



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2025 – 10:13 PM JST

PDB ID : 9UOZ / pdb_00009uoz
Title : Structure of Echinococcus multilocularis Cystatin B
Authors : Huang, S.Q.; Hong, W.B.
Deposited on : 2025-04-27
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

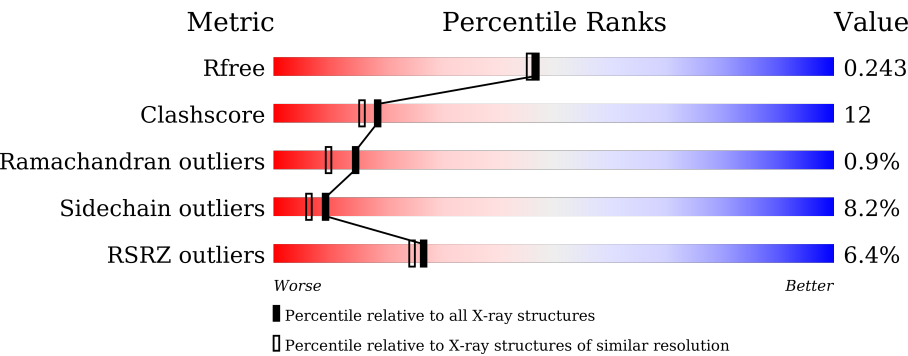
MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	106	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>76%17%... .</div></div>
1	B	106	<div><div></div><div></div><div></div><div></div><div></div></div> <div>4%72%19%..8%</div>
1	C	106	<div><div></div><div></div><div></div><div></div><div></div></div> <div>9%75%14%5%6%</div>
1	D	106	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%73%19%..6%</div>
1	E	106	<div><div></div><div></div><div></div><div></div><div></div></div> <div>4%67%24%5%5%</div>
1	F	106	<div><div></div><div></div><div></div><div></div><div></div></div> <div>5%72%19%..6%</div>

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Mol	Chain	Length	Quality of chain
1	G	106	<div><div></div><div>23%</div><div>49%</div><div>29%</div><div>8%</div><div>6%</div><div>8%</div></div>
1	H	106	<div>%<div><div></div><div>76%</div><div>14%</div><div>..</div><div>8%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6647 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	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	1	0
			824	516	153	151	4			
1	B	98	Total	C	N	O	S	0	0	0
			769	482	139	145	3			
1	D	100	Total	C	N	O	S	0	0	0
			784	492	141	147	4			
1	F	100	Total	C	N	O	S	0	0	0
			787	493	143	147	4			
1	C	100	Total	C	N	O	S	0	0	0
			787	493	143	147	4			
1	E	101	Total	C	N	O	S	0	0	0
			797	499	146	148	4			
1	G	98	Total	C	N	O	S	0	0	0
			769	482	139	145	3			
1	H	98	Total	C	N	O	S	0	0	0
			769	482	139	145	3			

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
B	99	LEU	-	expression tag	UNP A0A087VZV0
B	100	GLU	-	expression tag	UNP A0A087VZV0
B	101	HIS	-	expression tag	UNP A0A087VZV0
B	102	HIS	-	expression tag	UNP A0A087VZV0
B	103	HIS	-	expression tag	UNP A0A087VZV0

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

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

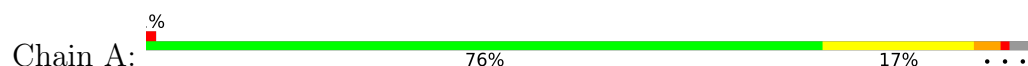
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	36	Total O 36 36	0	0
2	D	46	Total O 46 46	0	0
2	F	42	Total O 42 42	0	0
2	C	27	Total O 27 27	0	0
2	E	51	Total O 51 51	0	0
2	G	39	Total O 39 39	0	0
2	H	64	Total O 64 64	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: Cystatin B Stefin B



