



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 10:17 AM EDT

PDB ID : 7KE3
Title : Heavy chain ferritin with C-terminal EBNA1 epitope
Authors : Pederick, J.L.; Bruning, J.B.
Deposited on : 2020-10-10
Resolution : 2.20 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

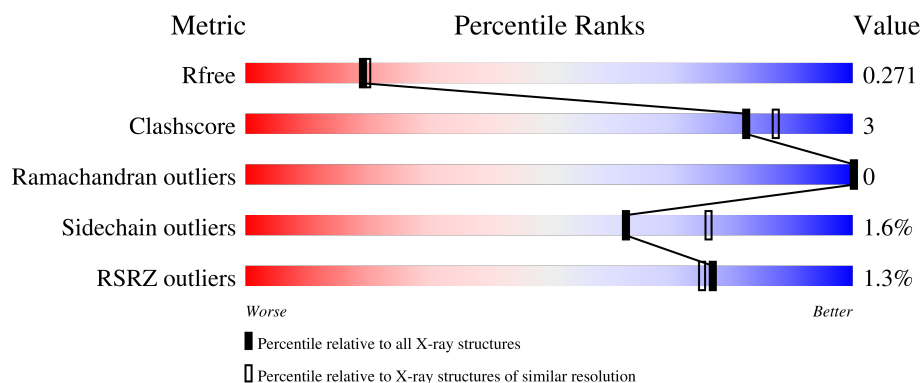
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	209	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>.</div> <div>21%</div> </div> </div>
1	B	209	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>6%</div> <div>21%</div> </div> </div>
1	C	209	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>.</div> <div>20%</div> </div> </div>
1	D	209	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>.</div> <div>21%</div> </div> </div>
1	E	209	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>8%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	209	<div><div><div>%</div><div><div></div><div>74%</div><div>6%</div><div>20%</div></div></div></div>
1	G	209	<div><div><div></div><div>73%</div><div>6%</div><div>20%</div></div></div>
1	H	209	<div><div><div>%</div><div><div></div><div>71%</div><div>9%</div><div>20%</div></div></div></div>
1	I	209	<div><div><div>%</div><div><div></div><div>74%</div><div>5%</div><div>20%</div></div></div></div>
1	J	209	<div><div><div>%</div><div><div></div><div>74%</div><div>6%</div><div>20%</div></div></div></div>
1	K	209	<div><div><div>%</div><div><div></div><div>77%</div><div>.</div><div>20%</div></div></div></div>
1	L	209	<div><div><div></div><div>77%</div><div>.</div><div>20%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17042 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 Ferritin heavy chain, Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	1	0
			1354	851	240	256	7			
1	B	166	Total	C	N	O	S	0	1	0
			1348	848	240	253	7			
1	C	167	Total	C	N	O	S	0	2	0
			1370	861	246	256	7			
1	D	166	Total	C	N	O	S	0	2	0
			1349	849	241	252	7			
1	E	167	Total	C	N	O	S	0	1	0
			1359	854	240	258	7			
1	F	167	Total	C	N	O	S	0	1	0
			1345	847	239	252	7			
1	G	167	Total	C	N	O	S	0	1	0
			1363	857	241	258	7			
1	H	167	Total	C	N	O	S	0	1	0
			1345	847	239	252	7			
1	I	167	Total	C	N	O	S	0	2	0
			1363	856	243	257	7			
1	J	167	Total	C	N	O	S	0	1	0
			1365	858	241	259	7			
1	K	167	Total	C	N	O	S	0	1	0
			1359	854	242	256	7			
1	L	167	Total	C	N	O	S	0	1	0
			1343	845	238	253	7			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLY	-	linker	UNP P02794
A	184	GLY	-	linker	UNP P02794
A	185	SER	-	linker	UNP P02794
A	186	GLY	-	linker	UNP P02794
A	187	GLY	-	linker	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	linker	UNP P02794
A	189	GLY	-	linker	UNP P02794
A	190	SER	-	linker	UNP P02794
A	191	GLY	-	linker	UNP P02794
A	192	GLY	-	linker	UNP P02794
A	193	GLY	-	linker	UNP P02794
A	194	GLY	-	linker	UNP P02794
A	195	SER	-	linker	UNP P02794
A	196	GLY	-	linker	UNP P02794
A	197	GLY	-	linker	UNP P02794
B	183	GLY	-	linker	UNP P02794
B	184	GLY	-	linker	UNP P02794
B	185	SER	-	linker	UNP P02794
B	186	GLY	-	linker	UNP P02794
B	187	GLY	-	linker	UNP P02794
B	188	GLY	-	linker	UNP P02794
B	189	GLY	-	linker	UNP P02794
B	190	SER	-	linker	UNP P02794
B	191	GLY	-	linker	UNP P02794
B	192	GLY	-	linker	UNP P02794
B	193	GLY	-	linker	UNP P02794
B	194	GLY	-	linker	UNP P02794
B	195	SER	-	linker	UNP P02794
B	196	GLY	-	linker	UNP P02794
B	197	GLY	-	linker	UNP P02794
C	183	GLY	-	linker	UNP P02794
C	184	GLY	-	linker	UNP P02794
C	185	SER	-	linker	UNP P02794
C	186	GLY	-	linker	UNP P02794
C	187	GLY	-	linker	UNP P02794
C	188	GLY	-	linker	UNP P02794
C	189	GLY	-	linker	UNP P02794
C	190	SER	-	linker	UNP P02794
C	191	GLY	-	linker	UNP P02794
C	192	GLY	-	linker	UNP P02794
C	193	GLY	-	linker	UNP P02794
C	194	GLY	-	linker	UNP P02794
C	195	SER	-	linker	UNP P02794
C	196	GLY	-	linker	UNP P02794
C	197	GLY	-	linker	UNP P02794
D	183	GLY	-	linker	UNP P02794
D	184	GLY	-	linker	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
D	185	SER	-	linker	UNP P02794
D	186	GLY	-	linker	UNP P02794
D	187	GLY	-	linker	UNP P02794
D	188	GLY	-	linker	UNP P02794
D	189	GLY	-	linker	UNP P02794
D	190	SER	-	linker	UNP P02794
D	191	GLY	-	linker	UNP P02794
D	192	GLY	-	linker	UNP P02794
D	193	GLY	-	linker	UNP P02794
D	194	GLY	-	linker	UNP P02794
D	195	SER	-	linker	UNP P02794
D	196	GLY	-	linker	UNP P02794
D	197	GLY	-	linker	UNP P02794
E	183	GLY	-	linker	UNP P02794
E	184	GLY	-	linker	UNP P02794
E	185	SER	-	linker	UNP P02794
E	186	GLY	-	linker	UNP P02794
E	187	GLY	-	linker	UNP P02794
E	188	GLY	-	linker	UNP P02794
E	189	GLY	-	linker	UNP P02794
E	190	SER	-	linker	UNP P02794
E	191	GLY	-	linker	UNP P02794
E	192	GLY	-	linker	UNP P02794
E	193	GLY	-	linker	UNP P02794
E	194	GLY	-	linker	UNP P02794
E	195	SER	-	linker	UNP P02794
E	196	GLY	-	linker	UNP P02794
E	197	GLY	-	linker	UNP P02794
F	183	GLY	-	linker	UNP P02794
F	184	GLY	-	linker	UNP P02794
F	185	SER	-	linker	UNP P02794
F	186	GLY	-	linker	UNP P02794
F	187	GLY	-	linker	UNP P02794
F	188	GLY	-	linker	UNP P02794
F	189	GLY	-	linker	UNP P02794
F	190	SER	-	linker	UNP P02794
F	191	GLY	-	linker	UNP P02794
F	192	GLY	-	linker	UNP P02794
F	193	GLY	-	linker	UNP P02794
F	194	GLY	-	linker	UNP P02794
F	195	SER	-	linker	UNP P02794
F	196	GLY	-	linker	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	197	GLY	-	linker	UNP P02794
G	183	GLY	-	linker	UNP P02794
G	184	GLY	-	linker	UNP P02794
G	185	SER	-	linker	UNP P02794
G	186	GLY	-	linker	UNP P02794
G	187	GLY	-	linker	UNP P02794
G	188	GLY	-	linker	UNP P02794
G	189	GLY	-	linker	UNP P02794
G	190	SER	-	linker	UNP P02794
G	191	GLY	-	linker	UNP P02794
G	192	GLY	-	linker	UNP P02794
G	193	GLY	-	linker	UNP P02794
G	194	GLY	-	linker	UNP P02794
G	195	SER	-	linker	UNP P02794
G	196	GLY	-	linker	UNP P02794
G	197	GLY	-	linker	UNP P02794
H	183	GLY	-	linker	UNP P02794
H	184	GLY	-	linker	UNP P02794
H	185	SER	-	linker	UNP P02794
H	186	GLY	-	linker	UNP P02794
H	187	GLY	-	linker	UNP P02794
H	188	GLY	-	linker	UNP P02794
H	189	GLY	-	linker	UNP P02794
H	190	SER	-	linker	UNP P02794
H	191	GLY	-	linker	UNP P02794
H	192	GLY	-	linker	UNP P02794
H	193	GLY	-	linker	UNP P02794
H	194	GLY	-	linker	UNP P02794
H	195	SER	-	linker	UNP P02794
H	196	GLY	-	linker	UNP P02794
H	197	GLY	-	linker	UNP P02794
I	183	GLY	-	linker	UNP P02794
I	184	GLY	-	linker	UNP P02794
I	185	SER	-	linker	UNP P02794
I	186	GLY	-	linker	UNP P02794
I	187	GLY	-	linker	UNP P02794
I	188	GLY	-	linker	UNP P02794
I	189	GLY	-	linker	UNP P02794
I	190	SER	-	linker	UNP P02794
I	191	GLY	-	linker	UNP P02794
I	192	GLY	-	linker	UNP P02794
I	193	GLY	-	linker	UNP P02794

