



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:41 AM UTC

PDB ID : 4QAW / pdb_00004qaw
Title : Structure of modular Xyn30D from *Paenibacillus barcinonensis*
Authors : Sainz-Polo, M.A.; Sanz-Aparicio, J.
Deposited on : 2014-05-06
Resolution : 2.40 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
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

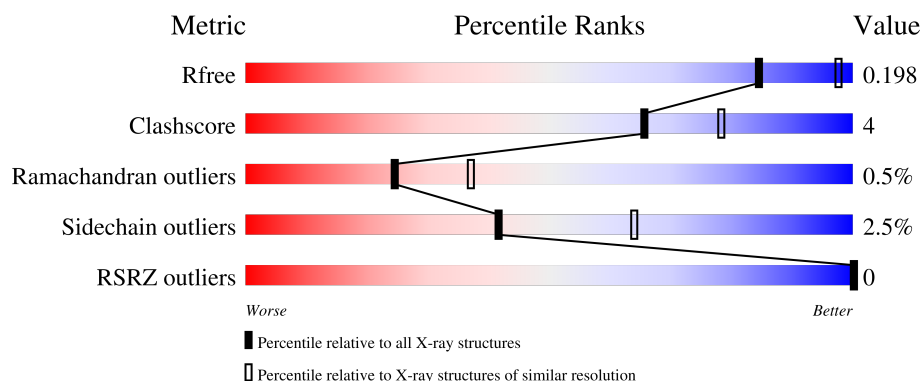
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	563	
1	B	563	
1	C	563	
1	D	563	
1	E	563	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	563	86% 8% • 6%
1	G	563	86% 7% •• 6%
1	H	563	83% 10% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33266 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 Xyn30D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4179	2623	723	820	13			
1	B	533	Total	C	N	O	S	0	0	0
			4146	2603	718	812	13			
1	C	532	Total	C	N	O	S	0	0	0
			4142	2601	716	812	13			
1	D	531	Total	C	N	O	S	0	0	0
			4138	2599	715	811	13			
1	E	529	Total	C	N	O	S	0	0	0
			4126	2593	712	808	13			
1	F	531	Total	C	N	O	S	0	0	0
			4138	2599	715	811	13			
1	G	531	Total	C	N	O	S	0	0	0
			4138	2599	715	811	13			
1	H	533	Total	C	N	O	S	0	0	0
			4148	2605	718	812	13			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	ALA	-	expression tag	UNP H6WCZ0
A	532	LYS	-	expression tag	UNP H6WCZ0
A	533	GLY	-	expression tag	UNP H6WCZ0
A	534	GLU	-	expression tag	UNP H6WCZ0
A	535	LEU	-	expression tag	UNP H6WCZ0
A	536	ASN	-	expression tag	UNP H6WCZ0
A	537	SER	-	expression tag	UNP H6WCZ0
A	538	LYS	-	expression tag	UNP H6WCZ0
A	539	LEU	-	expression tag	UNP H6WCZ0
A	540	GLU	-	expression tag	UNP H6WCZ0
A	541	GLY	-	expression tag	UNP H6WCZ0
A	542	LYS	-	expression tag	UNP H6WCZ0
A	543	PRO	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ILE	-	expression tag	UNP H6WCZ0
A	545	PRO	-	expression tag	UNP H6WCZ0
A	546	ASN	-	expression tag	UNP H6WCZ0
A	547	PRO	-	expression tag	UNP H6WCZ0
A	548	LEU	-	expression tag	UNP H6WCZ0
A	549	LEU	-	expression tag	UNP H6WCZ0
A	550	GLY	-	expression tag	UNP H6WCZ0
A	551	LEU	-	expression tag	UNP H6WCZ0
A	552	ASP	-	expression tag	UNP H6WCZ0
A	553	SER	-	expression tag	UNP H6WCZ0
A	554	THR	-	expression tag	UNP H6WCZ0
A	555	ARG	-	expression tag	UNP H6WCZ0
A	556	THR	-	expression tag	UNP H6WCZ0
A	557	GLY	-	expression tag	UNP H6WCZ0
A	558	HIS	-	expression tag	UNP H6WCZ0
A	559	HIS	-	expression tag	UNP H6WCZ0
A	560	HIS	-	expression tag	UNP H6WCZ0
A	561	HIS	-	expression tag	UNP H6WCZ0
A	562	HIS	-	expression tag	UNP H6WCZ0
A	563	HIS	-	expression tag	UNP H6WCZ0
B	531	ALA	-	expression tag	UNP H6WCZ0
B	532	LYS	-	expression tag	UNP H6WCZ0
B	533	GLY	-	expression tag	UNP H6WCZ0
B	534	GLU	-	expression tag	UNP H6WCZ0
B	535	LEU	-	expression tag	UNP H6WCZ0
B	536	ASN	-	expression tag	UNP H6WCZ0
B	537	SER	-	expression tag	UNP H6WCZ0
B	538	LYS	-	expression tag	UNP H6WCZ0
B	539	LEU	-	expression tag	UNP H6WCZ0
B	540	GLU	-	expression tag	UNP H6WCZ0
