W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 01:44 PM EDT

PDB ID	:	2IGO
Title	:	Crystal structure of pyranose 2-oxidase H167A mutant with 2-fluoro-2-deoxy-D-glucose
Authors	:	Divne, C.
Deposited on	:	unknown
Resolution	:	1.95 Å(reported)

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

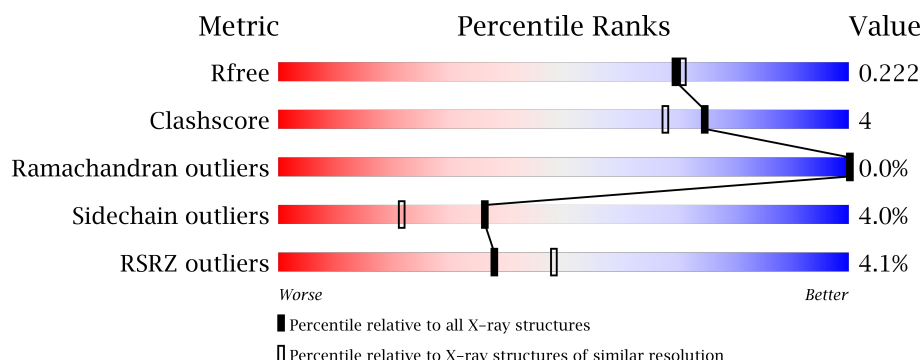|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		4
Ramachandran outliers		0.0%
Sidechain outliers		4.0%
RSRZ outliers		4.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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% / 80% 12% · 7%
1	B	623	3% / 82% 9% · 7%
1	C	623	4% / 82% 10% · 7%
1	D	623	3% / 80% 11% · 7%
1	E	623	4% / 82% 9% · 7%

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Mol	Chain	Length	Quality of chain
1	F	623	5% / 81% / 9% · 7%
1	G	623	4% / 80% / 11% · 7%
1	H	623	4% / 80% / 12% · 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
2	SHG	G	808	-	-	-	X
3	FAD	A	701	-	-	-	X
3	FAD	B	702	-	-	-	X
3	FAD	C	704	-	-	-	X
3	FAD	D	703	-	-	-	X
3	FAD	E	705	-	-	-	X
3	FAD	F	706	-	-	-	X
3	FAD	G	708	-	-	-	X
3	FAD	H	707	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 38602 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.
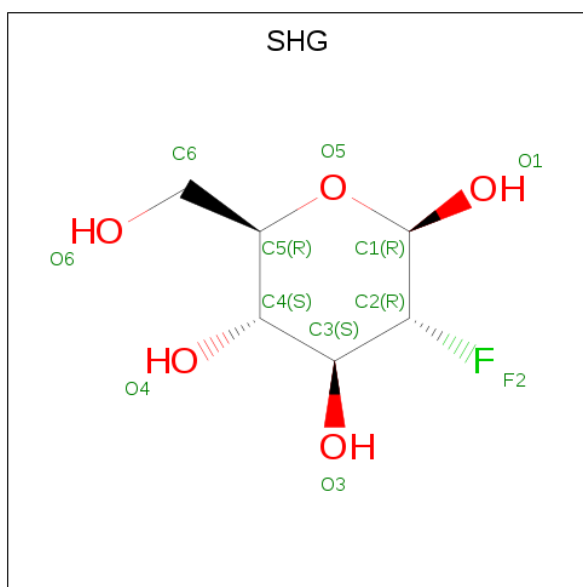
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
B	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
C	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
D	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
E	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
F	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
G	167	ALA	HIS	ENGINEERED	UNP Q7ZA32
H	167	ALA	HIS	ENGINEERED	UNP Q7ZA32

