

# Full wwPDB X-ray Structure Validation Report (i)

#### Jun 25, 2024 – 04:04 PM EDT

:	8SE7
:	HTRA-1 PDSA bound to CKP 1A8
:	Ultsch, M.H.; Kirchhofer, D.; Wei, Y.
:	2023-04-08
:	2.96  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
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.37.1
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)	:	2.37.1

# 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 2.96 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$	
$R_{free}$	130704	3104 (3.00-2.92)	
Clashscore	141614	3462 (3.00-2.92)	
Ramachandran outliers	138981	3340 (3.00-2.92)	
Sidechain outliers	138945	3343 (3.00-2.92)	
RSRZ outliers	127900	2986 (3.00-2.92)	

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	Δ	240	6%	110/ 100/			
1	11	240	%	1170 1070			
1	В	240	58%	20% • 21%			
1	С	240	5%	120/ 100/			
1	0	240	6%	13% •			
1	D	240	68%	11% 20%			
1	Б	0.40	10%				
	E	240	60%	12% 28%			



Mol	Chain	Length	Quality of chain		
1	F	240	73%	9%	18%
1	К	240	<sup>2%</sup> 69%	11% •	19%
1	L	240	66%	12% •	20%
1	М	240	64%	14%	22%
1	Q	240	68%	12%	20%
1	R	240	2% 68%	13%	20%
1	S	240	65%	14%	20%
2	G	40	78%	5%	• 15%
2	Н	40	72%	8% •	18%
2	Ι	40	65%	10% 5%	20%
2	J	40	70%	15%	15%
2	N	40	58%	25%	5% 12%
2	0	40	68%	15%	• 15%
2	Р	40	8% 62%	12%	25%
2	Т	40	5% 68%	5%	28%
2	U	40	70%	8% 5%	18%
2	V	40	78%	8%	6 15%
2	X	40	2% <b>8</b> 5%		5% • 8%
2	Y	40	78%	1	2% 10%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19018 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	А	196	Total C N O 1393 888 235 270	0	0	0
1	В	190	Total         C         N         O           1381         880         232         269	0	0	0
1	С	195	Total         C         N         O           1392         885         236         271	0	0	0
1	D	191	Total         C         N         O           1362         872         229         261	0	0	0
1	Е	173	Total         C         N         O           1169         739         200         230	0	0	0
1	F	197	Total C N O 1388 876 238 274	0	0	0
1	K	194	Total C N O 1377 877 226 274	0	1	0
1	L	191	Total         C         N         O         S           1369         870         231         267         1	0	0	0
1	М	188	Total         C         N         O           1307         830         220         257	0	0	0
1	Q	193	Total         C         N         O           1308         823         226         259	0	0	0
1	R	193	Total         C         N         O           1389         887         234         268	0	0	0
1	S	191	Total         C         N         O           1332         848         223         261	0	0	0

• Molecule 1 is a protein called Serine protease HTRA1.

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	140	MET	-	expression tag	UNP Q92743
А	141	GLY	-	expression tag	UNP Q92743
А	142	SER	-	expression tag	UNP Q92743
А	143	SER	-	expression tag	UNP Q92743
А	144	HIS	-	expression tag	UNP Q92743



Chain	Residue	Modelled	Actual	Comment	Reference
А	145	HIS	-	expression tag	UNP Q92743
А	146	HIS	-	expression tag	UNP Q92743
А	147	HIS	-	expression tag	UNP Q92743
А	148	HIS	-	expression tag	UNP Q92743
А	149	HIS	-	expression tag	UNP Q92743
А	150	SER	-	expression tag	UNP Q92743
А	151	SER	-	expression tag	UNP Q92743
А	152	GLY	-	expression tag	UNP Q92743
А	153	LEU	-	expression tag	UNP Q92743
А	154	VAL	-	expression tag	UNP Q92743
А	155	PRO	-	expression tag	UNP Q92743
А	156	ARG	-	expression tag	UNP Q92743
А	157	GLY	-	expression tag	UNP Q92743
А	158	SER	-	expression tag	UNP Q92743
А	159	HIS	-	expression tag	UNP Q92743
А	160	MET	-	expression tag	UNP Q92743
А	328	ALA	SER	engineered mutation	UNP Q92743
В	140	MET	-	expression tag	UNP Q92743
В	141	GLY	-	expression tag	UNP Q92743
В	142	SER	-	expression tag	UNP Q92743
В	143	SER	-	expression tag	UNP Q92743
В	144	HIS	-	expression tag	UNP Q92743
В	145	HIS	-	expression tag	UNP Q92743
В	146	HIS	-	expression tag	UNP Q92743
В	147	HIS	-	expression tag	UNP Q92743
В	148	HIS	-	expression tag	UNP Q92743
B	149	HIS	-	expression tag	UNP Q92743
B	150	SER	-	expression tag	UNP Q92743
B	151	SER	-	expression tag	UNP Q92743
B	152	GLY	-	expression tag	UNP Q92743
B	153	LEU	-	expression tag	UNP Q92743
B	154	VAL	-	expression tag	UNP Q92743
B	155	PRO	-	expression tag	UNP Q92743
B	156	ARG	-	expression tag	UNP Q92743
B	157	GLY	-	expression tag	UNP Q92743
B	158	SER	-	expression tag	UNP Q92743
B	159	HIS	-	expression tag	UNP Q92743
B	160	MET	-	expression tag	UNP Q92743
B	328	ALA	SER	engineered mutation	UNP Q92743
C	140	MET	-	expression tag	UNP Q92743
C	141	GLY	-	expression tag	UNP Q92743
C	142	SER	-	expression tag	UNP Q92743



Chain	Residue	Modelled	Actual	Comment	Reference
С	143	SER	-	expression tag	UNP Q92743
С	144	HIS	-	expression tag	UNP Q92743
С	145	HIS	-	expression tag	UNP Q92743
С	146	HIS	-	expression tag	UNP Q92743
С	147	HIS	-	expression tag	UNP Q92743
С	148	HIS	-	expression tag	UNP Q92743
С	149	HIS	-	expression tag	UNP Q92743
С	150	SER	-	expression tag	UNP Q92743
С	151	SER	-	expression tag	UNP Q92743
С	152	GLY	-	expression tag	UNP Q92743
С	153	LEU	-	expression tag	UNP Q92743
С	154	VAL	-	expression tag	UNP Q92743
С	155	PRO	-	expression tag	UNP Q92743
С	156	ARG	_	expression tag	UNP Q92743
С	157	GLY	_	expression tag	UNP Q92743
С	158	SER	-	expression tag	UNP Q92743
С	159	HIS	_	expression tag	UNP Q92743
С	160	MET	-	expression tag	UNP Q92743
С	328	ALA	SER	engineered mutation	UNP Q92743
D	140	MET	-	expression tag	UNP Q92743
D	141	GLY	-	expression tag	UNP Q92743
D	142	SER	-	expression tag	UNP Q92743
D	143	SER	-	expression tag	UNP Q92743
D	144	HIS	-	expression tag	UNP Q92743
D	145	HIS	-	expression tag	UNP Q92743
D	146	HIS	-	expression tag	UNP Q92743
D	147	HIS	-	expression tag	UNP Q92743
D	148	HIS	-	expression tag	UNP Q92743
D	149	HIS	_	expression tag	UNP Q92743
D	150	SER	_	expression tag	UNP Q92743
D	151	SER	_	expression tag	UNP Q92743
D	152	GLY	_	expression tag	UNP Q92743
D	153	LEU	_	expression tag	UNP Q92743
D	154	VAL	_	expression tag	UNP Q92743
D	155	PRO	_	expression tag	UNP Q92743
D	156	ARG	_	expression tag	UNP Q92743
D	157	GLY	_	expression tag	UNP Q92743
D	158	SER	_	expression tag	UNP Q92743
D	159	HIS	-	expression tag	UNP Q92743
D	160	MET	_	expression tag	UNP Q92743
D	328	ALA	SER	engineered mutation	UNP Q92743
E	140	MET	-	expression tag	UNP Q92743