- Molecule 1: Cystatin B Stefin B



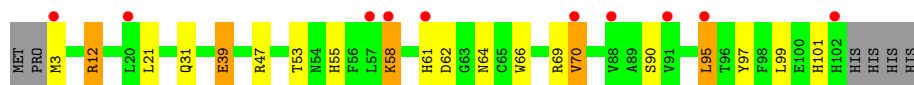
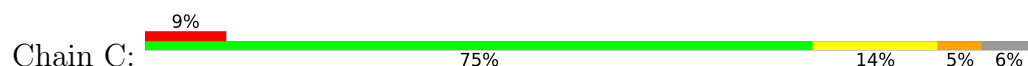
- Molecule 1: Cystatin B Stefin B



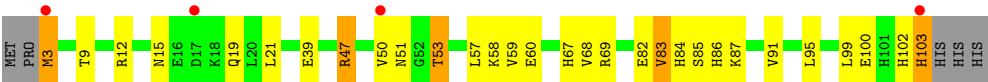
- Molecule 1: Cystatin B Stefin B



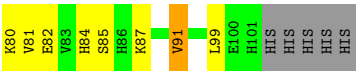
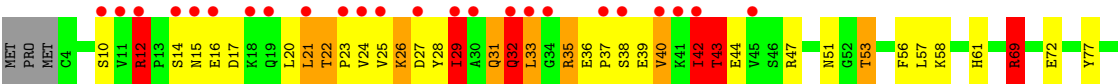
- Molecule 1: Cystatin B Stefin B



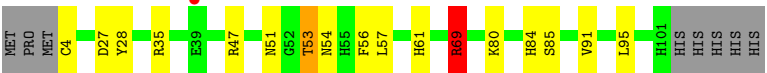
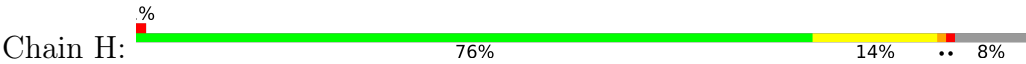
- Molecule 1: Cystatin B Stefin B



● Molecule 1: Cystatin B Stefin B



● Molecule 1: Cystatin B Stefin B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.77Å 66.11Å 92.60Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	37.25 – 2.00 37.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.25-2.00) 98.8 (37.25-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.211 , 0.240 0.216 , 0.243	Depositor DCC
R_{free} test set	2798 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/847	1.09	5/1150 (0.4%)
1	B	0.61	0/787	1.04	3/1069 (0.3%)
1	C	0.56	0/806	1.03	3/1094 (0.3%)
1	D	0.67	0/803	1.08	5/1090 (0.5%)
1	E	0.65	0/817	1.12	5/1109 (0.5%)
1	F	0.64	0/806	1.09	3/1094 (0.3%)
1	G	0.67	0/787	1.29	8/1069 (0.7%)
1	H	0.61	0/787	1.08	4/1069 (0.4%)
All	All	0.64	0/6440	1.10	36/8744 (0.4%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	3
1	H	0	1
All	All	0	10

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	ARG	CD-NE-CZ	9.72	138.01	124.40
1	H	69	ARG	CD-NE-CZ	8.91	136.87	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	HIS	CA-CB-CG	-7.83	105.97	113.80
1	F	69	ARG	NE-CZ-NH1	7.74	129.24	121.50
1	G	69	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	H	69	ARG	NE-CZ-NH1	7.54	129.04	121.50
1	G	69	ARG	CD-NE-CZ	7.47	134.86	124.40
1	F	69	ARG	NE-CZ-NH2	-7.12	112.79	119.20
1	H	69	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	E	83	VAL	N-CA-CB	7.00	118.16	110.53
1	C	69	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	G	69	ARG	NE-CZ-NH2	-6.78	113.10	119.20
1	B	69	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	D	69	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	E	60	GLU	CB-CG-CD	6.43	123.53	112.60
1	D	69	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	G	14	SER	CA-C-O	-6.33	115.69	119.55
1	D	69	ARG	CD-NE-CZ	6.32	133.25	124.40
1	G	43	THR	N-CA-CB	6.27	121.08	110.49
1	D	27	ASP	CA-CB-CG	6.24	118.84	112.60
1	E	69	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	B	69	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	61	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	D	93	ASP	CA-CB-CG	5.78	118.38	112.60
1	E	69	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	G	12	ARG	CA-CB-CG	5.54	125.18	114.10
1	B	83	VAL	N-CA-CB	5.48	116.51	110.53
1	G	87	LYS	CB-CG-CD	5.47	123.88	111.30
1	C	12	ARG	CA-CB-CG	5.30	124.71	114.10
1	C	69	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	91	VAL	N-CA-CB	5.18	119.51	110.65
1	G	36	GLU	CB-CA-C	5.09	120.20	110.17
1	H	69	ARG	CB-CG-CD	5.05	122.92	111.30
1	A	60	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	61	HIS	CB-CG-ND1	5.04	130.26	122.70
1	E	102	HIS	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	B	47	ARG	Sidechain
1	C	47	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	47	ARG	Sidechain
1	E	47	ARG	Sidechain
1	F	47	ARG	Sidechain
1	G	12	ARG	Sidechain
1	G	35	ARG	Sidechain
1	G	47	ARG	Sidechain
1	H	47	ARG	Sidechain

