Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 PM GMT

PDB ID	:	3UR7
Title	:	Higher-density crystal structure of potato endo-1,3-beta-glucanase
Authors	:	Wojtkowiak, A.; Witek, K.; Hennig, J.; Jaskolski, M.
Deposited on	:	2011-11-21
Resolution	:	1.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

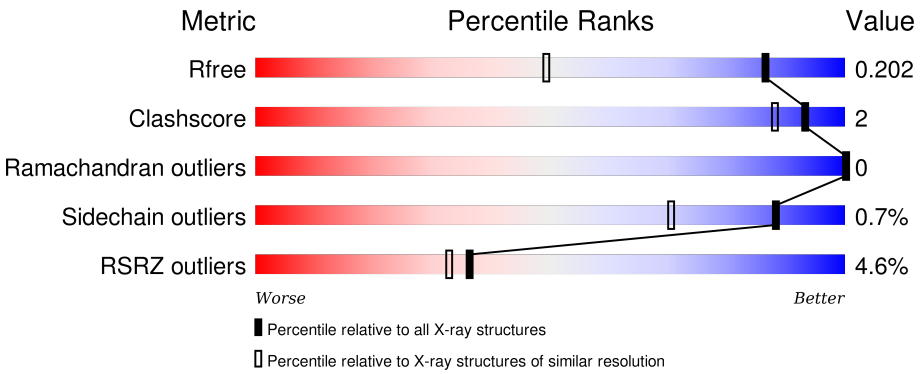
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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	323	4% 93%
1	B	323	5% 93% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5607 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 Glucan endo-1,3-beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2546	1624	439	476	7	0	7	0
1	B	316	2554	1630	441	476	7	0	10	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LEU	-	EXPRESSION TAG	UNP Q70C53
A	340	ASN	-	EXPRESSION TAG	UNP Q70C53
A	341	HIS	-	EXPRESSION TAG	UNP Q70C53
A	342	HIS	-	EXPRESSION TAG	UNP Q70C53
A	343	HIS	-	EXPRESSION TAG	UNP Q70C53
A	344	HIS	-	EXPRESSION TAG	UNP Q70C53
A	345	HIS	-	EXPRESSION TAG	UNP Q70C53
A	346	HIS	-	EXPRESSION TAG	UNP Q70C53
B	339	LEU	-	EXPRESSION TAG	UNP Q70C53
B	340	ASN	-	EXPRESSION TAG	UNP Q70C53
B	341	HIS	-	EXPRESSION TAG	UNP Q70C53
B	342	HIS	-	EXPRESSION TAG	UNP Q70C53
B	343	HIS	-	EXPRESSION TAG	UNP Q70C53
B	344	HIS	-	EXPRESSION TAG	UNP Q70C53
B	345	HIS	-	EXPRESSION TAG	UNP Q70C53
B	346	HIS	-	EXPRESSION TAG	UNP Q70C53

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	B	1	1	1	0	0

- Molecule 3 is water.

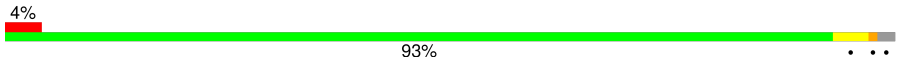
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	258	258	258	0	0
			Total	O		
3	B	248	248	248	0	0

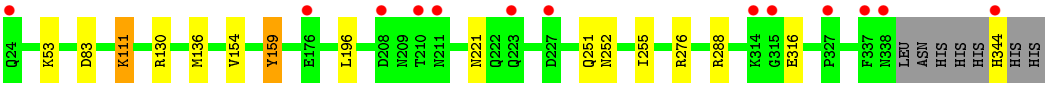
3 Residue-property plots (i)

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

- Molecule 1: Glucan endo-1,3-beta-D-glucosidase

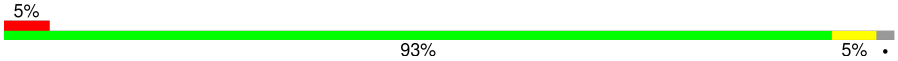
Chain A:

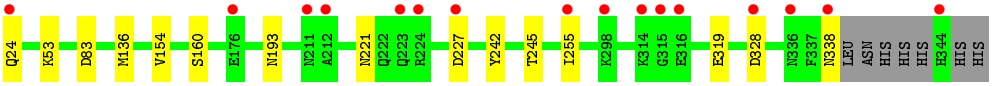




- Molecule 1: Glucan endo-1,3-beta-D-glucosidase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.13Å 49.13Å 80.50Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 19.92 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.40) 99.7 (19.92-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.161 , 0.186 0.174 , 0.202	Depositor DCC
R_{free} test set	1117 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	3 of 110951 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5607	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 38.90 % 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 3.4395e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.88	1/2643 (0.0%)	0.92	5/3586 (0.1%)
1	B	0.85	0/2667	0.88	3/3618 (0.1%)
All	All	0.87	1/5310 (0.0%)	0.90	8/7204 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	TYR	CE1-CZ	-5.85	1.30	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	276	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	83	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	288	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	276	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	328	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	130	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	227	ASP	CB-CG-OD2	5.20	122.98	118.30

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	2546	0	2470	7	0
1	B	2554	0	2480	13	0
2	B	1	0	0	0	0
3	A	258	0	0	1	0
3	B	248	0	0	6	0
All	All	5607	0	4950	19	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 2.

All (19) 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:160[B]:SER:OG	3:B:667:HOH:O	1.71	1.08
1:B:193[B]:ASN:OD1	3:B:662:HOH:O	1.75	1.04
1:A:53:LYS:HE3	1:A:53:LYS:HA	1.81	0.61
1:B:193[A]:ASN:ND2	3:B:661:HOH:O	2.34	0.60
1:B:53:LYS:HD2	3:B:579:HOH:O	2.02	0.59
1:A:344:HIS:HA	1:B:319:GLU:OE1	2.09	0.52
1:B:53:LYS:CD	3:B:579:HOH:O	2.57	0.50
1:A:316:GLU:HB3	3:A:621:HOH:O	2.15	0.46
1:A:196:LEU:HD23	1:A:255[B]:ILE:CD1	2.45	0.45
1:B:242:TYR:CE1	1:B:255[B]:ILE:HG12	2.51	0.45
1:B:24:GLN:NE2	1:B:338:ASN:HB3	2.32	0.45
1:B:160[A]:SER:HB3	3:B:667:HOH:O	2.17	0.44
1:B:24:GLN:NE2	1:B:24:GLN:HA	2.33	0.44
1:B:136[B]:MET:HG3	1:B:154:VAL:CG1	2.49	0.43
1:A:251:GLN:HG3	1:A:252:ASN:N	2.35	0.42
1:A:136[B]:MET:HG3	1:A:154:VAL:CG1	2.50	0.42
1:B:24:GLN:HE21	1:B:338:ASN:HB3	1.84	0.41
1:A:111:LYS:HA	1:A:111:LYS:HE3	2.02	0.41

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	320/323 (99%)	313 (98%)	7 (2%)	0	100	100
1	B	323/323 (100%)	315 (98%)	8 (2%)	0	100	100
All	All	643/646 (100%)	628 (98%)	15 (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	278/278 (100%)	275 (99%)	3 (1%)	80	56
1	B	281/278 (101%)	280 (100%)	1 (0%)	93	81
All	All	559/556 (100%)	555 (99%)	4 (1%)	88	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	159	TYR
1	A	221	ASN
1	B	221	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	284	ASN
1	B	24	GLN
1	B	221	ASN
1	B	222	GLN

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Mol	Chain	Res	Type
1	B	284	ASN
1	B	334	GLN

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	316/323 (97%)	0.10	13 (4%)	41	39	12, 16, 29, 37	2 (0%)
1	B	316/323 (97%)	0.26	16 (5%)	32	28	13, 18, 30, 39	1 (0%)
All	All	632/646 (97%)	0.18	29 (4%)	36	33	12, 17, 29, 39	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	GLN	5.7
1	A	338	ASN	5.3
1	A	223	GLN	5.3
1	B	24	GLN	5.2
1	A	24	GLN	4.7
1	A	210	THR	4.6
1	A	337	PHE	3.7
1	B	224	ARG	3.7
1	B	344	HIS	3.6
1	A	344	HIS	3.5
1	B	212	ALA	3.4
1	A	227	ASP	3.3
1	B	314	LYS	3.2
1	A	211	ASN	3.2
1	A	314	LYS	2.9
1	B	227	ASP	2.9
1	B	211	ASN	2.7
1	B	328	ASP	2.7
1	A	208	ASP	2.5
1	A	176	GLU	2.4
1	B	338	ASN	2.4
1	B	336	ASN	2.2
1	B	255[A]	ILE	2.2
1	B	315	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	176	GLU	2.1
1	A	315	GLY	2.1
1	A	327	PRO	2.0
1	B	316	GLU	2.0
1	B	298	LYS	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 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
2	NA	B	401	1/1	0.99	0.06	-1.25	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.