Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 06:37 pm BST

PDB ID	:	1S3B
Title	:	Crystal structure of MAOB in complex with N-methyl-N-propargyl-1(R)-aminoindan
Authors	:	Binda, C.; Hubalek, F.; Li, M.; Herzig, Y.; Sterling, J.; Edmondson, D.E.; Mattevi, A.
Deposited on	:	2004-01-13
Resolution	:	1.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

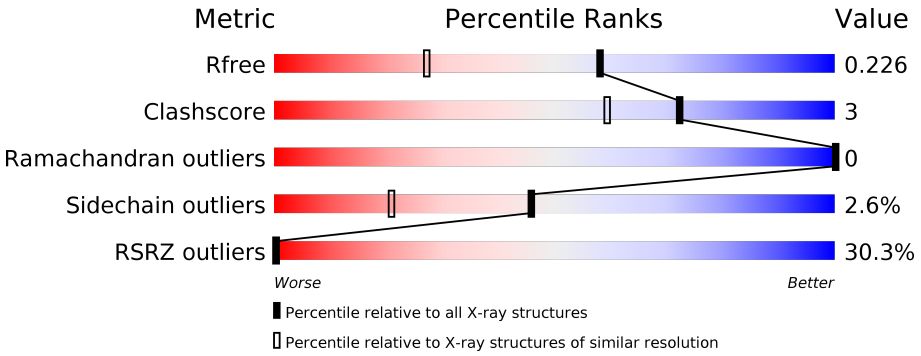
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	29% 88% 7% •
1	B	520	29% 85% 9% • 5%

2 Entry composition

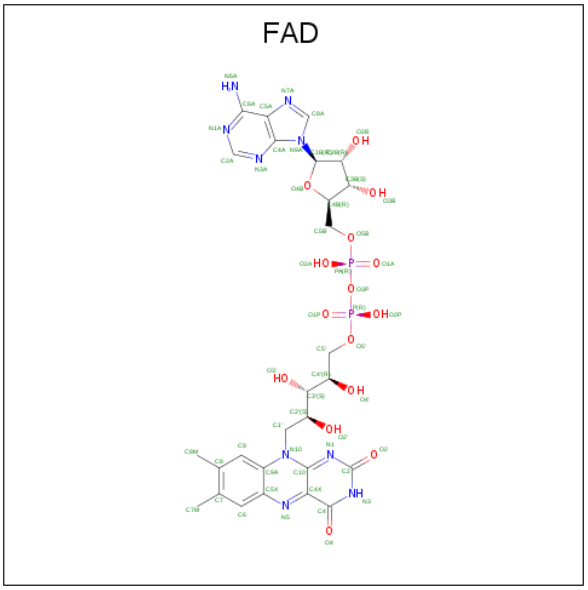
There are 4 unique types of molecules in this entry. The entry contains 8864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

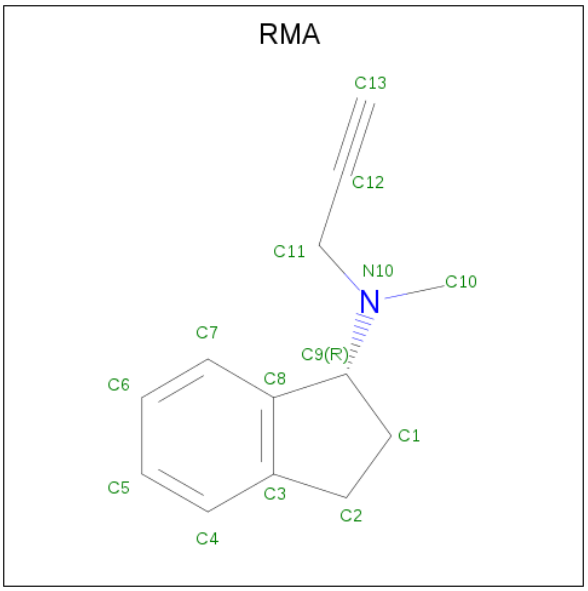
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3971	2538	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- 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 N-[(1S)-2,3-DIHYDRO-1H-INDEN-1-YL]-N-METHYL-N-PROP-2-YNYLAMINE (three-letter code: RMA) (formula: $C_{13}H_{15}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 14 13 1	0	0
3	B	1	Total C N 14 13 1	0	0

- Molecule 4 is water.

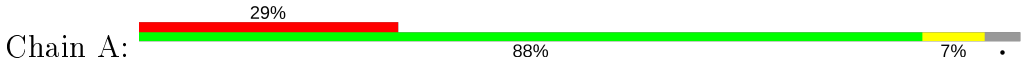
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	376	Total O 376 376	0	0
4	B	443	Total O 443 443	0	0

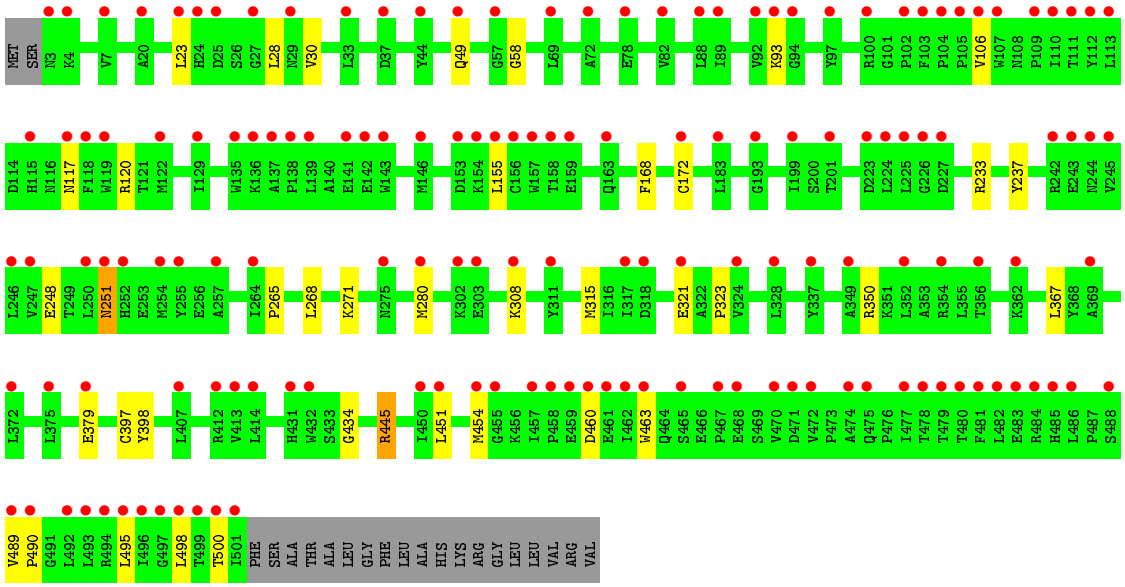
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