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Reference
Е	141	GLY	-	expression tag	UNP Q92743
Е	142	SER	-	expression tag	UNP Q92743
Е	143	SER	-	expression tag	UNP Q92743
Е	144	HIS	-	expression tag	UNP Q92743
Е	145	HIS	-	expression tag	UNP Q92743
Е	146	HIS	-	expression tag	UNP Q92743
Е	147	HIS	-	expression tag	UNP Q92743
Е	148	HIS	-	expression tag	UNP Q92743
Е	149	HIS	-	expression tag	UNP Q92743
Е	150	SER	-	expression tag	UNP Q92743
Е	151	SER	-	expression tag	UNP Q92743
E	152	GLY	-	expression tag	UNP Q92743
E	153	LEU	-	expression tag	UNP Q92743
E	154	VAL	-	expression tag	UNP Q92743
E	155	PRO	-	expression tag	UNP Q92743
E	156	ARG	-	expression tag	UNP Q92743
E	157	GLY	-	expression tag	UNP Q92743
Ε	158	SER	-	expression tag	UNP Q92743
E	159	HIS	-	expression tag	UNP Q92743
Ε	160	MET	-	expression tag	UNP Q92743
E	328	ALA	SER	engineered mutation	UNP Q92743
F	140	MET	-	expression tag	UNP Q92743
F	141	GLY	-	expression tag	UNP Q92743
F	142	SER	-	expression tag	UNP Q92743
F	143	SER	-	expression tag	UNP Q92743
F	144	HIS	-	expression tag	UNP Q92743
F	145	HIS	-	expression tag	UNP Q92743
F	146	HIS	-	expression tag	UNP Q92743
F	147	HIS	-	expression tag	UNP Q92743
F	148	HIS	-	expression tag	UNP Q92743
F	149	HIS	-	expression tag	UNP Q92743
F	150	SER	-	expression tag	UNP Q92743
F	151	SER	-	expression tag	UNP Q92743
F	152	GLY	-	expression tag	UNP Q92743
F	153	LEU	-	expression tag	UNP Q92743
F	154	VAL	-	expression tag	UNP Q92743
F	155	PRO	-	expression tag	UNP Q92743
F	156	ARG	-	expression tag	UNP Q92743
F	157	GLY	-	expression tag	UNP Q92743
F	158	SER	-	expression tag	UNP Q92743
F	159	HIS	-	expression tag	UNP Q92743
F	160	MET	-	expression tag	UNP Q92743



Chain	Residue	Modelled	Actual	Comment	Reference
F	328	ALA	SER	engineered mutation	UNP Q92743
K	140	MET	-	expression tag	UNP Q92743
K	141	GLY	-	expression tag	UNP Q92743
K	142	SER	-	expression tag	UNP Q92743
K	143	SER	_	expression tag	UNP Q92743
K	144	HIS	-	expression tag	UNP Q92743
K	145	HIS	-	expression tag	UNP Q92743
K	146	HIS	-	expression tag	UNP Q92743
K	147	HIS	-	expression tag	UNP Q92743
K	148	HIS	-	expression tag	UNP Q92743
K	149	HIS	-	expression tag	UNP Q92743
K	150	SER	-	expression tag	UNP Q92743
K	151	SER	-	expression tag	UNP Q92743
K	152	GLY	-	expression tag	UNP Q92743
K	153	LEU	-	expression tag	UNP Q92743
K	154	VAL	-	expression tag	UNP Q92743
K	155	PRO	-	expression tag	UNP Q92743
K	156	ARG	-	expression tag	UNP Q92743
K	157	GLY	-	expression tag	UNP Q92743
K	158	SER	-	expression tag	UNP Q92743
K	159	HIS	-	expression tag	UNP Q92743
K	160	MET	-	expression tag	UNP Q92743
K	328	ALA	SER	engineered mutation	UNP Q92743
L	140	MET	-	expression tag	UNP Q92743
L	141	GLY	-	expression tag	UNP Q92743
L	142	SER	-	expression tag	UNP Q92743
L	143	SER	-	expression tag	UNP Q92743
L	144	HIS	-	expression tag	UNP Q92743
L	145	HIS	-	expression tag	UNP Q92743
L	146	HIS	-	expression tag	UNP Q92743
L	147	HIS	-	expression tag	UNP Q92743
L	148	HIS	-	expression tag	UNP Q92743
L	149	HIS	-	expression tag	UNP Q92743
L	150	SER	-	expression tag	UNP Q92743
L	151	SER	-	expression tag	UNP Q92743
	152	GLY	-	expression tag	UNP Q92743
	153	LEU	-	expression tag	UNP Q92743
L	154	VAL	-	expression tag	UNP Q92743
	155	PRO	-	expression tag	UNP Q92743
	156	ARG	-	expression tag	UNP Q92743
	157	GLY	-	expression tag	UNP Q92743
L	158	SER	-	expression tag	UNP Q92743



Chain	Residue	Modelled	Actual	Comment	Reference
L	159	HIS	-	expression tag	UNP Q92743
L	160	MET	-	expression tag	UNP Q92743
L	328	ALA	SER	engineered mutation	UNP Q92743
М	140	MET	-	expression tag	UNP Q92743
М	141	GLY	-	expression tag	UNP Q92743
М	142	SER	-	expression tag	UNP Q92743
М	143	SER	-	expression tag	UNP Q92743
М	144	HIS	-	expression tag	UNP Q92743
M	145	HIS	-	expression tag	UNP Q92743
М	146	HIS	-	expression tag	UNP Q92743
М	147	HIS	-	expression tag	UNP Q92743
М	148	HIS	-	expression tag	UNP Q92743
М	149	HIS	-	expression tag	UNP Q92743
М	150	SER	-	expression tag	UNP Q92743
М	151	SER	-	expression tag	UNP Q92743
M	152	GLY	-	expression tag	UNP Q92743
М	153	LEU	-	expression tag	UNP Q92743
М	154	VAL	-	expression tag	UNP Q92743
М	155	PRO	-	expression tag	UNP Q92743
М	156	ARG	-	expression tag	UNP Q92743
М	157	GLY	-	expression tag	UNP Q92743
М	158	SER	-	expression tag	UNP Q92743
М	159	HIS	-	expression tag	UNP Q92743
М	160	MET	-	expression tag	UNP Q92743
М	328	ALA	SER	engineered mutation	UNP Q92743
Q	140	MET	-	expression tag	UNP Q92743
Q	141	GLY	-	expression tag	UNP Q92743
Q	142	SER	-	expression tag	UNP Q92743
Q	143	SER	-	expression tag	UNP Q92743
Q	144	HIS	-	expression tag	UNP Q92743
Q	145	HIS	-	expression tag	UNP Q92743
Q	146	HIS	-	expression tag	UNP Q92743
Q	147	HIS	-	expression tag	UNP Q92743
Q	148	HIS	-	expression tag	UNP Q92743
Q	149	HIS	-	expression tag	UNP Q92743
Q	150	SER	-	expression tag	UNP $Q9\overline{2743}$
Q	151	SER	-	expression tag	UNP Q92743
Q	152	GLY	-	expression tag	UNP Q92743
Q	153	LEU	-	expression tag	UNP Q92743
Q	154	VAL	-	expression tag	UNP Q92743
Q	155	PRO	-	expression tag	UNP Q92743
Q	156	ARG	-	expression tag	UNP Q92743

