Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

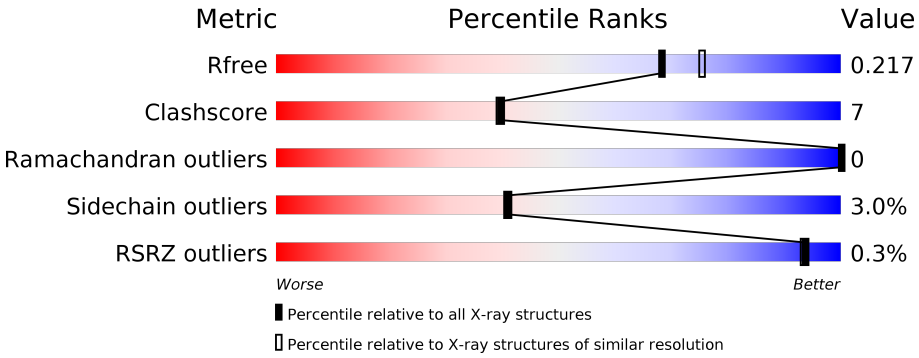
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 <=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	68% 7% • • 23%
1	B	200	64% 11% • • 22%
1	C	200	68% 9% • 23%
1	D	200	66% 11% • 22%
1	E	200	60% 17% • 23%
1	F	200	% 66% 10% • • 22%

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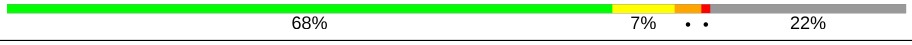
Mol	Chain	Length	Quality of chain
1	G	200	
1	H	200	
1	I	200	
1	J	200	
1	K	200	
1	L	200	

2 Entry composition

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

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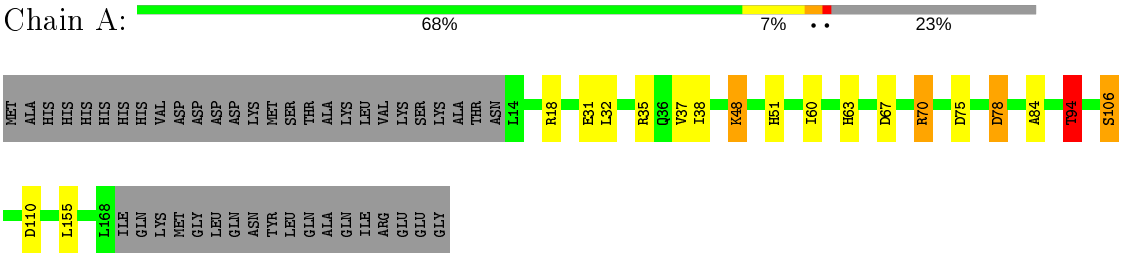
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	141	Total O 141 141	0	0
3	H	156	Total O 156 156	0	0
3	I	148	Total O 148 148	0	0
3	J	113	Total O 113 113	0	0
3	K	161	Total O 161 161	0	0
3	L	128	Total O 128 128	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

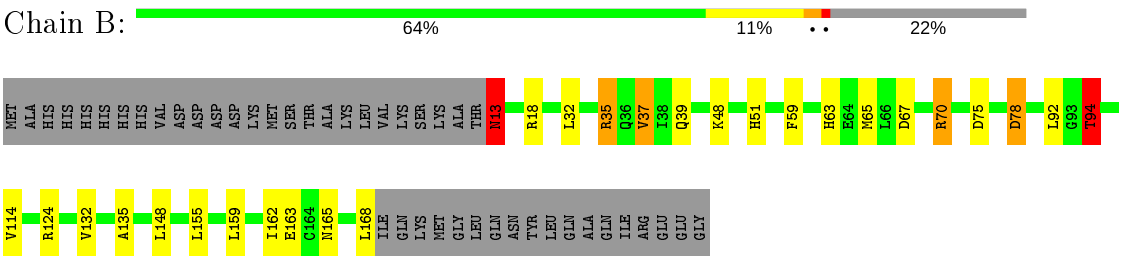
- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain A:



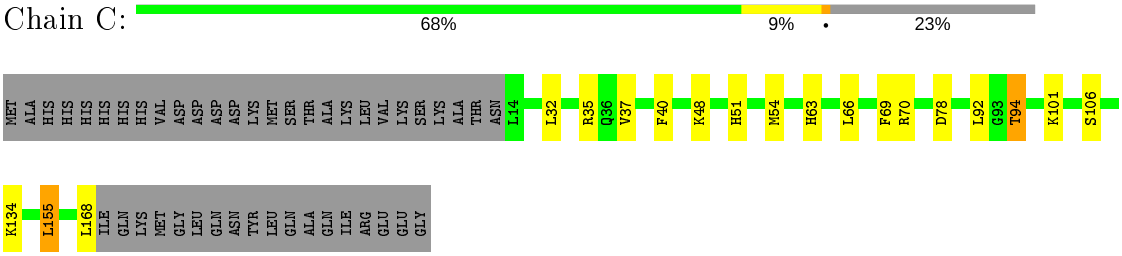
- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain B:



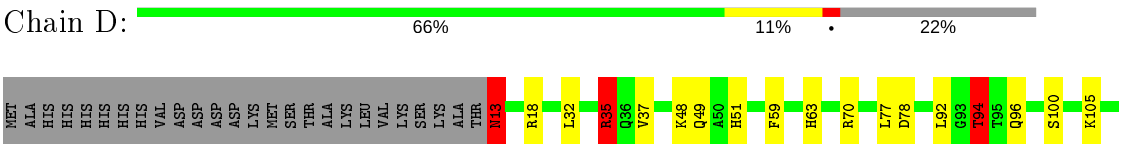
- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain C:



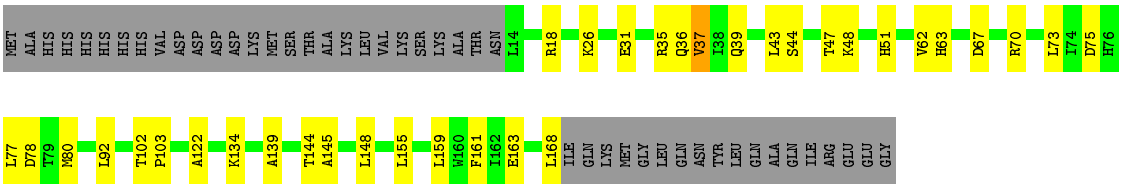
- Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain D:



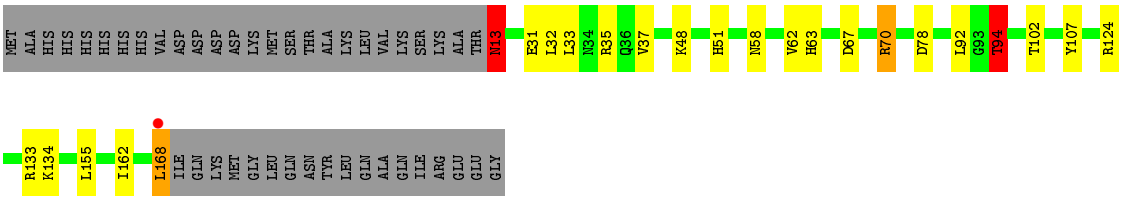
• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain E:



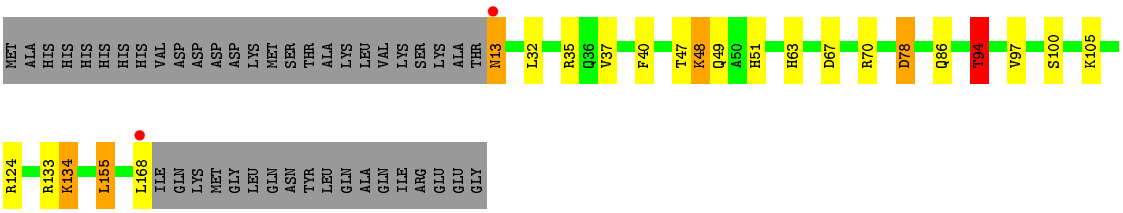
• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain F:



• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain G:

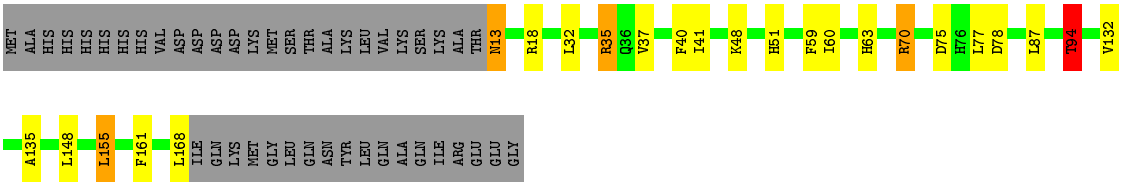


• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain H:

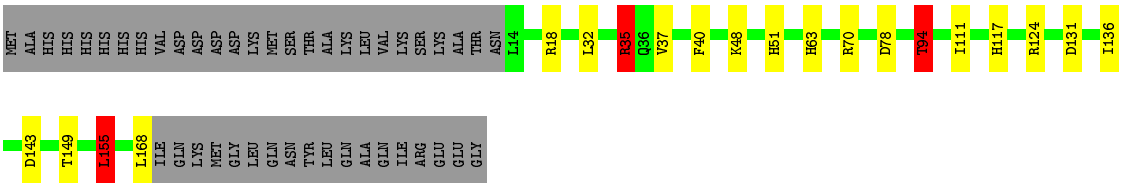
• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain I:



