



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:57 pm BST

PDB ID : 6P2V  
Title : RebH Variant 10S, Tryptamine 5-halogenase  
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Deposited on : 2019-05-22  
Resolution : 2.55 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](mailto: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.

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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

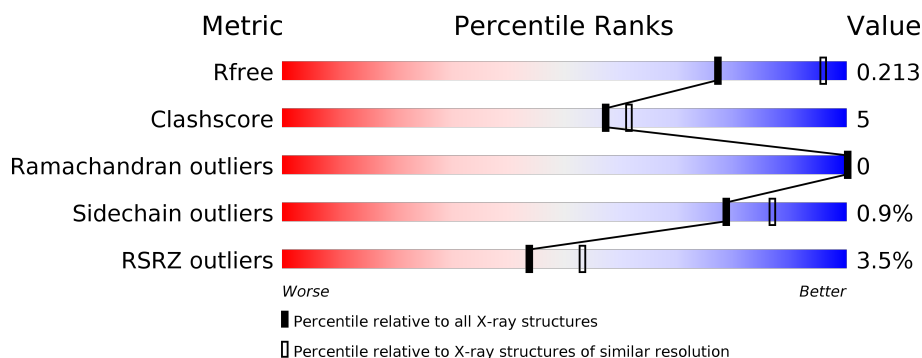
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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  $\geq 3$ , 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	550	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	B	550	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8885 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 Flavin-dependent tryptophan halogenase RebH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4185	2655	730	780	20			
1	B	521	Total	C	N	O	S	0	0	0
			4162	2642	727	773	20			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8KHZ8
A	-18	GLY	-	expression tag	UNP Q8KHZ8
A	-17	SER	-	expression tag	UNP Q8KHZ8
A	-16	SER	-	expression tag	UNP Q8KHZ8
A	-15	HIS	-	expression tag	UNP Q8KHZ8
A	-14	HIS	-	expression tag	UNP Q8KHZ8
A	-13	HIS	-	expression tag	UNP Q8KHZ8
A	-12	HIS	-	expression tag	UNP Q8KHZ8
A	-11	HIS	-	expression tag	UNP Q8KHZ8
A	-10	HIS	-	expression tag	UNP Q8KHZ8
A	-9	SER	-	expression tag	UNP Q8KHZ8
A	-8	SER	-	expression tag	UNP Q8KHZ8
A	-7	GLY	-	expression tag	UNP Q8KHZ8
A	-6	LEU	-	expression tag	UNP Q8KHZ8
A	-5	VAL	-	expression tag	UNP Q8KHZ8
A	-4	PRO	-	expression tag	UNP Q8KHZ8
A	-3	ARG	-	expression tag	UNP Q8KHZ8
A	-2	GLY	-	expression tag	UNP Q8KHZ8
A	-1	SER	-	expression tag	UNP Q8KHZ8
A	0	HIS	-	expression tag	UNP Q8KHZ8
A	52	HIS	ILE	engineered mutation	UNP Q8KHZ8
A	380	PHE	LEU	engineered mutation	UNP Q8KHZ8
A	465	CYS	PHE	engineered mutation	UNP Q8KHZ8
A	470	SER	ASN	engineered mutation	UNP Q8KHZ8
A	494	ARG	GLN	engineered mutation	UNP Q8KHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLN	ARG	engineered mutation	UNP Q8KHZ8
B	-19	MET	-	initiating methionine	UNP Q8KHZ8
B	-18	GLY	-	expression tag	UNP Q8KHZ8
B	-17	SER	-	expression tag	UNP Q8KHZ8
B	-16	SER	-	expression tag	UNP Q8KHZ8
B	-15	HIS	-	expression tag	UNP Q8KHZ8
B	-14	HIS	-	expression tag	UNP Q8KHZ8
B	-13	HIS	-	expression tag	UNP Q8KHZ8
B	-12	HIS	-	expression tag	UNP Q8KHZ8
B	-11	HIS	-	expression tag	UNP Q8KHZ8
B	-10	HIS	-	expression tag	UNP Q8KHZ8
B	-9	SER	-	expression tag	UNP Q8KHZ8
B	-8	SER	-	expression tag	UNP Q8KHZ8
B	-7	GLY	-	expression tag	UNP Q8KHZ8
B	-6	LEU	-	expression tag	UNP Q8KHZ8
B	-5	VAL	-	expression tag	UNP Q8KHZ8
B	-4	PRO	-	expression tag	UNP Q8KHZ8
B	-3	ARG	-	expression tag	UNP Q8KHZ8
B	-2	GLY	-	expression tag	UNP Q8KHZ8
B	-1	SER	-	expression tag	UNP Q8KHZ8
B	0	HIS	-	expression tag	UNP Q8KHZ8
B	52	HIS	ILE	engineered mutation	UNP Q8KHZ8
B	380	PHE	LEU	engineered mutation	UNP Q8KHZ8
B	465	CYS	PHE	engineered mutation	UNP Q8KHZ8
B	470	SER	ASN	engineered mutation	UNP Q8KHZ8
B	494	ARG	GLN	engineered mutation	UNP Q8KHZ8
B	509	GLN	ARG	engineered mutation	UNP Q8KHZ8

