



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 08:17 PM EDT

PDB ID : 3BG6  
Title : Pyranose 2-oxidase from *Trametes multicolor*, E542K mutant  
Authors : Tan, T.C.; Divne, C.  
Deposited on : 2007-11-26  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

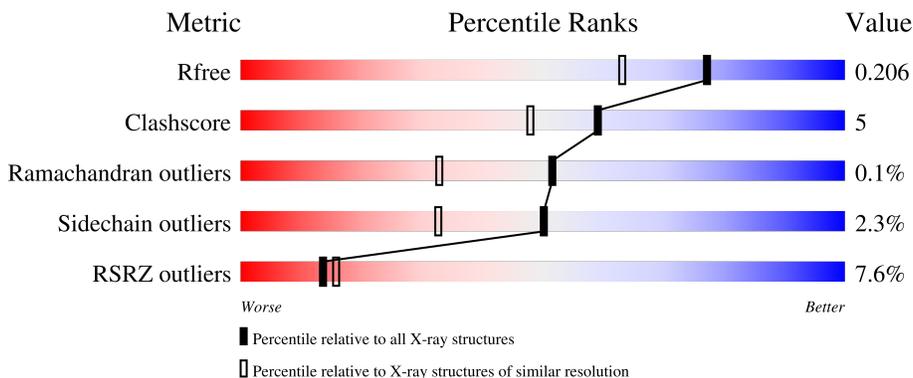
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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.



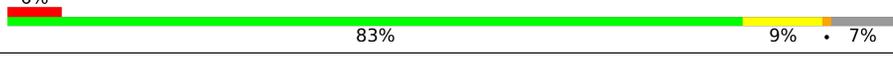
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	623	 7% 83% 8% • 7%
1	B	623	 5% 85% 7% • 7%
1	C	623	 8% 84% 7% • 7%
1	D	623	 6% 82% 10% • 7%
1	E	623	 9% 84% 8% • 7%

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Mol	Chain	Length	Quality of chain
1	F	623	 9% 83% 8% • 7%
1	G	623	 7% 83% 9% • 7%
1	H	623	 6% 83% 9% • 7%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 39362 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.

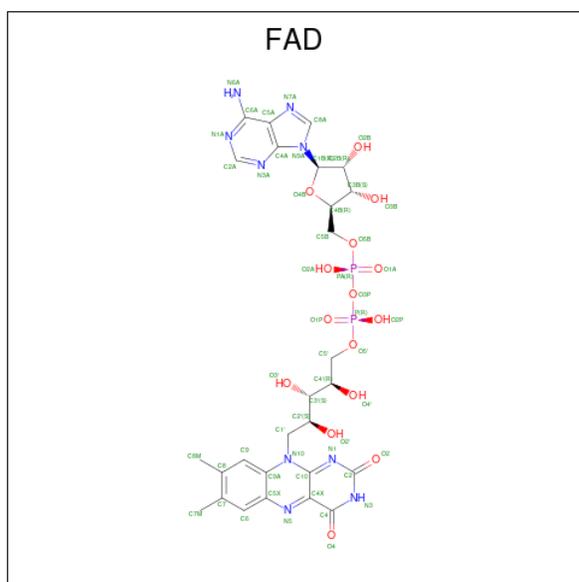
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4549	2873	779	872	25	0	0	0
1	B	577	4549	2873	779	872	25	0	0	0
1	C	577	4549	2873	779	872	25	0	0	0
1	D	577	4549	2873	779	872	25	0	0	0
1	E	577	4549	2873	779	872	25	0	0	0
1	F	577	4549	2873	779	872	25	0	0	0
1	G	577	4549	2873	779	872	25	0	0	0
1	H	577	4549	2873	779	872	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	LYS	GLU	engineered mutation	UNP Q7ZA32
B	542	LYS	GLU	engineered mutation	UNP Q7ZA32
C	542	LYS	GLU	engineered mutation	UNP Q7ZA32
D	542	LYS	GLU	engineered mutation	UNP Q7ZA32
E	542	LYS	GLU	engineered mutation	UNP Q7ZA32
F	542	LYS	GLU	engineered mutation	UNP Q7ZA32
G	542	LYS	GLU	engineered mutation	UNP Q7ZA32
H	542	LYS	GLU	engineered mutation	UNP Q7ZA32

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	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	359	Total	O	0	0
			359	359		
3	B	373	Total	O	0	0
			373	373		
3	C	267	Total	O	0	0
			267	267		
3	D	314	Total	O	0	0
			314	314		

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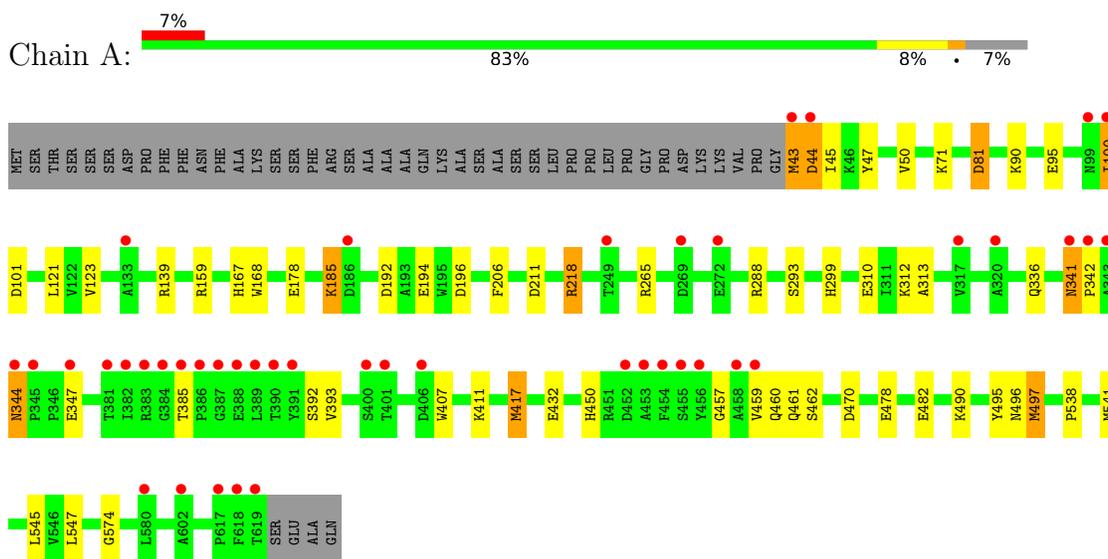
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	301	Total 301	O 301	0	0
3	F	262	Total 262	O 262	0	0
3	G	315	Total 315	O 315	0	0
3	H	355	Total 355	O 355	0	0

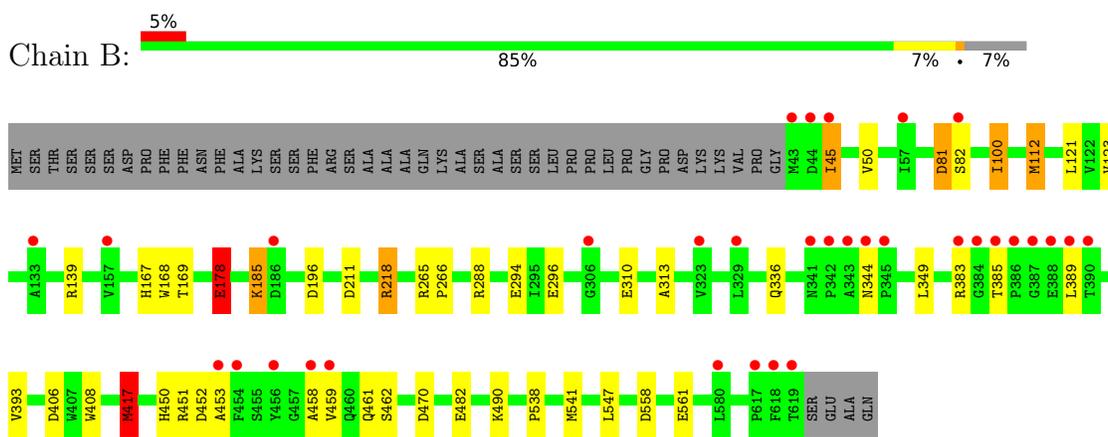
### 3 Residue-property plots i

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.