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	A	824	0	794	17	0
1	B	769	0	750	15	0
1	C	787	0	766	21	0
1	D	784	0	767	16	0
1	E	797	0	773	22	0
1	F	787	0	766	16	0
1	G	769	0	750	58	0
1	H	769	0	750	15	0
2	A	56	0	0	3	0
2	B	36	0	0	4	0
2	C	27	0	0	0	0
2	D	46	0	0	4	0
2	E	51	0	0	9	0
2	F	42	0	0	4	0
2	G	39	0	0	4	0
2	H	64	0	0	11	0
All	All	6647	0	6116	146	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 12.

All (146) 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:E:59:VAL:HB	2:E:246:HOH:O	1.25	1.36
1:C:66:TRP:CH2	1:G:33:LEU:HD13	1.78	1.17
1:G:20:LEU:O	1:G:23:PRO:HD2	1.49	1.13
1:C:66:TRP:HH2	1:G:33:LEU:HD13	1.21	0.95
1:E:87:LYS:HB2	1:E:100:GLU:HG3	1.49	0.93
1:G:32:GLN:HG3	1:G:33:LEU:HG	1.50	0.93
1:F:49:ILE:HD11	2:F:229:HOH:O	1.69	0.92
1:C:66:TRP:CZ3	1:G:33:LEU:HD13	2.07	0.90
1:A:55:HIS:HB2	1:A:70:VAL:CG2	2.02	0.89
1:G:29:ILE:HA	1:G:33:LEU:HD12	1.59	0.84
1:C:66:TRP:HH2	1:G:33:LEU:CD1	1.89	0.84
1:G:32:GLN:CG	1:G:33:LEU:HG	2.07	0.84
1:C:66:TRP:CH2	1:G:33:LEU:CD1	2.62	0.83
1:B:87:LYS:HB2	1:B:100:GLU:HG3	1.61	0.82
1:A:55:HIS:HB2	1:A:70:VAL:HG22	1.59	0.82
1:G:22:THR:HG23	1:G:23:PRO:HD3	1.63	0.81
1:F:87:LYS:HB3	1:F:100:GLU:HG3	1.59	0.80
1:C:58:LYS:HB2	1:C:95:LEU:CD2	2.12	0.78
1:H:4:CYS:HB2	2:H:224:HOH:O	1.83	0.77
1:B:101:HIS:C	2:B:220:HOH:O	2.27	0.76
1:H:80:LYS:HD2	2:H:261:HOH:O	1.88	0.73
1:C:61:HIS:HA	1:G:39:GLU:O	1.89	0.72
1:E:53:THR:HG22	2:E:249:HOH:O	1.87	0.72
1:C:58:LYS:HB2	1:C:95:LEU:HD21	1.71	0.71
1:G:25:VAL:HG23	1:G:40:VAL:HG21	1.71	0.70
1:G:29:ILE:HD11	1:G:37:PRO:HG3	1.74	0.70
1:E:103:HIS:HA	2:E:222:HOH:O	1.91	0.70
1:A:23:PRO:HB3	1:E:9:THR:HG21	1.75	0.69
1:C:66:TRP:HZ3	1:G:29:ILE:HG22	1.59	0.67
1:G:28:TYR:O	1:G:29:ILE:HG23	1.95	0.66
1:C:31:GLN:HE22	1:C:101:HIS:HB2	1.61	0.66
1:C:66:TRP:CZ3	1:G:29:ILE:HG22	2.31	0.66
1:A:61:HIS:HA	1:D:39:GLU:O	1.96	0.65
1:A:15:ASN:ND2	2:A:201:HOH:O	2.29	0.65
1:E:53:THR:CG2	2:E:249:HOH:O	2.44	0.64
1:E:21:LEU:HD13	1:H:57:LEU:HD21	1.80	0.63
1:C:97:TYR:CE1	1:G:80:LYS:HE2	2.35	0.62
