wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:41 PM GMT

PDB ID	:	1UP6
Title	:	STRUCTURE OF THE 6-PHOSPHO-BETA GLUCOSIDASE FROM THERMOTOGA MARITIMA AT 2.55 ANGSTROM RESOLUTION IN THE TETRAGONAL FORM WITH MANGANESE, NAD+ AND GLUCOSE-6-PHOSPHATE
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Deposited on	:	2003-09-29
Resolution	:	2.55 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
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:

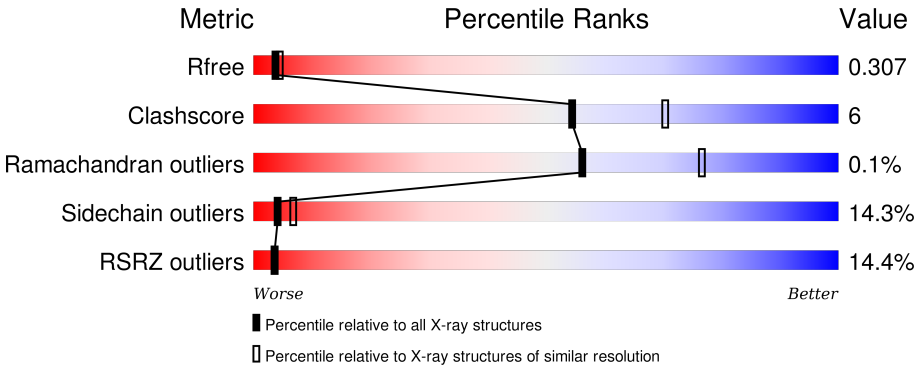
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	416	8% 74% 22%
1	B	416	11% 74% 21%
1	C	416	8% 75% 19%
1	D	416	7% 75% 19%
1	E	416	25% 67% 22% 5% 6%

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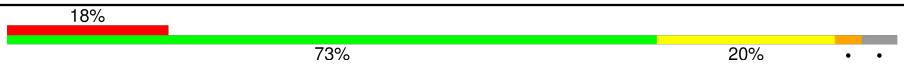
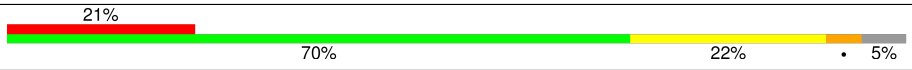
Mol	Chain	Length	Quality of chain
1	F	416	
1	G	416	
1	H	416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	A	1416	-	-	-	X
2	NAD	C	1416	-	-	-	X
2	NAD	G	1416	-	-	-	X
4	G6P	A	1418	X	-	-	-
4	G6P	C	1418	X	-	-	-
5	SO4	B	1416	-	-	-	X
5	SO4	D	1416	-	-	-	X

2 Entry composition (i)

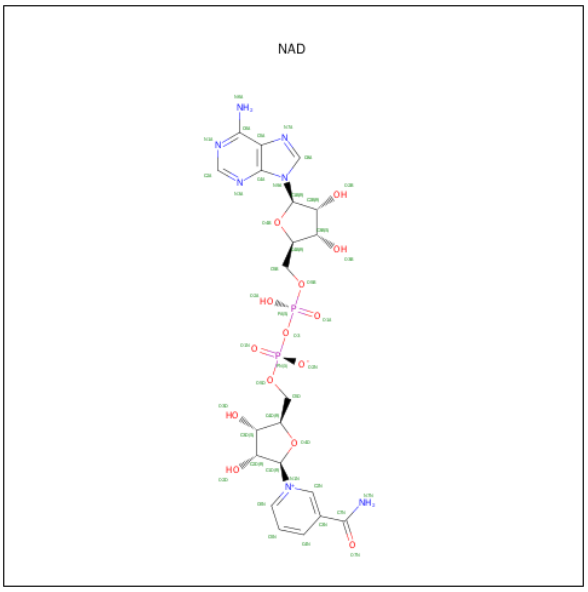
There are 6 unique types of molecules in this entry. The entry contains 26917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-PHOSPHO-BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	Se	0	1	0
			3356	2164	560	623	2	7			
1	B	410	Total	C	N	O	S	Se	39	0	0
			3331	2150	552	620	2	7			
1	C	407	Total	C	N	O	S	Se	14	0	0
			3303	2129	548	617	2	7			
1	D	404	Total	C	N	O	S	Se	10	0	0
			3276	2113	543	611	2	7			
1	E	390	Total	C	N	O	S	Se	121	0	0
			3165	2041	525	591	2	6			
1	F	399	Total	C	N	O	S	Se	80	0	0
			3240	2091	539	602	2	6			
1	G	404	Total	C	N	O	S	Se	20	0	0
			3280	2117	544	610	2	7			
1	H	395	Total	C	N	O	S	Se	104	0	0
			3209	2072	533	596	2	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

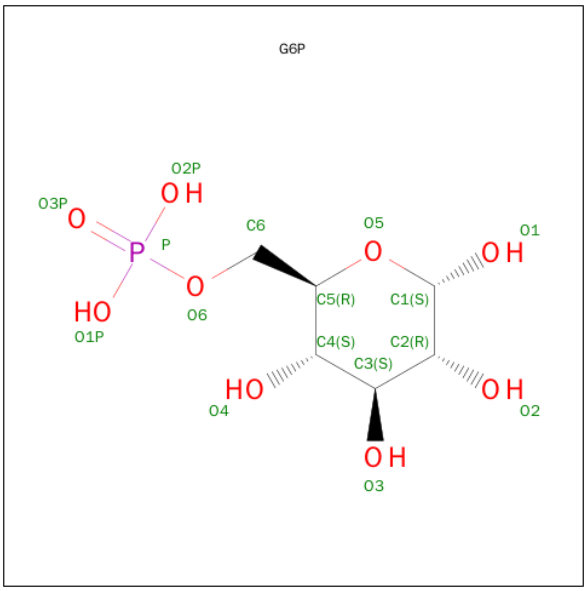


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

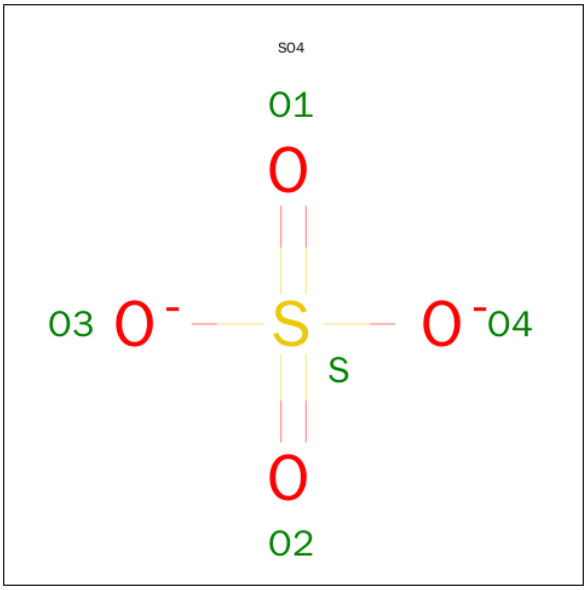
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	A	3	Total	Mn	0	0
			3	3		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 16 6 9 1	0	0
4	C	1	Total C O P 16 6 9 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