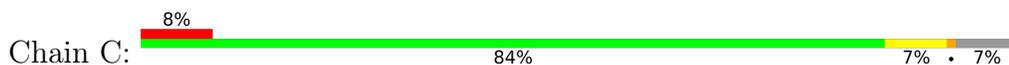
- Molecule 1: Pyranose oxidase

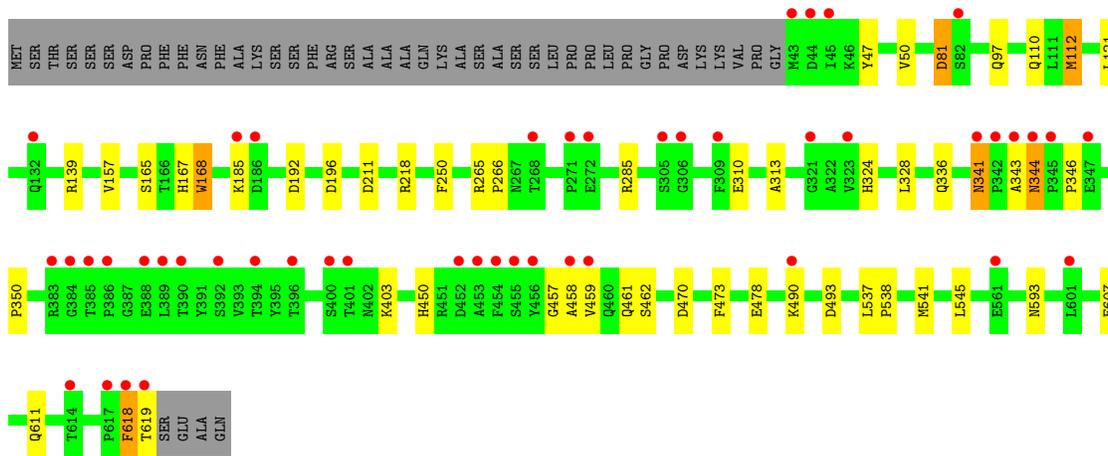


- Molecule 1: Pyranose oxidase

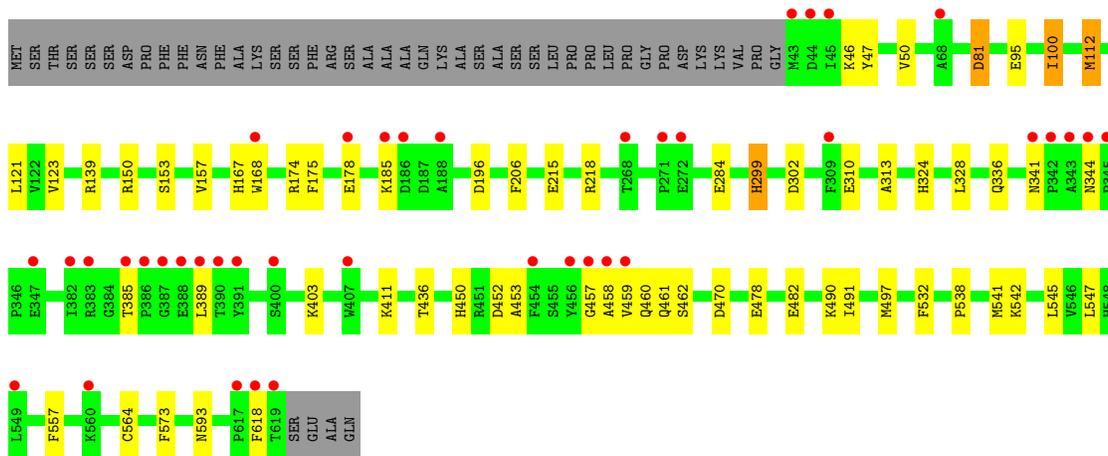
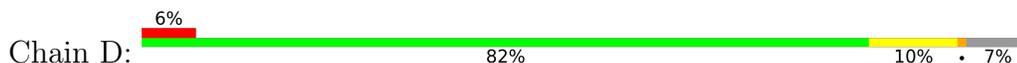


- Molecule 1: Pyranose oxidase

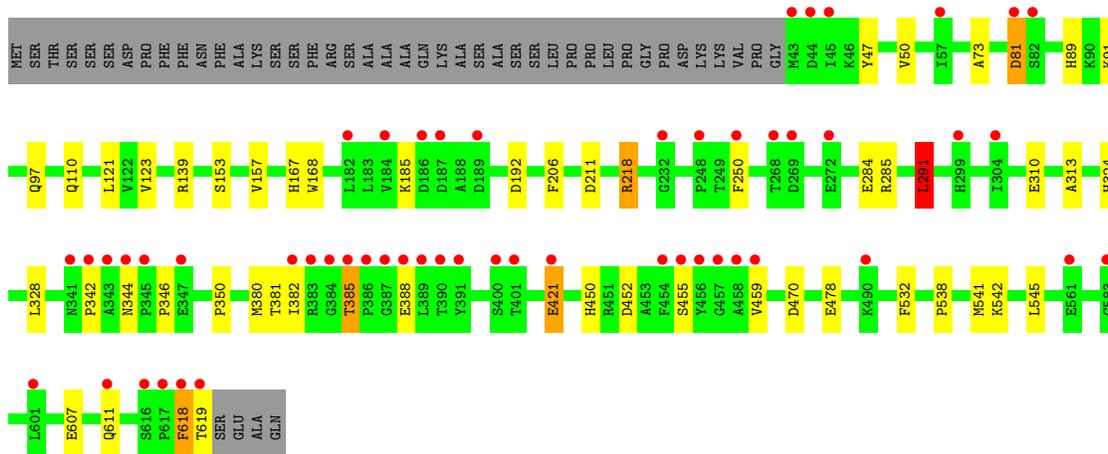
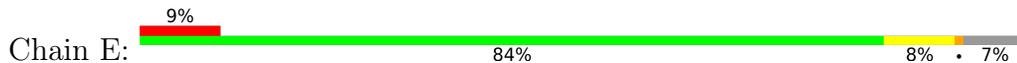




