



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 13, 2026 – 02:05 pm BST

PDB ID : 2BYB / pdb_00002byb
Title : Human Monoamine Oxidase B in complex with Deprenyl
Authors : Binda, C.; De Colibus, L.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2005-07-29
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

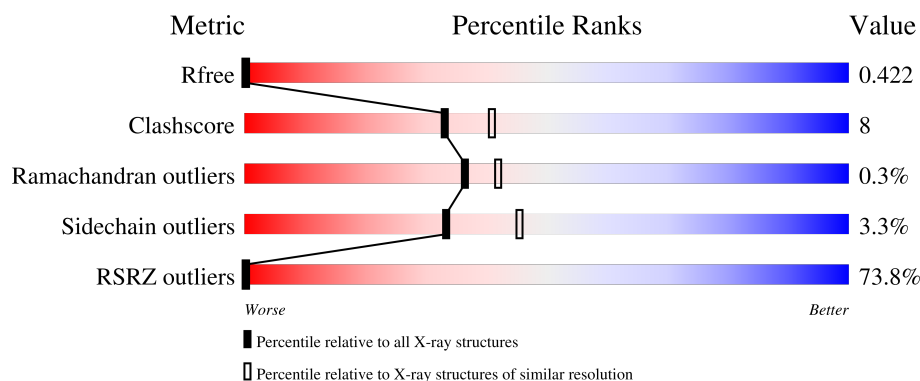
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of 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	520	
1	B	520	

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
2	FAD	A	600	-	-	X	-

2 Entry composition [i](#)

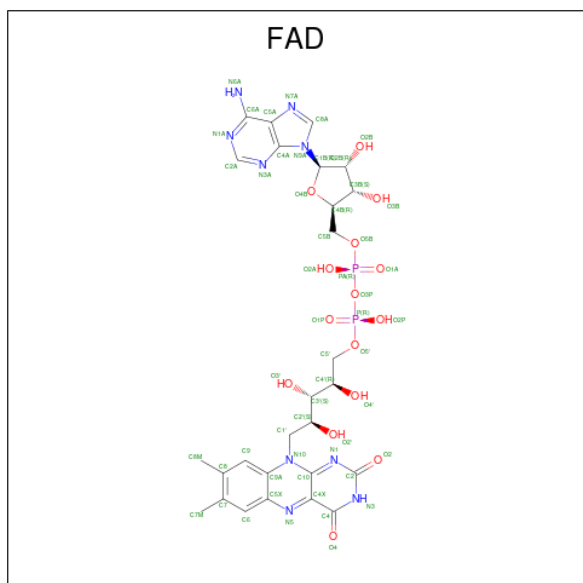
There are 4 unique types of molecules in this entry. The entry contains 8534 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

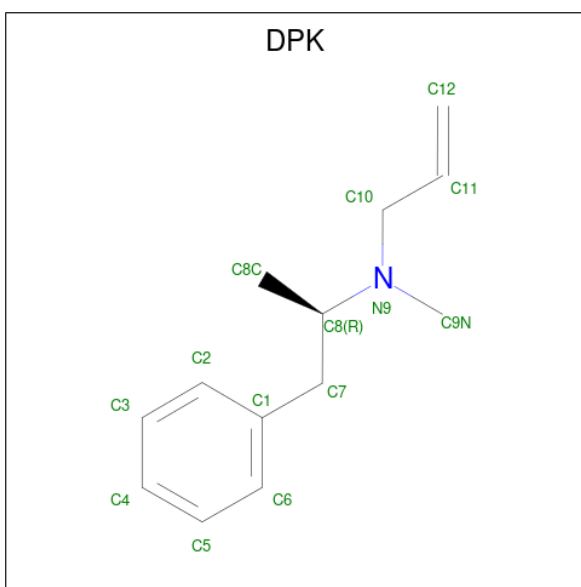
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3971	2538	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 DEPRENYL (CCD ID: DPK) (formula: $C_{13}H_{19}N$).