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total	O	0	0
			224	224		
3	B	208	Total	O	0	0
			208	208		



- Molecule 1: Flavin-dependent tryptophan halogenase RebH



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.16Å 115.16Å 230.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.73 – 2.55 49.87 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.73-2.55) 92.4 (49.87-2.55)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.171 , 0.210 0.174 , 0.213	Depositor DCC
$R_{free}$ test set	2786 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.48	0/4300	0.60	0/5834
1	B	0.44	0/4277	0.57	0/5805
All	All	0.46	0/8577	0.59	0/11639

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	4185	0	3978	42	0
1	B	4162	0	3949	41	0
2	A	53	0	30	6	0
2	B	53	0	30	4	0
3	A	224	0	0	3	0
3	B	208	0	0	0	0
All	All	8885	0	7987	80	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 5.

All (80) 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:387:ARG:HH12	1:A:390:ARG:HD2	1.17	1.08
1:A:12:GLY:HA2	2:A:601:FAD:H1B	1.37	1.06
1:A:387:ARG:NH1	1:A:390:ARG:HD2	1.75	1.01
1:A:488:ARG:HD2	1:B:372:VAL:O	1.76	0.83
1:A:348:THR:HG23	2:A:601:FAD:O3'	1.82	0.79
1:A:437:TYR:HB2	1:A:443:ILE:HD11	1.65	0.77
1:A:328:ILE:HD13	2:A:601:FAD:HM73	1.65	0.76
1:A:80:VAL:HB	1:A:150:LEU:HD21	1.71	0.72
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.77	0.67
1:A:519:SER:OG	1:A:522:GLU:HG3	1.95	0.65
1:B:49:GLU:HG3	1:B:173:ALA:HB2	1.79	0.64
1:A:348:THR:CG2	2:A:601:FAD:O3'	2.46	0.63
2:B:601:FAD:O4'	2:B:601:FAD:O2'	1.99	0.61
1:B:276:ILE:HG21	1:B:315:MET:CE	2.32	0.60
1:A:49:GLU:HG3	1:A:173:ALA:HB2	1.84	0.59
1:A:187:LYS:NZ	3:A:701:HOH:O	2.27	0.58
1:A:410:SER:O	1:A:422:LYS:NZ	2.37	0.58
1:B:276:ILE:HG21	1:B:315:MET:HE2	1.87	0.57
1:A:387:ARG:O	1:A:391:GLU:HG2	2.04	0.57
1:B:369:TYR:OH	1:B:459:GLU:HG2	2.06	0.56
1:B:49:GLU:OE2	2:B:601:FAD:O2'	2.23	0.55
1:B:18:TRP:CZ2	1:B:181:ARG:HG3	2.42	0.55
1:A:436:MET:SD	1:B:387:ARG:HD2	2.47	0.55
1:A:4:LYS:O	1:A:378:LYS:HE3	2.08	0.54
1:B:390:ARG:O	1:B:394:THR:HG23	2.10	0.52
1:B:170:HIS:CE1	1:B:287:PRO:HD2	2.45	0.51
1:B:215:THR:OG1	1:B:217:ARG:HD2	2.11	0.51
1:A:360:GLY:HA3	2:A:601:FAD:H2'	1.93	0.51
1:A:5:ILE:HG23	1:A:222:ASP:HB2	1.94	0.49
1:A:41:ASP:OD1	1:A:42:ILE:N	2.45	0.49
1:B:250:LEU:HD13	1:B:353:VAL:HG23	1.94	0.49
1:B:456:GLY:N	1:B:461:GLU:OE2	2.45	0.49
1:B:5:ILE:HG23	1:B:222:ASP:HB2	1.95	0.48
1:A:255:ALA:HA	1:A:296:TYR:O	2.13	0.48
