

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

Jun 3, 2024 – 03:30 PM JST

PDB ID : 8JOH

Title : structure of Echinococcus multilocularis Cystatin B

Authors: Huang, S.Q.; Hong, W.B.

Deposited on : 2023-06-07

Resolution : 2.04 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

EDS : 2.36.2

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)

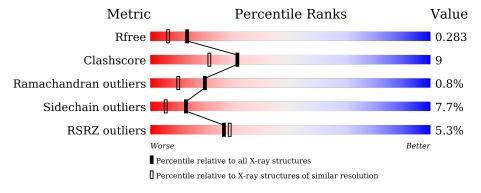
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 Å.

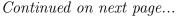
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
TVICTIE	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	A	106	79%	15%				
1	В	106	75%	17%	• 8%			
1	С	106	65%	22% •	11%			
1	D	106	70%	23%	• 7%			
1	Е	106	69%	26%	5%			
1	F	106	74%	19%	• 6%			





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Mol	Chain	Length		Qualit	y of chain			
1	G	106	22%	48%	35%	8%	•	8%
1	Н	106	2%	72%		19%	•	8%



# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Cystatin B Stefin B.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	102	Total	С	N	О	S	0	0	0
1	A	102	807	505	149	149	4	U		U
1	В	98	Total	С	N	О	S	0	0	0
1	Б	90	769	482	139	145	3	0	U	U
1	D	99	Total	С	N	О	S	0	0	0
1	D	99	777	487	140	146	4	0	U	
1	F	100	Total	С	N	О	S	0	0	0
1	I.	100	787	493	143	147	4	0		U
1	С	94	Total	С	N	О	S	0	0	0
1		94	747	468	137	138	4	0	U	0
1	Е	101	Total	С	N	О	S	0	0	0
1	12	101	797	499	146	148	4	0	U	U
1	G	98	Total	С	N	О	S	0	0	0
1	G	90	766	481	139	143	3	U		U
1	Н	98	Total	С	N	О	S	0	0	0
1	11	90	769	482	139	145	3	U	U	U

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	LEU	-	expression tag	UNP A0A087VZV0
A	100	GLU	-	expression tag	UNP A0A087VZV0
A	101	HIS	-	expression tag	UNP A0A087VZV0
A	102	HIS	-	expression tag	UNP A0A087VZV0
A	103	HIS	-	expression tag	UNP A0A087VZV0
A	104	HIS	-	expression tag	UNP A0A087VZV0
A	105	HIS	-	expression tag	UNP A0A087VZV0
A	106	HIS	-	expression tag	UNP A0A087VZV0
В	99	LEU	-	expression tag	UNP A0A087VZV0
В	100	GLU	-	expression tag	UNP A0A087VZV0
В	101	HIS	-	expression tag	UNP A0A087VZV0
В	102	HIS	-	expression tag	UNP A0A087VZV0
В	103	HIS	-	expression tag	UNP A0A087VZV0



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
В	104	HIS	-	expression tag	UNP A0A087VZV0
В	105	HIS	-	expression tag	UNP A0A087VZV0
В	106	HIS	-	expression tag	UNP A0A087VZV0
D	99	LEU	-	expression tag	UNP A0A087VZV0
D	100	GLU	-	expression tag	UNP A0A087VZV0
D	101	HIS	-	expression tag	UNP A0A087VZV0
D	102	HIS	-	expression tag	UNP A0A087VZV0
D	103	HIS	-	expression tag	UNP A0A087VZV0
D	104	HIS	-	expression tag	UNP A0A087VZV0
D	105	HIS	-	expression tag	UNP A0A087VZV0
D	106	HIS	-	expression tag	UNP A0A087VZV0
F	99	LEU	-	expression tag	UNP A0A087VZV0
F	100	GLU	-	expression tag	UNP A0A087VZV0
F	101	HIS	-	expression tag	UNP A0A087VZV0
F	102	HIS	-	expression tag	UNP A0A087VZV0
F	103	HIS	-	expression tag	UNP A0A087VZV0
F	104	HIS	-	expression tag	UNP A0A087VZV0
F	105	HIS	-	expression tag	UNP A0A087VZV0
F	106	HIS	-	expression tag	UNP A0A087VZV0
С	99	LEU	-	expression tag	UNP A0A087VZV0
С	100	GLU	-	expression tag	UNP A0A087VZV0
С	101	HIS	_	expression tag	UNP A0A087VZV0
С	102	HIS	-	expression tag	UNP A0A087VZV0
С	103	HIS	-	expression tag	UNP A0A087VZV0
С	104	HIS	_	expression tag	UNP A0A087VZV0
С	105	HIS	-	expression tag	UNP A0A087VZV0
С	106	HIS	-	expression tag	UNP A0A087VZV0
Е	99	LEU	-	expression tag	UNP A0A087VZV0
Е	100	GLU	-	expression tag	UNP A0A087VZV0
Е	101	HIS	-	expression tag	UNP A0A087VZV0
Е	102	HIS	-	expression tag	UNP A0A087VZV0
Е	103	HIS	-	expression tag	UNP A0A087VZV0
Е	104	HIS	-	expression tag	UNP A0A087VZV0
Е	105	HIS	-	expression tag	UNP A0A087VZV0
Е	106	HIS	-	expression tag	UNP A0A087VZV0
G	99	LEU	-	expression tag	UNP A0A087VZV0
G	100	GLU	-	expression tag	UNP A0A087VZV0
G	101	HIS	-	expression tag	UNP A0A087VZV0
G	102	HIS	-	expression tag	UNP A0A087VZV0
G	103	HIS	-	expression tag	UNP A0A087VZV0
G	104	HIS	-	expression tag	UNP A0A087VZV0
G	105	HIS	-	expression tag	timued on mort mass



