



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:19 PM GMT

PDB ID : 3Q0M  
Title : Crystal structure of the PUMILIO-homology domain from Human PUMILIO1  
in complex with p38alpha NREb  
Authors : Lu, G.; Hall, T.M.T.  
Deposited on : 2010-12-15  
Resolution : 2.71 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

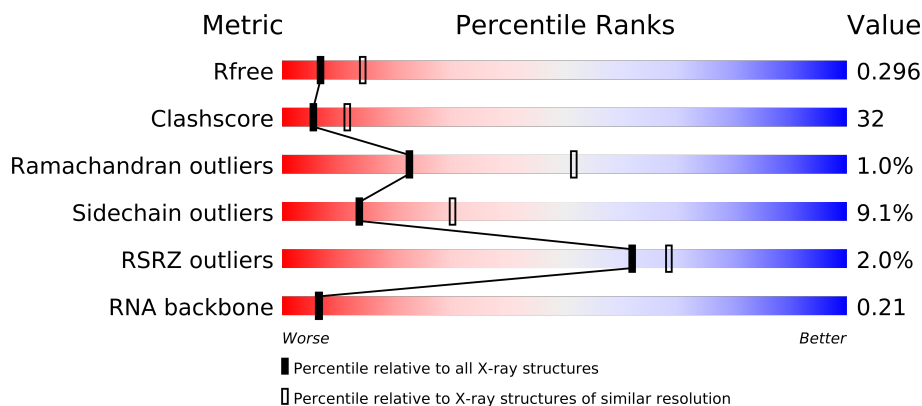
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.71 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
2	C	8	
2	D	8	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5912 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pumilio homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2738	1732	496	493	17			
1	B	338	Total	C	N	O	S	0	0	0
			2748	1741	495	495	17			

- Molecule 2 is a RNA chain called 5'-R(UP\*GP\*UP\*AP\*GP\*AP\*UP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			
2	D	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	39	Total	O	0	0
			39	39		
3	C	4	Total	O	0	0
			4	4		
3	D	6	Total	O	0	0
			6	6		



- Molecule 2: 5'-R(UP\*GP\*UP\*AP\*GP\*AP\*UP\*A)-3'

Chain C:



- Molecule 2: 5'-R(UP\*GP\*UP\*AP\*GP\*AP\*UP\*A)-3'

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.86Å 59.65Å 333.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.71 29.83 – 2.71	Depositor EDS
% Data completeness (in resolution range)	78.7 (29.80-2.71) 79.3 (29.83-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4.6)	Depositor
R, $R_{free}$	0.212 , 0.298 0.213 , 0.296	Depositor DCC
$R_{free}$ test set	804 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 16361 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5912	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 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0/2790	0.60	0/3763
1	B	0.42	0/2801	0.58	1/3778 (0.0%)
2	C	0.85	0/189	1.69	5/293 (1.7%)
2	D	0.82	0/189	1.98	7/293 (2.4%)
All	All	0.46	0/5969	0.76	13/8127 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	U	O4'-C1'-N1	9.95	116.16	108.20
2	C	6	A	P-O3'-C3'	-7.21	111.05	119.70
2	D	5	G	P-O3'-C3'	6.86	127.93	119.70
2	C	5	G	P-O3'-C3'	6.80	127.86	119.70
2	C	7	U	O5'-P-OP2	-6.68	99.69	105.70
2	D	7	U	N1-C1'-C2'	-6.27	105.11	112.00
2	D	1	U	O4'-C1'-N1	-6.13	103.30	108.20
2	D	6	A	N9-C1'-C2'	-5.62	105.81	112.00
2	D	6	A	C3'-C2'-C1'	5.59	105.97	101.50
2	C	7	U	N1-C1'-C2'	-5.58	105.86	112.00
2	C	7	U	C3'-C2'-C1'	5.37	105.80	101.50
2	D	6	A	P-O5'-C5'	-5.16	112.64	120.90
1	B	981	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2738	0	2756	178	0
1	B	2748	0	2765	182	0
2	C	169	0	87	8	0
2	D	169	0	87	12	0
3	A	39	0	0	4	0
3	B	39	0	0	10	0
3	C	4	0	0	1	0
3	D	6	0	0	0	0