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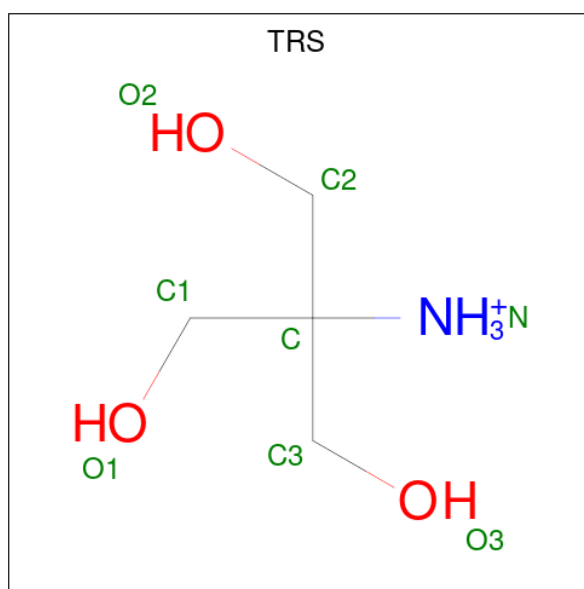
Chain	Residue	Modelled	Actual	Comment	Reference
I	194	GLY	-	linker	UNP P02794
I	195	SER	-	linker	UNP P02794
I	196	GLY	-	linker	UNP P02794
I	197	GLY	-	linker	UNP P02794
J	183	GLY	-	linker	UNP P02794
J	184	GLY	-	linker	UNP P02794
J	185	SER	-	linker	UNP P02794
J	186	GLY	-	linker	UNP P02794
J	187	GLY	-	linker	UNP P02794
J	188	GLY	-	linker	UNP P02794
J	189	GLY	-	linker	UNP P02794
J	190	SER	-	linker	UNP P02794
J	191	GLY	-	linker	UNP P02794
J	192	GLY	-	linker	UNP P02794
J	193	GLY	-	linker	UNP P02794
J	194	GLY	-	linker	UNP P02794
J	195	SER	-	linker	UNP P02794
J	196	GLY	-	linker	UNP P02794
J	197	GLY	-	linker	UNP P02794
K	183	GLY	-	linker	UNP P02794
K	184	GLY	-	linker	UNP P02794
K	185	SER	-	linker	UNP P02794
K	186	GLY	-	linker	UNP P02794
K	187	GLY	-	linker	UNP P02794
K	188	GLY	-	linker	UNP P02794
K	189	GLY	-	linker	UNP P02794
K	190	SER	-	linker	UNP P02794
K	191	GLY	-	linker	UNP P02794
K	192	GLY	-	linker	UNP P02794
K	193	GLY	-	linker	UNP P02794
K	194	GLY	-	linker	UNP P02794
K	195	SER	-	linker	UNP P02794
K	196	GLY	-	linker	UNP P02794
K	197	GLY	-	linker	UNP P02794
L	183	GLY	-	linker	UNP P02794
L	184	GLY	-	linker	UNP P02794
L	185	SER	-	linker	UNP P02794
L	186	GLY	-	linker	UNP P02794
L	187	GLY	-	linker	UNP P02794
L	188	GLY	-	linker	UNP P02794
L	189	GLY	-	linker	UNP P02794
L	190	SER	-	linker	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
L	191	GLY	-	linker	UNP P02794
L	192	GLY	-	linker	UNP P02794
L	193	GLY	-	linker	UNP P02794
L	194	GLY	-	linker	UNP P02794
L	195	SER	-	linker	UNP P02794
L	196	GLY	-	linker	UNP P02794
L	197	GLY	-	linker	UNP P02794

