



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:33 pm BST

PDB ID : 6BZZ
Title : Crystal structure of halogenase PltM in complex with partially bound FAD
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Deposited on : 2017-12-26
Resolution : 2.05 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

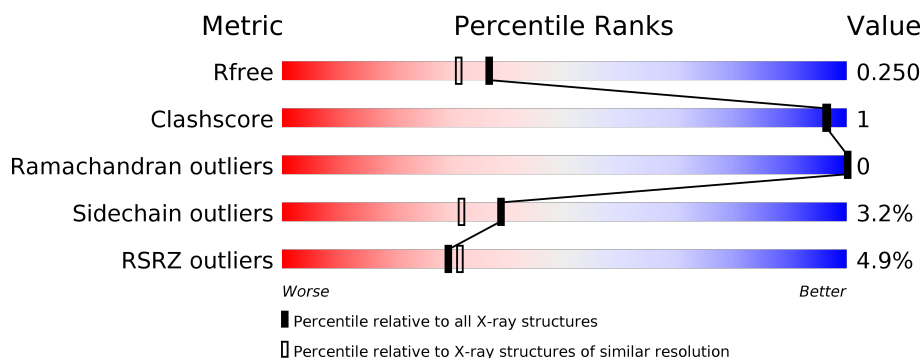
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 $\leq 5\%$. 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	522	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	522	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div></div> <div>.</div> </div> </div>
2	C	522	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div></div> <div>.</div> </div> </div>
2	D	522	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div></div> <div>.</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16332 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
1	A	500	Total	C	N	O	S	0	0	0
			3950	2521	697	721	11			
1	B	500	Total	C	N	O	S	0	0	0
			3943	2515	696	721	11			

There are 40 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Halogenase PltM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	500	Total	C	N	O	S	0	0	0
			3953	2521	697	724	11			
2	D	499	Total	C	N	O	S	0	1	0
			3955	2523	698	723	11			

There are 40 discrepancies between the modelled and reference sequences:

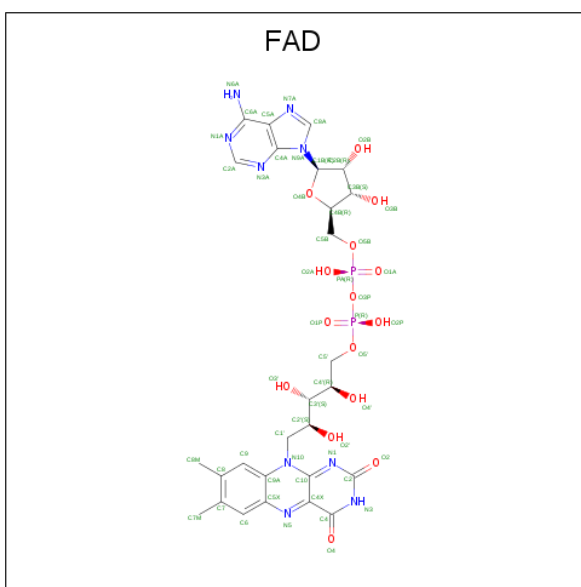
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP Q4KCZ3
C	-18	GLY	-	expression tag	UNP Q4KCZ3
C	-17	SER	-	expression tag	UNP Q4KCZ3
C	-16	SER	-	expression tag	UNP Q4KCZ3
C	-15	HIS	-	expression tag	UNP Q4KCZ3
C	-14	HIS	-	expression tag	UNP Q4KCZ3
C	-13	HIS	-	expression 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 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 18	C 12	N 4	O 2	0	0
3	B	1	Total 18	C 12	N 4	O 2	0	0
3	C	1	Total 18	C 12	N 4	O 2	0	0
3	D	1	Total 18	C 12	N 4	O 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	134	Total O 134 134	0	0

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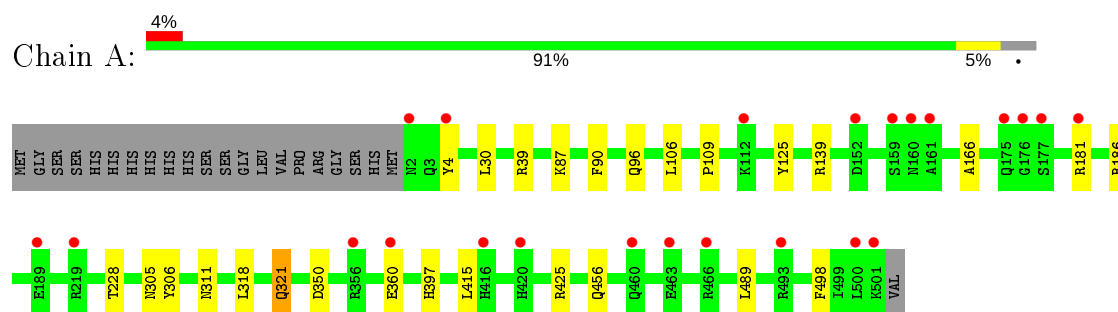
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	85	Total 85	O 85	0	0
5	C	121	Total 121	O 121	0	0
5	D	115	Total 115	O 115	0	0

