



Full wwPDB NMR Structure Validation Report ⓘ

Mar 2, 2021 – 08:04 PM EST

PDB ID : 7K7F
Title : Solution Structure of the Corynebacterium diphtheriae SpaA Pilin-Signal Peptide Complex
Authors : McConnell, S.A.; Clubb, R.T.
Deposited on : 2020-09-22

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 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)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.17.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1

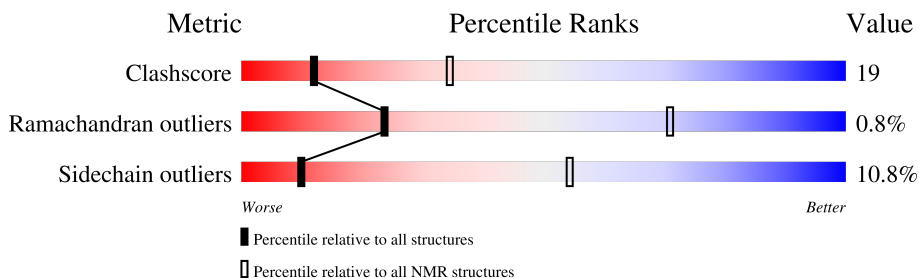
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	A	143	
2	B	10	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:54-A:193, B:487-B:494 (148)	0.35	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 9, 10, 12, 19
2	6, 15, 17, 20
3	7, 8, 14
4	11, 13, 16
Single-model clusters	18

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2328 atoms, of which 1167 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative surface-anchored fimbrial subunit.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	143	2172	687	1087	185	211	2	0

- Molecule 2 is a protein called SpaA sorting signal peptide.

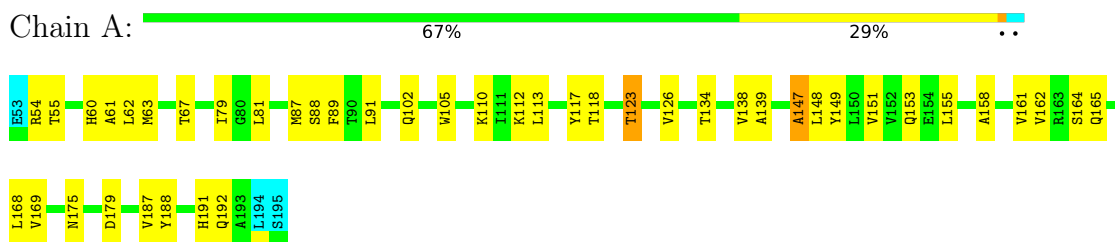
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	10	156	50	80	12	14	0

4 Residue-property plots [i](#)

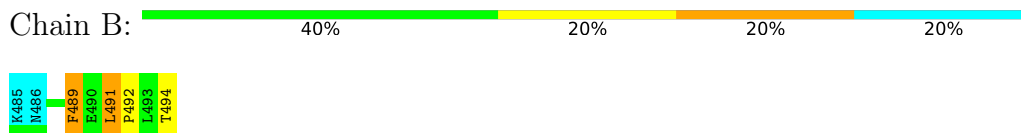
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Putative surface-anchored fimbrial subunit



- Molecule 2: SpaA sorting signal peptide

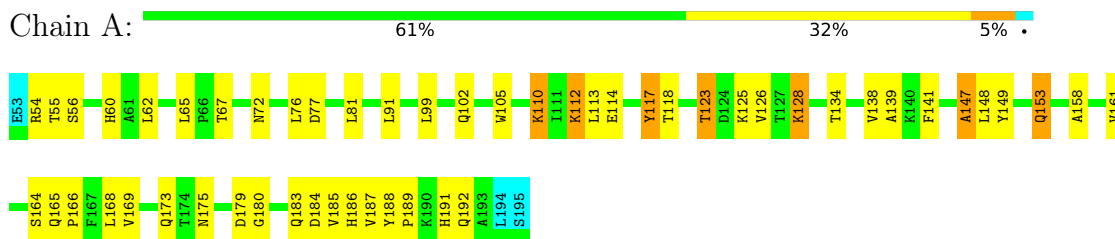


4.2 Scores per residue for each member of the ensemble

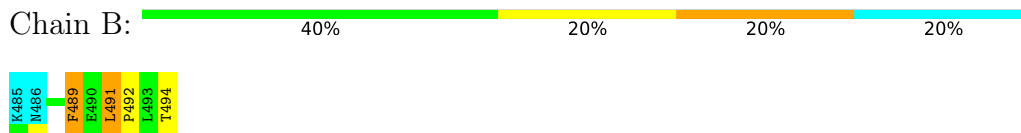
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Putative surface-anchored fimbrial subunit