1:B:84:PHE:O	1:B:106:HIS:HA	2.14	0.48
1:B:12:GLY:HA2	2:B:601:FAD:H1B	1.96	0.47
1:A:274:SER:HB2	1:A:285:LYS:HB3	1.96	0.47
1:A:18:TRP:CZ2	1:A:181:ARG:HG3	2.49	0.46
1:B:438:ARG:HA	1:B:482:PRO:HA	1.96	0.46
1:A:99:GLU:OE2	1:A:102:GLY:N	2.44	0.46
1:A:155:SER:HB2	1:A:520:LEU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:NH1	1:B:167:TYR:OH	2.49	0.46
1:A:383:VAL:HG21	1:B:435:ASP:HB3	1.98	0.45
1:B:137:GLU:OE2	1:B:507:LYS:NZ	2.41	0.45
1:A:271:PRO:HB3	1:A:520:LEU:HD22	1.99	0.44
1:B:140:ASP:OD1	1:B:140:ASP:N	2.50	0.44
1:A:243:PHE:CZ	1:A:331:ARG:HG2	2.53	0.44
1:A:339:TRP:CG	1:A:385:THR:HG23	2.53	0.44
1:A:88:ARG:HA	1:A:411:PRO:HG2	2.00	0.43
1:A:110:SER:HB3	3:A:880:HOH:O	2.17	0.43
1:A:436:MET:CG	1:B:387:ARG:HD2	2.49	0.43
1:A:84:PHE:O	1:A:106:HIS:HA	2.18	0.43
1:A:250:LEU:HD13	1:A:353:VAL:HG23	2.00	0.43
1:A:116:TYR:CD1	1:A:449:ASP:HB3	2.53	0.43
1:B:50:ALA:O	1:B:358:SER:HB3	2.18	0.43
1:B:80:VAL:HB	1:B:150:LEU:HD21	2.01	0.43
1:A:488:ARG:O	1:A:492:MET:HG3	2.19	0.42
1:B:212:ARG:HG3	1:B:218:VAL:HG22	2.00	0.42
1:B:155:SER:HB2	1:B:520:LEU:HA	2.00	0.42
1:B:38:GLN:O	1:B:194:GLU:HA	2.19	0.42
1:B:305:GLU:OE2	1:B:327:ARG:HD3	2.19	0.42
1:B:159:LEU:HG	1:B:518:PRO:HG3	2.01	0.42
1:A:436:MET:HG2	1:B:387:ARG:HD2	2.02	0.42
1:B:446:PRO:HB2	1:B:448:SER:O	2.20	0.42
1:B:144:TYR:OH	1:B:469:SER:HB3	2.19	0.42
2:A:601:FAD:H9	2:A:601:FAD:H1'1	1.88	0.42
1:B:357:GLU:OE2	1:B:406:HIS:NE2	2.37	0.42
1:B:401:ASP:HB3	1:B:430:MET:HB2	2.02	0.42
1:B:233:LEU:HD11	2:B:601:FAD:N7A	2.35	0.41
1:B:252:ASN:O	1:B:332:VAL:HG21	2.20	0.41
1:A:37:LEU:HD23	1:A:193:VAL:HB	2.03	0.41
1:A:132:ARG:HB2	1:A:132:ARG:HE	1.62	0.41
1:A:387:ARG:CZ	1:A:390:ARG:HD2	2.47	0.41
1:B:276:ILE:HG21	1:B:315:MET:HE1	2.01	0.41
1:B:94:THR:N	1:B:315:MET:HE3	2.36	0.41
1:A:151:ASP:HA	3:A:817:HOH:O	2.20	0.41
1:A:251:LEU:HD13	1:A:302:PHE:HE2	1.86	0.41
1:B:307:GLU:O	1:B:311:GLU:HG3	2.21	0.40
1:A:38:GLN:HG2	1:A:192:HIS:NE2	2.37	0.40
1:B:247:SER:HA	1:B:250:LEU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	519/550 (94%)	506 (98%)	13 (2%)	0	100	100
1	B	517/550 (94%)	505 (98%)	12 (2%)	0	100	100
All	All	1036/1100 (94%)	1011 (98%)	25 (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	439/463 (95%)	433 (99%)	6 (1%)	67	78
1	B	435/463 (94%)	433 (100%)	2 (0%)	88	93
All	All	874/926 (94%)	866 (99%)	8 (1%)	78	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	110	SER
1	A	178	ASP
1	A	390	ARG
1	A	425	ARG
1	A	488	ARG
1	B	330	PHE
1	B	509	GLN