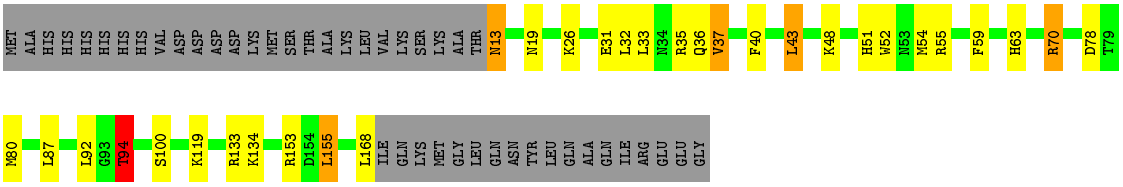
• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain J:



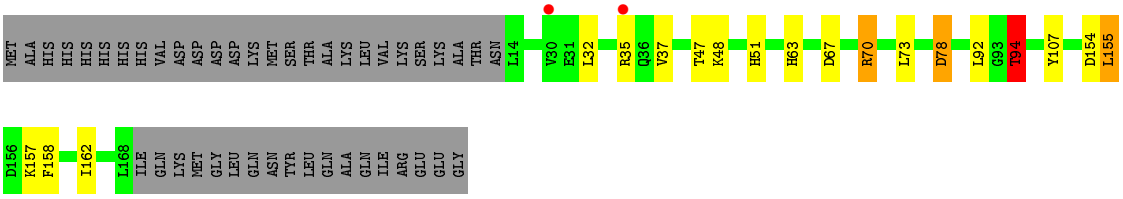
• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain K:



• Molecule 1: DNA protection during starvation protein,Bacterioferritin

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.50 (at 1.98Å)	Xtriage
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	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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%)

All (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
1	C	94	THR	CB-CG2	-6.35	1.31	1.52
1	D	94	THR	CB-CG2	-6.24	1.31	1.52
1	F	94	THR	CB-CG2	-6.23	1.31	1.52
1	D	100	SER	CB-OG	-6.08	1.34	1.42
1	E	31	GLU	CD-OE1	5.99	1.32	1.25
1	G	94	THR	CB-CG2	-5.94	1.32	1.52
1	I	94	THR	CB-CG2	-5.69	1.33	1.52
1	H	94	THR	CB-CG2	-5.68	1.33	1.52
1	F	31	GLU	CD-OE1	5.67	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	94	THR	CB-CG2	-5.66	1.33	1.52
1	A	94	THR	CB-CG2	-5.63	1.33	1.52
1	A	31	GLU	CD-OE2	5.39	1.31	1.25
1	G	100	SER	CB-OG	-5.11	1.35	1.42
1	A	31	GLU	CG-CD	5.10	1.59	1.51

