



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:07 am BST

PDB ID : 3BSB  
Title : Crystal Structure of Human Pumilio1 in Complex with CyclinB reverse RNA  
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Deposited on : 2007-12-23  
Resolution : 2.80 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.

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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	:	2.11
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)	:	2.11

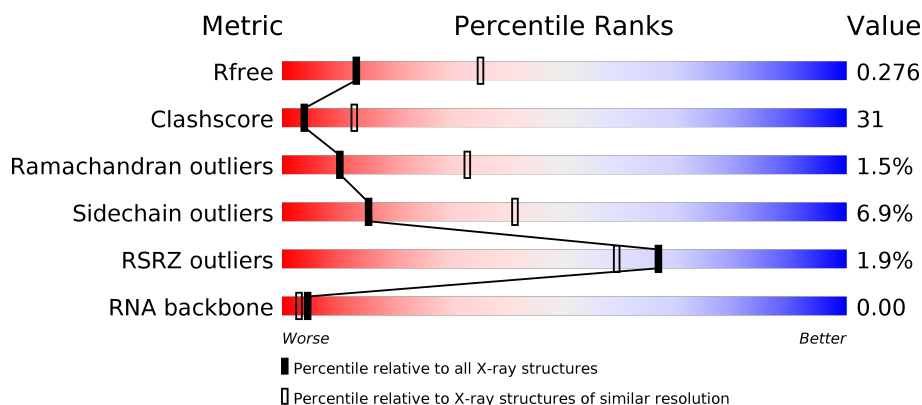
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 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	C	9	<div> <div>22%</div> <div>11% 89%</div> </div>
2	A	343	<div> <div>2%</div> <div>57% 39% ..</div> </div>
2	B	343	<div> <div>%</div> <div>56% 37% 6% ..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5820 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 RNA chain called 5'-R(\*UP\*UP\*UP\*AP\*AP\*UP\*GP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	9	Total	C	N	O	P	0	0	0
			184	84	27	65	8			

- Molecule 2 is a protein called Pumilio homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	340	Total	C	N	O	S	0	0	0
			2742	1741	490	494	17			
2	B	341	Total	C	N	O	S	0	0	0
			2749	1743	490	499	17			

- Molecule 3 is water.

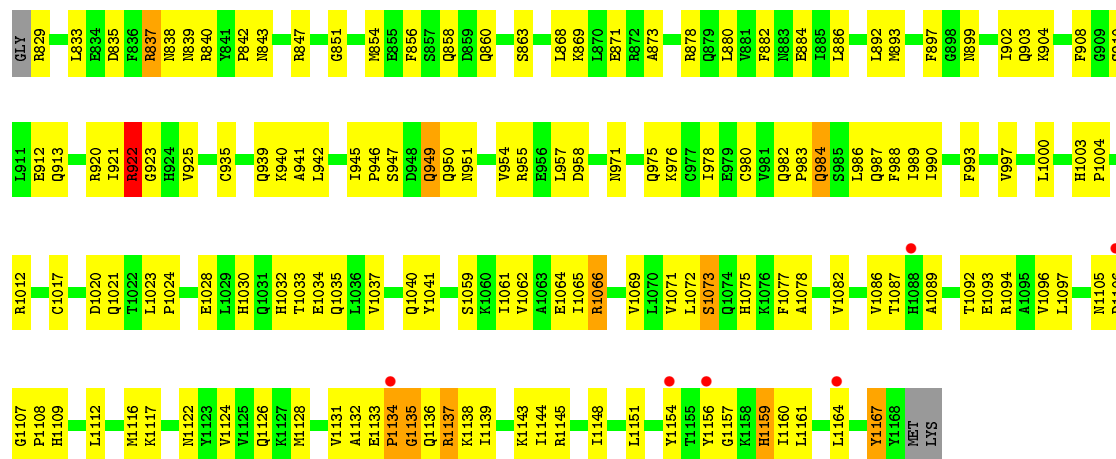
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	14	Total	O	0	0
			14	14		
3	A	48	Total	O	0	0
			48	48		
3	B	83	Total	O	0	0
			83	83		

These plots are drawn for all protein, RNA and DNA 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.

