



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:20 PM UTC

PDB ID : 6FDB / pdb_00006fdb
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 Full wwPDB X-ray Structure Validation 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

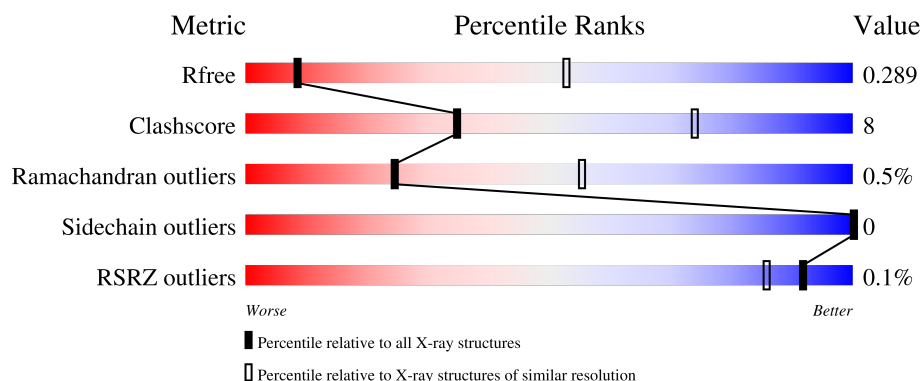
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	192	
1	B	192	
1	C	192	
1	D	192	
1	E	192	

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Mol	Chain	Length	Quality of chain
1	F	192	 77% 19% .
1	G	192	 79% 17% .
1	H	192	 79% 17% .

2 Entry composition

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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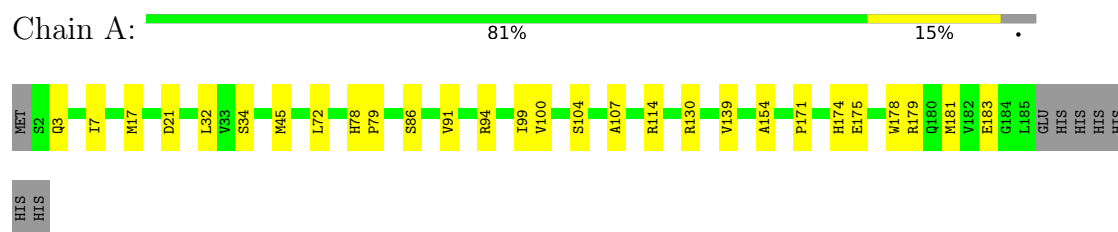
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Chain	Residue	Modelled	Actual	Comment	Reference
H	163	ARG	LEU	engineered mutation	UNP A0A0M0QF47
H	167	ALA	ARG	engineered mutation	UNP A0A0M0QF47
H	169	LEU	VAL	engineered mutation	UNP A0A0M0QF47
H	185	LEU	-	expression tag	UNP A0A0M0QF47
H	186	GLU	-	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

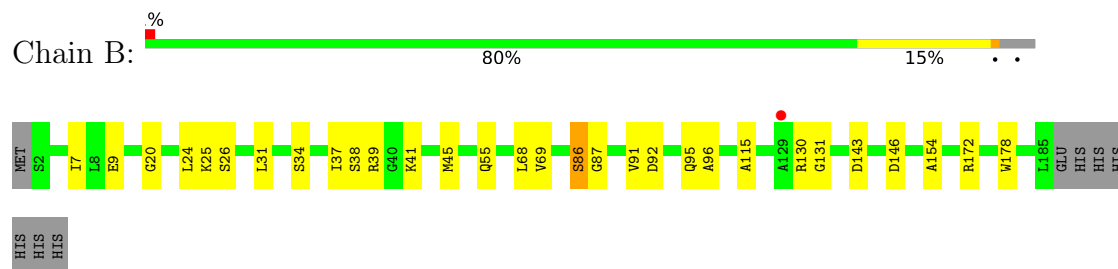
3 Residue-property plots

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.

