



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2022 – 12:22 AM JST

PDB ID : 7W43  
Title : Crystal structure of Bacillus subtilis YjoB N-terminal domain  
Authors : Dahal, P.; Kwon, E.; Kim, D.Y.  
Deposited on : 2021-11-26  
Resolution : 3.00 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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

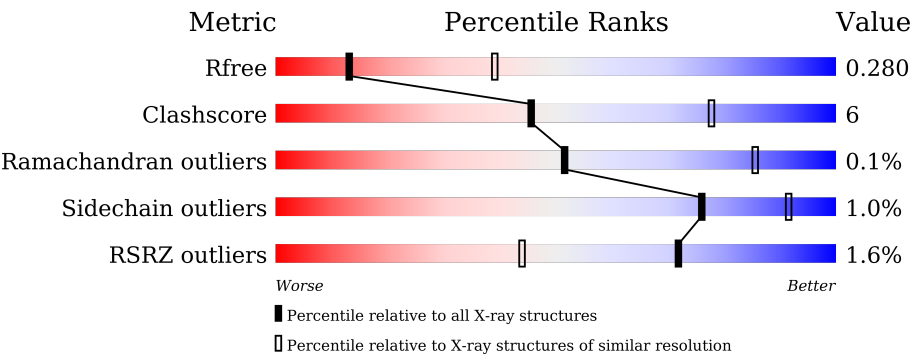
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>71%25%.</div>
1	B	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>79%17%.</div>
1	C	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>74%20%. .</div>
1	D	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>4%80%16%. .</div>
1	E	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>80%16%.</div>
1	F	161	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>81%15%. .</div>

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Mol	Chain	Length	Quality of chain
1	G	161	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>16%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	161	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>80%</div><div>15%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	I	161	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>81%</div><div>13%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	J	161	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>79%</div><div>16%</div><div>5%</div></div><div><div></div><div></div><div></div></div></div>
1	K	161	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>16%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	L	161	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>83%</div><div>14%</div><div></div></div><div><div></div><div></div><div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15526 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 Uncharacterized ATPase YjoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1299	841	202	253	3			
1	B	155	Total	C	N	O	S	0	0	0
			1299	841	202	253	3			
1	C	154	Total	C	N	O	S	0	0	0
			1290	835	200	252	3			
1	D	155	Total	C	N	O	S	0	0	0
			1298	839	202	254	3			
1	E	154	Total	C	N	O	S	0	0	0
			1290	835	200	252	3			
1	F	156	Total	C	N	O	S	0	0	0
			1307	845	204	255	3			
1	G	154	Total	C	N	O	S	0	0	0
			1290	835	200	252	3			
1	H	154	Total	C	N	O	S	0	0	0
			1290	835	200	252	3			
1	I	154	Total	C	N	O	S	0	0	0
			1290	835	200	252	3			
1	J	153	Total	C	N	O	S	0	0	0
			1284	830	200	251	3			
1	K	154	Total	C	N	O	S	0	0	0
			1291	835	201	252	3			
1	L	155	Total	C	N	O	S	0	0	0
			1298	839	202	254	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O34703
A	0	SER	-	expression tag	UNP O34703
B	-1	GLY	-	expression tag	UNP O34703
B	0	SER	-	expression tag	UNP O34703
C	-1	GLY	-	expression tag	UNP O34703

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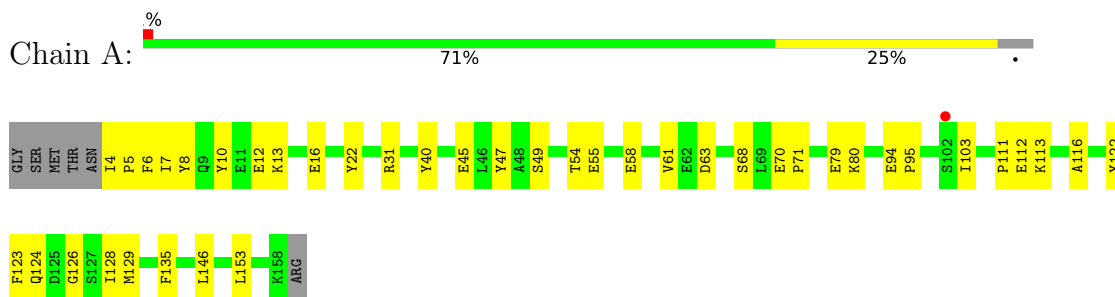
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP O34703
D	-1	GLY	-	expression tag	UNP O34703
D	0	SER	-	expression tag	UNP O34703
E	-1	GLY	-	expression tag	UNP O34703
E	0	SER	-	expression tag	UNP O34703
F	-1	GLY	-	expression tag	UNP O34703
F	0	SER	-	expression tag	UNP O34703
G	-1	GLY	-	expression tag	UNP O34703
G	0	SER	-	expression tag	UNP O34703
H	-1	GLY	-	expression tag	UNP O34703
H	0	SER	-	expression tag	UNP O34703
I	-1	GLY	-	expression tag	UNP O34703
I	0	SER	-	expression tag	UNP O34703
J	-1	GLY	-	expression tag	UNP O34703
J	0	SER	-	expression tag	UNP O34703
K	-1	GLY	-	expression tag	UNP O34703
K	0	SER	-	expression tag	UNP O34703
L	-1	GLY	-	expression tag	UNP O34703
L	0	SER	-	expression tag	UNP O34703