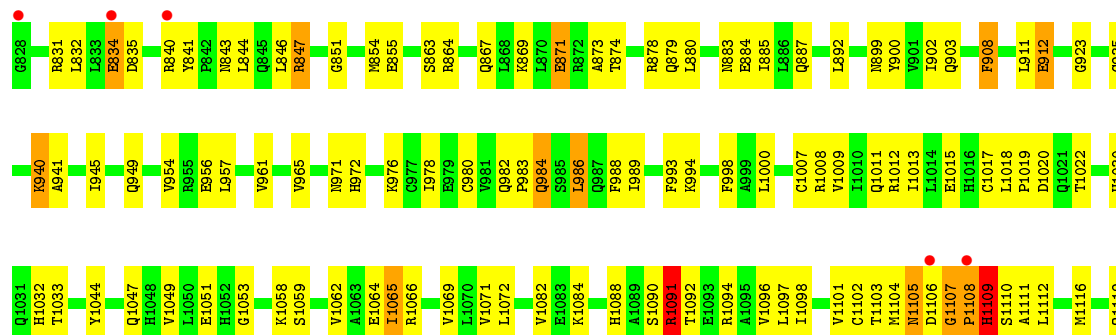
- Chain C:  11% 89%



- Chain A:  2% 57% 39%



- Chain B:  56% 37% 6%



V1124	V1125	Q1126	K1127	M1128	I1129	D1130	V1131	A1132	E1133	P1134	G1135	Q1136	R1137	K1138	I1139	V1140	M1141	H1142	K1143	I1144	R1145	P1146	H1147	I1148	A1149	T1150	L1151	R1152	K1153	Y1154	T1155	Y1156	G1157	K1158	H1159	I1160	L1161	A1162	K1163	L1164	E1165	K1166	Y1167	MET	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.87Å 64.29Å 321.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.87 – 2.80 25.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.3 (25.87-2.80) 89.6 (25.30-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.08 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.244 , 0.268 0.252 , 0.276	Depositor DCC
$R_{free}$ test set	1377 reflections (7.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.68% 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	C	1.33	1/204 (0.5%)	2.65	24/315 (7.6%)
2	A	0.42	0/2796	0.61	0/3776
2	B	0.59	0/2803	0.81	9/3786 (0.2%)
All	All	0.56	1/5803 (0.0%)	0.88	33/7877 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	U	C3'-O3'	6.25	1.50	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	U	N1-C1'-C2'	-13.22	96.81	114.00
1	C	3	U	P-O3'-C3'	10.59	132.41	119.70
1	C	2	U	O4'-C4'-C3'	-10.28	93.72	104.00
1	C	7	G	N9-C1'-C2'	-9.98	101.02	112.00
2	B	1108	PRO	CA-N-CD	-9.26	98.54	111.50
1	C	6	U	P-O3'-C3'	9.23	130.78	119.70
1	C	4	A	N9-C1'-C2'	-9.07	102.02	112.00
2	B	1167	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	C	6	U	O4'-C4'-C3'	-8.29	95.71	104.00
2	B	1109	HIS	CA-CB-CG	-7.45	100.94	113.60
1	C	4	A	OP1-P-OP2	-7.14	108.88	119.60
1	C	4	A	P-O3'-C3'	7.04	128.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	U	OP1-P-OP2	-6.83	109.36	119.60
1	C	3	U	OP1-P-OP2	-6.76	109.46	119.60
2	B	1134	PRO	CA-N-CD	-6.67	102.16	111.50
1	C	5	A	C8-N9-C4	-6.59	103.16	105.80
1	C	8	U	OP1-P-OP2	-6.36	110.07	119.60
1	C	9	U	OP1-P-OP2	-6.33	110.11	119.60
1	C	5	A	OP1-P-OP2	-6.13	110.41	119.60
1	C	6	U	O3'-P-O5'	-6.08	92.45	104.00
1	C	6	U	OP1-P-OP2	-5.86	110.81	119.60
2	B	834	GLU	CA-C-N	-5.85	104.32	117.20
1	C	5	A	P-O3'-C3'	5.85	126.72	119.70
2	B	1091	ARG	CB-CA-C	-5.84	98.72	110.40
1	C	1	U	O4'-C1'-N1	-5.83	103.54	108.20
1	C	4	A	O4'-C4'-C3'	-5.44	98.56	104.00
1	C	1	U	N1-C1'-C2'	5.43	121.06	114.00
1	C	4	A	C3'-C2'-C1'	-5.39	97.19	101.50
2	B	1158	LYS	CA-C-N	5.25	128.76	117.20
2	B	1152	ARG	C-N-CA	-5.23	108.62	121.70
2	B	1167	TYR	CB-CA-C	5.10	120.60	110.40
1	C	6	U	N1-C1'-C2'	5.03	120.54	114.00
1	C	3	U	P-O5'-C5'	-5.01	112.88	120.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	U	Sidechain
1	C	4	A	Sidechain
1	C	6	U	Sidechain

## 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	C	184	0	95	27	0
2	A	2742	0	2737	132	0
2	B	2749	0	2735	203	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	0	20	0
3	B	83	0	0	64	0
3	C	14	0	0	10	0
All	All	5820	0	5567	343	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 31.

