



Full wwPDB NMR Structure Validation Report ⓘ

Jun 12, 2024 – 02:29 PM EDT

PDB ID : 1E5U
Title : NMR Representative Structure of Intimin-190 (Int190) from Enteropathogenic E. coli
Authors : Prasannan, S.; Matthews, S.J.; Batchelor, M.; Daniell, S.; Reece, S.; Frankel, G.; Dougan, G.; Connerton, I.; Bloomberg, G.
Deposited on : 2000-08-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

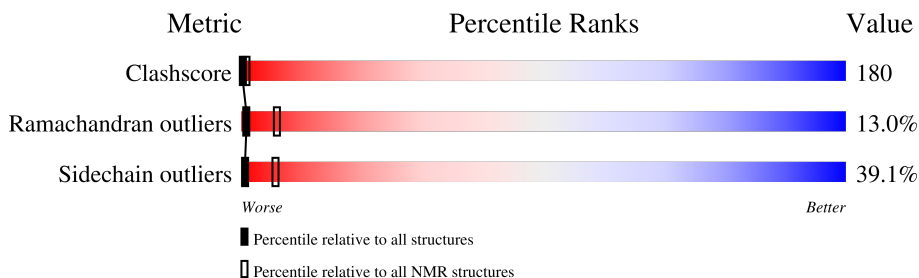
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	I	187	

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2813 atoms, of which 1401 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTIMIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	I	187	2813	881	1401	240	288	3	0

5 Refinement protocol and experimental data overview

The models were refined using the following method: *HYBRID TORSION ANGLE/ CARTESIAN CO-ORDINATE DYNAMICS*.

Of the 15 calculated structures, 1 were deposited, based on the following criterion: *LEAST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	
XWIN-NMR	structure solution	
AURELIA	structure solution	
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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	Planarity
1	I	0	1
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	I	44	ARG	Sidechain

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	I	1412	1401	1401	507
All	All	1412	1401	1401	507

