

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

Sep 11, 2024 – 04:13 pm BST

PDB ID	:	8R3E
Title	:	Huntingtin, 1-17, MBP-N
Authors	:	Steinbacher, S.; Toledo-Sherman, L.; Dominguez, C
Deposited on	:	2023-11-08
Resolution	:	2.91 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
$\mathrm{EDS}$	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 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 2.91 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.



Motria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
R <sub>free</sub>	164625	2797 (2.94-2.90)		
Clashscore	180529	3049 (2.94-2.90)		
Ramachandran outliers	177936	2981 (2.94-2.90)		
Sidechain outliers	177891	2983 (2.94-2.90)		
RSRZ outliers	164620	2799 (2.94-2.90)		

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	٨	000	3%		
	А	399	86%	12%	••
			2%		
1	В	399	86%	12%	•
			3%		
1	С	399	84%	16%	•
			5%		
1	D	399	80%	18%	•
			3%		
1	Е	399	84%	14%	••



Mol	Chain	Length	Quality of chain		
			5%		_
1	F	399	83%	16%	•



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18255 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	202	Total	С	Ν	0	S	18	0	0
	A		3035	1955	492	580	8	10	0	0
1	В	304	Total	С	Ν	0	S	0	0	0
	D	094	3044	1961	494	581	8	0		0
1	С	306	Total	С	Ν	0	S	12	0	0
	U	- 390	3061	1973	496	584	8	10	0	0
1	Л	202	Total	С	Ν	0	S	0	0	0
	D		3035	1955	492	580	8	0	0	0
1	F	202	Total	С	Ν	0	S	0	0	0
	Ľ		3035	1955	492	580	8	0	0	0
1	1 E	394	Total	С	Ν	0	S	17	0	0
	Г		3044	1961	494	581	8		U	U

• Molecule 1 is a protein called Maltodextrin-binding protein.

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
А	-1	GLY	-	expression tag	UNP A0A4P1LXE0
А	0	MET	-	expression tag	UNP A0A4P1LXE0
А	359	ALA	GLU	conflict	UNP A0A4P1LXE0
А	362	ALA	LYS	conflict	UNP A0A4P1LXE0
А	363	ALA	ASP	conflict	UNP A0A4P1LXE0
А	371	GLY	-	expression tag	UNP A0A4P1LXE0
А	372	SER	-	expression tag	UNP A0A4P1LXE0
А	373	GLU	-	expression tag	UNP A0A4P1LXE0
А	374	ASN	-	expression tag	UNP A0A4P1LXE0
А	375	LEU	-	expression tag	UNP A0A4P1LXE0
А	376	TYR	-	expression tag	UNP A0A4P1LXE0
А	377	PHE	-	expression tag	UNP A0A4P1LXE0
А	378	GLN	-	expression tag	UNP A0A4P1LXE0
А	379	GLY	-	expression tag	UNP A0A4P1LXE0
А	380	MET	-	expression tag	UNP A0A4P1LXE0
А	381	ALA	-	expression tag	UNP A0A4P1LXE0



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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	THR	-	expression tag	UNP A0A4P1LXE0
A	383	LEU	_	expression tag	UNP A0A4P1LXE0
A	384	GLU	_	expression tag	UNP A0A4P1LXE0
A	385	LYS	_	expression tag	UNP A0A4P1LXE0
A	386	LEU	-	expression tag	UNP A0A4P1LXE0
A	387	MET	-	expression tag	UNP A0A4P1LXE0
A	388	LYS	-	expression tag	UNP A0A4P1LXE0
А	389	ALA	-	expression tag	UNP A0A4P1LXE0
А	390	PHE	_	expression tag	UNP A0A4P1LXE0
А	391	GLU	-	expression tag	UNP A0A4P1LXE0
А	392	SER	-	expression tag	UNP A0A4P1LXE0
А	393	LEU	-	expression tag	UNP A0A4P1LXE0
А	394	LYS	-	expression tag	UNP A0A4P1LXE0
А	395	SER	-	expression tag	UNP A0A4P1LXE0
А	396	PHE	-	expression tag	UNP A0A4P1LXE0
В	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
В	-1	GLY	-	expression tag	UNP A0A4P1LXE0
В	0	MET	-	expression tag	UNP A0A4P1LXE0
В	359	ALA	GLU	conflict	UNP A0A4P1LXE0
В	362	ALA	LYS	conflict	UNP A0A4P1LXE0
В	363	ALA	ASP	conflict	UNP A0A4P1LXE0
В	371	GLY	-	expression tag	UNP A0A4P1LXE0
В	372	SER	-	expression tag	UNP A0A4P1LXE0
В	373	GLU	-	expression tag	UNP A0A4P1LXE0
В	374	ASN	-	expression tag	UNP A0A4P1LXE0
В	375	LEU	-	expression tag	UNP A0A4P1LXE0
В	376	TYR	-	expression tag	UNP A0A4P1LXE0
В	377	PHE	-	expression tag	UNP A0A4P1LXE0
В	378	GLN	-	expression tag	UNP A0A4P1LXE0
В	379	GLY	-	expression tag	UNP A0A4P1LXE0
В	380	MET	-	expression tag	UNP A0A4P1LXE0
В	381	ALA	-	expression tag	UNP A0A4P1LXE0
В	382	THR	-	expression tag	UNP A0A4P1LXE0
В	383	LEU	-	expression tag	UNP A0A4P1LXE0
В	384	GLU	-	expression tag	UNP A0A4P1LXE0
В	385	LYS	-	expression tag	UNP A0A4P1LXE0
B	386	LEU		expression tag	UNP A0A4P1LXE0
В	387	MET	-	expression tag	UNP A0A4P1LXE0
В	388	LYS	-	expression tag	UNP A0A4P1LXE0
B	389	ALA	-	expression tag	UNP A0A4P1LXE0
B	390	PHE	-	expression tag	UNP A0A4P1LXE0
В	391	GLU	_	expression tag	UNP A0A4P1LXE0



