Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2024 – 10:26 pm BST

PDB ID	:	8QVT
Title	:	Crystal structure of Zea mays cytokinin oxidase/dehydrogenase 5 (ZmCKX5)
Authors	:	Kopecny, D.; Briozzo, P.
Deposited on	:	2023-10-18
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 (i) 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 (i)) were used in the production of this report:

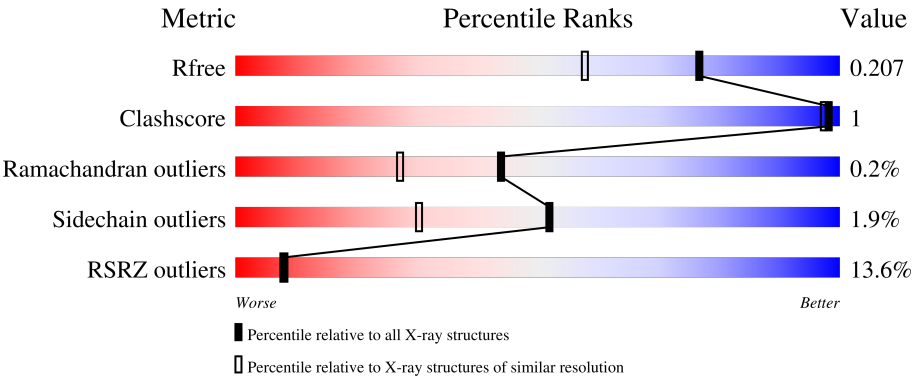
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (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 <=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	561	9% 89% · 8%
1	B	561	15% 87% · 11%

2 Entry composition

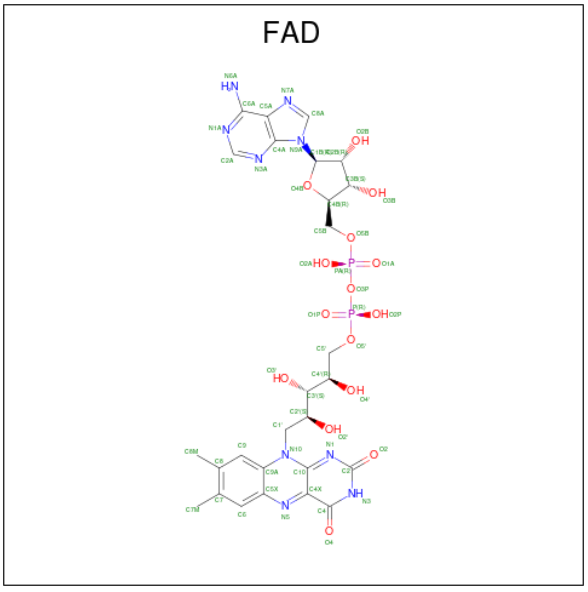
There are 5 unique types of molecules in this entry. The entry contains 8380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cytokinin dehydrogenase.

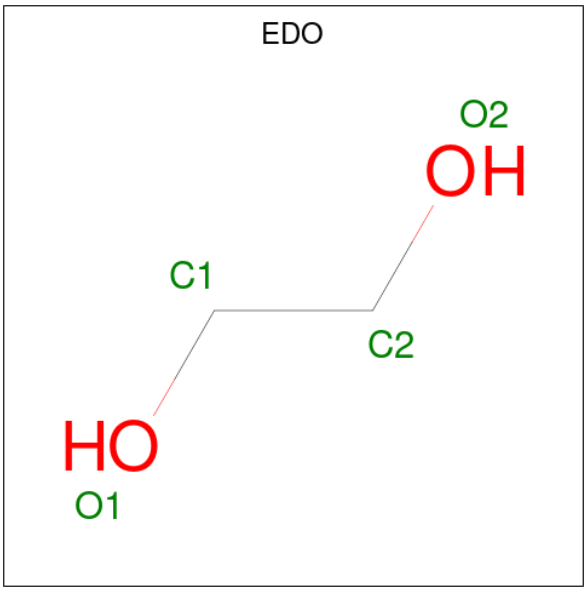
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	3	0
			3880	2428	706	735	11			
1	B	501	Total	C	N	O	S	0	2	0
			3785	2375	687	711	12			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



