wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:22 AM EDT

PDB ID	:	6FDB
Title	:	Positively supercharged variant of the computationally designed cage protein O3-33
Authors	:	Edwardson, T.; Mori, T.; Hilvert, D.
Deposited on	:	2017-12-22
Resolution	:	3.62 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:

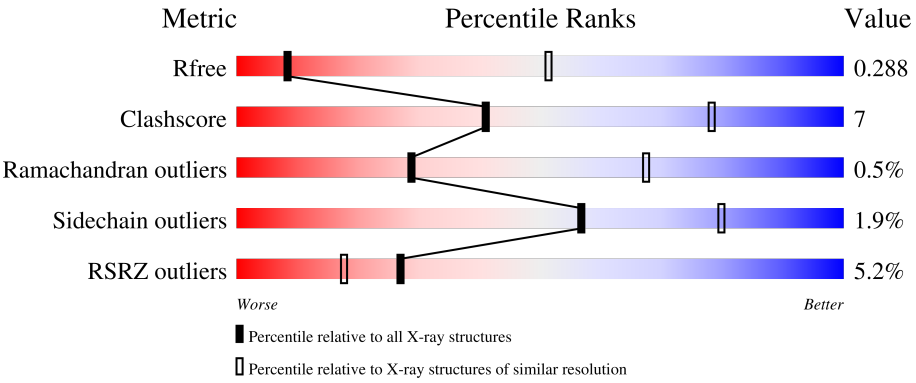
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.62 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 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	192	80% 16% .
1	B	192	4% 80% 15% . .
1	C	192	7% 79% 17% .
1	D	192	5% 79% 16% . .
1	E	192	% 79% 17% .

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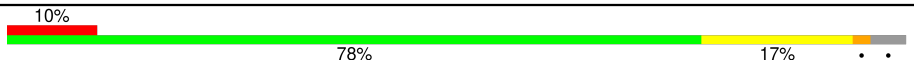
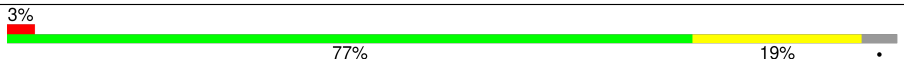
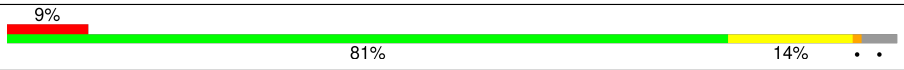
Mol	Chain	Length	Quality of chain
1	F	192	
1	G	192	
1	H	192	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10624 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 Propanediol utilization protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	B	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	C	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	D	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	E	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	F	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	G	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			
1	H	184	Total	C	N	O	S	0	0	0
			1328	830	240	249	9			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
A	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
A	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
A	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
A	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
A	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
A	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
A	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
A	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
A	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
A	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
A	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
A	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47

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Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
A	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
A	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
A	185	LEU	-	expression tag	UNP A0A0M0QF47
A	186	GLU	-	expression tag	UNP A0A0M0QF47
A	187	HIS	-	expression tag	UNP A0A0M0QF47
A	188	HIS	-	expression tag	UNP A0A0M0QF47
A	189	HIS	-	expression tag	UNP A0A0M0QF47
A	190	HIS	-	expression tag	UNP A0A0M0QF47
A	191	HIS	-	expression tag	UNP A0A0M0QF47
A	192	HIS	-	expression tag	UNP A0A0M0QF47
B	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
B	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
B	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
B	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
B	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
B	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
B	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
B	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
B	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
B	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
B	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
B	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
B	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
B	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
B	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
B	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
B	185	LEU	-	expression tag	UNP A0A0M0QF47
B	186	GLU	-	expression tag	UNP A0A0M0QF47
B	187	HIS	-	expression tag	UNP A0A0M0QF47
B	188	HIS	-	expression tag	UNP A0A0M0QF47
B	189	HIS	-	expression tag	UNP A0A0M0QF47
B	190	HIS	-	expression tag	UNP A0A0M0QF47
B	191	HIS	-	expression tag	UNP A0A0M0QF47
B	192	HIS	-	expression tag	UNP A0A0M0QF47
C	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
C	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
C	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
C	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
C	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
C	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
C	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47