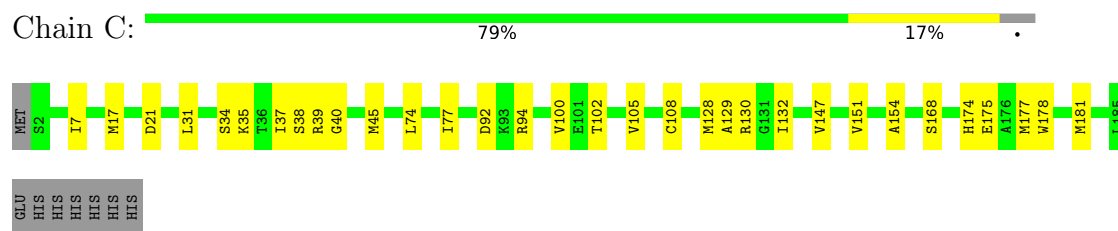
- Molecule 1: Propanediol utilization protein



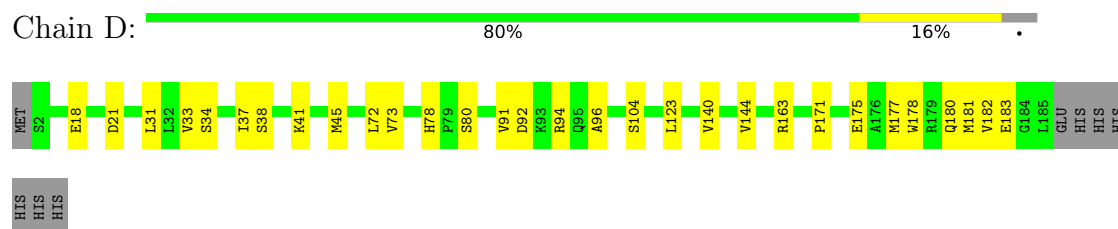
- Molecule 1: Propanediol utilization protein



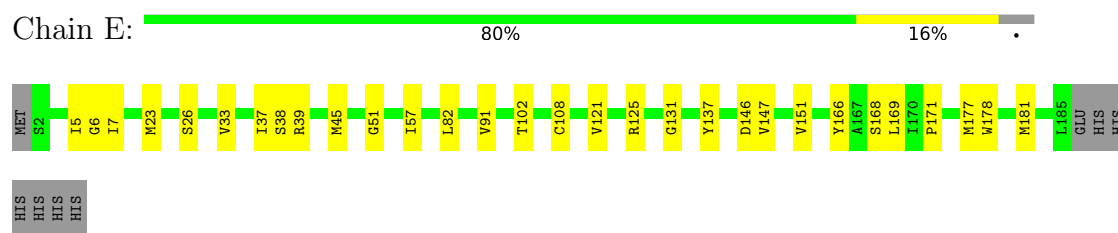
- Molecule 1: Propanediol utilization protein



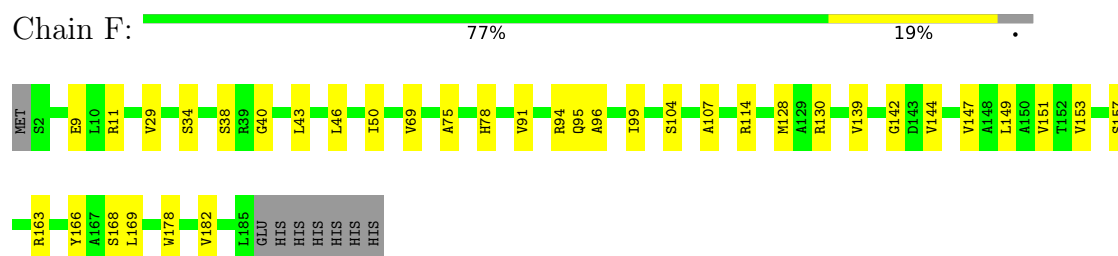
- Molecule 1: Propanediol utilization protein