All	All	5912	0	5695	370	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (370) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:863:SER:O	1:B:867:GLN:HG3	1.52	1.09
1:B:874:THR:HA	1:B:878:ARG:HD3	1.31	1.07
1:A:990:ILE:HG13	1:A:1021:GLN:HB3	1.43	0.99
2:D:2:G:OP1	2:D:2:G:H4'	1.66	0.95
1:A:1040:GLN:OE1	1:B:876:ALA:HB2	1.66	0.95
1:B:1075:HIS:HB3	1:B:1078:ALA:HB3	1.48	0.95
1:A:890:TYR:HA	1:A:893:MET:HE2	1.48	0.94
1:A:1047:GLN:HG3	1:A:1081:VAL:HG22	1.50	0.94
2:D:1:U:H3'	2:D:2:G:H5''	1.49	0.93
1:B:890:TYR:HB2	1:B:920:ARG:HH21	1.35	0.90
1:B:890:TYR:HB2	1:B:920:ARG:NH2	1.87	0.89
1:B:854:MET:CE	1:B:888:ALA:HB3	2.03	0.88
1:A:890:TYR:HA	1:A:893:MET:CE	2.04	0.88
1:A:1094:ARG:HH11	1:A:1094:ARG:HG3	1.40	0.86
1:A:1161:LEU:O	1:A:1161:LEU:HD22	1.77	0.85
1:A:945:ILE:HG13	1:A:950:GLN:HG3	1.57	0.84
1:B:1043:ASN:O	1:B:1047:GLN:HG3	1.78	0.83
1:A:1007:CYS:O	1:A:1011:GLN:HG2	1.79	0.83
1:A:1075:HIS:HB3	1:A:1078:ALA:HB3	1.61	0.83
2:D:1:U:H3'	2:D:2:G:C5'	2.10	0.81
1:A:1104:MET:O	1:A:1104:MET:HG2	1.80	0.81
1:B:854:MET:HE2	1:B:888:ALA:HB3	1.62	0.80
1:A:854:MET:SD	1:A:888:ALA:HB3	2.22	0.80
1:A:1050:LEU:O	1:A:1058:LYS:HE2	1.81	0.80

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:984:GLN:H	1:B:984:GLN:CD	1.84	0.80
1:A:1094:ARG:HH11	1:A:1094:ARG:CG	1.94	0.80
1:A:1161:LEU:O	1:A:1161:LEU:CD2	2.30	0.79
1:B:945:ILE:HD12	1:B:949:GLN:HB3	1.65	0.78
1:A:1021:GLN:O	1:A:1024:PRO:HD2	1.84	0.78
1:A:860:GLN:HG2	1:A:864:ARG:HH12	1.50	0.77
1:B:874:THR:HA	1:B:878:ARG:CD	2.13	0.77
1:A:1062:VAL:HG13	1:A:1097:LEU:HD11	1.67	0.77
1:B:1021:GLN:O	1:B:1024:PRO:HD2	1.85	0.76
1:B:1151:LEU:HD22	1:B:1161:LEU:HB2	1.66	0.76
1:A:950:GLN:O	1:A:954:VAL:HG23	1.85	0.75
1:B:1023:LEU:HB3	1:B:1024:PRO:HD3	1.68	0.75
1:A:1155:THR:HA	1:A:1158:LYS:NZ	2.01	0.75
1:B:911:LEU:HD13	1:B:915:LEU:HD11	1.68	0.75
1:A:1090:SER:HB3	1:A:1093:GLU:HG3	1.70	0.74
1:B:835:ASP:HB3	1:B:840:ARG:HB2	1.70	0.74
1:A:1098:ILE:HG12	1:A:1128:MET:HE2	1.68	0.74
1:A:993:PHE:CE2	1:A:1000:LEU:HD13	2.23	0.74
1:B:986:LEU:HB3	1:B:989:ILE:HD12	1.69	0.74
1:A:1122:ASN:HB2	1:A:1160:ILE:HD11	1.68	0.73
1:B:1092:THR:O	1:B:1096:VAL:HG23	1.89	0.73
1:B:840:ARG:HH11	1:B:840:ARG:HG2	1.53	0.73
1:B:912:GLU:HA	1:B:915:LEU:HD12	1.70	0.73
1:B:934:GLY:O	1:B:938:ILE:HG12	1.88	0.72
1:A:1155:THR:HA	1:A:1158:LYS:HZ3	1.54	0.72
1:B:1105:ASN:HA	1:B:1110:SER:HA	1.69	0.72
1:B:1073:SER:HB2	1:B:1124:VAL:HG21	1.71	0.72
1:A:1144:ILE:HG22	1:A:1164:LEU:HD21	1.71	0.71
1:B:835:ASP:HB2	1:B:841:TYR:CE2	2.24	0.71
1:B:840:ARG:HG2	1:B:840:ARG:NH1	2.05	0.71
1:B:860:GLN:O	1:B:864:ARG:HG3	1.90	0.71
1:A:903:GLN:HB3	1:A:940:LYS:NZ	2.06	0.70
1:B:911:LEU:O	1:B:915:LEU:HG	1.92	0.70
1:B:846:LEU:HD23	1:B:849:ILE:HD11	1.73	0.69
1:A:982:GLN:HB3	1:A:984:GLN:NE2	2.06	0.69
1:B:1140:VAL:O	1:B:1144:ILE:HG13	1.92	0.69
