wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:46 AM GMT

PDB ID	:	2IGM
Title	:	Crystal structure of recombinant pyranose 2-oxidase H548N mutant
Authors	:	Divne, C.
Deposited on	:	2006-09-22
Resolution	:	1.90 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

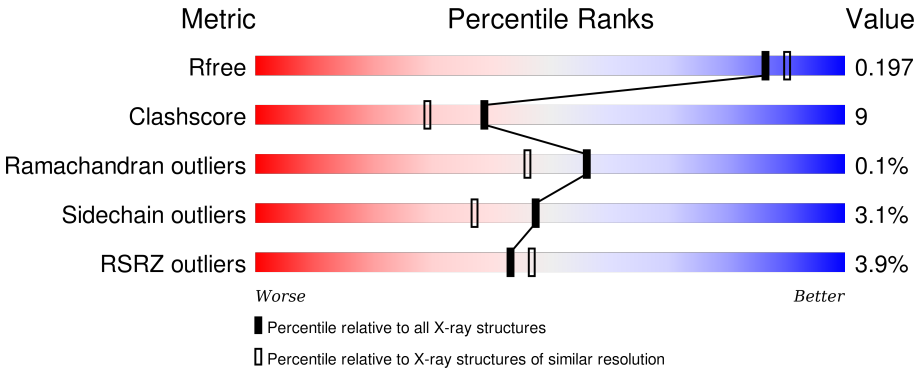
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	4% 81% 10% • 7%
1	B	623	3% 80% 11% • 7%
1	C	623	4% 81% 11% • 7%
1	D	623	3% 80% 12% 7%
1	E	623	4% 80% 11% • 7%

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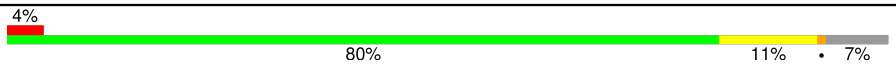
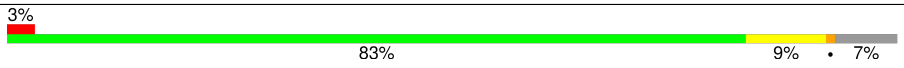
Mol	Chain	Length	Quality of chain
1	F	623	
1	G	623	
1	H	623	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41255 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.

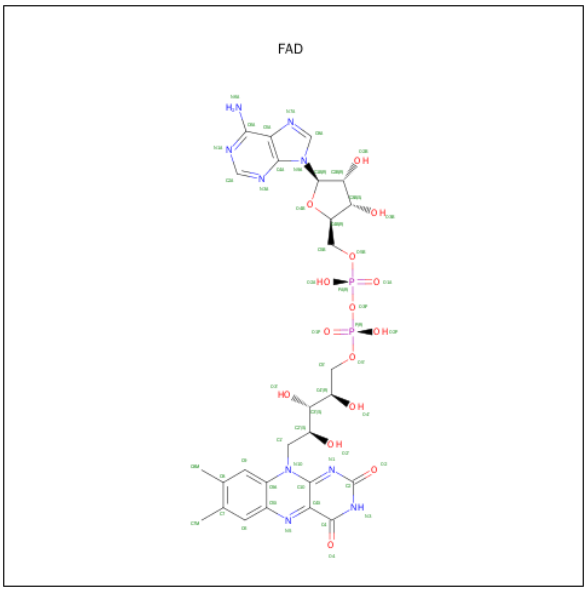
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	2	0
			4561	2879	779	878	25			
1	B	577	Total	C	N	O	S	0	2	0
			4562	2881	779	877	25			
1	D	577	Total	C	N	O	S	0	3	0
			4569	2883	780	881	25			
1	C	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			
1	E	577	Total	C	N	O	S	0	2	0
			4561	2879	779	878	25			
1	F	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			
1	G	577	Total	C	N	O	S	0	2	0
			4562	2881	779	877	25			
1	H	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			

There are 8 discrepancies between the modelled and reference sequences:

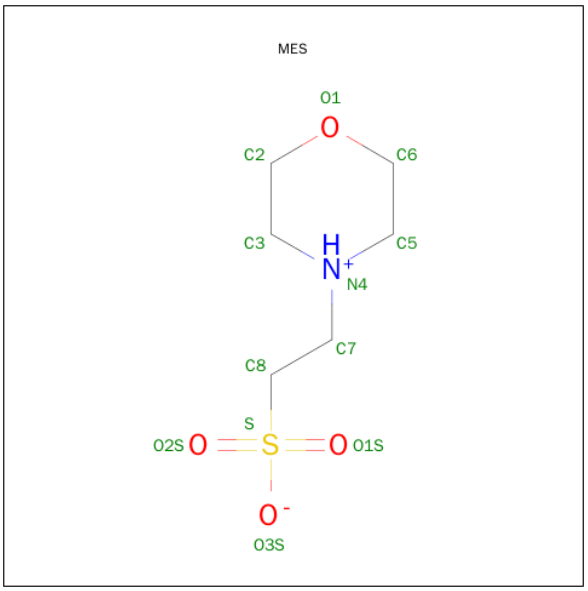
Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
B	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
C	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
D	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
E	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
F	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
G	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
H	548	ASN	HIS	ENGINEERED	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	D	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	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: $C_6H_{13}NO_4S$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	572	Total O 572 572	0	0
4	B	570	Total O 570 570	0	0
4	C	514	Total O 514 514	0	0
4	D	546	Total O 546 546	0	0

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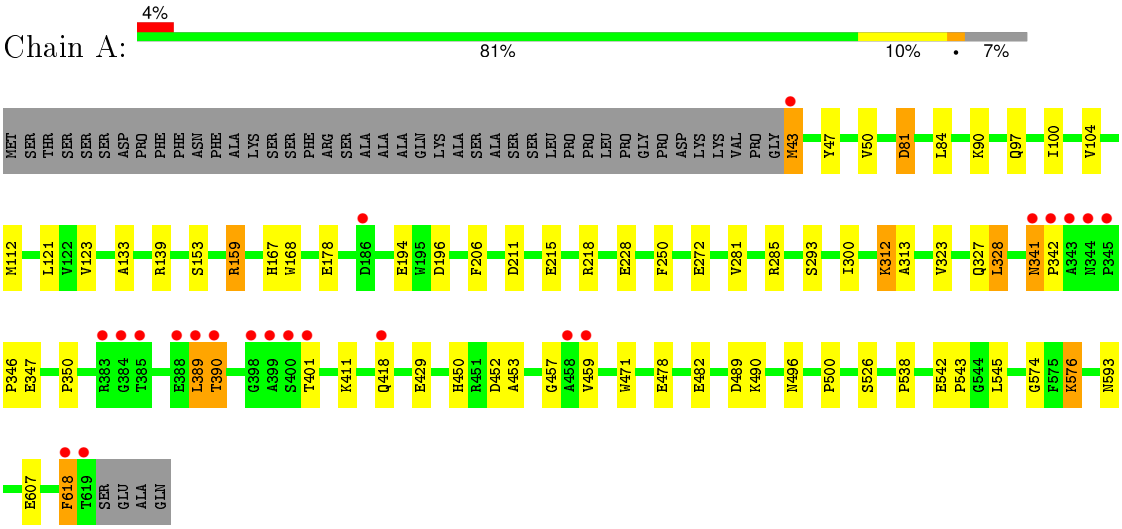
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	524	Total O 524 524	0	0
4	F	472	Total O 472 472	0	0
4	G	519	Total O 519 519	0	0
4	H	538	Total O 538 538	0	0

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 errors 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.

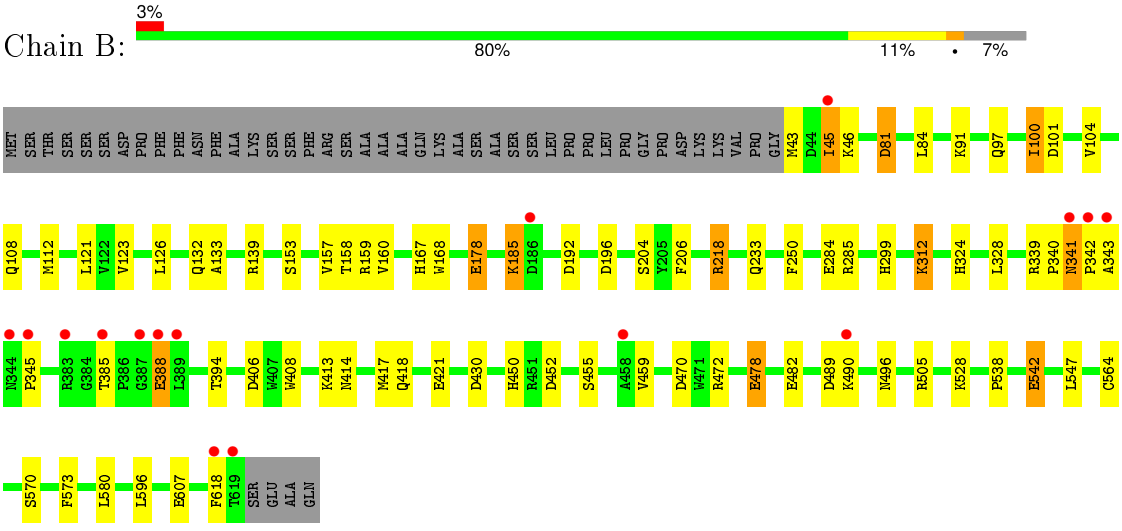
- Molecule 1: Pyranose oxidase

Chain A:



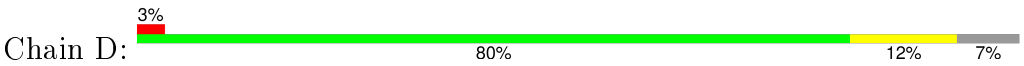
- Molecule 1: Pyranose oxidase

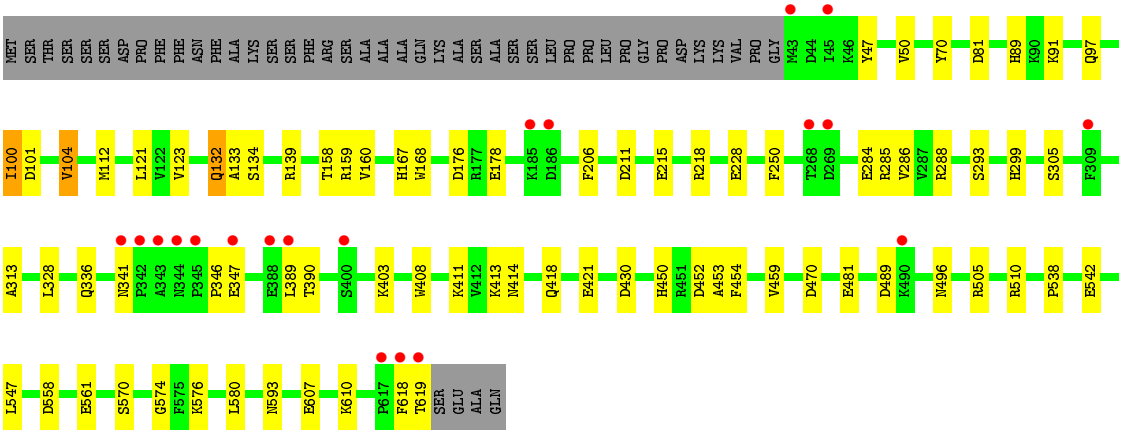
Chain B:



- Molecule 1: Pyranose oxidase

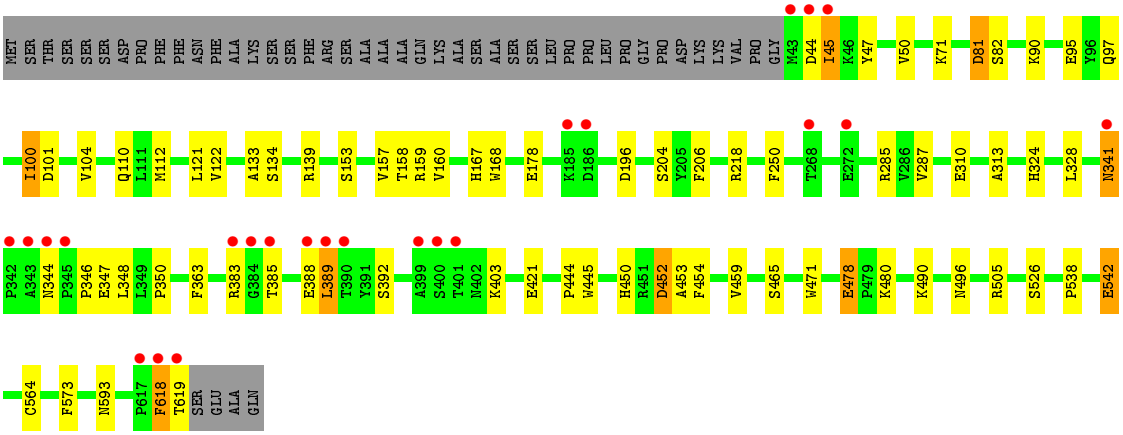
Chain D:





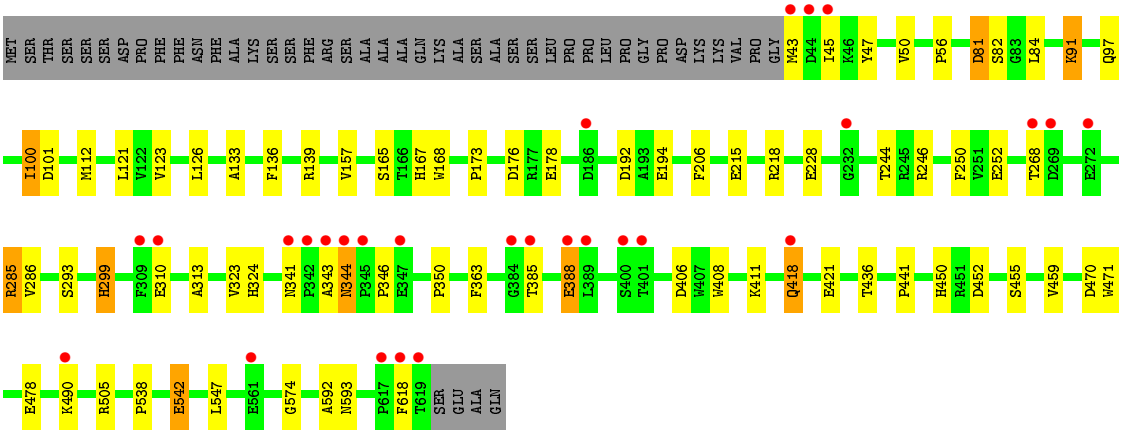
• Molecule 1: Pyranose oxidase

Chain C:



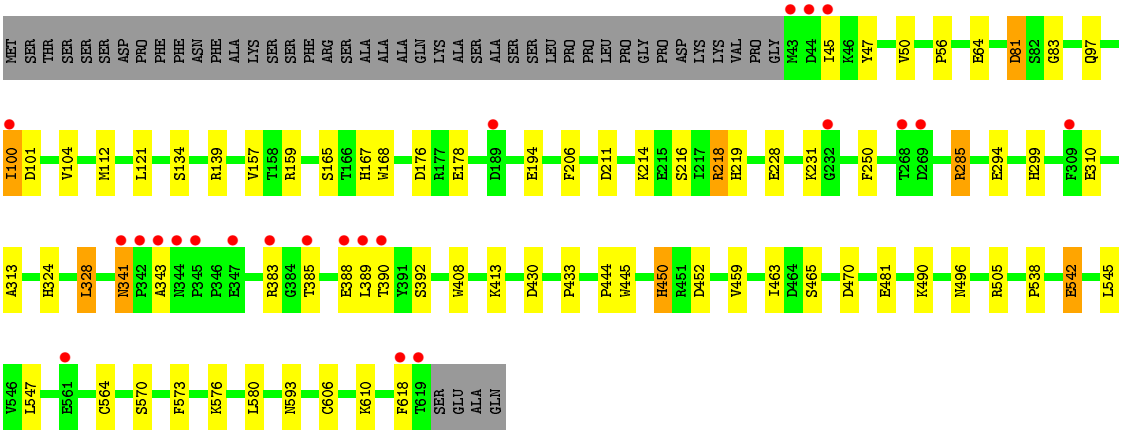
• Molecule 1: Pyranose oxidase

Chain E:



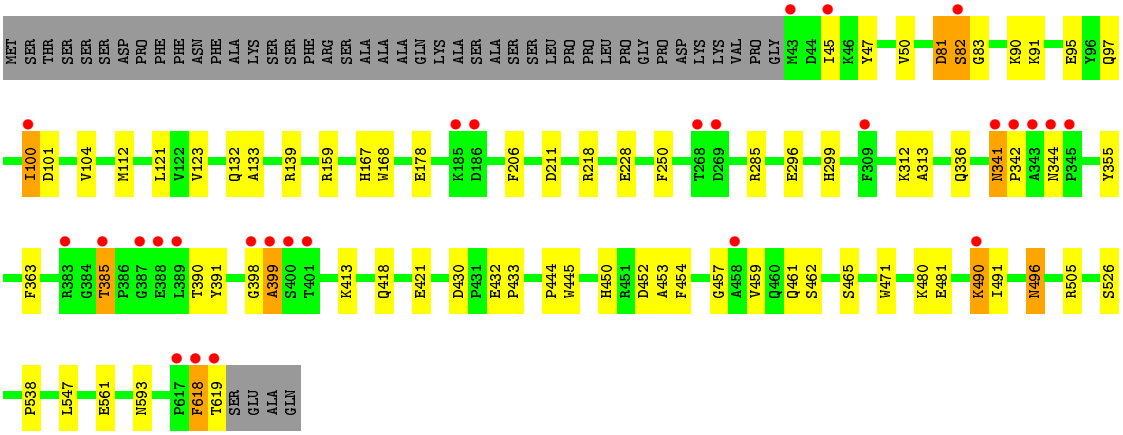
• Molecule 1: Pyranose oxidase

Chain F:



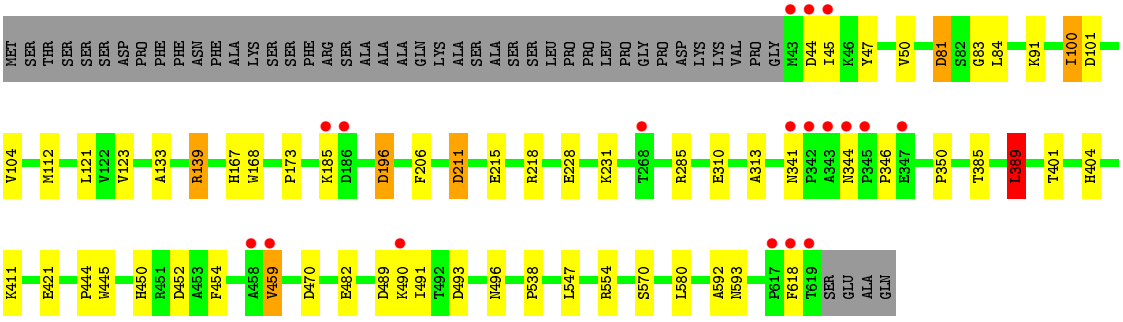
- Molecule 1: Pyranose oxidase

Chain G:



- Molecule 1: Pyranose oxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	168.43Å 103.14Å 168.91Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-1.90) 96.8 (19.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.152 , 0.189 0.160 , 0.197	Depositor DCC
R_{free} test set	4236 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 57.9	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 422213 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	41255	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.90	3/4676 (0.1%)	0.87	6/6358 (0.1%)
1	B	0.90	5/4677 (0.1%)	0.90	16/6360 (0.3%)
1	C	0.86	5/4670 (0.1%)	0.90	8/6350 (0.1%)
1	D	0.86	3/4684 (0.1%)	0.90	12/6369 (0.2%)
1	E	0.84	3/4676 (0.1%)	0.82	7/6358 (0.1%)
1	F	0.84	3/4670 (0.1%)	0.87	9/6350 (0.1%)
1	G	0.87	2/4677 (0.0%)	0.88	9/6360 (0.1%)
1	H	0.86	1/4670 (0.0%)	0.88	13/6350 (0.2%)
All	All	0.87	25/37400 (0.1%)	0.88	80/50855 (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	E	0	1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLU	CB-CG	-7.40	1.38	1.52
1	B	542	GLU	CG-CD	6.54	1.61	1.51
1	D	104	VAL	CB-CG2	-6.25	1.39	1.52
1	B	482	GLU	CG-CD	6.15	1.61	1.51
1	D	542	GLU	CB-CG	-6.08	1.40	1.52

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	ARG	NE-CZ-NH2	-23.67	108.46	120.30
1	C	139	ARG	NE-CZ-NH2	-23.61	108.49	120.30
1	F	139	ARG	NE-CZ-NH2	-22.77	108.92	120.30
1	G	139	ARG	NE-CZ-NH2	-21.96	109.32	120.30
1	H	139	ARG	NE-CZ-NH2	-19.62	110.49	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	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	4561	0	4408	91	0
1	B	4562	0	4412	112	0
1	C	4555	0	4404	85	0
1	D	4569	0	4411	87	0
1	E	4561	0	4408	100	0
1	F	4555	0	4404	93	0
1	G	4562	0	4412	104	0
1	H	4555	0	4404	74	0
2	A	53	0	30	6	0
2	B	53	0	29	13	0
2	C	53	0	28	5	0
2	D	53	0	29	8	0
2	E	53	0	30	11	0
2	F	53	0	29	9	0
2	G	53	0	29	10	0
2	H	53	0	28	6	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
3	D	12	0	12	2	0
3	E	12	0	12	4	0
3	F	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	12	0	12	2	0
3	H	12	0	12	1	0
4	A	572	0	0	40	0
4	B	570	0	0	37	0
4	C	514	0	0	22	0
4	D	546	0	0	46	0
4	E	524	0	0	43	0
4	F	472	0	0	30	0
4	G	519	0	0	38	0
4	H	538	0	0	30	0
All	All	41255	0	35591	648	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 9.

The worst 5 of 648 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:G:167:HIS:HE2	2:G:801:FAD:C8M	0.98	1.61
1:E:167:HIS:HE2	2:E:801:FAD:C8M	1.01	1.60
1:D:167:HIS:HE2	2:D:801:FAD:C8M	0.97	1.59
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.97	1.57
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.96	1.54

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	577/623 (93%)	557 (96%)	20 (4%)	0	100	100
1	B	577/623 (93%)	564 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	576/623 (92%)	561 (97%)	14 (2%)	1 (0%)	52 42
1	D	578/623 (93%)	564 (98%)	14 (2%)	0	100 100
1	E	577/623 (93%)	562 (97%)	14 (2%)	1 (0%)	52 42
1	F	576/623 (92%)	560 (97%)	16 (3%)	0	100 100
1	G	577/623 (93%)	561 (97%)	15 (3%)	1 (0%)	52 42
1	H	576/623 (92%)	559 (97%)	17 (3%)	0	100 100
All	All	4614/4984 (93%)	4488 (97%)	123 (3%)	3 (0%)	56 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	344	ASN
1	G	399	ALA
1	C	344	ASN

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	507/542 (94%)	490 (97%)	17 (3%)	44 33
1	B	507/542 (94%)	492 (97%)	15 (3%)	48 38
1	C	506/542 (93%)	491 (97%)	15 (3%)	48 38
1	D	508/542 (94%)	495 (97%)	13 (3%)	54 45
1	E	507/542 (94%)	488 (96%)	19 (4%)	41 29
1	F	506/542 (93%)	489 (97%)	17 (3%)	44 33
1	G	507/542 (94%)	490 (97%)	17 (3%)	44 33
1	H	506/542 (93%)	494 (98%)	12 (2%)	57 49
All	All	4054/4336 (94%)	3929 (97%)	125 (3%)	47 37

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	490	LYS
1	E	385	THR
1	H	168	TRP
1	C	593	ASN
1	E	168	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	341	ASN
1	E	611	GLN
1	H	460	GLN
1	E	418	GLN
1	B	461	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	MES	A	7003	-	11,12,12	0.55	0	14,16,16	6.20	7 (50%)
2	FAD	A	801	1	48,58,58	1.37	7 (14%)	54,89,89	4.46	19 (35%)
3	MES	B	7006	-	11,12,12	0.60	0	14,16,16	6.10	7 (50%)
2	FAD	B	801	1	48,58,58	1.22	5 (10%)	54,89,89	3.41	18 (33%)
3	MES	C	7005	-	11,12,12	0.54	0	14,16,16	5.93	8 (57%)
2	FAD	C	801	1	48,58,58	1.36	7 (14%)	54,89,89	3.70	16 (29%)
3	MES	D	7007	-	11,12,12	0.63	0	14,16,16	7.50	7 (50%)
2	FAD	D	801	1	48,58,58	1.29	7 (14%)	54,89,89	3.67	18 (33%)
3	MES	E	7004	-	11,12,12	0.80	0	14,16,16	7.75	7 (50%)
2	FAD	E	801	1	48,58,58	1.22	5 (10%)	54,89,89	4.00	22 (40%)
3	MES	F	7001	-	11,12,12	0.52	0	14,16,16	5.34	6 (42%)
2	FAD	F	801	1	48,58,58	1.32	8 (16%)	54,89,89	3.74	19 (35%)
3	MES	G	7008	-	11,12,12	0.54	0	14,16,16	6.57	6 (42%)
2	FAD	G	801	1	48,58,58	1.29	5 (10%)	54,89,89	3.93	17 (31%)
3	MES	H	7002	-	11,12,12	0.59	0	14,16,16	5.27	7 (50%)
2	FAD	H	801	1	48,58,58	1.14	3 (6%)	54,89,89	4.63	15 (27%)

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	MES	A	7003	-	-	0/6/14/14	0/1/1/1
2	FAD	A	801	1	-	0/30/50/50	0/6/6/6
3	MES	B	7006	-	-	0/6/14/14	0/1/1/1
2	FAD	B	801	1	-	0/30/50/50	0/6/6/6
3	MES	C	7005	-	-	0/6/14/14	0/1/1/1
2	FAD	C	801	1	-	0/30/50/50	0/6/6/6
3	MES	D	7007	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	1	-	0/30/50/50	0/6/6/6
3	MES	E	7004	-	-	0/6/14/14	0/1/1/1
2	FAD	E	801	1	-	0/30/50/50	0/6/6/6
3	MES	F	7001	-	-	0/6/14/14	0/1/1/1
2	FAD	F	801	1	-	0/30/50/50	0/6/6/6
3	MES	G	7008	-	-	0/6/14/14	0/1/1/1
2	FAD	G	801	1	-	0/30/50/50	0/6/6/6
3	MES	H	7002	-	-	0/6/14/14	0/1/1/1
2	FAD	H	801	1	-	0/30/50/50	0/6/6/6

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	O4B-C4B	-3.18	1.37	1.45
2	C	801	FAD	O3B-C3B	-2.79	1.36	1.43
2	D	801	FAD	O3B-C3B	-2.67	1.36	1.43
2	B	801	FAD	O2B-C2B	-2.52	1.36	1.43
2	F	801	FAD	O3B-C3B	-2.49	1.37	1.43

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	7004	MES	O2S-S-C8	-23.85	86.55	106.91
3	D	7007	MES	O2S-S-C8	-22.71	87.53	106.91
3	G	7008	MES	O1S-S-C8	-19.90	89.92	106.91
3	A	7003	MES	O1S-S-C8	-18.51	91.11	106.91
3	C	7005	MES	O2S-S-C8	-17.30	92.15	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7003	MES	1	0
2	A	801	FAD	6	0
3	B	7006	MES	1	0
2	B	801	FAD	13	0
2	C	801	FAD	5	0
3	D	7007	MES	2	0
2	D	801	FAD	8	0
3	E	7004	MES	4	0
2	E	801	FAD	11	0
2	F	801	FAD	9	0
3	G	7008	MES	2	0
2	G	801	FAD	10	0
3	H	7002	MES	1	0
2	H	801	FAD	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	577/623 (92%)	-0.28	22 (3%)	44	48	8, 13, 36, 57	0
1	B	577/623 (92%)	-0.32	16 (2%)	56	60	8, 14, 31, 49	0
1	C	577/623 (92%)	-0.17	24 (4%)	40	44	9, 17, 37, 54	0
1	D	577/623 (92%)	-0.25	20 (3%)	48	51	8, 15, 34, 54	0
1	E	577/623 (92%)	-0.20	28 (4%)	33	36	10, 17, 34, 53	0
1	F	577/623 (92%)	-0.20	23 (3%)	42	46	9, 18, 37, 53	0
1	G	577/623 (92%)	-0.19	28 (4%)	33	36	10, 16, 39, 52	0
1	H	577/623 (92%)	-0.29	18 (3%)	52	56	8, 15, 31, 53	0
All	All	4616/4984 (92%)	-0.24	179 (3%)	43	47	8, 16, 35, 57	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	619	THR	11.5
1	C	619	THR	10.0
1	A	619	THR	9.9
1	D	619	THR	9.5
1	B	619	THR	9.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{th} 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^2)	Q<0.9
3	MES	C	7005	12/12	0.96	0.10	0.24	17,20,22,23	0
3	MES	H	7002	12/12	0.96	0.09	-0.16	18,20,21,22	0
3	MES	G	7008	12/12	0.97	0.08	-0.35	19,22,24,24	0
3	MES	B	7006	12/12	0.96	0.09	-0.39	22,23,26,26	0
2	FAD	C	801	53/53	0.97	0.07	-0.43	9,13,16,19	0
3	MES	D	7007	12/12	0.98	0.07	-0.62	20,24,25,25	0
3	MES	E	7004	12/12	0.98	0.07	-0.70	19,22,25,27	0
2	FAD	F	801	53/53	0.98	0.06	-0.70	10,13,15,17	0
2	FAD	D	801	53/53	0.98	0.06	-0.71	10,12,14,16	0
2	FAD	A	801	53/53	0.98	0.06	-0.80	7,10,14,16	0
3	MES	F	7001	12/12	0.98	0.07	-0.86	14,18,19,19	0
3	MES	A	7003	12/12	0.98	0.06	-0.95	16,17,19,20	0
2	FAD	E	801	53/53	0.98	0.06	-0.99	9,13,15,18	0
2	FAD	H	801	53/53	0.98	0.06	-0.99	9,13,15,17	0
2	FAD	G	801	53/53	0.98	0.06	-1.02	10,12,15,17	0
2	FAD	B	801	53/53	0.98	0.06	-1.08	8,11,13,19	0

6.5 Other polymers

There are no such residues in this entry.