

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 03:12 AM EDT

PDB ID	:	7KE5
Title	:	Heavy chain ferritin with N-terminal EBNA1 epitope
Authors	:	Pederick, J.P.; Bruning, J.B.
Deposited on	:	2020-10-10
Resolution	:	2.80 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 (i) symbol.

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	3140 (2.80-2.80)		
Clashscore	141614	3569 (2.80-2.80)		
Ramachandran outliers	138981	3498 (2.80-2.80)		
Sidechain outliers	138945	3500 (2.80-2.80)		
RSRZ outliers	127900	3078 (2.80-2.80)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	209	^{2%}	9%	18%
		_00	% •	570	1070
1	В	209	70%	12%	18%
1	С	209	73%	8%	19%
1	р	209	2%	90/	1.00/
		205	2%	0%	10 %
1	Е	209	73%	8%	19%



Mol	Chain	Length	Quality of chain		
1	F	209	3% 72%	9%	19%
1	G	209	3% 72%	10%	18%
1	Н	209	3% 74%	7%	19%
1	Ι	209	3% 72%	11%	18%
1	J	209	^{2%} 74%	7%	19%
1	Κ	209	% 69%	11%	19%
1	L	209	^{2%} 71%	11%	18%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16674 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	179	Total	С	Ν	0	S	0	0	0
1	Λ	172	1380	870	240	264	6	0	0	0
1	В	179	Total	С	Ν	0	S	0	0	0
1	D	112	1391	876	246	262	7	0	0	0
1	C	160	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	U	105	1379	868	244	261	6	0	0	0
1	п	179	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	112	1396	878	244	267	7	0	0	0
1	E	169	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		105	1374	866	240	262	6	0	0	0
1	F	169	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	T,		1374	866	244	259	5	0		0
1	G	172	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	ŭ	112	1398	877	246	268	7	0	0	0
1	н	169	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	11	105	1372	864	243	259	6	0	0	0
1	Т	172	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	112	1386	869	244	266	7	0	0	0
1	Т	169	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	5	105	1368	861	241	260	6	0	0	0
1	K	160	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	17	103	1369	861	241	261	6	0	0	0
1	L	172	Total	С	Ν	0	S	0	0	0
1		112	1388	868	245	268	7	0	0	U

• Molecule 1 is a protein called Epstein-Barr nuclear antigen 1, Ferritin heavy chain.

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-26	MET	-	initiating methionine	UNP P03211
А	-14	GLY	-	linker	UNP P03211
А	-13	GLY	-	linker	UNP P03211
А	-12	SER	-	linker	UNP P03211
А	-11	GLY	-	linker	UNP P03211



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Chain	Residue	Modelled	Actual	Comment	Reference
А	-10	GLY	_	linker	UNP P03211
A	-9	GLY	-	linker	UNP P03211
A	-8	GLY	_	linker	UNP P03211
A	-7	SER	_	linker	UNP P03211
A	-6	GLY	_	linker	UNP P03211
A	-5	GLY	_	linker	UNP P03211
А	-4	GLY	_	linker	UNP P03211
А	-3	GLY	-	linker	UNP P03211
А	-2	SER	-	linker	UNP P03211
А	-1	GLY	-	linker	UNP P03211
А	0	GLY	-	linker	UNP P03211
В	-26	MET	-	initiating methionine	UNP P03211
В	-14	GLY	-	linker	UNP P03211
В	-13	GLY	-	linker	UNP P03211
В	-12	SER	-	linker	UNP P03211
В	-11	GLY	-	linker	UNP P03211
В	-10	GLY	-	linker	UNP P03211
В	-9	GLY	-	linker	UNP P03211
В	-8	GLY	-	linker	UNP P03211
В	-7	SER	-	linker	UNP P03211
В	-6	GLY	-	linker	UNP P03211
В	-5	GLY	-	linker	UNP P03211
В	-4	GLY	-	linker	UNP P03211
В	-3	GLY	-	linker	UNP P03211
В	-2	SER	-	linker	UNP P03211
В	-1	GLY	-	linker	UNP P03211
В	0	GLY	-	linker	UNP P03211
С	-26	MET	-	initiating methionine	UNP P03211
С	-14	GLY	_	linker	UNP P03211
С	-13	GLY	-	linker	UNP P03211
С	-12	SER	-	linker	UNP P03211
С	-11	GLY	-	linker	UNP P03211
С	-10	GLY	-	linker	UNP P03211
С	-9	GLY	-	linker	UNP P03211
С	-8	GLY	-	linker	UNP P03211
С	-7	SER	-	linker	UNP P03211
С	-6	GLY	-	linker	UNP P03211
С	-5	GLY	-	linker	UNP P03211
С	-4	GLY	-	linker	UNP P03211
С	-3	GLY	-	linker	UNP P03211
С	-2	SER	-	linker	UNP P03211
С	-1	GLY	-	linker	UNP P03211