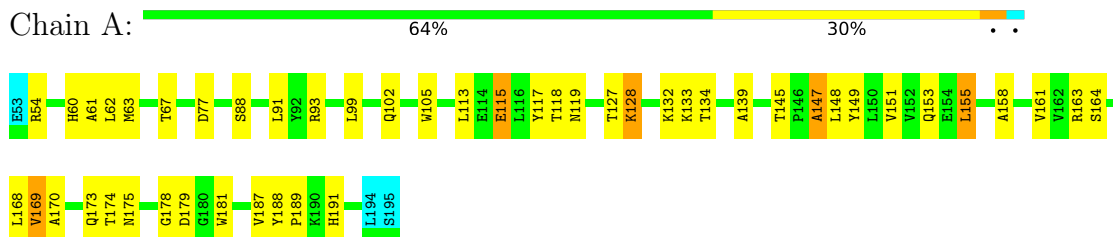


- Molecule 2: SpaA sorting signal peptide

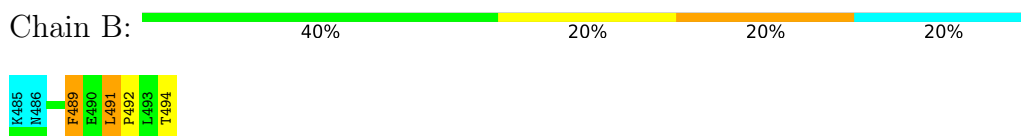


4.2.2 Score per residue for model 2

- Molecule 1: Putative surface-anchored fimbrial subunit



- Molecule 2: SpaA sorting signal peptide

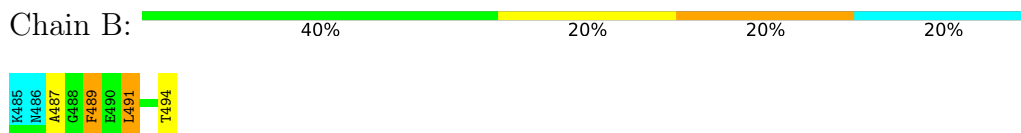


4.2.3 Score per residue for model 3

- Molecule 1: Putative surface-anchored fimbrial subunit

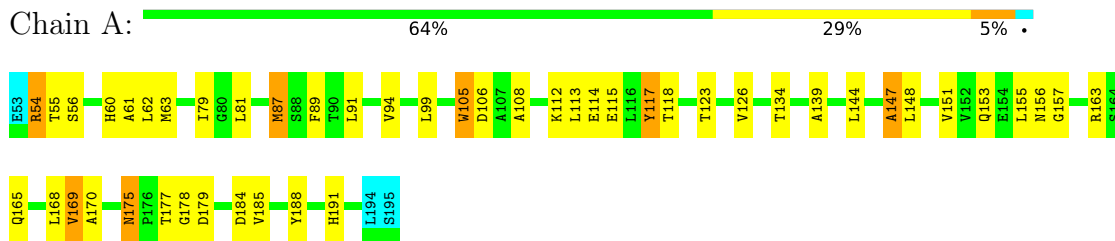


- Molecule 2: SpaA sorting signal peptide

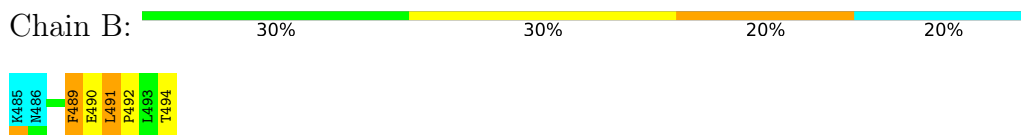


4.2.4 Score per residue for model 4

- Molecule 1: Putative surface-anchored fimbrial subunit

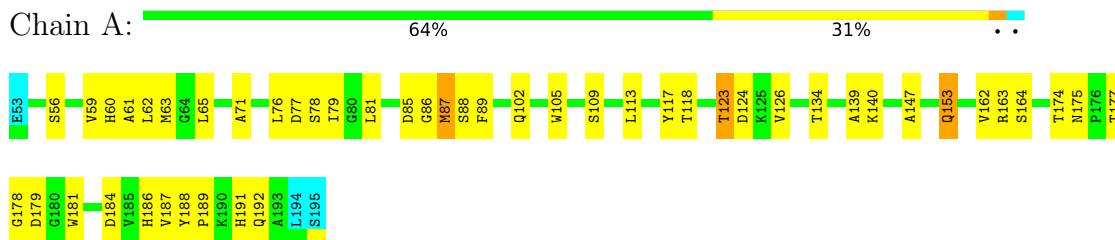


- Molecule 2: SpaA sorting signal peptide



4.2.5 Score per residue for model 5

- Molecule 1: Putative surface-anchored fimbrial subunit

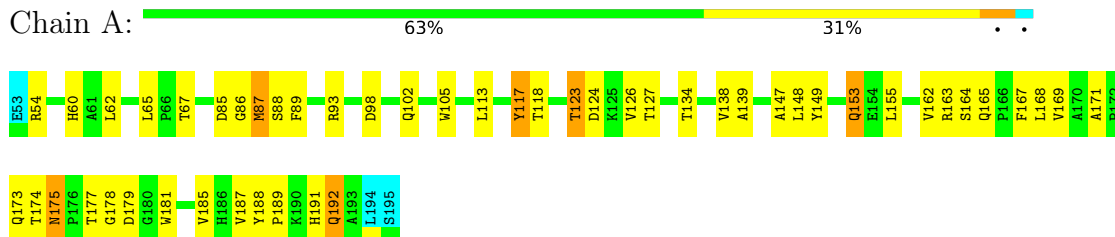


- Molecule 2: SpaA sorting signal peptide

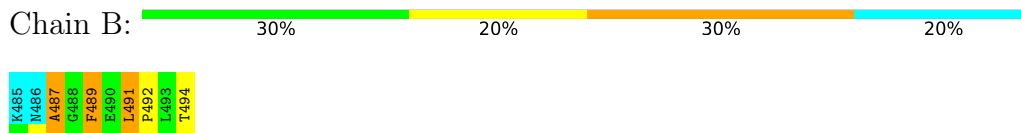


4.2.6 Score per residue for model 6

- Molecule 1: Putative surface-anchored fimbrial subunit

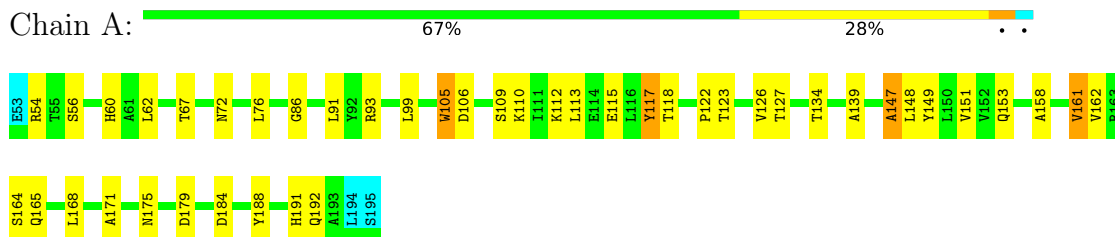


- Molecule 2: SpaA sorting signal peptide



4.2.7 Score per residue for model 7

- Molecule 1: Putative surface-anchored fimbrial subunit

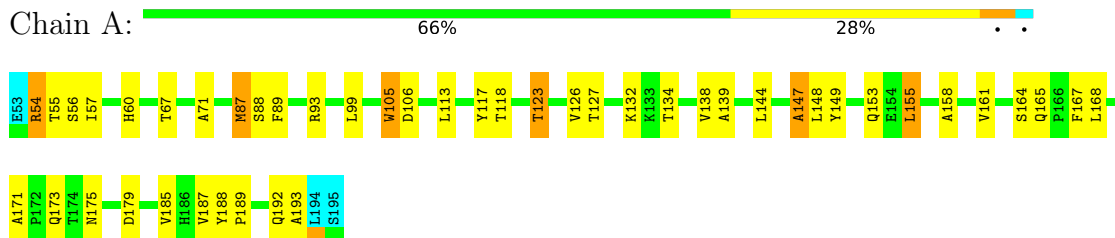


- Molecule 2: SpaA sorting signal peptide

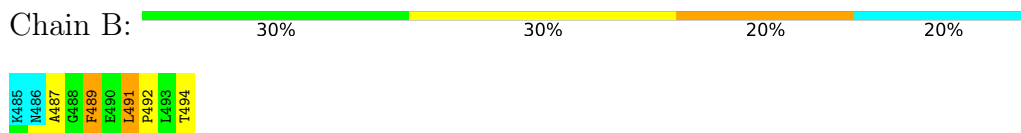


4.2.8 Score per residue for model 8

- Molecule 1: Putative surface-anchored fimbrial subunit

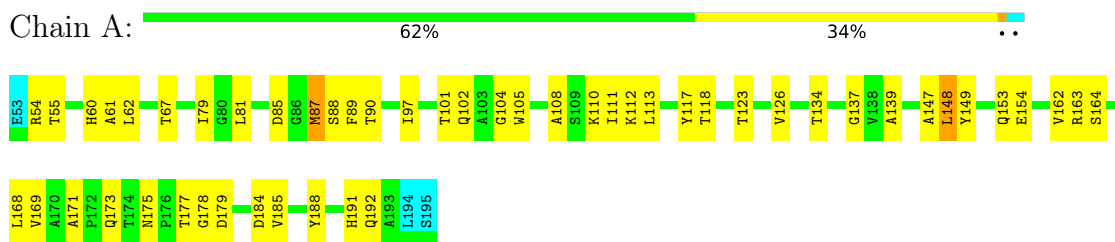


