



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 12:17 PM EST

PDB ID : 1TZL
Title : Crystal Structure of Pyranose 2-Oxidase from the White-Rot Fungus *Peniophora* sp.
Authors : Bannwarth, M.; Bastian, S.; Heckmann-Pohl, D.; Giffhorn, F.; Schulz, G.E.
Deposited on : 2004-07-10
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

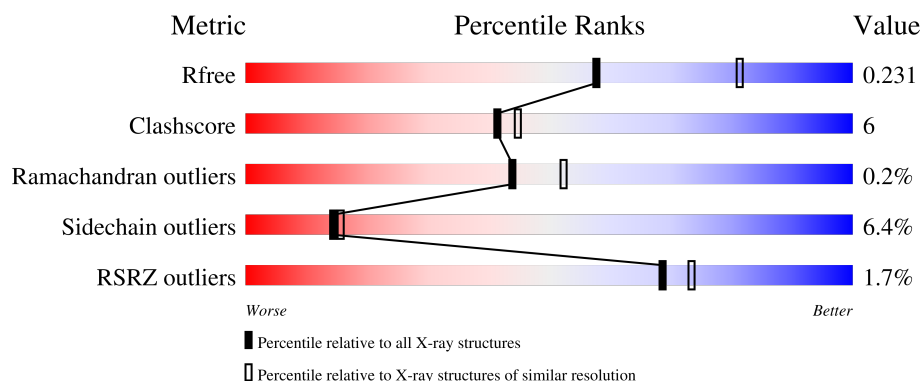
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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 ≥ 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	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 78%, yellow 78%, yellow 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 78% 14% • 7% </div> </div>
1	B	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 68%, yellow 68%, yellow 88%, grey 88%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 68% 20% • 7% </div> </div>
1	C	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 78%, yellow 78%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 78% 13% • 7% </div> </div>
1	D	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 76%, yellow 76%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 76% 15% • 7% </div> </div>
1	E	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 77%, yellow 77%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 77% 14% • 7% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	622	<p>75% 16% 7%</p>
1	G	622	<p>77% 14% 7%</p>
1	H	622	<p>77% 14% 7%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 38970 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	Se	0	0	0
			4549	2872	778	874	9	16			
1	B	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	C	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	D	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	E	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	F	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	G	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	H	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MSE	MET	modified residue	UNP Q8J136
A	74	MSE	MET	modified residue	UNP Q8J136
A	112	MSE	MET	modified residue	UNP Q8J136
A	164	MSE	MET	modified residue	UNP Q8J136
A	368	MSE	MET	modified residue	UNP Q8J136
A	380	MSE	MET	modified residue	UNP Q8J136
A	416	MSE	MET	modified residue	UNP Q8J136
A	417	MSE	MET	modified residue	UNP Q8J136
A	497	MSE	MET	modified residue	UNP Q8J136
A	518	MSE	MET	modified residue	UNP Q8J136
A	519	MSE	MET	modified residue	UNP Q8J136
A	522	MSE	MET	modified residue	UNP Q8J136
A	525	MSE	MET	modified residue	UNP Q8J136

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Chain	Residue	Modelled	Actual	Comment	Reference
A	541	MSE	MET	modified residue	UNP Q8J136
A	555	MSE	MET	modified residue	UNP Q8J136
A	599	MSE	MET	modified residue	UNP Q8J136
B	43	MSE	MET	modified residue	UNP Q8J136
B	74	MSE	MET	modified residue	UNP Q8J136
B	112	MSE	MET	modified residue	UNP Q8J136
B	164	MSE	MET	modified residue	UNP Q8J136
B	368	MSE	MET	modified residue	UNP Q8J136
B	380	MSE	MET	modified residue	UNP Q8J136
B	416	MSE	MET	modified residue	UNP Q8J136
B	417	MSE	MET	modified residue	UNP Q8J136
B	497	MSE	MET	modified residue	UNP Q8J136
B	518	MSE	MET	modified residue	UNP Q8J136
B	519	MSE	MET	modified residue	UNP Q8J136
B	522	MSE	MET	modified residue	UNP Q8J136
B	525	MSE	MET	modified residue	UNP Q8J136
B	541	MSE	MET	modified residue	UNP Q8J136
B	555	MSE	MET	modified residue	UNP Q8J136
B	599	MSE	MET	modified residue	UNP Q8J136
C	43	MSE	MET	modified residue	UNP Q8J136
C	74	MSE	MET	modified residue	UNP Q8J136
C	112	MSE	MET	modified residue	UNP Q8J136
C	164	MSE	MET	modified residue	UNP Q8J136
C	368	MSE	MET	modified residue	UNP Q8J136
C	380	MSE	MET	modified residue	UNP Q8J136
C	416	MSE	MET	modified residue	UNP Q8J136
C	417	MSE	MET	modified residue	UNP Q8J136
C	497	MSE	MET	modified residue	UNP Q8J136
C	518	MSE	MET	modified residue	UNP Q8J136
C	519	MSE	MET	modified residue	UNP Q8J136
C	522	MSE	MET	modified residue	UNP Q8J136
C	525	MSE	MET	modified residue	UNP Q8J136
C	541	MSE	MET	modified residue	UNP Q8J136
C	555	MSE	MET	modified residue	UNP Q8J136
C	599	MSE	MET	modified residue	UNP Q8J136
D	43	MSE	MET	modified residue	UNP Q8J136
D	74	MSE	MET	modified residue	UNP Q8J136
D	112	MSE	MET	modified residue	UNP Q8J136
D	164	MSE	MET	modified residue	UNP Q8J136
D	368	MSE	MET	modified residue	UNP Q8J136
D	380	MSE	MET	modified residue	UNP Q8J136
D	416	MSE	MET	modified residue	UNP Q8J136

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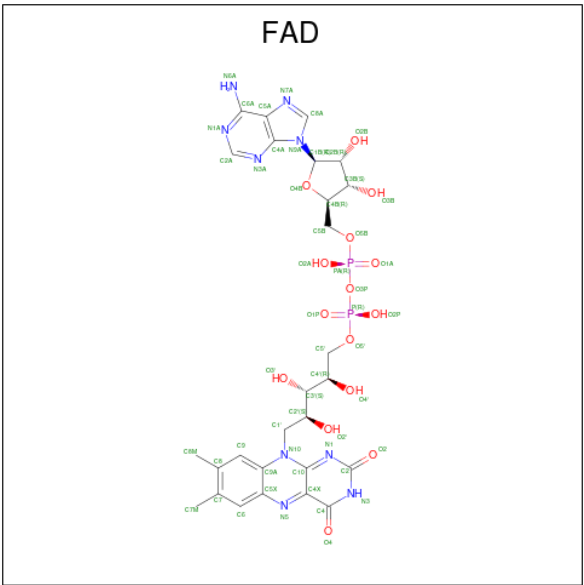
Chain	Residue	Modelled	Actual	Comment	Reference
D	417	MSE	MET	modified residue	UNP Q8J136
D	497	MSE	MET	modified residue	UNP Q8J136
D	518	MSE	MET	modified residue	UNP Q8J136
D	519	MSE	MET	modified residue	UNP Q8J136
D	522	MSE	MET	modified residue	UNP Q8J136
D	525	MSE	MET	modified residue	UNP Q8J136
D	541	MSE	MET	modified residue	UNP Q8J136
D	555	MSE	MET	modified residue	UNP Q8J136
D	599	MSE	MET	modified residue	UNP Q8J136
E	43	MSE	MET	modified residue	UNP Q8J136
E	74	MSE	MET	modified residue	UNP Q8J136
E	112	MSE	MET	modified residue	UNP Q8J136
E	164	MSE	MET	modified residue	UNP Q8J136
E	368	MSE	MET	modified residue	UNP Q8J136
E	380	MSE	MET	modified residue	UNP Q8J136
E	416	MSE	MET	modified residue	UNP Q8J136
E	417	MSE	MET	modified residue	UNP Q8J136
E	497	MSE	MET	modified residue	UNP Q8J136
E	518	MSE	MET	modified residue	UNP Q8J136
E	519	MSE	MET	modified residue	UNP Q8J136
E	522	MSE	MET	modified residue	UNP Q8J136
E	525	MSE	MET	modified residue	UNP Q8J136
E	541	MSE	MET	modified residue	UNP Q8J136
E	555	MSE	MET	modified residue	UNP Q8J136
E	599	MSE	MET	modified residue	UNP Q8J136
F	43	MSE	MET	modified residue	UNP Q8J136
F	74	MSE	MET	modified residue	UNP Q8J136
F	112	MSE	MET	modified residue	UNP Q8J136
F	164	MSE	MET	modified residue	UNP Q8J136
F	368	MSE	MET	modified residue	UNP Q8J136
F	380	MSE	MET	modified residue	UNP Q8J136
F	416	MSE	MET	modified residue	UNP Q8J136
F	417	MSE	MET	modified residue	UNP Q8J136
F	497	MSE	MET	modified residue	UNP Q8J136
F	518	MSE	MET	modified residue	UNP Q8J136
F	519	MSE	MET	modified residue	UNP Q8J136
F	522	MSE	MET	modified residue	UNP Q8J136
F	525	MSE	MET	modified residue	UNP Q8J136
F	541	MSE	MET	modified residue	UNP Q8J136
F	555	MSE	MET	modified residue	UNP Q8J136
F	599	MSE	MET	modified residue	UNP Q8J136
G	43	MSE	MET	modified residue	UNP Q8J136