Chain	Residue	Modelled	Actual	Comment	Reference
С	0	GLY	_	linker	UNP P03211
D	-26	MET	-	initiating methionine	UNP P03211
D	-14	GLY	-	linker	UNP P03211
D	-13	GLY	-	linker	UNP P03211
D	-12	SER	-	linker	UNP P03211
D	-11	GLY	-	linker	UNP P03211
D	-10	GLY	-	linker	UNP P03211
D	-9	GLY	-	linker	UNP P03211
D	-8	GLY	-	linker	UNP P03211
D	-7	SER	-	linker	UNP P03211
D	-6	GLY	-	linker	UNP P03211
D	-5	GLY	-	linker	UNP P03211
D	-4	GLY	-	linker	UNP P03211
D	-3	GLY	-	linker	UNP P03211
D	-2	SER	-	linker	UNP P03211
D	-1	GLY	-	linker	UNP P03211
D	0	GLY	-	linker	UNP P03211
Е	-26	MET	-	initiating methionine	UNP P03211
Е	-14	GLY	-	linker	UNP P03211
Е	-13	GLY	-	linker	UNP P03211
Е	-12	SER	_	linker	UNP P03211
Е	-11	GLY	-	linker	UNP P03211
Е	-10	GLY	-	linker	UNP P03211
E	-9	GLY	-	linker	UNP P03211
E	-8	GLY	-	linker	UNP P03211
E	-7	SER	-	linker	UNP P03211
E	-6	GLY	-	linker	UNP P03211
E	-5	GLY	-	linker	UNP P03211
E	-4	GLY	-	linker	UNP P03211
E	-3	GLY	_	linker	UNP P03211
E	-2	SER	_	linker	UNP P03211
E	-1	GLY	_	linker	UNP P03211
E	0	GLY	_	linker	UNP P03211
F	-26	MET	-	initiating methionine	UNP P03211
F	-14	GLY	-	linker	UNP P03211
F	-13	GLY	-	linker	UNP P03211
F	-12	SER	-	linker	UNP P03211
F	-11	GLY	-	linker	UNP P03211
F	-10	GLY	-	linker	UNP P03211
F	-9	GLY	-	linker	UNP P03211
F	-8	GLY	-	linker	UNP P03211
F	-7	SER	-	linker	UNP P03211



Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	GLY	-	linker	UNP P03211
F	-5	GLY	-	linker	UNP P03211
F	-4	GLY	-	linker	UNP P03211
F	-3	GLY	-	linker	UNP P03211
F	-2	SER	-	linker	UNP P03211
F	-1	GLY	-	linker	UNP P03211
F	0	GLY	-	linker	UNP P03211
G	-26	MET	-	initiating methionine	UNP P03211
G	-14	GLY	-	linker	UNP P03211
G	-13	GLY	-	linker	UNP P03211
G	-12	SER	-	linker	UNP P03211
G	-11	GLY	-	linker	UNP P03211
G	-10	GLY	-	linker	UNP P03211
G	-9	GLY	-	linker	UNP P03211
G	-8	GLY	-	linker	UNP P03211
G	-7	SER	-	linker	UNP P03211
G	-6	GLY	-	linker	UNP P03211
G	-5	GLY	-	linker	UNP P03211
G	-4	GLY	-	linker	UNP P03211
G	-3	GLY	-	linker	UNP P03211
G	-2	SER	-	linker	UNP P03211
G	-1	GLY	-	linker	UNP P03211
G	0	GLY	-	linker	UNP P03211
Н	-26	MET	-	initiating methionine	UNP P03211
Н	-14	GLY	-	linker	UNP P03211
Н	-13	GLY	-	linker	UNP P03211
Н	-12	SER	-	linker	UNP P03211
Н	-11	GLY	-	linker	UNP P03211
H	-10	GLY	-	linker	UNP P03211
Н	-9	GLY	-	linker	UNP P03211
Н	-8	GLY	-	linker	UNP P03211
Н	-7	SER	-	linker	UNP P03211
Н	-6	GLY	-	linker	UNP P03211
Н	-5	GLY	-	linker	UNP P03211
Н	-4	GLY	-	linker	UNP P03211
Н	-3	GLY	-	linker	UNP P03211
H	-2	SER	-	linker	UNP P03211
H	-1	GLY	-	linker	UNP P03211
H	0	GLY	-	linker	UNP P03211
I	-26	MET	-	initiating methionine	UNP P03211
Ι	-14	GLY	-	linker	UNP P03211
Ι	-13	GLY	-	linker	UNP P03211



