



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:19 PM UTC

PDB ID : 7QUZ / pdb_00007quz
Title : Crystal structure of the SeMet octameric C-terminal Big_2-CBM56 domains from *Paenibacillus illinoisensis* (*Bacillus circulans* IAM1165) beta-1,3-glucanase H
Authors : Najmudin, S.; Venditto, I.; Fontes, C.M.G.A.; Bule, P.
Deposited on : 2022-01-19
Resolution : 2.16 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

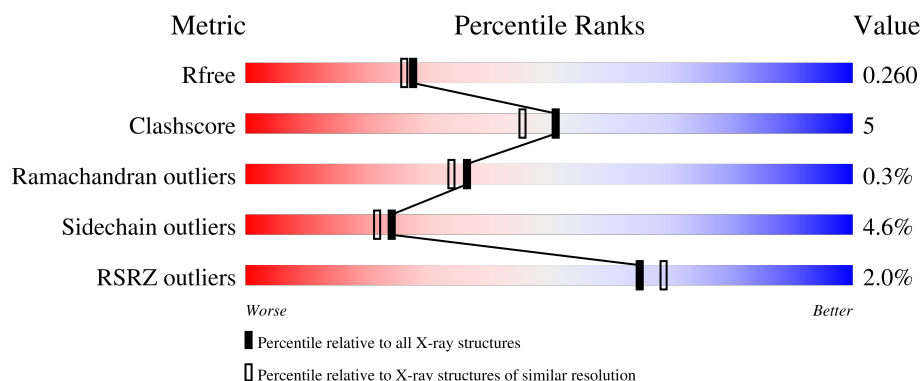
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	AAA	207	2% 77% 12% 11%
1	BBB	207	2% 76% 13% 10%
1	CCC	207	2% 77% 11% 11%
1	DDD	207	2% 80% 9% 10%
1	EEE	207	2% 73% 14% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	207	2% 71% 17% • 11%
1	GGG	207	3% 75% 13% • 11%
1	HHH	207	3% 75% 14% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22187 atoms, of which 10558 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 Beta-1,3-glucanase bglH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	184	Total	C	H	N	O	Se	51	1	0
			2660	847	1312	226	274	1			
1	BBB	186	Total	C	H	N	O	Se	52	1	0
			2681	853	1322	228	277	1			
1	CCC	184	Total	C	H	N	O	Se	51	1	0
			2660	847	1312	226	274	1			
1	DDD	187	Total	C	H	N	O	Se	52	1	0
			2699	858	1332	229	278	2			
1	EEE	184	Total	C	H	N	O	Se	52	1	0
			2647	839	1307	225	275	1			
1	FFF	184	Total	C	H	N	O	Se	51	0	0
			2640	837	1303	225	274	1			
1	GGG	184	Total	C	H	N	O	Se	51	0	0
			2640	837	1303	225	274	1			
1	HHH	184	Total	C	H	N	O	Se	51	0	0
			2640	837	1303	225	274	1			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MSE	-	initiating methionine	UNP Q45095
AAA	2	GLY	-	expression tag	UNP Q45095
AAA	3	SER	-	expression tag	UNP Q45095
AAA	4	SER	-	expression tag	UNP Q45095
AAA	5	HIS	-	expression tag	UNP Q45095
AAA	6	HIS	-	expression tag	UNP Q45095
AAA	7	HIS	-	expression tag	UNP Q45095
AAA	8	HIS	-	expression tag	UNP Q45095
AAA	9	HIS	-	expression tag	UNP Q45095
AAA	10	HIS	-	expression tag	UNP Q45095
AAA	11	SER	-	expression tag	UNP Q45095
AAA	12	SER	-	expression tag	UNP Q45095
AAA	13	GLY	-	expression tag	UNP Q45095

