Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:31 pm BST

PDB ID : 6BZA
Title : Crystal structure of halogenase PltM in complex with phloroglucinol and FAD
Authors : Pang, A.H.; Garneau-Tsodikova, S.; Tsodikov, O.V.
Deposited on : 2017-12-22
Resolution : 2.60 Å(reported)

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

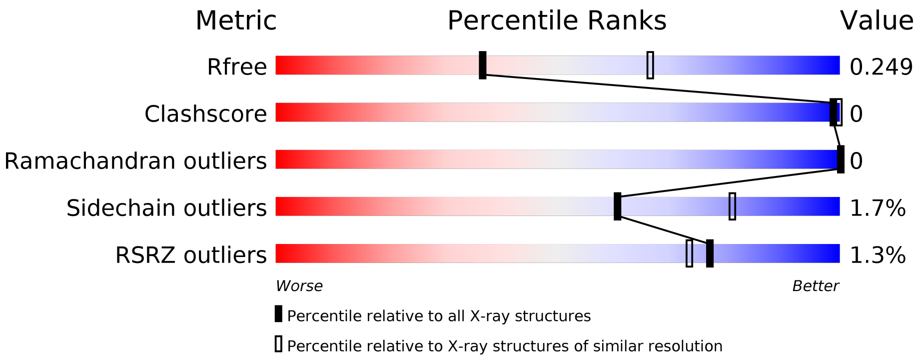
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance

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

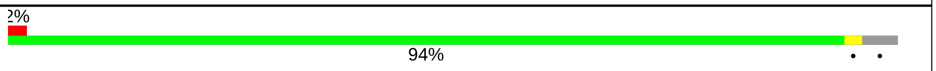
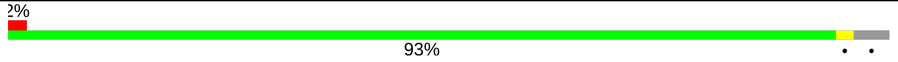
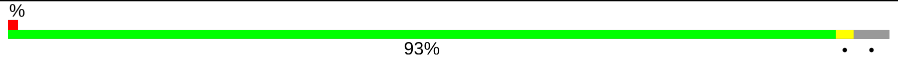
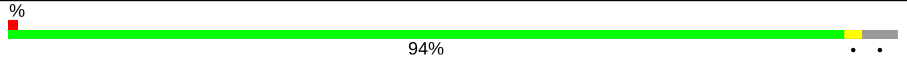
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	522	
1	B	522	
1	C	522	
1	D	522	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15979 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 Halogenase PltM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	3950	2521	697	721	11	0	0	0
1	B	500	3944	2518	694	721	11	0	0	0
1	C	501	3953	2524	697	721	11	0	0	0
1	D	500	3949	2520	697	721	11	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q4KCZ3
A	-18	GLY	-	expression tag	UNP Q4KCZ3
A	-17	SER	-	expression tag	UNP Q4KCZ3
A	-16	SER	-	expression tag	UNP Q4KCZ3
A	-15	HIS	-	expression tag	UNP Q4KCZ3
A	-14	HIS	-	expression tag	UNP Q4KCZ3
A	-13	HIS	-	expression tag	UNP Q4KCZ3
A	-12	HIS	-	expression tag	UNP Q4KCZ3
A	-11	HIS	-	expression tag	UNP Q4KCZ3
A	-10	HIS	-	expression tag	UNP Q4KCZ3
A	-9	SER	-	expression tag	UNP Q4KCZ3
A	-8	SER	-	expression tag	UNP Q4KCZ3
A	-7	GLY	-	expression tag	UNP Q4KCZ3
A	-6	LEU	-	expression tag	UNP Q4KCZ3
A	-5	VAL	-	expression tag	UNP Q4KCZ3
A	-4	PRO	-	expression tag	UNP Q4KCZ3
A	-3	ARG	-	expression tag	UNP Q4KCZ3
A	-2	GLY	-	expression tag	UNP Q4KCZ3
A	-1	SER	-	expression tag	UNP Q4KCZ3
A	0	HIS	-	expression tag	UNP Q4KCZ3
B	-19	MET	-	initiating methionine	UNP Q4KCZ3

Continued on next page...

Continued from previous page...