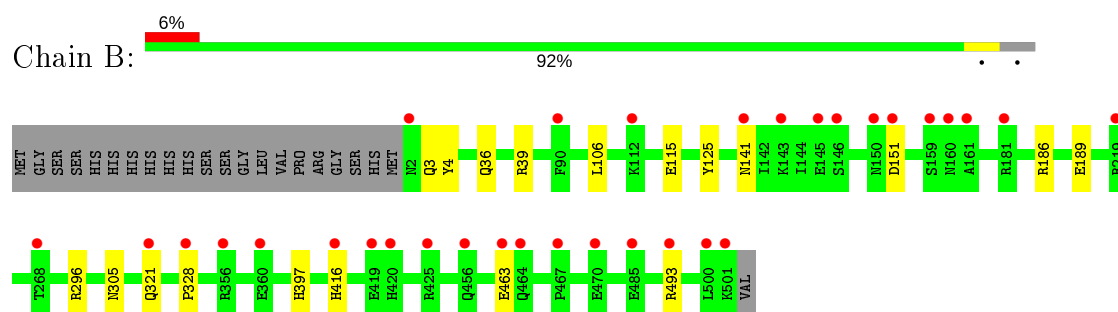
3 Residue-property plots [i](#)

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.

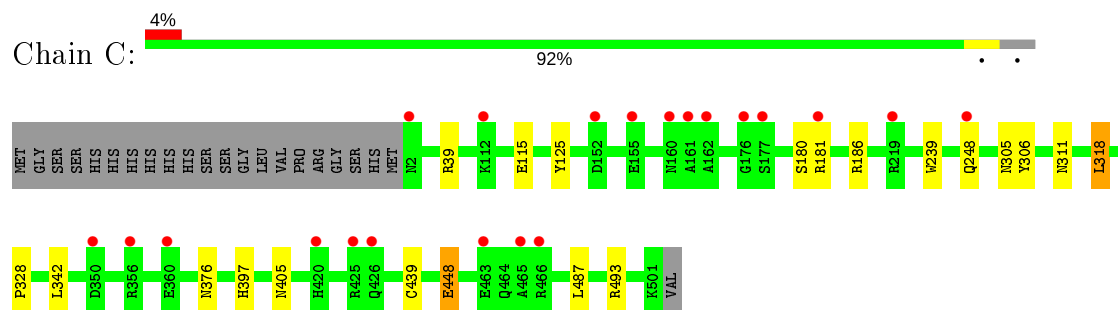
• Molecule 1: Halogenase PltM



• Molecule 1: Halogenase PltM

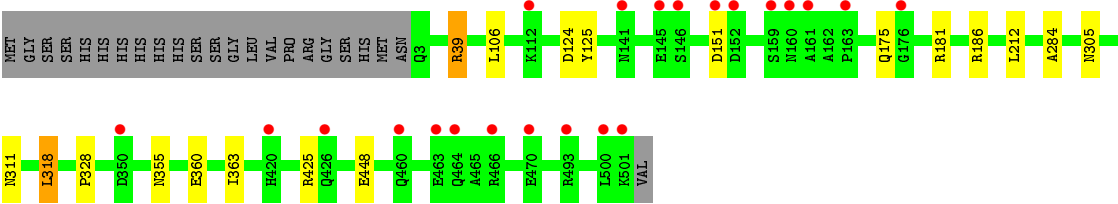


• Molecule 2: Halogenase PltM



• Molecule 2: 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	63.81Å 157.23Å 214.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 37.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.05) 97.7 (37.88-2.05)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.219 , 0.245 0.224 , 0.250	Depositor DCC
R_{free} test set	6596 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16332	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, OCS, 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	0.37	0/4050	0.64	0/5499
1	B	0.37	0/4043	0.62	0/5491
2	C	0.37	0/4043	0.62	0/5488
2	D	0.37	0/4046	0.63	0/5492
All	All	0.37	0/16182	0.63	0/21970