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Chain	Residue	Modelled	Actual	Comment	Reference		
В	392	SER	-	expression tag	UNP A0A4P1LXE0		
В	393	LEU	-	expression tag	UNP A0A4P1LXE0		
В	394	LYS	-	expression tag	UNP A0A4P1LXE0		
В	395	SER	-	expression tag	UNP A0A4P1LXE0		
В	396	PHE	-	expression tag	UNP A0A4P1LXE0		
С	-2	MET	-	initiating methionine	UNP A0A4P1LXE0		
С	-1	GLY	-	expression tag	UNP A0A4P1LXE0		
С	0	MET	-	expression tag	UNP A0A4P1LXE0		
С	359	ALA	GLU	conflict	UNP A0A4P1LXE0		
С	362	ALA	LYS	conflict	UNP A0A4P1LXE0		
С	363	ALA	ASP	conflict	UNP A0A4P1LXE0		
С	371	GLY	-	expression tag	UNP A0A4P1LXE0		
С	372	SER	-	expression tag	UNP A0A4P1LXE0		
С	373	GLU	_	expression tag	UNP A0A4P1LXE0		
С	374	ASN	-	expression tag	UNP A0A4P1LXE0		
С	375	LEU	-	expression tag	UNP A0A4P1LXE0		
С	376	TYR	-	expression tag	UNP A0A4P1LXE0		
С	377	PHE	-	expression tag	UNP A0A4P1LXE0		
С	378	GLN	-	expression tag	UNP A0A4P1LXE0		
С	379	GLY	-	expression tag	UNP A0A4P1LXE0		
С	380	MET	-	expression tag	UNP A0A4P1LXE0		
С	381	ALA	-	expression tag	UNP A0A4P1LXE0		
С	382	THR	-	expression tag	UNP A0A4P1LXE0		
С	383	LEU	-	expression tag	UNP A0A4P1LXE0		
С	384	GLU	-	expression tag	UNP A0A4P1LXE0		
С	385	LYS	-	expression tag	UNP A0A4P1LXE0		
С	386	LEU	-	expression tag	UNP A0A4P1LXE0		
С	387	MET	-	expression tag	UNP A0A4P1LXE0		
С	388	LYS	-	expression tag	UNP A0A4P1LXE0		
С	389	ALA	-	expression tag	UNP A0A4P1LXE0		
С	390	PHE	-	expression tag	UNP A0A4P1LXE0		
С	391	GLU	-	expression tag	UNP A0A4P1LXE0		
С	392	SER	-	expression tag	UNP A0A4P1LXE0		
С	393	LEU	-	expression tag	UNP A0A4P1LXE0		
С	394	LYS	-	expression tag	UNP A0A4P1LXE0		
C	395	SER	-	expression tag	UNP A0A4P1LXE0		
C	396	PHE	-	expression tag	UNP A0A4P1LXE0		
D	-2	MET	-	initiating methionine	UNP A0A4P1LXE0		
D	-1	GLY	-	expression tag	UNP A0A4P1LXE0		
D	0	MET	-	expression tag	UNP A0A4P1LXE0		
D	359	ALA	GLU	conflict	UNP A0A4P1LXE0		
D	362	ALA	LYS	conflict	UNP A0A4P1LXE0		