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

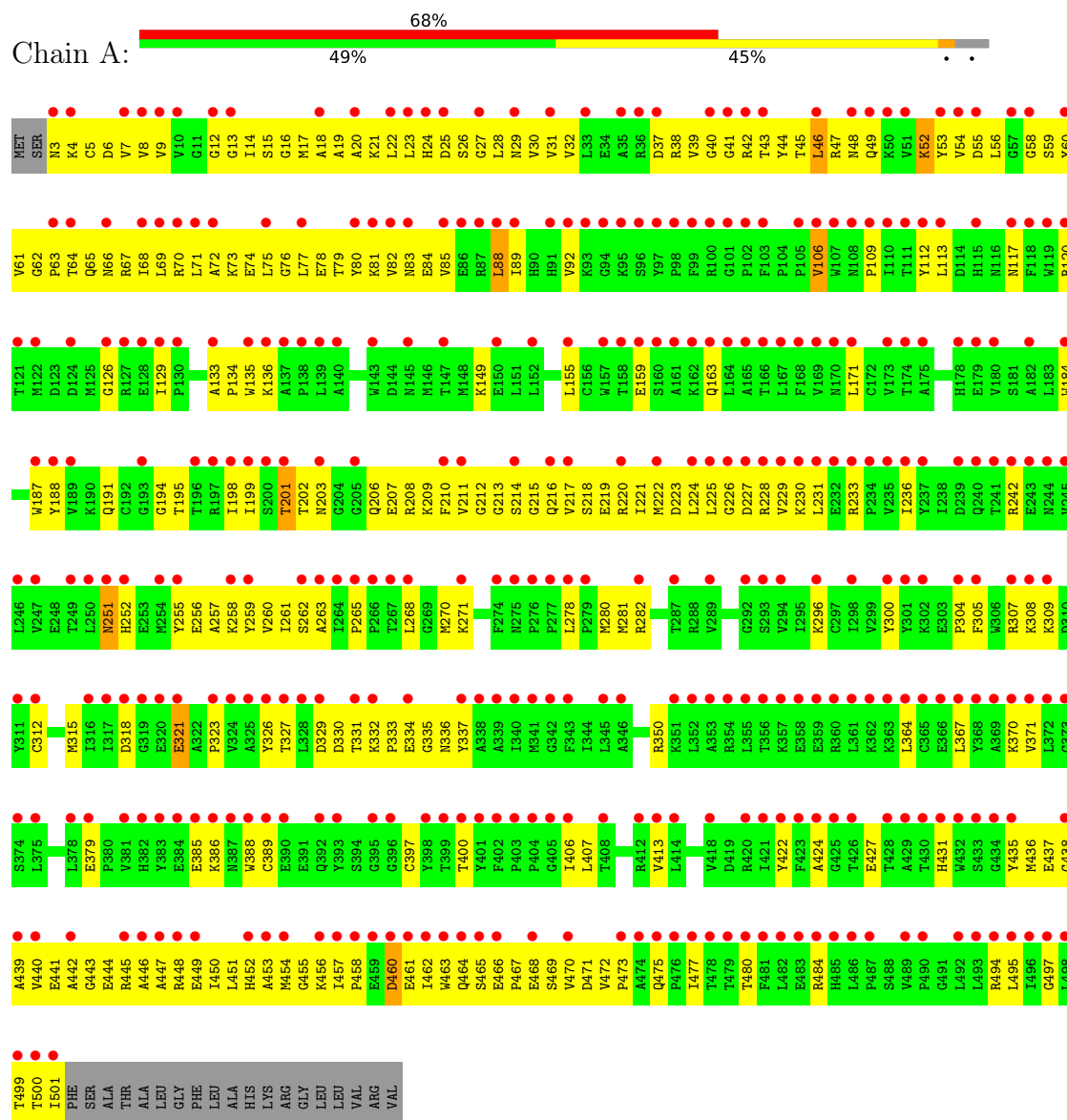
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		
4	B	256	Total	O	0	0
			256	256		

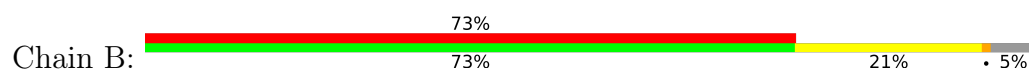
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