B	541	GLY	-	expression tag	UNP H6WCZ0
B	542	LYS	-	expression tag	UNP H6WCZ0
B	543	PRO	-	expression tag	UNP H6WCZ0
B	544	ILE	-	expression tag	UNP H6WCZ0
B	545	PRO	-	expression tag	UNP H6WCZ0
B	546	ASN	-	expression tag	UNP H6WCZ0
B	547	PRO	-	expression tag	UNP H6WCZ0
B	548	LEU	-	expression tag	UNP H6WCZ0
B	549	LEU	-	expression tag	UNP H6WCZ0
B	550	GLY	-	expression tag	UNP H6WCZ0
B	551	LEU	-	expression tag	UNP H6WCZ0
B	552	ASP	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	553	SER	-	expression tag	UNP H6WCZ0
B	554	THR	-	expression tag	UNP H6WCZ0
B	555	ARG	-	expression tag	UNP H6WCZ0
B	556	THR	-	expression tag	UNP H6WCZ0
B	557	GLY	-	expression tag	UNP H6WCZ0
B	558	HIS	-	expression tag	UNP H6WCZ0
B	559	HIS	-	expression tag	UNP H6WCZ0
B	560	HIS	-	expression tag	UNP H6WCZ0
B	561	HIS	-	expression tag	UNP H6WCZ0
B	562	HIS	-	expression tag	UNP H6WCZ0
B	563	HIS	-	expression tag	UNP H6WCZ0
C	531	ALA	-	expression tag	UNP H6WCZ0
C	532	LYS	-	expression tag	UNP H6WCZ0
C	533	GLY	-	expression tag	UNP H6WCZ0
C	534	GLU	-	expression tag	UNP H6WCZ0
C	535	LEU	-	expression tag	UNP H6WCZ0
C	536	ASN	-	expression tag	UNP H6WCZ0
C	537	SER	-	expression tag	UNP H6WCZ0
C	538	LYS	-	expression tag	UNP H6WCZ0
C	539	LEU	-	expression tag	UNP H6WCZ0
C	540	GLU	-	expression tag	UNP H6WCZ0
C	541	GLY	-	expression tag	UNP H6WCZ0
C	542	LYS	-	expression tag	UNP H6WCZ0
C	543	PRO	-	expression tag	UNP H6WCZ0
C	544	ILE	-	expression tag	UNP H6WCZ0
C	545	PRO	-	expression tag	UNP H6WCZ0
C	546	ASN	-	expression tag	UNP H6WCZ0
C	547	PRO	-	expression tag	UNP H6WCZ0
C	548	LEU	-	expression tag	UNP H6WCZ0
C	549	LEU	-	expression tag	UNP H6WCZ0
C	550	GLY	-	expression tag	UNP H6WCZ0
C	551	LEU	-	expression tag	UNP H6WCZ0
C	552	ASP	-	expression tag	UNP H6WCZ0
C	553	SER	-	expression tag	UNP H6WCZ0
C	554	THR	-	expression tag	UNP H6WCZ0
C	555	ARG	-	expression tag	UNP H6WCZ0
C	556	THR	-	expression tag	UNP H6WCZ0
C	557	GLY	-	expression tag	UNP H6WCZ0
C	558	HIS	-	expression tag	UNP H6WCZ0
C	559	HIS	-	expression tag	UNP H6WCZ0
C	560	HIS	-	expression tag	UNP H6WCZ0
C	561	HIS	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	562	HIS	-	expression tag	UNP H6WCZ0
C	563	HIS	-	expression tag	UNP H6WCZ0
D	531	ALA	-	expression tag	UNP H6WCZ0
D	532	LYS	-	expression tag	UNP H6WCZ0
D	533	GLY	-	expression tag	UNP H6WCZ0
D	534	GLU	-	expression tag	UNP H6WCZ0
D	535	LEU	-	expression tag	UNP H6WCZ0
D	536	ASN	-	expression tag	UNP H6WCZ0
D	537	SER	-	expression tag	UNP H6WCZ0
D	538	LYS	-	expression tag	UNP H6WCZ0
D	539	LEU	-	expression tag	UNP H6WCZ0
D	540	GLU	-	expression tag	UNP H6WCZ0
D	541	GLY	-	expression tag	UNP H6WCZ0
D	542	LYS	-	expression tag	UNP H6WCZ0
D	543	PRO	-	expression tag	UNP H6WCZ0
D	544	ILE	-	expression tag	UNP H6WCZ0
D	545	PRO	-	expression tag	UNP H6WCZ0
D	546	ASN	-	expression tag	UNP H6WCZ0
D	547	PRO	-	expression tag	UNP H6WCZ0
D	548	LEU	-	expression tag	UNP H6WCZ0