- Molecule 2: SpaA sorting signal peptide

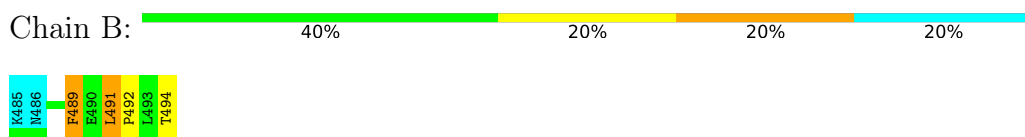


4.2.9 Score per residue for model 9

- Molecule 1: Putative surface-anchored fimbrial subunit

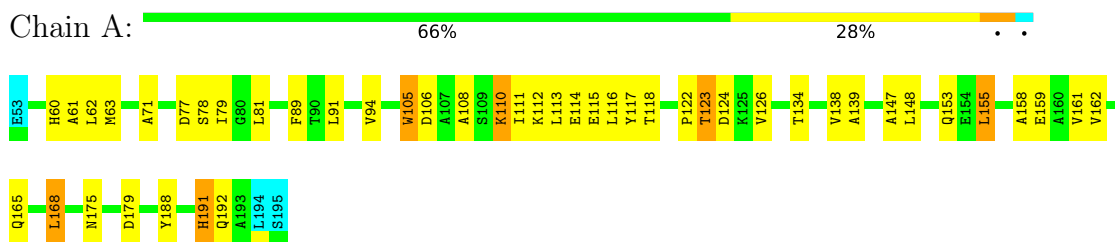


- Molecule 2: SpaA sorting signal peptide

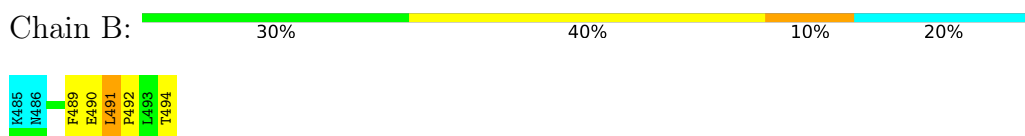


4.2.10 Score per residue for model 10

- Molecule 1: Putative surface-anchored fimbrial subunit

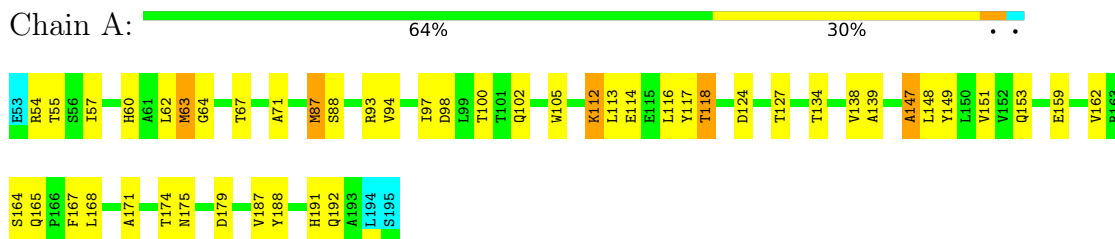


- Molecule 2: SpaA sorting signal peptide

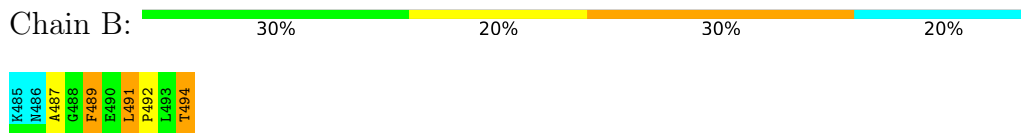


4.2.11 Score per residue for model 11

- Molecule 1: Putative surface-anchored fimbrial subunit

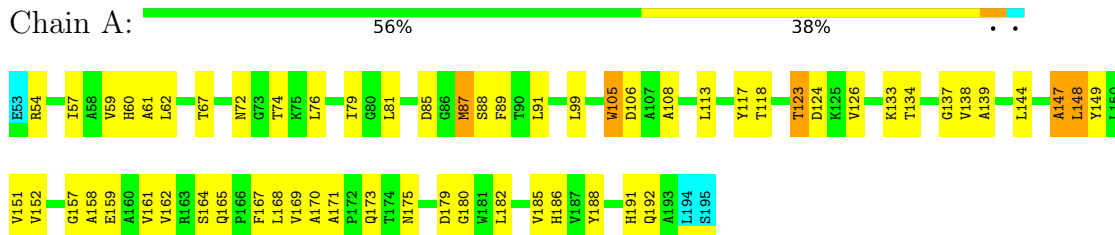


- Molecule 2: SpaA sorting signal peptide

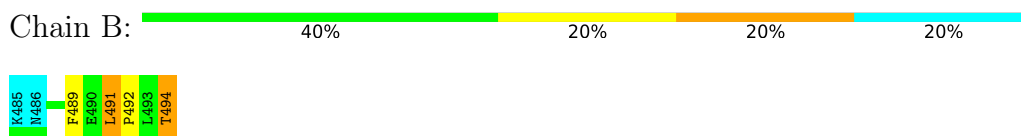


4.2.12 Score per residue for model 12

- Molecule 1: Putative surface-anchored fimbrial subunit

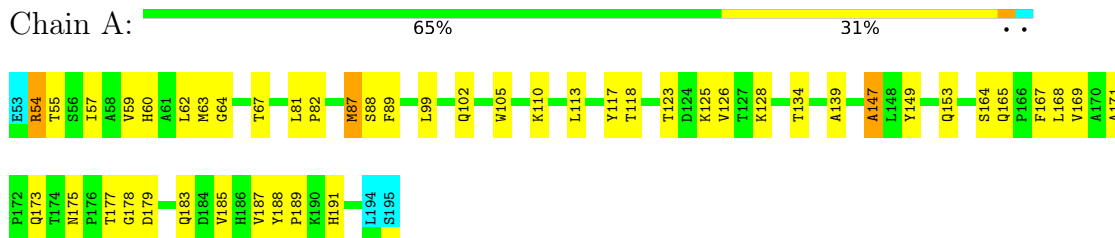


- Molecule 2: SpaA sorting signal peptide

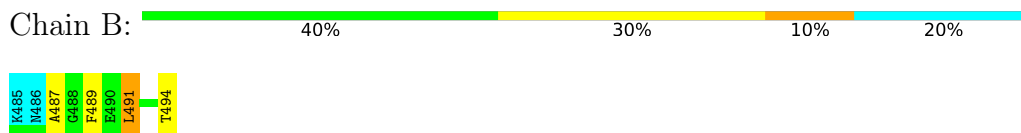


4.2.13 Score per residue for model 13

- Molecule 1: Putative surface-anchored fimbrial subunit

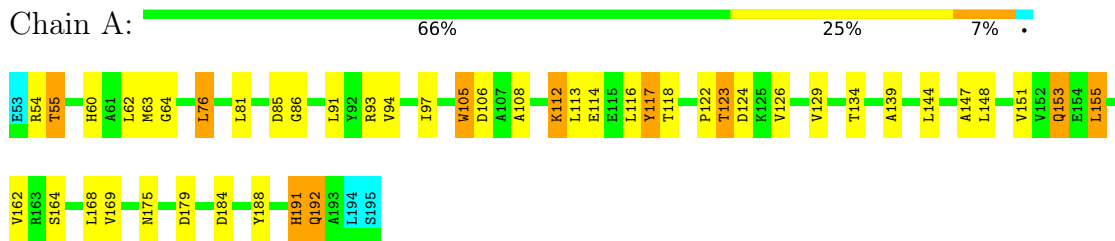


- Molecule 2: SpaA sorting signal peptide

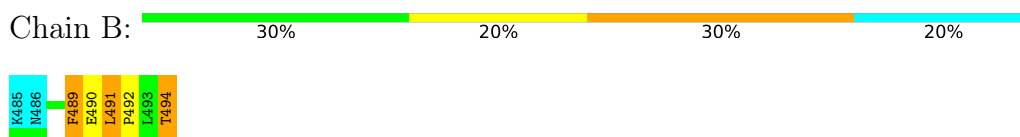


4.2.14 Score per residue for model 14

- Molecule 1: Putative surface-anchored fimbrial subunit

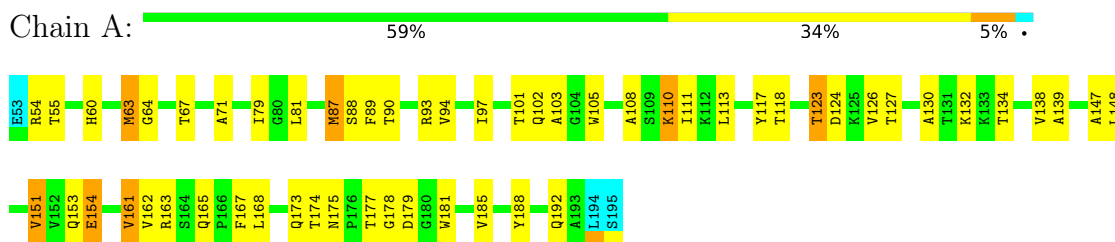


- Molecule 2: SpaA sorting signal peptide

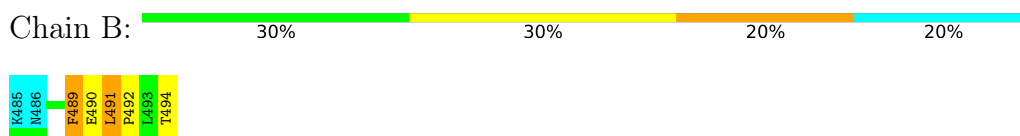


4.2.15 Score per residue for model 15

