



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:39 AM GMT

PDB ID : 2B9R  
Title : Crystal Structure of Human Cyclin B1  
Authors : Basavappa, R.; Petri, E.  
Deposited on : 2005-10-12  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

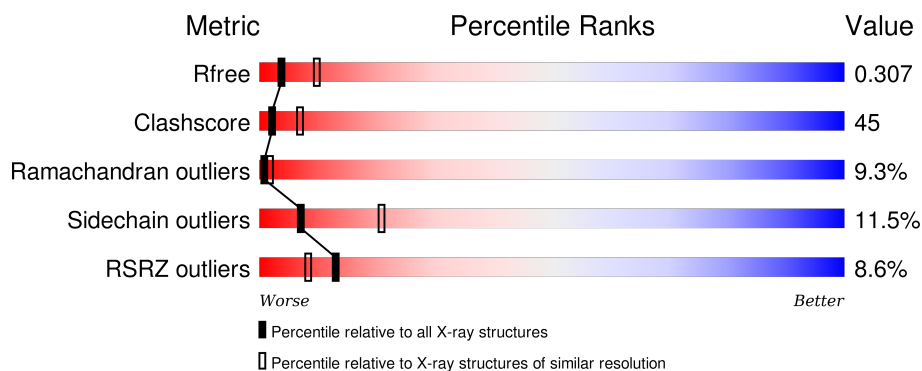
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	269	<div> <div>10%</div> <div> <div></div> <div>38%</div> <div>43%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	269	<div> <div>6%</div> <div> <div></div> <div>38%</div> <div>43%</div> <div>13%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4030 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 Human cyclin B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1952	1259	329	348	16			
1	B	255	Total	C	N	O	S	0	0	0
			1984	1280	336	352	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	ENGINEERED	UNP P14635
A	19	ALA	GLU	ENGINEERED	UNP P14635
A	20	ALA	GLU	ENGINEERED	UNP P14635
A	74	SER	CYS	ENGINEERED	UNP P14635
A	186	SER	CYS	ENGINEERED	UNP P14635
B	3	SER	CYS	ENGINEERED	UNP P14635
B	19	ALA	GLU	ENGINEERED	UNP P14635
B	20	ALA	GLU	ENGINEERED	UNP P14635
B	74	SER	CYS	ENGINEERED	UNP P14635
B	186	SER	CYS	ENGINEERED	UNP P14635

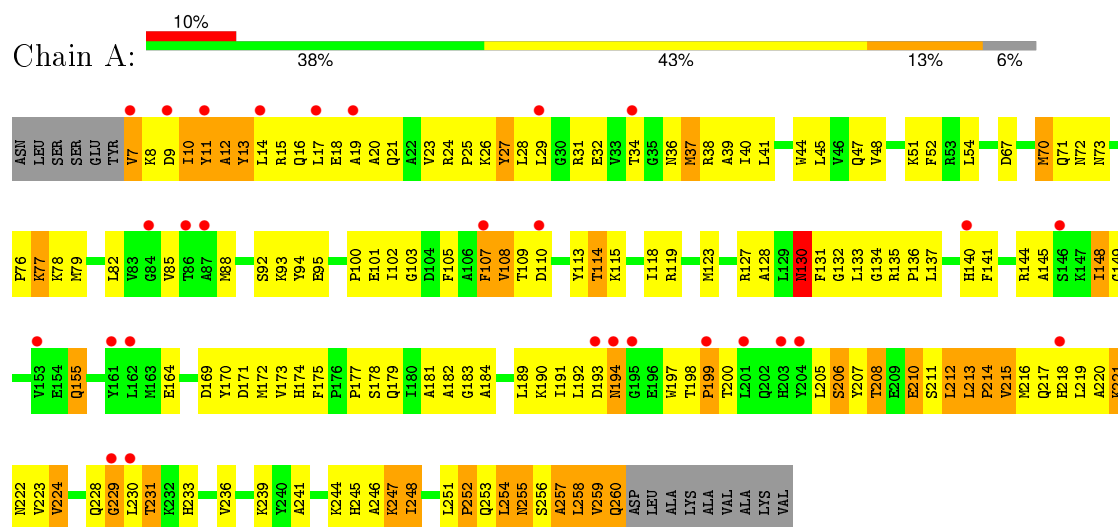
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	50	Total	O	0	0
			50	50		

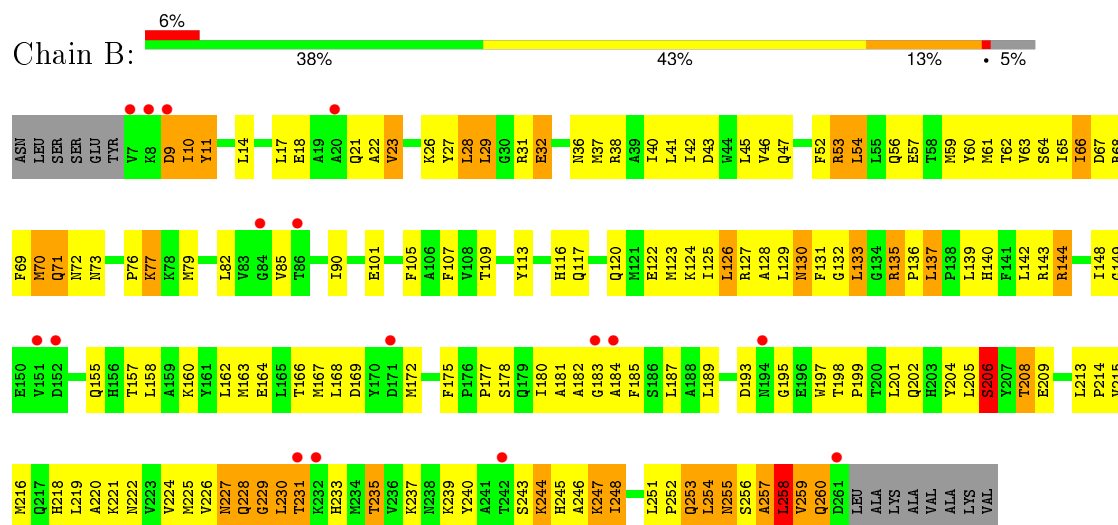
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Human cyclin B1



#### • Molecule 1: Human cyclin B1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.17Å 117.17Å 197.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.90) 98.2 (19.95-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.243 , 0.308 0.240 , 0.307	Depositor DCC
$R_{free}$ test set	1773 reflections (10.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 122.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 18051 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	2/1991 (0.1%)	0.65	0/2703
1	B	0.49	0/2025	0.71	1/2748 (0.0%)
All	All	0.52	2/4016 (0.0%)	0.68	1/5451 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	VAL	N-CA	8.52	1.63	1.46
1	A	7	VAL	C-N	5.43	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	CA-CB-CG	-5.20	103.33	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	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	1952	0	1942	176	0
1	B	1984	0	1989	184	0
2	A	44	0	0	13	0
2	B	50	0	0	17	0
All	All	4030	0	3931	352	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 45.