D	549	LEU	-	expression tag	UNP H6WCZ0
D	550	GLY	-	expression tag	UNP H6WCZ0
D	551	LEU	-	expression tag	UNP H6WCZ0
D	552	ASP	-	expression tag	UNP H6WCZ0
D	553	SER	-	expression tag	UNP H6WCZ0
D	554	THR	-	expression tag	UNP H6WCZ0
D	555	ARG	-	expression tag	UNP H6WCZ0
D	556	THR	-	expression tag	UNP H6WCZ0
D	557	GLY	-	expression tag	UNP H6WCZ0
D	558	HIS	-	expression tag	UNP H6WCZ0
D	559	HIS	-	expression tag	UNP H6WCZ0
D	560	HIS	-	expression tag	UNP H6WCZ0
D	561	HIS	-	expression tag	UNP H6WCZ0
D	562	HIS	-	expression tag	UNP H6WCZ0
D	563	HIS	-	expression tag	UNP H6WCZ0
E	531	ALA	-	expression tag	UNP H6WCZ0
E	532	LYS	-	expression tag	UNP H6WCZ0
E	533	GLY	-	expression tag	UNP H6WCZ0
E	534	GLU	-	expression tag	UNP H6WCZ0
E	535	LEU	-	expression tag	UNP H6WCZ0
E	536	ASN	-	expression tag	UNP H6WCZ0
E	537	SER	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	538	LYS	-	expression tag	UNP H6WCZ0
E	539	LEU	-	expression tag	UNP H6WCZ0
E	540	GLU	-	expression tag	UNP H6WCZ0
E	541	GLY	-	expression tag	UNP H6WCZ0
E	542	LYS	-	expression tag	UNP H6WCZ0
E	543	PRO	-	expression tag	UNP H6WCZ0
E	544	ILE	-	expression tag	UNP H6WCZ0
E	545	PRO	-	expression tag	UNP H6WCZ0
E	546	ASN	-	expression tag	UNP H6WCZ0
E	547	PRO	-	expression tag	UNP H6WCZ0
E	548	LEU	-	expression tag	UNP H6WCZ0
E	549	LEU	-	expression tag	UNP H6WCZ0
E	550	GLY	-	expression tag	UNP H6WCZ0
E	551	LEU	-	expression tag	UNP H6WCZ0
E	552	ASP	-	expression tag	UNP H6WCZ0
E	553	SER	-	expression tag	UNP H6WCZ0
E	554	THR	-	expression tag	UNP H6WCZ0
E	555	ARG	-	expression tag	UNP H6WCZ0
E	556	THR	-	expression tag	UNP H6WCZ0
E	557	GLY	-	expression tag	UNP H6WCZ0
E	558	HIS	-	expression tag	UNP H6WCZ0
E	559	HIS	-	expression tag	UNP H6WCZ0
E	560	HIS	-	expression tag	UNP H6WCZ0
E	561	HIS	-	expression tag	UNP H6WCZ0
E	562	HIS	-	expression tag	UNP H6WCZ0
E	563	HIS	-	expression tag	UNP H6WCZ0
F	531	ALA	-	expression tag	UNP H6WCZ0
F	532	LYS	-	expression tag	UNP H6WCZ0
F	533	GLY	-	expression tag	UNP H6WCZ0
F	534	GLU	-	expression tag	UNP H6WCZ0
F	535	LEU	-	expression tag	UNP H6WCZ0
F	536	ASN	-	expression tag	UNP H6WCZ0
F	537	SER	-	expression tag	UNP H6WCZ0
F	538	LYS	-	expression tag	UNP H6WCZ0
F	539	LEU	-	expression tag	UNP H6WCZ0
F	540	GLU	-	expression tag	UNP H6WCZ0
F	541	GLY	-	expression tag	UNP H6WCZ0
F	542	LYS	-	expression tag	UNP H6WCZ0
F	543	PRO	-	expression tag	UNP H6WCZ0
F	544	ILE	-	expression tag	UNP H6WCZ0
F	545	PRO	-	expression tag	UNP H6WCZ0
F	546	ASN	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	547	PRO	-	expression tag	UNP H6WCZ0
F	548	LEU	-	expression tag	UNP H6WCZ0
F	549	LEU	-	expression tag	UNP H6WCZ0
F	550	GLY	-	expression tag	UNP H6WCZ0
F	551	LEU	-	expression tag	UNP H6WCZ0
F	552	ASP	-	expression tag	UNP H6WCZ0
F	553	SER	-	expression tag	UNP H6WCZ0
F	554	THR	-	expression tag	UNP H6WCZ0
F	555	ARG	-	expression tag	UNP H6WCZ0
F	556	THR	-	expression tag	UNP H6WCZ0
F	557	GLY	-	expression tag	UNP H6WCZ0