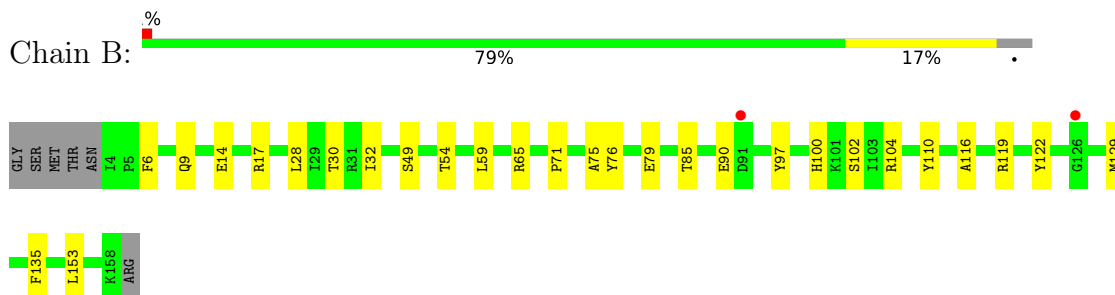
### 3 Residue-property plots [i](#)

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.

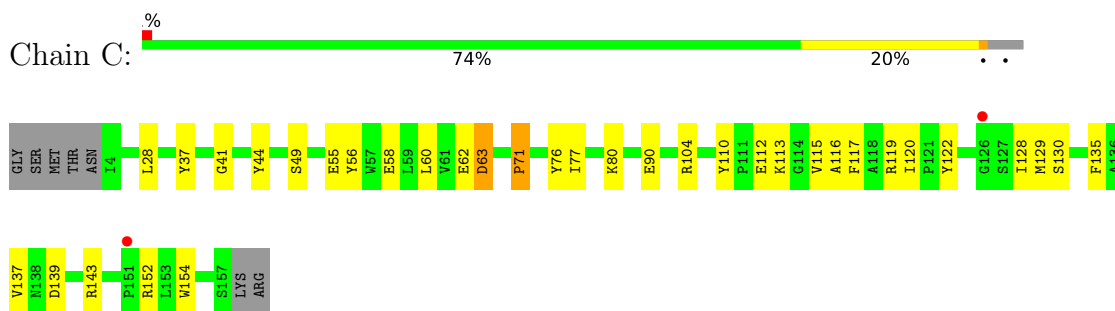
- Molecule 1: Uncharacterized ATPase YjoB



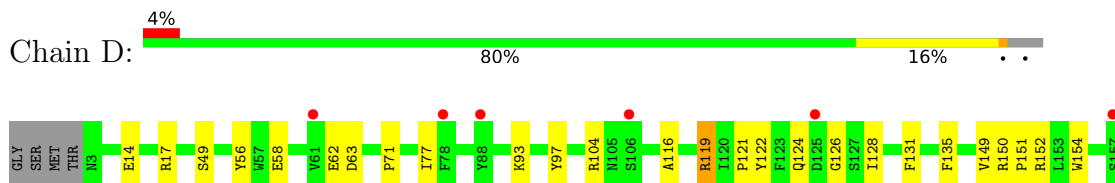
- Molecule 1: Uncharacterized ATPase YjoB