PHE	G442	G380	D318	T249	Y187	G126	Q65	MET
SER	G443	Y381	G319	L260	Y188	R127	N66	SER
ALA	E444	H382	E321	N251	V189	E128	R67	N3
THR	R445	Y383	E320	H252	K190	I129	I68	K4
ALA	A446	E384	A322	E253	Q191	P130	L69	C5
LEU	A447	E385	P323	M254	G192	S131	R70	D6
GLY	R448	K386	V324	Y255	G193	D132	L71	V7
PHE	E449	K387	A325	E256	G194	A133	A72	V8
LEU	L450	Y388	Y326	A257	T195	D133	K73	V9
ALA	L451	Q392	T327	K258	T196	A135	E74	
HIS	H452	Y393	L328	Y259	R197	K136	L75	I14
LYS	A453	Y394	D329	V260	I198	A137	G76	S15
ARG	M454	S394	D330	I261	I199	P138	L77	G16
GLY	G455	G395	T331	S262		L139	E78	M17
LEU	K456	G396	K332	A263	T202	A140	Y80	
LEU	L457	C397	P333	I264	N203	E141	X81	A20
VAL	P458	Y398	E334	P265	G204	E142	N82	K21
ARG	E459	T399	G335		G205	V143	Y82	L22
ARG	D460	T400	N336	L268	Q206	D144	N83	L23
VAL	E461	Y401	Y337	G269	E207	N145	E84	H24
	I462	F402	A338	M270	R208	M146	Y85	D25
	W463	P403	A339	K271	K209	T147	E86	S26
	Q464	P404	I340	I272		M148	R87	G27
	S465	G405		H273	G212	K149	L88	L28
	E466	I406	F343	F274	G213	E150	N89	N29
	P467	L407	I344	N275	S214	L151	H90	V30
	E468	T408	L345	P276	G215	L152	Y91	V31
	S469	Q409	A346	P277	Q216	D153	V92	V32
	V470	Y410	K347	L278	V217	K154	N93	L33
	D471	G411	K348	P279	S218	L155	G94	E34
	V472	R412	A349	M280	E219	C156	N95	A35
	P473	V413	R350	R281	R220	W157	S96	R36
	A474	L414	K351	N282	I221	T158	Y97	D37
	Q475	R415	L352	N283	M222	S159	F98	R38
	P476	Q416	A353		D223	S160	F99	V39
	I477	P417	R354	V289	L224	A161	G100	G40
	T478	V418	L355		L225	K162	G101	G41
	T479	D419	T356	V284	G226	Q163	P102	R42
	T480	R420	K357	I295	D227	L164	F103	T43
	F481	I421	E358	K296	R228	A165	P104	Y44
	L482	Y422	E359	C297	V229	T166	P105	T45
	E483	F423	R360	I298	K230	L167	V106	L46
	R484	A424	L361	V299	L231	F168	W107	R47
	H485	G425	K362	Y300	E232		N108	N48
	L486	T426	K363	Y301	R233	L171	P109	Q49
	P487	E427	L364	K302	P234	C172	I110	Q50
	S488	T428	C365	E303	V235	V173	T111	V51
	V489	A429	E366	P304	I236	T174	Y112	K52
	P490	T430	L367	F305	Y237	A175	L113	Y53
	G491	H431	Y368	Y306	I238	E176	D114	V54
	L492	W432	A369	R307	D239	T177	N115	D55
	L493	S433	K370	K308	Q240	H178	M116	L56
	R494	G434	V371	K309	T241	E179	N117	G57
	L495	Y435		D310	R242	V180	F118	G58
	T496	M436	S374	Y311	E243	S181	W119	S59
GLY		F437	L375	C312	N244	A182	R120	Y60
LEU		G438	E376		V245	L183	T121	V61
THR		A439	A377	M315	L246	W184	M22	G62
THR		V440	L378	I316	V247	F185	D123	P63
ILE		E441	E379	I317	E248	L186	T64	T64

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.84Å 225.84Å 85.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (15.00-2.20) 94.6 (15.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.299 0.400 , 0.422	Depositor DCC
R_{free} test set	2140 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	8534	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: DPK, 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	1.00	2/4068 (0.0%)	1.08	2/5522 (0.0%)
1	B	1.07	9/4037 (0.2%)	1.13	7/5479 (0.1%)
All	All	1.04	11/8105 (0.1%)	1.11	9/11001 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	VAL	CA-CB	6.83	1.63	1.54
1	B	182	ALA	CA-CB	5.98	1.62	1.53
1	B	206	GLN	N-CA	5.92	1.53	1.46
1	B	82	VAL	CA-CB	5.73	1.60	1.54
1	A	477	ILE	CA-CB	5.67	1.60	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	LEU	CA-C-N	-6.83	113.27	120.03
1	B	278	LEU	C-N-CA	-6.83	113.27	120.03
1	B	319	GLY	N-CA-C	6.30	117.93	111.95
1	A	236	ILE	CB-CA-C	-6.03	104.11	110.62
1	A	194	GLY	N-CA-C	5.97	118.13	112.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3971	0	3967	64	1344
1	B	3940	0	3937	64	22
2	A	53	0	29	2	60
2	B	53	0	29	2	0
3	A	14	0	17	0	0
3	B	14	0	17	1	0
4	A	233	0	0	7	132
4	B	256	0	0	16	3
All	All	8534	0	7996	125	1369

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 8.