All (343) 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)
2:A:829:ARG:NE	2:A:837:ARG:HH12	1.27	1.28
2:B:982:GLN:HB3	3:B:141:HOH:O	1.26	1.25
2:A:1138:LYS:HG2	3:A:166:HOH:O	1.37	1.22
2:A:829:ARG:NE	2:A:837:ARG:NH1	1.86	1.21
2:B:1098:ILE:HG12	3:B:145:HOH:O	1.43	1.14
2:A:829:ARG:HE	2:A:837:ARG:NH1	1.42	1.11
2:B:1128:MET:HB3	3:B:145:HOH:O	1.56	1.02
2:B:1166:LYS:HG2	2:B:1166:LYS:O	1.61	1.01
2:B:1009:VAL:HG11	3:B:140:HOH:O	1.58	1.00
2:B:1097:LEU:HD23	3:B:148:HOH:O	1.61	1.00
2:B:1129:ILE:HD11	3:B:149:HOH:O	1.62	0.99
2:A:1108:PRO:HG3	2:B:980:CYS:HB3	1.43	0.97
2:B:949:GLN:HG3	3:B:40:HOH:O	1.64	0.96
2:B:1069:VAL:HG21	3:B:148:HOH:O	1.66	0.95
2:B:989:ILE:HA	3:B:150:HOH:O	1.65	0.95
2:B:899:ASN:O	2:B:903:GLN:HG3	1.67	0.92
2:A:833:LEU:O	2:A:837:ARG:HB2	1.69	0.91
2:A:829:ARG:CZ	2:A:837:ARG:HH12	1.85	0.90
2:B:1033:THR:HG21	2:B:1064:GLU:HG3	1.53	0.89
1:C:6:U:H3'	3:C:116:HOH:O	1.73	0.88
2:B:1168:TYR:N	2:B:1168:TYR:CD2	2.31	0.88
2:A:835:ASP:OD1	2:A:840:ARG:CB	2.23	0.87
2:A:1138:LYS:CG	3:A:166:HOH:O	2.06	0.85
2:B:1090:SER:O	2:B:1091:ARG:C	2.13	0.85
2:A:986:LEU:HG	2:A:989:ILE:HD12	1.58	0.85
2:A:829:ARG:HE	2:A:837:ARG:HH12	0.99	0.83
2:B:961:VAL:HG11	3:B:150:HOH:O	1.76	0.83
2:B:1137:ARG:HB2	3:B:119:HOH:O	1.78	0.83
2:A:1138:LYS:HG2	2:A:1167:TYR:OH	1.79	0.82
2:B:1167:TYR:HD1	2:B:1167:TYR:C	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1167:TYR:CD1	2:B:1167:TYR:C	2.53	0.82
1:C:8:U:H4'	3:C:98:HOH:O	1.79	0.81
2:B:1164:LEU:HD12	2:B:1164:LEU:O	1.81	0.81
2:B:854:MET:SD	3:B:133:HOH:O	2.39	0.80
2:B:989:ILE:HG12	3:B:150:HOH:O	1.80	0.80
2:A:1156:TYR:HA	2:A:1159:HIS:NE2	1.97	0.78
2:A:1138:LYS:CD	3:A:166:HOH:O	2.31	0.78
2:B:879:GLN:HE21	2:B:883:ASN:HD21	1.30	0.78
2:B:993:PHE:HZ	3:B:140:HOH:O	1.67	0.77
2:A:1032:HIS:CE1	3:A:144:HOH:O	2.36	0.77
2:A:921:ILE:O	2:A:922:ARG:O	2.03	0.77
2:B:1017:CYS:SG	3:B:115:HOH:O	2.22	0.77
2:B:1017:CYS:SG	3:B:139:HOH:O	2.42	0.77
2:B:1133:GLU:C	3:B:119:HOH:O	2.23	0.76
2:B:841:TYR:HB3	2:B:844:LEU:HB2	1.67	0.76
1:C:2:U:H5'	3:C:109:HOH:O	1.86	0.75
2:B:1125:VAL:CG1	3:B:149:HOH:O	2.34	0.75
2:B:1110:SER:HB2	3:B:142:HOH:O	1.86	0.75
2:B:1159:HIS:O	2:B:1163:LYS:HD2	1.87	0.74
2:B:880:LEU:HD23	3:B:164:HOH:O	1.86	0.74
2:B:1013:ILE:HG12	3:B:139:HOH:O	1.87	0.74
2:B:1168:TYR:N	2:B:1168:TYR:HD2	1.85	0.73
2:B:864:ARG:HG3	3:B:157:HOH:O	1.88	0.73
2:B:1125:VAL:HG12	3:B:149:HOH:O	1.88	0.73
1:C:7:G:N2	2:B:935:CYS:SG	2.61	0.73
2:B:1030:HIS:HA	3:B:120:HOH:O	1.88	0.73
2:B:885:ILE:HG22	3:B:133:HOH:O	1.89	0.72
1:C:9:U:C6	2:B:900:TYR:CZ	2.77	0.72
2:A:1033:THR:HG21	2:A:1064:GLU:HG3	1.72	0.72
2:B:1137:ARG:CB	3:B:119:HOH:O	2.36	0.72
2:B:1098:ILE:HG23	3:B:145:HOH:O	1.89	0.72
2:B:984:GLN:HG2	3:B:141:HOH:O	1.89	0.71
1:C:6:U:H2'	3:C:116:HOH:O	1.90	0.71
2:A:951:ASN:O	2:A:955:ARG:HG3	1.91	0.71
1:C:6:U:C3'	3:C:116:HOH:O	2.32	0.71
2:B:1108:PRO:HD2	2:B:1109:HIS:N	2.05	0.70
2:B:1167:TYR:C	2:B:1168:TYR:CD2	2.65	0.70
2:B:965:VAL:CG2	3:B:140:HOH:O	2.39	0.70
2:B:1097:LEU:HA	3:B:148:HOH:O	1.92	0.69
3:C:186:HOH:O	2:B:1158:LYS:N	2.26	0.69