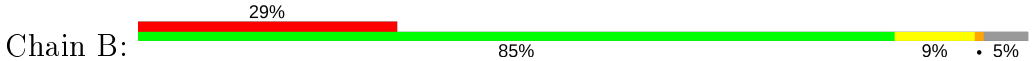
Chain A:

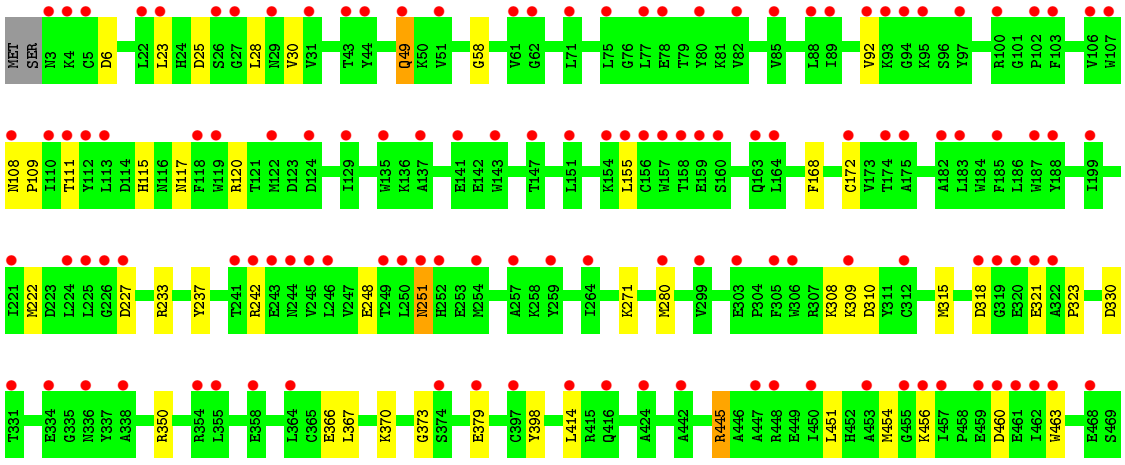


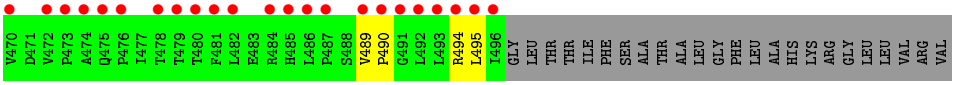


- Molecule 1: Amine oxidase [flavin-containing] B

Chain B:






V470
D471
V472
P473
A474
Q475
P476
I477
T478
T479
T480
F481
L482
E483
R484
H485
L486
P487
S488
V489
P490
G491
L492
L493
R494
L495
Y496
GLY
LEU
THR
THR
ILE
PHE
SER
ALA
THR
ALA
LEU
GLY
PHE
LEU
ALA
HIS
LYS
ARG
GLY
LEU
LEU
VAL
ARG
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.76Å 222.91Å 86.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.65 14.96 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-1.65) 98.1 (14.96-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.223 0.208 , 0.226	Depositor DCC
R_{free} test set	3732 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 80.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 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	8864	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RMA, 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	0.38	0/4068	0.65	2/5522 (0.0%)
1	B	0.36	0/4037	0.65	7/5479 (0.1%)
All	All	0.37	0/8105	0.65	9/11001 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	445	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	315	MET	CG-SD-CE	5.82	109.51	100.20
1	B	315	MET	CG-SD-CE	5.82	109.51	100.20
1	A	445	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	227	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	445	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	310	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	6	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	330	ASP	CB-CG-OD2	5.08	122.88	118.30

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	3971	0	3967	23	0
1	B	3940	0	3937	31	1
2	A	53	0	29	2	0
2	B	53	0	29	1	0
3	A	14	0	15	2	0
3	B	14	0	15	1	0
4	A	376	0	0	2	0
4	B	443	0	0	5	0
All	All	8864	0	7992	54	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 3.