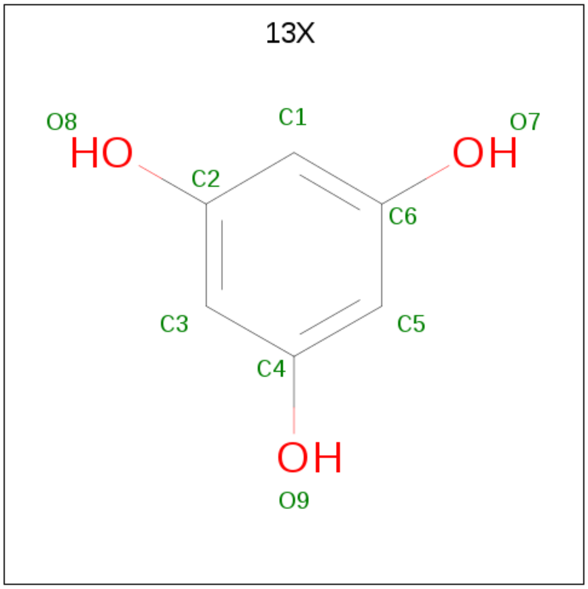
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q4KCZ3
B	-17	SER	-	expression tag	UNP Q4KCZ3
B	-16	SER	-	expression tag	UNP Q4KCZ3
B	-15	HIS	-	expression tag	UNP Q4KCZ3
B	-14	HIS	-	expression tag	UNP Q4KCZ3
B	-13	HIS	-	expression tag	UNP Q4KCZ3
B	-12	HIS	-	expression tag	UNP Q4KCZ3
B	-11	HIS	-	expression tag	UNP Q4KCZ3
B	-10	HIS	-	expression tag	UNP Q4KCZ3
B	-9	SER	-	expression tag	UNP Q4KCZ3
B	-8	SER	-	expression tag	UNP Q4KCZ3
B	-7	GLY	-	expression tag	UNP Q4KCZ3
B	-6	LEU	-	expression tag	UNP Q4KCZ3
B	-5	VAL	-	expression tag	UNP Q4KCZ3
B	-4	PRO	-	expression tag	UNP Q4KCZ3
B	-3	ARG	-	expression tag	UNP Q4KCZ3
B	-2	GLY	-	expression tag	UNP Q4KCZ3
B	-1	SER	-	expression tag	UNP Q4KCZ3
B	0	HIS	-	expression tag	UNP Q4KCZ3
C	-19	MET	-	initiating methionine	UNP Q4KCZ3
C	-18	GLY	-	expression tag	UNP Q4KCZ3
C	-17	SER	-	expression tag	UNP Q4KCZ3
C	-16	SER	-	expression tag	UNP Q4KCZ3
C	-15	HIS	-	expression tag	UNP Q4KCZ3
C	-14	HIS	-	expression tag	UNP Q4KCZ3
C	-13	HIS	-	expression tag	UNP Q4KCZ3
C	-12	HIS	-	expression tag	UNP Q4KCZ3
C	-11	HIS	-	expression tag	UNP Q4KCZ3
C	-10	HIS	-	expression tag	UNP Q4KCZ3
C	-9	SER	-	expression tag	UNP Q4KCZ3
C	-8	SER	-	expression tag	UNP Q4KCZ3
C	-7	GLY	-	expression tag	UNP Q4KCZ3
C	-6	LEU	-	expression tag	UNP Q4KCZ3
C	-5	VAL	-	expression tag	UNP Q4KCZ3
C	-4	PRO	-	expression tag	UNP Q4KCZ3
C	-3	ARG	-	expression tag	UNP Q4KCZ3
C	-2	GLY	-	expression tag	UNP Q4KCZ3
C	-1	SER	-	expression tag	UNP Q4KCZ3
C	0	HIS	-	expression tag	UNP Q4KCZ3
D	-19	MET	-	initiating methionine	UNP Q4KCZ3
D	-18	GLY	-	expression tag	UNP Q4KCZ3
D	-17	SER	-	expression tag	UNP Q4KCZ3

Continued on next page...

Continued from previous page...

