Full wwPDB NMR Structure Validation Report (i)

Mar 7, 2022 – 04:22 AM EST

PDB ID	:	2YSZ
Title	:	Solution structure of the chimera of the C-terminal PID domain of Fe65L and the C-terminal tail peptide of APP
Authors	:	Li, H.; Koshiba, S.; Watanabe, S.; Harada, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-05

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 (i) symbol.

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

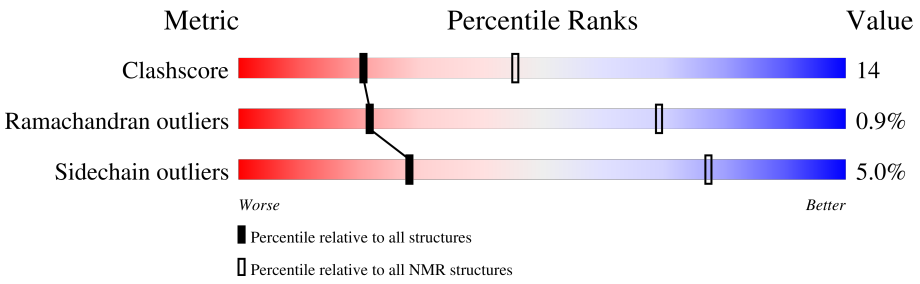
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	185	51% 16% • 32%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:15-A:103, A:107-A:130, A:163-A:174 (125)	0.23	10

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2718 atoms, of which 1322 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	185	2718	857	1322	240	287	12	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9DBR4
A	2	SER	-	expression tag	UNP Q9DBR4
A	3	SER	-	expression tag	UNP Q9DBR4
A	4	GLY	-	expression tag	UNP Q9DBR4
A	5	SER	-	expression tag	UNP Q9DBR4
A	6	SER	-	expression tag	UNP Q9DBR4
A	7	GLY	-	expression tag	UNP Q9DBR4
A	131	SER	-	linker	UNP Q9DBR4
A	132	GLY	-	linker	UNP Q9DBR4
A	133	PRO	-	linker	UNP Q9DBR4
A	134	SER	-	linker	UNP Q9DBR4
A	135	SER	-	linker	UNP Q9DBR4
A	136	GLY	-	linker	UNP Q9DBR4
A	137	ILE	-	linker	UNP Q9DBR4
A	138	GLU	-	linker	UNP Q9DBR4
A	139	GLY	-	linker	UNP Q9DBR4
A	140	ARG	-	linker	UNP Q9DBR4
A	141	GLY	-	linker	UNP Q9DBR4
A	142	SER	-	linker	UNP Q9DBR4
A	143	SER	-	linker	UNP Q9DBR4
A	144	GLY	-	linker	UNP Q9DBR4
A	145	SER	-	linker	UNP Q9DBR4
A	146	SER	-	linker	UNP Q9DBR4
A	147	GLY	-	linker	UNP Q9DBR4
A	148	SER	-	linker	UNP Q9DBR4
A	149	SER	-	linker	UNP Q9DBR4
A	150	GLY	-	linker	UNP Q9DBR4
A	151	SER	-	linker	UNP Q9DBR4
A	152	SER	-	linker	UNP Q9DBR4
A	153	GLY	-	linker	UNP Q9DBR4

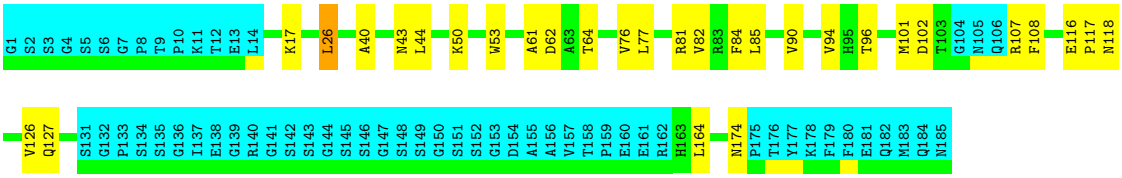
4 Residue-property plots (i)

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: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 51% 16% • 32%



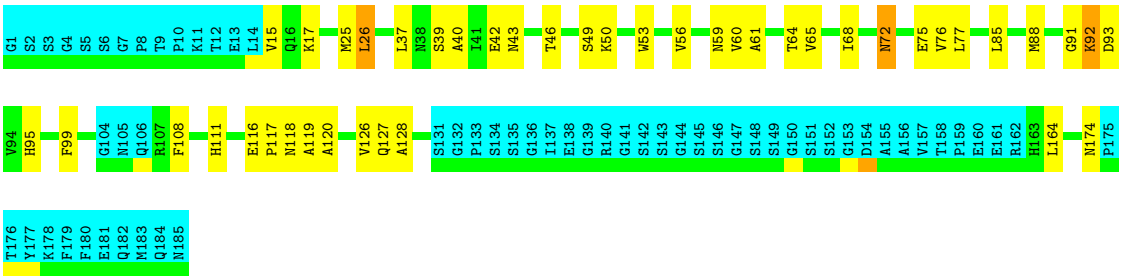
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