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Chain	Residue	Modelled	Actual	Comment	Reference
G	106	HIS	-	expression tag	UNP A0A087VZV0
Н	99	LEU	-	expression tag	UNP A0A087VZV0
Н	100	GLU	-	expression tag	UNP A0A087VZV0
Н	101	HIS	-	expression tag	UNP A0A087VZV0
Н	102	HIS	-	expression tag	UNP A0A087VZV0
Н	103	HIS	-	expression tag	UNP A0A087VZV0
Н	104	HIS	-	expression tag	UNP A0A087VZV0
Н	105	HIS	-	expression tag	UNP A0A087VZV0
Н	106	HIS	-	expression tag	UNP A0A087VZV0



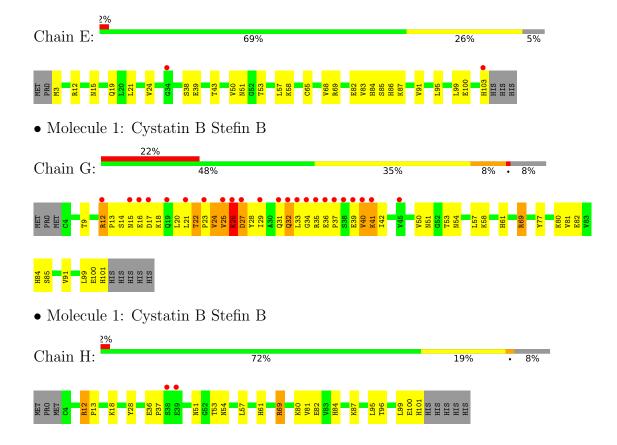
# 3 Residue-property plots (i)

• Molecule 1: Cystatin B Stefin B

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: Cystatin B Stefin B Chain A: 79% 15% • Molecule 1: Cystatin B Stefin B Chain B: • Molecule 1: Cystatin B Stefin B Chain D: 70% 23% 7% • Molecule 1: Cystatin B Stefin B Chain F: 74% • 6% 19% • Molecule 1: Cystatin B Stefin B Chain C: 22% 11%







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	72.72Å 65.99Å 92.71Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 103.38° 90.00°	Depositor
Resolution (Å)	53.31 - 2.04	Depositor
Resolution (A)	53.26 - 2.04	EDS
% Data completeness	99.5 (53.31-2.04)	Depositor
(in resolution range)	99.5 (53.26-2.04)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.97 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.250 , 0.282	Depositor
$R, R_{free}$	0.253 , $0.283$	DCC
$R_{free}$ test set	2726 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 35.8	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<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	Во	ond angles
WIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.70	0/828	0.90	0/1124
1	В	0.68	0/787	0.90	2/1069 (0.2%)
1	С	0.67	0/764	0.92	2/1034 (0.2%)
1	D	0.70	0/795	0.96	3/1079 (0.3%)
1	Е	0.69	0/817	0.96	2/1109 (0.2%)
1	F	0.69	0/806	1.04	3/1094 (0.3%)
1	G	0.72	0/784	1.06	2/1065~(0.2%)
1	Н	0.70	0/787	1.01	4/1069 (0.4%)
All	All	0.69	0/6368	0.97	18/8643 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