- Molecule 1: Uncharacterized ATPase YjoB

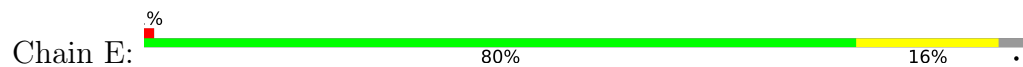


- Molecule 1: Uncharacterized ATPase YjoB

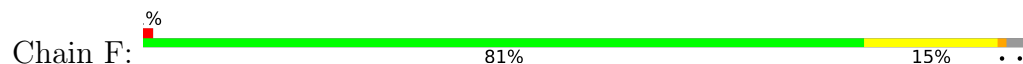


LYS  
ARG

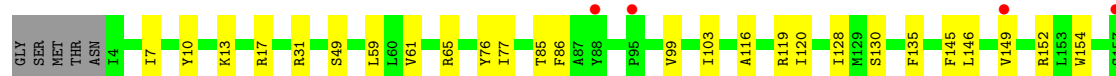
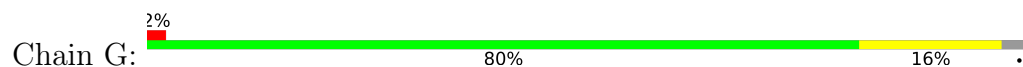
- Molecule 1: Uncharacterized ATPase YjoB



- Molecule 1: Uncharacterized ATPase YjoB

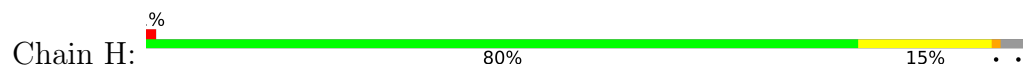


- Molecule 1: Uncharacterized ATPase YjoB

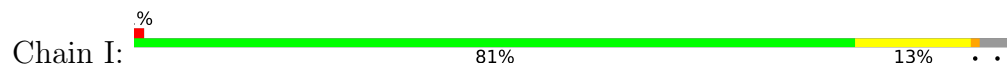


LYS  
ARG

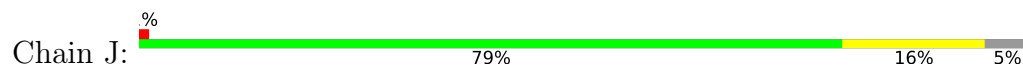
- Molecule 1: Uncharacterized ATPase YjoB



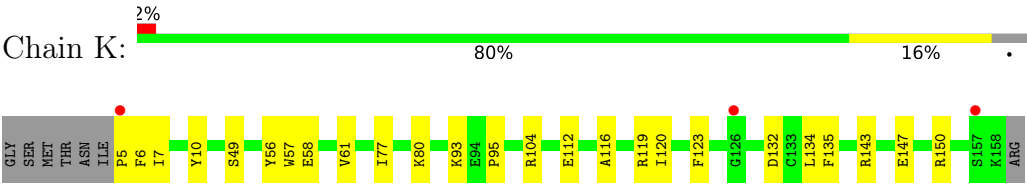
- Molecule 1: Uncharacterized ATPase YjoB



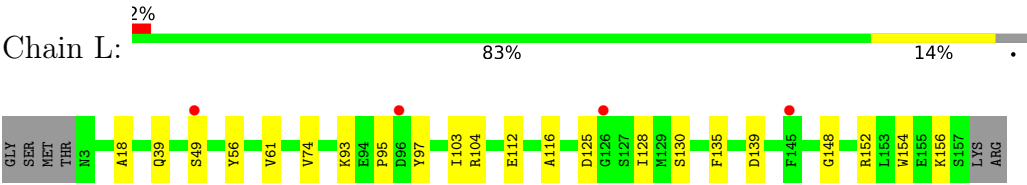
- Molecule 1: Uncharacterized ATPase YjoB



- Molecule 1: Uncharacterized ATPase YjoB



● Molecule 1: Uncharacterized ATPase YjoB





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.33Å 84.18Å 180.22Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	49.36 – 3.00 49.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.36-3.00) 96.6 (49.36-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, $R_{free}$	0.237 , 0.280 0.237 , 0.280	Depositor DCC
$R_{free}$ test set	1984 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1336	0.46	0/1808
1	B	0.25	0/1336	0.42	0/1808
1	C	0.26	0/1327	0.47	0/1797
1	D	0.27	0/1335	0.44	0/1808
1	E	0.26	0/1327	0.43	0/1797
1	F	0.26	0/1344	0.45	0/1819
1	G	0.26	0/1327	0.45	0/1797
1	H	0.28	0/1327	0.49	0/1797
1	I	0.27	0/1327	0.44	0/1797
1	J	0.27	0/1320	0.45	0/1785
1	K	0.26	0/1328	0.43	0/1796
1	L	0.26	0/1335	0.45	0/1808
All	All	0.26	0/15969	0.45	0/21617