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		
2	H	1	Total	C	N	O	0	0
			8	4	1	3		
2	I	1	Total	C	N	O	0	0
			8	4	1	3		
2	K	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Fe 2 2	0	1
3	B	2	Total Fe 2 2	0	0
3	C	3	Total Fe 3 3	0	1
3	D	2	Total Fe 2 2	0	0
3	E	3	Total Fe 3 3	0	1
3	F	1	Total Fe 1 1	0	0
3	G	2	Total Fe 2 2	0	1
3	H	1	Total Fe 1 1	0	0
3	I	1	Total Fe 1 1	0	0
3	J	1	Total Fe 1 1	0	0
3	K	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	59	Total O 59 59	0	0
4	C	61	Total O 61 61	0	0
4	D	60	Total O 60 60	0	0
4	E	64	Total O 64 64	0	0
4	F	63	Total O 63 63	0	0
4	G	58	Total O 58 58	0	0
4	H	64	Total O 64 64	0	0

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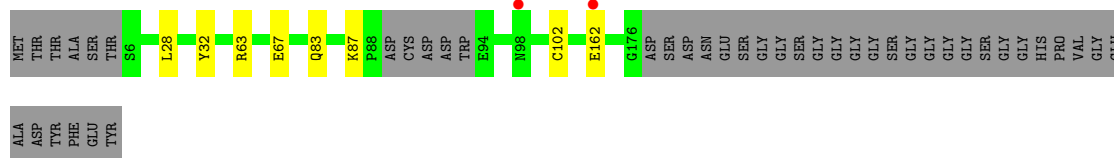
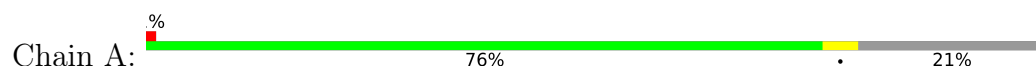
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	62	Total 62	O 62	0	0
4	J	61	Total 61	O 61	0	0
4	K	48	Total 48	O 48	0	0
4	L	59	Total 59	O 59	0	0

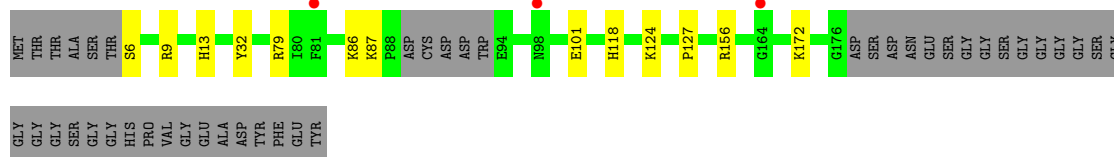
3 Residue-property plots

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.

