



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 02:29 PM EDT

PDB ID : 6XWX  
Title : Crystal structure of the Tof1-Csm3 complex  
Authors : Grabarczyk, D.B.  
Deposited on : 2020-01-24  
Resolution : 3.10 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:

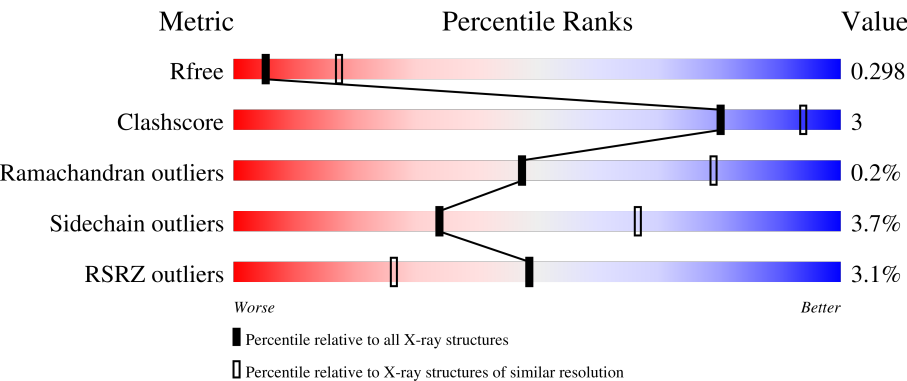
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.10 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 <sub>free</sub>	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	599	<div><div>2%</div><div><div></div><div>81%</div><div>12%</div><div>6%</div></div></div>
1	C	599	<div><div>3%</div><div><div></div><div>84%</div><div>10%</div><div>6%</div></div></div>
1	E	599	<div><div>3%</div><div><div></div><div>85%</div><div>9%</div><div>6%</div></div></div>
2	B	111	<div><div>3%</div><div><div></div><div>63%</div><div>10%</div><div>24%</div></div></div>
2	D	111	<div><div>3%</div><div><div></div><div>68%</div><div>6%</div><div>26%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	111	<div><div></div><div>5%</div><div>59%</div><div>5%</div><div>36%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15731 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 Uncharacterized protein,Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4580	2933	789	837	21			
1	C	562	Total	C	N	O	S	0	0	0
			4579	2930	788	840	21			
1	E	566	Total	C	N	O	S	0	0	0
			4623	2964	792	845	22			

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP G0S825
A	-17	LYS	-	expression tag	UNP G0S825
A	-16	HIS	-	expression tag	UNP G0S825
A	-15	HIS	-	expression tag	UNP G0S825
A	-14	HIS	-	expression tag	UNP G0S825
A	-13	HIS	-	expression tag	UNP G0S825
A	-12	HIS	-	expression tag	UNP G0S825
A	-11	HIS	-	expression tag	UNP G0S825
A	-10	SER	-	expression tag	UNP G0S825
A	-9	ALA	-	expression tag	UNP G0S825
A	-8	GLY	-	expression tag	UNP G0S825
A	-7	LEU	-	expression tag	UNP G0S825
A	-6	GLU	-	expression tag	UNP G0S825
A	-5	VAL	-	expression tag	UNP G0S825
A	-4	LEU	-	expression tag	UNP G0S825
A	-3	PHE	-	expression tag	UNP G0S825
A	-2	GLN	-	expression tag	UNP G0S825
A	-1	GLY	-	expression tag	UNP G0S825
A	0	PRO	-	expression tag	UNP G0S825
A	257	GLY	-	linker	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	GLN	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	VAL	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASN	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLN	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	437	GLY	ASP	conflict	UNP G0S825
C	-18	MET	-	initiating methionine	UNP G0S825
C	-17	LYS	-	expression tag	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP G0S825
C	-15	HIS	-	expression tag	UNP G0S825
C	-14	HIS	-	expression tag	UNP G0S825
C	-13	HIS	-	expression tag	UNP G0S825
C	-12	HIS	-	expression tag	UNP G0S825
C	-11	HIS	-	expression tag	UNP G0S825
C	-10	SER	-	expression tag	UNP G0S825
C	-9	ALA	-	expression tag	UNP G0S825
C	-8	GLY	-	expression tag	UNP G0S825
C	-7	LEU	-	expression tag	UNP G0S825
C	-6	GLU	-	expression tag	UNP G0S825
C	-5	VAL	-	expression tag	UNP G0S825
C	-4	LEU	-	expression tag	UNP G0S825
C	-3	PHE	-	expression tag	UNP G0S825
C	-2	GLN	-	expression tag	UNP G0S825
C	-1	GLY	-	expression tag	UNP G0S825
C	0	PRO	-	expression tag	UNP G0S825
C	257	GLY	-	linker	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	GLN	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	VAL	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASN	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLN	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	437	GLY	ASP	conflict	UNP G0S825
E	-18	MET	-	initiating methionine	UNP G0S825
E	-17	LYS	-	expression tag	UNP G0S825
E	-16	HIS	-	expression tag	UNP G0S825
E	-15	HIS	-	expression tag	UNP G0S825
E	-14	HIS	-	expression tag	UNP G0S825
E	-13	HIS	-	expression tag	UNP G0S825
E	-12	HIS	-	expression tag	UNP G0S825
E	-11	HIS	-	expression tag	UNP G0S825
E	-10	SER	-	expression tag	UNP G0S825
E	-9	ALA	-	expression tag	UNP G0S825
E	-8	GLY	-	expression tag	UNP G0S825
E	-7	LEU	-	expression tag	UNP G0S825
E	-6	GLU	-	expression tag	UNP G0S825
E	-5	VAL	-	expression tag	UNP G0S825
E	-4	LEU	-	expression tag	UNP G0S825
E	-3	PHE	-	expression tag	UNP G0S825
E	-2	GLN	-	expression tag	UNP G0S825
E	-1	GLY	-	expression tag	UNP G0S825
E	0	PRO	-	expression tag	UNP G0S825
E	257	GLY	-	linker	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	GLN	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	VAL	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASN	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLN	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	437	GLY	ASP	conflict	UNP G0S825

- Molecule 2 is a protein called Chromosome segregation in meiosis protein.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			693	447	125	119	2			
2	D	82	Total	C	N	O	S	0	0	0
			675	436	120	117	2			
2	F	71	Total	C	N	O	S	0	0	0
			581	378	104	97	2			

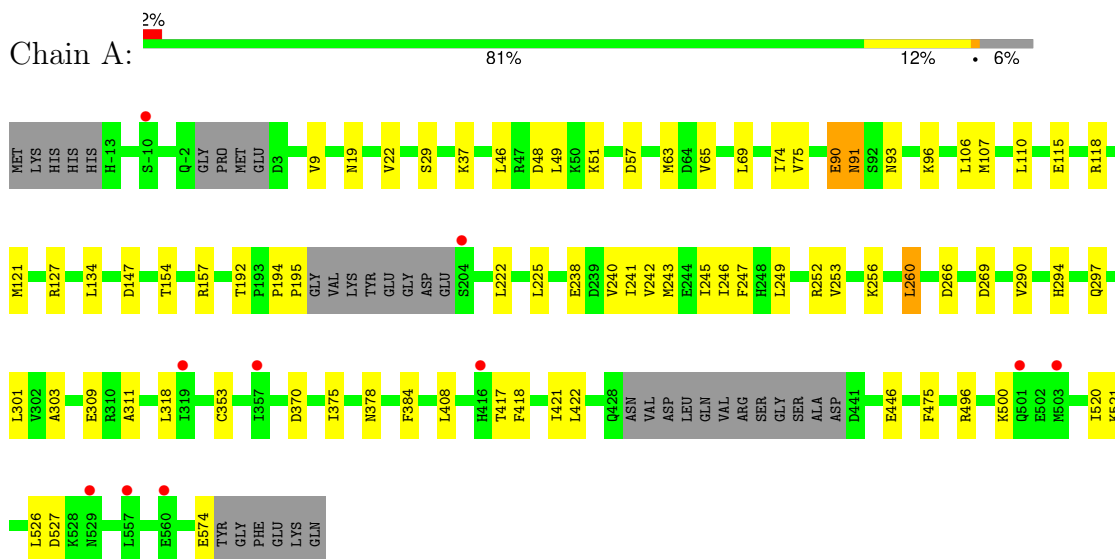
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	MET	-	initiating methionine	UNP G0S0S7
D	47	MET	-	initiating methionine	UNP G0S0S7
F	47	MET	-	initiating methionine	UNP G0S0S7

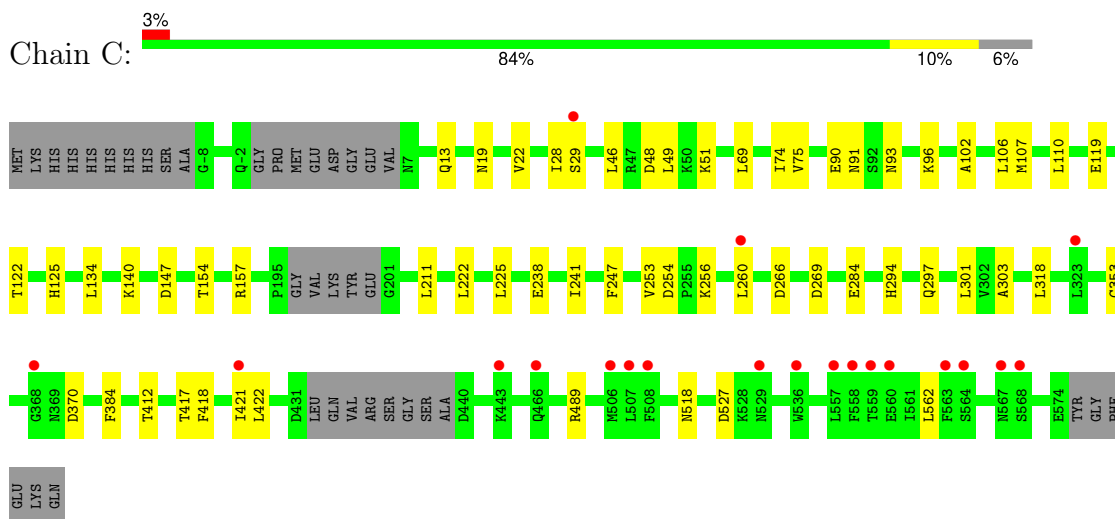
### 3 Residue-property plots [i](#)

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.

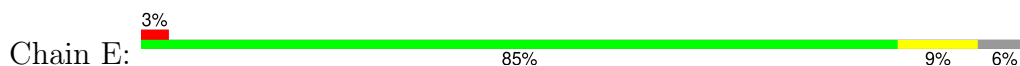
- Molecule 1: Uncharacterized protein,Uncharacterized protein

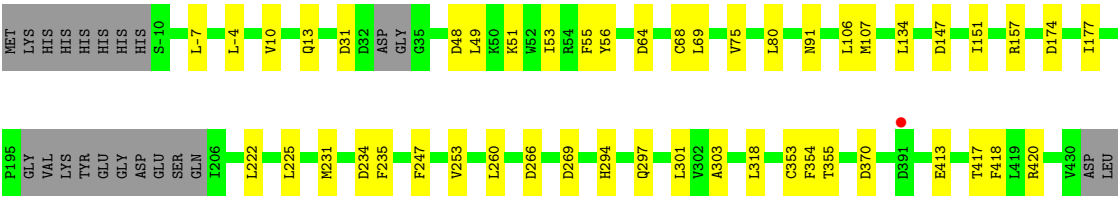


- Molecule 1: Uncharacterized protein,Uncharacterized protein



- Molecule 1: Uncharacterized protein,Uncharacterized protein





• Molecule 2: Chromosome segregation in meiosis protein



• Molecule 2: Chromosome segregation in meiosis protein



• Molecule 2: Chromosome segregation in meiosis protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.47Å 82.03Å 161.16Å 90.00° 124.85° 90.00°	Depositor
Resolution (Å)	45.73 – 3.10 76.74 – 3.09	Depositor EDS
% Data completeness (in resolution range)	52.3 (45.73-3.10) 52.1 (76.74-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.237 , 0.264 0.263 , 0.298	Depositor DCC
$R_{free}$ test set	1355 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 76.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	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.*

<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	0.41	0/4677	0.58	0/6322
1	C	0.41	0/4676	0.58	0/6320
1	E	0.41	0/4722	0.58	0/6382
2	B	0.38	0/708	0.55	0/948
2	D	0.39	0/689	0.54	0/922
2	F	0.40	0/595	0.54	0/796
All	All	0.41	0/16067	0.58	0/21690

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	4580	0	4534	34	0
1	C	4579	0	4535	22	0
1	E	4623	0	4607	22	0
2	B	693	0	720	5	0
2	D	675	0	700	2	0
2	F	581	0	604	3	0
All	All	15731	0	15700	85	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 3.

All (85) 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:A:9:VAL:HG11	1:A:127:ARG:HE	1.49	0.76
1:E:10:VAL:HG11	1:E:68:CYS:SG	2.35	0.67
1:E:91:ASN:HB3	1:E:157:ARG:HH11	1.65	0.61
1:C:238:GLU:HA	1:C:241:ILE:HD12	1.82	0.61
1:C:19:ASN:HA	1:C:22:VAL:HG22	1.83	0.61
1:A:19:ASN:HA	1:A:22:VAL:HG22	1.83	0.61
1:A:93:ASN:HB3	1:A:96:LYS:HB2	1.83	0.60
1:C:93:ASN:HB3	1:C:96:LYS:HB2	1.84	0.60
1:E:247:PHE:HB2	1:E:301:LEU:HD11	1.83	0.60
1:C:91:ASN:HB3	1:C:157:ARG:HH21	1.68	0.59
1:A:247:PHE:HB2	1:A:301:LEU:HD11	1.85	0.59
1:A:238:GLU:HA	1:A:241:ILE:HD12	1.83	0.58
2:B:98:HIS:CD2	2:B:101:SER:H	2.22	0.58
1:A:91:ASN:HB2	1:A:157:ARG:HH11	1.69	0.57
1:A:192:THR:HG21	1:A:252:ARG:HH22	1.70	0.56
1:C:75:VAL:HG13	1:C:107:MET:HG2	1.89	0.55
1:E:174:ASP:HA	1:E:177:ILE:HD12	1.91	0.53
1:E:355:THR:HG21	1:E:413:GLU:HG2	1.91	0.53
1:C:303:ALA:HB2	1:C:353:CYS:HA	1.90	0.53
1:C:28:ILE:HG13	1:C:29:SER:H	1.73	0.53
1:A:303:ALA:HB2	1:A:353:CYS:HA	1.92	0.51
1:E:75:VAL:HG13	1:E:107:MET:HG2	1.93	0.51
2:D:87:MET:HB3	2:D:109:PHE:HZ	1.76	0.50
2:B:85:ARG:HB3	2:B:146:TRP:HE1	1.76	0.50
1:C:253:VAL:HG21	1:C:260:LEU:HD21	1.93	0.50
1:E:303:ALA:HB2	1:E:353:CYS:HA	1.93	0.50
1:C:269:ASP:HA	1:C:318:LEU:HD22	1.94	0.49
1:C:294:HIS:HA	1:C:297:GLN:HE21	1.77	0.49
1:E:544:LEU:HB3	2:F:103:THR:HG21	1.93	0.49
1:E:269:ASP:HA	1:E:318:LEU:HD22	1.94	0.49
2:B:93:PHE:HD1	2:B:93:PHE:H	1.61	0.48
1:A:75:VAL:HG13	1:A:107:MET:HG2	1.95	0.48
1:A:242:VAL:HA	1:A:245:ILE:HD12	1.96	0.48
1:A:269:ASP:HA	1:A:318:LEU:HD22	1.95	0.47
1:C:412:THR:HG22	1:C:489:ARG:HE	1.80	0.46
1:A:154:THR:HA	1:A:157:ARG:HD3	1.97	0.46
2:F:81:ILE:HG13	2:F:82:PRO:HD3	1.98	0.46
1:A:49:LEU:HD22	1:A:69:LEU:HD21	1.98	0.45
1:A:118:ARG:HB2	1:A:121:MET:HG2	1.99	0.45
1:C:154:THR:HA	1:C:157:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:O	1:A:500:LYS:HB2	2.17	0.45
1:E:294:HIS:HA	1:E:297:GLN:HE21	1.81	0.45
1:E:503:MET:HG2	1:E:574:GLU:HG3	1.99	0.45
1:A:408:LEU:HD21	1:A:475:PHE:HA	1.99	0.45
1:A:240:VAL:HG11	1:A:290:VAL:HG12	1.98	0.44
1:A:294:HIS:HA	1:A:297:GLN:HE21	1.81	0.44
1:E:48:ASP:HA	1:E:51:LYS:HD3	1.99	0.44
1:C:140:LYS:HE3	1:C:211:LEU:HD13	1.98	0.44
1:C:384:PHE:HD1	1:C:422:LEU:HD22	1.83	0.44
1:A:520:ILE:HG22	1:A:521:LYS:HG3	1.98	0.44
1:C:49:LEU:HD22	1:C:69:LEU:HD21	1.99	0.44
1:E:417:THR:HG22	1:E:420:ARG:HH21	1.81	0.43
1:A:417:THR:O	1:A:421:ILE:HG12	2.18	0.43
1:A:384:PHE:HD1	1:A:422:LEU:HD22	1.84	0.43
1:A:48:ASP:HA	1:A:51:LYS:HD3	1.99	0.43
1:C:247:PHE:HB2	1:C:301:LEU:HD11	2.00	0.43
1:A:246:ILE:HA	1:A:249:LEU:HD12	2.00	0.43
1:C:417:THR:O	1:C:421:ILE:HG12	2.18	0.43
1:A:57:ASP:CG	1:A:65:VAL:HG22	2.39	0.43
1:C:48:ASP:HA	1:C:51:LYS:HD3	2.00	0.43
1:E:510:LEU:HG	1:E:561:ILE:HG12	2.01	0.43
1:E:49:LEU:HD22	1:E:69:LEU:HD21	2.01	0.43
1:A:90:GLU:HG2	1:A:96:LYS:HD2	2.01	0.42
1:E:-7:LEU:HB3	1:E:-4:LEU:HD12	2.01	0.42
1:C:19:ASN:HB2	1:E:55:PHE:HB3	2.01	0.42
1:C:119:GLU:HA	1:C:125:HIS:HB3	2.00	0.42
2:D:78:GLU:HG2	2:D:81:ILE:HB	2.01	0.42
1:A:256:LYS:HG2	1:A:311:ALA:HB2	2.01	0.42
1:A:194:PRO:HA	1:A:195:PRO:HD3	1.97	0.42
1:A:29:SER:HA	1:A:37:LYS:HE2	2.02	0.41
1:A:375:ILE:HD13	1:A:378:ASN:HD21	1.84	0.41
1:C:46:LEU:HB3	1:C:102:ALA:HB1	2.02	0.41
2:B:81:ILE:HA	2:B:84:LEU:HD12	2.02	0.41
1:E:253:VAL:HG11	1:E:260:LEU:HD13	2.03	0.41
1:A:69:LEU:HD13	1:A:110:LEU:HD11	2.03	0.41
1:A:526:LEU:HG	1:A:526:LEU:O	2.21	0.41
2:B:140:ARG:HD2	2:B:143:ARG:HH21	1.86	0.41
1:A:115:GLU:HB2	1:A:118:ARG:HE	1.86	0.41
1:A:253:VAL:HG11	1:A:260:LEU:HD21	2.03	0.40
1:E:56:TYR:HE2	1:E:64:ASP:HB2	1.86	0.40
1:E:509:ARG:HH12	2:F:131:GLU:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:HG2	1:A:301:LEU:HD13	2.04	0.40
1:C:69:LEU:HD13	1:C:110:LEU:HD11	2.04	0.40
1:E:80:LEU:HD22	1:E:151:ILE:HG13	2.03	0.40
1:E:231:MET:HA	1:E:235:PHE:HB2	2.03	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	556/599 (93%)	533 (96%)	22 (4%)	1 (0%)	47	79
1	C	554/599 (92%)	534 (96%)	19 (3%)	1 (0%)	47	79
1	E	558/599 (93%)	532 (95%)	24 (4%)	2 (0%)	34	69
2	B	82/111 (74%)	80 (98%)	2 (2%)	0	100	100
2	D	80/111 (72%)	78 (98%)	2 (2%)	0	100	100
2	F	69/111 (62%)	64 (93%)	5 (7%)	0	100	100
All	All	1899/2130 (89%)	1821 (96%)	74 (4%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	503	MET
1	A	527	ASP
1	C	527	ASP
1	E	527	ASP



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/528 (93%)	472 (96%)	17 (4%)	36	68
1	C	492/528 (93%)	475 (96%)	17 (4%)	36	68
1	E	500/528 (95%)	485 (97%)	15 (3%)	41	71
2	B	73/96 (76%)	65 (89%)	8 (11%)	6	25
2	D	71/96 (74%)	68 (96%)	3 (4%)	30	62
2	F	60/96 (62%)	58 (97%)	2 (3%)	38	69
All	All	1685/1872 (90%)	1623 (96%)	62 (4%)	34	66

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	63	MET
1	A	74	ILE
1	A	90	GLU
1	A	91	ASN
1	A	106	LEU
1	A	134	LEU
1	A	147	ASP
1	A	222	LEU
1	A	225	LEU
1	A	260	LEU
1	A	266	ASP
1	A	309	GLU
1	A	370	ASP
1	A	418	PHE
1	A	446	GLU
1	A	574	GLU
2	B	78	GLU
2	B	81	ILE
2	B	92	LYS
2	B	93	PHE
2	B	117	LEU

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Mol	Chain	Res	Type
2	B	144	LEU
2	B	146	TRP
2	B	150	LEU
1	C	13	GLN
1	C	74	ILE
1	C	90	GLU
1	C	106	LEU
1	C	122	THR
1	C	134	LEU
1	C	147	ASP
1	C	222	LEU
1	C	225	LEU
1	C	254	ASP
1	C	256	LYS
1	C	266	ASP
1	C	284	GLU
1	C	370	ASP
1	C	418	PHE
1	C	518	ASN
1	C	562	LEU
2	D	99	GLU
2	D	117	LEU
2	D	144	LEU
1	E	13	GLN
1	E	31	ASP
1	E	53	ILE
1	E	106	LEU
1	E	134	LEU
1	E	147	ASP
1	E	222	LEU
1	E	225	LEU
1	E	234	ASP
1	E	266	ASP
1	E	354	PHE
1	E	370	ASP
1	E	418	PHE
1	E	470	ASP
1	E	562	LEU
2	F	144	LEU
2	F	146	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	378	ASN
2	B	98	HIS
1	C	297	GLN
1	C	466	GLN
1	C	518	ASN
1	E	11	HIS
1	E	297	GLN
1	E	450	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 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

### 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<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	564/599 (94%)	-0.04	10 (1%)	68 47	65, 110, 152, 179	0
1	C	562/599 (93%)	0.11	20 (3%)	42 22	57, 121, 165, 194	0
1	E	566/599 (94%)	0.10	17 (3%)	50 27	58, 115, 183, 209	0
2	B	84/111 (75%)	0.18	3 (3%)	42 22	132, 174, 196, 201	0
2	D	82/111 (73%)	0.06	3 (3%)	41 21	154, 169, 191, 203	0
2	F	71/111 (63%)	0.37	6 (8%)	10 4	151, 160, 172, 188	0
All	All	1929/2130 (90%)	0.07	59 (3%)	49 26	57, 119, 181, 209	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	567	ASN	9.1
1	E	558	PHE	6.0
1	E	557	LEU	4.6
1	E	568	SER	4.4
1	C	508	PHE	4.0
1	C	507	LEU	4.0
2	B	90	ARG	3.8
2	F	84	LEU	3.8
1	A	501	GLN	3.6
1	C	563	PHE	3.4
1	C	567	ASN	3.3
2	B	71	ASP	3.2
1	E	497	VAL	3.2
1	C	564	SER	3.1
2	F	108	SER	3.0
1	C	559	THR	3.0
1	E	560	GLU	3.0
2	F	121	ALA	3.0
1	E	563	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	507	LEU	2.9
1	C	536	TRP	2.9
2	F	138	THR	2.8
1	A	557	LEU	2.8
1	C	560	GLU	2.7
1	C	368	GLY	2.7
1	C	558	PHE	2.7
1	C	260	LEU	2.7
1	E	510	LEU	2.7
1	C	323	LEU	2.7
1	E	529	ASN	2.7
1	C	466	GLN	2.6
1	C	557	LEU	2.6
2	D	136	LYS	2.6
1	C	443	LYS	2.6
1	E	559	THR	2.5
1	C	506	MET	2.5
1	E	391	ASP	2.5
1	E	496	ARG	2.5
1	E	511	ASP	2.4
2	F	94	LYS	2.4
1	C	421	ILE	2.4
1	C	29	SER	2.4
1	E	556	ALA	2.4
2	D	72	ASP	2.3
1	C	529	ASN	2.3
1	E	530	SER	2.3
1	A	204	SER	2.3
1	A	503	MET	2.3
1	A	560	GLU	2.2
2	B	93	PHE	2.2
2	F	123	PHE	2.2
1	A	416	HIS	2.2
1	A	357	ILE	2.1
1	A	-10	SER	2.1
2	D	140	ARG	2.1
1	E	555	PRO	2.1
1	C	568	SER	2.0
1	A	319	ILE	2.0
1	A	529	ASN	2.0

## 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.