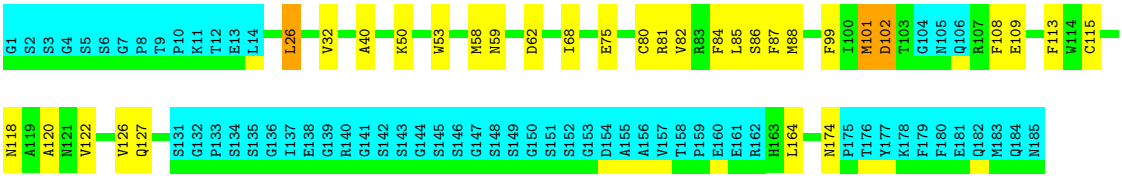
Chain A: 44% 22% • 32%



4.2.2 Score per residue for model 2

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

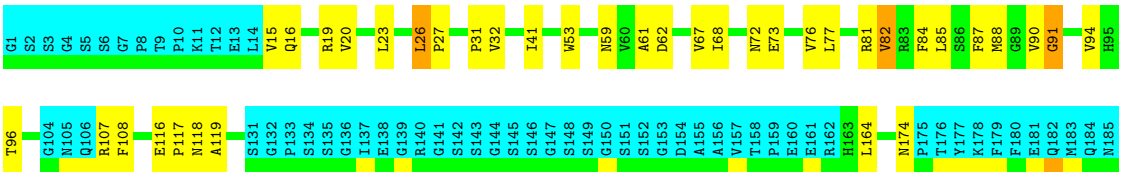
Chain A: 50% 16% • 32%



4.2.3 Score per residue for model 3

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

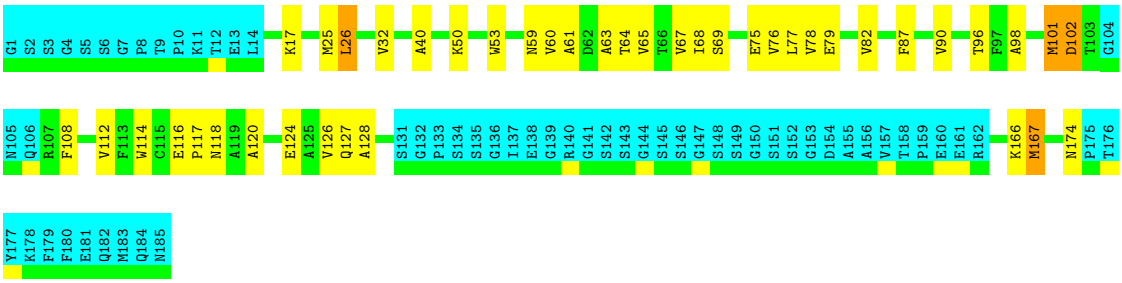
Chain A: 47% 19% • 32%



4.2.4 Score per residue for model 4

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 45% 21% • 32%



4.2.5 Score per residue for model 5

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 42% 24% • 32%

G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 K17 L23 G24 M25 L26 V32 N38 S39 A40 I41 L44 M45 T46 S47 N59 V60 A61 D62 A63 T64 I68 S69 E70 E75 V76 L77 V78 E79 C80 R81 V82 R83 F84 F87 V90

V94 H95 T96 F99 I100 M101 D102 T103 G104 N105 Q106 R107 F108 H111 V112 E116 P117 N118 A119 A120 E124 A125 V126 Q127 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161

R162 H163 L164 Y172 E173 N174 P175 T176 Y177 K178 F179 F180 E181 Q182 M183 Q184 N185

4.2.6 Score per residue for model 6

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 48% 19% • 32%

G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 K17 L23 L26 D29 R30 P31 V32 L37 A40 I41 E42 N43 L44 M45 S49 K50 W53 I68 E73 R81 V82 R83 F84 L85 S86 F87 T96 F97 A98 F99 G104 N105 Q106

R107 F108 H111 V112 F113 W114 C115 E116 P117 N118 V126 Q127 C130 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161 R162 N174 P175 T176 Y177 K178 F179 F180 E181 Q182 M183 Q184

N185

4.2.7 Score per residue for model 7

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 43% 23% • 32%

G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 K17 F18 R19 V20 L23 L26 P31 A40 I41 E42 N43 L44 M45 S48 S49 K50 W53 N57 V60 A61 T64 V65 I68 S69 E73 E74 E75 V76 L77 V78 E79 C80 R81 V82

V90 V94 H95 T96 F99 D102 T103 G104 N105 Q106 R107 F108 V112 C115 E116 P117 N118 V122 V126 Q127 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161

R162 H163 L164 P175 T176 Y177 K178 F179 F180 E181 Q182 M183 Q184 N185

4.2.8 Score per residue for model 8

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 45% 22% • 32%

G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 V15 Q16 K17 L26 M34 L37 N38 S39 A40 I41 E42 N43 L44 S47 S48 S49 K50 W53 A61 T64 V65 E70 V78 E79 C80 R81 F84 L85 K92 D93 V94 H95 A98

G104 N105 Q106 R107 F108 V112 C115 E116 P117 N118 V122 Q127 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161 R162 H163 L164 M167 Y172 E173 N174 P175 T176 Y177

K178 F179 F180 E181 Q182 M183 Q184 N185

4.2.9 Score per residue for model 9

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 45% 21% • 32%

G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 V15 Q16 K17 F18 R19 V20 L23 L26 P27 P31 M34 D52 N59 V60 A61 D62 A63 T64 V65 T66 V76 L77 V78 E79 C80 R81 V82 R83 F84 L85 M88 V94 H95 M101 G104

N105 Q106 R107 F108 H111 V112 F113 W114 C115 E116 P117 N118 A125 V126 Q127 A128 A129 C130 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161 R162 H163 L164 N174 P175 T176 Y177 K178

