wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1GOS
Title	:	Human Monoamine Oxidase B
Authors	:	Binda, C.; Newton-Vinson, P.; Hubalek, F.; Edmondson, D.E.; Mattevi, A.
Deposited on	:	2001-10-26
Resolution	:	3.00 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 (i) symbol.

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

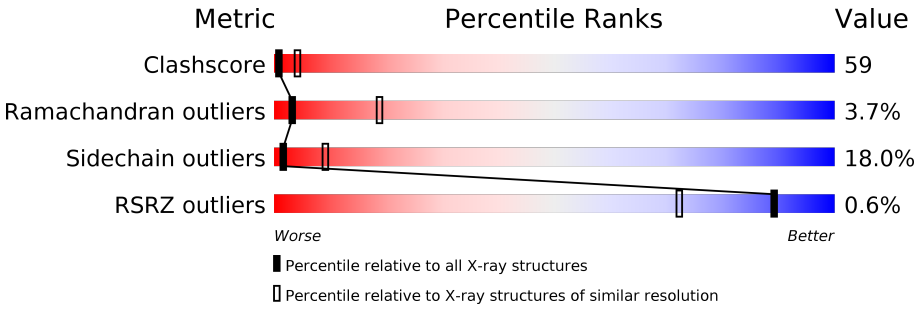
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	% 25% 55% 14%
1	B	520	31% 49% 13% 5%

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
3	NYP	A	601	X	-	X	-
3	NYP	B	601	X	-	X	-

2 Entry composition

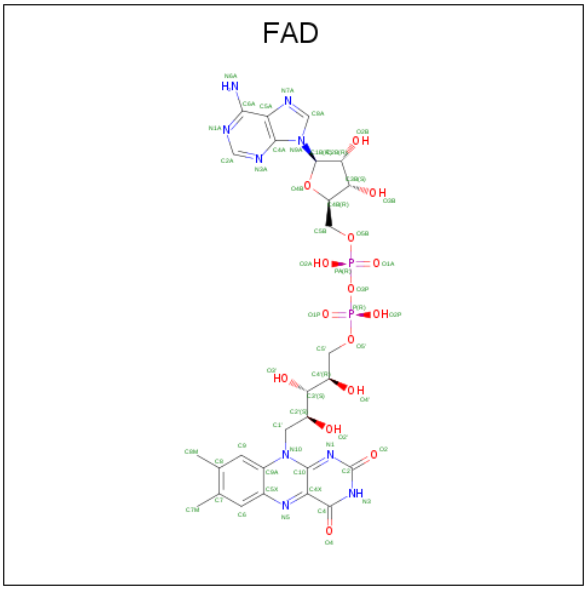
There are 3 unique types of molecules in this entry. The entry contains 8020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MONOAMINE OXIDASE.

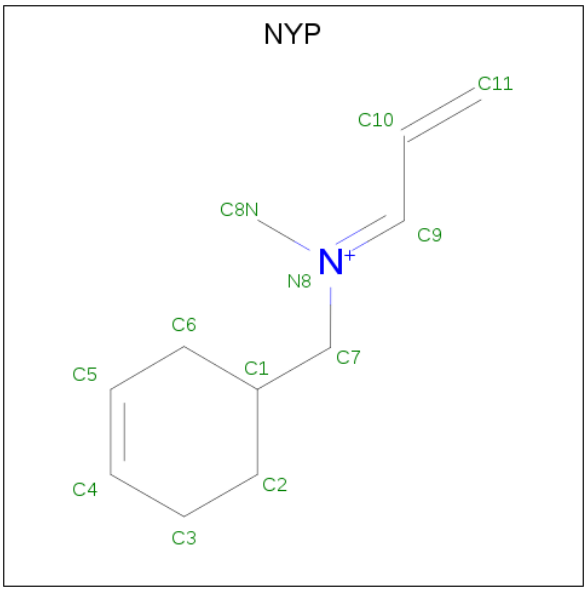
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	B	493	Total	C	N	O	S	0	0	0
			3932	2515	674	719	24			

- 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-[(E)-METHYL](PHENYL)-N-[(E)-2-PROPENYLIDENE]METHANAMINIUM (three-letter code: NYP) (formula: $C_{11}H_{18}N$).