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Chain	Residue	Modelled	Actual	Comment	Reference
D	363	ALA	ASP	conflict	UNP A0A4P1LXE0
D	371	GLY	-	expression tag	UNP A0A4P1LXE0
D	372	SER	-	expression tag	UNP A0A4P1LXE0
D	373	GLU	_	expression tag	UNP A0A4P1LXE0
D	374	ASN	_	expression tag	UNP A0A4P1LXE0
D	375	LEU	_	expression tag	UNP A0A4P1LXE0
D	376	TYR	_	expression tag	UNP A0A4P1LXE0
D	377	PHE	-	expression tag	UNP A0A4P1LXE0
D	378	GLN	-	expression tag	UNP A0A4P1LXE0
D	379	GLY	-	expression tag	UNP A0A4P1LXE0
D	380	MET	-	expression tag	UNP A0A4P1LXE0
D	381	ALA	_	expression tag	UNP A0A4P1LXE0
D	382	THR	-	expression tag	UNP A0A4P1LXE0
D	383	LEU	_	expression tag	UNP A0A4P1LXE0
D	384	GLU	-	expression tag	UNP A0A4P1LXE0
D	385	LYS	-	expression tag	UNP A0A4P1LXE0
D	386	LEU	-	expression tag	UNP A0A4P1LXE0
D	387	MET	-	expression tag	UNP A0A4P1LXE0
D	388	LYS	-	expression tag	UNP A0A4P1LXE0
D	389	ALA	-	expression tag	UNP A0A4P1LXE0
D	390	PHE	-	expression tag	UNP A0A4P1LXE0
D	391	GLU	-	expression tag	UNP A0A4P1LXE0
D	392	SER	-	expression tag	UNP A0A4P1LXE0
D	393	LEU	-	expression tag	UNP A0A4P1LXE0
D	394	LYS	-	expression tag	UNP A0A4P1LXE0
D	395	SER	-	expression tag	UNP A0A4P1LXE0
D	396	PHE	-	expression tag	UNP A0A4P1LXE0
Е	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
Е	-1	GLY	-	expression tag	UNP A0A4P1LXE0
Е	0	MET	-	expression tag	UNP A0A4P1LXE0
Е	359	ALA	GLU	conflict	UNP A0A4P1LXE0
Е	362	ALA	LYS	conflict	UNP A0A4P1LXE0
Е	363	ALA	ASP	conflict	UNP A0A4P1LXE0
Е	371	GLY	-	expression tag	UNP A0A4P1LXE0
Е	372	SER	-	expression tag	UNP A0A4P1LXE0
E	373	GLU	-	expression tag	UNP A0A4P1LXE0
E	374	ASN	-	expression tag	UNP A0A4P1LXE0
E	375	LEU	-	expression tag	UNP A0A4P1LXE0
E	376	TYR	-	expression tag	UNP A0A4P1LXE0
E	377	PHE	-	expression tag	UNP A0A4P1LXE0
E	378	GLN	-	expression tag	UNP A0A4P1LXE0
Е	379	GLY	-	expression tag	UNP A0A4P1LXE0



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Chain	Residue	Modelled	Actual	Comment	Reference
Е	380	MET	-	expression tag	UNP A0A4P1LXE0
Е	381	ALA	-	expression tag	UNP A0A4P1LXE0
Е	382	THR	-	expression tag	UNP A0A4P1LXE0
E	383	LEU	_	expression tag	UNP A0A4P1LXE0
Е	384	GLU	_	expression tag	UNP A0A4P1LXE0
Е	385	LYS	_	expression tag	UNP A0A4P1LXE0
Е	386	LEU	_	expression tag	UNP A0A4P1LXE0
Е	387	MET	-	expression tag	UNP A0A4P1LXE0
Е	388	LYS	-	expression tag	UNP A0A4P1LXE0
Е	389	ALA	-	expression tag	UNP A0A4P1LXE0
Е	390	PHE	-	expression tag	UNP A0A4P1LXE0
Е	391	GLU	-	expression tag	UNP A0A4P1LXE0
Е	392	SER	-	expression tag	UNP A0A4P1LXE0
Е	393	LEU	-	expression tag	UNP A0A4P1LXE0
Е	394	LYS	-	expression tag	UNP A0A4P1LXE0
Е	395	SER	-	expression tag	UNP A0A4P1LXE0
Е	396	PHE	-	expression tag	UNP A0A4P1LXE0
F	-2	MET	-	initiating methionine	UNP A0A4P1LXE0
F	-1	GLY	-	expression tag	UNP A0A4P1LXE0
F	0	MET	-	expression tag	UNP A0A4P1LXE0
F	359	ALA	GLU	conflict	UNP A0A4P1LXE0
F	362	ALA	LYS	conflict	UNP A0A4P1LXE0
F	363	ALA	ASP	conflict	UNP A0A4P1LXE0
F	371	GLY	-	expression tag	UNP A0A4P1LXE0
F	372	SER	-	expression tag	UNP A0A4P1LXE0
F	373	GLU	-	expression tag	UNP A0A4P1LXE0
F	374	ASN	-	expression tag	UNP A0A4P1LXE0
F	375	LEU	-	expression tag	UNP A0A4P1LXE0
F	376	TYR	-	expression tag	UNP A0A4P1LXE0
F	377	PHE	-	expression tag	UNP A0A4P1LXE0
F	378	GLN	-	expression tag	UNP A0A4P1LXE0
F	379	GLY	-	expression tag	UNP A0A4P1LXE0
F	380	MET	-	expression tag	UNP A0A4P1LXE0
F	381	ALA	-	expression tag	UNP A0A4P1LXE0
F	382	THR	-	expression tag	UNP A0A4P1LXE0
F	383	LEU	-	expression tag	UNP A0A4P1LXE0
F	384	GLU	-	expression tag	UNP A0A4P1LXE0
F	385	LYS	-	expression tag	UNP A0A4P1LXE0
F	386	LEU	-	expression tag	UNP A0A4P1LXE0
F	387	MET	-	expression tag	UNP A0A4P1LXE0
F	388	LYS	-	expression tag	UNP A0A4P1LXE0
F	389	ALA	-	expression tag	UNP A0A4P1LXE0