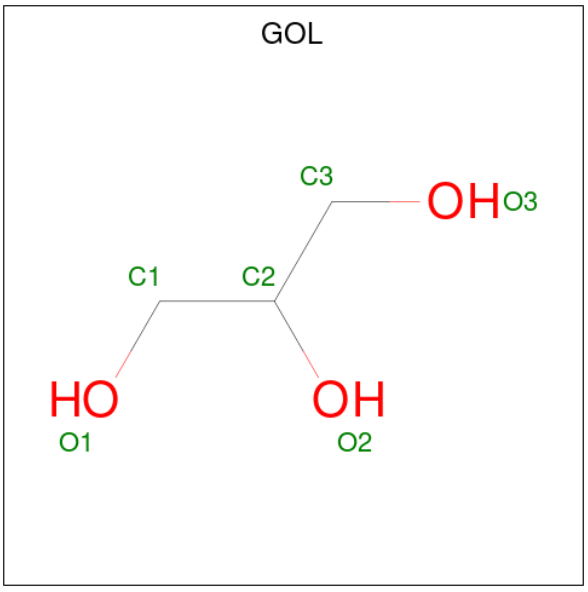
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

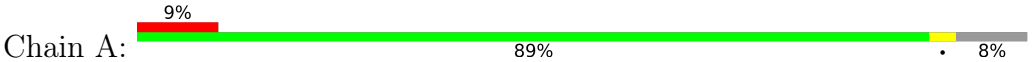
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	387	Total O 387 387	0	0
5	B	198	Total O 198 198	0	0

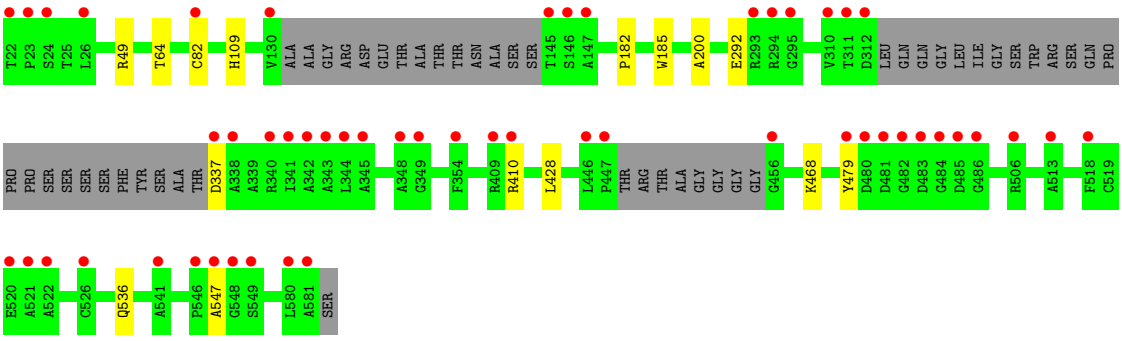
3 Residue-property plots (i)

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: cytokinin dehydrogenase

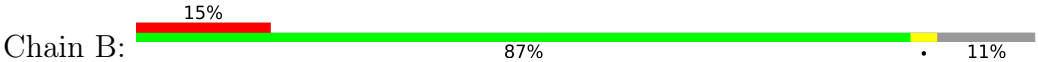
Chain A:

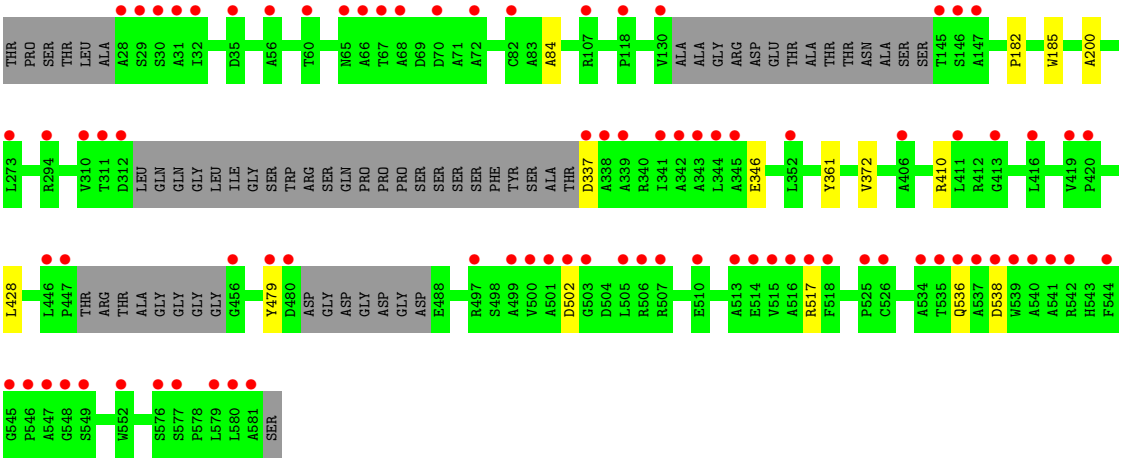




• Molecule 1: cytokinin dehydrogenase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.34Å 132.40Å 185.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.87 – 1.65 53.87 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.87-1.65) 99.9 (53.87-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.181 , 0.201 0.187 , 0.207	Depositor DCC
R_{free} test set	6756 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8380	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 4.33% 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: GOL, FAD, EDO

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	0.50	0/3966	0.58	0/5390
1	B	0.45	0/3866	0.58	0/5252
All	All	0.48	0/7832	0.58	0/10642

There are no bond length outliers.

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	3880	0	3806	7	0
1	B	3785	0	3721	3	0
2	A	53	0	30	1	0
2	B	53	0	29	0	0
3	A	8	0	12	1	0
3	B	4	0	6	0	0
4	A	12	0	16	0	0
5	A	387	0	0	2	0
5	B	198	0	0	0	0
All	All	8380	0	7620	9	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 1.

All (9) 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:A:49:ARG:HH22	3:A:602:EDO:H12	1.55	0.71
1:A:479:TYR:O	1:A:547:ALA:HA	2.12	0.50
1:B:361:TYR:CD1	1:B:372:VAL:HG21	2.51	0.46
1:A:109:HIS:CE1	2:A:600:FAD:HM71	2.54	0.43
1:A:64:THR:HG22	5:A:841:HOH:O	2.20	0.42
1:B:182:PRO:HD2	1:B:185:TRP:CZ2	2.54	0.41
1:A:82:CYS:SG	1:B:84:ALA:HB3	2.61	0.41
1:A:182:PRO:HD2	1:A:185:TRP:CZ2	2.55	0.41
1:A:468:LYS:HE3	5:A:926:HOH:O	2.21	0.40

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	509/561 (91%)	496 (97%)	12 (2%)	1 (0%)	44	27
1	B	493/561 (88%)	478 (97%)	14 (3%)	1 (0%)	44	27
All	All	1002/1122 (89%)	974 (97%)	26 (3%)	2 (0%)	44	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ALA
1	B	200	ALA

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	385/416 (92%)	380 (99%)	5 (1%)	65 47
1	B	375/416 (90%)	366 (98%)	9 (2%)	44 21
All	All	760/832 (91%)	746 (98%)	14 (2%)	52 32

