Full wwPDB NMR Structure Validation Report (i)

Mar 7, 2022 – 12:35 AM EST

PDB ID	:	2RPB
Title	:	The solution structure of membrane protein
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Deposited on	:	2008-05-13

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:

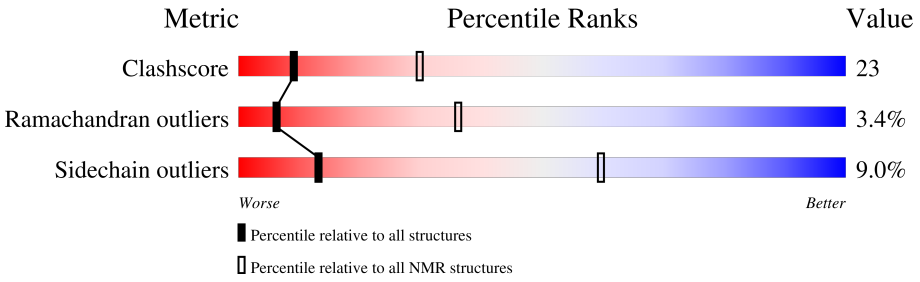
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	113	52% 38% • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:69-A:172 (104)	0.25	3

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1825 atoms, of which 923 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical membrane protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	113	1825	569	923	156	174	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	expression tag	UNP O58205
A	63	SER	-	expression tag	UNP O58205
A	64	ASP	-	expression tag	UNP O58205
A	65	HIS	-	expression tag	UNP O58205

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: hypothetical membrane protein

Chain A: 52% 38% • 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 C82 V87 V90 D91 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 L123 R124 A125 I126 I127 M130 E131 L132 D133 E134 T135 L136 N143 D151 K152 I153 T154 D155 R156

W157 G158 V159 K160 I161 T162 I169 D170 K173 D174

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: hypothetical membrane protein

Chain A: 43% 45% • 8%

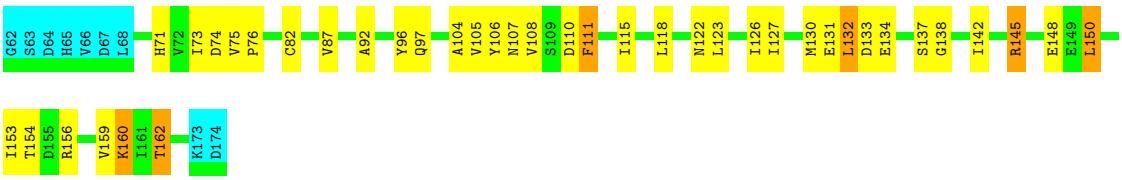
G62 S63 D64 H65 V66 D67 L68 R69 E70 I73 D74 V75 P76 P77 C82 V87 V88 T89 V90 D91 A92 V93 Y96 Q97 D100 P101 V102 K103 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 K117 L118 T121 N122 L123 R124 I127 M130 E131 L132 D133 L136

S137 N143 A144 R145 L146 R147 L150 D151 K152 I153 T154 D155 R156 W157 G158 V159 K160 I161 T162 R163 V164 E165 I166 I169 D170 K173 D174

4.2.2 Score per residue for model 2

• Molecule 1: hypothetical membrane protein

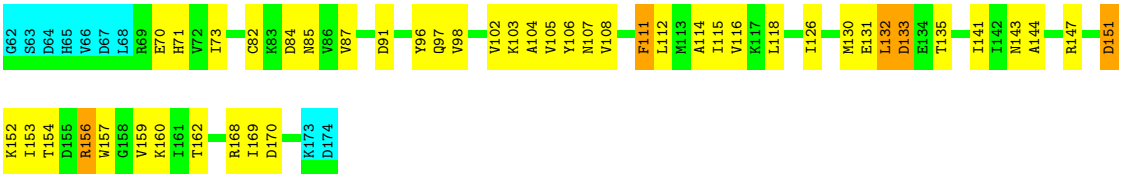
Chain A: 57% 30% 5% 8%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: hypothetical membrane protein