All (54) 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:92:VAL:HB	1:B:318:ASP:OD2	1.79	0.83
1:A:28:LEU:HD11	1:A:454:MET:HE1	1.64	0.78
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.67	0.75
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.37	0.72
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.38	0.71
1:B:92:VAL:CG2	1:B:318:ASP:OD2	2.42	0.68
1:B:414:LEU:HD12	4:B:811:HOH:O	1.95	0.67
1:B:251:ASN:H	1:B:251:ASN:HD22	1.44	0.66
1:B:92:VAL:CB	1:B:318:ASP:OD2	2.44	0.65
1:A:251:ASN:H	1:A:251:ASN:HD22	1.43	0.64
1:A:451:LEU:HA	1:A:454:MET:HE2	1.81	0.60
1:B:451:LEU:HA	1:B:454:MET:HE2	1.83	0.60
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.39	0.58
1:B:92:VAL:HG23	1:B:318:ASP:OD2	2.04	0.57
1:B:445:ARG:HD3	4:B:616:HOH:O	2.04	0.56
1:B:445:ARG:HD2	1:B:463:TRP:CH2	2.40	0.56
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.42	0.54
1:A:271:LYS:HE2	4:A:767:HOH:O	2.12	0.50
1:A:445:ARG:HD3	4:A:623:HOH:O	2.11	0.50
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.46	0.50
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.77	0.50
1:B:233:ARG:HG3	1:B:251:ASN:HD21	1.77	0.50
1:B:168:PHE:CE1	1:B:172:CYS:SG	3.05	0.50
1:A:321:GLU:H	1:A:321:GLU:CD	2.15	0.49
1:B:321:GLU:CD	1:B:321:GLU:H	2.17	0.48
1:A:58:GLY:HA2	2:A:600:FAD:C4X	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:CZ	3:A:601:RMA:H111	2.48	0.48
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.46	0.46
1:B:222:MET:HE3	4:B:859:HOH:O	2.15	0.46
1:B:237:TYR:HB3	1:B:248:GLU:HB3	1.98	0.45
1:B:398:TYR:CZ	3:B:601:RMA:H111	2.51	0.45
1:A:168:PHE:CE1	1:A:172:CYS:SG	3.09	0.45
1:B:308:LYS:HE2	1:B:308:LYS:HB2	1.88	0.45
1:B:366:GLU:O	1:B:370:LYS:HG3	2.17	0.44
1:A:237:TYR:HB3	1:A:248:GLU:HB3	1.99	0.44
1:A:265:PRO:HD2	1:A:268:LEU:HD12	2.00	0.44
1:B:111:THR:HG22	1:B:115:HIS:CD2	2.52	0.43
1:A:308:LYS:HB2	1:A:308:LYS:HE2	1.87	0.43
1:B:323:PRO:HD2	1:B:367:LEU:HD22	2.00	0.43
1:A:323:PRO:HD2	1:A:367:LEU:HD22	2.00	0.43
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.12	0.43
1:A:251:ASN:ND2	1:A:251:ASN:H	2.13	0.43
1:B:251:ASN:H	1:B:251:ASN:ND2	2.13	0.43
1:A:172:CYS:SG	3:A:601:RMA:H6	2.59	0.42
1:B:454:MET:HE3	1:B:456:LYS:HG3	2.02	0.42
1:B:489:VAL:N	1:B:490:PRO:HD2	2.35	0.42
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.87	0.42
1:B:309:LYS:NZ	1:B:373:GLY:O	2.53	0.41
1:B:271:LYS:HE2	4:B:858:HOH:O	2.20	0.41
1:A:489:VAL:N	1:A:490:PRO:HD2	2.35	0.41
1:A:23:LEU:HB2	1:A:30:VAL:HG11	2.03	0.41
1:B:494:ARG:NH1	4:B:926:HOH:O	2.54	0.40
1:A:434:GLY:O	2:A:600:FAD:H1'2	2.21	0.40
1:B:23:LEU:HB2	1:B:30:VAL:HG11	2.02	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)
1:B:25:ASP:O	1:B:49:GLN:NE2[4_565]	2.01	0.19

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%)	486 (98%)	11 (2%)	0	100	100
1	B	492/520 (95%)	480 (98%)	12 (2%)	0	100	100
All	All	989/1040 (95%)	966 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/444 (96%)	414 (97%)	13 (3%)	41	15
1	B	424/444 (96%)	415 (98%)	9 (2%)	53	29
All	All	851/888 (96%)	829 (97%)	22 (3%)	46	21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	93	LYS
1	A	106	VAL
1	A	155	LEU
1	A	251	ASN
1	A	280	MET
1	A	350	ARG
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	397	CYS
1	A	460	ASP
1	A	495	LEU
1	A	498	LEU
1	A	500	THR
1	B	49	GLN
1	B	155	LEU
1	B	242	ARG
1	B	251	ASN
1	B	280	MET
1	B	350	ARG
1	B	379	GLU
1	B	460	ASP
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

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)

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	B	600	1,3	51,58,58	1.34	6 (11%)	60,89,89	1.71	11 (18%)
3	RMA	A	601	2	13,15,15	3.04	3 (23%)	14,20,20	8.64	5 (35%)
3	RMA	B	601	2	13,15,15	3.09	3 (23%)	14,20,20	8.56	6 (42%)
2	FAD	A	600	1,3	51,58,58	1.38	7 (13%)	60,89,89	1.66	10 (16%)