- Molecule 1: Putative surface-anchored fimbrial subunit

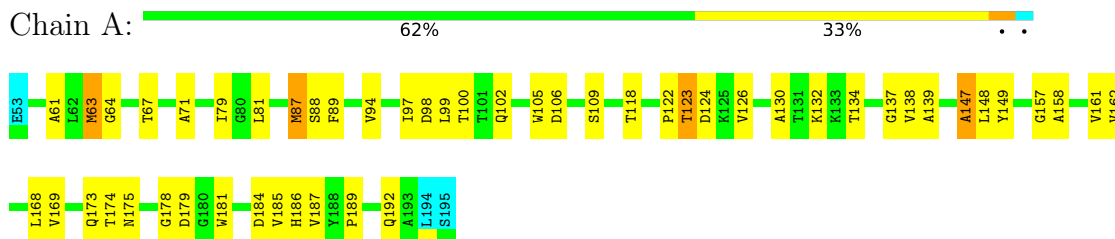


- Molecule 2: SpaA sorting signal peptide

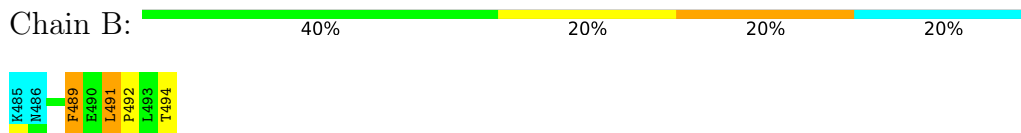


4.2.16 Score per residue for model 16

- Molecule 1: Putative surface-anchored fimbrial subunit

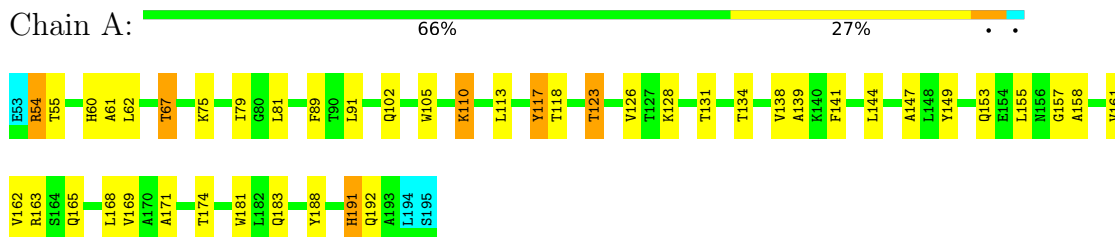


- Molecule 2: SpaA sorting signal peptide

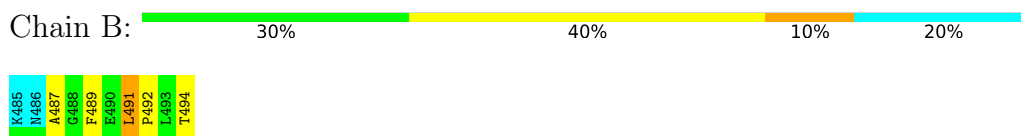


4.2.17 Score per residue for model 17

- Molecule 1: Putative surface-anchored fimbrial subunit

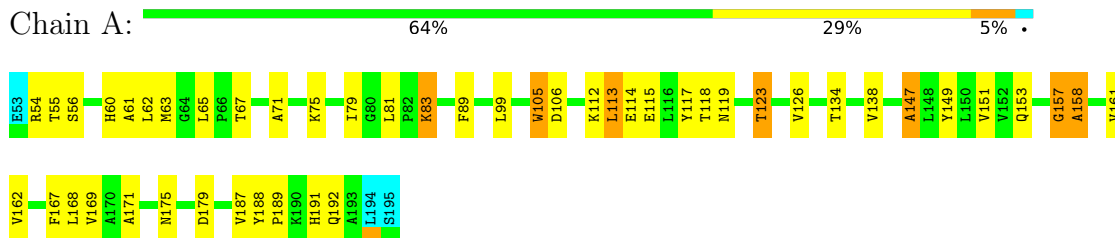


- Molecule 2: SpaA sorting signal peptide

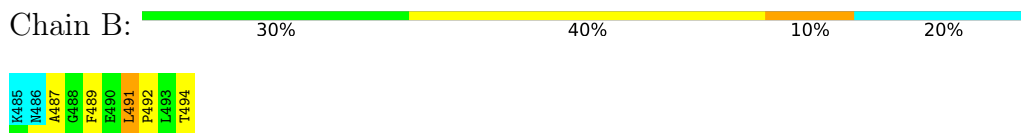


4.2.18 Score per residue for model 18

- Molecule 1: Putative surface-anchored fimbrial subunit

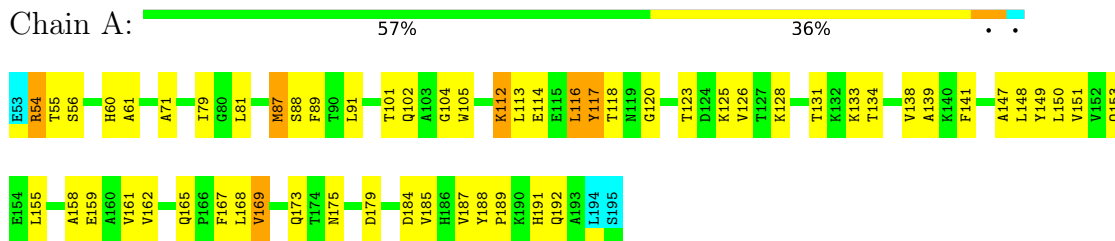


- Molecule 2: SpaA sorting signal peptide

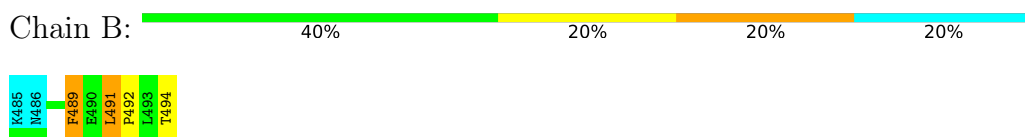


4.2.19 Score per residue for model 19

- Molecule 1: Putative surface-anchored fimbrial subunit

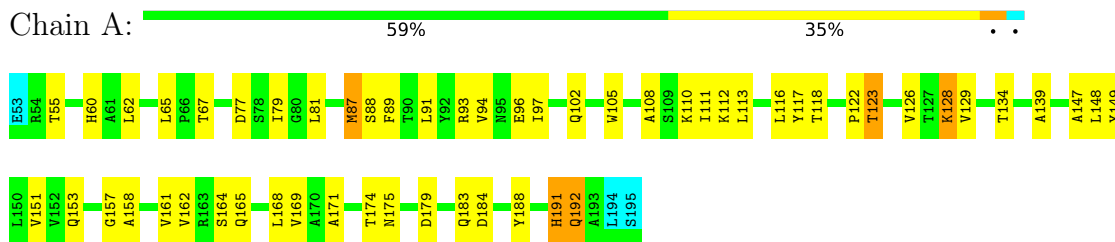


- Molecule 2: SpaA sorting signal peptide

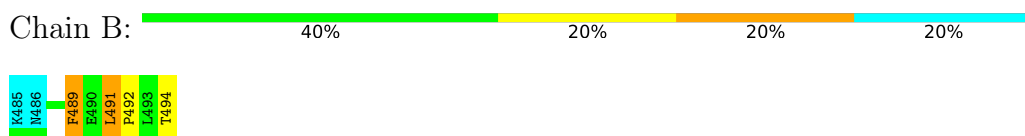


4.2.20 Score per residue for model 20

- Molecule 1: Putative surface-anchored fimbrial subunit



- Molecule 2: SpaA sorting signal peptide



GLOBAL-STATISTICS INFOmissingINFO

5 Model quality

5.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 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	A	1061	1063	1063	40±6
2	B	59	59	59	6±2
All	All	22400	22440	22440	869