2:B:986:LEU:HG	2:B:989:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:U:C2'	3:C:116:HOH:O	2.41	0.69
2:B:1167:TYR:C	2:B:1168:TYR:HD2	1.95	0.69
2:B:1160:ILE:O	2:B:1161:LEU:C	2.31	0.69
2:B:1066:ARG:NH1	2:B:1096:VAL:HG11	2.08	0.69
2:A:903:GLN:HB3	2:A:940:LYS:HD2	1.75	0.68
2:A:920:ARG:CZ	3:A:163:HOH:O	2.39	0.68
2:B:1051:GLU:OE1	2:B:1084:LYS:NZ	2.26	0.68
2:B:1092:THR:HB	3:B:88:HOH:O	1.94	0.68
2:B:961:VAL:HG21	3:B:150:HOH:O	1.94	0.68
2:B:1110:SER:CB	3:B:142:HOH:O	2.41	0.68
2:A:893:MET:HG3	2:A:902:ILE:HD13	1.76	0.67
2:A:1034:GLU:HB3	2:A:1035:GLN:HE21	1.60	0.67
2:A:1073:SER:OG	2:A:1124:VAL:HG21	1.94	0.66
1:C:9:U:H1'	2:B:900:TYR:CE1	2.29	0.66
2:A:1105:ASN:HB2	3:A:176:HOH:O	1.95	0.66
2:A:935:CYS:O	2:A:939:GLN:HG3	1.96	0.66
2:A:1136:GLN:O	2:A:1137:ARG:C	2.34	0.66
2:B:961:VAL:CG1	3:B:150:HOH:O	2.37	0.66
2:A:1069:VAL:O	2:A:1073:SER:HB2	1.95	0.66
2:A:1167:TYR:CD1	2:A:1167:TYR:C	2.69	0.66
2:B:1161:LEU:HB3	3:B:108:HOH:O	1.94	0.66
2:A:971:ASN:O	2:A:975:GLN:HG3	1.97	0.65
2:B:1066:ARG:HH11	2:B:1066:ARG:HG2	1.62	0.65
2:A:921:ILE:O	2:A:922:ARG:C	2.36	0.64
2:B:1112:LEU:O	2:B:1116:MET:HG2	1.98	0.64
2:A:1105:ASN:HB2	3:A:152:HOH:O	1.97	0.63
2:B:1058:LYS:HE3	2:B:1088:HIS:HB3	1.79	0.63
2:A:1138:LYS:HD3	3:A:166:HOH:O	1.98	0.63
2:B:965:VAL:HG21	3:B:140:HOH:O	1.96	0.62
2:A:833:LEU:O	2:A:837:ARG:CB	2.45	0.62
2:B:854:MET:HE1	2:B:892:LEU:HG	1.81	0.62
2:B:1013:ILE:HG23	3:B:139:HOH:O	1.99	0.62
2:B:1160:ILE:O	2:B:1163:LYS:N	2.31	0.62
1:C:5:A:H5''	3:B:56:HOH:O	1.99	0.62
2:A:1124:VAL:O	2:A:1128:MET:HG3	1.99	0.62
2:B:892:LEU:HB2	2:B:902:ILE:HD11	1.82	0.62
2:B:1090:SER:O	2:B:1091:ARG:O	2.18	0.61
2:B:1106:ASP:CG	2:B:1107:GLY:H	2.04	0.61
2:A:1107:GLY:N	3:A:176:HOH:O	2.25	0.61
2:A:892:LEU:HB2	2:A:902:ILE:HD11	1.83	0.61
2:A:893:MET:CG	2:A:902:ILE:HD13	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1167:TYR:C	2:A:1167:TYR:HD1	2.03	0.61
2:B:1107:GLY:C	2:B:1109:HIS:H	2.04	0.61
2:B:1124:VAL:O	2:B:1128:MET:HG3	2.01	0.60
2:B:1111:ALA:HA	3:B:137:HOH:O	1.99	0.60
2:B:1168:TYR:HA	3:B:113:HOH:O	2.00	0.60
2:A:1059:SER:HA	2:A:1062:VAL:HG12	1.82	0.60
2:A:1138:LYS:HD3	3:A:147:HOH:O	2.01	0.60
2:B:879:GLN:NE2	2:B:883:ASN:HD21	1.97	0.60
2:A:1108:PRO:HG3	2:B:980:CYS:CB	2.25	0.60
2:B:1033:THR:HB	3:B:120:HOH:O	2.02	0.60
2:A:941:ALA:O	2:A:945:ILE:HG12	2.02	0.59
2:B:1069:VAL:CG2	3:B:148:HOH:O	2.38	0.59
2:A:829:ARG:CD	2:A:837:ARG:NH1	2.65	0.59
2:B:1104:MET:HG2	2:B:1105:ASN:N	2.18	0.59
2:B:1165:GLU:O	2:B:1167:TYR:N	2.35	0.59
2:A:869:LYS:O	2:A:873:ALA:HB2	2.04	0.58
2:A:1145:ARG:HA	2:A:1164:LEU:HD11	1.85	0.58
2:A:1108:PRO:CG	2:B:980:CYS:HB3	2.26	0.58
2:A:1034:GLU:HB3	2:A:1035:GLN:NE2	2.18	0.58
1:C:4:A:H1'	2:B:1044:TYR:CE2	2.38	0.58
2:B:831:ARG:O	2:B:835:ASP:CG	2.42	0.58
2:B:940:LYS:HA	2:B:940:LYS:HE3	1.86	0.58
2:A:976:LYS:CD	3:A:110:HOH:O	2.50	0.58
2:B:912:GLU:CD	2:B:912:GLU:H	2.07	0.57
2:B:884:GLU:HG3	3:B:164:HOH:O	2.03	0.57
2:A:833:LEU:O	2:A:837:ARG:N	2.32	0.57
2:A:1032:HIS:HE1	3:A:144:HOH:O	1.76	0.57
2:A:1092:THR:O	2:A:1096:VAL:HG23	2.04	0.57
2:A:1148:ILE:HG23	2:A:1161:LEU:HD11	1.87	0.57
2:A:976:LYS:HD3	3:A:110:HOH:O	2.04	0.57