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	B	600	1,3	-	2/30/50/50	0/6/6/6
3	RMA	A	601	2	-	4/5/16/16	0/2/2/2
3	RMA	B	601	2	-	4/5/16/16	0/2/2/2
2	FAD	A	600	1,3	-	2/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	RMA	C10-N10	-8.47	1.29	1.46
3	A	601	RMA	C10-N10	-8.42	1.29	1.46
3	B	601	RMA	C11-C12	5.55	1.54	1.47
3	A	601	RMA	C11-C12	5.39	1.54	1.47
2	A	600	FAD	C10-N1	4.70	1.39	1.33
2	A	600	FAD	C4X-N5	4.19	1.39	1.33
2	B	600	FAD	C10-N1	4.12	1.38	1.33
3	B	601	RMA	C12-C13	4.08	1.30	1.18
3	A	601	RMA	C12-C13	4.02	1.30	1.18
2	B	600	FAD	C4X-N5	3.90	1.38	1.33
2	A	600	FAD	C2A-N3A	3.46	1.37	1.32
2	B	600	FAD	C2A-N3A	3.34	1.37	1.32
2	A	600	FAD	C4-N3	2.99	1.38	1.33
2	B	600	FAD	C1'-N10	2.86	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C4-N3	2.73	1.37	1.33
2	A	600	FAD	C1'-N10	2.52	1.50	1.48
2	B	600	FAD	C2A-N1A	2.45	1.38	1.33
2	A	600	FAD	C2A-N1A	2.44	1.38	1.33
2	A	600	FAD	C5X-N5	2.20	1.39	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	RMA	C11-C12-C13	-31.28	125.19	177.67
3	B	601	RMA	C11-C12-C13	-30.94	125.76	177.67
2	B	600	FAD	C4-N3-C2	6.72	120.81	115.14
2	A	600	FAD	C4-N3-C2	5.93	120.15	115.14
2	A	600	FAD	N3A-C2A-N1A	-5.57	119.98	128.68
2	B	600	FAD	N3A-C2A-N1A	-5.54	120.02	128.68
3	A	601	RMA	C12-C11-N10	5.19	121.69	112.14
3	B	601	RMA	C12-C11-N10	5.02	121.39	112.14
2	A	600	FAD	C9A-N10-C10	-4.46	116.07	121.91
2	B	600	FAD	C9A-N10-C10	-4.29	116.30	121.91
3	A	601	RMA	C11-N10-C9	3.63	118.63	113.65
3	B	601	RMA	C11-N10-C9	3.59	118.57	113.65
2	B	600	FAD	C9A-C5X-N5	-2.79	118.00	122.36
2	B	600	FAD	C1'-N10-C9A	2.74	120.45	118.29
3	B	601	RMA	C6-C7-C8	-2.73	117.53	121.01
2	A	600	FAD	C5'-C4'-C3'	-2.61	107.16	112.20
2	B	600	FAD	C4X-C4-N3	-2.59	119.89	123.43
3	A	601	RMA	C2-C1-C9	2.58	108.58	105.91
3	A	601	RMA	C6-C7-C8	-2.57	117.75	121.01
2	A	600	FAD	C10-C4X-N5	-2.50	119.53	121.26
3	B	601	RMA	C2-C1-C9	2.49	108.49	105.91
2	B	600	FAD	C4X-N5-C5X	2.48	119.25	116.77
2	B	600	FAD	C5'-C4'-C3'	-2.45	107.46	112.20
2	A	600	FAD	C1B-N9A-C4A	-2.38	122.46	126.64
2	A	600	FAD	C1'-N10-C9A	2.35	120.14	118.29
2	A	600	FAD	C4X-C4-N3	-2.33	120.25	123.43
2	A	600	FAD	C4-C4X-N5	2.30	121.22	118.60
2	A	600	FAD	C9A-C5X-N5	-2.24	118.85	122.36
3	B	601	RMA	C5-C4-C3	-2.21	117.59	120.89
2	B	600	FAD	C4-C4X-N5	2.21	121.12	118.60
2	B	600	FAD	C10-C4X-N5	-2.17	119.75	121.26
2	B	600	FAD	C1B-N9A-C4A	-2.09	122.97	126.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	RMA	C12-C11-N10-C10
3	A	601	RMA	C12-C11-N10-C9
3	A	601	RMA	C8-C9-N10-C11
3	B	601	RMA	C12-C11-N10-C10
3	B	601	RMA	C12-C11-N10-C9
2	B	600	FAD	PA-O3P-P-O5'
3	A	601	RMA	C1-C9-N10-C11
3	B	601	RMA	C1-C9-N10-C11
3	B	601	RMA	C8-C9-N10-C11
2	A	600	FAD	PA-O3P-P-O5'
2	B	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	O4B-C4B-C5B-O5B

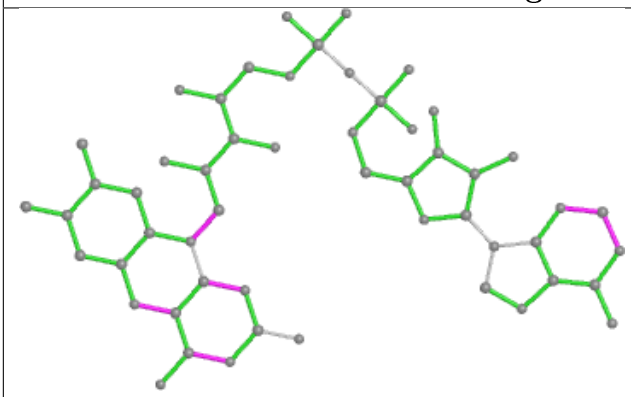
There are no ring outliers.

4 monomers are involved in 6 short contacts:

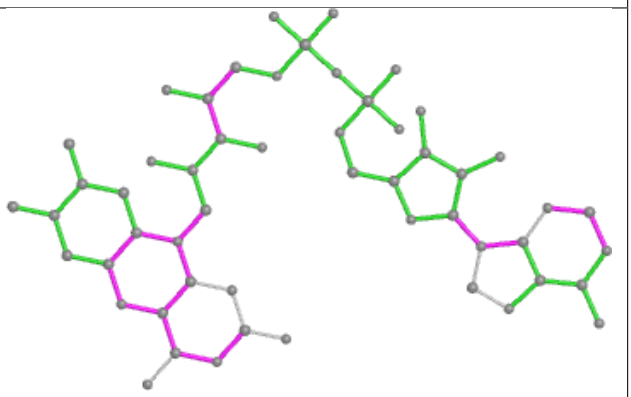
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	1	0
3	A	601	RMA	2	0
3	B	601	RMA	1	0
2	A	600	FAD	2	0