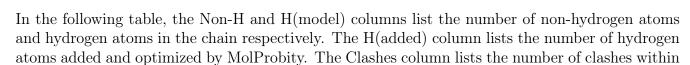
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\operatorname{Ideal}({}^{o})$
1	F	69	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	G	69	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	Н	69	ARG	NE-CZ-NH1	12.51	126.55	120.30
1	Е	69	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	Н	69	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	В	69	ARG	NE-CZ-NH1	-9.28	115.66	120.30
1	С	69	ARG	NE-CZ-NH1	-9.27	115.67	120.30
1	D	69	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	G	69	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	F	69	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	D	69	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	F	4	CYS	CB-CA-C	7.48	125.36	110.40
1	В	69	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	С	69	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	Е	69	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	D	12	ARG	CB-CG-CD	5.85	126.82	111.60
1	Н	12	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	Н	12	ARG	NE-CZ-NH1	-5.21	117.69	120.30



There are no chirality outliers.

There are no planarity outliers.

#### 5.2 Too-close contacts (i)



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	807	0	780	17	0
1	В	769	0	750	12	0
1	С	747	0	726	16	0
1	D	777	0	759	15	0
1	Ε	797	0	773	17	0
1	F	787	0	766	12	0
1	G	766	0	748	41	0
1	Н	769	0	750	15	0
All	All	6219	0	6052	111	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 9.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:THR:O	1:G:26:LYS:HB3	1.74	0.87
1:D:87:LYS:HB3	1:D:100:GLU:HG3	1.61	0.81
1:C:66:TRP:CZ2	1:G:33:LEU:HD22	2.14	0.81
1:H:87:LYS:HB3	1:H:100:GLU:HG3	1.62	0.80
1:A:55:HIS:HB2	1:A:70:VAL:HG22	1.63	0.79
1:A:55:HIS:HB2	1:A:70:VAL:CG2	2.13	0.79
1:G:25:VAL:HA	1:G:29:ILE:HG12	1.66	0.78
1:C:66:TRP:HZ2	1:G:33:LEU:HD22	1.49	0.78
1:E:87:LYS:HB2	1:E:100:GLU:HG3	1.65	0.77
1:C:55:HIS:HB2	1:C:70:VAL:HG13	1.67	0.75
1:C:31:GLN:HE22	1:C:101:HIS:HB2	1.50	0.75
1:A:61:HIS:HA	1:D:39:GLU:O	1.89	0.72
1:G:25:VAL:HG11	1:G:40:VAL:HG21	1.77	0.66
1:A:31:GLN:HB3	1:A:103:HIS:CG	2.31	0.66
1:E:15:ASN:O	1:E:19:GLN:HG2	1.95	0.66