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 180.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:44:ARG:O	1:I:70:ILE:HD13	1.09	1.47
1:I:12:VAL:HA	1:I:29:GLN:O	1.08	1.49
1:I:24:TRP:C	1:I:25:LEU:HD13	1.06	1.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:12:VAL:HG21	1:I:24:TRP:CE3	1.06	1.86
1:I:144:ILE:HD12	1:I:165:LEU:HD11	0.98	1.29
1:I:12:VAL:HG22	1:I:29:GLN:N	0.97	1.73
1:I:45:SER:CB	1:I:60:VAL:HG13	0.97	1.90
1:I:116:PRO:CG	1:I:122:LEU:HD11	0.96	1.90
1:I:89:SER:O	1:I:90:LEU:HD23	0.94	1.61
1:I:12:VAL:HG21	1:I:24:TRP:CZ3	0.91	1.99
1:I:9:ILE:O	1:I:17:LYS:HA	0.91	1.66
1:I:9:ILE:O	1:I:9:ILE:HD12	0.90	1.66
1:I:12:VAL:CA	1:I:29:GLN:O	0.90	2.19
1:I:147:TRP:HD1	1:I:181:ALA:HB3	0.90	1.26
1:I:84:ILE:HG23	1:I:88:ASN:OD1	0.89	1.67
1:I:12:VAL:HG23	1:I:30:VAL:HG12	0.89	1.43
1:I:12:VAL:HG22	1:I:28:GLY:C	0.88	1.89
1:I:24:TRP:CH2	1:I:62:LEU:HD21	0.88	2.03
1:I:144:ILE:CD1	1:I:165:LEU:HD11	0.88	1.98
1:I:132:ALA:HA	1:I:165:LEU:HD13	0.87	1.45
1:I:11:ILE:O	1:I:13:GLY:N	0.86	2.08
1:I:147:TRP:CD1	1:I:181:ALA:HB3	0.85	2.06
1:I:25:LEU:O	1:I:26:GLN:CB	0.85	2.25
1:I:104:ALA:HB1	1:I:183:ALA:HB2	0.85	1.46
1:I:145:ILE:HA	1:I:163:TYR:O	0.84	1.73
1:I:23:VAL:HG13	1:I:91:ILE:HD11	0.83	1.47
1:I:162:THR:CG2	1:I:174:ILE:HG21	0.83	2.03
1:I:50:ILE:HD13	1:I:50:ILE:O	0.82	1.73
1:I:25:LEU:HD13	1:I:25:LEU:N	0.82	1.89
1:I:24:TRP:HB2	1:I:89:SER:O	0.81	1.74
1:I:162:THR:HG21	1:I:174:ILE:HG21	0.80	1.52
1:I:168:GLN:O	1:I:169:ASN:HB2	0.80	1.74
1:I:104:ALA:HB1	1:I:183:ALA:CB	0.80	2.06
1:I:177:SER:O	1:I:178:GLU:CB	0.79	2.29
1:I:46:ALA:N	1:I:69:THR:O	0.79	2.15
1:I:25:LEU:O	1:I:26:GLN:HB2	0.79	1.75
1:I:46:ALA:CB	1:I:68:THR:HG22	0.79	2.07
1:I:138:TYR:CE1	1:I:166:VAL:HG22	0.78	2.13
1:I:95:MET:HB3	1:I:182:TYR:HB2	0.78	1.56
1:I:45:SER:HA	1:I:70:ILE:HG12	0.77	1.56
1:I:24:TRP:CE3	1:I:90:LEU:HD22	0.77	2.14
1:I:11:ILE:HD11	1:I:20:LEU:HD12	0.77	1.55
1:I:126:PHE:HB3	1:I:132:ALA:HB2	0.77	1.56
1:I:168:GLN:O	1:I:169:ASN:CB	0.76	2.31
1:I:150:GLN:HG3	1:I:155:ALA:HB2	0.76	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:95:MET:HE2	1:I:95:MET:O	0.76	1.80
1:I:89:SER:C	1:I:90:LEU:HD23	0.76	2.02
1:I:11:ILE:HG22	1:I:13:GLY:H	0.75	1.41
1:I:181:ALA:O	1:I:182:TYR:HB3	0.75	1.81
1:I:165:LEU:HD12	1:I:166:VAL:HG23	0.75	1.59
1:I:12:VAL:CG1	1:I:28:GLY:HA2	0.74	2.11
1:I:12:VAL:HG13	1:I:28:GLY:HA2	0.74	1.59
1:I:174:ILE:CG2	1:I:180:ASN:CB	0.74	2.65
1:I:23:VAL:HG11	1:I:129:TRP:CZ2	0.73	2.17
1:I:99:VAL:O	1:I:179:SER:HA	0.73	1.84
1:I:116:PRO:HG2	1:I:122:LEU:HD11	0.73	1.60
1:I:138:TYR:CE1	1:I:166:VAL:CG2	0.73	2.71
1:I:45:SER:HB3	1:I:60:VAL:HG22	0.73	1.61
1:I:144:ILE:HD12	1:I:165:LEU:CD1	0.72	2.11
1:I:143:THR:HG23	1:I:167:LYS:CB	0.72	2.14
1:I:104:ALA:CB	1:I:183:ALA:HB2	0.72	2.13
1:I:40:LYS:C	1:I:75:SER:HA	0.71	2.06
1:I:29:GLN:HG3	1:I:61:THR:HG22	0.71	1.62
1:I:34:ALA:O	1:I:43:TRP:CH2	0.71	2.44
1:I:25:LEU:O	1:I:26:GLN:CG	0.70	2.39
1:I:178:GLU:O	1:I:179:SER:CB	0.70	2.39
1:I:24:TRP:CZ3	1:I:62:LEU:HD11	0.70	2.21
1:I:95:MET:CB	1:I:182:TYR:CB	0.69	2.70
1:I:53:VAL:HA	1:I:59:GLN:O	0.69	1.87
1:I:2:LEU:O	1:I:2:LEU:HD23	0.68	1.88
1:I:72:VAL:O	1:I:80:ALA:HB3	0.68	1.87
1:I:46:ALA:HB1	1:I:68:THR:HG22	0.68	1.65
1:I:13:GLY:HA2	1:I:25:LEU:O	0.68	1.89
1:I:5:ASP:N	1:I:33:LYS:O	0.67	2.27
1:I:70:ILE:HG22	1:I:82:TYR:CB	0.67	2.19
1:I:46:ALA:HB3	1:I:51:ALA:HB3	0.67	1.65
1:I:2:LEU:CD1	1:I:72:VAL:HG12	0.67	2.20
1:I:24:TRP:CB	1:I:89:SER:O	0.66	2.43
1:I:24:TRP:CZ3	1:I:62:LEU:HD21	0.66	2.24
1:I:76:ASP:O	1:I:77:ASN:CB	0.66	2.43
1:I:145:ILE:HD11	1:I:162:THR:CB	0.66	2.20
1:I:24:TRP:CE3	1:I:90:LEU:CD2	0.66	2.79