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Reference
Q	157	GLY	-	expression tag	UNP Q92743
Q	158	SER	-	expression tag	UNP Q92743
Q	159	HIS	-	expression tag	UNP Q92743
Q	160	MET	-	expression tag	UNP Q92743
Q	328	ALA	SER	engineered mutation	UNP Q92743
R	140	MET	-	expression tag	UNP Q92743
R	141	GLY	-	expression tag	UNP Q92743
R	142	SER	-	expression tag	UNP Q92743
R	143	SER	-	expression tag	UNP Q92743
R	144	HIS	-	expression tag	UNP Q92743
R	145	HIS	-	expression tag	UNP Q92743
R	146	HIS	-	expression tag	UNP Q92743
R	147	HIS	-	expression tag	UNP Q92743
R	148	HIS	-	expression tag	UNP Q92743
R	149	HIS	-	expression tag	UNP Q92743
R	150	SER	-	expression tag	UNP Q92743
R	151	SER	-	expression tag	UNP Q92743
R	152	GLY	-	expression tag	UNP Q92743
R	153	LEU	-	expression tag	UNP Q92743
R	154	VAL	-	expression tag	UNP Q92743
R	155	PRO	-	expression tag	UNP Q92743
R	156	ARG	-	expression tag	UNP Q92743
R	157	GLY	-	expression tag	UNP Q92743
R	158	SER	-	expression tag	UNP Q92743
R	159	HIS	-	expression tag	UNP Q92743
R	160	MET	-	expression tag	UNP Q92743
R	328	ALA	SER	engineered mutation	UNP Q92743
S	140	MET	-	expression tag	UNP Q92743
S	141	GLY	-	expression tag	UNP Q92743
S	142	SER	-	expression tag	UNP Q92743
S	143	SER	-	expression tag	UNP Q92743
S	144	HIS	-	expression tag	UNP Q92743
S	145	HIS	-	expression tag	UNP Q92743
S	146	HIS	-	expression tag	UNP Q92743
S	147	HIS	-	expression tag	UNP Q92743
S	148	HIS	-	expression tag	UNP Q92743
S	149	HIS	-	expression tag	UNP Q92743
S	150	SER	-	expression tag	UNP Q92743
S	151	SER	-	expression tag	UNP Q92743
S	152	GLY	-	expression tag	UNP Q92743
S	153	LEU	-	expression tag	UNP Q92743
S	154	VAL	-	expression tag	UNP Q92743

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Reference
S	155	PRO	-	expression tag	UNP Q92743
S	156	ARG	-	expression tag	UNP Q92743
S	157	GLY	-	expression tag	UNP Q92743
S	158	SER	-	expression tag	UNP Q92743
S	159	HIS	-	expression tag	UNP Q92743
S	160	MET	-	expression tag	UNP Q92743
S	328	ALA	SER	engineered mutation	UNP Q92743

Continued from previous page...

• Molecule 2 is a protein called Cysteine knot peptide.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace	
0	т	20	Total	С	Ν	Ο	S	0	0	0	
	1	52	212	127	37	42	6	0	0	0	
9	v	37	Total	С	Ν	Ο	S	0	0	0	
	Λ	51	277	174	46	51	6	0	0	0	
2	v	36	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
2	L	50	260	159	46	49	6	0	0	0	
2	G	34	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
	u	04	240	147	43	44	6	0	0	0	
2	н	33	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
	11		226	139	38	43	6	0			
2	Т	34	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0	
	0	, v	04	249	159	40	44	6	0	0	0
2	N	35	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
			267	168	45	48	6	0	0	0	
2	0	34	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
			245	152	42	45	6	0	0	0	
2	Р	30	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
	1	50	195	118	33	38	6	0	0	0	
2	Т	29	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0	
		25	197	119	34	38	6	0	0	0	
2 II	U	33	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0	
	Ŭ	00	233	142	39	46	6		0	U U	
2	V	34	Total	$\mathbf{C}$	Ν	Ο	S	0	0	0	
	v	94	243	153	40	44	6		U	U	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	О	1	Total O 1 1	0	0
3	Q	1	Total O 1 1	0	0
3	R	2	Total O 2 2	0	0
3	U	1	Total O 1 1	0	0



# 3 Residue-property plots (i)

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



• Molecule 1: Serine protease HTRA1



















## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	116.03Å 152.72Å 165.85Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(Å)	54.23 - 2.96	Depositor
Resolution (A)	54.23 - 2.96	EDS
% Data completeness	77.6 (54.23-2.96)	Depositor
(in resolution range)	77.6 (54.23-2.96)	EDS
R <sub>merge</sub>	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.29 (at 2.96 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D .	0.270 , $0.296$	Depositor
$\Lambda, \Lambda_{free}$	0.271 , $0.295$	DCC
$R_{free}$ test set	1990 reflections $(4.15\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	86.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.26 , $43.6$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	19018	wwPDB-VP
Average B, all atoms $(Å^2)$	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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

Mol Chain		Bond	lengths	Bond angles	
IVIOI	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/1416	0.45	0/1937
1	В	0.25	0/1404	0.48	0/1919
1	С	0.25	0/1414	0.48	0/1932
1	D	0.24	0/1385	0.47	0/1895
1	Ε	0.24	0/1182	0.47	0/1616
1	F	0.25	0/1409	0.47	0/1929
1	Κ	0.25	0/1398	0.47	0/1917
1	L	0.24	0/1391	0.48	0/1904
1	М	0.24	0/1325	0.47	0/1811
1	Q	0.24	0/1325	0.47	0/1820
1	R	0.24	0/1413	0.47	0/1933
1	S	0.24	0/1351	0.46	0/1848
2	G	0.25	0/248	0.51	0/340
2	Н	0.27	0/234	0.48	0/321
2	Ι	0.26	0/218	0.43	0/299
2	J	0.24	0/260	0.45	0/359
2	Ν	0.38	0/278	0.46	0/382
2	0	0.28	0/254	0.52	0/347
2	Р	0.24	0/200	0.49	0/274
2	Т	0.25	0/202	0.42	0/276
2	U	0.24	0/241	0.48	0/331
2	V	0.23	0/253	0.45	0/350
2	Х	0.24	0/288	0.49	0/396
2	Y	0.24	0/268	0.50	0/368
All	All	0.25	0/19357	0.47	0/26504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1393	0	1303	16	0
1	В	1381	0	1329	26	0
1	С	1392	0	1326	20	0
1	D	1362	0	1279	13	0
1	Е	1169	0	1065	14	0
1	F	1388	0	1297	11	0
1	Κ	1377	0	1296	18	0
1	L	1369	0	1287	17	0
1	М	1307	0	1223	22	0
1	Q	1308	0	1174	15	0
1	R	1389	0	1320	17	0
1	S	1332	0	1235	20	0
2	G	240	0	184	1	0
2	Н	226	0	162	2	0
2	Ι	212	0	152	3	0
2	J	249	0	187	3	0
2	N	267	0	214	6	0
2	0	245	0	187	3	0
2	Р	195	0	127	4	0
2	Т	197	0	138	1	0
2	U	233	0	176	2	0
2	V	243	0	180	2	0
2	Х	277	0	222	2	0
2	Y	260	0	204	3	0
3	В	1	0	0	0	0
3	D	1	0	0	0	0
3	0	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	2	0	0	0	0
3	U	1	0	0	0	0
All	All	19018	0	$17\overline{267}$	213	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 6.