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	14	LEU	-	expression tag	UNP Q45095
AAA	15	VAL	-	expression tag	UNP Q45095
AAA	16	PRO	-	expression tag	UNP Q45095
AAA	17	ARG	-	expression tag	UNP Q45095
AAA	18	GLY	-	expression tag	UNP Q45095
AAA	19	SER	-	expression tag	UNP Q45095
AAA	20	HIS	-	expression tag	UNP Q45095
AAA	21	MSE	-	expression tag	UNP Q45095
AAA	22	ALA	-	expression tag	UNP Q45095
AAA	23	SER	-	expression tag	UNP Q45095
BBB	1	MSE	-	initiating methionine	UNP Q45095
BBB	2	GLY	-	expression tag	UNP Q45095
BBB	3	SER	-	expression tag	UNP Q45095
BBB	4	SER	-	expression tag	UNP Q45095
BBB	5	HIS	-	expression tag	UNP Q45095
BBB	6	HIS	-	expression tag	UNP Q45095
BBB	7	HIS	-	expression tag	UNP Q45095
BBB	8	HIS	-	expression tag	UNP Q45095
BBB	9	HIS	-	expression tag	UNP Q45095
BBB	10	HIS	-	expression tag	UNP Q45095
BBB	11	SER	-	expression tag	UNP Q45095
BBB	12	SER	-	expression tag	UNP Q45095
BBB	13	GLY	-	expression tag	UNP Q45095
BBB	14	LEU	-	expression tag	UNP Q45095
BBB	15	VAL	-	expression tag	UNP Q45095
BBB	16	PRO	-	expression tag	UNP Q45095
BBB	17	ARG	-	expression tag	UNP Q45095
BBB	18	GLY	-	expression tag	UNP Q45095
BBB	19	SER	-	expression tag	UNP Q45095
BBB	20	HIS	-	expression tag	UNP Q45095
BBB	21	MSE	-	expression tag	UNP Q45095
BBB	22	ALA	-	expression tag	UNP Q45095
BBB	23	SER	-	expression tag	UNP Q45095
CCC	1	MSE	-	initiating methionine	UNP Q45095
CCC	2	GLY	-	expression tag	UNP Q45095
CCC	3	SER	-	expression tag	UNP Q45095
CCC	4	SER	-	expression tag	UNP Q45095
CCC	5	HIS	-	expression tag	UNP Q45095
CCC	6	HIS	-	expression tag	UNP Q45095
CCC	7	HIS	-	expression tag	UNP Q45095
CCC	8	HIS	-	expression tag	UNP Q45095
CCC	9	HIS	-	expression tag	UNP Q45095

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	10	HIS	-	expression tag	UNP Q45095
CCC	11	SER	-	expression tag	UNP Q45095
CCC	12	SER	-	expression tag	UNP Q45095
CCC	13	GLY	-	expression tag	UNP Q45095
CCC	14	LEU	-	expression tag	UNP Q45095
CCC	15	VAL	-	expression tag	UNP Q45095
CCC	16	PRO	-	expression tag	UNP Q45095
CCC	17	ARG	-	expression tag	UNP Q45095
CCC	18	GLY	-	expression tag	UNP Q45095
CCC	19	SER	-	expression tag	UNP Q45095
CCC	20	HIS	-	expression tag	UNP Q45095
CCC	21	MSE	-	expression tag	UNP Q45095
CCC	22	ALA	-	expression tag	UNP Q45095
CCC	23	SER	-	expression tag	UNP Q45095
DDD	1	MSE	-	initiating methionine	UNP Q45095
DDD	2	GLY	-	expression tag	UNP Q45095
DDD	3	SER	-	expression tag	UNP Q45095
DDD	4	SER	-	expression tag	UNP Q45095
DDD	5	HIS	-	expression tag	UNP Q45095
DDD	6	HIS	-	expression tag	UNP Q45095
DDD	7	HIS	-	expression tag	UNP Q45095
DDD	8	HIS	-	expression tag	UNP Q45095
DDD	9	HIS	-	expression tag	UNP Q45095
DDD	10	HIS	-	expression tag	UNP Q45095
DDD	11	SER	-	expression tag	UNP Q45095
DDD	12	SER	-	expression tag	UNP Q45095
DDD	13	GLY	-	expression tag	UNP Q45095
DDD	14	LEU	-	expression tag	UNP Q45095
DDD	15	VAL	-	expression tag	UNP Q45095
DDD	16	PRO	-	expression tag	UNP Q45095
DDD	17	ARG	-	expression tag	UNP Q45095
DDD	18	GLY	-	expression tag	UNP Q45095
DDD	19	SER	-	expression tag	UNP Q45095
DDD	20	HIS	-	expression tag	UNP Q45095
DDD	21	MSE	-	expression tag	UNP Q45095
DDD	22	ALA	-	expression tag	UNP Q45095
DDD	23	SER	-	expression tag	UNP Q45095
EEE	1	MSE	-	initiating methionine	UNP Q45095
EEE	2	GLY	-	expression tag	UNP Q45095
EEE	3	SER	-	expression tag	UNP Q45095
EEE	4	SER	-	expression tag	UNP Q45095
EEE	5	HIS	-	expression tag	UNP Q45095