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

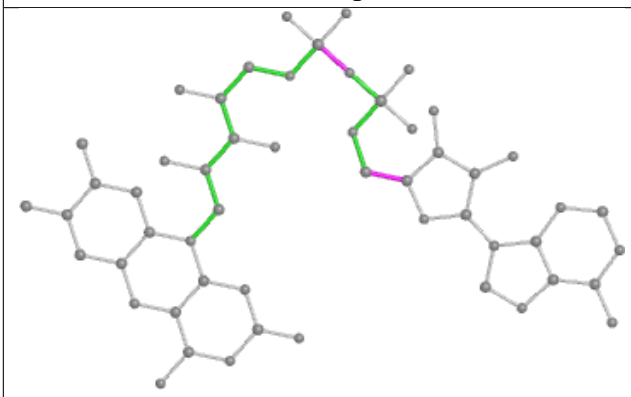
Ligand FAD B 600



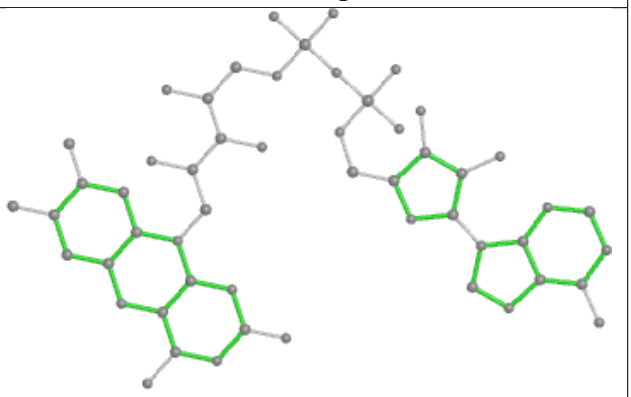
Bond lengths



Bond angles

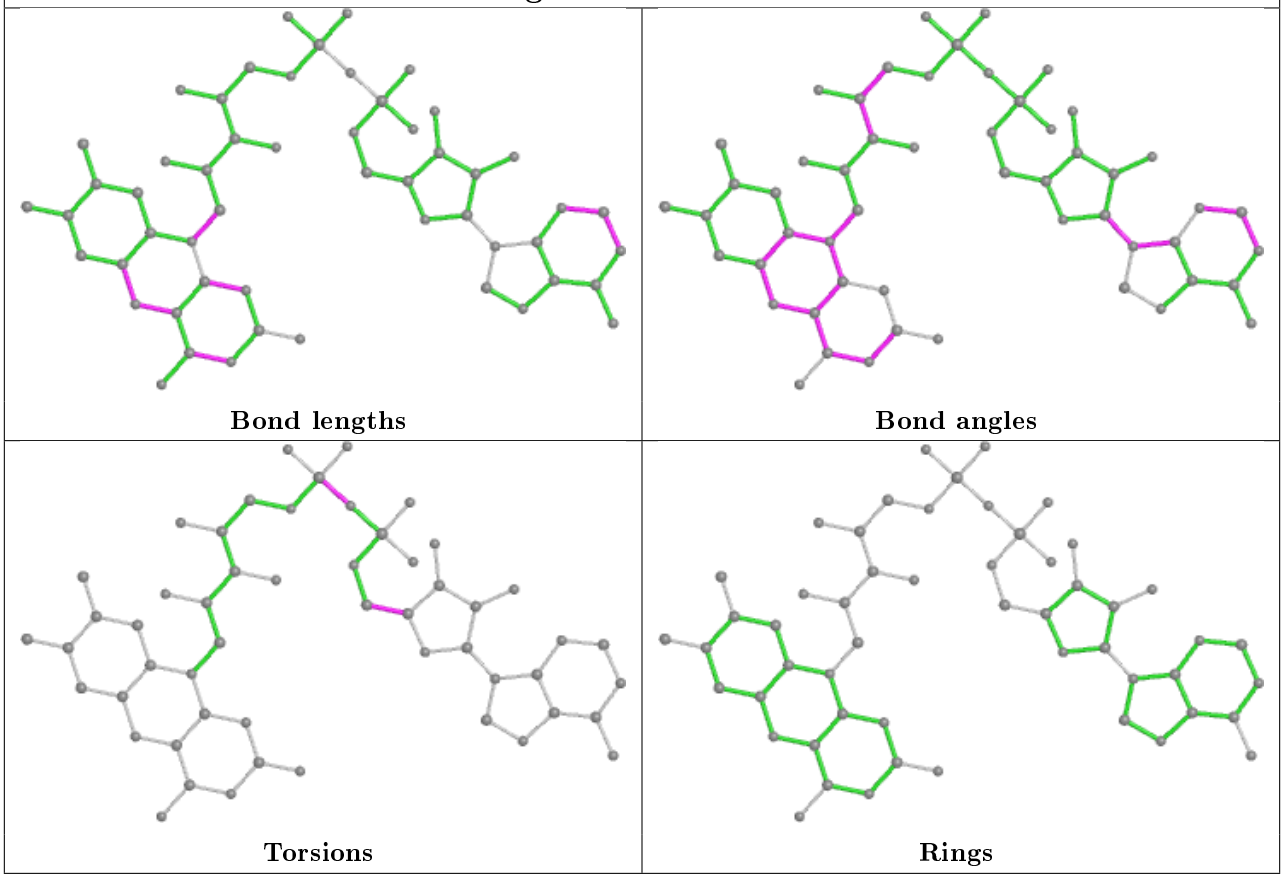


Torsions



Rings

Ligand FAD A 600



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	499/520 (95%)	1.83	151 (30%)	0	0	28, 37, 55, 78	0
1	B	494/520 (95%)	1.77	150 (30%)	0	0	28, 37, 52, 72	0
All	All	993/1040 (95%)	1.80	301 (30%)	0	0	28, 37, 53, 78	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	ILE	11.5
1	A	499	THR	11.1
1	A	500	THR	10.4
1	B	496	ILE	8.9
1	A	107	TRP	8.8
1	A	103	PHE	8.5
1	A	479	THR	8.2
1	A	496	ILE	8.1
1	A	498	LEU	8.0
1	A	497	GLY	7.6
1	B	494	ARG	7.6
1	A	478	THR	7.1
1	A	480	THR	7.1
1	B	495	LEU	6.9
1	A	354	ARG	6.7
1	B	103	PHE	6.7
1	B	107	TRP	6.5
1	B	157	TRP	6.5
1	B	119	TRP	6.5
1	A	252	HIS	6.4
1	B	492	LEU	6.3
1	B	482	LEU	6.2
1	A	3	ASN	6.0
1	A	460	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	93	LYS	5.8
1	A	245	VAL	5.7
1	B	242	ARG	5.6
1	B	481	PHE	5.6
1	A	105	PRO	5.4
1	B	252	HIS	5.3
1	A	106	VAL	5.2
1	B	243	GLU	5.2
1	A	242	ARG	5.2
1	A	494	ARG	5.1
1	A	102	PRO	5.0
1	B	319	GLY	5.0
1	B	475	GLN	4.9
1	B	3	ASN	4.8
1	A	93	LYS	4.8
1	B	89	ILE	4.7
1	A	29	ASN	4.7
1	A	243	GLU	4.7
1	B	95	LYS	4.6
1	A	78	GLU	4.5
1	A	470	VAL	4.4
1	B	241	THR	4.4
1	B	110	ILE	4.4
1	A	251	ASN	4.3
1	A	246	LEU	4.3
1	B	92	VAL	4.3
1	B	470	VAL	4.2
1	B	244	ASN	4.2
1	A	482	LEU	4.2
1	B	85	VAL	4.2
1	A	454	MET	4.2
1	A	159	GLU	4.2
1	A	227	ASP	4.1
1	A	155	LEU	4.1
1	A	486	LEU	4.1
1	A	493	LEU	4.1
1	B	460	ASP	4.1
1	B	254	MET	4.0
1	A	321	GLU	4.0
1	B	303	GLU	4.0
1	A	110	ILE	4.0
1	A	459	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	TRP	4.0
1	B	491	GLY	4.0
1	A	89	ILE	4.0
1	A	163	GLN	3.9
1	B	354	ARG	3.9
1	A	4	LYS	3.9
1	A	223	ASP	3.8
1	B	172	CYS	3.8
1	A	154	LYS	3.8
1	B	155	LEU	3.8
1	B	49	GLN	3.7
1	A	254	MET	3.7
1	B	474	ALA	3.7