2:B:961:VAL:O	2:B:965:VAL:HG23	2.05	0.57
2:B:885:ILE:C	2:B:885:ILE:HD12	2.25	0.57
2:B:961:VAL:CG2	3:B:150:HOH:O	2.52	0.56
2:A:1109:HIS:HB3	3:A:1:HOH:O	2.05	0.56
2:A:1112:LEU:CD2	2:A:1143:LYS:HB3	2.35	0.56
2:B:1155:THR:C	2:B:1157:GLY:H	2.09	0.56
1:C:9:U:N1	2:B:900:TYR:CZ	2.73	0.56
2:B:984:GLN:NE2	3:B:141:HOH:O	2.24	0.56
2:A:1040:GLN:HA	2:A:1077:PHE:CD2	2.41	0.56
2:B:1102:CYS:SG	2:B:1140:VAL:HG22	2.45	0.56
2:B:878:ARG:HG3	2:B:878:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1125:VAL:HG12	2:B:1160:ILE:HD12	1.88	0.56
2:B:887:GLN:HA	2:B:887:GLN:NE2	2.21	0.56
2:A:921:ILE:C	2:A:922:ARG:O	2.42	0.56
2:B:1135:GLY:O	2:B:1139:ILE:HG13	2.06	0.55
2:B:1145:ARG:HB3	2:B:1146:PRO:HD3	1.87	0.55
2:B:879:GLN:HE21	2:B:883:ASN:ND2	2.01	0.55
2:A:842:PRO:HG2	2:A:843:ASN:OD1	2.06	0.55
2:A:984:GLN:H	2:A:984:GLN:CD	2.09	0.55
2:B:1066:ARG:NH1	2:B:1096:VAL:CG1	2.69	0.55
2:B:1106:ASP:HB3	3:B:137:HOH:O	2.06	0.55
2:B:1158:LYS:C	3:B:108:HOH:O	2.44	0.55
2:A:1116:MET:SD	2:A:1144:ILE:HG23	2.46	0.55
2:A:1107:GLY:CA	3:A:176:HOH:O	2.53	0.55
2:A:920:ARG:NH2	3:A:163:HOH:O	2.40	0.55
2:B:1108:PRO:CD	2:B:1109:HIS:N	2.63	0.55
1:C:9:U:C6	2:B:900:TYR:OH	2.59	0.55
2:A:854:MET:O	2:A:858:GLN:HG3	2.07	0.54
2:A:912:GLU:OE1	2:A:912:GLU:N	2.38	0.54
2:B:965:VAL:HG22	3:B:140:HOH:O	2.06	0.54
2:A:910:SER:H	2:A:913:GLN:NE2	2.06	0.54
2:B:840:ARG:HA	2:B:840:ARG:NE	2.23	0.54
2:B:911:LEU:HB3	2:B:912:GLU:OE1	2.08	0.54
2:B:941:ALA:O	2:B:945:ILE:HG12	2.08	0.54
2:B:1059:SER:O	2:B:1062:VAL:HG12	2.07	0.53
2:B:1103:THR:O	2:B:1103:THR:HG22	2.09	0.53
2:B:912:GLU:N	2:B:912:GLU:OE1	2.36	0.53
2:B:1138:LYS:O	2:B:1139:ILE:C	2.44	0.53
2:B:846:LEU:HG	2:B:869:LYS:HB3	1.91	0.53
2:A:1030:HIS:O	2:A:1033:THR:HG22	2.08	0.53
2:B:1018:LEU:O	2:B:1022:THR:HG23	2.09	0.53
1:C:9:U:C4	2:B:900:TYR:CE2	2.96	0.53
2:A:1167:TYR:CD1	2:A:1167:TYR:O	2.62	0.53
2:A:1094:ARG:HD2	2:A:1131:VAL:HB	1.91	0.53
2:A:1133:GLU:O	2:A:1135:GLY:N	2.42	0.53
2:B:1159:HIS:N	3:B:108:HOH:O	2.42	0.52
2:A:860:GLN:HG3	2:A:897:PHE:CE2	2.44	0.52
2:B:1134:PRO:HD3	3:B:156:HOH:O	2.09	0.52
2:B:982:GLN:C	3:B:141:HOH:O	2.47	0.52
2:A:942:LEU:O	2:A:950:GLN:NE2	2.43	0.52
2:A:987:GLN:OE1	2:A:1021:GLN:HG2	2.10	0.52
2:A:1071:VAL:HG23	2:A:1072:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:GLU:HA	2:B:871:GLU:OE1	2.09	0.52
2:A:829:ARG:HG3	2:A:829:ARG:HH11	1.76	0.51
2:B:831:ARG:O	2:B:835:ASP:CB	2.59	0.51
2:B:854:MET:HE3	2:B:892:LEU:HD21	1.92	0.51
2:B:984:GLN:H	2:B:984:GLN:CD	2.13	0.51
2:A:954:VAL:HA	2:A:957:LEU:HD13	1.92	0.51
2:B:1047:GLN:OE1	2:B:1084:LYS:NZ	2.34	0.51
1:C:9:U:C2	2:B:900:TYR:CE1	2.99	0.51
2:B:840:ARG:HA	2:B:840:ARG:HE	1.76	0.51
2:B:1098:ILE:HD13	2:B:1132:ALA:HB2	1.92	0.50
1:C:9:U:C1'	2:B:900:TYR:CE1	2.94	0.50
2:A:829:ARG:HG3	2:A:829:ARG:NH1	2.25	0.50
2:B:1091:ARG:O	2:B:1094:ARG:HB2	2.11	0.50
2:A:1093:GLU:O	2:A:1097:LEU:HG	2.12	0.50
2:B:1106:ASP:CG	2:B:1107:GLY:N	2.63	0.50
2:A:829:ARG:HB3	2:A:833:LEU:HD23	1.92	0.50
2:B:831:ARG:O	2:B:835:ASP:HB2	2.12	0.50
2:A:1003:HIS:CG	2:A:1004:PRO:HD2	2.47	0.50
2:A:1033:THR:O	2:A:1037:VAL:HG13	2.12	0.49
2:A:1136:GLN:O	2:A:1139:ILE:N	2.44	0.49