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	6	HIS	-	expression tag	UNP Q45095
EEE	7	HIS	-	expression tag	UNP Q45095
EEE	8	HIS	-	expression tag	UNP Q45095
EEE	9	HIS	-	expression tag	UNP Q45095
EEE	10	HIS	-	expression tag	UNP Q45095
EEE	11	SER	-	expression tag	UNP Q45095
EEE	12	SER	-	expression tag	UNP Q45095
EEE	13	GLY	-	expression tag	UNP Q45095
EEE	14	LEU	-	expression tag	UNP Q45095
EEE	15	VAL	-	expression tag	UNP Q45095
EEE	16	PRO	-	expression tag	UNP Q45095
EEE	17	ARG	-	expression tag	UNP Q45095
EEE	18	GLY	-	expression tag	UNP Q45095
EEE	19	SER	-	expression tag	UNP Q45095
EEE	20	HIS	-	expression tag	UNP Q45095
EEE	21	MSE	-	expression tag	UNP Q45095
EEE	22	ALA	-	expression tag	UNP Q45095
EEE	23	SER	-	expression tag	UNP Q45095
FFF	1	MSE	-	initiating methionine	UNP Q45095
FFF	2	GLY	-	expression tag	UNP Q45095
FFF	3	SER	-	expression tag	UNP Q45095
FFF	4	SER	-	expression tag	UNP Q45095
FFF	5	HIS	-	expression tag	UNP Q45095
FFF	6	HIS	-	expression tag	UNP Q45095
FFF	7	HIS	-	expression tag	UNP Q45095
FFF	8	HIS	-	expression tag	UNP Q45095
FFF	9	HIS	-	expression tag	UNP Q45095
FFF	10	HIS	-	expression tag	UNP Q45095
FFF	11	SER	-	expression tag	UNP Q45095
FFF	12	SER	-	expression tag	UNP Q45095
FFF	13	GLY	-	expression tag	UNP Q45095
FFF	14	LEU	-	expression tag	UNP Q45095
FFF	15	VAL	-	expression tag	UNP Q45095
FFF	16	PRO	-	expression tag	UNP Q45095
FFF	17	ARG	-	expression tag	UNP Q45095
FFF	18	GLY	-	expression tag	UNP Q45095
FFF	19	SER	-	expression tag	UNP Q45095
FFF	20	HIS	-	expression tag	UNP Q45095
FFF	21	MSE	-	expression tag	UNP Q45095
FFF	22	ALA	-	expression tag	UNP Q45095
FFF	23	SER	-	expression tag	UNP Q45095
GGG	1	MSE	-	initiating methionine	UNP Q45095

Continued on next page...

Continued from previous page...