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Chain	Residue	Modelled	Actual	Comment	Reference
G	74	MSE	MET	modified residue	UNP Q8J136
G	112	MSE	MET	modified residue	UNP Q8J136
G	164	MSE	MET	modified residue	UNP Q8J136
G	368	MSE	MET	modified residue	UNP Q8J136
G	380	MSE	MET	modified residue	UNP Q8J136
G	416	MSE	MET	modified residue	UNP Q8J136
G	417	MSE	MET	modified residue	UNP Q8J136
G	497	MSE	MET	modified residue	UNP Q8J136
G	518	MSE	MET	modified residue	UNP Q8J136
G	519	MSE	MET	modified residue	UNP Q8J136
G	522	MSE	MET	modified residue	UNP Q8J136
G	525	MSE	MET	modified residue	UNP Q8J136
G	541	MSE	MET	modified residue	UNP Q8J136
G	555	MSE	MET	modified residue	UNP Q8J136
G	599	MSE	MET	modified residue	UNP Q8J136
H	43	MSE	MET	modified residue	UNP Q8J136
H	74	MSE	MET	modified residue	UNP Q8J136
H	112	MSE	MET	modified residue	UNP Q8J136
H	164	MSE	MET	modified residue	UNP Q8J136
H	368	MSE	MET	modified residue	UNP Q8J136
H	380	MSE	MET	modified residue	UNP Q8J136
H	416	MSE	MET	modified residue	UNP Q8J136
H	417	MSE	MET	modified residue	UNP Q8J136
H	497	MSE	MET	modified residue	UNP Q8J136
H	518	MSE	MET	modified residue	UNP Q8J136
H	519	MSE	MET	modified residue	UNP Q8J136
H	522	MSE	MET	modified residue	UNP Q8J136
H	525	MSE	MET	modified residue	UNP Q8J136
H	541	MSE	MET	modified residue	UNP Q8J136
H	555	MSE	MET	modified residue	UNP Q8J136
H	599	MSE	MET	modified residue	UNP Q8J136

- 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	290	Total	O	0	0
			290	290		
3	B	221	Total	O	0	0
			221	221		
3	C	274	Total	O	0	0
			274	274		
3	D	172	Total	O	0	0
			172	172		

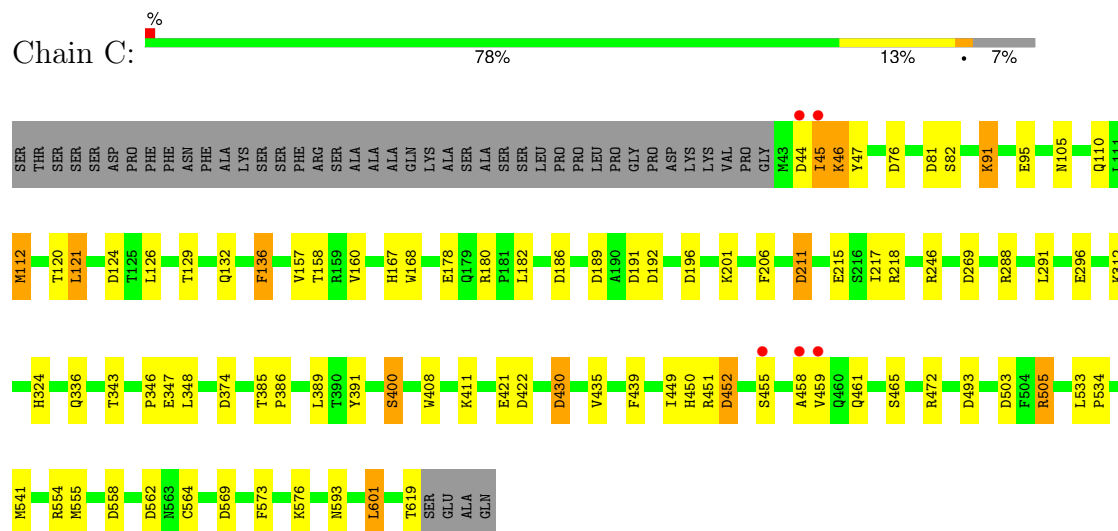
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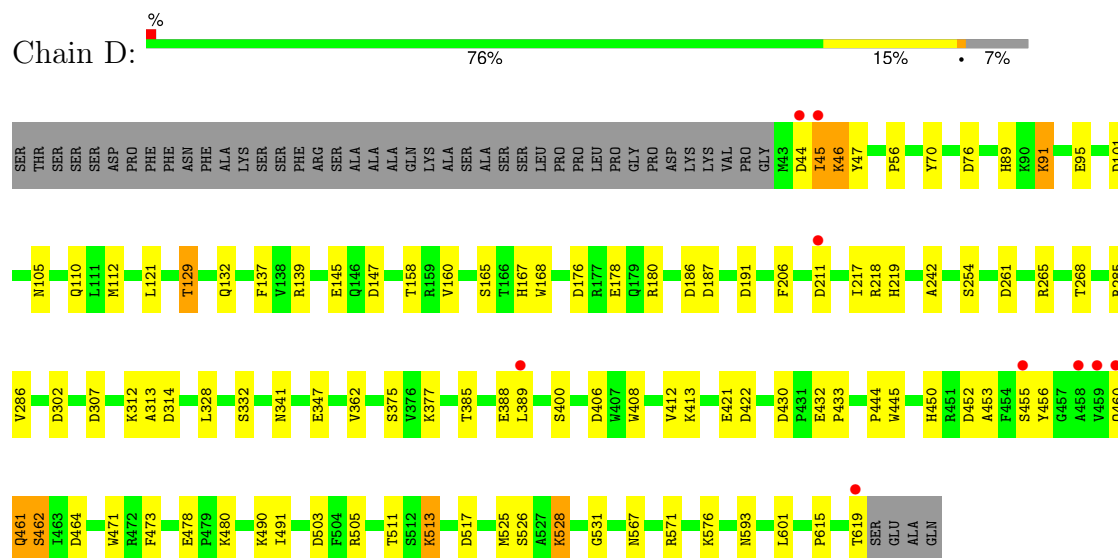
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	303	Total 303	O 303	0	0
3	F	317	Total 317	O 317	0	0
3	G	251	Total 251	O 251	0	0
3	H	326	Total 326	O 326	0	0

GLN

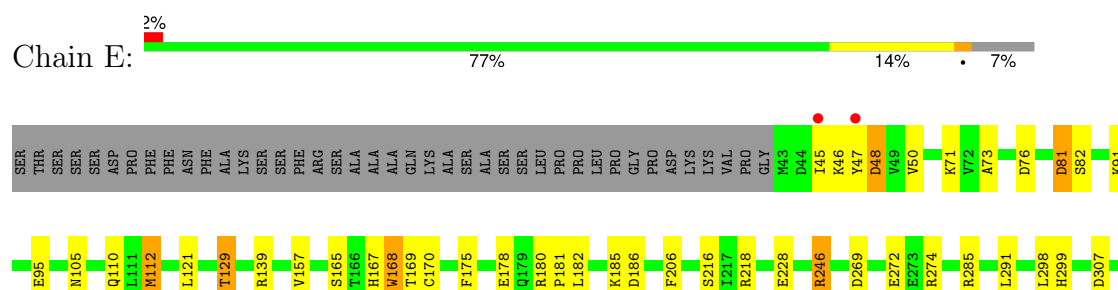
- Molecule 1: pyranose oxidase

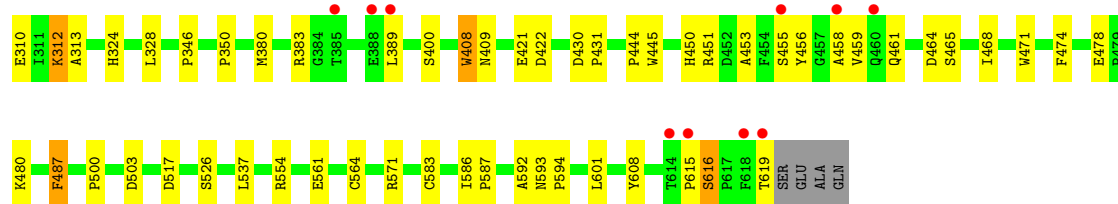


- Molecule 1: pyranose oxidase

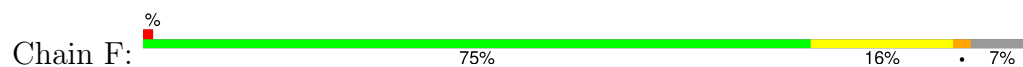


- Molecule 1: pyranose oxidase

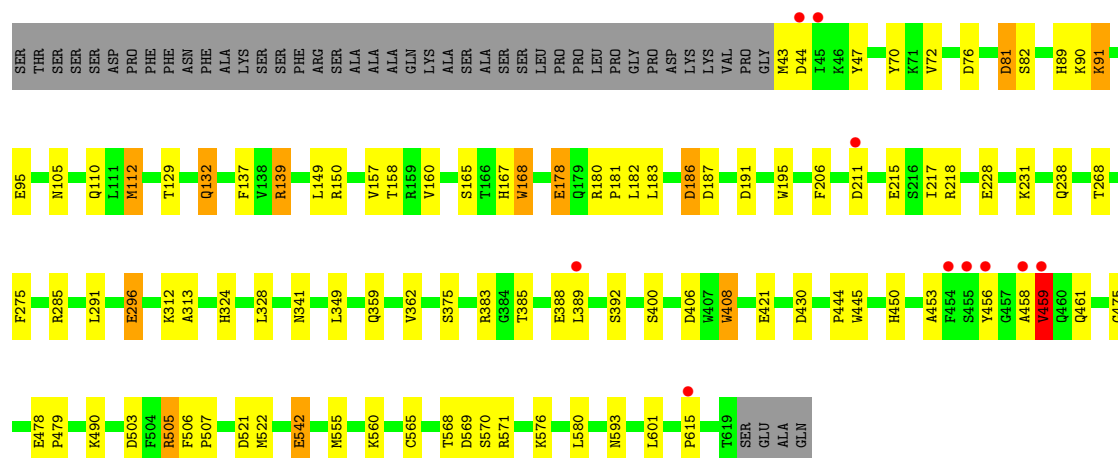
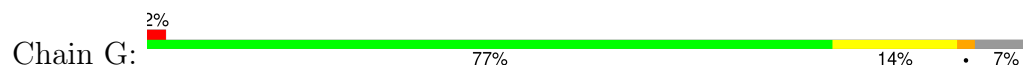