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	C	155	LEU	CB-CG-CD1	12.46	132.18	111.00
1	A	155	LEU	CB-CG-CD1	12.00	131.40	111.00
1	K	155	LEU	CB-CG-CD1	11.75	130.97	111.00
1	H	155	LEU	CB-CG-CD1	11.51	130.57	111.00
1	D	155	LEU	CB-CG-CD1	11.33	130.27	111.00
1	J	155	LEU	CB-CG-CD1	11.33	130.26	111.00
1	I	35	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	H	70	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	A	70	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	C	70	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	D	70	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	H	70	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	J	70	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	E	70	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	C	155	LEU	CA-CB-CG	-8.65	95.41	115.30
1	L	78	ASP	CB-CG-OD1	8.65	126.08	118.30
1	G	70	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	I	70	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	F	70	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	I	155	LEU	CA-CB-CG	-8.55	95.64	115.30
1	J	155	LEU	CA-CB-CG	-8.47	95.81	115.30
1	K	155	LEU	CA-CB-CG	-8.33	96.13	115.30
1	A	155	LEU	CA-CB-CG	-8.32	96.17	115.30
1	F	155	LEU	CA-CB-CG	-8.31	96.19	115.30
1	L	70	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	H	155	LEU	CA-CB-CG	-8.25	96.32	115.30
1	K	70	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	C	78	ASP	CB-CG-OD1	8.16	125.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	155	LEU	CB-CG-CD1	-8.14	97.17	111.00
1	D	78	ASP	CB-CG-OD1	8.12	125.61	118.30
1	D	155	LEU	CA-CB-CG	-8.08	96.71	115.30
1	F	35	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	J	70	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	J	35	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	I	35	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	I	78	ASP	CB-CG-OD1	7.81	125.33	118.30
1	J	35	ARG	CD-NE-CZ	7.69	134.37	123.60
1	A	70	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	G	70	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	K	78	ASP	CB-CG-OD1	7.63	125.17	118.30
1	J	78	ASP	CB-CG-OD1	7.60	125.14	118.30
1	G	155	LEU	CA-CB-CG	-7.55	97.94	115.30
1	B	70	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	155	LEU	CB-CG-CD1	-7.51	98.23	111.00
1	E	78	ASP	CB-CG-OD1	7.36	124.92	118.30
1	E	70	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	L	35	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	B	78	ASP	CB-CG-OD1	7.19	124.78	118.30
1	L	155	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	F	78	ASP	CB-CG-OD1	7.08	124.67	118.30
1	I	35	ARG	CD-NE-CZ	7.03	133.44	123.60
1	H	78	ASP	CB-CG-OD1	6.87	124.48	118.30
1	L	70	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	106	SER	CB-CA-C	-6.84	97.11	110.10
1	B	70	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	78	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	70	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	G	78	ASP	CB-CG-OD1	6.50	124.15	118.30
1	K	70	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	70	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	48	LYS	CD-CE-NZ	6.32	126.23	111.70