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3950	0	3894	12	0
1	B	3943	0	3874	6	0
2	C	3953	0	3893	5	0
2	D	3955	0	3893	7	0
3	A	18	0	9	1	0
3	B	18	0	9	1	0
3	C	18	0	9	2	0
3	D	18	0	9	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	134	0	0	0	0
5	B	85	0	0	1	0
5	C	121	0	0	0	0
5	D	115	0	0	0	0
All	All	16332	0	15590	30	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 (30) 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:4:TYR:O	1:A:166:ALA:HA	1.96	0.66
1:B:493:ARG:NE	1:B:493:ARG:HA	2.16	0.61
1:A:306:TYR:OH	1:A:321:GLN:O	2.20	0.59
2:D:212:LEU:HD21	2:D:284:ALA:O	2.03	0.57
2:C:439:OCS:OD1	2:C:448:GLU:HB2	2.09	0.53
1:A:106:LEU:HD12	1:A:106:LEU:C	2.30	0.52
2:D:39:ARG:NH2	2:D:124:ASP:OD2	2.44	0.51
2:D:328:PRO:HB3	3:D:601:FAD:HM73	1.94	0.50
1:B:328:PRO:HB3	3:B:601:FAD:HM73	1.94	0.50
1:A:106:LEU:HD11	1:A:498:PHE:CE1	2.47	0.50
1:B:493:ARG:HE	1:B:493:ARG:HA	1.76	0.49
2:C:328:PRO:HB3	3:C:601:FAD:HM73	1.94	0.49
1:A:311:ASN:HB2	1:A:318:LEU:HB2	1.96	0.47
2:D:311:ASN:HB2	2:D:318:LEU:HB2	1.98	0.46
1:A:321:GLN:HB3	3:A:601:FAD:HN3	1.81	0.45
2:C:311:ASN:HB2	2:C:318:LEU:HB2	1.99	0.44
1:A:90:PHE:CD1	1:A:228:THR:HB	2.52	0.44
1:B:3:GLN:HB3	1:B:4:TYR:CD2	2.54	0.43
2:C:306:TYR:OH	3:C:601:FAD:O2	2.25	0.43
2:D:181:ARG:HD3	2:D:186:ARG:HD2	2.01	0.42
2:D:360:GLU:HA	2:D:363:ILE:HG12	2.01	0.42
1:A:30:LEU:HD11	1:A:139:ARG:HD3	2.00	0.42
1:B:36:GLN:OE1	1:B:141:ASN:ND2	2.52	0.42
2:C:405:ASN:HB3	2:C:487:LEU:HD12	2.01	0.42
1:A:90:PHE:HD1	1:A:228:THR:HB	1.84	0.42
1:A:87:LYS:HE3	1:A:90:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:CD1	1:A:498:PHE:CE1	3.02	0.41
2:D:212:LEU:HD23	2:D:212:LEU:HA	1.87	0.41
1:A:106:LEU:HD11	1:A:498:PHE:CZ	2.56	0.41
1:B:36:GLN:NE2	5:B:701:HOH:O	2.51	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%)	488 (98%)	10 (2%)	0	100	100
1	B	498/522 (95%)	488 (98%)	10 (2%)	0	100	100
2	C	497/522 (95%)	487 (98%)	10 (2%)	0	100	100
2	D	497/522 (95%)	489 (98%)	8 (2%)	0	100	100
All	All	1990/2088 (95%)	1952 (98%)	38 (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	421/440 (96%)	406 (96%)	15 (4%)	35	28
1	B	419/440 (95%)	406 (97%)	13 (3%)	40	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	420/439 (96%)	405 (96%)	15 (4%)	35	28
2	D	420/439 (96%)	410 (98%)	10 (2%)	49	42
All	All	1680/1758 (96%)	1627 (97%)	53 (3%)	39	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	96	GLN
1	A	109	PRO
1	A	125	TYR
1	A	181	ARG
1	A	186	ARG
1	A	305	ASN
1	A	321	GLN
1	A	350	ASP
1	A	360	GLU
1	A	397	HIS
1	A	415	LEU
1	A	425	ARG
1	A	456	GLN
1	A	489	LEU
1	B	39	ARG
1	B	106	LEU
1	B	115	GLU
1	B	125	TYR
1	B	151	ASP
1	B	186	ARG
1	B	189	GLU
1	B	296	ARG
1	B	305	ASN
1	B	321	GLN
1	B	397	HIS
1	B	416	HIS
1	B	463	GLU
2	C	39	ARG
2	C	115	GLU
2	C	125	TYR
2	C	180	SER
2	C	181	ARG
2	C	186	ARG

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Mol	Chain	Res	Type
2	C	239	TRP
2	C	248	GLN
2	C	305	ASN
2	C	318	LEU
2	C	342	LEU
2	C	376	ASN
2	C	397	HIS
2	C	448	GLU
2	C	493	ARG
2	D	39	ARG
2	D	106	LEU
2	D	125	TYR
2	D	151	ASP
2	D	175	GLN
2	D	305	ASN
2	D	318	LEU
2	D	355	ASN
2	D	425	ARG
2	D	448	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	98	ASN
1	A	140	GLN
1	B	98	ASN
1	B	405	ASN
2	C	98	ASN
2	C	175	GLN
2	C	405	ASN
2	D	3	GLN
2	D	98	ASN
2	D	246	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	OCS	D	439	2	7,8,9	2.62	2 (28%)	6,11,13	3.11	3 (50%)
2	OCS	C	439	2	7,8,9	2.45	2 (28%)	6,11,13	2.12	3 (50%)

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	OCS	D	439	2	-	1/4/7/9	-
2	OCS	C	439	2	-	4/4/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	439	OCS	OD3-SG	6.22	1.63	1.45
2	C	439	OCS	OD1-SG	5.80	1.62	1.45
2	D	439	OCS	CB-SG	-2.65	1.67	1.77
2	C	439	OCS	CB-SG	-2.51	1.68	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	439	OCS	OD1-SG-CB	6.26	114.38	106.94
2	C	439	OCS	OD3-SG-CB	3.72	111.36	106.94
2	D	439	OCS	OD2-SG-CB	3.26	110.93	105.74
2	C	439	OCS	OD2-SG-CB	2.89	110.35	105.74
2	C	439	OCS	OD3-SG-OD1	-2.14	106.53	113.95
2	D	439	OCS	OD3-SG-OD1	-2.04	106.90	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	439	OCS	N-CA-CB-SG
2	C	439	OCS	N-CA-CB-SG
2	C	439	OCS	CA-CB-SG-OD1
2	C	439	OCS	CA-CB-SG-OD2
2	C	439	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	439	OCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	FAD	C	601	-	19,20,58	2.42	6 (31%)	24,30,89	2.68	7 (29%)
3	FAD	D	601	-	19,20,58	2.45	6 (31%)	24,30,89	2.70	7 (29%)
3	FAD	A	601	-	19,20,58	2.45	9 (47%)	24,30,89	2.51	6 (25%)
3	FAD	B	601	-	19,20,58	2.38	6 (31%)	24,30,89	2.57	7 (29%)