All (352) 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:70:MET:O	1:A:72:ASN:N	1.58	1.34
1:B:70:MET:O	1:B:72:ASN:N	1.63	1.31
1:B:143:ARG:HH21	1:B:160:LYS:NZ	1.29	1.30
1:A:252:PRO:HG2	2:A:273:HOH:O	1.32	1.27
1:B:253:GLN:HA	1:B:255:ASN:ND2	1.64	1.11
1:B:53:ARG:HH11	1:B:53:ARG:CG	1.65	1.09
1:B:79:MET:HG3	2:B:293:HOH:O	1.53	1.06
1:B:53:ARG:NH1	1:B:53:ARG:HG3	1.51	1.03
1:B:253:GLN:HA	1:B:255:ASN:HD21	1.15	1.02
1:B:254:LEU:O	1:B:256:SER:N	1.94	1.01
1:B:177:PRO:HA	2:B:308:HOH:O	1.62	0.99
1:B:79:MET:HE1	2:B:317:HOH:O	1.63	0.99
1:A:131:PHE:HA	2:B:313:HOH:O	1.63	0.97
1:B:178:SER:N	2:B:308:HOH:O	1.96	0.97
1:B:143:ARG:HH21	1:B:160:LYS:HZ2	1.04	0.97
1:B:43:ASP:OD1	1:B:235:THR:HG23	1.67	0.94
1:B:79:MET:CE	2:B:317:HOH:O	2.16	0.94
1:B:143:ARG:HH21	1:B:160:LYS:HZ1	1.09	0.93
1:B:253:GLN:C	1:B:255:ASN:H	1.69	0.93
1:B:47:GLN:HE21	1:B:235:THR:HG21	1.33	0.93
1:B:143:ARG:NH2	1:B:160:LYS:NZ	2.15	0.93
1:B:64:SER:O	1:B:68:ARG:HG3	1.70	0.92
1:B:124:LYS:NZ	2:B:283:HOH:O	2.02	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TYR:HB3	1:A:212:LEU:HD21	1.54	0.89
1:B:253:GLN:CA	1:B:255:ASN:ND2	2.35	0.89
1:B:77:LYS:HE2	1:B:77:LYS:H	1.36	0.88
1:B:18:GLU:OE2	1:B:177:PRO:HD2	1.72	0.88
1:B:177:PRO:O	1:B:178:SER:HB2	1.71	0.87
1:A:251:LEU:HB3	1:A:252:PRO:HD2	1.54	0.86
1:A:251:LEU:C	1:A:253:GLN:H	1.76	0.86
1:A:254:LEU:O	1:A:256:SER:N	2.08	0.86
1:B:132:GLY:N	2:B:273:HOH:O	2.09	0.85
1:A:216:MET:HA	1:A:219:LEU:HD12	1.57	0.85
1:B:57:GLU:N	1:B:57:GLU:OE2	2.08	0.85
1:A:253:GLN:C	1:A:255:ASN:H	1.78	0.84
1:B:32:GLU:H	1:B:32:GLU:CD	1.80	0.83
1:B:143:ARG:NH2	1:B:160:LYS:HZ2	1.74	0.83
1:A:257:ALA:O	1:A:259:VAL:N	2.13	0.82
1:B:26:LYS:O	1:B:29:LEU:HB2	1.80	0.82
1:A:77:LYS:HE2	1:A:78:LYS:H	1.44	0.82
1:A:133:LEU:H	1:B:131:PHE:CB	1.93	0.82
1:B:23:VAL:HA	1:B:71:GLN:OE1	1.78	0.82
1:B:228:GLN:HG3	1:B:229:GLY:H	1.45	0.80
1:B:70:MET:C	1:B:72:ASN:H	1.83	0.79
1:B:256:SER:O	1:B:259:VAL:HG23	1.83	0.79
1:B:199:PRO:HA	1:B:202:GLN:HG2	1.64	0.79
1:A:27:TYR:C	1:A:27:TYR:HD2	1.86	0.79
1:B:177:PRO:CA	2:B:308:HOH:O	2.22	0.77
1:A:13:TYR:HA	2:A:310:HOH:O	1.85	0.77
1:B:248:ILE:HD13	1:B:248:ILE:O	1.85	0.76
1:B:257:ALA:O	1:B:259:VAL:N	2.12	0.76
1:A:17:LEU:HD23	1:A:136:PRO:HD3	1.69	0.75
1:B:169:ASP:HB3	1:B:172:MET:HG2	1.69	0.75
1:B:253:GLN:C	1:B:255:ASN:N	2.38	0.75
1:A:155:GLN:HE22	1:A:189:LEU:HD12	1.51	0.74
1:B:40:ILE:HG13	1:B:41:LEU:N	2.02	0.74
1:A:131:PHE:O	1:B:132:GLY:HA2	1.87	0.74
1:A:27:TYR:C	1:A:27:TYR:CD2	2.58	0.74
1:B:227:ASN:HD22	1:B:254:LEU:HG	1.53	0.73
1:B:254:LEU:HD13	2:B:318:HOH:O	1.89	0.73
1:A:193:ASP:O	1:A:194:ASN:HB3	1.87	0.73
