



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:27 AM UTC

PDB ID : 1S3B / pdb_00001s3b
Title : Crystal structure of MAOB in complex with N-methyl-N-propargyl-1(R)-aminindan
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 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

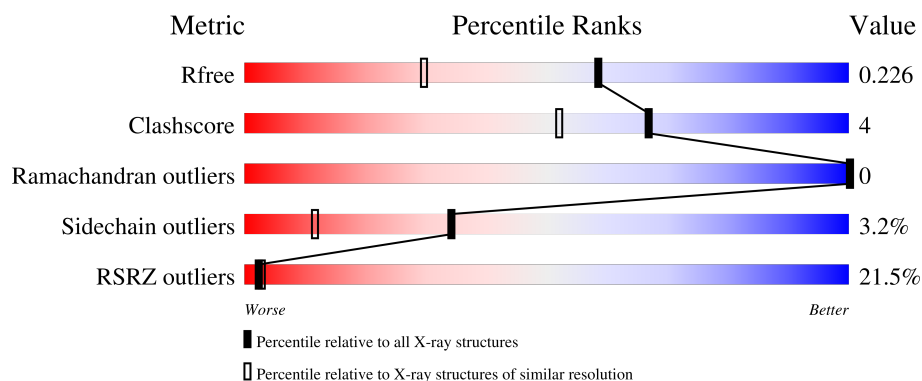
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	21% 88% 7% . .
1	B	520	20% 86% 8% . 5%

2 Entry composition [i](#)

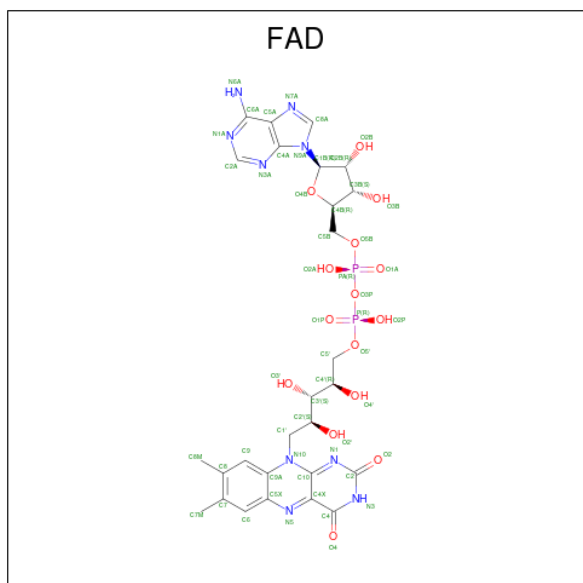
There are 4 unique types of molecules in this entry. The entry contains 8864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

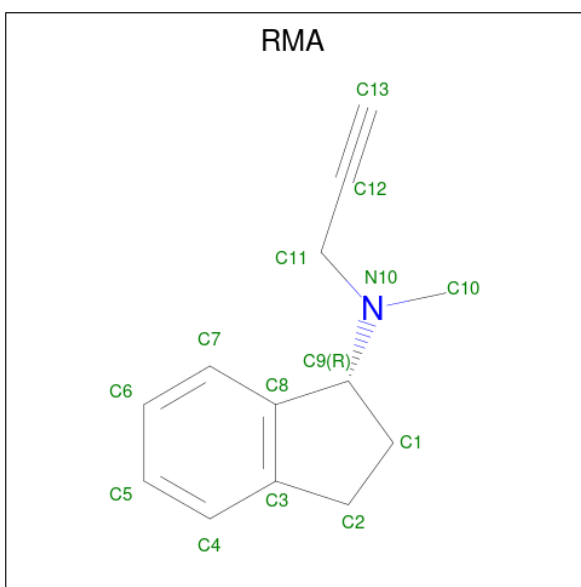
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3971	2538	681	728	24			
1	B	494	Total	C	N	O	S	0	0	0
			3940	2519	676	721	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (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 N-[(1S)-2,3-DIHYDRO-1H-INDEN-1-YL]-N-METHYL-N-PROP-2-YNYLAMINE (CCD ID: RMA) (formula: $C_{13}H_{15}N$).



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		

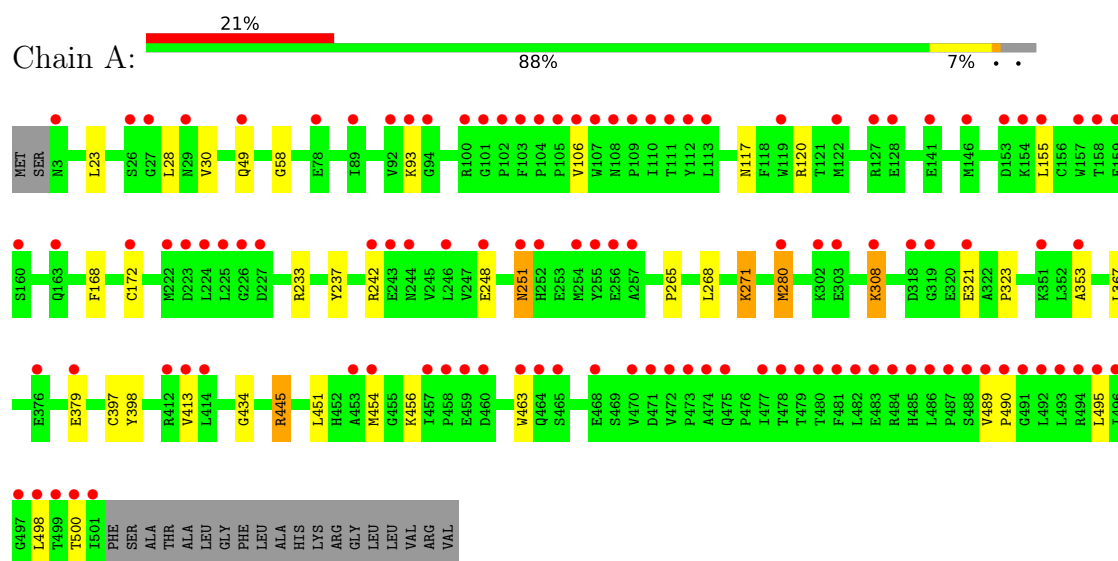
- Molecule 4 is water.

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

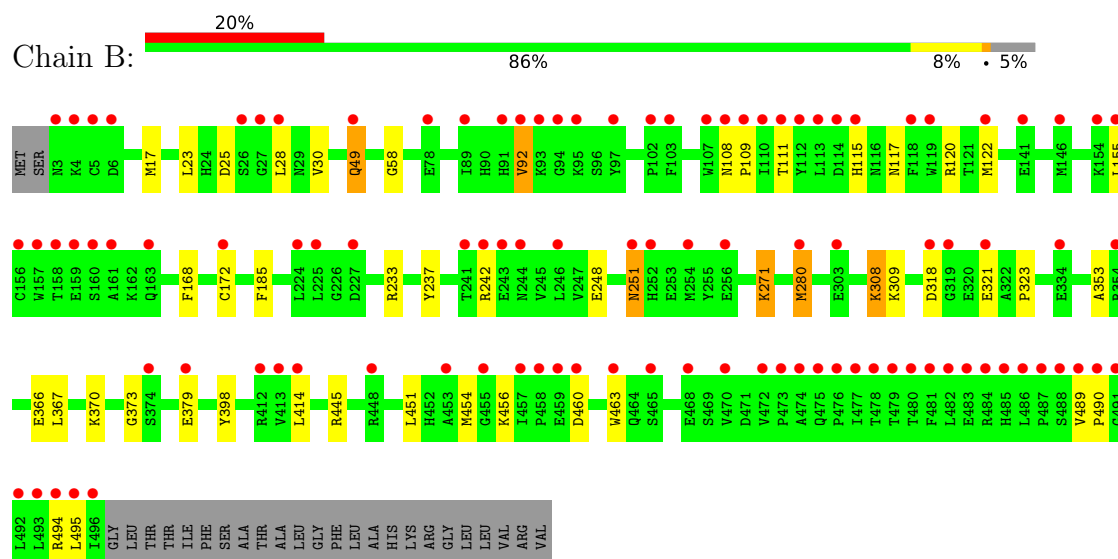
3 Residue-property plots

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



4 Data and refinement statistics

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 15.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-1.65) 97.9 (15.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.223 0.207 , 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)	0.42 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, RMA

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	0.46	0/4068	0.78	0/5522
1	B	0.44	1/4037 (0.0%)	0.76	0/5479
All	All	0.45	1/8105 (0.0%)	0.77	0/11001

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	MET	SD-CE	-6.15	1.64	1.79

There are no bond angle outliers.

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	27	0
1	B	3940	0	3937	34	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	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8864	0	7992	59	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 4.

All (59) 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	1.67	0.75
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.69	0.73
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:HD22	1:B:251:ASN:H	1.44	0.66
1:B:92:VAL:CB	1:B:318:ASP:OD2	2.44	0.65
1:A:251:ASN:HD22	1:A:251:ASN:H	1.43	0.64
1:A:451:LEU:HA	1:A:454:MET:HE2	1.80	0.63
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:B:321:GLU:H	1:B:321:GLU:CD	2.17	0.53
1:A:321:GLU:H	1:A:321:GLU:CD	2.15	0.52
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:58:GLY:HA2	2:A:600:FAD:C4X	2.44	0.48
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:A:280:MET:HE1	1:B:353:ALA:HB1	1.97	0.46
1:A:280:MET:HE2	1:A:280:MET:HB3	1.83	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:HB2	1:B:308:LYS:HE2	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:B:280:MET:HE2	1:B:280:MET:HB3	1.80	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:353:ALA:HB1	1:B:280:MET:HE1	1.99	0.43
1:B:454:MET:HE3	1:B:456:LYS:HG3	2.01	0.43
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.12	0.43
1:A:251:ASN:H	1:A:251:ASN:ND2	2.13	0.43
1:B:251:ASN:H	1:B:251:ASN:ND2	2.13	0.43
1:B:122:MET:HE1	1:B:185:PHE:HE2	1.85	0.42
1:A:172:CYS:SG	3:A:601:RMA:H6	2.59	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:A:454:MET:HE3	1:A:456:LYS:HG3	2.02	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 ⓘ

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%)	411 (96%)	16 (4%)	30	8
1	B	424/444 (96%)	413 (97%)	11 (3%)	40	17
All	All	851/888 (96%)	824 (97%)	27 (3%)	34	12

All (27) 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	242	ARG
1	A	251	ASN
1	A	271	LYS
1	A	280	MET
1	A	308	LYS
1	A	379	GLU
1	A	397	CYS
1	A	413	VAL
1	A	445	ARG
1	A	495	LEU
1	A	498	LEU

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Mol	Chain	Res	Type
1	A	500	THR
1	B	49	GLN
1	B	92	VAL
1	B	155	LEU
1	B	242	ARG
1	B	251	ASN
1	B	271	LYS
1	B	280	MET
1	B	308	LYS
1	B	379	GLU
1	B	460	ASP
1	B	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	244	ASN
1	A	251	ASN
1	B	117	ASN
1	B	145	ASN
1	B	244	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 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
2	FAD	A	600	3,1	58,58,58	1.08	5 (8%)	85,89,89	1.57	15 (17%)
3	RMA	A	601	2	14,15,15	2.82	3 (21%)	15,20,20	8.64	7 (46%)
2	FAD	B	600	3,1	58,58,58	1.03	3 (5%)	85,89,89	1.59	16 (18%)
3	RMA	B	601	2	14,15,15	2.86	3 (21%)	15,20,20	8.56	7 (46%)

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	3,1	-	2/34/50/50	0/6/6/6
3	RMA	A	601	2	-	4/6/16/16	0/2/2/2
2	FAD	B	600	3,1	-	2/34/50/50	0/6/6/6
3	RMA	B	601	2	-	4/6/16/16	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	RMA	C10-N10	-8.17	1.29	1.46
3	A	601	RMA	C10-N10	-8.13	1.29	1.46
3	B	601	RMA	C11-C12	5.00	1.54	1.46
3	A	601	RMA	C11-C12	4.86	1.54	1.46
3	B	601	RMA	C12-C13	4.16	1.30	1.18
3	A	601	RMA	C12-C13	4.09	1.30	1.18
2	A	600	FAD	C4X-N5	3.97	1.39	1.30
2	B	600	FAD	C4X-N5	3.78	1.38	1.30
2	A	600	FAD	C10-N1	3.01	1.39	1.33
2	B	600	FAD	C10-N1	2.64	1.38	1.33
2	B	600	FAD	C2A-N1A	2.55	1.38	1.33
2	A	600	FAD	C2A-N1A	2.54	1.38	1.33
2	A	600	FAD	C2A-N3A	2.11	1.37	1.33
2	A	600	FAD	C8A-N7A	2.09	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	RMA	C11-C12-C13	-32.33	125.19	177.63
3	B	601	RMA	C11-C12-C13	-31.98	125.76	177.63
2	A	600	FAD	N3A-C2A-N1A	-5.68	119.98	128.58
2	B	600	FAD	N3A-C2A-N1A	-5.66	120.02	128.58
3	A	601	RMA	C12-C11-N10	5.24	121.69	112.19
3	B	601	RMA	C12-C11-N10	5.07	121.39	112.19
2	B	600	FAD	C9A-C5X-N5	-4.19	118.00	122.45
2	B	600	FAD	N9A-C8A-N7A	-4.10	108.12	113.94
2	A	600	FAD	N9A-C8A-N7A	-3.97	108.30	113.94
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	C5A-C4A-N3A	-3.44	121.98	126.72
2	A	600	FAD	C5A-C4A-N3A	-3.40	122.04	126.72
2	A	600	FAD	C9A-C5X-N5	-3.39	118.85	122.45
2	B	600	FAD	C5A-N7A-C8A	3.39	108.78	103.45
2	A	600	FAD	C5A-N7A-C8A	3.33	108.68	103.45
2	A	600	FAD	C4-N3-C2	-3.09	120.15	125.64
2	A	600	FAD	C9A-N10-C10	-3.07	116.07	120.75
2	A	600	FAD	C2A-N3A-C4A	2.96	119.06	111.83
2	B	600	FAD	C9A-N10-C10	-2.92	116.30	120.75
2	B	600	FAD	C2A-N3A-C4A	2.91	118.94	111.83
3	B	601	RMA	C6-C7-C8	-2.88	117.53	120.99
2	A	600	FAD	C4X-C4-N3	2.75	120.25	113.25
2	B	600	FAD	C4-N3-C2	-2.72	120.81	125.64
3	A	601	RMA	C6-C7-C8	-2.71	117.75	120.99
2	A	600	FAD	C5'-C4'-C3'	-2.68	107.16	112.22
3	A	601	RMA	C2-C1-C9	2.65	108.58	105.91
2	B	600	FAD	C4X-C4-N3	2.61	119.89	113.25
2	A	600	FAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	A	600	FAD	C10-C4X-N5	-2.58	119.53	124.81
3	B	601	RMA	C2-C1-C9	2.56	108.49	105.91
3	B	601	RMA	C3-C8-C9	2.54	112.22	110.62
2	B	600	FAD	C5'-C4'-C3'	-2.52	107.46	112.22
2	B	600	FAD	C10-C4X-N5	-2.48	119.75	124.81
3	A	601	RMA	C3-C8-C9	2.46	112.17	110.62
2	B	600	FAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	B	600	FAD	O4-C4-C4X	-2.35	120.32	126.53
3	B	601	RMA	C5-C4-C3	-2.24	117.59	120.88
2	B	600	FAD	C4A-N9A-C8A	2.20	108.05	105.74
2	A	600	FAD	C4-C4X-N5	2.18	121.22	118.21
2	B	600	FAD	N3A-C4A-N9A	2.17	130.85	127.17
2	A	600	FAD	O4-C4-C4X	-2.12	120.94	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4-C4X-N5	2.11	121.12	118.21
2	A	600	FAD	C4A-N9A-C8A	2.10	107.94	105.74
3	A	601	RMA	C5-C4-C3	-2.01	117.94	120.88

There are no chirality outliers.

All (12) torsion outliers are listed below:

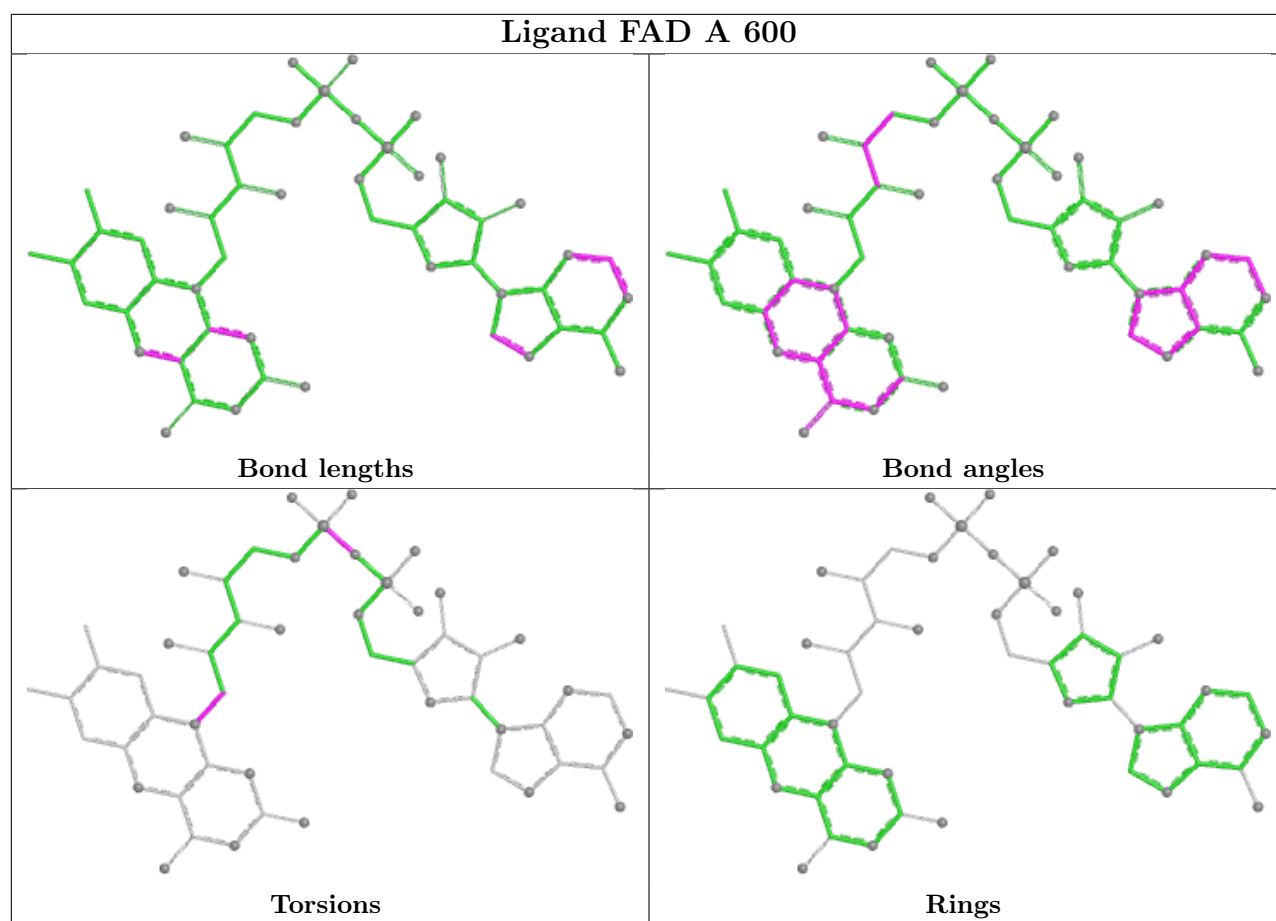
Mol	Chain	Res	Type	Atoms
3	A	601	RMA	C12-C11-N10-C10
3	A	601	RMA	C12-C11-N10-C9
3	A	601	RMA	C8-C9-N10-C11
3	B	601	RMA	C12-C11-N10-C10
3	B	601	RMA	C12-C11-N10-C9
2	B	600	FAD	PA-O3P-P-O5'
3	B	601	RMA	C1-C9-N10-C11
2	A	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	C2'-C1'-N10-C10
3	B	601	RMA	C8-C9-N10-C11
2	A	600	FAD	PA-O3P-P-O5'
3	A	601	RMA	C1-C9-N10-C11

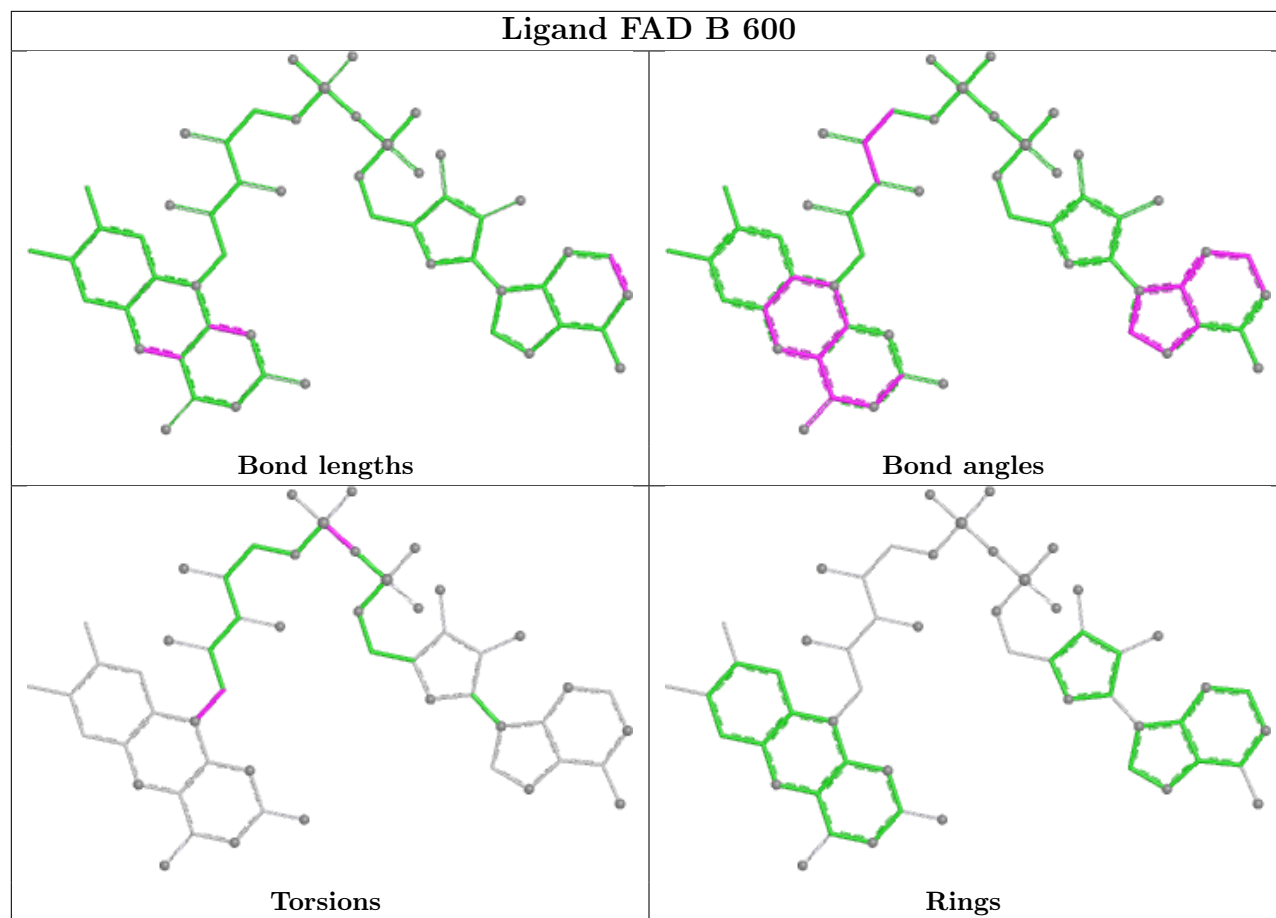
There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/520 (95%)	1.24	111 (22%) 2 3	28, 37, 55, 78	0
1	B	494/520 (95%)	1.27	102 (20%) 2 3	28, 37, 52, 72	0
All	All	993/1040 (95%)	1.26	213 (21%) 2 3	28, 37, 53, 78	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	ILE	8.1
1	B	495	LEU	6.8
1	A	501	ILE	6.4
1	B	92	VAL	6.3
1	B	481	PHE	5.7
1	B	157	TRP	5.4
1	A	497	GLY	5.3
1	A	103	PHE	5.3
1	A	252	HIS	5.2
1	B	103	PHE	5.2
1	A	498	LEU	5.1
1	A	480	THR	5.0
1	A	481	PHE	5.0
1	B	493	LEU	4.9
1	B	494	ARG	4.9
1	A	460	ASP	4.9
1	B	482	LEU	4.8
1	B	107	TRP	4.8
1	B	93	LYS	4.8
1	A	111	THR	4.8
1	A	500	THR	4.7
1	A	479	THR	4.7
1	A	482	LEU	4.7
1	B	89	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	95	LYS	4.7
1	B	49	GLN	4.6
1	A	499	THR	4.5
1	A	107	TRP	4.5
1	B	110	ILE	4.5
1	B	492	LEU	4.5
1	A	413	VAL	4.4
1	B	460	ASP	4.4
1	A	486	LEU	4.4
1	B	489	VAL	4.3
1	A	470	VAL	4.2
1	A	492	LEU	4.2
1	B	119	TRP	4.2
1	B	254	MET	4.2
1	B	3	ASN	4.2
1	B	158	THR	4.2
1	A	157	TRP	4.1
1	B	243	GLU	4.1
1	A	496	ILE	4.0
1	B	224	LEU	4.0
1	B	112	TYR	4.0
1	B	252	HIS	4.0
1	A	92	VAL	4.0
1	A	224	LEU	3.9
1	A	319	GLY	3.9
1	A	494	ARG	3.9
1	A	227	ASP	3.9
1	B	490	PRO	3.9
1	B	479	THR	3.8
1	A	105	PRO	3.8
1	B	246	LEU	3.8
1	B	475	GLN	3.8
1	B	455	GLY	3.8
1	A	471	ASP	3.7
1	B	111	THR	3.7
1	A	495	LEU	3.7
1	A	493	LEU	3.7
1	B	155	LEU	3.7
1	A	89	ILE	3.6
1	A	109	PRO	3.6
1	B	172	CYS	3.6
1	A	489	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	118	PHE	3.6
1	B	26	SER	3.6
1	B	491	GLY	3.5
1	A	155	LEU	3.5
1	A	3	ASN	3.5
1	A	483	GLU	3.5
1	A	484	ARG	3.5
1	A	475	GLN	3.5
1	A	321	GLU	3.5
1	A	478	THR	3.5
1	B	474	ALA	3.4
1	A	49	GLN	3.4
1	B	227	ASP	3.3
1	B	318	ASP	3.3
1	B	303	GLU	3.3
1	A	93	LYS	3.3
1	B	473	PRO	3.3
1	A	488	SER	3.2
1	B	244	ASN	3.2
1	A	154	LYS	3.2
1	B	485	HIS	3.2
1	B	321	GLU	3.2
1	A	474	ALA	3.2
1	B	141	GLU	3.2
1	B	457	ILE	3.1
1	B	486	LEU	3.1
1	B	319	GLY	3.1
1	B	241	THR	3.1
1	A	477	ILE	3.1
1	B	154	LYS	3.1
1	B	242	ARG	3.1
1	B	160	SER	3.1
1	A	491	GLY	3.1
1	A	254	MET	3.1
1	B	122	MET	3.1
1	A	29	ASN	3.0
1	A	243	GLU	3.0
1	B	379	GLU	3.0
1	B	94	GLY	3.0
1	B	114	ASP	2.9
1	B	413	VAL	2.9
1	A	487	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	112	TYR	2.9
1	A	414	LEU	2.9
1	A	110	ILE	2.9
1	B	476	PRO	2.9
1	A	141	GLU	2.9
1	A	251	ASN	2.9
1	B	97	TYR	2.9
1	A	101	GLY	2.9
1	A	242	ARG	2.9
1	B	113	LEU	2.9
1	B	251	ASN	2.9
1	A	473	PRO	2.8
1	B	109	PRO	2.8
1	B	463	TRP	2.8
1	A	226	GLY	2.8
1	A	246	LEU	2.8
1	B	477	ILE	2.8
1	A	412	ARG	2.7
1	B	27	GLY	2.7
1	B	484	ARG	2.7
1	A	128	GLU	2.7
1	A	244	ASN	2.7
1	A	113	LEU	2.7
1	A	303	GLU	2.7
1	B	280	MET	2.7
1	B	354	ARG	2.6
1	B	78	GLU	2.6
1	A	102	PRO	2.6
1	B	374	SER	2.6
1	B	488	SER	2.6
1	B	472	VAL	2.6
1	A	490	PRO	2.6
1	B	483	GLU	2.6
1	B	480	THR	2.5
1	A	472	VAL	2.5
1	B	459	GLU	2.5
1	B	91	HIS	2.5
1	A	122	MET	2.5
1	A	100	ARG	2.5
1	A	256	GLU	2.5
1	B	487	PRO	2.5
1	A	308	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	351	LYS	2.5
1	B	108	ASN	2.5
1	A	223	ASP	2.5
1	A	104	PRO	2.5
1	B	412	ARG	2.5
1	A	302	LYS	2.4
1	A	159	GLU	2.4
1	B	163	GLN	2.4
1	A	318	ASP	2.4
1	A	459	GLU	2.4
1	A	94	GLY	2.4
1	A	225	LEU	2.4
1	A	158	THR	2.4
1	A	465	SER	2.4
1	A	485	HIS	2.4
1	A	26	SER	2.3
1	A	172	CYS	2.3
1	A	458	PRO	2.3
1	B	458	PRO	2.3
1	B	159	GLU	2.3
1	A	153	ASP	2.3
1	A	353	ALA	2.3
1	B	4	LYS	2.3
1	A	457	ILE	2.3
1	A	27	GLY	2.3
1	B	5	CYS	2.3
1	A	280	MET	2.3
1	B	115	HIS	2.3
1	A	78	GLU	2.3
1	B	28	LEU	2.3
1	B	414	LEU	2.3
1	A	127	ARG	2.3
1	B	448	ARG	2.3
1	A	255	TYR	2.3
1	A	119	TRP	2.2
1	A	163	GLN	2.2
1	A	379	GLU	2.2
1	A	108	ASN	2.2
1	B	334	GLU	2.2
1	B	470	VAL	2.2
1	A	463	TRP	2.2
1	A	160	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	ASP	2.2
1	A	146	MET	2.2
1	A	248	GLU	2.2
1	B	256	GLU	2.2
1	A	454	MET	2.2
1	B	102	PRO	2.2
1	B	478	THR	2.2
1	A	257	ALA	2.1
1	B	146	MET	2.1
1	A	106	VAL	2.1
1	B	156	CYS	2.1
1	A	464	GLN	2.1
1	A	453	ALA	2.1
1	B	161	ALA	2.1
1	B	453	ALA	2.1
1	A	376	GLU	2.1
1	B	465	SER	2.1
1	A	222	MET	2.0
1	B	225	LEU	2.0
1	A	468	GLU	2.0
1	B	468	GLU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

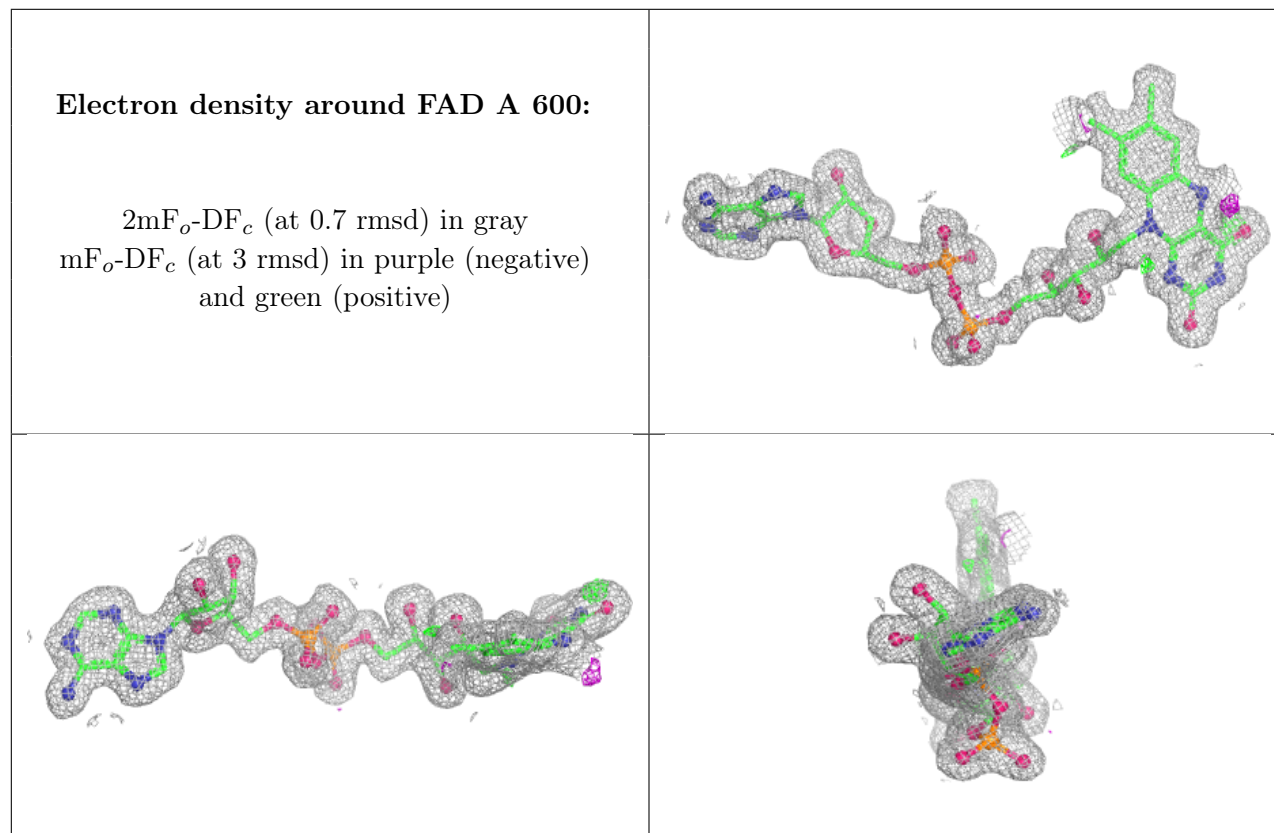
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RMA	A	601	14/14	0.88	0.13	37,43,44,44	0
3	RMA	B	601	14/14	0.91	0.11	38,42,43,44	0

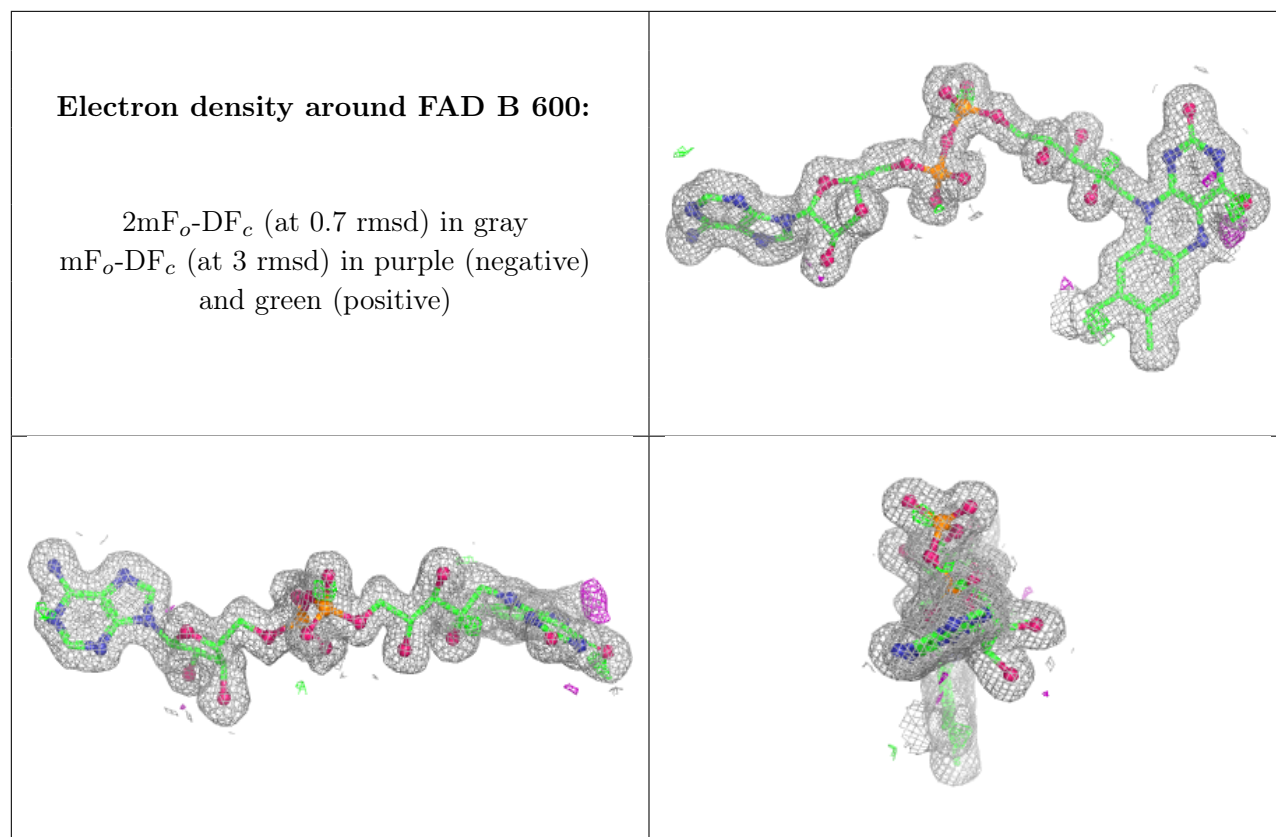
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	600	53/53	0.98	0.07	29,31,33,33	0
2	FAD	B	600	53/53	0.98	0.07	28,31,33,33	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.