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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	-12	SER	-	linker	UNP P03211
Ι	-11	GLY	-	linker	UNP P03211
Ι	-10	GLY	-	linker	UNP P03211
Ι	-9	GLY	-	linker	UNP P03211
Ι	-8	GLY	-	linker	UNP P03211
Ι	-7	SER	-	linker	UNP P03211
Ι	-6	GLY	-	linker	UNP P03211
Ι	-5	GLY	-	linker	UNP P03211
Ι	-4	GLY	-	linker	UNP P03211
Ι	-3	GLY	-	linker	UNP P03211
Ι	-2	SER	-	linker	UNP P03211
Ι	-1	GLY	-	linker	UNP P03211
Ι	0	GLY	-	linker	UNP P03211
J	-26	MET	-	initiating methionine	UNP P03211
J	-14	GLY	-	linker	UNP P03211
J	-13	GLY	-	linker	UNP P03211
J	-12	SER	-	linker	UNP P03211
J	-11	GLY	-	linker	UNP P03211
J	-10	GLY	-	linker	UNP P03211
J	-9	GLY	-	linker	UNP P03211
J	-8	GLY	_	linker	UNP P03211
J	-7	SER	-	linker	UNP P03211
J	-6	GLY	_	linker	UNP P03211
J	-5	GLY	-	linker	UNP P03211
J	-4	GLY	-	linker	UNP P03211
J	-3	GLY	_	linker	UNP P03211
J	-2	SER	-	linker	UNP P03211
J	-1	GLY	-	linker	UNP P03211
J	0	GLY	-	linker	UNP P03211
Κ	-26	MET	-	initiating methionine	UNP P03211
K	-14	GLY	-	linker	UNP P03211
K	-13	GLY	-	linker	UNP P03211
K	-12	SER	-	linker	UNP P03211
K	-11	GLY	-	linker	UNP P03211
K	-10	GLY	-	linker	UNP P03211
Κ	-9	GLY	-	linker	UNP P03211
К	-8	GLY	-	linker	UNP P03211
K	-7	SER	-	linker	UNP P03211
K	-6	GLY	-	linker	UNP P03211
K	-5	GLY	-	linker	UNP P03211
K	-4	GLY	-	linker	UNP P03211

-3

Κ

GLY

-

Continued on next page...

UNP P03211



linker

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	SER	-	linker	UNP P03211
K	-1	GLY	-	linker	UNP P03211
K	0	GLY	-	linker	UNP P03211
L	-26	MET	-	initiating methionine	UNP P03211
L	-14	GLY	-	linker	UNP P03211
L	-13	GLY	-	linker	UNP P03211
L	-12	SER	-	linker	UNP P03211
L	-11	GLY	-	linker	UNP P03211
L	-10	GLY	-	linker	UNP P03211
L	-9	GLY	-	linker	UNP P03211
L	-8	GLY	-	linker	UNP P03211
L	-7	SER	-	linker	UNP P03211
L	-6	GLY	-	linker	UNP P03211
L	-5	GLY	-	linker	UNP P03211
L	-4	GLY	-	linker	UNP P03211
L	-3	GLY	-	linker	UNP P03211
L	-2	SER	-	linker	UNP P03211
L	-1	GLY	-	linker	UNP P03211
L	0	GLY	-	linker	UNP P03211

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



Mol	Chain	Residues	А	ton	ns		ZeroOcc	AltConf
2	А	1	Total 8	С 4	N 1	O 3	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	Total C N O	0	0
			0 4 1 3		
0	Б	1	Total C N O	0	0
	E	L	8 4 1 3	0	0
2	н	1	Total C N O	0	0
2	11	T	8 4 1 3	0	0
0	т	1	Total C N O	0	0
	1	L	8 4 1 3	0	0
9	т	1	Total C N O	0	0
		L	8 4 1 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Fe 2 2	0	0
3	В	1	Total Fe 1 1	0	0
3	С	2	Total Fe 2 2	0	0
3	D	2	Total Fe 2 2	0	0
3	Ε	2	Total Fe 2 2	0	0
3	F	1	Total Fe 1 1	0	0
3	G	1	Total Fe 1 1	0	0
3	Н	1	Total Fe 1 1	0	0
3	Ι	1	Total Fe 1 1	0	0
3	J	1	Total Fe 1 1	0	0
3	К	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	А	2	Total O 2 2	0	0
4	В	6	Total O 6 6	0	0
4	С	2	Total O 2 2	0	0
4	D	3	Total O 3 3	0	0
4	Е	4	Total O 4 4	0	0
4	F	5	Total O 5 5	0	0
4	G	3	Total O 3 3	0	0
4	Н	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	K	2	Total O 2 2	0	0
4	L	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0



3 Residue-property plots (i)

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

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





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

Chain J:	74%		7%	19%	
MET HIS PRO VAL GLY GLV ALA ALA ALA ALP FYR PHE GLU	TYR GLY SER GLY GLY GLY GLY GLY THR THR THR THR THR THR THR THR THR THR	86 07 014 132 133 132 141	F55 HG0 RG3	F81 D89 CYS ASP ASP	w93 L106 H118



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



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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	219.32Å 219.32Å 148.56Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.82 - 2.80	Depositor
Resolution (A)	48.82 - 2.80	EDS
% Data completeness	91.0 (48.82-2.80)	Depositor
(in resolution range)	92.8 (48.82-2.80)	EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.70 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
P. P.	0.274 , 0.317	Depositor
n, n_{free}	0.273 , 0.315	DCC
R_{free} test set	4320 reflections (5.06%)	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 28.9	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16674	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 51.94 % 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 5.2217e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: 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).