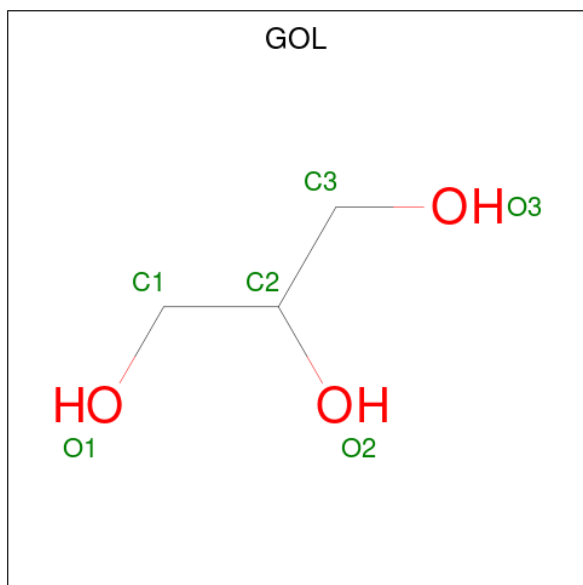
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	2	GLY	-	expression tag	UNP Q45095
GGG	3	SER	-	expression tag	UNP Q45095
GGG	4	SER	-	expression tag	UNP Q45095
GGG	5	HIS	-	expression tag	UNP Q45095
GGG	6	HIS	-	expression tag	UNP Q45095
GGG	7	HIS	-	expression tag	UNP Q45095
GGG	8	HIS	-	expression tag	UNP Q45095
GGG	9	HIS	-	expression tag	UNP Q45095
GGG	10	HIS	-	expression tag	UNP Q45095
GGG	11	SER	-	expression tag	UNP Q45095
GGG	12	SER	-	expression tag	UNP Q45095
GGG	13	GLY	-	expression tag	UNP Q45095
GGG	14	LEU	-	expression tag	UNP Q45095
GGG	15	VAL	-	expression tag	UNP Q45095
GGG	16	PRO	-	expression tag	UNP Q45095
GGG	17	ARG	-	expression tag	UNP Q45095
GGG	18	GLY	-	expression tag	UNP Q45095
GGG	19	SER	-	expression tag	UNP Q45095
GGG	20	HIS	-	expression tag	UNP Q45095
GGG	21	MSE	-	expression tag	UNP Q45095
GGG	22	ALA	-	expression tag	UNP Q45095
GGG	23	SER	-	expression tag	UNP Q45095
HHH	1	MSE	-	initiating methionine	UNP Q45095
HHH	2	GLY	-	expression tag	UNP Q45095
HHH	3	SER	-	expression tag	UNP Q45095
HHH	4	SER	-	expression tag	UNP Q45095
HHH	5	HIS	-	expression tag	UNP Q45095
HHH	6	HIS	-	expression tag	UNP Q45095
HHH	7	HIS	-	expression tag	UNP Q45095
HHH	8	HIS	-	expression tag	UNP Q45095
HHH	9	HIS	-	expression tag	UNP Q45095
HHH	10	HIS	-	expression tag	UNP Q45095
HHH	11	SER	-	expression tag	UNP Q45095
HHH	12	SER	-	expression tag	UNP Q45095
HHH	13	GLY	-	expression tag	UNP Q45095
HHH	14	LEU	-	expression tag	UNP Q45095
HHH	15	VAL	-	expression tag	UNP Q45095
HHH	16	PRO	-	expression tag	UNP Q45095
HHH	17	ARG	-	expression tag	UNP Q45095
HHH	18	GLY	-	expression tag	UNP Q45095
HHH	19	SER	-	expression tag	UNP Q45095
HHH	20	HIS	-	expression tag	UNP Q45095

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
HHH	21	MSE	-	expression tag	UNP Q45095
HHH	22	ALA	-	expression tag	UNP Q45095
HHH	23	SER	-	expression tag	UNP Q45095

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
2	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
2	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
2	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
2	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
2	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
2	FFF	1	Total	C	H	O	2	0
			14	3	8	3		
2	HHH	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	2	Total 2	Cl 2	0	0
3	BBB	1	Total 1	Cl 1	0	0
3	CCC	1	Total 1	Cl 1	0	0
3	DDD	2	Total 2	Cl 2	0	0
3	EEE	2	Total 2	Cl 2	0	0
3	FFF	1	Total 1	Cl 1	0	0
3	GGG	2	Total 2	Cl 2	0	0
3	HHH	1	Total 1	Cl 1	0	0