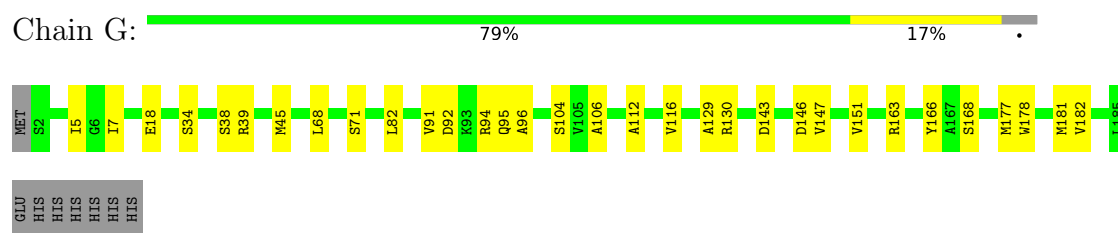
- Molecule 1: Propanediol utilization protein



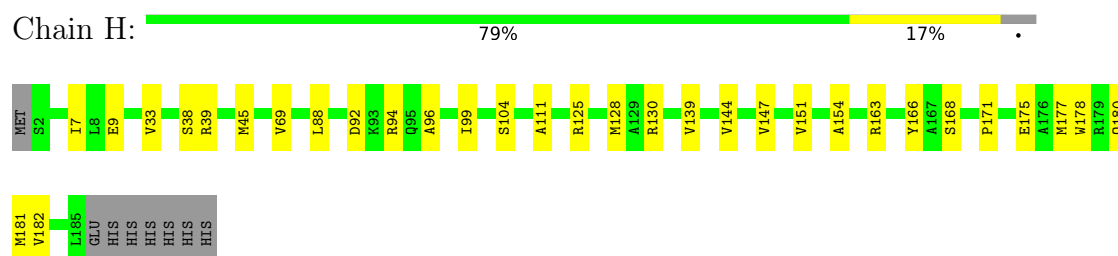
- Molecule 1: Propanediol utilization protein



- Molecule 1: Propanediol utilization protein



- Molecule 1: Propanediol utilization protein



4 Data and refinement statistics

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) 99.5 (47.59-3.62)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.225 , 0.288 0.230 , 0.289	Depositor DCC
R_{free} test set	1175 reflections (4.98%)	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)	0.36 , 110.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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.*

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](#)

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	0.17	0/1340	0.39	0/1812
1	B	0.16	0/1340	0.37	0/1812
1	C	0.16	0/1340	0.37	0/1812
1	D	0.17	0/1340	0.38	0/1812
1	E	0.17	0/1340	0.39	0/1812
1	F	0.15	0/1340	0.33	0/1812
1	G	0.16	0/1340	0.36	0/1812
1	H	0.15	0/1340	0.34	0/1812
All	All	0.16	0/10720	0.37	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 [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	1328	0	1394	21	0
1	B	1328	0	1394	26	0
1	C	1328	0	1394	21	0
1	D	1328	0	1394	23	0
1	E	1328	0	1394	16	0
1	F	1328	0	1394	24	0
1	G	1328	0	1394	24	0
1	H	1328	0	1394	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10624	0	11152	164	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 8.

All (164) 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
1:D:177:MET:HB3	1:D:181:MET:HE3	1.73	0.69
1:A:130:ARG:NH1	1:C:38:SER:OG	2.27	0.68
1:E:177:MET:HB3	1:E:181:MET:HE3	1.76	0.67
1:F:114:ARG:HG2	1:F:153:VAL:HG12	1.79	0.64
1:C:35:LYS:HE3	1:C:37:ILE:HD11	1.79	0.64
1:A:91:VAL:HG11	1:A:178:TRP:CZ2	2.33	0.63
1:A:3:GLN:HG3	1:A:79:PRO:HG3	1.81	0.63
1:F:91:VAL:HG11	1:F:178:TRP:CZ2	2.34	0.63
1:A:21:ASP:HB2	1:D:177:MET:HG3	1.79	0.63
1:B:172:ARG:O	1:B:172:ARG:HD3	2.01	0.61
1:F:96:ALA:HB2	1:F:144:VAL:HG22	1.83	0.60
1:G:104:SER:HB3	1:G:163:ARG:HD3	1.81	0.60
1:H:9:GLU:HG2	1:H:69:VAL:HB	1.84	0.59
1:D:78:HIS:ND1	1:D:80:SER:OG	2.32	0.58
1:H:99:ILE:HG12	1:H:139:VAL:HG22	1.85	0.58
1:H:7:ILE:HG12	1:H:45:MET:HG2	1.84	0.58
1:H:33:VAL:HG21	1:H:128:MET:HE1	1.85	0.58
1:F:91:VAL:HG11	1:F:178:TRP:HZ2	1.67	0.57
1:D:91:VAL:HG11	1:D:178:TRP:HH2	1.68	0.57
1:B:25:LYS:O	1:B:25:LYS:HG3	2.04	0.56
1:H:94:ARG:HH12	1:H:175:GLU:HG3	1.70	0.56
1:D:94:ARG:HH12	1:D:175:GLU:HG3	1.69	0.56
1:B:172:ARG:O	1:B:172:ARG:HD2	2.05	0.56
1:A:94:ARG:HH12	1:A:175:GLU:HG3	1.71	0.56
1:A:78:HIS:CD2	1:A:79:PRO:HD2	2.41	0.56
1:D:94:ARG:HH22	1:D:175:GLU:HG3	1.71	0.55
1:F:104:SER:HB3	1:F:163:ARG:HD3	1.88	0.55
1:G:7:ILE:HG12	1:G:45:MET:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:OG	1:B:87:GLY:N	2.40	0.55
1:G:34:SER:O	1:H:180:GLN:NE2	2.40	0.55
1:A:7:ILE:HG12	1:A:45:MET:HE3	1.88	0.55
1:E:102:THR:HG21	1:E:108:CYS:HB2	1.88	0.55
1:G:166:TYR:HE2	1:G:168:SER:HB3	1.73	0.54
1:A:17:MET:HB3	1:D:181:MET:HE2	1.90	0.54
1:F:114:ARG:HD2	1:F:157:SER:HB2	1.90	0.53
1:B:92:ASP:OD1	1:B:92:ASP:N	2.41	0.53
1:G:178:TRP:O	1:G:182:VAL:HG22	2.09	0.53
1:A:174:HIS:HB2	1:C:21:ASP:OD1	2.09	0.53
1:F:147:VAL:HG12	1:F:169:LEU:HD12	1.90	0.53
1:F:50:ILE:HD13	1:F:75:ALA:HB2	1.91	0.52
1:A:32:LEU:HD22	1:A:86:SER:HB3	1.91	0.52
1:H:94:ARG:HH22	1:H:175:GLU:HG3	1.74	0.52
1:E:5:ILE:HD11	1:E:82:LEU:HG	1.91	0.51
1:B:9:GLU:HG2	1:B:69:VAL:HB	1.93	0.51
1:D:37:ILE:O	1:D:41:LYS:N	2.44	0.51
1:C:31:LEU:HD11	1:C:34:SER:HB2	1.93	0.51
1:F:107:ALA:HB2	1:F:163:ARG:HD2	1.93	0.51
1:D:92:ASP:OD1	1:D:92:ASP:N	2.42	0.50
1:G:91:VAL:HG11	1:G:178:TRP:CH2	2.46	0.50
1:B:37:ILE:HD12	1:B:131:GLY:H	1.76	0.50
1:H:92:ASP:OD1	1:H:92:ASP:N	2.42	0.50
1:G:18:GLU:HB2	1:H:168:SER:HB2	1.94	0.50