1	A	481	PHE	3.7
1	A	224	LEU	3.7
1	B	4	LYS	3.7
1	A	226	GLY	3.7
1	B	227	ASP	3.7
1	A	472	VAL	3.7
1	B	31	VAL	3.7
1	A	118	PHE	3.7
1	A	302	LYS	3.7
1	B	111	THR	3.7
1	B	485	HIS	3.7
1	B	490	PRO	3.6
1	B	414	LEU	3.6
1	A	157	TRP	3.6
1	A	477	ILE	3.6
1	A	49	GLN	3.6
1	A	142	GLU	3.6
1	B	321	GLU	3.6
1	B	225	LEU	3.6
1	A	109	PRO	3.5
1	A	308	LYS	3.5
1	A	474	ALA	3.5
1	A	458	PRO	3.4
1	B	455	GLY	3.4
1	A	413	VAL	3.4
1	B	246	LEU	3.4
1	A	483	GLU	3.4
1	B	5	CYS	3.4
1	A	44	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	97	TYR	3.4
1	A	100	ARG	3.4
1	A	141	GLU	3.4
1	A	250	LEU	3.3
1	A	489	VAL	3.3
1	B	88	LEU	3.3
1	B	493	LEU	3.3
1	B	112	TYR	3.3
1	B	468	GLU	3.3
1	A	111	THR	3.3
1	A	465	SER	3.2
1	B	122	MET	3.2
1	B	478	THR	3.2
1	B	459	GLU	3.2
1	A	72	ALA	3.2
1	B	309	LYS	3.2
1	B	476	PRO	3.2
1	A	247	VAL	3.2
1	A	156	CYS	3.2
1	A	485	HIS	3.2
1	B	224	LEU	3.1
1	B	318	ASP	3.1
1	B	44	TYR	3.1
1	A	468	GLU	3.1
1	A	112	TYR	3.1
1	B	245	VAL	3.1
1	A	135	TRP	3.0
1	A	97	TYR	3.0
1	B	118	PHE	3.0
1	B	113	LEU	3.0
1	A	484	ARG	3.0
1	A	129	ILE	3.0
1	B	479	THR	3.0
1	A	495	LEU	3.0
1	A	462	ILE	3.0
1	A	471	ASP	3.0
1	A	225	LEU	3.0
1	B	486	LEU	2.9
1	B	453	ALA	2.9
1	B	251	ASN	2.9
1	B	374	SER	2.9
1	A	92	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	472	VAL	2.8
1	A	153	ASP	2.8
1	B	163	GLN	2.8
1	B	338	ALA	2.8
1	A	37	ASP	2.8
1	A	244	ASN	2.8
1	A	362	LYS	2.8
1	B	71	LEU	2.8
1	B	160	SER	2.8
1	B	484	ARG	2.8
1	B	141	GLU	2.8
1	B	473	PRO	2.8
1	B	29	ASN	2.8
1	B	135	TRP	2.8
1	A	158	THR	2.7
1	A	379	GLU	2.7
1	A	172	CYS	2.7
1	A	414	LEU	2.7
1	B	164	LEU	2.7
1	A	467	PRO	2.7
1	B	106	VAL	2.7
1	B	158	THR	2.7
1	A	328	LEU	2.7
1	A	324	VAL	2.6
1	B	22	LEU	2.6
1	B	379	GLU	2.6
1	B	462	ILE	2.6
1	B	183	LEU	2.6
1	B	250	LEU	2.6
1	B	147	THR	2.6
1	B	480	THR	2.6
1	B	457	ILE	2.6
1	B	61	VAL	2.6
1	A	69	LEU	2.6
1	B	27	GLY	2.5
1	B	336	ASN	2.5
1	A	457	ILE	2.5
1	B	280	MET	2.5
1	A	372	LEU	2.5
1	A	451	LEU	2.5
1	B	102	PRO	2.5
