



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 10:20 AM EDT

PDB ID : 4MIG
Title : Pyranose 2-oxidase from Phanerochaete chrysosporium, recombinant wild type
Authors : Hassan, N.; Tan, T.C.; Spadiut, O.; Pisanelli, I.; Fusco, L.; Haltrich, D.; Peterbauer, C.; Divne, C.
Deposited on : 2013-08-31
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

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

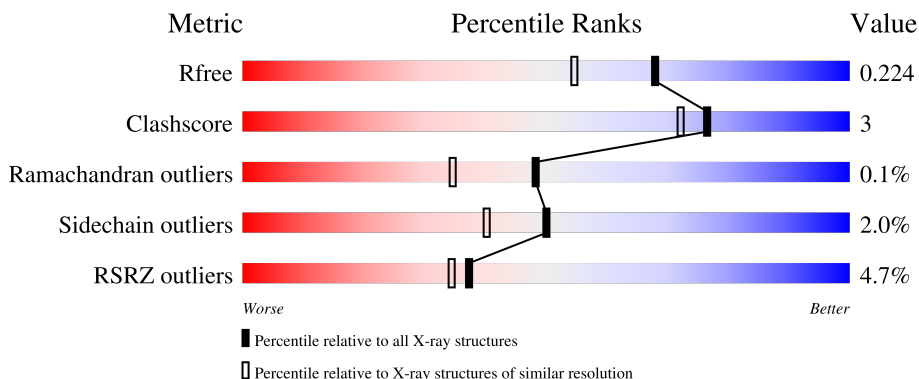
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


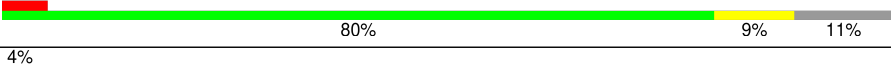
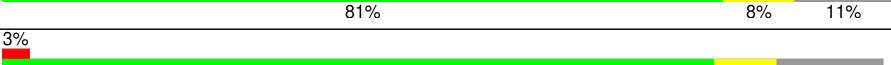

The reported resolution of this entry is 1.80 Å.

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 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	648	
1	B	648	
1	C	648	
1	D	648	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20096 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 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	5	0
			4524	2879	781	838	26			
1	B	574	Total	C	N	O	S	0	3	0
			4543	2889	783	845	26			
1	C	579	Total	C	N	O	S	0	6	0
			4598	2923	796	853	26			
1	D	570	Total	C	N	O	S	0	4	0
			4519	2876	780	837	26			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q6QWR1
A	-12	ALA	-	expression tag	UNP Q6QWR1
A	-11	SER	-	expression tag	UNP Q6QWR1
A	-10	MET	-	expression tag	UNP Q6QWR1
A	-9	THR	-	expression tag	UNP Q6QWR1
A	-8	GLY	-	expression tag	UNP Q6QWR1
A	-7	GLY	-	expression tag	UNP Q6QWR1
A	-6	GLN	-	expression tag	UNP Q6QWR1
A	-5	GLN	-	expression tag	UNP Q6QWR1
A	-4	MET	-	expression tag	UNP Q6QWR1
A	-3	GLY	-	expression tag	UNP Q6QWR1
A	-2	ARG	-	expression tag	UNP Q6QWR1
A	-1	GLY	-	expression tag	UNP Q6QWR1
A	0	SER	-	expression tag	UNP Q6QWR1
A	622	LYS	-	expression tag	UNP Q6QWR1
A	623	LEU	-	expression tag	UNP Q6QWR1
A	624	ALA	-	expression tag	UNP Q6QWR1
A	625	ALA	-	expression tag	UNP Q6QWR1
A	626	ALA	-	expression tag	UNP Q6QWR1
A	627	LEU	-	expression tag	UNP Q6QWR1
A	628	GLU	-	expression tag	UNP Q6QWR1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	629	HIS	-	expression tag	UNP Q6QWR1
A	630	HIS	-	expression tag	UNP Q6QWR1
A	631	HIS	-	expression tag	UNP Q6QWR1
A	632	HIS	-	expression tag	UNP Q6QWR1
A	633	HIS	-	expression tag	UNP Q6QWR1
A	634	HIS	-	expression tag	UNP Q6QWR1
B	-13	MET	-	initiating methionine	UNP Q6QWR1
B	-12	ALA	-	expression tag	UNP Q6QWR1
B	-11	SER	-	expression tag	UNP Q6QWR1
B	-10	MET	-	expression tag	UNP Q6QWR1
B	-9	THR	-	expression tag	UNP Q6QWR1
B	-8	GLY	-	expression tag	UNP Q6QWR1
B	-7	GLY	-	expression tag	UNP Q6QWR1
B	-6	GLN	-	expression tag	UNP Q6QWR1
B	-5	GLN	-	expression tag	UNP Q6QWR1
B	-4	MET	-	expression tag	UNP Q6QWR1
B	-3	GLY	-	expression tag	UNP Q6QWR1
B	-2	ARG	-	expression tag	UNP Q6QWR1
B	-1	GLY	-	expression tag	UNP Q6QWR1
B	0	SER	-	expression tag	UNP Q6QWR1
B	622	LYS	-	expression tag	UNP Q6QWR1
B	623	LEU	-	expression tag	UNP Q6QWR1
B	624	ALA	-	expression tag	UNP Q6QWR1
B	625	ALA	-	expression tag	UNP Q6QWR1
B	626	ALA	-	expression tag	UNP Q6QWR1
B	627	LEU	-	expression tag	UNP Q6QWR1
B	628	GLU	-	expression tag	UNP Q6QWR1
B	629	HIS	-	expression tag	UNP Q6QWR1
B	630	HIS	-	expression tag	UNP Q6QWR1
B	631	HIS	-	expression tag	UNP Q6QWR1
B	632	HIS	-	expression tag	UNP Q6QWR1
B	633	HIS	-	expression tag	UNP Q6QWR1
B	634	HIS	-	expression tag	UNP Q6QWR1
C	-13	MET	-	initiating methionine	UNP Q6QWR1
C	-12	ALA	-	expression tag	UNP Q6QWR1
C	-11	SER	-	expression tag	UNP Q6QWR1
C	-10	MET	-	expression tag	UNP Q6QWR1
C	-9	THR	-	expression tag	UNP Q6QWR1
C	-8	GLY	-	expression tag	UNP Q6QWR1
C	-7	GLY	-	expression tag	UNP Q6QWR1
C	-6	GLN	-	expression tag	UNP Q6QWR1
C	-5	GLN	-	expression tag	UNP Q6QWR1