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Chain	Residue	Modelled	Actual	Comment	Reference
C	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
C	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
C	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
C	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
C	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
C	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
C	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
C	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
C	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
C	185	LEU	-	expression tag	UNP A0A0M0QF47
C	186	GLU	-	expression tag	UNP A0A0M0QF47
C	187	HIS	-	expression tag	UNP A0A0M0QF47
C	188	HIS	-	expression tag	UNP A0A0M0QF47
C	189	HIS	-	expression tag	UNP A0A0M0QF47
C	190	HIS	-	expression tag	UNP A0A0M0QF47
C	191	HIS	-	expression tag	UNP A0A0M0QF47
C	192	HIS	-	expression tag	UNP A0A0M0QF47
D	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
D	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
D	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
D	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
D	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
D	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
D	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
D	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
D	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
D	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
D	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
D	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
D	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
D	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
D	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
D	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
D	185	LEU	-	expression tag	UNP A0A0M0QF47
D	186	GLU	-	expression tag	UNP A0A0M0QF47
D	187	HIS	-	expression tag	UNP A0A0M0QF47
D	188	HIS	-	expression tag	UNP A0A0M0QF47
D	189	HIS	-	expression tag	UNP A0A0M0QF47
D	190	HIS	-	expression tag	UNP A0A0M0QF47
D	191	HIS	-	expression tag	UNP A0A0M0QF47
D	192	HIS	-	expression tag	UNP A0A0M0QF47
E	11	ARG	THR	engineered mutation	UNP A0A0M0QF47

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Chain	Residue	Modelled	Actual	Comment	Reference
E	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
E	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
E	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
E	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
E	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
E	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
E	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
E	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
E	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
E	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
E	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
E	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
E	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
E	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
E	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
E	185	LEU	-	expression tag	UNP A0A0M0QF47
E	186	GLU	-	expression tag	UNP A0A0M0QF47
E	187	HIS	-	expression tag	UNP A0A0M0QF47
E	188	HIS	-	expression tag	UNP A0A0M0QF47
E	189	HIS	-	expression tag	UNP A0A0M0QF47
E	190	HIS	-	expression tag	UNP A0A0M0QF47
E	191	HIS	-	expression tag	UNP A0A0M0QF47
E	192	HIS	-	expression tag	UNP A0A0M0QF47
F	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
F	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
F	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
F	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
F	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
F	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
F	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
F	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
F	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
F	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
F	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
F	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
F	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
F	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
F	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
F	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
F	185	LEU	-	expression tag	UNP A0A0M0QF47
F	186	GLU	-	expression tag	UNP A0A0M0QF47
F	187	HIS	-	expression tag	UNP A0A0M0QF47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	188	HIS	-	expression tag	UNP A0A0M0QF47
F	189	HIS	-	expression tag	UNP A0A0M0QF47
F	190	HIS	-	expression tag	UNP A0A0M0QF47
F	191	HIS	-	expression tag	UNP A0A0M0QF47
F	192	HIS	-	expression tag	UNP A0A0M0QF47
G	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
G	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
G	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
G	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
G	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
G	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
G	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
G	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
G	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
G	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
G	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
G	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
G	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47
G	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
G	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
G	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
G	185	LEU	-	expression tag	UNP A0A0M0QF47
G	186	GLU	-	expression tag	UNP A0A0M0QF47
G	187	HIS	-	expression tag	UNP A0A0M0QF47
G	188	HIS	-	expression tag	UNP A0A0M0QF47
G	189	HIS	-	expression tag	UNP A0A0M0QF47
G	190	HIS	-	expression tag	UNP A0A0M0QF47
G	191	HIS	-	expression tag	UNP A0A0M0QF47
G	192	HIS	-	expression tag	UNP A0A0M0QF47
H	11	ARG	THR	engineered mutation	UNP A0A0M0QF47
H	15	ALA	LYS	engineered mutation	UNP A0A0M0QF47
H	38	SER	CYS	engineered mutation	UNP A0A0M0QF47
H	39	ARG	PRO	engineered mutation	UNP A0A0M0QF47
H	66	ARG	GLU	engineered mutation	UNP A0A0M0QF47
H	67	LEU	MET	engineered mutation	UNP A0A0M0QF47
H	103	ARG	TRP	engineered mutation	UNP A0A0M0QF47
H	130	ARG	PHE	engineered mutation	UNP A0A0M0QF47
H	148	ALA	ASN	engineered mutation	UNP A0A0M0QF47
H	149	LEU	ASN	engineered mutation	UNP A0A0M0QF47
H	156	SER	GLU	engineered mutation	UNP A0A0M0QF47
H	160	ALA	GLU	engineered mutation	UNP A0A0M0QF47
H	161	TYR	LYS	engineered mutation	UNP A0A0M0QF47