The worst 5 of 125 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:464:GLN:NE2	4:B:2244:HOH:O	1.79	1.14
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.12	0.96
1:A:92:VAL:HG22	1:A:318:ASP:OD2	1.75	0.84
1:B:414:LEU:HD12	4:B:2217:HOH:O	1.78	0.83
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.29	0.80

The worst 5 of 1369 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:A:67:ARG:NE	1:A:222:MET:CB[3_655]	0.21	1.99
1:A:76:GLY:C	2:A:600:FAD:N1[3_655]	0.29	1.91
1:A:223:ASP:O	1:A:441:GLU:OE2[3_655]	0.32	1.88
1:A:223:ASP:CA	1:A:441:GLU:OE1[3_655]	0.37	1.83
1:A:228:ARG:CB	1:A:462:ILE:O[3_655]	0.37	1.83

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/520 (96%)	476 (96%)	20 (4%)	1 (0%)	43	51
1	B	492/520 (95%)	470 (96%)	20 (4%)	2 (0%)	30	34
All	All	989/1040 (95%)	946 (96%)	40 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	LYS
1	A	52	LYS
1	B	460	ASP

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	427/444 (96%)	413 (97%)	14 (3%)	33	45
1	B	424/444 (96%)	410 (97%)	14 (3%)	33	45
All	All	851/888 (96%)	823 (97%)	28 (3%)	33	45

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	LEU
1	B	495	LEU
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	397	CYS
1	B	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	ASN
1	B	117	ASN
1	B	431	HIS
1	B	251	ASN
1	A	416	GLN

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 oligosaccharides 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	$\# Z > 2$
3	DPK	A	601	2	14,14,14	0.53	0	15,17,17	2.34	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DPK	B	601	2	14,14,14	0.60	0	15,17,17	2.28	3 (20%)
2	FAD	B	600	3,1	56,58,58	1.34	8 (14%)	81,89,89	2.01	23 (28%)
2	FAD	A	600	3,1	56,58,58	1.37	7 (12%)	81,89,89	1.84	22 (27%)

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	DPK	A	601	2	-	6/11/11/11	0/1/1/1
3	DPK	B	601	2	-	6/11/11/11	0/1/1/1
2	FAD	B	600	3,1	-	3/34/50/50	0/6/6/6
2	FAD	A	600	3,1	-	4/34/50/50	0/6/6/6

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4X-N5	4.69	1.39	1.30
2	B	600	FAD	C4X-N5	4.55	1.39	1.30
2	B	600	FAD	C2A-N1A	3.19	1.39	1.33
2	A	600	FAD	C8A-N7A	3.01	1.37	1.31
2	B	600	FAD	C10-N1	2.91	1.39	1.33

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	DPK	C9N-N9-C10	7.02	119.16	110.20
3	A	601	DPK	C9N-N9-C10	6.64	118.67	110.20
2	B	600	FAD	N3A-C2A-N1A	-6.00	119.22	128.60
2	B	600	FAD	C9A-C5X-N5	-5.22	116.75	122.43
2	A	600	FAD	C5A-C4A-N3A	-5.12	120.06	126.75

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	PA-O3P-P-O5'