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	GLU
1	A	337	ASP
1	A	410	ARG
1	A	428	LEU
1	A	536	GLN
1	B	337	ASP
1	B	346	GLU
1	B	410	ARG
1	B	428	LEU
1	B	479	TYR
1	B	502	ASP
1	B	517	ARG
1	B	536	GLN
1	B	538	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

7 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	EDO	A	602	-	3,3,3	0.58	0	2,2,2	0.41	0
4	GOL	A	604	-	5,5,5	0.06	0	5,5,5	0.15	0
2	FAD	A	600	1	53,58,58	0.57	0	68,89,89	0.66	2 (2%)
2	FAD	B	600	1	53,58,58	0.54	0	68,89,89	0.66	2 (2%)
3	EDO	A	601	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	B	601	-	3,3,3	0.46	0	2,2,2	0.35	0
4	GOL	A	603	-	5,5,5	0.07	0	5,5,5	0.19	0

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	EDO	A	602	-	-	1/1/1/1	-
4	GOL	A	604	-	-	0/4/4/4	-
2	FAD	A	600	1	-	2/30/50/50	0/6/6/6
2	FAD	B	600	1	-	3/30/50/50	0/6/6/6
3	EDO	A	601	-	-	0/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-
4	GOL	A	603	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	C4'-C3'-C2'	2.52	118.61	113.36
2	B	600	FAD	C5A-C6A-N6A	2.40	124.00	120.35
2	A	600	FAD	O5'-P-O1P	2.28	117.99	109.07
2	A	600	FAD	C5A-C6A-N6A	2.24	123.76	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	EDO	O1-C1-C2-O2
2	B	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	PA-O3P-P-O1P
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	PA-O3P-P-O1P
2	B	600	FAD	O3'-C3'-C4'-C5'

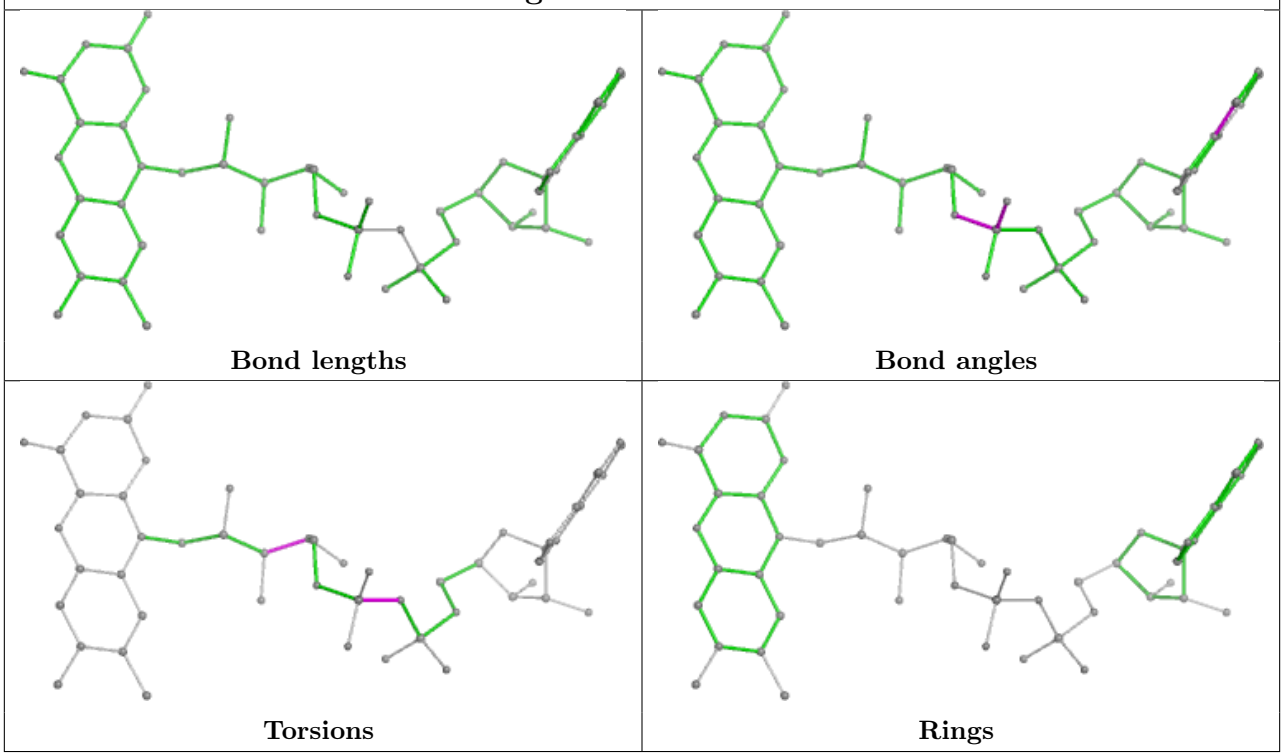
There are no ring outliers.