1	J	48	LYS	CD-CE-NZ	6.25	126.06	111.70
1	F	70	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	K	48	LYS	CD-CE-NZ	6.22	126.00	111.70
1	I	70	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	G	35	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	G	134	LYS	CG-CD-CE	6.13	130.30	111.90
1	F	35	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	94	THR	N-CA-CB	-6.11	98.70	110.30
1	A	106	SER	CB-CA-C	-6.05	98.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	35	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	F	35	ARG	CG-CD-NE	6.01	124.43	111.80
1	C	48	LYS	CD-CE-NZ	5.92	125.31	111.70
1	G	35	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	H	153	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	18	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	I	48	LYS	CD-CE-NZ	5.74	124.91	111.70
1	L	35	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	13	ASN	CB-CA-C	5.69	121.78	110.40
1	B	155	LEU	CB-CG-CD2	5.68	120.66	111.00
1	C	69	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	E	161	PHE	CB-CG-CD1	5.62	124.73	120.80
1	K	43	LEU	CB-CG-CD2	5.60	120.52	111.00
1	B	37	VAL	CG1-CB-CG2	5.58	119.82	110.90
1	J	18	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	H	124	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	124	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	G	133	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	I	161	PHE	CB-CG-CD1	5.51	124.65	120.80
1	J	124	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	94	THR	N-CA-CB	-5.47	99.91	110.30
1	F	94	THR	N-CA-CB	-5.41	100.03	110.30
1	D	105	LYS	CG-CD-CE	-5.37	95.81	111.90
1	F	124	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	35	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	18	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	35	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	110	ASP	CB-CG-OD1	5.27	123.04	118.30
1	I	13	ASN	CB-CA-C	5.25	120.89	110.40
1	D	13	ASN	CB-CA-C	5.24	120.87	110.40
1	L	155	LEU	CB-CG-CD2	5.22	119.88	111.00
1	G	13	ASN	CB-CA-C	5.21	120.82	110.40
1	D	94	THR	N-CA-CB	-5.21	100.41	110.30
1	E	18	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	48	LYS	CG-CD-CE	5.14	127.33	111.90
1	K	94	THR	N-CA-CB	-5.13	100.55	110.30
1	L	94	THR	N-CA-CB	-5.12	100.58	110.30
1	B	124	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	H	48	LYS	CG-CD-CE	5.09	127.17	111.90
1	G	48	LYS	CG-CD-CE	5.08	127.15	111.90
1	D	94	THR	OG1-CB-CG2	5.08	121.67	110.00
1	F	13	ASN	CB-CA-C	5.07	120.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	37	VAL	CG1-CB-CG2	5.06	119.00	110.90
1	H	13	ASN	CB-CA-C	5.04	120.49	110.40
1	E	31	GLU	OE1-CD-OE2	5.03	129.33	123.30
1	I	18	ARG	NE-CZ-NH1	5.01	122.81	120.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:B:75:ASP:HB2	3:B:328:HOH:O	1.68	0.92
1:E:122:ALA:HB1	3:E:206:HOH:O	1.71	0.90
1:K:54:MET:SD	3:K:215:HOH:O	2.27	0.90
1:E:148:LEU:HD12	3:E:204:HOH:O	1.75	0.86
1:D:18:ARG:HD2	3:E:206:HOH:O	1.75	0.85
1:E:144:THR:HG22	3:E:204:HOH:O	1.77	0.83
1:B:78:ASP:HB2	3:G:268:HOH:O	1.81	0.81
1:K:70:ARG:NH1	3:K:201:HOH:O	2.09	0.80
1:B:70:ARG:NH1	3:B:201:HOH:O	2.03	0.80
1:I:60:ILE:HD12	3:I:310:HOH:O	1.84	0.77