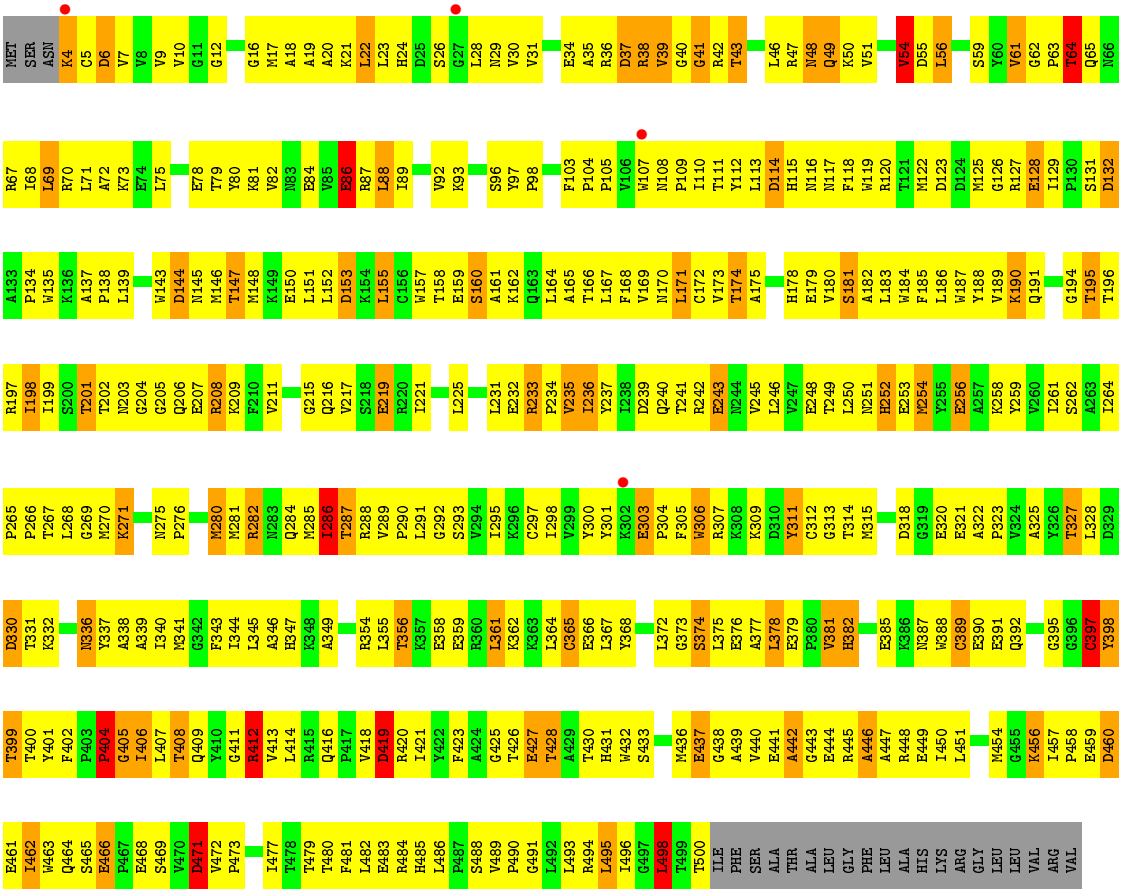
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 12 11 1	0	0
3	B	1	Total C N 12 11 1	0	0

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.

