



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2017 – 08:15 PM EDT

PDB ID : 2IGK  
Title : Crystal structure of recombinant pyranose 2-oxidase  
Authors : Divne, C.  
Deposited on : unknown  
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

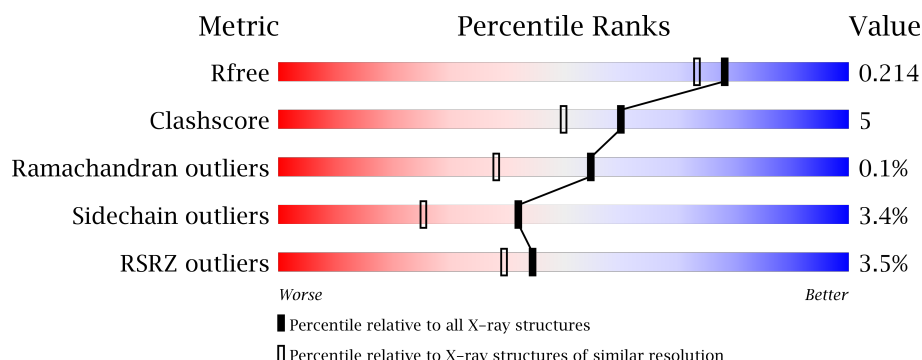
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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. 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	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	623	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	C	623	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	623	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	E	623	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	623	 3% 82% 9% • 7%
1	G	623	 4% 82% 10% • 7%
1	H	623	 2% 83% 8% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	A	902	-	-	X	X
3	MES	B	901	-	-	X	X
3	MES	C	904	-	-	X	X
3	MES	D	903	-	-	X	X
3	MES	E	905	-	-	-	X
3	MES	E	906	-	-	X	X
3	MES	G	908	-	-	X	X
3	MES	H	907	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39837 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
1	A	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4549	2872	778	874	25			

- 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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	417	Total	O	0	0
			417	417		
4	B	418	Total	O	0	0
			418	418		
4	C	307	Total	O	0	0
			307	307		
4	D	354	Total	O	0	0
			354	354		

Continued on next page...

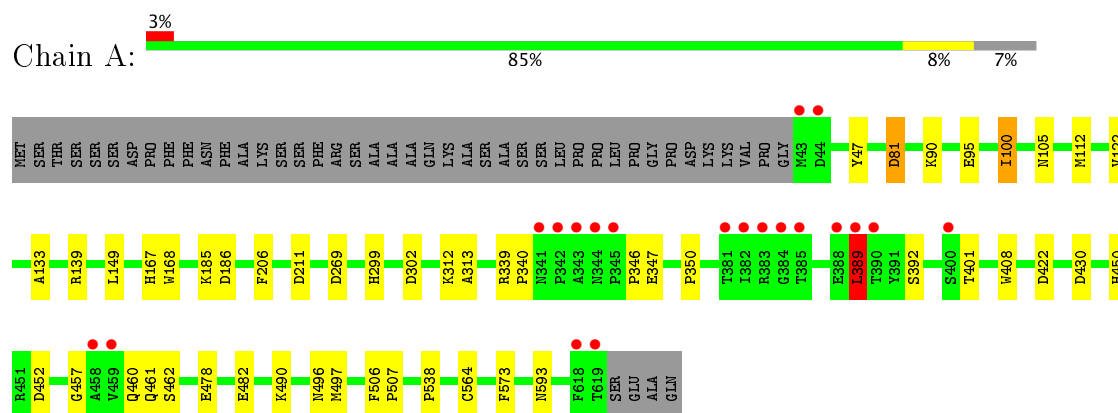
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	336	Total 336	O 336	0	0
4	F	318	Total 318	O 318	0	0
4	G	379	Total 379	O 379	0	0
4	H	396	Total 396	O 396	0	0

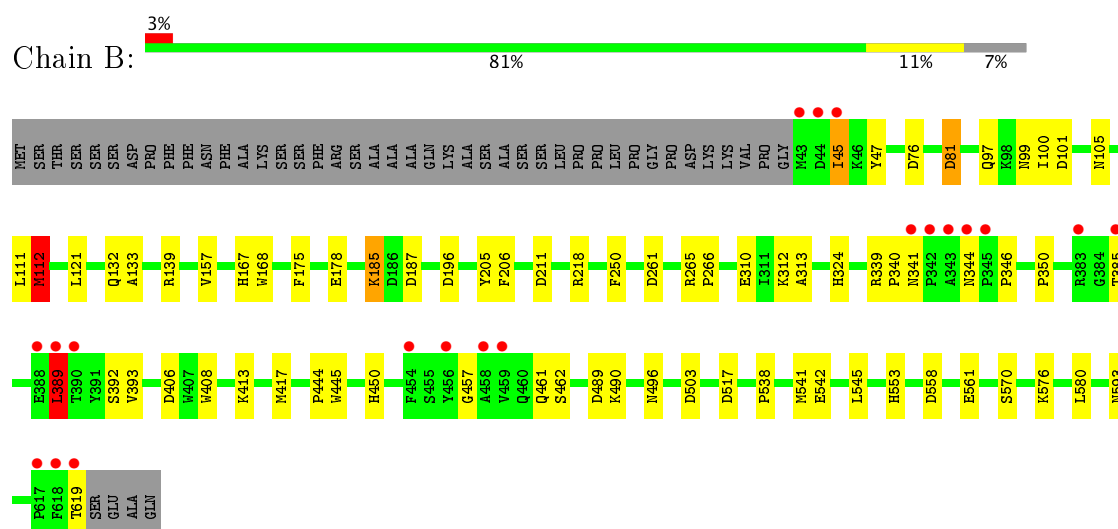
### 3 Residue-property plots [i](#)

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.

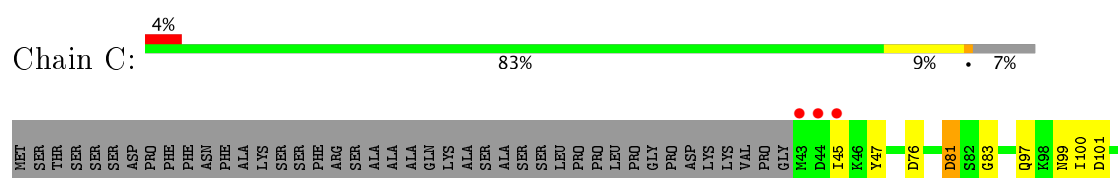
#### • Molecule 1: Pyranose oxidase



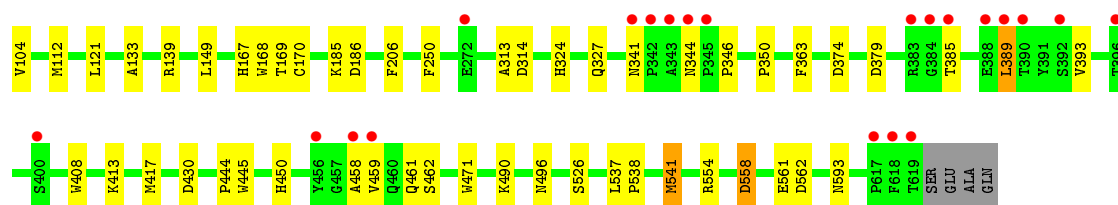
#### • Molecule 1: Pyranose oxidase



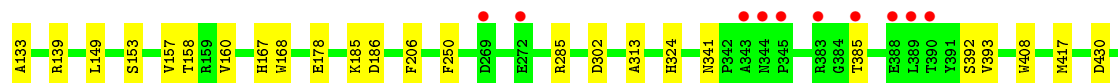
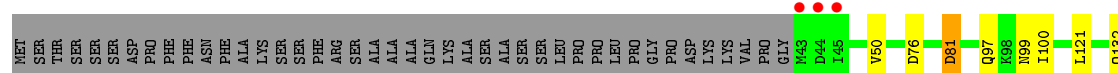
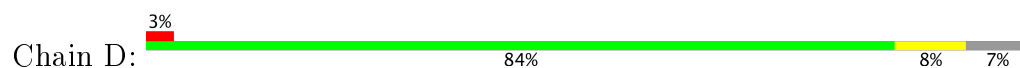
#### • Molecule 1: Pyranose oxidase



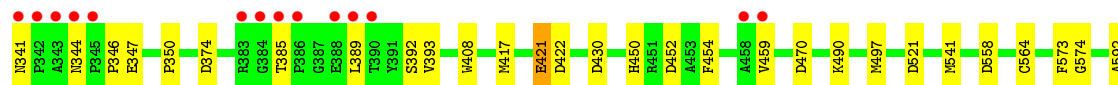
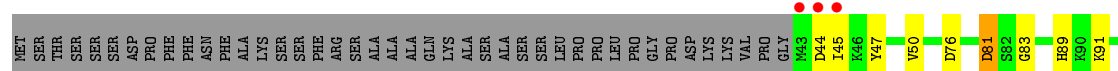
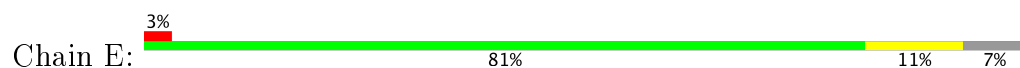




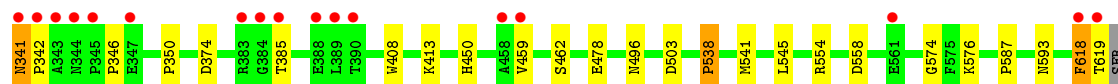
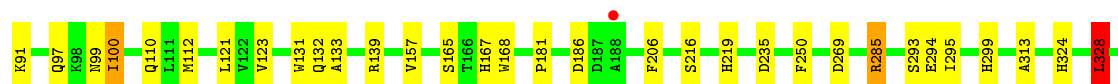
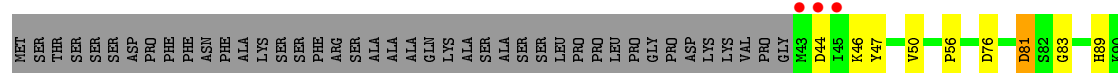
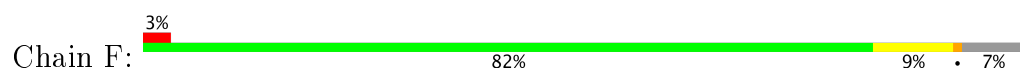
• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase

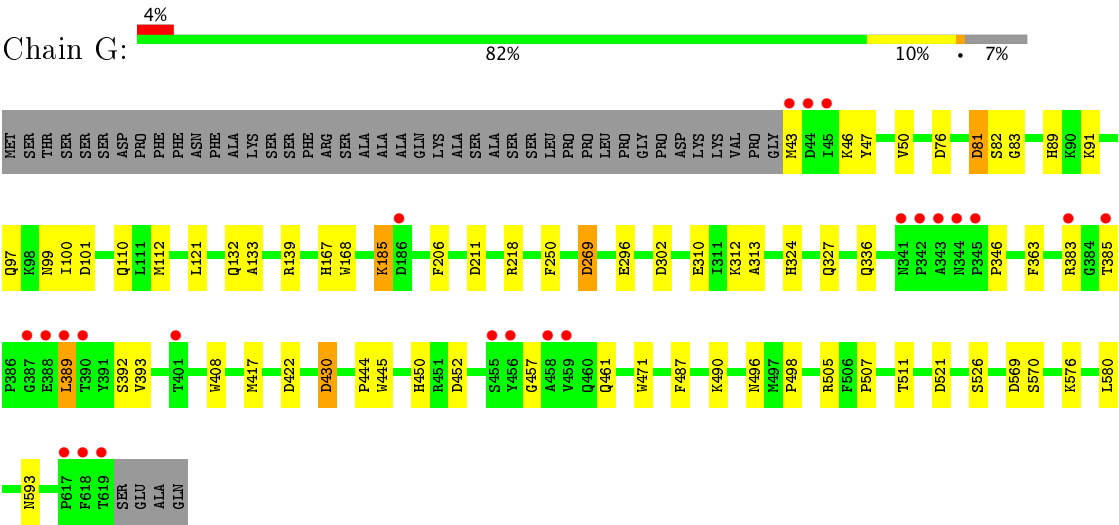


• Molecule 1: Pyranose oxidase

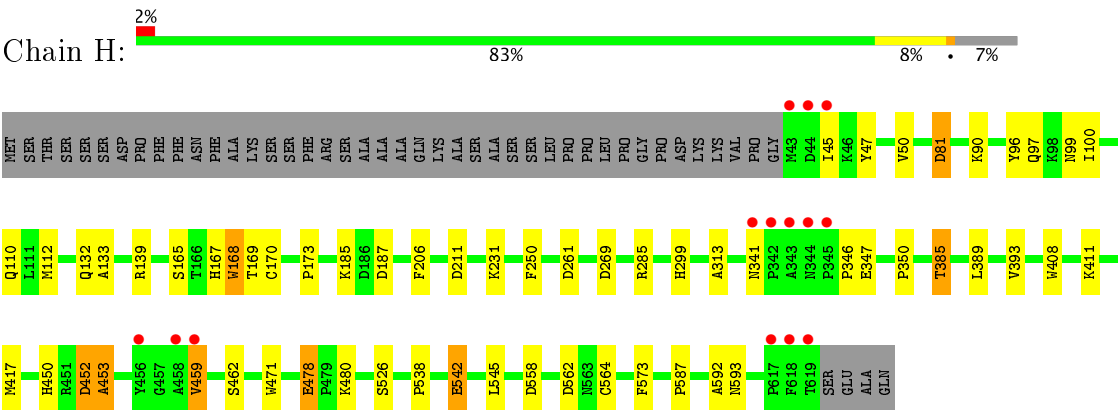


GLU  
ALA  
GLN

• 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, $\alpha$ , $\beta$ , $\gamma$	168.78Å 103.86Å 169.26Å 90.00° 106.36° 90.00°	Depositor
Resolution (Å)	39.20 – 1.80 39.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.20-1.80) 99.9 (39.17-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.177 , 0.214 0.177 , 0.214	Depositor DCC
$R_{free}$ test set	5182 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	39837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.94% 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, MES

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	1.01	3/4665 (0.1%)	0.95	13/6343 (0.2%)
1	B	0.97	3/4665 (0.1%)	0.98	15/6343 (0.2%)
1	C	0.87	0/4665	0.91	13/6343 (0.2%)
1	D	0.90	2/4665 (0.0%)	0.91	12/6343 (0.2%)
1	E	0.89	0/4665	0.90	14/6343 (0.2%)
1	F	0.88	1/4665 (0.0%)	0.92	14/6343 (0.2%)
1	G	0.95	1/4665 (0.0%)	0.96	14/6343 (0.2%)
1	H	0.96	2/4665 (0.0%)	0.97	13/6343 (0.2%)
All	All	0.93	12/37320 (0.0%)	0.94	108/50744 (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	B	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	MET	CB-CG	6.50	1.72	1.51
1	D	478	GLU	CD-OE1	5.70	1.31	1.25
1	B	205	TYR	CD1-CE1	5.67	1.47	1.39
1	H	96	TYR	CD2-CE2	-5.54	1.31	1.39
1	B	175	PHE	CE2-CZ	5.48	1.47	1.37

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	ARG	NE-CZ-NH2	-19.04	110.78	120.30
1	B	139	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	G	139	ARG	NE-CZ-NH2	-14.95	112.83	120.30
1	H	389	LEU	CA-CB-CG	14.62	148.93	115.30
1	B	139	ARG	NE-CZ-NH1	13.94	127.27	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	553	HIS	Peptide

## 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	4549	0	4395	37	0
1	B	4549	0	4395	53	0
1	C	4549	0	4395	44	0
1	D	4549	0	4395	37	0
1	E	4549	0	4395	68	1
1	F	4549	0	4395	52	0
1	G	4549	0	4395	57	0
1	H	4549	0	4395	48	0
2	A	53	0	31	8	0
2	B	53	0	31	8	0
2	C	53	0	31	4	0
2	D	53	0	31	6	0
2	E	53	0	31	7	0
2	F	53	0	30	3	0
2	G	53	0	30	0	0
2	H	53	0	30	3	0
3	A	12	0	13	9	0
3	B	12	0	13	15	0
3	C	12	0	13	12	0
3	D	12	0	13	14	0
3	E	24	0	26	13	0
3	G	12	0	13	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	12	0	13	13	0
4	A	417	0	0	4	0
4	B	418	0	0	6	0
4	C	307	0	0	3	0
4	D	354	0	0	2	1
4	E	336	0	0	14	0
4	F	318	0	0	9	0
4	G	379	0	0	21	0
4	H	396	0	0	5	0
All	All	39837	0	35509	379	1