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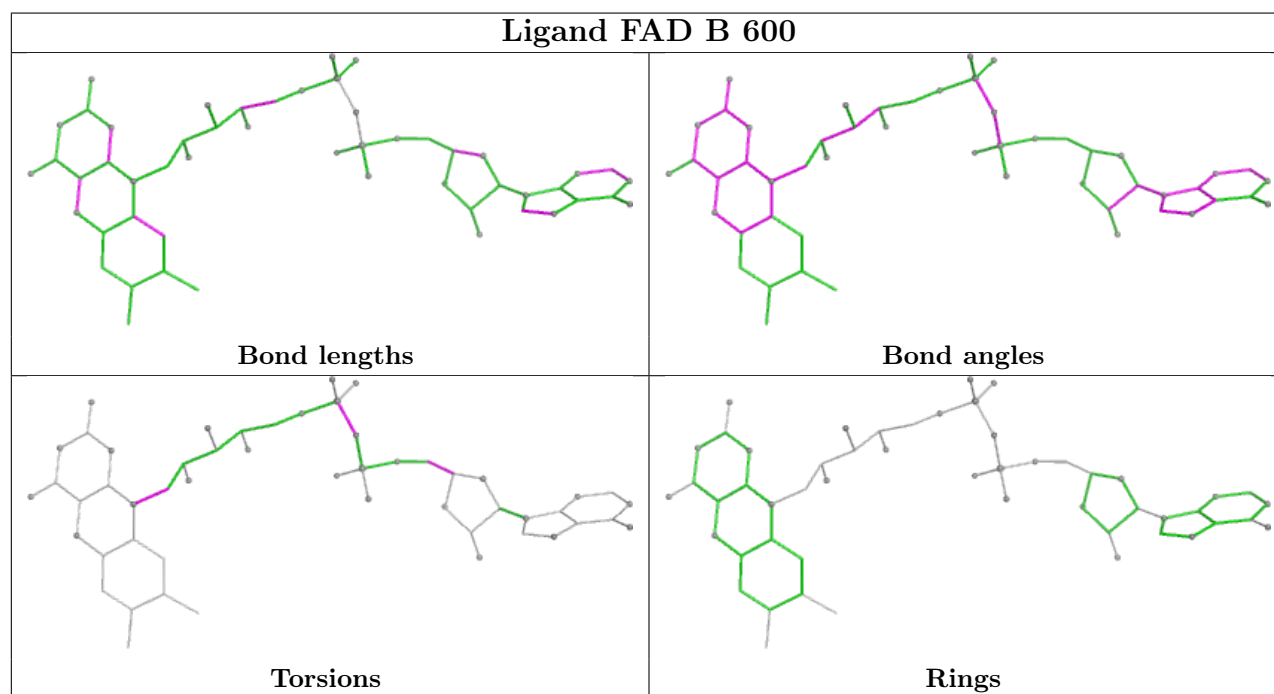
Mol	Chain	Res	Type	Atoms
3	A	601	DPK	C11-C10-N9-C9N
3	A	601	DPK	C11-C10-N9-C8

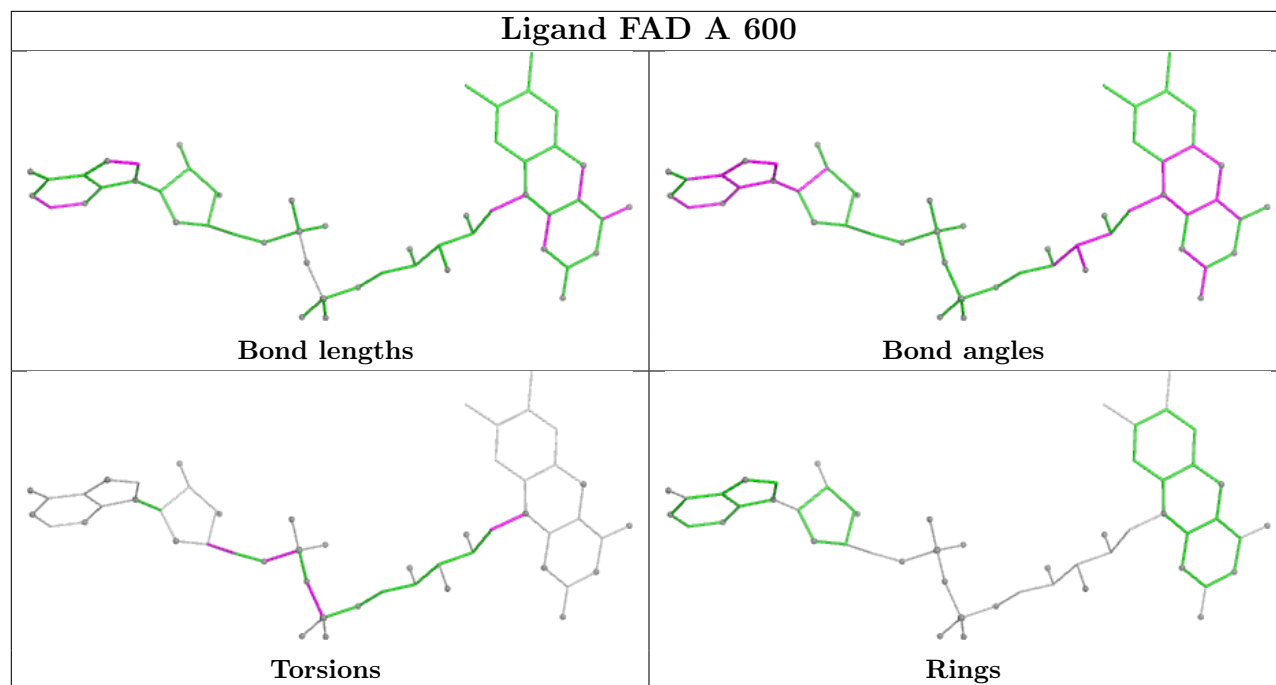
There are no ring outliers.