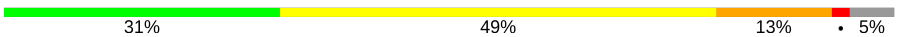
- Molecule 1: MONOAMINE OXIDASE

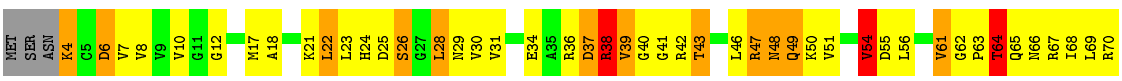
Chain A:

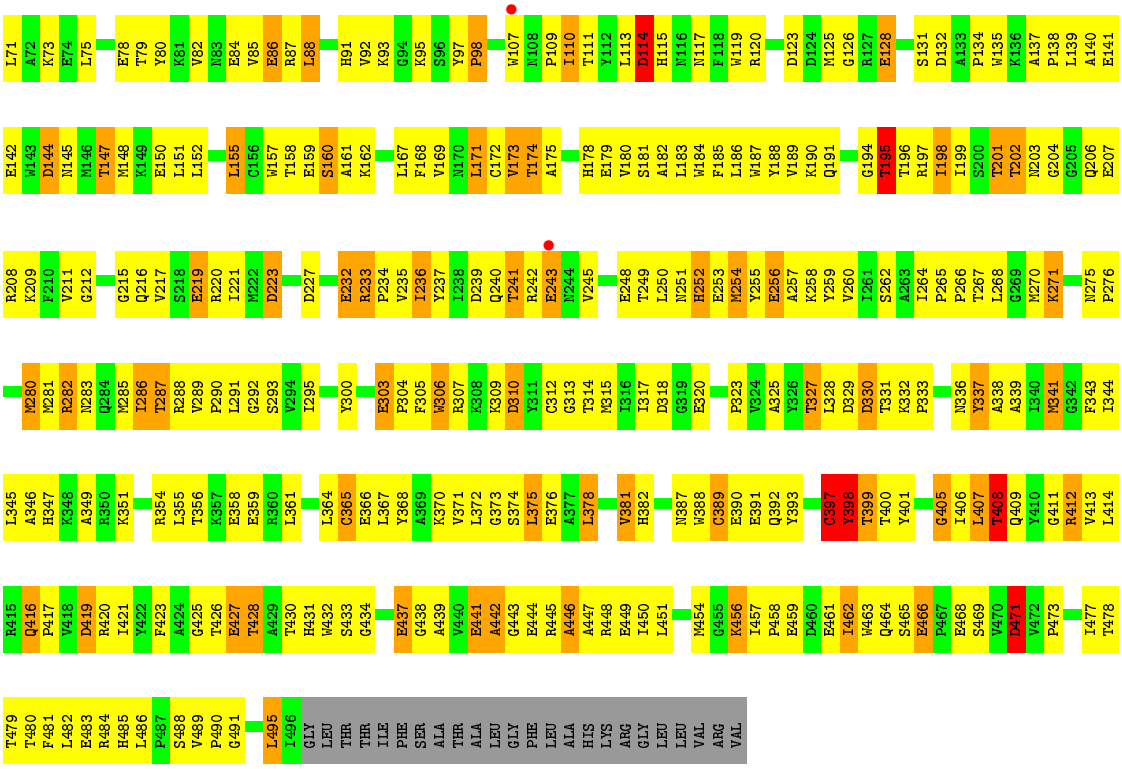


- Molecule 1: MONOAMINE OXIDASE

Chain B:






L71 A72 K73 E74 L75
E78 T79 Y80 K81 V82 N83 E84 V85 E86 R87 L88
H91 V92 K93 G94 K95 S96 Y97 P98
W107 N108 P109 I110 T111 Y112 L113 D114 H115 N116 N117 F118 W119 R120
D123 D124 M125 G126 R127 E128
S131 D132 A133 P134 W135 K136 A137 P138 L139 A140 E141
E142 W143 D144 N145 M146 T147 M148 K149 E150 L151 L152
L155 C156 W157 T158 E159 S160 A161 K162
L167 F168 V169 N170 L171 C172 V173 T174 A175
H178 E179 V180 S181 A182 L183 W184 F185 L186 W187 Y188 V189 K190 Q191
G194 T195 T196 R197 I198 I199 S200 T201 T202 N203 G204 G205 Q206 E207
R208 K209 F210 V211 G212
G215 Q216 V217 S218 E219 R220 I221 M222 D223 D227
E232 R233 P234 V235 I236 Y237 I238 D239 Q240 T241 R242 E243 N244 V245
E248 T249 L250 N251 H252 E253 M254 Y255 E256 A257 K258 Y259 V260 I261 S262 A263 I264 P265 P266 T267 L268 G269 M270 K271
N275 P276
M280 M281 R282 N283 Q284 M285 I286 T287 R288 V289 P290 L291 G292 S293 V294 I295
Y300
E303 P304 F305 W306 R307 K308 K309 D310 Y311 C312 G313 T314 M315 I316 I317 D318 G319 E320
P323 V324 A325 Y326 T327 L328 D329 D330 T331 K332 P333
N336 Y337 A338 A339 I340 M341 G342 F343 I344
L345 A346 H347 K348 A349 R350 K351
R354 L355 T356 K357 E358 E359 R360 L361
L364 C365 E366 L367 Y368 A369 K370 V371 L372 G373 S374 L375 E376 A377 L378
V381 H382
N387 W388 C389 E390 E391 Q392 Y393
G397 Y398 T399 T400 Y401
G405 I406 L407 T408 Q409 Y410 G411 R412 V413 L414
R415 Q416 P417 V418 D419 R420 I421 Y422 F423
A424 G425 T426 E427 T428 A429 T430 H431 W432 S433 G434
E437 G438 A439 V440 E441 A442 G443 E444 R445 A446 A447 R448 E449 I450 L451
M454 G455 K456 I457 P458 E459 D460 E461 I462 W463 Q464 S465 E466 P467 E468 S469 V470 D471 V472 P473
I477 T478
T479 T480 F481 L482 E483 R484 H485 L486 P487 S488 V489 P490 G491
L495 I496 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	138.80Å 224.30Å 87.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 14.90 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.3 (40.00-3.00) 94.5 (14.90-3.08)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.271 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NYP, 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	0.71	0/4055	1.17	20/5504 (0.4%)
1	B	0.79	1/4029 (0.0%)	1.21	27/5468 (0.5%)
All	All	0.75	1/8084 (0.0%)	1.19	47/10972 (0.4%)

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
1	A	1	2
1	B	0	2
All	All	1	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	TRP	CB-CG	-5.13	1.41	1.50

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	123	ASP	CB-CG-OD2	10.68	127.92	118.30
1	B	310	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	54	VAL	CB-CA-C	-7.89	96.41	111.40
1	A	419	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	471	ASP	CB-CG-OD2	7.64	125.18	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	CYS	Peptide
1	A	405	GLY	Peptide
1	B	397	CYS	Peptide
1	B	405	GLY	Peptide

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	3958	0	3959	533	0
1	B	3932	0	3931	435	0
2	A	53	0	29	7	0
2	B	53	0	29	3	0
3	A	12	0	16	12	0
3	B	12	0	16	8	0
All	All	8020	0	7980	945	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 59.

The worst 5 of 945 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:79:THR:CG2	1:B:208:ARG:HD3	1.66	1.25
1:A:79:THR:CG2	1:A:208:ARG:HD3	1.70	1.20
1:B:175:ALA:HB1	1:B:179:GLU:OE1	1.40	1.19
1:A:82:VAL:HG23	1:A:207:GLU:O	1.43	1.19
1:A:22:LEU:O	1:A:22:LEU:HD12	1.37	1.18

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	495/520 (95%)	391 (79%)	83 (17%)	21 (4%)	3 16
1	B	491/520 (94%)	400 (82%)	76 (16%)	15 (3%)	4 23
All	All	986/1040 (95%)	791 (80%)	159 (16%)	36 (4%)	3 19