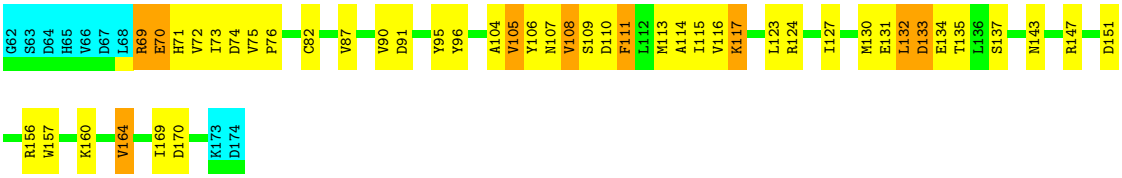
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: hypothetical membrane protein

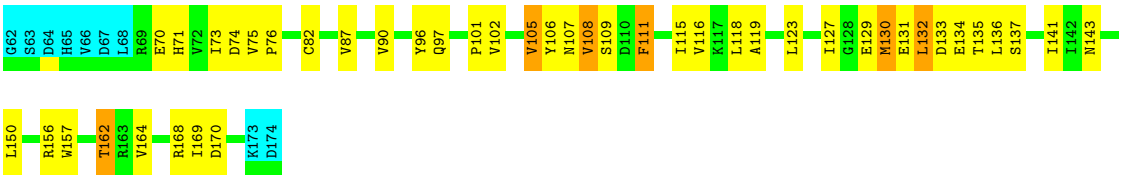
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: hypothetical membrane protein

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical membrane protein

Chain A: 47% 42% • 8%

G62 S63 D64 H65 V66 D67 L68 H71 V72 I73 D74 V75 P76 E79 C82 K83 V87 V90 D91 A92 V93 V94 Y95 Y96 Q97 V98 P101 A104 V105 Y106 N107 V108 F111 I115 L123 I126 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 I141 I142

N143 A144 E149 I153 R156 W157 G158 V159 K160 I161 T162 R163 V164 E165 I166 I169 D170 K173 D174

4.2.7 Score per residue for model 7

- Molecule 1: hypothetical membrane protein

Chain A: 42% 45% • 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 I81 C82 V86 V90 D91 A92 Y95 Y96 Q97 P101 V102 K103 A104 V105 Y106 N107 V108 F111 I115 L118 A119 Q120 T121 N122 L123 R124 A125 I126 I127 G128 E129 M130 E131 L132 D133 L136

S137 G138 R139 D140 I141 I142 N143 A144 L150 D151 K152 I153 T154 W157 G158 V159 K160 I161 T162 I169 D170 P171 P172 K173 D174

4.2.8 Score per residue for model 8

- Molecule 1: hypothetical membrane protein

Chain A: 52% 36% • 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 P77 Q78 I81 C82 V87 V88 T89 V90 Y95 Y96 Q97 V98 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 L123 R124 I127 E131 L132 D133 E134 T135 L136 N143 L150 D151 K152

I153 T154 D155 R156 W157 G158 V159 T162 I166 Q167 R168 I169 D170 K173 D174

4.2.9 Score per residue for model 9

- Molecule 1: hypothetical membrane protein

Chain A: 47% 38% 7% 8%

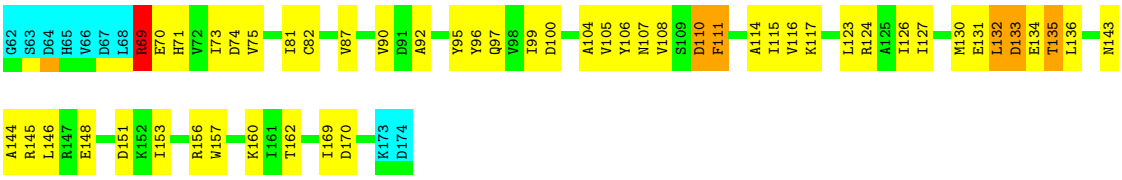
G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 P77 Q78 I81 C82 V87 V90 D91 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 K117 L118 A119 Q120 T121 N122 L123 R124 A125 I126 M130 E131 L132 D133 E134 T135 L136 I141