3 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	DPK	1	0
2	B	600	FAD	2	0
2	A	600	FAD	2	60

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 [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%)	2.76	355 (71%) 0 0	24, 31, 46, 64	0
1	B	494/520 (95%)	3.00	378 (76%) 0 0	23, 31, 42, 60	0
All	All	993/1040 (95%)	2.88	733 (73%) 0 0	23, 31, 44, 64	0

The worst 5 of 733 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	13.6
1	B	212	GLY	11.1
1	B	495	LEU	9.2
1	B	496	ILE	8.6
1	A	496	ILE	7.3

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](#)

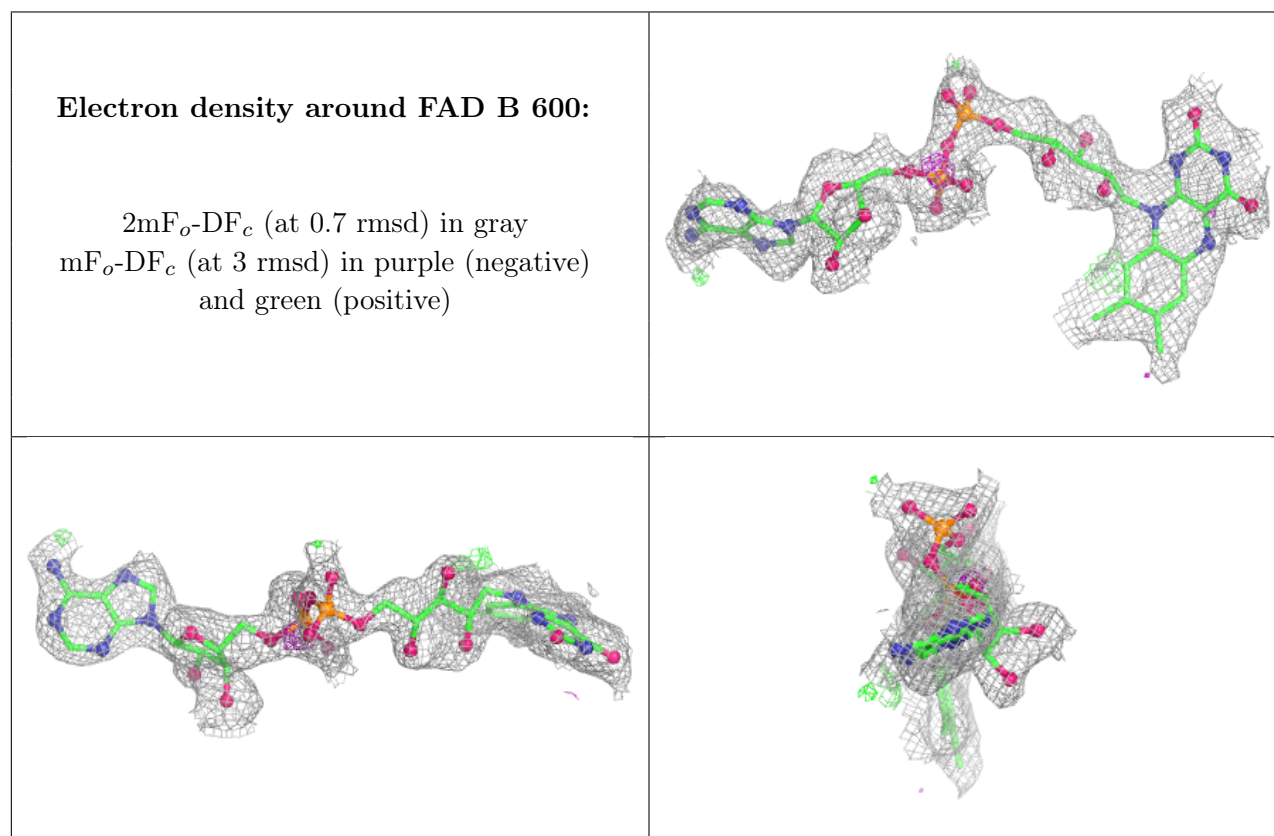
There are no oligosaccharides in this entry.