1:G:27:ASP:O	1:G:31:GLN:HB2	2.00	0.62
1:G:27:ASP:O	1:G:31:GLN:N	2.28	0.62
1:F:53:THR:HG23	2:F:207:HOH:O	1.99	0.62
1:C:58:LYS:HB2	1:C:95:LEU:HD23	1.82	0.61
1:H:85:SER:HB3	2:H:207:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ASN:O	1:E:19:GLN:HG2	2.01	0.60
1:C:62:ASP:OD1	1:G:38:SER:HB3	2.01	0.60
1:A:84:HIS:C	1:A:84:HIS:ND1	2.59	0.60
1:A:50:VAL:HG21	1:D:54:ASN:ND2	2.17	0.59
1:C:66:TRP:HH2	1:G:33:LEU:CG	2.15	0.59
1:E:86:HIS:HD2	1:H:28:TYR:OH	1.88	0.57
1:G:29:ILE:HA	1:G:33:LEU:CD1	2.31	0.57
1:G:53:THR:HG23	2:G:214:HOH:O	2.05	0.56
1:H:80:LYS:CD	2:H:261:HOH:O	2.51	0.56
1:H:84:HIS:HD2	2:H:211:HOH:O	1.87	0.56
1:C:66:TRP:CH2	1:G:33:LEU:HD22	2.41	0.55
1:E:47:ARG:NE	2:E:201:HOH:O	2.37	0.55
1:G:84:HIS:HD2	2:G:216:HOH:O	1.89	0.55
1:B:53:THR:HG23	2:B:213:HOH:O	2.06	0.55
1:G:51:ASN:HD21	1:H:51:ASN:HD21	1.54	0.54
1:G:85:SER:HB3	2:G:227:HOH:O	2.08	0.54
1:E:85:SER:HB2	2:E:214:HOH:O	2.08	0.54
1:A:31:GLN:HB3	1:A:103:HIS:CG	2.44	0.53
1:C:55:HIS:HB2	1:C:70:VAL:HG13	1.89	0.53
1:G:32:GLN:HG2	1:G:33:LEU:HG	1.87	0.53
1:F:58:LYS:HE2	1:F:91:VAL:O	2.08	0.53
1:B:86:HIS:HD2	1:F:28:TYR:OH	1.91	0.53
1:G:31:GLN:HE22	1:G:35:ARG:CZ	2.21	0.53
1:B:85:SER:HB2	2:B:215:HOH:O	2.10	0.52
1:G:20:LEU:C	1:G:23:PRO:HD2	2.30	0.52
1:B:71:HIS:HD2	2:B:224:HOH:O	1.91	0.52
1:H:80:LYS:HE2	2:H:218:HOH:O	2.07	0.52
1:G:24:VAL:O	1:G:28:TYR:O	2.28	0.52
1:C:21:LEU:HD13	1:G:57:LEU:HD21	1.92	0.51
1:E:57:LEU:HB2	1:E:68:VAL:CG1	2.39	0.51
1:D:81:VAL:HG23	1:D:81:VAL:O	2.10	0.51
1:A:12:ARG:NH1	2:A:206:HOH:O	2.44	0.51
1:G:29:ILE:CD1	1:G:37:PRO:HG3	2.39	0.51
1:H:53:THR:HG23	2:H:225:HOH:O	2.11	0.51
1:A:58:LYS:HE2	1:A:91:VAL:O	2.11	0.50
1:G:42:ILE:O	1:G:43:THR:OG1	2.23	0.50
1:G:81:VAL:HG23	1:G:81:VAL:O	2.12	0.49
1:G:58:LYS:HE2	1:G:91:VAL:O	2.13	0.49
1:E:84:HIS:HD2	2:E:219:HOH:O	1.96	0.48
1:G:31:GLN:C	1:G:32:GLN:O	2.57	0.48
1:E:91:VAL:HG23	2:E:224:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:TRP:CZ2	1:G:33:LEU:HD22	2.49	0.48