I142 N143 E148 D151 K152 I153 T154 D155 R156 W157 G158 V159 K160 I161 T162 I166 I169 D170 K173 D174

4.2.10 Score per residue for model 10

- Molecule 1: hypothetical membrane protein

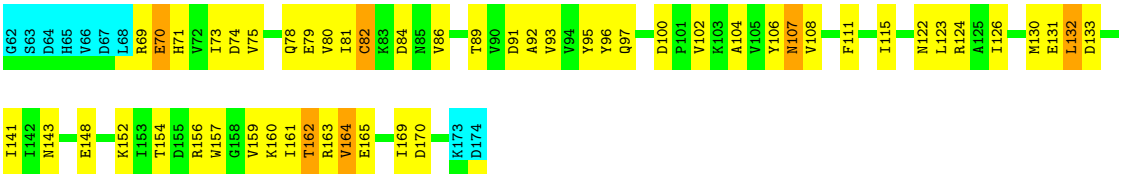
Chain A: 47% 40% • • 8%



4.2.11 Score per residue for model 11

- Molecule 1: hypothetical membrane protein

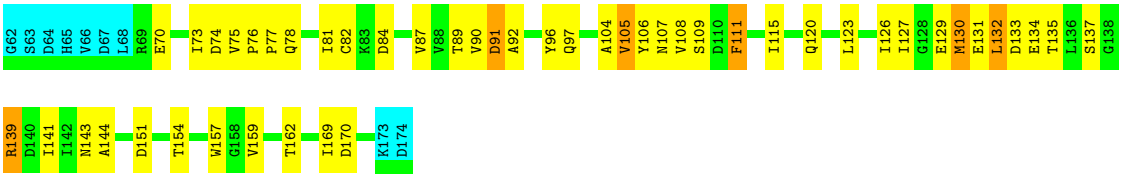
Chain A: 46% 41% 5% 8%



4.2.12 Score per residue for model 12

- Molecule 1: hypothetical membrane protein

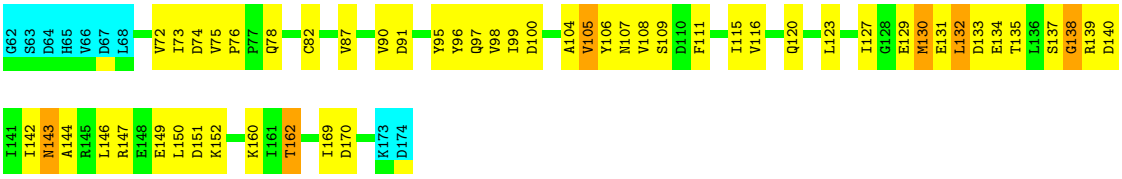
Chain A: 50% 37% 5% 8%



4.2.13 Score per residue for model 13

- Molecule 1: hypothetical membrane protein

Chain A: 46% 41% 5% 8%



4.2.14 Score per residue for model 14

- Molecule 1: hypothetical membrane protein

Chain A: 48% 40% • 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 C82 V90 D91 A92 V93 V94 Y95 Y96 Q97 V102 V105 Y106 N107 V108 S109 D110 F111 A114 I115 L123 R124 A125 I126 I127 M130 E131 L132 D133 E134 T135 L136 S137 G138 I141 I142 N143 A144 R145

L146 R147 E148 E149 L150 D151 K152 I153 R156 W157 K160 I161 T162 R163 I166 I169 D170 K173 D174

4.2.15 Score per residue for model 15

- Molecule 1: hypothetical membrane protein

Chain A: 46% 40% 6% 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 C82 N85 V86 V87 V90 Y95 Y96 Q97 V98 I99 A104 V105 Y106 N107 V108 S109 D110 F111 I115 L118 L123 R124 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 S137 G138 R139

I142 N143 A144 R145 E148 D151 K152 I153 T154 D155 R156 W157 G158 V159 T162 R168 I169 D170 K173 D174

4.2.16 Score per residue for model 16

- Molecule 1: hypothetical membrane protein

Chain A: 50% 38% • 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 P77 C82 V87 V88 T89 V90 D91 A92 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 Q120 L123 R124 I127 M130 E131 L132 D133 E134 R139 N143 L146 E149

L150 D151 K152 I153 T154 D155 R156 V159 T162 R163 V164 E165 I166 I169 D170 K173 D174

4.2.17 Score per residue for model 17

- Molecule 1: hypothetical membrane protein

Chain A: 46% 41% 5% 8%

G62 S63 D64 H65 V66 D67 L68 I73 D74 V75 P76 P77 I81 C82 K83 D84 N85 V86 V87 V88 T89 V90 Q97 V98 I99 D100 P101 V102 K103 A104 V105 Y106 N107 V108 S109 D110 F111 L112 M113 A114 I115 V116 K117 Q120 L123 I126 I127 M130 E131 L132 D133 E134