2:B:1098:ILE:CG2	3:B:145:HOH:O	2.53	0.49
2:B:1129:ILE:CD1	3:B:149:HOH:O	2.37	0.49
2:B:832:LEU:O	2:B:835:ASP:HB2	2.13	0.49
2:B:1141:MET:CB	2:B:1167:TYR:OH	2.61	0.49
1:C:9:U:N1	2:B:900:TYR:CE1	2.79	0.49
2:B:940:LYS:CE	2:B:940:LYS:HA	2.42	0.49
1:C:1:U:C4	3:C:186:HOH:O	2.53	0.49
2:B:874:THR:O	2:B:878:ARG:HG3	2.11	0.49
2:A:1017:CYS:SG	3:A:68:HOH:O	2.37	0.49
2:A:1126:GLN:HG2	2:A:1160:ILE:HD13	1.94	0.49
1:C:4:A:H1'	2:B:1044:TYR:HE2	1.75	0.49
2:B:883:ASN:ND2	3:B:161:HOH:O	2.45	0.49
2:A:1028:GLU:O	2:A:1032:HIS:HD2	1.96	0.49
2:B:878:ARG:HG3	2:B:878:ARG:NH1	2.28	0.49
2:B:1148:ILE:O	2:B:1149:ALA:C	2.48	0.48
2:B:976:LYS:HE3	2:B:980:CYS:SG	2.53	0.48
2:A:1117:LYS:HG3	3:A:138:HOH:O	2.12	0.48
2:B:887:GLN:HA	2:B:887:GLN:HE21	1.78	0.48
1:C:7:G:H2'	1:C:7:G:N3	2.28	0.48
2:B:1130:ASP:OD1	2:B:1163:LYS:NZ	2.47	0.48
2:B:880:LEU:HD23	2:B:880:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1061:ILE:O	2:A:1065:ILE:HD13	2.14	0.48
2:B:1091:ARG:HH21	2:B:1133:GLU:CD	2.16	0.48
2:B:854:MET:HA	3:B:133:HOH:O	2.13	0.48
2:A:1089:ALA:HB1	2:A:1093:GLU:OE2	2.14	0.48
2:B:1011:GLN:O	2:B:1015:GLU:HG3	2.14	0.47
2:A:880:LEU:O	2:A:880:LEU:HD23	2.14	0.47
2:A:982:GLN:HB3	2:A:984:GLN:HE21	1.78	0.47
1:C:5:A:C2	2:B:972:HIS:CE1	3.02	0.47
2:A:868:LEU:O	2:A:871:GLU:CB	2.62	0.47
2:B:993:PHE:CE2	2:B:1000:LEU:HD13	2.50	0.47
2:A:1033:THR:CG2	2:A:1064:GLU:HG3	2.42	0.47
2:A:946:PRO:HB2	2:A:949:GLN:HE21	1.79	0.47
2:B:1107:GLY:C	2:B:1109:HIS:N	2.68	0.47
2:A:1075:HIS:HB3	2:A:1078:ALA:HB3	1.96	0.47
2:B:1012:ARG:NH1	2:B:1012:ARG:HG2	2.30	0.46
2:B:1137:ARG:N	3:B:119:HOH:O	2.38	0.46
2:B:1164:LEU:C	2:B:1164:LEU:HD12	2.36	0.46
2:B:892:LEU:HB2	2:B:902:ILE:CD1	2.44	0.46
2:A:868:LEU:O	2:A:871:GLU:HB2	2.16	0.46
1:C:9:U:C5	2:B:900:TYR:CE2	3.04	0.46
2:B:998:PHE:HB2	2:B:1032:HIS:CD2	2.51	0.46
2:B:1030:HIS:O	2:B:1033:THR:HG22	2.16	0.46
2:A:1040:GLN:HA	2:A:1077:PHE:CE2	2.51	0.45
2:A:983:PRO:O	2:A:986:LEU:HB2	2.15	0.45
2:B:1119:GLN:HG3	2:B:1156:TYR:CZ	2.51	0.45
2:A:878:ARG:HG3	2:A:878:ARG:HH11	1.82	0.45
2:B:1160:ILE:HG12	3:B:14:HOH:O	2.17	0.45
2:B:869:LYS:O	2:B:873:ALA:HB2	2.16	0.45
2:A:851:GLY:H	2:A:884:GLU:CD	2.20	0.45
2:B:978:ILE:HA	2:B:986:LEU:CD2	2.46	0.45
2:A:1138:LYS:HG2	2:A:1167:TYR:HH	1.81	0.45
2:B:1094:ARG:O	2:B:1098:ILE:HG13	2.16	0.45
2:B:1071:VAL:HG23	2:B:1072:LEU:N	2.31	0.45
1:C:1:U:O4	2:B:1159:HIS:HB2	2.17	0.45
2:A:1107:GLY:HA2	3:A:176:HOH:O	2.14	0.44
2:A:1145:ARG:O	2:A:1148:ILE:HG13	2.17	0.44
2:A:978:ILE:HA	2:A:986:LEU:HD21	1.99	0.44
2:B:1007:CYS:O	2:B:1011:GLN:HG3	2.17	0.44
2:B:1141:MET:HB3	2:B:1167:TYR:OH	2.17	0.44
1:C:9:U:C2	2:B:900:TYR:CD1	3.05	0.44
2:A:947:SER:O	2:A:951:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1145:ARG:NH2	3:B:113:HOH:O	2.50	0.44
2:B:851:GLY:H	2:B:884:GLU:CD	2.20	0.44
2:B:899:ASN:OD1	2:B:903:GLN:NE2	2.51	0.44
2:B:1091:ARG:O	2:B:1094:ARG:N	2.50	0.44
2:B:993:PHE:CZ	3:B:140:HOH:O	2.54	0.44
2:B:986:LEU:HG	2:B:989:ILE:CD1	2.44	0.44
2:A:1087:THR:O	2:A:1087:THR:HG22	2.18	0.43
2:B:847:ARG:HH11	2:B:880:LEU:HD12	1.83	0.43
2:B:1091:ARG:HA	2:B:1094:ARG:NH2	2.34	0.43