All (213) 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 $(\text{\AA})$	overlap (Å)	
1:L:258:HIS:HB3	1:L:262:LEU:HD11	1.70	0.73	
1:B:171:PHE:HB2	1:C:165:LEU:HD21	1.72	0.70	
1:M:188:LEU:HD11	1:M:221:VAL:HG23	1.73	0.69	
1:D:214:LEU:HD22	1:D:253:LEU:HD21	1.75	0.67	
1:C:246:ASP:HB3	1:C:251:ILE:HG22	1.78	0.66	
1:L:231:GLU:HG2	1:L:237:THR:HG22	1.77	0.66	
1:L:188:LEU:HB2	1:L:202:ALA:HB3	1.77	0.65	
1:M:344:THR:HG21	1:M:355:ILE:HG12	1.78	0.65	
1:D:186:ILE:HG12	1:D:230:VAL:HG12	1.79	0.65	
1:S:231:GLU:HG2	1:S:237:THR:HG22	1.79	0.64	
1:B:282:ILE:HG13	1:B:292:VAL:HG22	1.81	0.63	
1:Q:214:LEU:HB3	1:Q:253:LEU:HD11	1.80	0.63	
1:C:193:PRO:HB2	1:M:223:THR:HA	1.79	0.63	
1:K:219:ALA:HA	1:K:252:ALA:HB2	1.80	0.63	
1:C:318:GLN:HB3	1:C:351:ILE:HD11	1.80	0.63	
1:F:231:GLU:HG2	1:F:237:THR:HG22	1.81	0.63	
1:D:357:SER:HA	1:D:360:ILE:HD12	1.80	0.62	
1:F:188:LEU:HD12	1:F:202:ALA:HB3	1.82	0.62	
2:Y:5:ILE:HD12	2:Y:19:ALA:HB2	1.81	0.61	
1:D:219:ALA:HA	1:D:252:ALA:HB2	1.81	0.61	
1:L:282:ILE:HG13	1:L:292:VAL:HG22	1.83	0.61	
2:N:3:ASP:OD1	2:N:3:ASP:N	2.34	0.60	
1:M:219:ALA:HA	1:M:252:ALA:HB2	1.83	0.59	
1:C:193:PRO:HG3	1:M:225:LYS:HE2	1.84	0.59	
1:C:282:ILE:HG13	1:C:292:VAL:HG22	1.84	0.59	
1:A:214:LEU:HB3	1:A:253:LEU:HD11	1.83	0.59	
2:0:10:CYS:SG	2:O:11:LYS:N	2.76	0.59	
1:Q:240:ALA:HB2	1:Q:256:ILE:HG23	1.85	0.58	
2:T:10:CYS:SG	2:T:11:LYS:N	2.76	0.58	
1:A:186:ILE:HG12	1:A:230:VAL:HG12	1.86	0.58	
1:F:219:ALA:HA	1:F:252:ALA:HB2	1.85	0.58	
2:X:10:CYS:SG	2:X:11:LYS:N	2.77	0.58	
1:D:230:VAL:HG21	1:D:256:ILE:HG21	1.86	0.57	
2:U:10:CYS:SG	2:U:11:LYS:N	2.76	0.57	
1:R:188:LEU:HB2	1:R:202:ALA:HB3	1.86	0.57	
1:B:262:LEU:HD12	1:B:263:PRO:HD2	1.86	0.57	
1:D:282:ILE:HG13	1:D:292:VAL:HG22	1.86	0.57	
1:R:282:ILE:HG13	1:R:292:VAL:HG22	1.86	0.57	
1:A:219:ALA:HA	1:A:252:ALA:HB2	1.85	0.57	
1:M:217:THR:OG1	1:M:218:ASN:N	2.37	0.56	
1:Q:219:ALA:HA	1:Q:252:ALA:HB2	1.88	0.56	
1:Q:242:ILE:HA	1:Q:254:ILE:HG22	1.88	0.56	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:S:348:THR:HG1	1:S:350:GLY:N	2.04	0.56
1:B:333:VAL:HG12	1:B:339:VAL:HA	1.89	0.55
2:O:24:THR:HG22	2:O:35:GLY:HA2	1.88	0.55
1:R:256:ILE:HD11	1:R:262:LEU:HD11	1.90	0.54
2:I:6:CYS:N	2:I:22:CYS:SG	2.81	0.54
2:I:10:CYS:SG	2:I:11:LYS:N	2.81	0.54
2:H:10:CYS:SG	2:H:11:LYS:N	2.81	0.54
1:K:165:LEU:HD21	1:M:171:PHE:HB2	1.89	0.54
1:R:267:LEU:HD23	1:R:339:VAL:HB	1.88	0.54
1:B:188:LEU:HB2	1:B:202:ALA:HB3	1.90	0.54
1:C:195:SER:OG	1:C:196:LYS:N	2.37	0.54
1:E:242:ILE:HA	1:E:254:ILE:HG22	1.90	0.53
1:E:270:SER:HB2	1:E:317:ILE:HD11	1.89	0.53
2:J:5:ILE:HD12	2:J:19:ALA:HB2	1.89	0.53
1:R:219:ALA:HA	1:R:252:ALA:HB2	1.91	0.53
2:G:10:CYS:SG	2:G:11:LYS:N	2.82	0.53
1:S:188:LEU:HD11	1:S:221:VAL:HG23	1.89	0.53
1:S:219:ALA:HA	1:S:252:ALA:HB2	1.91	0.53
1:A:163:ASN:OD1	1:A:164:SER:N	2.38	0.52
1:B:219:ALA:HA	1:B:252:ALA:HB2	1.91	0.52
1:L:186:ILE:HG13	1:L:230:VAL:HG22	1.92	0.52
1:A:184:VAL:HG21	1:A:215:ILE:HD13	1.91	0.52
1:E:322:ILE:O	1:E:327:ASN:ND2	2.43	0.52
1:E:342:ILE:HG23	1:E:355:ILE:HB	1.92	0.52
1:Q:323:ILE:HD12	1:Q:352:SER:HB3	1.91	0.52
2:O:23:GLN:H	2:O:35:GLY:HA3	1.74	0.52
1:Q:282:ILE:HG13	1:Q:292:VAL:HG22	1.91	0.52
1:D:192:LEU:N	1:D:197:ARG:O	2.38	0.51
1:M:282:ILE:HG13	1:M:292:VAL:HG22	1.91	0.51
1:R:232:LEU:HD12	1:R:236:ALA:HB3	1.92	0.51
1:R:274:ARG:NH1	1:S:174:ASP:OD1	2.38	0.51
1:L:223:THR:HA	1:R:193:PRO:HG3	1.93	0.51
1:A:262:LEU:HD12	1:A:263:PRO:HD2	1.92	0.51
1:A:317:ILE:HG13	1:A:356:PRO:HG3	1.92	0.51
1:B:189:PHE:HA	1:B:201:VAL:HG13	1.93	0.51
1:C:192:LEU:HD13	1:M:247:GLU:HG3	1.92	0.51
1:E:319:THR:O	1:E:352:SER:OG	2.24	0.51
1:R:171:PHE:HB2	1:S:165:LEU:HD23	1.93	0.50
1:S:282:ILE:HG13	1:S:292:VAL:HG22	1.93	0.50
1:F:255:LYS:NZ	1:F:257:ASP:OD1	2.43	0.50
2:N:10:CYS:SG	2:N:11:LYS:N	2.84	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:166:ARG:HD2	1:M:336:ASP:HB2	1.94	0.50
1:K:222:VAL:HA	1:K:242:ILE:HD13	1.94	0.49
1:D:273:LEU:HD21	1:D:340:ILE:HG21	1.94	0.49
1:Q:317:ILE:HG12	1:Q:356:PRO:HG3	1.95	0.49
1:Q:166:ARG:O	1:Q:170:ASN:ND2	2.39	0.49
1:K:267:LEU:HD23	1:K:339:VAL:HB	1.95	0.49
1:C:208:ILE:HD13	1:C:262:LEU:HD13	1.94	0.49
2:P:22:CYS:HA	2:P:34:TRP:HA	1.95	0.48
1:E:342:ILE:HG22	1:E:360:ILE:HD11	1.95	0.48
1:A:286:PHE:HZ	2:I:35:GLY:HA2	1.78	0.48
1:S:270:SER:HB2	1:S:317:ILE:HD11	1.96	0.48
1:L:222:VAL:HG21	1:L:245:VAL:HG21	1.96	0.48
1:C:243:LYS:HD2	1:C:255:LYS:HB2	1.95	0.48
1:K:357:SER:HA	1:K:360:ILE:HD12	1.96	0.48
1:M:218:ASN:O	1:M:221:VAL:HG12	2.13	0.48
1:C:188:LEU:HD12	1:C:202:ALA:HB3	1.95	0.47
1:K:282:ILE:HG13	1:K:292:VAL:HG22	1.96	0.47
1:A:323:ILE:HD12	1:A:352:SER:HB3	1.95	0.47
2:N:24:THR:OG1	2:N:37:ARG:NH1	2.47	0.47