1:B:874:THR:O	1:B:878:ARG:HB2	1.94	0.68
1:B:943:GLU:HB2	1:B:976:LYS:HZ1	1.59	0.68
1:B:1139:ILE:O	1:B:1143:LYS:HG2	1.93	0.68
1:A:903:GLN:OE1	1:A:940:LYS:NZ	2.26	0.67
1:B:882:PHE:HA	1:B:885:ILE:HG12	1.76	0.67
1:B:1079:SER:O	1:B:1082:VAL:HG22	1.95	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:864:ARG:O	1:B:868:LEU:HG	1.95	0.67
1:A:998:PHE:O	1:A:1002:THR:HG23	1.95	0.66
1:A:1022:THR:O	1:A:1026:LEU:HG	1.96	0.66
1:A:1113:TYR:O	1:A:1117:LYS:HG3	1.96	0.66
1:A:899:ASN:O	1:A:903:GLN:HG3	1.96	0.65
1:A:1008:ARG:HA	1:A:1011:GLN:HG3	1.79	0.65
1:A:867:GLN:HB3	1:A:904:LYS:HE2	1.79	0.64
1:A:993:PHE:HE2	1:A:1000:LEU:HD13	1.62	0.64
1:A:903:GLN:HB3	1:A:940:LYS:HZ2	1.61	0.64
1:B:900:TYR:O	1:B:904:LYS:HG2	1.98	0.64
1:A:1003:HIS:CG	1:A:1004:PRO:HD2	2.33	0.63
1:B:873:ALA:HB3	1:B:877:GLU:CD	2.18	0.63
1:A:1136:GLN:O	1:A:1140:VAL:HG23	1.97	0.63
1:B:859:ASP:HB3	1:B:862:GLY:HA3	1.80	0.63
1:B:874:THR:HB	1:B:875:PRO:HD3	1.80	0.63
1:A:1031:GLN:HB3	1:A:1032:HIS:CD2	2.34	0.63
1:A:906:PHE:O	1:A:914:LYS:HE2	1.98	0.62
1:A:989:ILE:O	1:A:993:PHE:HD1	1.83	0.62
1:B:1010:ILE:O	1:B:1014:LEU:HG	2.00	0.62
1:B:911:LEU:HB3	1:B:912:GLU:OE2	2.01	0.61
1:A:1122:ASN:O	1:A:1126:GLN:HG3	2.00	0.61
1:B:984:GLN:N	1:B:984:GLN:CD	2.53	0.61
1:B:981:VAL:HG12	1:B:982:GLN:H	1.66	0.61
1:A:984:GLN:H	1:A:984:GLN:CD	2.03	0.61
1:A:1119:GLN:HG2	3:A:69:HOH:O	1.99	0.61
1:B:890:TYR:O	1:B:894:VAL:HG22	2.00	0.60
1:B:846:LEU:HD12	1:B:877:GLU:OE2	2.02	0.60
1:A:990:ILE:HG13	1:A:1021:GLN:CB	2.26	0.60
1:A:1118:ASP:HB3	1:A:1121:ALA:HB3	1.83	0.60
1:A:975:GLN:OE1	1:A:1012:ARG:NH1	2.32	0.60
1:B:862:GLY:O	1:B:866:ILE:HG13	2.02	0.59
1:A:916:ALA:O	1:A:919:GLU:HB3	2.02	0.59
1:B:943:GLU:HB2	1:B:976:LYS:NZ	2.17	0.59
1:B:1119:GLN:HB2	1:B:1156:TYR:CE1	2.37	0.59
1:B:1159:HIS:HB3	3:B:81:HOH:O	2.02	0.59
1:B:854:MET:HE1	1:B:888:ALA:HB3	1.81	0.59
1:A:1147:HIS:O	1:A:1150:THR:HB	2.02	0.59
1:B:975:GLN:OE1	1:B:1012:ARG:NH1	2.36	0.59
1:B:920:ARG:HD2	3:B:22:HOH:O	2.03	0.59
2:D:2:G:C4'	2:D:2:G:OP1	2.47	0.58
1:B:1112:LEU:HD21	1:B:1140:VAL:HG13	1.85	0.58
1:A:1039:ASP:O	1:A:1043:ASN:ND2	2.35	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1040:GLN:CD	1:B:876:ALA:HB2	2.23	0.58
1:B:1056:GLU:O	1:B:1059:SER:HB2	2.03	0.58
1:A:882:PHE:CD2	1:A:885:ILE:HD11	2.39	0.58
1:A:1125:VAL:HA	1:A:1128:MET:HG3	1.85	0.58
1:A:1094:ARG:NH1	1:A:1094:ARG:HB2	2.19	0.58
1:A:1033:THR:O	1:A:1037:VAL:HG13	2.04	0.58
1:B:990:ILE:HG13	1:B:1021:GLN:HB3	1.86	0.58
1:A:1065:ILE:HG21	1:A:1082:VAL:HG12	1.84	0.57
1:A:1023:LEU:N	1:A:1024:PRO:CD	2.66	0.57
1:A:863:SER:O	1:A:867:GLN:HG3	2.04	0.57
1:B:852:HIS:HD2	3:B:61:HOH:O	1.86	0.57
1:B:1140:VAL:O	1:B:1143:LYS:HB2	2.04	0.57
1:B:912:GLU:CD	1:B:912:GLU:N	2.58	0.57
1:B:982:GLN:HB3	1:B:984:GLN:NE2	2.20	0.56