2 monomers are involved in 2 short contacts:

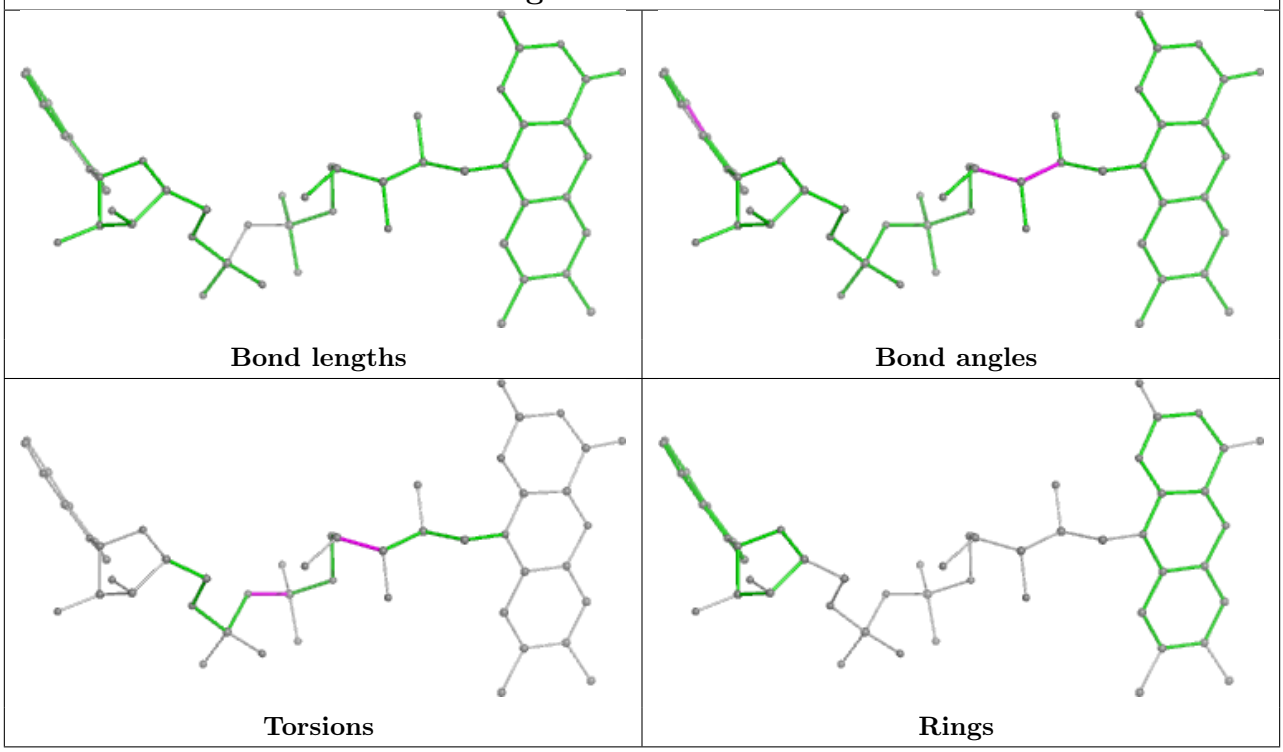
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	EDO	1	0
2	A	600	FAD	1	0