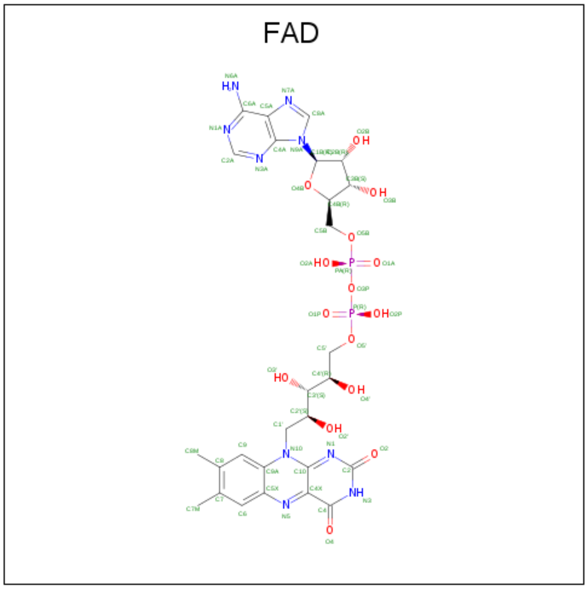
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q4KCZ3
D	-15	HIS	-	expression tag	UNP Q4KCZ3
D	-14	HIS	-	expression tag	UNP Q4KCZ3
D	-13	HIS	-	expression tag	UNP Q4KCZ3
D	-12	HIS	-	expression tag	UNP Q4KCZ3
D	-11	HIS	-	expression tag	UNP Q4KCZ3
D	-10	HIS	-	expression tag	UNP Q4KCZ3
D	-9	SER	-	expression tag	UNP Q4KCZ3
D	-8	SER	-	expression tag	UNP Q4KCZ3
D	-7	GLY	-	expression tag	UNP Q4KCZ3
D	-6	LEU	-	expression tag	UNP Q4KCZ3
D	-5	VAL	-	expression tag	UNP Q4KCZ3
D	-4	PRO	-	expression tag	UNP Q4KCZ3
D	-3	ARG	-	expression tag	UNP Q4KCZ3
D	-2	GLY	-	expression tag	UNP Q4KCZ3
D	-1	SER	-	expression tag	UNP Q4KCZ3
D	0	HIS	-	expression tag	UNP Q4KCZ3

- Molecule 2 is benzene-1,3,5-triol (three-letter code: 13X) (formula: $C_6H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 6 3	0	0
2	B	1	Total C O 9 6 3	0	0
2	C	1	Total C O 9 6 3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 17 4 9 1	0	0
3	B	1	Total C N O 19 13 4 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

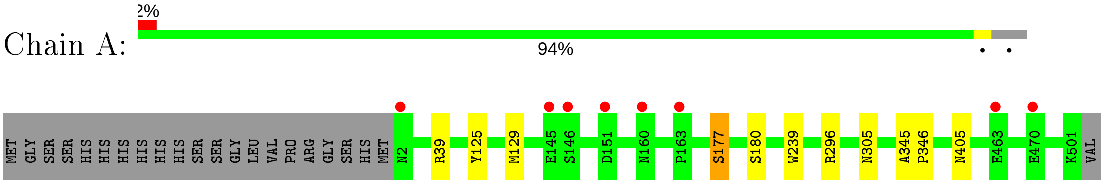
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	29	Total O 29 29	0	0
5	B	21	Total O 21 21	0	0
5	C	23	Total O 23 23	0	0
5	D	31	Total O 31 31	0	0

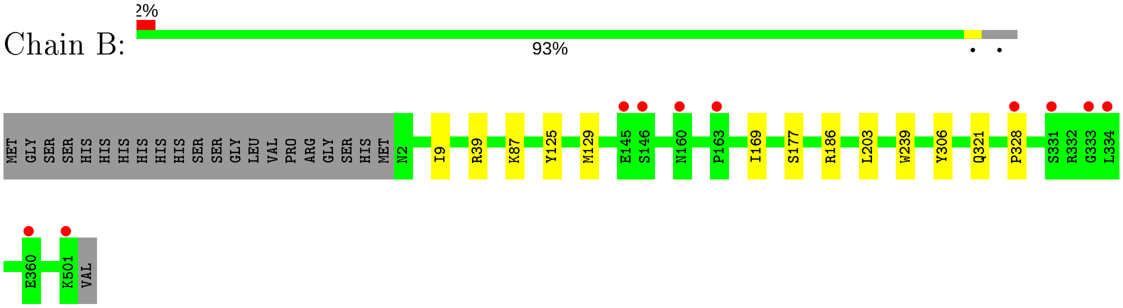
3 Residue-property plots

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.

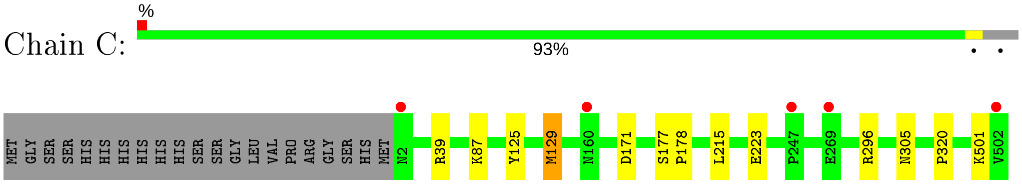
- Molecule 1: Halogenase PltM



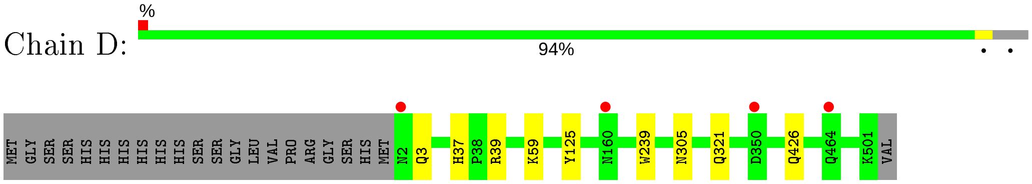
- Molecule 1: Halogenase PltM



- Molecule 1: Halogenase PltM



- Molecule 1: Halogenase PltM



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.24Å 156.98Å 213.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 35.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.60) 97.4 (35.25-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.203 , 0.253 0.203 , 0.249	Depositor DCC
R_{free} test set	3336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 16.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15979	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: 13X, FAD, CL

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	0.39	0/4050	0.62	0/5499
1	B	0.39	0/4044	0.60	0/5492
1	C	0.39	0/4053	0.61	0/5504
1	D	0.39	0/4049	0.61	0/5497
All	All	0.39	0/16196	0.61	0/21992

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	3950	0	3894	4	0
1	B	3944	0	3883	4	0
1	C	3953	0	3897	4	0
1	D	3949	0	3890	1	0
2	A	9	0	6	1	0
2	B	9	0	6	0	0
2	C	9	0	4	0	0
3	A	31	0	19	1	0
3	B	19	0	9	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	29	0	0	0	0
5	B	21	0	0	0	0
5	C	23	0	0	0	0
5	D	31	0	0	0	0
All	All	15979	0	15608	12	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 0.

All (12) 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:177:SER:HB2	1:A:180:SER:HB3	1.83	0.61
1:B:328:PRO:HB3	3:B:601:FAD:HM73	1.85	0.58
3:A:602:FAD:O4'	3:A:602:FAD:O1P	2.30	0.50
1:C:171:ASP:OD2	1:C:177:SER:HB2	2.14	0.47
1:B:306:TYR:OH	1:B:321:GLN:O	2.33	0.46
1:A:405:ASN:OD1	2:A:601:13X:H4	2.17	0.43
1:B:9:ILE:HD11	1:B:169:ILE:HD11	2.00	0.43
1:C:215:LEU:HD21	1:C:223:GLU:HA	1.99	0.42
1:A:345:ALA:HB3	1:A:346:PRO:HD3	2.02	0.42
1:C:177:SER:HA	1:C:178:PRO:HD3	1.85	0.42
1:A:296:ARG:NH2	1:D:37:HIS:O	2.53	0.41
1:B:203:LEU:HD21	1:C:129:MET:HG3	2.03	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	498/522 (95%)	486 (98%)	12 (2%)	0	100	100
1	B	498/522 (95%)	487 (98%)	11 (2%)	0	100	100
1	C	499/522 (96%)	490 (98%)	9 (2%)	0	100	100
1	D	498/522 (95%)	488 (98%)	10 (2%)	0	100	100
All	All	1993/2088 (96%)	1951 (98%)	42 (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	421/440 (96%)	415 (99%)	6 (1%)	67	85
1	B	420/440 (96%)	413 (98%)	7 (2%)	60	81
1	C	421/440 (96%)	413 (98%)	8 (2%)	57	79
1	D	421/440 (96%)	413 (98%)	8 (2%)	57	79
All	All	1683/1760 (96%)	1654 (98%)	29 (2%)	60	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	125	TYR
1	A	129	MET
1	A	177	SER
1	A	239	TRP
1	A	305	ASN
1	B	39	ARG
1	B	87	LYS
1	B	125	TYR
1	B	129	MET
1	B	177	SER
1	B	186	ARG
1	B	239	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	39	ARG
1	C	87	LYS
1	C	125	TYR
1	C	129	MET
1	C	296	ARG
1	C	305	ASN
1	C	320	PRO
1	C	501	LYS
1	D	3	GLN
1	D	39	ARG
1	D	59	LYS
1	D	125	TYR
1	D	239	TRP
1	D	305	ASN
1	D	321	GLN
1	D	426	GLN

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	294	ASN
1	B	459	GLN
1	C	160	ASN
1	C	321	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	13X	C	601	-	9,9,9	0.67	0	12,12,12	0.47	0
2	13X	B	602	-	9,9,9	0.54	0	12,12,12	0.72	0
3	FAD	B	601	-	19,21,58	3.44	5 (26%)	24,32,89	2.85	9 (37%)
3	FAD	A	602	-	31,33,58	2.50	5 (16%)	40,50,89	2.26	8 (20%)
2	13X	A	601	-	9,9,9	0.55	0	12,12,12	0.72	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
2	13X	C	601	-	-	-	0/1/1/1
2	13X	B	602	-	-	-	0/1/1/1
3	FAD	A	602	-	-	7/18/18/50	0/3/3/6
3	FAD	B	601	-	-	-	0/3/3/6
2	13X	A	601	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C4X-C10	11.38	1.50	1.38
3	A	602	FAD	C4X-C10	10.59	1.49	1.38
3	B	601	FAD	C4-C4X	4.85	1.49	1.41
3	B	601	FAD	C9A-N10	4.78	1.43	1.37
3	A	602	FAD	C9A-C5X	4.46	1.51	1.42
3	A	602	FAD	C4-C4X	4.45	1.49	1.41
3	B	601	FAD	C9A-C5X	4.43	1.51	1.42
3	B	601	FAD	C8-C7	3.76	1.50	1.40
3	A	602	FAD	C8-C7	3.41	1.49	1.40
3	A	602	FAD	C9A-N10	3.04	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	8.31	122.16	115.14
3	A	602	FAD	C4-N3-C2	8.04	121.93	115.14
3	A	602	FAD	C1'-N10-C9A	6.51	123.42	118.29
3	A	602	FAD	C4-C4X-C10	-5.06	116.60	119.95
3	B	601	FAD	C1'-N10-C9A	4.93	123.76	119.06
3	B	601	FAD	C4-C4X-C10	-4.69	116.85	119.95
3	B	601	FAD	C9A-N10-C10	-4.46	117.86	121.79
3	B	601	FAD	C4X-C4-N3	-4.08	117.86	123.43
3	B	601	FAD	C4X-N5-C5X	4.03	120.80	116.77
3	A	602	FAD	C4X-N5-C5X	3.87	120.64	116.77
3	A	602	FAD	C4X-C4-N3	-3.63	118.46	123.43
3	B	601	FAD	C4-C4X-N5	3.44	122.53	118.60
3	A	602	FAD	C4-C4X-N5	3.29	122.36	118.60
3	A	602	FAD	C9A-N10-C10	-3.22	117.70	121.91
3	A	602	FAD	O2P-P-O1P	2.60	120.86	110.68
3	B	601	FAD	C4X-C10-N10	2.06	120.50	118.25
3	B	601	FAD	C5X-C9A-N10	2.02	118.87	117.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	FAD	O4'-C4'-C5'-O5'
3	A	602	FAD	O3'-C3'-C4'-O4'
3	A	602	FAD	C2'-C3'-C4'-O4'
3	A	602	FAD	O3'-C3'-C4'-C5'
3	A	602	FAD	C2'-C3'-C4'-C5'
3	A	602	FAD	C4'-C5'-O5'-P
3	A	602	FAD	C3'-C4'-C5'-O5'