1:I:95:MET:CB	1:I:99:VAL:HG21	0.66	2.21
1:I:99:VAL:C	1:I:179:SER:HA	0.66	2.10
1:I:12:VAL:O	1:I:13:GLY:O	0.65	2.14
1:I:25:LEU:N	1:I:25:LEU:CD1	0.65	2.59
1:I:159:VAL:HA	1:I:175:LYS:HB3	0.65	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:125:VAL:O	1:I:129:TRP:CE2	0.65	2.50
1:I:132:ALA:O	1:I:166:VAL:HG23	0.65	1.90
1:I:163:TYR:HA	1:I:170:PRO:HA	0.65	1.69
1:I:146:SER:CA	1:I:181:ALA:HB1	0.65	2.22
1:I:22:THR:O	1:I:89:SER:CB	0.65	2.44
1:I:12:VAL:HG21	1:I:24:TRP:CD2	0.64	2.27
1:I:45:SER:HA	1:I:70:ILE:CG1	0.64	2.21
1:I:50:ILE:CG1	1:I:65:LYS:HB2	0.64	2.22
1:I:95:MET:HB3	1:I:182:TYR:CB	0.64	2.23
1:I:154:ASP:O	1:I:157:SER:HB2	0.64	1.93
1:I:116:PRO:HG3	1:I:122:LEU:HD11	0.64	1.68
1:I:159:VAL:HB	1:I:173:ASN:HA	0.64	1.68
1:I:22:THR:O	1:I:89:SER:HB3	0.64	1.92
1:I:95:MET:CB	1:I:182:TYR:HB2	0.64	2.22
1:I:45:SER:HB2	1:I:60:VAL:HG13	0.63	1.67
1:I:43:TRP:CZ3	1:I:55:ALA:O	0.63	2.51
1:I:162:THR:O	1:I:171:LEU:N	0.63	2.21
1:I:12:VAL:HA	1:I:29:GLN:C	0.63	2.13
1:I:68:THR:OG1	1:I:84:ILE:HD12	0.63	1.94
1:I:43:TRP:CE3	1:I:55:ALA:O	0.62	2.51
1:I:51:ALA:CB	1:I:61:THR:O	0.62	2.47
1:I:23:VAL:HG13	1:I:91:ILE:CD1	0.62	2.24
1:I:116:PRO:CG	1:I:122:LEU:CD1	0.62	2.74
1:I:134:LYS:HB3	1:I:137:TYR:CB	0.62	2.24
1:I:95:MET:HB2	1:I:99:VAL:CG2	0.62	2.25
1:I:101:TYR:O	1:I:105:VAL:HG23	0.62	1.93
1:I:101:TYR:CB	1:I:147:TRP:CZ3	0.62	2.82
1:I:145:ILE:HD11	1:I:162:THR:HB	0.62	1.70
1:I:44:ARG:O	1:I:70:ILE:HA	0.62	1.94
1:I:37:GLY:H	1:I:75:SER:CB	0.61	2.08
1:I:11:ILE:C	1:I:13:GLY:N	0.61	2.53
1:I:45:SER:HB3	1:I:60:VAL:HG13	0.61	1.68
1:I:168:GLN:O	1:I:168:GLN:CG	0.61	2.49
1:I:181:ALA:O	1:I:182:TYR:CB	0.61	2.49
1:I:13:GLY:HA3	1:I:25:LEU:HD23	0.61	1.72
1:I:100:THR:HG23	1:I:103:ASP:CB	0.61	2.25
1:I:144:ILE:HB	1:I:165:LEU:HD21	0.61	1.73
1:I:162:THR:CG2	1:I:174:ILE:CG2	0.61	2.79
1:I:23:VAL:CG1	1:I:91:ILE:CG1	0.60	2.79
1:I:95:MET:CG	1:I:182:TYR:CB	0.60	2.79
1:I:138:TYR:CG	1:I:166:VAL:HG11	0.60	2.31
1:I:12:VAL:HG13	1:I:28:GLY:CA	0.60	2.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:141:SER:O	1:I:142:GLN:C	0.60	2.40
1:I:147:TRP:HD1	1:I:181:ALA:CB	0.60	2.07
1:I:159:VAL:HB	1:I:174:ILE:N	0.60	2.11
1:I:22:THR:HG23	1:I:23:VAL:HG23	0.60	1.72
1:I:46:ALA:O	1:I:47:ASN:CB	0.60	2.49
1:I:4:ILE:CA	1:I:33:LYS:O	0.60	2.50
1:I:119:GLN:HB2	1:I:163:TYR:CD2	0.60	2.31
1:I:50:ILE:CG1	1:I:65:LYS:CB	0.60	2.80
1:I:122:LEU:HD12	1:I:122:LEU:H	0.59	1.56
1:I:95:MET:SD	1:I:182:TYR:CD2	0.59	2.95
1:I:172:ASN:O	1:I:173:ASN:CB	0.59	2.48
1:I:47:ASN:OD1	1:I:49:ALA:N	0.59	2.35
1:I:11:ILE:C	1:I:13:GLY:H	0.59	2.01
1:I:144:ILE:CG1	1:I:165:LEU:HD11	0.59	2.26
1:I:68:THR:OG1	1:I:84:ILE:HB	0.59	1.98
1:I:91:ILE:HD12	1:I:186:VAL:HG12	0.59	1.73
1:I:125:VAL:O	1:I:129:TRP:CD2	0.59	2.56
1:I:99:VAL:HG23	1:I:182:TYR:HA	0.58	1.74
1:I:145:ILE:O	1:I:182:TYR:CE2	0.58	2.56
1:I:13:GLY:CA	1:I:25:LEU:O	0.58	2.51
1:I:150:GLN:HB3	1:I:160:ALA:HA	0.58	1.74
1:I:63:LYS:O	1:I:64:GLU:HB3	0.58	1.98
1:I:169:ASN:CG	1:I:170:PRO:CD	0.58	2.72
1:I:141:SER:O	1:I:143:THR:N	0.58	2.37
1:I:146:SER:CB	1:I:182:TYR:CZ	0.58	2.86
1:I:46:ALA:HB2	1:I:60:VAL:HG12	0.58	1.75
1:I:57:SER:O	1:I:59:GLN:N	0.58	2.36
1:I:69:THR:O	1:I:69:THR:CG2	0.58	2.52
1:I:129:TRP:N	1:I:129:TRP:CE3	0.58	2.71
1:I:138:TYR:O	1:I:141:SER:N	0.58	2.35
1:I:135:TYR:O	1:I:138:TYR:CG	0.58	2.56
1:I:162:THR:OG1	1:I:174:ILE:CG1	0.58	2.52
1:I:167:LYS:O	1:I:168:GLN:HB2	0.58	1.99
1:I:11:ILE:HD11	1:I:20:LEU:CD1	0.57	2.28
1:I:101:TYR:HB2	1:I:147:TRP:CZ3	0.57	2.34
1:I:157:SER:HB3	1:I:159:VAL:CG2	0.57	2.29
1:I:70:ILE:HG22	1:I:82:TYR:O	0.57	1.98