1:A:867:GLN:NE2	1:A:900:TYR:HB2	2.20	0.56
1:A:939:GLN:HE22	2:C:6:A:H2	1.53	0.56
1:B:1047:GLN:NE2	1:B:1080:ASN:HB3	2.20	0.56
1:B:831:ARG:HD2	1:B:832:LEU:N	2.20	0.56
1:A:829:ARG:HD3	1:A:833:LEU:HD23	1.86	0.56
1:A:890:TYR:CA	1:A:893:MET:HE2	2.31	0.56
1:A:1110:SER:OG	1:A:1111:ALA:N	2.37	0.56
1:A:986:LEU:HD22	1:A:989:ILE:HD11	1.86	0.56
1:B:1018:LEU:O	1:B:1022:THR:HG23	2.06	0.55
1:B:1089:ALA:HB1	1:B:1093:GLU:HB2	1.88	0.55
1:B:834:GLU:O	1:B:838:ASN:OD1	2.25	0.55
1:A:882:PHE:O	1:A:885:ILE:HG13	2.06	0.55
1:B:982:GLN:HB3	1:B:984:GLN:HE22	1.72	0.55
1:A:1094:ARG:HH11	1:A:1094:ARG:HB2	1.72	0.55
1:A:869:LYS:O	1:A:873:ALA:HB2	2.06	0.55
1:B:844:LEU:HD12	1:B:845:GLN:H	1.72	0.55
1:B:983:PRO:O	1:B:986:LEU:N	2.37	0.55
2:D:7:U:H4'	2:D:7:U:OP1	2.06	0.55
1:B:866:ILE:O	1:B:870:LEU:HG	2.07	0.55
1:B:847:ARG:HA	1:B:847:ARG:HE	1.71	0.55
1:A:1161:LEU:HD23	1:A:1164:LEU:HD12	1.89	0.54
1:A:854:MET:O	1:A:857:SER:N	2.40	0.54
1:B:1020:ASP:HB2	3:B:74:HOH:O	2.07	0.54
1:B:1137:ARG:O	1:B:1141:MET:HG2	2.08	0.54
1:A:1094:ARG:HH11	1:A:1094:ARG:CB	2.19	0.54
1:B:1084:LYS:HD2	1:B:1084:LYS:N	2.22	0.54
1:B:983:PRO:CB	1:B:1018:LEU:HG	2.38	0.54
1:A:1014:LEU:HD22	1:A:1026:LEU:HD21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:961:VAL:HG12	1:A:962:LEU:HD23	1.89	0.54
1:B:1052:HIS:HB2	3:B:50:HOH:O	2.08	0.54
1:B:918:ALA:HA	1:B:921:ILE:HD12	1.90	0.54
1:B:950:GLN:O	1:B:954:VAL:HG23	2.07	0.54
1:A:982:GLN:HB3	1:A:984:GLN:HE21	1.71	0.53
1:A:860:GLN:HG2	1:A:864:ARG:NH1	2.21	0.53
1:B:840:ARG:HH11	1:B:840:ARG:CG	2.18	0.53
1:A:1033:THR:HB	1:A:1064:GLU:HG3	1.91	0.53
1:A:1144:ILE:HG22	1:A:1144:ILE:O	2.08	0.53
1:A:1161:LEU:HA	1:A:1164:LEU:HD12	1.89	0.53
1:A:882:PHE:CD1	1:A:913:GLN:HG2	2.44	0.53
1:A:1112:LEU:O	1:A:1116:MET:HG3	2.09	0.53
1:A:1161:LEU:O	1:A:1161:LEU:HD23	2.08	0.53
1:B:1143:LYS:HB3	1:B:1143:LYS:HZ3	1.74	0.53
1:B:863:SER:OG	1:B:867:GLN:NE2	2.42	0.53
1:B:860:GLN:NE2	2:D:8:A:O2'	2.42	0.52
1:B:1030:HIS:HA	1:B:1033:THR:OG1	2.09	0.52
1:B:1076:LYS:HG3	1:B:1120:TYR:CZ	2.45	0.52
1:A:1125:VAL:HA	1:A:1128:MET:CG	2.39	0.52
1:A:935:CYS:SG	1:A:969:ASN:HB3	2.49	0.52
1:B:1075:HIS:CB	1:B:1078:ALA:HB3	2.31	0.52
1:A:947:SER:HA	1:A:950:GLN:HB2	1.91	0.52
1:B:1099:ASP:N	1:B:1136:GLN:HE22	2.08	0.51
1:B:1077:PHE:HE2	2:D:3:U:H1'	1.74	0.51
1:A:1075:HIS:HE1	1:A:1077:PHE:HD1	1.58	0.51
1:B:989:ILE:O	1:B:993:PHE:HD1	1.93	0.51
1:A:850:ALA:O	1:A:852:HIS:HD2	1.93	0.51
1:A:1051:GLU:HB2	1:A:1052:HIS:CD2	2.45	0.51
1:A:981:VAL:HG12	1:A:982:GLN:O	2.09	0.51
1:B:977:CYS:O	1:B:981:VAL:HG23	2.10	0.51
1:A:1014:LEU:CD2	1:A:1026:LEU:HD21	2.41	0.51
1:B:1023:LEU:HB3	1:B:1024:PRO:CD	2.39	0.51
1:A:1098:ILE:HG12	1:A:1128:MET:CE	2.39	0.51
1:B:1159:HIS:H	1:B:1159:HIS:CD2	2.28	0.51