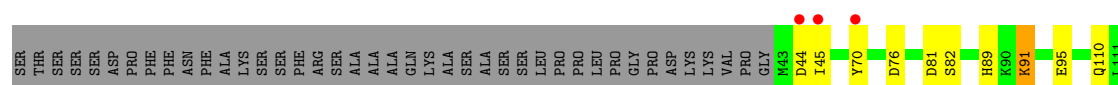
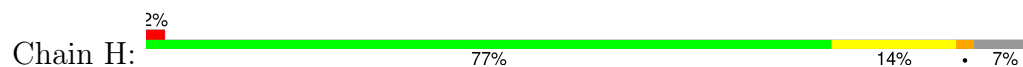
• Molecule 1: pyranose oxidase

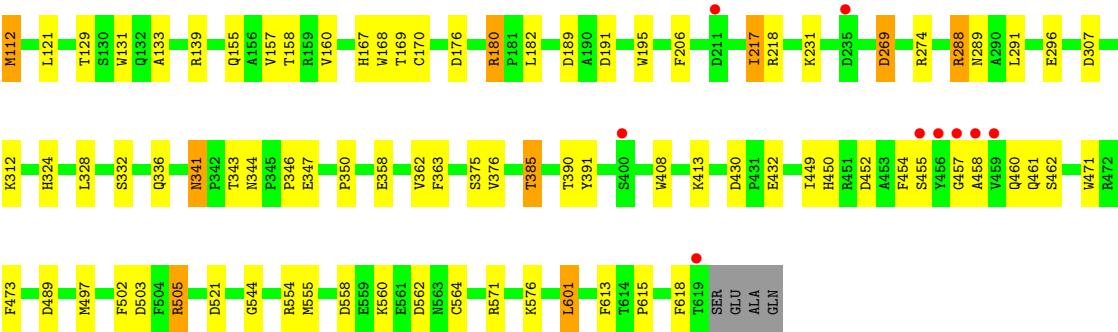


• Molecule 1: pyranose oxidase



• Molecule 1: pyranose oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.88Å 103.60Å 169.17Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	19.70 – 2.35 19.70 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.70-2.35) 99.8 (19.70-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.226 0.196 , 0.231	Depositor DCC
R_{free} test set	9088 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38970	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0477e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/4650	0.85	12/6298 (0.2%)
1	B	1.20	34/4650 (0.7%)	1.01	23/6298 (0.4%)
1	C	0.68	2/4650 (0.0%)	0.83	19/6298 (0.3%)
1	D	0.59	0/4650	0.80	16/6298 (0.3%)
1	E	0.86	7/4650 (0.2%)	0.87	11/6298 (0.2%)
1	F	0.72	1/4650 (0.0%)	0.85	13/6298 (0.2%)
1	G	0.69	0/4650	0.83	11/6298 (0.2%)
1	H	0.73	0/4650	0.86	18/6298 (0.3%)
All	All	0.79	44/37200 (0.1%)	0.86	123/50384 (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	2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	TYR	CG-CD1	15.59	1.59	1.39
1	B	195	TRP	CD2-CE3	13.34	1.60	1.40
1	E	608	TYR	CE2-CZ	13.32	1.55	1.38
1	B	608	TYR	CE2-CZ	12.58	1.54	1.38
1	B	199	TYR	CG-CD1	11.92	1.54	1.39

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ASP	CB-CG-OD2	9.06	126.45	118.30
1	B	575	PHE	CB-CG-CD1	-8.74	114.68	120.80
1	H	503	ASP	CB-CG-OD2	8.53	125.98	118.30
1	C	288	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	H	288	ARG	NE-CZ-NH2	-7.85	116.37	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	PRO	Peptide
1	B	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	4549	0	4395	55	0
1	B	4549	0	4395	111	0
1	C	4549	0	4395	40	0
1	D	4549	0	4395	44	0
1	E	4549	0	4395	51	0
1	F	4549	0	4395	63	0
1	G	4549	0	4395	57	0
1	H	4549	0	4395	44	0
2	A	53	0	30	0	0
2	B	53	0	30	6	0
2	C	53	0	30	0	0
2	D	53	0	30	1	0
2	E	53	0	30	1	0
2	F	53	0	30	0	0
2	G	53	0	30	0	0
2	H	53	0	30	0	0
3	A	290	0	0	16	0
3	B	221	0	0	8	0
3	C	274	0	0	10	0
3	D	172	0	0	9	0
3	E	303	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	317	0	0	12	0
3	G	251	0	0	12	0
3	H	326	0	0	9	0
All	All	38970	0	35400	452	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 6.

The worst 5 of 452 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:B:164:MSE:HB3	1:B:167:HIS:CE1	1.66	1.31
1:B:548:HIS:CE1	1:B:593:ASN:HA	1.87	1.09
1:B:167:HIS:CD2	2:B:625:FAD:C8M	2.41	1.02
1:E:71:LYS:HB2	1:E:274:ARG:NH1	1.74	1.01
1:B:167:HIS:NE2	2:B:625:FAD:HM81	1.74	0.99

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	575/622 (92%)	554 (96%)	21 (4%)	0	100	100
1	B	575/622 (92%)	549 (96%)	25 (4%)	1 (0%)	44	52
1	C	575/622 (92%)	555 (96%)	18 (3%)	2 (0%)	37	43
1	D	575/622 (92%)	551 (96%)	24 (4%)	0	100	100
1	E	575/622 (92%)	554 (96%)	21 (4%)	0	100	100
1	F	575/622 (92%)	556 (97%)	19 (3%)	0	100	100
1	G	575/622 (92%)	557 (97%)	17 (3%)	1 (0%)	44	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	575/622 (92%)	551 (96%)	21 (4%)	3 (0%)	25	28
All	All	4600/4976 (92%)	4427 (96%)	166 (4%)	7 (0%)	44	52

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	231	LYS
1	H	454	PHE
1	B	455	SER
1	C	455	SER
1	G	459	VAL

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	505/525 (96%)	478 (95%)	27 (5%)	19	23
1	B	505/525 (96%)	474 (94%)	31 (6%)	15	17
1	C	505/525 (96%)	475 (94%)	30 (6%)	16	18
1	D	505/525 (96%)	466 (92%)	39 (8%)	10	10
1	E	505/525 (96%)	474 (94%)	31 (6%)	15	17
1	F	505/525 (96%)	470 (93%)	35 (7%)	13	13
1	G	505/525 (96%)	466 (92%)	39 (8%)	10	10
1	H	505/525 (96%)	478 (95%)	27 (5%)	19	23
All	All	4040/4200 (96%)	3781 (94%)	259 (6%)	14	16

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	601	LEU
1	H	168	TRP
1	D	180	ARG
1	D	129	THR

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Mol	Chain	Res	Type
1	H	269	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	440	GLN
1	F	461	GLN
1	E	460	GLN
1	F	324	HIS
1	G	324	HIS

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 oligosaccharides 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	D	625	1	54,58,58	1.28	5 (9%)	71,89,89	1.50	14 (19%)
2	FAD	E	625	1	54,58,58	1.59	6 (11%)	71,89,89	1.63	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	625	1	54,58,58	1.49	7 (12%)	71,89,89	1.45	11 (15%)
2	FAD	A	625	1	54,58,58	1.24	6 (11%)	71,89,89	1.63	13 (18%)
2	FAD	F	625	1	54,58,58	1.17	4 (7%)	71,89,89	1.54	13 (18%)
2	FAD	H	625	1	54,58,58	1.27	8 (14%)	71,89,89	1.36	10 (14%)
2	FAD	B	625	1	54,58,58	2.32	8 (14%)	71,89,89	1.53	15 (21%)
2	FAD	G	625	1	54,58,58	1.51	6 (11%)	71,89,89	1.49	11 (15%)