1:A:257:ALA:C	1:A:259:VAL:H	1.91	0.72
1:B:143:ARG:NH2	1:B:160:LYS:HZ1	1.84	0.71
1:B:228:GLN:O	1:B:229:GLY:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:C	1:A:214:PRO:HD2	2.12	0.70
1:A:132:GLY:N	2:B:273:HOH:O	2.24	0.70
1:A:253:GLN:HA	1:A:255:ASN:ND2	2.06	0.70
1:A:123:MET:CE	1:A:127:ARG:HH22	2.05	0.69
1:B:193:ASP:HB3	1:B:195:GLY:H	1.58	0.68
1:A:257:ALA:C	1:A:259:VAL:N	2.46	0.68
1:B:256:SER:OG	1:B:258:LEU:HA	1.94	0.67
1:B:260:GLN:HE21	1:B:260:GLN:N	1.90	0.67
1:B:253:GLN:O	1:B:255:ASN:N	2.28	0.67
1:B:43:ASP:CG	1:B:235:THR:HG23	2.15	0.67
1:B:53:ARG:HH11	1:B:53:ARG:HG3	0.71	0.67
1:A:70:MET:C	1:A:72:ASN:N	2.48	0.67
1:B:226:VAL:HG13	1:B:237:LYS:HD2	1.76	0.67
1:B:163:MET:O	1:B:166:THR:OG1	2.12	0.66
1:B:187:LEU:HB2	1:B:216:MET:HG2	1.78	0.66
1:B:253:GLN:CA	1:B:255:ASN:HD21	1.99	0.66
1:A:212:LEU:HD23	1:A:212:LEU:N	2.10	0.66
1:B:243:SER:O	1:B:245:HIS:N	2.30	0.65
1:A:251:LEU:C	1:A:253:GLN:N	2.48	0.65
1:A:198:THR:C	1:A:200:THR:H	1.99	0.65
1:B:123:MET:HE3	1:B:127:ARG:HH12	1.62	0.65
1:A:179:GLN:HB2	1:A:207:TYR:OH	1.96	0.64
1:A:219:LEU:O	1:A:223:VAL:HG23	1.96	0.64
1:A:193:ASP:O	1:A:194:ASN:CB	2.45	0.64
1:B:251:LEU:HB3	1:B:252:PRO:HD2	1.79	0.64
1:A:245:HIS:O	1:A:248:ILE:HB	1.97	0.64
1:A:37:MET:O	1:A:40:ILE:HG12	1.98	0.64
1:A:253:GLN:C	1:A:255:ASN:N	2.48	0.63
1:B:177:PRO:O	1:B:178:SER:CB	2.43	0.63
1:B:82:LEU:HB2	1:B:113:TYR:CE1	2.34	0.63
1:A:241:ALA:O	1:A:247:LYS:HG2	1.98	0.62
1:A:213:LEU:N	1:A:214:PRO:CD	2.62	0.62
1:A:82:LEU:HB2	1:A:113:TYR:CZ	2.35	0.62
1:B:137:LEU:HB2	1:B:140:HIS:CD2	2.35	0.62
1:B:213:LEU:HB3	1:B:214:PRO:HD3	1.80	0.61
1:A:256:SER:C	1:A:258:LEU:N	2.52	0.61
1:A:169:ASP:HB3	1:A:172:MET:HG2	1.82	0.61
1:A:255:ASN:O	1:A:256:SER:HB3	2.00	0.61
1:B:27:TYR:CE2	1:B:28:LEU:HD13	2.35	0.61
1:A:179:GLN:HB2	1:A:207:TYR:CZ	2.35	0.61
1:B:77:LYS:N	1:B:77:LYS:HE2	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HB3	1:A:252:PRO:CD	2.26	0.61
1:A:191:ILE:HG22	1:A:192:LEU:HD23	1.83	0.61
1:A:93:LYS:O	1:B:123:MET:HG2	2.01	0.61
1:B:135:ARG:HG2	1:B:136:PRO:HD2	1.82	0.61
1:B:228:GLN:CG	1:B:229:GLY:H	2.12	0.60
1:A:38:ARG:HB3	2:A:289:HOH:O	2.02	0.60
1:B:53:ARG:NH1	1:B:53:ARG:CG	2.35	0.60
1:A:131:PHE:CB	1:B:133:LEU:H	2.15	0.60
1:B:47:GLN:NE2	1:B:235:THR:HG21	2.12	0.60
1:B:42:ILE:CG2	1:B:168:LEU:HD23	2.32	0.60
1:A:256:SER:O	1:A:259:VAL:N	2.35	0.59
1:A:101:GLU:CD	1:A:102:ILE:HG22	2.23	0.59
1:A:128:ALA:C	1:A:130:ASN:H	2.05	0.59
1:A:253:GLN:O	1:A:255:ASN:N	2.36	0.59
1:A:251:LEU:CB	1:A:252:PRO:HD2	2.32	0.58
1:A:253:GLN:HA	1:A:255:ASN:HD21	1.66	0.58
1:B:254:LEU:C	1:B:256:SER:N	2.56	0.58