1:A:230:VAL:HG21	1:A:256:ILE:HG21	1.97	0.47
1:E:219:ALA:HA	1:E:252:ALA:HB2	1.96	0.47
1:R:258:HIS:CD2	1:R:260:GLY:H	2.33	0.47
1:F:273:LEU:HD11	1:F:340:ILE:HD12	1.97	0.47
1:S:258:HIS:CG	1:S:259:GLN:N	2.83	0.47
1:M:317:ILE:HG12	1:M:356:PRO:HG3	1.97	0.47
1:D:334:ASN:HD21	1:D:338:GLU:HB2	1.80	0.46
1:S:286:PHE:HZ	2:V:35:GLY:HA2	1.79	0.46
1:B:344:THR:HG21	1:B:355:ILE:HG12	1.98	0.46
1:B:357:SER:O	1:B:361:LYS:HG2	2.14	0.46
1:B:189:PHE:O	1:B:227:ARG:HB2	2.16	0.46
1:B:349:ALA:C	1:B:351:ILE:H	2.18	0.46
1:M:189:PHE:O	1:M:227:ARG:CB	2.63	0.46
1:K:277:GLU:OE2	1:L:166:ARG:NE	2.49	0.46
1:C:176:VAL:HG21	1:C:292:VAL:HG11	1.98	0.46
1:F:180:ALA:O	1:F:183:VAL:HG22	2.16	0.46
1:M:244:ASP:OD1	1:M:245:VAL:N	2.49	0.46
1:F:176:VAL:HG21	1:F:292:VAL:HG21	1.98	0.46
2:N:5:ILE:HB	2:N:19:ALA:HB2	1.98	0.46
1:Q:166:ARG:NE	1:S:277:GLU:OE2	2.48	0.46
1:D:346:LYS:HB2	1:D:353:PHE:HD2	1.81	0.45
1:S:242:ILE:HG13	1:S:254:ILE:HG22	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:328:ALA:HB2	1:C:345:LEU:HD12	1.98	0.45
1:E:330:GLY:O	1:E:343:ASN:ND2	2.50	0.45
1:L:219:ALA:HA	1:L:252:ALA:HB2	1.99	0.45
1:E:333:VAL:HG22	1:E:339:VAL:HA	1.99	0.45
1:B:334:ASN:HD21	1:B:338:GLU:HB2	1.82	0.45
1:M:253:LEU:HB2	1:M:363:PHE:HE2	1.81	0.45
1:R:210:SER:OG	1:R:212:ASP:OD1	2.21	0.44
1:B:214:LEU:HB3	1:B:253:LEU:HD11	1.98	0.44
1:C:214:LEU:HB3	1:C:253:LEU:HD11	1.98	0.44
1:C:273:LEU:HD11	1:C:340:ILE:HD12	1.99	0.44
1:K:188:LEU:O	1:K:201:VAL:HG22	2.18	0.44
1:S:273:LEU:HD21	1:S:340:ILE:HG21	1.98	0.44
1:L:283:GLY:HA3	1:L:326:GLY:O	2.18	0.44
1:Q:296:ILE:HD13	1:R:294:THR:HB	1.99	0.44
1:B:258:HIS:CD2	1:B:262:LEU:HD13	2.53	0.43
1:E:182:ALA:HB3	1:E:265:LEU:HG	1.99	0.43
1:L:267:LEU:HD23	1:L:339:VAL:HB	2.00	0.43
1:M:220:HIS:HB3	2:P:30:TRP:NE1	2.33	0.43
1:M:334:ASN:HD21	1:M:338:GLU:HB2	1.84	0.43
1:B:323:ILE:HG22	1:B:345:LEU:HD12	2.01	0.43
1:M:267:LEU:HD23	1:M:339:VAL:HB	2.00	0.43
1:Q:294:THR:HB	1:S:296:ILE:HD13	1.98	0.43
1:S:242:ILE:HA	1:S:254:ILE:HG22	1.99	0.43
1:E:208:ILE:HG12	1:E:215:ILE:HD12	1.99	0.43
1:B:299:THR:HG22	1:B:318:GLN:HB2	2.01	0.43
1:C:163:ASN:OD1	1:C:163:ASN:N	2.40	0.43
1:D:299:THR:HG22	1:D:318:GLN:HB2	1.99	0.43
1:R:283:GLY:HA3	1:R:326:GLY:O	2.19	0.43
1:S:348:THR:OG1	1:S:350:GLY:N	2.52	0.43
1:B:345:LEU:O	1:B:347:VAL:N	2.52	0.43
1:D:323:ILE:HD12	1:D:352:SER:HB3	2.01	0.43
1:E:267:LEU:HD23	1:E:339:VAL:HB	2.01	0.43
2:H:14:ASP:OD1	2:H:14:ASP:N	2.50	0.43
1:L:185:HIS:CE1	1:L:187:GLU:HG2	2.53	0.43
1:M:208:ILE:HD13	1:M:262:LEU:HD23	2.01	0.43
1:B:244:ASP:OD1	1:B:245:VAL:N	2.52	0.42
1:R:360:ILE:O	1:R:364:LEU:HG	2.19	0.42
1:B:218:ASN:ND2	1:B:250:ASP:OD2	2.52	0.42
1:L:201:VAL:HG21	1:L:226:HIS:ND1	2.35	0.42
2:Y:24:THR:OG1	2:Y:35:GLY:HA3	2.20	0.42
1:S:246:ASP:HB3	1:S:251:ILE:HG13	2.02	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:K:188:LEU:HB2	1:K:202:ALA:HB3	2.01	0.42	
1:K:351:ILE:HD13	1:K:351:ILE:HA	1.96	0.42	
1:Q:165:LEU:HD22	1:S:335:LEU:HB3	2.01	0.42	
1:Q:259:GLN:O	1:Q:262:LEU:HG	2.19	0.42	
1:A:333:VAL:HG22	1:A:339:VAL:HA	2.01	0.42	
1:B:182:ALA:HB3	1:B:265:LEU:HG	2.00	0.42	
1:C:219:ALA:HA	1:C:252:ALA:HB2	2.00	0.42	
1:E:277:GLU:OE2	1:F:166:ARG:NH1	2.53	0.42	
1:A:323:ILE:HD13	1:A:343:ASN:HB3	2.02	0.42	
1:K:295:GLY:HA3	1:K:321:ALA:HB2	2.02	0.42	
1:K:296:ILE:HD13	1:L:294:THR:HB	2.02	0.42	
1:Q:211:GLU:HA	1:Q:262:LEU:HB2	2.02	0.42	
2:U:23:GLN:HB3	2:U:36:LEU:HA	2.02	0.42	
1:C:203:SER:O	2:Y:26:TYR:HA	2.20	0.42	
1:B:273:LEU:HD21	1:B:340:ILE:HG21	2.02	0.41	
1:D:208:ILE:HG12	1:D:215:ILE:HG12	2.02	0.41	
1:K:327:ASN:HB3	1:K:343:ASN:ND2	2.35	0.41	
1:Q:190:ARG:O	1:Q:199:VAL:N	2.53	0.41	
1:B:246:ASP:HB3	1:B:251:ILE:HG22	2.02	0.41	
1:F:235:GLY:HA2	1:F:288:LEU:HD11	2.03	0.41	
1:R:273:LEU:HD21	1:R:340:ILE:HG21	2.01	0.41	
1:K:217:THR:OG1	1:K:218:ASN:N	2.54	0.41	
2:X:3:ASP:OD1	2:X:3:ASP:N	2.48	0.41	
2:J:13:HIS:CE1	2:J:25:CYS:H	2.38	0.41	
1:L:222:VAL:HG12	1:L:242:ILE:HG12	2.03	0.41	
1:M:221:VAL:HB	2:P:27:TYR:CE1	2.56	0.41	
1:A:327:ASN:HB3	1:A:343:ASN:ND2	2.36	0.41	
1:F:220:HIS:HB3	2:J:30:TRP:HE1	1.86	0.41	
1:L:190:ARG:O	1:L:198:GLU:HA	2.21	0.41	
1:K:204:GLY:HA3	2:N:27:TYR:CZ	2.55	0.41	
1:S:332:LEU:HB2	1:S:343:ASN:OD1	2.20	0.41	
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.92	0.41	
1:A:334:ASN:HD21	1:A:338:GLU:HB2	1.86	0.41	
1:C:244:ASP:OD1	1:C:245:VAL:N	2.54	0.41	
1:L:217:THR:OG1	1:L:218:ASN:N	2.54	0.41	
1:B:281:ALA:O	1:B:327:ASN:ND2	2.54	0.40	
1:M:203:SER:O	2:P:26:TYR:HA	2.21	0.40	
2:V:24:THR:HB	2:V:26:TYR:CE2	2.56	0.40	
1:A:296:ILE:HD13	1:B:294:THR:HB	2.02	0.40	
1:B:296:ILE:HD13	1:C:294:THR:HB	2.03	0.40	
1:E:280:VAL:HG13	1:E:292:VAL:HG23	2.04	0.40	