1:G:28:TYR:O	1:G:29:ILE:HG12	2.14	0.47
1:G:21:LEU:C	1:G:21:LEU:HD13	2.39	0.47
1:G:22:THR:O	1:G:25:VAL:HG12	2.15	0.47
1:H:27:ASP:HB2	2:H:209:HOH:O	2.13	0.47
1:D:84:HIS:HD2	2:D:225:HOH:O	1.97	0.46
1:A:86:HIS:HD2	1:D:28:TYR:OH	1.98	0.46
1:B:57:LEU:HD22	1:F:45:VAL:HG12	1.97	0.46
1:A:70:VAL:HG21	1:D:21:LEU:HD22	1.96	0.46
1:D:58:LYS:NZ	1:D:67:HIS:HE1	2.14	0.46
1:B:97:TYR:CE1	1:F:80:LYS:HE2	2.51	0.46
1:D:58:LYS:HE2	1:D:91:VAL:O	2.17	0.45
1:A:35:ARG:NH1	2:A:209:HOH:O	2.49	0.45
1:F:13:PRO:HG2	1:F:18:LYS:HE3	1.99	0.45
1:G:32:GLN:C	1:G:33:LEU:HG	2.42	0.45
1:D:49:ILE:HD13	1:D:50:VAL:N	2.33	0.44
1:G:32:GLN:O	1:G:33:LEU:CB	2.63	0.44
1:H:56:PHE:CE1	1:H:69:ARG:HG3	2.52	0.44
1:F:31:GLN:NE2	1:F:32:GLN:OE1	2.50	0.44
1:A:39:GLU:O	1:D:61:HIS:HA	2.18	0.44
1:B:97:TYR:OH	1:F:82:GLU:OE2	2.36	0.44
1:B:58:LYS:NZ	1:B:67:HIS:HE1	2.16	0.43
1:D:72:GLU:HG3	1:D:81:VAL:HG12	1.98	0.43
1:F:84:HIS:HD2	2:F:209:HOH:O	1.99	0.43
1:F:56:PHE:CE1	1:F:69:ARG:HG3	2.53	0.43
1:G:15:ASN:O	1:G:17:ASP:N	2.51	0.43
1:G:28:TYR:C	1:G:29:ILE:HG23	2.43	0.43
1:B:58:LYS:HE2	1:B:91:VAL:O	2.19	0.43
1:H:35:ARG:NH2	2:H:203:HOH:O	2.51	0.43
1:F:69:ARG:HD3	2:F:209:HOH:O	2.18	0.43
1:G:42:ILE:O	1:G:43:THR:CB	2.66	0.43
1:E:58:LYS:NZ	1:E:67:HIS:HE1	2.17	0.43
1:C:66:TRP:CH2	1:G:33:LEU:CD2	3.02	0.42
1:G:25:VAL:HG23	1:G:40:VAL:CG2	2.44	0.42
1:G:42:ILE:HG22	1:G:43:THR:H	1.83	0.42
1:E:50:VAL:HG21	1:H:54:ASN:ND2	2.35	0.42
1:G:42:ILE:HG22	1:G:43:THR:N	2.34	0.42
1:A:101:HIS:HE1	1:D:83:VAL:O	2.01	0.42
1:E:82:GLU:OE2	1:E:84:HIS:HE1	2.01	0.42
1:G:25:VAL:CG2	1:G:40:VAL:HG21	2.43	0.42
1:D:51:ASN:C	1:D:51:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:HD3	2:D:225:HOH:O	2.19	0.42
1:E:58:LYS:HE2	1:E:91:VAL:O	2.19	0.42
1:G:56:PHE:CE1	1:G:69:ARG:HG3	2.55	0.42
1:E:39:GLU:HG2	2:H:239:HOH:O	2.20	0.42
1:E:57:LEU:HB2	1:E:68:VAL:HG12	2.01	0.42
1:D:84:HIS:CD2	2:D:225:HOH:O	2.73	0.42
1:G:26:LYS:O	1:G:28:TYR:N	2.52	0.42
1:G:72:GLU:HG3	1:G:81:VAL:HG12	2.02	0.42
1:H:61:HIS:HD2	2:H:235:HOH:O	2.02	0.41