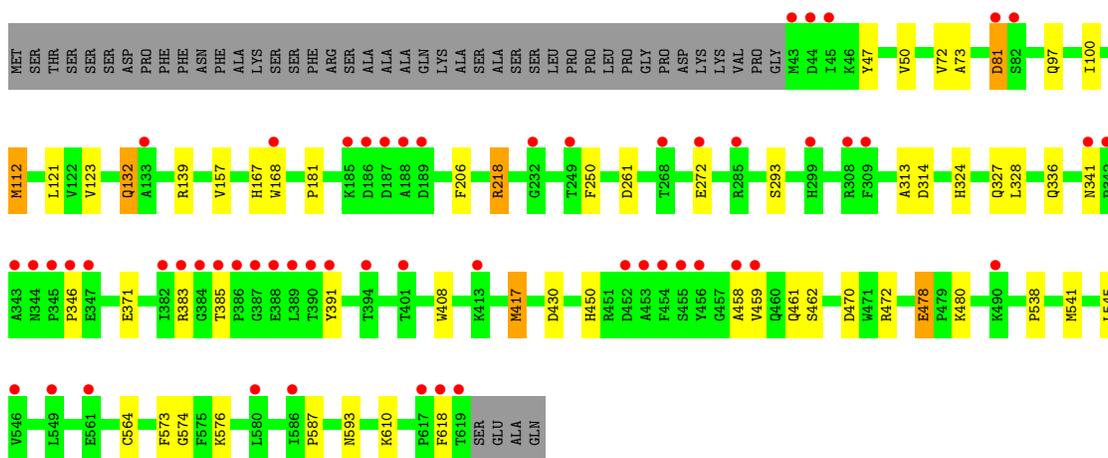
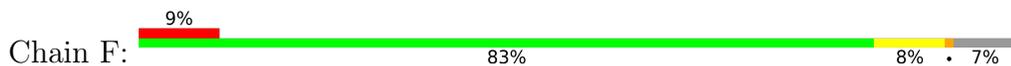
• Molecule 1: Pyranose oxidase



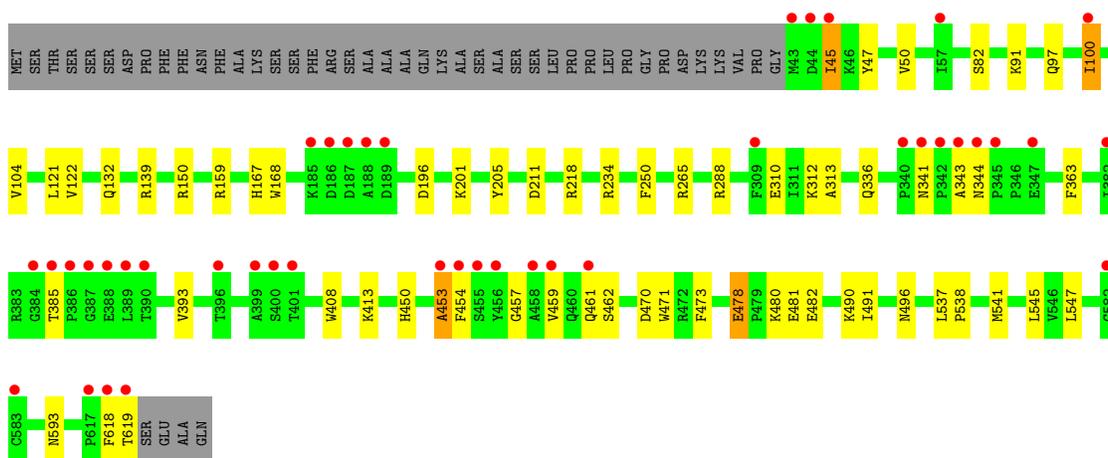
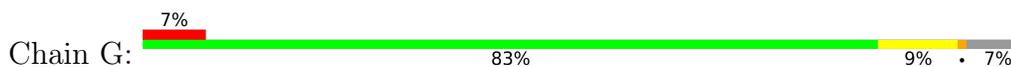
• Molecule 1: Pyranose oxidase



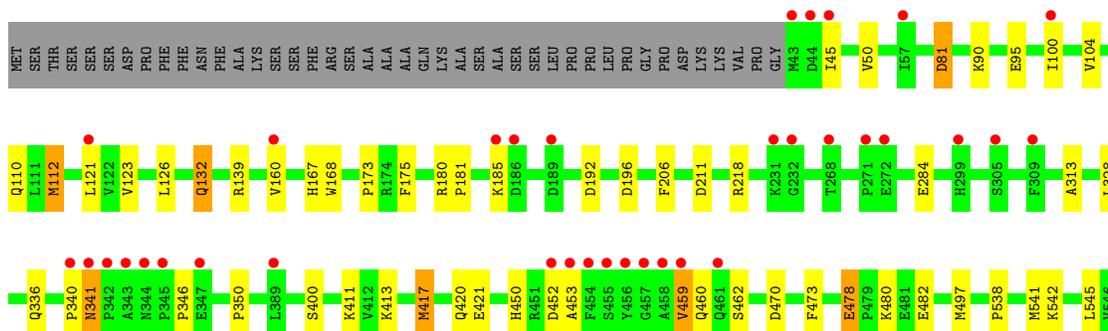
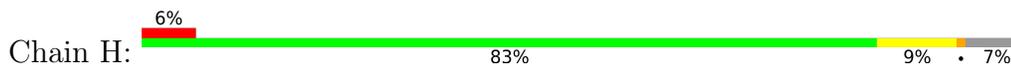
- Molecule 1: Pyranose oxidase

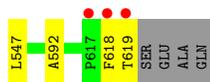


- Molecule 1: Pyranose oxidase



- Molecule 1: Pyranose oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.86Å 103.75Å 169.33Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 39.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-1.70) 98.3 (39.18-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.198 0.177 , 0.206	Depositor DCC
$R_{free}$ test set	6061 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	39362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	1.09	11/4665 (0.2%)	1.03	18/6342 (0.3%)
1	B	1.11	7/4665 (0.2%)	1.05	17/6342 (0.3%)
1	C	0.91	2/4665 (0.0%)	0.94	13/6342 (0.2%)
1	D	0.97	6/4665 (0.1%)	0.96	13/6342 (0.2%)
1	E	0.98	5/4665 (0.1%)	0.96	10/6342 (0.2%)
1	F	0.96	5/4665 (0.1%)	0.99	10/6342 (0.2%)
1	G	1.01	6/4665 (0.1%)	0.96	11/6342 (0.2%)
1	H	1.07	11/4665 (0.2%)	1.03	18/6342 (0.3%)
All	All	1.01	53/37320 (0.1%)	0.99	110/50736 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	LEU	CG-CD1	12.75	1.99	1.51
1	A	194	GLU	CG-CD	-8.00	1.40	1.51
1	H	478	GLU	CD-OE1	7.85	1.34	1.25
1	B	482	GLU	CD-OE1	7.83	1.34	1.25
1	E	478	GLU	CD-OE1	7.68	1.34	1.25

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	ARG	NE-CZ-NH2	-23.75	108.43	120.30
1	B	139	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	E	139	ARG	NE-CZ-NH1	18.29	129.44	120.30
1	F	139	ARG	NE-CZ-NH1	18.25	129.43	120.30
1	D	139	ARG	NE-CZ-NH2	-18.23	111.18	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	MET	Peptide
1	D	436	THR	Peptide

## 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	4549	0	4402	46	0
1	B	4549	0	4402	43	0
1	C	4549	0	4402	42	0
1	D	4549	0	4402	46	0
1	E	4549	0	4402	49	0
1	F	4549	0	4402	42	0
1	G	4549	0	4402	46	0
1	H	4549	0	4402	43	0
2	A	53	0	30	11	0
2	B	53	0	31	12	0
2	C	53	0	29	4	0
2	D	53	0	31	10	0
2	E	53	0	30	5	0
2	F	53	0	29	8	0
2	G	53	0	31	13	0
2	H	53	0	30	5	0
3	A	359	0	0	5	0
3	B	373	0	0	6	0
3	C	267	0	0	3	0
3	D	314	0	0	2	0
3	E	301	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	262	0	0	5	0
3	G	315	0	0	6	0
3	H	355	0	0	4	0
All	All	39362	0	35457	330	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.