1:B:1072:LEU:HD22	1:B:1078:ALA:HB1	1.92	0.51
1:B:983:PRO:HB2	1:B:1018:LEU:HG	1.91	0.51
1:B:951:ASN:O	1:B:954:VAL:HB	2.10	0.51
1:B:1003:HIS:CG	1:B:1004:PRO:HD2	2.46	0.51
1:A:1082:VAL:O	1:A:1085:CYS:HB2	2.11	0.50
1:B:1090:SER:HB3	1:B:1093:GLU:HG3	1.93	0.50
1:B:1074:GLN:O	1:B:1120:TYR:HD1	1.95	0.50
1:B:1120:TYR:O	1:B:1123:TYR:HB2	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1128:MET:HA	1:A:1128:MET:HE2	1.92	0.50
1:B:1148:ILE:HA	1:B:1151:LEU:HB2	1.93	0.50
1:A:993:PHE:CE2	1:A:1000:LEU:CD1	2.93	0.50
1:B:952:GLU:HB2	3:B:29:HOH:O	2.11	0.50
1:B:1032:HIS:O	1:B:1034:GLU:N	2.45	0.50
1:A:1163:LYS:C	1:A:1165:GLU:H	2.14	0.50
1:A:835:ASP:OD1	1:A:840:ARG:CZ	2.60	0.50
1:B:847:ARG:NE	1:B:847:ARG:HA	2.27	0.50
1:A:1047:GLN:OE1	1:A:1084:LYS:HD3	2.11	0.49
1:A:1075:HIS:HE1	1:A:1077:PHE:CD1	2.30	0.49
1:B:941:ALA:O	1:B:945:ILE:HG12	2.12	0.49
1:A:1024:PRO:O	1:A:1028:GLU:HG3	2.12	0.49
1:B:906:PHE:HB3	1:B:940:LYS:HG3	1.94	0.49
1:B:1030:HIS:CE1	1:B:1060:LYS:HB2	2.47	0.49
1:A:1032:HIS:HB3	1:A:1035:GLN:OE1	2.13	0.49
1:A:1061:ILE:O	1:A:1064:GLU:N	2.45	0.49
1:A:845:GLN:HB2	1:A:848:GLU:HG3	1.93	0.49
1:B:1023:LEU:CB	1:B:1024:PRO:HD3	2.41	0.49
1:A:1147:HIS:O	1:A:1151:LEU:HG	2.13	0.49
1:A:1065:ILE:CG2	1:A:1082:VAL:HG12	2.43	0.49
1:A:1158:LYS:HB2	1:A:1158:LYS:NZ	2.28	0.49
1:B:865:PHE:CD2	1:B:865:PHE:C	2.85	0.49
2:D:6:A:C2'	2:D:7:U:O5'	2.61	0.48
2:D:5:G:O2'	2:D:6:A:H5''	2.13	0.48
1:A:1094:ARG:NH1	1:A:1094:ARG:CB	2.76	0.48
1:A:1161:LEU:C	1:A:1161:LEU:CD2	2.80	0.48
1:A:860:GLN:HB2	1:A:897:PHE:CZ	2.49	0.48
1:A:882:PHE:CE1	1:A:913:GLN:HG2	2.48	0.48
1:B:889:ALA:HB1	1:B:893:MET:CE	2.44	0.48
1:B:972:HIS:CE1	2:D:5:G:C8	3.01	0.48
1:B:978:ILE:HA	1:B:986:LEU:CD1	2.44	0.48
1:B:1073:SER:HB3	1:B:1082:VAL:HG21	1.96	0.48
1:B:1063:ALA:HA	1:B:1066:ARG:CZ	2.44	0.48
1:B:996:GLN:NE2	3:B:5:HOH:O	2.47	0.47
1:B:1143:LYS:HB3	1:B:1143:LYS:NZ	2.30	0.47
1:B:1003:HIS:CD2	1:B:1004:PRO:HD2	2.50	0.47
1:A:1141:MET:HE2	1:A:1141:MET:HA	1.97	0.47
1:B:1065:ILE:HG13	1:B:1085:CYS:SG	2.54	0.47
1:B:1164:LEU:HD23	1:B:1164:LEU:HA	1.72	0.47
1:A:1002:THR:HB	1:A:1039:ASP:OD2	2.15	0.47
1:A:1104:MET:HE1	3:A:35:HOH:O	2.15	0.47
1:B:1099:ASP:H	1:B:1136:GLN:HE22	1.63	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1018:LEU:HB2	1:B:1021:GLN:OE1	2.15	0.47
1:A:1003:HIS:CD2	1:A:1004:PRO:HD2	2.49	0.47
1:A:1104:MET:O	1:A:1111:ALA:HB2	2.15	0.46
1:A:854:MET:O	1:A:855:GLU:C	2.53	0.46
1:B:940:LYS:HB2	1:B:940:LYS:HE2	1.55	0.46
2:C:8:A:H4'	3:C:65:HOH:O	2.15	0.46
1:A:1145:ARG:N	1:A:1146:PRO:CD	2.79	0.46
1:B:994:LYS:NZ	1:B:1024:PRO:HG2	2.31	0.46
1:B:850:ALA:HB2	1:B:880:LEU:HD11	1.98	0.46
1:A:939:GLN:NE2	2:C:6:A:C2	2.79	0.46
1:A:1113:TYR:CE2	1:A:1117:LYS:HD2	2.50	0.46
1:B:1013:ILE:HG22	1:B:1014:LEU:N	2.29	0.46