1:B:62:THR:O	1:B:66:ILE:HG22	2.03	0.58
1:A:217:GLN:O	1:A:220:ALA:HB3	2.03	0.58
1:A:132:GLY:HA2	1:B:131:PHE:O	2.03	0.58
1:B:243:SER:C	1:B:245:HIS:N	2.56	0.58
1:A:37:MET:O	1:A:40:ILE:CG1	2.51	0.58
1:A:164:GLU:HG2	1:A:236:VAL:CG1	2.33	0.58
1:A:244:LYS:O	1:A:244:LYS:HG2	2.03	0.57
1:A:198:THR:HB	1:A:199:PRO:HD2	1.86	0.57
1:B:123:MET:HB3	1:B:127:ARG:NH1	2.19	0.57
1:B:255:ASN:O	1:B:256:SER:HB3	2.03	0.57
1:A:212:LEU:C	1:A:214:PRO:CD	2.72	0.57
1:A:246:ALA:O	1:A:248:ILE:N	2.38	0.57
1:B:254:LEU:CD1	2:B:318:HOH:O	2.48	0.56
1:B:260:GLN:NE2	1:B:260:GLN:N	2.53	0.56
1:A:14:LEU:HD22	1:A:136:PRO:HB3	1.86	0.56
1:B:257:ALA:C	1:B:259:VAL:H	2.07	0.56
1:A:208:THR:HB	1:A:211:SER:H	1.71	0.56
1:B:256:SER:C	1:B:258:LEU:N	2.57	0.56
1:B:46:VAL:HG22	1:B:59:MET:HE2	1.88	0.56
1:B:202:GLN:O	1:B:206:SER:HA	2.06	0.56
1:B:243:SER:C	1:B:245:HIS:H	2.09	0.56
1:B:21:GLN:CB	1:B:135:ARG:HD2	2.35	0.56
1:B:63:VAL:HA	1:B:66:ILE:CG2	2.36	0.56
1:B:253:GLN:O	1:B:255:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:HG23	1:B:129:LEU:HD11	1.88	0.55
1:B:131:PHE:C	2:B:273:HOH:O	2.40	0.55
1:A:172:MET:SD	1:A:218:HIS:HB3	2.47	0.55
1:A:134:GLY:H	1:B:131:PHE:CB	2.19	0.55
1:A:11:TYR:O	1:A:14:LEU:HB2	2.07	0.55
1:B:227:ASN:O	1:B:228:GLN:HB3	2.06	0.55
1:B:253:GLN:C	1:B:255:ASN:ND2	2.60	0.55
1:B:128:ALA:C	1:B:130:ASN:H	2.08	0.55
1:A:103:GLY:HA2	1:A:115:LYS:HE2	1.89	0.55
1:B:197:TRP:CE3	1:B:201:LEU:HD13	2.42	0.55
1:B:70:MET:O	1:B:73:ASN:N	2.35	0.54
1:A:123:MET:CE	1:A:127:ARG:NH2	2.70	0.54
1:A:251:LEU:O	1:A:253:GLN:N	2.39	0.54
1:A:27:TYR:HE2	1:A:28:LEU:HD13	1.72	0.54
1:B:63:VAL:HA	1:B:66:ILE:HG23	1.89	0.54
1:A:198:THR:O	1:A:200:THR:N	2.41	0.54
1:B:42:ILE:HG21	1:B:168:LEU:HD23	1.90	0.54
1:A:48:VAL:HA	1:A:51:LYS:HD3	1.89	0.54
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.73	0.54
1:A:40:ILE:HG13	1:A:41:LEU:N	2.23	0.54
1:A:70:MET:O	1:A:73:ASN:N	2.38	0.54
1:B:244:LYS:HG3	1:B:245:HIS:CE1	2.43	0.53
1:B:228:GLN:HG3	1:B:229:GLY:N	2.18	0.53
1:B:76:PRO:HD2	1:B:79:MET:HE2	1.91	0.53
1:A:132:GLY:HA2	1:B:131:PHE:C	2.29	0.53
1:B:155:GLN:HE22	1:B:189:LEU:N	2.07	0.53
1:A:44:TRP:HA	1:A:47:GLN:HE21	1.72	0.53
1:A:36:ASN:HA	1:A:39:ALA:HB3	1.90	0.53
1:B:148:ILE:O	1:B:148:ILE:HG13	2.09	0.53
1:A:27:TYR:HD2	1:A:28:LEU:N	2.07	0.53
1:A:177:PRO:O	1:A:178:SER:CB	2.56	0.52
1:B:158:LEU:O	1:B:162:LEU:HG	2.09	0.52
1:B:14:LEU:HD23	1:B:136:PRO:HG3	1.91	0.52
1:A:102:ILE:HD11	1:A:118:ILE:HB	1.91	0.52
1:A:18:GLU:O	1:A:21:GLN:N	2.21	0.52
1:A:79:MET:HG3	2:A:304:HOH:O	2.09	0.52
1:A:215:VAL:HB	2:A:284:HOH:O	2.08	0.52