Chain	Residue	Modelled	Actual	Comment	Reference
F	390	PHE	-	expression tag	UNP A0A4P1LXE0
F	391	GLU	-	expression tag	UNP A0A4P1LXE0
F	392	SER	-	expression tag	UNP A0A4P1LXE0
F	393	LEU	-	expression tag	UNP A0A4P1LXE0
F	394	LYS	-	expression tag	UNP A0A4P1LXE0
F	395	SER	-	expression tag	UNP A0A4P1LXE0
F	396	PHE	-	expression tag	UNP A0A4P1LXE0

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf
2	С	1	Total 1	Zn 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: Maltodextrin-binding protein

• Molecule 1: Maltodextrin-binding protein







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	96.04Å 96.11Å 97.67Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$76.40^{\circ}$ $80.72^{\circ}$ $63.19^{\circ}$	Depositor
Resolution(A)	45.79 - 2.91	Depositor
Resolution (A)	45.79 - 2.91	EDS
% Data completeness	48.0 (45.79-2.91)	Depositor
(in resolution range)	48.0 (45.79-2.91)	EDS
R <sub>merge</sub>	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.252 , $0.329$	Depositor
$\Lambda, \Lambda_{free}$	0.254 , $0.323$	DCC
$R_{free}$ test set	3273 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 22.2	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	18255	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.44% 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)

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

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		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.74	0/3107	0.90	1/4216~(0.0%)	
1	В	0.73	0/3116	0.88	0/4227	
1	С	0.73	0/3134	0.88	0/4251	
1	D	0.72	0/3107	0.87	0/4216	
1	Е	0.73	0/3107	0.88	0/4216	
1	F	0.73	0/3116	0.89	0/4227	
All	All	0.73	0/18687	0.88	1/25353~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	320	THR	CA-CB-OG1	-5.47	97.51	109.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	142	LYS	Peptide
	0		7	



Continued from previous page...

Mol	Chain	$\operatorname{Res}$	Type	Group
1	F	368	ALA	Peptide

### 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	3035	0	3008	19	1
1	В	3044	0	3021	23	0
1	С	3061	0	3035	28	0
1	D	3035	0	3008	33	1
1	Е	3035	0	3008	35	0
1	F	3044	0	3021	37	1
2	С	1	0	0	0	1
All	All	18255	0	18101	164	2

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 5.

All (164) 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:F:184:ASP:HB2	1:F:365:GLN:HG3	1.56	0.85
1:F:181:VAL:HG21	1:F:369:ALA:HA	1.73	0.71
1:D:342:ALA:HB1	1:D:364:ALA:HA	1.77	0.67
1:D:39:HIS:CG	1:D:39:HIS:O	2.48	0.66
1:E:380:MET:CE	1:F:382:THR:HG21	2.26	0.65
1:F:192:LEU:HD23	1:F:357:VAL:HG13	1.80	0.64
1:E:122:LEU:HD21	1:E:126:PRO:HD3	1.80	0.63
1:E:152:GLN:HA	1:E:348:ILE:HD11	1.79	0.63
1:C:115:LEU:HB2	1:C:247:LEU:HD23	1.80	0.63
1:E:380:MET:HE2	1:F:382:THR:HG21	1.82	0.61
1:A:51:ALA:HB3	1:A:75:LEU:HD13	1.82	0.61
1:C:8:VAL:HG13	1:C:57:PRO:HA	1.82	0.61
1:D:122:LEU:HD21	1:D:126:PRO:HD3	1.83	0.61
1:E:39:HIS:CG	1:E:39:HIS:O	2.54	0.61
1:D:115:LEU:HD11	1:D:224:MET:HB3	1.83	0.61



Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
1.E.342.ALA.HB1	1.E.364.ALA.HA	1.84	0.60	
1.E.012.HER.HB1 1.F.184:ASP:HB2	1:F:365:GLN:CG	2.31	0.60	
1.C.89.LEU.HD12	$1 \cdot C \cdot 94 \cdot TBP \cdot CZ2$	2.31	0.60	
1.D.136.ASP.HA	1.D.146.ALA.HB2	1.84	0.50	
1.D.109.ALA.HB3	1.D.262.LEU.HB3	1.81	0.59	
1.C.122.LEU.HD22	1.C.135.LEU.HD11	1.81	0.59	
1.E.109.ALA.HB3	1.E.262.LEU.HB3	1.86	0.57	
1.C.39.HIS.O	1.C·39·HIS·CG	2.58	0.56	
1:A:97:VAL:HG21	1.A.107.PRO.HD3	1.87	0.56	
1.C.136.ASP.HA	1.C.146.ALA.HB2	1.81	0.56	
1.E.100.ALA·HB3	1.E.110.HEILIID2	1.00	0.56	
1.R.89.LEU.HD12	1.1.202.EE0.IIB0 1.8.94.TRP.CZ2	2.41	0.55	
1.D.39.HIS.O	1.D.39.HIS.CD2	2.59	0.55	
1.B.39.HIS.O	1.D.39.HIS.CD2	2.59	0.55	
1.B.108.ILE.HD11	$1 \cdot B \cdot 264 \cdot \Delta L \Delta \cdot HB2$	1.00	0.54	
1.D.108.ILE.IID11 1.D.178.ILE.HD11	1:D:371:CLV:CA	2.38	0.53	
1.E.170.IEE.IID11 1.F.80.LEU.HD12	1.E.971.0E1.0A 1.F.94.TRP.CZ2	2.30	0.55	
1.F.80.I FU.HD12	1.F.04.TRP.CZ2	2.44	0.52	
1.E.05.EE0.HD12	1.E.94.1101.022	2.44	0.52	
$1 \cdot \Delta \cdot 136 \cdot \Delta \text{SP-H} \Delta$	1.1.236.1  HL.012 $1.4.146.4  L  A  HB 2$	1.02	0.52	
1.F.50.ILE.HD11	$\frac{1.1.140.140.11D1.11D2}{1.1.1276.\Delta L\Delta \cdot CB}$	2.40	0.52	
1.D.178.ILE.HC22	1.D.270.MLA.OD	1 01	0.52	
1.D.170.ILL.II022	1.D.935.11D.11D12	2.40	0.52	
1.C.192.LEU.HD22	1.D.270.RLA.OD	1 91	0.52	
1.0.192.EE0.HD22	1.0.001.EE0.HD21 1.D.57.PRO.HΔ	1.01	0.51	
1.E.0. VAL.HU13	$1 \cdot F \cdot 230 \cdot TBP \cdot CZ3$	2.46	0.51	
1.R.158.TRP.CD1	1.R.258.PHE.CE2	2.40	0.51	
1.E.116.ILE.HD12	1.E.116.ILE.N	2.35	0.51	
1.C.228.CLV.HA3	$1 \cdot C \cdot 230 \cdot TBP \cdot CZ3$	2.25	0.51	
1.E.85.PHE.HA	1.C.290.11(1.C20	1.92	0.50	
1.C.329.ILE.N	1.E.00.E15.HQ2	2.27	0.50	
1.0.020.1111.1.1 1.D.35.VAL.HG12	1.0.320.HLL.HD12	1 94	0.50	
1.D.97.VAL:HG21	1.D.107.PRO.HD3	1.91	0.50	
1.D.311.LEU.HB3	1.D.317.ILE.HD13	1.01	0.50	
1.A.89.LEU.HD12	$1 \cdot A \cdot 94 \cdot TRP \cdot CZ2$	2.47	0.50	
1:C:205:ASN·HB3	1:C:208·THB·HG23	1.94	0.50	
1.D.158.TRP.CD1	1.D.258.PHE.CE2	2.99	0.50	
1:B:122:LEU·HD21	1:B:126·PRO·HD3	1.93	0.49	
1.E.112.LEU.HD11	1:E:125:TVB:CE1	2.47	0.49	
1:A:139.LEU:HD13	1:A:146·ALA·HA	1 94	0.49	
1:D:47:PHE:HB3	1:D:48:PRO:HD3	1.95	0.49	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:59:ILE:HD11	1:D:276:ALA:HB1	1.94	0.49
1:D:184:ASP:HB2	1:D:365:GLN:HB2	1.95	0.49
1:F:158:TRP:CD1	1:F:258:PHE:CE2	3.01	0.49
1:B:33:ILE:HD13	1:B:275:LEU:HD22	1.93	0.48
1:E:136:ASP:HA	1:E:146:ALA:HB2	1.94	0.48
1:F:191:GLY:HA2	1:F:250:PHE:CE2	2.48	0.48
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.01	0.48
1:B:90:TYB:CE2	1:B:305:LYS:HA	2.48	0.48
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.48	0.48
1:E:24:GLY:HA2	1:E:35:VAL:HG21	1.94	0.48
1:E:330:MET:HE3	1:E:330:MET:HA	1.96	0.48
1:F:152:GLN:HA	1:F:348:ILE:HD11	1.94	0.48
1:D:256:LYS:HA	1:D:327:GLY:HA2	1.96	0.48
1:C:139:LEU:HD13	1:C:146:ALA:HA	1.96	0.48
1:F:39:HIS:O	1:F:39:HIS:CD2	2.67	0.48
1:F:64:HIS:CE1	1:F:330:MET:O	2.67	0.48
1:A:158:TRP:CD1	1:A:258:PHE:CE2	3.01	0.47
1:B:5:GLY:O	1:B:33:ILE:HG23	2.14	0.47
1:B:68:GLY:CA	1:B:332:ASN:HD22	2.28	0.47
1:B:259:VAL:HG12	1:B:261:VAL:HG23	1.96	0.47
1:F:342:ALA:HB1	1:F:364:ALA:HA	1.95	0.47
1:F:131:GLU:O	1:F:131:GLU:HG2	2.14	0.47
1:A:72:GLN:HG2	1:A:99:TYR:CE2	2.49	0.47
1:A:72:GLN:HG2	1:A:99:TYR:CZ	2.50	0.47
1:D:342:ALA:HB2	1:D:367:ASN:HB3	1.97	0.47
1:B:89:LEU:HD13	1:B:107:PRO:HG2	1.96	0.47
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.97	0.46
1:E:153:GLU:OE1	1:E:344:ARG:NH1	2.48	0.46
1:C:307:TYR:CE2	1:C:311:LEU:HD11	2.50	0.46
1:F:259:VAL:HG12	1:F:261:VAL:HG23	1.97	0.46
1:B:178:ILE:HD13	1:B:372:SER:OG	2.15	0.46
1:C:51:ALA:HB3	1:C:75:LEU:HD13	1.96	0.46
1:E:329:ILE:HD12	1:E:329:ILE:N	2.30	0.46
1:E:380:MET:HE1	1:F:382:THR:HG21	1.97	0.46
1:A:5:GLY:O	1:A:33:ILE:HG23	2.15	0.46
1:C:110:VAL:HG13	1:C:259:VAL:HG13	1.97	0.46
1:A:43:LEU:HD11	1:A:62:TRP:CE3	2.51	0.46
1:D:89:LEU:HD12	1:D:94:TRP:CZ2	2.51	0.46
1:D:5:GLY:O	1:D:33:ILE:HG23	2.16	0.45
1:A:302:VAL:HG22	1:A:311:LEU:HD12	1.97	0.45
1:F:108:ILE:HG12	1:F:263:SER:HA	1.98	0.45