The worst 5 of 330 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:D:167:HIS:HE2	2:D:801:FAD:C8M	0.96	1.56
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.92	1.55
1:G:167:HIS:HE2	2:G:801:FAD:C8M	0.90	1.51
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.89	1.51
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.88	1.51

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	575/623 (92%)	557 (97%)	17 (3%)	1 (0%)	47	30
1	B	575/623 (92%)	555 (96%)	18 (3%)	2 (0%)	41	24
1	C	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	D	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	E	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	F	575/623 (92%)	562 (98%)	13 (2%)	0	100	100
1	G	575/623 (92%)	558 (97%)	15 (3%)	2 (0%)	41	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	575/623 (92%)	557 (97%)	18 (3%)	0	100	100
All	All	4600/4984 (92%)	4468 (97%)	127 (3%)	5 (0%)	51	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	389	LEU
1	G	453	ALA
1	A	44	ASP
1	B	461	GLN
1	G	45	ILE

### 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	505/542 (93%)	491 (97%)	14 (3%)	43	25
1	B	505/542 (93%)	494 (98%)	11 (2%)	52	34
1	C	505/542 (93%)	495 (98%)	10 (2%)	55	38
1	D	505/542 (93%)	493 (98%)	12 (2%)	49	31
1	E	505/542 (93%)	496 (98%)	9 (2%)	59	43
1	F	505/542 (93%)	489 (97%)	16 (3%)	39	20
1	G	505/542 (93%)	495 (98%)	10 (2%)	55	38
1	H	505/542 (93%)	493 (98%)	12 (2%)	49	31
All	All	4040/4336 (93%)	3946 (98%)	94 (2%)	50	33

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	112	MET
1	F	618	PHE
1	F	168	TRP

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Mol	Chain	Res	Type
1	F	408	TRP
1	G	385	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	341	ASN
1	H	341	ASN
1	E	611	GLN
1	G	341	ASN
1	E	461	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	C	801	1	53,58,58	1.48	10 (18%)	68,89,89	1.82	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	A	801	1	53,58,58	1.49	11 (20%)	68,89,89	1.68	15 (22%)
2	FAD	D	801	1	53,58,58	1.26	5 (9%)	68,89,89	1.90	21 (30%)
2	FAD	E	801	1	53,58,58	1.48	11 (20%)	68,89,89	1.67	12 (17%)
2	FAD	F	801	1	53,58,58	1.38	8 (15%)	68,89,89	1.75	16 (23%)
2	FAD	G	801	1	53,58,58	1.43	9 (16%)	68,89,89	1.69	14 (20%)
2	FAD	H	801	1	53,58,58	1.36	5 (9%)	68,89,89	1.54	14 (20%)
2	FAD	B	801	1	53,58,58	1.66	9 (16%)	68,89,89	2.08	18 (26%)

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	C	801	1	-	3/30/50/50	0/6/6/6
2	FAD	A	801	1	-	3/30/50/50	0/6/6/6
2	FAD	D	801	1	-	4/30/50/50	0/6/6/6
2	FAD	E	801	1	-	1/30/50/50	0/6/6/6
2	FAD	F	801	1	-	3/30/50/50	0/6/6/6
2	FAD	G	801	1	-	2/30/50/50	0/6/6/6
2	FAD	H	801	1	-	2/30/50/50	0/6/6/6
2	FAD	B	801	1	-	2/30/50/50	0/6/6/6

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C4X-N5	4.85	1.40	1.30
2	B	801	FAD	C8A-N7A	-4.08	1.27	1.34
2	A	801	FAD	C4X-N5	3.76	1.38	1.30
2	B	801	FAD	O4B-C4B	-3.75	1.36	1.45
2	G	801	FAD	O4B-C1B	3.71	1.46	1.41

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-6.57	118.41	128.68
2	A	801	FAD	N3A-C2A-N1A	-5.65	119.85	128.68
2	B	801	FAD	C4-C4X-N5	5.28	125.75	118.23
2	C	801	FAD	N3A-C2A-N1A	-5.20	120.55	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O3B-C3B-C4B	4.85	125.08	111.05

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

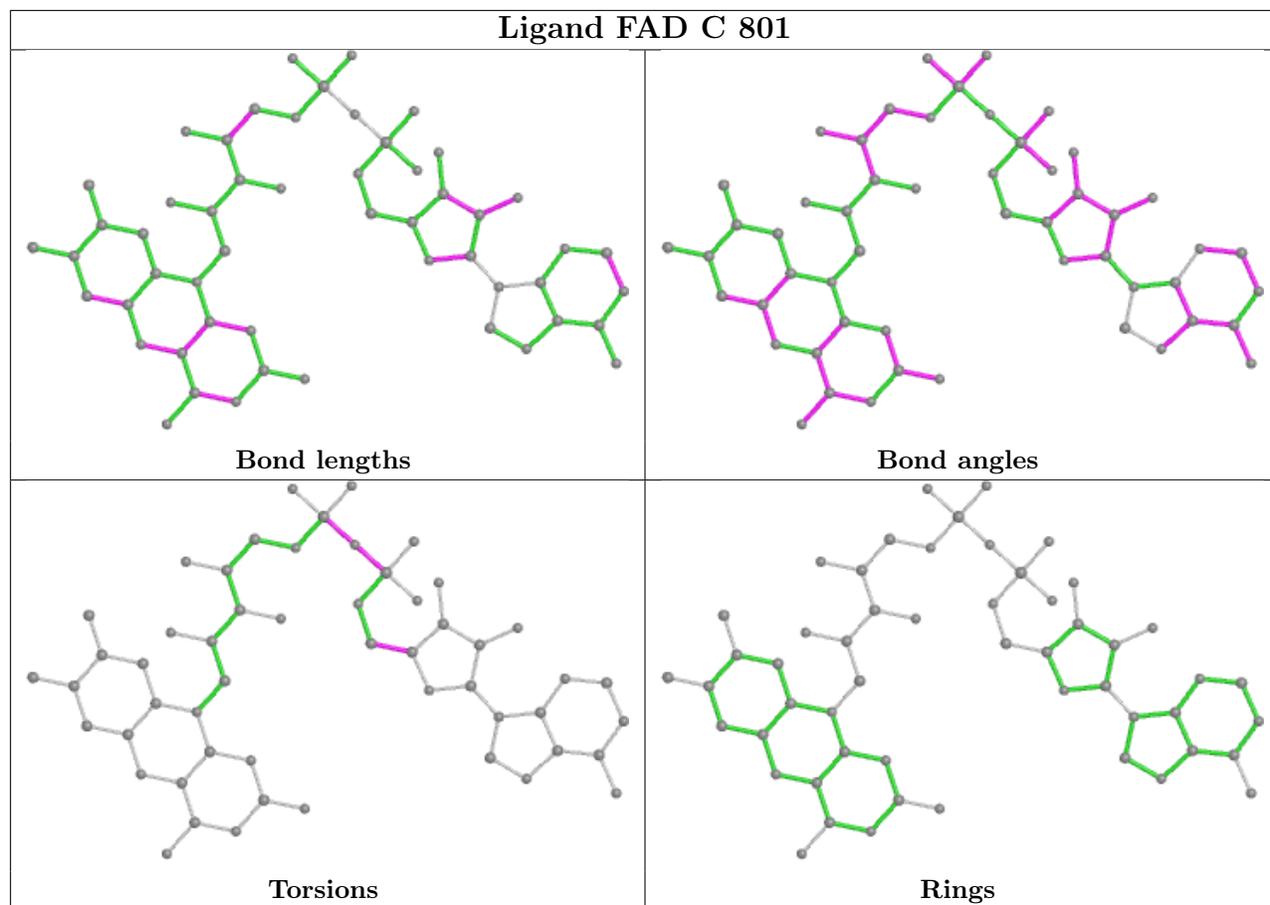
Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	PA-O3P-P-O5'

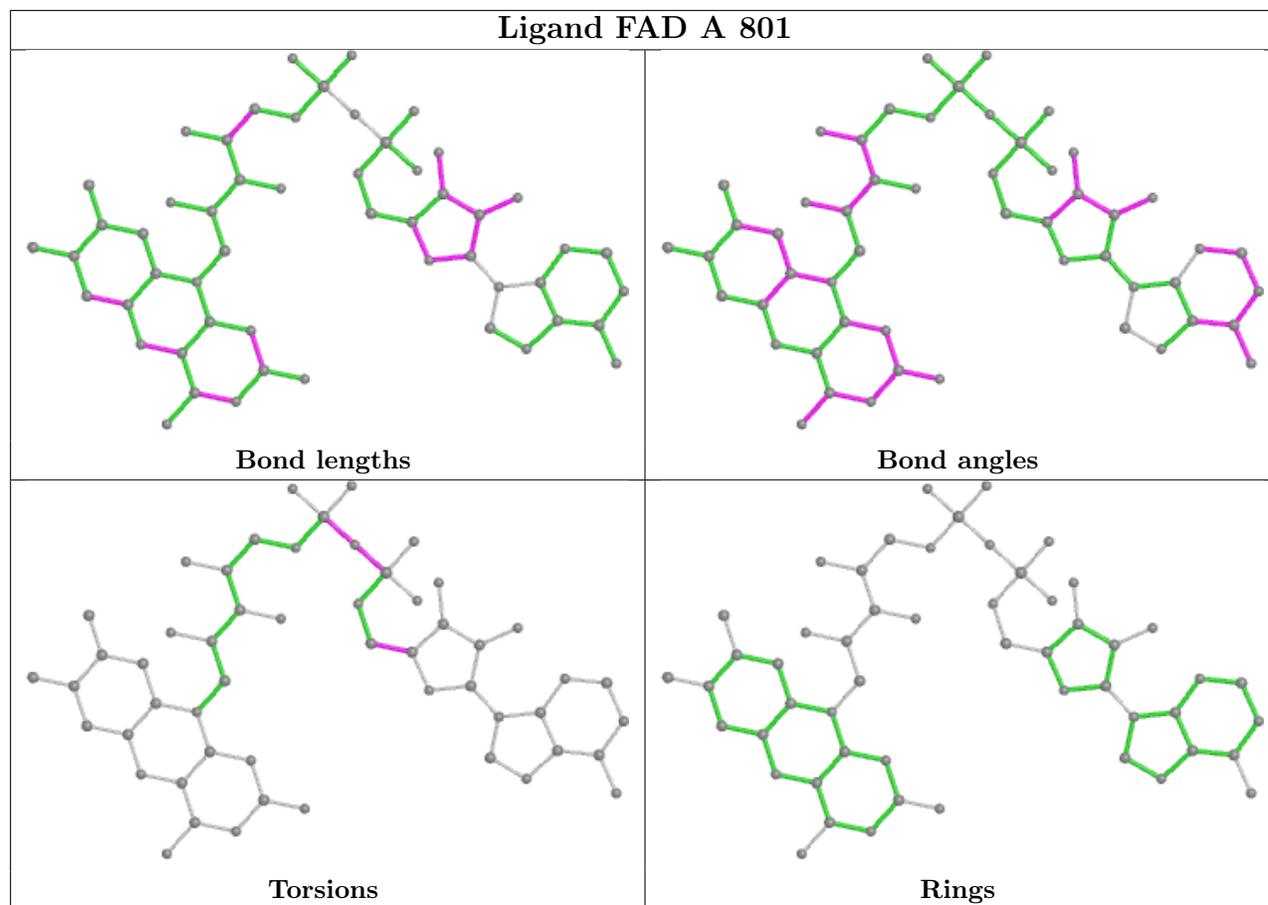
There are no ring outliers.

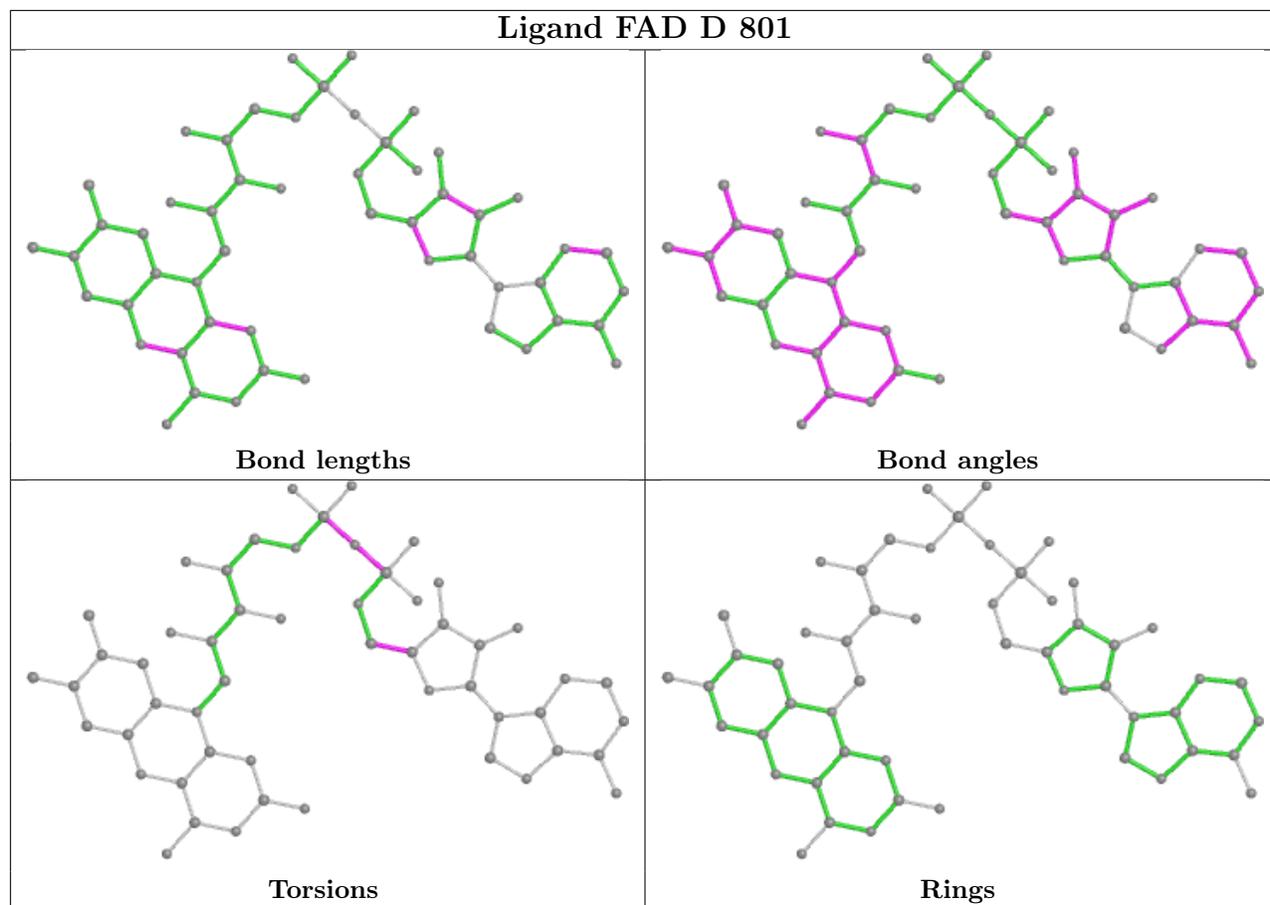
8 monomers are involved in 68 short contacts:

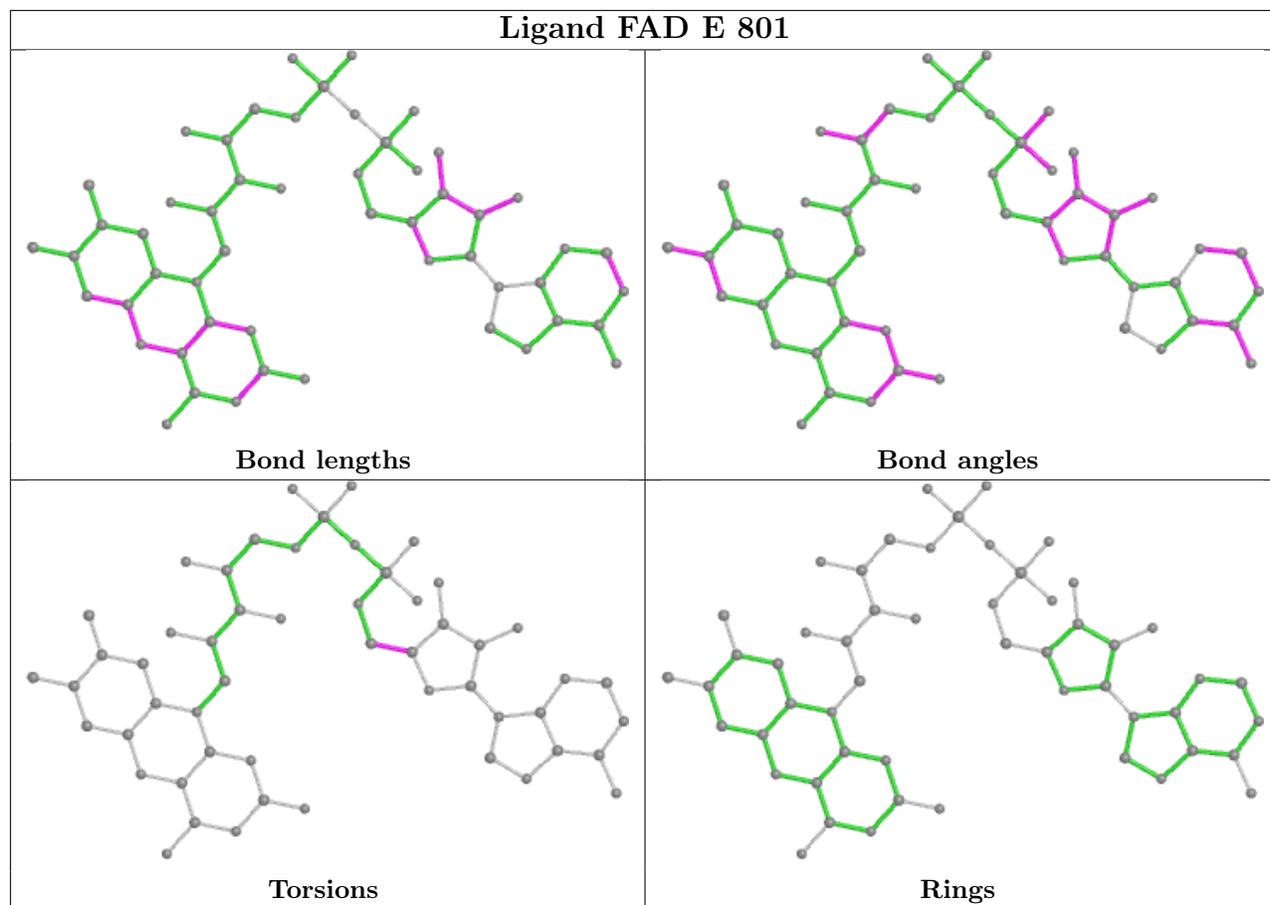
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	4	0
2	A	801	FAD	11	0
2	D	801	FAD	10	0
2	E	801	FAD	5	0
2	F	801	FAD	8	0
2	G	801	FAD	13	0
2	H	801	FAD	5	0
2	B	801	FAD	12	0

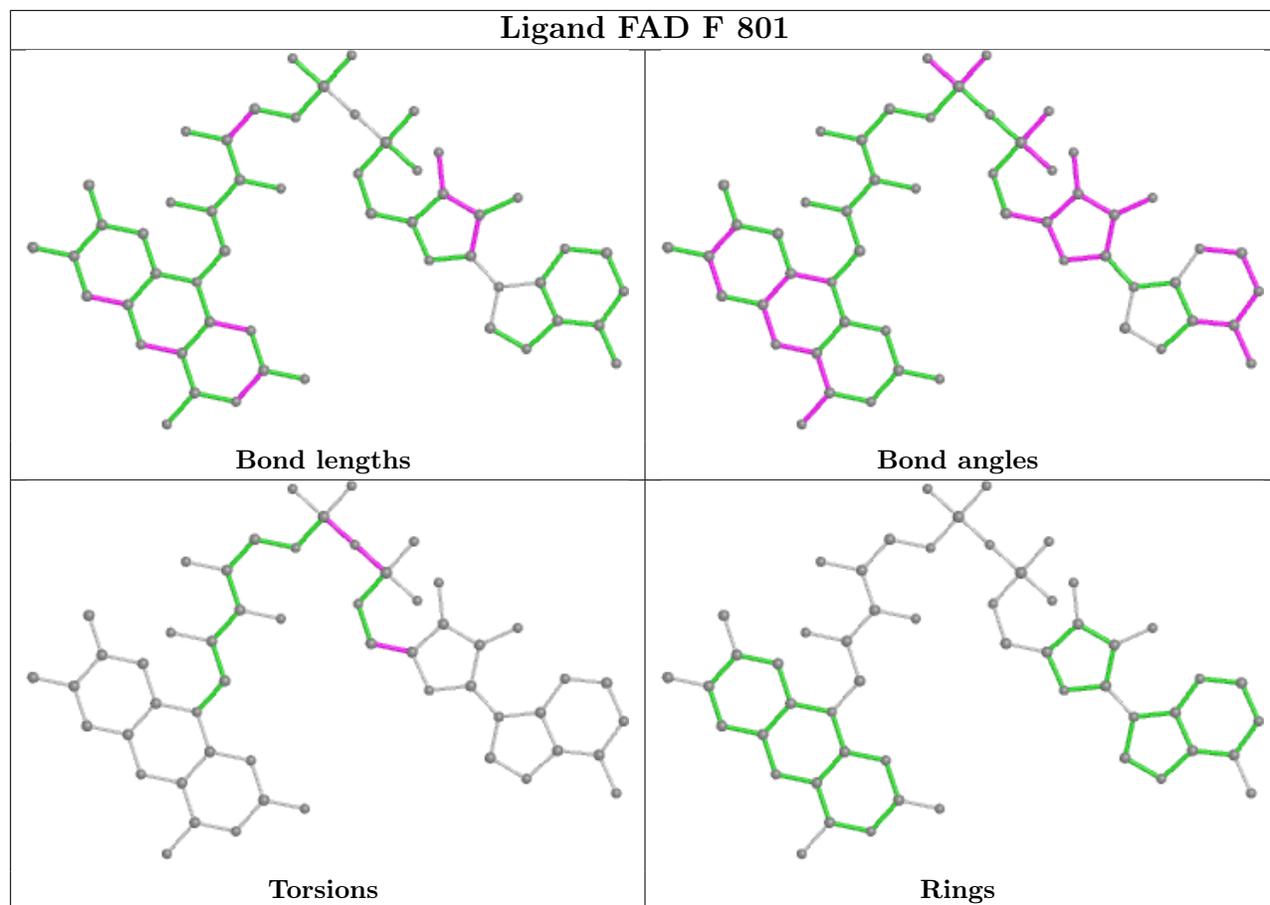
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