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	601	-	51,58,58	4.69	18 (35%)	60,89,89	2.39	13 (21%)
2	FAD	B	601	-	51,58,58	4.70	18 (35%)	60,89,89	2.36	12 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	9/30/50/50	0/6/6/6
2	FAD	B	601	-	-	16/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4B-C1B	15.50	1.62	1.41
2	B	601	FAD	C2B-C1B	-15.36	1.30	1.53
2	B	601	FAD	O4B-C1B	15.29	1.62	1.41
2	A	601	FAD	C2B-C1B	-14.88	1.31	1.53
2	A	601	FAD	C10-N1	10.56	1.46	1.33
2	B	601	FAD	C10-N1	10.52	1.46	1.33
2	B	601	FAD	C4X-N5	8.77	1.45	1.33
2	A	601	FAD	C4X-N5	8.76	1.45	1.33
2	A	601	FAD	C5X-N5	8.51	1.49	1.35
2	B	601	FAD	C5X-N5	8.50	1.49	1.35
2	B	601	FAD	C9A-N10	8.49	1.50	1.38
2	A	601	FAD	C9A-N10	8.48	1.50	1.38
2	B	601	FAD	C4-N3	7.59	1.46	1.33
2	A	601	FAD	C4-N3	7.56	1.46	1.33
2	A	601	FAD	C4X-C10	7.20	1.46	1.38
2	B	601	FAD	C4X-C10	7.13	1.45	1.38
2	A	601	FAD	O4B-C4B	-6.39	1.30	1.45
2	B	601	FAD	O4B-C4B	-6.18	1.31	1.45
2	A	601	FAD	C4-C4X	6.00	1.51	1.41
2	B	601	FAD	C4-C4X	6.00	1.51	1.41
2	A	601	FAD	C2-N3	5.69	1.49	1.38
2	B	601	FAD	C2-N3	5.67	1.49	1.38
2	B	601	FAD	C2-N1	5.28	1.48	1.38
2	A	601	FAD	C2-N1	5.28	1.48	1.38
2	A	601	FAD	O2B-C2B	3.11	1.50	1.43
2	B	601	FAD	O2B-C2B	3.04	1.50	1.43
2	B	601	FAD	C6A-N6A	3.00	1.45	1.34
2	A	601	FAD	C6A-N6A	3.00	1.45	1.34
2	B	601	FAD	O3B-C3B	-2.93	1.36	1.43
2	A	601	FAD	O3B-C3B	-2.92	1.36	1.43
2	A	601	FAD	C5A-C4A	-2.71	1.33	1.40
2	B	601	FAD	C5A-C4A	-2.69	1.33	1.40
2	A	601	FAD	O4-C4	-2.31	1.18	1.24
2	B	601	FAD	O4-C4	-2.29	1.18	1.24
2	A	601	FAD	C2A-N3A	2.26	1.35	1.32
2	B	601	FAD	C2A-N3A	2.25	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-C6A-N6A	9.86	135.33	120.35
2	A	601	FAD	C5A-C6A-N6A	9.82	135.28	120.35
2	B	601	FAD	N6A-C6A-N1A	-6.71	104.64	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N6A-C6A-N1A	-6.71	104.65	118.57
2	B	601	FAD	C7M-C7-C8	5.56	132.13	120.74
2	B	601	FAD	N3A-C2A-N1A	-5.53	120.03	128.68
2	A	601	FAD	C4-N3-C2	5.53	119.81	115.14
2	A	601	FAD	N3A-C2A-N1A	-5.52	120.06	128.68
2	A	601	FAD	C7M-C7-C8	5.50	132.01	120.74
2	B	601	FAD	C4-N3-C2	5.46	119.75	115.14
2	B	601	FAD	C7M-C7-C6	-5.21	107.87	120.34
2	A	601	FAD	C7M-C7-C6	-5.20	107.90	120.34
2	A	601	FAD	C3B-C2B-C1B	3.54	106.30	100.98
2	A	601	FAD	C4X-N5-C5X	3.32	120.08	116.77
2	B	601	FAD	C4X-N5-C5X	3.27	120.04	116.77
2	B	601	FAD	C5X-C9A-N10	3.26	120.08	117.72
2	A	601	FAD	C5X-C9A-N10	3.17	120.01	117.72
2	B	601	FAD	C4X-C4-N3	-2.71	119.72	123.43
2	A	601	FAD	C4X-C4-N3	-2.70	119.74	123.43
2	A	601	FAD	P-O3P-PA	-2.68	123.62	132.83
2	B	601	FAD	P-O3P-PA	-2.68	123.63	132.83
2	A	601	FAD	C1'-N10-C9A	2.42	120.20	118.29
2	B	601	FAD	C3B-C2B-C1B	2.10	104.14	100.98
2	A	601	FAD	C10-C4X-N5	-2.08	119.82	121.26
2	B	601	FAD	C1'-N10-C9A	2.07	119.92	118.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'