R139 I142 N143 A144 E148 D151 T154 V159 T162 R163 I166 I169 D170 K173 D174

4.2.18 Score per residue for model 18

- Molecule 1: hypothetical membrane protein

Chain A: 47% 40% 5% 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 P77 Q78 C82 K83 D84 N85 V86 V87 V90 D91 A92 V93 Y96 Q97 V98 V105 Y106 N107 V108 S109 D110 F111 A114 I115 V116 K117 L118 T121 N122 L123 R124 A125 I126 I127 M130 E131 L132 D133

E134 T135 L136 D140 I141 I142 E149 L150 D151 K152 I153 T154 D155 R156 K160 I161 T162 E165 I169 D170 K173 D174

4.2.19 Score per residue for model 19

- Molecule 1: hypothetical membrane protein

Chain A: 48% 39% 5% 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 V80 I81 C82 D91 A92 Y95 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 K117 L118 A119 Q120 L123 R124 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 N143 A144

L150 D151 K152 I153 R156 W157 G158 V159 K160 I161 T162 R163 V164 E165 I166 I169 D170 K173 D174

4.2.20 Score per residue for model 20

- Molecule 1: hypothetical membrane protein

Chain A: 45% 42% • 8%

G62 S63 D64 H65 V66 D67 L68 H71 V72 I73 D74 V75 P76 P77 C82 K83 D84 V87 V88 T89 V90 D91 A92 V93 Y96 Q97 V98 P101 V102 K103 A104 V105 Y106 N107 V108 S109 D110 F111 L112 M113 A114 I115 V116 K117 Q120 L123 R124 I127 G128 E129 M130 E131

L132 D133 E134 G138 R139 N143 L146 R147 I153 T154 D155 V159 K160 I161 T162 E165 R168 I169 D170 K173 D174

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, torsion angle dynamics, rigid body restrained molecular dynamics.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *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
MOLMOL	refinement	2K.2
Sparky	refinement	3.106

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	834	862	861	39±5
All	All	16680	17240	17220	781