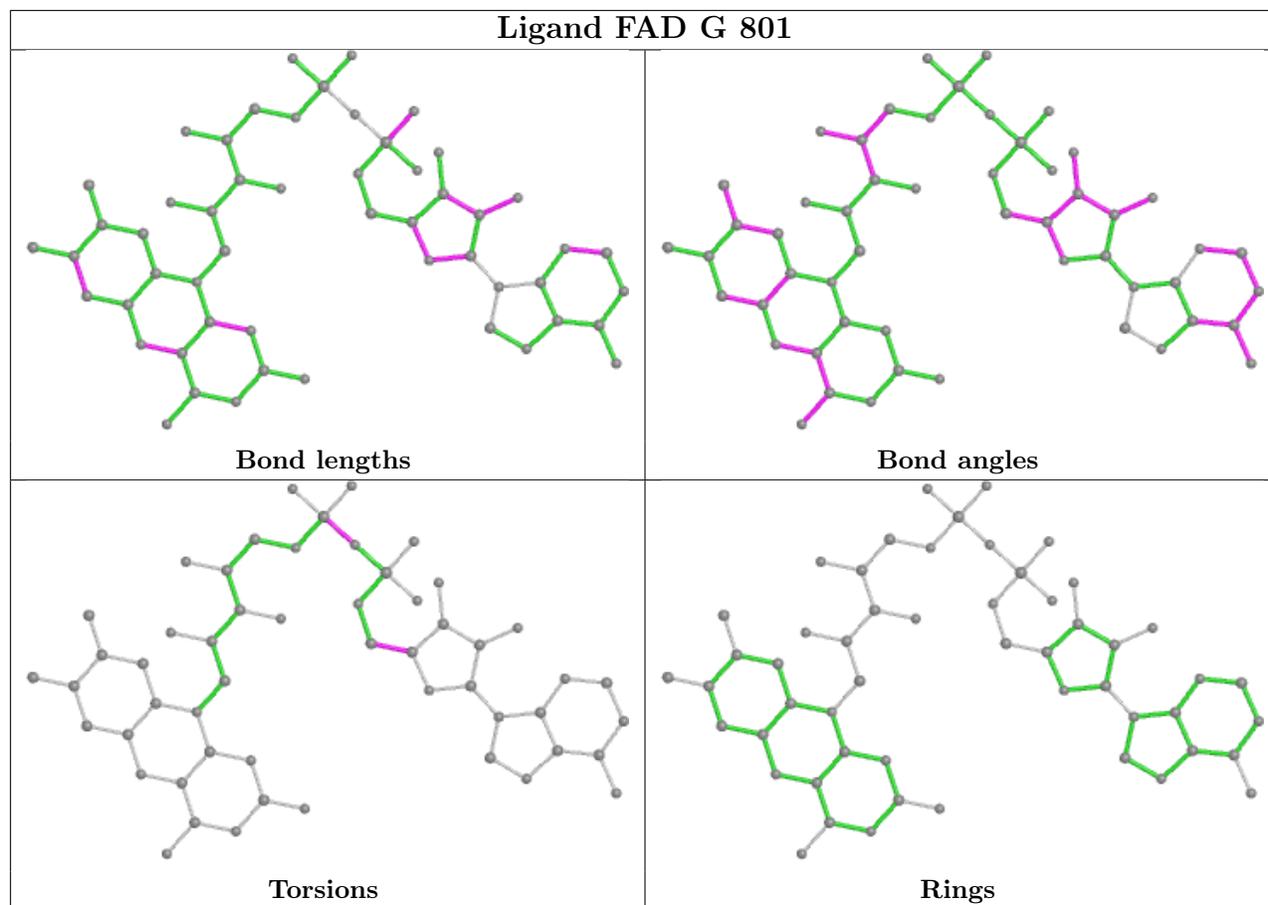


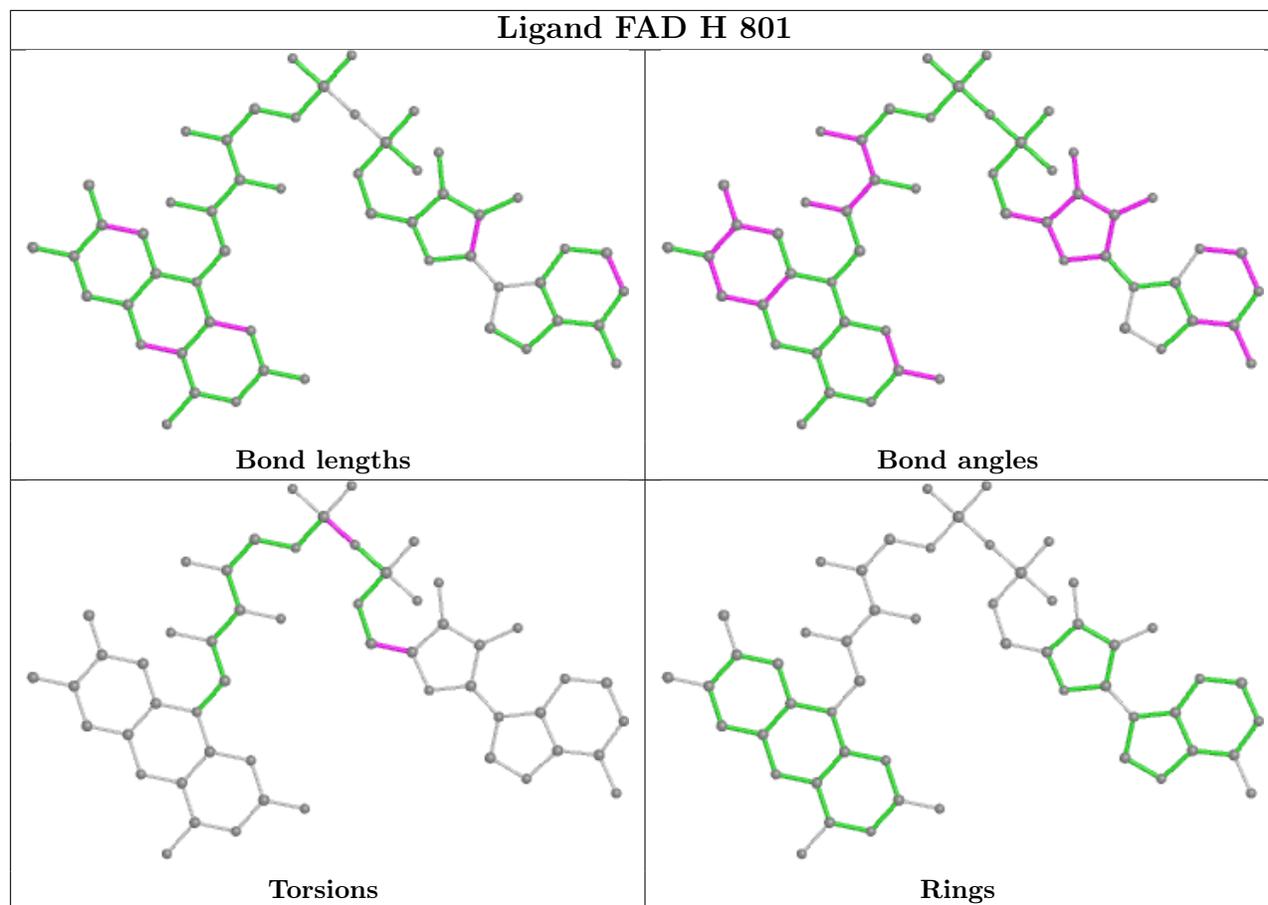


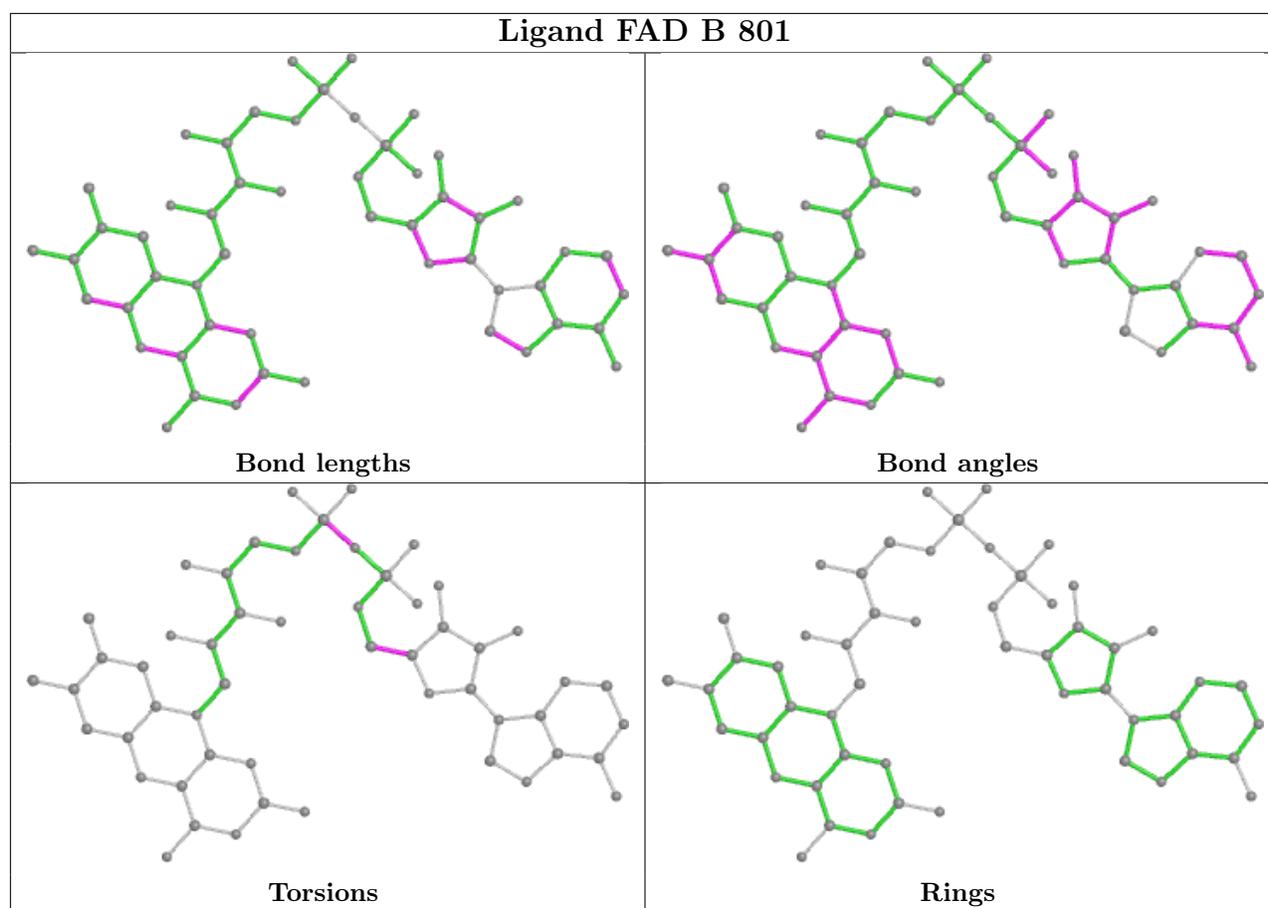












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	577/623 (92%)	0.65	43 (7%) 14 16	15, 21, 40, 56	0
1	B	577/623 (92%)	0.60	33 (5%) 23 26	17, 22, 39, 65	0
1	C	577/623 (92%)	0.75	47 (8%) 12 14	20, 27, 45, 65	0
1	D	577/623 (92%)	0.63	40 (6%) 16 19	19, 25, 41, 62	0
1	E	577/623 (92%)	0.71	53 (9%) 9 10	18, 26, 42, 63	0
1	F	577/623 (92%)	0.78	56 (9%) 7 8	19, 27, 42, 64	0
1	G	577/623 (92%)	0.63	42 (7%) 15 17	18, 24, 42, 59	0
1	H	577/623 (92%)	0.60	38 (6%) 18 20	18, 23, 38, 61	0
All	All	4616/4984 (92%)	0.67	352 (7%) 13 16	15, 25, 42, 65	0

The worst 5 of 352 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	619	THR	15.2
1	E	389	LEU	15.1
1	C	619	THR	14.3
1	A	459	VAL	14.0
1	B	619	THR	12.9

### 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<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	E	801	53/53	0.93	0.12	14,18,21,22	0
2	FAD	C	801	53/53	0.94	0.14	7,16,21,24	0
2	FAD	D	801	53/53	0.94	0.16	14,17,20,20	0
2	FAD	B	801	53/53	0.94	0.17	10,15,17,21	0
2	FAD	F	801	53/53	0.94	0.12	16,19,21,22	0
2	FAD	A	801	53/53	0.95	0.15	12,17,21,23	0
2	FAD	G	801	53/53	0.95	0.12	14,18,20,21	0
2	FAD	H	801	53/53	0.95	0.14	11,15,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.