



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:56 AM EDT

PDB ID : 3ZQP  
Title : Crystal structure of the small terminase oligomerization domain from a SPP1-like bacteriophage  
Authors : Buttner, C.R.; Chechik, M.; Ortiz-Lombardia, M.; Smits, C.; Chechik, V.; Jeschke, G.; Dykeman, E.; Benini, S.; Alonso, J.C.; Antson, A.A.  
Deposited on : 2011-06-10  
Resolution : 3.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 2.36.2  
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) : 2.36.2

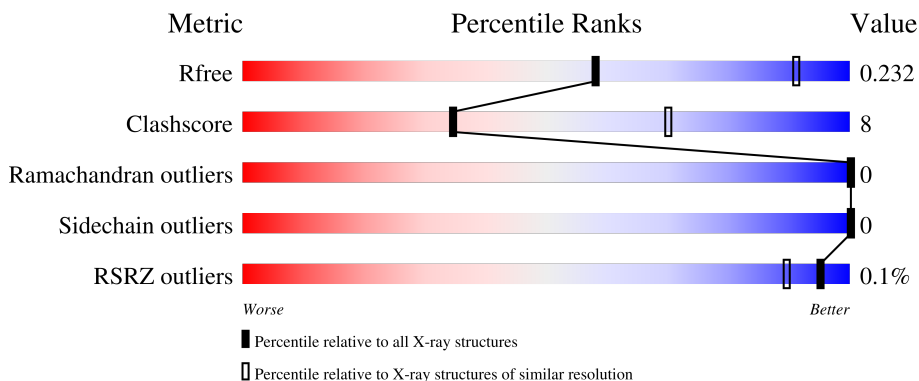
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	164	
1	B	164	
1	C	164	
1	D	164	
1	E	164	

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Mol	Chain	Length	Quality of chain
1	F	164	 37% 9% 54%
1	G	164	 42% 1% 54%
1	H	164	 41% 6% 53%
1	I	164	 41% 5% 54%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 5289 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 TERMINASE SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	75	581	365	103	112	1	0	0	0
1	B	76	587	368	104	114	1	0	0	0
1	C	77	596	374	106	115	1	0	0	0
1	D	75	581	365	103	112	1	0	0	0
1	E	76	590	371	105	113	1	0	0	0
1	F	75	581	365	103	112	1	0	0	0
1	G	76	587	368	104	114	1	0	0	0
1	H	77	596	374	106	115	1	0	0	0
1	I	76	590	371	105	113	1	0	0	0