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	A	1299	0	1218	30	0
1	B	1299	0	1218	21	0
1	C	1290	0	1205	28	0
1	D	1298	0	1211	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1290	0	1205	18	0
1	F	1307	0	1224	18	0
1	G	1290	0	1205	19	0
1	H	1290	0	1205	20	1
1	I	1290	0	1205	18	0
1	J	1284	0	1200	17	0
1	K	1291	0	1208	17	0
1	L	1298	0	1211	17	0
All	All	15526	0	14515	193	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (193) 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:C:63:ASP:HB3	1:C:71:PRO:HG2	1.62	0.79
1:B:116:ALA:HB3	1:B:135:PHE:HB2	1.65	0.78
1:H:14:GLU:N	1:H:14:GLU:OE1	2.21	0.73
1:C:143:ARG:NH1	1:D:97:TYR:O	2.22	0.72
1:K:104:ARG:HA	1:K:119:ARG:HB3	1.71	0.72
1:C:112:GLU:HG3	1:C:113:LYS:HG3	1.74	0.70
1:C:49:SER:HB2	1:D:128:ILE:HD12	1.72	0.69
1:J:119:ARG:HG2	1:J:130:SER:HB2	1.74	0.68
1:A:13:LYS:HG2	1:A:16:GLU:HG3	1.74	0.68
1:D:116:ALA:HB3	1:D:135:PHE:HB2	1.74	0.68
1:L:116:ALA:HB3	1:L:135:PHE:HB2	1.75	0.68
1:F:63:ASP:HB3	1:F:71:PRO:HG2	1.74	0.68
1:C:116:ALA:HB3	1:C:135:PHE:HB2	1.77	0.67
1:G:61:VAL:HG22	1:G:103:ILE:HD13	1.77	0.66
1:D:58:GLU:O	1:D:62:GLU:HG2	1.95	0.66
1:H:12:GLU:HG2	1:I:23:GLY:HA3	1.77	0.66
1:H:116:ALA:HB3	1:H:135:PHE:HB2	1.77	0.66
1:G:85:THR:HG22	1:G:86:PHE:H	1.61	0.66
1:F:116:ALA:HB3	1:F:135:PHE:HB2	1.77	0.65
1:J:116:ALA:HB3	1:J:135:PHE:HB2	1.79	0.65
1:I:116:ALA:HB3	1:I:135:PHE:HB2	1.80	0.64
1:B:14:GLU:O	1:B:17:ARG:HG2	1.99	0.63
1:K:77:ILE:HD13	1:K:120:ILE:HA	1.81	0.62
1:E:14:GLU:HA	1:E:17:ARG:HB2	1.79	0.62
1:E:40:TYR:O	1:E:42:VAL:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:CZ	1:B:129:MET:HB2	2.35	0.61
1:L:61:VAL:HG22	1:L:103:ILE:HG21	1.83	0.61
1:G:99:VAL:HG11	1:L:139:ASP:HB2	1.81	0.61
1:F:89:ASP:HB3	1:F:92:GLU:HB2	1.84	0.60
1:G:49:SER:HB3	1:H:128:ILE:HD12	1.84	0.60
1:F:150:ARG:HD2	1:F:154:TRP:HZ3	1.67	0.60
1:G:119:ARG:HG2	1:G:130:SER:HB2	1.86	0.58
1:J:110:TYR:HB3	1:J:113:LYS:HG3	1.85	0.57
1:K:147:GLU:HG2	1:L:97:TYR:CD1	2.40	0.57
1:D:131:PHE:HE1	1:E:127:SER:HA	1.70	0.56
1:J:47:TYR:OH	1:J:139:ASP:OD1	2.14	0.56
1:C:154:TRP:HD1	1:G:154:TRP:HB2	1.70	0.56
1:A:116:ALA:HB3	1:A:135:PHE:HB2	1.87	0.56
1:B:49:SER:HB2	1:C:128:ILE:HD12	1.88	0.55