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	CYS
1	B	286	ILE
1	B	442	ALA
1	B	446	ALA
1	A	252	HIS

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	426/444 (96%)	353 (83%)	73 (17%)	2 10
1	B	423/444 (95%)	343 (81%)	80 (19%)	1 8
All	All	849/888 (96%)	696 (82%)	153 (18%)	1 9

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	THR

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Mol	Chain	Res	Type
1	B	64	THR
1	B	437	GLU
1	A	498	LEU
1	B	38	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	431	HIS
1	B	206	GLN
1	A	206	GLN
1	A	216	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	$\#\|Z\|>2$
3	NYP	B	601	2	9,12,12	3.59	8 (88%)	8,14,14	3.49	4 (50%)
2	FAD	B	600	1,3	51,58,58	1.47	6 (11%)	60,89,89	2.51	19 (31%)
2	FAD	A	600	1,3	51,58,58	1.44	8 (15%)	60,89,89	2.19	17 (28%)
3	NYP	A	601	2	9,12,12	3.44	8 (88%)	8,14,14	3.45	4 (50%)

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
3	NYP	B	601	2	1/1/2/6	3/4/15/15	0/1/1/1
2	FAD	B	600	1,3	-	6/30/50/50	0/6/6/6
2	FAD	A	600	1,3	-	7/30/50/50	0/6/6/6
3	NYP	A	601	2	1/1/2/6	3/4/15/15	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NYP	C9-N8	5.44	1.33	1.30
3	A	601	NYP	C2-C3	-5.39	1.40	1.52
3	B	601	NYP	C2-C3	-5.18	1.40	1.52
3	A	601	NYP	C2-C1	-4.75	1.39	1.52
2	B	600	FAD	C2A-N3A	4.53	1.39	1.32

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	O4B-C1B-C2B	-8.76	94.13	106.93
2	A	600	FAD	P-O3P-PA	-8.15	104.85	132.83
3	B	601	NYP	C2-C1-C6	7.31	121.52	109.36
2	B	600	FAD	C4-N3-C2	7.05	121.10	115.14
2	B	600	FAD	P-O3P-PA	-6.89	109.17	132.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	NYP	C1
3	A	601	NYP	C1

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NYP	C2-C1-C7-N8
3	B	601	NYP	C6-C1-C7-N8
2	B	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	O3'-C3'-C4'-O4'

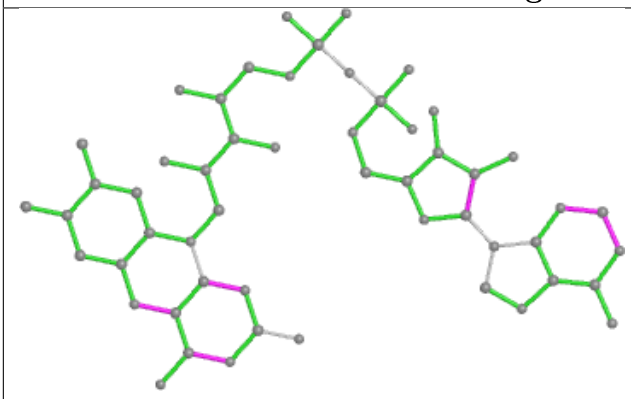
There are no ring outliers.

4 monomers are involved in 30 short contacts:

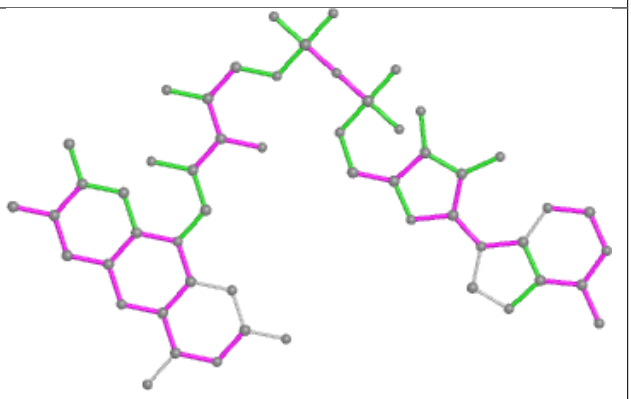
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NYP	8	0
2	B	600	FAD	3	0
2	A	600	FAD	7	0
3	A	601	NYP	12	0

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 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.

