Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:08 am BST

PDB ID	:	1S3E
Title	:	Crystal structure of MAOB in complex with 6-hydroxy-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	:	1.60 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:

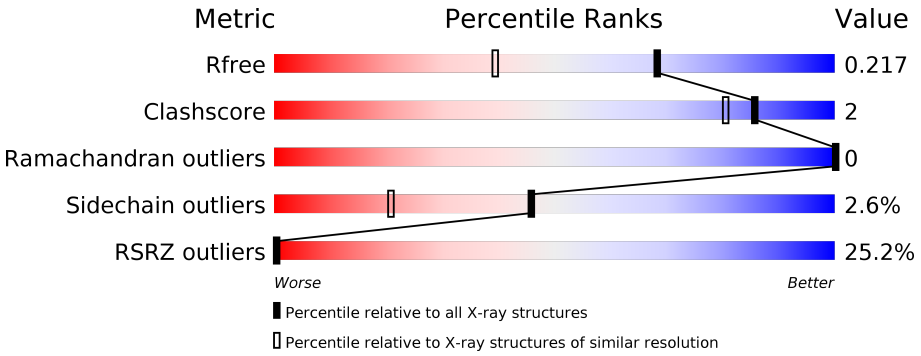
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	23% 91%
1	B	520	25% 89% 5% 5%

2 Entry composition

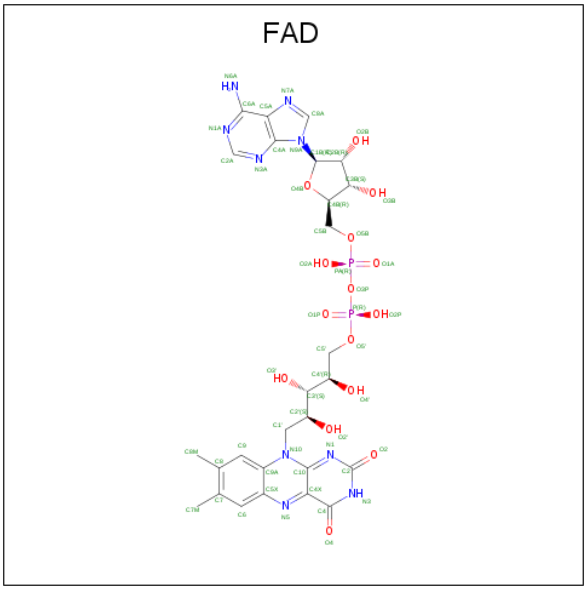
There are 4 unique types of molecules in this entry. The entry contains 8838 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

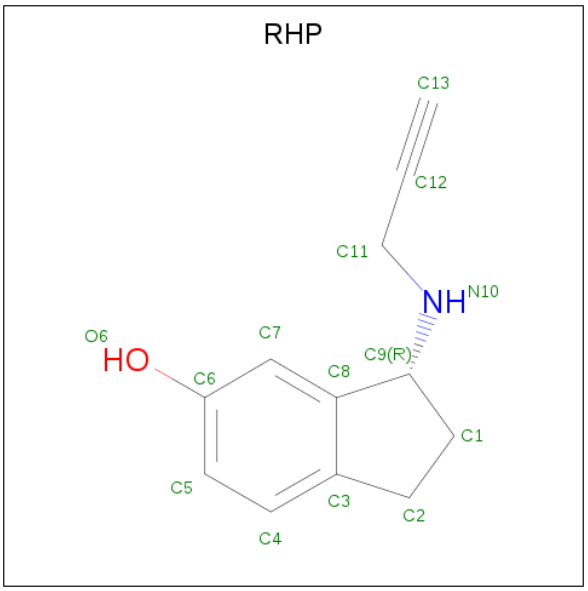
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	1	0
			3972	2538	681	728	25			
1	B	494	Total	C	N	O	S	0	1	0
			3941	2519	676	721	25			

- 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 (3R)-3-(PROP-2-YNYLAMINO)INDAN-5-OL (three-letter code: RHP) (formula: $C_{12}H_{13}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 12 1 1	0	0
3	B	1	Total C N O 14 12 1 1	0	0

- Molecule 4 is water.