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ILE:HG22	1:A:81:LEU:HD13	0.82	1.51	15	9
1:A:113:LEU:HD12	1:A:113:LEU:O	0.80	1.77	18	1
2:B:491:LEU:N	2:B:491:LEU:HD23	0.80	1.92	7	20
1:A:173:GLN:NE2	1:A:185:VAL:HG13	0.80	1.92	6	2
1:A:99:LEU:HD12	1:A:147:ALA:O	0.78	1.78	8	4
1:A:173:GLN:OE1	1:A:185:VAL:HG13	0.77	1.80	8	7
1:A:99:LEU:HD22	1:A:147:ALA:O	0.74	1.83	2	2
1:A:175:ASN:HD21	1:A:179:ASP:H	0.73	1.26	13	7
1:A:155:LEU:HD23	1:A:155:LEU:N	0.71	1.97	2	3
1:A:123:THR:O	1:A:126:VAL:HG22	0.70	1.85	12	18
1:A:148:LEU:HD11	2:B:489:PHE:CZ	0.69	2.22	16	8
1:A:59:VAL:CG1	1:A:139:ALA:HB3	0.68	2.18	13	3
1:A:55:THR:HG23	1:A:183:GLN:O	0.68	1.88	17	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ASP:OD1	1:A:100:THR:HG23	0.68	1.87	11	2
1:A:158:ALA:HB1	1:A:161:VAL:HG13	0.68	1.65	2	7
1:A:71:ALA:HB1	2:B:492:PRO:O	0.68	1.89	19	6
1:A:105:TRP:CD1	1:A:106:ASP:N	0.68	2.62	12	8
1:A:79:ILE:HG22	1:A:81:LEU:HD23	0.67	1.66	5	1
1:A:175:ASN:HD21	1:A:179:ASP:N	0.67	1.87	6	5
1:A:81:LEU:HD12	1:A:81:LEU:C	0.67	2.10	14	2
2:B:491:LEU:HD23	2:B:491:LEU:H	0.67	1.48	15	20
1:A:108:ALA:HB1	2:B:489:PHE:CZ	0.66	2.25	14	3
1:A:65:LEU:HD11	1:A:192:GLN:OE1	0.65	1.92	1	1
1:A:83:LYS:N	1:A:83:LYS:CD	0.64	2.60	18	1
1:A:102:GLN:NE2	1:A:105:TRP:HE1	0.63	1.91	2	1
1:A:175:ASN:ND2	1:A:178:GLY:N	0.63	2.46	4	2
1:A:60:HIS:CD2	1:A:188:TYR:CE2	0.63	2.87	5	18
1:A:59:VAL:HG13	1:A:59:VAL:O	0.63	1.93	5	3
1:A:153:GLN:NE2	1:A:164:SER:H	0.63	1.91	7	4
1:A:134:THR:OG1	1:A:139:ALA:HB2	0.62	1.93	5	18
1:A:102:GLN:NE2	1:A:105:TRP:NE1	0.62	2.47	2	1
1:A:87:MET:SD	1:A:88:SER:N	0.62	2.73	5	11
1:A:72:ASN:HD22	1:A:76:LEU:HD22	0.62	1.54	7	2
1:A:102:GLN:O	1:A:105:TRP:CD1	0.62	2.53	6	12
1:A:101:THR:HG23	1:A:104:GLY:H	0.62	1.55	19	2
1:A:102:GLN:HE21	1:A:105:TRP:HE1	0.61	1.38	2	1
1:A:153:GLN:NE2	1:A:164:SER:N	0.61	2.47	7	1
1:A:175:ASN:ND2	1:A:179:ASP:H	0.61	1.94	4	4
1:A:89:PHE:CE2	1:A:153:GLN:NE2	0.61	2.68	10	1
1:A:151:VAL:HG11	1:A:167:PHE:CZ	0.61	2.31	11	4
1:A:87:MET:SD	1:A:89:PHE:CZ	0.61	2.94	3	10
1:A:162:VAL:HG12	1:A:192:GLN:O	0.60	1.96	5	2
1:A:151:VAL:HG11	1:A:167:PHE:CE1	0.60	2.31	15	1
1:A:148:LEU:HD21	2:B:489:PHE:CE1	0.60	2.30	12	2
1:A:153:GLN:HE22	1:A:164:SER:H	0.60	1.40	7	2
1:A:87:MET:SD	1:A:153:GLN:NE2	0.60	2.75	19	2
1:A:148:LEU:HD23	1:A:149:TYR:N	0.60	2.12	2	7
2:B:491:LEU:N	2:B:491:LEU:CD2	0.60	2.65	5	20
1:A:175:ASN:OD1	1:A:182:LEU:HD21	0.60	1.96	12	1
1:A:149:TYR:CD1	1:A:171:ALA:HB3	0.59	2.32	8	9
1:A:87:MET:SD	1:A:89:PHE:CE1	0.59	2.95	5	5
1:A:153:GLN:HE22	1:A:164:SER:N	0.59	1.96	7	1
1:A:67:THR:O	1:A:67:THR:HG23	0.59	1.97	16	8
1:A:54:ARG:N	1:A:54:ARG:CD	0.58	2.66	8	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:GLY:O	1:A:158:ALA:HB2	0.58	1.97	18	1
1:A:175:ASN:OD1	1:A:179:ASP:N	0.58	2.37	5	7
1:A:162:VAL:N	1:A:192:GLN:O	0.58	2.36	3	9
1:A:165:GLN:HE22	1:A:192:GLN:NE2	0.58	1.97	10	1
1:A:79:ILE:CG2	1:A:81:LEU:HD13	0.58	2.29	4	6
1:A:63:MET:SD	1:A:64:GLY:N	0.58	2.76	16	4
1:A:113:LEU:HD12	1:A:113:LEU:C	0.58	2.19	18	1
2:B:491:LEU:N	2:B:492:PRO:CD	0.57	2.67	15	16
1:A:93:ARG:NH2	1:A:147:ALA:CB	0.57	2.67	11	2
1:A:54:ARG:HE	1:A:54:ARG:CA	0.57	2.12	19	1
1:A:94:VAL:CG1	1:A:97:ILE:HD12	0.57	2.28	11	4
1:A:175:ASN:ND2	1:A:179:ASP:O	0.57	2.37	13	17
1:A:175:ASN:ND2	1:A:177:THR:OG1	0.57	2.38	13	5
1:A:174:THR:OG1	2:B:487:ALA:HB2	0.56	1.99	3	1
1:A:61:ALA:O	1:A:62:LEU:HD22	0.56	1.99	17	5
1:A:76:LEU:HD23	1:A:76:LEU:H	0.56	1.59	14	1
1:A:102:GLN:O	1:A:105:TRP:NE1	0.56	2.39	15	7
1:A:91:LEU:CD2	1:A:151:VAL:HG22	0.55	2.32	14	7
1:A:118:THR:HG23	1:A:119:ASN:N	0.55	2.16	2	2
1:A:153:GLN:NE2	1:A:166:PRO:N	0.55	2.54	1	1
1:A:128:LYS:H	1:A:128:LYS:CD	0.55	2.14	20	1
1:A:148:LEU:HD23	1:A:148:LEU:C	0.55	2.21	4	6
1:A:54:ARG:CA	1:A:54:ARG:NE	0.55	2.70	19	2
1:A:122:PRO:HB3	1:A:126:VAL:HG21	0.55	1.79	10	5
1:A:99:LEU:HD11	1:A:147:ALA:O	0.55	2.00	13	1
1:A:65:LEU:HD21	1:A:192:GLN:OE1	0.55	2.00	6	2
1:A:76:LEU:HD23	1:A:76:LEU:N	0.55	2.17	14	1
1:A:99:LEU:HD21	1:A:170:ALA:HB1	0.55	1.77	2	1
1:A:153:GLN:NE2	1:A:164:SER:OG	0.55	2.40	8	6
1:A:57:ILE:HD11	1:A:171:ALA:HB2	0.55	1.78	8	4
1:A:89:PHE:CE2	1:A:153:GLN:OE1	0.55	2.60	17	4
1:A:59:VAL:HG12	1:A:139:ALA:HB3	0.55	1.79	13	3
1:A:153:GLN:NE2	1:A:165:GLN:O	0.55	2.39	20	2
1:A:164:SER:CB	1:A:192:GLN:HE21	0.54	2.15	6	1
1:A:64:GLY:N	1:A:191:HIS:O	0.54	2.41	14	2
1:A:108:ALA:HB1	2:B:489:PHE:CE1	0.54	2.37	14	3
1:A:153:GLN:O	1:A:163:ARG:NH2	0.54	2.41	15	1
1:A:85:ASP:OD1	1:A:86:GLY:N	0.54	2.40	14	3
1:A:155:LEU:HD22	1:A:163:ARG:HH22	0.54	1.63	6	1
1:A:192:GLN:NE2	1:A:193:ALA:O	0.54	2.41	8	1
1:A:153:GLN:N	1:A:153:GLN:OE1	0.54	2.41	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:ASN:OD1	1:A:178:GLY:N	0.54	2.41	5	7