F179 F180 E181 Q182 M183 Q184 N185

4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 48% 18% • 32%

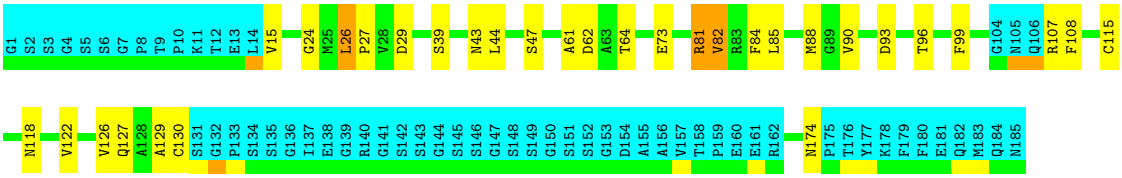
G1 S2 S3 G4 S5 S6 G7 P8 T9 P10 K11 T12 E13 L14 V15 Q16 K17 F18 L23 L26 M34 N38 V60 A61 D62 A63 T64 V65 V82 R83 F84 L85 V90 G91 K92 D93 V94 A98 D102 T103 G104 N105 Q106 R107 F108 V112 E116 P117 N118

V126 Q127 A128 A129 C130 S131 G132 P133 S134 S135 G136 I137 E138 G139 R140 G141 S142 S143 G144 S145 S146 G147 S148 S149 G150 S151 S152 G153 D154 A155 A156 V157 T158 P159 E160 E161 R162 H163 L164 S165 K166 M167 Q168 Q169 N170 N174 P175 T176 Y177 K178 F179 F180 E181 Q182 M183 Q184 N185

4.2.11 Score per residue for model 11

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

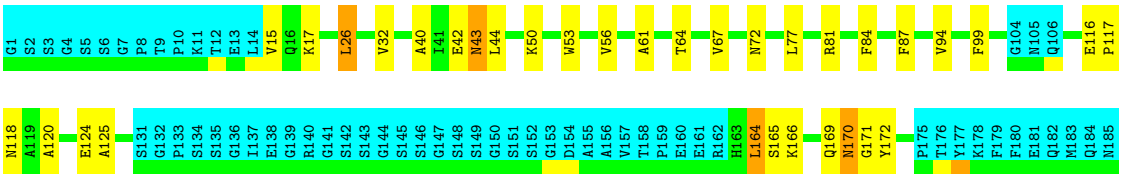
Chain A: 50% 16% • 32%



4.2.12 Score per residue for model 12

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

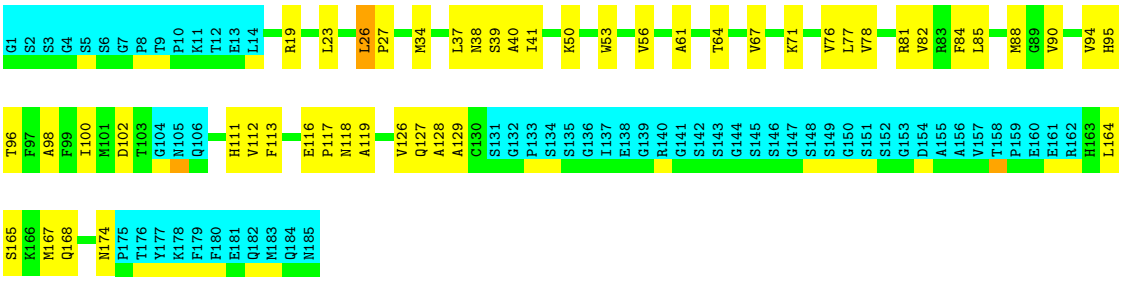
Chain A: 49% 16% • 32%



4.2.13 Score per residue for model 13

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

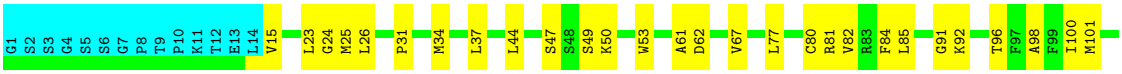
Chain A: 42% 25% • 32%

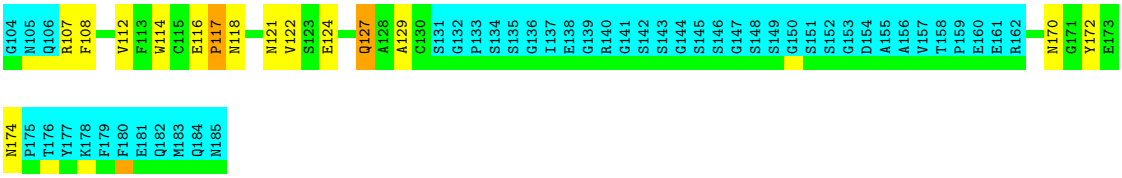


4.2.14 Score per residue for model 14

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 44% 22% • 32%





4.2.15 Score per residue for model 15

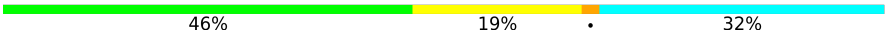
• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

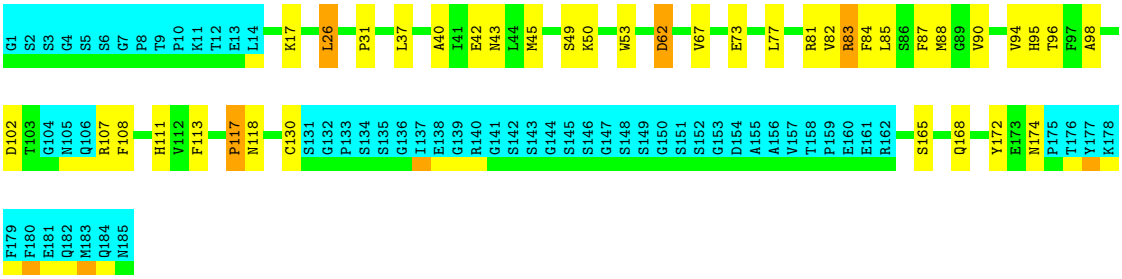
Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A:

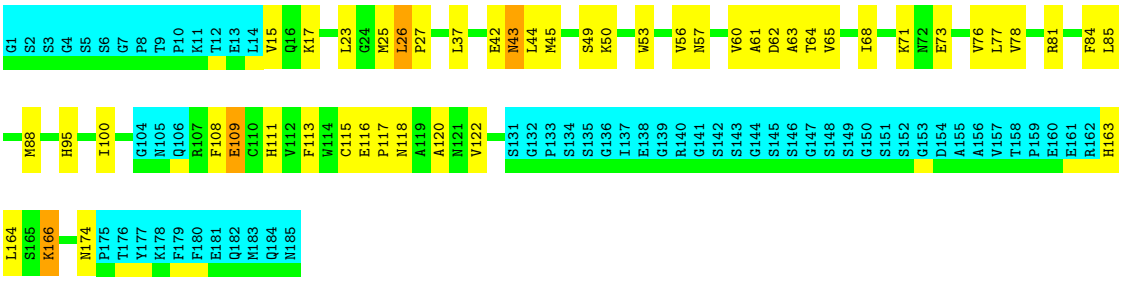




4.2.17 Score per residue for model 17

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

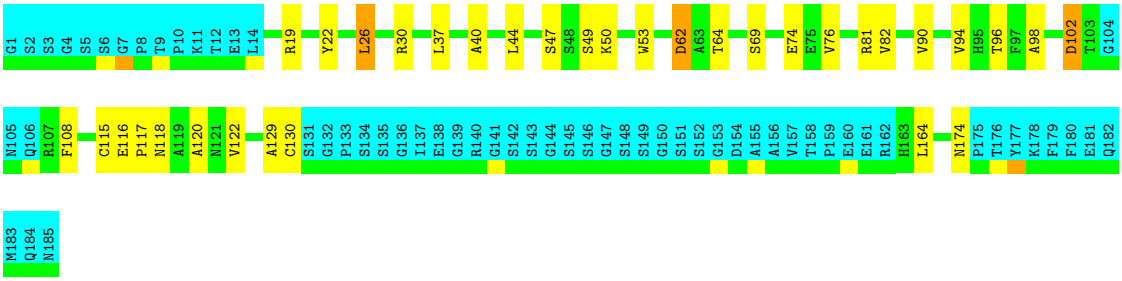
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

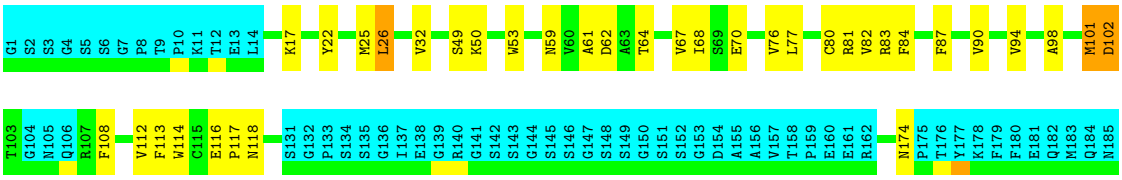
Chain A: 49% 17% • 32%



4.2.19 Score per residue for model 19

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 48% 18% • 32%



4.2.20 Score per residue for model 20

• Molecule 1: Amyloid beta A4 precursor protein-binding family B member 2 and Amyloid beta A4 protein

Chain A: 43% 23% • 32%

G1
S2
S3
G4
S5
S6
G7
P8
T9
P10
K11
T12
E13
L14
L23
G24
M25
L26
A40
I41
E42
N43
L44
M45
T46
K50
W53
N57
A61
T64
V67
I68
S69
V76
L77
V82
L85
M88
G89
V90
G91
K92
D93
V94
H95
T96
M101
D102
T103
G104
N105
Q106
R107
F108
V112
E116
P117
N118
A119
A120
V126
C130
S131
G132
P133
S134
S135
G136
I137
E138
G139
R140
G141
S142
S143
G144
S145
S146
G147
S148
S149
G150
S151
S152
G153
D154
A155
A156
V157
T158
P159
E160
E161
R162
H163
L164
S165
K166
M167
Q168
G171
Y172
E173
N174
P175
T176
Y177
K178
F179
F180
E181
Q182
M183
Q184
N185

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	984	949	948	26±6
All	All	19680	18980	18960	522

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD13	1:A:112:VAL:HG12	0.89	1.43	13	6
1:A:62:ASP:O	1:A:129:ALA:HB1	0.82	1.74	18	5
1:A:37:LEU:HD21	1:A:98:ALA:HB3	0.76	1.57	13	6
1:A:90:VAL:HG13	1:A:96:THR:O	0.72	1.83	20	10
1:A:26:LEU:HB3	1:A:40:ALA:HB1	0.68	1.65	1	11
1:A:59:ASN:ND2	1:A:68:ILE:HD12	0.68	2.04	19	7
1:A:67:VAL:HG12	1:A:77:LEU:HD12	0.67	1.64	4	7
1:A:32:VAL:HG12	1:A:87:PHE:HB2	0.66	1.67	2	7
1:A:82:VAL:HG21	1:A:129:ALA:HB1	0.64	1.68	15	1
1:A:120:ALA:HB2	1:A:164:LEU:HD11	0.63	1.68	20	1
1:A:119:ALA:C	1:A:164:LEU:HD21	0.63	2.14	5	4
1:A:15:VAL:HG22	1:A:61:ALA:HB2	0.63	1.69	14	2
1:A:76:VAL:O	1:A:76:VAL:HG13	0.62	1.93	4	6
1:A:64:THR:HG23	1:A:81:ARG:HG3	0.62	1.70	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:VAL:HG12	1:A:115:CYS:HA	0.62	1.71	9	2
1:A:68:ILE:HG23	1:A:73:GLU:O	0.62	1.94	7	2
1:A:37:LEU:HD12	1:A:100:ILE:CD1	0.61	2.26	17	2
1:A:56:VAL:HG11	1:A:77:LEU:CD1	0.61	2.25	12	4
1:A:94:VAL:HB	1:A:164:LEU:HD22	0.60	1.70	13	4
1:A:60:VAL:HG13	1:A:65:VAL:HG22	0.60	1.72	1	5
1:A:25:MET:SD	1:A:111:HIS:CE1	0.60	2.95	5	1
1:A:95:HIS:CD2	1:A:117:PRO:O	0.60	2.55	16	8
1:A:109:GLU:OE2	1:A:111:HIS:CE1	0.59	2.55	17	1
1:A:76:VAL:O	1:A:76:VAL:HG22	0.59	1.96	13	3
1:A:120:ALA:N	1:A:164:LEU:HD21	0.59	2.12	18	2
1:A:94:VAL:HB	1:A:164:LEU:HD13	0.59	1.73	3	1
1:A:101:MET:SD	1:A:103:THR:HG23	0.59	2.37	5	1
1:A:90:VAL:HG11	1:A:94:VAL:HA	0.58	1.75	5	7
1:A:49:SER:O	1:A:53:TRP:CD1	0.58	2.57	17	9
1:A:98:ALA:CB	1:A:112:VAL:HG22	0.58	2.28	4	2
1:A:15:VAL:CG2	1:A:61:ALA:HB2	0.57	2.29	3	1
1:A:72:ASN:ND2	1:A:72:ASN:H	0.57	1.97	15	1
1:A:118:ASN:ND2	1:A:120:ALA:HB2	0.57	2.14	17	1
1:A:59:ASN:CG	1:A:68:ILE:HD12	0.56	2.20	19	3
1:A:85:LEU:HD21	1:A:88:MET:HB3	0.56	1.77	15	8
1:A:42:GLU:O	1:A:46:THR:HG22	0.56	2.01	20	1
1:A:75:GLU:OE2	1:A:77:LEU:HD23	0.55	2.00	5	2
1:A:82:VAL:HG13	1:A:130:CYS:SG	0.55	2.42	6	1
1:A:99:PHE:CD1	1:A:99:PHE:O	0.55	2.59	6	4
1:A:98:ALA:HB2	1:A:112:VAL:HG22	0.55	1.79	19	3
1:A:67:VAL:CG1	1:A:77:LEU:HD12	0.54	2.33	3	2
1:A:120:ALA:HB2	1:A:164:LEU:HD21	0.54	1.79	12	1
1:A:166:LYS:CG	1:A:167:MET:N	0.54	2.71	4	1
1:A:87:PHE:CD1	1:A:172:TYR:O	0.54	2.61	5	3
1:A:126:VAL:HG13	1:A:127:GLN:N	0.53	2.17	4	10
1:A:115:CYS:SG	1:A:122:VAL:HG21	0.53	2.43	8	6
1:A:170:ASN:HD22	1:A:171:GLY:N	0.53	2.02	12	1
1:A:80:CYS:HA	1:A:101:MET:HE3	0.53	1.81	14	1
1:A:26:LEU:HD13	1:A:27:PRO:N	0.52	2.19	9	4
1:A:59:ASN:OD1	1:A:68:ILE:HD12	0.52	2.04	3	1
1:A:56:VAL:HG11	1:A:77:LEU:HD11	0.52	1.79	13	1
1:A:16:GLN:HE22	1:A:125:ALA:HB1	0.52	1.64	9	1
1:A:15:VAL:HG22	1:A:61:ALA:CB	0.52	2.34	3	1
1:A:78:VAL:HG11	1:A:111:HIS:CE1	0.52	2.40	17	2
1:A:102:ASP:OD2	1:A:108:PHE:CE1	0.52	2.62	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:HG21	1:A:111:HIS:CE1	0.51	2.40	17	2
1:A:42:GLU:O	1:A:44:LEU:N	0.51	2.44	6	4
1:A:87:PHE:C	1:A:87:PHE:CD1	0.51	2.84	15	1
1:A:99:PHE:C	1:A:99:PHE:CD1	0.51	2.84	12	1
1:A:16:GLN:HG2	1:A:18:PHE:CZ	0.50	2.41	10	1
1:A:24:GLY:HA3	1:A:44:LEU:HD22	0.50	1.83	11	4
1:A:163:HIS:O	1:A:166:LYS:N	0.50	2.45	20	2
1:A:164:LEU:HD12	1:A:164:LEU:H	0.50	1.66	7	1
1:A:76:VAL:HG12	1:A:76:VAL:O	0.50	2.06	19	1
1:A:75:GLU:OE1	1:A:76:VAL:N	0.50	2.45	1	1
1:A:42:GLU:O	1:A:45:MET:N	0.50	2.45	6	1
1:A:58:MET:CE	1:A:113:PHE:CG	0.50	2.95	2	1
1:A:82:VAL:O	1:A:174:ASN:ND2	0.50	2.45	4	7
1:A:49:SER:O	1:A:53:TRP:NE1	0.50	2.45	14	7
1:A:34:MET:O	1:A:38:ASN:ND2	0.50	2.45	13	2
1:A:165:SER:O	1:A:169:GLN:N	0.49	2.45	12	1
1:A:74:GLU:OE1	1:A:74:GLU:N	0.49	2.45	18	1
1:A:16:GLN:HG3	1:A:18:PHE:CE2	0.49	2.42	9	1
1:A:72:ASN:OD1	1:A:73:GLU:N	0.49	2.45	3	1
1:A:15:VAL:HG23	1:A:61:ALA:HA	0.49	1.83	10	2
1:A:94:VAL:HG12	1:A:164:LEU:HB3	0.49	1.83	12	1
1:A:57:ASN:ND2	1:A:69:SER:O	0.49	2.46	20	1
1:A:165:SER:O	1:A:168:GLN:N	0.49	2.46	10	1
1:A:94:VAL:HG12	1:A:168:GLN:OE1	0.49	2.07	20	1
1:A:15:VAL:HG23	1:A:61:ALA:CA	0.49	2.37	10	5
1:A:25:MET:CG	1:A:109:GLU:OE2	0.49	2.60	17	1
1:A:44:LEU:O	1:A:47:SER:N	0.49	2.46	14	5
1:A:44:LEU:HD12	1:A:112:VAL:HG21	0.48	1.85	7	1
1:A:85:LEU:O	1:A:174:ASN:ND2	0.48	2.46	8	4
1:A:111:HIS:HB3	1:A:113:PHE:CE2	0.48	2.43	17	1
1:A:61:ALA:N	1:A:64:THR:O	0.48	2.47	17	13
1:A:107:ARG:O	1:A:107:ARG:CG	0.48	2.61	3	3
1:A:25:MET:SD	1:A:26:LEU:N	0.48	2.87	4	3
1:A:127:GLN:OE1	1:A:163:HIS:CE1	0.48	2.66	10	1
1:A:39:SER:O	1:A:43:ASN:ND2	0.48	2.47	1	3
1:A:88:MET:SD	1:A:126:VAL:HG22	0.48	2.48	20	1
1:A:38:ASN:O	1:A:41:ILE:N	0.48	2.47	13	2
1:A:26:LEU:HD13	1:A:26:LEU:C	0.48	2.29	9	3
1:A:23:LEU:HD12	1:A:23:LEU:N	0.48	2.24	7	1
1:A:50:LYS:HA	1:A:53:TRP:CH2	0.47	2.44	16	1
1:A:81:ARG:O	1:A:84:PHE:N	0.47	2.47	9	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLN:NE2	1:A:125:ALA:HB1	0.47	2.23	9	1
1:A:69:SER:CB	1:A:75:GLU:CD	0.47	2.83	4	2
1:A:62:ASP:O	1:A:129:ALA:CB	0.47	2.63	14	1
1:A:25:MET:CG	1:A:109:GLU:CD	0.47	2.83	17	1
1:A:26:LEU:CD1	1:A:27:PRO:O	0.47	2.63	9	2
1:A:80:CYS:SG	1:A:99:PHE:CE1	0.47	3.08	5	3
1:A:50:LYS:HA	1:A:53:TRP:CZ3	0.47	2.45	16	3
1:A:99:PHE:CD1	1:A:99:PHE:C	0.47	2.88	6	5
1:A:34:MET:CE	1:A:37:LEU:HD22	0.47	2.39	15	1
1:A:50:LYS:HA	1:A:53:TRP:CE3	0.47	2.45	18	14
1:A:45:MET:HE2	1:A:53:TRP:CH2	0.47	2.45	16	3
1:A:31:PRO:HB3	1:A:108:PHE:CE2	0.46	2.45	16	5
1:A:31:PRO:HB3	1:A:108:PHE:CD2	0.46	2.45	14	1
1:A:96:THR:HG22	1:A:114:TRP:CE3	0.46	2.44	4	3
1:A:120:ALA:O	1:A:124:GLU:CB	0.46	2.64	4	2
1:A:19:ARG:O	1:A:20:VAL:CG1	0.46	2.63	3	2
1:A:25:MET:O	1:A:44:LEU:HD21	0.46	2.10	14	1
1:A:87:PHE:CD1	1:A:88:MET:N	0.46	2.84	15	1
1:A:59:ASN:ND2	1:A:68:ILE:CD1	0.46	2.79	3	2
1:A:68:ILE:HG21	1:A:73:GLU:HA	0.46	1.87	6	2
1:A:173:GLU:CD	1:A:173:GLU:O	0.46	2.55	20	1
1:A:127:GLN:NE2	1:A:172:TYR:CG	0.46	2.84	14	1
1:A:15:VAL:HG23	1:A:61:ALA:N	0.45	2.26	12	3
1:A:166:LYS:CG	1:A:167:MET:SD	0.45	3.04	4	1
1:A:85:LEU:O	1:A:174:ASN:CB	0.45	2.64	9	1
1:A:23:LEU:HD21	1:A:45:MET:HE2	0.45	1.88	17	1
1:A:127:GLN:CG	1:A:128:ALA:N	0.45	2.79	4	2
1:A:38:ASN:O	1:A:40:ALA:N	0.45	2.50	13	2
1:A:109:GLU:OE2	1:A:111:HIS:NE2	0.45	2.50	17	1
1:A:81:ARG:O	1:A:82:VAL:C	0.45	2.55	14	11
1:A:67:VAL:O	1:A:77:LEU:N	0.45	2.50	12	1
1:A:26:LEU:C	1:A:26:LEU:CD1	0.45	2.84	9	2
1:A:16:GLN:CD	1:A:18:PHE:CZ	0.45	2.90	10	1
1:A:102:ASP:O	1:A:102:ASP:CG	0.45	2.55	2	1
1:A:85:LEU:O	1:A:174:ASN:CG	0.45	2.55	6	1
1:A:111:HIS:HB3	1:A:113:PHE:CE1	0.45	2.47	6	4
1:A:84:PHE:O	1:A:85:LEU:C	0.44	2.55	16	4
1:A:78:VAL:CG1	1:A:79:GLU:N	0.44	2.80	7	2
1:A:50:LYS:HA	1:A:53:TRP:CZ2	0.44	2.48	16	1
1:A:129:ALA:O	1:A:130:CYS:C	0.44	2.55	18	1
1:A:44:LEU:HD12	1:A:112:VAL:CG2	0.44	2.42	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:GLU:O	1:A:174:ASN:C	0.44	2.55	20	2
1:A:88:MET:CE	1:A:130:CYS:SG	0.44	3.05	16	1
1:A:25:MET:HG3	1:A:111:HIS:CE1	0.44	2.47	1	1
1:A:15:VAL:CG1	1:A:16:GLN:N	0.44	2.80	3	1
1:A:116:GLU:HA	1:A:117:PRO:C	0.44	2.32	17	17
1:A:63:ALA:O	1:A:82:VAL:HG22	0.44	2.13	4	1
1:A:50:LYS:HA	1:A:53:TRP:CE2	0.44	2.48	16	1
1:A:78:VAL:CG1	1:A:111:HIS:CE1	0.44	3.01	17	1
1:A:91:GLY:O	1:A:92:LYS:C	0.44	2.56	14	2
1:A:98:ALA:HB2	1:A:112:VAL:HG13	0.44	1.87	4	1
1:A:78:VAL:CG2	1:A:111:HIS:CE1	0.44	3.01	17	1
1:A:101:MET:SD	1:A:102:ASP:C	0.44	2.96	2	2
1:A:53:TRP:N	1:A:53:TRP:CD1	0.44	2.85	3	1