8SE7
------

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:LEU:HD22	1:M:335:LEU:HB3	2.04	0.40
1:K:201:VAL:HB	2:N:12:THR:HG23	2.02	0.40
1:R:265:LEU:HB3	1:R:339:VAL:HG23	2.04	0.40
1:B:283:GLY:HA3	1:B:326:GLY:O	2.21	0.40
1:F:332:LEU:HB2	1:F:343:ASN:OD1	2.22	0.40
1:R:281:ALA:O	1:R:327:ASN:ND2	2.55	0.40
1:S:323:ILE:HD12	1:S:352:SER:HB3	2.03	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	ntiles
1	А	188/240~(78%)	180 (96%)	7 (4%)	1 (0%)	29	64
1	В	184/240~(77%)	170 (92%)	12 (6%)	2 (1%)	14	46
1	С	191/240~(80%)	179 (94%)	11 (6%)	1 (0%)	29	64
1	D	185/240~(77%)	180 (97%)	4 (2%)	1 (0%)	29	64
1	Е	163/240~(68%)	158 (97%)	5 (3%)	0	100	100
1	F	193/240~(80%)	185 (96%)	8 (4%)	0	100	100
1	Κ	191/240~(80%)	186 (97%)	4 (2%)	1 (0%)	29	64
1	L	185/240~(77%)	177 (96%)	6 (3%)	2 (1%)	14	46
1	М	182/240~(76%)	176 (97%)	6 (3%)	0	100	100
1	Q	185/240~(77%)	177 (96%)	8 (4%)	0	100	100
1	R	187/240~(78%)	185 (99%)	2 (1%)	0	100	100
1	S	183/240~(76%)	174 (95%)	8 (4%)	1 (0%)	29	64
2	G	32/40~(80%)	27 (84%)	5 (16%)	0	100	100
2	Н	31/40~(78%)	26 (84%)	5 (16%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Ι	30/40~(75%)	26~(87%)	4 (13%)	0	100 100
2	J	32/40~(80%)	29 (91%)	3~(9%)	0	100 100
2	Ν	33/40~(82%)	28 (85%)	5 (15%)	0	100 100
2	Ο	32/40~(80%)	27 (84%)	5 (16%)	0	100 100
2	Р	26/40~(65%)	23~(88%)	3 (12%)	0	100 100
2	Т	25/40~(62%)	23~(92%)	2 (8%)	0	100 100
2	U	31/40 (78%)	30~(97%)	1 (3%)	0	100 100
2	V	32/40~(80%)	27 (84%)	5 (16%)	0	100 100
2	Х	35/40~(88%)	32 (91%)	3~(9%)	0	100 100
2	Y	34/40~(85%)	28 (82%)	6 (18%)	0	100 100
All	All	2590/3360~(77%)	2453 (95%)	128 (5%)	9~(0%)	41 73

All (9) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	В	346	LYS
1	D	328	ALA
1	Κ	328	ALA
1	S	347	VAL
1	С	196	LYS
1	В	163	ASN
1	А	328	ALA
1	L	165	LEU
1	L	198	GLU

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	138/202~(68%)	138 (100%)	0	100	100
1	В	143/202~(71%)	139~(97%)	4(3%)	43	74

Continued on next page...



Rotameric

Outliers

Percentiles

Continued from previous page...MolChainAnalysed

1	С	139/202~(69%)	134~(96%)	5(4%)	35	67
1	D	134/202~(66%)	133 (99%)	1 (1%)	84	93
1	Е	107/202~(53%)	103 (96%)	4 (4%)	34	66
1	F	137/202~(68%)	135 (98%)	2 (2%)	65	85
1	Κ	137/202~(68%)	133~(97%)	4 (3%)	42	73
1	L	138/202~(68%)	134~(97%)	4 (3%)	42	73
1	М	126/202~(62%)	123~(98%)	3~(2%)	49	77
1	Q	121/202~(60%)	114 (94%)	7~(6%)	20	51
1	R	141/202~(70%)	139~(99%)	2(1%)	67	86
1	S	128/202~(63%)	125~(98%)	3~(2%)	50	78
2	G	22/34~(65%)	20~(91%)	2 (9%)	9	31
2	Η	20/34~(59%)	18 (90%)	2(10%)	7	26
2	Ι	19/34~(56%)	16~(84%)	3~(16%)	2	10
2	J	23/34~(68%)	22~(96%)	1 (4%)	29	62
2	Ν	27/34~(79%)	22 (82%)	5(18%)	1	7
2	Ο	23/34~(68%)	20~(87%)	3(13%)	4	16
2	Р	16/34~(47%)	16 (100%)	0	100	100
2	Т	18/34~(53%)	18 (100%)	0	100	100
2	U	23/34~(68%)	20~(87%)	3~(13%)	4	16
2	V	22/34~(65%)	22~(100%)	0	100	100
2	Х	27/34~(79%)	26~(96%)	1 (4%)	34	66
2	Y	25/34 (74%)	$25 \ (100\%)$	0	100	100
All	All	1854/2832 (66%)	1795 (97%)	59 (3%)	39	71

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	166	ARG
1	В	201	VAL
1	В	209	VAL
1	В	346	LYS
1	С	161	ASP
1	С	163	ASN
1	С	212	ASP



Mol	Chain	Res	Type
1	С	345	LEU
1	С	352	SER
2	Ι	10	CYS
2	Ι	16	CYS
2	Ι	22	CYS
2	Х	10	CYS
1	D	315	ASP
1	Е	166	ARG
1	Е	256	ILE
1	Е	344	THR
1	Е	351	ILE
1	F	212	ASP
1	F	364	LEU
2	G	10	CYS
2	G	37	ARG
2	Н	10	CYS
2	Н	36	LEU
2	J	20	TRP
1	K	165	LEU
1	Κ	166	ARG
1	Κ	299	THR
1	K	333	VAL
1	L	166	ARG
1	L	201	VAL
1	L	209	VAL
1	L	347	VAL
1	М	209	VAL
1	М	217	THR
1	М	297	VAL
2	N	3	ASP
2	N	6	CYS
2	N	10	CYS
2	N	23	GLN
2	N	29	THR
2	0	10	CYS
2	Ō	29	THR
2	0	36	LEU
1	Q	161	ASP
1	Q	201	VAL
1	Q	209	VAL
1	Q	245	VAL
1	Q	256	ILE



Mol	Chain	Res	Type
1	Q	299	THR
1	Q	362	LYS
1	R	209	VAL
1	R	336	ASP
1	S	187	GLU
1	S	209	VAL
1	S	299	THR
2	U	10	CYS
2	U	13	HIS
2	U	36	LEU

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

Mol	Chain	Res	Type
2	Ν	23	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)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.



### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	$\# RSRZ {>}2$	$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	196/240~(81%)	0.48	14 (7%) 16 9	49, 82, 117, 170	0
1	В	190/240~(79%)	0.37	3 (1%) 72 55	46, 63, 92, 115	0
1	С	195/240~(81%)	0.37	12 (6%) 20 12	51, 71, 100, 112	0
1	D	191/240~(79%)	0.42	14 (7%) 15 8	65, 86, 113, 145	0
1	Ε	173/240~(72%)	0.69	24 (13%) 2 1	77,105,133,146	0
1	F	197/240~(82%)	0.23	5 (2%) 57 40	54, 73, 98, 132	0
1	K	194/240~(80%)	0.22	5 (2%) 56 39	56, 72, 98, 118	0
1	L	191/240~(79%)	0.49	17 (8%) 9 5	62, 82, 109, 150	0
1	М	188/240~(78%)	0.46	18 (9%) 8 4	69, 88, 110, 120	0
1	Q	193/240~(80%)	0.67	25 (12%) 3 2	67, 101, 145, 198	0
1	R	193/240~(80%)	0.27	6 (3%) 49 32	60, 77, 104, 125	0
1	S	191/240~(79%)	0.36	13 (6%) 17 10	71, 87, 108, 121	0
2	G	34/40~(85%)	0.27	1 (2%) 51 35	87, 108, 121, 125	0
2	Н	33/40~(82%)	0.16	0 100 100	101, 117, 125, 129	0
2	Ι	32/40~(80%)	0.29	2 (6%) 20 11	96, 120, 141, 145	0
2	J	34/40~(85%)	0.21	3 (8%) 10 5	80, 106, 124, 131	0
2	Ν	35/40~(87%)	-0.01	2 (5%) 23 14	76, 91, 107, 111	0
2	Ο	34/40~(85%)	0.50	6 (17%) 1 1	87, 109, 116, 118	0
2	Р	30/40~(75%)	0.53	3 (10%) 7 4	102, 138, 159, 163	0
2	Т	29/40~(72%)	1.09	2 (6%) 16 10	120, 146, 152, 157	0
2	U	33/40~(82%)	-0.14	0 100 100	71, 90, 103, 105	0
2	V	34/40 (85%)	0.15	2 (5%) 22 13	86, 96, 109, 119	0
2	X	$37/40\ \overline{(92\%)}$	0.17	1 (2%) 54 38	$67, 88, \overline{108, 114}$	0
2	Y	36/40~(90%)	0.20	2 (5%) 24 15	75, 98, 113, 117	0



Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
All	All	2693/3360~(80%)	0.39	180 (6%) 17 10	46, 85, 127, 198	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	THR	7.6
1	K	223	THR	7.0
1	Е	360	ILE	6.3
2	J	20	TRP	5.6
1	Е	285	PRO	5.2
1	А	223	THR	5.1
1	Е	240	ALA	5.0
1	Q	316	TYR	5.0
1	М	223	THR	4.9
1	S	316	TYR	4.7
1	Е	179	ILE	4.5
2	Х	20	TRP	4.5
2	V	20	TRP	4.5
1	Е	209	VAL	4.3
1	S	223	THR	4.3
2	Ι	18	GLY	4.3
1	А	189	PHE	4.2
1	М	200	PRO	4.0
1	L	300	THR	4.0
1	Е	355	ILE	3.9
1	Е	245	VAL	3.8
1	Е	210	SER	3.8
1	Е	265	LEU	3.8
1	S	183	VAL	3.8
1	С	349	ALA	3.7
1	F	223	THR	3.7
1	E	226	HIS	3.5
1	L	226	HIS	3.5
1	Q	165	LEU	3.5
1	D	245	VAL	3.5
1	L	230	VAL	3.5
1	F	346	LYS	3.4
1	L	223	THR	3.4
1	М	189	PHE	3.4
1	Е	317	ILE	3.4
2	V	36	LEU	3.4
1	С	348	THR	3.4



Mol	Chain	Res	Type	RSRZ
2	Т	14	ASP	3.4
1	А	345	LEU	3.4
2	0	20	TRP	3.4
1	D	248	LYS	3.3
1	Q	238	TYR	3.3
1	L	364	LEU	3.3
1	Q	236	ALA	3.3
2	Ι	35	GLY	3.3
1	Q	325	TYR	3.3
1	L	360	ILE	3.3
1	Q	285	PRO	3.2
1	L	254	ILE	3.2
2	0	37	ARG	3.2
1	М	224	ASN	3.2
1	М	171	PHE	3.2
1	Q	230	VAL	3.2
1	Е	344	THR	3.2
1	Е	248	LYS	3.2
1	S	207	PHE	3.1
1	М	340	ILE	3.1
1	М	251	ILE	3.0
1	Q	192	LEU	3.0
1	F	345	LEU	3.0
1	Е	342	ILE	3.0
1	А	316	TYR	3.0
2	J	34	TRP	3.0
2	0	17	SER	3.0
1	Е	247	GLU	3.0
1	Q	260	GLY	3.0
1	М	249	ALA	3.0
1	Q	189	PHE	3.0
2	Т	30	TRP	3.0
1	Κ	348	THR	3.0
1	S	228	VAL	3.0
1	М	165	LEU	2.9
1	Q	262	LEU	2.9
1	М	199	VAL	2.9
1	М	323	ILE	2.9
1	А	192	LEU	2.9
1	Е	316	TYR	2.9
1	Q	193	PRO	2.9
1	R	369	ASP	2.9