Interatomic (			
Atom-1	Atom-2	distance (Å)	overlap (Å)
1·E·301·ALA·HA	1·E·317·ILE·HG23	1.97	0.45
1:D:1:LYS:HB2	1:D:55:ASP:HB3	1.98	0.45
1.D.354.ABG.O	1·F·53·THR·HG22	2.17	0.45
1:E:38:GLU:C	1:E:40:PRO:HD3	2.37	0.44
1:B:185:ASN:OD1	1:B:186:ALA:N	2.51	0.44
1:E:72:GLN:HG2	1:E:99:TYR:CE2	2.52	0.44
1:E:181:VAL:CG1	1:E:183:VAL:HG23	2.46	0.44
1:D:171:TYR:CZ	1:D:174:GLY:HA2	2.53	0.44
1:F:329:ILE:HD12	1:F:329:ILE:N	2.32	0.44
1:F:192:LEU:HD22	1:F:361:LEU:CD1	2.47	0.44
1:F:382:THR:HG22	1:F:385:LYS:NZ	2.33	0.44
1:E:112:ALA:HB2	1:E:324:ALA:HB2	1.99	0.44
1:B:129:TRP:CE2	1:B:248:PRO:HG2	2.52	0.44
1:B:342:ALA:HB1	1:B:364:ALA:HA	1.98	0.44
1:D:118:ASN:CG	1:D:121:LEU:HD12	2.38	0.44
1:D:9:ILE:HB	1:D:37:VAL:HG22	2.00	0.44
1:D:240:VAL:HG23	1:D:242:TYR:HB3	1.99	0.43
1:E:64:HIS:HE2	1:E:330:MET:HB3	1.83	0.43
1:F:7:LEU:HD21	1:F:275:LEU:HB2	2.00	0.43
1:B:115:LEU:HD22	1:B:248:PRO:HD3	1.99	0.43
1:B:122:LEU:HD21	1:B:126:PRO:CD	2.48	0.43
1:C:383:LEU:HD23	1:C:386:LEU:HD12	2.00	0.43
1:A:53:THR:HG22	1:B:354:ARG:O	2.19	0.43
1:E:59:ILE:HD11	1:E:276:ALA:HB1	2.01	0.43
1:F:307:TYR:CD2	1:F:311:LEU:HD11	2.54	0.43
1:C:18:ASN:O	1:C:22:GLU:HG2	2.19	0.43
1:F:181:VAL:HG21	1:F:369:ALA:CA	2.46	0.43
1:A:342:ALA:HB1	1:A:364:ALA:HA	2.00	0.43
1:D:379:GLY:HA2	1:E:380:MET:HG3	2.01	0.43
1:E:72:GLN:HG2	1:E:99:TYR:CZ	2.53	0.43
1:B:52:ALA:O	1:C:356:THR:N	2.51	0.42
1:C:349:ASN:OD1	1:C:354:ARG:NH2	2.52	0.42
1:E:214:GLU:OE1	1:E:227:ASN:ND2	2.52	0.42
1:F:136:ASP:HA	1:F:146:ALA:HB2	2.01	0.42
1:E:115:LEU:HB2	1:E:247:LEU:HD23	2.01	0.42
1:F:113:LEU:HD11	1:F:155:TYR:CE1	2.53	0.42
1:D:380:MET:HE1	1:F:338:ALA:HB2	2.00	0.42
1:B:39:HIS:O	1:B:39:HIS:ND1	2.52	0.42
1:A:129:TRP:HA	1:A:132:ILE:HD12	2.00	0.42
1:C:189:LYS:HA	1:C:361:LEU:HD12	2.02	0.42
1:D:38:GLU:C	1:D:40:PRO:HD3	2.39	0.42



