wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 10:47 PM EDT

PDB ID	:	4QAW
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

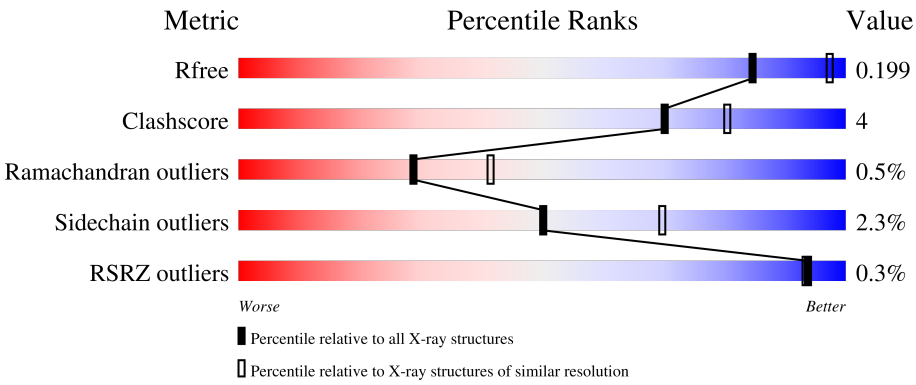
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	% 84% 11% • 5%
1	B	563	85% 10% 5%
1	C	563	84% 10% • 6%
1	D	563	86% 8% 6%
1	E	563	86% 8% 6%

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Mol	Chain	Length	Quality of chain
1	F	563	85% 8% • 6%
1	G	563	87% 7% • 6%
1	H	563	.% 84% 9% • 5%

2 Entry composition (i)

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

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

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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

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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

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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

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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

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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

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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 (three-letter code: 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.

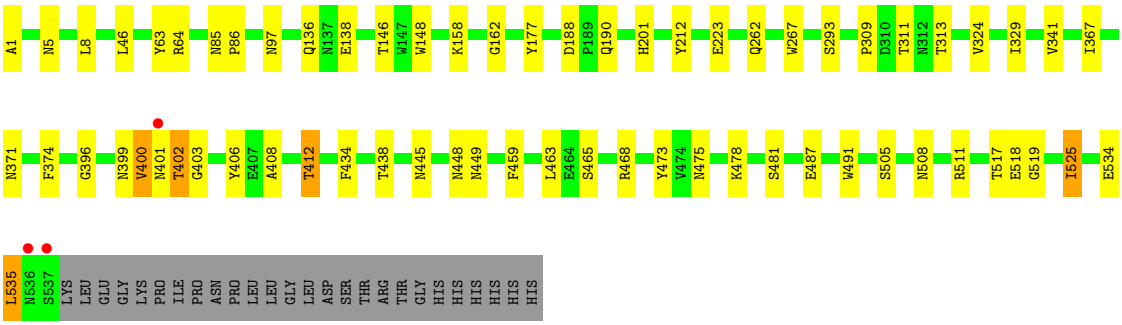
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	21	Total O 21 21	0	0
3	C	10	Total O 10 10	0	0
3	D	11	Total O 11 11	0	0
3	E	18	Total O 18 18	0	0
3	F	6	Total O 6 6	0	0
3	G	6	Total O 6 6	0	0
3	H	13	Total O 13 13	0	0

3 Residue-property plots (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.

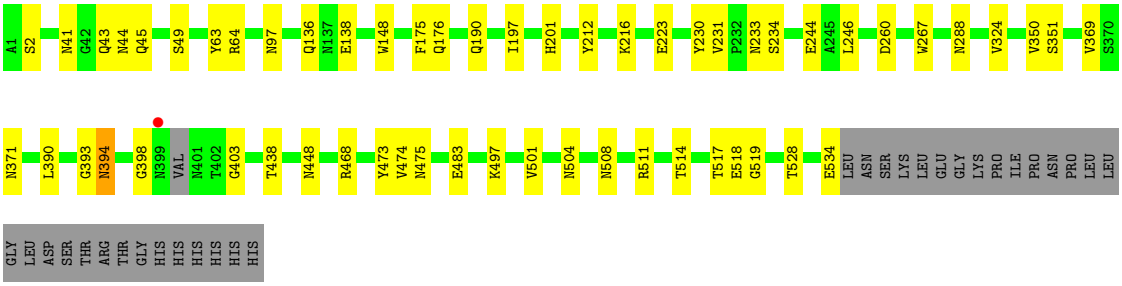
• Molecule 1: Xyn30D

Chain A:



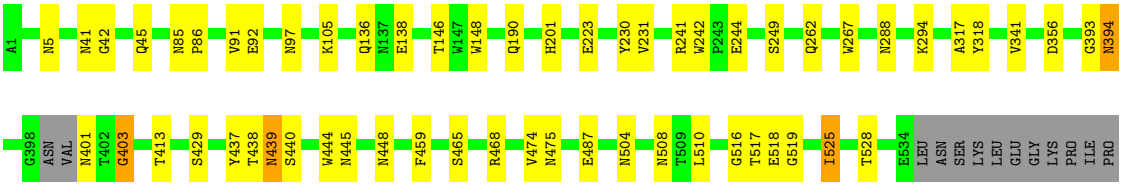
• Molecule 1: Xyn30D

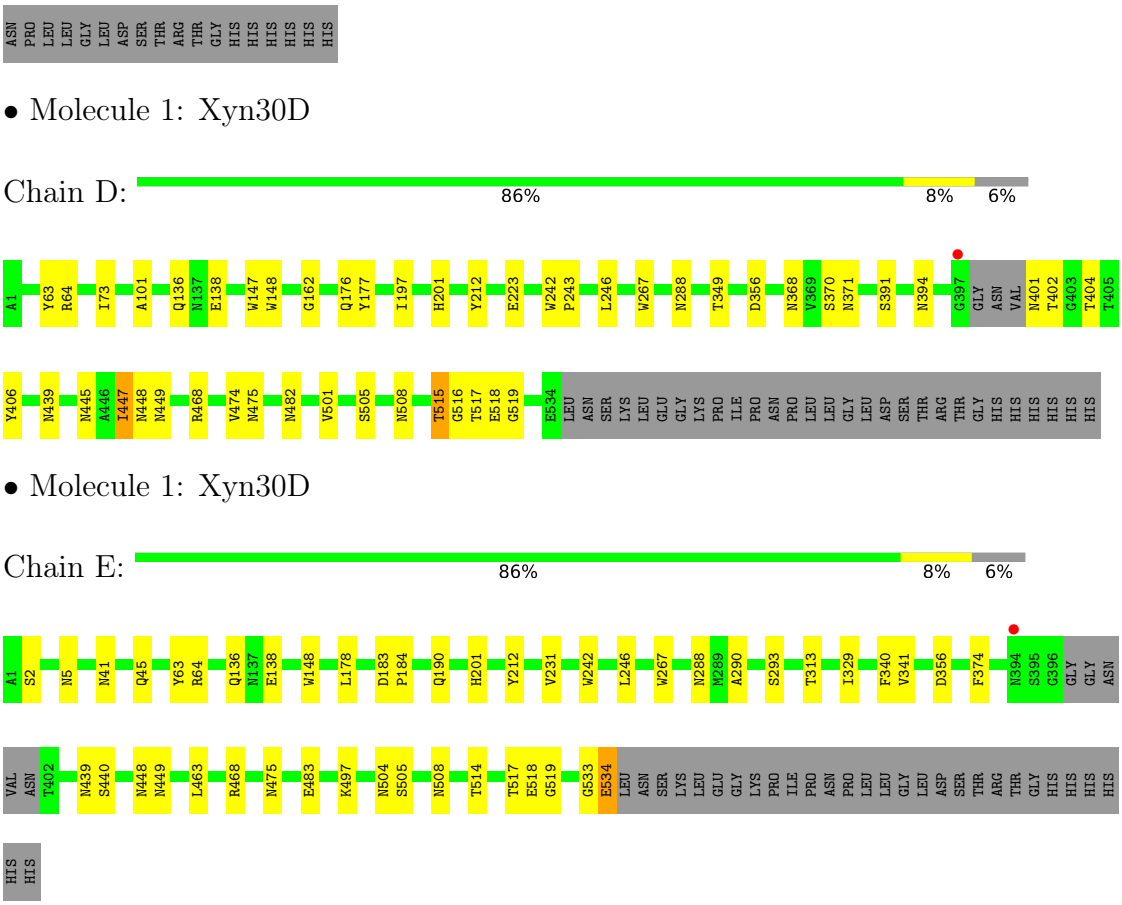
Chain B:



• Molecule 1: Xyn30D

Chain C:




ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS HIS HIS
• Molecule 1: Xyn30D
Chain D:
86%
8%
6%
A1 Y63 R64 I73 A101 Q136 N137 E138 W147 W148 G162 Q176 Y177 I197 H201 Y212 E223 W242 P243 L246 W267 N288 T349 D356 N368 V369 S370 N371 S391 N394 G397 GLY ASN VAL N401 T402 G403 T404 T405
Y406 N439 N445 A446 I447 N448 N449 R468 V474 N475 N482 V501 S505 N508 T515 G516 T517 E518 G519 E534 LEU ASN SER LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: Xyn30D
Chain E:
86%
8%
6%
A1 S2 N5 N41 Q45 Y63 R64 Q136 N137 E138 W148 L178 D183 P184 Q190 H201 Y212 V231 W242 L246 W267 N288 M289 A290 S293 T313 I329 F340 V341 D356 F374 N394 S395 G396 GLY GLY ASN
VAL ASN T402 N439 S440 N448 N449 L463 R468 N475 E483 K497 N504 S505 N508 T514 T517 E518 G519 G533 E534 LEU ASN SER LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS
HIS HIS
• Molecule 1: Xyn30D
Chain F:
85%
8%
• 6%
A1 S2 N5 G19 N41 Q45 I50 Y63 R64 N95 G98 Q136 N137 E138 W148 D183 P184 H201 Y212 V231 W242 P243 W267 S283 A328 V341 N371 V383 N394 S395 G396 G397 GLY ASN VAL N401 T402 G403
Y406 Y437 T438 I447 N448 N449 R468 N469 N475 S490 N504 S505 N508 T515 G516 T517 E518 G519 E534 LEU ASN SER LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS HIS HIS
• Molecule 1: Xyn30D
Chain G:
87%
7%
• 6%
A1 G19 H23 W26 I50 Y63 R64 L130 Q136 N137 E138 W148 T167 Q190 H201 V229 W242 P243 W267 S352 G397 GLY ASN VAL N401 T402 Y406 D416 F434 T438 N439 S440 I447 N448 N449 L463 R468
Y473 E483 K497 S505 R511 I512 V513 T514 T515 G516 T517 E518 G519 T528 E534 LEU ASN SER LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS
• Molecule 1: Xyn30D
Chain H:
%
84%
9%
• 5%

A1
N5
K12
G19
I50
R59
W62
Y63
R64
F94
N95
R96
E138
G162
Y177
D183
P184
I197
H201
E223
Y230
S234
W242
P243
L246
W267
N288
M289
A290
S293
V324
V341
T349
L390
G398
N399
V400
N401
T402
G403
D416
T427
Y437
T438
N439
S440
N448
R468
Y473
V474
N475
N482
S490
N504
N508
R511
T514
T515
G516
T517
E518
G519
N524
I525
T528
A529
S530
G533
GLU
LEU
ASN
SER
LYS
LEU
GLU
GLY
LYS
PRO
ILE
PRO
ASN
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THR
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4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.202 0.190 , 0.199	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)	0.33 , -12.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	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	0.92	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/4278	0.60	0/5826
1	B	0.37	0/4244	0.62	0/5777
1	C	0.35	0/4240	0.58	0/5772
1	D	0.36	0/4236	0.60	0/5767
1	E	0.37	0/4224	0.60	0/5751
1	F	0.35	0/4236	0.58	0/5767
1	G	0.37	0/4236	0.60	1/5767 (0.0%)
1	H	0.37	0/4247	0.62	1/5784 (0.0%)
All	All	0.36	0/33941	0.60	2/46211 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	439	ASN	N-CA-C	6.57	128.74	111.00
1	H	438	THR	N-CA-C	-5.80	95.34	111.00

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	38	0
1	B	4146	0	3957	33	0
1	C	4142	0	3954	32	0
1	D	4138	0	3951	26	0
1	E	4126	0	3942	24	0
1	F	4138	0	3951	28	0
1	G	4138	0	3951	27	0
1	H	4148	0	3964	28	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
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	234	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 234 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%)	34	48
1	B	529/563 (94%)	507 (96%)	19 (4%)	3 (1%)	25	36
1	C	528/563 (94%)	505 (96%)	19 (4%)	4 (1%)	19	29
1	D	527/563 (94%)	510 (97%)	15 (3%)	2 (0%)	34	48
1	E	525/563 (93%)	504 (96%)	20 (4%)	1 (0%)	47	62
1	F	527/563 (94%)	504 (96%)	19 (4%)	4 (1%)	19	29
1	G	527/563 (94%)	501 (95%)	24 (5%)	2 (0%)	34	48
1	H	531/563 (94%)	509 (96%)	19 (4%)	3 (1%)	25	36
All	All	4229/4504 (94%)	4051 (96%)	157 (4%)	21 (0%)	29	41

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	ASN

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Mol	Chain	Res	Type
1	C	439	ASN
1	A	267	TRP
1	A	403	GLY
1	B	398	GLY

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	442/465 (95%)	428 (97%)	14 (3%)	39	59
1	B	437/465 (94%)	426 (98%)	11 (2%)	47	67
1	C	437/465 (94%)	427 (98%)	10 (2%)	50	70
1	D	437/465 (94%)	427 (98%)	10 (2%)	50	70
1	E	436/465 (94%)	428 (98%)	8 (2%)	59	76
1	F	437/465 (94%)	428 (98%)	9 (2%)	53	72
1	G	437/465 (94%)	430 (98%)	7 (2%)	62	79
1	H	438/465 (94%)	426 (97%)	12 (3%)	44	65
All	All	3501/3720 (94%)	3420 (98%)	81 (2%)	50	70

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	394	ASN
1	H	177	TYR
1	F	448	ASN
1	G	402	THR
1	H	448	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	5	ASN

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Mol	Chain	Res	Type
1	H	136	GLN
1	G	136	GLN
1	G	508	ASN
1	H	508	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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%)	-0.74	3 (0%)	89	88	2, 14, 31, 64	0
1	B	533/563 (94%)	-0.83	1 (0%)	95	94	2, 9, 20, 65	0
1	C	532/563 (94%)	-0.79	0	100	100	2, 13, 25, 55	0
1	D	531/563 (94%)	-0.76	1 (0%)	95	94	2, 12, 29, 60	0
1	E	529/563 (93%)	-0.84	1 (0%)	95	94	2, 10, 21, 41	0
1	F	531/563 (94%)	-0.70	1 (0%)	95	94	3, 16, 33, 54	0
1	G	531/563 (94%)	-0.75	1 (0%)	95	94	2, 14, 26, 51	0
1	H	533/563 (94%)	-0.78	3 (0%)	89	88	2, 11, 25, 62	0
All	All	4257/4504 (94%)	-0.77	11 (0%)	94	93	2, 12, 27, 65	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	399	ASN	4.3
1	H	398	GLY	3.1
1	D	397	GLY	2.9
1	B	399	ASN	2.8
1	H	400	VAL	2.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	CA	E	1001	1/1	0.91	0.08	41,41,41,41	0
2	CA	A	1001	1/1	0.93	0.07	46,46,46,46	0
2	CA	F	1001	1/1	0.94	0.08	51,51,51,51	0
2	CA	D	1001	1/1	0.95	0.06	44,44,44,44	0
2	CA	C	1001	1/1	0.96	0.06	21,21,21,21	0
2	CA	G	1001	1/1	0.96	0.10	34,34,34,34	0
2	CA	H	1001	1/1	0.96	0.08	50,50,50,50	0
2	CA	B	1001	1/1	0.97	0.04	23,23,23,23	0
2	CA	G	1000	1/1	0.99	0.04	13,13,13,13	0
2	CA	D	1000	1/1	0.99	0.06	16,16,16,16	0
2	CA	E	1000	1/1	0.99	0.06	14,14,14,14	0
2	CA	C	1000	1/1	1.00	0.08	6,6,6,6	0
2	CA	B	1000	1/1	1.00	0.08	7,7,7,7	0
2	CA	A	1000	1/1	1.00	0.07	12,12,12,12	0
2	CA	H	1000	1/1	1.00	0.08	10,10,10,10	0
2	CA	F	1000	1/1	1.00	0.06	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.