1	A	455	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	456	LYS	2.5
1	A	463	TRP	2.5
1	A	475	GLN	2.5
1	B	259	TYR	2.5
1	B	78	GLU	2.5
1	A	349	ALA	2.5
1	B	182	ALA	2.5
1	B	129	ILE	2.5
1	A	139	LEU	2.5
1	A	280	MET	2.5
1	A	88	LEU	2.5
1	B	355	LEU	2.5
1	B	364	LEU	2.5
1	B	100	ARG	2.4
1	B	80	TYR	2.4
1	B	448	ARG	2.4
1	B	77	LEU	2.4
1	A	20	ALA	2.4
1	B	175	ALA	2.4
1	A	311	TYR	2.4
1	B	299	VAL	2.4
1	B	424	ALA	2.4
1	B	108	ASN	2.4
1	B	94	GLY	2.4
1	B	156	CYS	2.4
1	A	7	VAL	2.4
1	A	82	VAL	2.4
1	B	489	VAL	2.4
1	A	303	GLU	2.4
1	B	320	GLU	2.4
1	A	488	SER	2.4
1	A	275	ASN	2.4
1	A	25	ASP	2.4
1	A	199	ILE	2.3
1	A	412	ARG	2.3
1	A	94	GLY	2.3
1	A	264	ILE	2.3
1	A	146	MET	2.3
1	A	57	GLY	2.3
1	A	113	LEU	2.3
1	A	356	THR	2.3
1	B	322	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	331	THR	2.3
1	B	442	ALA	2.3
1	A	337	TYR	2.3
1	A	117	ASN	2.3
1	B	151	LEU	2.2
1	A	317	ILE	2.2
1	A	24	HIS	2.2
1	B	51	VAL	2.2
1	A	33	LEU	2.2
1	B	221	ILE	2.2
1	B	26	SER	2.2
1	B	312	CYS	2.2
1	A	193	GLY	2.2
1	A	257	ALA	2.2
1	A	136	LYS	2.2
1	B	264	ILE	2.2
1	A	104	PRO	2.2
1	A	143	TRP	2.2
1	B	306	TRP	2.2
1	A	255	TYR	2.2
1	B	159	GLU	2.2
1	B	23	LEU	2.2
1	B	199	ILE	2.2
1	A	27	GLY	2.2
1	A	201	THR	2.2
1	A	432	TRP	2.2
1	B	463	TRP	2.2
1	B	416	GLN	2.1
1	A	431	HIS	2.1
1	A	450	ILE	2.1
1	B	334	GLU	2.1
1	A	122	MET	2.1
1	B	154	LYS	2.1
1	B	187	TRP	2.1
1	B	226	GLY	2.1
1	A	461	GLU	2.1
1	B	82	VAL	2.1
1	A	183	LEU	2.1
1	A	375	LEU	2.1
1	A	137	ALA	2.1
1	B	450	ILE	2.1
1	A	490	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	115	HIS	2.1
1	B	124	ASP	2.1
1	B	358	GLU	2.1
1	B	137	ALA	2.1
1	B	397	CYS	2.1
1	B	43	THR	2.1
1	B	185	PHE	2.1
1	A	138	PRO	2.0
1	B	461	GLU	2.0
1	B	487	PRO	2.0
1	B	257	ALA	2.0
1	B	305	PHE	2.0
1	A	23	LEU	2.0
1	B	143	TRP	2.0
1	B	249	THR	2.0
1	B	62	GLY	2.0
1	A	369	ALA	2.0
1	B	447	ALA	2.0
1	B	188	TYR	2.0
1	A	352	LEU	2.0
1	A	407	LEU	2.0
1	A	492	LEU	2.0
1	B	75	LEU	2.0
1	A	318	ASP	2.0
1	B	174	THR	2.0