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	D	625	1	-	2/30/50/50	0/6/6/6
2	FAD	E	625	1	-	6/30/50/50	0/6/6/6
2	FAD	C	625	1	-	2/30/50/50	0/6/6/6
2	FAD	A	625	1	-	4/30/50/50	0/6/6/6
2	FAD	F	625	1	-	4/30/50/50	0/6/6/6
2	FAD	H	625	1	-	2/30/50/50	0/6/6/6
2	FAD	B	625	1	-	4/30/50/50	0/6/6/6
2	FAD	G	625	1	-	1/30/50/50	0/6/6/6

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	FAD	P-O3P	12.91	1.73	1.59
2	G	625	FAD	P-O3P	7.57	1.67	1.59
2	E	625	FAD	P-O3P	7.04	1.67	1.59
2	B	625	FAD	PA-O3P	-6.47	1.52	1.59
2	C	625	FAD	P-O3P	5.16	1.65	1.59

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	625	FAD	N3A-C2A-N1A	-6.28	120.15	128.67
2	A	625	FAD	N3A-C2A-N1A	-5.98	120.56	128.67
2	D	625	FAD	N3A-C2A-N1A	-5.46	121.26	128.67
2	C	625	FAD	N3A-C2A-N1A	-5.43	121.30	128.67
2	E	625	FAD	N3A-C2A-N1A	-5.39	121.36	128.67

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

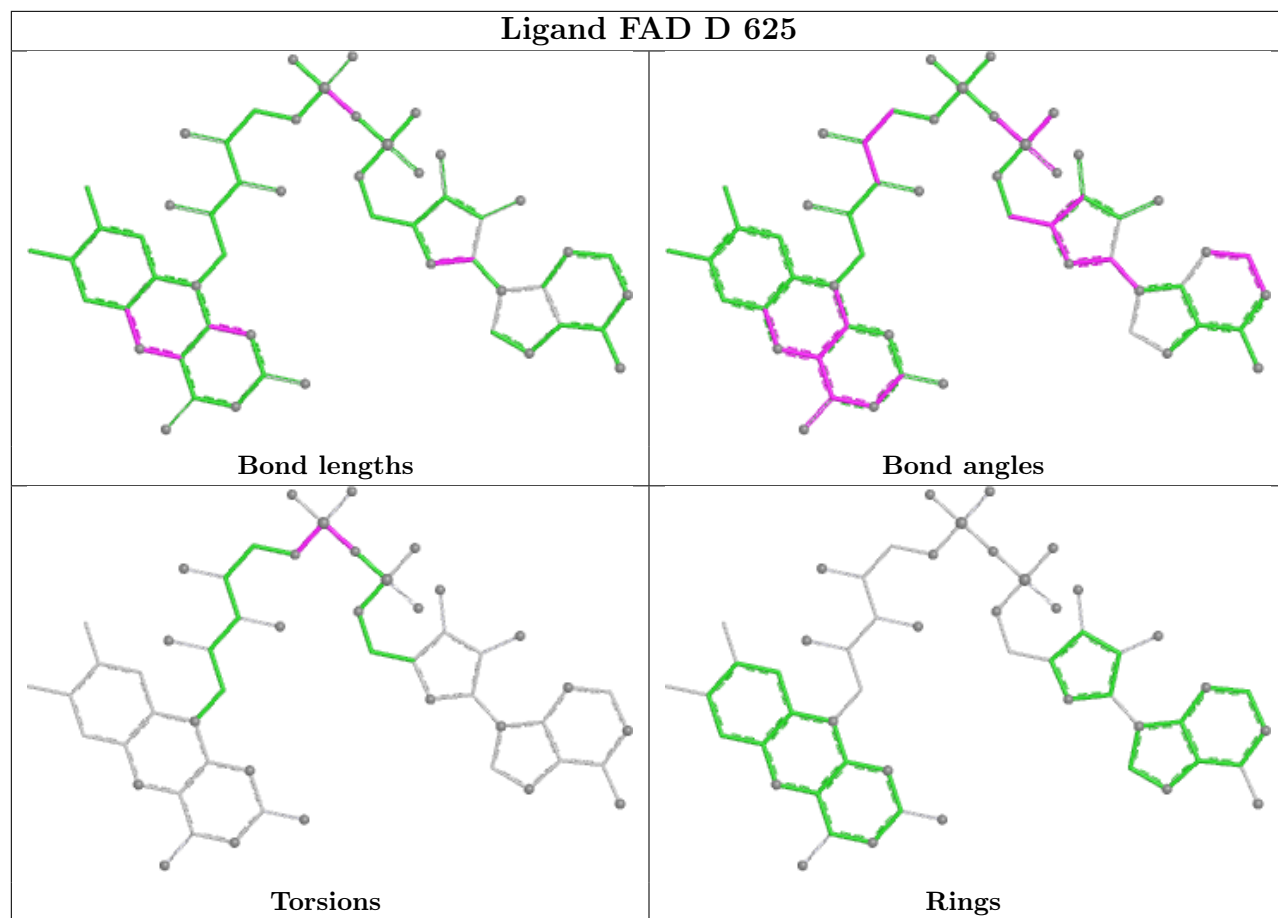
Mol	Chain	Res	Type	Atoms
2	A	625	FAD	C5'-O5'-P-O1P
2	B	625	FAD	C5'-O5'-P-O1P
2	C	625	FAD	C5'-O5'-P-O1P
2	C	625	FAD	C5'-O5'-P-O3P
2	E	625	FAD	C5'-O5'-P-O1P

There are no ring outliers.

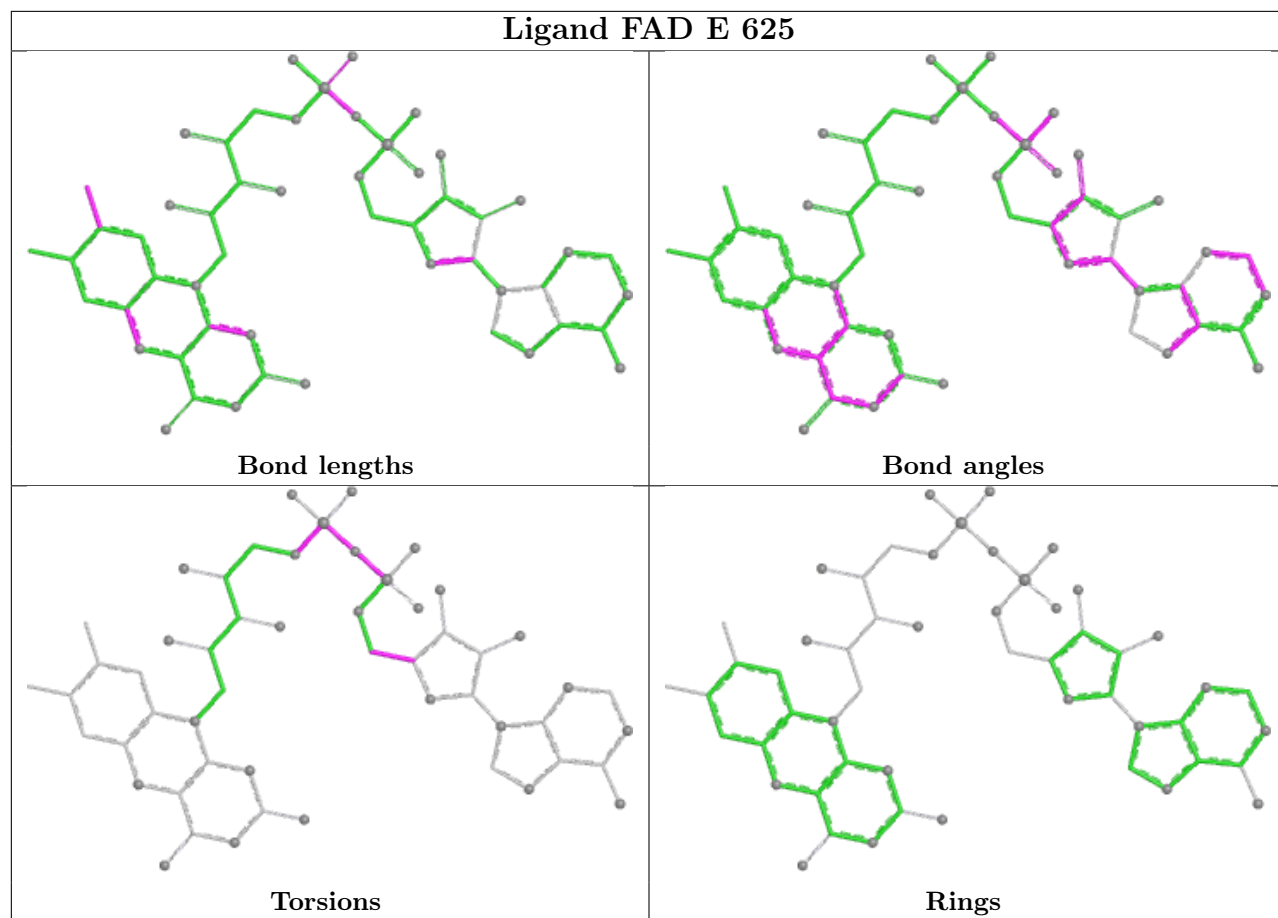
3 monomers are involved in 8 short contacts:

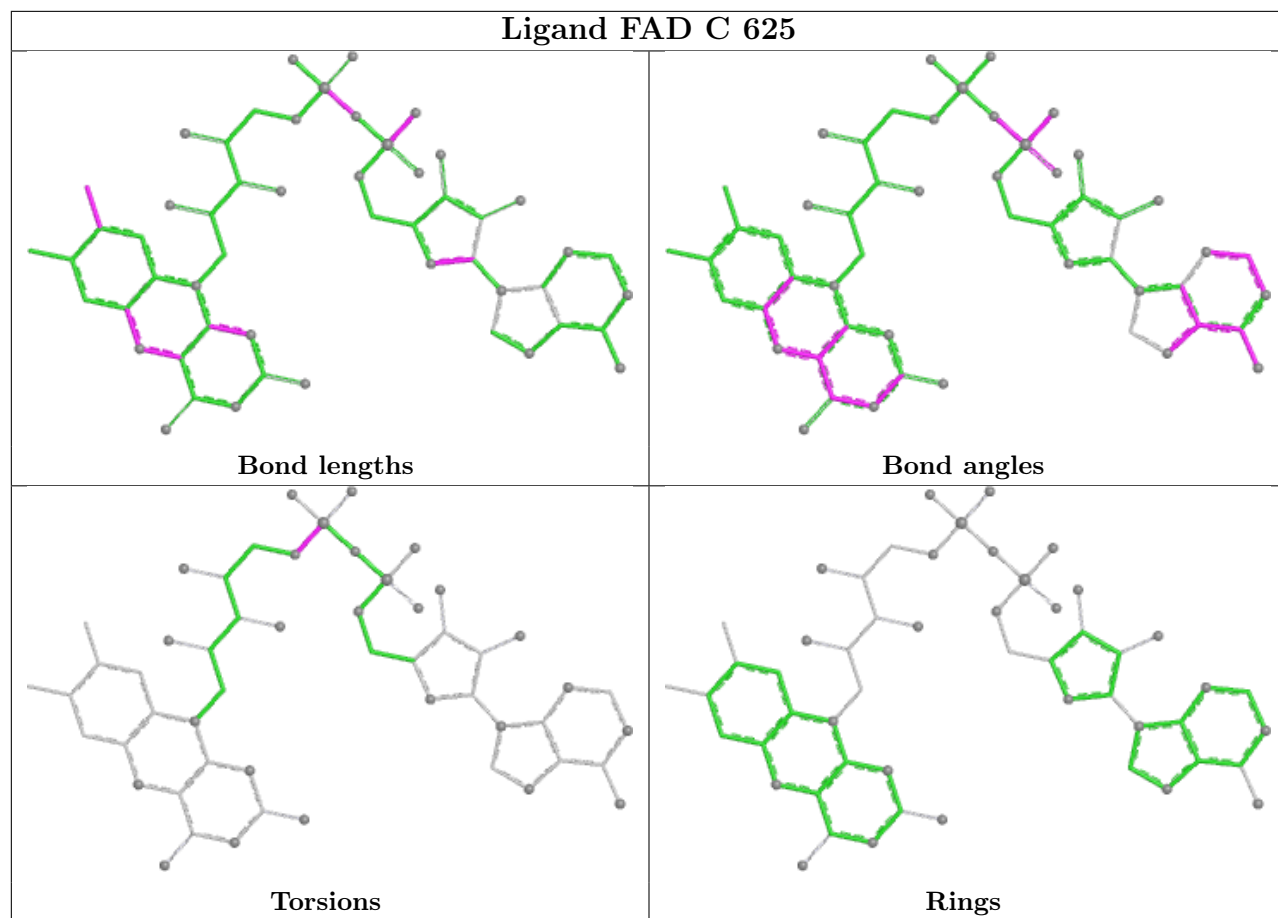
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	625	FAD	1	0
2	E	625	FAD	1	0
2	B	625	FAD	6	0

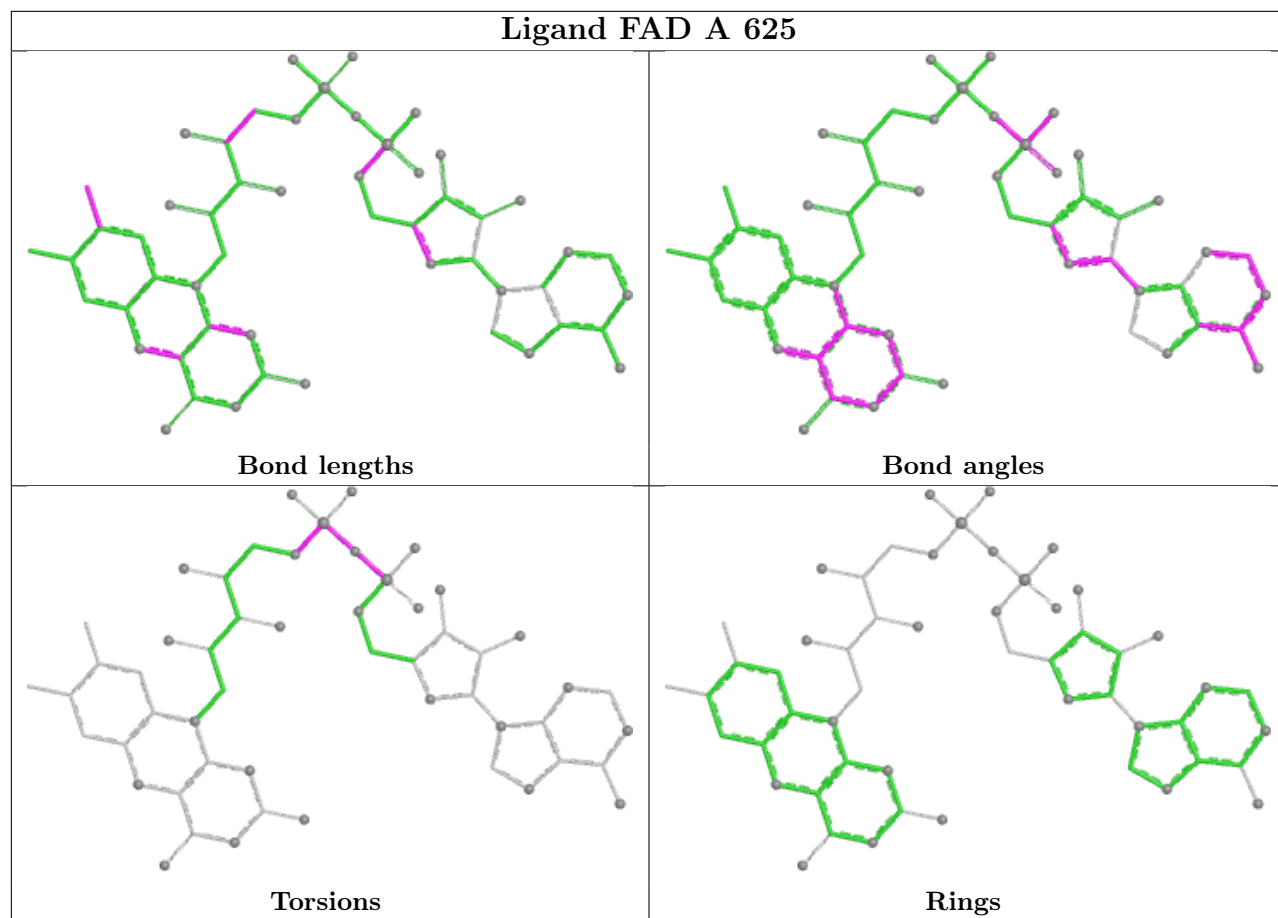
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