8SE7

MolChainResTypeRSRZ1A325TYR2.81M335LEU2.81S298SER2.81Q370ARG2.81Q370ARG2.82Y38GLN2.81A363PHE2.82P14ASP2.81A363PHE2.82P14ASP2.81S266LEU2.72Y35GLY2.71M344THR2.71Q350GLY2.71Q350GLY2.71R370ARG2.71Q350GLY2.71R370ARG2.71R370ARG2.71R370ARG2.71R370ARG2.61R370ARG2.71S353PHE2.61C249ALA2.71S353PHE2.61M298SER2.61A193PRO2.61A193PRO2.61A193PRO2.61A256ILE2.61B	Conti	nued fron	Continued from previous page					
1       A       325       TYR       2.8         1       M       335       LEU       2.8         1       S       298       SER       2.8         1       Q       370       ARG       2.8         2       Y       38       GLN       2.8         2       Y       38       GLN       2.8         1       A       363       PHE       2.8         2       P       14       ASP       2.8         1       S       266       LEU       2.7         2       Y       35       GLY       2.7         1       M       344       THR       2.7         1       Q       350       GLY       2.7         1       Q       256       ILE       2.7         1       Q       256       ILE       2.7         1       R       370       ARG       2.7         1       R       370<	Mol	Chain	Res	Type	RSRZ			
1         M         335         LEU         2.8           1         S         298         SER         2.8           1         Q         370         ARG         2.8           2         Y         38         GLN         2.8           2         Y         38         GLN         2.8           2         P         14         ASP         2.8           1         A         363         PHE         2.8           2         P         14         ASP         2.8           1         S         266         LEU         2.7           2         Y         35         GLY         2.7           1         Q         350         GLY         2.7           1         Q         256         ILE         2.7           1         R         370         ARG         2.7           1         R         370         ARG         2.7           1         R         370         ARG         2.7           1         R         353         PHE         2.6           1         C         252         ALA         2.6	1	А	325	TYR	2.8			
1         S         298         SER         2.8           1         C         316         TYR         2.8           1         Q         370         ARG         2.8           2         Y         38         GLN         2.8           1         A         363         PHE         2.8           2         P         14         ASP         2.8           1         S         266         LEU         2.7           2         Y         35         GLY         2.7           1         M         344         THR         2.7           1         Q         350         GLY         2.7           1         Q         256         ILE         2.7           1         Q         256         ILE         2.7           1         R         370         ARG         2.7           1         R         370         ARG         2.7           1         R         370         ARG         2.7           1         R         353         PHE         2.6           1         C         252         ALA         2.6 <t< td=""><td>1</td><td>М</td><td>335</td><td>LEU</td><td>2.8</td></t<>	1	М	335	LEU	2.8			
1         C         316         TYR         2.8           1         Q         370         ARG         2.8           2         Y         38         GLN         2.8           1         A         363         PHE         2.8           2         P         14         ASP         2.8           1         S         266         LEU         2.7           2         Y         35         GLY         2.7           1         M         344         THR         2.7           1         Q         350         GLY         2.7           1         Q         350         GLY         2.7           1         Q         256         ILE         2.7           1         R         370         ARG         2.7           1         S         353         PHE         2.6           1         C         252         ALA         2.6 <t< td=""><td>1</td><td>S</td><td>298</td><td>SER</td><td>2.8</td></t<>	1	S	298	SER	2.8			
1         Q $370$ ARG $2.8$ 2         Y $38$ GLN $2.8$ 1         A $363$ PHE $2.8$ 2         P $14$ ASP $2.8$ 1         S $266$ LEU $2.7$ 2         Y $35$ GLY $2.7$ 1         M $344$ THR $2.7$ 1         Q $350$ GLY $2.7$ 1         Q $350$ GLY $2.7$ 1         Q $256$ ILE $2.7$ 1         R $370$ ARG $2.7$ 1         C $249$ ALA $2.7$ 1         C $252$ ALA $2.6$ 1         Q $28$	1	С	316	TYR	2.8			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Q	370	ARG	2.8			
1       A $363$ PHE $2.8$ 2       P       14       ASP $2.8$ 1       S $266$ LEU $2.7$ 2       Y $35$ GLY $2.7$ 1       M $344$ THR $2.7$ 1       Q $350$ GLY $2.7$ 1       Q $256$ ILE $2.7$ 1       Q $256$ ILE $2.7$ 1       Q $256$ ILE $2.7$ 1       R $370$ ARG $2.7$ 1       R $370$ ARG $2.7$ 1       C $249$ ALA $2.7$ 1       C $249$ ALA $2.7$ 1       S $353$ PHE $2.6$ 1       C $252$ ALA $2.6$ 1       D $325$ TYR $2.6$ 1       Q $283$ GLY $2.6$ 1       A $256$ ILE $2.6$ <	2	Y	38	GLN	2.8			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	363	PHE	2.8			
1       S       266       LEU $2.7$ 2       Y       35       GLY $2.7$ 1       M       344       THR $2.7$ 1       Q       350       GLY $2.7$ 1       Q       353       PHE $2.7$ 1       Q       256       ILE $2.7$ 1       R       370       ARG $2.7$ 1       C       249       ALA $2.7$ 1       C       353       PHE $2.6$ 1       C       350       GLY $2.6$ 1       D       325       TYR $2.6$ 1       Q       283       GLY $2.6$ 1       A       193       PRO $2.6$ 1       A       256       ILE $2.6$ 1       D       317       ILE $2.6$ <td< td=""><td>2</td><td>Р</td><td>14</td><td>ASP</td><td>2.8</td></td<>	2	Р	14	ASP	2.8			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	S	266	LEU	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Y	35	GLY	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	М	344	THR	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Q	350	GLY	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	353	PHE	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Q	256	ILE	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	R	370	ARG	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	249	ALA	2.7			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	S	353	PHE	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	350	GLY	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	252	ALA	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	М	298	SER	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	325	TYR	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	367	SER	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Q	283	GLY	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	193	PRO	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	162	PRO	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	256	ILE	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	317	ILE	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	279	VAL	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Q	287	SER	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	0	16	CYS	2.6			
1       B       353       PHE       2.6         2       N       21       PHE       2.6         1       D       170       ASN       2.6         1       K       347       VAL       2.5         1       L       228       VAL       2.5         1       S       253       LEU       2.5         1       F       353       PHE       2.5         1       F       353       PHE       2.5         1       F       353       LEU       2.5         1       C       251       ILE       2.5         1       E       241       LYS       2.5         1       E       332       LEU       2.5         1       D       351       ILE       2.5	1	L	345	LEU	2.6			
2       N       21       PHE       2.6         1       D       170       ASN       2.6         1       K       347       VAL       2.5         1       L       228       VAL       2.5         1       S       253       LEU       2.5         1       F       353       PHE       2.5         1       F       353       PHE       2.5         1       C       251       ILE       2.5         1       E       241       LYS       2.5         1       E       332       LEU       2.5         1       D       351       ILE       2.5	1	В	353	PHE	2.6			
1         D         170         ASN         2.6           1         K         347         VAL         2.5           1         L         228         VAL         2.5           1         S         253         LEU         2.5           1         F         353         PHE         2.5           1         F         251         ILE         2.5           1         C         251         ILE         2.5           1         E         241         LYS         2.5           1         E         332         LEU         2.5           1         D         351         ILE         2.5	2	N	21	PHE	2.6			
1       K       347       VAL       2.5         1       L       228       VAL       2.5         1       S       253       LEU       2.5         1       F       353       PHE       2.5         1       F       251       ILE       2.5         1       C       251       ILE       2.5         1       E       241       LYS       2.5         1       E       332       LEU       2.5         1       D       351       ILE       2.5	1	D	170	ASN	2.6			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	K	347	VAL	2.5			
1         S         253         LEU         2.5           1         F         353         PHE         2.5           1         C         251         ILE         2.5           1         E         241         LYS         2.5           1         E         332         LEU         2.5           1         D         351         ILE         2.5	1	L	228	VAL	2.5			
1         F         353         PHE         2.5           1         C         251         ILE         2.5           1         E         241         LYS         2.5           1         E         332         LEU         2.5           1         D         351         ILE         2.5	1	S	253	LEU	2.5			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	F	353	PHE	2.5			
1         E         241         LYS         2.5           1         E         332         LEU         2.5           1         D         351         ILE         2.5	1	С	251	ILE	2.5			
1         E         332         LEU         2.5           1         D         351         ILE         2.5	1	Е	241	LYS	2.5			
1 D 351 ILE 2.5	1	Е	332	LEU	2.5			
	1	D	351	ILE	2.5			



Mol	Chain	Res	Type	RSRZ
1	М	353	PHE	2.5
2	G	20	TRP	2.5
1	Е	250	ASP	2.5
1	А	353	PHE	2.4
2	Р	30	TRP	2.4
1	K	346	LYS	2.4
1	L	222	VAL	2.4
1	А	235	GLY	2.4
1	D	244	ASP	2.4
1	Е	353	PHE	2.4
1	D	230	VAL	2.4
1	Q	324	ASN	2.4
1	L	250	ASP	2.4
1	Q	369	ASP	2.4
1	R	193	PRO	2.4
1	L	240	ALA	2.4
1	D	242	ILE	2.4
1	Q	263	PRO	2.3
1	L	193	PRO	2.3
1	В	315	ASP	2.3
1	L	334	ASN	2.3
2	0	21	PHE	2.3
1	S	288	LEU	2.3
2	J	21	PHE	2.3
1	Е	176	VAL	2.3
1	К	349	ALA	2.3
1	А	215	ILE	2.3
2	Р	27	TYR	2.3
1	В	189	PHE	2.3
1	С	163	ASN	2.2
1	М	228	VAL	2.2
2	N	37	ARG	2.2
1	Q	223	THR	2.2
1	М	169	TYR	2.2
1	S	224	ASN	2.2
1	Е	205	SER	2.2
1	Q	203	SER	2.2
1	М	250	ASP	2.2
1	D	209	VAL	2.2
1	Q	209	VAL	2.1
1	R	316	TYR	2.1
1	D	249	ALA	2.1



Mol	Chain	Res	Type	RSRZ
1	L	224	ASN	2.1
1	R	190	ARG	2.1
1	L	251	ILE	2.1
2	0	23	GLN	2.1
1	D	316	TYR	2.1
1	А	221	VAL	2.1
1	Е	356	PRO	2.1
1	F	230	VAL	2.1
1	D	222	VAL	2.1
1	S	267	LEU	2.1
1	С	347	VAL	2.1
1	Q	182	ALA	2.0
1	S	355	ILE	2.0
1	L	218	ASN	2.0
1	R	188	LEU	2.0
1	Q	208	ILE	2.0
1	А	236	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)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