2:B:923:GLY:H	2:B:956:GLU:CD	2.21	0.43
2:A:1071:VAL:HG23	2:A:1072:LEU:H	1.83	0.43
2:A:1151:LEU:HD22	2:A:1157:GLY:HA2	2.00	0.43
2:A:1112:LEU:HD23	2:A:1143:LYS:HB3	2.00	0.43
2:B:1106:ASP:CB	3:B:137:HOH:O	2.64	0.43
2:A:1106:ASP:O	2:A:1108:PRO:HD2	2.19	0.43
2:A:899:ASN:O	2:A:903:GLN:HG3	2.19	0.43
2:A:958:ASP:HA	2:A:988:PHE:CD1	2.53	0.43
2:B:863:SER:O	2:B:867:GLN:HG3	2.19	0.43
2:A:1012:ARG:NE	2:A:1012:ARG:HA	2.34	0.43
2:A:880:LEU:C	2:A:880:LEU:HD23	2.39	0.43
2:B:1128:MET:CG	3:B:145:HOH:O	2.64	0.43
2:B:832:LEU:C	2:B:835:ASP:HB2	2.39	0.43
1:C:9:U:H5"	3:C:22:HOH:O	2.19	0.43
2:B:1165:GLU:C	2:B:1167:TYR:H	2.22	0.42
2:B:954:VAL:CG1	2:B:988:PHE:HE2	2.32	0.42
2:A:1133:GLU:O	2:A:1134:PRO:C	2.56	0.42
2:B:1153:LYS:HE2	2:B:1153:LYS:HB3	1.45	0.42
2:A:997:VAL:HG21	2:A:1028:GLU:HB2	2.01	0.42
1:C:9:U:P	3:C:175:HOH:O	2.77	0.42
2:B:1007:CYS:SG	2:B:1008:ARG:N	2.93	0.42
2:B:1012:ARG:HH11	2:B:1012:ARG:HG2	1.85	0.42
2:A:1040:GLN:HG3	2:A:1041:TYR:CD1	2.55	0.42
2:A:835:ASP:C	2:A:838:ASN:H	2.23	0.42
2:A:904:LYS:HG3	2:A:908:PHE:CD1	2.55	0.42
2:A:957:LEU:HD12	2:A:957:LEU:N	2.35	0.42
2:B:1145:ARG:O	2:B:1148:ILE:HG13	2.20	0.42
2:A:1122:ASN:O	2:A:1126:GLN:HG3	2.20	0.41
2:A:993:PHE:CE2	2:A:1000:LEU:HD13	2.55	0.41
2:A:1117:LYS:HD2	2:A:1154:TYR:HE1	1.86	0.41
2:A:983:PRO:HG2	2:A:984:GLN:NE2	2.36	0.41
2:B:983:PRO:HG2	2:B:984:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1132:ALA:O	2:A:1137:ARG:NH1	2.54	0.41
2:B:1101:VAL:O	2:B:1111:ALA:HB3	2.20	0.41
2:B:1129:ILE:HD12	2:B:1163:LYS:HD3	2.03	0.41
2:B:1049:VAL:O	2:B:1053:GLY:N	2.52	0.41
2:B:989:ILE:CG1	3:B:150:HOH:O	2.55	0.41
2:A:886:LEU:HD11	3:A:163:HOH:O	2.20	0.41
2:B:1098:ILE:CG1	3:B:145:HOH:O	2.24	0.41
2:A:1066:ARG:NH2	2:A:1096:VAL:HG11	2.35	0.41
2:B:1134:PRO:HA	3:B:156:HOH:O	2.20	0.41
2:B:1168:TYR:CD2	2:B:1168:TYR:C	2.88	0.41
2:A:990:ILE:HG13	2:A:1021:GLN:HB3	2.03	0.41
2:A:882:PHE:CE1	2:A:886:LEU:HD22	2.56	0.41
2:B:1065:ILE:HA	2:B:1065:ILE:HD12	1.88	0.41
2:A:925:VAL:CG1	2:A:957:LEU:HD11	2.51	0.40
2:B:1145:ARG:N	2:B:1146:PRO:CD	2.84	0.40
2:A:1059:SER:O	2:A:1062:VAL:HG12	2.22	0.40
2:A:1082:VAL:O	2:A:1086:VAL:HG23	2.21	0.40
2:B:1152:ARG:HG2	2:B:1152:ARG:HH11	1.86	0.40
2:B:1167:TYR:HD1	2:B:1168:TYR:N	2.19	0.40
2:A:1023:LEU:N	2:A:1024:PRO:HD2	2.36	0.40
2:A:856:PHE:O	2:A:863:SER:N	2.54	0.40
2:B:1096:VAL:O	2:B:1096:VAL:HG12	2.20	0.40
2:B:978:ILE:HA	2:B:986:LEU:HD21	2.03	0.40
1:C:4:A:C1'	2:B:1044:TYR:CE2	3.04	0.40
2:B:835:ASP:O	2:B:840:ARG:HB2	2.20	0.40
2:B:908:PHE:CD1	2:B:908:PHE:N	2.89	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	
2	A	338/343 (98%)	315 (93%)	18 (5%)	5 (2%)	10	33
2	B	339/343 (99%)	313 (92%)	21 (6%)	5 (2%)	10	33
All	All	677/686 (99%)	628 (93%)	39 (6%)	10 (2%)	10	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	922	ARG
2	A	1134	PRO
2	B	1107	GLY
2	B	1134	PRO
2	B	1166	LYS
2	B	1091	ARG
2	A	839	ASN
2	A	923	GLY
2	A	1135	GLY
2	B	1160	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	298/306 (97%)	286 (96%)	12 (4%)	31	65
2	B	299/306 (98%)	270 (90%)	29 (10%)	8	24
All	All	597/612 (98%)	556 (93%)	41 (7%)	15	41