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



Ligand FAD B 600



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, 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	514/561 (91%)	0.23	53 (10%) 13 14	15, 27, 65, 100	3 (0%)
1	B	501/561 (89%)	0.85	85 (16%) 5 5	18, 41, 88, 121	2 (0%)
All	All	1015/1122 (90%)	0.53	138 (13%) 8 8	15, 34, 81, 121	5 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	VAL	7.2
1	A	146	SER	6.9
1	B	580	LEU	6.7
1	B	581	ALA	6.3
1	A	547	ALA	6.2
1	A	130	VAL	6.1
1	A	147	ALA	6.1
1	A	479	TYR	5.6
1	B	547	ALA	5.5
1	B	28	ALA	5.4
1	A	23	PRO	5.3
1	A	581	ALA	5.0
1	A	145	THR	4.9
1	A	482	GLY	4.9
1	B	146	SER	4.8
1	A	22	THR	4.7
1	B	145	THR	4.4
1	A	341	ILE	4.4
1	B	517	ARG	4.3
1	B	312	ASP	4.3
1	B	479	TYR	4.3
1	B	503	GLY	4.2
1	B	67	THR	4.2
1	B	541	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	546	PRO	4.2
1	B	501	ALA	4.2
1	A	344	LEU	4.2
1	A	456	GLY	4.2
1	B	502	ASP	4.2
1	B	456	GLY	4.2
1	B	311	THR	4.1
1	A	485	ASP	4.1
1	B	535	THR	4.0
1	B	447	PRO	3.9
1	B	500	VAL	3.9
1	B	537	ALA	3.9
1	B	480	ASP	3.8
1	B	32	ILE	3.7
1	B	506	ARG	3.7
1	A	337	ASP	3.7
1	B	310	VAL	3.7
1	A	24	SER	3.7
1	B	546	PRO	3.6
1	B	526	CYS	3.6
1	A	484	GLY	3.6
1	B	70	ASP	3.5
1	A	311	THR	3.5
1	B	339	ALA	3.4
1	B	66	ALA	3.4
1	B	337	ASP	3.4
1	B	505	LEU	3.4
1	A	513	ALA	3.4
1	A	447	PRO	3.3
1	A	343	ALA	3.3
1	B	338	ALA	3.3
1	B	516	ALA	3.2
1	B	446	LEU	3.2
1	B	549	SER	3.2
1	A	26	LEU	3.2
1	A	518	PHE	3.2
1	B	343	ALA	3.2
1	B	540	ALA	3.1
1	B	342	ALA	3.1
1	B	147	ALA	3.0
1	B	341	ILE	3.0
1	A	446	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	31	ALA	3.0
1	B	499	ALA	3.0
1	A	348	ALA	2.9
1	B	344	LEU	2.9
1	B	411	LEU	2.9
1	A	312	ASP	2.9
1	A	548	GLY	2.9
1	B	294	ARG	2.8
1	A	526	CYS	2.8
1	A	294	ARG	2.8
1	A	480	ASP	2.8
1	A	340	ARG	2.8
1	B	416	LEU	2.7
1	A	522	ALA	2.6
1	B	68	ALA	2.6
1	B	513	ALA	2.6
1	B	510	GLU	2.6
1	B	497	ARG	2.6
1	A	342	ALA	2.5
1	A	345	ALA	2.5
1	B	514	GLU	2.5
1	B	545	GLY	2.5
1	B	548	GLY	2.5
1	B	536	GLN	2.5
1	A	486	GLY	2.5
1	B	515	VAL	2.5
1	A	338	ALA	2.5
1	B	534	ALA	2.5
1	B	30	SER	2.4
1	B	107	ARG	2.4
1	A	82	CYS	2.4
1	A	354	PHE	2.4
1	A	409	ARG	2.4
1	A	521	ALA	2.4
1	B	345	ALA	2.4
1	B	507	ARG	2.4
1	B	542	ARG	2.4
1	B	579	LEU	2.4
1	B	60	THR	2.4
1	B	35	ASP	2.4
1	B	576	SER	2.3
1	B	56	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	310	VAL	2.3
1	B	419	VAL	2.3
1	B	273	LEU	2.3
1	B	118	PRO	2.3
1	A	295	GLY	2.3
1	B	413	GLY	2.3
1	A	410	ARG	2.3
1	A	580	LEU	2.3
1	A	549	SER	2.2
1	B	538	ASP	2.2
1	B	82	CYS	2.2
1	B	65	ASN	2.2
1	B	544	PHE	2.2
1	B	577	SER	2.2
1	A	481	ASP	2.2
1	B	525	PRO	2.2
1	B	552	TRP	2.2
1	B	352	LEU	2.2
1	A	506	ARG	2.1
1	B	539	TRP	2.1
1	A	293	ARG	2.1
1	B	420	PRO	2.1
1	A	520	GLU	2.1
1	B	406	ALA	2.1
1	B	518	PHE	2.1
1	B	29	SER	2.1
1	A	483	ASP	2.1
1	A	541	ALA	2.0
1	B	72	ALA	2.0
1	A	349	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