1:A:205:LEU:O	1:A:206:SER:C	2.48	0.52
1:A:164:GLU:HG2	1:A:236:VAL:HG13	1.91	0.52
1:A:24:ARG:O	1:A:27:TYR:HB3	2.09	0.52
1:B:185:PHE:HD2	1:B:197:TRP:HZ3	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:C	1:A:200:THR:N	2.64	0.51
1:B:259:VAL:O	1:B:260:GLN:HG3	2.10	0.51
1:A:101:GLU:CD	1:A:102:ILE:H	2.13	0.51
1:A:172:MET:HB2	1:A:175:PHE:HD1	1.76	0.51
1:B:227:ASN:O	1:B:228:GLN:CB	2.59	0.51
1:B:9:ASP:O	1:B:10:ILE:C	2.49	0.51
1:B:157:THR:HG22	1:B:248:ILE:HG21	1.94	0.50
1:A:12:ALA:C	1:A:14:LEU:H	2.14	0.50
1:B:177:PRO:C	2:B:308:HOH:O	2.28	0.50
1:B:130:ASN:O	1:B:131:PHE:CB	2.60	0.50
1:A:244:LYS:CG	1:A:244:LYS:O	2.59	0.50
1:A:76:PRO:O	1:A:77:LYS:C	2.49	0.50
1:A:27:TYR:CD2	1:A:28:LEU:N	2.80	0.50
1:A:12:ALA:O	1:A:14:LEU:N	2.44	0.50
1:B:17:LEU:HD23	1:B:136:PRO:HD3	1.93	0.50
1:A:130:ASN:O	1:A:131:PHE:CB	2.60	0.49
1:B:172:MET:HB2	1:B:175:PHE:CD1	2.47	0.49
1:B:105:PHE:O	1:B:109:THR:HG23	2.12	0.49
1:A:85:VAL:HG21	1:A:109:THR:HG22	1.92	0.49
1:B:18:GLU:OE2	1:B:177:PRO:CD	2.55	0.49
1:B:43:ASP:OD2	1:B:235:THR:CG2	2.60	0.49
1:A:101:GLU:OE2	1:A:102:ILE:HG22	2.12	0.49
1:A:9:ASP:O	1:A:10:ILE:CB	2.60	0.49
1:A:220:ALA:O	1:A:224:VAL:HG23	2.13	0.48
1:A:220:ALA:HB1	1:A:260:GLN:NE2	2.28	0.48
1:B:254:LEU:HD22	2:B:318:HOH:O	2.12	0.48
1:A:215:VAL:CG2	1:A:216:MET:N	2.76	0.48
1:A:31:ARG:NH1	1:A:31:ARG:HG3	2.28	0.48
1:A:115:LYS:HB3	1:A:119:ARG:HH21	1.77	0.48
1:B:41:LEU:HG	1:B:45:LEU:HD12	1.96	0.48
1:B:21:GLN:CB	1:B:135:ARG:CD	2.92	0.48
1:B:205:LEU:O	1:B:206:SER:C	2.52	0.48
1:A:25:PRO:HD3	1:A:174:HIS:HB3	1.96	0.47
1:A:181:ALA:O	1:A:182:ALA:C	2.51	0.47
1:A:107:PHE:O	1:A:110:ASP:N	2.45	0.47
1:A:255:ASN:C	1:A:257:ALA:N	2.67	0.47
1:B:158:LEU:HB2	1:B:248:ILE:HD11	1.96	0.47
1:A:82:LEU:HB2	1:A:113:TYR:CE1	2.50	0.47
1:B:231:THR:C	1:B:233:HIS:N	2.67	0.47
1:B:256:SER:O	1:B:257:ALA:C	2.52	0.47
1:A:220:ALA:O	1:A:221:LYS:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:CE	1:B:77:LYS:H	2.20	0.47
1:B:52:PHE:HB3	1:B:54:LEU:HD13	1.96	0.47
1:B:219:LEU:O	1:B:220:ALA:C	2.53	0.47
1:B:260:GLN:HE21	1:B:260:GLN:H	1.62	0.47
1:A:255:ASN:C	1:A:257:ALA:H	2.18	0.46
1:B:144:ARG:NH2	1:B:204:TYR:HD2	2.14	0.46
1:B:189:LEU:O	1:B:193:ASP:HB2	2.15	0.46
1:A:220:ALA:CB	1:A:260:GLN:NE2	2.78	0.46
1:A:82:LEU:HD13	1:A:113:TYR:CG	2.50	0.46
1:B:90:ILE:HD13	1:B:126:LEU:HD13	1.97	0.46
1:A:172:MET:HB2	1:A:175:PHE:CD1	2.49	0.46
1:B:189:LEU:O	1:B:193:ASP:CB	2.64	0.46
1:A:257:ALA:O	1:A:258:LEU:C	2.53	0.46
1:B:38:ARG:NH1	1:B:67:ASP:OD1	2.48	0.46
1:B:204:TYR:O	1:B:205:LEU:HD23	2.16	0.46
1:B:246:ALA:O	1:B:247:LYS:C	2.53	0.46
