



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 12:04 PM EST

PDB ID : 3HIB  
Title : Crystal structure of the second Sec63 domain of yeast Brr2  
Authors : Zhang, L.; Xu, T.; Zhao, R.  
Deposited on : 2009-05-19  
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](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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

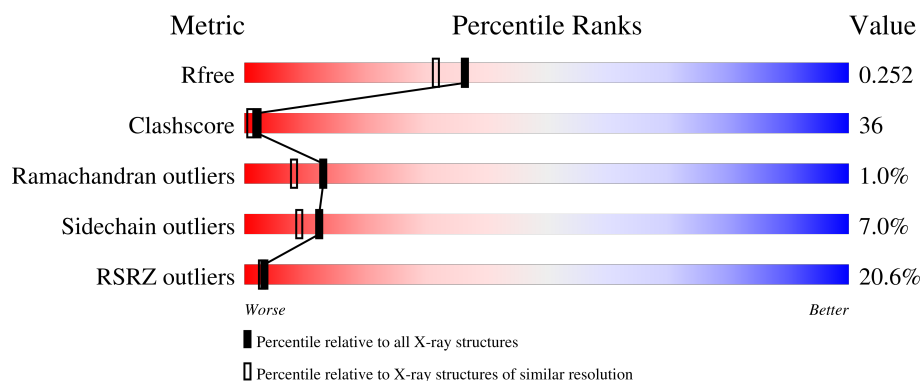
# 1 Overall quality at a glance

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  $\geq 3$ , 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	318	<div> <div>20%</div> <div>60%</div> <div>33%</div> <div>...</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2674 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 Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	Se	0	0	1
			2482	1593	399	483	3	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1846	GLY	-	expression tag	UNP P32639
A	1847	PRO	-	expression tag	UNP P32639
A	1848	LEU	-	expression tag	UNP P32639
A	1849	GLY	-	expression tag	UNP P32639
A	1850	SER	-	expression tag	UNP P32639

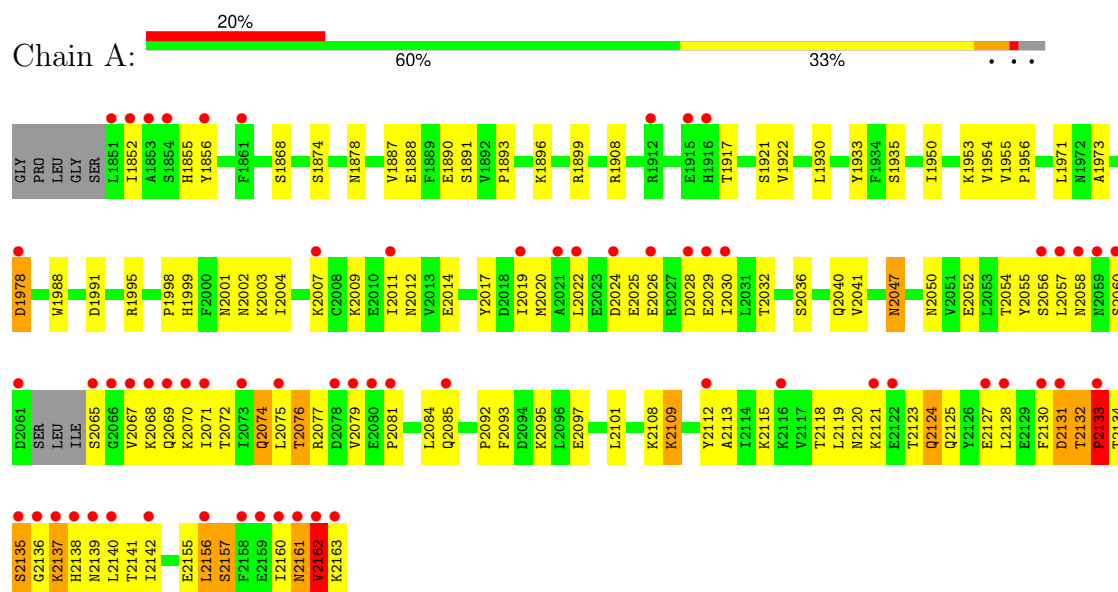
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	192	Total	O	0	0
			192	192		