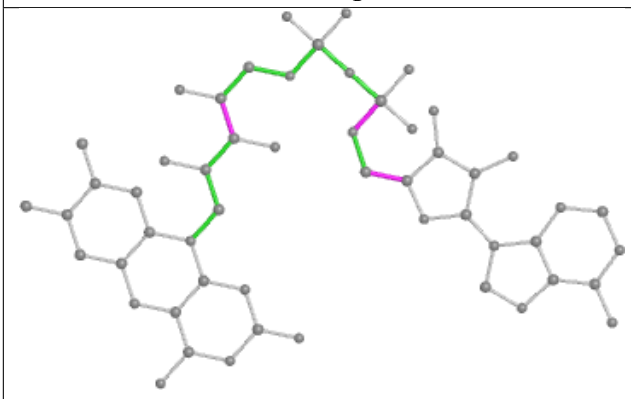
Ligand FAD B 600



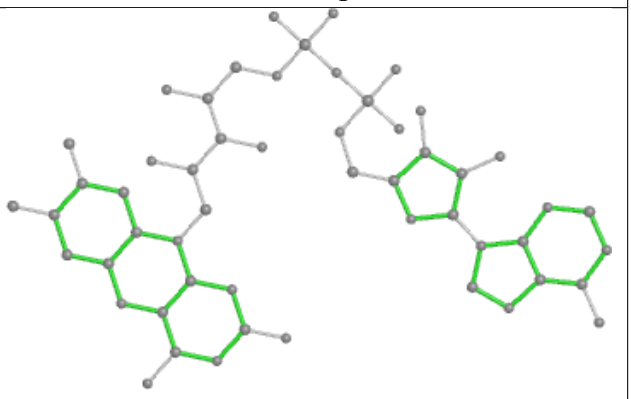
Bond lengths



Bond angles

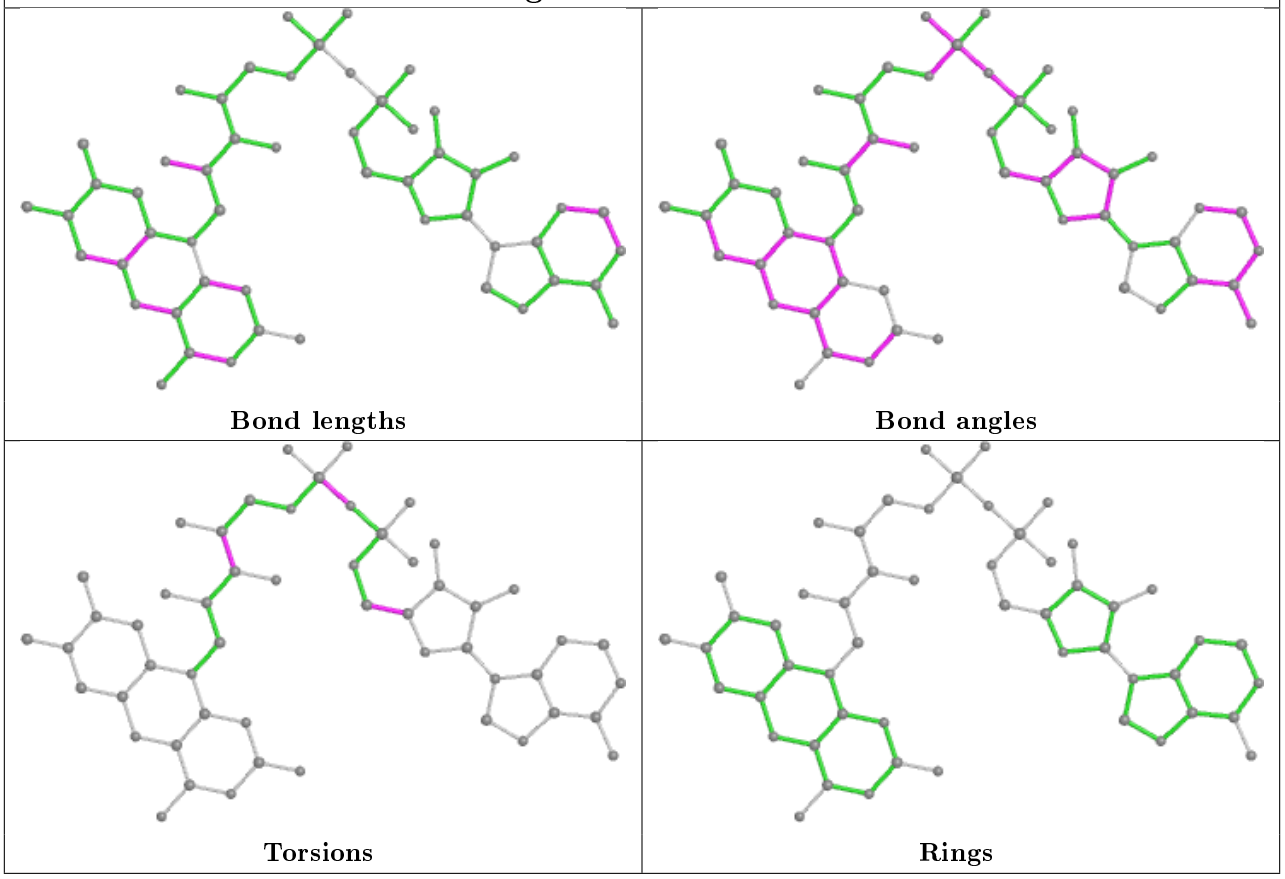


Torsions



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	497/520 (95%)	-0.15	4 (0%)	86	65	27, 44, 74, 100	0
1	B	493/520 (94%)	-0.40	2 (0%)	92	79	27, 44, 73, 91	0
All	All	990/1040 (95%)	-0.28	6 (0%)	89	72	27, 44, 74, 100	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	2.9