- Molecule 2 is 2-deoxy-2-fluoro-beta-D-glucopyranose (three-letter code: SHG) (formula: $C_6H_{11}FO_5$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 12	C 6	F 1	O 5	0	0
2	B	1	Total 12	C 6	F 1	O 5	0	0
2	D	1	Total 12	C 6	F 1	O 5	0	0
2	C	1	Total 12	C 6	F 1	O 5	0	0
2	E	1	Total 12	C 6	F 1	O 5	0	0
2	F	1	Total 12	C 6	F 1	O 5	0	0
2	H	1	Total 12	C 6	F 1	O 5	0	0
2	G	1	Total 12	C 6	F 1	O 5	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	B	251	Total	O	0	0
			251	251		
4	D	222	Total	O	0	0
			222	222		
4	C	199	Total	O	0	0
			199	199		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	195	Total 195	O 195	0	0
4	F	192	Total 192	O 192	0	0
4	H	217	Total 217	O 217	0	0
4	G	210	Total 210	O 210	0	0

3 Residue-property plots ⓘ

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.
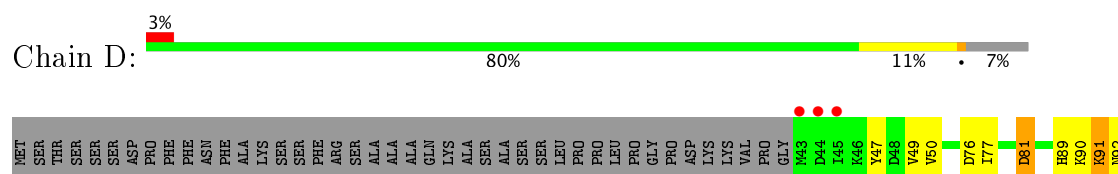
- Molecule 1: Pyranose oxidase
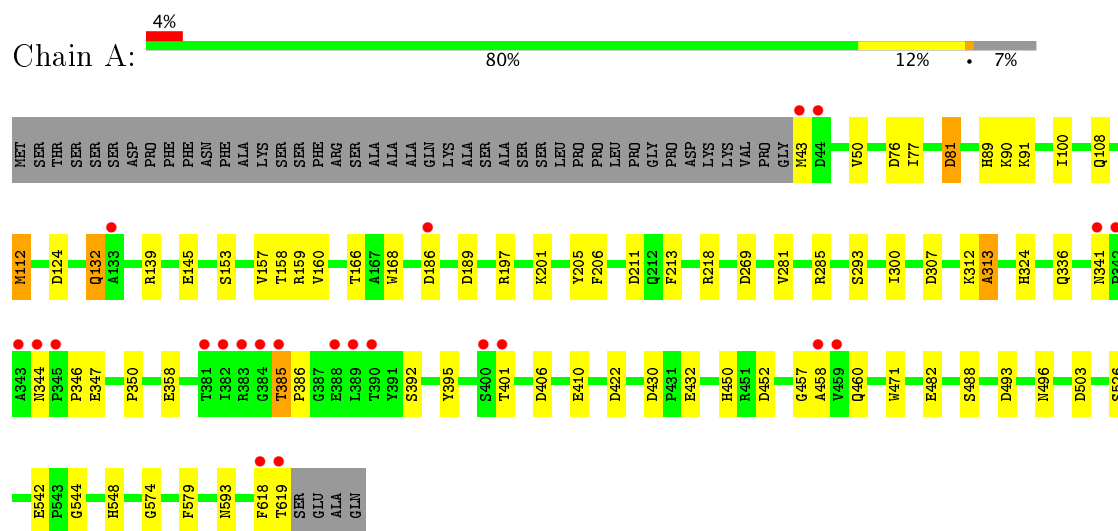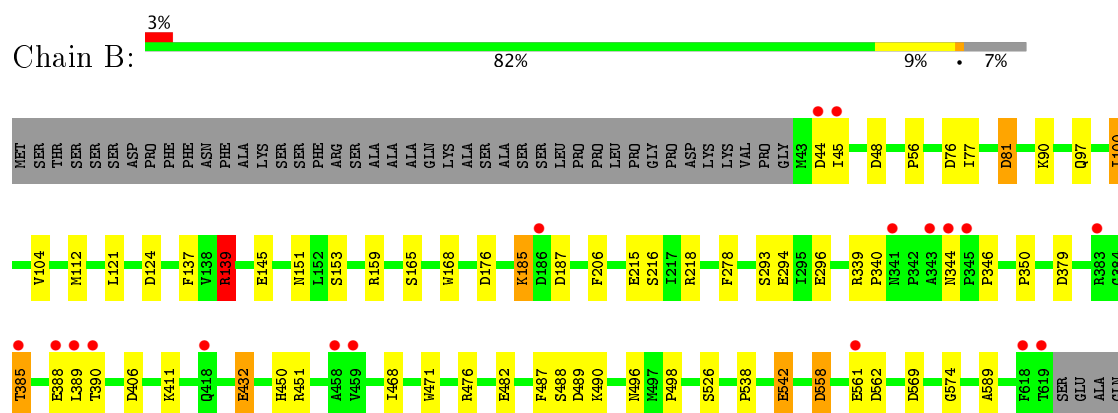
- Molecule 1: Pyranose oxidase
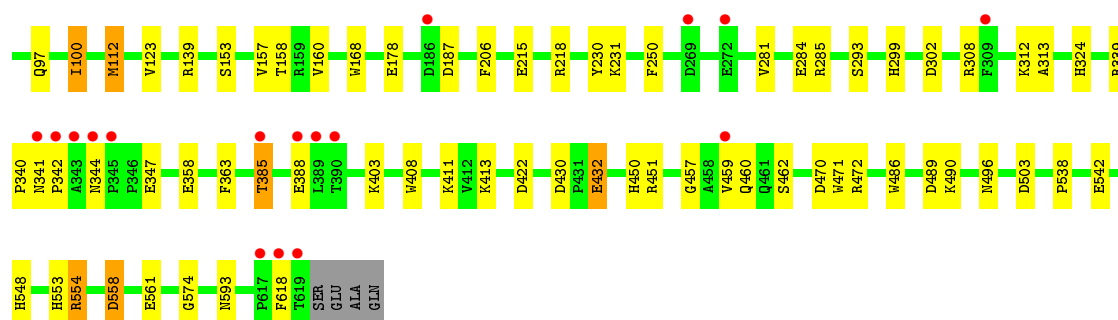