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Continuea from pre-		Interatomic	Clash	
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)	
1:C:66:TRP:CZ2	1:G:33:LEU:CD2	2.80	0.65	
1:C:97:TYR:CE1	1:G:80:LYS:HE2	2.31	0.65	
1:A:31:GLN:HE21	1:H:96:THR:HG22	1.62	0.65	
1:G:32:GLN:HG3	1:G:33:LEU:HG	1.80	0.63	
1:C:58:LYS:HE2	1:C:65:CYS:SG	2.40	0.62	
1:G:31:GLN:O	1:G:32:GLN:HG2	1.99	0.61	
1:E:86:HIS:HD2	1:H:28:TYR:OH	1.83	0.60	
1:E:58:LYS:HE2	1:E:91:VAL:HA	1.83	0.60	
1:D:81:VAL:HG23	1:D:81:VAL:O	2.01	0.60	
1:G:82:GLU:HG3	1:G:84:HIS:CE1	2.37	0.59	
1:A:70:VAL:HG21	1:D:21:LEU:HD22	1.84	0.59	
1:G:81:VAL:HG23	1:G:81:VAL:O	2.03	0.58	
1:G:22:THR:HG23	1:G:23:PRO:HD3	1.84	0.58	
1:G:23:PRO:O	1:G:24:VAL:HG23	2.03	0.58	
1:A:50:VAL:HG21	1:D:54:ASN:ND2	2.18	0.57	
1:C:61:HIS:HA	1:G:39:GLU:O	2.04	0.57	
1:G:34:GLY:O	1:G:35:ARG:HG2	2.04	0.57	
1:E:21:LEU:HD13	1:H:57:LEU:HD21	1.87	0.57	
1:G:51:ASN:HD21	1:H:51:ASN:HD21	1.53	0.56	
1:A:57:LEU:HB2	1:A:68:VAL:CG1	2.35	0.56	
1:G:23:PRO:HA	1:G:26:LYS:HD2	1.89	0.55	
1:F:58:LYS:HE2	1:F:91:VAL:O	2.08	0.53	
1:C:58:LYS:CE	1:C:65:CYS:SG	2.97	0.53	
1:G:22:THR:O	1:G:24:VAL:N	2.42	0.53	
1:D:58:LYS:HE3	1:D:65:CYS:SG	2.50	0.52	
1:C:21:LEU:HD13	1:G:57:LEU:HD21	1.93	0.52	
1:A:86:HIS:HD2	1:D:28:TYR:OH	1.93	0.51	
1:B:57:LEU:HB2	1:B:68:VAL:CG1	2.40	0.51	
1:E:57:LEU:HB2	1:E:68:VAL:CG1	2.39	0.51	
1:A:58:LYS:HE2	1:A:91:VAL:O	2.11	0.51	
1:G:58:LYS:HE2	1:G:91:VAL:O	2.10	0.50	
1:G:29:ILE:HD11	1:G:37:PRO:CB	2.42	0.50	
1:D:82:GLU:HG3	1:D:84:HIS:CE1	2.46	0.49	
1:B:97:TYR:OH	1:F:82:GLU:OE2	2.16	0.49	
1:E:83:VAL:O	1:H:101:HIS:HE1	1.95	0.49	
1:G:12:ARG:H	1:G:12:ARG:CD	2.26	0.49	
1:B:86:HIS:HD2	1:F:28:TYR:OH	1.95	0.48	
1:G:31:GLN:NE2	1:G:32:GLN:HE21	2.11	0.48	
1:B:39:GLU:O	1:F:61:HIS:HA	2.14	0.48	
1:G:22:THR:HG23	1:G:23:PRO:CD	2.44	0.47	
1:E:51:ASN:ND2	1:G:77:TYR:OH	2.40	0.47	



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Continuea from pre		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:F:100:GLU:O	1:F:101:HIS:HB2	2.14	0.47
1:C:83:VAL:O	1:G:101:HIS:HE1	1.98	0.47
1:E:58:LYS:HE3	1:E:65:CYS:SG	2.55	0.47
1:F:36:GLU:OE2	1:F:37:PRO:O	2.32	0.47
1:D:81:VAL:O	1:D:81:VAL:CG2	2.63	0.46
1:A:44:GLU:HB2	1:D:58:LYS:HB3	1.97	0.46
1:G:15:ASN:O	1:G:18:LYS:N	2.47	0.45
1:C:54:ASN:ND2	1:G:50:VAL:HG21	2.31	0.45
1:G:28:TYR:O	1:G:31:GLN:O	2.34	0.45
1:G:17:ASP:O	1:G:21:LEU:HB3	2.17	0.45
1:G:23:PRO:HA	1:G:26:LYS:CD	2.46	0.45
1:A:57:LEU:HB2	1:A:68:VAL:HG12	1.98	0.45
1:A:84:HIS:ND1	1:A:84:HIS:C	2.69	0.45
1:E:50:VAL:HG21	1:H:54:ASN:ND2	2.32	0.45
1:E:84:HIS:O	1:E:85:SER:HB3	2.17	0.45
1:F:84:HIS:O	1:F:85:SER:HB3	2.17	0.45
1:D:72:GLU:HG3	1:D:81:VAL:HG12	1.99	0.44
1:D:58:LYS:NZ	1:D:67:HIS:HE1	2.15	0.44
1:B:74:LEU:HB3	1:D:4:CYS:SG	2.58	0.44
1:C:39:GLU:O	1:G:61:HIS:HA	2.18	0.44
1:E:83:VAL:O	1:H:101:HIS:CE1	2.70	0.44
1:G:39:GLU:HB3	1:G:41:LYS:HE2	2.00	0.44
1:F:26:LYS:HE3	1:F:36:GLU:HG3	2.00	0.44
1:C:50:VAL:HG21	1:G:54:ASN:ND2	2.33	0.43
1:B:83:VAL:HG11	1:F:28:TYR:CB	2.48	0.43
1:A:84:HIS:CE1	1:A:85:SER:HB3	2.53	0.43
1:E:12:ARG:HD2	1:E:43:THR:O	2.19	0.43
1:E:39:GLU:O	1:H:61:HIS:HA	2.19	0.43
1:A:39:GLU:O	1:D:61:HIS:HA	2.18	0.43
1:G:84:HIS:O	1:G:85:SER:HB3	2.19	0.43
1:E:82:GLU:OE2	1:E:84:HIS:HE1	2.02	0.42
1:H:69:ARG:HD2	1:H:84:HIS:HB2	2.01	0.42
1:A:57:LEU:HB2	1:A:68:VAL:HG13	2.01	0.42
1:B:82:GLU:OE2	1:B:84:HIS:HE1	2.02	0.42
1:G:69:ARG:HD2	1:G:84:HIS:HB2	2.02	0.42
1:G:17:ASP:O	1:G:21:LEU:CB	2.68	0.42
1:H:80:LYS:HE3	1:H:82:GLU:OE2	2.19	0.42
1:G:20:LEU:O	1:G:23:PRO:HD2	2.19	0.42
1:B:13:PRO:HG2	1:B:18:LYS:HE2	2.01	0.42
1:B:58:LYS:HE3	1:B:65:CYS:SG	2.59	0.42
1:E:86:HIS:CD2	1:H:28:TYR:OH	2.70	0.41