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	FAD	C	601	-	-	-	0/3/3/6
3	FAD	D	601	-	-	-	0/3/3/6
3	FAD	A	601	-	-	-	0/3/3/6
3	FAD	B	601	-	-	-	0/3/3/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	FAD	C4X-C10	4.73	1.49	1.40
3	C	601	FAD	C4X-C10	4.72	1.49	1.40
3	C	601	FAD	C4-C4X	4.71	1.49	1.41
3	D	601	FAD	C4-C4X	4.71	1.49	1.41
3	A	601	FAD	C4-C4X	4.66	1.49	1.41
3	A	601	FAD	C4X-C10	4.63	1.49	1.40
3	B	601	FAD	C4X-C10	4.63	1.49	1.40
3	B	601	FAD	C4-C4X	4.23	1.48	1.41
3	A	601	FAD	C9A-C5X	4.19	1.50	1.42
3	C	601	FAD	C9A-C5X	4.08	1.50	1.42
3	D	601	FAD	C9A-C5X	4.04	1.50	1.42
3	B	601	FAD	C9A-N10	4.04	1.42	1.35
3	B	601	FAD	C9A-C5X	3.98	1.50	1.42
3	D	601	FAD	C9A-N10	3.90	1.41	1.35
3	D	601	FAD	C8-C7	3.73	1.50	1.40
3	B	601	FAD	C8-C7	3.72	1.50	1.40
3	C	601	FAD	C8-C7	3.71	1.50	1.40
3	C	601	FAD	C9A-N10	3.63	1.41	1.35
3	A	601	FAD	C6-C5X	-3.47	1.36	1.41
3	B	601	FAD	C10-N10	3.41	1.41	1.35
3	D	601	FAD	C10-N10	3.34	1.41	1.35
3	C	601	FAD	C10-N10	3.17	1.41	1.35
3	A	601	FAD	C8-C7	2.76	1.47	1.40
3	A	601	FAD	C2-N1	-2.67	1.32	1.38
3	A	601	FAD	C10-N10	2.64	1.40	1.35
3	A	601	FAD	C10-N1	-2.51	1.30	1.35
3	A	601	FAD	C9-C9A	-2.08	1.38	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	FAD	C4-N3-C2	8.62	122.42	115.14
3	C	601	FAD	C4-N3-C2	8.51	122.33	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	8.42	122.25	115.14
3	A	601	FAD	C4-N3-C2	6.63	120.74	115.14
3	C	601	FAD	C4-C4X-C10	-5.50	116.31	119.95
3	A	601	FAD	C4-C4X-C10	-5.49	116.32	119.95
3	D	601	FAD	C4-C4X-C10	-5.28	116.46	119.95
3	A	601	FAD	C4-C4X-N5	4.98	124.30	118.60
3	D	601	FAD	C4X-N5-C5X	4.24	121.01	116.77
3	B	601	FAD	C4-C4X-C10	-4.18	117.19	119.95
3	A	601	FAD	C4X-C4-N3	-4.17	117.73	123.43
3	C	601	FAD	C4X-N5-C5X	4.12	120.89	116.77
3	B	601	FAD	C4X-N5-C5X	4.07	120.84	116.77
3	B	601	FAD	C4X-C4-N3	-3.97	118.00	123.43
3	C	601	FAD	C4X-C4-N3	-3.95	118.03	123.43
3	C	601	FAD	C4-C4X-N5	3.84	122.99	118.60
3	D	601	FAD	C4X-C4-N3	-3.83	118.20	123.43
3	D	601	FAD	C4-C4X-N5	3.62	122.73	118.60
3	B	601	FAD	N10-C10-N1	3.25	122.11	116.81
3	A	601	FAD	C4X-N5-C5X	3.19	119.96	116.77
3	D	601	FAD	N10-C10-N1	2.80	121.38	116.81
3	A	601	FAD	C10-C4X-N5	-2.62	119.36	122.33
3	B	601	FAD	C4-C4X-N5	2.47	121.42	118.60
3	C	601	FAD	N10-C10-N1	2.39	120.71	116.81
3	B	601	FAD	C5X-C9A-N10	-2.33	119.48	121.42
3	D	601	FAD	C5X-C9A-N10	-2.30	119.50	121.42
3	C	601	FAD	C5X-C9A-N10	-2.13	119.65	121.42

There are no chirality outliers.

There are no torsion outliers.