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	837	ARG
2	A	847	ARG
2	A	922	ARG
2	A	949	GLN
2	A	980	CYS
2	A	984	GLN

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Mol	Chain	Res	Type
2	A	1020	ASP
2	A	1066	ARG
2	A	1073	SER
2	A	1137	ARG
2	A	1159	HIS
2	A	1167	TYR
2	B	834	GLU
2	B	843	ASN
2	B	847	ARG
2	B	855	GLU
2	B	871	GLU
2	B	908	PHE
2	B	912	GLU
2	B	940	LYS
2	B	957	LEU
2	B	971	ASN
2	B	984	GLN
2	B	986	LEU
2	B	994	LYS
2	B	1019	PRO
2	B	1020	ASP
2	B	1065	ILE
2	B	1082	VAL
2	B	1105	ASN
2	B	1109	HIS
2	B	1127	LYS
2	B	1134	PRO
2	B	1143	LYS
2	B	1151	LEU
2	B	1153	LYS
2	B	1161	LEU
2	B	1163	LYS
2	B	1166	LYS
2	B	1167	TYR
2	B	1168	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	860	GLN
2	A	883	ASN
2	A	891	GLN

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Mol	Chain	Res	Type
2	A	913	GLN
2	A	949	GLN
2	A	984	GLN
2	A	1031	GLN
2	A	1032	HIS
2	A	1035	GLN
2	A	1136	GLN
2	B	839	ASN
2	B	858	GLN
2	B	860	GLN
2	B	883	ASN
2	B	887	GLN
2	B	891	GLN
2	B	913	GLN
2	B	949	GLN
2	B	968	GLN
2	B	972	HIS
2	B	984	GLN
2	B	1031	GLN
2	B	1032	HIS
2	B	1074	GLN
2	B	1109	HIS
2	B	1119	GLN
2	B	1147	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	9/9 (100%)	8 (88%)	4 (44%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	U
1	C	3	U
1	C	4	A
1	C	5	A
1	C	6	U
1	C	7	G
1	C	8	U
1	C	9	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	1	U
1	C	2	U
1	C	4	A
1	C	6	U

#### 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 [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<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	C	9/9 (100%)	1.22	2 (22%) 0 0	58, 70, 86, 90	0
2	A	340/343 (99%)	0.16	6 (1%) 68 61	25, 47, 73, 87	0
2	B	341/343 (99%)	-0.04	5 (1%) 73 68	19, 37, 69, 87	0
All	All	690/695 (99%)	0.07	13 (1%) 66 59	19, 42, 73, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	828	GLY	3.9
2	A	1156	TYR	3.6
2	B	840	ARG	3.4
2	A	1106	ASP	2.8
2	A	1088	HIS	2.6
2	A	1154	TYR	2.5
1	C	7	G	2.5
2	A	1164	LEU	2.4
2	A	1134	PRO	2.4
2	B	1106	ASP	2.2
1	C	9	U	2.1
2	B	834	GLU	2.1
2	B	1108	PRO	2.1

### 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.