F	558	HIS	-	expression tag	UNP H6WCZ0
F	559	HIS	-	expression tag	UNP H6WCZ0
F	560	HIS	-	expression tag	UNP H6WCZ0
F	561	HIS	-	expression tag	UNP H6WCZ0
F	562	HIS	-	expression tag	UNP H6WCZ0
F	563	HIS	-	expression tag	UNP H6WCZ0
G	531	ALA	-	expression tag	UNP H6WCZ0
G	532	LYS	-	expression tag	UNP H6WCZ0
G	533	GLY	-	expression tag	UNP H6WCZ0
G	534	GLU	-	expression tag	UNP H6WCZ0
G	535	LEU	-	expression tag	UNP H6WCZ0
G	536	ASN	-	expression tag	UNP H6WCZ0
G	537	SER	-	expression tag	UNP H6WCZ0
G	538	LYS	-	expression tag	UNP H6WCZ0
G	539	LEU	-	expression tag	UNP H6WCZ0
G	540	GLU	-	expression tag	UNP H6WCZ0
G	541	GLY	-	expression tag	UNP H6WCZ0
G	542	LYS	-	expression tag	UNP H6WCZ0
G	543	PRO	-	expression tag	UNP H6WCZ0
G	544	ILE	-	expression tag	UNP H6WCZ0
G	545	PRO	-	expression tag	UNP H6WCZ0
G	546	ASN	-	expression tag	UNP H6WCZ0
G	547	PRO	-	expression tag	UNP H6WCZ0
G	548	LEU	-	expression tag	UNP H6WCZ0
G	549	LEU	-	expression tag	UNP H6WCZ0
G	550	GLY	-	expression tag	UNP H6WCZ0
G	551	LEU	-	expression tag	UNP H6WCZ0
G	552	ASP	-	expression tag	UNP H6WCZ0
G	553	SER	-	expression tag	UNP H6WCZ0
G	554	THR	-	expression tag	UNP H6WCZ0
G	555	ARG	-	expression tag	UNP H6WCZ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	556	THR	-	expression tag	UNP H6WCZ0
G	557	GLY	-	expression tag	UNP H6WCZ0
G	558	HIS	-	expression tag	UNP H6WCZ0
G	559	HIS	-	expression tag	UNP H6WCZ0
G	560	HIS	-	expression tag	UNP H6WCZ0
G	561	HIS	-	expression tag	UNP H6WCZ0
G	562	HIS	-	expression tag	UNP H6WCZ0
G	563	HIS	-	expression tag	UNP H6WCZ0
H	531	ALA	-	expression tag	UNP H6WCZ0
H	532	LYS	-	expression tag	UNP H6WCZ0
H	533	GLY	-	expression tag	UNP H6WCZ0
H	534	GLU	-	expression tag	UNP H6WCZ0
H	535	LEU	-	expression tag	UNP H6WCZ0
H	536	ASN	-	expression tag	UNP H6WCZ0
H	537	SER	-	expression tag	UNP H6WCZ0
H	538	LYS	-	expression tag	UNP H6WCZ0
H	539	LEU	-	expression tag	UNP H6WCZ0
H	540	GLU	-	expression tag	UNP H6WCZ0
H	541	GLY	-	expression tag	UNP H6WCZ0
H	542	LYS	-	expression tag	UNP H6WCZ0
H	543	PRO	-	expression tag	UNP H6WCZ0
H	544	ILE	-	expression tag	UNP H6WCZ0
H	545	PRO	-	expression tag	UNP H6WCZ0
H	546	ASN	-	expression tag	UNP H6WCZ0
H	547	PRO	-	expression tag	UNP H6WCZ0
H	548	LEU	-	expression tag	UNP H6WCZ0
H	549	LEU	-	expression tag	UNP H6WCZ0
H	550	GLY	-	expression tag	UNP H6WCZ0
H	551	LEU	-	expression tag	UNP H6WCZ0
H	552	ASP	-	expression tag	UNP H6WCZ0
H	553	SER	-	expression tag	UNP H6WCZ0
H	554	THR	-	expression tag	UNP H6WCZ0
H	555	ARG	-	expression tag	UNP H6WCZ0
H	556	THR	-	expression tag	UNP H6WCZ0
H	557	GLY	-	expression tag	UNP H6WCZ0
H	558	HIS	-	expression tag	UNP H6WCZ0
H	559	HIS	-	expression tag	UNP H6WCZ0
H	560	HIS	-	expression tag	UNP H6WCZ0
H	561	HIS	-	expression tag	UNP H6WCZ0
H	562	HIS	-	expression tag	UNP H6WCZ0
H	563	HIS	-	expression tag	UNP H6WCZ0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0
2	G	2	Total Ca 2 2	0	0
2	H	2	Total Ca 2 2	0	0