1:A:54:ARG:HE	1:A:54:ARG:N	0.54	2.00	19	1
1:A:62:LEU:O	1:A:191:HIS:CG	0.53	2.61	13	9
1:A:88:SER:OG	1:A:133:LYS:NZ	0.53	2.42	19	2
1:A:170:ALA:O	1:A:173:GLN:NE2	0.53	2.41	2	1
1:A:62:LEU:O	1:A:191:HIS:ND1	0.53	2.41	2	10
1:A:77:ASP:OD1	1:A:78:SER:N	0.53	2.42	5	2
1:A:91:LEU:HD11	1:A:141:PHE:CD1	0.53	2.38	17	1
1:A:155:LEU:N	1:A:155:LEU:CD2	0.53	2.64	2	1
1:A:155:LEU:H	1:A:155:LEU:HD23	0.53	1.64	8	3
1:A:85:ASP:OD1	1:A:137:GLY:N	0.53	2.42	12	2
1:A:165:GLN:OE1	1:A:192:GLN:NE2	0.53	2.42	10	1
1:A:157:GLY:O	1:A:158:ALA:CB	0.53	2.57	18	1
1:A:91:LEU:HD21	1:A:151:VAL:HG22	0.52	1.80	20	5
1:A:156:ASN:OD1	1:A:157:GLY:N	0.52	2.42	4	1
1:A:148:LEU:HD13	2:B:489:PHE:CD1	0.52	2.39	14	1
1:A:86:GLY:N	1:A:134:THR:O	0.52	2.42	7	1
1:A:113:LEU:O	1:A:117:TYR:N	0.52	2.43	15	10
1:A:61:ALA:HB1	1:A:191:HIS:CE1	0.52	2.39	18	6
1:A:122:PRO:CB	1:A:126:VAL:HG21	0.52	2.34	10	5
1:A:158:ALA:O	1:A:161:VAL:HG22	0.52	2.04	20	1
1:A:99:LEU:HD23	1:A:147:ALA:O	0.52	2.04	1	1
1:A:162:VAL:HG22	1:A:163:ARG:N	0.52	2.19	6	2
1:A:148:LEU:HD13	2:B:489:PHE:CE1	0.52	2.38	11	1
1:A:93:ARG:NH2	1:A:149:TYR:OH	0.52	2.43	20	1
1:A:94:VAL:HG11	1:A:97:ILE:HD12	0.52	1.82	20	3
1:A:60:HIS:CD2	1:A:188:TYR:CZ	0.52	2.97	15	11
1:A:175:ASN:ND2	1:A:177:THR:H	0.52	2.03	4	1
1:A:72:ASN:HD22	1:A:76:LEU:HD13	0.52	1.65	12	1
1:A:72:ASN:ND2	1:A:76:LEU:HD22	0.52	2.20	7	1
1:A:148:LEU:HD11	2:B:489:PHE:CE1	0.52	2.39	20	3
1:A:153:GLN:CD	1:A:153:GLN:H	0.52	2.07	1	1
1:A:128:LYS:NZ	1:A:131:THR:OG1	0.52	2.43	17	2
1:A:153:GLN:NE2	1:A:164:SER:O	0.51	2.43	1	2
1:A:134:THR:HG22	1:A:139:ALA:HB2	0.51	1.81	7	1
1:A:93:ARG:N	1:A:127:THR:O	0.51	2.43	7	3
1:A:153:GLN:CD	1:A:164:SER:HG	0.51	2.09	9	1
1:A:63:MET:H	1:A:81:LEU:HD11	0.51	1.65	14	1
1:A:164:SER:OG	1:A:192:GLN:NE2	0.50	2.44	6	2
1:A:62:LEU:O	1:A:191:HIS:N	0.50	2.44	6	2
1:A:99:LEU:HD11	1:A:170:ALA:HB1	0.50	1.84	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:GLN:NE2	1:A:165:GLN:C	0.50	2.65	1	3
1:A:150:LEU:HD13	1:A:168:LEU:CD1	0.50	2.37	19	1
1:A:93:ARG:O	1:A:127:THR:N	0.49	2.45	8	3
1:A:91:LEU:N	1:A:91:LEU:CD2	0.49	2.75	10	1
1:A:155:LEU:H	1:A:155:LEU:CD2	0.49	2.19	8	3
1:A:76:LEU:N	1:A:76:LEU:CD2	0.49	2.75	14	1
1:A:162:VAL:HG11	1:A:192:GLN:NE2	0.49	2.22	15	1
1:A:63:MET:SD	1:A:63:MET:C	0.49	2.91	16	10
1:A:118:THR:CG2	1:A:119:ASN:N	0.49	2.76	2	1
1:A:57:ILE:HD11	1:A:171:ALA:CB	0.49	2.37	8	2
1:A:123:THR:OG1	1:A:124:ASP:N	0.49	2.42	12	7
1:A:110:LYS:O	1:A:110:LYS:NZ	0.49	2.42	1	2
1:A:175:ASN:HD22	1:A:180:GLY:C	0.48	2.12	12	2
1:A:128:LYS:CD	1:A:128:LYS:O	0.48	2.61	2	1
1:A:116:LEU:HD12	1:A:116:LEU:C	0.48	2.28	19	1
1:A:175:ASN:ND2	1:A:179:ASP:N	0.48	2.60	4	4
1:A:112:LYS:O	1:A:115:GLU:N	0.48	2.41	18	4
1:A:65:LEU:CD1	1:A:192:GLN:OE1	0.48	2.62	1	1
1:A:175:ASN:ND2	1:A:178:GLY:H	0.48	2.07	6	1
1:A:165:GLN:NE2	1:A:192:GLN:NE2	0.48	2.61	10	1
1:A:170:ALA:HB3	1:A:173:GLN:HE22	0.48	1.67	2	1
1:A:165:GLN:N	1:A:165:GLN:CD	0.48	2.67	19	10
1:A:62:LEU:CD1	1:A:81:LEU:O	0.48	2.61	5	1
1:A:112:LYS:C	1:A:114:GLU:N	0.48	2.67	18	7
1:A:134:THR:HG23	1:A:138:VAL:C	0.48	2.28	10	12
1:A:148:LEU:HD22	2:B:489:PHE:CE1	0.48	2.43	14	1
1:A:91:LEU:HD11	1:A:141:PHE:CG	0.47	2.44	19	3
1:A:79:ILE:HD12	1:A:79:ILE:H	0.47	1.69	18	1
1:A:81:LEU:O	1:A:83:LYS:CD	0.47	2.62	18	1
1:A:87:MET:SD	1:A:153:GLN:OE1	0.47	2.72	19	1
1:A:175:ASN:ND2	1:A:177:THR:N	0.47	2.62	4	1
1:A:155:LEU:HD13	1:A:163:ARG:NH2	0.47	2.24	6	1
1:A:62:LEU:O	1:A:191:HIS:CE1	0.47	2.67	17	3
1:A:116:LEU:O	1:A:123:THR:HG23	0.47	2.09	20	1
1:A:81:LEU:C	1:A:81:LEU:CD1	0.47	2.82	14	2
1:A:175:ASN:HD21	1:A:178:GLY:N	0.47	2.08	6	2
1:A:98:ASP:OD1	1:A:100:THR:CG2	0.47	2.62	11	2
1:A:175:ASN:OD1	1:A:182:LEU:CD2	0.47	2.61	12	1
1:A:108:ALA:O	1:A:111:ILE:CG1	0.47	2.62	3	5
1:A:59:VAL:CG1	1:A:59:VAL:O	0.47	2.62	5	3
1:A:167:PHE:CE1	1:A:187:VAL:HG11	0.47	2.45	11	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:MET:O	1:A:81:LEU:HD11	0.47	2.10	13	1
1:A:175:ASN:ND2	1:A:180:GLY:C	0.47	2.68	1	1
1:A:174:THR:OG1	2:B:487:ALA:HB1	0.47	2.10	11	1
1:A:62:LEU:N	1:A:191:HIS:CE1	0.47	2.83	18	1
1:A:148:LEU:CD1	2:B:489:PHE:CE2	0.47	2.98	4	1
1:A:71:ALA:HB1	2:B:492:PRO:HA	0.47	1.87	8	2
1:A:115:GLU:CD	1:A:115:GLU:N	0.46	2.68	2	1
1:A:173:GLN:HE21	1:A:185:VAL:HG22	0.46	1.70	13	2
1:A:170:ALA:HB2	2:B:489:PHE:CD1	0.46	2.45	3	3
1:A:113:LEU:O	1:A:117:TYR:O	0.46	2.34	11	12
1:A:93:ARG:HH22	1:A:147:ALA:CB	0.46	2.23	11	1
2:B:489:PHE:O	2:B:490:GLU:CB	0.46	2.63	14	1
1:A:174:THR:OG1	2:B:487:ALA:CB	0.46	2.64	17	1
1:A:184:ASP:OD2	1:A:186:HIS:NE2	0.46	2.49	5	1
1:A:162:VAL:CG2	1:A:163:ARG:N	0.46	2.79	6	1
1:A:175:ASN:ND2	1:A:175:ASN:C	0.46	2.66	6	1