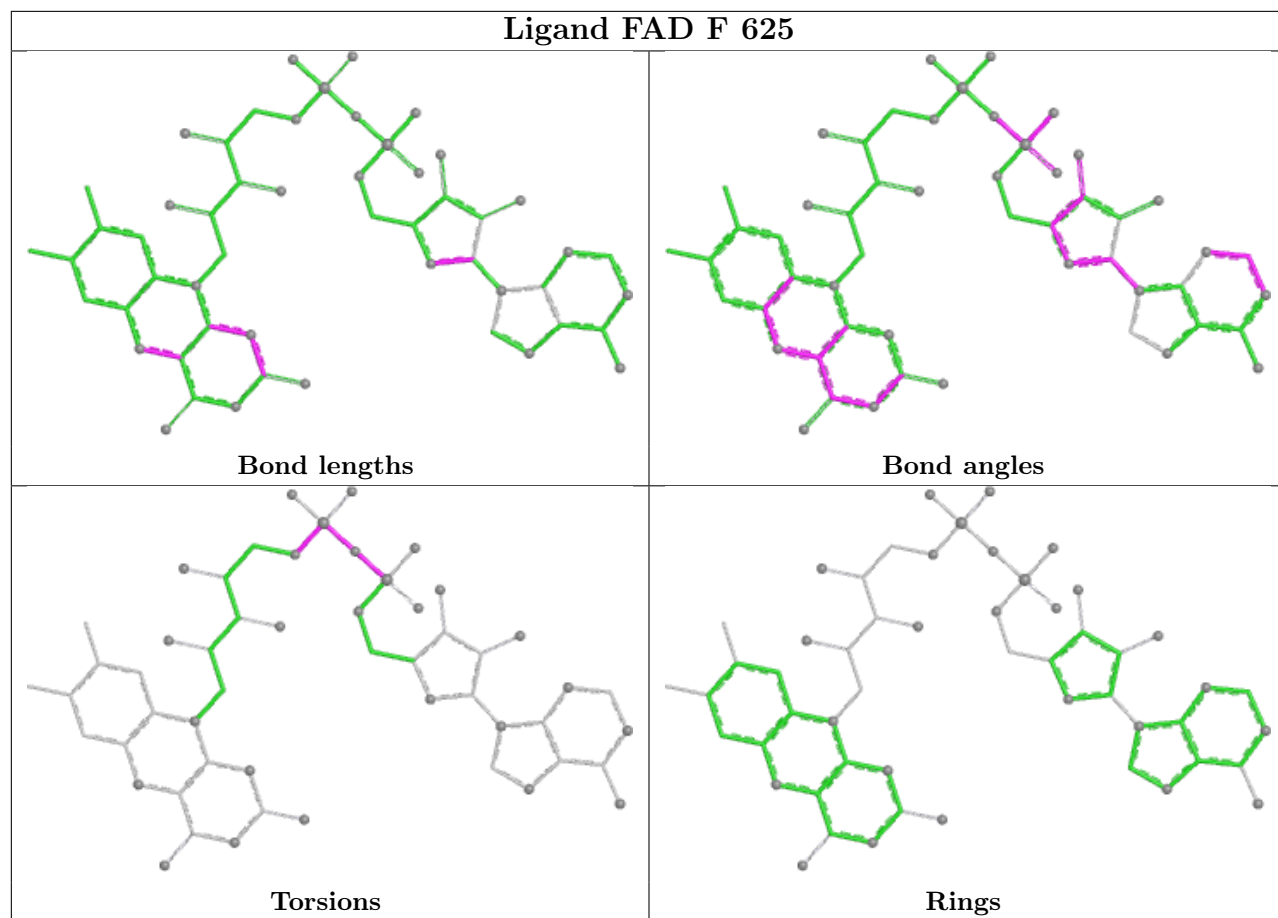
Ligand FAD E 625

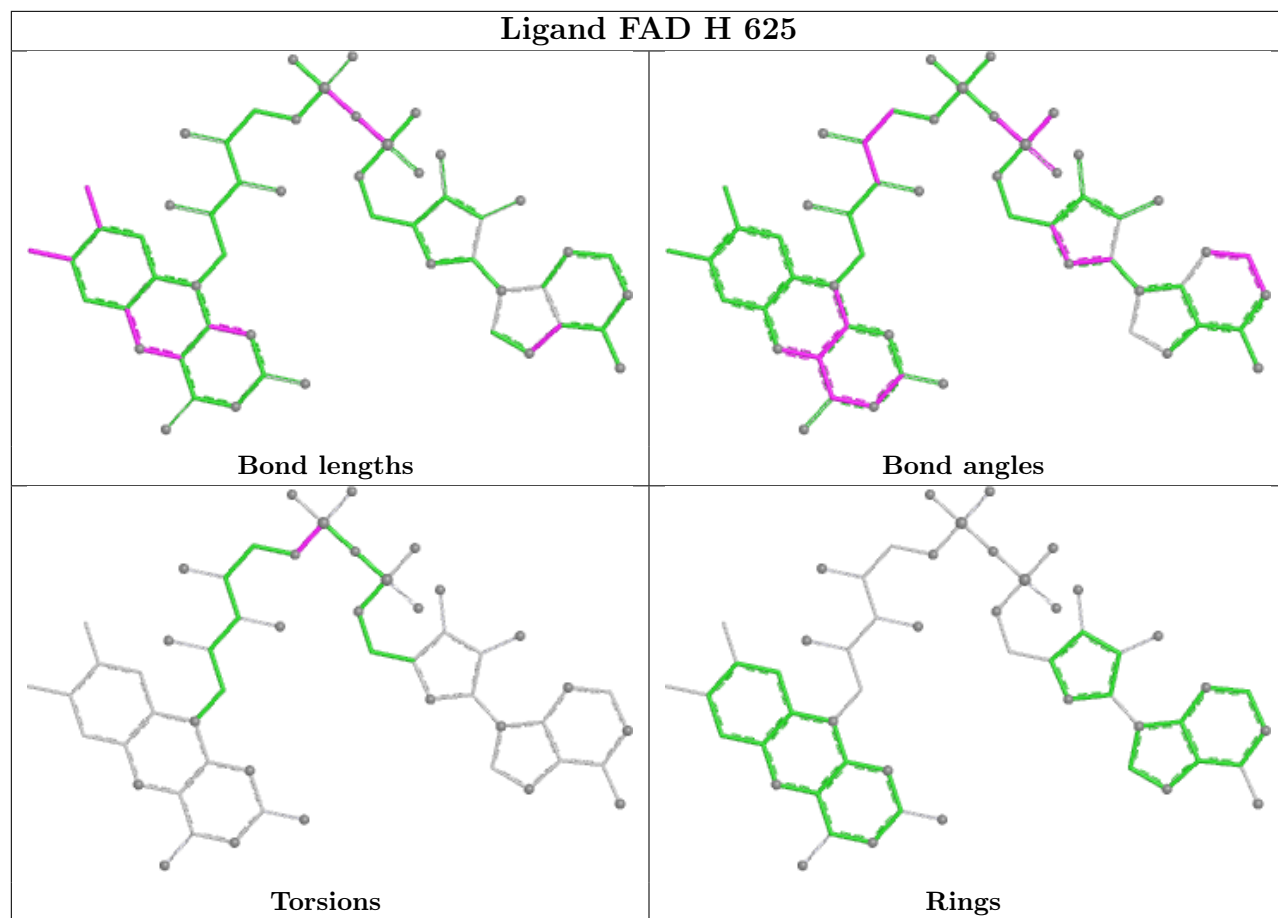


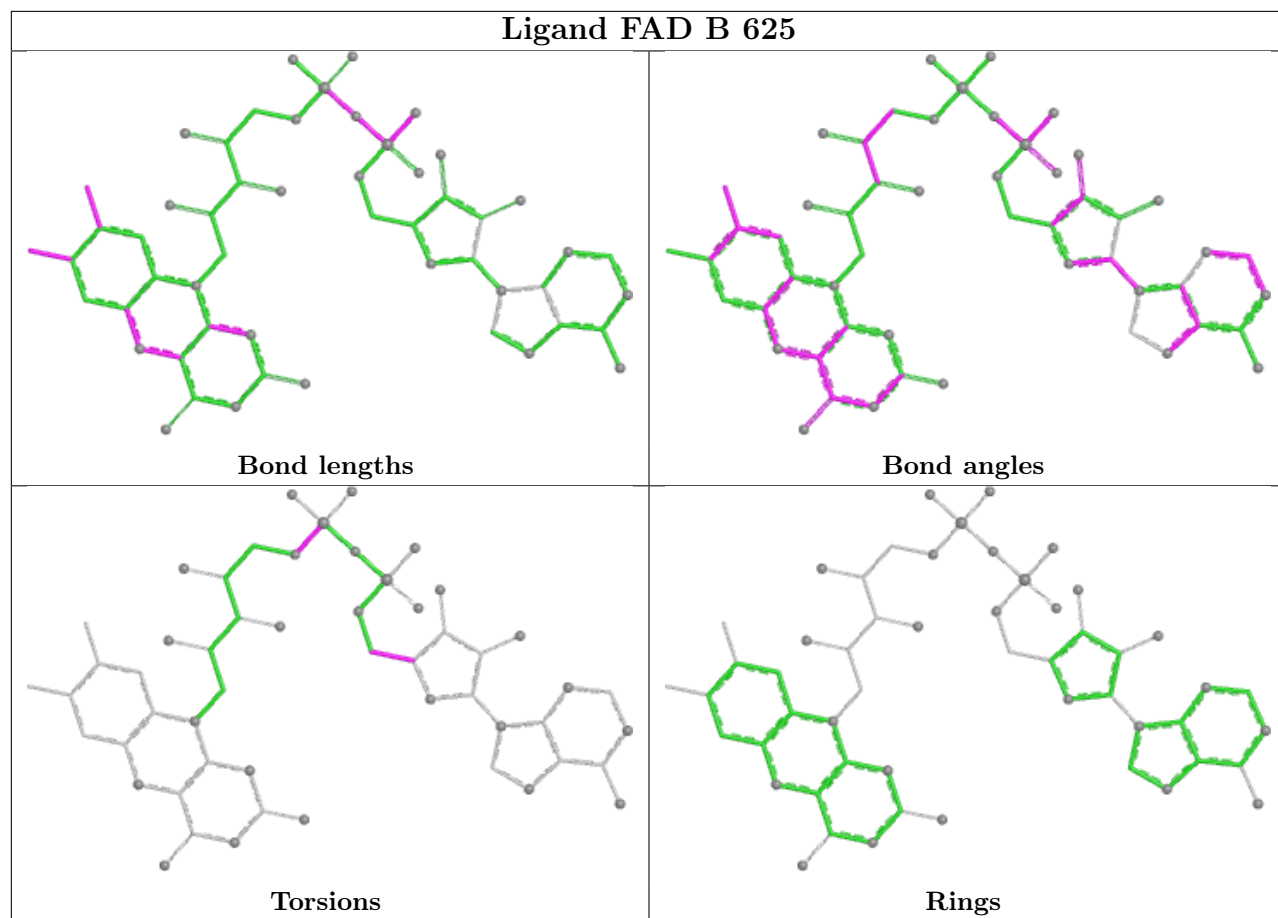


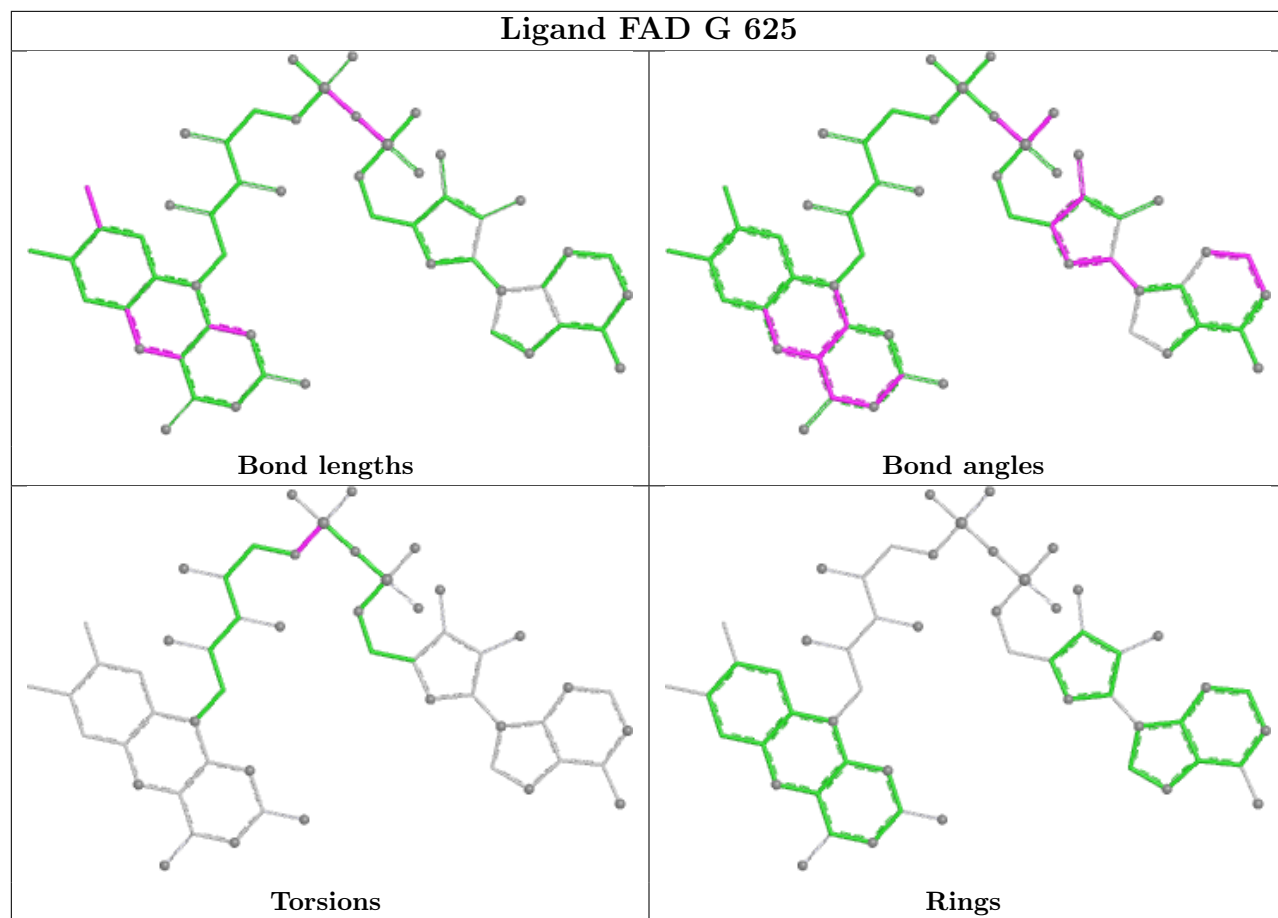


Ligand FAD F 625









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(Å ²)	Q<0.9
1	A	561/622 (90%)	-0.40	8 (1%) 73 77	8, 16, 31, 51	0
1	B	561/622 (90%)	0.19	18 (3%) 50 57	12, 23, 38, 58	0
1	C	561/622 (90%)	-0.37	5 (0%) 81 84	8, 16, 32, 57	0
1	D	561/622 (90%)	-0.16	9 (1%) 70 75	8, 23, 40, 63	0
1	E	561/622 (90%)	-0.28	12 (2%) 63 68	5, 16, 36, 56	0
1	F	561/622 (90%)	-0.43	4 (0%) 84 86	4, 14, 31, 50	0