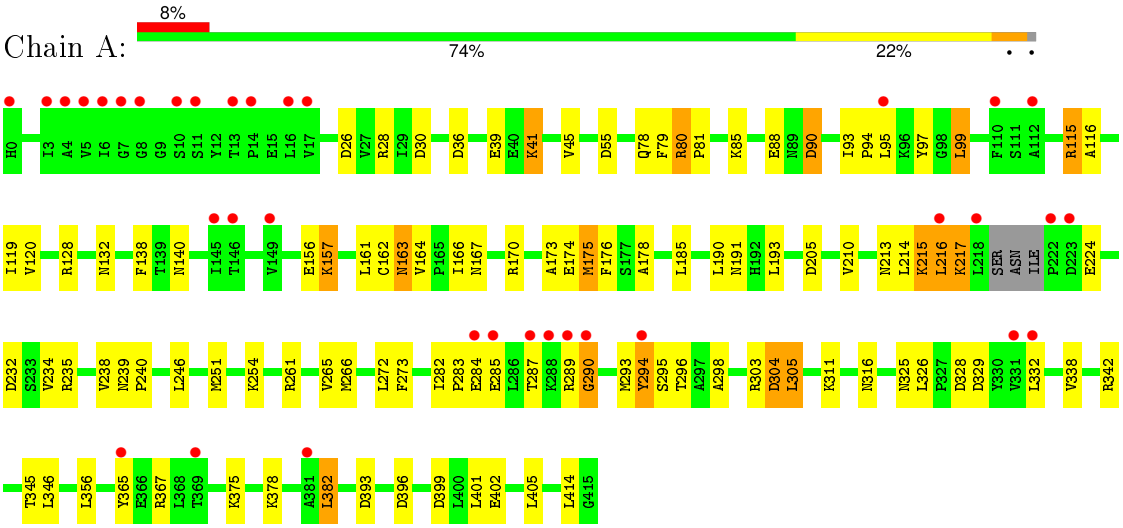
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	136	Total O 136 136	0	0
6	B	83	Total O 83 83	0	0
6	C	106	Total O 106 106	0	0
6	D	95	Total O 95 95	0	0
6	E	23	Total O 23 23	0	0
6	F	36	Total O 36 36	0	0
6	G	59	Total O 59 59	0	0
6	H	30	Total O 30 30	0	0

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.

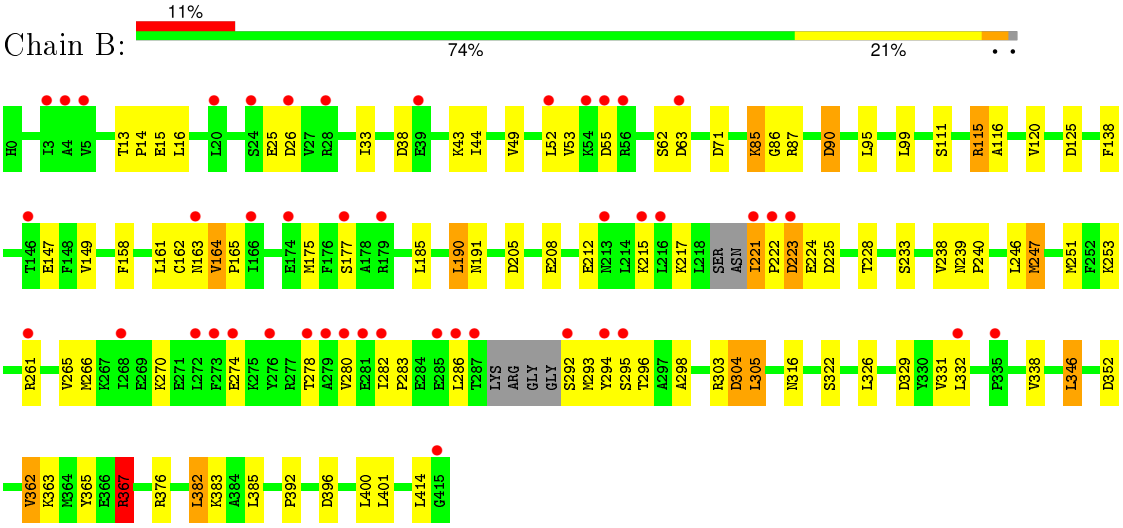
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain A:



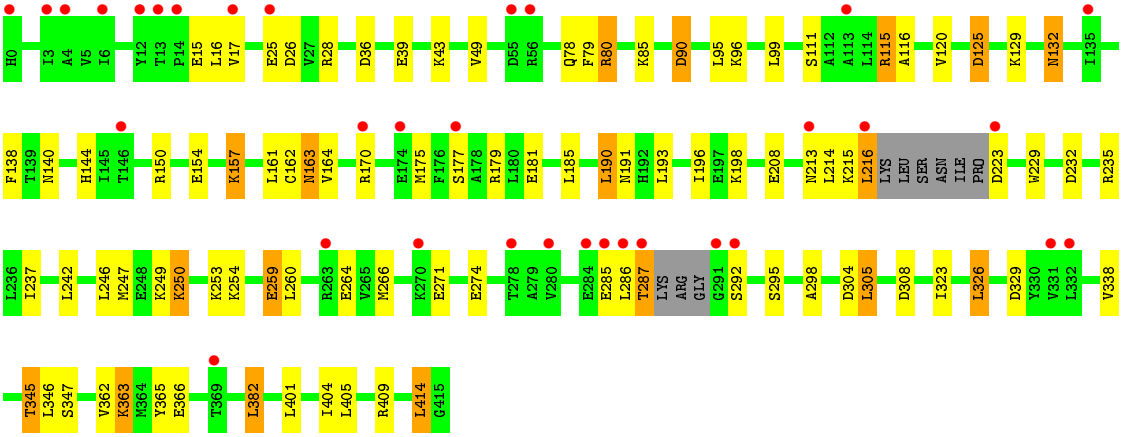
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain B:



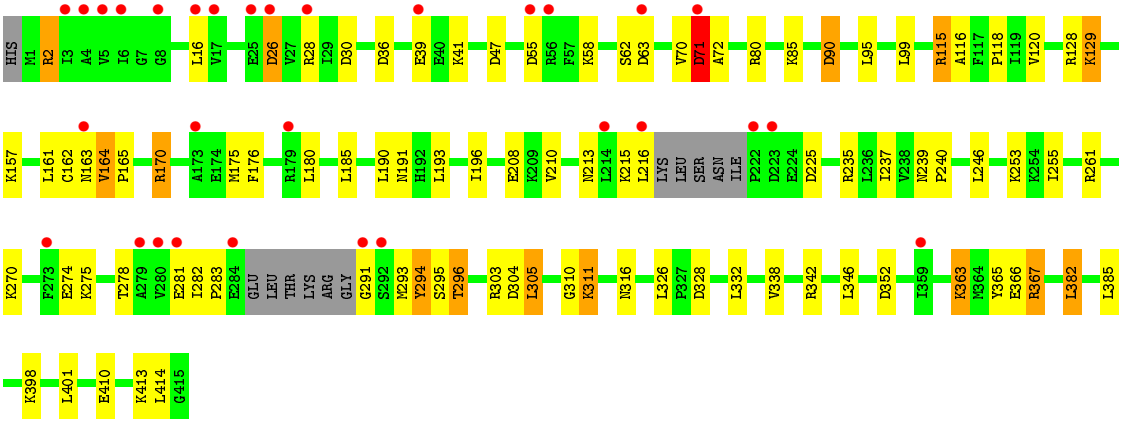
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain C:



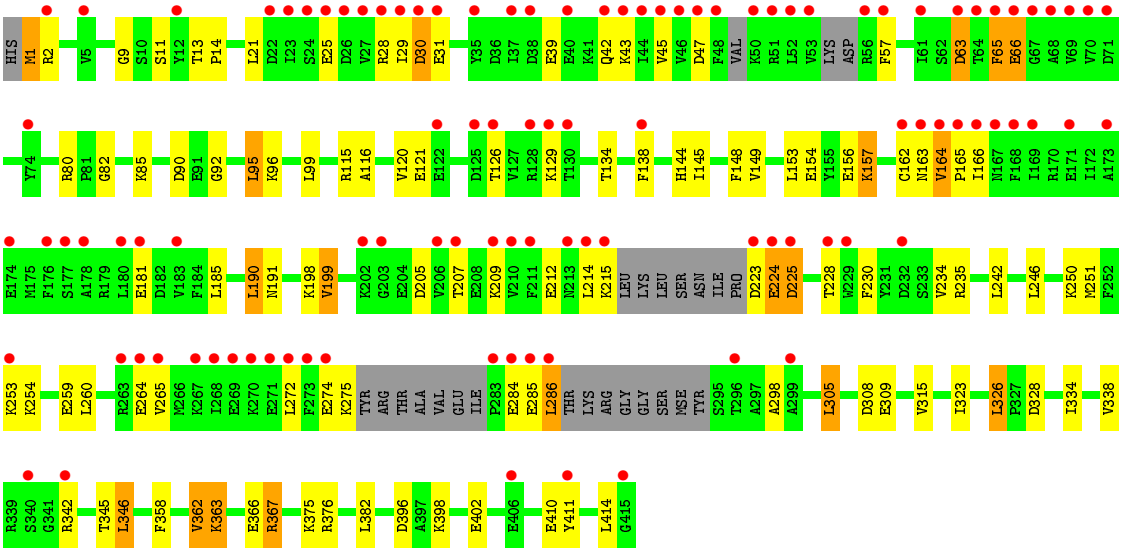
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain D:



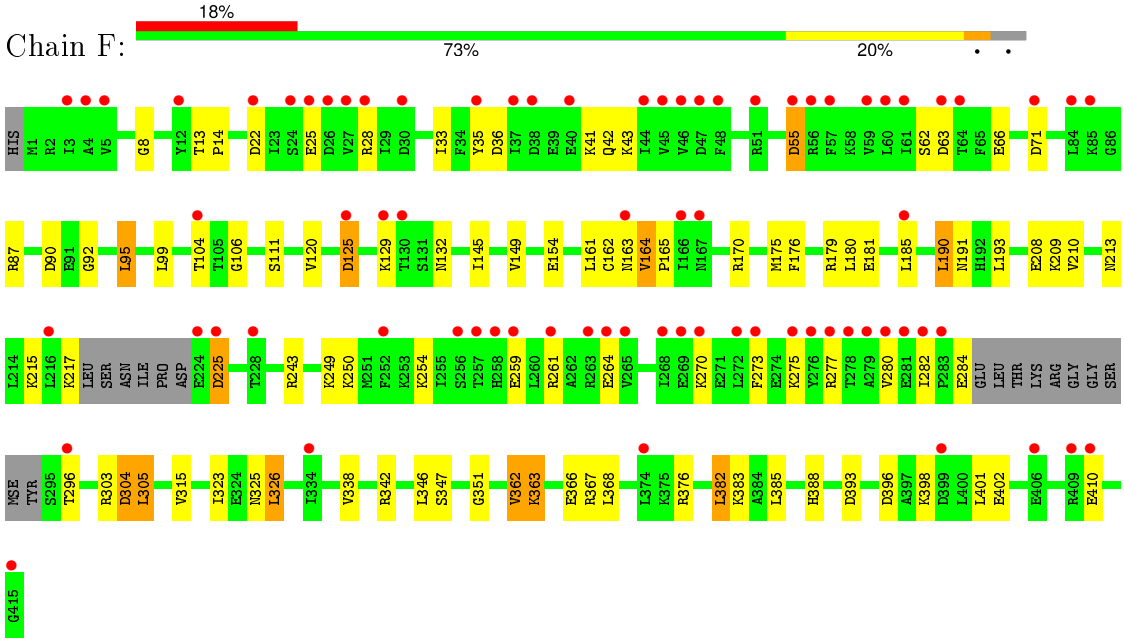
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain E:



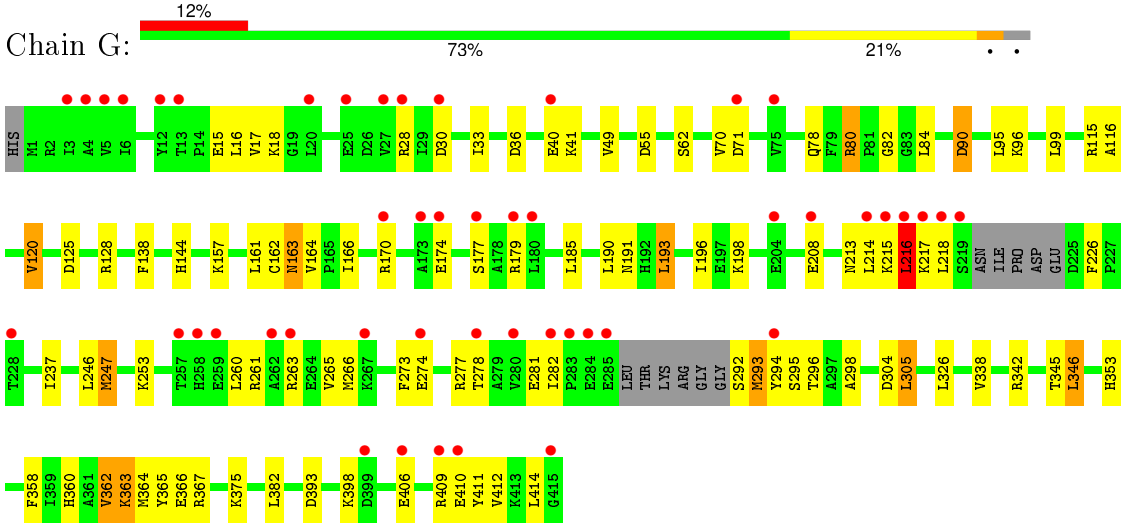
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain F:



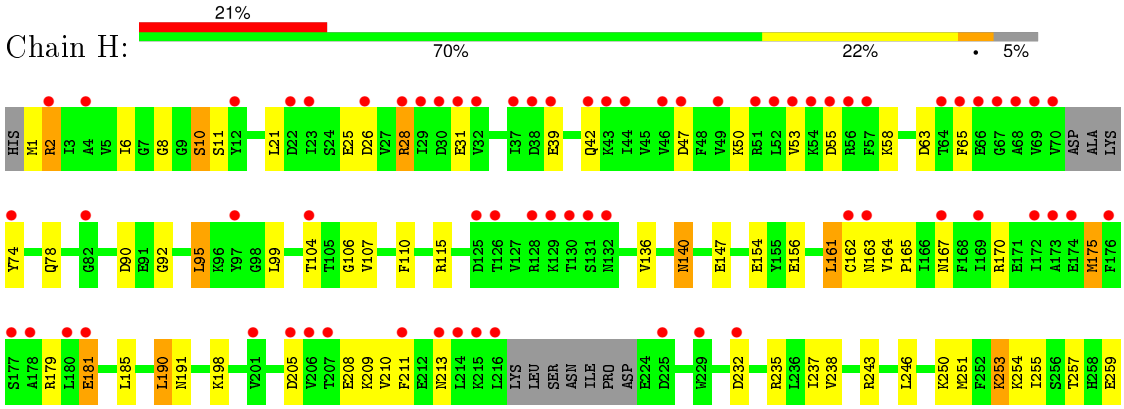
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

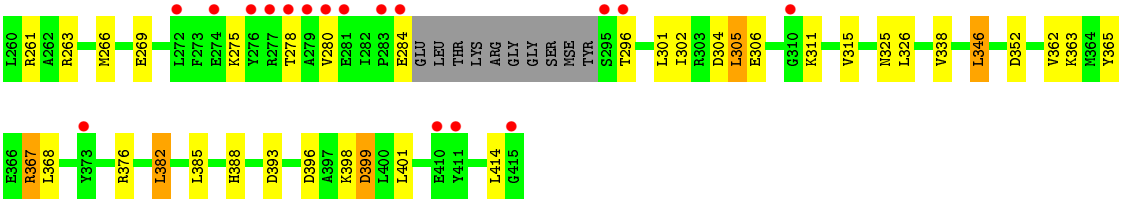
Chain G:



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain H:




L260
R261
A262
R263
M266
E269
L272
F273
E274
K275
Y276
R277
T278
A279
V280
E281
I282
P283
E284
GLU
LEU
THR
LYS
ARG
GLY
GLY
SER
MSE
TYR
S295
T296
L301
I302
R303
D304
L305
E306
G310
K311
V315
N325
L326
V338
L346
D352
V362
K363
M364
Y365
E366
R367
L368
Y373
R376
L382
L385
H388
D393
D396
A397
K398
D399
L400
L401
E410
Y411
L414
G415

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	179.44Å 179.44Å 282.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.55 19.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.55) 99.8 (19.98-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.95 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.250 0.272 , 0.307	Depositor DCC
R_{free} test set	7464 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 286743 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26917	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: G6P, MN, SO4, NAD

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	0.75	1/3420 (0.0%)	0.88	15/4595 (0.3%)
1	B	0.67	0/3390	0.89	13/4558 (0.3%)
1	C	0.72	0/3361	0.88	10/4518 (0.2%)
1	D	0.70	0/3335	0.89	12/4484 (0.3%)
1	E	0.51	0/3219	0.77	8/4323 (0.2%)
1	F	0.51	0/3298	0.78	9/4435 (0.2%)
1	G	0.59	0/3338	0.81	8/4487 (0.2%)
1	H	0.49	0/3266	0.77	11/4392 (0.3%)
All	All	0.63	1/26627 (0.0%)	0.84	86/35792 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ASN	CG-OD1	5.05	1.35	1.24

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	115	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	90	ASP	CB-CG-OD2	8.03	125.53	118.30
1	D	115	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	367	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	304	ASP	CB-CG-OD2	7.44	125.00	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3356	0	3393	54	0
1	B	3331	0	3362	46	0
1	C	3303	0	3322	47	0
1	D	3276	0	3300	36	0
1	E	3165	0	3184	43	0
1	F	3240	0	3275	38	0
1	G	3280	0	3313	45	0
1	H	3209	0	3239	37	0
2	A	44	0	26	5	0
2	C	44	0	26	2	0
2	G	44	0	26	3	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
4	A	16	0	9	1	0
4	C	16	0	10	1	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	136	0	0	1	0
6	B	83	0	0	1	0
6	C	106	0	0	2	0
6	D	95	0	0	2	0
6	E	23	0	0	0	0
6	F	36	0	0	0	0
6	G	59	0	0	0	0
6	H	30	0	0	0	0
All	All	26917	0	26485	334	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 334 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:G:41:LYS:HE2	1:G:273:PHE:CZ	1.75	1.22
1:F:175:MSE:HE3	1:F:213:ASN:ND2	1.62	1.15
1:F:175:MSE:HE3	1:F:213:ASN:HD22	1.05	1.15
1:G:41:LYS:HE2	1:G:273:PHE:CE2	1.85	1.11
1:D:175:MSE:HE3	1:D:213:ASN:HD22	0.92	1.07

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	410/416 (99%)	398 (97%)	10 (2%)	2 (0%)	34	54
1	B	404/416 (97%)	393 (97%)	11 (3%)	0	100	100
1	C	401/416 (96%)	395 (98%)	6 (2%)	0	100	100
1	D	398/416 (96%)	387 (97%)	11 (3%)	0	100	100
1	E	378/416 (91%)	372 (98%)	5 (1%)	1 (0%)	46	66
1	F	393/416 (94%)	383 (98%)	10 (2%)	0	100	100
1	G	398/416 (96%)	386 (97%)	11 (3%)	1 (0%)	46	66
1	H	387/416 (93%)	379 (98%)	8 (2%)	0	100	100
All	All	3169/3328 (95%)	3093 (98%)	72 (2%)	4 (0%)	56	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	290	GLY
1	E	285	GLU
1	G	216	LEU

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	366/361 (101%)	327 (89%)	39 (11%)	8 14
1	B	364/361 (101%)	319 (88%)	45 (12%)	6 10
1	C	360/361 (100%)	312 (87%)	48 (13%)	5 8
1	D	357/361 (99%)	306 (86%)	51 (14%)	4 7
1	E	345/361 (96%)	280 (81%)	65 (19%)	2 3
1	F	353/361 (98%)	302 (86%)	51 (14%)	4 6
1	G	358/361 (99%)	305 (85%)	53 (15%)	4 6
1	H	350/361 (97%)	295 (84%)	55 (16%)	3 5
All	All	2853/2888 (99%)	2446 (86%)	407 (14%)	4 7

5 of 407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	11	SER
1	E	274	GLU
1	H	213	ASN
1	E	43	LYS
1	E	166	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	191	ASN
1	F	42	GLN
1	H	300	HIS
1	E	320	ASN
1	F	213	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	NAD	A	1416	3	38,48,48	1.72	3 (7%)	47,73,73	1.93	5 (10%)
4	G6P	A	1418	3	16,16,16	0.95	1 (6%)	23,24,24	1.22	3 (13%)
5	SO4	B	1416	-	4,4,4	1.03	0	6,6,6	0.47	0
2	NAD	C	1416	3	38,48,48	1.70	3 (7%)	47,73,73	1.93	7 (14%)
4	G6P	C	1418	3	16,16,16	0.55	0	23,24,24	1.05	1 (4%)
5	SO4	D	1416	-	4,4,4	1.04	0	6,6,6	0.34	0
5	SO4	E	1416	-	4,4,4	0.35	0	6,6,6	0.27	0
2	NAD	G	1416	3	38,48,48	1.67	3 (7%)	47,73,73	2.15	6 (12%)
5	SO4	G	1418	-	4,4,4	0.22	0	6,6,6	0.19	0

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	NAD	A	1416	3	-	0/22/62/62	0/5/5/5
4	G6P	A	1418	3	1/1/6/6	0/6/26/26	0/1/1/1
5	SO4	B	1416	-	-	0/0/0/0	0/0/0/0
2	NAD	C	1416	3	-	0/22/62/62	0/5/5/5
4	G6P	C	1418	3	1/1/6/6	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	1416	-	-	0/0/0/0	0/0/0/0
5	SO4	E	1416	-	-	0/0/0/0	0/0/0/0
2	NAD	G	1416	3	-	0/22/62/62	0/5/5/5
5	SO4	G	1418	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1418	G6P	P-O2P	-2.27	1.46	1.54
2	G	1416	NAD	C2A-N1A	2.37	1.38	1.33
2	A	1416	NAD	C2A-N1A	2.49	1.38	1.33
2	C	1416	NAD	C2A-N1A	2.53	1.38	1.33
2	A	1416	NAD	C2A-N3A	3.54	1.38	1.32

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1416	NAD	N3A-C2A-N1A	-12.15	119.59	128.89
2	A	1416	NAD	N3A-C2A-N1A	-9.91	121.30	128.89
2	C	1416	NAD	N3A-C2A-N1A	-9.73	121.45	128.89
2	G	1416	NAD	PN-O3-PA	-4.40	120.36	132.73
2	C	1416	NAD	PN-O3-PA	-3.70	122.34	132.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1418	G6P	C1
4	C	1418	G6P	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1416	NAD	5	0
4	A	1418	G6P	1	0
2	C	1416	NAD	2	0
4	C	1418	G6P	1	0
2	G	1416	NAD	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	406/416 (97%)	0.75	35 (8%) 13 14	13, 19, 32, 51	3 (0%)
1	B	403/416 (96%)	0.74	45 (11%) 7 8	12, 19, 32, 54	18 (4%)
1	C	400/416 (96%)	0.63	33 (8%) 14 15	14, 19, 29, 52	11 (2%)
1	D	397/416 (95%)	0.67	30 (7%) 17 19	13, 19, 29, 45	11 (2%)
1	E	384/416 (92%)	1.30	104 (27%) 1 0	16, 19, 28, 47	42 (10%)
1	F	393/416 (94%)	0.94	75 (19%) 2 1	15, 19, 29, 49	36 (9%)
1	G	397/416 (95%)	0.66	48 (12%) 6 6	14, 19, 37, 46	26 (6%)
1	H	389/416 (93%)	1.14	86 (22%) 1 1	15, 19, 29, 49	47 (12%)
All	All	3169/3328 (95%)	0.85	456 (14%) 3 3	12, 19, 32, 54	194 (6%)

The worst 5 of 456 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	213	ASN	6.6
1	F	280	VAL	6.6
1	A	218	LEU	6.2
1	E	37	ILE	6.1
1	E	42	GLN	6.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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
5	SO4	B	1416	5/5	0.80	0.27	3.90	42,43,45,50	0
5	SO4	D	1416	5/5	0.74	0.27	3.71	41,42,45,49	0
2	NAD	G	1416	44/44	0.76	0.34	2.60	10,16,18,18	44
2	NAD	C	1416	44/44	0.81	0.34	2.45	11,16,19,19	44
2	NAD	A	1416	44/44	0.84	0.32	2.35	11,16,18,19	44
4	G6P	C	1418	16/16	0.82	0.30	1.56	14,20,23,24	16
4	G6P	A	1418	16/16	0.88	0.30	0.97	13,24,27,28	16
3	MN	A	1420	1/1	0.62	0.22	0.27	42,42,42,42	0
5	SO4	G	1418	5/5	0.90	0.16	0.02	54,54,55,57	0
3	MN	C	1417	1/1	0.79	0.18	-0.07	35,35,35,35	1
5	SO4	E	1416	5/5	0.95	0.14	-0.77	40,40,41,43	0
3	MN	G	1417	1/1	0.77	0.12	-1.63	45,45,45,45	1
3	MN	A	1417	1/1	0.80	0.12	-1.67	35,35,35,35	1
3	MN	A	1419	1/1	0.94	0.10	-1.90	35,35,35,35	1

6.5 Other polymers

There are no such residues in this entry.