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:HD13	1:A:115:ILE:HG21	1.00	1.31	7	17
1:A:81:ILE:CD1	1:A:87:VAL:HG22	0.87	1.98	9	4
1:A:72:VAL:HG12	1:A:95:TYR:CE1	0.86	2.05	8	3
1:A:154:THR:HB	1:A:159:VAL:HG13	0.81	1.52	3	9
1:A:123:LEU:HB2	1:A:127:ILE:HD13	0.79	1.53	17	5
1:A:90:VAL:HG21	1:A:127:ILE:HG21	0.77	1.55	8	4
1:A:90:VAL:HG11	1:A:127:ILE:HG21	0.77	1.55	18	8
1:A:115:ILE:HD13	1:A:150:LEU:HD12	0.75	1.57	19	5
1:A:111:PHE:CE2	1:A:115:ILE:HD11	0.73	2.19	17	2
1:A:123:LEU:HD12	1:A:124:ARG:N	0.72	2.00	4	12
1:A:76:PRO:HD2	1:A:116:VAL:HG13	0.69	1.65	9	3
1:A:108:VAL:HG13	1:A:108:VAL:O	0.69	1.86	5	1
1:A:153:ILE:O	1:A:153:ILE:HG22	0.68	1.89	9	9
1:A:113:MET:O	1:A:116:VAL:HG22	0.68	1.88	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:GLN:HG2	1:A:162:THR:HG23	0.66	1.68	6	16
1:A:105:VAL:O	1:A:105:VAL:HG13	0.66	1.89	13	4
1:A:73:ILE:CD1	1:A:115:ILE:HG21	0.65	2.19	3	4
1:A:123:LEU:C	1:A:123:LEU:HD12	0.65	2.11	10	6
1:A:102:VAL:O	1:A:105:VAL:HG13	0.65	1.92	14	2
1:A:71:HIS:CB	1:A:96:TYR:CZ	0.65	2.80	20	3
1:A:123:LEU:HD12	1:A:123:LEU:C	0.64	2.12	16	8
1:A:108:VAL:HG12	1:A:108:VAL:O	0.64	1.93	3	7
1:A:73:ILE:HD11	1:A:111:PHE:CE1	0.63	2.27	8	5
1:A:149:GLU:O	1:A:153:ILE:HD12	0.63	1.94	18	2
1:A:143:ASN:OD1	1:A:164:VAL:HG12	0.62	1.94	5	2
1:A:73:ILE:HD11	1:A:111:PHE:CZ	0.62	2.29	15	16
1:A:111:PHE:CD1	1:A:111:PHE:C	0.62	2.73	19	8
1:A:150:LEU:O	1:A:154:THR:HG23	0.62	1.94	7	3
1:A:71:HIS:CB	1:A:96:TYR:CE2	0.62	2.83	2	5
1:A:97:GLN:NE2	1:A:162:THR:HG21	0.61	2.10	12	6
1:A:141:ILE:HG22	1:A:145:ARG:NE	0.61	2.10	14	1
1:A:114:ALA:O	1:A:118:LEU:HD12	0.61	1.94	3	1
1:A:108:VAL:HG22	1:A:108:VAL:O	0.61	1.96	4	3
1:A:143:ASN:HB3	1:A:166:ILE:HD11	0.59	1.74	9	2
1:A:93:VAL:HG23	1:A:165:GLU:HB2	0.59	1.74	6	5
1:A:123:LEU:HB3	1:A:146:LEU:HD21	0.59	1.73	20	1
1:A:123:LEU:CB	1:A:146:LEU:HD21	0.59	2.27	20	1
1:A:140:ASP:O	1:A:144:ALA:HB2	0.59	1.98	13	1
1:A:73:ILE:HD13	1:A:115:ILE:CG2	0.58	2.24	3	2
1:A:143:ASN:CB	1:A:164:VAL:HG21	0.58	2.29	11	1
1:A:99:ILE:HD12	1:A:100:ASP:HB2	0.57	1.74	17	3
1:A:126:ILE:HD12	1:A:126:ILE:H	0.57	1.59	3	10
1:A:133:ASP:HA	1:A:136:LEU:HD21	0.56	1.76	18	1
1:A:78:GLN:HE21	1:A:123:LEU:HD11	0.56	1.60	18	1
1:A:87:VAL:O	1:A:87:VAL:HG13	0.56	2.01	2	11
1:A:78:GLN:NE2	1:A:123:LEU:HD11	0.56	2.16	18	2
1:A:157:TRP:O	1:A:159:VAL:HG23	0.56	2.00	19	1
1:A:123:LEU:HD13	1:A:127:ILE:HD12	0.56	1.78	7	1
1:A:111:PHE:CE2	1:A:115:ILE:CD1	0.56	2.89	17	1
1:A:127:ILE:HD11	1:A:142:ILE:HG23	0.55	1.78	15	4
1:A:105:VAL:O	1:A:105:VAL:HG22	0.55	2.01	10	6