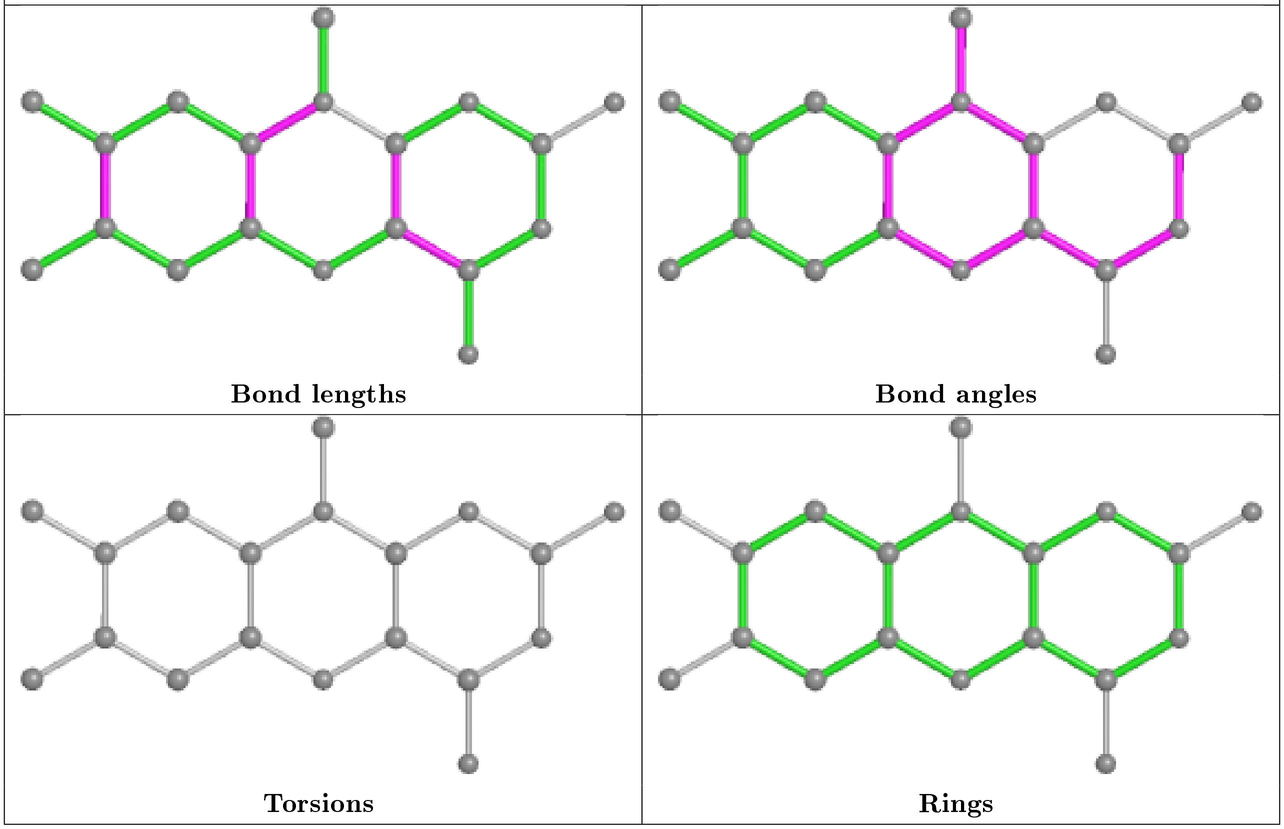
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FAD	1	0
3	A	602	FAD	1	0
2	A	601	13X	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 B 601



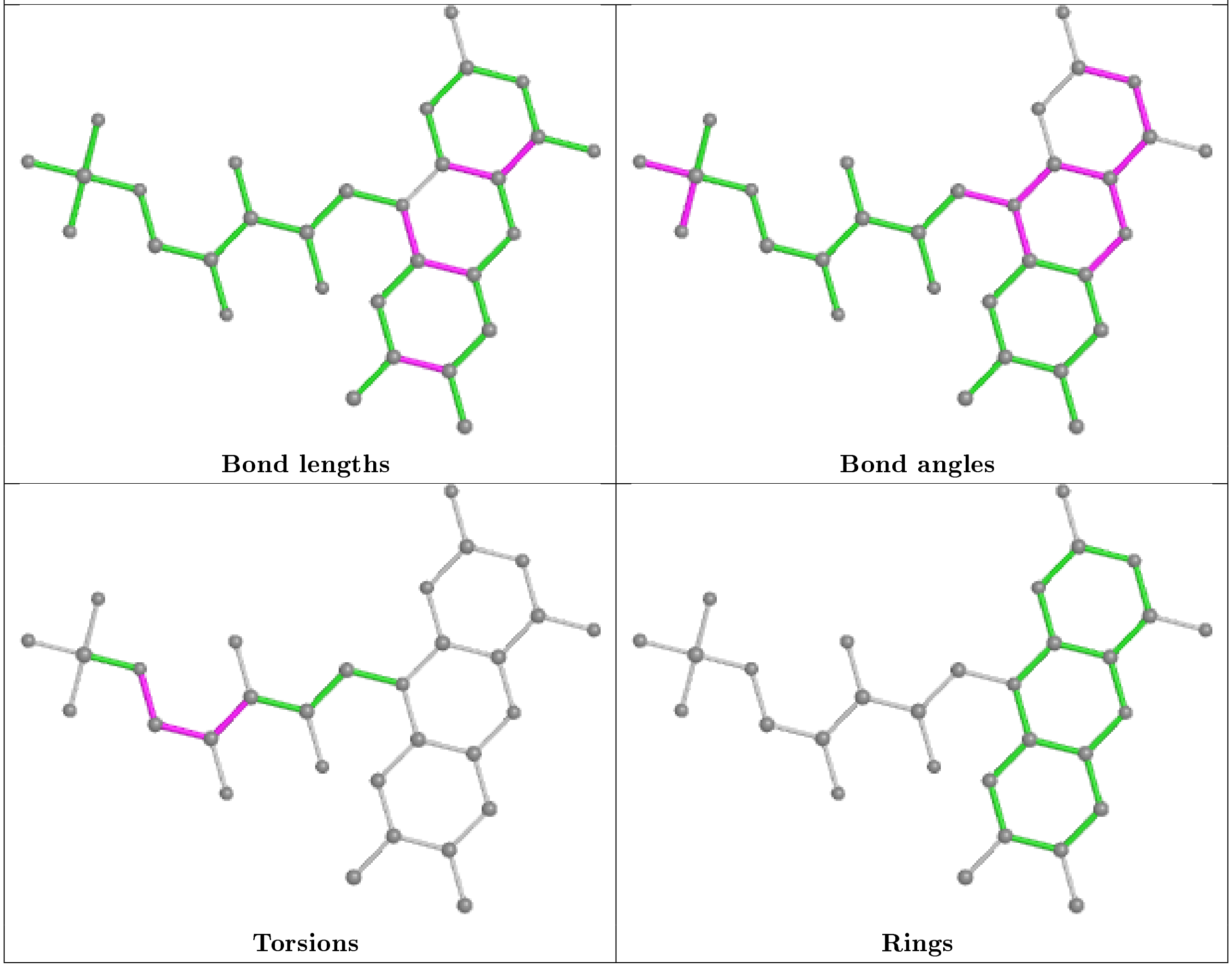
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 602