1:A:130:ALA:HB1	1:A:132:LYS:NZ	0.46	2.26	15	2
1:A:87:MET:SD	1:A:89:PHE:CE2	0.46	3.09	12	4
1:A:88:SER:OG	1:A:133:LYS:CD	0.46	2.64	12	1
1:A:56:SER:CB	1:A:140:LYS:HZ2	0.45	2.24	5	1
1:A:112:LYS:O	1:A:114:GLU:N	0.45	2.49	18	2
1:A:187:VAL:HG12	1:A:189:PRO:HD3	0.45	1.88	5	10
1:A:188:TYR:O	2:B:494:THR:O	0.45	2.34	12	4
1:A:110:LYS:O	1:A:110:LYS:CG	0.45	2.65	15	2
1:A:158:ALA:O	1:A:161:VAL:O	0.45	2.34	16	6
1:A:148:LEU:HD22	2:B:489:PHE:CZ	0.45	2.46	14	1
1:A:108:ALA:O	2:B:489:PHE:CZ	0.45	2.69	9	1
1:A:150:LEU:HD12	1:A:167:PHE:O	0.45	2.12	19	1
1:A:87:MET:SD	1:A:87:MET:C	0.45	2.95	3	4
1:A:184:ASP:O	1:A:184:ASP:OD1	0.45	2.35	20	5
1:A:99:LEU:CD1	1:A:147:ALA:O	0.45	2.65	12	1
1:A:55:THR:OG1	1:A:144:LEU:O	0.45	2.32	14	2
1:A:60:HIS:HD1	1:A:138:VAL:HG22	0.45	1.71	12	1
1:A:101:THR:HG22	1:A:103:ALA:H	0.45	1.72	15	1
1:A:77:ASP:O	1:A:77:ASP:OD1	0.44	2.35	1	3
1:A:153:GLN:OE1	1:A:164:SER:OG	0.44	2.36	7	3
1:A:168:LEU:CD1	2:B:490:GLU:OE1	0.44	2.65	10	1
1:A:170:ALA:HB3	1:A:173:GLN:NE2	0.44	2.27	2	1
1:A:133:LYS:O	1:A:135:GLU:OE1	0.44	2.36	3	1
1:A:56:SER:OG	1:A:184:ASP:OD1	0.44	2.36	1	3
1:A:175:ASN:OD1	1:A:178:GLY:CA	0.44	2.66	15	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ARG:NH1	1:A:129:VAL:HG13	0.44	2.27	14	2
1:A:113:LEU:C	1:A:113:LEU:CD1	0.44	2.85	18	1
1:A:153:GLN:OE1	1:A:164:SER:O	0.44	2.36	14	1
1:A:113:LEU:HD11	2:B:490:GLU:OE2	0.44	2.13	4	1
1:A:158:ALA:CB	1:A:161:VAL:HG13	0.44	2.42	7	2
1:A:175:ASN:CG	1:A:177:THR:H	0.44	2.17	4	1
1:A:162:VAL:CG1	1:A:192:GLN:HE21	0.44	2.25	14	1
1:A:161:VAL:HG23	1:A:162:VAL:N	0.44	2.28	15	1
1:A:81:LEU:HD12	1:A:81:LEU:O	0.43	2.12	14	2
1:A:174:THR:HG23	1:A:181:TRP:CZ3	0.43	2.48	6	1
1:A:124:ASP:O	1:A:124:ASP:OD1	0.43	2.36	11	1
1:A:153:GLN:HE21	1:A:164:SER:C	0.43	2.15	11	2
1:A:158:ALA:HB1	1:A:161:VAL:HG23	0.43	1.90	8	1
1:A:155:LEU:CD2	1:A:155:LEU:H	0.43	2.26	2	1
1:A:169:VAL:O	1:A:169:VAL:CG2	0.43	2.65	19	3
1:A:87:MET:SD	1:A:88:SER:O	0.43	2.76	5	1
1:A:175:ASN:OD1	1:A:177:THR:OG1	0.43	2.36	6	1
1:A:117:TYR:OH	1:A:152:VAL:HG13	0.43	2.13	12	1
1:A:184:ASP:OD1	1:A:185:VAL:N	0.43	2.51	4	1
1:A:56:SER:HA	1:A:144:LEU:HD12	0.43	1.91	4	3
1:A:67:THR:O	1:A:67:THR:OG1	0.43	2.37	17	1
1:A:174:THR:CG2	1:A:181:TRP:CZ3	0.43	3.02	3	6
1:A:90:THR:OG1	1:A:154:GLU:OE2	0.43	2.36	9	1
2:B:489:PHE:O	2:B:490:GLU:OE1	0.43	2.36	15	1
1:A:163:ARG:O	1:A:163:ARG:CG	0.42	2.66	4	1
1:A:162:VAL:O	1:A:192:GLN:O	0.42	2.36	7	1
1:A:94:VAL:HG21	1:A:148:LEU:HD23	0.42	1.89	15	2
1:A:151:VAL:CG1	1:A:167:PHE:CE1	0.42	3.01	15	1
1:A:157:GLY:O	1:A:158:ALA:HB3	0.42	2.14	16	1
1:A:61:ALA:N	1:A:137:GLY:O	0.42	2.47	16	2
1:A:155:LEU:HD22	1:A:163:ARG:NH2	0.42	2.28	6	1
1:A:192:GLN:N	1:A:192:GLN:CD	0.42	2.72	16	1
1:A:110:LYS:O	1:A:110:LYS:CD	0.42	2.68	15	2
1:A:94:VAL:HG23	1:A:94:VAL:O	0.42	2.14	4	1
1:A:114:GLU:O	1:A:118:THR:HG21	0.42	2.15	11	1
1:A:105:TRP:O	1:A:109:SER:OG	0.42	2.37	5	2
1:A:174:THR:CG2	1:A:181:TRP:CH2	0.42	3.02	6	1
1:A:97:ILE:HD12	1:A:108:ALA:HB2	0.42	1.91	15	1
1:A:116:LEU:HD12	1:A:116:LEU:O	0.42	2.15	19	1
1:A:175:ASN:ND2	1:A:175:ASN:O	0.42	2.53	6	1
1:A:144:LEU:HD22	1:A:149:TYR:CE2	0.42	2.50	17	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LYS:CD	1:A:128:LYS:N	0.41	2.83	1	1
1:A:155:LEU:HD22	1:A:163:ARG:HD2	0.41	1.91	2	1
1:A:97:ILE:HG13	1:A:108:ALA:HB2	0.41	1.92	9	1
1:A:81:LEU:HD12	1:A:82:PRO:O	0.41	2.16	13	1
1:A:155:LEU:O	1:A:156:ASN:C	0.41	2.59	4	1
1:A:133:LYS:O	1:A:135:GLU:CD	0.41	2.58	3	1
1:A:153:GLN:OE1	1:A:165:GLN:O	0.41	2.37	15	2
1:A:54:ARG:CA	1:A:54:ARG:HE	0.41	2.29	13	1
1:A:93:ARG:NH2	1:A:145:THR:CG2	0.41	2.83	2	1
1:A:157:GLY:O	1:A:158:ALA:C	0.41	2.58	12	3
1:A:65:LEU:HD21	1:A:192:GLN:CG	0.41	2.46	18	1
1:A:105:TRP:O	1:A:109:SER:CB	0.41	2.69	7	1
1:A:162:VAL:HG11	1:A:192:GLN:HE21	0.41	1.75	15	1
1:A:89:PHE:CZ	1:A:153:GLN:OE1	0.41	2.74	17	1
1:A:117:TYR:CE2	1:A:120:GLY:C	0.41	2.94	19	1
1:A:65:LEU:HD21	1:A:192:GLN:HG2	0.41	1.92	3	2
1:A:77:ASP:O	1:A:78:SER:C	0.41	2.59	10	1
1:A:174:THR:HG22	1:A:181:TRP:CZ3	0.41	2.51	15	1
1:A:158:ALA:HB1	1:A:161:VAL:O	0.41	2.16	16	1
1:A:55:THR:HG22	1:A:56:SER:N	0.41	2.31	18	1
1:A:153:GLN:HE22	1:A:164:SER:CA	0.41	2.29	7	1
1:A:151:VAL:HG11	1:A:167:PHE:CE2	0.40	2.51	11	1
1:A:90:THR:N	1:A:154:GLU:OE2	0.40	2.54	15	1
1:A:175:ASN:OD1	1:A:179:ASP:O	0.40	2.40	6	1
1:A:158:ALA:HB1	1:A:161:VAL:CG1	0.40	2.46	12	1
1:A:170:ALA:C	1:A:173:GLN:HE21	0.40	2.20	2	1
1:A:57:ILE:HD11	1:A:149:TYR:CD1	0.40	2.52	3	1
1:A:148:LEU:C	1:A:148:LEU:CD2	0.40	2.88	4	1
1:A:165:GLN:NE2	1:A:192:GLN:HE22	0.40	2.15	10	1
1:A:106:ASP:O	1:A:109:SER:OG	0.40	2.38	16	1
1:A:150:LEU:HD12	1:A:151:VAL:N	0.40	2.31	19	1