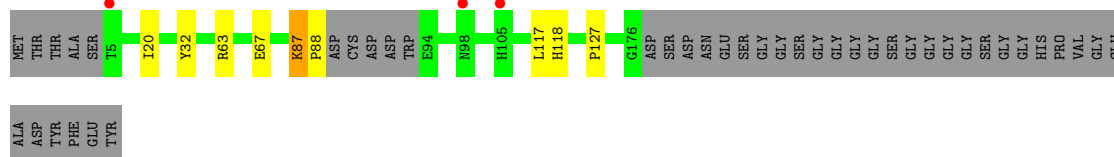
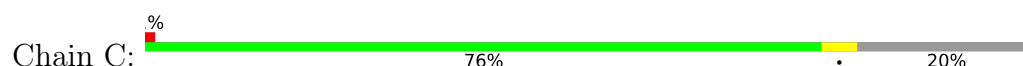
- Molecule 1: Ferritin heavy chain,Epstein-Barr nuclear antigen 1



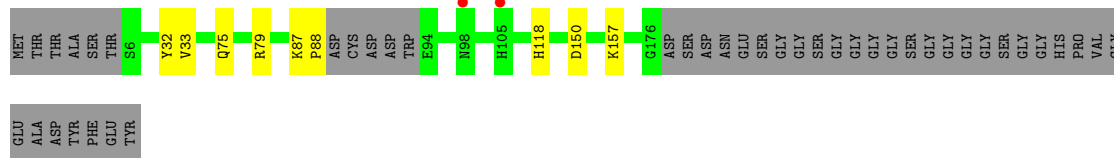
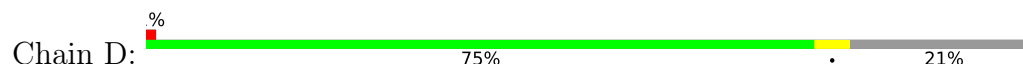
- Molecule 1: Ferritin heavy chain,Epstein-Barr nuclear antigen 1



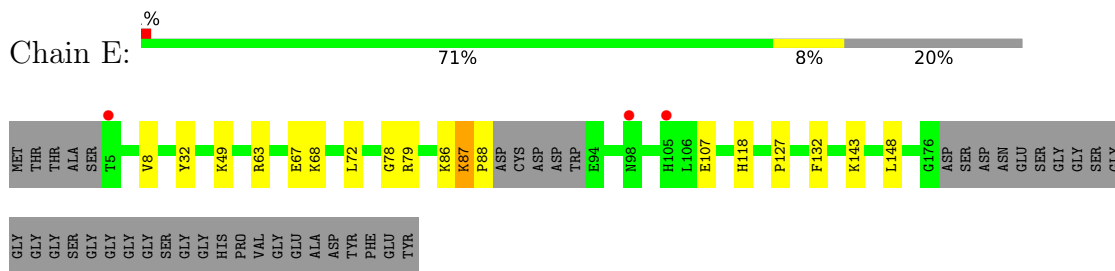
- Molecule 1: Ferritin heavy chain,Epstein-Barr nuclear antigen 1



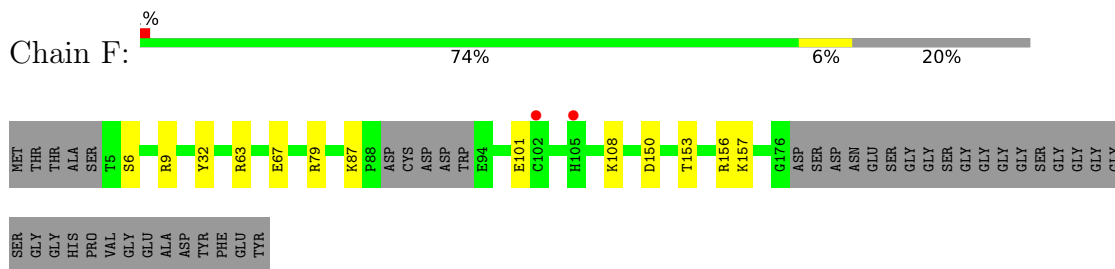
- Molecule 1: Ferritin heavy chain,Epstein-Barr nuclear antigen 1



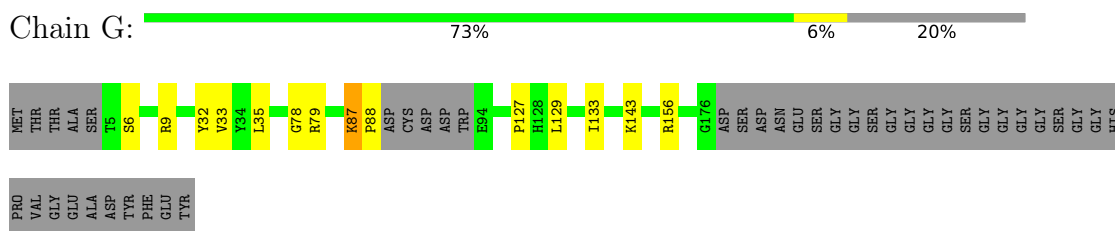
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



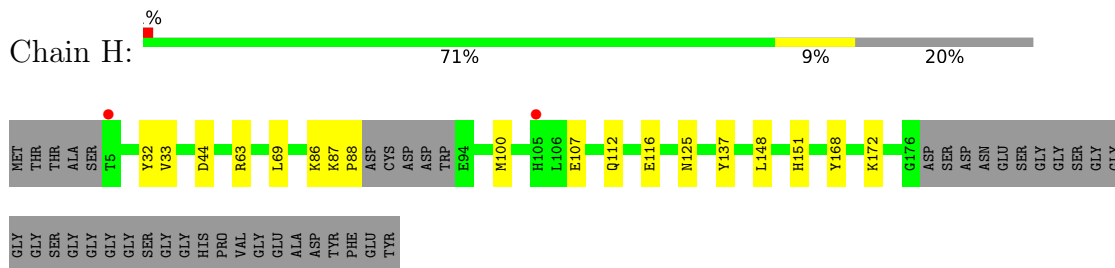
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