1:I:167:LYS:O	1:I:168:GLN:CB	0.57	2.52
1:I:87:PRO:O	1:I:88:ASN:CB	0.57	2.52
1:I:63:LYS:O	1:I:64:GLU:CB	0.57	2.53
1:I:101:TYR:CE1	1:I:105:VAL:HG21	0.57	2.34
1:I:38:ASN:N	1:I:75:SER:HB2	0.57	2.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:70:ILE:HG22	1:I:82:TYR:HB3	0.56	1.77
1:I:130:GLY:O	1:I:134:LYS:CD	0.56	2.52
1:I:13:GLY:HA3	1:I:25:LEU:CD2	0.56	2.29
1:I:68:THR:OG1	1:I:84:ILE:CB	0.56	2.53
1:I:164:ASP:O	1:I:169:ASN:N	0.56	2.39
1:I:12:VAL:CG2	1:I:29:GLN:N	0.56	2.62
1:I:35:SER:O	1:I:36:GLY:O	0.56	2.22
1:I:95:MET:CB	1:I:182:TYR:HB3	0.56	2.31
1:I:123:GLU:HB2	1:I:163:TYR:CZ	0.56	2.36
1:I:50:ILE:CG2	1:I:51:ALA:N	0.56	2.69
1:I:177:SER:O	1:I:178:GLU:HB3	0.56	2.00
1:I:24:TRP:O	1:I:25:LEU:HD13	0.56	1.99
1:I:45:SER:HB3	1:I:60:VAL:CG2	0.56	2.31
1:I:174:ILE:HG21	1:I:180:ASN:HB3	0.56	1.78
1:I:101:TYR:O	1:I:105:VAL:CG2	0.56	2.54
1:I:173:ASN:O	1:I:174:ILE:CD1	0.56	2.53
1:I:10:GLU:O	1:I:30:VAL:HA	0.56	2.01
1:I:45:SER:C	1:I:47:ASN:H	0.56	2.04
1:I:51:ALA:HB1	1:I:61:THR:O	0.56	2.01
1:I:143:THR:HG23	1:I:167:LYS:HB2	0.56	1.77
1:I:173:ASN:N	1:I:173:ASN:OD1	0.56	2.39
1:I:101:TYR:HB2	1:I:147:TRP:CE3	0.55	2.35
1:I:138:TYR:CD1	1:I:138:TYR:N	0.55	2.70
1:I:177:SER:CB	1:I:180:ASN:ND2	0.55	2.69
1:I:25:LEU:HD12	1:I:129:TRP:CE2	0.55	2.37
1:I:13:GLY:C	1:I:25:LEU:O	0.55	2.45
1:I:23:VAL:HG11	1:I:129:TRP:HZ2	0.55	1.58
1:I:165:LEU:HD12	1:I:166:VAL:N	0.55	2.16
1:I:169:ASN:CB	1:I:170:PRO:CD	0.55	2.85
1:I:12:VAL:CG2	1:I:24:TRP:CE3	0.55	2.77
1:I:50:ILE:HG13	1:I:65:LYS:CB	0.55	2.32
1:I:95:MET:O	1:I:95:MET:CG	0.55	2.54
1:I:94:ASN:O	1:I:95:MET:HB3	0.55	2.00
1:I:173:ASN:O	1:I:174:ILE:HD13	0.55	2.01
1:I:116:PRO:HG3	1:I:122:LEU:CD1	0.55	2.32
1:I:40:LYS:O	1:I:75:SER:HA	0.55	2.02
1:I:121:GLU:O	1:I:125:VAL:CG2	0.55	2.55
1:I:45:SER:O	1:I:47:ASN:N	0.55	2.40
1:I:174:ILE:CG2	1:I:180:ASN:HB2	0.54	2.31
1:I:12:VAL:N	1:I:29:GLN:O	0.54	2.40
1:I:46:ALA:CB	1:I:60:VAL:HG12	0.54	2.33
1:I:174:ILE:CG2	1:I:180:ASN:HB3	0.54	2.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:72:VAL:O	1:I:80:ALA:CB	0.54	2.56
1:I:100:THR:HG23	1:I:103:ASP:HB2	0.54	1.77
1:I:24:TRP:HZ3	1:I:62:LEU:HD11	0.54	1.62
1:I:135:TYR:HA	1:I:138:TYR:CE2	0.54	2.38
1:I:23:VAL:CG1	1:I:129:TRP:CZ2	0.54	2.90
1:I:99:VAL:HG23	1:I:182:TYR:CA	0.54	2.32
1:I:157:SER:HB3	1:I:159:VAL:HG22	0.54	1.77
1:I:119:GLN:CG	1:I:120:ASN:N	0.54	2.70
1:I:9:ILE:HD12	1:I:9:ILE:C	0.54	2.23
1:I:146:SER:C	1:I:181:ALA:CB	0.54	2.77
1:I:70:ILE:CG2	1:I:70:ILE:O	0.54	2.56
1:I:99:VAL:CG2	1:I:182:TYR:HA	0.54	2.32
1:I:146:SER:C	1:I:181:ALA:HB1	0.54	2.23
1:I:177:SER:O	1:I:178:GLU:HB2	0.54	2.00
1:I:47:ASN:OD1	1:I:47:ASN:C	0.53	2.45
1:I:100:THR:CG2	1:I:103:ASP:HB2	0.53	2.34
1:I:143:THR:OG1	1:I:167:LYS:CG	0.53	2.56
1:I:150:GLN:CB	1:I:160:ALA:HA	0.53	2.33
1:I:23:VAL:HB	1:I:129:TRP:CH2	0.53	2.38
1:I:138:TYR:CG	1:I:166:VAL:CG1	0.53	2.92
1:I:159:VAL:HA	1:I:175:LYS:CB	0.53	2.34
1:I:12:VAL:CG1	1:I:24:TRP:HB3	0.53	2.34
1:I:123:GLU:HB2	1:I:163:TYR:CE2	0.53	2.39
1:I:42:THR:C	1:I:43:TRP:HD1	0.53	2.08
1:I:162:THR:OG1	1:I:174:ILE:HG13	0.53	2.03
1:I:45:SER:CA	1:I:70:ILE:HG12	0.52	2.32
1:I:148:VAL:HG12	1:I:149:GLN:N	0.52	2.18
1:I:164:ASP:O	1:I:169:ASN:CA	0.52	2.57
1:I:149:GLN:O	1:I:161:SER:CB	0.52	2.57
1:I:4:ILE:HD12	1:I:4:ILE:C	0.52	2.25
1:I:89:SER:C	1:I:90:LEU:CD2	0.52	2.78
1:I:121:GLU:O	1:I:125:VAL:HG23	0.52	2.04
1:I:99:VAL:O	1:I:179:SER:CA	0.52	2.57
1:I:47:ASN:OD1	1:I:49:ALA:HB3	0.52	2.04
1:I:12:VAL:HG11	1:I:24:TRP:HB3	0.52	1.80
1:I:41:TYR:HB3	1:I:75:SER:CA	0.52	2.34
1:I:24:TRP:CG	1:I:89:SER:O	0.52	2.63
1:I:50:ILE:HD13	1:I:50:ILE:C	0.52	2.24
