Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 01:26 am GMT

PDB ID	:	6RZN
Title	:	Crystal structure of the N-terminal carbohydrate binding module family 48 and ferulic acid esterase from the multi-enzyme CE1-GH62-GH10
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Deposited on	:	2019-06-13
Resolution	:	1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

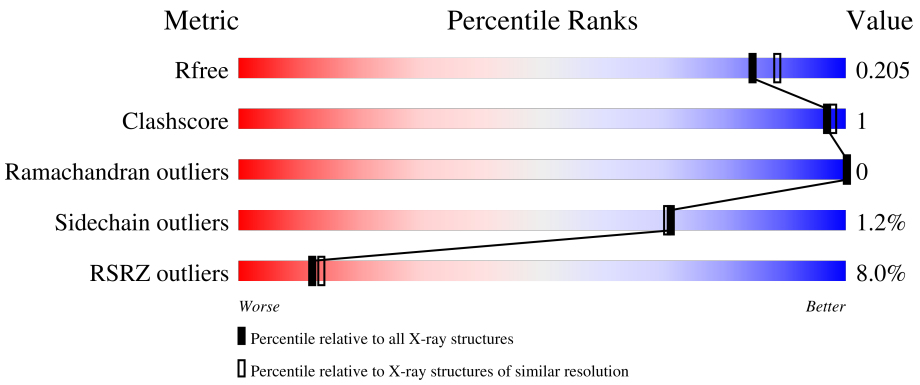
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.91 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	386	8% 85% • 12%
1	B	386	6% 85% • 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11532 atoms, of which 5224 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 Ferulic acid esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	338	5273	1710	2599	453	499	12	0	0	0
1	B	340	5317	1721	2625	456	503	12	0	0	0

- Molecule 2 is water.

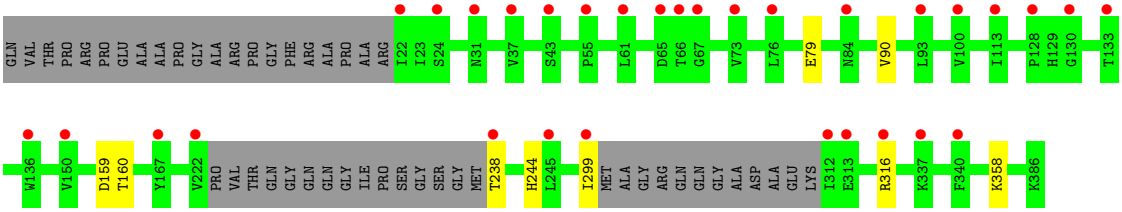
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	468	468	468	0	0
2	B	474	474	474	0	0

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.

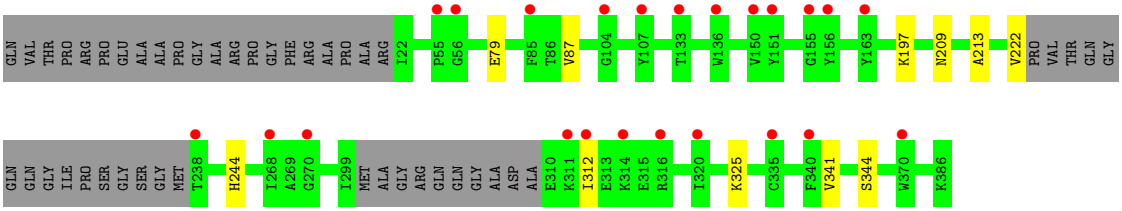
- Molecule 1: Ferulic acid esterase

Chain A:



- Molecule 1: Ferulic acid esterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.65Å 99.90Å 133.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.86 – 1.91 79.94 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.86-1.91) 98.5 (79.94-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.91Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.176 , 0.205 0.175 , 0.205	Depositor DCC
R_{free} test set	3490 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11532	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.27	0/2741	0.48	0/3710
1	B	0.27	0/2759	0.47	0/3733
All	All	0.27	0/5500	0.48	0/7443

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2674	2599	2607	5	0
1	B	2692	2625	2626	6	0
2	A	468	0	0	3	2
2	B	474	0	0	3	2
All	All	6308	5224	5233	10	2

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 1.