1:B:31:ARG:HG3	1:B:31:ARG:HH11	1.80	0.46
1:B:199:PRO:HA	1:B:202:GLN:CG	2.40	0.46
1:A:27:TYR:HE1	1:A:67:ASP:OD2	1.99	0.46
1:A:77:LYS:NZ	2:A:306:HOH:O	2.02	0.46
1:B:14:LEU:CD2	1:B:136:PRO:HB3	2.46	0.46
1:A:241:ALA:O	1:A:247:LYS:HA	2.16	0.45
1:B:213:LEU:N	1:B:214:PRO:HD2	2.31	0.45
1:A:123:MET:HE1	1:A:127:ARG:HH22	1.82	0.45
1:B:27:TYR:OH	1:B:67:ASP:OD2	2.31	0.45
1:A:24:ARG:HA	1:A:25:PRO:HD2	1.76	0.45
1:A:254:LEU:C	1:A:256:SER:N	2.70	0.45
1:A:258:LEU:HD12	2:A:286:HOH:O	2.15	0.45
1:B:175:PHE:HB2	1:B:180:ILE:HD11	1.99	0.45
1:B:181:ALA:O	1:B:182:ALA:C	2.55	0.45
1:A:135:ARG:CB	2:A:293:HOH:O	2.63	0.45
1:A:135:ARG:HG3	2:A:293:HOH:O	2.17	0.45
1:B:239:LYS:HD3	1:B:240:TYR:CE1	2.52	0.45
1:B:224:VAL:HG12	1:B:225:MET:N	2.32	0.45
1:B:28:LEU:O	1:B:29:LEU:C	2.55	0.45
1:A:246:ALA:O	1:A:247:LYS:C	2.55	0.45
1:A:175:PHE:HB3	1:A:179:GLN:OE1	2.16	0.45
1:B:22:ALA:O	1:B:23:VAL:HB	2.17	0.45
1:A:170:TYR:HA	1:A:173:VAL:CG2	2.47	0.45
1:A:94:TYR:CE2	1:B:126:LEU:HB3	2.52	0.45
1:A:144:ARG:O	1:A:148:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:HG2	1:B:126:LEU:HD22	1.98	0.44
1:B:69:PHE:CD1	1:B:125:ILE:HG12	2.52	0.44
1:B:228:GLN:CG	1:B:229:GLY:N	2.79	0.44
1:A:135:ARG:HB2	2:A:293:HOH:O	2.17	0.44
1:B:140:HIS:N	1:B:140:HIS:CD2	2.86	0.44
1:A:141:PHE:HB3	2:A:288:HOH:O	2.18	0.44
1:A:100:PRO:HG2	1:A:105:PHE:CE2	2.53	0.44
1:A:256:SER:HB3	1:A:258:LEU:HD23	1.99	0.44
1:B:116:HIS:CE1	1:B:120:GLN:OE1	2.70	0.44
1:B:218:HIS:O	1:B:221:LYS:HB3	2.18	0.44
1:A:210:GLU:OE1	1:A:210:GLU:N	2.51	0.44
1:A:256:SER:O	1:A:257:ALA:C	2.56	0.44
1:B:158:LEU:HB2	1:B:248:ILE:CD1	2.48	0.44
1:A:133:LEU:HD22	1:A:133:LEU:N	2.32	0.44
1:A:95:GLU:HA	1:A:95:GLU:OE2	2.17	0.44
1:B:113:TYR:HA	1:B:117:GLN:OE1	2.18	0.43
1:A:39:ALA:O	1:A:40:ILE:C	2.56	0.43
1:A:220:ALA:HB1	1:A:260:GLN:HE21	1.82	0.43
1:A:108:VAL:C	1:A:110:ASP:H	2.21	0.43
1:B:139:LEU:O	1:B:143:ARG:HG2	2.18	0.43
1:A:211:SER:C	1:A:212:LEU:HD23	2.38	0.43
1:B:172:MET:HB2	1:B:175:PHE:HD1	1.83	0.43
1:B:243:SER:O	1:B:244:LYS:C	2.56	0.43
1:A:228:GLN:HG3	1:A:229:GLY:N	2.33	0.43
1:A:14:LEU:O	1:A:16:GLN:N	2.51	0.43
1:A:101:GLU:CG	1:A:102:ILE:H	2.31	0.43
1:A:101:GLU:CG	1:A:102:ILE:N	2.81	0.43
1:A:190:LYS:HD2	2:A:290:HOH:O	2.17	0.43
1:B:56:GLN:HB3	1:B:139:LEU:HD11	2.00	0.43
1:A:40:ILE:HG13	1:A:41:LEU:H	1.84	0.43
1:A:231:THR:C	1:A:233:HIS:H	2.22	0.43
1:B:252:PRO:HG2	1:B:255:ASN:OD1	2.18	0.43
1:A:230:LEU:O	1:A:231:THR:O	2.36	0.43
1:B:208:THR:O	1:B:209:GLU:C	2.56	0.43
1:A:88:MET:O	1:A:92:SER:OG	2.33	0.43
1:A:25:PRO:HD3	1:A:174:HIS:CB	2.49	0.42