### 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: Pre-mRNA-splicing helicase BRR2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.15Å 75.68Å 83.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.00) 98.3 (30.00-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.246 , 0.257 0.239 , 0.252	Depositor DCC
$R_{free}$ test set	2362 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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

### 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	0.43	0/2524	0.80	3/3423 (0.1%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2162	VAL	CA-C-N	-13.28	87.99	117.20
1	A	2133	PRO	CA-N-CD	-5.77	103.43	111.50
1	A	2162	VAL	O-C-N	-5.30	114.22	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2162	VAL	Mainchain

### 5.2 Too-close contacts

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	2482	0	2490	180	1
2	A	192	0	0	88	1
All	All	2674	0	2490	180	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 36.

All (180) 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:A:2135:SER:HA	1:A:2162:VAL:CG2	1.34	1.51
1:A:2135:SER:CA	1:A:2162:VAL:HG21	1.70	1.20
1:A:2161:ASN:O	1:A:2162:VAL:HG12	1.38	1.19
1:A:2135:SER:CA	1:A:2162:VAL:CG2	2.25	1.15
1:A:1988:TRP:HB2	2:A:134:HOH:O	1.45	1.12
1:A:2156:LEU:HB2	2:A:139:HOH:O	1.50	1.11
1:A:1890:GLU:HB2	2:A:170:HOH:O	1.51	1.11
1:A:2085:GLN:HB2	2:A:89:HOH:O	1.50	1.10
1:A:1978:ASP:HB2	2:A:24:HOH:O	1.50	1.10
1:A:2022:LEU:HD22	2:A:173:HOH:O	1.54	1.08
1:A:2135:SER:HA	1:A:2162:VAL:HG23	1.13	1.07
1:A:2135:SER:HA	1:A:2162:VAL:HG21	1.12	1.04
1:A:2052:GLU:HB2	1:A:2076:THR:HG22	1.37	1.02
1:A:2019:ILE:HG22	1:A:2020:MSE:HE2	1.44	0.97
1:A:2054:THR:HA	2:A:111:HOH:O	1.63	0.97
1:A:1953:LYS:HE3	2:A:106:HOH:O	1.66	0.94
1:A:2025:GLU:HG2	2:A:138:HOH:O	1.67	0.93
1:A:2161:ASN:O	1:A:2162:VAL:CG1	2.15	0.93
1:A:2140:LEU:HD23	2:A:162:HOH:O	1.71	0.89
1:A:2138:HIS:CD2	2:A:72:HOH:O	2.28	0.87
1:A:2067:VAL:O	1:A:2132:THR:OG1	1.94	0.84
1:A:2133:PRO:HB2	2:A:72:HOH:O	1.78	0.84
1:A:2134:THR:HB	2:A:125:HOH:O	1.78	0.83
1:A:2032:THR:CG2	2:A:116:HOH:O	2.28	0.81
1:A:2056:SER:HB2	1:A:2072:THR:CG2	2.10	0.80
1:A:2136:GLY:H	1:A:2162:VAL:HG21	1.47	0.79
1:A:2070:LYS:HD3	2:A:160:HOH:O	1.83	0.79