- Molecule 3 is water.

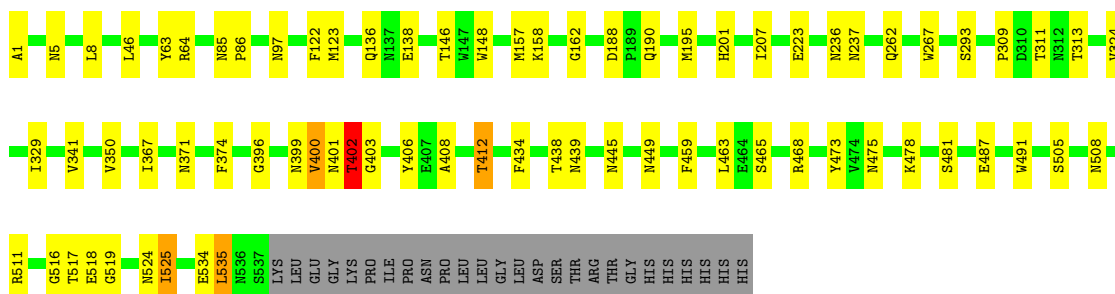
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	21	Total O 21 21	0	0
3	C	10	Total O 10 10	0	0
3	D	11	Total O 11 11	0	0
3	E	18	Total O 18 18	0	0
3	F	6	Total O 6 6	0	0
3	G	6	Total O 6 6	0	0
3	H	13	Total O 13 13	0	0