All (10) 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:238:THR:OG1	2:A:401:HOH:O	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:NZ	2:B:402:HOH:O	2.28	0.66
1:A:159:ASP:OD1	1:A:160:THR:N	2.44	0.51
1:B:213:ALA:HB2	1:B:222:VAL:HG11	1.95	0.47
1:B:325:LYS:NZ	2:B:409:HOH:O	2.50	0.44
1:A:90:VAL:HG11	1:B:87:VAL:HG21	1.99	0.43
1:B:209:ASN:OD1	2:B:401:HOH:O	2.22	0.42
1:A:358:LYS:NZ	2:A:418:HOH:O	2.53	0.41
1:B:341:VAL:HG22	1:B:344:SER:HB3	2.01	0.41
1:A:238:THR:N	2:A:417:HOH:O	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:708:HOH:O	2:B:402:HOH:O[3_656]	2.00	0.20
2:A:837:HOH:O	2:B:772:HOH:O[1_455]	2.16	0.04

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	332/386 (86%)	327 (98%)	5 (2%)	0	100	100
1	B	334/386 (86%)	328 (98%)	6 (2%)	0	100	100
All	All	666/772 (86%)	655 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	283/315 (90%)	279 (99%)	4 (1%)	67	65
1	B	285/315 (90%)	282 (99%)	3 (1%)	73	73
All	All	568/630 (90%)	561 (99%)	7 (1%)	71	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	244	HIS
1	A	299	ILE
1	A	316	ARG
1	B	79	GLU
1	B	244	HIS
1	B	312	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	338/386 (87%)	0.97	31 (9%)	9	10	12, 19, 39, 88	0
1	B	340/386 (88%)	0.91	23 (6%)	17	19	11, 19, 43, 81	0
All	All	678/772 (87%)	0.94	54 (7%)	12	13	11, 19, 41, 88	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ILE	8.4
1	A	222	VAL	5.9
1	A	238	THR	4.7
1	A	22	ILE	4.2
1	B	55	PRO	3.9
1	B	107	TYR	3.7
1	A	93	LEU	3.7
1	A	37	VAL	3.5
1	B	312	ILE	3.3
1	B	340	PHE	3.3
1	B	268	ILE	3.2
1	A	130	GLY	3.2
1	B	311	LYS	3.1
1	B	155	GLY	3.1
1	B	156	TYR	3.1
1	A	55	PRO	2.9
1	A	167	TYR	2.9
1	A	113	ILE	2.9
1	B	270	GLY	2.8
1	A	245	LEU	2.7
1	A	299	ILE	2.7
1	B	104	GLY	2.7
1	A	340	PHE	2.7
1	A	67	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	316	ARG	2.7
1	B	133	THR	2.5
1	B	320	ILE	2.5
1	A	128	PRO	2.4
1	B	238	THR	2.4
1	B	150	VAL	2.4
1	B	151	TYR	2.3
1	A	73	VAL	2.3
1	A	150	VAL	2.3
1	B	314	LYS	2.3
1	A	337	LYS	2.2
1	B	163	TYR	2.2
1	A	65	ASP	2.2
1	B	56	GLY	2.2
1	A	24	SER	2.1
1	A	100	VAL	2.1
1	B	370	TRP	2.1
1	A	133	THR	2.1
1	B	316	ARG	2.1
1	A	31	ASN	2.1
1	B	335	CYS	2.1
1	B	85	PHE	2.1
1	A	43	SER	2.1
1	A	61	LEU	2.1
1	A	66	THR	2.0
1	A	76	LEU	2.0
1	A	313	GLU	2.0
1	A	136	TRP	2.0
1	B	136	TRP	2.0
1	A	84	ASN	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.