1:I:132:ALA:O	1:I:166:VAL:CG2	0.52	2.58
1:I:154:ASP:O	1:I:159:VAL:CG2	0.52	2.58
1:I:159:VAL:CB	1:I:173:ASN:HA	0.52	2.33
1:I:173:ASN:O	1:I:174:ILE:CG1	0.52	2.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:95:MET:O	1:I:95:MET:CE	0.52	2.57
1:I:95:MET:CB	1:I:99:VAL:CG2	0.51	2.88
1:I:31:ASN:HA	1:I:58:GLY:O	0.51	2.06
1:I:128:ALA:C	1:I:129:TRP:CE3	0.51	2.83
1:I:157:SER:CB	1:I:159:VAL:HG22	0.51	2.35
1:I:165:LEU:HD12	1:I:166:VAL:CG2	0.51	2.33
1:I:25:LEU:HG	1:I:129:TRP:CE3	0.51	2.40
1:I:46:ALA:O	1:I:50:ILE:HG22	0.51	2.06
1:I:45:SER:C	1:I:60:VAL:HG13	0.51	2.25
1:I:99:VAL:C	1:I:179:SER:CA	0.51	2.79
1:I:87:PRO:O	1:I:88:ASN:HB2	0.51	2.05
1:I:28:GLY:O	1:I:62:LEU:N	0.51	2.42
1:I:70:ILE:O	1:I:82:TYR:N	0.51	2.41
1:I:37:GLY:C	1:I:75:SER:HB2	0.51	2.25
1:I:76:ASP:O	1:I:77:ASN:HB3	0.51	2.04
1:I:147:TRP:HE1	1:I:180:ASN:N	0.51	2.04
1:I:40:LYS:N	1:I:75:SER:O	0.51	2.44
1:I:74:SER:HB3	1:I:78:GLN:CB	0.51	2.36
1:I:100:THR:HA	1:I:147:TRP:CZ2	0.50	2.40
1:I:13:GLY:HA2	1:I:25:LEU:CB	0.50	2.37
1:I:54:ASP:HB3	1:I:59:GLN:CB	0.50	2.36
1:I:70:ILE:CG2	1:I:82:TYR:CB	0.50	2.90
1:I:146:SER:HB2	1:I:182:TYR:OH	0.50	2.07
1:I:95:MET:HB3	1:I:99:VAL:HG21	0.50	1.82
1:I:164:ASP:O	1:I:169:ASN:O	0.50	2.28
1:I:90:LEU:C	1:I:91:ILE:HD13	0.50	2.26
1:I:137:TYR:O	1:I:137:TYR:CD1	0.50	2.64
1:I:29:GLN:CG	1:I:61:THR:HG22	0.50	2.35
1:I:138:TYR:CE2	1:I:166:VAL:HG13	0.50	2.41
1:I:159:VAL:HB	1:I:173:ASN:CA	0.50	2.35
1:I:172:ASN:O	1:I:173:ASN:HB2	0.50	2.06
1:I:146:SER:OG	1:I:182:TYR:CZ	0.50	2.63
1:I:12:VAL:CG2	1:I:24:TRP:CD2	0.50	2.95
1:I:145:ILE:CD1	1:I:162:THR:HG22	0.50	2.36
1:I:13:GLY:HA2	1:I:25:LEU:CA	0.50	2.37
1:I:100:THR:HB	1:I:178:GLU:O	0.50	2.06
1:I:173:ASN:O	1:I:174:ILE:HG12	0.50	2.06
1:I:4:ILE:CB	1:I:34:ALA:HA	0.50	2.37
1:I:119:GLN:HG3	1:I:120:ASN:N	0.50	2.22
1:I:122:LEU:HD12	1:I:122:LEU:N	0.50	2.20
1:I:4:ILE:CG2	1:I:34:ALA:CB	0.49	2.90
1:I:68:THR:OG1	1:I:84:ILE:CG2	0.49	2.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:146:SER:HA	1:I:181:ALA:HB1	0.49	1.84
1:I:9:ILE:HD13	1:I:11:ILE:HG12	0.49	1.83
1:I:37:GLY:N	1:I:75:SER:CB	0.49	2.75
1:I:76:ASP:O	1:I:77:ASN:OD1	0.49	2.31
1:I:123:GLU:HG3	1:I:163:TYR:CZ	0.49	2.42
1:I:143:THR:CB	1:I:167:LYS:HB2	0.49	2.36
1:I:45:SER:OG	1:I:53:VAL:HB	0.49	2.07
1:I:114:LYS:O	1:I:186:VAL:HG23	0.49	2.08
1:I:151:THR:OG1	1:I:154:ASP:OD2	0.49	2.30
1:I:10:GLU:O	1:I:30:VAL:CA	0.49	2.61
1:I:68:THR:OG1	1:I:84:ILE:CD1	0.49	2.61
1:I:148:VAL:CG1	1:I:149:GLN:N	0.49	2.75
1:I:13:GLY:HA2	1:I:25:LEU:HB2	0.49	1.83
1:I:70:ILE:HG22	1:I:70:ILE:O	0.49	2.07
1:I:84:ILE:HG12	1:I:88:ASN:ND2	0.49	2.23
1:I:95:MET:SD	1:I:182:TYR:HB3	0.49	2.48
1:I:145:ILE:CA	1:I:163:TYR:O	0.49	2.57
1:I:159:VAL:CG2	1:I:173:ASN:HA	0.49	2.37
1:I:86:THR:OG1	1:I:87:PRO:CD	0.49	2.61
1:I:137:TYR:CD1	1:I:137:TYR:C	0.49	2.85
1:I:146:SER:HA	1:I:182:TYR:CE2	0.49	2.43
1:I:76:ASP:O	1:I:77:ASN:CG	0.49	2.50
1:I:45:SER:HB3	1:I:60:VAL:CG1	0.49	2.35
1:I:45:SER:C	1:I:47:ASN:N	0.49	2.64
1:I:148:VAL:HB	1:I:161:SER:O	0.49	2.08
1:I:178:GLU:O	1:I:179:SER:HB3	0.49	2.07
1:I:46:ALA:HB2	1:I:60:VAL:CG1	0.48	2.38
1:I:134:LYS:HB3	1:I:137:TYR:HB2	0.48	1.84
1:I:4:ILE:HB	1:I:33:LYS:O	0.48	2.08
1:I:45:SER:C	1:I:60:VAL:CG1	0.48	2.82
1:I:39:GLY:N	1:I:75:SER:HB3	0.48	2.23
1:I:43:TRP:CD1	1:I:43:TRP:N	0.48	2.80
1:I:138:TYR:CD2	1:I:166:VAL:HG13	0.48	2.43
1:I:37:GLY:N	1:I:75:SER:OG	0.48	2.40
1:I:116:PRO:HG3	1:I:122:LEU:CG	0.48	2.37
1:I:25:LEU:N	1:I:25:LEU:HD22	0.48	2.22
1:I:54:ASP:CB	1:I:59:GLN:HB3	0.48	2.37
1:I:70:ILE:CG2	1:I:82:TYR:HB3	0.48	2.38
1:I:134:LYS:HB3	1:I:137:TYR:HB3	0.48	1.84
1:I:41:TYR:N	1:I:75:SER:HA	0.48	2.23