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 379 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	0.98	1.61
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.98	1.58
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.91	1.56
1:E:167:HIS:HE2	2:E:801:FAD:C8M	0.92	1.56
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.92	1.55

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:LEU:CD2	4:D:3818:HOH:O[2_665]	1.77	0.43

## 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%)	556 (97%)	19 (3%)	0	100	100
1	B	575/623 (92%)	562 (98%)	12 (2%)	1 (0%)	51	35
1	C	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	D	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	E	575/623 (92%)	555 (96%)	20 (4%)	0	100	100
1	F	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	G	575/623 (92%)	557 (97%)	17 (3%)	1 (0%)	51	35
1	H	575/623 (92%)	561 (98%)	12 (2%)	2 (0%)	44	29
All	All	4600/4984 (92%)	4470 (97%)	126 (3%)	4 (0%)	55	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	46	LYS
1	H	187	ASP
1	H	453	ALA
1	B	389	LEU

### 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	505/542 (93%)	490 (97%)	15 (3%)	46	30
1	B	505/542 (93%)	486 (96%)	19 (4%)	38	21
1	C	505/542 (93%)	487 (96%)	18 (4%)	40	23
1	D	505/542 (93%)	488 (97%)	17 (3%)	42	25
1	E	505/542 (93%)	487 (96%)	18 (4%)	40	23
1	F	505/542 (93%)	487 (96%)	18 (4%)	40	23
1	G	505/542 (93%)	490 (97%)	15 (3%)	46	30
1	H	505/542 (93%)	488 (97%)	17 (3%)	42	25
All	All	4040/4336 (93%)	3903 (97%)	137 (3%)	42	25

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	408	TRP
1	E	341	ASN
1	H	231	LYS
1	D	490	LYS
1	E	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	460	GLN
1	E	324	HIS
1	H	341	ASN
1	E	99	ASN
1	E	341	ASN

### 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 ⓘ

16 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	801	1	51,58,58	1.71	8 (15%)	54,89,89	2.71	9 (16%)
3	MES	A	902	-	12,12,12	1.21	2 (16%)	14,16,16	15.65	9 (64%)
2	FAD	B	801	1	51,58,58	1.43	8 (15%)	54,89,89	2.22	11 (20%)
3	MES	B	901	-	12,12,12	1.26	2 (16%)	14,16,16	17.65	8 (57%)
2	FAD	C	801	1	51,58,58	1.53	8 (15%)	54,89,89	2.53	9 (16%)
3	MES	C	904	-	12,12,12	1.34	1 (8%)	14,16,16	18.37	9 (64%)
2	FAD	D	801	1	51,58,58	1.48	7 (13%)	54,89,89	2.13	11 (20%)
3	MES	D	903	-	12,12,12	1.14	1 (8%)	14,16,16	20.09	9 (64%)
2	FAD	E	801	1	51,58,58	1.55	8 (15%)	54,89,89	2.01	5 (9%)
3	MES	E	905	-	12,12,12	1.11	1 (8%)	14,16,16	16.83	8 (57%)
3	MES	E	906	-	12,12,12	0.88	1 (8%)	14,16,16	17.72	9 (64%)
2	FAD	F	801	1	51,58,58	1.51	7 (13%)	54,89,89	2.32	12 (22%)
2	FAD	G	801	1	51,58,58	1.54	7 (13%)	54,89,89	2.33	9 (16%)
3	MES	G	908	-	12,12,12	1.09	2 (16%)	14,16,16	17.96	10 (71%)
2	FAD	H	801	1	51,58,58	1.50	8 (15%)	54,89,89	2.43	7 (12%)
3	MES	H	907	-	12,12,12	0.95	1 (8%)	14,16,16	16.25	8 (57%)

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	801	1	-	0/28/50/50	0/6/6/6
3	MES	A	902	-	-	0/6/14/14	0/1/1/1
2	FAD	B	801	1	-	0/28/50/50	0/6/6/6
3	MES	B	901	-	-	0/6/14/14	0/1/1/1
2	FAD	C	801	1	-	0/28/50/50	0/6/6/6
3	MES	C	904	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	1	-	0/28/50/50	0/6/6/6
3	MES	D	903	-	-	0/6/14/14	0/1/1/1
2	FAD	E	801	1	-	0/28/50/50	0/6/6/6
3	MES	E	905	-	-	0/6/14/14	0/1/1/1
3	MES	E	906	-	-	0/6/14/14	0/1/1/1
2	FAD	F	801	1	-	0/28/50/50	0/6/6/6
2	FAD	G	801	1	-	0/28/50/50	0/6/6/6
3	MES	G	908	-	-	0/6/14/14	0/1/1/1
2	FAD	H	801	1	-	0/28/50/50	0/6/6/6
3	MES	H	907	-	-	0/6/14/14	0/1/1/1