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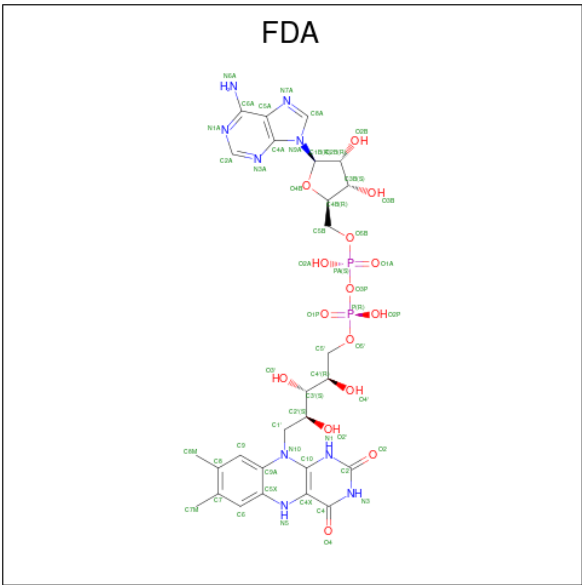
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	expression tag	UNP Q6QWR1
C	-3	GLY	-	expression tag	UNP Q6QWR1
C	-2	ARG	-	expression tag	UNP Q6QWR1
C	-1	GLY	-	expression tag	UNP Q6QWR1
C	0	SER	-	expression tag	UNP Q6QWR1
C	622	LYS	-	expression tag	UNP Q6QWR1
C	623	LEU	-	expression tag	UNP Q6QWR1
C	624	ALA	-	expression tag	UNP Q6QWR1
C	625	ALA	-	expression tag	UNP Q6QWR1
C	626	ALA	-	expression tag	UNP Q6QWR1
C	627	LEU	-	expression tag	UNP Q6QWR1
C	628	GLU	-	expression tag	UNP Q6QWR1
C	629	HIS	-	expression tag	UNP Q6QWR1
C	630	HIS	-	expression tag	UNP Q6QWR1
C	631	HIS	-	expression tag	UNP Q6QWR1
C	632	HIS	-	expression tag	UNP Q6QWR1
C	633	HIS	-	expression tag	UNP Q6QWR1
C	634	HIS	-	expression tag	UNP Q6QWR1
D	-13	MET	-	initiating methionine	UNP Q6QWR1
D	-12	ALA	-	expression tag	UNP Q6QWR1
D	-11	SER	-	expression tag	UNP Q6QWR1
D	-10	MET	-	expression tag	UNP Q6QWR1
D	-9	THR	-	expression tag	UNP Q6QWR1
D	-8	GLY	-	expression tag	UNP Q6QWR1
D	-7	GLY	-	expression tag	UNP Q6QWR1
D	-6	GLN	-	expression tag	UNP Q6QWR1
D	-5	GLN	-	expression tag	UNP Q6QWR1
D	-4	MET	-	expression tag	UNP Q6QWR1
D	-3	GLY	-	expression tag	UNP Q6QWR1
D	-2	ARG	-	expression tag	UNP Q6QWR1
D	-1	GLY	-	expression tag	UNP Q6QWR1
D	0	SER	-	expression tag	UNP Q6QWR1
D	622	LYS	-	expression tag	UNP Q6QWR1
D	623	LEU	-	expression tag	UNP Q6QWR1
D	624	ALA	-	expression tag	UNP Q6QWR1
D	625	ALA	-	expression tag	UNP Q6QWR1
D	626	ALA	-	expression tag	UNP Q6QWR1
D	627	LEU	-	expression tag	UNP Q6QWR1
D	628	GLU	-	expression tag	UNP Q6QWR1
D	629	HIS	-	expression tag	UNP Q6QWR1
D	630	HIS	-	expression tag	UNP Q6QWR1
D	631	HIS	-	expression tag	UNP Q6QWR1

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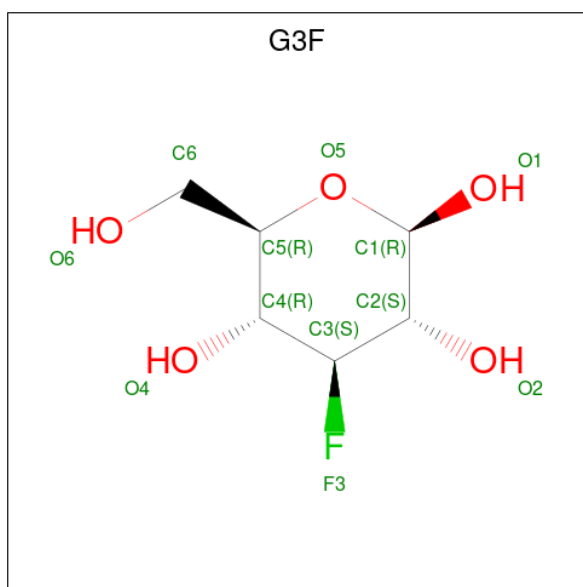
Chain	Residue	Modelled	Actual	Comment	Reference
D	632	HIS	-	expression tag	UNP Q6QWR1
D	633	HIS	-	expression tag	UNP Q6QWR1
D	634	HIS	-	expression tag	UNP Q6QWR1

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



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		

- Molecule 3 is 3-deoxy-3-fluoro-beta-D-glucopyranose (three-letter code: G3F) (formula: C₆H₁₁FO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	D	3	Total	Mn	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	467	Total	O	0	0
			467	467		

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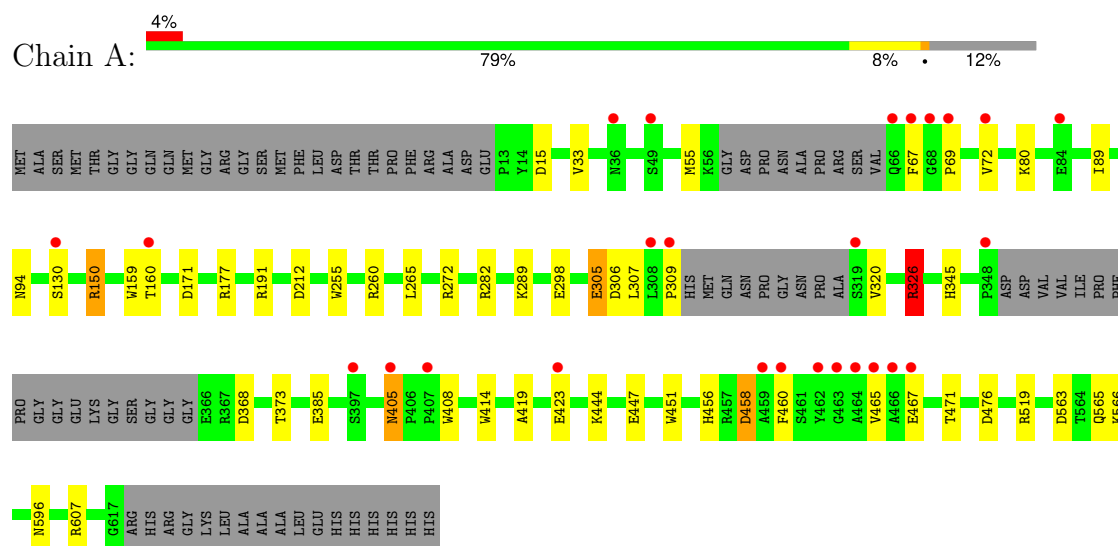
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	380	Total 380	O 380	0	0
5	C	340	Total 340	O 340	0	0
5	D	457	Total 457	O 457	0	0