1:B:248:ILE:HD11	1:B:251:LEU:HD11	2.01	0.42
1:B:164:GLU:HG3	1:B:167:MET:HE2	2.00	0.42
1:A:215:VAL:HG22	1:A:216:MET:N	2.34	0.42
1:A:12:ALA:C	1:A:14:LEU:N	2.72	0.42
1:A:14:LEU:C	1:A:16:GLN:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:OG1	1:A:115:LYS:N	2.52	0.42
1:A:183:GLY:O	1:A:184:ALA:C	2.57	0.42
1:B:216:MET:O	1:B:219:LEU:HB2	2.19	0.42
1:B:251:LEU:C	1:B:253:GLN:H	2.22	0.42
1:A:26:LYS:HA	1:A:170:TYR:CZ	2.55	0.42
1:B:60:TYR:O	1:B:61:MET:C	2.57	0.42
1:B:28:LEU:HD12	1:B:28:LEU:HA	1.78	0.42
1:A:123:MET:HB3	1:A:123:MET:HE2	1.67	0.42
1:B:254:LEU:CD2	2:B:318:HOH:O	2.67	0.42
1:A:216:MET:HE3	1:A:216:MET:HB3	1.95	0.42
1:B:226:VAL:HG12	1:B:227:ASN:N	2.35	0.42
1:A:36:ASN:HA	1:A:39:ALA:CB	2.50	0.42
1:B:82:LEU:HB2	1:B:113:TYR:CD1	2.54	0.41
1:A:258:LEU:HD23	1:A:258:LEU:H	1.84	0.41
1:A:18:GLU:O	1:A:20:ALA:N	2.52	0.41
1:B:11:TYR:C	1:B:11:TYR:CD1	2.94	0.41
1:A:164:GLU:HG2	1:A:236:VAL:HG11	2.02	0.41
1:B:142:LEU:HA	1:B:142:LEU:HD12	1.81	0.41
1:B:257:ALA:C	1:B:259:VAL:N	2.70	0.41
1:B:79:MET:HE2	2:B:317:HOH:O	2.03	0.41
1:A:135:ARG:HG2	1:A:136:PRO:HD2	2.02	0.41
1:B:101:GLU:OE1	1:B:101:GLU:HA	2.20	0.41
1:B:158:LEU:HG	1:B:162:LEU:HD11	2.03	0.41
1:A:218:HIS:O	1:A:219:LEU:C	2.57	0.41
1:A:28:LEU:HA	1:A:31:ARG:HG2	2.03	0.41
1:B:183:GLY:O	1:B:184:ALA:C	2.59	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.89	0.41
1:A:212:LEU:N	1:A:212:LEU:CD2	2.81	0.41
1:A:248:ILE:O	1:A:248:ILE:HD13	2.21	0.40
1:B:198:THR:O	1:B:201:LEU:N	2.53	0.40
1:A:52:PHE:CE2	1:A:108:VAL:HG11	2.56	0.40
1:A:137:LEU:H	1:A:140:HIS:HD2	1.68	0.40
1:B:107:PHE:C	1:B:107:PHE:CD1	2.94	0.40
1:B:128:ALA:C	1:B:130:ASN:N	2.74	0.40
1:A:217:GLN:CB	1:A:260:GLN:HG2	2.51	0.40
1:B:259:VAL:C	1:B:260:GLN:HG3	2.42	0.40
1:A:82:LEU:HB2	1:A:113:TYR:CE2	2.56	0.40
1:B:231:THR:C	1:B:233:HIS:H	2.23	0.40
1:A:128:ALA:C	1:A:130:ASN:N	2.73	0.40
1:A:169:ASP:OD1	1:A:171:ASP:N	2.41	0.40
1:B:219:LEU:O	1:B:222:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ALA:CB	2:A:307:HOH:O	2.70	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	252/269 (94%)	188 (75%)	38 (15%)	26 (10%)	1	1
1	B	253/269 (94%)	204 (81%)	28 (11%)	21 (8%)	1	2
All	All	505/538 (94%)	392 (78%)	66 (13%)	47 (9%)	1	2

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	71	GLN
1	A	206	SER
1	A	247	LYS
1	A	255	ASN
1	A	258	LEU
1	A	259	VAL
1	B	9	ASP
1	B	10	ILE
1	B	29	LEU
1	B	71	GLN
1	B	206	SER
1	B	228	GLN
1	B	229	GLY
1	B	244	LYS
1	B	253	GLN
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	255	ASN
1	B	258	LEU
1	A	8	LYS
1	A	12	ALA
1	A	13	TYR
1	A	231	THR
1	A	254	LEU
1	A	257	ALA