1:A:128:ALA:O	1:A:129:ALA:C	0.44	2.56	9	2
1:A:50:LYS:HD2	1:A:53:TRP:CZ3	0.44	2.48	19	2
1:A:82:VAL:O	1:A:85:LEU:N	0.44	2.50	20	1
1:A:76:VAL:O	1:A:76:VAL:CG1	0.44	2.64	4	2
1:A:91:GLY:O	1:A:93:ASP:N	0.44	2.50	1	1
1:A:42:GLU:O	1:A:43:ASN:C	0.44	2.55	17	6
1:A:41:ILE:CD1	1:A:91:GLY:CA	0.43	2.95	3	1
1:A:34:MET:HE3	1:A:34:MET:HA	0.43	1.90	15	1
1:A:83:ARG:NH2	1:A:84:PHE:CZ	0.43	2.86	19	1
1:A:61:ALA:O	1:A:62:ASP:C	0.43	2.56	19	1
1:A:50:LYS:CD	1:A:53:TRP:CZ3	0.43	3.01	18	1
1:A:22:TYR:CD1	1:A:113:PHE:CE2	0.43	3.06	19	1
1:A:82:VAL:HG11	1:A:130:CYS:HA	0.43	1.91	6	2
1:A:23:LEU:HD13	1:A:112:VAL:CG1	0.43	2.30	13	1
1:A:88:MET:SD	1:A:126:VAL:CG2	0.43	3.06	20	1
1:A:72:ASN:OD1	1:A:72:ASN:N	0.43	2.51	1	1
1:A:78:VAL:HG12	1:A:79:GLU:N	0.43	2.27	7	2
1:A:163:HIS:O	1:A:164:LEU:C	0.43	2.57	8	2
1:A:52:ASP:OD1	1:A:52:ASP:C	0.43	2.57	9	1
1:A:56:VAL:CG1	1:A:77:LEU:CD1	0.43	2.95	12	1
1:A:31:PRO:O	1:A:100:ILE:CD1	0.43	2.67	14	1
1:A:50:LYS:HD2	1:A:53:TRP:CE3	0.43	2.48	18	1
1:A:42:GLU:O	1:A:46:THR:HG23	0.42	2.14	1	1
1:A:121:ASN:O	1:A:124:GLU:N	0.42	2.53	14	1
1:A:86:SER:OG	1:A:87:PHE:N	0.42	2.52	2	1
1:A:166:LYS:HG3	1:A:167:MET:N	0.42	2.29	4	1
1:A:42:GLU:C	1:A:44:LEU:N	0.42	2.72	6	1
1:A:124:GLU:CG	1:A:125:ALA:N	0.42	2.82	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:CG1	1:A:130:CYS:SG	0.42	3.07	10	1
1:A:68:ILE:CG2	1:A:73:GLU:O	0.42	2.67	3	1
1:A:64:THR:HG22	1:A:65:VAL:N	0.42	2.30	8	1
1:A:70:GLU:CD	1:A:70:GLU:C	0.42	2.77	8	1
1:A:163:HIS:CE1	1:A:167:MET:SD	0.42	3.12	8	1
1:A:37:LEU:C	1:A:37:LEU:HD23	0.42	2.35	1	1
1:A:41:ILE:CD1	1:A:91:GLY:HA3	0.42	2.44	3	1
1:A:165:SER:O	1:A:168:GLN:CG	0.42	2.67	13	2
1:A:44:LEU:O	1:A:45:MET:C	0.42	2.58	5	1
1:A:49:SER:O	1:A:53:TRP:CE2	0.42	2.73	1	1
1:A:94:VAL:CG2	1:A:95:HIS:N	0.42	2.83	5	1
1:A:19:ARG:NH1	1:A:116:GLU:OE2	0.42	2.53	13	1
1:A:82:VAL:HG21	1:A:129:ALA:CB	0.42	2.42	15	1
1:A:58:MET:HE1	1:A:113:PHE:CD1	0.41	2.49	2	1
1:A:59:ASN:O	1:A:66:THR:N	0.41	2.53	9	1
1:A:118:ASN:OD1	1:A:164:LEU:HD11	0.41	2.15	2	1
1:A:62:ASP:CG	1:A:63:ALA:N	0.41	2.74	17	1
1:A:23:LEU:HD12	1:A:23:LEU:H	0.41	1.75	9	1
1:A:16:GLN:HG2	1:A:18:PHE:CE1	0.41	2.50	10	1
1:A:126:VAL:CG1	1:A:127:GLN:N	0.41	2.83	4	2
1:A:53:TRP:CD1	1:A:53:TRP:N	0.41	2.86	6	3
1:A:41:ILE:HG23	1:A:112:VAL:HG11	0.41	1.92	8	1
1:A:26:LEU:HD13	1:A:27:PRO:CD	0.41	2.46	13	1
1:A:36:THR:O	1:A:39:SER:CB	0.41	2.69	15	1
1:A:78:VAL:HG11	1:A:111:HIS:CD2	0.41	2.51	9	1
1:A:80:CYS:SG	1:A:101:MET:CB	0.41	3.08	9	2
1:A:76:VAL:O	1:A:76:VAL:CG2	0.41	2.67	13	1
1:A:118:ASN:ND2	1:A:164:LEU:HD11	0.41	2.29	17	1
1:A:101:MET:HE2	1:A:103:THR:HG22	0.41	1.93	20	1
1:A:118:ASN:OD1	1:A:120:ALA:N	0.41	2.54	2	1
1:A:102:ASP:OD1	1:A:102:ASP:N	0.41	2.53	10	1
1:A:120:ALA:CB	1:A:164:LEU:HD21	0.41	2.45	12	1
1:A:37:LEU:HD12	1:A:100:ILE:HD12	0.41	1.92	13	1
1:A:82:VAL:O	1:A:83:ARG:C	0.41	2.58	16	1
1:A:50:LYS:HE2	1:A:114:TRP:CE2	0.41	2.51	19	1
1:A:23:LEU:HG	1:A:53:TRP:CD2	0.41	2.51	6	4
1:A:167:MET:O	1:A:171:GLY:CA	0.41	2.68	20	1
1:A:127:GLN:OE1	1:A:172:TYR:CD2	0.41	2.73	8	1
1:A:127:GLN:OE1	1:A:172:TYR:CE2	0.41	2.73	8	1
1:A:50:LYS:HA	1:A:53:TRP:CD2	0.41	2.51	16	2
1:A:88:MET:HE3	1:A:127:GLN:HA	0.41	1.92	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ALA:HB3	1:A:64:THR:HB	0.41	1.94	19	1
1:A:19:ARG:C	1:A:20:VAL:HG13	0.40	2.37	3	1
1:A:127:GLN:NE2	1:A:167:MET:SD	0.40	2.95	13	1
1:A:72:ASN:ND2	1:A:72:ASN:N	0.40	2.61	15	1
1:A:121:ASN:O	1:A:122:VAL:C	0.40	2.59	14	1
1:A:165:SER:O	1:A:166:LYS:C	0.40	2.60	10	1
1:A:37:LEU:HD12	1:A:100:ILE:HD11	0.40	1.93	17	1
1:A:45:MET:O	1:A:48:SER:O	0.40	2.40	7	1