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:B:22:THR:HB	1:B:23:PRO:HD3	2.01	0.41
1:F:35:ARG:HE	1:F:35:ARG:HB3	1.66	0.41
1:H:13:PRO:HG2	1:H:18:LYS:HE3	2.02	0.41
1:A:84:HIS:ND1	1:A:85:SER:HB3	2.36	0.41
1:B:83:VAL:HG11	1:F:28:TYR:HB2	2.02	0.41
1:C:10:SER:HB3	1:C:44:GLU:OE2	2.21	0.41
1:G:81:VAL:O	1:G:81:VAL:CG2	2.66	0.41
1:C:57:LEU:HD13	1:G:42:ILE:HD13	2.02	0.41
1:G:26:LYS:HD3	1:G:27:ASP:CB	2.49	0.41
1:E:24:VAL:HG21	1:H:81:VAL:CG1	2.51	0.41
1:B:57:LEU:HB2	1:B:68:VAL:HG13	2.03	0.40
1:D:22:THR:HB	1:D:23:PRO:HD3	2.03	0.40
1:F:22:THR:HB	1:F:23:PRO:HD3	2.02	0.40
1:H:36:GLU:OE1	1:H:37:PRO:HD2	2.21	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	A	100/106 (94%)	100 (100%)	0	0	100	100
1	В	96/106 (91%)	96 (100%)	0	0	100	100
1	С	90/106 (85%)	90 (100%)	0	0	100	100
1	D	97/106 (92%)	97 (100%)	0	0	100	100
1	E	99/106 (93%)	99 (100%)	0	0	100	100
1	F	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
1	G	96/106 (91%)	86 (90%)	4 (4%)	6 (6%)	1	0
1	Н	96/106 (91%)	96 (100%)	0	0	100	100
All	All	772/848 (91%)	760 (98%)	6 (1%)	6 (1%)	19	10



All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	24	VAL
1	G	14	SER
1	G	26	LYS
1	G	16	GLU
1	G	13	PRO
1	G	27	ASP

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	91/95 (96%)	86 (94%)	5 (6%)	21 13
1	В	87/95~(92%)	83 (95%)	4 (5%)	27 19
1	C	84/95 (88%)	75 (89%)	9 (11%)	6 2
1	D	88/95 (93%)	81 (92%)	7 (8%)	12 5
1	E	90/95~(95%)	84 (93%)	6 (7%)	16 9
1	F	89/95 (94%)	82 (92%)	7 (8%)	12 5
1	G	86/95 (90%)	74 (86%)	12 (14%)	3 1
1	Н	87/95 (92%)	83 (95%)	4 (5%)	27 19
All	All	702/760~(92%)	648 (92%)	54 (8%)	13 5

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	58	LYS
1	A	65	CYS
1	A	76	CYS
1	A	91	VAL
1	В	53	THR
1	В	83	VAL
1	В	95	LEU