1:I:45:SER:O	1:I:46:ALA:HB3	0.48	2.09
1:I:84:ILE:CG2	1:I:88:ASN:OD1	0.48	2.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:70:ILE:O	1:I:82:TYR:O	0.48	2.32
1:I:169:ASN:CG	1:I:170:PRO:HD3	0.48	2.29
1:I:122:LEU:CD2	1:I:184:THR:OG1	0.48	2.62
1:I:2:LEU:HB2	1:I:74:SER:CB	0.47	2.39
1:I:143:THR:CG2	1:I:167:LYS:HB2	0.47	2.39
1:I:162:THR:HG21	1:I:174:ILE:CG2	0.47	2.34
1:I:91:ILE:HA	1:I:185:CYS:O	0.47	2.09
1:I:143:THR:CG2	1:I:167:LYS:CB	0.47	2.91
1:I:178:GLU:O	1:I:179:SER:OG	0.47	2.32
1:I:13:GLY:CA	1:I:25:LEU:CD2	0.47	2.92
1:I:25:LEU:HD12	1:I:129:TRP:CD2	0.47	2.44
1:I:32:LEU:N	1:I:58:GLY:O	0.47	2.47
1:I:68:THR:OG1	1:I:84:ILE:HG21	0.47	2.08
1:I:25:LEU:HD22	1:I:25:LEU:H	0.47	1.70
1:I:91:ILE:HD13	1:I:91:ILE:N	0.47	2.24
1:I:162:THR:HG23	1:I:174:ILE:CG2	0.47	2.40
1:I:45:SER:CB	1:I:53:VAL:HB	0.47	2.40
1:I:86:THR:OG1	1:I:87:PRO:HD3	0.47	2.10
1:I:50:ILE:C	1:I:50:ILE:CD1	0.47	2.83
1:I:62:LEU:HD22	1:I:68:THR:HG21	0.47	1.86
1:I:153:GLN:O	1:I:156:LYS:HG3	0.47	2.09
1:I:165:LEU:CD1	1:I:166:VAL:HG23	0.47	2.37
1:I:46:ALA:CB	1:I:51:ALA:HB3	0.46	2.38
1:I:130:GLY:O	1:I:134:LYS:HD2	0.46	2.10
1:I:41:TYR:HD2	1:I:75:SER:HG	0.46	1.51
1:I:64:GLU:O	1:I:65:LYS:HB2	0.46	2.09
1:I:95:MET:O	1:I:95:MET:HG3	0.46	2.10
1:I:86:THR:CB	1:I:87:PRO:CD	0.46	2.93
1:I:154:ASP:CG	1:I:173:ASN:OD1	0.46	2.54
1:I:4:ILE:HA	1:I:33:LYS:O	0.46	2.09
1:I:46:ALA:O	1:I:47:ASN:CG	0.46	2.54
1:I:46:ALA:HA	1:I:69:THR:N	0.46	2.26
1:I:148:VAL:CG2	1:I:163:TYR:HB2	0.46	2.40
1:I:146:SER:N	1:I:163:TYR:O	0.46	2.45
1:I:157:SER:CB	1:I:159:VAL:CG2	0.46	2.94
1:I:158:GLY:O	1:I:175:LYS:HG3	0.46	2.11
1:I:10:GLU:CB	1:I:31:ASN:HB3	0.46	2.41
1:I:50:ILE:HG12	1:I:65:LYS:CB	0.46	2.41
1:I:45:SER:HB2	1:I:53:VAL:CG1	0.46	2.41
1:I:106:ASN:O	1:I:110:ASN:HB2	0.46	2.10
1:I:41:TYR:HB3	1:I:75:SER:OG	0.45	2.10
1:I:74:SER:OG	1:I:78:GLN:HB2	0.45	2.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:162:THR:CG2	1:I:174:ILE:CB	0.45	2.94
1:I:168:GLN:O	1:I:168:GLN:HG3	0.45	2.11
1:I:12:VAL:HG11	1:I:24:TRP:CE3	0.45	2.46
1:I:31:ASN:OD1	1:I:58:GLY:O	0.45	2.35
1:I:86:THR:N	1:I:87:PRO:HD2	0.45	2.27
1:I:138:TYR:O	1:I:142:GLN:N	0.45	2.50
1:I:177:SER:HB2	1:I:180:ASN:ND2	0.45	2.25
1:I:13:GLY:CA	1:I:25:LEU:HB2	0.45	2.41
1:I:50:ILE:HG12	1:I:65:LYS:CG	0.45	2.40
1:I:149:GLN:O	1:I:161:SER:HB3	0.45	2.11
1:I:160:ALA:N	1:I:175:LYS:HB3	0.45	2.27
1:I:24:TRP:CH2	1:I:62:LEU:CD2	0.45	2.90
1:I:42:THR:CB	1:I:73:ILE:HD12	0.45	2.42
1:I:156:LYS:HG3	1:I:157:SER:N	0.45	2.26
1:I:37:GLY:N	1:I:75:SER:H	0.45	2.09
1:I:172:ASN:C	1:I:173:ASN:OD1	0.45	2.55
1:I:12:VAL:HA	1:I:29:GLN:N	0.45	2.27
1:I:25:LEU:O	1:I:26:GLN:HG3	0.45	2.10
1:I:134:LYS:O	1:I:135:TYR:HB3	0.45	2.11
1:I:74:SER:HB3	1:I:78:GLN:HB3	0.45	1.89
1:I:129:TRP:CE3	1:I:129:TRP:CA	0.45	3.00
1:I:142:GLN:O	1:I:166:VAL:HG12	0.45	2.12
1:I:46:ALA:O	1:I:50:ILE:CG2	0.44	2.64
1:I:121:GLU:O	1:I:125:VAL:CB	0.44	2.65
1:I:143:THR:OG1	1:I:167:LYS:HB2	0.44	2.12
1:I:12:VAL:HA	1:I:29:GLN:H	0.44	1.71
1:I:12:VAL:CB	1:I:24:TRP:CD2	0.44	3.00
1:I:42:THR:C	1:I:43:TRP:CD1	0.44	2.90
1:I:77:ASN:OD1	1:I:77:ASN:C	0.44	2.55
1:I:121:GLU:O	1:I:125:VAL:HB	0.44	2.11
1:I:145:ILE:HD11	1:I:162:THR:CG2	0.44	2.42
1:I:145:ILE:O	1:I:145:ILE:CG2	0.44	2.65
1:I:147:TRP:CD1	1:I:181:ALA:CB	0.44	2.91
1:I:169:ASN:OD1	1:I:170:PRO:HD2	0.44	2.12
1:I:11:ILE:O	1:I:12:VAL:C	0.44	2.54
1:I:23:VAL:HA	1:I:89:SER:HB3	0.44	1.88
1:I:45:SER:CA	1:I:60:VAL:HG13	0.44	2.40
1:I:47:ASN:N	1:I:69:THR:HG22	0.44	2.28
1:I:97:LYS:O	1:I:98:ARG:C	0.44	2.54
1:I:148:VAL:CG1	1:I:161:SER:HB3	0.44	2.42
1:I:135:TYR:N	1:I:138:TYR:CE1	0.44	2.84