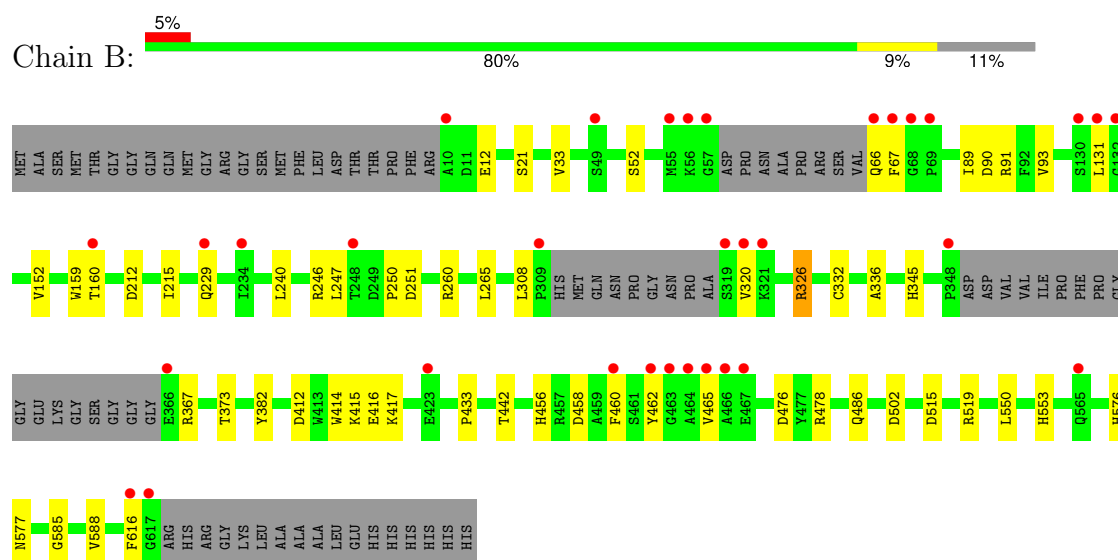
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

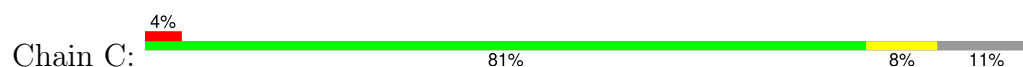
• Molecule 1: Pyranose 2-oxidase

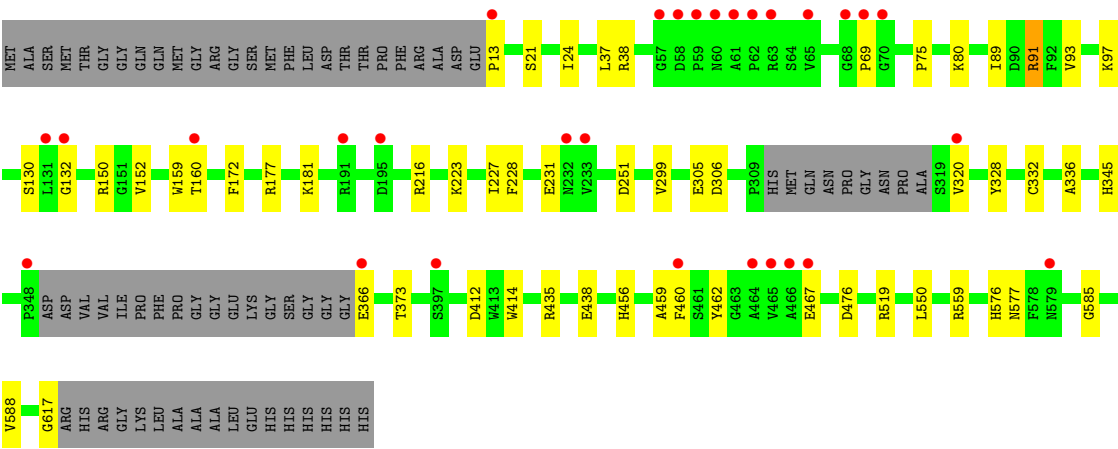


• Molecule 1: Pyranose 2-oxidase

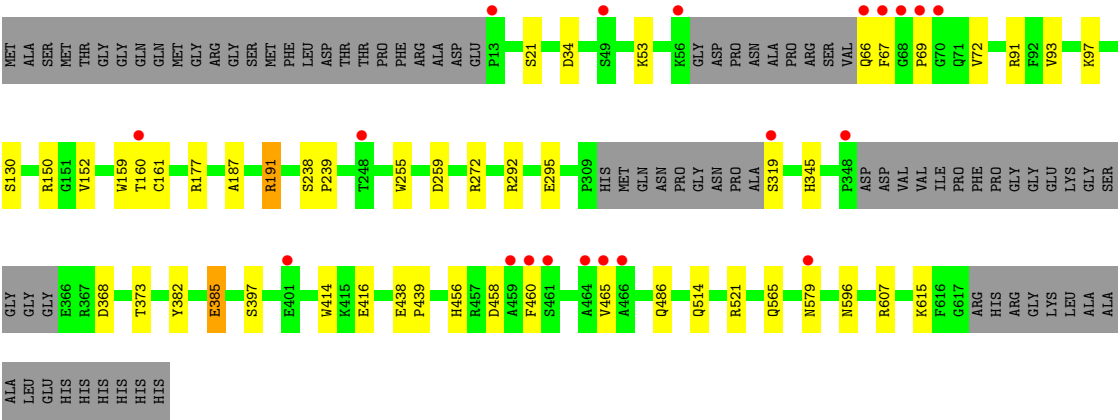
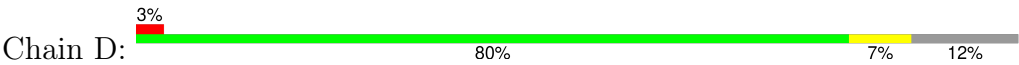