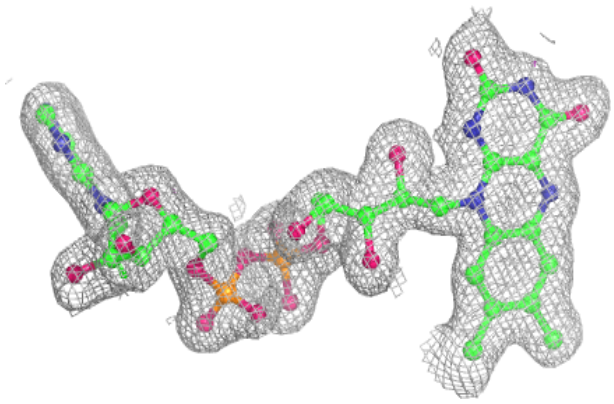
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

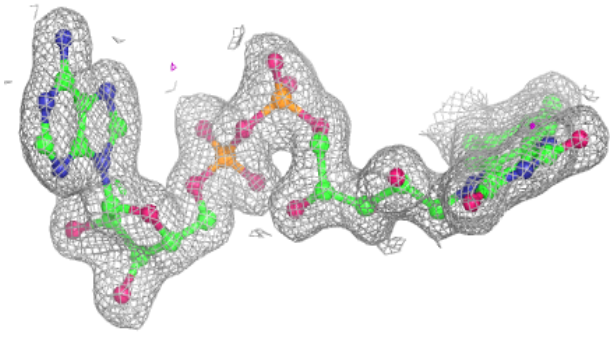
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	602	4/4	0.81	0.20	33,36,42,52	0
3	EDO	B	601	4/4	0.87	0.18	58,60,60,61	0
4	GOL	A	604	6/6	0.87	0.16	65,68,70,71	0
4	GOL	A	603	6/6	0.91	0.10	32,36,41,42	0
3	EDO	A	601	4/4	0.92	0.13	41,42,45,45	0
2	FAD	B	600	53/53	0.98	0.06	24,28,32,34	0
2	FAD	A	600	53/53	0.99	0.04	15,19,23,24	0

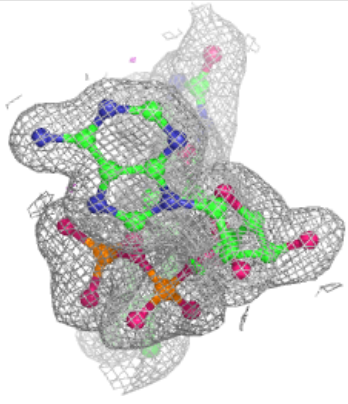
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

