

wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2023 – 08:05 AM EDT

PDB ID : 5U1B

Title: Ferritin with Gc MtrE loop2 inserted at the N-terminus

Authors : Wang, S. Deposited on : 2016-11-28

Resolution : 2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

MolProbity: 4.02b-467 Xtriage (Phenix): 1.13

EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

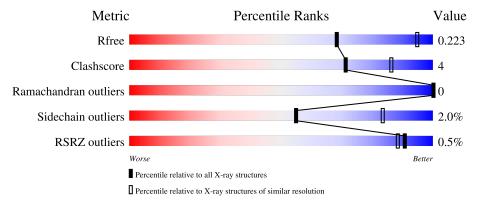
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.81 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	189	78%	,)	11%
1	В	189	81%	•	12%
1	С	189	76% 12%		12%
1	D	189	82%	%	12%
1	Е	189	79% 8%		12%



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Mol	Chain	Length	Quality of chain	
1	F	189	81%	6% • 12%
1	G	189	83%	5% • 12%
1	Н	189	80%	8% • 11%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10895 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 MtrE protein, Ferritin chimera.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	168	Total	С	N	О	S	0	0	0
1	A	100	1374	875	229	265	5	0	0	U
1	В	166	Total	С	N	О	S	0	0	0
1	Ъ	100	1356	865	225	261	5	0	0	U
1	С	166	Total	С	N	О	S	0	0	0
1		100	1356	865	225	261	5	0	0	U
1	D	166	Total	С	N	О	S	0	0	0
1	D	100	1356	865	225	261	5	U	U	
1	Е	166	Total	С	N	О	S	0	0	0
1	<u> </u>	100	1356	865	225	261	5	0	0	U
1	F	166	Total	С	N	О	S	0	0	0
1	I.	100	1356	865	225	261	5	0	0	U
1	G	166	Total	С	N	О	S	0	0	0
1	G	100	1356	865	225	261	5	0	0	U
1	Н	168	Total	С	N	О	S	0	0	0
1	Н	100	1374	875	229	265	5	0		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q51006
A	-20	ALA	-	expression tag	UNP Q51006
A	-19	ARG	_	expression tag	UNP Q51006
A	-18	CYS	-	expression tag	UNP Q51006
A	-2	CYS	-	linker	UNP Q51006
A	-1	ASP	-	linker	UNP Q51006
A	0	HIS	-	linker	UNP Q51006
A	125	SER	ALA	conflict	UNP O69434
В	-21	MET	-	initiating methionine	UNP Q51006
В	-20	ALA	-	expression tag	UNP Q51006
В	-19	ARG	-	expression tag	UNP Q51006
В	-18	CYS	-	expression tag	UNP Q51006
В	-2	CYS	-	linker	UNP Q51006



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B	Chain	Residue	Modelled Modelled	Actual	Comment	Reference
B 125 SER ALA conflict UNP 069 C -21 MET - initiating methionine UNP Q510 C -20 ALA - expression tag UNP Q510 C -19 ARG - expression tag UNP Q510 C -18 CYS - expression tag UNP Q510 C -18 CYS - expression tag UNP Q510 C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - expression tag UNP Q510 D -1 ASP - linker UNP Q510 D -1 ASP -	В	-1	ASP	-	linker	UNP Q51006
C -21 MET - initiating methionine UNP Q510 C -20 ALA - expression tag UNP Q510 C -19 ARG - expression tag UNP Q510 C -18 CYS - expression tag UNP Q510 C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -21 MET - expression tag UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - expression tag UNP Q510 D -1 ASP - linker UNP Q510 D	В	0	HIS	-	linker	UNP Q51006
C -20 ALA - expression tag UNP Q510 C -19 ARG - expression tag UNP Q510 C -18 CYS - expression tag UNP Q510 C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -21 MET - initiating methionine UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D -1 ASP - linker UNP Q510 E -21 <td>В</td> <td>125</td> <td>SER</td> <td>ALA</td> <td>conflict</td> <td>UNP O69434</td>	В	125	SER	ALA	conflict	UNP O69434
C -19 ARG - expression tag UNP Q510 C -18 CYS - expression tag UNP Q510 C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -20 ALA - expression tag UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - expression tag UNP Q510 D -18 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D -1 ASP - linitating methionine UNP Q510 E <td< td=""><td>С</td><td>-21</td><td>MET</td><td>-</td><td>initiating methionine</td><td>UNP Q51006</td></td<>	С	-21	MET	-	initiating methionine	UNP Q51006
C -18 CYS - expression tag UNP Q510 C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -20 ALA - expression tag UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - expression tag UNP Q510 D -18 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D -1 ASP - linitiating methionine UNP Q510 E -21 MET - initiating methionine UNP Q510 E	С	-20	ALA	-	expression tag	UNP Q51006
C -2 CYS - linker UNP Q510 C -1 ASP - linker UNP Q510 C 0 HIS - linker UNP Q510 C 125 SER ALA conflict UNP Q510 D -21 MET - initiating methionine UNP Q510 D -20 ALA - expression tag UNP Q510 D -19 ARG - expression tag UNP Q510 D -18 CYS - expression tag UNP Q510 D -18 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D -1 ASP - linitiating methionine UNP Q510 E -21 MET - initiating methionine UNP Q510 E -19 ARG - expression tag UNP Q510 E	С	-19	ARG	-	expression tag	UNP Q51006
C -1 ASP (C) -1 linker (UNP Q510) C 0 HIS (C) -1 linker (UNP Q510) C 125 (SER) (SER) (SER) (SER) (SER) (SER) ALA (C) (SER) (S	С	-18	CYS	-	expression tag	UNP Q51006
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D	С	125	SER	ALA	conflict	UNP O69434
D	D	-21	MET	_	initiating methionine	UNP Q51006
D -18 CYS - expression tag UNP Q510 D -2 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D 0 HIS - linker UNP Q510 D 125 SER ALA conflict UNP Q510 E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 125 SER ALA conflict UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -19 <td>D</td> <td>-20</td> <td>ALA</td> <td>_</td> <td>expression tag</td> <td>UNP Q51006</td>	D	-20	ALA	_	expression tag	UNP Q51006
D -2 CYS - linker UNP Q510 D -1 ASP - linker UNP Q510 D 0 HIS - linker UNP Q510 D 125 SER ALA conflict UNP Q510 E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - linker UNP Q510 E -2 CYS - linker UNP Q510 E 125 SER ALA conflict UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -18 <td>D</td> <td>-19</td> <td>ARG</td> <td>-</td> <td>expression tag</td> <td>UNP Q51006</td>	D	-19	ARG	-	expression tag	UNP Q51006
D -1 ASP - linker UNP Q510 D 0 HIS - linker UNP Q510 D 125 SER ALA conflict UNP Q510 E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - linker UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -1	D	-18	CYS	-	expression tag	UNP Q51006
D 0 HIS - linker UNP Q510 D 125 SER ALA conflict UNP 0690 E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 125 SER ALA conflict UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -19 ARG - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F	D	-2	CYS	_	linker	UNP Q51006
D 125 SER ALA conflict UNP 0694 E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 125 SER ALA conflict UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - expression tag UNP Q510	D	-1	ASP	-	linker	UNP Q51006
E -21 MET - initiating methionine UNP Q510 E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	D	0	HIS	-	linker	UNP Q51006
E -20 ALA - expression tag UNP Q510 E -19 ARG - expression tag UNP Q510 E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP O690 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	D	125	SER	ALA	conflict	UNP O69434
E -19 ARG - expression tag UNP Q510 E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP Q690 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-21	MET	-	initiating methionine	UNP Q51006
E -18 CYS - expression tag UNP Q510 E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP O694 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-20	ALA	-	expression tag	UNP Q51006
E -2 CYS - linker UNP Q510 E -1 ASP - linker UNP Q510 E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-19	ARG	-	expression tag	UNP Q51006
E -1 ASP - linker UNP Q510 E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP Q510 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-18	CYS	-	expression tag	UNP Q51006
E 0 HIS - linker UNP Q510 E 125 SER ALA conflict UNP Q690 F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-2	CYS	-	linker	UNP Q51006
E 125 SER ALA conflict UNP 069- F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	-1	ASP	-	linker	UNP Q51006
F -21 MET - initiating methionine UNP Q510 F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	0	HIS	-	linker	UNP Q51006
F -20 ALA - expression tag UNP Q510 F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	Е	125	SER	ALA	conflict	UNP O69434
F -19 ARG - expression tag UNP Q510 F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	F	-21	MET	-	initiating methionine	UNP Q51006
F -18 CYS - expression tag UNP Q510 F -2 CYS - linker UNP Q510	F	-20	ALA	-	expression tag	UNP Q51006
F -2 CYS - linker UNP Q510	F	-19	ARG	-	expression tag	UNP Q51006
	F	-18	CYS	-	expression tag	UNP Q51006
E 1 ACD 11.1 IIND OF 1	F	-2	CYS	-	linker	UNP Q51006
r -1 ASP - linker UNP Q510	F	-1	ASP	-	linker	UNP Q51006
F 0 HIS - linker UNP Q510	F	0	HIS	-	linker	UNP Q51006
F 125 SER ALA conflict UNP O694	F	125	SER	ALA	conflict	UNP O69434
G -21 MET - initiating methionine UNP Q510	G	-21	MET	-	initiating methionine	UNP Q51006
G -20 ALA - expression tag UNP Q510	G	-20	ALA	-	expression tag	UNP Q51006
G -19 ARG - expression tag UNP Q510	G	-19	ARG	-	expression tag	UNP Q51006
G -18 CYS - expression tag UNP Q510	G	-18	CYS	-	expression tag	UNP Q51006
G -2 CYS - linker UNP Q510	G	-2	CYS	-	linker	UNP Q51006
G -1 ASP - linker UNP Q510	G	-1	ASP	-	linker	UNP Q51006
G 0 HIS - linker UNP Q510	G	0	HIS	-	linker	UNP Q51006



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Chain	Residue	Modelled	Actual Comment		Reference
G	125	SER	ALA	conflict	UNP O69434
Н	-21	MET	-	initiating methionine	UNP Q51006
Н	-20	ALA	-	expression tag	UNP Q51006
Н	-19	ARG	-	expression tag	UNP Q51006
Н	-18	CYS	-	expression tag	UNP Q51006
Н	-2	CYS	-	linker	UNP Q51006
Н	-1	ASP	-	linker	UNP Q51006
Н	0	HIS	-	linker	UNP Q51006
Н	125	SER	ALA	conflict	UNP O69434

• Molecule 2 is water.

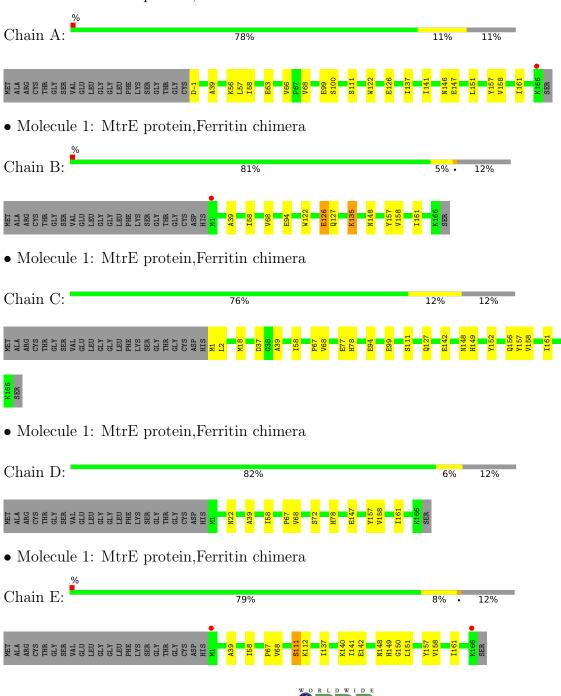
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	В	1	Total O 1 1	0	0
2	С	1	Total O 1 1	0	0
2	G	3	Total O 3 3	0	0
2	Н	1	Total O 1 1	0	0



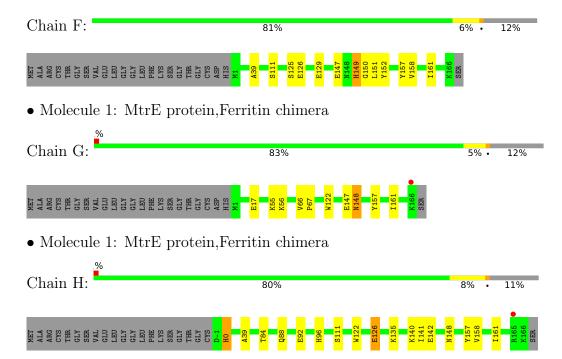
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MtrE protein, Ferritin chimera



• Molecule 1: MtrE protein, Ferritin chimera





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	124.51Å 124.51Å 314.88Å	Donogiton
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	$egin{array}{cccc} 19.89 & - & 2.81 \ 19.89 & - & 2.81 \end{array}$	Depositor EDS
% Data completeness	92.4 (19.89-2.81)	Depositor
(in resolution range)	92.7 (19.89-2.81)	EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.19 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D	0.177 , 0.225	Depositor
R, R_{free}	0.178 , 0.223	DCC
R_{free} test set	2273 reflections $(5.52%)$	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.27 \; , 9.6$	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	$\begin{array}{c} 0.056 \text{ for } -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/\\ 3*k+1/3*l \\ 0.079 \text{ for } -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+\\ 1/3*l,-4/3*h+4/3*k+1/3*l \\ 0.057 \text{ for } -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k \\ +1/3*l \\ 0.056 \text{ for } -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 \\ *k-1/3*l \\ 0.056 \text{ for } 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l \\ 0.080 \text{ for } -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l \\ 0.437 \text{ for } -h-k,k,-l \end{array}$	Xtriage
Reported twinning fraction Outliers	0.545 for H, K, L 0.455 for K, H, -L 0 of 41193 reflections	Depositor
F_o, F_c correlation	0 of 41195 reflections 0.94	Xtriage EDS
Γ_o, Γ_c correlation Total number of atoms	10895	wwPDB-VP
	62.0	wwPDB-VP wwPDB-VP
Average B, all atoms (\mathring{A}^2)	02.0	WWLDD-VL

¹Intensities estimated from amplitudes.



²Theoretical 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.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.



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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	1.06	1/1405 (0.1%)	0.84	1/1895 (0.1%)	
1	В	0.98	0/1386	0.80	0/1869	
1	С	0.99	0/1386	0.80	0/1869	
1	D	0.92	0/1386	0.83	0/1869	
1	Е	0.90	0/1386	0.80	0/1869	
1	F	0.90	0/1386	0.79	1/1869 (0.1%)	
1	G	1.05	0/1386	0.81	0/1869	
1	Н	1.04	0/1405	0.78	0/1895	
All	All	0.98	1/11126 (0.0%)	0.81	2/15004 (0.0%)	

All (1) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$[Ideal(\AA)]$
1	A	63	GLU	CG-CD	5.17	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	A	147	GLU	N-CA-C	5.13	124.86	111.00
1	F	149	HIS	C-N-CA	-5.03	111.74	122.30

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	1374	0	1326	8	0
1	В	1356	0	1315	11	0
1	С	1356	0	1315	13	0
1	D	1356	0	1315	5	0
1	Е	1356	0	1315	10	0
1	F	1356	0	1315	7	0
1	G	1356	0	1315	8	0
1	Н	1374	0	1326	14	0
2	A	5	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	G	3	0	0	0	0
2	Н	1	0	0	0	0
All	All	10895	0	10542	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 75 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:E:137:ILE:O	1:E:141:ILE:HG13	1.75	0.86
1:C:18:MET:HE1	1:D:22:ASN:OD1	1.81	0.80
1:F:149:HIS:O	1:F:150:GLY:C	2.17	0.80
1:F:149:HIS:O	1:F:152:TYR:N	2.20	0.74
1:H:96:HIS:O	1:H:96:HIS:ND1	2.25	0.69

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	Perce	ntiles
1	A	166/189 (88%)	162 (98%)	4 (2%)	0	100	100
1	В	164/189 (87%)	160 (98%)	4 (2%)	0	100	100
1	C	164/189 (87%)	160 (98%)	4 (2%)	0	100	100
1	D	164/189 (87%)	159 (97%)	5 (3%)	0	100	100
1	E	164/189 (87%)	160 (98%)	4 (2%)	0	100	100
1	F	164/189 (87%)	159 (97%)	5 (3%)	0	100	100
1	G	164/189 (87%)	160 (98%)	4 (2%)	0	100	100
1	Н	166/189 (88%)	162 (98%)	4 (2%)	0	100	100
All	All	1316/1512 (87%)	1282 (97%)	34 (3%)	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	Perce	ntiles
1	A	152/167 (91%)	147 (97%)	5 (3%)	38	70
1	В	150/167 (90%)	148 (99%)	2 (1%)	69	90
1	С	150/167 (90%)	146 (97%)	4 (3%)	44	77
1	D	150/167 (90%)	147 (98%)	3 (2%)	55	83
1	E	150/167 (90%)	148 (99%)	2 (1%)	69	90
1	F	150/167 (90%)	148 (99%)	2 (1%)	69	90
1	G	150/167 (90%)	148 (99%)	2 (1%)	69	90
1	Н	152/167 (91%)	148 (97%)	4 (3%)	46	78
All	All	1204/1336 (90%)	1180 (98%)	24 (2%)	55	83

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	67	PRO
1	F	126	GLU



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Mol	Chain	Res	Type
1	F	111	SER
1	G	17	GLU
1	В	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	65	ASN
1	Н	0	HIS
1	Н	148	ASN
1	С	148	ASN
1	С	149	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^{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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	168/189 (88%)	-0.55	1 (0%) 89 86	36, 56, 92, 137	2 (1%)
1	В	166/189 (87%)	-0.51	1 (0%) 89 86	31, 57, 87, 109	2 (1%)
1	С	166/189 (87%)	-0.53	0 100 100	37, 60, 89, 122	2 (1%)
1	D	166/189 (87%)	-0.54	0 100 100	37, 59, 82, 123	0
1	Е	166/189 (87%)	-0.52	2 (1%) 79 73	44, 64, 93, 126	0
1	F	166/189 (87%)	-0.46	0 100 100	44, 64, 93, 120	4 (2%)
1	G	166/189 (87%)	-0.53	1 (0%) 89 86	35, 55, 92, 136	2 (1%)
1	Н	168/189 (88%)	-0.54	1 (0%) 89 86	39, 55, 98, 124	1 (0%)
All	All	1332/1512 (88%)	-0.52	6 (0%) 91 88	31, 59, 93, 137	13 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	166	LYS	4.1
1	Е	166	LYS	2.7
1	Н	165	ARG	2.2
1	В	1	MET	2.2
1	Е	1	MET	2.1

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.