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q1EJR8
A	-17	GLY	-	expression tag	UNP Q1EJR8
A	-16	SER	-	expression tag	UNP Q1EJR8
A	-15	SER	-	expression tag	UNP Q1EJR8
A	-14	HIS	-	expression tag	UNP Q1EJR8
A	-13	HIS	-	expression tag	UNP Q1EJR8
A	-12	HIS	-	expression tag	UNP Q1EJR8
A	-11	HIS	-	expression tag	UNP Q1EJR8
A	-10	HIS	-	expression tag	UNP Q1EJR8
A	-9	HIS	-	expression tag	UNP Q1EJR8
A	-8	SER	-	expression tag	UNP Q1EJR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP Q1EJR8
A	-6	GLY	-	expression tag	UNP Q1EJR8
A	-5	LEU	-	expression tag	UNP Q1EJR8
A	-4	VAL	-	expression tag	UNP Q1EJR8
A	-3	PRO	-	expression tag	UNP Q1EJR8
A	-2	ARG	-	expression tag	UNP Q1EJR8
A	-1	GLY	-	expression tag	UNP Q1EJR8
A	0	SER	-	expression tag	UNP Q1EJR8
B	-18	MET	-	expression tag	UNP Q1EJR8
B	-17	GLY	-	expression tag	UNP Q1EJR8
B	-16	SER	-	expression tag	UNP Q1EJR8
B	-15	SER	-	expression tag	UNP Q1EJR8
B	-14	HIS	-	expression tag	UNP Q1EJR8
B	-13	HIS	-	expression tag	UNP Q1EJR8
B	-12	HIS	-	expression tag	UNP Q1EJR8
B	-11	HIS	-	expression tag	UNP Q1EJR8
B	-10	HIS	-	expression tag	UNP Q1EJR8
B	-9	HIS	-	expression tag	UNP Q1EJR8
B	-8	SER	-	expression tag	UNP Q1EJR8
B	-7	SER	-	expression tag	UNP Q1EJR8
B	-6	GLY	-	expression tag	UNP Q1EJR8
B	-5	LEU	-	expression tag	UNP Q1EJR8
B	-4	VAL	-	expression tag	UNP Q1EJR8
B	-3	PRO	-	expression tag	UNP Q1EJR8
B	-2	ARG	-	expression tag	UNP Q1EJR8
B	-1	GLY	-	expression tag	UNP Q1EJR8
B	0	SER	-	expression tag	UNP Q1EJR8
C	-18	MET	-	expression tag	UNP Q1EJR8
C	-17	GLY	-	expression tag	UNP Q1EJR8
C	-16	SER	-	expression tag	UNP Q1EJR8
C	-15	SER	-	expression tag	UNP Q1EJR8
C	-14	HIS	-	expression tag	UNP Q1EJR8
C	-13	HIS	-	expression tag	UNP Q1EJR8
C	-12	HIS	-	expression tag	UNP Q1EJR8
C	-11	HIS	-	expression tag	UNP Q1EJR8
C	-10	HIS	-	expression tag	UNP Q1EJR8
C	-9	HIS	-	expression tag	UNP Q1EJR8
C	-8	SER	-	expression tag	UNP Q1EJR8
C	-7	SER	-	expression tag	UNP Q1EJR8
C	-6	GLY	-	expression tag	UNP Q1EJR8
C	-5	LEU	-	expression tag	UNP Q1EJR8
C	-4	VAL	-	expression tag	UNP Q1EJR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	PRO	-	expression tag	UNP Q1EJR8
C	-2	ARG	-	expression tag	UNP Q1EJR8
C	-1	GLY	-	expression tag	UNP Q1EJR8
C	0	SER	-	expression tag	UNP Q1EJR8
D	-18	MET	-	expression tag	UNP Q1EJR8
D	-17	GLY	-	expression tag	UNP Q1EJR8
D	-16	SER	-	expression tag	UNP Q1EJR8
D	-15	SER	-	expression tag	UNP Q1EJR8
D	-14	HIS	-	expression tag	UNP Q1EJR8
D	-13	HIS	-	expression tag	UNP Q1EJR8
D	-12	HIS	-	expression tag	UNP Q1EJR8
D	-11	HIS	-	expression tag	UNP Q1EJR8
D	-10	HIS	-	expression tag	UNP Q1EJR8
D	-9	HIS	-	expression tag	UNP Q1EJR8
D	-8	SER	-	expression tag	UNP Q1EJR8
D	-7	SER	-	expression tag	UNP Q1EJR8
D	-6	GLY	-	expression tag	UNP Q1EJR8
D	-5	LEU	-	expression tag	UNP Q1EJR8
D	-4	VAL	-	expression tag	UNP Q1EJR8
D	-3	PRO	-	expression tag	UNP Q1EJR8
D	-2	ARG	-	expression tag	UNP Q1EJR8
D	-1	GLY	-	expression tag	UNP Q1EJR8
D	0	SER	-	expression tag	UNP Q1EJR8
E	-18	MET	-	expression tag	UNP Q1EJR8
E	-17	GLY	-	expression tag	UNP Q1EJR8
E	-16	SER	-	expression tag	UNP Q1EJR8
E	-15	SER	-	expression tag	UNP Q1EJR8