3 Residue-property plots

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.

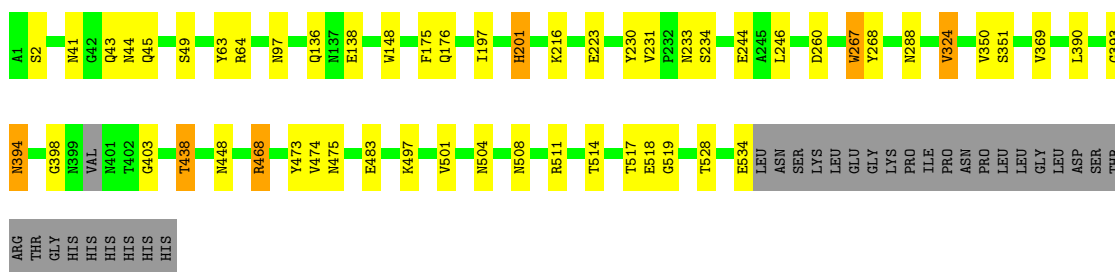
• Molecule 1: Xyn30D

Chain A: 



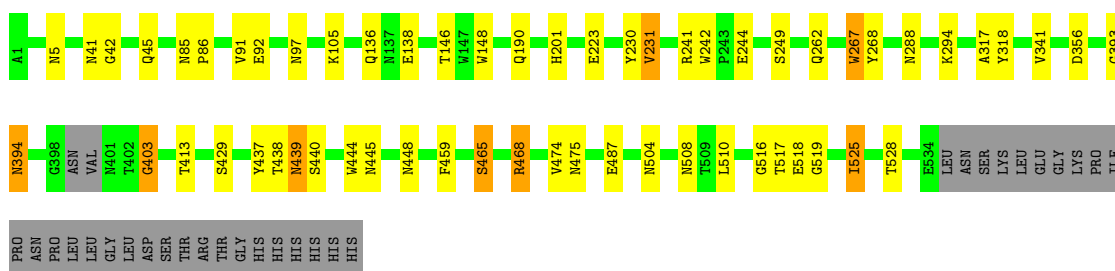
• Molecule 1: Xyn30D

Chain B: 

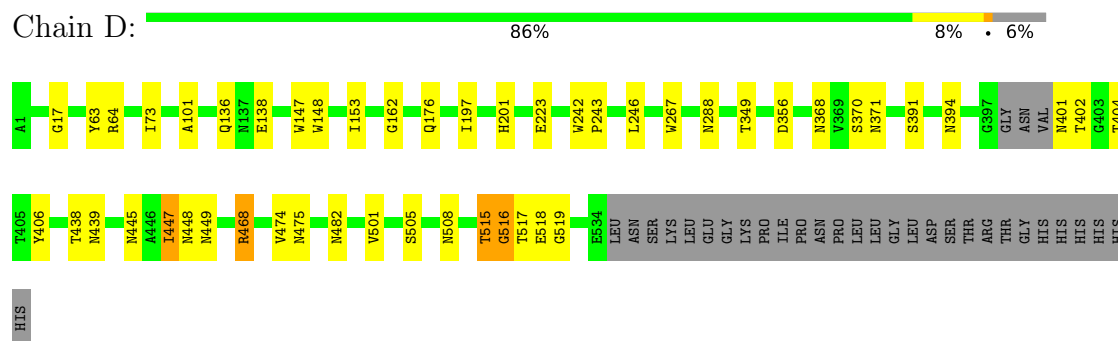


• Molecule 1: Xyn30D

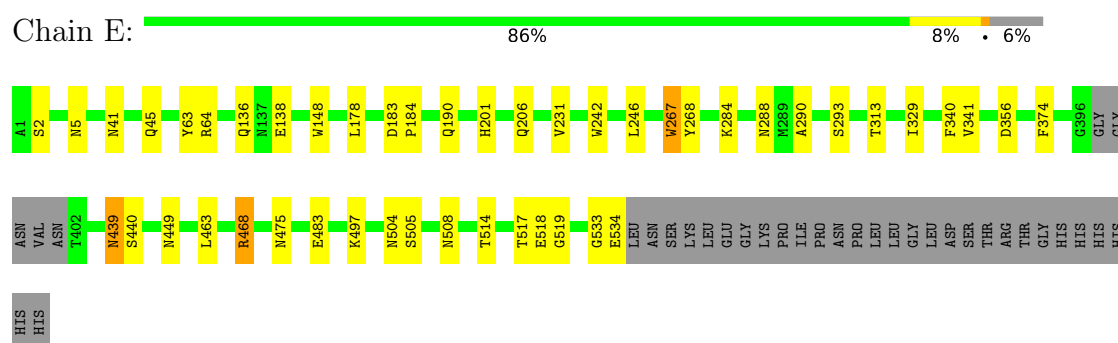
Chain C: 