Mal	Chain	Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/1409	0.58	0/1903	
1	В	0.43	0/1420	0.57	0/1914	
1	С	0.43	0/1407	0.55	0/1895	
1	D	0.44	0/1425	0.57	0/1921	
1	Ε	0.47	0/1402	0.57	0/1889	
1	F	0.46	0/1402	0.58	0/1889	
1	G	0.49	0/1427	0.59	0/1925	
1	Н	0.44	0/1400	0.56	0/1887	
1	Ι	0.43	0/1415	0.60	1/1912~(0.1%)	
1	J	0.47	0/1396	0.56	0/1883	
1	Κ	0.45	0/1397	0.55	0/1885	
1	L	0.46	0/1416	0.58	0/1912	
All	All	0.45	0/16916	0.57	1/22815~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ι	117	LEU	CA-CB-CG	7.49	132.52	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



(KE5

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1380	0	1302	9	0
1	В	1391	0	1333	16	0
1	С	1379	0	1324	10	0
1	D	1396	0	1334	9	0
1	Е	1374	0	1313	13	0
1	F	1374	0	1317	11	0
1	G	1398	0	1329	14	0
1	Н	1372	0	1311	11	0
1	Ι	1386	0	1303	11	0
1	J	1368	0	1298	9	0
1	Κ	1369	0	1295	14	0
1	L	1388	0	1311	13	0
2	А	8	0	12	0	0
2	С	8	0	12	0	0
2	Е	8	0	12	1	0
2	Н	8	0	12	1	0
2	Ι	8	0	12	0	0
2	L	8	0	12	0	0
3	А	2	0	0	0	0
3	В	1	0	0	0	0
3	С	2	0	0	0	0
3	D	2	0	0	0	0
3	Ε	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Η	1	0	0	0	0
3	Ι	1	0	0	0	0
3	J	1	0	0	0	0
3	Κ	1	0	0	0	0
3	L	1	0	0	0	0
4	А	2	0	0	0	0
4	В	6	0	0	0	0
4	С	2	0	0	0	0
4	D	3	0	0	0	0
4	E	4	0	0	0	0
4	F	5	0	0	1	0
4	G	3	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
4	Κ	2	0	0	0	0
4	L	5	0	0	0	0
All	All	16674	0	15842	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 4.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:117:LEU:HD22	1:A:133:ILE:HD11	1.55	0.89	
1:D:117:LEU:HD22	1:D:133:ILE:HD11	1.58	0.86	
1:E:60:HIS:HD2	1:E:63:ARG:HH22	1.32	0.77	
1:G:78:GLY:O	1:G:79:ARG:NH1	2.20	0.74	
1:I:154:ASN:O	1:I:158:MET:HG3	1.89	0.72	
1:D:78:GLY:O	1:D:79:ARG:NH1	2.25	0.70	
1:L:101:GLU:OE1	1:L:156:ARG:NH2	2.24	0.70	
1:L:154:ASN:O	1:L:158:MET:HG3	1.91	0.69	
1:J:60:HIS:CD2	1:J:63:ARG:HH22	2.12	0.68	
1:B:101:GLU:OE1	1:B:156:ARG:NH1	2.26	0.68	
1:C:157:LYS:NZ	1:K:46:VAL:O	2.26	0.67	
1:A:154:ASN:O	1:A:158:MET:HG3	1.95	0.67	
1:F:78:GLY:O	1:F:79:ARG:NH1	2.28	0.66	
1:H:154:ASN:O	1:H:158:MET:HG3	1.94	0.66	
1:G:101:GLU:OE1	1:G:156:ARG:NH2	2.28	0.65	
1:D:154:ASN:O	1:D:158:MET:HG3	1.97	0.64	
1:C:154:ASN:O	1:C:158:MET:HG3	1.98	0.64	
1:F:154:ASN:O	1:F:158:MET:HG3	1.99	0.63	
1:L:78:GLY:O	1:L:79:ARG:NH1	2.32	0.62	
1:L:114:LEU:HD13	1:L:137:TYR:HB3	1.81	0.62	
1:F:101:GLU:OE1	1:F:156:ARG:NH2	2.32	0.62	
1:E:154:ASN:O	1:E:158:MET:HG3	2.01	0.61	
1:G:114:LEU:HD13	1:G:137:TYR:HB3	1.83	0.60	
1:H:20:ILE:HD11	1:H:129:LEU:HD11	1.84	0.59	
1:E:60:HIS:HD2	1:E:63:ARG:NH2	2.00	0.59	
1:B:6:SER:OG	1:B:9:ARG:HB2	2.02	0.59	
1:J:127:PRO:HB3	1:L:118:HIS:CE1	2.38	0.58	
1:I:76:ARG:NH2	1:I:126:ASP:OD1	2.36	0.58	
1:J:154:ASN:O	1:J:158:MET:HG3	2.02	0.58	
1:G:63:ARG:NH1	1:H:60:HIS:HD2	2.02	0.58	
1:B:154:ASN:O	1:B:158:MET:HG3	2.04	0.57	
1:G:154:ASN:O	1:G:158:MET:HG3	2.03	0.57	
1:K:154:ASN:O	1:K:158:MET:HG3	2.04	0.57	
1:L:13:HIS:CD2	1:L:124:LYS:HD2	2.40	0.56	
1:B:127:PRO:HB3	1:E:118:HIS:CE1	2.42	0.54	
1:H:20:ILE:HD13	1:H:117:LEU:HD21	1.89	0.54	
1:K:20:ILE:HD11	1:K:129:LEU:HD11	1.88	0.54	
1:B:118:HIS:CE1	1:I:127:PRO:HB3	2.43	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlan (Å)	
1.G.63.ABG.HH11	1.H.60.HIS.CD2	2.26	0.54	
1:A:114:LEU:HD13	1:A:137:TYR:HB3	1.89	0.53	
$2 \cdot \text{E} \cdot 201 \cdot \text{TBS} \cdot \text{H} 32$	1.F.28.LEU.HD22	1.90	0.53	
1:E:63:ARG:HD3	1:F:63:ARG:NH2	2.25	0.52	
1:B:50:ASN:HA	1:B:53:LYS:HG2	1.92	0.52	
1:I:101:GLU:OE1	1:I:156:ARG:NH1	2.39	0.51	
1:I:114:LEU:HD13	1:I:137:TYR:HB3	1.93	0.51	
1:C:8:VAL:HB	1:J:145:ILE:HG22	1.93	0.51	
1:I:78:GLY:O	1:I:79:ARG:NH1	2.44	0.50	
1:H:85:ILE:HD13	2:H:201:TRS:H32	1.94	0.50	
1:C:127:PRO:HB3	1:J:118:HIS:CE1	2.46	0.49	
1:K:63:ARG:NH2	1:L:59:SER:OG	2.41	0.49	
1:B:8:VAL:HB	1:E:145:ILE:HG22	1.95	0.49	
1:A:79:ARG:NH2	1:B:45:ASP:OD2	2.47	0.48	
1:E:117:LEU:HG	1:E:133:ILE:HD11	1.95	0.48	
1:G:63:ARG:HH11	1:H:60:HIS:HD2	1.62	0.48	
1:H:79:ARG:HD3	1:H:79:ARG:HA	1.69	0.48	
1:A:6:SER:HB3	1:A:9:ARG:HB2	1.96	0.48	
1:C:19:ALA:HB1	1:C:117:LEU:HD13	1.96	0.48	
1:D:117:LEU:HD22	1:D:133:ILE:CD1	2.37	0.48	
1:H:78:GLY:O	1:H:79:ARG:NH2	2.41	0.48	
1:J:8:VAL:HB	1:L:145:ILE:HG22	1.96	0.48	
1:B:9:ARG:NH2	1:B:17:GLU:OE2	2.34	0.48	
1:H:65:HIS:HB3	1:H:137:TYR:HE1	1.80	0.47	
1:B:19:ALA:HB1	1:B:117:LEU:HD13	1.95	0.47	
1:E:8:VAL:HB	1:I:145:ILE:HG22	1.97	0.47	
1:B:78:GLY:O	1:B:79:ARG:NH1	2.48	0.47	
1:B:114:LEU:HD13	1:B:137:TYR:HB3	1.97	0.47	
1:L:20:ILE:HD13	1:L:117:LEU:HD21	1.97	0.46	
1:B:90:CYS:HB3	1:B:93:TRP:CH2	2.49	0.46	
1:E:127:PRO:HB3	1:I:118:HIS:CE1	2.50	0.46	
1:A:97:LEU:HD21	1:A:156:ARG:HG2	1.98	0.46	
1:I:138:LEU:HD23	1:I:138:LEU:HA	1.73	0.45	
1:K:129:LEU:O	1:K:133:ILE:HG12	2.16	0.45	
1:K:69:LEU:HG	1:K:137:TYR:OH	2.17	0.45	
1:F:79:ARG:HD3	1:F:79:ARG:HA	1.65	0.45	
1:F:139:ASN:ND2	4:F:301:HOH:O	2.49	0.45	
1:K:71:LYS:O	1:K:75:GLN:HG3	2.17	0.45	
1:F:56:LEU:O	1:F:60:HIS:HD2	2.00	0.45	
1:G:33:VAL:HG22	1:G:88:PRO:HB3	1.97	0.45	
1:L:138:LEU:HA	1:L:138:LEU:HD23	1.68	0.44	



	le de pagen	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:133:ILE:HG22	1:G:138:LEU:HG	2.00	0.44	
1:C:79:ARG:HD3	1:C:79:ARG:HA	1.78	0.44	
1:D:118:HIS:CE1	1:G:127:PRO:HB3	2.53	0.44	
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.63	0.44	
1:E:29:TYR:O	1:E:33:VAL:HG23	2.17	0.44	
1:F:24:ILE:HD13	1:F:70:MET:HG2	1.99	0.44	
1:I:140:GLU:HA	1:I:143:LYS:HZ3	1.83	0.43	
1:H:13:HIS:CD2	1:H:124:LYS:HD2	2.53	0.43	
1:C:6:SER:OG	1:C:9:ARG:HB2	2.18	0.43	
1:I:79:ARG:HD3	1:I:79:ARG:HA	1.84	0.42	
1:K:43:ARG:NH2	1:K:45:ASP:OD2	2.42	0.42	
1:B:124:LYS:HD3	1:B:124:LYS:HA	1.71	0.42	
1:J:138:LEU:HD23	1:J:138:LEU:HA	1.79	0.42	
1:C:133:ILE:HG22	1:C:138:LEU:HG	2.01	0.42	
1:E:72:LEU:HD22	1:E:132:PHE:CE2	2.54	0.42	
1:D:114:LEU:HD13	1:D:137:TYR:HB3	2.02	0.42	
1:B:79:ARG:HD3	1:B:79:ARG:HA	1.73	0.42	
1:C:114:LEU:HD13	1:C:137:TYR:HB3	2.01	0.42	
1:E:60:HIS:CD2	1:E:63:ARG:NH2	2.85	0.42	
1:G:90:CYS:HB2	1:G:93:TRP:CZ3	2.55	0.42	
1:K:16:SER:O	1:K:20:ILE:HG12	2.20	0.42	
1:L:133:ILE:HG22	1:L:138:LEU:HG	2.01	0.42	
1:A:155:LEU:HD21	1:A:170:PHE:CD2	2.55	0.41	
1:B:72:LEU:HD13	1:B:132:PHE:CD1	2.56	0.41	
1:J:33:VAL:HG11	1:J:106:LEU:HD22	2.01	0.41	
1:J:41:PHE:CE2	1:J:55:PHE:HE2	2.39	0.41	
1:K:24:ILE:HD13	1:K:70:MET:HG2	2.02	0.41	
1:K:114:LEU:HD13	1:K:137:TYR:HB3	2.03	0.41	
1:L:79:ARG:HA	1:L:79:ARG:HD3	1.77	0.41	
1:K:79:ARG:HA	1:K:79:ARG:HD3	1.92	0.41	
1:A:33:VAL:HG11	1:A:106:LEU:HD22	2.02	0.40	
1:L:24:ILE:HD13	1:L:70:MET:HG2	2.03	0.40	
1:D:104:LEU:HA	1:D:148:LEU:HD13	2.03	0.40	
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.89	0.40	
1:D:33:VAL:HG22	1:D:88:PRO:HB3	2.02	0.40	
1:E:87:LYS:HD2	1:F:82:LEU:O	2.20	0.40	
1:C:158:MET:HB2	1:C:166:ALA:HB1	2.04	0.40	
1:D:145:ILE:HG22	1:G:8:VAL:HB	2.03	0.40	
1:G:24:ILE:HD13	1:G:70:MET:HG2	2.02	0.40	
1:K:148:LEU:HD23	1:K:148:LEU:HA	1.96	0.40	
1:F:33:VAL:HG22	1:F:88:PRO:HB3	2.02	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:K:101:GLU:OE1	1:K: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	Perce	entiles
1	А	170/209~(81%)	167 (98%)	3~(2%)	0	100	100
1	В	170/209~(81%)	166 (98%)	4 (2%)	0	100	100
1	С	165/209~(79%)	163 (99%)	2(1%)	0	100	100
1	D	170/209~(81%)	168 (99%)	2(1%)	0	100	100
1	Е	165/209~(79%)	164 (99%)	1 (1%)	0	100	100
1	F	165/209~(79%)	162 (98%)	3 (2%)	0	100	100
1	G	170/209~(81%)	167 (98%)	3 (2%)	0	100	100
1	Н	165/209~(79%)	163 (99%)	2(1%)	0	100	100
1	Ι	170/209~(81%)	168 (99%)	2 (1%)	0	100	100
1	J	165/209~(79%)	163 (99%)	2(1%)	0	100	100
1	Κ	165/209~(79%)	163 (99%)	2 (1%)	0	100	100
1	L	170/209~(81%)	168 (99%)	2 (1%)	0	100	100
All	All	2010/2508~(80%)	1982 (99%)	28 (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.