1:B:94:THR:OG1	3:B:202:HOH:O	2.03	0.76
1:F:13:ASN:ND2	3:F:201:HOH:O	2.16	0.76
1:I:60:ILE:HA	3:I:310:HOH:O	1.85	0.76
1:L:155:LEU:HD22	3:L:242:HOH:O	1.86	0.76
1:L:154:ASP:HB3	3:L:242:HOH:O	1.86	0.76
1:B:94:THR:HG21	3:G:291:HOH:O	1.85	0.74
1:D:134:LYS:NZ	3:D:202:HOH:O	2.20	0.74
1:K:37:VAL:HA	3:K:294:HOH:O	1.86	0.74
1:I:77:LEU:HB2	3:I:203:HOH:O	1.88	0.74
1:K:94:THR:HG21	3:K:300:HOH:O	1.88	0.73
1:B:13:ASN:N	3:B:204:HOH:O	2.21	0.73
1:E:44:SER:HB3	3:E:264:HOH:O	1.87	0.73
1:B:59:PHE:HD1	3:B:276:HOH:O	1.71	0.72
1:C:54:MET:SD	3:C:247:HOH:O	2.46	0.72
1:K:13:ASN:ND2	3:K:202:HOH:O	2.22	0.71
1:D:59:PHE:HD1	3:D:241:HOH:O	1.73	0.70
1:D:94:THR:HG21	3:H:369:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:PHE:HB2	3:K:294:HOH:O	1.90	0.70
1:H:37:VAL:HA	3:H:401:HOH:O	1.89	0.70
3:J:266:HOH:O	1:L:94:THR:HG21	1.91	0.70
1:E:102:THR:OG1	3:E:203:HOH:O	2.09	0.69
1:K:32:LEU:HD12	3:K:258:HOH:O	1.91	0.69
1:L:158:PHE:CE2	3:L:242:HOH:O	2.44	0.69
1:H:94:THR:OG1	3:H:301:HOH:O	2.10	0.69
1:I:148:LEU:HB3	3:I:202:HOH:O	1.92	0.69
1:D:13:ASN:OD1	3:D:201:HOH:O	2.11	0.69
3:F:275:HOH:O	1:I:94:THR:HG21	1.91	0.69
1:H:142:ASP:HB3	3:J:202:HOH:O	1.94	0.68
1:K:52:TRP:HA	3:K:316:HOH:O	1.95	0.67
1:A:51:HIS:HE1	3:E:218:HOH:O	1.77	0.67
1:I:94:THR:OG1	3:I:201:HOH:O	2.14	0.66
1:B:148:LEU:HB3	3:B:203:HOH:O	1.95	0.65
1:A:78:ASP:HB2	3:E:292:HOH:O	1.94	0.65
1:I:59:PHE:CE2	3:I:310:HOH:O	2.50	0.65
1:B:65:MET:HE1	3:B:208:HOH:O	1.97	0.64
1:C:134:LYS:NZ	3:C:201:HOH:O	2.30	0.64
1:H:80:MET:HE3	3:H:401:HOH:O	1.96	0.64
1:C:32:LEU:HG	3:C:310:HOH:O	1.97	0.64
1:C:66:LEU:HD12	3:C:247:HOH:O	1.98	0.64
1:A:70:ARG:NH1	3:A:301:HOH:O	2.26	0.64
1:B:132:VAL:O	3:B:203:HOH:O	2.15	0.63
1:D:114:VAL:CG2	3:D:241:HOH:O	2.45	0.63
1:F:94:THR:HG21	3:I:287:HOH:O	1.98	0.62
1:D:35:ARG:NH2	3:D:203:HOH:O	2.31	0.62
1:C:63:HIS:HA	3:C:247:HOH:O	1.99	0.61
1:K:134:LYS:NZ	3:K:204:HOH:O	2.33	0.61
1:E:144:THR:C	3:E:204:HOH:O	2.38	0.61
1:K:55:ARG:NH1	3:K:203:HOH:O	2.32	0.61
1:L:157:LYS:HD3	3:L:205:HOH:O	2.01	0.61
1:B:114:VAL:CG2	3:B:276:HOH:O	2.49	0.61
3:B:302:HOH:O	1:G:94:THR:HG21	2.00	0.60
1:E:92:LEU:HB2	3:E:283:HOH:O	2.01	0.60
1:F:32:LEU:HD12	3:F:271:HOH:O	2.02	0.60
1:G:105:LYS:N	3:G:202:HOH:O	2.34	0.60
1:E:36:GLN:HB2	3:E:230:HOH:O	2.02	0.59
1:K:80:MET:HE3	3:K:294:HOH:O	2.02	0.59
1:H:105:LYS:N	3:H:302:HOH:O	2.35	0.59
1:H:124:ARG:NE	3:H:302:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:LEU:HA	3:K:257:HOH:O	2.02	0.59
1:A:94:THR:HG21	3:E:262:HOH:O	2.03	0.58
3:J:281:HOH:O	1:L:78:ASP:HB2	2.02	0.58
1:H:32:LEU:HD12	3:H:303:HOH:O	2.02	0.58
1:L:158:PHE:CD2	3:L:242:HOH:O	2.57	0.58
1:A:75:ASP:HB2	3:A:392:HOH:O	2.05	0.57
1:B:162:ILE:HA	3:B:208:HOH:O	2.04	0.57
1:H:40:PHE:HB2	3:H:401:HOH:O	2.02	0.57
1:I:132:VAL:O	3:I:202:HOH:O	2.17	0.57
1:E:51:HIS:HD2	1:E:63:HIS:O	1.88	0.57
1:K:36:GLN:HB2	3:K:282:HOH:O	2.03	0.57
1:E:62:VAL:HG22	3:E:214:HOH:O	2.04	0.57
1:B:32:LEU:HD12	3:B:256:HOH:O	2.05	0.57
1:J:51:HIS:HE1	3:L:219:HOH:O	1.87	0.56
1:D:51:HIS:HD2	1:D:63:HIS:O	1.88	0.56
1:H:35:ARG:NH2	3:H:303:HOH:O	2.37	0.56
1:K:51:HIS:HD2	1:K:63:HIS:O	1.89	0.56
1:D:96:GLN:NE2	3:D:204:HOH:O	2.38	0.56
1:B:51:HIS:HE1	3:G:203:HOH:O	1.89	0.55
1:J:149:THR:HG23	3:J:202:HOH:O	2.06	0.55