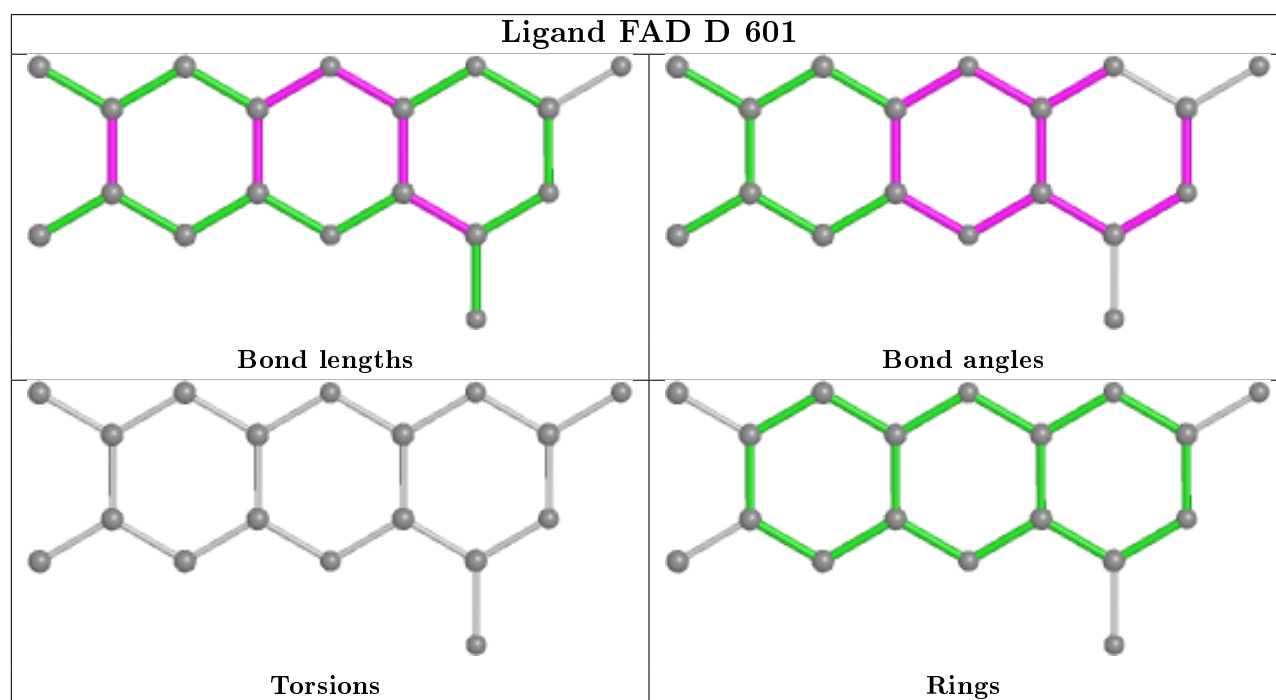
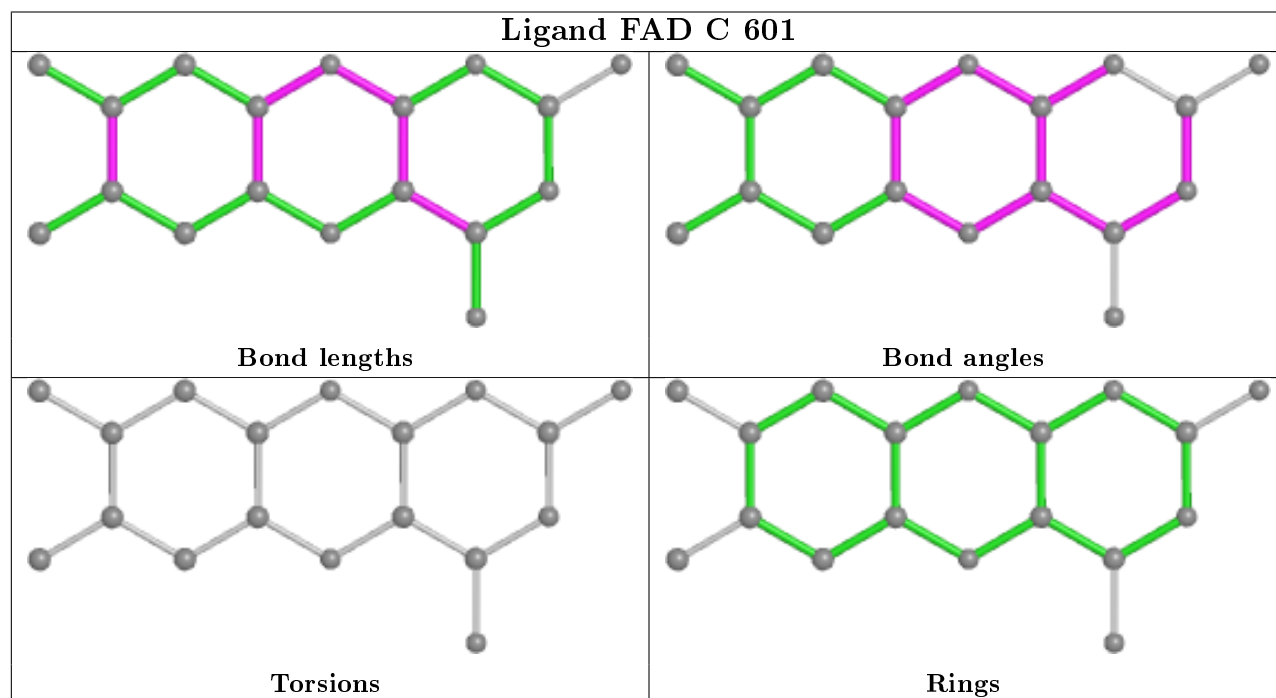
There are no ring outliers.