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)

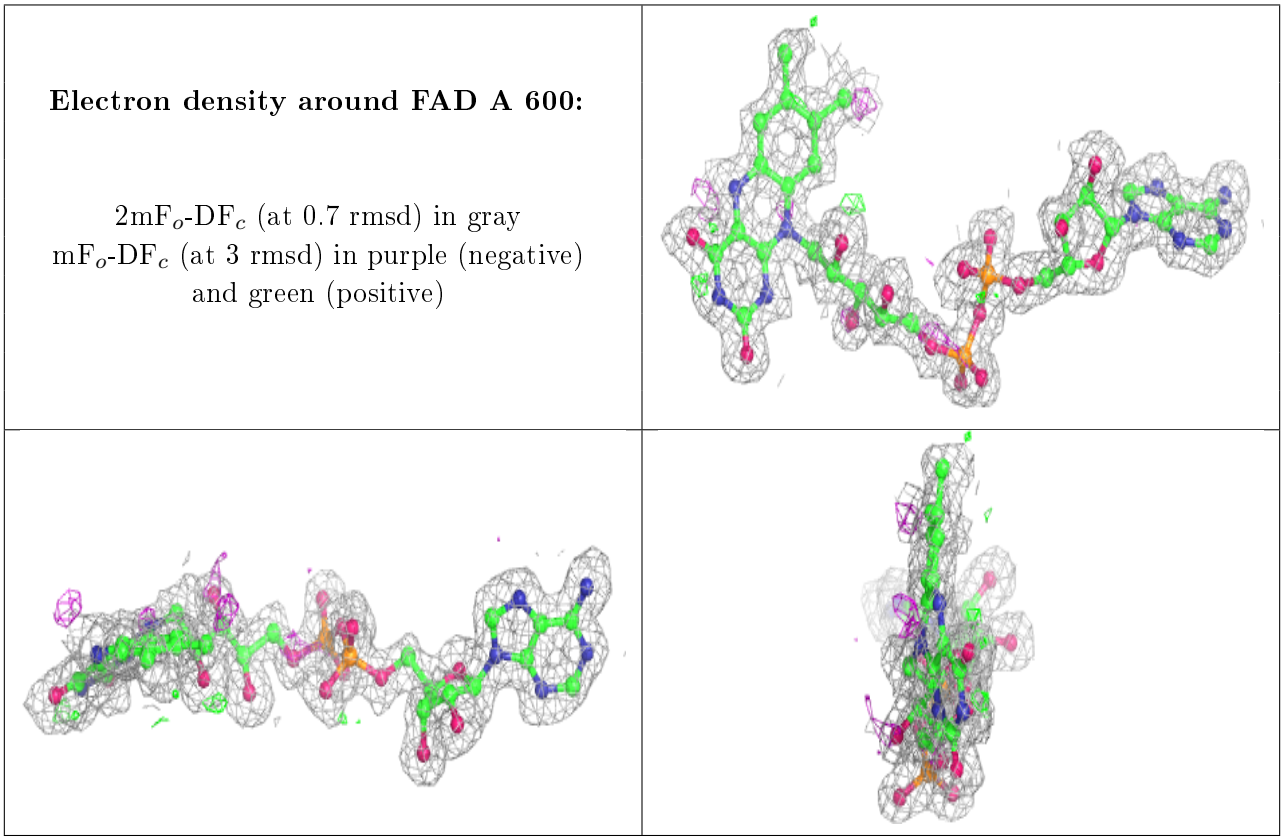
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RMA	A	601	14/14	0.76	0.20	37,43,44,44	0
3	RMA	B	601	14/14	0.80	0.20	38,42,43,44	0
2	FAD	A	600	53/53	0.92	0.13	29,31,33,33	0
2	FAD	B	600	53/53	0.94	0.13	28,31,33,33	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.

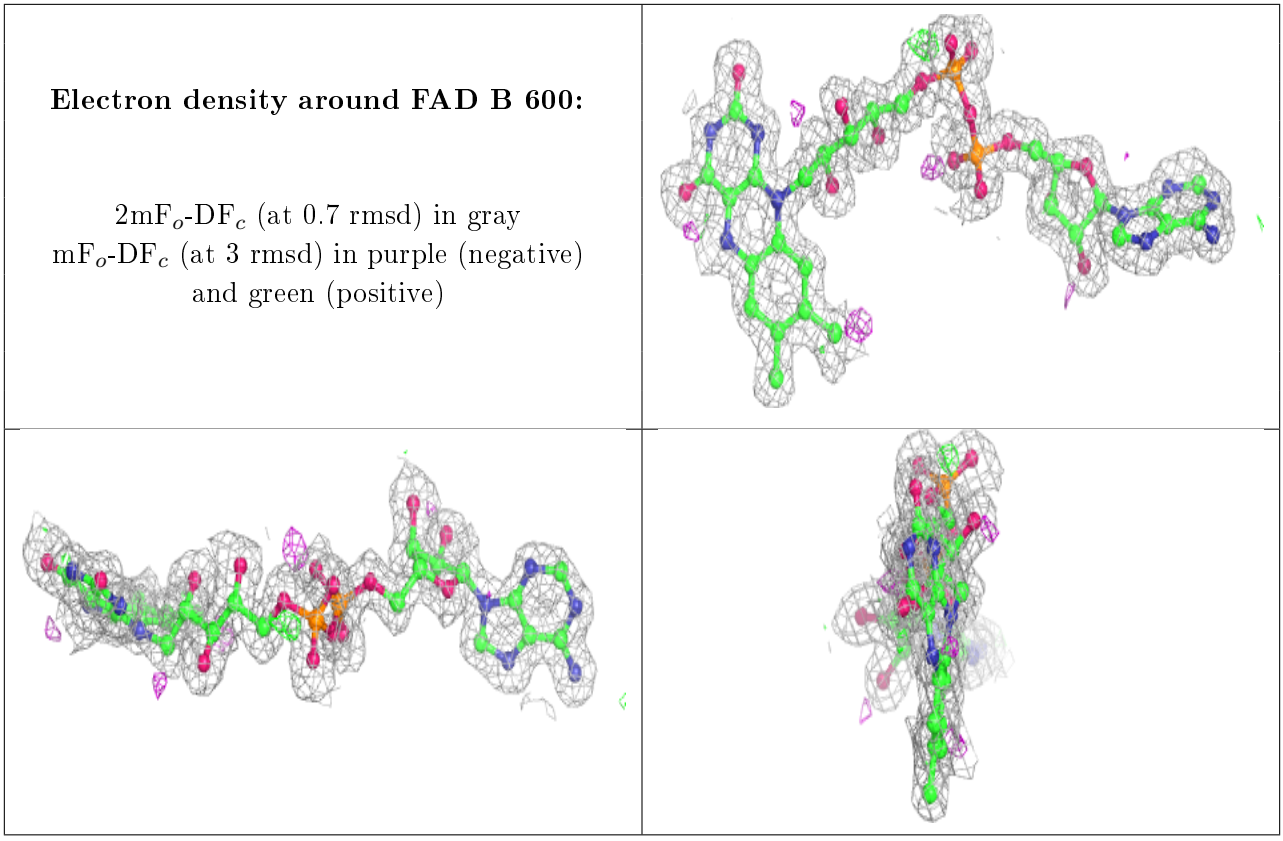
Electron density around FAD A 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD B 600:

$2mF_o$-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.