.53	0.41
1:B:489:VAL:N	1:B:490:PRO:HD2	2.35	0.41
1:A:239:ASP:HB3	1:A:246:LEU:HB2	2.01	0.41
1:B:243:GLU:O	1:B:420:ARG:NH1	2.54	0.41
1:A:298:ILE:N	1:A:298:ILE:HD12	2.36	0.41
1:B:448:ARG:HD3	4:B:708:HOH:O	2.19	0.41
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.68	0.40
1:B:296:LYS:NZ	4:B:709:HOH:O	2.55	0.40

All (1) 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)
4:B:802:HOH:O	4:B:802:HOH:O[4_565]	0.56	1.64

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	497/520 (96%)	476 (96%)	20 (4%)	1 (0%)	52	69
1	B	492/520 (95%)	477 (97%)	13 (3%)	2 (0%)	39	54
All	All	989/1040 (95%)	953 (96%)	33 (3%)	3 (0%)	46	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ASN

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Mol	Chain	Res	Type
1	A	52	LYS
1	B	52	LYS

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	428/444 (96%)	422 (99%)	6 (1%)	74	88
1	B	424/444 (96%)	414 (98%)	10 (2%)	57	76
All	All	852/888 (96%)	836 (98%)	16 (2%)	65	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	ARG
1	A	379	GLU
1	A	397	CYS
1	A	412	ARG
1	A	495	LEU
1	A	501	ILE
1	B	92	VAL
1	B	93	LYS
1	B	155	LEU
1	B	190	LYS
1	B	251	ASN
1	B	350	ARG
1	B	374	SER
1	B	379	GLU
1	B	397	CYS
1	B	482	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	170	ASN
1	A	251	ASN
1	B	117	ASN
1	B	251	ASN
1	B	464	GLN

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 ⓘ

4 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	$\# Z > 2$
2	FAD	A	600	1,3	52,58,58	0.83	1 (1%)	52,89,89	2.03	12 (23%)
3	F2M	A	601	2	9,11,11	4.15	6 (66%)	8,13,13	2.72	4 (50%)
2	FAD	B	600	1,3	52,58,58	1.08	4 (7%)	52,89,89	2.37	13 (25%)
3	F2M	B	601	2	9,11,11	4.96	5 (55%)	8,13,13	1.57	1 (12%)

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
2	FAD	A	600	1,3	-	0/30/50/50	0/6/6/6
3	F2M	A	601	2	-	0/6/7/7	0/0/1/1
2	FAD	B	600	1,3	-	0/30/50/50	0/6/6/6
3	F2M	B	601	2	-	0/6/7/7	0/0/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	F2M	CAB-NAL	-12.72	1.29	1.46
3	A	601	F2M	CAB-NAL	-9.48	1.34	1.46
2	B	600	FAD	C10-N10	-3.87	1.34	1.39
3	B	601	F2M	CAH-CAK	-3.86	1.32	1.39
3	A	601	F2M	CAC-CAD	-3.74	1.36	1.49
3	A	601	F2M	CAF-CAG	-3.17	1.33	1.39
3	B	601	F2M	CAF-CAG	-2.95	1.33	1.39
2	A	600	FAD	C10-N10	-2.89	1.35	1.39
3	A	601	F2M	CAH-CAK	-2.80	1.34	1.39
3	B	601	F2M	CAC-CAD	-2.66	1.40	1.49
2	B	600	FAD	O4B-C4B	-2.01	1.40	1.45
3	A	601	F2M	CAI-CAK	2.31	1.54	1.51
2	B	600	FAD	C4-N3	2.32	1.37	1.33
2	B	600	FAD	C4X-N5	2.45	1.37	1.33
3	B	601	F2M	CAE-CAD	4.62	1.47	1.32
3	A	601	F2M	CAE-CAD	5.08	1.49	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	N3A-C2A-N1A	-9.23	121.62	128.87
2	A	600	FAD	N3A-C2A-N1A	-7.60	122.90	128.87
2	A	600	FAD	C1B-N9A-C4A	-5.56	120.59	126.81
2	B	600	FAD	N3-C2-N1	-4.90	119.44	127.69
2	B	600	FAD	C4X-C10-N10	-4.72	117.09	120.52
2	B	600	FAD	C9A-C5X-N5	-3.78	116.03	122.18
2	A	600	FAD	N3-C2-N1	-3.46	121.86	127.69
2	A	600	FAD	C9A-C5X-N5	-3.13	117.08	122.18
3	A	601	F2M	CAC-CAD-CAE	-3.06	118.06	125.50
3	A	601	F2M	CAI-CAK-CAH	-2.84	123.18	128.48
2	A	600	FAD	O3'-C3'-C4'	-2.80	101.45	108.73
3	B	601	F2M	CAC-CAD-CAE	-2.67	119.00	125.50
2	B	600	FAD	C4-C4X-C10	-2.49	118.34	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C1B-N9A-C4A	-2.37	124.16	126.81
2	B	600	FAD	C4X-C4-N3	-2.30	120.52	123.52
2	A	600	FAD	O5'-P-O1P	-2.17	100.31	109.21
2	A	600	FAD	C9-C9A-C5X	-2.02	116.02	119.65
2	B	600	FAD	C2B-C1B-N9A	2.05	118.94	113.47
2	A	600	FAD	C6-C5X-C9A	2.07	121.39	119.11
2	B	600	FAD	C8M-C8-C7	2.11	125.26	120.73
2	A	600	FAD	C1'-N10-C9A	2.40	121.61	118.83
2	B	600	FAD	C4-C4X-N5	2.55	121.80	118.70
2	B	600	FAD	C1'-N10-C9A	2.65	121.90	118.83
2	A	600	FAD	C8M-C8-C7	2.74	126.62	120.73
3	A	601	F2M	CAB-NAL-CAI	3.33	122.35	114.64
2	A	600	FAD	C4-N3-C2	3.89	118.40	115.16
2	A	600	FAD	C4X-N5-C5X	4.01	121.45	116.72
2	B	600	FAD	C4X-N5-C5X	4.62	122.17	116.72
3	A	601	F2M	CAF-CAH-CAK	4.76	110.37	106.72
2	B	600	FAD	C4-N3-C2	7.25	121.21	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/520 (95%)	-0.42	6 (1%) 81 81	14, 24, 46, 85	0
1	B	494/520 (95%)	-0.45	2 (0%) 93 93	10, 20, 40, 78	0
All	All	993/1040 (95%)	-0.44	8 (0%) 87 87	10, 22, 44, 85	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	THR	4.8
1	B	496	ILE	4.2
1	A	499	THR	3.9
1	A	501	ILE	3.6
1	A	498	LEU	2.9
1	B	495	LEU	2.4
1	A	3	ASN	2.3
1	A	494	ARG	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(\AA^2)	Q<0.9
3	F2M	A	601	11/11	0.89	0.21	7.85	40,55,68,71	0
3	F2M	B	601	11/11	0.90	0.21	7.11	33,52,64,65	0
2	FAD	B	600	53/53	0.98	0.12	-0.17	11,14,16,17	0
2	FAD	A	600	53/53	0.98	0.10	-0.36	16,19,21,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.