1:I:45:SER:HA	1:I:70:ILE:CD1	0.44	2.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:143:THR:OG1	1:I:167:LYS:HD3	0.44	2.13
1:I:126:PHE:HA	1:I:129:TRP:CD1	0.44	2.48
1:I:160:ALA:O	1:I:174:ILE:N	0.44	2.51
1:I:163:TYR:CD1	1:I:170:PRO:HB3	0.44	2.48
1:I:174:ILE:HG23	1:I:180:ASN:CB	0.44	2.41
1:I:13:GLY:HA2	1:I:25:LEU:C	0.44	2.34
1:I:25:LEU:CD1	1:I:129:TRP:CD2	0.44	3.01
1:I:162:THR:HG23	1:I:174:ILE:CB	0.44	2.43
1:I:108:CYS:SG	1:I:184:THR:C	0.44	2.96
1:I:84:ILE:HG23	1:I:88:ASN:CG	0.43	2.32
1:I:159:VAL:CA	1:I:175:LYS:HB3	0.43	2.42
1:I:4:ILE:HG22	1:I:34:ALA:HA	0.43	1.91
1:I:46:ALA:CB	1:I:51:ALA:CB	0.43	2.96
1:I:50:ILE:HG12	1:I:65:LYS:HB2	0.43	1.88
1:I:154:ASP:HB3	1:I:173:ASN:OD1	0.43	2.14
1:I:40:LYS:O	1:I:75:SER:CA	0.43	2.66
1:I:62:LEU:O	1:I:63:LYS:HD2	0.43	2.13
1:I:100:THR:CA	1:I:179:SER:HA	0.43	2.43
1:I:178:GLU:C	1:I:179:SER:OG	0.43	2.56
1:I:77:ASN:CG	1:I:77:ASN:O	0.43	2.55
1:I:40:LYS:O	1:I:75:SER:C	0.43	2.57
1:I:64:GLU:O	1:I:65:LYS:CB	0.43	2.67
1:I:94:ASN:OD1	1:I:94:ASN:N	0.43	2.51
1:I:50:ILE:O	1:I:50:ILE:CD1	0.43	2.56
1:I:42:THR:CB	1:I:73:ILE:HB	0.43	2.44
1:I:46:ALA:HB3	1:I:51:ALA:CB	0.43	2.38
1:I:101:TYR:HB3	1:I:147:TRP:CZ3	0.43	2.49
1:I:154:ASP:OD2	1:I:172:ASN:HB2	0.43	2.14
1:I:2:LEU:CD1	1:I:72:VAL:CG1	0.42	2.96
1:I:28:GLY:O	1:I:62:LEU:O	0.42	2.37
1:I:147:TRP:N	1:I:181:ALA:CB	0.42	2.82
1:I:165:LEU:HD12	1:I:166:VAL:H	0.42	1.73
1:I:39:GLY:C	1:I:75:SER:HB3	0.42	2.35
1:I:162:THR:HG21	1:I:174:ILE:HG13	0.42	1.90
1:I:23:VAL:CG1	1:I:91:ILE:HG13	0.42	2.44
1:I:45:SER:CB	1:I:60:VAL:CG1	0.42	2.80
1:I:155:ALA:O	1:I:158:GLY:N	0.42	2.47
1:I:123:GLU:CB	1:I:163:TYR:CZ	0.42	3.02
1:I:129:TRP:CD2	1:I:129:TRP:N	0.42	2.83
1:I:54:ASP:CB	1:I:59:GLN:CB	0.42	2.97
1:I:100:THR:CG2	1:I:103:ASP:CB	0.42	2.98
1:I:172:ASN:C	1:I:173:ASN:CG	0.42	2.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:146:SER:OG	1:I:182:TYR:CE1	0.42	2.53
1:I:13:GLY:HA2	1:I:25:LEU:N	0.42	2.30
1:I:117:SER:C	1:I:118:SER:OG	0.42	2.58
1:I:42:THR:HB	1:I:73:ILE:HD12	0.42	1.91
1:I:100:THR:HA	1:I:179:SER:HA	0.42	1.92
1:I:145:ILE:O	1:I:182:TYR:CD2	0.42	2.72
1:I:146:SER:CA	1:I:182:TYR:CE2	0.42	3.03
1:I:46:ALA:CA	1:I:68:THR:HG22	0.41	2.45
1:I:108:CYS:O	1:I:111:PHE:HB2	0.41	2.15
1:I:4:ILE:CB	1:I:33:LYS:O	0.41	2.67
1:I:12:VAL:HB	1:I:24:TRP:CG	0.41	2.50
1:I:46:ALA:CB	1:I:60:VAL:CG1	0.41	2.98
1:I:134:LYS:O	1:I:135:TYR:CB	0.41	2.69
1:I:186:VAL:O	1:I:187:LYS:HB3	0.41	2.15
1:I:95:MET:CG	1:I:182:TYR:HB2	0.41	2.45
1:I:2:LEU:HD11	1:I:72:VAL:CG1	0.41	2.45
1:I:54:ASP:HB3	1:I:59:GLN:HB2	0.41	1.92
1:I:116:PRO:CB	1:I:121:GLU:HB3	0.41	2.46
1:I:162:THR:N	1:I:171:LEU:O	0.41	2.49
1:I:169:ASN:CB	1:I:170:PRO:HD2	0.41	2.46
1:I:186:VAL:O	1:I:187:LYS:CB	0.41	2.66
1:I:12:VAL:HG21	1:I:24:TRP:CH2	0.41	2.49
1:I:23:VAL:CG1	1:I:91:ILE:CD1	0.41	2.98
1:I:62:LEU:O	1:I:63:LYS:CG	0.41	2.68
1:I:74:SER:CB	1:I:78:GLN:HB2	0.41	2.46
1:I:94:ASN:OD1	1:I:185:CYS:SG	0.41	2.79
1:I:154:ASP:O	1:I:157:SER:CB	0.41	2.69
1:I:4:ILE:HG22	1:I:34:ALA:CB	0.40	2.45
1:I:41:TYR:CA	1:I:75:SER:HA	0.40	2.46
1:I:63:LYS:C	1:I:64:GLU:HG2	0.40	2.36
1:I:147:TRP:N	1:I:181:ALA:HB3	0.40	2.31
1:I:163:TYR:CG	1:I:170:PRO:HB3	0.40	2.51
1:I:2:LEU:HD11	1:I:72:VAL:HG12	0.40	1.92
1:I:9:ILE:CD1	1:I:11:ILE:HG12	0.40	2.46
1:I:138:TYR:CD1	1:I:166:VAL:HG11	0.40	2.52
1:I:138:TYR:CD1	1:I:166:VAL:HG21	0.40	2.50
1:I:138:TYR:CD2	1:I:166:VAL:CG1	0.40	3.04
1:I:37:GLY:CA	1:I:75:SER:HB2	0.40	2.46
1:I:4:ILE:CA	1:I:34:ALA:HA	0.40	2.45
1:I:62:LEU:O	1:I:63:LYS:HG3	0.40	2.16
1:I:4:ILE:HA	1:I:34:ALA:HA	0.40	1.93
1:I:123:GLU:HG3	1:I:163:TYR:OH	0.40	2.16