1:J:104:ARG:HA	1:J:119:ARG:HB3	1.88	0.55
1:H:13:LYS:HD2	1:H:14:GLU:OE1	2.07	0.55
1:C:44:TYR:HA	1:C:137:VAL:HA	1.89	0.54
1:H:7:ILE:HB	1:J:77:ILE:HA	1.89	0.54
1:A:55:GLU:O	1:A:58:GLU:HG2	2.07	0.54
1:G:128:ILE:HD12	1:L:49:SER:HB2	1.89	0.54
1:H:12:GLU:HG2	1:I:23:GLY:CA	2.37	0.53
1:J:104:ARG:HD3	1:J:130:SER:HB3	1.90	0.53
1:E:119:ARG:HG2	1:E:130:SER:HB2	1.90	0.53
1:B:59:LEU:HD11	1:B:153:LEU:HG	1.90	0.53
1:I:4:ILE:HG13	1:I:5:PRO:HD3	1.91	0.52
1:A:79:GLU:HG2	1:A:80:LYS:HE2	1.91	0.52
1:G:116:ALA:HB3	1:G:135:PHE:HB2	1.90	0.52
1:C:55:GLU:O	1:C:58:GLU:HG2	2.09	0.52
1:A:58:GLU:O	1:A:61:VAL:HG22	2.10	0.51
1:C:122:TYR:CE2	1:D:126:GLY:HA3	2.45	0.51
1:G:77:ILE:HA	1:K:7:ILE:HB	1.93	0.51
1:I:62:GLU:OE1	1:I:156:LYS:HD2	2.10	0.51
1:A:123:PHE:CE1	1:A:128:ILE:HG12	2.46	0.50
1:C:122:TYR:CZ	1:C:129:MET:HB2	2.46	0.50
1:D:122:TYR:OH	1:E:126:GLY:O	2.30	0.50
1:G:59:LEU:HD13	1:G:152:ARG:HD2	1.92	0.50
1:I:77:ILE:HD13	1:I:120:ILE:HA	1.93	0.50
1:C:37:TYR:O	1:C:41:GLY:N	2.42	0.50
1:H:13:LYS:HB3	1:H:16:GLU:HG3	1.93	0.49
1:E:112:GLU:H	1:E:112:GLU:CD	2.16	0.49
1:J:57:TRP:CZ2	1:J:132:ASP:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ARG:HA	1:C:119:ARG:HB3	1.95	0.49
1:F:61:VAL:HG22	1:F:103:ILE:HG12	1.94	0.49
1:D:104:ARG:HA	1:D:119:ARG:HB3	1.94	0.49
1:E:116:ALA:HB3	1:E:135:PHE:HB2	1.95	0.49
1:F:70:GLU:OE2	1:F:111:PRO:HD2	2.13	0.49
1:H:63:ASP:HB3	1:H:71:PRO:HG2	1.96	0.48
1:I:69:LEU:H	1:I:69:LEU:HD23	1.77	0.48
1:I:89:ASP:HB3	1:I:92:GLU:HG2	1.96	0.48
1:C:112:GLU:HG3	1:C:113:LYS:N	2.28	0.48
1:J:30:THR:HG22	1:K:80:LYS:HE3	1.95	0.48
1:H:61:VAL:HG12	1:H:103:ILE:HG13	1.95	0.48
1:I:139:ASP:HB3	1:J:99:VAL:HG11	1.96	0.48
1:A:153:LEU:HD23	1:I:154:TRP:NE1	2.28	0.48
1:E:49:SER:HB2	1:F:128:ILE:HD12	1.95	0.48
1:J:61:VAL:HG22	1:J:103:ILE:HG13	1.95	0.47
1:A:40:TYR:CE1	1:A:111:PRO:HB3	2.49	0.47
1:I:57:TRP:CZ2	1:I:132:ASP:HB3	2.49	0.47
1:A:112:GLU:HG2	1:A:113:LYS:HG3	1.95	0.47
1:B:6:PHE:O	1:B:9:GLN:NE2	2.46	0.47
1:K:143:ARG:HG3	1:L:97:TYR:O	2.14	0.47
1:B:65:ARG:HG2	1:B:100:HIS:CD2	2.49	0.47
1:H:4:ILE:HG12	1:H:5:PRO:HD2	1.96	0.47
1:C:58:GLU:O	1:C:62:GLU:HG2	2.15	0.47
1:J:60:LEU:HD12	1:J:117:PHE:CG	2.50	0.47