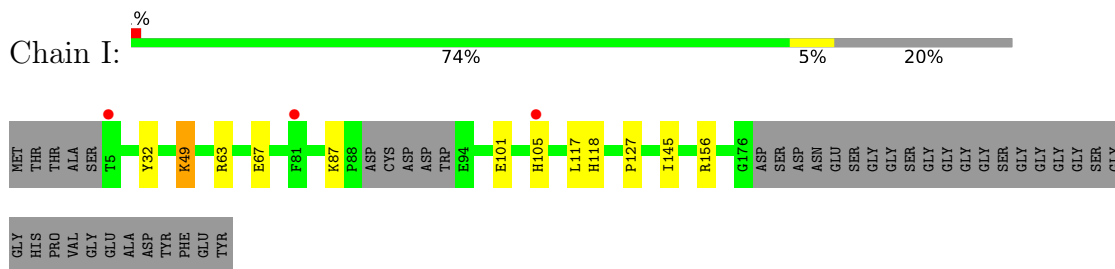
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



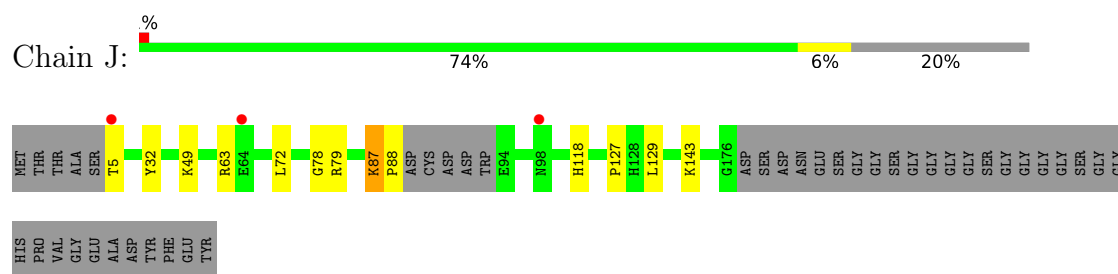
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



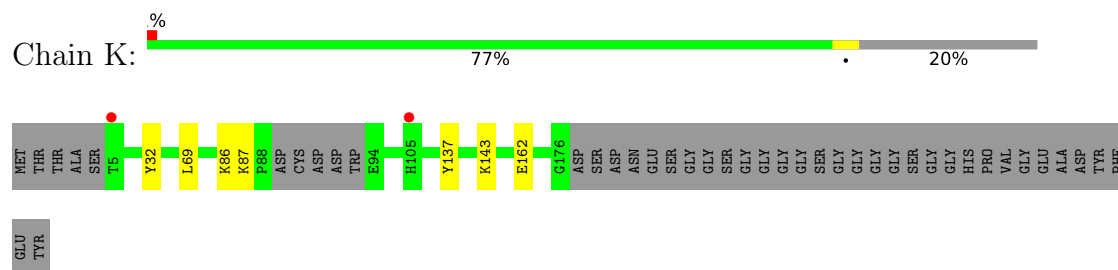
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



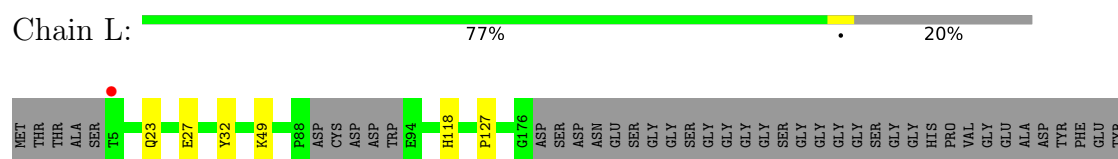
- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



- Molecule 1: Ferritin heavy chain, Epstein-Barr nuclear antigen 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	217.88Å 217.88Å 147.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.20 48.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.72-2.20) 99.8 (48.72-2.20)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.241 , 0.271 0.242 , 0.271	Depositor DCC
R_{free} test set	8906 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9699e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/1380	0.52	0/1857
1	B	0.37	0/1374	0.50	0/1849
1	C	0.38	0/1396	0.51	0/1877
1	D	0.38	0/1375	0.52	0/1851
1	E	0.38	0/1385	0.53	0/1864
1	F	0.38	0/1371	0.53	1/1847 (0.1%)
1	G	0.38	0/1389	0.52	0/1868
1	H	0.39	0/1371	0.52	0/1847
1	I	0.37	0/1389	0.52	0/1871
1	J	0.39	0/1391	0.53	0/1871
1	K	0.37	0/1385	0.52	0/1864
1	L	0.38	0/1369	0.52	0/1846
All	All	0.38	0/16575	0.52	1/22312 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	150	ASP	CB-CG-OD1	5.38	123.14	118.30