1:A:2052:GLU:HB2	1:A:2076:THR:CG2	2.12	0.78
1:A:2070:LYS:CD	2:A:160:HOH:O	2.30	0.78
1:A:2108:LYS:O	1:A:2109:LYS:HG2	1.84	0.77
1:A:2113:ALA:HB1	2:A:86:HOH:O	1.85	0.76
1:A:2026:GLU:O	1:A:2030:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2056:SER:HB2	1:A:2072:THR:HG22	1.68	0.75
1:A:1852:ILE:HG12	2:A:182:HOH:O	1.87	0.74
1:A:2136:GLY:N	1:A:2162:VAL:HG21	2.02	0.74
1:A:2128:LEU:HB2	2:A:108:HOH:O	1.86	0.74
1:A:2135:SER:CB	1:A:2162:VAL:HG21	2.17	0.74
1:A:1922:VAL:HG23	2:A:98:HOH:O	1.88	0.73
1:A:2047:ASN:ND2	2:A:155:HOH:O	2.20	0.73
1:A:1953:LYS:CE	2:A:106:HOH:O	2.32	0.72
1:A:1978:ASP:CB	2:A:24:HOH:O	2.22	0.71
1:A:1991:ASP:CG	2:A:134:HOH:O	2.28	0.71
1:A:2139:ASN:C	2:A:162:HOH:O	2.28	0.70
1:A:2032:THR:HG23	2:A:116:HOH:O	1.90	0.70
1:A:2127:GLU:CD	2:A:160:HOH:O	2.29	0.70
1:A:2140:LEU:CD2	2:A:162:HOH:O	2.35	0.69
1:A:2025:GLU:CG	2:A:138:HOH:O	2.31	0.68
1:A:2019:ILE:HG22	1:A:2020:MSE:CE	2.23	0.68
1:A:2067:VAL:CG1	1:A:2068:LYS:N	2.57	0.67
1:A:2007:LYS:HE3	1:A:2030:ILE:O	1.96	0.67
1:A:2025:GLU:OE2	2:A:105:HOH:O	2.13	0.66
1:A:2014:GLU:OE1	2:A:177:HOH:O	2.13	0.66
1:A:1868:SER:O	2:A:115:HOH:O	2.13	0.66
1:A:2135:SER:CA	1:A:2162:VAL:HG23	2.08	0.66
1:A:2071:ILE:HG23	2:A:108:HOH:O	1.96	0.65
1:A:2028:ASP:O	2:A:116:HOH:O	2.14	0.65
1:A:2032:THR:HG22	2:A:116:HOH:O	1.94	0.65
1:A:2055:TYR:N	2:A:111:HOH:O	2.29	0.65
1:A:2067:VAL:HG12	1:A:2068:LYS:N	2.09	0.65
1:A:2022:LEU:CD2	2:A:173:HOH:O	2.27	0.65
1:A:2109:LYS:NZ	2:A:180:HOH:O	2.24	0.64
1:A:2120:ASN:OD1	2:A:169:HOH:O	2.15	0.64
1:A:2040:GLN:HB3	2:A:42:HOH:O	1.98	0.64
1:A:2125:GLN:N	2:A:191:HOH:O	2.25	0.63
1:A:2054:THR:CA	2:A:111:HOH:O	2.33	0.63
1:A:2069:GLN:CA	2:A:154:HOH:O	2.46	0.63
1:A:2058:ASN:HA	2:A:189:HOH:O	1.98	0.63
1:A:2140:LEU:HD11	1:A:2160:ILE:HD13	1.81	0.62
1:A:2128:LEU:CB	2:A:108:HOH:O	2.45	0.62
1:A:2069:GLN:C	2:A:154:HOH:O	2.38	0.62
1:A:2024:ASP:C	1:A:2025:GLU:HG3	2.20	0.62
1:A:2007:LYS:NZ	1:A:2032:THR:HG23	2.15	0.61
1:A:2007:LYS:HZ2	1:A:2032:THR:HG23	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:LEU:HD11	1:A:2101:LEU:HD21	1.81	0.61
1:A:1887:VAL:HG22	2:A:170:HOH:O	2.00	0.61
1:A:2029:GLU:HA	2:A:116:HOH:O	2.00	0.61
1:A:1978:ASP:OD1	1:A:1978:ASP:C	2.39	0.61
1:A:2124:GLN:HG2	2:A:62:HOH:O	2.01	0.60
1:A:2136:GLY:H	1:A:2162:VAL:CG2	2.14	0.60
