

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

#### Sep 4, 2024 – 06:10 PM JST

PDB ID	:	8X0U
Title	:	Crystal structure of cupin-like fold protein StrC from Stachybotrys sp.g12
Authors	:	Wang, H.; Wang, W.G.
Deposited on	:	2023-11-06
Resolution	:	2.65  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 2.65 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	164625	$1003 \ (2.66-2.66)$
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	007	3%		
	A	207	77%	14%	9%
	- E		.% ■		
1	В	207	78%	.0% •	11%
			.% •		
1	С	207	81%	7%	12%
	-		2%		
1	D	207	77%	.2%	11%
			2%		
1	Ε	207	79%	13%	9%
			<u>%</u>		
1	F	207	81%	7%	11%



Contr	nued fron	<i>i</i> previous	page		
Mol	Chain	Length	Quality of chain		
1	G	207	78%	9%	12%
1	Н	207	75%	13%	12%
1	Ι	207	<b>% 7</b> 9%	11%	10%
1	J	207	75%	14%	11%
1	Κ	207	80%	9%	12%
1	L	207	.% <b>78</b> %	10%	12%





# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	190	Total	С	Ν	0	S	0	0	0
	A	169	1473	924	264	278	7	0	0	0
1	р	194	Total	С	Ν	0	S	0	0	0
	D	104	1427	894	258	268	7	0	0	0
1	С	189	Total	С	Ν	Ο	S	0	0	0
1	U	102	1411	884	256	264	7	0	0	0
1	а	184	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	104	1427	894	258	268	7	0	0	0
1	E	180	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
T	Ľ	105	1473	924	264	278	7	0	0	0
1	F	184	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Ľ	104	1427	894	258	268	7	0	0	0
1	G	182	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
-	u	102	1411	884	256	264	7	0	0	0
1	н	182	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	11	102	1411	884	256	264	7	0	0	0
1	т	186	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	T	100	1445	905	261	272	7	0	0	0
1	Т	184	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	0	104	1427	894	258	268	7	0	0	0
1	K	183	Total	$\mathbf{C}$	N	Ο	S	0	0	0
	17	100	1419	888	257	267	7	U	U	0
1	L	183	Total	C	Ν	Ο	S	0	0	0
		100	1419	888	257	267	7			U

• Molecule 1 is a protein called Cupin conserved barrel domain protein.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	6	Total O 6 6	0	0
2	В	14	Total         O           14         14	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	8	Total O 8 8	0	0
2	D	8	Total O 8 8	0	0
2	Е	5	Total O 5 5	0	0
2	F	13	Total         O           13         13	0	0
2	G	10	Total         O           10         10	0	0
2	Н	8	Total O 8 8	0	0
2	Ι	8	Total O 8 8	0	0
2	J	4	Total O 4 4	0	0
2	K	8	Total O 8 8	0	0
2	L	14	Total         O           14         14	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: Cupin conserved barrel domain protein







#### GLY ALA SER LYS





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	73.70Å 253.98Å 73.83Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $102.79^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	46.03 - 2.65	Depositor
Resolution (A)	46.03 - 2.65	EDS
% Data completeness	99.7(46.03-2.65)	Depositor
(in resolution range)	99.6 (46.03 - 2.65)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.65 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
P. P.	0.187 , $0.233$	Depositor
$n, n_{free}$	0.187 , $0.233$	DCC
$R_{free}$ test set	3711 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, $33.8$	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17276	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.13% 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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/1506	0.46	0/2045
1	В	0.25	0/1459	0.47	0/1982
1	С	0.25	0/1443	0.47	0/1960
1	D	0.25	0/1459	0.49	0/1982
1	Ε	0.25	0/1506	0.46	0/2045
1	F	0.25	0/1459	0.46	0/1982
1	G	0.25	0/1443	0.46	0/1960
1	Н	0.25	0/1443	0.47	0/1960
1	Ι	0.25	0/1477	0.47	0/2005
1	J	0.26	0/1459	0.48	0/1982
1	Κ	0.25	0/1451	0.47	0/1971
1	L	0.25	0/1451	0.46	0/1971
All	All	0.25	0/17556	0.47	0/23845