1:E:51:ASN:ND2	1:G:77:TYR:OH	2.45	0.41
1:G:84:HIS:CD2	2:G:216:HOH:O	2.69	0.41
1:A:70:VAL:O	1:A:70:VAL:HG23	2.21	0.41
1:B:39:GLU:O	1:F:61:HIS:HA	2.21	0.41
1:E:3:MET:N	2:E:205:HOH:O	2.53	0.41
1:G:10:SER:HB3	1:G:44:GLU:HG2	2.03	0.41
1:C:39:GLU:O	1:G:61:HIS:HA	2.21	0.40
1:B:82:GLU:OE2	1:B:84:HIS:HE1	2.04	0.40
1:B:83:VAL:HG11	1:F:28:TYR:CB	2.51	0.40
1:D:53:THR:HG23	2:D:215:HOH:O	2.21	0.40
1:A:71[B]:HIS:CE1	1:A:84:HIS:HB2	2.56	0.40
1:B:13:PRO:HG2	1:B:18:LYS:HE3	2.04	0.40
1:F:87:LYS:CB	1:F:100:GLU:HG3	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
1	B	96/106 (91%)	96 (100%)	0	0	100	100
1	C	98/106 (92%)	98 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	98/106 (92%)	98 (100%)	0	0	100	100
1	E	99/106 (93%)	99 (100%)	0	0	100	100
1	F	98/106 (92%)	98 (100%)	0	0	100	100
1	G	96/106 (91%)	85 (88%)	4 (4%)	7 (7%)	1	0
1	H	96/106 (91%)	96 (100%)	0	0	100	100
All	All	783/848 (92%)	771 (98%)	5 (1%)	7 (1%)	14	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	16	GLU
1	G	32	GLN
1	G	26	LYS
1	G	43	THR
1	G	33	LEU
1	G	42	ILE
1	G	29	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	93/95 (98%)	88 (95%)	5 (5%)	18	16
1	B	87/95 (92%)	83 (95%)	4 (5%)	23	21
1	C	89/95 (94%)	79 (89%)	10 (11%)	5	3
1	D	89/95 (94%)	83 (93%)	6 (7%)	13	10
1	E	90/95 (95%)	83 (92%)	7 (8%)	10	7
1	F	89/95 (94%)	80 (90%)	9 (10%)	6	3
1	G	87/95 (92%)	74 (85%)	13 (15%)	2	1
1	H	87/95 (92%)	83 (95%)	4 (5%)	23	21
All	All	711/760 (94%)	653 (92%)	58 (8%)	9	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	53	THR
1	A	59	VAL
1	A	91	VAL
1	A	99	LEU
1	B	53	THR
1	B	80	LYS
1	B	83	VAL
1	B	95	LEU
1	D	3	MET
1	D	35	ARG
1	D	49	ILE
1	D	53	THR
1	D	69	ARG
1	D	99	LEU
1	F	3	MET
1	F	35	ARG
1	F	36	GLU
1	F	49	ILE
1	F	53	THR
1	F	58	LYS
1	F	69	ARG
1	F	95	LEU
1	F	99	LEU
1	C	3	MET
1	C	12	ARG
1	C	39	GLU
1	C	53	THR
1	C	58	LYS
1	C	64	ASN
1	C	70	VAL
1	C	90	SER
1	C	95	LEU
1	C	99	LEU
1	E	3	MET
1	E	12	ARG
1	E	53	THR
1	E	83	VAL
1	E	95	LEU
1	E	99	LEU
1	E	103	HIS
1	G	12	ARG

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Mol	Chain	Res	Type
1	G	21	LEU
1	G	22	THR
1	G	29	ILE
1	G	31	GLN
1	G	32	GLN
1	G	40	VAL
1	G	42	ILE
1	G	53	THR
1	G	69	ARG
1	G	82	GLU
1	G	91	VAL
1	G	99	LEU
1	H	53	THR
1	H	69	ARG
1	H	91	VAL
1	H	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	61	HIS
1	A	86	HIS
1	A	101	HIS
1	B	51	ASN
1	B	61	HIS
1	B	67	HIS
1	B	71	HIS
1	B	84	HIS
1	B	86	HIS
1	B	101	HIS
1	D	51	ASN
1	D	61	HIS
1	D	64	ASN
1	D	67	HIS
1	D	84	HIS
1	F	31	GLN
1	F	32	GLN
1	F	51	ASN
1	F	84	HIS
1	F	101	HIS
1	F	102	HIS

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	31	GLN
1	C	48	GLN
1	C	101	HIS
1	E	51	ASN
1	E	61	HIS
1	E	67	HIS
1	E	84	HIS
1	E	86	HIS
1	E	101	HIS
1	G	51	ASN
1	G	54	ASN
1	G	67	HIS
1	G	84	HIS
1	G	101	HIS
1	H	51	ASN
1	H	55	HIS
1	H	84	HIS
1	H	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	103/106 (97%)	0.29	1 (0%) 79 78	13, 34, 58, 66	1 (0%)
1	B	98/106 (92%)	0.56	4 (4%) 42 40	25, 42, 69, 82	0
1	C	100/106 (94%)	0.75	10 (10%) 14 13	28, 47, 84, 89	0
1	D	100/106 (94%)	0.32	2 (2%) 64 63	22, 36, 69, 101	0
1	E	101/106 (95%)	0.39	4 (3%) 43 41	26, 37, 64, 88	0
1	F	100/106 (94%)	0.49	5 (5%) 35 33	23, 41, 83, 118	0
1	G	98/106 (92%)	1.18	24 (24%) 2 2	26, 49, 110, 118	0
1	H	98/106 (92%)	0.21	1 (1%) 79 78	22, 35, 65, 99	0
All	All	798/848 (94%)	0.52	51 (6%) 27 25	13, 39, 84, 118	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	33	LEU	7.3
1	G	29	ILE	5.3
1	G	42	ILE	5.1
1	A	2	PRO	4.3
1	G	25	VAL	4.3
1	F	37	PRO	4.1
1	G	21	LEU	4.0
1	G	37	PRO	3.7
1	B	20	LEU	3.6
1	G	34	GLY	3.5
1	C	91	VAL	3.5
1	C	95	LEU	3.4
1	G	40	VAL	3.3
1	G	15	ASN	3.3
1	G	16	GLU	3.2
1	G	45	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	27	ASP	3.0
1	F	38	SER	3.0
1	G	11	VAL	3.0
1	G	41	LYS	3.0
1	G	19	GLN	3.0
1	E	103	HIS	2.9
1	F	40	VAL	2.8
1	F	36	GLU	2.8
1	G	32	GLN	2.7
1	B	91	VAL	2.6
1	C	102	HIS	2.6
1	G	23	PRO	2.6
1	C	88	VAL	2.5
1	E	17	ASP	2.4
1	F	3	MET	2.4
1	E	3	MET	2.4
1	G	10	SER	2.4
1	G	14	SER	2.4
1	G	24	VAL	2.4
1	G	18	LYS	2.3
1	G	30	ALA	2.3
1	B	90	SER	2.3
1	C	20	LEU	2.3
1	C	61	HIS	2.3
1	D	92	GLY	2.3
1	C	3	MET	2.3
1	E	50	VAL	2.3
1	C	70	VAL	2.2
1	G	12	ARG	2.2
1	G	38	SER	2.2
1	B	62	ASP	2.2
1	C	57	LEU	2.2
1	D	37	PRO	2.1
1	C	58	LYS	2.1
1	H	39	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.