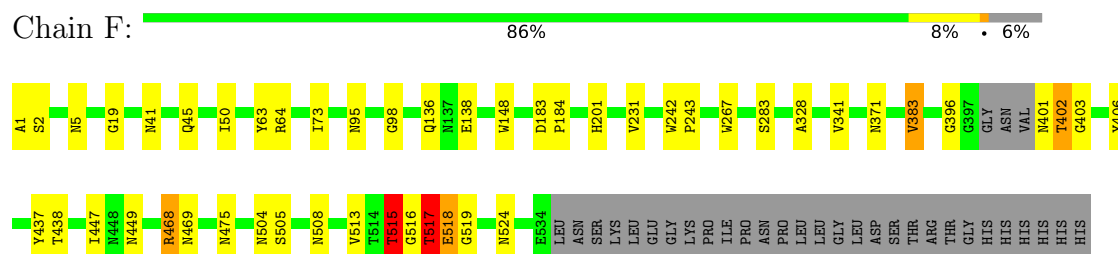
• Molecule 1: Xyn30D



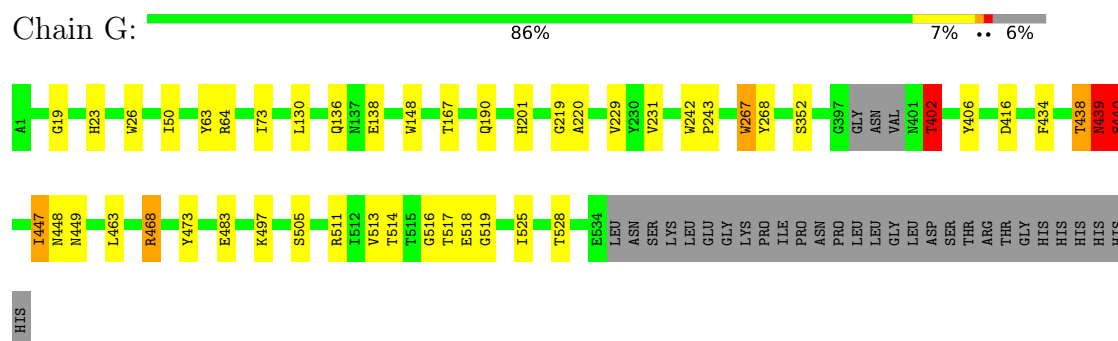
• Molecule 1: Xyn30D



• Molecule 1: Xyn30D



• Molecule 1: Xyn30D



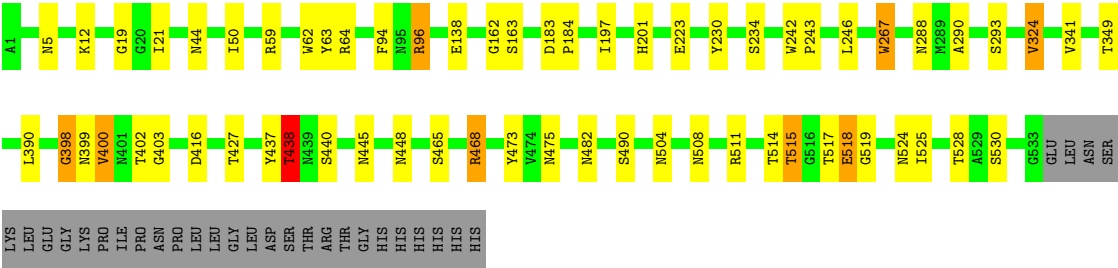
• Molecule 1: Xyn30D

Chain H:

83%

10%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	174.06Å 174.06Å 183.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.77 – 2.40 40.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.77-2.40) 100.0 (40.77-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.202 0.190 , 0.198	Depositor DCC
R_{free} test set	12151 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l 0.469 for h,-h-k,-l 0.064 for -k,-h,-l	Xtriage
Reported twinning fraction	0.510 for H, K, L 0.490 for K, H, -L	Depositor
Outliers	0 of 243712 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33266	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 31.41 % 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 1.1121e-03. 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: CA

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	0.49	0/4278	0.79	3/5826 (0.1%)
1	B	0.52	0/4244	0.79	2/5777 (0.0%)
1	C	0.49	0/4240	0.76	0/5772
1	D	0.49	0/4236	0.78	3/5767 (0.1%)
1	E	0.51	0/4224	0.77	1/5751 (0.0%)
1	F	0.48	0/4236	0.75	2/5767 (0.0%)
1	G	0.52	1/4236 (0.0%)	0.79	3/5767 (0.1%)
1	H	0.50	0/4247	0.79	3/5784 (0.1%)
All	All	0.50	1/33941 (0.0%)	0.78	17/46211 (0.0%)

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	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	440	SER	C-O	-5.13	1.17	1.23

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	438	THR	N-CA-C	-9.04	95.34	109.07
1	G	439	ASN	N-CA-C	8.42	128.74	110.80
1	A	439	ASN	N-CA-C	8.36	122.93	111.39
1	E	439	ASN	N-CA-C	8.16	122.76	111.74
1	F	515	THR	N-CA-C	7.89	120.47	110.61

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Peptide
1	D	162	GLY	Peptide
1	F	515	THR	Peptide
1	G	402	THR	Peptide
1	H	162	GLY	Peptide

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	4179	0	3992	42	0
1	B	4146	0	3957	34	0
1	C	4142	0	3954	33	0
1	D	4138	0	3951	26	0
1	E	4126	0	3942	26	0
1	F	4138	0	3951	29	0
1	G	4138	0	3951	29	0
1	H	4148	0	3964	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	10	0	0	0	0
3	B	21	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	0	0	0
3	D	11	0	0	0	0
3	E	18	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	13	0	0	0	0
All	All	33266	0	31662	247	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 4.