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	1354	0	1300	8	0
1	B	1348	0	1297	9	0
1	C	1370	0	1327	5	0
1	D	1349	0	1294	6	0
1	E	1359	0	1306	11	0
1	F	1345	0	1287	6	0
1	G	1363	0	1317	10	0
1	H	1345	0	1287	12	0
1	I	1363	0	1299	8	0
1	J	1365	0	1316	8	0
1	K	1359	0	1310	4	0
1	L	1343	0	1275	4	0
2	A	8	0	12	3	0
2	C	8	0	12	0	0
2	F	8	0	12	1	0
2	H	8	0	12	0	0
2	I	8	0	12	0	0
2	K	8	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	52	0	0	3	0
4	B	59	0	0	2	0
4	C	61	0	0	0	0
4	D	60	0	0	1	0
4	E	64	0	0	1	0
4	F	63	0	0	1	0
4	G	58	0	0	1	0
4	H	64	0	0	2	0
4	I	62	0	0	0	0
4	J	61	0	0	1	0
4	K	48	0	0	0	0
4	L	59	0	0	0	0
All	All	17042	0	15687	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HH21	2:A:301:TRS:H31	1.54	0.70
1:A:102[B]:CYS:SG	4:A:452:HOH:O	2.50	0.69
1:A:83:GLN:NE2	4:A:401:HOH:O	2.21	0.69
1:I:101:GLU:O	1:I:105:HIS:ND1	2.20	0.67
1:F:6:SER:HB3	1:F:9:ARG:HB2	1.78	0.66
1:G:6:SER:HB3	1:G:9:ARG:HB2	1.80	0.64
1:B:172:LYS:NZ	4:B:401:HOH:O	2.31	0.64
1:J:5:THR:N	4:J:401:HOH:O	2.31	0.63
1:B:101:GLU:OE2	1:B:156:ARG:NH2	2.31	0.60
1:F:108:LYS:NZ	4:F:401:HOH:O	2.35	0.60
1:B:6:SER:HB3	1:B:9:ARG:HB2	1.84	0.59
1:I:49:LYS:N	1:I:49:LYS:HD2	2.20	0.56
1:B:118:HIS:CE1	1:I:127:PRO:HB3	2.43	0.54
1:D:118:HIS:CE1	1:G:127:PRO:HB3	2.43	0.53
1:H:100:MET:HE2	1:H:151:HIS:HB2	1.90	0.53
1:D:75:GLN:NE2	4:D:403:HOH:O	2.42	0.53
1:F:63:ARG:NE	1:F:67:GLU:OE1	2.34	0.52
1:H:107:GLU:HG3	1:H:148:LEU:CD1	2.39	0.52
1:B:127:PRO:HB3	1:E:118:HIS:CE1	2.44	0.52
1:I:63[B]:ARG:NH1	1:J:63:ARG:HG2	2.26	0.51
1:A:63:ARG:NH2	2:A:301:TRS:H31	2.24	0.51
1:E:86:LYS:NZ	4:E:403:HOH:O	2.43	0.50
1:E:78:GLY:O	1:E:79:ARG:NH1	2.44	0.50
1:G:78:GLY:O	1:G:79:ARG:NH1	2.43	0.50
1:C:127:PRO:HB3	1:J:118:HIS:CE1	2.46	0.50
1:A:63:ARG:NE	1:A:67:GLU:OE1	2.43	0.49
1:K:69:LEU:HG	1:K:137:TYR:OH	2.13	0.48
1:H:100:MET:HE1	1:H:148:LEU:HD23	1.96	0.47
1:J:127:PRO:HB3	1:L:118:HIS:CE1	2.49	0.47
1:A:102[A]:CYS:SG	4:A:452:HOH:O	2.61	0.47
1:C:63:ARG:NE	1:C:67:GLU:OE2	2.36	0.47
1:C:118:HIS:CE1	1:L:127:PRO:HB3	2.48	0.47
1:E:8:VAL:HB	1:I:145:ILE:HG22	1.96	0.47
1:B:86:LYS:HG2	4:B:423:HOH:O	2.14	0.47
1:E:127:PRO:HB3	1:I:118:HIS:CE1	2.50	0.46
1:J:143:LYS:HB2	1:J:143:LYS:HE3	1.65	0.46
1:A:28:LEU:HD22	2:A:301:TRS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:GLN:O	1:H:116:GLU:HG2	2.16	0.46
1:L:23:GLN:O	1:L:27:GLU:HG2	2.16	0.46
1:C:20:ILE:HD13	1:C:117:LEU:HD21	1.98	0.46
1:D:33:VAL:HG22	1:D:88:PRO:HB3	1.98	0.45
1:I:63[A]:ARG:NE	1:I:67:GLU:OE1	2.40	0.45
1:A:162:GLU:H	1:A:162:GLU:CD	2.20	0.45
1:H:125:ASN:ND2	4:H:401:HOH:O	2.33	0.44
1:F:79:ARG:HA	1:F:79:ARG:HD3	1.79	0.44
1:B:87:LYS:HE3	1:B:87:LYS:HB2	1.72	0.44
1:G:79:ARG:HD3	1:G:79:ARG:HA	1.71	0.44
1:J:72:LEU:HD21	1:J:129:LEU:HD13	1.99	0.44
1:E:107:GLU:HG3	1:E:148:LEU:CD1	2.47	0.44
1:F:101:GLU:OE1	1:F:156:ARG:NH2	2.50	0.44
1:E:63:ARG:NE	1:E:67:GLU:OE1	2.48	0.44
1:L:49:LYS:HA	1:L:49:LYS:HD3	1.71	0.43
1:H:33:VAL:HG22	1:H:88:PRO:HB3	1.99	0.43
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.54	0.43
1:D:79:ARG:HD3	1:D:79:ARG:HA	1.81	0.42
1:G:33:VAL:HG22	1:G:88:PRO:HB3	2.00	0.42
1:G:156:ARG:NE	4:G:405:HOH:O	2.51	0.42
1:K:143:LYS:HE3	1:K:143:LYS:HB2	1.83	0.42
1:E:72:LEU:HD22	1:E:132:PHE:CE2	2.54	0.42
1:K:86:LYS:HD3	1:K:86:LYS:HA	1.87	0.42
1:B:79:ARG:HD3	1:B:79:ARG:HA	1.77	0.42
1:H:168:TYR:O	1:H:172:LYS:HG2	2.20	0.41
1:D:33:VAL:HA	1:D:88:PRO:HB3	2.03	0.41
1:F:153:THR:O	1:F:157:LYS:HG3	2.21	0.41
2:F:301:TRS:O3	2:F:301:TRS:O2	2.28	0.41
1:D:150:ASP:OD1	1:H:44:ASP:HA	2.21	0.41
1:E:87:LYS:HA	1:E:88:PRO:HD3	1.90	0.41
1:G:35:LEU:HD13	1:H:63:ARG:HH21	1.85	0.41
1:B:13:HIS:CE1	1:B:124:LYS:NZ	2.89	0.41
1:C:87:LYS:HA	1:C:88:PRO:HD3	1.91	0.41
1:J:87:LYS:HA	1:J:88:PRO:HD3	1.87	0.41
1:G:143:LYS:HB2	1:G:143:LYS:HE3	1.69	0.41
1:E:68:LYS:HG2	1:E:132:PHE:HZ	1.86	0.40
1:H:69:LEU:HG	1:H:137:TYR:OH	2.20	0.40
1:K:162:GLU:H	1:K:162:GLU:CD	2.24	0.40
1:G:87:LYS:HA	1:G:88:PRO:HD3	1.90	0.40
1:G:129:LEU:O	1:G:133:ILE:HG12	2.21	0.40
1:J:78:GLY:O	1:J:79:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:LYS:HE3	4:H:446:HOH:O	2.20	0.40
1:H:107:GLU:HG3	1:H:148:LEU:HD11	2.04	0.40
1:I:101:GLU:OE1	1:I:156:ARG:NH2	2.54	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	163/209 (78%)	161 (99%)	2 (1%)	0	100	100
1	B	163/209 (78%)	161 (99%)	2 (1%)	0	100	100
1	C	165/209 (79%)	163 (99%)	2 (1%)	0	100	100
1	D	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	E	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	F	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	G	164/209 (78%)	161 (98%)	3 (2%)	0	100	100
1	H	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	I	165/209 (79%)	163 (99%)	2 (1%)	0	100	100
1	J	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	K	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
1	L	164/209 (78%)	162 (99%)	2 (1%)	0	100	100
All	All	1968/2508 (78%)	1943 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/175 (82%)	142 (99%)	2 (1%)	67	80
1	B	143/175 (82%)	142 (99%)	1 (1%)	84	91
1	C	146/175 (83%)	144 (99%)	2 (1%)	67	80
1	D	142/175 (81%)	139 (98%)	3 (2%)	53	67
1	E	145/175 (83%)	141 (97%)	4 (3%)	43	56
1	F	141/175 (81%)	139 (99%)	2 (1%)	67	80
1	G	146/175 (83%)	144 (99%)	2 (1%)	67	80
1	H	141/175 (81%)	139 (99%)	2 (1%)	67	80
1	I	143/175 (82%)	139 (97%)	4 (3%)	43	56
1	J	146/175 (83%)	143 (98%)	3 (2%)	53	67
1	K	145/175 (83%)	143 (99%)	2 (1%)	67	80
1	L	140/175 (80%)	139 (99%)	1 (1%)	84	91
All	All	1722/2100 (82%)	1694 (98%)	28 (2%)	62	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	87	LYS
1	B	32	TYR
1	C	32	TYR
1	C	87	LYS
1	D	32	TYR
1	D	87	LYS
1	D	157	LYS
1	E	32	TYR
1	E	49	LYS
1	E	87	LYS
1	E	143	LYS
1	F	32	TYR
1	F	87	LYS

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Mol	Chain	Res	Type
1	G	32	TYR
1	G	87	LYS
1	H	32	TYR
1	H	87	LYS
1	I	32	TYR
1	I	49	LYS
1	I	87	LYS
1	I	117	LEU
1	J	32	TYR
1	J	49	LYS
1	J	87	LYS
1	K	32	TYR
1	K	87	LYS
1	L	32	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	75	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRS	F	301	-	7,7,7	0.51	0	9,9,9	0.98	0
2	TRS	I	301	-	7,7,7	0.51	0	9,9,9	1.18	1 (11%)
2	TRS	K	301	-	7,7,7	0.46	0	9,9,9	0.73	0
2	TRS	A	301	-	7,7,7	0.55	0	9,9,9	1.19	1 (11%)
2	TRS	C	301	-	7,7,7	0.46	0	9,9,9	1.07	0
2	TRS	H	301	-	7,7,7	0.46	0	9,9,9	0.96	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	F	301	-	-	3/9/9/9	-
2	TRS	I	301	-	-	2/9/9/9	-
2	TRS	K	301	-	-	9/9/9/9	-
2	TRS	A	301	-	-	6/9/9/9	-
2	TRS	C	301	-	-	8/9/9/9	-
2	TRS	H	301	-	-	3/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	TRS	O2-C2-C	-2.42	103.32	111.00
2	A	301	TRS	O1-C1-C	-2.31	103.68	111.00
2	H	301	TRS	O3-C3-C	-2.03	104.55	111.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	TRS	N-C-C3-O3
2	K	301	TRS	C2-C-C1-O1