1:E:168:LEU:C	3:E:250:HOH:O	2.44	0.55
1:E:77:LEU:HD23	3:E:264:HOH:O	2.07	0.55
1:H:51:HIS:HD2	1:H:63:HIS:O	1.90	0.55
1:K:133:ARG:NH1	3:K:204:HOH:O	2.40	0.55
1:A:51:HIS:HD2	1:A:63:HIS:O	1.90	0.55
1:I:70:ARG:NH1	3:I:205:HOH:O	2.30	0.55
1:K:13:ASN:ND2	3:K:208:HOH:O	2.40	0.55
1:F:51:HIS:HD2	1:F:63:HIS:O	1.90	0.55
1:I:32:LEU:HD12	3:I:218:HOH:O	2.06	0.55
1:I:51:HIS:HD2	1:I:63:HIS:O	1.90	0.54
1:E:43:LEU:HG	3:E:201:HOH:O	2.06	0.54
1:K:119:LYS:HG2	3:K:205:HOH:O	2.07	0.54
1:D:35:ARG:NH2	3:D:205:HOH:O	2.40	0.54
1:G:124:ARG:HG2	3:G:202:HOH:O	2.07	0.54
1:G:32:LEU:HD12	3:G:257:HOH:O	2.07	0.54
1:D:133:ARG:NH1	3:D:202:HOH:O	2.40	0.54
1:E:80:MET:HB3	3:E:230:HOH:O	2.07	0.54
1:J:51:HIS:HD2	1:J:63:HIS:O	1.90	0.54
1:F:102:THR:HG21	3:F:276:HOH:O	2.07	0.53
1:G:51:HIS:HD2	1:G:63:HIS:O	1.91	0.53
1:F:92:LEU:HB2	3:F:213:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG22	3:B:276:HOH:O	2.06	0.53
1:C:51:HIS:HD2	1:C:63:HIS:O	1.92	0.53
1:D:162:ILE:HG22	3:D:296:HOH:O	2.08	0.53
1:D:92:LEU:HB2	3:D:258:HOH:O	2.09	0.53
1:D:49:GLN:HG2	3:H:301:HOH:O	2.08	0.52
1:L:51:HIS:HD2	1:L:63:HIS:O	1.92	0.52
1:E:73:LEU:HB3	3:E:264:HOH:O	2.09	0.52
1:D:114:VAL:HG22	3:D:241:HOH:O	2.06	0.52
3:A:386:HOH:O	1:F:168:LEU:HD22	2.09	0.52
1:E:73:LEU:HD11	3:E:201:HOH:O	2.10	0.51
1:A:38:ILE:HD11	3:A:416:HOH:O	2.10	0.51
1:I:63:HIS:HB3	3:I:310:HOH:O	2.10	0.51
1:E:39:GLN:HA	3:E:203:HOH:O	2.11	0.51
1:G:47:THR:HG21	3:G:207:HOH:O	2.11	0.51
1:B:51:HIS:HD2	1:B:63:HIS:O	1.93	0.51
1:L:162:ILE:HG22	3:L:260:HOH:O	2.10	0.50
1:A:32:LEU:HD12	3:A:319:HOH:O	2.11	0.50
1:L:70:ARG:HA	3:L:276:HOH:O	2.11	0.50
1:I:37:VAL:O	3:I:203:HOH:O	2.19	0.50
1:L:92:LEU:HB2	3:L:258:HOH:O	2.11	0.50
1:F:134:LYS:NZ	3:F:202:HOH:O	2.43	0.50
1:H:13:ASN:N	3:H:304:HOH:O	2.45	0.50
1:B:39:GLN:HA	3:B:207:HOH:O	2.12	0.49
1:B:92:LEU:HB2	3:B:285:HOH:O	2.11	0.49
1:I:135:ALA:HB3	3:I:202:HOH:O	2.12	0.49
1:G:124:ARG:NE	3:G:202:HOH:O	2.45	0.49
1:K:26:LYS:HB3	3:K:207:HOH:O	2.12	0.49
1:B:159:LEU:HD12	3:B:278:HOH:O	2.12	0.49
1:E:47:THR:HG21	3:E:210:HOH:O	2.12	0.49
1:F:107:TYR:HB3	3:I:201:HOH:O	2.11	0.49
1:H:124:ARG:HG2	3:H:302:HOH:O	2.12	0.49
1:J:94:THR:OG1	3:J:201:HOH:O	2.20	0.49
1:I:87:LEU:HD12	3:I:227:HOH:O	2.12	0.49
1:L:73:LEU:HD12	3:L:276:HOH:O	2.13	0.48
1:C:168:LEU:HD22	3:E:284:HOH:O	2.13	0.48
3:J:284:HOH:O	1:K:153:ARG:HG2	2.14	0.48
1:K:92:LEU:HB2	3:K:295:HOH:O	2.12	0.48
1:I:41:ILE:HG13	3:I:203:HOH:O	2.14	0.48
1:A:51:HIS:CE1	3:E:218:HOH:O	2.59	0.48
1:F:70:ARG:NH1	3:I:205:HOH:O	2.31	0.47
1:H:80:MET:CE	3:H:401:HOH:O	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:THR:CG2	3:J:202:HOH:O	2.63	0.47
1:E:139:ALA:CB	3:E:204:HOH:O	2.63	0.47
1:E:48:LYS:HE3	1:E:67:ASP:OD1	2.15	0.47
1:B:48:LYS:HE3	1:B:67:ASP:OD1	2.15	0.47
1:L:48:LYS:HE3	1:L:67:ASP:OD1	2.16	0.46
1:H:94:THR:HB	3:H:301:HOH:O	2.16	0.46
1:F:162:ILE:HG12	3:F:349:HOH:O	2.16	0.46
1:G:48:LYS:HE3	1:G:67:ASP:OD1	2.16	0.46
3:J:210:HOH:O	1:L:51:HIS:HE1	1.99	0.46
3:J:201:HOH:O	1:L:107:TYR:HB3	2.16	0.46
1:I:40:PHE:CZ	1:I:155:LEU:HD13	2.52	0.45
1:F:62:VAL:HG22	3:F:256:HOH:O	2.15	0.45
1:J:32:LEU:HD12	3:J:205:HOH:O	2.17	0.45
1:B:135:ALA:HB3	3:B:203:HOH:O	2.16	0.45
3:A:404:HOH:O	1:F:58:ASN:HB2	2.17	0.45
1:D:32:LEU:CD1	3:D:203:HOH:O	2.64	0.45
1:E:103:PRO:HD2	3:E:203:HOH:O	2.17	0.45
1:F:33:LEU:HG	3:F:251:HOH:O	2.16	0.45
1:K:40:PHE:CZ	1:K:155:LEU:HD13	2.53	0.45
1:J:111:ILE:HB	3:J:231:HOH:O	2.17	0.44
1:J:35:ARG:NH2	1:J:131:ASP:OD2	2.50	0.44
1:A:48:LYS:HE3	1:A:67:ASP:OD1	2.17	0.44
1:D:32:LEU:HD12	3:D:205:HOH:O	2.16	0.44
1:E:26:LYS:HB3	3:E:205:HOH:O	2.17	0.44
1:F:48:LYS:HE3	1:F:67:ASP:OD1	2.17	0.44
1:C:40:PHE:CZ	1:C:155:LEU:HD13	2.52	0.44
1:J:143:ASP:HB3	3:J:284:HOH:O	2.17	0.44
1:J:117:HIS:CD2	3:J:231:HOH:O	2.71	0.44
1:F:133:ARG:NH1	3:F:202:HOH:O	2.50	0.43
1:C:92:LEU:HB2	3:C:272:HOH:O	2.18	0.43
1:H:48:LYS:HE3	1:H:67:ASP:OD1	2.18	0.43
1:A:60:ILE:HG21	3:F:256:HOH:O	2.18	0.43
1:E:159:LEU:HD11	3:E:206:HOH:O	2.17	0.43
1:B:165:ASN:HB2	3:B:208:HOH:O	2.18	0.43
1:E:145:ALA:N	3:E:204:HOH:O	2.49	0.43
1:D:35:ARG:NH1	3:D:207:HOH:O	2.48	0.43
1:H:92:LEU:HB2	3:H:383:HOH:O	2.18	0.43
1:B:32:LEU:HG	3:B:335:HOH:O	2.19	0.43
1:H:70:ARG:NH1	3:H:306:HOH:O	2.52	0.42
1:K:19:ASN:HB3	3:K:257:HOH:O	2.20	0.42
1:J:136:ILE:HD13	3:J:202:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:202:HOH:O	1:G:49:GLN:HG2	2.20	0.42
1:E:73:LEU:CD1	3:E:201:HOH:O	2.68	0.42
1:H:40:PHE:CZ	1:H:155:LEU:HD13	2.54	0.42
1:K:31:GLU:HG3	3:K:329:HOH:O	2.19	0.41
1:K:33:LEU:HA	3:K:282:HOH:O	2.21	0.41
1:L:47:THR:HB	3:L:276:HOH:O	2.19	0.41
1:A:84:ALA:HA	3:A:373:HOH:O	2.20	0.41
1:E:148:LEU:CD1	3:E:204:HOH:O	2.48	0.41
1:J:51:HIS:CE1	3:L:219:HOH:O	2.68	0.41
1:C:101:LYS:HE2	3:C:333:HOH:O	2.21	0.41
1:G:40:PHE:CZ	1:G:155:LEU:HD13	2.56	0.41
1:K:59:PHE:HA	3:K:215:HOH:O	2.20	0.41
1:J:40:PHE:CZ	1:J:155:LEU:HD13	2.56	0.41
1:G:94:THR:HG22	1:G:97:VAL:HG23	2.03	0.40
1:L:32:LEU:HG	3:L:278:HOH:O	2.20	0.40
1:B:163:GLU:HG3	3:B:278:HOH:O	2.20	0.40
1:G:86:GLN:HG3	3:G:201:HOH:O	2.21	0.40
1:D:77:LEU:HD13	3:D:323:HOH:O	2.22	0.40
1:E:163:GLU:CG	3:E:206:HOH:O	2.69	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	37	VAL
1	A	94	THR
1	A	106	SER
1	B	13	ASN
1	B	35	ARG
1	B	37	VAL
1	B	94	THR
1	B	168	LEU
1	C	35	ARG
1	C	37	VAL
1	C	94	THR
1	D	13	ASN
1	D	35	ARG
1	D	37	VAL
1	D	94	THR
1	D	168	LEU
1	E	37	VAL
1	F	13	ASN
1	F	37	VAL
1	F	94	THR
1	F	168	LEU
1	G	13	ASN
1	G	37	VAL
1	G	94	THR
1	G	134	LYS
1	G	168	LEU
1	H	13	ASN
1	H	35	ARG
1	H	94	THR
1	H	168	LEU
1	I	13	ASN
1	I	35	ARG
1	I	94	THR
1	I	168	LEU
1	J	35	ARG
1	J	37	VAL
1	J	94	THR
1	J	155	LEU
1	J	168	LEU
1	K	13	ASN
1	K	35	ARG

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Mol	Chain	Res	Type
1	K	37	VAL
1	K	43	LEU
1	K	94	THR
1	K	168	LEU
1	L	37	VAL
1	L	94	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	51	HIS
1	B	51	HIS
1	C	39	GLN
1	C	51	HIS
1	C	112	HIS
1	D	13	ASN
1	D	39	GLN
1	D	51	HIS
1	E	39	GLN
1	E	51	HIS
1	F	39	GLN
1	F	51	HIS
1	F	112	HIS
1	G	39	GLN
1	G	51	HIS
1	H	39	GLN
1	H	51	HIS
1	I	39	GLN
1	I	51	HIS
1	J	39	GLN
1	J	51	HIS
1	K	39	GLN
1	K	51	HIS
1	K	112	HIS
1	L	39	GLN
1	L	51	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{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>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

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, 95^{th} 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.