1:A:2067:VAL:CG1	1:A:2068:LYS:H	2.14	0.60
1:A:2134:THR:CB	2:A:125:HOH:O	2.41	0.60
1:A:2161:ASN:C	1:A:2162:VAL:HG12	2.17	0.60
1:A:2077:ARG:NH2	1:A:2097:GLU:OE2	2.33	0.59
1:A:2029:GLU:HA	1:A:2029:GLU:OE1	2.01	0.59
1:A:2142:ILE:HB	1:A:2156:LEU:CD1	2.33	0.59
1:A:2026:GLU:CD	2:A:173:HOH:O	2.40	0.58
1:A:1995:ARG:NH2	1:A:2002:ASN:OD1	2.38	0.57
1:A:2071:ILE:CG2	2:A:108:HOH:O	2.51	0.57
1:A:2070:LYS:N	2:A:154:HOH:O	2.37	0.56
1:A:2072:THR:O	1:A:2072:THR:HG23	2.04	0.56
1:A:2011:ILE:HG22	1:A:2011:ILE:O	2.04	0.56
1:A:2055:TYR:HA	1:A:2072:THR:O	2.05	0.56
1:A:2135:SER:C	1:A:2162:VAL:HG21	2.26	0.56
1:A:2140:LEU:HD12	1:A:2160:ILE:HG23	1.87	0.56
1:A:2156:LEU:HD12	1:A:2156:LEU:N	2.21	0.55
1:A:2156:LEU:C	2:A:139:HOH:O	2.44	0.55
1:A:1874:SER:HA	1:A:1878:ASN:HD22	1.71	0.55
1:A:2047:ASN:HB2	2:A:75:HOH:O	2.07	0.55
1:A:2011:ILE:O	1:A:2012:ASN:HB2	2.07	0.55
1:A:2007:LYS:NZ	1:A:2032:THR:CG2	2.70	0.54
1:A:2081:PRO:HG3	1:A:2084:LEU:HD21	1.90	0.54
1:A:2134:THR:CG2	2:A:125:HOH:O	2.56	0.53
1:A:2056:SER:O	1:A:2071:ILE:HG13	2.09	0.53
1:A:1953:LYS:HG2	2:A:106:HOH:O	2.09	0.53
1:A:2136:GLY:N	1:A:2162:VAL:CG2	2.72	0.53
1:A:2136:GLY:C	1:A:2162:VAL:HB	2.29	0.53
1:A:2115:LYS:HB2	1:A:2128:LEU:CD2	2.38	0.52
1:A:1888:GLU:O	1:A:1953:LYS:HE2	2.08	0.52
1:A:2128:LEU:N	2:A:108:HOH:O	2.27	0.52
1:A:2131:ASP:CG	2:A:178:HOH:O	2.48	0.52
1:A:1899:ARG:NH2	2:A:67:HOH:O	2.42	0.51
1:A:2047:ASN:HD22	1:A:2047:ASN:N	2.07	0.51
1:A:2127:GLU:N	2:A:185:HOH:O	2.12	0.50
1:A:2074:GLN:HB2	1:A:2125:GLN:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2019:ILE:CG2	1:A:2020:MSE:HE2	2.29	0.50
1:A:1971:LEU:C	1:A:1973:ALA:H	2.15	0.50
1:A:2142:ILE:O	1:A:2155:GLU:HA	2.12	0.50
1:A:1891:SER:O	2:A:143:HOH:O	2.20	0.50
1:A:2029:GLU:CA	2:A:116:HOH:O	2.58	0.49
1:A:2067:VAL:HG13	1:A:2068:LYS:H	1.77	0.49
1:A:2004:ILE:HA	1:A:2007:LYS:HG2	1.94	0.49
1:A:2056:SER:HB2	1:A:2072:THR:HG21	1.93	0.49
1:A:2140:LEU:CG	2:A:162:HOH:O	2.60	0.49
1:A:1855:HIS:CG	1:A:1856:TYR:N	2.81	0.49
1:A:2140:LEU:N	2:A:162:HOH:O	2.42	0.49
1:A:2012:ASN:ND2	2:A:164:HOH:O	2.40	0.48
1:A:1890:GLU:CB	2:A:170:HOH:O	2.32	0.48
1:A:2141:THR:N	2:A:92:HOH:O	2.45	0.48
1:A:1887:VAL:O	2:A:170:HOH:O	2.20	0.48
1:A:2113:ALA:CB	2:A:86:HOH:O	2.52	0.48
1:A:2108:LYS:C	1:A:2109:LYS:HG2	2.34	0.48