E	-14	HIS	-	expression tag	UNP Q1EJR8
E	-13	HIS	-	expression tag	UNP Q1EJR8
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E	-9	HIS	-	expression tag	UNP Q1EJR8
E	-8	SER	-	expression tag	UNP Q1EJR8
E	-7	SER	-	expression tag	UNP Q1EJR8
E	-6	GLY	-	expression tag	UNP Q1EJR8
E	-5	LEU	-	expression tag	UNP Q1EJR8
E	-4	VAL	-	expression tag	UNP Q1EJR8
E	-3	PRO	-	expression tag	UNP Q1EJR8
E	-2	ARG	-	expression tag	UNP Q1EJR8
E	-1	GLY	-	expression tag	UNP Q1EJR8
E	0	SER	-	expression tag	UNP Q1EJR8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	MET	-	expression tag	UNP Q1EJR8
F	-17	GLY	-	expression tag	UNP Q1EJR8
F	-16	SER	-	expression tag	UNP Q1EJR8
F	-15	SER	-	expression tag	UNP Q1EJR8
F	-14	HIS	-	expression tag	UNP Q1EJR8
F	-13	HIS	-	expression tag	UNP Q1EJR8
F	-12	HIS	-	expression tag	UNP Q1EJR8
F	-11	HIS	-	expression tag	UNP Q1EJR8
F	-10	HIS	-	expression tag	UNP Q1EJR8
F	-9	HIS	-	expression tag	UNP Q1EJR8
F	-8	SER	-	expression tag	UNP Q1EJR8
F	-7	SER	-	expression tag	UNP Q1EJR8
F	-6	GLY	-	expression tag	UNP Q1EJR8
F	-5	LEU	-	expression tag	UNP Q1EJR8
F	-4	VAL	-	expression tag	UNP Q1EJR8
F	-3	PRO	-	expression tag	UNP Q1EJR8
F	-2	ARG	-	expression tag	UNP Q1EJR8
F	-1	GLY	-	expression tag	UNP Q1EJR8
F	0	SER	-	expression tag	UNP Q1EJR8
G	-18	MET	-	expression tag	UNP Q1EJR8
G	-17	GLY	-	expression tag	UNP Q1EJR8
G	-16	SER	-	expression tag	UNP Q1EJR8
G	-15	SER	-	expression tag	UNP Q1EJR8
G	-14	HIS	-	expression tag	UNP Q1EJR8
G	-13	HIS	-	expression tag	UNP Q1EJR8
G	-12	HIS	-	expression tag	UNP Q1EJR8
G	-11	HIS	-	expression tag	UNP Q1EJR8
G	-10	HIS	-	expression tag	UNP Q1EJR8
G	-9	HIS	-	expression tag	UNP Q1EJR8
G	-8	SER	-	expression tag	UNP Q1EJR8
G	-7	SER	-	expression tag	UNP Q1EJR8
G	-6	GLY	-	expression tag	UNP Q1EJR8
G	-5	LEU	-	expression tag	UNP Q1EJR8
G	-4	VAL	-	expression tag	UNP Q1EJR8
G	-3	PRO	-	expression tag	UNP Q1EJR8
G	-2	ARG	-	expression tag	UNP Q1EJR8
G	-1	GLY	-	expression tag	UNP Q1EJR8
G	0	SER	-	expression tag	UNP Q1EJR8
H	-18	MET	-	expression tag	UNP Q1EJR8
H	-17	GLY	-	expression tag	UNP Q1EJR8
H	-16	SER	-	expression tag	UNP Q1EJR8
H	-15	SER	-	expression tag	UNP Q1EJR8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	HIS	-	expression tag	UNP Q1EJR8
H	-13	HIS	-	expression tag	UNP Q1EJR8
H	-12	HIS	-	expression tag	UNP Q1EJR8
H	-11	HIS	-	expression tag	UNP Q1EJR8
H	-10	HIS	-	expression tag	UNP Q1EJR8
H	-9	HIS	-	expression tag	UNP Q1EJR8
H	-8	SER	-	expression tag	UNP Q1EJR8
H	-7	SER	-	expression tag	UNP Q1EJR8
H	-6	GLY	-	expression tag	UNP Q1EJR8
H	-5	LEU	-	expression tag	UNP Q1EJR8
H	-4	VAL	-	expression tag	UNP Q1EJR8
H	-3	PRO	-	expression tag	UNP Q1EJR8
H	-2	ARG	-	expression tag	UNP Q1EJR8
H	-1	GLY	-	expression tag	UNP Q1EJR8
H	0	SER	-	expression tag	UNP Q1EJR8
I	-18	MET	-	expression tag	UNP Q1EJR8
I	-17	GLY	-	expression tag	UNP Q1EJR8
I	-16	SER	-	expression tag	UNP Q1EJR8
I	-15	SER	-	expression tag	UNP Q1EJR8
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I	-4	VAL	-	expression tag	UNP Q1EJR8
I	-3	PRO	-	expression tag	UNP Q1EJR8
I	-2	ARG	-	expression tag	UNP Q1EJR8
I	-1	GLY	-	expression tag	UNP Q1EJR8
I	0	SER	-	expression tag	UNP Q1EJR8