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	1473	0	1434	16	0
1	В	1427	0	1391	14	0
1	С	1411	0	1376	8	0
1	D	1427	0	1391	12	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	1473	0	1434	15	0
1	F	1427	0	1391	10	0
1	G	1411	0	1376	15	0
1	Н	1411	0	1376	15	0
1	Ι	1445	0	1410	13	0
1	J	1427	0	1391	16	0
1	Κ	1419	0	1380	11	0
1	L	1419	0	1380	12	0
2	А	6	0	0	0	0
2	В	14	0	0	1	0
2	С	8	0	0	0	0
2	D	8	0	0	0	0
2	Ε	5	0	0	0	0
2	F	13	0	0	1	0
2	G	10	0	0	0	0
2	Н	8	0	0	0	0
2	Ι	8	0	0	0	0
2	J	4	0	0	0	0
2	Κ	8	0	0	0	0
2	L	14	0	0	1	0
All	All	17276	0	16730	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (134) 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:E:193:LEU:HB2	1:E:197:GLU:HG3	1.65	0.78
1:A:40:ASP:OD2	1:A:44:LYS:HB2	1.88	0.74
1:A:103:VAL:HG22	1:A:175:ILE:HG13	1.80	0.63
1:K:113:GLU:HG3	1:K:160:ILE:HG12	1.83	0.61
1:G:113:GLU:HG2	1:G:160:ILE:HG12	1.84	0.60
1:B:113:GLU:HG2	1:B:160:ILE:HG12	1.82	0.60
1:F:118:ARG:HG2	1:F:191:GLY:HA2	1.83	0.59
1:J:18:ASN:HA	1:J:62:LYS:HB2	1.83	0.59
1:E:95:LEU:O	1:E:104:ARG:NH2	2.36	0.58
1:G:96:HIS:HA	1:G:102:ILE:HD12	1.86	0.58
1:D:69:LEU:HD12	1:D:103:VAL:HG12	1.87	0.57
1:E:70:TYR:OH	1:E:84:ASP:OD2	2.21	0.56
1:H:68:ILE:HG21	1:H:93:PRO:HG3	1.88	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:115:PRO:HB3	1:L:195:ASP:HB2	1.89	0.54
1:E:122:ILE:HG23	1:E:177:LEU:HB2	1.90	0.54
1:E:83:VAL:HG12	1:E:87:LYS:HD2	1.90	0.53
1:D:74:GLU:OE1	1:D:87:LYS:NZ	2.41	0.53
1:A:113:GLU:HG2	1:A:160:ILE:HG23	1.90	0.53
1:F:96:HIS:NE2	1:F:178:ASP:HA	2.24	0.52
1:G:18:ASN:HA	1:G:62:LYS:HB2	1.90	0.52
1:E:180:HIS:CE1	1:F:76:PRO:HG2	2.45	0.52
1:J:87:LYS:HA	1:J:90:LYS:HE3	1.92	0.52
1:E:96:HIS:NE2	1:E:178:ASP:HA	2.25	0.52
1:J:96:HIS:HA	1:J:102:ILE:HD12	1.92	0.52
1:A:152:GLN:OE1	1:A:155:THR:OG1	2.26	0.51
1:K:69:LEU:HD13	1:L:149:VAL:HG21	1.92	0.51
1:A:26:ALA:HB3	1:A:29:LEU:HD12	1.93	0.51
1:F:122:ILE:HG23	1:F:177:LEU:HB2	1.91	0.51
1:I:90:LYS:HG3	1:I:91:GLU:HG3	1.94	0.50
1:K:68:ILE:HG21	1:K:93:PRO:HG3	1.94	0.50
1:B:52:HIS:HD2	2:B:301:HOH:O	1.95	0.50
1:I:180:HIS:NE2	1:J:76:PRO:HG2	2.27	0.50
1:B:95:LEU:HD21	1:B:119:ALA:HB1	1.94	0.50
1:B:87:LYS:HA	1:B:90:LYS:HE2	1.94	0.49
1:C:128:VAL:HB	1:C:171:ARG:HG2	1.94	0.49
1:H:18:ASN:HA	1:H:62:LYS:HB2	1.94	0.49
1:I:128:VAL:HB	1:I:171:ARG:HG2	1.95	0.49
1:I:14:LEU:HD23	1:I:17:LEU:HD22	1.94	0.49
1:I:18:ASN:HA	1:I:62:LYS:HB2	1.96	0.48
1:I:179:CYS:HA	1:J:77:VAL:H	1.79	0.48
1:C:138:SER:HB3	1:D:44:LYS:HB3	1.94	0.48
1:J:113:GLU:HG3	1:J:160:ILE:HG12	1.96	0.48
1:A:79:LEU:HD13	1:B:153:ARG:HB3	1.95	0.48
1:G:62:LYS:NZ	1:J:187:GLN:OE1	2.46	0.48
1:A:180:HIS:NE2	1:B:76:PRO:HG2	2.28	0.47
1:F:73:GLN:NE2	2:F:301:HOH:O	2.47	0.47
1:H:34:ARG:NH1	1:H:69:LEU:O	2.36	0.47
1:A:149:VAL:HG21	1:B:69:LEU:HD13	1.94	0.47
1:B:38:GLY:HA3	1:B:48:LEU:HD11	1.96	0.47
1:G:127:VAL:HG22	1:G:172:MET:SD	2.55	0.47
1:G:138:SER:HB3	1:H:44:LYS:HB3	1.97	0.47
1:A:165:ASN:OD1	1:F:165:ASN:ND2	2.48	0.47
1:H:14:LEU:HD22	1:H:63:GLN:NE2	2.30	0.47
1:K:109:ALA:HB3	1:K:112:VAL:HG21	1.97	0.47