• Molecule 1: Pyranose 2-oxidase





● Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.54Å 166.45Å 91.84Å 90.00° 106.41° 90.00°	Depositor
Resolution (Å)	44.05 – 1.80 44.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.05-1.80) 99.0 (44.05-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.173 , 0.214 0.183 , 0.224	Depositor DCC
R_{free} test set	1514 reflections (0.64%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.107 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20096	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, G3F, FDA

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	1.08	4/4661 (0.1%)	1.02	18/6342 (0.3%)
1	B	1.00	1/4674 (0.0%)	0.98	10/6360 (0.2%)
1	C	0.99	2/4741 (0.0%)	0.96	10/6453 (0.2%)
1	D	1.09	3/4653 (0.1%)	1.01	10/6331 (0.2%)
All	All	1.04	10/18729 (0.1%)	0.99	48/25486 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	385	GLU	CD-OE2	-9.93	1.14	1.25
1	A	255	TRP	NE1-CE2	-5.80	1.30	1.37
1	C	412	ASP	CB-CG	5.52	1.63	1.51
1	A	385	GLU	CD-OE2	5.51	1.31	1.25
1	D	255	TRP	CD2-CE2	5.34	1.47	1.41

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	D	191	ARG	NE-CZ-NH1	8.05	124.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	C	91	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	A	368	ASP	CB-CG-OD1	7.80	125.32	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ARG	Sidechain
1	A	69	PRO	Peptide
1	C	132	GLY	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	4524	0	4424	27	0
1	B	4543	0	4430	26	0
1	C	4598	0	4496	24	0
1	D	4519	0	4418	19	0
2	A	53	0	32	2	0
2	B	53	0	29	1	0
2	C	53	0	30	3	0
2	D	53	0	31	3	0
3	A	12	0	11	1	0
3	B	12	0	11	3	0
3	C	12	0	11	1	0
3	D	12	0	11	3	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
5	A	467	0	0	8	0
5	B	380	0	0	7	0
5	C	340	0	0	5	0
5	D	457	0	0	7	0
All	All	20096	0	17934	100	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 3.

The worst 5 of 100 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:A:160[B]:THR:HG22	5:A:1007:HOH:O	1.57	1.03
1:B:160[B]:THR:HG22	5:B:1257:HOH:O	1.59	1.01
1:D:160[B]:THR:HG22	5:D:1044:HOH:O	1.74	0.87
1:A:15:ASP:HA	1:A:326:ARG:HG3	1.64	0.76
1:A:419:ALA:O	1:A:423:GLU:HG2	1.84	0.76

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	567/648 (88%)	553 (98%)	14 (2%)	0	100	100
1	B	569/648 (88%)	556 (98%)	12 (2%)	1 (0%)	44	31
1	C	579/648 (89%)	565 (98%)	14 (2%)	0	100	100
1	D	566/648 (87%)	553 (98%)	11 (2%)	2 (0%)	30	19
All	All	2281/2592 (88%)	2227 (98%)	51 (2%)	3 (0%)	48	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	465	VAL
1	D	69	PRO
1	D	67	PHE

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	495/548 (90%)	485 (98%)	10 (2%)	50	40
1	B	495/548 (90%)	483 (98%)	12 (2%)	44	32
1	C	503/548 (92%)	495 (98%)	8 (2%)	58	50
1	D	494/548 (90%)	483 (98%)	11 (2%)	47	36
All	All	1987/2192 (91%)	1946 (98%)	41 (2%)	50	38

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	460	PHE
1	D	397[B]	SER
1	C	467	GLU
1	D	272	ARG
1	D	456	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	B	66	GLN
1	B	405	ASN
1	D	427	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	G3F	A	802	-	12,12,12	1.21	2 (16%)	17,17,17	2.69	4 (23%)
3	G3F	C	802	-	12,12,12	1.28	1 (8%)	17,17,17	3.03	8 (47%)
2	FDA	B	801	1	53,58,58	1.61	11 (20%)	64,89,89	1.99	13 (20%)
2	FDA	D	801	1	53,58,58	1.60	11 (20%)	64,89,89	1.84	9 (14%)
2	FDA	A	801	1	53,58,58	1.86	13 (24%)	64,89,89	2.22	17 (26%)
2	FDA	C	801	1	53,58,58	1.74	13 (24%)	64,89,89	2.07	18 (28%)
3	G3F	D	802	-	12,12,12	1.04	0	17,17,17	2.48	8 (47%)
3	G3F	B	802	-	12,12,12	1.22	1 (8%)	17,17,17	2.19	4 (23%)

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	G3F	A	802	-	-	0/2/22/22	0/1/1/1
3	G3F	C	802	-	-	0/2/22/22	0/1/1/1
2	FDA	B	801	1	-	1/30/50/50	0/6/6/6
2	FDA	D	801	1	-	1/30/50/50	0/6/6/6
2	FDA	A	801	1	-	2/30/50/50	0/6/6/6
2	FDA	C	801	1	-	1/30/50/50	0/6/6/6
3	G3F	D	802	-	-	0/2/22/22	0/1/1/1
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FDA	C2A-N3A	5.36	1.40	1.32
2	A	801	FDA	C9-C8	5.04	1.46	1.39
2	D	801	FDA	C5X-N5	-4.97	1.31	1.39
2	A	801	FDA	C6-C5X	4.90	1.47	1.39
2	B	801	FDA	C6-C5X	4.54	1.46	1.39

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	N3A-C2A-N1A	-9.01	116.44	128.67
3	A	802	G3F	F3-C3-C2	8.32	116.01	108.81
2	B	801	FDA	N3A-C2A-N1A	-8.28	117.43	128.67
2	A	801	FDA	O4B-C1B-N9A	7.95	119.29	108.75
2	C	801	FDA	N3A-C2A-N1A	-7.46	118.54	128.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FDA	PA-O3P-P-O5'
2	C	801	FDA	PA-O3P-P-O5'
2	D	801	FDA	PA-O3P-P-O5'
2	B	801	FDA	O4B-C4B-C5B-O5B
2	A	801	FDA	P-O3P-PA-O2A