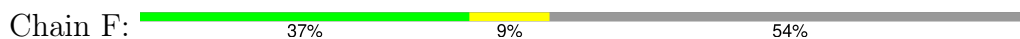




MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	ARG	GLY	SER	MET	PRO	GLU	PRO	GLU	LEU	SER	PRO	GLN	GLU	ARG	PHE	ILE	GLU	TYR	PHE	ILE	ASN	ASP	ASN	MET	ASN	ALA	THR	LYS	ALA	ALA	ALA	ALA	ALA	GLY	TYR	SER	LYS	ASN	SER	ALA	ALA	ALA	ILE
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GLY	ALA	GLU	ASN	LEU	GLN	LYS	PRO	ALA	ILE	ARG	ALA	ARG	ILE	ASP	ALA	ARG	LEU	LEU	LYS	GLU	ILE	LYS	ASN	PRO	GLU	LEU	K65	K66	I67	L68	T78	Q88	V89	L90	E104	I136	D140	SER	GLY	ASP	ALA	GLU
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• Molecule 1: TERMINASE SMALL SUBUNIT



MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	ARG	GLY	SER	MET	PRO	GLU	PRO	GLU	LEU	SER	PRO	GLN	GLU	ARG	PHE	ILE	GLU	TYR	PHE	ILE	ASN	ASP	ASN	MET	ASN	ALA	THR	LYS	ALA	ALA	ALA	ALA	ILE	ILE	GLY	TYR	SER	LYS	ASN	SER	ALA	ALA	ALA	ILE
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GLY	ALA	GLU	ASN	LEU	GLN	LYS	PRO	ALA	ILE	ARG	ALA	ARG	ILE	ASP	ALA	ARG	LEU	LEU	LYS	GLU	ILE	LYS	ASN	PRO	GLU	LEU	K66	I67	L68	V73	E72	T78	Q88	V89	L90	E104	H121	E131	I136	V138	D139	D140	SER	GLY	ASP	ALA	GLU
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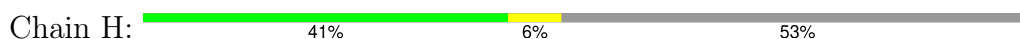
• Molecule 1: TERMINASE SMALL SUBUNIT



MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	ARG	GLY	SER	MET	PRO	GLU	PRO	GLU	LEU	SER	PRO	GLN	GLU	ARG	PHE	ILE	GLU	TYR	PHE	ILE	ASN	ASP	ASN	MET	ASN	ALA	THR	LYS	ALA	ALA	ALA	ALA	ILE	ILE	GLY	TYR	SER	LYS	ASN	SER	ALA	ALA	ALA	ILE
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GLY	ALA	GLU	ASN	LEU	GLN	LYS	PRO	ALA	ILE	ARG	ALA	ARG	ILE	ASP	ALA	ARG	LEU	LEU	LYS	GLU	ILE	LYS	ASN	PRO	GLU	LEU	K66	I67	L68	L74	Q88	V89	L90	E104	K129	I136	S141	GLY	ASP	ALA	GLU
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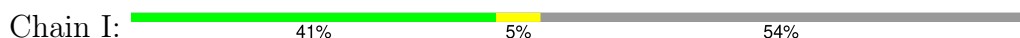
• Molecule 1: TERMINASE SMALL SUBUNIT



MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	ARG	GLY	SER	MET	PRO	GLU	PRO	GLU	LEU	SER	PRO	GLN	GLU	ARG	PHE	ILE	GLU	TYR	PHE	ILE	ASN	ASP	ASN	MET	ASN	ALA	THR	LYS	ALA	ALA	ALA	ALA	ILE	ILE	GLY	TYR	SER	LYS	ASN	SER	ALA	ALA	ALA	ILE
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GLY	ALA	GLU	ASN	LEU	GLN	LYS	PRO	ALA	ILE	ARG	ALA	ARG	ILE	ASP	ALA	ARG	LEU	LEU	LYS	GLU	ILE	LYS	ASN	PRO	GLU	LEU	K65	K66	I67	L68	Q88	V89	L90	E104	K129	V130	E131	T132	N133	Q134	S141	GLY	ASP	ALA	GLU
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• Molecule 1: TERMINASE SMALL SUBUNIT



MET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	ARG	GLY	SER	MET	PRO	GLU	PRO	GLU	LEU	SER	PRO	GLN	GLU	ARG	PHE	ILE	GLU	TYR	PHE	ILE	ASN	ASP	ASN	MET	ASN	ALA	THR	LYS	ALA	ALA	ALA	ALA	ILE	ILE	GLY	TYR	SER	LYS	ASN	SER	ALA	ALA	ALA	ILE
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GLY	ALA	GLU	ASN	LEU	GLN	LYS	PRO	ALA	ILE	ARG	ALA	ARG	ILE	ASP	ALA	ARG	LEU	LEU	LYS	GLU	ILE	LYS	ASN	PRO	GLU	LEU	K65	L68	E72	V73	Q88	V89	L90	E104	K127	G128	K129	I136	D140	SER	GLY	ASP	ALA	GLU
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## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.27Å 74.27Å 119.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.00 43.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-3.00) 100.0 (43.80-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.185 , 0.226 0.191 , 0.232	Depositor DCC
$R_{free}$ test set	748 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 13.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l 0.048 for h,-h-k,-l 0.026 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.76	0/584	0.66	0/783
1	B	0.78	0/590	0.66	0/791
1	C	0.80	0/599	0.64	0/802
1	D	0.79	0/584	0.69	0/783
1	E	0.79	0/593	0.66	0/794
1	F	0.75	0/584	0.67	1/783 (0.1%)
1	G	0.77	0/590	0.65	0/791
1	H	0.77	0/599	0.64	0/802
1	I	0.80	0/593	0.65	0/794
All	All	0.78	0/5316	0.66	1/7123 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	F	139	ASP	CB-CG-OD1	5.23	123.01	118.30

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	581	0	613	14	0
1	B	587	0	618	12	0
1	C	596	0	631	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	581	0	613	16	0
1	E	590	0	626	11	0
1	F	581	0	613	21	0
1	G	587	0	618	16	0
1	H	596	0	631	18	0
1	I	590	0	626	16	0
All	All	5289	0	5589	90	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 (90) 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:F:78:THR:HG23	1:G:68:LEU:HD12	1.24	1.13
1:F:78:THR:HG23	1:G:68:LEU:CD1	1.86	1.05
1:H:132:THR:HG22	1:H:134:GLN:HG3	1.51	0.91
1:A:78:THR:HG21	1:B:67:ILE:HA	1.56	0.88
1:D:78:THR:HG21	1:E:67:ILE:HA	1.54	0.88
1:A:74:LEU:O	1:A:78:THR:HG23	1.74	0.86
1:H:132:THR:CG2	1:H:134:GLN:HG3	2.09	0.81
1:D:74:LEU:O	1:D:78:THR:HG23	1.81	0.79
1:F:78:THR:CG2	1:G:68:LEU:HD12	2.10	0.76
1:F:138:VAL:HG12	1:G:136:ILE:HB	1.68	0.73
1:I:68:LEU:HD22	1:I:73:VAL:CG2	2.20	0.71
1:H:132:THR:CG2	1:H:134:GLN:CG	2.70	0.70
1:I:68:LEU:HD22	1:I:73:VAL:HG23	1.74	0.69
1:D:68:LEU:CD1	1:D:72:GLU:HB3	2.25	0.65
1:H:132:THR:HG21	1:H:134:GLN:CG	2.28	0.64
1:D:68:LEU:HD11	1:D:72:GLU:HB3	1.80	0.62
1:B:66:LYS:HG2	1:B:67:ILE:N	2.14	0.60
1:F:68:LEU:HD21	1:F:73:VAL:N	2.16	0.60
1:D:139:ASP:O	1:D:139:ASP:OD1	2.20	0.59
1:E:90:LEU:N	1:E:90:LEU:HD12	2.18	0.59
1:H:132:THR:HG22	1:H:133:ASN:N	2.18	0.59
1:F:90:LEU:HD12	1:F:90:LEU:N	2.18	0.58
1:F:68:LEU:CD2	1:F:73:VAL:HG23	2.35	0.57
1:G:90:LEU:HD12	1:G:90:LEU:N	2.20	0.57
1:I:90:LEU:HD12	1:I:90:LEU:N	2.20	0.57
1:H:90:LEU:N	1:H:90:LEU:HD12	2.20	0.56
1:C:90:LEU:HD12	1:C:90:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:HIS:HE1	1:E:68:LEU:O	1.89	0.56
1:G:74:LEU:CB	1:H:67:ILE:HD13	2.37	0.55
1:F:104:GLU:H	1:G:88:GLN:NE2	2.06	0.54
1:I:68:LEU:CD2	1:I:73:VAL:HG23	2.37	0.54
1:A:121:HIS:HE1	1:B:68:LEU:O	1.90	0.54
1:C:104:GLU:H	1:D:88:GLN:HE21	1.55	0.53
1:C:104:GLU:H	1:D:88:GLN:NE2	2.06	0.53
1:G:104:GLU:H	1:H:88:GLN:HE21	1.57	0.53
1:H:104:GLU:H	1:I:88:GLN:NE2	2.07	0.53
1:E:104:GLU:H	1:F:88:GLN:NE2	2.05	0.52
1:H:104:GLU:H	1:I:88:GLN:HE21	1.58	0.52
1:G:74:LEU:HB2	1:H:67:ILE:HD13	1.92	0.52
1:A:88:GLN:NE2	1:I:104:GLU:H	2.07	0.51
1:A:88:GLN:HE21	1:I:104:GLU:H	1.59	0.51
1:I:68:LEU:HD22	1:I:73:VAL:HG22	1.91	0.51
1:G:104:GLU:H	1:H:88:GLN:NE2	2.09	0.51
1:H:132:THR:CG2	1:H:133:ASN:N	2.74	0.51
1:F:68:LEU:HD23	1:F:73:VAL:HG23	1.93	0.50
1:B:104:GLU:H	1:C:88:GLN:NE2	2.11	0.49
1:D:68:LEU:HD12	1:D:72:GLU:HB3	1.94	0.48
1:F:138:VAL:CG1	1:G:136:ILE:HB	2.39	0.48
1:D:68:LEU:CD1	1:D:72:GLU:CB	2.90	0.48
1:F:104:GLU:H	1:G:88:GLN:HE21	1.61	0.48
1:A:68:LEU:HD23	1:A:73:VAL:HG22	1.96	0.47
1:A:136:ILE:HD12	1:I:136:ILE:HG23	1.97	0.47
1:D:104:GLU:H	1:E:88:GLN:NE2	2.11	0.47
1:E:104:GLU:H	1:F:88:GLN:HE21	1.63	0.47
1:E:136:ILE:HG23	1:F:136:ILE:HD12	1.96	0.47
1:A:138:VAL:HG12	1:A:139:ASP:N	2.30	0.47
1:B:104:GLU:H	1:C:88:GLN:HE21	1.63	0.46
1:D:68:LEU:HD12	1:D:72:GLU:CB	2.46	0.46
1:H:131:GLU:OE2	1:I:129:LYS:HE3	2.15	0.46
1:A:127:LYS:HD2	1:B:122:ALA:O	2.16	0.45
1:A:78:THR:CG2	1:B:68:LEU:H	2.30	0.45
1:D:104:GLU:H	1:E:88:GLN:HE21	1.65	0.45
1:C:78:THR:HG23	1:D:68:LEU:HB2	2.00	0.44
1:I:68:LEU:HD23	1:I:72:GLU:HB2	1.98	0.44
1:B:127:LYS:HD2	1:C:122:ALA:O	2.18	0.43
1:G:74:LEU:HB3	1:H:67:ILE:HD13	2.00	0.43
1:B:78:THR:HG21	1:C:65:LYS:O	2.18	0.43
1:F:121:HIS:HE1	1:G:68:LEU:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:O	1:A:70:ALA:C	2.57	0.42
1:A:78:THR:HG21	1:B:68:LEU:H	1.84	0.42
1:D:78:THR:CG2	1:E:68:LEU:H	2.33	0.42
1:F:68:LEU:HD21	1:F:72:GLU:C	2.39	0.42
1:E:78:THR:HG23	1:F:68:LEU:HB2	2.02	0.41
1:F:66:LYS:HG3	1:F:67:ILE:N	2.35	0.41
1:F:90:LEU:N	1:F:90:LEU:CD1	2.83	0.41
1:A:104:GLU:H	1:B:88:GLN:NE2	2.18	0.41
1:C:68:LEU:HD11	1:C:72:GLU:HB3	2.02	0.41
1:F:131:GLU:OE2	1:G:129:LYS:HE2	2.20	0.41
1:H:90:LEU:N	1:H:90:LEU:CD1	2.83	0.41
1:E:90:LEU:N	1:E:90:LEU:CD1	2.82	0.41
1:A:104:GLU:H	1:B:88:GLN:HE21	1.69	0.41
1:I:90:LEU:N	1:I:90:LEU:CD1	2.83	0.41
1:F:68:LEU:CD2	1:F:73:VAL:CG2	2.99	0.41
1:H:129:LYS:O	1:I:127:LYS:HA	2.20	0.41
1:D:66:LYS:CG	1:D:67:ILE:N	2.84	0.41
1:G:90:LEU:N	1:G:90:LEU:CD1	2.83	0.41
1:H:67:ILE:HG22	1:H:68:LEU:O	2.21	0.41
1:C:90:LEU:N	1:C:90:LEU:CD1	2.83	0.40
1:I:68:LEU:CD2	1:I:72:GLU:HB2	2.51	0.40
1:I:68:LEU:HD21	1:I:73:VAL:N	2.35	0.40

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	73/164 (44%)	71 (97%)	2 (3%)	0	100	100
1	B	74/164 (45%)	74 (100%)	0	0	100	100
1	C	75/164 (46%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	73/164 (44%)	73 (100%)	0	0	100	100
1	E	74/164 (45%)	73 (99%)	1 (1%)	0	100	100
1	F	73/164 (44%)	73 (100%)	0	0	100	100
1	G	74/164 (45%)	73 (99%)	1 (1%)	0	100	100
1	H	75/164 (46%)	74 (99%)	1 (1%)	0	100	100
1	I	74/164 (45%)	73 (99%)	1 (1%)	0	100	100
All	All	665/1476 (45%)	658 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	63/134 (47%)	63 (100%)	0	100	100
1	B	64/134 (48%)	64 (100%)	0	100	100
1	C	65/134 (48%)	65 (100%)	0	100	100
1	D	63/134 (47%)	63 (100%)	0	100	100
1	E	64/134 (48%)	64 (100%)	0	100	100
1	F	63/134 (47%)	63 (100%)	0	100	100
1	G	64/134 (48%)	64 (100%)	0	100	100
1	H	65/134 (48%)	65 (100%)	0	100	100
1	I	64/134 (48%)	64 (100%)	0	100	100
All	All	575/1206 (48%)	575 (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 (28) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	84	GLN
1	A	88	GLN
1	A	121	HIS
1	B	84	GLN
1	B	88	GLN
1	B	121	HIS
1	C	84	GLN
1	C	88	GLN
1	C	121	HIS
1	D	84	GLN
1	D	88	GLN
1	D	121	HIS
1	E	84	GLN
1	E	88	GLN
1	E	121	HIS
1	F	69	GLN
1	F	84	GLN
1	F	88	GLN
1	F	121	HIS
1	G	84	GLN
1	G	88	GLN
1	G	134	GLN
1	H	84	GLN
1	H	88	GLN
1	H	121	HIS
1	I	84	GLN
1	I	88	GLN
1	I	121	HIS

### 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	75/164 (45%)	-0.55	0 <a href="#">100</a> <a href="#">100</a>	18, 25, 42, 59	0
1	B	76/164 (46%)	-0.53	0 <a href="#">100</a> <a href="#">100</a>	19, 25, 39, 63	0
1	C	77/164 (46%)	-0.42	0 <a href="#">100</a> <a href="#">100</a>	19, 27, 47, 73	0
1	D	75/164 (45%)	-0.50	1 (1%) <a href="#">77</a> <a href="#">51</a>	19, 27, 42, 94	0
1	E	76/164 (46%)	-0.57	0 <a href="#">100</a> <a href="#">100</a>	21, 27, 49, 73	0
1	F	75/164 (45%)	-0.54	0 <a href="#">100</a> <a href="#">100</a>	20, 28, 47, 85	0
1	G	76/164 (46%)	-0.55	0 <a href="#">100</a> <a href="#">100</a>	19, 28, 51, 82	0
1	H	77/164 (46%)	-0.42	0 <a href="#">100</a> <a href="#">100</a>	19, 27, 49, 87	0
1	I	76/164 (46%)	-0.50	0 <a href="#">100</a> <a href="#">100</a>	18, 27, 48, 75	0
All	All	683/1476 (46%)	-0.51	1 (0%) <a href="#">95</a> <a href="#">89</a>	18, 27, 48, 94	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	140	ASP	3.0

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.