1	G	561/622 (90%)	-0.25	10 (1%) 67 72	3, 15, 33, 53	0
1	H	561/622 (90%)	-0.41	12 (2%) 63 68	3, 14, 30, 55	0
All	All	4488/4976 (90%)	-0.26	78 (1%) 69 73	3, 17, 36, 63	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	ALA	5.9
1	E	47	TYR	5.9
1	D	455	SER	5.4
1	B	445	TRP	5.3
1	G	44	ASP	5.1

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](#)

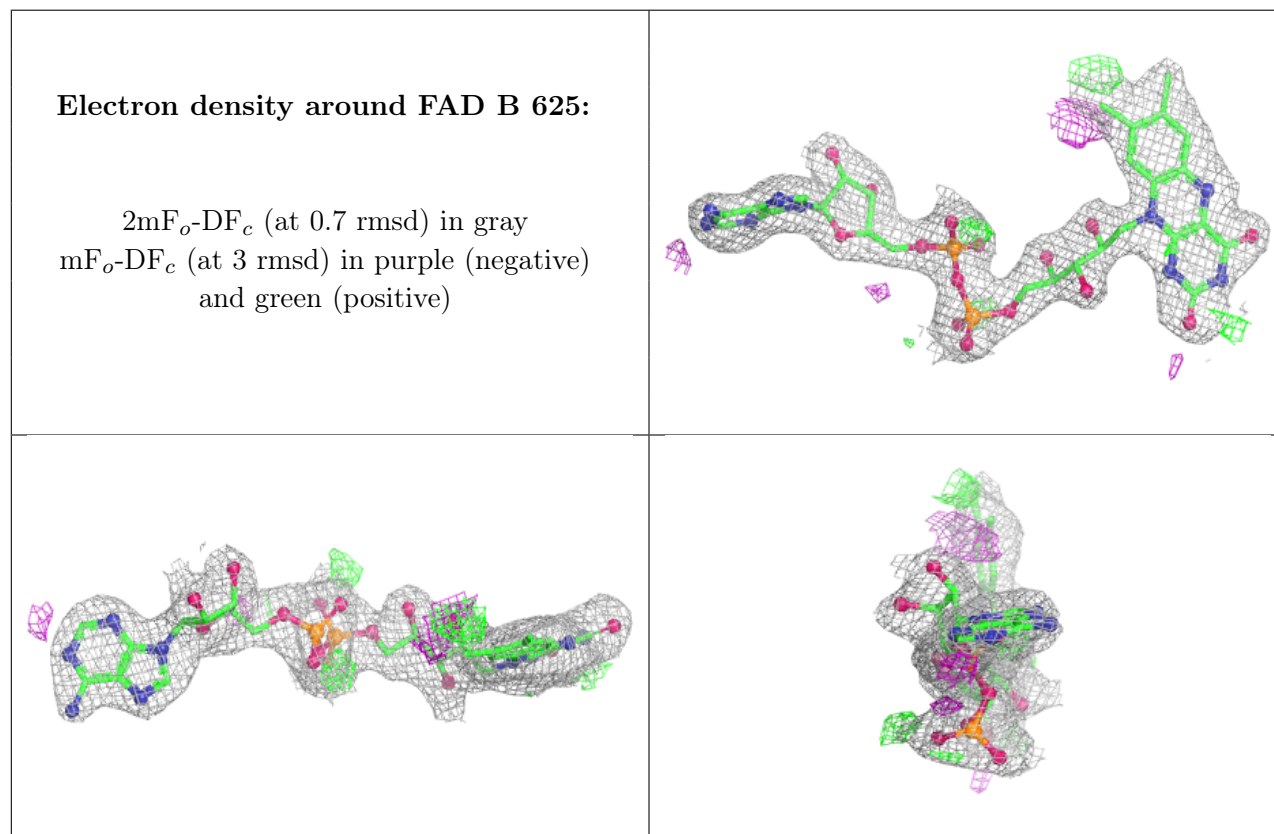
There are no monosaccharides in this entry.

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, 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.