1	B	230	LEU
1	B	247	LYS
1	B	257	ALA
1	B	259	VAL
1	A	19	ALA
1	A	130	ASN
1	A	197	TRP
1	A	214	PRO
1	B	130	ASN
1	B	227	ASN
1	A	15	ARG
1	A	149	GLY
1	A	194	ASN
1	A	199	PRO
1	A	229	GLY
1	A	252	PRO
1	B	23	VAL
1	B	70	MET
1	B	149	GLY
1	A	23	VAL
1	A	70	MET
1	A	221	LYS

### 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	202/237 (85%)	178 (88%)	24 (12%)	6 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/237 (88%)	185 (89%)	23 (11%)	8	22
All	All	410/474 (86%)	363 (88%)	47 (12%)	7	21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	27	TYR
1	A	29	LEU
1	A	32	GLU
1	A	34	THR
1	A	37	MET
1	A	54	LEU
1	A	77	LYS
1	A	107	PHE
1	A	108	VAL
1	A	114	THR
1	A	130	ASN
1	A	148	ILE
1	A	155	GLN
1	A	208	THR
1	A	210	GLU
1	A	212	LEU
1	A	213	LEU
1	A	215	VAL
1	A	222	ASN
1	A	224	VAL
1	A	239	LYS
1	A	248	ILE
1	A	260	GLN
1	B	11	TYR
1	B	28	LEU
1	B	32	GLU
1	B	36	ASN
1	B	37	MET
1	B	53	ARG
1	B	54	LEU
1	B	66	ILE
1	B	77	LYS
1	B	85	VAL
1	B	126	LEU
1	B	133	LEU

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Mol	Chain	Res	Type
1	B	135	ARG
1	B	137	LEU
1	B	144	ARG
1	B	206	SER
1	B	208	THR
1	B	215	VAL
1	B	230	LEU
1	B	231	THR
1	B	235	THR
1	B	248	ILE
1	B	260	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	81	GLN
1	A	130	ASN
1	A	140	HIS
1	A	155	GLN
1	A	218	HIS
1	A	233	HIS
1	A	255	ASN
1	A	260	GLN
1	B	47	GLN
1	B	72	ASN
1	B	116	HIS
1	B	130	ASN
1	B	140	HIS
1	B	155	GLN
1	B	227	ASN
1	B	233	HIS
1	B	260	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	254/269 (94%)	0.53	28 (11%) 7 4	69, 87, 119, 150	0
1	B	255/269 (94%)	0.25	16 (6%) 23 17	68, 86, 117, 150	0
All	All	509/538 (94%)	0.39	44 (8%) 13 8	68, 86, 118, 150	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ASN	10.0
1	A	195	GLY	8.1
1	B	194	ASN	4.6
1	A	199	PRO	4.5
1	B	231	THR	4.0
1	A	110	ASP	3.9
1	A	146	SER	3.9
1	A	9	ASP	3.8
1	B	152	ASP	3.5
1	A	11	TYR	3.4
1	A	84	GLY	3.4
1	A	218	HIS	3.3
1	B	9	ASP	3.3
1	A	14	LEU	3.2
1	A	153	VAL	3.1
1	A	230	LEU	3.1
1	A	204	TYR	3.0
1	B	86	THR	3.0
1	B	20	ALA	2.9
1	A	203	HIS	2.9
1	A	29	LEU	2.9
1	B	184	ALA	2.9
1	B	84	GLY	2.8
1	A	34	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	2.8
1	B	8	LYS	2.7
1	A	162	LEU	2.7
1	A	107	PHE	2.6
1	A	17	LEU	2.5
1	A	87	ALA	2.4
1	B	261	ASP	2.4
1	B	7	VAL	2.4
1	A	229	GLY	2.3
1	A	7	VAL	2.2
1	A	161	TYR	2.2
1	A	201	LEU	2.2
1	A	193	ASP	2.2
1	A	140	HIS	2.1
1	A	86	THR	2.1
1	B	171	ASP	2.1
1	B	151	VAL	2.1
1	B	242	THR	2.1
1	B	232	LYS	2.1
1	B	183	GLY	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 carbohydrates 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.