A + 1	A +	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:389:ALA:HB2	1:E:387:MET:CE	2.50	0.42
1:E:154:PRO:HG3	1:E:344:ARG:HA	2.02	0.42
1:D:162:ALA:HA	1:D:166:GLY:HA3	2.01	0.42
1:F:307:TYR:CE2	1:F:311:LEU:HD11	2.55	0.42
1:A:8:VAL:HG13	1:A:57:PRO:HA	2.02	0.41
1:C:189:LYS:HA	1:C:361:LEU:CD1	2.50	0.41
1:A:376:TYR:OH	1:C:375:LEU:HG	2.20	0.41
1:B:118:ASN:ND2	1:B:121:LEU:HD12	2.34	0.41
1:A:82:ASP:OD1	1:A:83:LYS:N	2.53	0.41
1:C:112:ALA:HB2	1:C:324:ALA:HB2	2.02	0.41
1:E:39:HIS:O	1:E:39:HIS:ND1	2.53	0.41
1:C:39:HIS:O	1:C:39:HIS:ND1	2.53	0.41
1:F:222:THR:HG22	1:F:224:MET:H	1.85	0.41
1:F:266:ILE:HD11	1:F:280:LEU:HD12	2.01	0.41
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.56	0.41
1:C:89:LEU:HB2	1:C:94:TRP:HE1	1.86	0.41
1:C:109:ALA:HB3	1:C:262:LEU:HB3	2.01	0.41
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.02	0.41
1:F:39:HIS:O	1:F:39:HIS:CG	2.73	0.41
1:F:89:LEU:HD13	1:F:107:PRO:HG2	2.02	0.41
1:F:129:TRP:CE3	1:F:132:ILE:HD12	2.56	0.41
1:C:181:VAL:CG1	1:C:183:VAL:HG23	2.51	0.41
1:E:5:GLY:O	1:E:33:ILE:HG23	2.21	0.41
1:B:68:GLY:HA2	1:B:332:ASN:HD22	1.86	0.40
1:E:183:VAL:HG11	1:E:364:ALA:HB3	2.04	0.40
1:E:53:THR:HG22	1:F:354:ARG:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:ND1	2:C:401:ZN:ZN[1_545]	1.61	0.59
1:D:15:LYS:O	$1:F:124:ASN:ND2[1_455]$	2.08	0.12

#### 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	391/399~(98%)	367 (94%)	23 (6%)	1 (0%)	37	65
1	В	392/399~(98%)	370 (94%)	21 (5%)	1 (0%)	37	65
1	С	394/399~(99%)	373 (95%)	20 (5%)	1 (0%)	37	65
1	D	391/399~(98%)	365 (93%)	24 (6%)	2 (0%)	25	55
1	Е	391/399~(98%)	369 (94%)	21 (5%)	1 (0%)	37	65
1	F	392/399~(98%)	366 (93%)	25 (6%)	1 (0%)	37	65
All	All	2351/2394 (98%)	2210 (94%)	134 (6%)	7 (0%)	37	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	239	LYS
1	А	165	GLY
1	С	165	GLY
1	D	165	GLY
1	F	165	GLY
1	Е	165	GLY
1	В	165	GLY

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	310/315~(98%)	294~(95%)	16~(5%)	19 49
1	В	311/315~(99%)	297~(96%)	14 (4%)	23 54
1	С	313/315~(99%)	297~(95%)	16 (5%)	20 50
1	D	310/315~(98%)	292 (94%)	18 (6%)	17 44
1	Ε	310/315~(98%)	300~(97%)	10 (3%)	34 67



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	F	311/315~(99%)	301~(97%)	10 (3%)	34	67
All	All	1865/1890~(99%)	1781 (96%)	84 (4%)	23	54

All (84) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	25	LYS
1	А	55	ASP
1	А	99	TYR
1	А	114	SER
1	А	145	SER
1	А	184	ASP
1	А	209	ASP
1	А	227	ASN
1	А	236	ASP
1	А	263	SER
1	А	287	ASP
1	А	297	LYS
1	А	320	THR
1	А	333	ILE
1	А	336	MET
1	А	383	LEU
1	В	55	ASP
1	В	72	GLN
1	В	145	SER
1	В	148	MET
1	В	184	ASP
1	В	193	THR
1	В	202	LYS
1	В	209	ASP
1	В	287	ASP
1	В	330	MET
1	В	341	TYR
1	В	345	THR
1	В	358	ASP
1	В	383	LEU
1	С	41	ASP
1	C	42	LYS
1	C	114	SER
1	С	145	SER
1	С	153	GLU
1	С	178	ILE