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	I	185/187 (99%)	144 (78%)	17 (9%)	24 (13%)	1	6
All	All	185/187 (99%)	144 (78%)	17 (9%)	24 (13%)	1	6

All 24 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	I	12	VAL
1	I	13	GLY
1	I	21	PRO
1	I	26	GLN
1	I	28	GLY
1	I	36	GLY
1	I	46	ALA
1	I	47	ASN
1	I	58	GLY
1	I	64	GLU
1	I	65	LYS
1	I	77	ASN
1	I	87	PRO
1	I	95	MET
1	I	135	TYR
1	I	141	SER
1	I	142	GLN
1	I	168	GLN
1	I	169	ASN
1	I	173	ASN
1	I	175	LYS
1	I	178	GLU
1	I	179	SER
1	I	182	TYR

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	I	156/156 (100%)	95 (61%)	61 (39%)	0 5
All	All	156/156 (100%)	95 (61%)	61 (39%)	0 5

All 61 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	I	1	THR
1	I	2	LEU
1	I	4	ILE
1	I	14	THR
1	I	19	LYS
1	I	25	LEU
1	I	30	VAL
1	I	35	SER
1	I	38	ASN
1	I	42	THR
1	I	44	ARG
1	I	45	SER
1	I	47	ASN
1	I	50	ILE
1	I	53	VAL
1	I	56	SER
1	I	60	VAL
1	I	62	LEU
1	I	63	LYS
1	I	65	LYS
1	I	67	THR
1	I	68	THR
1	I	69	THR
1	I	70	ILE
1	I	77	ASN
1	I	78	GLN
1	I	79	THR
1	I	81	THR
1	I	82	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	84	ILE
1	I	86	THR
1	I	90	LEU
1	I	95	MET
1	I	97	LYS
1	I	99	VAL
1	I	100	THR
1	I	109	LYS
1	I	117	SER
1	I	118	SER
1	I	120	ASN
1	I	123	GLU
1	I	126	PHE
1	I	129	TRP
1	I	133	ASN
1	I	134	LYS
1	I	139	LYS
1	I	144	ILE
1	I	145	ILE
1	I	151	THR
1	I	156	LYS
1	I	157	SER
1	I	162	THR
1	I	163	TYR
1	I	164	ASP
1	I	165	LEU
1	I	167	LYS
1	I	169	ASN
1	I	173	ASN
1	I	175	LYS
1	I	184	THR
1	I	186	VAL

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided