



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:54 am BST

PDB ID : 5XGO
Title : The Ferritin E-Domain: Toward Understanding Its Role in Protein Cage Assembly Through the Crystal Structure of a Maxi-/Mini-Ferritin Chimera
Authors : Cornell, T.A.; Srivastava, Y.; Jauch, R.; Fan, R.; Orner, B.P.
Deposited on : 2017-04-14
Resolution : 1.99 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

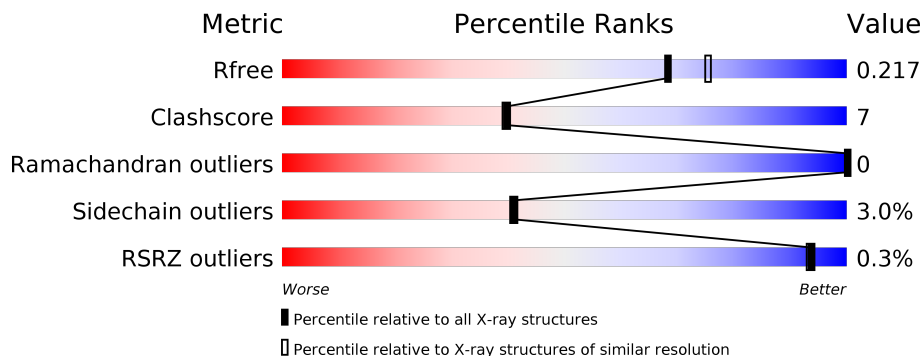
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	200	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	

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Mol	Chain	Length	Quality of chain
1	G	200	<p>%</p> <p>67% 9% •• 22%</p>
1	H	200	<p>68% 7% •• 22%</p>
1	I	200	<p>66% 10% •• 22%</p>
1	J	200	<p>68% 9% • 23%</p>
1	K	200	<p>63% 13% •• 22%</p>
1	L	200	<p>%</p> <p>68% 8% •• 23%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16563 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 DNA protection during starvation protein, Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1227	773	214	236	4	0	0	0
1	B	156	1235	777	216	238	4	0	0	0
1	C	155	1227	773	214	236	4	0	0	0
1	D	156	1235	777	216	238	4	0	0	0
1	E	155	1227	773	214	236	4	0	0	0
1	F	156	1235	777	216	238	4	0	0	0
1	G	156	1235	777	216	238	4	0	0	0
1	H	156	1235	777	216	238	4	0	0	0
1	I	156	1235	777	216	238	4	0	0	0
1	J	155	1227	773	214	236	4	0	0	0
1	K	156	1235	777	216	238	4	0	0	0
1	L	155	1227	773	214	236	4	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P0ABT2
A	-12	ALA	-	expression tag	UNP P0ABT2
A	-11	HIS	-	expression tag	UNP P0ABT2
A	-10	HIS	-	expression tag	UNP P0ABT2
A	-9	HIS	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP P0ABT2
A	-7	HIS	-	expression tag	UNP P0ABT2
A	-6	HIS	-	expression tag	UNP P0ABT2
A	-5	VAL	-	expression tag	UNP P0ABT2
A	-4	ASP	-	expression tag	UNP P0ABT2
A	-3	ASP	-	expression tag	UNP P0ABT2
A	-2	ASP	-	expression tag	UNP P0ABT2
A	-1	ASP	-	expression tag	UNP P0ABT2
A	0	LYS	-	expression tag	UNP P0ABT2
A	164	CYS	-	linker	UNP P0ABT2
A	165	ASN	-	linker	UNP P0ABT2
B	-13	MET	-	expression tag	UNP P0ABT2
B	-12	ALA	-	expression tag	UNP P0ABT2
B	-11	HIS	-	expression tag	UNP P0ABT2
B	-10	HIS	-	expression tag	UNP P0ABT2
B	-9	HIS	-	expression tag	UNP P0ABT2
B	-8	HIS	-	expression tag	UNP P0ABT2
B	-7	HIS	-	expression tag	UNP P0ABT2
B	-6	HIS	-	expression tag	UNP P0ABT2
B	-5	VAL	-	expression tag	UNP P0ABT2
B	-4	ASP	-	expression tag	UNP P0ABT2
B	-3	ASP	-	expression tag	UNP P0ABT2
B	-2	ASP	-	expression tag	UNP P0ABT2
B	-1	ASP	-	expression tag	UNP P0ABT2
B	0	LYS	-	expression tag	UNP P0ABT2
B	164	CYS	-	linker	UNP P0ABT2
B	165	ASN	-	linker	UNP P0ABT2
C	-13	MET	-	expression tag	UNP P0ABT2
C	-12	ALA	-	expression tag	UNP P0ABT2
C	-11	HIS	-	expression tag	UNP P0ABT2
C	-10	HIS	-	expression tag	UNP P0ABT2
C	-9	HIS	-	expression tag	UNP P0ABT2
C	-8	HIS	-	expression tag	UNP P0ABT2
C	-7	HIS	-	expression tag	UNP P0ABT2
C	-6	HIS	-	expression tag	UNP P0ABT2
C	-5	VAL	-	expression tag	UNP P0ABT2
C	-4	ASP	-	expression tag	UNP P0ABT2
C	-3	ASP	-	expression tag	UNP P0ABT2
C	-2	ASP	-	expression tag	UNP P0ABT2
C	-1	ASP	-	expression tag	UNP P0ABT2
C	0	LYS	-	expression tag	UNP P0ABT2
C	164	CYS	-	linker	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	ASN	-	linker	UNP P0ABT2
D	-13	MET	-	expression tag	UNP P0ABT2
D	-12	ALA	-	expression tag	UNP P0ABT2
D	-11	HIS	-	expression tag	UNP P0ABT2
D	-10	HIS	-	expression tag	UNP P0ABT2
D	-9	HIS	-	expression tag	UNP P0ABT2
D	-8	HIS	-	expression tag	UNP P0ABT2
D	-7	HIS	-	expression tag	UNP P0ABT2
D	-6	HIS	-	expression tag	UNP P0ABT2
D	-5	VAL	-	expression tag	UNP P0ABT2
D	-4	ASP	-	expression tag	UNP P0ABT2
D	-3	ASP	-	expression tag	UNP P0ABT2
D	-2	ASP	-	expression tag	UNP P0ABT2
D	-1	ASP	-	expression tag	UNP P0ABT2
D	0	LYS	-	expression tag	UNP P0ABT2
D	164	CYS	-	linker	UNP P0ABT2
D	165	ASN	-	linker	UNP P0ABT2
E	-13	MET	-	expression tag	UNP P0ABT2
E	-12	ALA	-	expression tag	UNP P0ABT2
E	-11	HIS	-	expression tag	UNP P0ABT2
E	-10	HIS	-	expression tag	UNP P0ABT2
E	-9	HIS	-	expression tag	UNP P0ABT2
E	-8	HIS	-	expression tag	UNP P0ABT2
E	-7	HIS	-	expression tag	UNP P0ABT2
E	-6	HIS	-	expression tag	UNP P0ABT2
E	-5	VAL	-	expression tag	UNP P0ABT2
E	-4	ASP	-	expression tag	UNP P0ABT2
E	-3	ASP	-	expression tag	UNP P0ABT2
E	-2	ASP	-	expression tag	UNP P0ABT2
E	-1	ASP	-	expression tag	UNP P0ABT2
E	0	LYS	-	expression tag	UNP P0ABT2
E	164	CYS	-	linker	UNP P0ABT2
E	165	ASN	-	linker	UNP P0ABT2
F	-13	MET	-	expression tag	UNP P0ABT2
F	-12	ALA	-	expression tag	UNP P0ABT2
F	-11	HIS	-	expression tag	UNP P0ABT2
F	-10	HIS	-	expression tag	UNP P0ABT2
F	-9	HIS	-	expression tag	UNP P0ABT2
F	-8	HIS	-	expression tag	UNP P0ABT2
F	-7	HIS	-	expression tag	UNP P0ABT2
F	-6	HIS	-	expression tag	UNP P0ABT2
F	-5	VAL	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASP	-	expression tag	UNP P0ABT2
F	-3	ASP	-	expression tag	UNP P0ABT2
F	-2	ASP	-	expression tag	UNP P0ABT2
F	-1	ASP	-	expression tag	UNP P0ABT2
F	0	LYS	-	expression tag	UNP P0ABT2
F	164	CYS	-	linker	UNP P0ABT2
F	165	ASN	-	linker	UNP P0ABT2
G	-13	MET	-	expression tag	UNP P0ABT2
G	-12	ALA	-	expression tag	UNP P0ABT2
G	-11	HIS	-	expression tag	UNP P0ABT2
G	-10	HIS	-	expression tag	UNP P0ABT2
G	-9	HIS	-	expression tag	UNP P0ABT2
G	-8	HIS	-	expression tag	UNP P0ABT2
G	-7	HIS	-	expression tag	UNP P0ABT2
G	-6	HIS	-	expression tag	UNP P0ABT2
G	-5	VAL	-	expression tag	UNP P0ABT2
G	-4	ASP	-	expression tag	UNP P0ABT2
G	-3	ASP	-	expression tag	UNP P0ABT2
G	-2	ASP	-	expression tag	UNP P0ABT2
G	-1	ASP	-	expression tag	UNP P0ABT2
G	0	LYS	-	expression tag	UNP P0ABT2
G	164	CYS	-	linker	UNP P0ABT2
G	165	ASN	-	linker	UNP P0ABT2
H	-13	MET	-	expression tag	UNP P0ABT2
H	-12	ALA	-	expression tag	UNP P0ABT2
H	-11	HIS	-	expression tag	UNP P0ABT2
H	-10	HIS	-	expression tag	UNP P0ABT2
H	-9	HIS	-	expression tag	UNP P0ABT2
H	-8	HIS	-	expression tag	UNP P0ABT2
H	-7	HIS	-	expression tag	UNP P0ABT2
H	-6	HIS	-	expression tag	UNP P0ABT2
H	-5	VAL	-	expression tag	UNP P0ABT2
H	-4	ASP	-	expression tag	UNP P0ABT2
H	-3	ASP	-	expression tag	UNP P0ABT2
H	-2	ASP	-	expression tag	UNP P0ABT2
H	-1	ASP	-	expression tag	UNP P0ABT2
H	0	LYS	-	expression tag	UNP P0ABT2
H	164	CYS	-	linker	UNP P0ABT2
H	165	ASN	-	linker	UNP P0ABT2
I	-13	MET	-	expression tag	UNP P0ABT2
I	-12	ALA	-	expression tag	UNP P0ABT2
I	-11	HIS	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P0ABT2
I	-9	HIS	-	expression tag	UNP P0ABT2
I	-8	HIS	-	expression tag	UNP P0ABT2
I	-7	HIS	-	expression tag	UNP P0ABT2
I	-6	HIS	-	expression tag	UNP P0ABT2
I	-5	VAL	-	expression tag	UNP P0ABT2
I	-4	ASP	-	expression tag	UNP P0ABT2
I	-3	ASP	-	expression tag	UNP P0ABT2
I	-2	ASP	-	expression tag	UNP P0ABT2
I	-1	ASP	-	expression tag	UNP P0ABT2
I	0	LYS	-	expression tag	UNP P0ABT2
I	164	CYS	-	linker	UNP P0ABT2
I	165	ASN	-	linker	UNP P0ABT2
J	-13	MET	-	expression tag	UNP P0ABT2
J	-12	ALA	-	expression tag	UNP P0ABT2
J	-11	HIS	-	expression tag	UNP P0ABT2
J	-10	HIS	-	expression tag	UNP P0ABT2
J	-9	HIS	-	expression tag	UNP P0ABT2
J	-8	HIS	-	expression tag	UNP P0ABT2
J	-7	HIS	-	expression tag	UNP P0ABT2
J	-6	HIS	-	expression tag	UNP P0ABT2
J	-5	VAL	-	expression tag	UNP P0ABT2
J	-4	ASP	-	expression tag	UNP P0ABT2
J	-3	ASP	-	expression tag	UNP P0ABT2
J	-2	ASP	-	expression tag	UNP P0ABT2
J	-1	ASP	-	expression tag	UNP P0ABT2
J	0	LYS	-	expression tag	UNP P0ABT2
J	164	CYS	-	linker	UNP P0ABT2
J	165	ASN	-	linker	UNP P0ABT2
K	-13	MET	-	expression tag	UNP P0ABT2
K	-12	ALA	-	expression tag	UNP P0ABT2
K	-11	HIS	-	expression tag	UNP P0ABT2
K	-10	HIS	-	expression tag	UNP P0ABT2
K	-9	HIS	-	expression tag	UNP P0ABT2
K	-8	HIS	-	expression tag	UNP P0ABT2
K	-7	HIS	-	expression tag	UNP P0ABT2
K	-6	HIS	-	expression tag	UNP P0ABT2
K	-5	VAL	-	expression tag	UNP P0ABT2
K	-4	ASP	-	expression tag	UNP P0ABT2
K	-3	ASP	-	expression tag	UNP P0ABT2
K	-2	ASP	-	expression tag	UNP P0ABT2
K	-1	ASP	-	expression tag	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	LYS	-	expression tag	UNP P0ABT2
K	164	CYS	-	linker	UNP P0ABT2
K	165	ASN	-	linker	UNP P0ABT2
L	-13	MET	-	expression tag	UNP P0ABT2
L	-12	ALA	-	expression tag	UNP P0ABT2
L	-11	HIS	-	expression tag	UNP P0ABT2
L	-10	HIS	-	expression tag	UNP P0ABT2
L	-9	HIS	-	expression tag	UNP P0ABT2
L	-8	HIS	-	expression tag	UNP P0ABT2
L	-7	HIS	-	expression tag	UNP P0ABT2
L	-6	HIS	-	expression tag	UNP P0ABT2
L	-5	VAL	-	expression tag	UNP P0ABT2
L	-4	ASP	-	expression tag	UNP P0ABT2
L	-3	ASP	-	expression tag	UNP P0ABT2
L	-2	ASP	-	expression tag	UNP P0ABT2
L	-1	ASP	-	expression tag	UNP P0ABT2
L	0	LYS	-	expression tag	UNP P0ABT2
L	164	CYS	-	linker	UNP P0ABT2
L	165	ASN	-	linker	UNP P0ABT2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

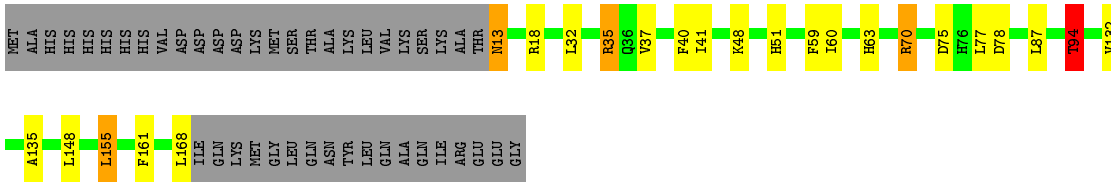
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	129	Total O 129 129	0	0
3	B	171	Total O 171 171	0	0
3	C	158	Total O 158 158	0	0
3	D	152	Total O 152 152	0	0
3	E	173	Total O 173 173	0	0
3	F	151	Total O 151 151	0	0

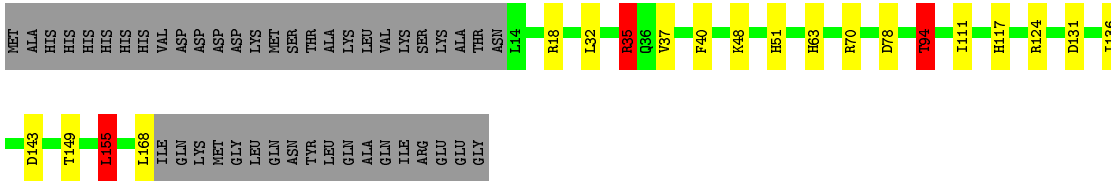
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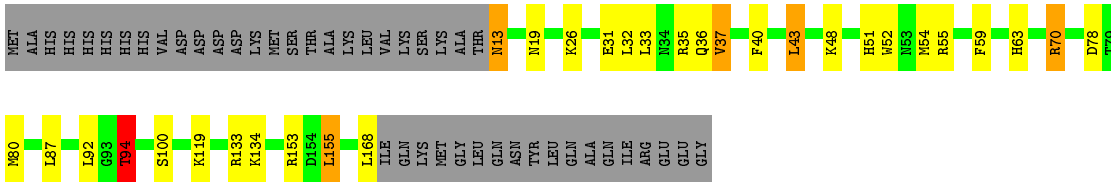
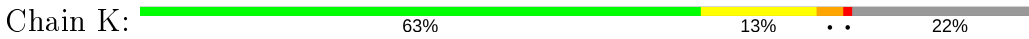
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	141	Total 141	O 141	0	0
3	H	156	Total 156	O 156	0	0
3	I	148	Total 148	O 148	0	0
3	J	113	Total 113	O 113	0	0
3	K	161	Total 161	O 161	0	0
3	L	128	Total 128	O 128	0	0



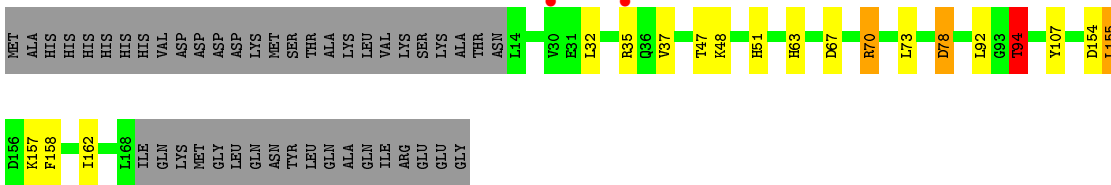
• Molecule 1: DNA protection during starvation protein, Bacterioferritin



• Molecule 1: DNA protection during starvation protein, Bacterioferritin



• Molecule 1: DNA protection during starvation protein, Bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.14Å 104.72Å 207.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 1.99 46.76 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.76-1.99) 91.8 (46.76-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.207 0.188 , 0.217	Depositor DCC
R_{free} test set	7167 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16563	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	1.06	4/1245 (0.3%)	1.04	10/1687 (0.6%)
1	B	0.95	1/1253 (0.1%)	1.02	12/1698 (0.7%)
1	C	0.98	2/1245 (0.2%)	1.04	8/1687 (0.5%)
1	D	0.98	2/1253 (0.2%)	1.06	11/1698 (0.6%)
1	E	0.96	1/1245 (0.1%)	1.13	10/1687 (0.6%)
1	F	0.93	2/1253 (0.2%)	1.07	11/1698 (0.6%)
1	G	0.94	2/1253 (0.2%)	1.06	11/1698 (0.6%)
1	H	0.92	1/1253 (0.1%)	1.05	9/1698 (0.5%)
1	I	0.90	1/1253 (0.1%)	1.08	12/1698 (0.7%)
1	J	0.78	1/1245 (0.1%)	1.03	11/1687 (0.7%)
1	K	0.90	2/1253 (0.2%)	1.02	8/1698 (0.5%)
1	L	0.79	0/1245	0.96	8/1687 (0.5%)
All	All	0.93	19/14996 (0.1%)	1.05	121/20321 (0.6%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	SER	CB-OG	-10.46	1.28	1.42
1	A	106	SER	CB-OG	-10.37	1.28	1.42
1	B	94	THR	CB-CG2	-7.52	1.27	1.52
1	K	100	SER	CB-OG	-6.75	1.33	1.42
1	K	94	THR	CB-CG2	-6.61	1.30	1.52

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	ARG	NE-CZ-NH1	14.99	127.80	120.30
1	E	35	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	G	155	LEU	CB-CG-CD1	12.91	132.94	111.00
1	I	155	LEU	CB-CG-CD1	12.74	132.66	111.00
1	F	155	LEU	CB-CG-CD1	12.56	132.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1227	0	1228	12	0
1	B	1235	0	1234	24	0
1	C	1227	0	1228	10	0
1	D	1235	0	1234	19	0
1	E	1227	0	1228	30	0
1	F	1235	0	1234	16	0
1	G	1235	0	1234	13	0
1	H	1235	0	1234	18	0
1	I	1235	0	1234	18	0
1	J	1227	0	1228	13	0
1	K	1235	0	1234	25	0
1	L	1227	0	1228	17	0
2	A	1	0	0	0	0
2	H	1	0	0	0	0
3	A	129	0	0	7	0
3	B	171	0	0	22	0
3	C	158	0	0	7	0
3	D	152	0	0	15	0
3	E	173	0	0	34	0
3	F	151	0	0	11	0
3	G	141	0	0	9	0
3	H	156	0	0	16	0
3	I	148	0	0	18	0
3	J	113	0	0	14	0
3	K	161	0	0	22	0
3	L	128	0	0	13	0
All	All	16563	0	14778	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 215 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:E:75:ASP:HB2	3:E:329:HOH:O	1.46	1.14
1:E:47:THR:OG1	3:E:201:HOH:O	1.76	1.03
1:E:134:LYS:NZ	3:E:202:HOH:O	1.79	0.98
3:B:281:HOH:O	1:G:78:ASP:HB2	1.60	0.98
1:I:75:ASP:HB2	3:I:300:HOH:O	1.61	0.97

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	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	B	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	C	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	D	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	E	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	F	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	G	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	H	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	I	154/200 (77%)	152 (99%)	2 (1%)	0	100	100
1	J	153/200 (76%)	152 (99%)	1 (1%)	0	100	100
1	K	154/200 (77%)	153 (99%)	1 (1%)	0	100	100
1	L	153/200 (76%)	151 (99%)	2 (1%)	0	100	100
All	All	1843/2400 (77%)	1827 (99%)	16 (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	133/172 (77%)	129 (97%)	4 (3%)	41	41
1	B	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	C	133/172 (77%)	130 (98%)	3 (2%)	50	53
1	D	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	E	133/172 (77%)	132 (99%)	1 (1%)	81	86
1	F	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	G	134/172 (78%)	129 (96%)	5 (4%)	34	32
1	H	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	I	134/172 (78%)	130 (97%)	4 (3%)	41	41
1	J	133/172 (77%)	128 (96%)	5 (4%)	33	31
1	K	134/172 (78%)	128 (96%)	6 (4%)	27	24
1	L	133/172 (77%)	131 (98%)	2 (2%)	65	69
All	All	1603/2064 (78%)	1555 (97%)	48 (3%)	41	41

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	168	LEU
1	G	168	LEU
1	K	94	THR
1	G	13	ASN
1	G	94	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	51	HIS
1	G	51	HIS
1	K	112	HIS
1	F	112	HIS

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Mol	Chain	Res	Type
1	C	51	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	155/200 (77%)	-0.27	0 100 100	20, 26, 38, 49	0
1	B	156/200 (78%)	-0.42	0 100 100	21, 28, 42, 54	0
1	C	155/200 (77%)	-0.27	0 100 100	20, 27, 41, 50	0
1	D	156/200 (78%)	-0.23	0 100 100	22, 29, 43, 50	0
1	E	155/200 (77%)	-0.31	0 100 100	21, 26, 40, 51	0
1	F	156/200 (78%)	-0.36	1 (0%) 89 88	23, 29, 44, 53	0
1	G	156/200 (78%)	-0.15	2 (1%) 77 76	22, 29, 48, 59	0
1	H	156/200 (78%)	-0.23	0 100 100	23, 30, 47, 56	0
1	I	156/200 (78%)	-0.28	0 100 100	26, 32, 45, 56	0
1	J	155/200 (77%)	-0.20	0 100 100	30, 39, 54, 62	0
1	K	156/200 (78%)	-0.30	0 100 100	25, 32, 46, 66	0
1	L	155/200 (77%)	-0.08	2 (1%) 77 76	29, 38, 57, 64	0
All	All	1867/2400 (77%)	-0.26	5 (0%) 94 93	20, 30, 47, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	ASN	2.7
1	L	30	VAL	2.6
1	G	168	LEU	2.3
1	L	35	ARG	2.1
1	F	168	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	201	1/1	0.98	0.36	35,35,35,35	0
2	CL	H	201	1/1	0.99	0.34	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.