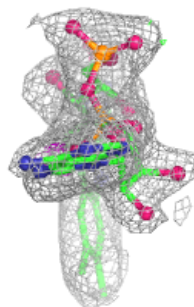
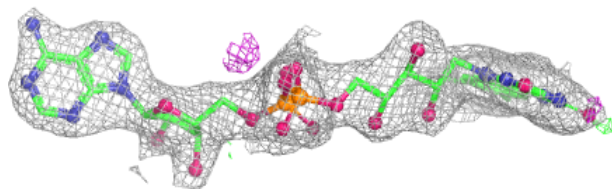
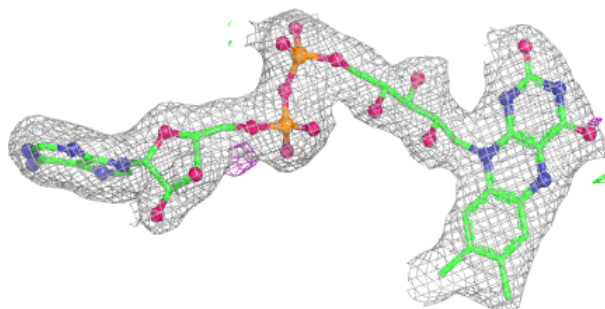
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	625	53/53	0.95	0.07	12,23,28,33	0
2	FAD	D	625	53/53	0.95	0.07	17,21,26,27	0
2	FAD	G	625	53/53	0.96	0.06	10,15,20,22	0
2	FAD	A	625	53/53	0.97	0.06	6,14,17,19	0
2	FAD	E	625	53/53	0.97	0.06	10,16,19,23	0
2	FAD	C	625	53/53	0.97	0.06	8,15,18,20	0
2	FAD	H	625	53/53	0.97	0.05	9,13,16,19	0
2	FAD	F	625	53/53	0.98	0.06	10,13,17,20	0

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

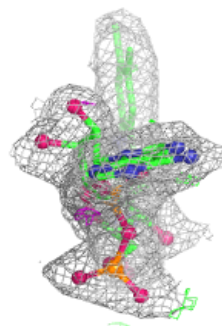
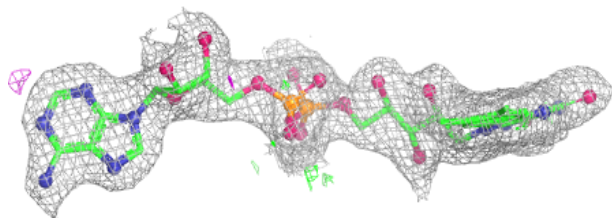
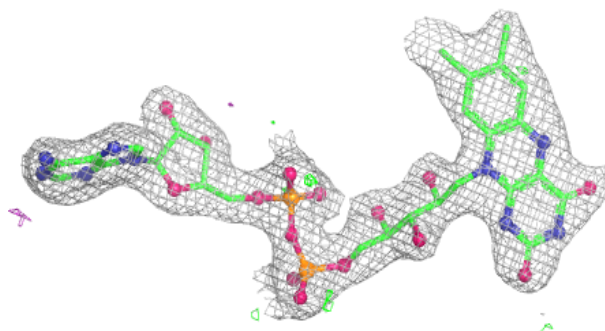


Electron density around FAD D 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

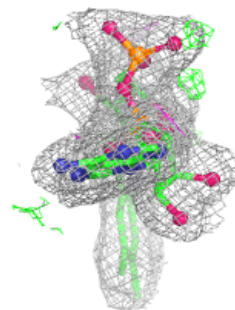
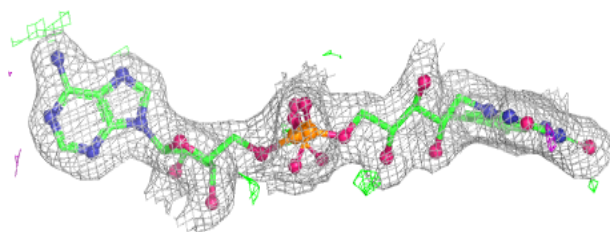
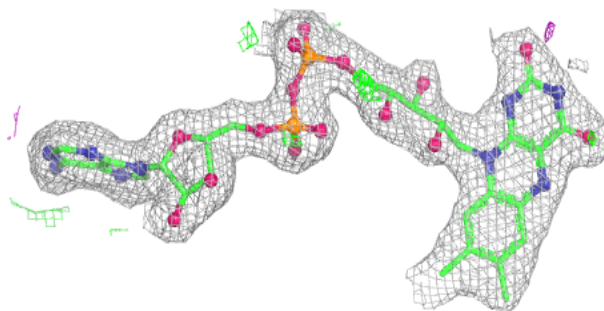
**Electron density around FAD G 625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

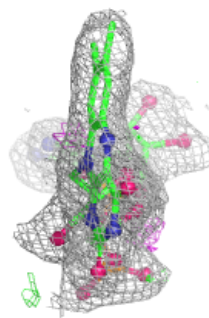
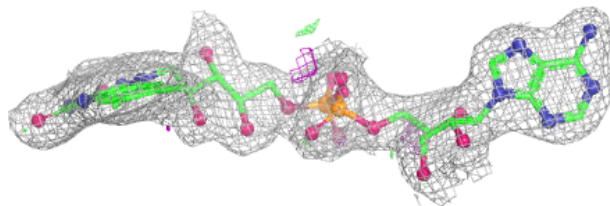
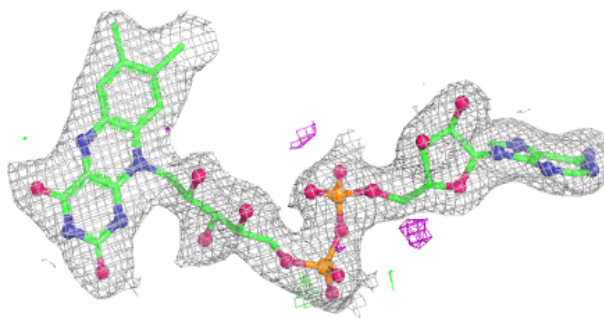


Electron density around FAD A 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

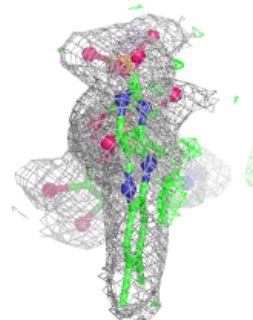
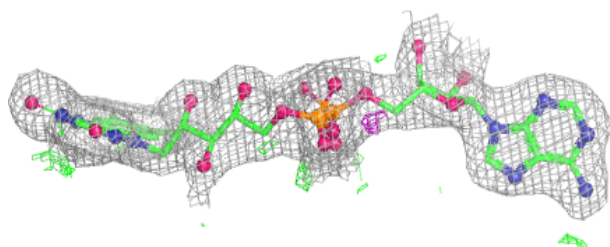
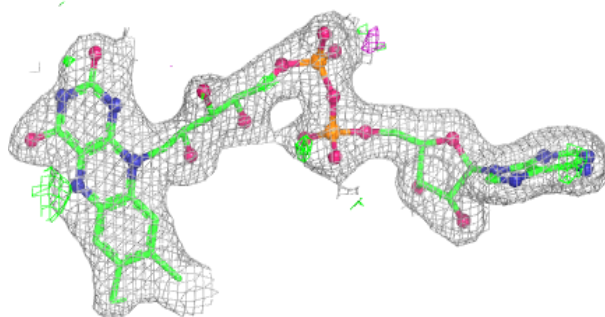
**Electron density around FAD E 625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

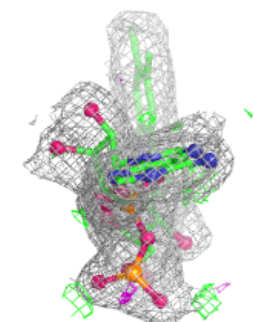
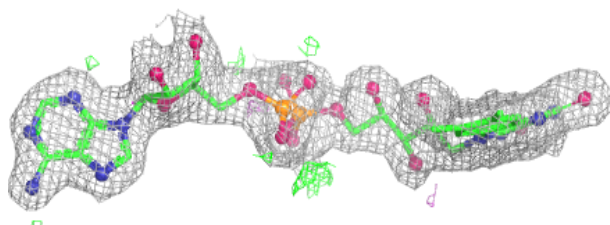
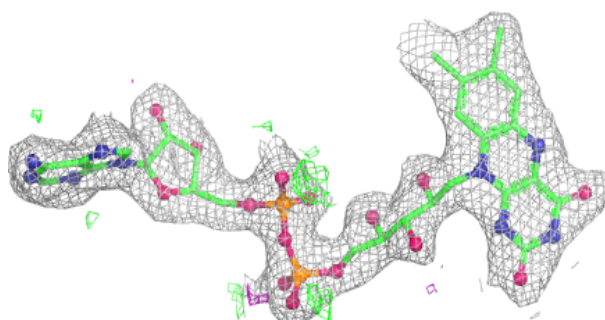


Electron density around FAD C 625:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

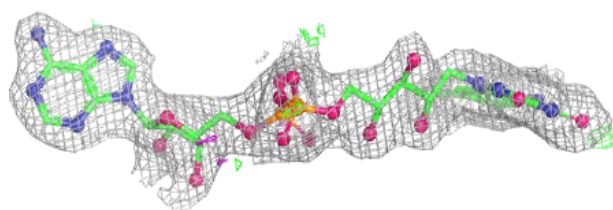
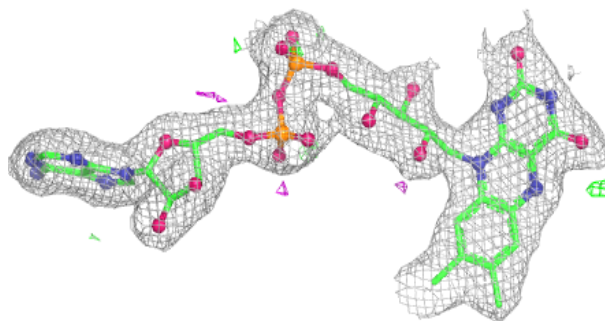
**Electron density around FAD H 625:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD F 625:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.