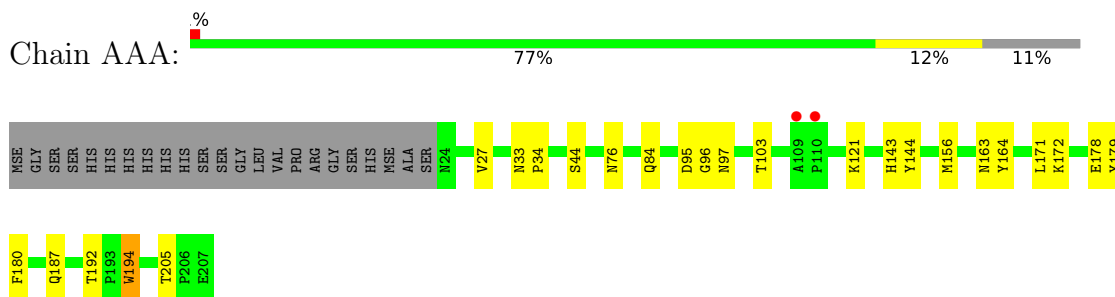
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	140	Total 140	O 140	0	0
4	BBB	114	Total 114	O 114	0	0
4	CCC	121	Total 121	O 121	0	0
4	DDD	114	Total 114	O 114	0	0
4	EEE	81	Total 81	O 81	0	0
4	FFF	67	Total 67	O 67	0	0
4	GGG	86	Total 86	O 86	0	0
4	HHH	73	Total 73	O 73	0	0

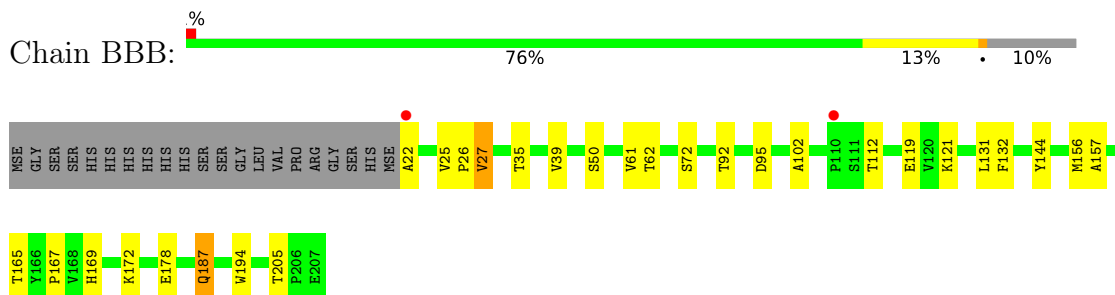
3 Residue-property plots [i](#)

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.