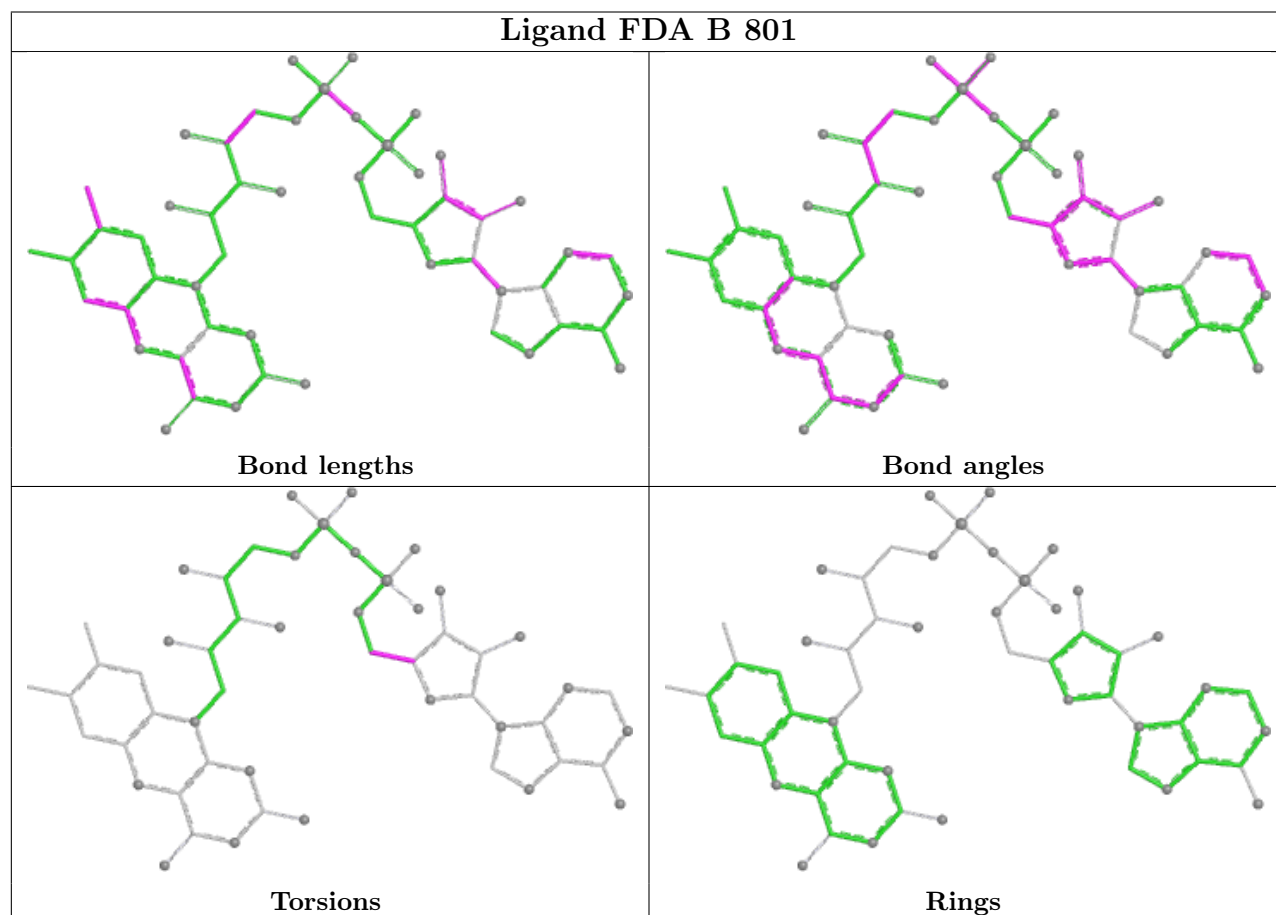
There are no ring outliers.

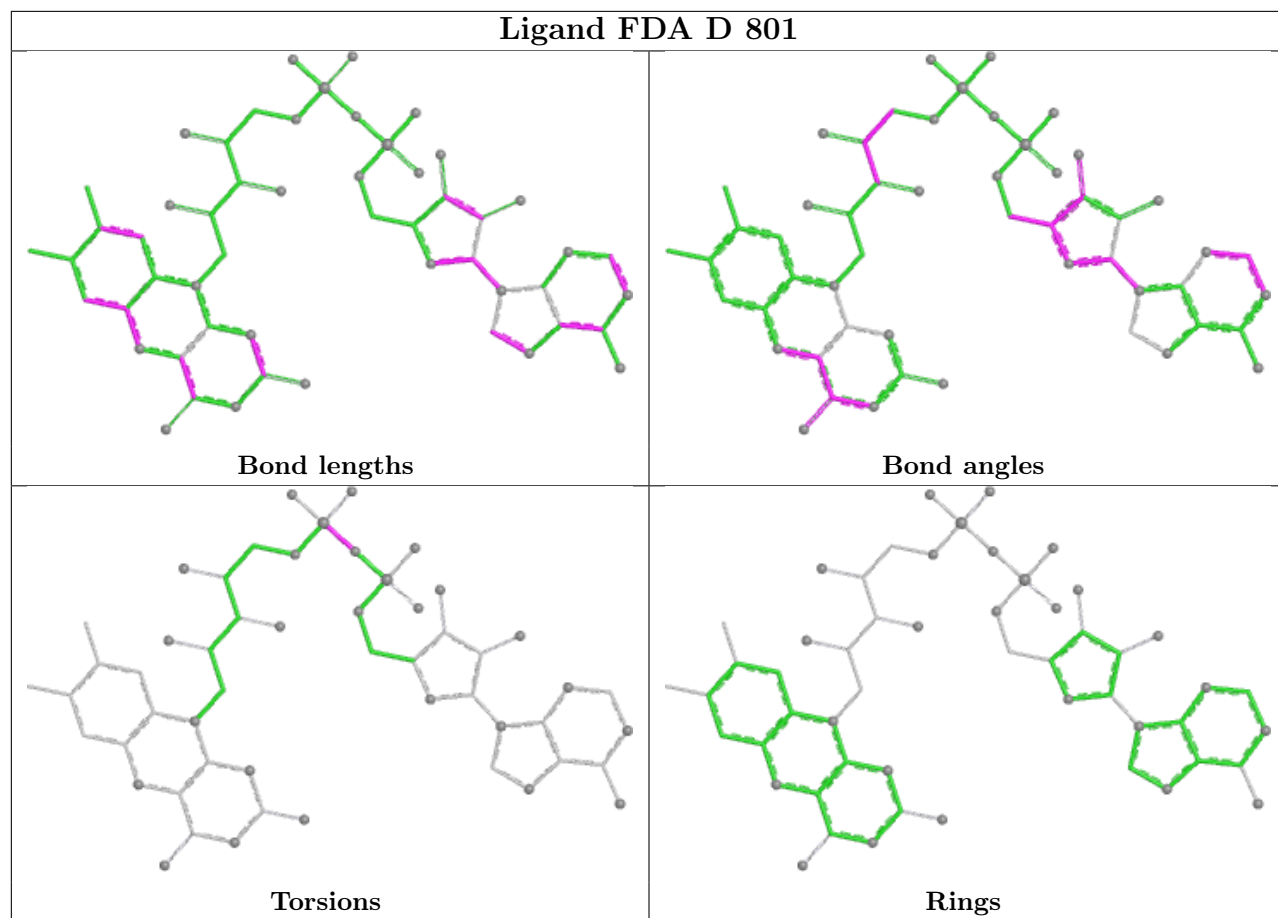
8 monomers are involved in 12 short contacts:

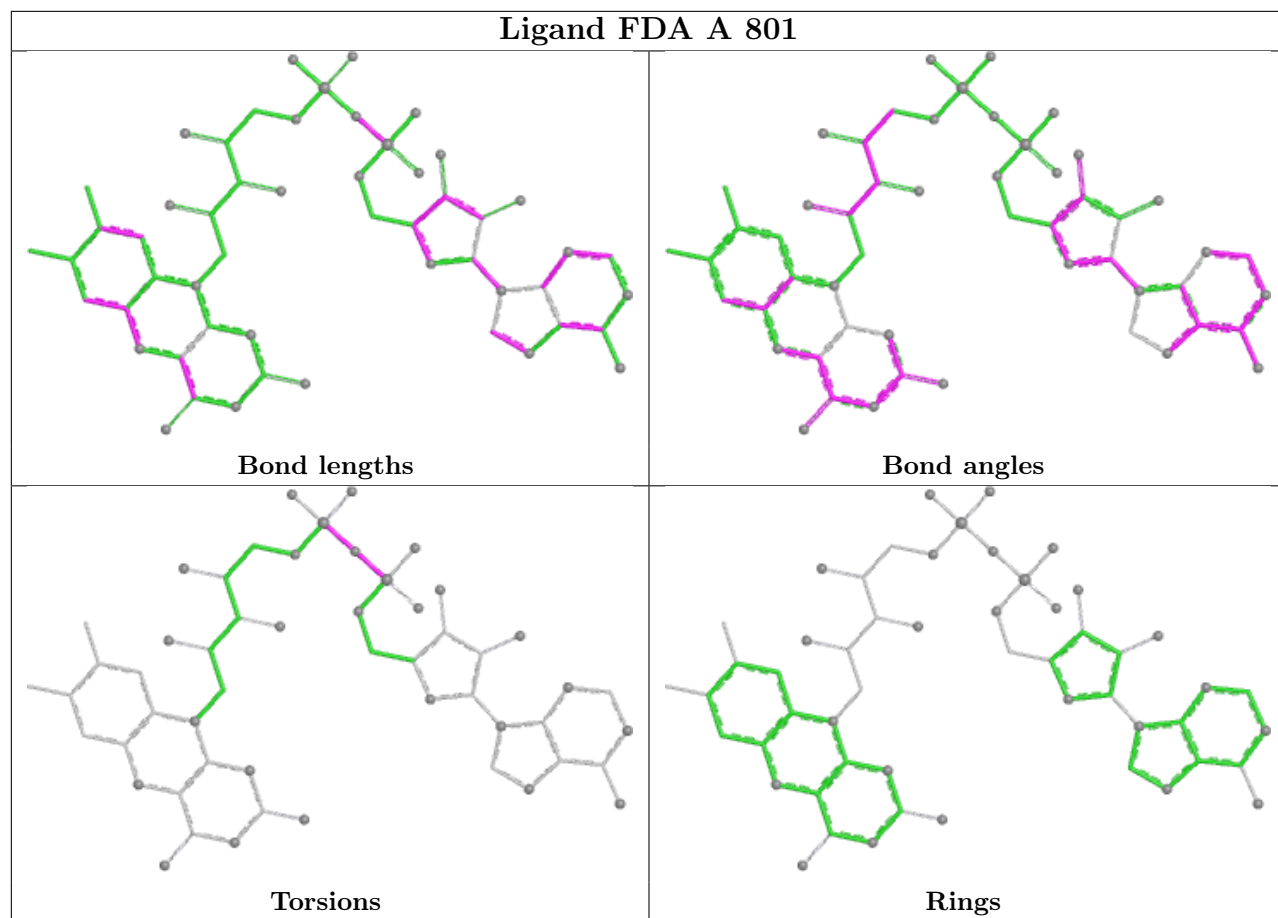
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G3F	1	0
3	C	802	G3F	1	0
2	B	801	FDA	1	0
2	D	801	FDA	3	0
2	A	801	FDA	2	0
2	C	801	FDA	3	0
3	D	802	G3F	3	0
3	B	802	G3F	3	0