1:E:121:VAL:HG12	1:E:146:ASP:HB3	1.93	0.50
1:B:143:ASP:HB2	1:B:146:ASP:HB2	1.92	0.49
1:F:11:ARG:HG2	1:F:69:VAL:HG22	1.94	0.49
1:C:100:VAL:HG21	1:C:154:ALA:HB3	1.95	0.49
1:C:105:VAL:HG12	1:C:132:ILE:O	2.12	0.49
1:E:169:LEU:HD23	1:E:171:PRO:HD3	1.95	0.49
1:H:111:ALA:HB1	1:H:154:ALA:HB1	1.95	0.49
1:F:147:VAL:O	1:F:151:VAL:HG23	2.13	0.48
1:G:166:TYR:CE2	1:G:168:SER:HB3	2.47	0.48
1:D:182:VAL:HG23	1:D:183:GLU:HG2	1.96	0.48
1:H:147:VAL:O	1:H:151:VAL:HG23	2.12	0.48
1:C:74:LEU:HB3	1:C:77:ILE:HD11	1.95	0.48
1:G:143:ASP:HB2	1:G:146:ASP:H	1.79	0.47
1:D:33:VAL:HB	1:D:45:MET:HB2	1.95	0.47
1:D:96:ALA:HB2	1:D:144:VAL:HG22	1.96	0.47
1:H:177:MET:HB3	1:H:181:MET:HE3	1.96	0.47
1:F:149:LEU:O	1:F:153:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG12	1:C:45:MET:HG2	1.95	0.47
1:B:31:LEU:HD11	1:B:34:SER:HB2	1.97	0.47
1:B:115:ALA:HB2	1:B:154:ALA:HB2	1.95	0.47
1:E:37:ILE:HG21	1:E:131:GLY:HA2	1.97	0.47
1:G:94:ARG:HA	1:G:178:TRP:CH2	2.50	0.47
1:C:92:ASP:OD1	1:C:92:ASP:N	2.44	0.47
1:G:112:ALA:O	1:G:116:VAL:HG22	2.15	0.47
1:B:37:ILE:HG23	1:B:131:GLY:H	1.80	0.46
1:F:166:TYR:HE2	1:F:168:SER:HB3	1.80	0.46
1:G:106:ALA:HB3	1:G:163:ARG:NH1	2.31	0.46
1:G:147:VAL:O	1:G:151:VAL:HG23	2.16	0.46
1:B:38:SER:HA	1:B:39:ARG:C	2.40	0.46
1:F:9:GLU:HG2	1:F:69:VAL:HB	1.96	0.46
1:F:38:SER:HB3	1:F:130:ARG:NH2	2.30	0.46
1:E:125:ARG:NH2	1:E:137:TYR:OH	2.49	0.46
1:H:104:SER:HB3	1:H:163:ARG:HD3	1.98	0.46
1:H:38:SER:HA	1:H:39:ARG:HA	1.63	0.45
1:C:128:MET:O	1:C:130:ARG:N	2.50	0.45
1:H:175:GLU:H	1:H:175:GLU:CD	2.25	0.45
1:D:91:VAL:HG11	1:D:178:TRP:CH2	2.50	0.45
1:G:177:MET:HE3	1:G:177:MET:HB3	1.82	0.45
1:F:99:ILE:HG12	1:F:139:VAL:HG22	1.97	0.45
1:A:94:ARG:NH1	1:A:175:GLU:HG3	2.31	0.44
1:E:147:VAL:O	1:E:151:VAL:HG23	2.18	0.44
1:B:38:SER:HB3	1:B:130:ARG:HE	1.82	0.44
1:E:51:GLY:HA3	1:F:78:HIS:CE1	2.53	0.44
1:E:7:ILE:HG23	1:E:45:MET:HG2	1.99	0.44
1:H:94:ARG:HA	1:H:178:TRP:CH2	2.51	0.44
1:F:29:VAL:HG21	1:F:46:LEU:HD13	1.99	0.44
1:G:5:ILE:HD11	1:G:82:LEU:HG	1.99	0.44
1:G:92:ASP:OD1	1:G:92:ASP:N	2.46	0.44
1:F:128:MET:HE3	1:F:128:MET:HB2	1.87	0.44
1:D:72:LEU:HD12	1:D:73:VAL:H	1.82	0.43
1:A:114:ARG:HE	1:A:114:ARG:HB2	1.71	0.43
1:C:94:ARG:NH1	1:C:175:GLU:HG3	2.32	0.43
1:F:34:SER:HA	1:F:43:LEU:O	2.17	0.43
1:A:34:SER:O	1:D:180:GLN:NE2	2.43	0.43
1:A:179:ARG:O	1:A:183:GLU:HB2	2.18	0.43
1:C:174:HIS:N	1:D:21:ASP:OD1	2.44	0.43
1:F:166:TYR:CE2	1:F:168:SER:HB3	2.52	0.43
1:B:68:LEU:HD12	1:B:69:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:MET:O	1:C:181:MET:HG2	2.18	0.43
1:E:91:VAL:HG11	1:E:178:TRP:HH2	1.83	0.43
1:G:38:SER:HA	1:G:39:ARG:HA	1.61	0.43
1:B:68:LEU:HD12	1:B:69:VAL:N	2.33	0.43
1:B:91:VAL:HG11	1:B:178:TRP:CH2	2.54	0.43
1:G:91:VAL:HG11	1:G:178:TRP:HH2	1.84	0.43
1:C:102:THR:OG1	1:C:108:CYS:HB2	2.19	0.42
1:B:45:MET:HE2	1:B:45:MET:HB3	1.92	0.42
1:C:94:ARG:HH12	1:C:175:GLU:HG3	1.84	0.42
1:A:104:SER:HB2	1:A:107:ALA:H	1.85	0.42
1:B:26:SER:O	1:B:55:GLN:NE2	2.53	0.42
1:B:95:GLN:HB3	1:B:96:ALA:H	1.70	0.42
1:B:25:LYS:O	1:B:25:LYS:CG	2.68	0.42
1:B:20:GLY:O	1:B:24:LEU:HG	2.20	0.42
1:D:104:SER:OG	1:D:163:ARG:HD3	2.19	0.42
1:G:68:LEU:HD11	1:G:71:SER:HB3	2.01	0.42
1:G:95:GLN:HB3	1:G:96:ALA:H	1.70	0.41
1:C:37:ILE:HD12	1:C:130:ARG:HA	2.02	0.41
1:G:39:ARG:NH1	1:H:130:ARG:HD3	2.34	0.41
1:H:166:TYR:HE2	1:H:168:SER:HB3	1.85	0.41
1:H:178:TRP:CE2	1:H:182:VAL:HG21	2.55	0.41
1:B:7:ILE:HG12	1:B:45:MET:HG2	2.02	0.41
1:A:7:ILE:HD12	1:A:72:LEU:HD23	2.03	0.41
1:E:6:GLY:HA3	1:E:57:ILE:HD11	2.01	0.41
1:C:39:ARG:HG2	1:C:39:ARG:O	2.21	0.41
1:C:147:VAL:O	1:C:151:VAL:HG23	2.20	0.41
1:G:95:GLN:HE21	1:G:95:GLN:HB2	1.63	0.41
1:H:178:TRP:O	1:H:182:VAL:HG22	2.20	0.41
1:A:17:MET:SD	1:D:181:MET:HG2	2.61	0.41
1:B:91:VAL:HG11	1:B:178:TRP:HH2	1.86	0.41
1:C:168:SER:HB2	1:D:18:GLU:OE1	2.19	0.41
1:G:177:MET:O	1:G:181:MET:HG3	2.20	0.41
1:E:23:MET:HA	1:E:26:SER:HB3	2.02	0.41
1:G:129:ALA:O	1:G:130:ARG:HB3	2.21	0.41
1:A:100:VAL:HG21	1:A:154:ALA:HB3	2.01	0.41
1:A:181:MET:HE2	1:C:17:MET:HB3	2.01	0.41
1:B:37:ILE:HD13	1:B:37:ILE:HA	1.87	0.41
1:B:41:LYS:HB2	1:B:41:LYS:HE3	1.88	0.41
1:C:94:ARG:HA	1:C:178:TRP:CH2	2.55	0.41
1:F:94:ARG:HD2	1:F:178:TRP:CD2	2.55	0.41
1:E:38:SER:HA	1:E:39:ARG:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG12	1:A:139:VAL:HG22	2.02	0.40
1:F:178:TRP:O	1:F:182:VAL:HG22	2.21	0.40
1:D:175:GLU:H	1:D:175:GLU:CD	2.29	0.40
1:F:95:GLN:HB3	1:F:142:GLY:O	2.21	0.40
1:H:88:LEU:HD22	1:H:125:ARG:HB3	2.03	0.40
1:D:37:ILE:HG22	1:D:38:SER:O	2.21	0.40
1:D:123:LEU:HA	1:D:140:VAL:HG12	2.03	0.40
1:E:166:TYR:CE2	1:E:168:SER:HB3	2.57	0.40

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	A	182/192 (95%)	165 (91%)	16 (9%)	1 (0%)	24	55
1	B	182/192 (95%)	172 (94%)	9 (5%)	1 (0%)	24	55
1	C	182/192 (95%)	162 (89%)	18 (10%)	2 (1%)	11	40
1	D	182/192 (95%)	170 (93%)	11 (6%)	1 (0%)	24	55
1	E	182/192 (95%)	170 (93%)	12 (7%)	0	100	100
1	F	182/192 (95%)	167 (92%)	14 (8%)	1 (0%)	24	55
1	G	182/192 (95%)	171 (94%)	11 (6%)	0	100	100
1	H	182/192 (95%)	167 (92%)	14 (8%)	1 (0%)	24	55
All	All	1456/1536 (95%)	1344 (92%)	105 (7%)	7 (0%)	24	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	SER
1	C	129	ALA

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Mol	Chain	Res	Type
1	C	40	GLY
1	D	171	PRO
1	H	171	PRO
1	F	40	GLY
1	A	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%)	140 (100%)	0	100	100
1	B	140/148 (95%)	140 (100%)	0	100	100
1	C	140/148 (95%)	140 (100%)	0	100	100
1	D	140/148 (95%)	140 (100%)	0	100	100
1	E	140/148 (95%)	140 (100%)	0	100	100
1	F	140/148 (95%)	140 (100%)	0	100	100
1	G	140/148 (95%)	140 (100%)	0	100	100
1	H	140/148 (95%)	140 (100%)	0	100	100
All	All	1120/1184 (95%)	1120 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	C	76	ASN
1	H	3	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	184/192 (95%)	-0.45	0 100 100	100, 129, 165, 180	0
1	B	184/192 (95%)	-0.49	1 (0%) 87 67	110, 135, 164, 184	0
1	C	184/192 (95%)	-0.46	0 100 100	118, 143, 175, 191	0
1	D	184/192 (95%)	-0.42	0 100 100	109, 137, 168, 180	0
1	E	184/192 (95%)	-0.36	0 100 100	110, 138, 170, 188	0
1	F	184/192 (95%)	-0.39	0 100 100	123, 154, 185, 197	0
1	G	184/192 (95%)	-0.38	0 100 100	121, 146, 170, 186	0
1	H	184/192 (95%)	-0.51	0 100 100	115, 139, 172, 195	0
All	All	1472/1536 (95%)	-0.43	1 (0%) 92 86	100, 141, 174, 197	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	ALA	2.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.