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:18:ASN:HA	1:B:62:LYS:HB2	1.98	0.46
1:G:68:ILE:HG21	1:G:93:PRO:HG3	1.98	0.46
1:C:135:VAL:HB	1:C:158:LYS:HG2	1.98	0.46
1:K:96:HIS:HA	1:K:102:ILE:HD12	1.96	0.46
1:J:152:GLN:OE1	1:J:157:HIS:CG	2.69	0.46
1:L:152:GLN:OE1	1:L:157:HIS:CG	2.69	0.46
1:B:152:GLN:OE1	1:B:155:THR:OG1	2.31	0.46
1:A:96:HIS:HA	1:A:102:ILE:HD12	1.98	0.46
1:B:128:VAL:HB	1:B:171:ARG:HG2	1.98	0.46
1:J:93:PRO:HB3	1:J:97:TYR:CE2	2.51	0.46
1:L:18:ASN:HA	1:L:62:LYS:HB2	1.97	0.46
1:I:69:LEU:HD13	1:J:149:VAL:HG21	1.97	0.45
1:A:23:GLY:HA2	1:A:58:ILE:HD11	1.97	0.45
1:E:197:GLU:O	1:E:201:VAL:HG13	2.17	0.45
1:E:120:VAL:O	1:E:120:VAL:HG23	2.17	0.45
1:L:109:ALA:HB3	1:L:112:VAL:HG21	1.99	0.45
1:E:113:GLU:HG3	1:E:160:ILE:HG23	1.98	0.45
1:G:44:LYS:HB3	1:H:138:SER:HB3	1.99	0.44
1:G:76:PRO:HG2	1:H:180:HIS:NE2	2.33	0.44
1:G:185:ASN:ND2	1:G:185:ASN:O	2.50	0.44
1:F:109:ALA:HB3	1:F:112:VAL:HG21	2.00	0.44
1:A:183:VAL:HG22	1:A:188:VAL:HG22	1.99	0.44
1:D:34:ARG:O	1:D:50:THR:HA	2.18	0.44
1:L:95:LEU:HD22	1:L:193:LEU:HD11	2.00	0.44
1:F:127:VAL:HG22	1:F:172:MET:SD	2.58	0.44
1:G:152:GLN:OE1	1:G:155:THR:OG1	2.27	0.44
1:J:118:ARG:HG2	1:J:191:GLY:HA2	2.00	0.44
1:A:128:VAL:HB	1:A:171:ARG:HG2	2.00	0.44
1:L:179:CYS:O	2:L:301:HOH:O	2.21	0.44
1:B:109:ALA:HB3	1:B:112:VAL:HG21	2.00	0.44
1:H:105:MET:HB2	1:H:173:MET:HG3	2.00	0.43
1:I:34:ARG:NH1	1:I:69:LEU:O	2.37	0.43
1:E:18:ASN:HA	1:E:62:LYS:HB2	2.00	0.43
1:I:153:ARG:HD3	1:J:37:THR:O	2.18	0.43
1:A:18:ASN:HA	1:A:62:LYS:HB2	1.99	0.43
1:G:113:GLU:HG2	1:G:160:ILE:HG23	2.00	0.43
1:I:15:PRO:O	1:I:63:GLN:HG2	2.18	0.43
1:L:57:ARG:NH1	1:L:92:GLU:OE2	2.52	0.43
1:A:37:THR:O	1:B:153:ARG:HD3	2.18	0.43
1:D:127:VAL:HG22	1:D:172:MET:SD	2.59	0.43
1:I:127:VAL:HG22	1:I:172:MET:SD	2.58	0.43