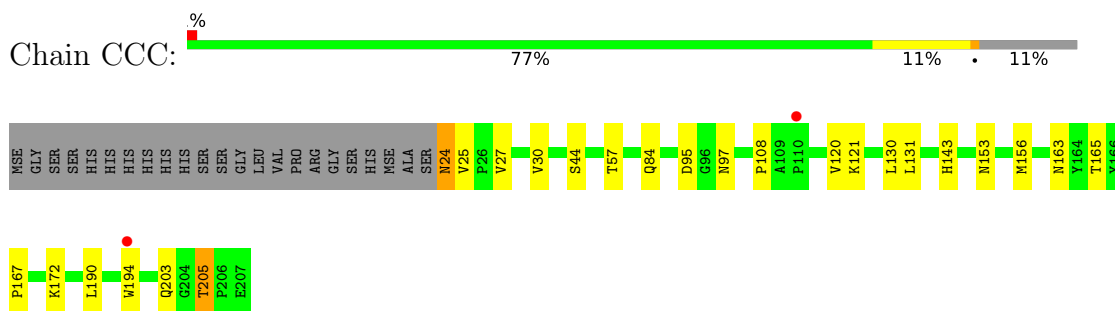
- Molecule 1: Beta-1,3-glucanase bglH



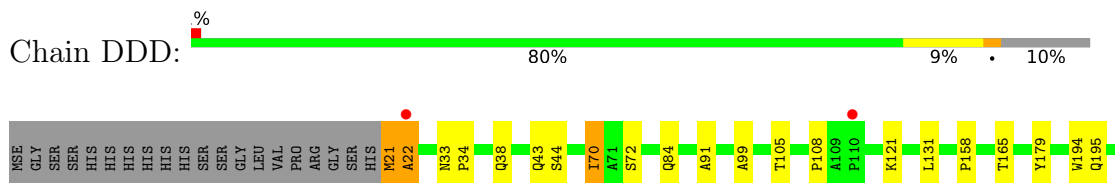
- Molecule 1: Beta-1,3-glucanase bglH



- Molecule 1: Beta-1,3-glucanase bglH



- Molecule 1: Beta-1,3-glucanase bglH





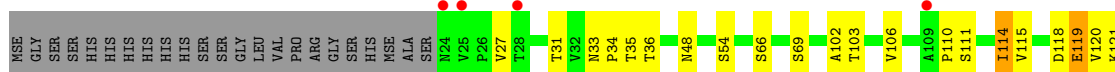
- Molecule 1: Beta-1,3-glucanase bglH

Chain EEE:



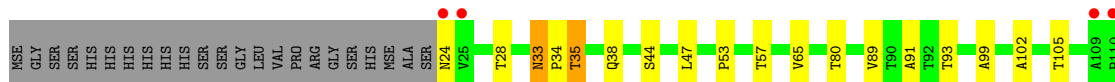
- Molecule 1: Beta-1,3-glucanase bglH

Chain FFF:



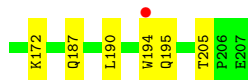
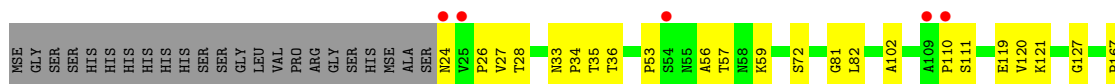
- Molecule 1: Beta-1,3-glucanase bglH

Chain GGG:



- Molecule 1: Beta-1,3-glucanase bglH

Chain HHH:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.12Å 51.72Å 168.66Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	48.77 – 2.16 48.77 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.77-2.16) 98.3 (48.77-2.16)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.240 , 0.292 (Not available) , 0.260	Depositor DCC
R_{free} test set	4801 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22187	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 57.75 % 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 2.2625e-05. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	AAA	1.16	0/1381	1.42	1/1899 (0.1%)
1	BBB	1.23	1/1392 (0.1%)	1.47	7/1914 (0.4%)
1	CCC	1.21	1/1381 (0.1%)	1.43	6/1899 (0.3%)
1	DDD	1.20	1/1400 (0.1%)	1.40	3/1924 (0.2%)
1	EEE	1.17	1/1371 (0.1%)	1.42	3/1884 (0.2%)
1	FFF	1.18	1/1365 (0.1%)	1.48	8/1876 (0.4%)
1	GGG	1.14	0/1365	1.44	3/1876 (0.2%)
1	HHH	1.15	0/1365	1.42	5/1876 (0.3%)
All	All	1.18	5/11020 (0.0%)	1.43	36/15148 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	158	PRO	C-O	-5.89	1.17	1.23
1	DDD	158	PRO	C-O	-5.85	1.17	1.23
1	CCC	25	VAL	N-CA	5.76	1.50	1.46
1	BBB	25	VAL	N-CA	5.51	1.50	1.46
1	EEE	25	VAL	N-CA	5.43	1.50	1.46

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	205	THR	CB-CA-C	9.56	121.15	110.15
1	EEE	112	THR	CA-CB-OG1	-8.36	97.07	109.60
1	BBB	62	THR	CA-CB-OG1	-6.70	99.56	109.60
1	BBB	156	MSE	CG-SE-CE	6.62	113.49	98.92
1	DDD	21	MSE	CG-SE-CE	6.52	113.28	98.92

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	AAA	1348	1312	1308	13	0
1	BBB	1359	1322	1318	14	0
1	CCC	1348	1312	1308	12	0
1	DDD	1367	1332	1327	11	0
1	EEE	1340	1307	1303	18	0
1	FFF	1337	1303	1298	16	0
1	GGG	1337	1303	1298	16	0
1	HHH	1337	1303	1298	12	0
2	AAA	12	16	16	4	0
2	BBB	12	16	16	2	0
2	CCC	6	8	8	3	0
2	DDD	6	8	8	1	0
2	FFF	6	8	8	0	0
2	HHH	6	8	8	0	0
3	AAA	2	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	2	0	0	0	0
3	EEE	2	0	0	2	0
3	FFF	1	0	0	0	0
3	GGG	2	0	0	0	0
3	HHH	1	0	0	0	0
4	AAA	140	0	0	3	0
4	BBB	114	0	0	0	0
4	CCC	121	0	0	0	0
4	DDD	114	0	0	0	0
4	EEE	81	0	0	0	0
4	FFF	67	0	0	4	0
4	GGG	86	0	0	1	0
4	HHH	73	0	0	2	0
All	All	11629	10558	10522	111	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 5.

The worst 5 of 111 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:EEE:180:PHE:HD1	1:EEE:194:TRP:HE1	1.10	0.99
1:EEE:180:PHE:HD1	1:EEE:194:TRP:NE1	1.79	0.79
1:EEE:180:PHE:CD1	1:EEE:194:TRP:NE1	2.52	0.76
1:AAA:97:ASN:HD22	2:AAA:302:GOL:C1	2.04	0.71
1:DDD:84:GLN:NE2	1:DDD:108:PRO:HB3	2.07	0.68

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	AAA	183/207 (88%)	174 (95%)	9 (5%)	0	100	100
1	BBB	185/207 (89%)	177 (96%)	8 (4%)	0	100	100
1	CCC	183/207 (88%)	176 (96%)	7 (4%)	0	100	100
1	DDD	186/207 (90%)	179 (96%)	6 (3%)	1 (0%)	24	20
1	EEE	183/207 (88%)	173 (94%)	10 (6%)	0	100	100
1	FFF	182/207 (88%)	170 (93%)	10 (6%)	2 (1%)	11	7
1	GGG	182/207 (88%)	164 (90%)	17 (9%)	1 (0%)	24	20
1	HHH	182/207 (88%)	171 (94%)	10 (6%)	1 (0%)	24	20
All	All	1466/1656 (88%)	1384 (94%)	77 (5%)	5 (0%)	36	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	119	GLU
1	GGG	57	THR
1	DDD	22	ALA
1	FFF	206	PRO
1	HHH	127	GLY

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	AAA	147/162 (91%)	140 (95%)	7 (5%)	23	20
1	BBB	148/162 (91%)	142 (96%)	6 (4%)	27	26
1	CCC	147/162 (91%)	139 (95%)	8 (5%)	20	16
1	DDD	149/162 (92%)	143 (96%)	6 (4%)	28	27
1	EEE	147/162 (91%)	140 (95%)	7 (5%)	23	20
1	FFF	146/162 (90%)	136 (93%)	10 (7%)	14	10
1	GGG	146/162 (90%)	141 (97%)	5 (3%)	32	33
1	HHH	146/162 (90%)	139 (95%)	7 (5%)	23	20
All	All	1176/1296 (91%)	1120 (95%)	56 (5%)	24	20