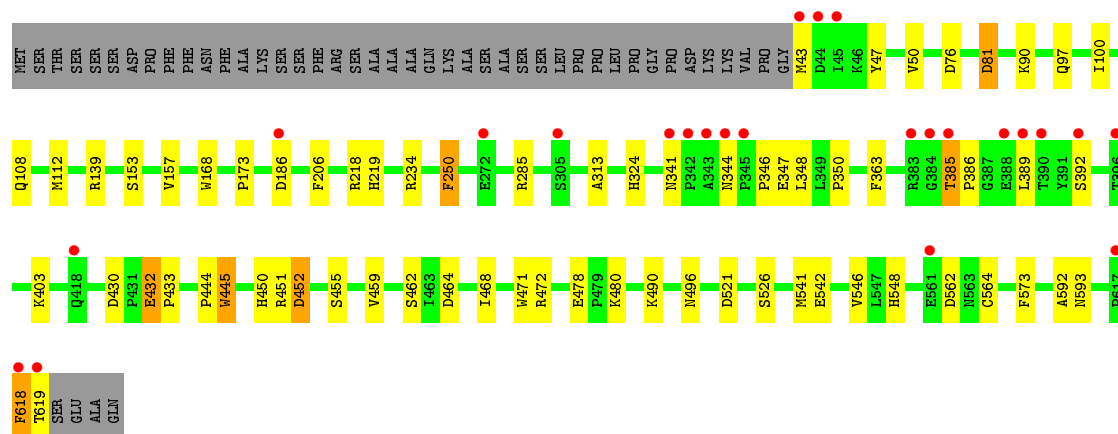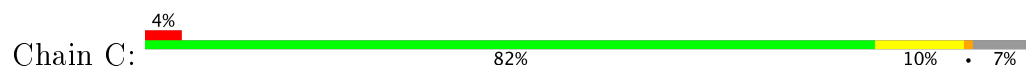- Molecule 1: Pyranose oxidase