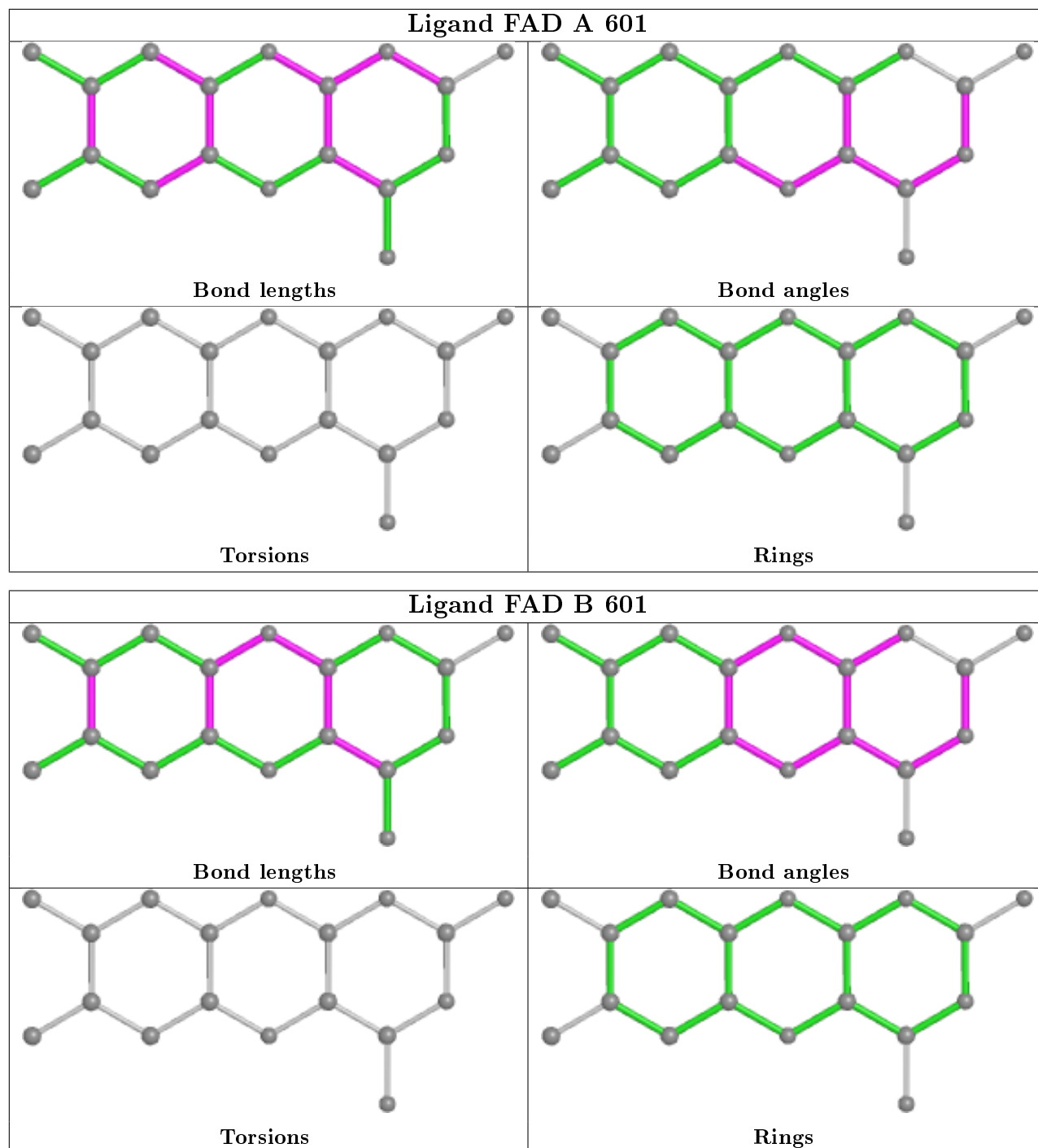
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	FAD	2	0
3	D	601	FAD	1	0
3	A	601	FAD	1	0
3	B	601	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 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	500/522 (95%)	0.29	23 (4%) 32 35	10, 18, 34, 46	0
1	B	500/522 (95%)	0.49	32 (6%) 19 21	13, 22, 40, 54	0
2	C	499/522 (95%)	0.28	21 (4%) 36 39	10, 19, 33, 46	0
2	D	498/522 (95%)	0.41	22 (4%) 34 37	10, 20, 40, 52	0
All	All	1997/2088 (95%)	0.37	98 (4%) 29 31	10, 20, 38, 54	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ASN	6.7
1	B	160	ASN	6.6
2	C	160	ASN	5.3
2	D	160	ASN	4.7
1	A	2	ASN	4.7
1	B	181	ARG	4.1
1	A	176	GLY	4.1
1	A	177	SER	4.0
1	B	159	SER	3.9
1	A	500	LEU	3.9
2	D	151	ASP	3.9
1	B	500	LEU	3.9
2	C	162	ALA	3.8
2	C	177	SER	3.7
1	B	463	GLU	3.7
1	B	161	ALA	3.6
2	D	470	GLU	3.5
2	C	466	ARG	3.5
1	B	470	GLU	3.5
2	C	176	GLY	3.3
2	C	463	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	493	ARG	3.3
1	B	145	GLU	3.3
2	D	500	LEU	3.2
2	D	176	GLY	3.2
2	D	420	HIS	3.2
1	B	112	LYS	3.1
2	D	501	LYS	3.1
1	B	360	GLU	3.1
1	B	425	ARG	3.1
2	D	159	SER	3.1
1	A	219	ARG	3.1
1	B	219	ARG	3.1
1	B	501	LYS	3.0
2	D	493	ARG	3.0
1	A	189	GLU	3.0
2	C	181	ARG	3.0
2	D	463	GLU	2.9
2	D	163	PRO	2.9
1	A	501	LYS	2.8
1	B	268	THR	2.8
1	B	416	HIS	2.8
2	D	466	ARG	2.7
2	C	425	ARG	2.7
2	C	161	ALA	2.7
2	C	248	GLN	2.7
2	D	146	SER	2.7
1	A	360	GLU	2.6
2	D	112	LYS	2.6
2	D	145	GLU	2.6
1	A	4	TYR	2.6
1	B	146	SER	2.6
2	D	464	GLN	2.6
1	A	161	ALA	2.6
2	C	219	ARG	2.6
1	A	416	HIS	2.6
1	A	152	ASP	2.5
1	A	466	ARG	2.5
2	D	152	ASP	2.5
1	B	143	LYS	2.5
1	A	181	ARG	2.5
1	A	493	ARG	2.4
2	C	152	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	464	GLN	2.4
2	D	426	GLN	2.4
2	D	161	ALA	2.4
1	B	356	ARG	2.3
1	B	456	GLN	2.3
2	C	2	ASN	2.3
1	A	460	GLN	2.3
1	A	420	HIS	2.3
2	C	112	LYS	2.3
1	B	321	GLN	2.2
2	C	426	GLN	2.2
2	C	465	ALA	2.2
2	C	360	GLU	2.2
2	D	460	GLN	2.2
1	A	463	GLU	2.2
1	B	328	PRO	2.2
1	B	485	GLU	2.2
1	B	419	GLU	2.2
1	A	112	LYS	2.2
1	A	175	GLN	2.2
2	C	155	GLU	2.1
2	C	420	HIS	2.1
2	D	350	ASP	2.1
1	B	467	PRO	2.1
1	B	141	ASN	2.1
1	B	151	ASP	2.1
1	A	159	SER	2.1
1	B	2	ASN	2.1
2	D	141	ASN	2.1
2	C	350	ASP	2.1
2	C	356	ARG	2.1
1	B	420	HIS	2.1
1	A	356	ARG	2.0
1	B	150	ASN	2.0
1	B	90	PHE	2.0

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

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(\AA^2)	Q<0.9
2	OCS	D	439	9/10	0.84	0.19	22,23,25,25	3
2	OCS	C	439	9/10	0.85	0.19	19,20,21,22	3

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

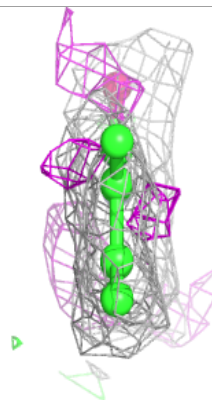
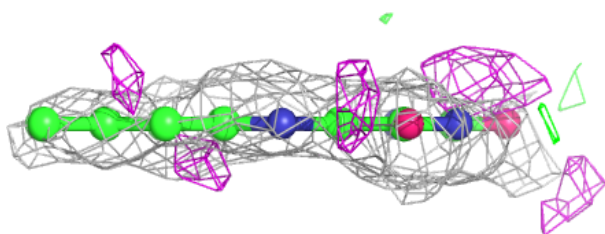
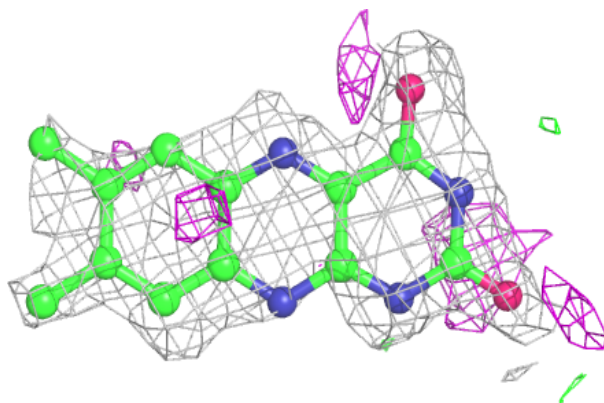
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	C	601	18/53	0.77	0.27	34,35,35,35	0
3	FAD	B	601	18/53	0.77	0.22	34,35,36,36	0
3	FAD	A	601	18/53	0.78	0.24	32,33,34,35	0
3	FAD	D	601	18/53	0.84	0.20	31,32,32,32	0
4	CA	A	602	1/1	0.88	0.09	24,24,24,24	0
4	CA	B	602	1/1	0.95	0.06	24,24,24,24	0
4	CA	C	602	1/1	0.96	0.06	22,22,22,22	0
4	CA	D	602	1/1	0.97	0.07	23,23,23,23	0