Bond lengths

Bond angles

Torsions

Rings

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	500/522 (95%)	-0.13	8 (1%)	72	68	28, 44, 73, 96	0
1	B	500/522 (95%)	-0.03	10 (2%)	65	60	31, 49, 75, 95	0
1	C	501/522 (95%)	-0.17	5 (0%)	82	80	29, 44, 64, 85	1 (0%)
1	D	500/522 (95%)	-0.24	4 (0%)	86	84	28, 42, 63, 87	0
All	All	2001/2088 (95%)	-0.14	27 (1%)	77	73	28, 45, 70, 96	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ASN	4.4
1	B	501	LYS	3.9
1	D	2	ASN	3.1
1	D	160	ASN	3.1
1	A	160	ASN	3.1
1	A	463	GLU	3.1
1	C	2	ASN	3.0
1	C	502	VAL	2.9
1	B	331	SER	2.8
1	A	151	ASP	2.8
1	C	160	ASN	2.7
1	A	2	ASN	2.6
1	B	334	LEU	2.5
1	A	163	PRO	2.5
1	C	247	PRO	2.3
1	B	145	GLU	2.3
1	A	145	GLU	2.3
1	D	350	ASP	2.3
1	D	464	GLN	2.2
1	A	470	GLU	2.2
1	B	333	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	146	SER	2.2
1	B	146	SER	2.1
1	B	328	PRO	2.1
1	B	163	PRO	2.0
1	B	360	GLU	2.0
1	C	269	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 carbohydrates in this entry.

6.4 Ligands ⓘ

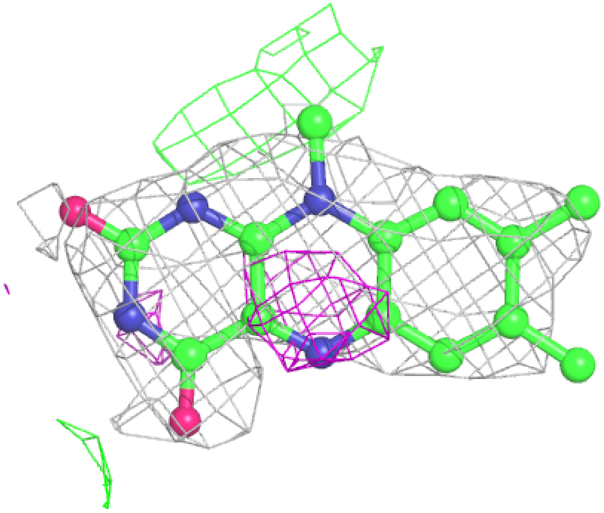
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