1:D:93:LYS:H	1:D:93:LYS:HD2	1.80	0.47
1:A:31:ARG:HD3	1:E:7:ILE:O	2.15	0.46
1:A:68:SER:HB3	1:A:70:GLU:HG3	1.97	0.46
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.68	0.46
1:B:28:LEU:O	1:B:32:ILE:HG13	2.16	0.46
1:E:109:ALA:HA	1:E:116:ALA:HA	1.98	0.46
1:H:77:ILE:HD13	1:H:120:ILE:HA	1.96	0.46
1:B:30:THR:HG22	1:C:80:LYS:HE3	1.98	0.46
1:L:104:ARG:HD2	1:L:130:SER:HB3	1.96	0.46
1:E:145:PHE:O	1:E:149:VAL:HG23	2.15	0.46
1:G:99:VAL:HG11	1:L:139:ASP:CB	2.46	0.46
1:K:116:ALA:HB3	1:K:135:PHE:HB2	1.97	0.46
1:A:22:TYR:OH	1:B:79:GLU:HG2	2.15	0.46
1:A:54:THR:N	1:B:90:GLU:OE1	2.34	0.46
1:A:45:GLU:HG3	1:A:47:TYR:HE1	1.81	0.46
1:K:10:TYR:CE2	1:L:18:ALA:HB2	2.50	0.46
1:C:113:LYS:HE3	1:C:152:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:GLU:OE2	1:F:112:GLU:HG3	2.15	0.45
1:B:85:THR:HG22	1:B:102:SER:HA	1.99	0.45
1:C:77:ILE:HD13	1:C:120:ILE:HA	1.98	0.45
1:A:63:ASP:HB3	1:A:71:PRO:HD3	1.97	0.45
1:B:104:ARG:HA	1:B:119:ARG:HB3	1.99	0.45
1:H:143:ARG:HH11	1:I:97:TYR:HB2	1.81	0.45
1:H:93:LYS:O	1:H:95:PRO:HD3	2.17	0.45
1:G:145:PHE:O	1:G:149:VAL:HG23	2.17	0.45
1:B:71:PRO:HG3	1:B:110:TYR:CZ	2.52	0.45
1:G:76:TYR:O	1:K:6:PHE:HA	2.17	0.45
1:D:150:ARG:HB3	1:D:151:PRO:HD3	1.98	0.45
1:G:10:TYR:CE2	1:H:18:ALA:HB2	2.52	0.44
1:I:4:ILE:CG1	1:I:5:PRO:HD3	2.47	0.44
1:D:77:ILE:HD12	1:D:121:PRO:HD3	1.98	0.44
1:G:77:ILE:HD13	1:G:120:ILE:HA	1.99	0.44
1:A:10:TYR:CE2	1:A:12:GLU:HA	2.52	0.44
1:C:56:TYR:HD2	1:C:117:PHE:CE2	2.35	0.44
1:D:154:TRP:CD1	1:L:154:TRP:HB2	2.53	0.44
1:F:13:LYS:HD3	1:F:13:LYS:HA	1.76	0.44
1:A:122:TYR:CE1	1:A:129:MET:HB2	2.53	0.44
1:A:124:GLN:C	1:A:126:GLY:H	2.22	0.44
1:A:126:GLY:O	1:F:122:TYR:OH	2.27	0.44
1:D:49:SER:OG	1:E:104:ARG:NH2	2.50	0.44
1:G:146:LEU:HD12	1:H:88:TYR:CD2	2.53	0.44
1:L:93:LYS:O	1:L:95:PRO:HD3	2.18	0.44
1:A:7:ILE:HB	1:C:77:ILE:HA	2.00	0.43
1:J:59:LEU:HD13	1:J:152:ARG:NE	2.32	0.43
1:H:145:PHE:O	1:H:149:VAL:HG23	2.18	0.43
1:C:119:ARG:HG3	1:C:130:SER:HB2	2.00	0.43
1:E:148:GLY:O	1:E:152:ARG:HG3	2.18	0.43
1:K:49:SER:HB2	1:L:128:ILE:HD12	2.01	0.43
1:K:56:TYR:CE2	1:K:134:LEU:HD11	2.54	0.43
1:D:14:GLU:O	1:D:17:ARG:HG2	2.18	0.43
1:E:77:ILE:HD13	1:E:120:ILE:HA	2.01	0.43
1:B:76:TYR:O	1:F:6:PHE:HA	2.19	0.43
1:D:63:ASP:CB	1:D:71:PRO:HG2	2.49	0.43
1:E:112:GLU:HG2	1:E:113:LYS:HG3	2.00	0.43
1:A:70:GLU:HG3	1:A:70:GLU:H	1.55	0.43
1:H:13:LYS:HD2	1:H:13:LYS:HA	1.68	0.43
1:I:138:ASN:HD21	1:I:141:LYS:HG3	1.84	0.43
1:K:93:LYS:O	1:K:95:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:PHE:HB3	1:F:99:VAL:HG22	2.01	0.42
1:G:7:ILE:HB	1:I:77:ILE:HA	2.01	0.42
1:G:13:LYS:O	1:G:17:ARG:HG3	2.19	0.42
1:J:29:ILE:O	1:J:33:GLU:HG2	2.19	0.42
1:E:40:TYR:O	1:E:42:VAL:HG23	2.19	0.42
1:F:70:GLU:HB3	1:F:71:PRO:HD3	2.02	0.42
1:F:109:ALA:HA	1:F:116:ALA:HA	2.01	0.42
1:J:116:ALA:O	1:J:134:LEU:HD12	2.20	0.42
1:C:139:ASP:N	1:C:139:ASP:OD1	2.53	0.42
1:K:57:TRP:CZ2	1:K:132:ASP:HB3	2.54	0.42
1:L:112:GLU:H	1:L:112:GLU:HG2	1.57	0.42
1:L:148:GLY:O	1:L:152:ARG:HG3	2.20	0.42
1:L:156:LYS:N	1:L:156:LYS:HD2	2.34	0.42
1:A:49:SER:OG	1:B:104:ARG:NH2	2.52	0.42
1:B:102:SER:HB2	1:B:104:ARG:O	2.19	0.42
1:A:4:ILE:HB	1:A:5:PRO:HD3	2.00	0.42
1:J:20:ALA:O	1:K:123:PHE:HB2	2.19	0.42
1:D:56:TYR:HB3	1:D:149:VAL:HG21	2.02	0.42
1:B:30:THR:HG23	1:C:80:LYS:HG3	2.02	0.41
1:J:145:PHE:O	1:J:149:VAL:HG23	2.20	0.41
1:K:58:GLU:O	1:K:61:VAL:HG22	2.21	0.41
1:B:75:ALA:HA	1:F:4:ILE:HG22	2.01	0.41
1:C:60:LEU:HD12	1:C:117:PHE:CD2	2.55	0.41
1:F:85:THR:HG22	1:F:102:SER:HA	2.02	0.41
1:K:147:GLU:HG2	1:L:97:TYR:CG	2.55	0.41
1:A:112:GLU:HG2	1:A:113:LYS:N	2.35	0.41
1:A:61:VAL:HG12	1:A:103:ILE:HG13	2.02	0.41
1:A:146:LEU:HB3	1:B:97:TYR:CD1	2.55	0.41
1:G:85:THR:HG22	1:G:86:PHE:N	2.31	0.41
1:I:123:PHE:CE1	1:I:128:ILE:HG12	2.56	0.41
1:L:39:GLN:HG3	1:L:74:VAL:HG13	2.02	0.41
1:D:104:ARG:HG2	1:D:121:PRO:HG3	2.02	0.41
1:I:80:LYS:HA	1:I:80:LYS:HD3	1.83	0.41
1:C:110:TYR:HB2	1:C:115:VAL:HG23	2.03	0.41
1:E:42:VAL:HG12	1:E:43:PHE:N	2.36	0.40
1:E:141:LYS:HA	1:E:141:LYS:HD2	1.81	0.40
1:H:17:ARG:HD3	1:I:27:TYR:CG	2.56	0.40
1:A:6:PHE:HA	1:C:76:TYR:O	2.22	0.40
1:A:8:TYR:HB2	1:C:28:LEU:HD21	2.02	0.40
1:B:54:THR:H	1:C:90:GLU:CD	2.24	0.40
1:F:80:LYS:HD3	1:F:80:LYS:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:LYS:HA	1:H:80:LYS:HD3	1.86	0.40
1:K:5:PRO:HB2	1:K:6:PHE:H	1.55	0.40
1:A:94:GLU:HA	1:A:95:PRO:HD3	1.91	0.40
1:F:156:LYS:C	1:F:156:LYS:HD3	2.42	0.40