• Molecule 1: Pyranose oxidase
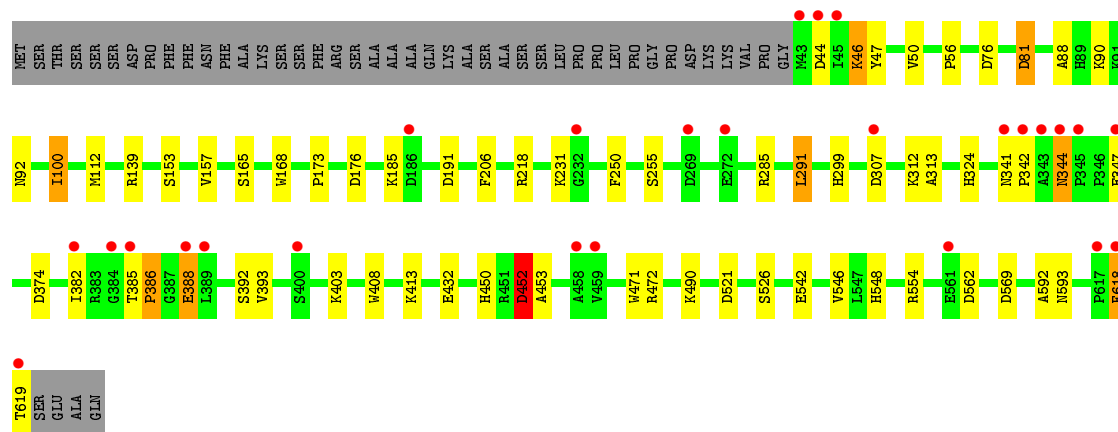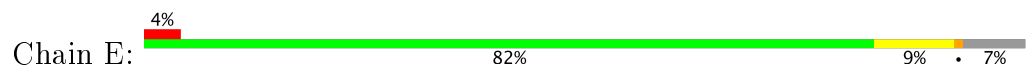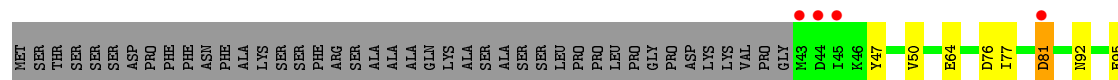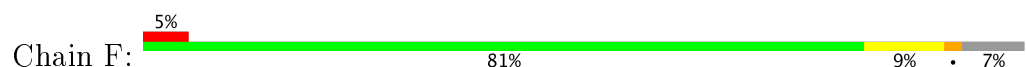