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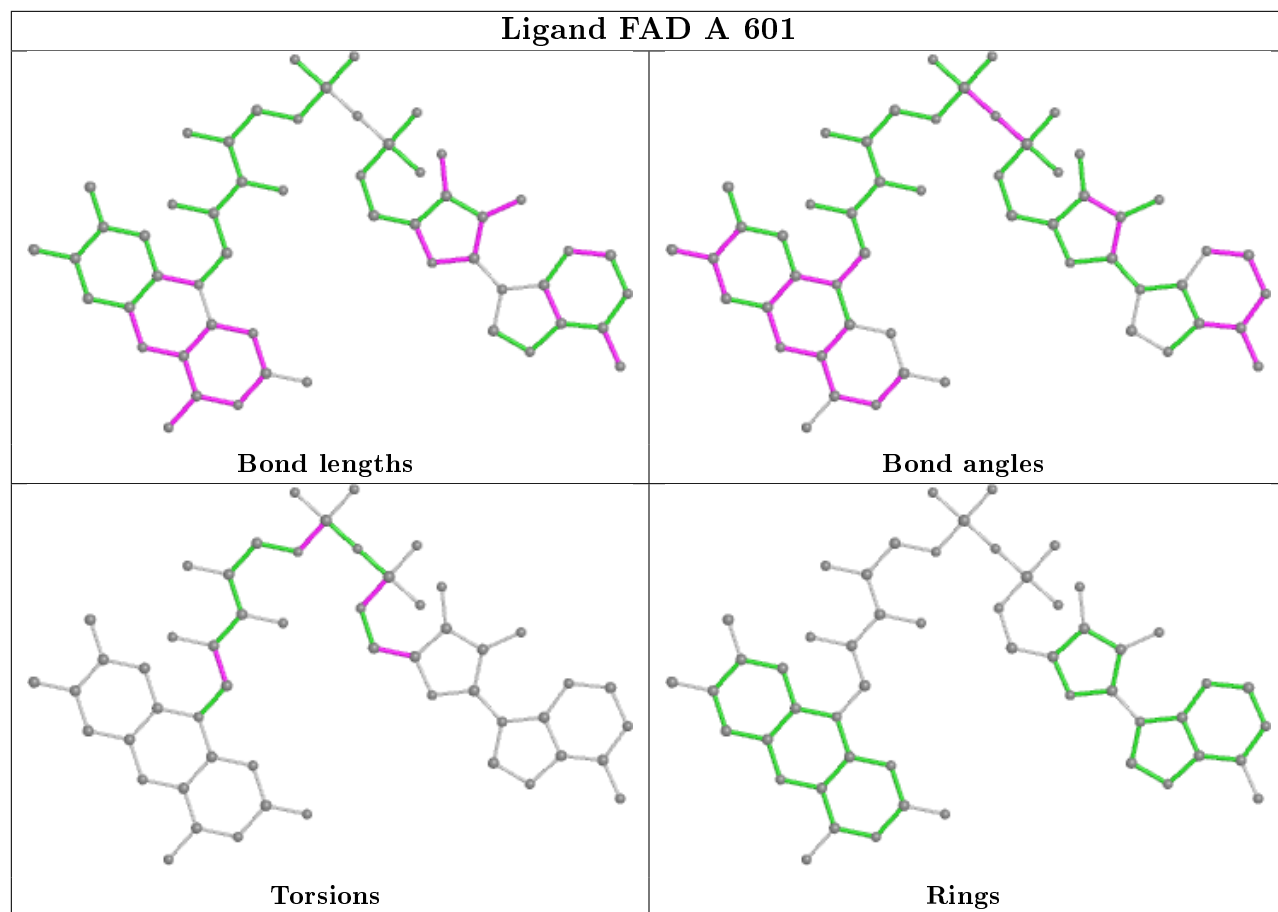
Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	PA-O3P-P-O2P
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	PA-O3P-P-O1P