All (1) 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:H:14:GLU:OE2	1:H:17:ARG:NH1[2_556]	1.95	0.25

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	153/161 (95%)	147 (96%)	6 (4%)	0	100	100
1	B	153/161 (95%)	149 (97%)	4 (3%)	0	100	100
1	C	152/161 (94%)	148 (97%)	3 (2%)	1 (1%)	22	60
1	D	153/161 (95%)	148 (97%)	5 (3%)	0	100	100
1	E	152/161 (94%)	145 (95%)	6 (4%)	1 (1%)	22	60
1	F	154/161 (96%)	149 (97%)	5 (3%)	0	100	100
1	G	152/161 (94%)	144 (95%)	8 (5%)	0	100	100
1	H	152/161 (94%)	148 (97%)	4 (3%)	0	100	100
1	I	152/161 (94%)	148 (97%)	4 (3%)	0	100	100
1	J	151/161 (94%)	145 (96%)	6 (4%)	0	100	100
1	K	152/161 (94%)	146 (96%)	6 (4%)	0	100	100
1	L	153/161 (95%)	147 (96%)	6 (4%)	0	100	100
All	All	1829/1932 (95%)	1764 (96%)	63 (3%)	2 (0%)	51	85



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	41	GLY
1	C	71	PRO

### 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	136/141 (96%)	136 (100%)	0	100	100
1	B	136/141 (96%)	136 (100%)	0	100	100
1	C	135/141 (96%)	134 (99%)	1 (1%)	84	94
1	D	136/141 (96%)	133 (98%)	3 (2%)	52	81
1	E	135/141 (96%)	134 (99%)	1 (1%)	84	94
1	F	137/141 (97%)	134 (98%)	3 (2%)	52	81
1	G	135/141 (96%)	133 (98%)	2 (2%)	65	87
1	H	135/141 (96%)	134 (99%)	1 (1%)	84	94
1	I	135/141 (96%)	133 (98%)	2 (2%)	65	87
1	J	134/141 (95%)	134 (100%)	0	100	100
1	K	135/141 (96%)	133 (98%)	2 (2%)	65	87
1	L	136/141 (96%)	134 (98%)	2 (2%)	65	87
All	All	1625/1692 (96%)	1608 (99%)	17 (1%)	76	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	ASP
1	D	119	ARG
1	D	124	GLN
1	D	152	ARG
1	E	80	LYS
1	F	44	TYR
1	F	92	GLU

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Mol	Chain	Res	Type
1	F	112	GLU
1	G	31	ARG
1	G	65	ARG
1	H	143	ARG
1	I	69	LEU
1	I	139	ASP
1	K	112	GLU
1	K	150	ARG
1	L	56	TYR
1	L	125	ASP

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

Mol	Chain	Res	Type
1	G	39	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	155/161 (96%)	-0.17	1 (0%) 89 72	56, 74, 108, 123	0
1	B	155/161 (96%)	-0.06	2 (1%) 77 51	52, 75, 108, 123	0
1	C	154/161 (95%)	0.12	2 (1%) 77 51	57, 90, 118, 131	0
1	D	155/161 (96%)	0.18	6 (3%) 39 15	60, 81, 125, 136	0
1	E	154/161 (95%)	-0.13	1 (0%) 89 72	56, 74, 112, 121	0
1	F	156/161 (96%)	-0.02	1 (0%) 89 72	58, 83, 118, 127	0
1	G	154/161 (95%)	0.20	4 (2%) 56 27	66, 94, 124, 142	0
1	H	154/161 (95%)	-0.12	2 (1%) 77 51	57, 74, 114, 128	0
1	I	154/161 (95%)	-0.09	2 (1%) 77 51	56, 77, 104, 118	0
1	J	153/161 (95%)	-0.06	1 (0%) 87 69	54, 77, 115, 128	0
1	K	154/161 (95%)	-0.01	3 (1%) 66 37	57, 78, 113, 131	0
1	L	155/161 (96%)	-0.01	4 (2%) 56 27	63, 87, 111, 125	0
All	All	1853/1932 (95%)	-0.01	29 (1%) 72 44	52, 80, 115, 142	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	SER	5.6
1	D	157	SER	4.9
1	I	157	SER	4.1
1	L	49	SER	3.3
1	L	96	ASP	3.3
1	G	157	SER	3.3
1	D	61	VAL	3.1
1	D	88	TYR	2.9
1	K	126	GLY	2.9
1	G	88	TYR	2.7
1	B	91	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	126	GLY	2.6
1	K	157	SER	2.6
1	K	5	PRO	2.6
1	F	56	TYR	2.5
1	D	78	PHE	2.4
1	G	95	PRO	2.3
1	B	126	GLY	2.3
1	I	25	PHE	2.3
1	L	126	GLY	2.2
1	C	151	PRO	2.2
1	J	88	TYR	2.1
1	H	97	TYR	2.1
1	D	125	ASP	2.1
1	H	157	SER	2.1
1	L	145	PHE	2.1
1	A	102	SER	2.0
1	D	106	SER	2.0
1	G	149	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.