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 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	A	140/143 (98%)	132±1 (94±1%)	7±1 (5±1%)	1±0 (1±0%)	24	71
2	B	7/10 (70%)	4±1 (64±8%)	2±1 (35±8%)	0±0 (1±4%)	15	61
All	All	2940/3060 (96%)	2727 (93%)	189 (6%)	24 (1%)	24	71

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	147	ALA	20
2	B	487	ALA	2
1	A	157	GLY	1
1	A	158	ALA	1

5.3.2 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	A	114/117 (97%)	104±3 (91±2%)	10±3 (9±2%)	13	60
2	B	6/8 (75%)	3±0 (52±5%)	3±0 (48±5%)	0	1
All	All	2400/2500 (96%)	2140 (89%)	260 (11%)	10	54

All 42 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	491	LEU	20
2	B	494	THR	20
1	A	118	THR	18
1	A	168	LEU	18
2	B	489	PHE	18
1	A	54	ARG	16
1	A	169	VAL	14
1	A	87	MET	13
1	A	123	THR	12
1	A	110	LYS	9
1	A	117	TYR	8
1	A	105	TRP	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	112	LYS	7
1	A	155	LEU	7
1	A	55	THR	7
1	A	67	THR	7
1	A	128	LYS	5
1	A	191	HIS	5
1	A	153	GLN	4
1	A	63	MET	4
1	A	116	LEU	4
1	A	125	LYS	3
1	A	186	HIS	3
1	A	192	GLN	3
1	A	132	LYS	2
1	A	74	THR	2
1	A	96	GLU	2
1	A	175	ASN	2
1	A	76	LEU	2
1	A	161	VAL	2
1	A	148	LEU	2
1	A	163	ARG	2
1	A	75	LYS	2
1	A	115	GLU	1
1	A	98	ASP	1
1	A	164	SER	1
1	A	151	VAL	1
1	A	154	GLU	1
1	A	162	VAL	1
1	A	83	LYS	1
1	A	113	LEU	1
1	A	174	THR	1

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such molecules in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

CHEMICAL-SHIFTS INFOmissingINFO