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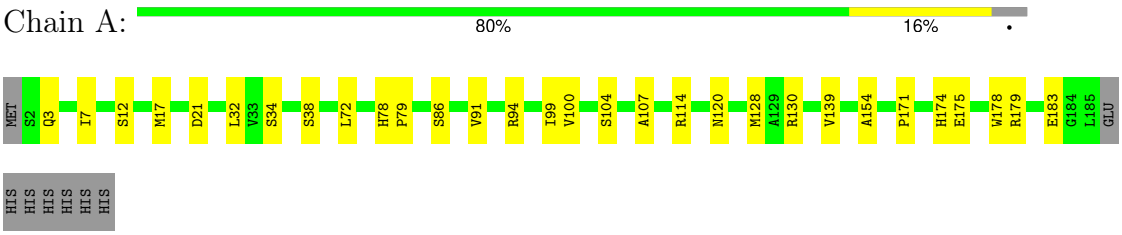
Chain	Residue	Modelled	Actual	Comment	Reference
H	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
H	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
H	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
H	185	LEU	-	expression tag	UNP A0A0M0QF47
H	186	GLU	-	expression tag	UNP A0A0M0QF47
H	187	HIS	-	expression tag	UNP A0A0M0QF47
H	188	HIS	-	expression tag	UNP A0A0M0QF47
H	189	HIS	-	expression tag	UNP A0A0M0QF47
H	190	HIS	-	expression tag	UNP A0A0M0QF47
H	191	HIS	-	expression tag	UNP A0A0M0QF47
H	192	HIS	-	expression tag	UNP A0A0M0QF47

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.

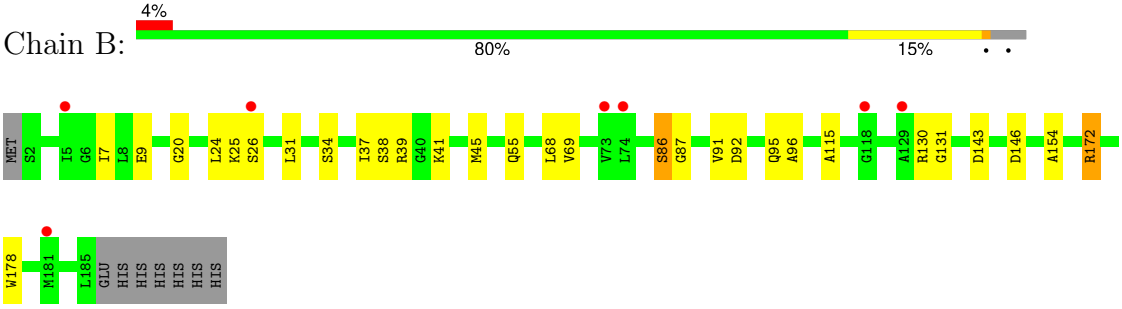
• Molecule 1: Propanediol utilization protein

Chain A:



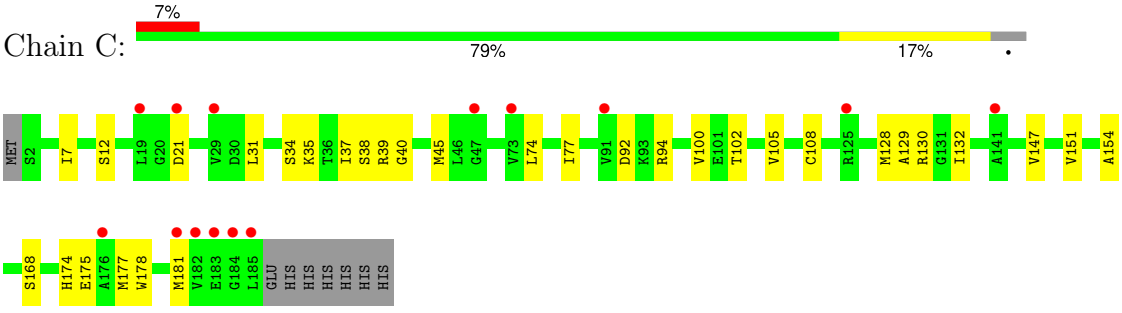
• Molecule 1: Propanediol utilization protein

Chain B:



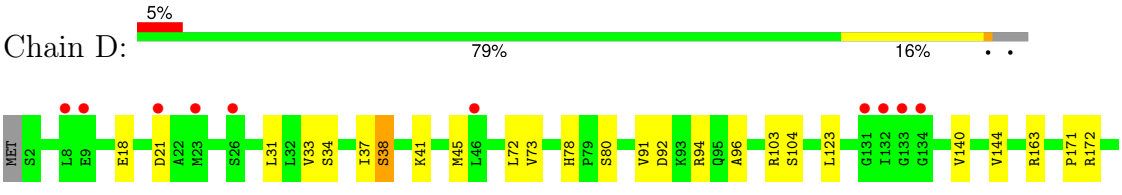
• Molecule 1: Propanediol utilization protein

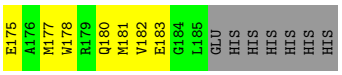
Chain C:



• Molecule 1: Propanediol utilization protein

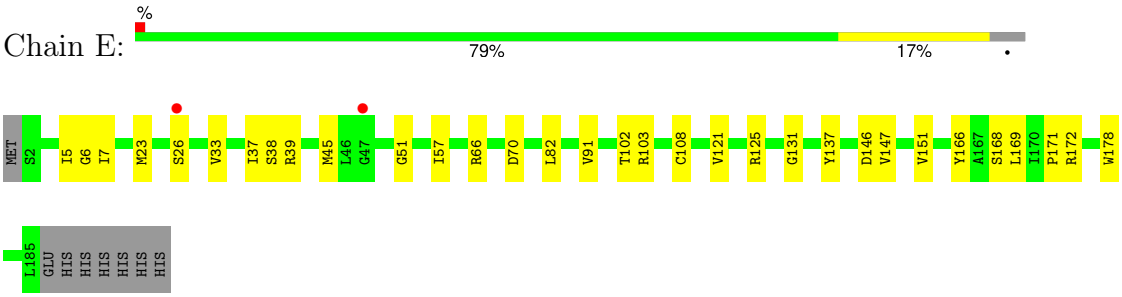
Chain D:





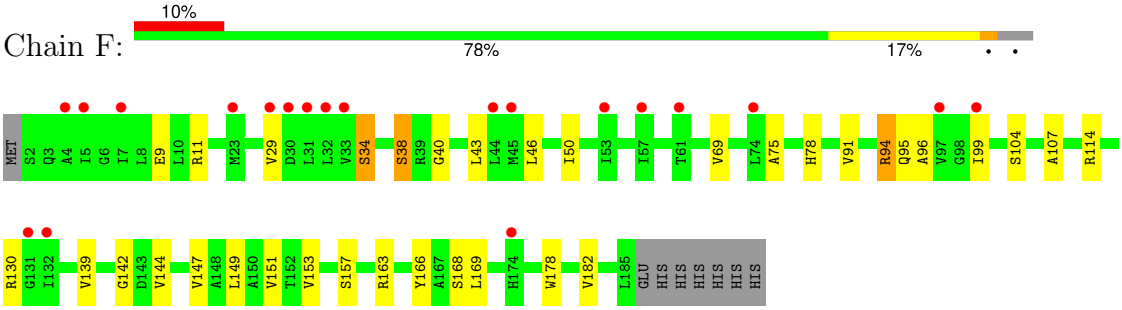
• Molecule 1: Propanediol utilization protein

Chain E:



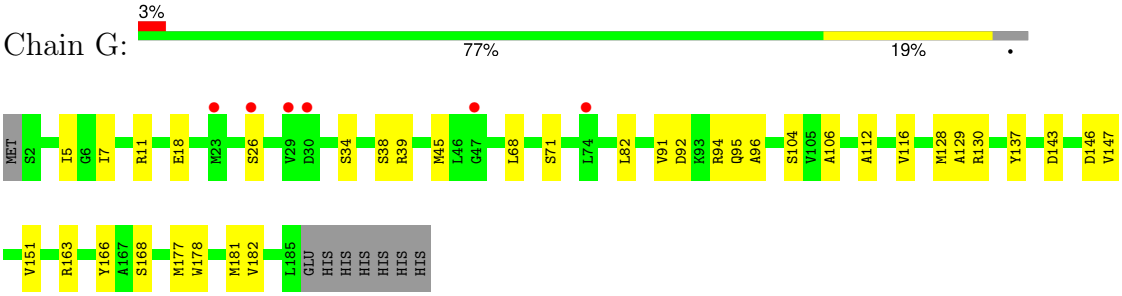
• Molecule 1: Propanediol utilization protein

Chain F:



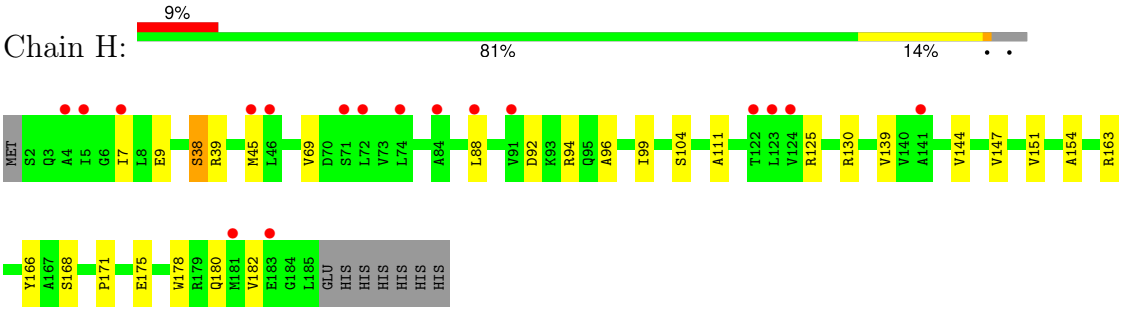
• Molecule 1: Propanediol utilization protein

Chain G:



• Molecule 1: Propanediol utilization protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	136.87Å 136.87Å 559.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.59 – 3.62 47.59 – 3.62	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.59-3.62) 99.6 (47.59-3.62)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.225 , 0.288 0.230 , 0.288	Depositor DCC
R_{free} test set	1175 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	158.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 104.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10624	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.26	0/1340	0.46	0/1812
1	B	0.25	0/1340	0.47	0/1812
1	C	0.25	0/1340	0.45	0/1812
1	D	0.26	0/1340	0.46	0/1812
1	E	0.26	0/1340	0.48	0/1812
1	F	0.25	0/1340	0.44	0/1812
1	G	0.25	0/1340	0.45	0/1812
1	H	0.25	0/1340	0.43	0/1812
All	All	0.26	0/10720	0.46	0/14496

There are no bond length outliers.

There are no bond angle outliers.

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	1328	0	1394	18	0
1	B	1328	0	1394	25	0
1	C	1328	0	1394	21	0
1	D	1328	0	1394	20	0
1	E	1328	0	1394	15	0
1	F	1328	0	1394	23	0
1	G	1328	0	1394	23	0
1	H	1328	0	1394	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10624	0	11152	154	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 7.

The worst 5 of 154 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:H:96:ALA:HB2	1:H:144:VAL:HG22	1.67	0.76
1:E:33:VAL:HB	1:E:45:MET:HB2	1.70	0.74
1:A:91:VAL:HG11	1:A:178:TRP:HZ2	1.55	0.72
1:D:31:LEU:HD11	1:D:34:SER:HB2	1.73	0.71
1:B:172:ARG:CD	1:B:172:ARG:O	2.40	0.70

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	182/192 (95%)	165 (91%)	16 (9%)	1 (0%)	29	67
1	B	182/192 (95%)	172 (94%)	9 (5%)	1 (0%)	29	67
1	C	182/192 (95%)	162 (89%)	18 (10%)	2 (1%)	14	53
1	D	182/192 (95%)	170 (93%)	11 (6%)	1 (0%)	29	67
1	E	182/192 (95%)	170 (93%)	12 (7%)	0	100	100
1	F	182/192 (95%)	167 (92%)	14 (8%)	1 (0%)	29	67
1	G	182/192 (95%)	171 (94%)	11 (6%)	0	100	100
1	H	182/192 (95%)	167 (92%)	14 (8%)	1 (0%)	29	67
All	All	1456/1536 (95%)	1344 (92%)	105 (7%)	7 (0%)	29	67

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	SER
1	C	129	ALA
1	C	40	GLY
1	D	171	PRO
1	H	171	PRO

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	140/148 (95%)	136 (97%)	4 (3%)	42	71
1	B	140/148 (95%)	139 (99%)	1 (1%)	84	92
1	C	140/148 (95%)	139 (99%)	1 (1%)	84	92
1	D	140/148 (95%)	137 (98%)	3 (2%)	53	78
1	E	140/148 (95%)	136 (97%)	4 (3%)	42	71
1	F	140/148 (95%)	137 (98%)	3 (2%)	53	78
1	G	140/148 (95%)	136 (97%)	4 (3%)	42	71
1	H	140/148 (95%)	139 (99%)	1 (1%)	84	92
All	All	1120/1184 (95%)	1099 (98%)	21 (2%)	57	80

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	SER
1	G	26	SER
1	H	38	SER
1	G	128	MET
1	G	11	ARG

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	184/192 (95%)	0.14	0 100 100	100, 129, 165, 180	0
1	B	184/192 (95%)	0.44	7 (3%) 40 27	110, 135, 164, 184	0
1	C	184/192 (95%)	0.45	14 (7%) 13 8	118, 143, 175, 191	0
1	D	184/192 (95%)	0.41	10 (5%) 25 16	109, 137, 168, 180	0
1	E	184/192 (95%)	0.17	2 (1%) 80 68	110, 138, 170, 188	0
1	F	184/192 (95%)	0.67	20 (10%) 5 3	123, 154, 185, 197	0
1	G	184/192 (95%)	0.36	6 (3%) 46 31	121, 146, 170, 186	0
1	H	184/192 (95%)	0.60	17 (9%) 9 5	115, 139, 172, 195	0
All	All	1472/1536 (95%)	0.40	76 (5%) 27 18	100, 141, 174, 197	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	LEU	4.3
1	F	131	GLY	4.3
1	F	132	ILE	3.9
1	C	184	GLY	3.8
1	G	23	MET	3.6

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.