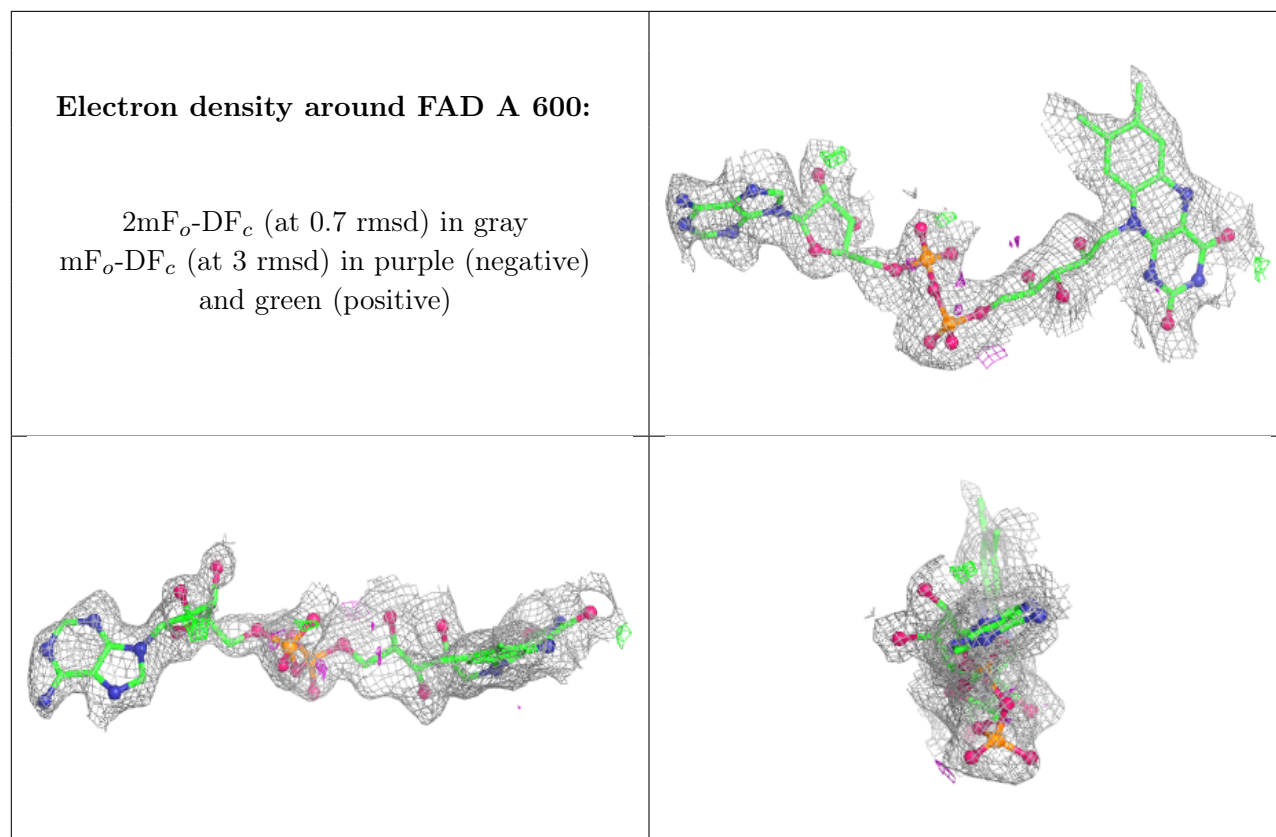
6.4 Ligands [i](#)

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, 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($\text{\AA}^2$)	Q<0.9
3	DPK	A	601	14/14	0.66	0.28	49,57,64,64	0
3	DPK	B	601	14/14	0.67	0.28	49,57,64,64	0
2	FAD	B	600	53/53	0.81	0.13	22,29,32,33	0
2	FAD	A	600	53/53	0.83	0.15	23,29,32,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.