Mol	Chain	Res	Type
1	С	200	LYS
1	С	209	ASP
1	С	227	ASN
1	С	255	SER
1	С	263	SER
1	С	287	ASP
1	С	313	LYS
1	С	345	THR
1	С	358	ASP
1	С	394	LYS
1	D	39	HIS
1	D	83	LYS
1	D	114	SER
1	D	137	LYS
1	D	148	MET
1	D	189	LYS
1	D	197	ASP
1	D	209	ASP
1	D	226	ILE
1	D	227	ASN
1	D	234	ASN
1	D	251	LYS
1	D	263	SER
1	D	310	GLU
1	D	341	TYR
1	D	345	THR
1	D	374	ASN
1	D	378	GLN
1	Е	39	HIS
1	Е	87	ASP
1	Е	114	SER
1	Е	127	LYS
1	Е	145	SER
1	Е	180	ASP
1	Е	227	ASN
1	Ε	297	LYS
1	E	345	THR
1	E	372	SER
1	F	46	LYS
1	F	114	SER
1	F	142	LYS
1	F	145	SER



Continued from previous page...

Mol	Chain	Res	Type
1	F	209	ASP
1	F	227	ASN
1	F	287	ASP
1	F	288	GLU
1	F	345	THR
1	F	390	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	D	12	ASN
1	D	39	HIS
1	D	374	ASN
1	F	227	ASN

#### 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 oligosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	393/399~(98%)	0.39	10 (2%) 58 52	15, 45, 74, 106	5 (1%)
1	В	394/399~(98%)	0.35	9 (2%) 61 55	17, 45, 73, 96	0
1	С	396/399~(99%)	0.49	12 (3%) 52 47	22, 49, 83, 120	4 (1%)
1	D	393/399~(98%)	0.48	18 (4%) 38 32	19, 46, 84, 129	0
1	Е	393/399~(98%)	0.55	11 (2%) 55 49	19, 55, 82, 119	0
1	F	394/399~(98%)	0.49	18 (4%) 38 32	27, 49, 79, 130	5 (1%)
All	All	2363/2394~(98%)	0.46	78 (3%) 49 43	15, 48, 81, 130	14 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	371	GLY	5.2
1	D	370	ALA	4.1
1	С	396	PHE	3.6
1	D	99	TYR	3.4
1	D	147	LEU	3.3
1	Е	393	LEU	3.2
1	F	258	PHE	3.1
1	Е	372	SER	3.1
1	А	361	LEU	3.0
1	А	383	LEU	3.0
1	Е	134	ALA	2.9
1	F	39	HIS	2.8
1	D	393	LEU	2.7
1	D	376	TYR	2.7
1	F	331	PRO	2.7
1	В	206	ALA	2.6
1	С	36	THR	2.6
1	Е	338	ALA	2.6
1	С	171	TYR	2.6



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Mol	Chain	Res   Type		RSRZ
1	С	176	TYR	2.6
1	D	68	GLY	2.5
1	С	370	ALA	2.5
1	С	383	LEU	2.5
1	D	8	VAL	2.5
1	С	213	ALA	2.5
1	F	74	GLY	2.4
1	F	369	ALA	2.4
1	D	179	LYS	2.4
1	А	184	ASP	2.4
1	Е	184	ASP	2.4
1	А	2	ILE	2.4
1	F	97	VAL	2.3
1	D	392	SER	2.3
1	F	372	SER	2.3
1	В	213	ALA	2.3
1	С	185	ASN	2.3
1	А	381	ALA	2.3
1	Е	178	ILE	2.3
1	А	269	ALA	2.3
1	F	370	ALA	2.3
1	С	118	ASN	2.2
1	D	11	ILE	2.2
1	F	354	ARG	2.2
1	А	76	LEU	2.2
1	D	383	LEU	2.2
1	D	181	VAL	2.2
1	Е	67	PHE	2.2
1	F	27	PHE	2.2
1	С	329	ILE	2.2
1	Е	330	MET	2.2
1	А	386	LEU	2.2
1	D	76	LEU	2.2
1	D	31	THR	2.2
1	F	226	ILE	2.2
1	Е	135	LEU	2.2
1	D	340	TRP	2.2
1	А	382	THR	2.1
1	Е	92	PHE	2.1
1	В	393	LEU	2.1
1	В	394	LYS	2.1
1	D	375	LEU	2.1



Mol	Chain	Res	Type	RSRZ
1	С	187	GLY	2.1
1	В	174	GLY	2.1
1	F	378	GLN	2.1
1	F	184	ASP	2.1
1	F	222	THR	2.1
1	С	324	ALA	2.1
1	В	1	LYS	2.1
1	А	280	LEU	2.0
1	Е	337	SER	2.0
1	В	104	ILE	2.0
1	В	101	GLY	2.0
1	В	156	PHE	2.0
1	F	85	PHE	2.0
1	F	228	GLY	2.0
1	F	269	ALA	2.0
1	D	104	ILE	2.0
1	D	244	VAL	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	ZN	С	401	1/1	0.97	0.04	32,32,32,32	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