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Mol	Chain	Res	Type	Atoms
2	K	301	TRS	C3-C-C1-O1
2	K	301	TRS	N-C-C1-O1
2	K	301	TRS	C1-C-C2-O2
2	K	301	TRS	N-C-C2-O2
2	K	301	TRS	C1-C-C3-O3
2	A	301	TRS	C1-C-C3-O3
2	C	301	TRS	C1-C-C2-O2
2	C	301	TRS	C2-C-C3-O3
2	F	301	TRS	C2-C-C3-O3
2	I	301	TRS	C3-C-C2-O2
2	K	301	TRS	C2-C-C3-O3
2	A	301	TRS	C3-C-C2-O2
2	A	301	TRS	N-C-C2-O2
2	A	301	TRS	N-C-C3-O3
2	C	301	TRS	N-C-C1-O1
2	C	301	TRS	N-C-C2-O2
2	C	301	TRS	N-C-C3-O3
2	H	301	TRS	N-C-C2-O2
2	I	301	TRS	N-C-C2-O2
2	K	301	TRS	C3-C-C2-O2
2	A	301	TRS	C2-C-C3-O3
2	C	301	TRS	C2-C-C1-O1
2	C	301	TRS	C3-C-C2-O2
2	C	301	TRS	C1-C-C3-O3
2	H	301	TRS	C1-C-C2-O2
2	A	301	TRS	C1-C-C2-O2
2	F	301	TRS	C1-C-C3-O3
2	H	301	TRS	C3-C-C2-O2
2	K	301	TRS	N-C-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	TRS	1	0
2	A	301	TRS	3	0

5.7 Other polymers [i](#)

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, 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	166/209 (79%)	-0.20	2 (1%) 79 77	20, 24, 36, 50	0
1	B	166/209 (79%)	-0.19	3 (1%) 68 66	20, 25, 34, 41	0
1	C	167/209 (79%)	-0.23	3 (1%) 68 66	20, 25, 34, 50	0
1	D	166/209 (79%)	-0.29	2 (1%) 79 77	19, 25, 33, 43	0
1	E	167/209 (79%)	-0.20	3 (1%) 68 66	20, 25, 36, 53	0
1	F	167/209 (79%)	-0.10	2 (1%) 79 77	21, 25, 34, 52	0
1	G	167/209 (79%)	-0.14	0 100 100	20, 25, 35, 50	0
1	H	167/209 (79%)	-0.22	2 (1%) 79 77	19, 25, 34, 53	0
1	I	167/209 (79%)	-0.15	3 (1%) 68 66	20, 25, 36, 63	0
1	J	167/209 (79%)	-0.18	3 (1%) 68 66	20, 24, 37, 58	0
1	K	167/209 (79%)	-0.25	2 (1%) 79 77	20, 25, 37, 55	0
1	L	167/209 (79%)	-0.15	1 (0%) 89 88	20, 25, 35, 56	0
All	All	2001/2508 (79%)	-0.19	26 (1%) 77 75	19, 25, 36, 63	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	5	THR	4.3
1	E	105	HIS	3.6
1	A	162	GLU	3.3
1	A	98	ASN	3.2
1	E	5	THR	3.1
1	E	98	ASN	3.0
1	C	5	THR	3.0
1	J	64	GLU	3.0
1	K	5	THR	2.8
1	C	105	HIS	2.7
1	L	5	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	98	ASN	2.7
1	B	164	GLY	2.6
1	H	105	HIS	2.5
1	I	5	THR	2.5
1	F	102[A]	CYS	2.4
1	D	105	HIS	2.4
1	K	105	HIS	2.4
1	H	5	THR	2.4
1	C	98	ASN	2.4
1	I	81	PHE	2.3
1	J	98	ASN	2.3
1	I	105	HIS	2.3
1	F	105	HIS	2.2
1	B	98	ASN	2.2
1	B	81	PHE	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](#)

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	TRS	K	301	8/8	0.72	0.31	26,32,34,43	8
2	TRS	C	301	8/8	0.77	0.18	33,34,37,39	0
2	TRS	H	301	8/8	0.78	0.27	28,32,37,42	8
2	TRS	A	301	8/8	0.80	0.22	29,35,40,41	0
2	TRS	F	301	8/8	0.86	0.23	30,34,37,37	8
2	TRS	I	301	8/8	0.88	0.22	30,32,36,38	8
3	FE	C	302	1/1	0.90	0.09	35,35,35,35	1
3	FE	C	304[A]	1/1	0.92	0.08	31,31,31,31	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FE	E	303	1/1	0.94	0.12	34,34,34,34	1
3	FE	B	302	1/1	0.96	0.12	25,25,25,25	1
3	FE	D	301	1/1	0.96	0.11	36,36,36,36	1
3	FE	D	302	1/1	0.96	0.11	31,31,31,31	0
3	FE	E	301[A]	1/1	0.96	0.09	25,25,25,25	1
3	FE	A	302	1/1	0.96	0.13	30,30,30,30	0
3	FE	G	302	1/1	0.97	0.09	32,32,32,32	0
3	FE	I	302	1/1	0.97	0.14	27,27,27,27	0
3	FE	L	301	1/1	0.97	0.11	27,27,27,27	0
3	FE	G	301[A]	1/1	0.98	0.07	31,31,31,31	1
3	FE	B	301	1/1	0.98	0.09	27,27,27,27	1
3	FE	E	302	1/1	0.98	0.14	32,32,32,32	0
3	FE	A	303[A]	1/1	0.98	0.18	34,34,34,34	1
3	FE	C	303	1/1	0.99	0.08	27,27,27,27	1
3	FE	J	301	1/1	0.99	0.13	33,33,33,33	0
3	FE	K	302	1/1	0.99	0.12	29,29,29,29	0
3	FE	H	302	1/1	0.99	0.14	25,25,25,25	1
3	FE	F	302	1/1	1.00	0.14	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.