1	B	243	GLU	2.8
1	A	27	GLY	2.7
1	B	107	TRP	2.1
1	A	4	LYS	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

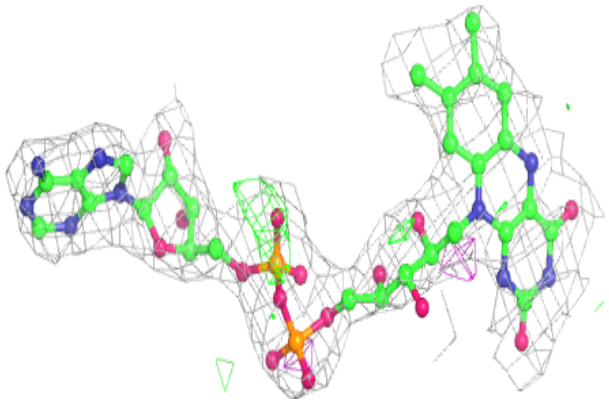
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

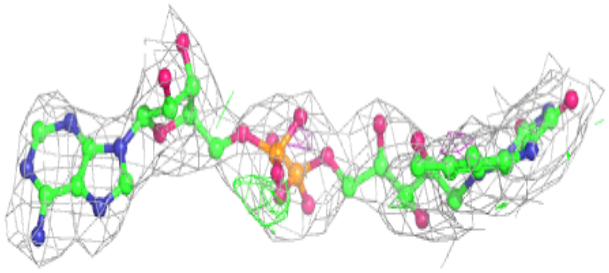
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NYP	A	601	12/12	0.86	0.27	46,53,58,59	0
2	FAD	A	600	53/53	0.90	0.21	24,35,45,49	0
3	NYP	B	601	12/12	0.91	0.21	46,53,58,58	0
2	FAD	B	600	53/53	0.96	0.14	23,35,45,50	0