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	A	125/185 (68%)	110±3 (88±2%)	14±2 (11±2%)	1±1 (1±1%)	21	69
All	All	2500/3700 (68%)	2207 (88%)	271 (11%)	22 (1%)	21	69

All 9 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	62	ASP	5
1	A	117	PRO	4
1	A	75	GLU	3
1	A	82	VAL	3
1	A	43	ASN	3
1	A	92	LYS	1
1	A	91	GLY	1
1	A	39	SER	1
1	A	85	LEU	1

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	A	111/157 (71%)	106±1 (95±1%)	6±1 (5±1%)	28 77
All	All	2220/3140 (71%)	2110 (95%)	110 (5%)	28 77

All 31 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)
1	A	26	LEU	20
1	A	118	ASN	18
1	A	17	LYS	11
1	A	102	ASP	9
1	A	101	MET	5
1	A	34	MET	4
1	A	72	ASN	3
1	A	57	ASN	3
1	A	92	LYS	3
1	A	93	ASP	3
1	A	170	ASN	3
1	A	109	GLU	2
1	A	70	GLU	2
1	A	29	ASP	2
1	A	19	ARG	2
1	A	107	ARG	2
1	A	73	GLU	2
1	A	166	LYS	2
1	A	71	LYS	2
1	A	167	MET	1
1	A	74	GLU	1
1	A	52	ASP	1
1	A	81	ARG	1
1	A	164	LEU	1
1	A	127	GLN	1
1	A	62	ASP	1
1	A	83	ARG	1
1	A	88	MET	1
1	A	22	TYR	1
1	A	30	ARG	1
1	A	69	SER	1

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 (i)

No chemical shift data were provided