1:A:2121:LYS:N	1:A:2124:GLN:OE1	2.40	0.48
1:A:2134:THR:O	1:A:2138:HIS:NE2	2.46	0.48
1:A:2134:THR:HG22	2:A:125:HOH:O	2.14	0.47
1:A:1908:ARG:NH2	2:A:97:HOH:O	2.35	0.47
1:A:2132:THR:HA	1:A:2133:PRO:HD2	1.55	0.47
1:A:2124:GLN:CG	2:A:62:HOH:O	2.61	0.46
1:A:1893:PRO:HD3	2:A:143:HOH:O	2.16	0.46
1:A:1998:PRO:HG2	1:A:2041:VAL:HA	1.96	0.46
1:A:2135:SER:CB	1:A:2162:VAL:CG2	2.88	0.46
1:A:2069:GLN:HA	2:A:154:HOH:O	2.15	0.46
1:A:2057:LEU:HB3	1:A:2058:ASN:H	1.47	0.46
1:A:2140:LEU:HA	2:A:92:HOH:O	2.15	0.45
1:A:1908:ARG:NE	2:A:97:HOH:O	2.41	0.45
1:A:2007:LYS:HE3	1:A:2030:ILE:HA	1.99	0.45
1:A:2068:LYS:H	1:A:2068:LYS:HG3	1.43	0.45
1:A:1999:HIS:NE2	1:A:2040:GLN:OE1	2.41	0.45
1:A:2118:THR:OG1	2:A:169:HOH:O	2.20	0.44
1:A:2127:GLU:HG2	2:A:185:HOH:O	2.17	0.44
1:A:2124:GLN:HE21	1:A:2124:GLN:N	2.16	0.44
1:A:2052:GLU:OE1	2:A:83:HOH:O	2.21	0.44
1:A:1935:SER:O	2:A:110:HOH:O	2.21	0.44
1:A:2136:GLY:O	1:A:2137:LYS:HB3	2.17	0.44
1:A:2112:TYR:HD2	1:A:2130:PHE:CD1	2.36	0.44
1:A:2136:GLY:H	1:A:2162:VAL:CB	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1930:LEU:O	1:A:1933:TYR:HB3	2.19	0.43
1:A:2115:LYS:CB	1:A:2128:LEU:HD21	2.48	0.43
1:A:1955:VAL:HB	1:A:1956:PRO:HD3	2.01	0.43
1:A:2128:LEU:CA	2:A:108:HOH:O	2.65	0.43
1:A:1971:LEU:C	1:A:1973:ALA:N	2.72	0.43
1:A:2092:PRO:HG2	1:A:2093:PHE:CE2	2.54	0.43
1:A:2163:LYS:N	2:A:153:HOH:O	2.51	0.43
1:A:2007:LYS:O	1:A:2030:ILE:CD1	2.67	0.43
1:A:2055:TYR:CD1	1:A:2071:ILE:HD11	2.53	0.42
1:A:2138:HIS:H	1:A:2160:ILE:HG13	1.84	0.42
1:A:1950:ILE:O	1:A:1954:VAL:HG13	2.20	0.42
1:A:1917:THR:HG22	2:A:181:HOH:O	2.18	0.42
1:A:2007:LYS:CE	1:A:2030:ILE:O	2.66	0.42
1:A:2113:ALA:CA	2:A:86:HOH:O	2.67	0.42
1:A:2076:THR:CG2	1:A:2076:THR:O	2.68	0.41
1:A:2047:ASN:ND2	1:A:2047:ASN:N	2.67	0.41
1:A:2141:THR:HA	1:A:2157:SER:HA	2.02	0.41
1:A:1890:GLU:CG	2:A:170:HOH:O	2.67	0.41
1:A:2017:TYR:CE2	1:A:2050:ASN:ND2	2.85	0.41
1:A:2024:ASP:O	1:A:2025:GLU:HG3	2.20	0.40
1:A:2072:THR:CG2	1:A:2072:THR:O	2.69	0.40
1:A:1921:SER:HB2	2:A:79:HOH:O	2.21	0.40
1:A:2112:TYR:CE2	1:A:2133:PRO:HG3	2.57	0.40
1:A:2001:ASN:OD1	1:A:2003:LYS:HB2	2.22	0.40
1:A:2127:GLU:OE2	2:A:160:HOH:O	2.22	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:A:1896:LYS:NZ	2:A:24:HOH:O[4_466]	2.15	0.05