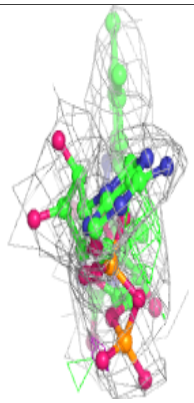
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

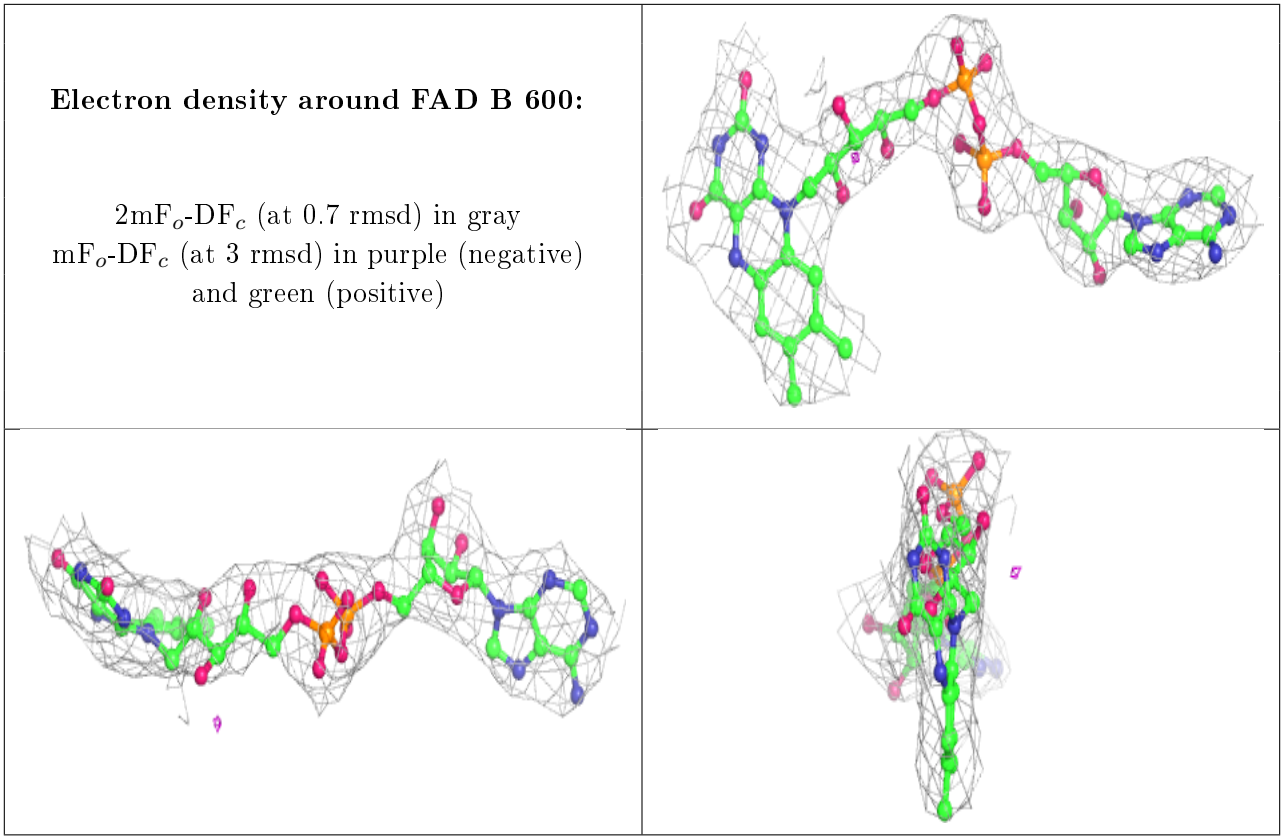






Electron density around FAD B 600:

$2mF_o$-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.