1:A:1144:ILE:CG2	1:A:1164:LEU:HD21	2.42	0.46
1:A:831:ARG:HA	1:A:834:GLU:HB2	1.97	0.46
1:B:1099:ASP:CG	1:B:1136:GLN:HE21	2.18	0.46
1:A:1022:THR:O	1:A:1026:LEU:CG	2.63	0.46
1:A:919:GLU:HA	1:A:922:ARG:CZ	2.46	0.46
1:A:1002:THR:HA	1:A:1039:ASP:OD2	2.16	0.46
1:B:946:PRO:O	1:B:950:GLN:HG3	2.16	0.46
1:A:1029:LEU:HA	1:A:1029:LEU:HD23	1.75	0.46
1:B:1072:LEU:HD22	1:B:1078:ALA:CB	2.46	0.45
1:B:1136:GLN:O	1:B:1140:VAL:HG23	2.17	0.45
1:A:962:LEU:HD11	1:A:996:GLN:HG3	1.98	0.45
1:A:835:ASP:OD1	1:A:840:ARG:HD2	2.16	0.45
1:A:1125:VAL:O	1:A:1128:MET:HB2	2.16	0.45
2:D:7:U:O2'	2:D:8:A:H5'	2.17	0.45
1:B:906:PHE:CZ	1:B:921:ILE:HD11	2.50	0.45
1:A:1141:MET:CE	1:A:1141:MET:HA	2.46	0.45
1:A:1065:ILE:O	1:A:1066:ARG:C	2.54	0.45
1:B:1124:VAL:O	1:B:1128:MET:HG3	2.16	0.45
1:B:975:GLN:O	1:B:979:GLU:HG3	2.16	0.45
1:A:1061:ILE:O	1:A:1064:GLU:HB2	2.16	0.45
1:A:854:MET:HB3	1:A:854:MET:HE3	1.89	0.45
1:B:978:ILE:HA	1:B:986:LEU:HD11	1.99	0.45
1:B:912:GLU:CD	1:B:912:GLU:H	2.18	0.45
1:B:1073:SER:CB	1:B:1124:VAL:HG21	2.43	0.45
1:B:1122:ASN:CG	1:B:1123:TYR:N	2.69	0.45
1:B:896:VAL:HA	1:B:933:TYR:CD2	2.52	0.45
1:A:911:LEU:O	1:A:915:LEU:HG	2.17	0.45
1:A:1161:LEU:HD23	1:A:1164:LEU:CD1	2.47	0.44
1:A:1127:LYS:O	1:A:1128:MET:C	2.55	0.44
1:A:986:LEU:HD22	1:A:989:ILE:CD1	2.46	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1148:ILE:C	1:A:1150:THR:H	2.21	0.44
1:B:1104:MET:HB3	1:B:1111:ALA:HB2	1.98	0.44
1:B:957:LEU:HA	1:B:957:LEU:HD23	1.73	0.44
1:A:936:ARG:HG3	2:C:7:U:C4	2.52	0.44
1:B:832:LEU:O	1:B:833:LEU:C	2.56	0.44
1:B:886:LEU:HG	1:B:886:LEU:O	2.17	0.44
1:A:972:HIS:O	1:A:976:LYS:HB2	2.17	0.44
1:A:1008:ARG:HG3	2:C:5:G:C8	2.53	0.44
1:A:939:GLN:NE2	2:C:6:A:H2	2.16	0.44
1:A:854:MET:SD	1:A:888:ALA:CB	3.01	0.44
1:A:954:VAL:HG21	1:A:981:VAL:HG21	2.00	0.44
1:B:974:VAL:O	1:B:977:CYS:HB2	2.17	0.44
1:A:1163:LYS:O	1:A:1165:GLU:N	2.40	0.44
1:B:879:GLN:HE21	1:B:883:ASN:ND2	2.16	0.44
1:B:1099:ASP:N	1:B:1136:GLN:NE2	2.65	0.44
1:B:1068:ASN:O	1:B:1072:LEU:HB2	2.17	0.44
1:B:890:TYR:HD1	1:B:890:TYR:O	2.01	0.44
1:B:840:ARG:C	1:B:842:PRO:HD3	2.38	0.44
1:B:949:GLN:C	3:B:29:HOH:O	2.56	0.44
1:A:1046:ILE:HG23	1:A:1061:ILE:HD13	1.99	0.44
1:B:962:LEU:HD22	1:B:1000:LEU:HD11	2.00	0.44
2:D:1:U:O5'	2:D:2:G:C5'	2.66	0.43
1:B:874:THR:CB	1:B:875:PRO:HD3	2.48	0.43
1:B:852:HIS:HB3	1:B:856:PHE:CD1	2.53	0.43
1:A:918:ALA:O	1:A:921:ILE:N	2.44	0.43
1:B:1157:GLY:C	1:B:1159:HIS:H	2.21	0.43
1:B:1003:HIS:HA	1:B:1004:PRO:HD3	1.82	0.43
1:B:1040:GLN:CD	1:B:1040:GLN:H	2.16	0.43
1:A:920:ARG:HD2	1:A:920:ARG:HA	1.52	0.43
1:A:989:ILE:HG22	1:A:993:PHE:HE1	1.83	0.43
1:A:1113:TYR:CZ	1:A:1117:LYS:HD2	2.54	0.43
1:A:919:GLU:HG2	1:A:922:ARG:HH22	1.84	0.43
1:B:1099:ASP:CG	1:B:1136:GLN:NE2	2.73	0.43
1:A:1094:ARG:HD3	1:A:1131:VAL:HG23	2.01	0.42
1:A:947:SER:HB3	3:A:87:HOH:O	2.19	0.42
1:A:1039:ASP:HB3	1:A:1042:GLY:HA3	2.00	0.42
1:A:1104:MET:CE	3:A:35:HOH:O	2.66	0.42
1:B:1098:ILE:HG12	1:B:1128:MET:HB3	2.02	0.42
1:B:966:LYS:HA	1:B:1003:HIS:CE1	2.54	0.42
1:B:879:GLN:HE21	1:B:883:ASN:HD21	1.66	0.42
1:B:1127:LYS:HA	1:B:1127:LYS:HD3	1.74	0.42
1:B:882:PHE:HE2	1:B:917:LEU:HG	1.85	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:6:A:H8	2:C:6:A:H5'	1.84	0.42
1:B:907:GLU:HG3	1:B:940:LYS:HD2	2.01	0.42
1:A:1082:VAL:HG23	1:A:1124:VAL:CG2	2.50	0.42
1:B:1098:ILE:O	1:B:1101:VAL:HG23	2.19	0.42
1:B:1155:THR:C	1:B:1157:GLY:H	2.23	0.42
1:A:829:ARG:NH2	1:A:837:ARG:HH12	2.18	0.42
1:B:880:LEU:O	1:B:880:LEU:HD12	2.19	0.42
1:A:910:SER:H	1:A:913:GLN:HE21	1.68	0.42
1:B:1151:LEU:HD21	1:B:1160:ILE:HB	2.02	0.42
1:A:1039:ASP:HB3	1:A:1042:GLY:H	1.84	0.42
1:B:1072:LEU:O	1:B:1075:HIS:HB3	2.19	0.42
1:A:1161:LEU:C	1:A:1161:LEU:HD22	2.39	0.41
1:A:1100:GLU:CG	1:A:1104:MET:HE3	2.49	0.41
1:A:940:LYS:HD2	1:A:944:PHE:HE1	1.85	0.41
2:C:1:U:O5'	2:C:1:U:H6	2.02	0.41
1:A:1023:LEU:N	1:A:1024:PRO:HD2	2.35	0.41
1:A:1094:ARG:NH1	1:A:1094:ARG:CG	2.64	0.41
1:B:1018:LEU:N	1:B:1021:GLN:OE1	2.53	0.41
1:A:1082:VAL:O	1:A:1083:GLU:C	2.57	0.41
1:B:877:GLU:O	1:B:880:LEU:HB3	2.19	0.41
1:B:926:LEU:HD22	1:B:960:HIS:CD2	2.56	0.41
1:A:1124:VAL:O	1:A:1128:MET:HG2	2.20	0.41
1:A:913:GLN:HE21	1:A:913:GLN:HB2	1.61	0.41
1:A:1163:LYS:C	1:A:1165:GLU:N	2.73	0.41
1:B:1108:PRO:HB2	1:B:1109:HIS:CD2	2.55	0.41
1:B:1109:HIS:CD2	3:B:79:HOH:O	2.72	0.41
1:A:919:GLU:HA	1:A:922:ARG:NH2	2.35	0.41
1:B:1157:GLY:O	1:B:1159:HIS:N	2.53	0.41
1:A:910:SER:H	1:A:913:GLN:NE2	2.18	0.41
1:B:1100:GLU:O	1:B:1104:MET:HB2	2.21	0.41
1:A:1011:GLN:O	1:A:1015:GLU:HG3	2.20	0.41
1:A:860:GLN:CG	1:A:864:ARG:HH12	2.26	0.41
1:B:1094:ARG:NH2	3:B:94:HOH:O	2.52	0.41
1:B:1023:LEU:HA	1:B:1023:LEU:HD12	1.80	0.41
1:B:1101:VAL:HG11	1:B:1115:MET:SD	2.61	0.41
1:B:853:ILE:HG13	1:B:884:GLU:CD	2.40	0.41
1:A:1035:GLN:HG3	1:A:1035:GLN:H	1.68	0.41
1:B:1125:VAL:O	1:B:1126:GLN:C	2.59	0.41
1:B:896:VAL:HG23	1:B:933:TYR:CE2	2.56	0.40
1:A:832:LEU:HA	1:A:832:LEU:HD12	1.81	0.40
1:A:836:PHE:CZ	1:A:865:PHE:HB2	2.56	0.40
1:A:1094:ARG:NH1	1:A:1094:ARG:HG3	2.18	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:847:ARG:CA	1:B:847:ARG:NE	2.85	0.40
1:A:951:ASN:HD22	1:A:951:ASN:HA	1.65	0.40
1:B:839:ASN:HA	1:B:839:ASN:HD22	1.62	0.40
1:B:924:HIS:O	1:B:928:LEU:HG	2.20	0.40
1:A:882:PHE:CG	1:A:913:GLN:HG2	2.56	0.40
1:B:1032:HIS:HB3	1:B:1035:GLN:HG3	2.03	0.40
1:A:1101:VAL:O	1:A:1111:ALA:HB3	2.22	0.40
1:A:989:ILE:HG22	1:A:993:PHE:CE1	2.57	0.40
1:B:907:GLU:CG	1:B:940:LYS:HD2	2.51	0.40
1:A:886:LEU:HA	1:A:886:LEU:HD12	1.91	0.40

There are no symmetry-related clashes.

## 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	335/349 (96%)	292 (87%)	40 (12%)	3 (1%)	25	55
1	B	336/349 (96%)	285 (85%)	47 (14%)	4 (1%)	19	45
All	All	671/698 (96%)	577 (86%)	87 (13%)	7 (1%)	22	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1033	THR
1	A	854	MET
1	A	919	GLU
1	A	920	ARG
1	B	1158	LYS
1	B	981	VAL
1	B	983	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	301/310 (97%)	271 (90%)	30 (10%)	11	25
1	B	302/310 (97%)	277 (92%)	25 (8%)	16	35
All	All	603/620 (97%)	548 (91%)	55 (9%)	14	30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	843	ASN
1	A	854	MET
1	A	868	LEU
1	A	920	ARG
1	A	937	VAL
1	A	940	LYS
1	A	942	LEU
1	A	947	SER
1	A	984	GLN
1	A	1011	GLN
1	A	1021	GLN
1	A	1033	THR
1	A	1035	GLN
1	A	1041	TYR
1	A	1066	ARG
1	A	1070	LEU
1	A	1083	GLU
1	A	1084	LYS
1	A	1094	ARG
1	A	1103	THR
1	A	1106	ASP
1	A	1112	LEU
1	A	1131	VAL
1	A	1133	GLU
1	A	1147	HIS
1	A	1153	LYS
1	A	1158	LYS
1	A	1161	LEU
1	A	1163	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1165	GLU
1	B	831	ARG
1	B	832	LEU
1	B	839	ASN
1	B	840	ARG
1	B	845	GLN
1	B	887	GLN
1	B	890	TYR
1	B	891	GLN
1	B	907	GLU
1	B	911	LEU
1	B	927	SER
1	B	940	LYS
1	B	949	GLN
1	B	958	ASP
1	B	985	SER
1	B	1035	GLN
1	B	1040	GLN
1	B	1084	LYS
1	B	1090	SER
1	B	1092	THR
1	B	1101	VAL
1	B	1148	ILE
1	B	1151	LEU
1	B	1159	HIS
1	B	1163	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	838	ASN
1	A	852	HIS
1	A	879	GLN
1	A	883	ASN
1	A	913	GLN
1	A	939	GLN
1	A	951	ASN
1	A	1031	GLN
1	A	1052	HIS
1	A	1119	GLN
1	A	1159	HIS
1	B	838	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	839	ASN
1	B	845	GLN
1	B	852	HIS
1	B	860	GLN
1	B	883	ASN
1	B	887	GLN
1	B	939	GLN
1	B	950	GLN
1	B	960	HIS
1	B	984	GLN
1	B	996	GLN
1	B	1031	GLN
1	B	1088	HIS
1	B	1109	HIS
1	B	1136	GLN
1	B	1147	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	7/8 (87%)	4 (57%)	3 (42%)
2	D	8/8 (100%)	5 (62%)	5 (62%)
All	All	15/16 (93%)	9 (60%)	8 (53%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	5	G
2	C	6	A
2	C	7	U
2	C	8	A
2	D	2	G
2	D	4	A
2	D	6	A
2	D	7	U
2	D	8	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	5	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	6	A
2	C	7	U
2	D	1	U
2	D	2	G
2	D	5	G
2	D	6	A
2	D	7	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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	337/349 (96%)	-0.21	9 (2%) 52 57	23, 27, 84, 178	0
1	B	338/349 (96%)	-0.25	5 (1%) 70 75	23, 29, 76, 239	0
2	C	8/8 (100%)	-0.59	0 100 100	25, 27, 32, 34	0
2	D	8/8 (100%)	-0.08	0 100 100	24, 25, 29, 34	0
All	All	691/714 (96%)	-0.23	14 (2%) 62 68	23, 28, 79, 239	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	PRO	6.1
1	B	1104	MET	5.6
1	B	1152	ARG	4.8
1	A	1148	ILE	4.3
1	A	1151	LEU	3.8
1	A	1109	HIS	3.7
1	B	875	PRO	2.9
1	A	1105	ASN	2.7
1	B	1165	GLU	2.7
1	A	1110	SER	2.7
1	A	888	ALA	2.5
1	B	874	THR	2.4
1	A	840	ARG	2.2
1	A	854	MET	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.