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	101	SER
1	HHH	187	GLN
1	FFF	36	THR
1	HHH	172	LYS
1	HHH	27	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 20 ligands modelled in this entry, 12 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	$\# Z > 2$
2	GOL	DDD	302	-	5,5,5	0.14	0	5,5,5	0.33	0
2	GOL	AAA	302	-	5,5,5	0.12	0	5,5,5	0.44	0
2	GOL	BBB	601	-	5,5,5	0.11	0	5,5,5	0.35	0
2	GOL	CCC	301	-	5,5,5	0.14	0	5,5,5	0.41	0
2	GOL	HHH	301	-	5,5,5	0.16	0	5,5,5	0.17	0
2	GOL	BBB	602	-	5,5,5	0.11	0	5,5,5	0.37	0
2	GOL	AAA	301	-	5,5,5	0.14	0	5,5,5	0.34	0
2	GOL	FFF	301	-	5,5,5	0.10	0	5,5,5	0.27	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	GOL	DDD	302	-	-	2/4/4/4	-
2	GOL	AAA	302	-	-	3/4/4/4	-
2	GOL	BBB	601	-	-	4/4/4/4	-
2	GOL	CCC	301	-	-	0/4/4/4	-
2	GOL	HHH	301	-	-	2/4/4/4	-
2	GOL	BBB	602	-	-	2/4/4/4	-
2	GOL	AAA	301	-	-	2/4/4/4	-
2	GOL	FFF	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	GOL	C1-C2-C3-O3
2	AAA	301	GOL	O2-C2-C3-O3
2	AAA	302	GOL	C1-C2-C3-O3
2	BBB	601	GOL	O1-C1-C2-C3
2	BBB	602	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	302	GOL	1	0
2	AAA	302	GOL	3	0
2	BBB	601	GOL	1	0
2	CCC	301	GOL	3	0
2	BBB	602	GOL	1	0
2	AAA	301	GOL	1	0

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	AAA	183/207 (88%)	-0.19	2 (1%) 78 80	14, 21, 40, 57	1 (0%)
1	BBB	185/207 (89%)	-0.06	2 (1%) 78 80	15, 25, 40, 60	1 (0%)
1	CCC	183/207 (88%)	-0.20	2 (1%) 78 80	14, 23, 38, 54	1 (0%)
1	DDD	185/207 (89%)	-0.06	2 (1%) 78 80	14, 26, 42, 69	1 (0%)
1	EEE	183/207 (88%)	0.08	5 (2%) 56 60	13, 28, 49, 63	1 (0%)
1	FFF	183/207 (88%)	0.24	5 (2%) 56 60	19, 31, 56, 70	0
1	GGG	183/207 (88%)	0.16	6 (3%) 49 53	18, 28, 50, 72	0
1	HHH	183/207 (88%)	0.22	6 (3%) 49 53	21, 30, 53, 68	0
All	All	1468/1656 (88%)	0.02	30 (2%) 65 69	13, 26, 49, 72	5 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	22	ALA	8.3
1	FFF	194	TRP	6.6
1	EEE	194	TRP	5.2
1	DDD	22	ALA	4.4
1	HHH	194	TRP	4.1

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 oligosaccharides 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. 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	GOL	AAA	301	6/6	0.70	0.18	42,43,46,49	2
2	GOL	AAA	302	6/6	0.74	0.19	42,45,47,51	2
2	GOL	CCC	301	6/6	0.79	0.15	36,41,46,46	2
2	GOL	HHH	301	6/6	0.87	0.15	42,44,46,47	2
2	GOL	BBB	601	6/6	0.89	0.12	41,43,50,51	2
2	GOL	FFF	301	6/6	0.91	0.10	36,41,42,44	2
2	GOL	DDD	302	6/6	0.91	0.12	40,41,42,42	2
2	GOL	BBB	602	6/6	0.92	0.10	32,33,42,42	2
3	CL	DDD	301	1/1	0.95	0.06	25,25,25,25	0
3	CL	DDD	303	1/1	0.95	0.06	21,21,21,21	0
3	CL	EEE	302	1/1	0.95	0.07	33,33,33,33	0
3	CL	GGG	302	1/1	0.95	0.06	29,29,29,29	0
3	CL	HHH	302	1/1	0.95	0.06	33,33,33,33	0
3	CL	EEE	301	1/1	0.96	0.05	23,23,23,23	0
3	CL	GGG	301	1/1	0.97	0.06	28,28,28,28	0
3	CL	AAA	303	1/1	0.97	0.04	26,26,26,26	0
3	CL	BBB	603	1/1	0.97	0.04	20,20,20,20	0
3	CL	AAA	304	1/1	0.98	0.06	26,26,26,26	0
3	CL	CCC	302	1/1	0.98	0.03	25,25,25,25	0
3	CL	FFF	302	1/1	0.98	0.04	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.