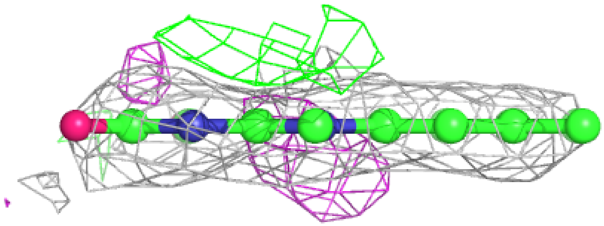
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	13X	B	602	9/9	0.78	0.37	89,91,93,94	0
2	13X	A	601	9/9	0.82	0.26	80,81,83,83	0
2	13X	C	601	9/9	0.82	0.31	72,76,78,81	0
3	FAD	B	601	19/53	0.86	0.24	53,67,69,70	0
3	FAD	A	602	31/53	0.87	0.22	52,66,67,68	12
4	CL	C	602	1/1	0.94	0.06	47,47,47,47	0
4	CL	D	601	1/1	0.95	0.05	50,50,50,50	0

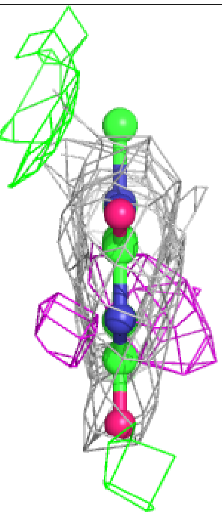
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

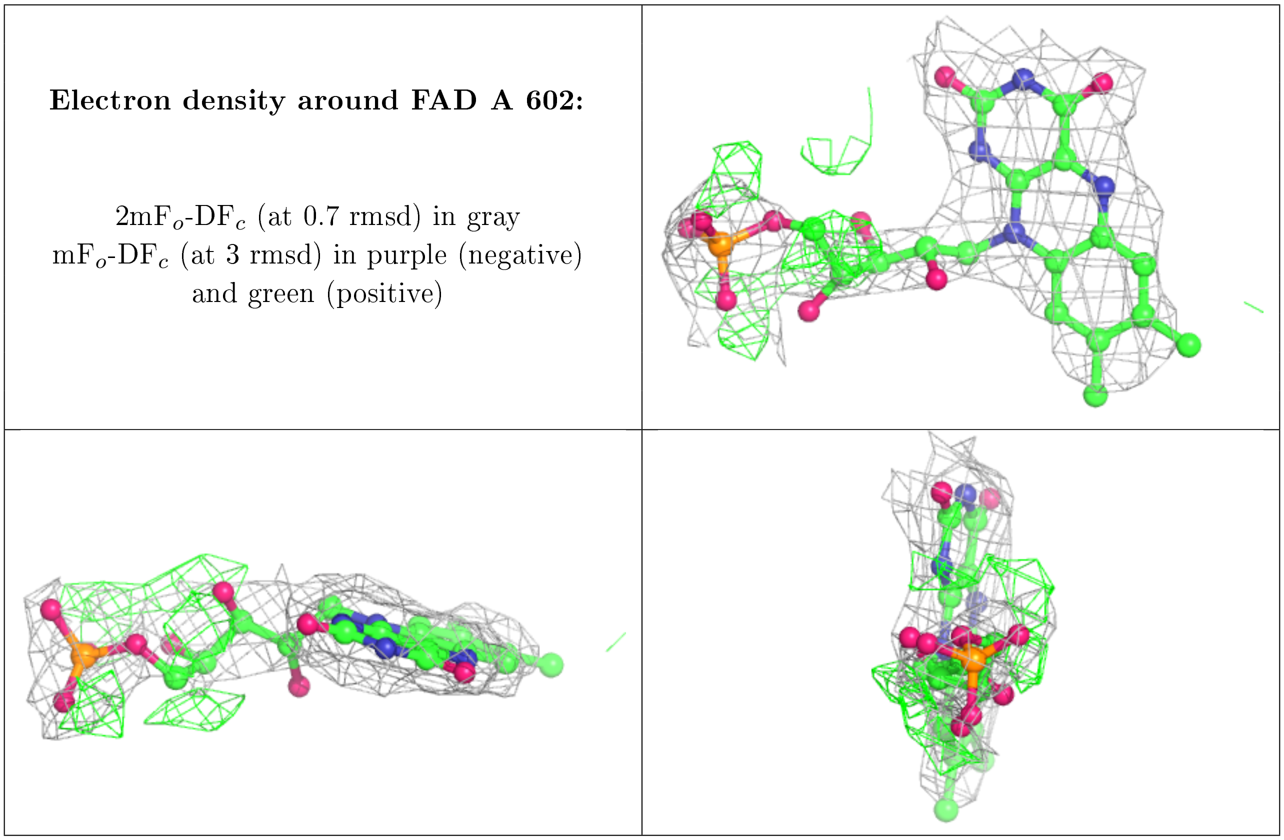






Electron density around FAD A 602:

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 ⓘ

There are no such residues in this entry.