	lo de page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:J:127:VAL:HG22	1:J:172:MET:SD	2.59	0.43	
1:H:55:HIS:HB3	1:H:92:GLU:HG3	2.00	0.43	
1:I:37:THR:O	1:J:153:ARG:HD3	2.19	0.42	
1:D:57:ARG:HD2	1:D:92:GLU:OE1	2.19	0.42	
1:G:190:GLU:H	1:G:190:GLU:HG3	1.69	0.42	
1:H:14:LEU:HD22	1:H:63:GLN:HE22	1.83	0.42	
1:J:122:ILE:HG23	1:J:177:LEU:HB2	2.00	0.42	
1:J:152:GLN:OE1	1:J:157:HIS:ND1	2.52	0.42	
1:G:153:ARG:HD3	1:H:37:THR:O	2.20	0.42	
1:H:165:ASN:HD21	1:K:165:ASN:CG	2.23	0.42	
1:A:40:ASP:OD1	1:A:44:LYS:N	2.45	0.42	
1:C:41:ASP:OD1	1:C:41:ASP:N	2.52	0.42	
1:F:93:PRO:HB3	1:F:97:TYR:CE2	2.54	0.42	
1:K:34:ARG:NE	1:K:51:ASP:OD1	2.52	0.42	
1:K:149:VAL:HG21	1:L:69:LEU:HD13	2.02	0.42	
1:D:18:ASN:HA	1:D:62:LYS:HB2	2.01	0.42	
1:D:122:ILE:HG23	1:D:177:LEU:HB2	2.02	0.42	
1:C:120:VAL:HG23	1:C:120:VAL:O	2.20	0.42	
1:D:120:VAL:O	1:D:120:VAL:HG13	2.19	0.42	
1:G:180:HIS:NE2	1:H:76:PRO:HG2	2.35	0.42	
1:C:75:THR:OG1	1:C:99:ASN:O	2.32	0.41	
1:L:117:HIS:HB2	1:L:193:LEU:HA	2.02	0.41	
1:D:79:LEU:HD23	1:D:84:ASP:OD2	2.20	0.41	
1:E:15:PRO:O	1:E:63:GLN:NE2	2.49	0.41	
1:K:18:ASN:HA	1:K:62:LYS:HB2	2.02	0.41	
1:E:95:LEU:HD21	1:E:119:ALA:HB2	2.01	0.41	
1:H:80:ASN:O	1:H:83:VAL:HG22	2.20	0.41	
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.87	0.41	
1:D:78:GLN:OE1	1:D:80:ASN:ND2	2.47	0.41	
1:K:180:HIS:CE1	1:L:76:PRO:HG2	2.55	0.41	
1:D:152:GLN:HE21	1:D:152:GLN:HB2	1.70	0.40	
1:I:54:ASP:OD1	1:I:55:HIS:N	2.54	0.40	
1:E:95:LEU:HD22	1:E:193:LEU:HD21	2.02	0.40	
1:E:180:HIS:NE2	1:F:76:PRO:HG2	2.37	0.40	
1:K:14:LEU:HD12	1:K:14:LEU:HA	1.92	0.40	
1:C:103:VAL:HG22	1:C:175:ILE:HG13	2.02	0.40	
1:C:127:VAL:HG22	1:C:172:MET:SD	2.62	0.40	
1:H:127:VAL:HG22	1:H:172:MET:SD	2.62	0.40	
1:L:90:LYS:HA	1:L:90:LYS:HD2	1.88	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	187/207~(90%)	185~(99%)	2(1%)	0	100	100
1	В	182/207~(88%)	176 (97%)	6 (3%)	0	100	100
1	С	180/207~(87%)	176 (98%)	4 (2%)	0	100	100
1	D	182/207~(88%)	177 (97%)	5(3%)	0	100	100
1	Е	187/207~(90%)	180 (96%)	7 (4%)	0	100	100
1	F	182/207~(88%)	176 (97%)	6 (3%)	0	100	100
1	G	180/207~(87%)	177 (98%)	3 (2%)	0	100	100
1	Н	180/207~(87%)	175 (97%)	5(3%)	0	100	100
1	Ι	184/207~(89%)	181 (98%)	3 (2%)	0	100	100
1	J	182/207~(88%)	178 (98%)	4 (2%)	0	100	100
1	K	181/207~(87%)	177 (98%)	4 (2%)	0	100	100
1	L	181/207~(87%)	177 (98%)	4 (2%)	0	100	100
All	All	2188/2484 (88%)	2135 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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

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	А	160/174~(92%)	155~(97%)	5(3%)	35 55
1	В	155/174~(89%)	150 (97%)	5(3%)	34 54



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	С	153/174~(88%)	150 (98%)	3(2%)	50	71
1	D	155/174~(89%)	150 (97%)	5 (3%)	34	54
1	Е	160/174~(92%)	156 (98%)	4 (2%)	42	64
1	F	155/174~(89%)	153 (99%)	2 (1%)	65	80
1	G	153/174 (88%)	151 (99%)	2 (1%)	65	80
1	Н	153/174~(88%)	149 (97%)	4 (3%)	41	63
1	Ι	157/174~(90%)	154 (98%)	3 (2%)	52	72
1	J	155/174~(89%)	149 (96%)	6 (4%)	27	45
1	Κ	154/174~(88%)	153 (99%)	1 (1%)	84	92
1	L	154/174~(88%)	151 (98%)	3 (2%)	52	72
All	All	1864/2088~(89%)	1821 (98%)	43 (2%)	45	67

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	52	HIS
1	А	57	ARG
1	А	61	GLU
1	А	165	ASN
1	А	198	LYS
1	В	52	HIS
1	В	95	LEU
1	В	97	TYR
1	В	152	GLN
1	В	190	GLU
1	С	41	ASP
1	С	57	ARG
1	С	114	SER
1	D	44	LYS
1	D	52	HIS
1	D	56	HIS
1	D	158	LYS
1	D	190	GLU
1	Е	52	HIS
1	Е	57	ARG
1	Е	114	SER
1	Е	181	ASP
1	F	52	HIS



Mol	Chain	Res	Type
1	F	97	TYR
1	G	52	HIS
1	G	152	GLN
1	Н	30	ARG
1	Н	49	SER
1	Н	97	TYR
1	Н	193	LEU
1	Ι	57	ARG
1	Ι	97	TYR
1	Ι	195	ASP
1	J	40	ASP
1	J	52	HIS
1	J	57	ARG
1	J	123	ASP
1	J	146	GLN
1	J	152	GLN
1	Κ	145	ARG
1	L	52	HIS
1	L	97	TYR
1	L	187	GLN

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

Mol	Chain	Res	Type
1	Е	73	GLN
1	F	56	HIS
1	Н	165	ASN
1	К	165	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)

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	$OWAB(Å^2)$	Q<0.9
1	А	189/207~(91%)	-0.05	7 (3%) 45 43	26, 41, 75, 119	0
1	В	184/207~(88%)	-0.18	3 (1%) 70 68	27, 42, 66, 111	0
1	С	182/207~(87%)	0.05	2 (1%) 77 75	30, 46, 74, 94	0
1	D	184/207~(88%)	0.16	5 (2%) 56 54	29, 48, 84, 116	0
1	Ε	189/207~(91%)	-0.01	4 (2%) 63 61	28, 45, 82, 124	0
1	F	184/207~(88%)	-0.13	3 (1%) 70 68	28, 43, 70, 114	0
1	G	182/207~(87%)	-0.05	3 (1%) 70 68	25, 44, 73, 94	0
1	Н	182/207~(87%)	-0.08	3 (1%) 70 68	27, 46, 70, 88	0
1	Ι	186/207~(89%)	-0.02	3 (1%) 70 68	27, 48, 76, 113	0
1	J	184/207~(88%)	0.13	6 (3%) 49 46	27, 50, 79, 104	0
1	Κ	183/207~(88%)	-0.13	1 (0%) 87 86	25, 41, 69, 101	0
1	L	183/207~(88%)	-0.13	3 (1%) 70 68	27, 43, 64, 94	0
All	All	2212/2484 (89%)	-0.04	43 (1%) 66 64	25, 45, 74, 124	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	13	VAL	5.3
1	D	196	LEU	4.5
1	С	13	VAL	4.5
1	G	13	VAL	4.1
1	А	201	VAL	3.6
1	Н	194	GLY	3.5
1	Е	201	VAL	3.5
1	В	13	VAL	3.4
1	D	13	VAL	3.2
1	L	13	VAL	3.0
1	F	13	VAL	3.0



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Mol	Chain	Res	Type	RSRZ
1	J	196	LEU	2.9
1	В	193	LEU	2.9
1	А	13	VAL	2.7
1	F	190	GLU	2.7
1	D	188	VAL	2.6
1	Н	193	LEU	2.6
1	J	189	MET	2.6
1	G	74	GLU	2.6
1	F	195	ASP	2.5
1	Е	96	HIS	2.5
1	А	200	TYR	2.5
1	А	40	ASP	2.5
1	С	193	LEU	2.5
1	D	15	PRO	2.4
1	Н	13	VAL	2.4
1	А	193	LEU	2.4
1	Е	113	GLU	2.3
1	Ι	129	GLU	2.3
1	G	54	ASP	2.2
1	J	164	ASP	2.2
1	А	197	GLU	2.2
1	Е	13	VAL	2.2
1	D	43	GLY	2.2
1	Ι	164	ASP	2.2
1	L	41	ASP	2.1
1	J	13	VAL	2.1
1	В	41	ASP	2.1
1	K	86	ASP	2.1
1	A	74	GLU	2.0
1	J	123	ASP	2.0
1	J	96	HIS	2.0
1	L	98	HIS	2.0

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### 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.