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Mol	Chain	Res	Type
1	В	99	LEU
1	D	3	MET
1	D	12	ARG
1	D	26	LYS
1	D	35	ARG
1	D	51	ASN
1	D	99	LEU
1	D	101	HIS
1	F	31	GLN
1	F F F F	35	ARG
1	F	50	VAL
1	F	53	THR
1	F	58	LYS
1	F	95	LYS LEU
1	F C C C C C C C C C C C E	99	LEU
1	С	12	ARG
1	С	62	ASP
1	С	64	ASP ASN CYS
1	С	65	CYS
1	С	70	VAL
1	С	76	CYS
1	С	87	LYS
1	С	99	LEU
1	С	102	HIS
1	Е	3	MET
1	Е	38	SER
1	Е	53	THR
1	Е	95	LEU
1	Е	99	LEU
1	Е	103	HIS
1	G	9	THR
1	G	12	ARG
1	G G	22	THR
1	G	25	VAL LYS
1	G	26	LYS
1	G	32	GLN
1	G	36	GLU
1	G	40	VAL
1	G	41	LYS
1	G	53	THR
1	G	99	LEU
1	G	100	GLU



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Mol	Chain	Res	Type
1	Н	12	ARG
1	Н	53	THR
1	Н	95	LEU
1	Н	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	32	GLN
1	A	55	HIS
1	A A A	86	HIS HIS
1	A B	103	HIS HIS
1	В	67	HIS
1	B B	84	HIS HIS
1	В	86	HIS
1	В	101	HIS
1	D	51	ASN
1	D D	61	HIS
1	D	67	HIS
1	D	84	HIS
1	F	31	GLN
1	F	32	GLN
1	F	61	HIS
1	F F F C C C C	84	GLN HIS HIS
1	С	31	GLN
1	С	51	GLN ASN
1	С	55	HIS HIS
1	С	61	HIS
1	Е	51	ASN
1	Е	67	HIS
1	Е	84	HIS
1	Е	86	HIS
1	Е	101	HIS
1	G	31	GLN
1	G	51	ASN
1	G	61	HIS
1	G	67	HIS
1	G	84	HIS
1	G	101	HIS
1	Н	55	HIS
1	Н	61	HIS



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Mol	Chain	Res	Type
1	Н	84	HIS
1	Н	101	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)

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	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	102/106~(96%)	0.23	4 (3%) 39 42	31, 41, 59, 70	0
1	В	98/106 (92%)	0.29	2 (2%) 65 69	30, 48, 78, 90	0
1	С	94/106 (88%)	0.38	5 (5%) 26 28	34, 52, 83, 98	0
1	D	99/106 (93%)	0.21	1 (1%) 82 84	27, 43, 77, 97	0
1	E	101/106 (95%)	0.15	2 (1%) 65 69	29, 43, 67, 92	0
1	F	100/106 (94%)	0.35	3 (3%) 50 54	29, 46, 90, 122	0
1	G	98/106 (92%)	1.02	23 (23%) 0 0	33, 56, 113, 124	0
1	Н	98/106 (92%)	0.21	2 (2%) 65 69	28, 41, 79, 102	0
All	All	790/848 (93%)	0.35	42 (5%) 26 28	27, 46, 87, 124	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	33	LEU	10.4
1	G	39	GLU	5.5
1	G	25	VAL	4.3
1	Н	39	GLU	4.3
1	G	29	ILE	4.3
1	G	16	GLU	4.2
1	G	26	LYS	4.2
1	F	38	SER	4.0
1	G	17	ASP	3.8
1	G	23	PRO	3.8
1	G	41	LYS	3.8
1	G	38	SER	3.6
1	Е	103	HIS	3.5
1	G	37	PRO	3.4
1	G	40	VAL	3.3
1	С	58	LYS	3.2



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Mol	Chain	Res	Type	RSRZ
1	G	31	GLN	3.1
1	G	12	ARG	3.1
1	G	21	LEU	3.0
1	С	61	HIS	2.9
1	G	36	GLU	2.9
1	С	60	GLU	2.8
1	Е	34	GLY	2.8
1	F	37	PRO	2.7
1	A	65	CYS	2.7
1	С	39	GLU	2.6
1	G	27	ASP	2.5
1	G	32	GLN	2.5
1	G	35	ARG	2.4
1	G	19	GLN	2.4
1	G	34	GLY	2.4
1	G	45	VAL	2.3
1	Н	38	SER	2.3
1	A	84	HIS	2.2
1	В	89	ALA	2.2
1	В	31	GLN	2.2
1	A	35	ARG	2.2
1	F	39	GLU	2.1
1	A	4	CYS	2.1
1	С	65	CYS	2.1
1	G	15	ASN	2.0
1	D	49	ILE	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.