There are no ring outliers.

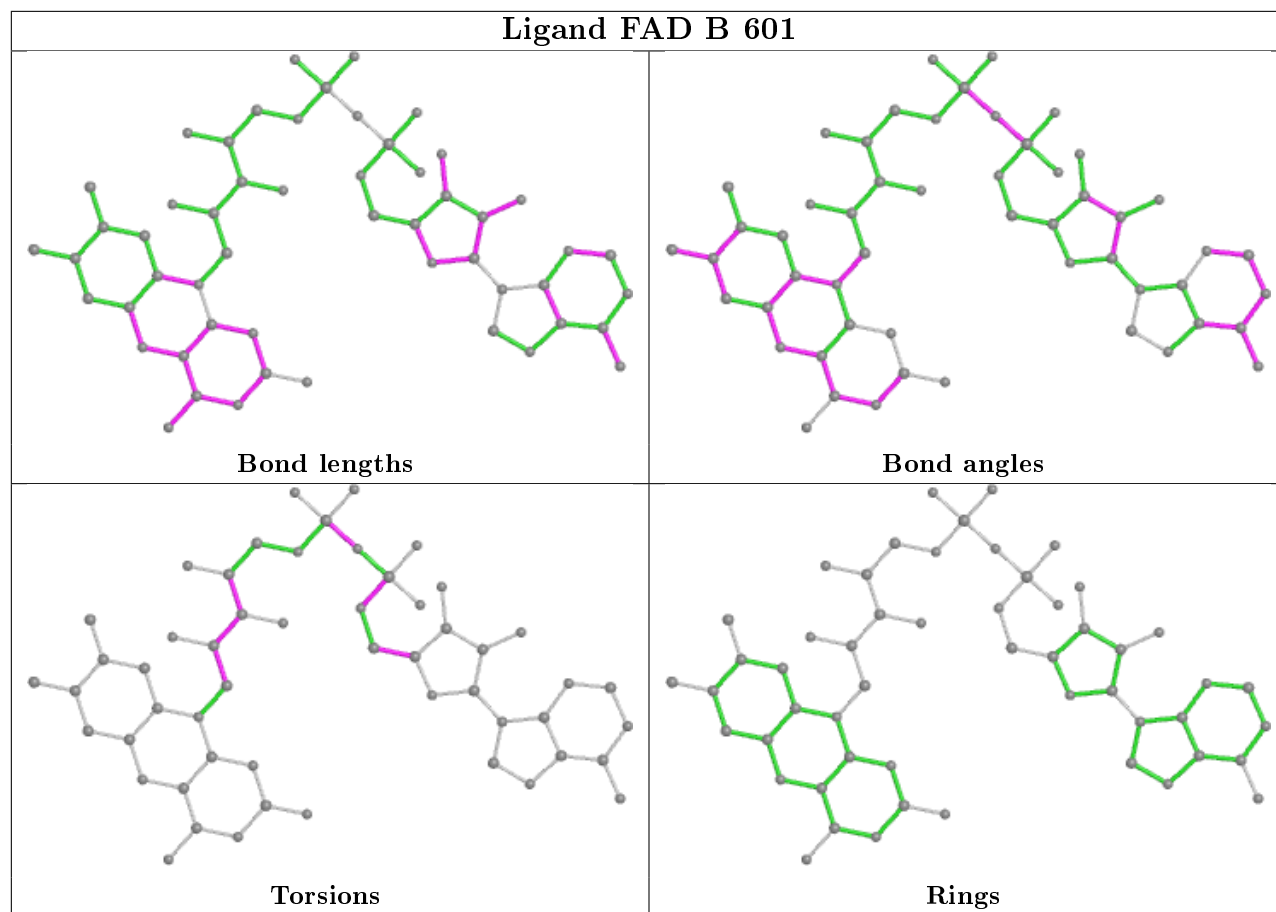
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	6	0
2	B	601	FAD	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	523/550 (95%)	0.01	22 (4%)	36 45	24, 36, 59, 94	0
1	B	521/550 (94%)	0.06	15 (2%)	51 61	25, 38, 60, 104	0
All	All	1044/1100 (94%)	0.03	37 (3%)	44 53	24, 37, 60, 104	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	GLY	4.1
1	B	159	LEU	3.9
1	A	512	ASN	3.3
1	A	527	GLN	3.2
1	A	526	GLN	3.1
1	A	162	SER	3.0
1	A	159	LEU	3.0
1	A	501	GLU	2.8
1	B	132	ARG	2.8
1	A	515	GLU	2.7
1	A	497	GLU	2.6
1	A	301	ARG	2.6
1	A	505	ALA	2.6
1	B	512	ASN	2.5
1	A	161	GLY	2.5
1	B	133	GLY	2.5
1	B	515	GLU	2.5
1	A	506	VAL	2.5
1	A	528	HIS	2.4
1	A	509	GLN	2.4
1	A	499	VAL	2.4
1	A	511	ARG	2.3
1	A	525	ARG	2.3
1	A	329	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	164	VAL	2.2
1	B	100	LEU	2.2
1	B	522	GLU	2.2
1	A	498	SER	2.2
1	B	516	THR	2.1
1	B	527	GLN	2.1
1	A	160	ASP	2.1
1	A	495	ALA	2.1
1	B	505	ALA	2.1
1	B	162	SER	2.1
1	B	204	ALA	2.1
1	B	101	ASP	2.1
1	B	463	ARG	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](#)