Mol	Chain	Analysed	Rotameric Outliers		Perce	ntiles
1	А	144/175~(82%)	141 (98%)	3~(2%)	53	84
1	В	147/175~(84%)	146 (99%)	1 (1%)	84	95
1	С	147/175~(84%)	145 (99%)	2 (1%)	67	90
1	D	149/175~(85%)	147 (99%)	2 (1%)	69	91
1	Е	146/175~(83%)	145 (99%)	1 (1%)	84	95
1	F	145/175~(83%)	143 (99%)	2 (1%)	67	90
1	G	149/175~(85%)	147 (99%)	2 (1%)	69	91
1	Н	145/175~(83%)	144 (99%)	1 (1%)	84	95
1	Ι	146/175~(83%)	141 (97%)	5(3%)	37	71
1	J	144/175~(82%)	143 (99%)	1 (1%)	84	95
1	Κ	144/175~(82%)	140 (97%)	4 (3%)	43	77
1	L	147/175 (84%)	143 (97%)	4 (3%)	44	78
All	All	1753/2100 (84%)	1725 (98%)	28 (2%)	62	88

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

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

Mol	Chain	Res	Type
1	А	32	TYR
1	А	68	LYS
1	А	84	ASP
1	В	32	TYR
1	С	32	TYR
1	С	49	LYS
1	D	32	TYR
1	D	90	CYS
1	Е	32	TYR
1	F	32	TYR
1	F	171	ASP
1	G	32	TYR
1	G	102	CYS
1	Н	32	TYR
1	Ι	32	TYR
1	Ι	87	LYS
1	Ι	90	CYS
1	Ι	116	GLU



Mol	Chain	Res	Type
1	Ι	171	ASP
1	J	32	TYR
1	K	32	TYR
1	K	63	ARG
1	K	86	LYS
1	K	143	LYS
1	L	5	THR
1	L	32	TYR
1	L	102	CYS
1	L	171	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ε	60	HIS
1	F	139	ASN
1	G	60	HIS
1	Н	60	HIS
1	J	60	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 16 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 Turo		Chain	Dog	Res Link	Bond lengths			Bond angles		
Moi Type	nes		Counts		RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	TRS	L	201	-	7,7,7	0.36	0	9,9,9	0.57	0
2	TRS	А	201	-	7,7,7	0.44	0	9,9,9	0.63	0
2	TRS	Ι	201	-	7,7,7	0.40	0	9,9,9	0.75	0
2	TRS	E	201	-	7,7,7	0.36	0	$9,\!9,\!9$	0.81	0
2	TRS	С	201	-	7,7,7	0.40	0	$9,\!9,\!9$	1.28	1 (11%)
2	TRS	Н	201	-	7,7,7	0.75	0	9,9,9	1.49	3 (33%)

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	L	201	-	-	3/9/9/9	-
2	TRS	А	201	-	-	4/9/9/9	-
2	TRS	Ι	201	-	-	0/9/9/9	-
2	TRS	Е	201	-	-	4/9/9/9	-
2	TRS	С	201	-	-	0/9/9/9	-
2	TRS	Н	201	-	_	6/9/9/9	_

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	201	TRS	O2-C2-C	-2.91	101.77	111.00
2	Н	201	TRS	01-C1-C	-2.70	102.42	111.00
2	Н	201	TRS	O2-C2-C	-2.10	104.35	111.00
2	Н	201	TRS	C3-C-C1	2.02	117.08	110.81

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	201	TRS	N-C-C1-O1
2	Н	201	TRS	C2-C-C1-O1



Mol	Chain	Res	Type	Atoms
2	Н	201	TRS	C3-C-C1-O1
2	L	201	TRS	C2-C-C1-O1
2	L	201	TRS	C3-C-C1-O1
2	Е	201	TRS	C3-C-C1-O1
2	Н	201	TRS	C2-C-C3-O3
2	А	201	TRS	C2-C-C1-O1
2	А	201	TRS	N-C-C1-O1
2	Е	201	TRS	N-C-C3-O3
2	Н	201	TRS	N-C-C1-O1
2	Н	201	TRS	C1-C-C2-O2
2	Н	201	TRS	N-C-C2-O2
2	L	201	TRS	N-C-C1-O1
2	А	201	TRS	C3-C-C1-O1
2	Е	201	TRS	C1-C-C3-O3
2	А	201	TRS	C3-C-C2-O2