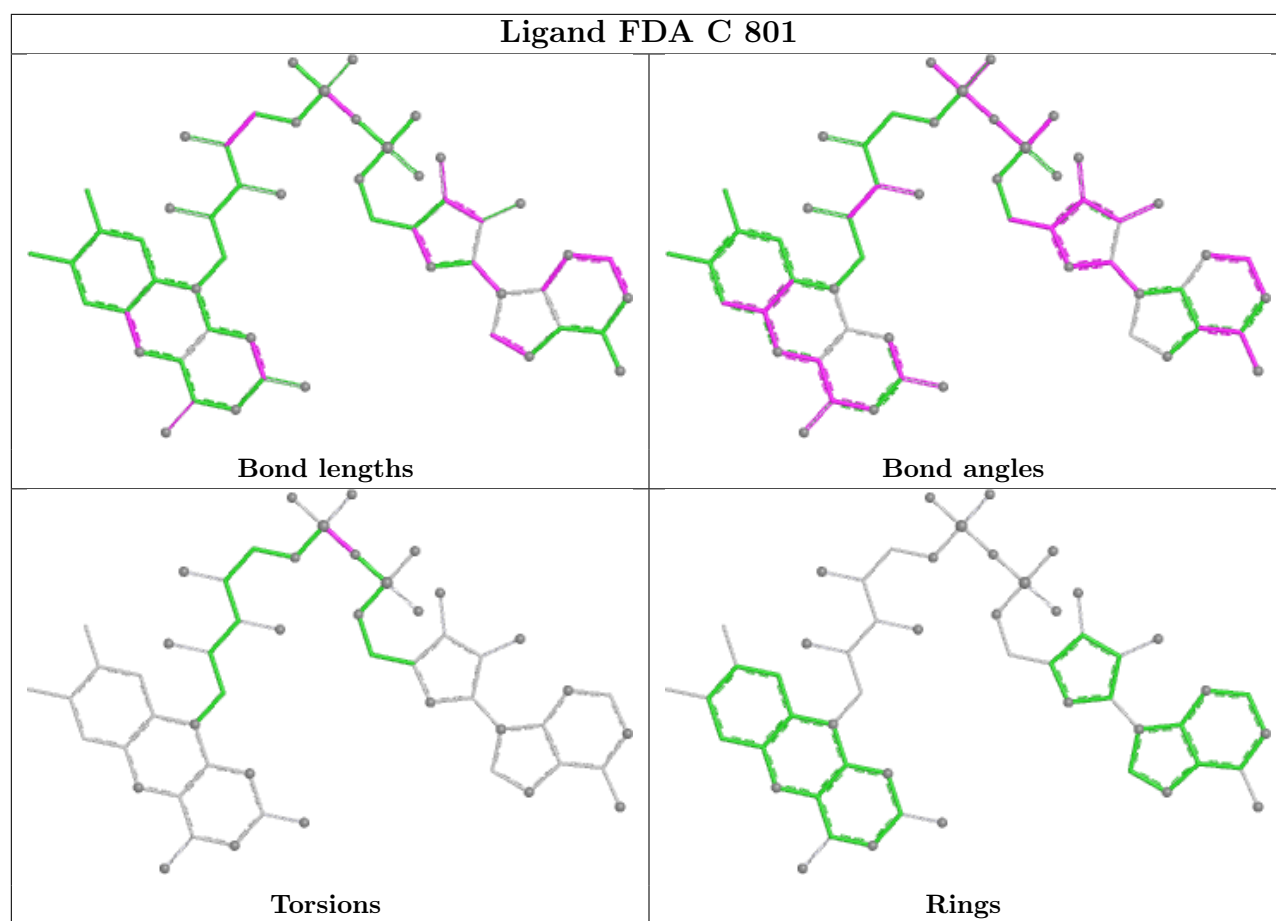
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	570/648 (87%)	-0.23	26 (4%)	38	35	6, 16, 39, 69	5 (0%)
1	B	574/648 (88%)	-0.06	33 (5%)	30	28	6, 20, 42, 72	3 (0%)
1	C	579/648 (89%)	-0.04	29 (5%)	35	32	6, 20, 45, 71	6 (1%)
1	D	570/648 (87%)	-0.25	20 (3%)	47	45	5, 16, 37, 78	4 (0%)
All	All	2293/2592 (88%)	-0.15	108 (4%)	37	34	5, 18, 41, 78	18 (0%)

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	VAL	6.5
1	D	68	GLY	5.6
1	D	69	PRO	5.4
1	A	68	GLY	5.1
1	D	466	ALA	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](#)

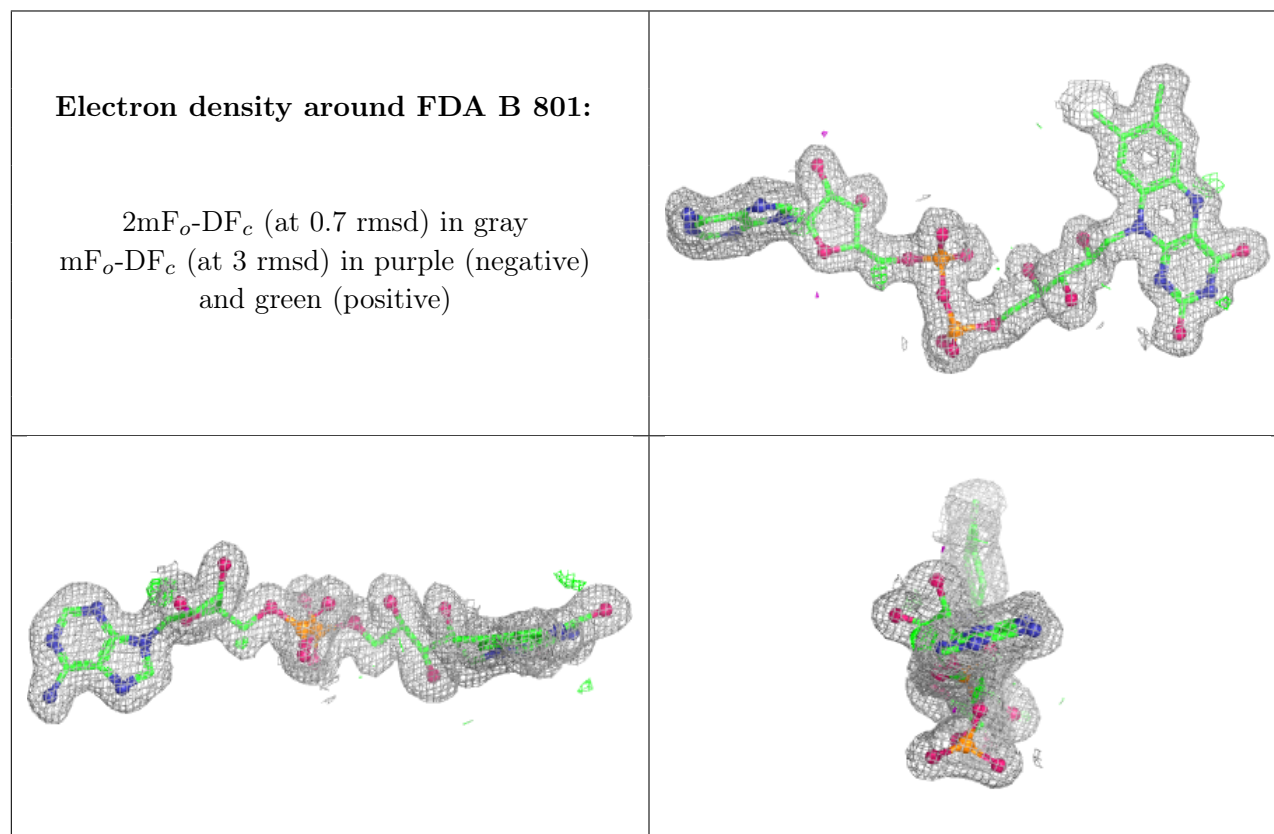
There are no monosaccharides in this entry.

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.