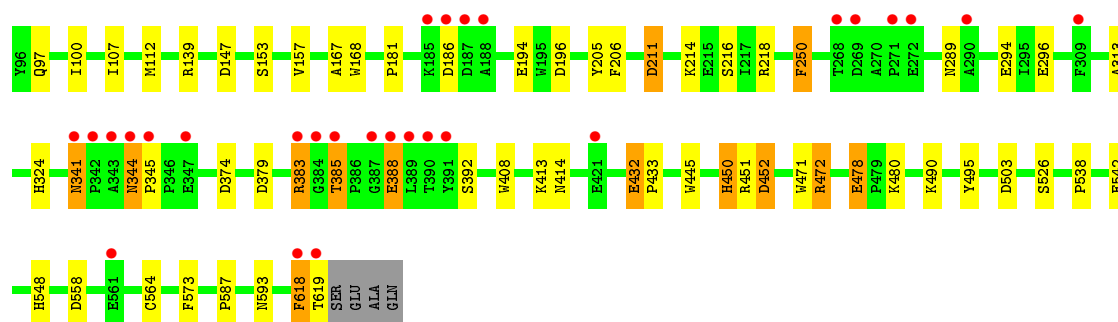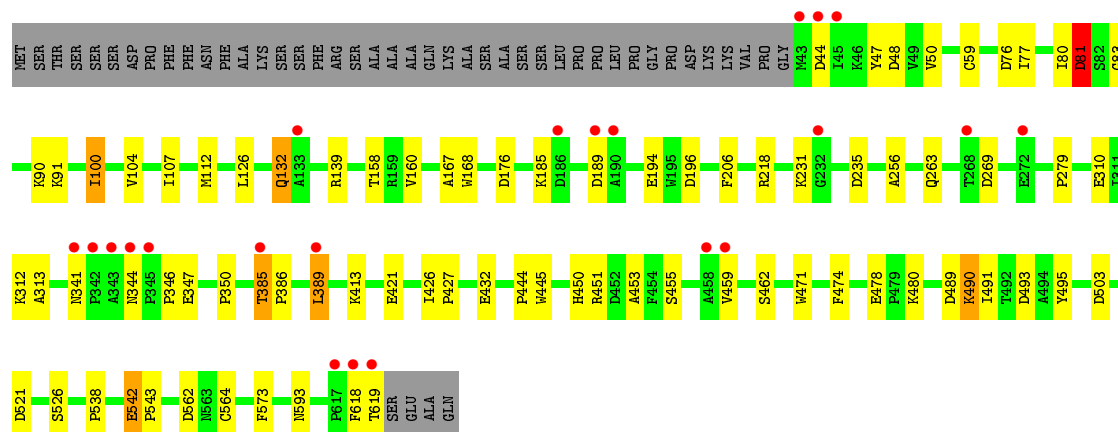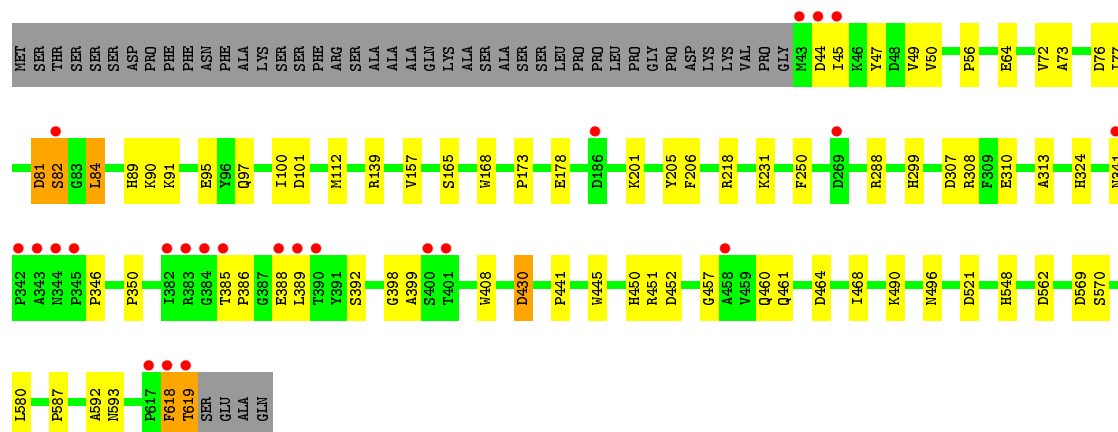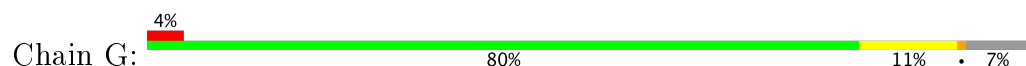
Chain C:

• Molecule 1: Pyranose oxidase

Chain E:

• Molecule 1: Pyranose oxidase

Chain F:

- Molecule 1: Pyranose oxidase

Chain H:

- Molecule 1: Pyranose oxidase

Chain G:
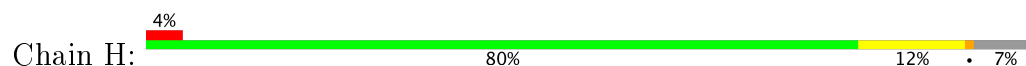
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	168.59Å 103.08Å 169.04Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	38.90 – 1.95 38.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.90-1.95) 99.9 (38.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.221 0.188 , 0.222	Depositor DCC
R_{free} test set	4042 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	38602	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

wwPDB X-ray Structure Validation Summary Report

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, SHG

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	1.14	7/4659 (0.2%)	1.08	20/6335 (0.3%)
1	B	1.10	4/4659 (0.1%)	1.08	19/6335 (0.3%)
1	C	1.04	3/4659 (0.1%)	1.04	13/6335 (0.2%)
1	D	1.08	5/4659 (0.1%)	1.05	19/6335 (0.3%)
1	E	1.04	1/4659 (0.0%)	1.04	20/6335 (0.3%)
1	F	1.03	3/4659 (0.1%)	1.07	18/6335 (0.3%)
1	G	1.05	0/4659	1.06	18/6335 (0.3%)
1	H	1.07	3/4659 (0.1%)	1.05	23/6335 (0.4%)
All	All	1.07	26/37272 (0.1%)	1.06	150/50680 (0.3%)

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
1	D	0	1
All	All	0	2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	LEU	CG-CD1	7.79	1.80	1.51
1	C	541	MET	CG-SD	6.66	1.98	1.81
1	A	482	GLU	CD-OE1	6.66	1.32	1.25
1	A	313	ALA	CA-CB	6.29	1.65	1.52
1	A	112	MET	CB-CG	5.91	1.70	1.51

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	139	ARG	NE-CZ-NH2	-24.01	108.29	120.30
1	D	139	ARG	NE-CZ-NH2	-20.93	109.83	120.30
1	B	139	ARG	NE-CZ-NH2	-20.35	110.12	120.30
1	E	139	ARG	NE-CZ-NH2	-19.12	110.74	120.30
1	G	139	ARG	NE-CZ-NH2	-18.89	110.86	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	151	ASN	Peptide
1	D	553	HIS	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	4544	0	4393	28	0
1	B	4544	0	4393	31	0
1	C	4544	0	4393	33	0
1	D	4544	0	4393	32	0
1	E	4544	0	4393	36	0
1	F	4544	0	4393	35	0
1	G	4544	0	4393	42	0
1	H	4544	0	4393	30	0
2	A	12	0	11	4	0
2	B	12	0	11	1	0
2	C	12	0	11	5	0
2	D	12	0	11	3	0
2	E	12	0	11	4	0
2	F	12	0	10	2	0
2	G	12	0	11	4	0
2	H	12	0	11	0	0
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	C	53	0	31	1	0
3	D	53	0	31	2	0
3	E	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	53	0	31	0	0
3	G	53	0	31	2	0
3	H	53	0	31	0	0
4	A	244	0	0	3	0
4	B	251	0	0	1	0
4	C	199	0	0	2	0
4	D	222	0	0	1	0
4	E	195	0	0	2	0
4	F	192	0	0	1	0
4	G	210	0	0	6	0
4	H	217	0	0	3	0
All	All	38602	0	35479	269	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 4.

The worst 5 of 269 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:E:291:LEU:CG	1:E:291:LEU:CD1	1.80	1.56
1:G:81:ASP:HA	4:G:2497:HOH:O	1.42	1.16
1:C:432:GLU:HG3	4:C:2381:HOH:O	1.48	1.12
1:G:81:ASP:CA	4:G:2497:HOH:O	2.04	0.98
1:E:291:LEU:CD1	1:E:291:LEU:HG	2.01	0.88

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	575/623 (92%)	558 (97%)	17 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	575/623 (92%)	563 (98%)	11 (2%)	1 (0%)	51	41
1	C	575/623 (92%)	554 (96%)	21 (4%)	0	100	100
1	D	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	E	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	F	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	G	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	H	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
All	All	4600/4984 (92%)	4470 (97%)	129 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP

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	504/541 (93%)	485 (96%)	19 (4%)	38	24
1	B	504/541 (93%)	489 (97%)	15 (3%)	46	34
1	C	504/541 (93%)	483 (96%)	21 (4%)	34	20
1	D	504/541 (93%)	483 (96%)	21 (4%)	34	20
1	E	504/541 (93%)	482 (96%)	22 (4%)	33	18
1	F	504/541 (93%)	485 (96%)	19 (4%)	38	24
1	G	504/541 (93%)	483 (96%)	21 (4%)	34	20
1	H	504/541 (93%)	480 (95%)	24 (5%)	30	14
All	All	4032/4328 (93%)	3870 (96%)	162 (4%)	36	21

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	593	ASN
1	E	408	TRP
1	G	231	LYS
1	C	619	THR
1	E	231	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	263	GLN
1	E	341	ASN
1	H	460	GLN
1	D	460	GLN
1	C	341	ASN

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)

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	FAD	A	701	-	51,58,58	1.73	9 (17%)	54,89,89	2.67	9 (16%)
2	SHG	A	801	-	11,12,12	0.85	0	14,17,17	4.64	8 (57%)
3	FAD	B	702	-	51,58,58	1.51	6 (11%)	54,89,89	2.38	8 (14%)
2	SHG	B	802	-	11,12,12	0.86	1 (9%)	14,17,17	3.73	7 (50%)
3	FAD	C	704	-	51,58,58	1.65	9 (17%)	54,89,89	2.34	7 (12%)
2	SHG	C	804	-	11,12,12	0.62	0	14,17,17	5.36	9 (64%)
3	FAD	D	703	-	51,58,58	1.48	6 (11%)	54,89,89	2.14	8 (14%)
2	SHG	D	803	-	11,12,12	1.04	1 (9%)	14,17,17	3.69	7 (50%)
3	FAD	E	705	-	51,58,58	1.38	7 (13%)	54,89,89	2.67	8 (14%)
2	SHG	E	805	-	11,12,12	0.80	0	14,17,17	4.78	7 (50%)
3	FAD	F	706	-	51,58,58	1.34	7 (13%)	54,89,89	2.42	11 (20%)
2	SHG	F	806	-	11,12,12	0.75	0	14,17,17	4.34	7 (50%)
3	FAD	G	708	-	51,58,58	1.59	8 (15%)	54,89,89	2.31	6 (11%)
2	SHG	G	808	-	11,12,12	0.89	0	14,17,17	5.30	7 (50%)
3	FAD	H	707	-	51,58,58	1.43	5 (9%)	54,89,89	2.33	8 (14%)
2	SHG	H	807	-	11,12,12	0.55	0	14,17,17	4.09	11 (78%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	701	-	-	0/28/50/50	0/6/6/6
2	SHG	A	801	-	-	0/2/22/22	0/1/1/1
3	FAD	B	702	-	-	0/28/50/50	0/6/6/6
2	SHG	B	802	-	-	0/2/22/22	0/1/1/1
3	FAD	C	704	-	-	0/28/50/50	0/6/6/6
2	SHG	C	804	-	-	0/2/22/22	0/1/1/1
3	FAD	D	703	-	-	0/28/50/50	0/6/6/6
2	SHG	D	803	-	-	0/2/22/22	0/1/1/1
3	FAD	E	705	-	-	0/28/50/50	0/6/6/6
2	SHG	E	805	-	-	0/2/22/22	0/1/1/1
3	FAD	F	706	-	-	0/28/50/50	0/6/6/6
2	SHG	F	806	-	-	0/2/22/22	0/1/1/1
3	FAD	G	708	-	-	0/28/50/50	0/6/6/6
2	SHG	G	808	-	-	0/2/22/22	0/1/1/1
3	FAD	H	707	-	-	0/28/50/50	0/6/6/6
2	SHG	H	807	-	-	0/2/22/22	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	SHG	C2-C3	-2.50	1.50	1.52
3	C	704	FAD	P-O1P	-2.15	1.42	1.50
2	B	802	SHG	O3-C3	-2.11	1.38	1.43
3	F	706	FAD	O4B-C4B	-2.09	1.40	1.45
3	E	705	FAD	C2A-N1A	2.02	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	FAD	N3A-C2A-N1A	-11.63	118.73	128.86
3	H	707	FAD	N3A-C2A-N1A	-11.12	119.18	128.86
3	E	705	FAD	N3A-C2A-N1A	-10.89	119.37	128.86
3	G	708	FAD	N3A-C2A-N1A	-10.85	119.41	128.86
3	D	703	FAD	N3A-C2A-N1A	-10.59	119.64	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	FAD	4	0
2	A	801	SHG	4	0
3	B	702	FAD	4	0
2	B	802	SHG	1	0
3	C	704	FAD	1	0
2	C	804	SHG	5	0
3	D	703	FAD	2	0
2	D	803	SHG	3	0
3	E	705	FAD	1	0
2	E	805	SHG	4	0
2	F	806	SHG	2	0
3	G	708	FAD	2	0
2	G	808	SHG	4	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	577/623 (92%)	-0.07	23 (3%)	39	49	16, 22, 45, 69	0
1	B	577/623 (92%)	-0.10	18 (3%)	49	60	15, 23, 42, 67	0
1	C	577/623 (92%)	0.03	24 (4%)	37	47	18, 26, 46, 71	0
1	D	577/623 (92%)	-0.05	20 (3%)	44	55	16, 25, 45, 72	0
1	E	577/623 (92%)	-0.00	26 (4%)	34	44	18, 26, 45, 72	0
1	F	577/623 (92%)	0.06	32 (5%)	26	36	17, 27, 47, 71	0
1	G	577/623 (92%)	-0.02	24 (4%)	37	47	18, 25, 48, 67	0
1	H	577/623 (92%)	-0.08	22 (3%)	41	51	16, 24, 43, 71	0
All	All	4616/4984 (92%)	-0.03	189 (4%)	38	48	15, 25, 45, 72	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	619	THR	13.2
1	H	619	THR	12.9
1	E	619	THR	11.0
1	A	619	THR	10.5
1	D	619	THR	9.5

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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FAD	D	703	53/53	0.88	0.22	5.08	16,20,105,106	0
3	FAD	C	704	53/53	0.86	0.21	4.94	16,23,113,114	0
3	FAD	E	705	53/53	0.89	0.22	4.47	15,21,119,120	0
3	FAD	G	708	53/53	0.88	0.21	4.39	16,21,101,103	0
3	FAD	B	702	53/53	0.89	0.21	4.35	14,19,107,107	0
3	FAD	H	707	53/53	0.89	0.22	4.25	15,21,119,120	0
3	FAD	F	706	53/53	0.89	0.20	4.23	16,21,115,116	0
3	FAD	A	701	53/53	0.88	0.21	3.69	12,18,94,95	0
2	SHG	G	808	12/12	0.89	0.16	2.46	27,35,39,42	0
2	SHG	C	804	12/12	0.89	0.12	0.38	29,37,41,41	0
2	SHG	E	805	12/12	0.91	0.11	0.06	31,37,40,41	0
2	SHG	H	807	12/12	0.94	0.10	-0.04	28,35,38,41	0
2	SHG	D	803	12/12	0.93	0.12	-0.18	30,35,40,41	0
2	SHG	A	801	12/12	0.94	0.10	-0.24	24,35,41,44	0
2	SHG	F	806	12/12	0.94	0.11	-0.35	31,34,40,42	0
2	SHG	B	802	12/12	0.96	0.07	-1.90	24,29,35,39	0

6.5 Other polymers (i)

There are no such residues in this entry.