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There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	201	TRS	1	0
2	Н	201	TRS	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	172/209~(82%)	0.27	5 (2%) 51 41	17, 23, 45, 70	0
1	В	172/209~(82%)	0.23	3 (1%) 70 63	18, 24, 40, 76	0
1	С	169/209~(80%)	0.09	0 100 100	17, 24, 39, 64	0
1	D	172/209~(82%)	0.22	5 (2%) 51 41	18, 25, 46, 87	0
1	Е	169/209~(80%)	0.27	5 (2%) 50 40	17, 25, 44, 70	0
1	F	169/209~(80%)	0.40	7 (4%) 37 27	15, 24, 40, 61	0
1	G	172/209~(82%)	0.40	7 (4%) 37 27	16, 24, 45, 84	0
1	Н	169/209~(80%)	0.22	6 (3%) 42 32	17, 24, 41, 78	0
1	Ι	172/209~(82%)	0.39	7 (4%) 37 27	18, 24, 45, 77	0
1	J	169/209~(80%)	0.23	5 (2%) 50 40	18, 24, 40, 56	0
1	K	169/209~(80%)	0.20	3 (1%) 68 61	19, 24, 40, 57	0
1	L	172/209~(82%)	0.37	5 (2%) 51 41	19, 24, 47, 82	0
All	All	2046/2508~(81%)	0.27	58 (2%) 53 43	15, 24, 43, 87	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ε	93	TRP	3.9
1	А	14	GLN	3.8
1	Ι	90	CYS	3.7
1	Ι	91	ASP	3.6
1	G	102	CYS	3.6
1	В	90	CYS	3.4
1	G	90	CYS	3.2
1	F	102	CYS	3.1
1	Н	161	PRO	3.1
1	L	164	GLY	3.1
1	E	26	LEU	3.1



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Mol	Chain	Res	Type	RSRZ
1	Ι	164	GLY	3.1
1	G	165	LEU	3.0
1	Е	63	ARG	3.0
1	А	164	GLY	3.0
1	В	164	GLY	3.0
1	G	91	ASP	3.0
1	G	164	GLY	2.9
1	Ι	109	ASN	2.9
1	А	105	HIS	2.8
1	Е	6	SER	2.8
1	G	168	TYR	2.8
1	J	93	TRP	2.8
1	Н	93	TRP	2.8
1	Н	162	GLU	2.7
1	L	90	CYS	2.7
1	F	164	GLY	2.7
1	Н	6	SER	2.6
1	Κ	5	THR	2.6
1	D	93	TRP	2.6
1	J	5	THR	2.5
1	D	92	ASP	2.5
1	J	81	PHE	2.5
1	Е	113	SER	2.5
1	D	162	GLU	2.4
1	D	91	ASP	2.4
1	В	22	ARG	2.4
1	А	163	SER	2.4
1	F	63	ARG	2.4
1	Ι	81	PHE	2.3
1	Κ	6	SER	2.3
1	F	144	ALA	2.3
1	Н	14	GLN	2.3
1	D	90	CYS	2.3
1	Η	5	THR	2.2
1	F	113	SER	2.2
1	F	109	ASN	2.2
1	Κ	161	PRO	2.2
1	J	6	SER	2.2
1	L	89	ASP	2.2
1	L	109	ASN	2.2
1	F	81	PHE	2.2
1	Ι	154	ASN	2.2



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Mol	Chain	Res	Type	RSRZ
1	G	123	ASP	2.1
1	А	81	PHE	2.1
1	J	14	GLN	2.1
1	L	166	ALA	2.1
1	Ι	166	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	TRS	С	201	8/8	0.78	0.24	30,32,37,42	0
2	TRS	Ι	201	8/8	0.81	0.34	22,26,28,31	8
2	TRS	Н	201	8/8	0.85	0.34	23,30,33,34	8
2	TRS	Е	201	8/8	0.85	0.30	24,30,37,39	0
2	TRS	А	201	8/8	0.87	0.29	22,25,28,29	0
2	TRS	L	201	8/8	0.87	0.39	23,28,36,37	8
3	FE	Е	203	1/1	0.88	0.11	40,40,40,40	1
3	FE	J	201	1/1	0.90	0.13	15,15,15,15	0
3	FE	А	203	1/1	0.91	0.08	36,36,36,36	1
3	FE	С	203	1/1	0.91	0.12	42,42,42,42	1
3	FE	D	202	1/1	0.92	0.08	38,38,38,38	0
3	FE	Е	202	1/1	0.92	0.14	18,18,18,18	0
3	FE	Н	202	1/1	0.95	0.13	18,18,18,18	0
3	FE	Ι	202	1/1	0.96	0.11	7,7,7,7	0
3	FE	F	201	1/1	0.96	0.17	13,13,13,13	0
3	FE	K	201	1/1	0.96	0.11	16,16,16,16	0
3	FE	D	201	1/1	0.97	0.11	11,11,11,11	0
3	FE	G	201	1/1	0.97	0.19	25,25,25,25	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	FE	А	202	1/1	0.98	0.09	9,9,9,9	0
3	FE	С	202	1/1	0.99	0.05	9,9,9,9	0
3	FE	В	201	1/1	0.99	0.10	16, 16, 16, 16	0
3	FE	L	202	1/1	0.99	0.11	$15,\!15,\!15,\!15$	0

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6.5 Other polymers (i)

There are no such residues in this entry.