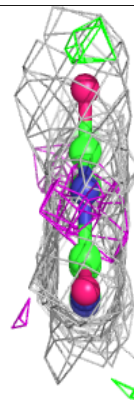
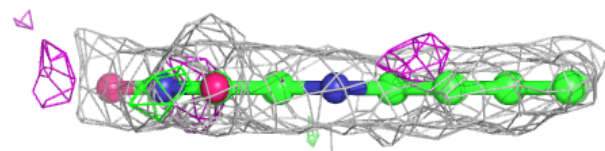
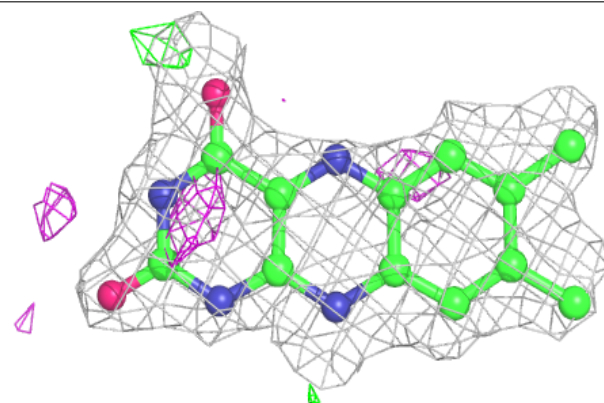
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 601:

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

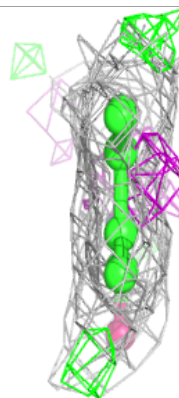
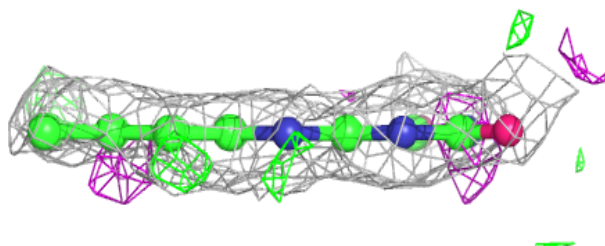
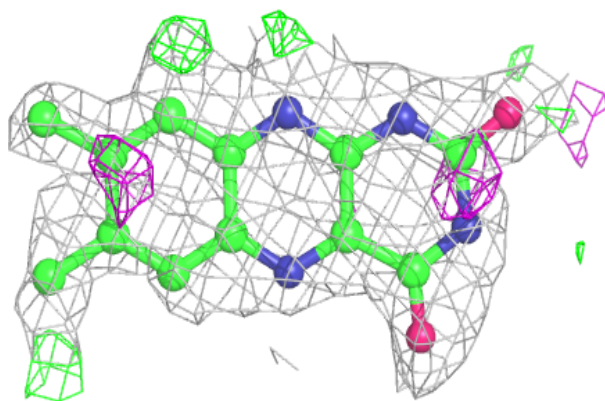
**Electron density around FAD B 601:**

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

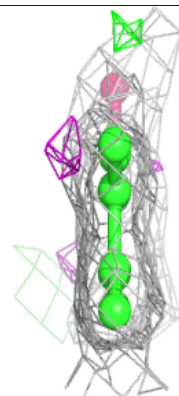
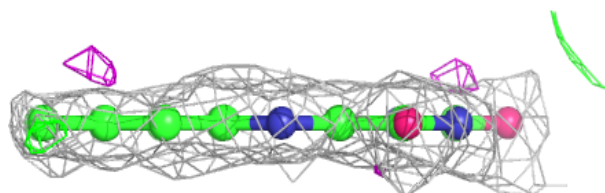
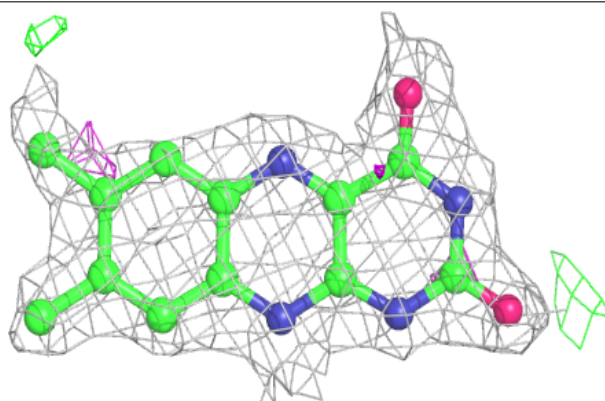


Electron density around FAD A 601:

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

**Electron density around FAD D 601:**

$2mF_o-DF_c$ (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.