1:A:71:HIS:HB2	1:A:96:TYR:CE2	0.55	2.37	14	13
1:A:101:PRO:O	1:A:105:VAL:HG12	0.55	2.02	7	2
1:A:143:ASN:CB	1:A:164:VAL:CG2	0.55	2.85	11	1
1:A:100:ASP:OD1	1:A:102:VAL:HG22	0.55	2.02	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ARG:O	1:A:71:HIS:CE1	0.54	2.61	4	1
1:A:145:ARG:CD	1:A:145:ARG:N	0.54	2.70	2	1
1:A:107:ASN:O	1:A:108:VAL:C	0.53	2.47	1	20
1:A:71:HIS:HB3	1:A:96:TYR:CE2	0.53	2.39	2	2
1:A:102:VAL:O	1:A:105:VAL:HG23	0.53	2.04	5	1
1:A:80:VAL:HG12	1:A:124:ARG:NH1	0.52	2.19	19	1
1:A:86:VAL:HG13	1:A:172:PRO:HG3	0.52	1.81	7	1
1:A:127:ILE:HD11	1:A:142:ILE:CG2	0.52	2.34	2	2
1:A:143:ASN:OD1	1:A:144:ALA:N	0.52	2.43	3	6
1:A:153:ILE:H	1:A:153:ILE:HD12	0.52	1.65	19	1
1:A:123:LEU:CA	1:A:146:LEU:HD21	0.52	2.35	20	1
1:A:107:ASN:O	1:A:109:SER:N	0.52	2.43	5	11
1:A:73:ILE:CG2	1:A:116:VAL:HG12	0.52	2.34	3	1
1:A:105:VAL:HG12	1:A:105:VAL:O	0.51	2.05	1	2
1:A:71:HIS:HB2	1:A:96:TYR:CZ	0.51	2.41	20	7
1:A:75:VAL:HG22	1:A:116:VAL:HA	0.51	1.81	20	4
1:A:111:PHE:CE1	1:A:115:ILE:HG13	0.51	2.41	13	2
1:A:108:VAL:O	1:A:108:VAL:CG1	0.51	2.58	5	2
1:A:73:ILE:HD11	1:A:111:PHE:HZ	0.51	1.65	19	3
1:A:169:ILE:CG2	1:A:170:ASP:N	0.51	2.74	12	19
1:A:116:VAL:O	1:A:120:GLN:NE2	0.51	2.44	20	2
1:A:131:GLU:O	1:A:133:ASP:N	0.51	2.44	18	20
1:A:134:GLU:O	1:A:136:LEU:N	0.50	2.44	19	3
1:A:75:VAL:CG1	1:A:92:ALA:O	0.50	2.59	7	9
1:A:75:VAL:HG23	1:A:76:PRO:HD2	0.50	1.82	5	8
1:A:97:GLN:O	1:A:99:ILE:HG23	0.50	2.06	13	2
1:A:154:THR:O	1:A:157:TRP:N	0.50	2.44	1	6
1:A:102:VAL:CG1	1:A:103:LYS:N	0.50	2.74	3	1
1:A:114:ALA:O	1:A:118:LEU:CD1	0.50	2.60	3	1
1:A:101:PRO:O	1:A:104:ALA:N	0.50	2.45	17	2
1:A:90:VAL:HG11	1:A:127:ILE:CG2	0.50	2.36	17	1
1:A:143:ASN:OD1	1:A:166:ILE:CD1	0.50	2.59	14	4
1:A:105:VAL:O	1:A:105:VAL:CG1	0.50	2.60	13	1
1:A:71:HIS:CD2	1:A:96:TYR:CE1	0.50	3.00	2	1
1:A:98:VAL:HG12	1:A:98:VAL:O	0.50	2.06	6	1
1:A:106:TYR:CE1	1:A:108:VAL:HA	0.49	2.42	1	14
1:A:139:ARG:O	1:A:143:ASN:ND2	0.49	2.45	13	3
1:A:143:ASN:OD1	1:A:166:ILE:HD11	0.49	2.06	17	3
1:A:130:MET:SD	1:A:142:ILE:HD11	0.49	2.47	9	1
1:A:70:GLU:OE2	1:A:97:GLN:NE2	0.49	2.45	3	4
1:A:106:TYR:CE2	1:A:108:VAL:HA	0.49	2.43	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:GLU:O	1:A:153:ILE:CD1	0.49	2.60	6	2
1:A:118:LEU:HD22	1:A:153:ILE:HD13	0.49	1.84	7	2
1:A:81:ILE:HD13	1:A:87:VAL:HG22	0.49	1.83	9	3
1:A:112:LEU:O	1:A:116:VAL:HG13	0.49	2.07	3	1
1:A:141:ILE:HD12	1:A:141:ILE:H	0.49	1.67	9	4
1:A:131:GLU:O	1:A:135:THR:HG23	0.49	2.07	12	1
1:A:111:PHE:CE2	1:A:115:ILE:HG13	0.49	2.43	5	9
1:A:76:PRO:O	1:A:120:GLN:NE2	0.49	2.46	7	5