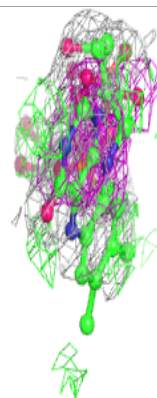
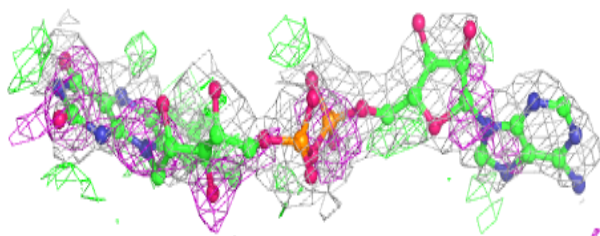
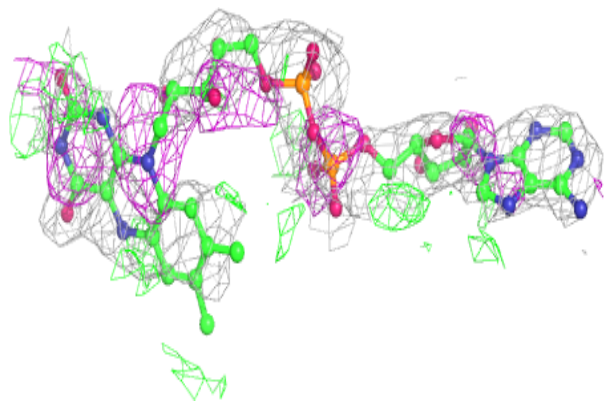
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	601	53/53	0.78	0.30	41,64,81,104	0
2	FAD	B	601	53/53	0.78	0.28	47,65,86,103	0

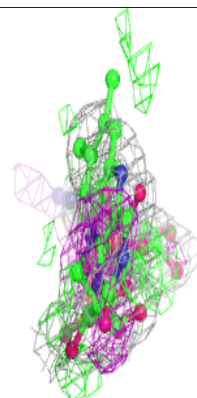
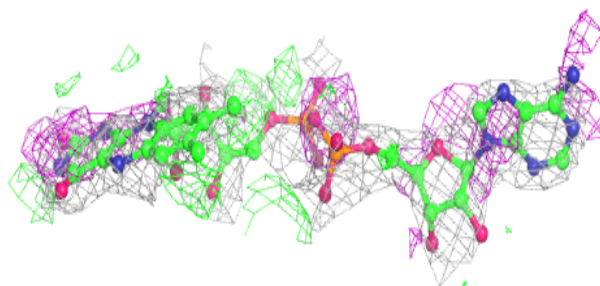
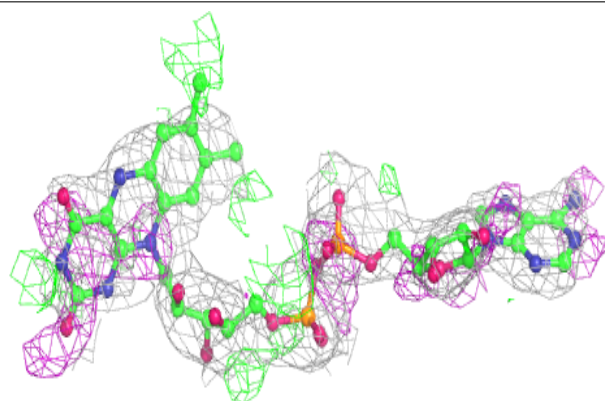
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD A 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)



## 6.5 Other polymers

There are no such residues in this entry.