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	PA-O1A	-2.04	1.43	1.50
2	G	801	FAD	C2A-N1A	2.03	1.37	1.33
3	B	901	MES	O1S-S	2.03	1.51	1.45
3	A	902	MES	O1S-S	2.06	1.51	1.45
3	E	906	MES	C8-S	2.07	1.80	1.77

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	N3A-C2A-N1A	-14.68	116.08	128.86
3	G	908	MES	O3S-S-C8	-12.76	90.37	106.06
3	D	903	MES	O3S-S-C8	-12.05	91.23	106.06
2	H	801	FAD	N3A-C2A-N1A	-11.87	118.52	128.86
3	C	904	MES	O3S-S-C8	-10.90	92.65	106.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	8	0
3	A	902	MES	9	0
2	B	801	FAD	8	0
3	B	901	MES	15	0
2	C	801	FAD	4	0
3	C	904	MES	12	0
2	D	801	FAD	6	0
3	D	903	MES	14	0
2	E	801	FAD	7	0
3	E	905	MES	2	0
3	E	906	MES	11	0
2	F	801	FAD	3	0
3	G	908	MES	13	0
2	H	801	FAD	3	0
3	H	907	MES	13	0

## 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	577/623 (92%)	-0.44	20 (3%) 44 39	10, 17, 42, 61	0
1	B	577/623 (92%)	-0.45	20 (3%) 44 39	10, 17, 39, 61	0
1	C	577/623 (92%)	-0.23	24 (4%) 37 31	13, 23, 47, 67	0
1	D	577/623 (92%)	-0.36	20 (3%) 44 39	12, 21, 42, 63	0
1	E	577/623 (92%)	-0.33	21 (3%) 43 38	13, 21, 43, 64	0
1	F	577/623 (92%)	-0.32	21 (3%) 43 38	11, 22, 43, 65	0
1	G	577/623 (92%)	-0.38	23 (3%) 39 33	12, 19, 43, 66	0
1	H	577/623 (92%)	-0.49	14 (2%) 59 55	11, 18, 39, 62	0
All	All	4616/4984 (92%)	-0.38	163 (3%) 44 39	10, 20, 43, 67	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	619	THR	11.2
1	H	619	THR	10.2
1	A	619	THR	9.6
1	G	619	THR	8.6
1	B	619	THR	8.6

### 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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	C	904	12/12	0.85	0.32	7.77	27,37,45,46	0
3	MES	D	903	12/12	0.89	0.29	7.32	32,37,41,44	0
3	MES	G	908	12/12	0.85	0.28	6.95	28,37,41,41	0
3	MES	E	906	12/12	0.85	0.28	6.27	31,38,41,42	0
3	MES	B	901	12/12	0.88	0.27	5.95	28,35,38,39	0
3	MES	A	902	12/12	0.92	0.20	3.60	24,29,34,34	0
3	MES	H	907	12/12	0.92	0.19	3.43	29,33,37,37	0
3	MES	E	905	12/12	0.95	0.18	2.17	21,29,32,32	0
2	FAD	D	801	53/53	0.98	0.10	0.11	14,17,20,22	0
2	FAD	F	801	53/53	0.98	0.09	0.01	15,18,21,21	0
2	FAD	H	801	53/53	0.98	0.09	-0.03	11,14,17,19	0
2	FAD	A	801	53/53	0.98	0.09	-0.09	9,13,17,18	0
2	FAD	G	801	53/53	0.98	0.08	-0.20	12,14,18,19	0
2	FAD	B	801	53/53	0.99	0.09	-0.20	9,14,16,17	0
2	FAD	C	801	53/53	0.98	0.09	-0.21	16,20,22,24	0
2	FAD	E	801	53/53	0.97	0.09	-0.22	15,18,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.