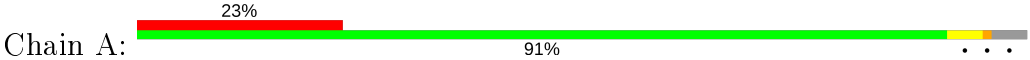
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	359	Total O 359 359	0	0
4	B	432	Total O 432 432	0	0

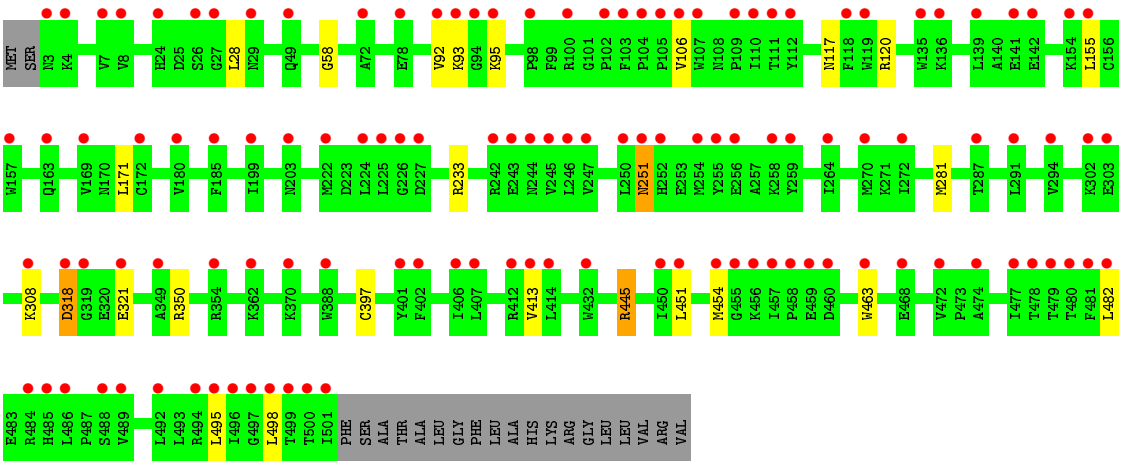
3 Residue-property plots (i)

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

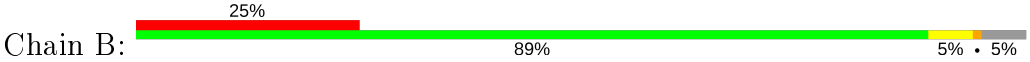
Chain A:

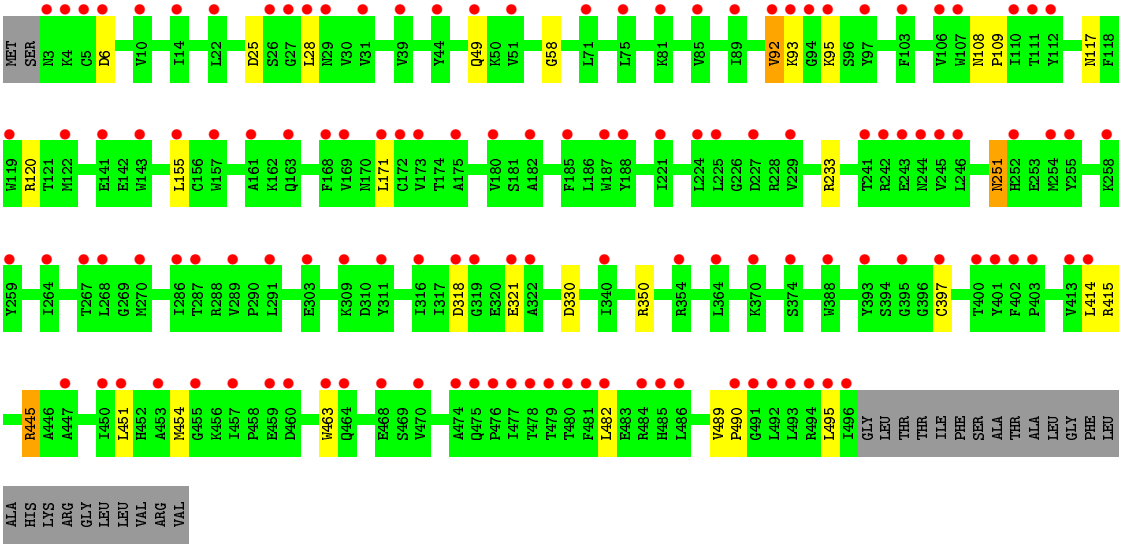




- Molecule 1: Amine oxidase [flavin-containing] B

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.96Å 224.06Å 86.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 47.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.6 (15.00-1.60) 88.6 (47.04-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.216 0.199 , 0.217	Depositor DCC
R_{free} test set	3823 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 76.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: RHP, 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	0.36	0/4074	0.64	3/5530 (0.1%)
1	B	0.36	0/4043	0.64	4/5487 (0.1%)
All	All	0.36	0/8117	0.64	7/11017 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	445	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	445	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	445	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	445	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	6	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	330	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	318	ASP	CB-CG-OD2	5.15	122.93	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	3972	0	3968	16	0
1	B	3941	0	3938	19	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	1	0
2	B	53	0	29	1	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
4	A	359	0	0	1	0
4	B	432	0	0	4	0
All	All	8838	0	7990	35	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (35) 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	4:B:1022:HOH:O	1.55	1.06
1:A:117:ASN:HD22	1:A:120:ARG:HH21	1.39	0.69
1:B:117:ASN:HD22	1:B:120:ARG:HH21	1.39	0.68
1:B:251:ASN:H	1:B:251:ASN:HD22	1.43	0.66
1:A:251:ASN:H	1:A:251:ASN:HD22	1.43	0.66
1:A:445:ARG:HD2	1:A:463:TRP:CH2	2.34	0.63
1:B:445:ARG:HD2	1:B:463:TRP:CH2	2.34	0.61
1:B:445:ARG:HD3	4:B:602:HOH:O	2.01	0.61
1:A:451:LEU:HD23	1:A:454:MET:HE1	1.83	0.58
1:B:451:LEU:HD23	1:B:454:MET:HE1	1.86	0.56
1:B:445:ARG:HD2	1:B:463:TRP:CZ2	2.42	0.54
1:B:233:ARG:HG3	1:B:251:ASN:HD21	1.73	0.53
1:A:445:ARG:HD3	4:A:628:HOH:O	2.09	0.52
1:A:445:ARG:HD2	1:A:463:TRP:CZ2	2.44	0.51
1:A:233:ARG:HG3	1:A:251:ASN:HD21	1.76	0.51
1:B:414:LEU:HD12	4:B:859:HOH:O	2.12	0.49
1:A:321:GLU:H	1:A:321:GLU:CD	2.20	0.46
1:B:321:GLU:CD	1:B:321:GLU:H	2.19	0.45
1:B:454:MET:HB2	1:B:454:MET:HE2	1.56	0.45
1:A:58:GLY:HA2	2:A:600:FAD:C4X	2.47	0.44
1:A:171:LEU:HD21	3:A:601:RHP:H21	1.99	0.44
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.88	0.44
1:A:28:LEU:HD11	1:A:454:MET:HE1	2.00	0.43
1:A:308:LYS:HB2	1:A:308:LYS:HE2	1.78	0.43
1:A:251:ASN:H	1:A:251:ASN:ND2	2.15	0.43
1:B:171:LEU:HD21	3:B:601:RHP:H21	2.00	0.42
1:B:28:LEU:HD11	1:B:454:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:HD22	1:A:120:ARG:NH2	2.11	0.42
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.50	0.42
1:B:117:ASN:HD22	1:B:120:ARG:NH2	2.13	0.41
1:B:415:ARG:NH1	4:B:897:HOH:O	2.52	0.41
1:B:251:ASN:H	1:B:251:ASN:ND2	2.15	0.41
1:A:454:MET:HB2	1:A:454:MET:HE2	1.57	0.41
1:B:489:VAL:N	1:B:490:PRO:HD2	2.36	0.41
1:A:281:MET:HB3	1:A:413:VAL:HG21	2.04	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]	1.59	0.61

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	498/520 (96%)	487 (98%)	11 (2%)	0	100	100
1	B	493/520 (95%)	481 (98%)	12 (2%)	0	100	100
All	All	991/1040 (95%)	968 (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	428/444 (96%)	416 (97%)	12 (3%)	43	18
1	B	425/444 (96%)	415 (98%)	10 (2%)	49	24
All	All	853/888 (96%)	831 (97%)	22 (3%)	46	21

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

Mol	Chain	Res	Type
1	A	92	VAL
1	A	93	LYS
1	A	95	LYS
1	A	106	VAL
1	A	155	LEU
1	A	251	ASN
1	A	318	ASP
1	A	350	ARG
1	A	397	CYS
1	A	482	LEU
1	A	495	LEU
1	A	498	LEU
1	B	92	VAL
1	B	93	LYS
1	B	95	LYS
1	B	155	LEU
1	B	251	ASN
1	B	318	ASP
1	B	350	ARG
1	B	397	CYS
1	B	482	LEU
1	B	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

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	RHP	B	601	2	14,15,15	1.56	2 (14%)	17,20,20	4.13	4 (23%)
2	FAD	A	600	1,3	51,58,58	1.37	7 (13%)	60,89,89	1.63	9 (15%)
2	FAD	B	600	1,3	51,58,58	1.41	6 (11%)	60,89,89	1.65	9 (15%)
3	RHP	A	601	2	14,15,15	1.55	2 (14%)	17,20,20	4.11	4 (23%)

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	RHP	B	601	2	-	2/3/13/13	0/2/2/2
2	FAD	A	600	1,3	-	1/30/50/50	0/6/6/6
2	FAD	B	600	1,3	-	2/30/50/50	0/6/6/6
3	RHP	A	601	2	-	2/3/13/13	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C10-N1	4.50	1.39	1.33
2	A	600	FAD	C4X-N5	4.44	1.39	1.33
2	B	600	FAD	C4X-N5	4.36	1.39	1.33
2	A	600	FAD	C10-N1	4.30	1.38	1.33
3	B	601	RHP	C12-C13	4.14	1.30	1.18
3	A	601	RHP	C12-C13	4.12	1.30	1.18
2	B	600	FAD	C2A-N3A	3.65	1.38	1.32
2	A	600	FAD	C2A-N3A	3.51	1.37	1.32
3	A	601	RHP	C11-C12	3.40	1.54	1.46
3	B	601	RHP	C11-C12	3.35	1.53	1.46
2	B	600	FAD	C1'-N10	3.06	1.51	1.48
2	A	600	FAD	C4-N3	2.84	1.38	1.33
2	B	600	FAD	C4-N3	2.78	1.37	1.33
2	A	600	FAD	C1'-N10	2.67	1.51	1.48
2	B	600	FAD	C2A-N1A	2.42	1.38	1.33
2	A	600	FAD	C2A-N1A	2.36	1.38	1.33
2	A	600	FAD	C5X-N5	2.07	1.38	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	RHP	C11-C12-C13	-15.98	125.76	177.79
3	B	601	RHP	C11-C12-C13	-15.97	125.81	177.79
2	B	600	FAD	C4-N3-C2	6.73	120.83	115.14
2	A	600	FAD	C4-N3-C2	6.49	120.62	115.14
2	B	600	FAD	N3A-C2A-N1A	-5.40	120.23	128.68
2	A	600	FAD	N3A-C2A-N1A	-5.31	120.37	128.68
2	A	600	FAD	C9A-N10-C10	-4.28	116.31	121.91
2	B	600	FAD	C9A-N10-C10	-4.02	116.65	121.91
3	B	601	RHP	C5-C4-C3	-2.88	117.59	121.39
2	B	600	FAD	C10-C4X-N5	-2.85	119.28	121.26
2	B	600	FAD	C4X-N5-C5X	2.78	119.55	116.77
3	A	601	RHP	C5-C4-C3	-2.68	117.86	121.39
2	B	600	FAD	C4-C4X-N5	2.61	121.58	118.60
3	A	601	RHP	C11-N10-C9	2.58	119.05	113.85
2	B	600	FAD	C4X-C4-N3	-2.56	119.93	123.43
3	B	601	RHP	C11-N10-C9	2.55	119.00	113.85
2	A	600	FAD	C1'-N10-C9A	2.50	120.26	118.29
2	A	600	FAD	C4X-C4-N3	-2.46	120.06	123.43
2	B	600	FAD	C9A-C5X-N5	-2.42	118.58	122.36
3	A	601	RHP	C12-C11-N10	2.32	120.50	112.71
2	A	600	FAD	C4-C4X-N5	2.23	121.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	RHP	C12-C11-N10	2.22	120.18	112.71
2	A	600	FAD	C9A-C5X-N5	-2.19	118.94	122.36
2	A	600	FAD	C1B-N9A-C4A	-2.10	122.94	126.64
2	A	600	FAD	C10-C4X-N5	-2.10	119.81	121.26
2	B	600	FAD	C4A-C5A-N7A	-2.03	107.28	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

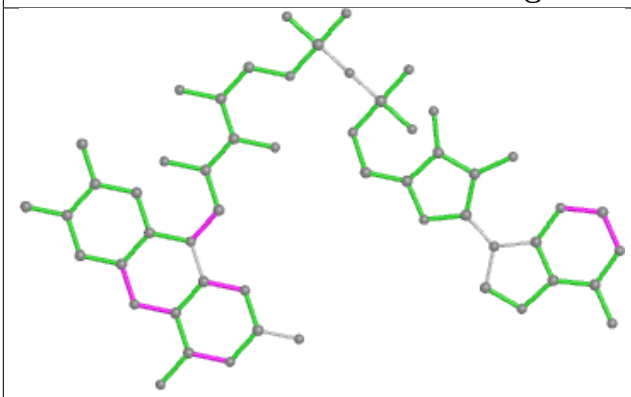
There are no ring outliers.

4 monomers are involved in 4 short contacts:

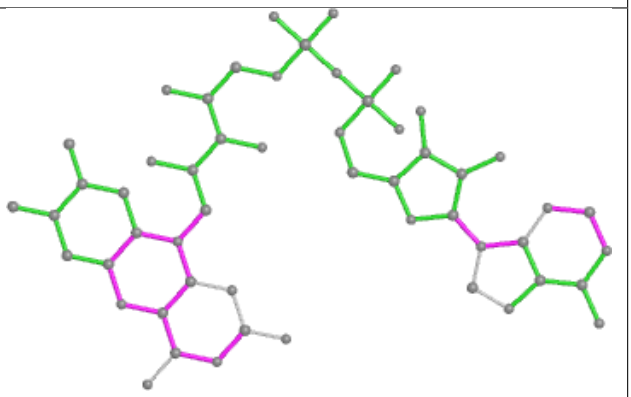
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	RHP	1	0
2	A	600	FAD	1	0
2	B	600	FAD	1	0
3	A	601	RHP	1	0

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 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.

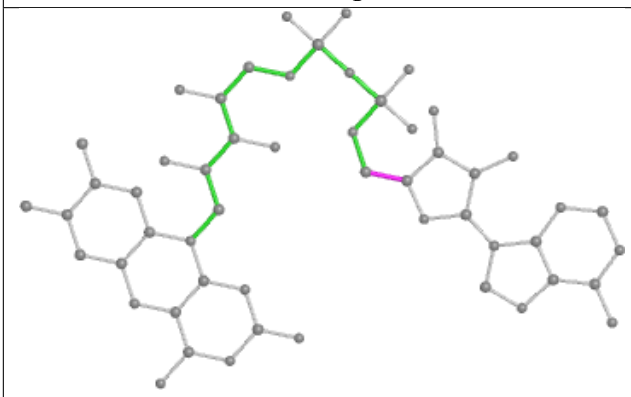
Ligand FAD A 600



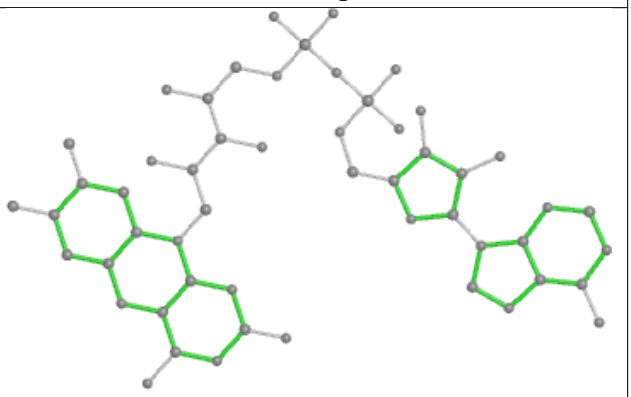
Bond lengths



Bond angles

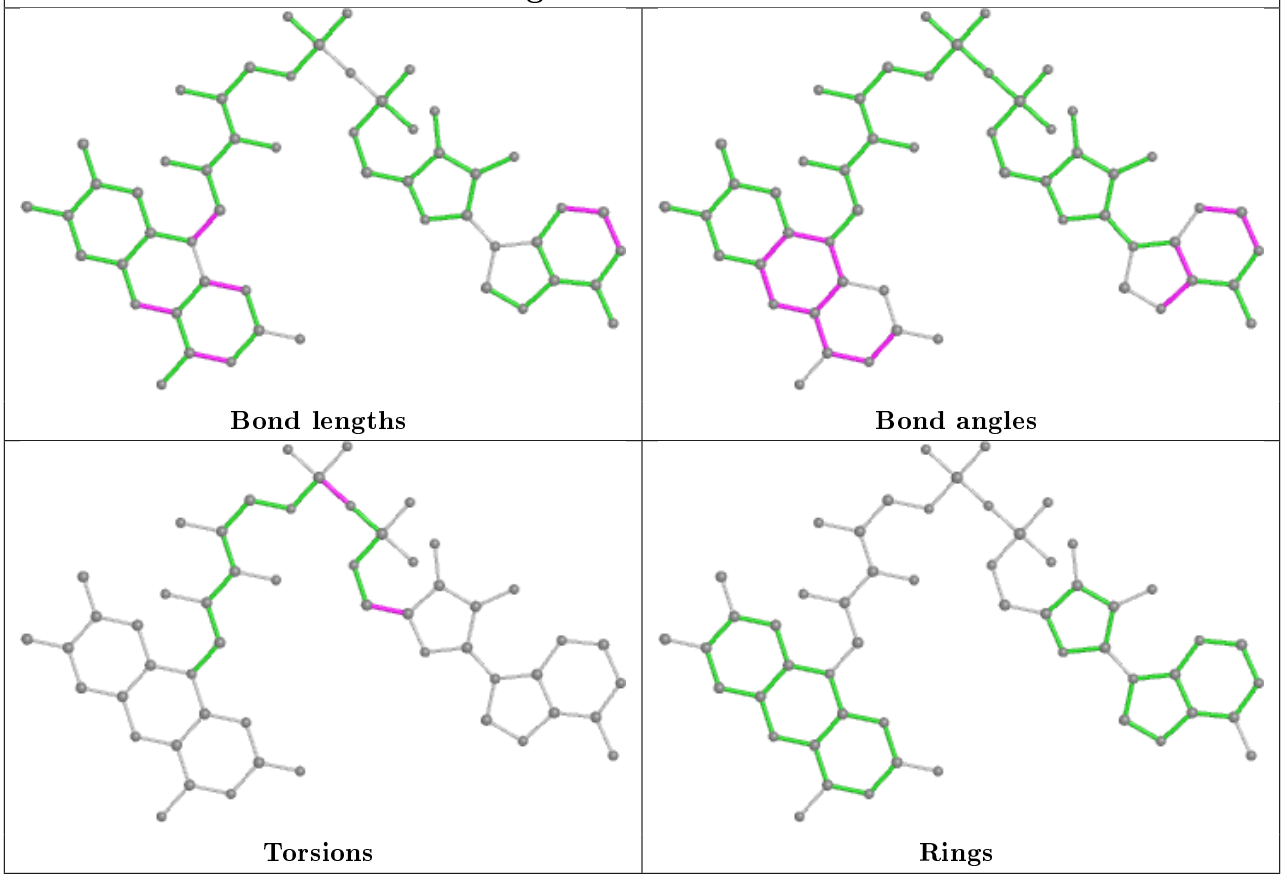


Torsions



Rings

Ligand FAD B 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%)	1.53	121 (24%)	0	0	28, 34, 51, 77	1 (0%)
1	B	494/520 (95%)	1.58	129 (26%)	0	0	26, 34, 48, 69	1 (0%)
All	All	993/1040 (95%)	1.55	250 (25%)	0	0	26, 34, 49, 77	2 (0%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	LEU	11.5
1	B	496	ILE	9.7
1	A	500	THR	9.6
1	A	499	THR	9.1
1	A	501	ILE	7.7
1	A	252	HIS	7.6
1	A	107	TRP	7.5
1	B	494	ARG	6.7
1	A	498	LEU	6.6
1	B	107	TRP	6.5
1	A	103	PHE	6.2
1	B	244	ASN	6.1
1	A	354	ARG	6.1
1	B	492	LEU	6.0
1	A	478	THR	5.9
1	B	481	PHE	5.9
1	A	246	LEU	5.6
1	B	243	GLU	5.6
1	B	242	ARG	5.6
1	B	482	LEU	5.6
1	A	482	LEU	5.5
1	B	252	HIS	5.3
1	A	496	ILE	5.3
1	A	479	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	243	GLU	5.0
1	B	93	LYS	5.0
1	B	493	LEU	4.8
1	A	480	THR	4.7
1	A	495	LEU	4.7
1	A	242	ARG	4.6
1	A	494	ARG	4.4
1	B	3	ASN	4.3
1	A	484	ARG	4.2
1	B	478	THR	4.2
1	B	459	GLU	4.1
1	B	157	TRP	4.1
1	A	4	LYS	4.0
1	A	3	ASN	4.0
1	A	106	VAL	4.0
1	A	92	VAL	3.9
1	A	251	ASN	3.9
1	B	119	TRP	3.9
1	A	93	LYS	3.8
1	B	303	GLU	3.8
1	A	226	GLY	3.8
1	B	103	PHE	3.7
1	B	491	GLY	3.7
1	B	490	PRO	3.7
1	A	49	GLN	3.7
1	A	459	GLU	3.7
1	A	105	PRO	3.7
1	A	227	ASP	3.6
1	B	95	LYS	3.6
1	B	354	ARG	3.6
1	B	110	ILE	3.6
1	A	110	ILE	3.6
1	B	49	GLN	3.5
1	B	475	GLN	3.5
1	A	497	GLY	3.5
1	A	458	PRO	3.4
1	A	451	LEU	3.4
1	B	453	ALA	3.4
1	B	27	GLY	3.4
1	B	414	LEU	3.4
1	A	302	LYS	3.4
1	B	254	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	481	PHE	3.3
1	B	5	CYS	3.3
1	A	112	TYR	3.3
1	B	479	THR	3.3
1	B	457	ILE	3.3
1	A	78	GLU	3.3
1	A	259	TYR	3.2
1	A	308	LYS	3.2
1	B	477	ILE	3.1
1	A	163	GLN	3.1
1	B	319	GLY	3.1
1	A	245	VAL	3.1
1	A	318	ASP	3.1
1	B	224	LEU	3.1
1	A	406	ILE	3.0
1	B	485	HIS	3.0
1	A	457	ILE	3.0
1	A	104	PRO	3.0
1	B	229	VAL	3.0
1	A	142	GLU	3.0
1	B	241	THR	3.0
1	B	4	LYS	3.0
1	A	486	LEU	3.0
1	B	92	VAL	3.0
1	A	460	ASP	2.9
1	B	267	THR	2.9
1	A	100	ARG	2.9
1	A	244	ASN	2.9
1	B	270	MET	2.9
1	B	318	ASP	2.9
1	B	28	LEU	2.9
1	B	289	VAL	2.9
1	B	450	ILE	2.9
1	A	119	TRP	2.9
1	A	468	GLU	2.9
1	A	454	MET	2.9
1	B	155	LEU	2.8
1	B	268	LEU	2.8
1	A	256	GLU	2.8
1	A	224	LEU	2.8
1	A	26	SER	2.8
1	B	112	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	393	TYR	2.8
1	A	169	VAL	2.8
1	A	321	GLU	2.8
1	A	349	ALA	2.7
1	B	39	VAL	2.7
1	A	118	PHE	2.7
1	B	225	LEU	2.7
1	B	246	LEU	2.7
1	B	480	THR	2.7
1	B	476	PRO	2.7
1	A	264	ILE	2.6
1	B	259	TYR	2.6
1	A	155	LEU	2.6
1	B	474	ALA	2.6
1	A	463	TRP	2.6
1	A	456	LYS	2.6
1	A	29	ASN	2.6
1	B	468	GLU	2.6
1	B	321	GLU	2.6
1	B	455	GLY	2.6
1	A	272	ILE	2.6
1	A	414	LEU	2.6
1	B	97	TYR	2.6
1	B	397	CYS	2.6
1	A	94	GLY	2.5
1	A	270	MET	2.5
1	B	163	GLN	2.5
1	A	102	PRO	2.5
1	B	168	PHE	2.5
1	A	319	GLY	2.5
1	B	264	ILE	2.5
1	A	492	LEU	2.5
1	A	154	LYS	2.5
1	B	402	PHE	2.5
1	A	157	TRP	2.5
1	B	31	VAL	2.5
1	B	169	VAL	2.5
1	B	340	ILE	2.5
1	A	488	SER	2.5
1	A	109	PRO	2.5
1	B	175	ALA	2.5
1	A	413	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	2.5
1	B	85	VAL	2.5
1	B	89	ILE	2.5
1	B	470	VAL	2.5
1	B	143	TRP	2.5
1	B	171	LEU	2.5
1	B	44	TYR	2.4
1	B	188	TYR	2.4
1	B	141	GLU	2.4
1	B	227	ASP	2.4
1	A	250	LEU	2.4
1	B	75	LEU	2.4
1	A	141	GLU	2.4
1	A	72	ALA	2.4
1	B	484	ARG	2.4
1	B	29	ASN	2.4
1	B	370	LYS	2.4
1	B	221	ILE	2.4
1	B	309	LYS	2.4
1	B	182	ALA	2.4
1	B	464	GLN	2.4
1	A	258	LYS	2.4
1	B	180	VAL	2.3
1	A	95	LYS	2.3
1	A	401	TYR	2.3
1	A	27	GLY	2.3
1	A	474	ALA	2.3
1	A	24	HIS	2.3
1	A	111	THR	2.3
1	B	51	VAL	2.3
1	B	245	VAL	2.3
1	B	291	LEU	2.3
1	B	286	ILE	2.3
1	B	122	MET	2.3
1	B	185	PHE	2.3
1	B	463	TRP	2.3
1	A	136	LYS	2.3
1	A	489	VAL	2.3
1	A	402	PHE	2.3
1	B	374	SER	2.3
1	A	455	GLY	2.3
1	B	173	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	LYS	2.3
1	B	111	THR	2.3
1	B	447	ALA	2.3
1	B	94	GLY	2.3
1	B	460	ASP	2.3
1	A	203	ASN	2.3
1	B	403	PRO	2.2
1	A	135	TRP	2.2
1	B	71	LEU	2.2
1	B	364	LEU	2.2
1	B	486	LEU	2.2
1	B	14	ILE	2.2
1	B	258	LYS	2.2
1	A	180	VAL	2.2
1	A	303	GLU	2.2
1	B	311	TYR	2.2
1	A	407	LEU	2.2
1	B	22	LEU	2.2
1	A	199	ILE	2.2
1	A	388	TRP	2.2
1	A	485	HIS	2.2
1	B	388	TRP	2.2
1	A	255	TYR	2.2
1	A	254	MET	2.2
1	B	6	ASP	2.2
1	B	26	SER	2.1
1	A	185	PHE	2.1
1	B	255	TYR	2.1
1	B	172[A]	CYS	2.1
1	B	316	ILE	2.1
1	A	432	TRP	2.1
1	B	395	GLY	2.1
1	A	477	ILE	2.1
1	A	222	MET	2.1
1	B	287	THR	2.1
1	B	413	VAL	2.1
1	A	139	LEU	2.1
1	A	412	ARG	2.1
1	A	450	ILE	2.1
1	B	400	THR	2.1
1	B	401	TYR	2.1
1	A	7	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	294	VAL	2.1
1	B	10	VAL	2.1
1	B	106	VAL	2.1
1	A	172[A]	CYS	2.1
1	A	287	THR	2.0
1	B	161	ALA	2.0
1	B	322	ALA	2.0
1	A	8	VAL	2.0
1	A	225	LEU	2.0
1	A	291	LEU	2.0
1	B	451	LEU	2.0
1	A	98	PRO	2.0
1	A	362	LYS	2.0
1	B	81	LYS	2.0
1	A	247	VAL	2.0
1	B	187	TRP	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.

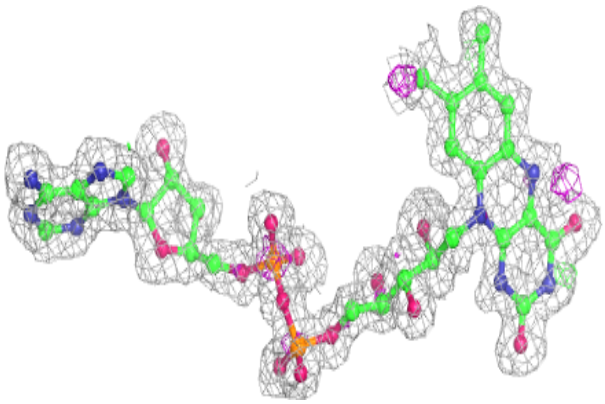
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RHP	B	601	14/14	0.67	0.25	38,44,45,46	0
3	RHP	A	601	14/14	0.77	0.21	38,44,45,46	0
2	FAD	A	600	53/53	0.91	0.14	27,29,31,31	0
2	FAD	B	600	53/53	0.94	0.14	27,29,31,31	0

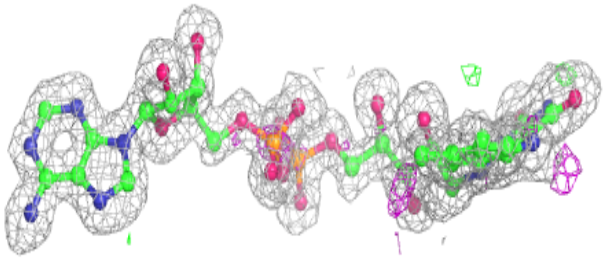
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

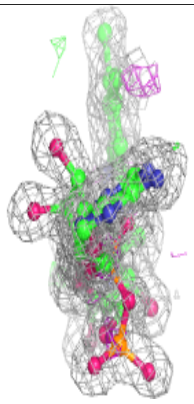
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

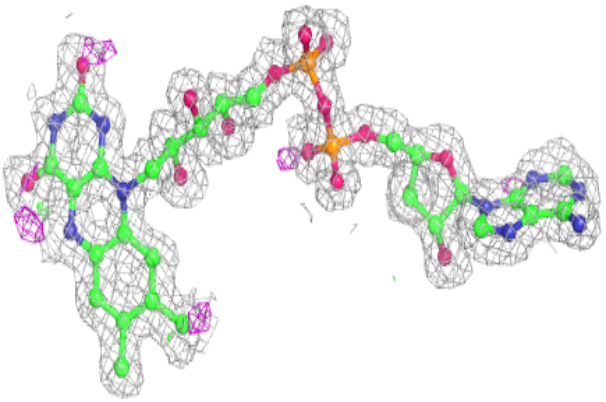


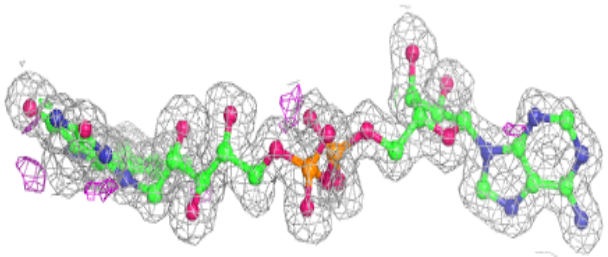


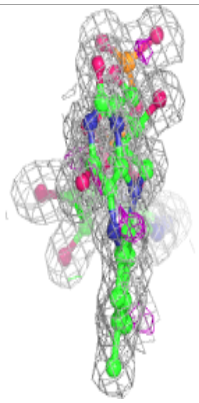


Electron density around FAD B 600:

$2mF_o$-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.