1:A:94:VAL:CG1	1:A:161:ILE:HD12	0.49	2.37	6	1
1:A:122:ASN:O	1:A:126:ILE:HD12	0.49	2.08	11	1
1:A:153:ILE:O	1:A:153:ILE:CG2	0.48	2.60	9	4
1:A:102:VAL:HG13	1:A:103:LYS:N	0.48	2.22	3	1
1:A:97:GLN:NE2	1:A:162:THR:CG2	0.48	2.75	12	4
1:A:139:ARG:HA	1:A:142:ILE:HD12	0.48	1.85	17	1
1:A:147:ARG:O	1:A:151:ASP:CB	0.48	2.61	1	2
1:A:110:ASP:O	1:A:114:ALA:CB	0.48	2.61	17	6
1:A:96:TYR:CG	1:A:111:PHE:CZ	0.48	3.01	5	6
1:A:71:HIS:HB3	1:A:96:TYR:CZ	0.48	2.44	20	2
1:A:83:LYS:CB	1:A:130:MET:O	0.48	2.61	6	1
1:A:95:TYR:O	1:A:161:ILE:HG23	0.48	2.07	7	3
1:A:111:PHE:CZ	1:A:115:ILE:HG13	0.48	2.44	3	5
1:A:123:LEU:CD1	1:A:124:ARG:N	0.48	2.76	16	4
1:A:134:GLU:O	1:A:135:THR:C	0.48	2.52	4	8
1:A:78:GLN:CG	1:A:120:GLN:OE1	0.48	2.61	9	1
1:A:159:VAL:CG2	1:A:160:LYS:N	0.47	2.77	2	1
1:A:156:ARG:HG3	1:A:157:TRP:CD1	0.47	2.44	1	11
1:A:71:HIS:HB2	1:A:96:TYR:CE1	0.47	2.44	7	3
1:A:113:MET:O	1:A:117:LYS:CD	0.47	2.62	4	1
1:A:96:TYR:CE1	1:A:108:VAL:HG21	0.47	2.45	8	1
1:A:106:TYR:C	1:A:107:ASN:CG	0.47	2.73	11	1
1:A:143:ASN:HB2	1:A:164:VAL:CG2	0.47	2.39	11	1
1:A:134:GLU:O	1:A:137:SER:N	0.47	2.47	5	6
1:A:91:ASP:N	1:A:91:ASP:OD1	0.47	2.47	12	3
1:A:102:VAL:HG23	1:A:103:LYS:HG2	0.47	1.86	17	1
1:A:96:TYR:CD2	1:A:111:PHE:CE1	0.47	3.03	1	3
1:A:114:ALA:O	1:A:118:LEU:CG	0.47	2.62	3	1
1:A:72:VAL:HG23	1:A:95:TYR:CE1	0.47	2.45	4	1
1:A:131:GLU:O	1:A:134:GLU:N	0.47	2.47	14	5
1:A:138:GLY:O	1:A:142:ILE:CD1	0.47	2.63	15	2
1:A:79:GLU:OE2	1:A:89:THR:HG23	0.47	2.10	11	1
1:A:104:ALA:HA	1:A:106:TYR:CE2	0.47	2.45	6	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ILE:HD12	1:A:153:ILE:H	0.47	1.70	18	1
1:A:90:VAL:HG22	1:A:91:ASP:N	0.46	2.25	13	2
1:A:116:VAL:CG2	1:A:117:LYS:N	0.46	2.77	10	2
1:A:78:GLN:CD	1:A:120:GLN:CD	0.46	2.74	12	1
1:A:131:GLU:O	1:A:132:LEU:C	0.46	2.54	12	17
1:A:145:ARG:O	1:A:148:GLU:N	0.46	2.48	10	1
1:A:123:LEU:O	1:A:127:ILE:N	0.46	2.48	8	8
1:A:143:ASN:OD1	1:A:143:ASN:C	0.46	2.54	12	8
1:A:150:LEU:CD1	1:A:150:LEU:N	0.46	2.78	2	1
1:A:118:LEU:HB2	1:A:150:LEU:HD11	0.46	1.87	19	1
1:A:129:GLU:O	1:A:130:MET:CG	0.46	2.64	15	8
1:A:150:LEU:O	1:A:154:THR:CG2	0.46	2.63	16	1
1:A:101:PRO:O	1:A:103:LYS:N	0.46	2.49	17	1
1:A:113:MET:CG	1:A:114:ALA:N	0.46	2.79	17	1
1:A:82:CYS:HG	1:A:130:MET:C	0.46	2.12	6	1
1:A:102:VAL:O	1:A:105:VAL:CG1	0.45	2.63	7	2
1:A:154:THR:C	1:A:159:VAL:O	0.45	2.55	11	3
1:A:70:GLU:CD	1:A:70:GLU:O	0.45	2.55	8	2
1:A:96:TYR:C	1:A:96:TYR:CD1	0.45	2.90	11	3
1:A:138:GLY:O	1:A:142:ILE:HD12	0.45	2.12	13	2
1:A:148:GLU:CD	1:A:148:GLU:O	0.45	2.55	14	1