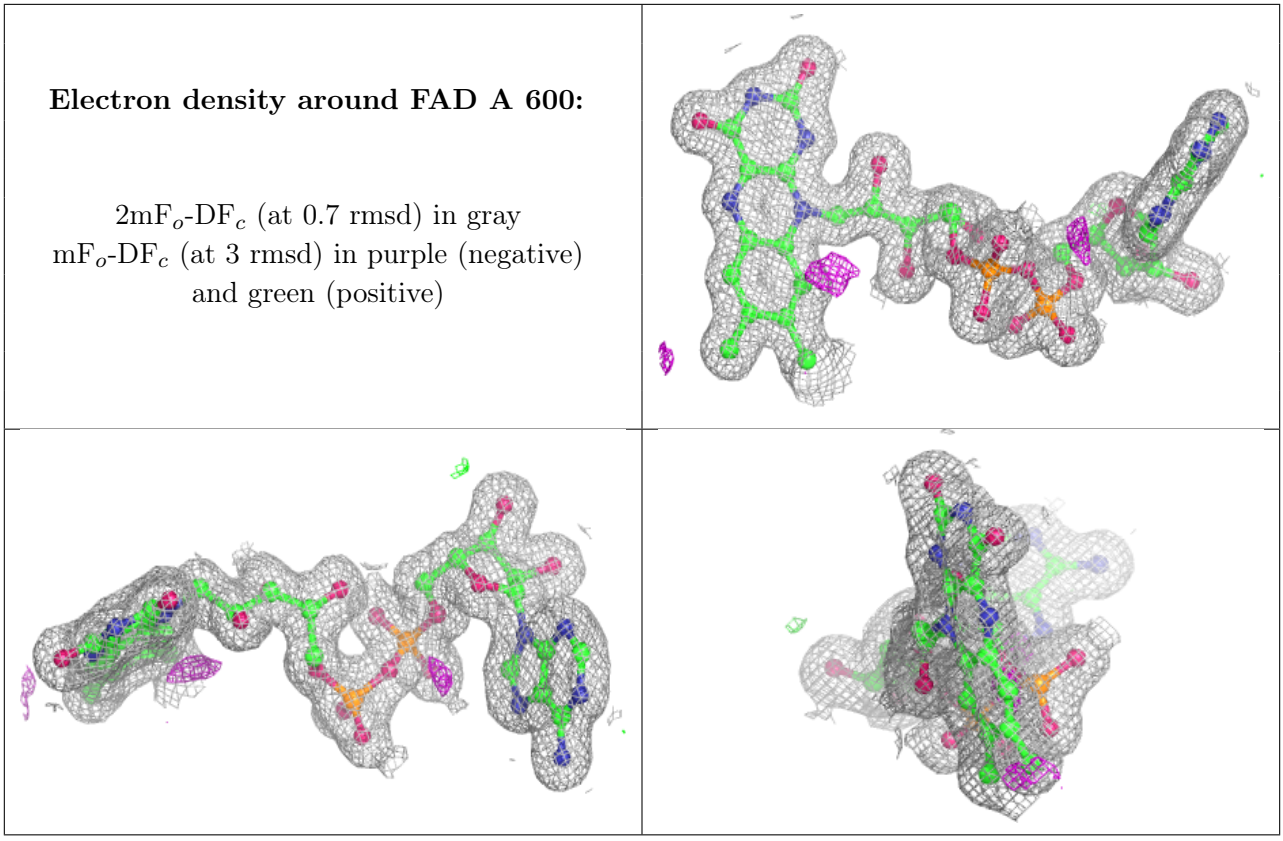






Electron density around FAD A 600:

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



6.5 Other polymers (i)

There are no such residues in this entry.