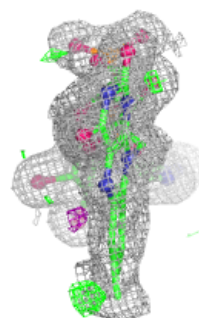
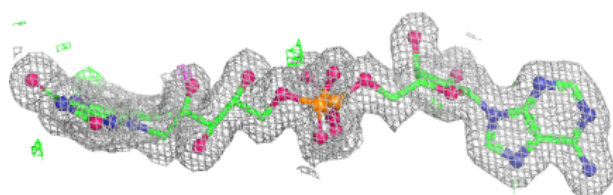
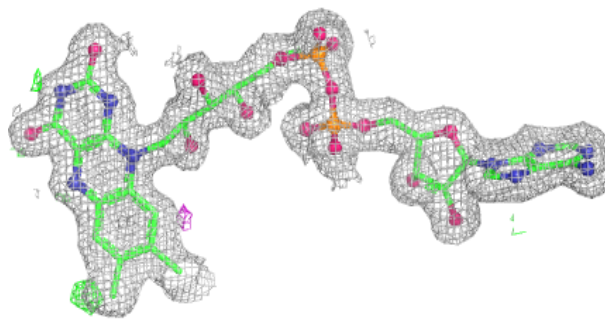
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	G3F	B	802	12/12	0.81	0.12	29,32,34,38	0
3	G3F	A	802	12/12	0.83	0.12	27,30,33,34	0
3	G3F	D	802	12/12	0.84	0.10	23,31,33,35	0
3	G3F	C	802	12/12	0.87	0.10	26,30,32,36	0
4	MN	D	803	1/1	0.97	0.04	13,13,13,13	1
2	FDA	B	801	53/53	0.98	0.05	10,15,17,18	0
2	FDA	C	801	53/53	0.98	0.05	10,14,17,18	0
2	FDA	D	801	53/53	0.98	0.04	9,11,15,15	0
4	MN	A	803	1/1	0.98	0.12	33,33,33,33	0
4	MN	A	805	1/1	0.98	0.12	34,34,34,34	0
4	MN	B	803	1/1	0.98	0.19	38,38,38,38	0
2	FDA	A	801	53/53	0.98	0.04	8,11,15,16	0
4	MN	C	803	1/1	0.99	0.14	35,35,35,35	0
4	MN	A	804	1/1	0.99	0.11	30,30,30,30	0
4	MN	D	804	1/1	0.99	0.07	32,32,32,32	0
4	MN	D	805	1/1	0.99	0.15	33,33,33,33	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.

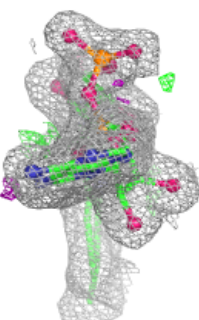
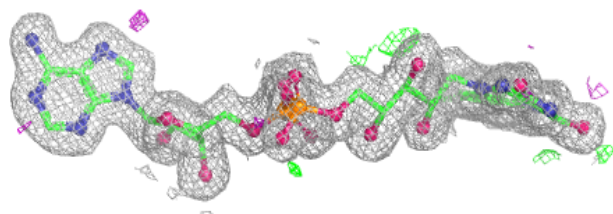
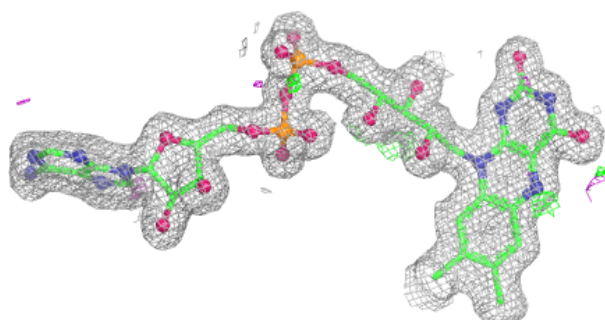


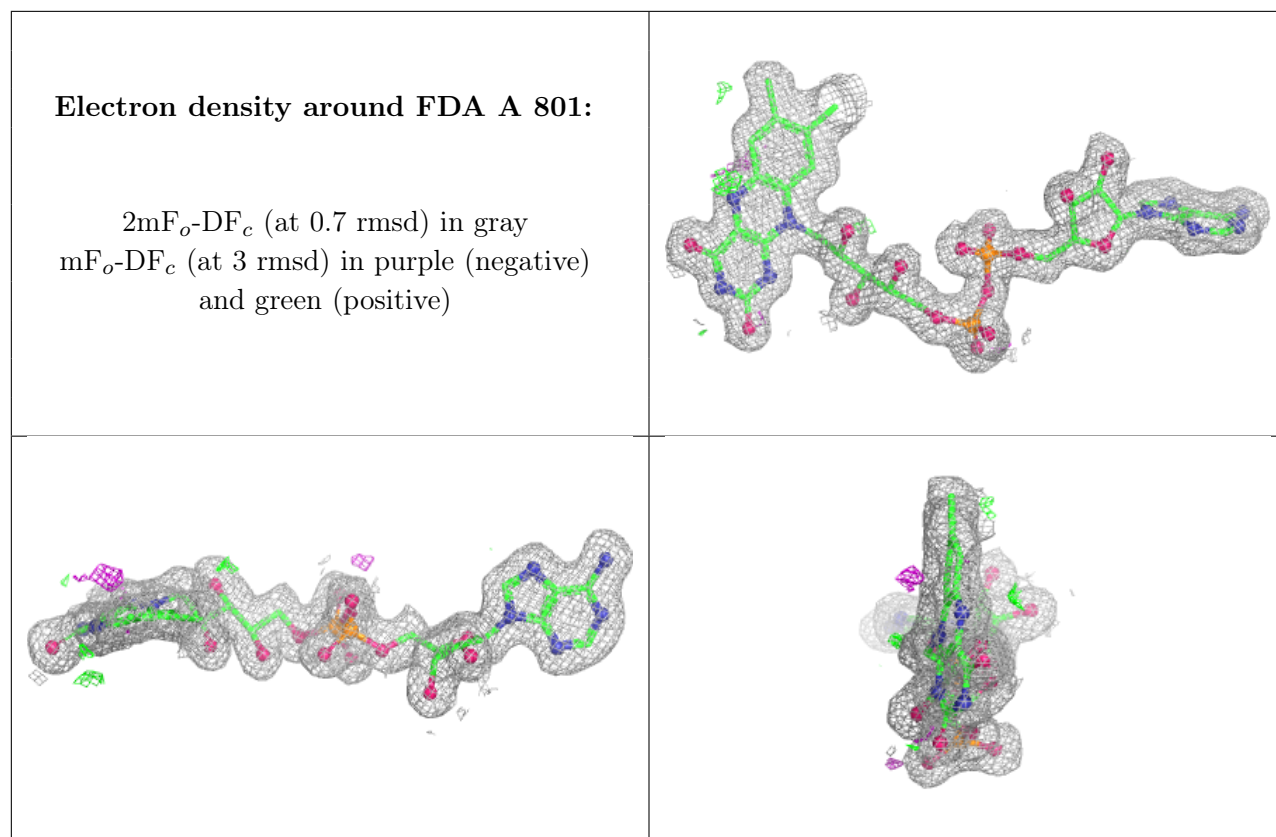
Electron density around FDA C 801:

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

**Electron density around FDA D 801:**

$2mF_o-DF_c$ (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.