## 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	306/318 (96%)	287 (94%)	16 (5%)	3 (1%)	13 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2133	PRO
1	A	2135	SER
1	A	2162	VAL

### 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	287/290 (99%)	267 (93%)	20 (7%)	12 9

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1978	ASP
1	A	2009	LYS
1	A	2036	SER
1	A	2047	ASN
1	A	2060	SER
1	A	2065	SER
1	A	2074	GLN
1	A	2076	THR
1	A	2079	VAL
1	A	2095	LYS
1	A	2109	LYS
1	A	2119	LEU
1	A	2123	THR
1	A	2124	GLN
1	A	2131	ASP
1	A	2132	THR

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Mol	Chain	Res	Type
1	A	2137	LYS
1	A	2156	LEU
1	A	2157	SER
1	A	2161	ASN

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

Mol	Chain	Res	Type
1	A	1855	HIS
1	A	1878	ASN
1	A	2047	ASN
1	A	2161	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

### 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	306/318 (96%)	0.81	63 (20%) <b>3</b> <b>3</b>	14, 31, 65, 71	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2163	LYS	6.0
1	A	1851	LEU	5.6
1	A	2160	ILE	5.1
1	A	2162	VAL	5.1
1	A	2139	ASN	4.6
1	A	2067	VAL	4.6
1	A	1978	ASP	4.0
1	A	2057	LEU	4.0
1	A	2140	LEU	3.8
1	A	1915	GLU	3.7
1	A	2069	GLN	3.6
1	A	2080	GLU	3.5
1	A	2128	LEU	3.5
1	A	2079	VAL	3.3
1	A	1853	ALA	3.2
1	A	2011	ILE	3.2
1	A	2056	SER	3.1
1	A	2158	PHE	3.1
1	A	2081	PRO	3.0
1	A	2112	TYR	3.0
1	A	1852	ILE	3.0
1	A	2073	ILE	3.0
1	A	2078	ASP	2.9
1	A	2059	ASN	2.9
1	A	1856	TYR	2.9
1	A	1854	SER	2.8
1	A	2136	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2133	PRO	2.8
1	A	2066	GLY	2.7
1	A	2060	SER	2.6
1	A	2156	LEU	2.6
1	A	2068	LYS	2.6
1	A	2138	HIS	2.6
1	A	2159	GLU	2.6
1	A	1861	PHE	2.6
1	A	2075	LEU	2.6
1	A	2061	ASP	2.5
1	A	2028	ASP	2.5
1	A	2161	ASN	2.5
1	A	2130	PHE	2.4
1	A	2137	LYS	2.4
1	A	1916	HIS	2.4
1	A	2131	ASP	2.4
1	A	2021	ALA	2.4
1	A	2024	ASP	2.4
1	A	2030	ILE	2.4
1	A	2026	GLU	2.3
1	A	2122	GLU	2.3
1	A	2065	SER	2.3
1	A	2127	GLU	2.3
1	A	2058	ASN	2.3
1	A	2135	SER	2.3
1	A	2121	LYS	2.2
1	A	1912	ARG	2.2
1	A	2071	ILE	2.2
1	A	2085	GLN	2.2
1	A	2029	GLU	2.2
1	A	2019	ILE	2.1
1	A	2142	ILE	2.1
1	A	2007	LYS	2.1
1	A	2022	LEU	2.1
1	A	2070	LYS	2.0
1	A	2116	LYS	2.0

## 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 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.