The worst 5 of 247 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:518:GLU:HG2	1:B:519:GLY:H	1.22	1.01
1:G:518:GLU:HG2	1:G:519:GLY:H	1.36	0.89
1:A:468:ARG:HG2	1:A:517:THR:O	1.75	0.86
1:E:468:ARG:HG2	1:E:517:THR:O	1.77	0.84
1:D:401:ASN:N	1:D:402:THR:HA	1.93	0.83

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	535/563 (95%)	511 (96%)	22 (4%)	2 (0%)	30	43
1	B	529/563 (94%)	507 (96%)	19 (4%)	3 (1%)	21	32
1	C	528/563 (94%)	505 (96%)	19 (4%)	4 (1%)	16	25
1	D	527/563 (94%)	510 (97%)	15 (3%)	2 (0%)	30	43
1	E	525/563 (93%)	504 (96%)	20 (4%)	1 (0%)	43	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	527/563 (94%)	504 (96%)	19 (4%)	4 (1%)	16	25
1	G	527/563 (94%)	501 (95%)	24 (5%)	2 (0%)	30	43
1	H	531/563 (94%)	509 (96%)	19 (4%)	3 (1%)	21	32
All	All	4229/4504 (94%)	4051 (96%)	157 (4%)	21 (0%)	24	37

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	ASN
1	C	439	ASN
1	A	267	TRP
1	A	403	GLY
1	B	398	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	A	442/465 (95%)	429 (97%)	13 (3%)	37	60
1	B	437/465 (94%)	427 (98%)	10 (2%)	44	66
1	C	437/465 (94%)	425 (97%)	12 (3%)	39	62
1	D	437/465 (94%)	427 (98%)	10 (2%)	44	66
1	E	436/465 (94%)	429 (98%)	7 (2%)	55	76
1	F	437/465 (94%)	428 (98%)	9 (2%)	47	69
1	G	437/465 (94%)	425 (97%)	12 (3%)	39	62
1	H	438/465 (94%)	423 (97%)	15 (3%)	32	54
All	All	3501/3720 (94%)	3413 (98%)	88 (2%)	42	64

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	402	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	525	ILE
1	F	513	VAL
1	G	352	SER
1	H	96	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	508	ASN
1	G	45	GLN
1	F	44	ASN
1	F	322	ASN
1	G	176	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are 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	537/563 (95%)	-1.66	0 100 100	2, 14, 31, 64	0
1	B	533/563 (94%)	-1.71	0 100 100	2, 9, 20, 65	0
1	C	532/563 (94%)	-1.68	0 100 100	2, 13, 25, 55	0
1	D	531/563 (94%)	-1.67	0 100 100	2, 12, 29, 60	0
1	E	529/563 (93%)	-1.72	0 100 100	2, 10, 21, 41	0
1	F	531/563 (94%)	-1.63	0 100 100	3, 16, 33, 54	0
1	G	531/563 (94%)	-1.68	0 100 100	2, 14, 26, 51	0
1	H	533/563 (94%)	-1.70	0 100 100	2, 11, 25, 62	0
All	All	4257/4504 (94%)	-1.68	0 100 100	2, 12, 27, 65	0

There are no RSRZ outliers to report.

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 [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($\text{\AA}^2$)	Q<0.9
2	CA	A	1001	1/1	0.99	0.03	46,46,46,46	0
2	CA	D	1001	1/1	0.99	0.02	44,44,44,44	0
2	CA	E	1001	1/1	0.99	0.03	41,41,41,41	0
2	CA	H	1001	1/1	0.99	0.03	50,50,50,50	0
2	CA	C	1000	1/1	1.00	0.01	6,6,6,6	0
2	CA	C	1001	1/1	1.00	0.01	21,21,21,21	0
2	CA	D	1000	1/1	1.00	0.01	16,16,16,16	0
2	CA	A	1000	1/1	1.00	0.01	12,12,12,12	0
2	CA	E	1000	1/1	1.00	0.01	14,14,14,14	0
2	CA	B	1000	1/1	1.00	0.00	7,7,7,7	0
2	CA	F	1000	1/1	1.00	0.01	11,11,11,11	0
2	CA	F	1001	1/1	1.00	0.02	51,51,51,51	0
2	CA	G	1000	1/1	1.00	0.02	13,13,13,13	0
2	CA	G	1001	1/1	1.00	0.06	34,34,34,34	0
2	CA	H	1000	1/1	1.00	0.01	10,10,10,10	0
2	CA	B	1001	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.