1:A:99:ILE:HD13	1:A:159:VAL:HA	0.45	1.88	15	1
1:A:139:ARG:O	1:A:143:ASN:CG	0.45	2.55	20	3
1:A:104:ALA:HA	1:A:106:TYR:CE1	0.45	2.46	16	2
1:A:146:LEU:O	1:A:149:GLU:N	0.45	2.50	13	2
1:A:118:LEU:O	1:A:122:ASN:ND2	0.45	2.50	9	3
1:A:126:ILE:HG23	1:A:145:ARG:NH2	0.45	2.27	14	1
1:A:135:THR:O	1:A:136:LEU:C	0.44	2.56	14	2
1:A:97:GLN:CG	1:A:162:THR:HG23	0.44	2.42	11	4
1:A:153:ILE:O	1:A:156:ARG:CG	0.44	2.65	3	1
1:A:106:TYR:O	1:A:107:ASN:CG	0.44	2.56	11	1
1:A:126:ILE:CG2	1:A:145:ARG:NH2	0.44	2.80	14	1
1:A:144:ALA:O	1:A:148:GLU:CD	0.44	2.55	17	1
1:A:111:PHE:CE1	1:A:115:ILE:CG1	0.44	3.01	13	1
1:A:92:ALA:HB1	1:A:166:ILE:HD13	0.44	1.89	6	1
1:A:94:VAL:HG21	1:A:150:LEU:CD1	0.44	2.43	14	1
1:A:101:PRO:O	1:A:102:VAL:C	0.44	2.56	20	2
1:A:84:ASP:CG	1:A:84:ASP:O	0.44	2.56	20	1
1:A:131:GLU:C	1:A:133:ASP:N	0.44	2.72	19	10
1:A:97:GLN:O	1:A:99:ILE:N	0.44	2.50	17	1
1:A:144:ALA:O	1:A:145:ARG:C	0.43	2.56	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:GLU:OE1	1:A:79:GLU:N	0.43	2.51	6	1
1:A:111:PHE:CE2	1:A:159:VAL:HG11	0.43	2.48	6	1
1:A:84:ASP:O	1:A:84:ASP:CG	0.43	2.57	18	1
1:A:143:ASN:OD1	1:A:164:VAL:HG23	0.43	2.13	19	1
1:A:93:VAL:HG23	1:A:165:GLU:CB	0.43	2.43	18	1
1:A:70:GLU:HG3	1:A:162:THR:HG21	0.43	1.91	5	1
1:A:101:PRO:O	1:A:105:VAL:HG22	0.43	2.13	5	1
1:A:90:VAL:C	1:A:91:ASP:OD1	0.43	2.57	9	1
1:A:84:ASP:O	1:A:86:VAL:HG23	0.43	2.13	11	1
1:A:76:PRO:CD	1:A:116:VAL:HG13	0.43	2.42	9	1
1:A:115:ILE:CD1	1:A:150:LEU:HD12	0.43	2.35	19	1
1:A:78:GLN:OE1	1:A:124:ARG:CZ	0.43	2.67	11	1
1:A:146:LEU:O	1:A:147:ARG:C	0.43	2.57	13	2
1:A:123:LEU:C	1:A:123:LEU:CD1	0.43	2.84	16	1
1:A:151:ASP:CG	1:A:151:ASP:O	0.43	2.57	19	1
1:A:156:ARG:CZ	1:A:156:ARG:HB2	0.43	2.44	16	1
1:A:115:ILE:O	1:A:116:VAL:C	0.42	2.58	8	3
1:A:141:ILE:O	1:A:144:ALA:N	0.42	2.52	6	2
1:A:154:THR:CB	1:A:159:VAL:O	0.42	2.67	7	1
1:A:154:THR:CB	1:A:159:VAL:HG13	0.42	2.33	20	3
1:A:78:GLN:CD	1:A:123:LEU:HD11	0.42	2.34	13	1
1:A:84:ASP:OD1	1:A:84:ASP:N	0.42	2.50	17	1
1:A:133:ASP:O	1:A:135:THR:N	0.42	2.53	18	1
1:A:159:VAL:HG22	1:A:160:LYS:N	0.42	2.29	20	1
1:A:118:LEU:O	1:A:121:THR:N	0.42	2.51	18	2
1:A:115:ILE:HD11	1:A:154:THR:CG2	0.42	2.44	18	1
1:A:127:ILE:HD12	1:A:127:ILE:N	0.42	2.29	18	1
1:A:96:TYR:CD1	1:A:96:TYR:C	0.42	2.93	2	3
1:A:70:GLU:HG3	1:A:95:TYR:CD2	0.42	2.49	10	1
1:A:108:VAL:O	1:A:112:LEU:HD12	0.42	2.14	20	1
1:A:136:LEU:C	1:A:136:LEU:HD12	0.42	2.35	7	3
1:A:147:ARG:O	1:A:151:ASP:N	0.42	2.53	3	1
1:A:147:ARG:HB2	1:A:164:VAL:HG21	0.42	1.91	4	1
1:A:91:ASP:OD1	1:A:92:ALA:N	0.42	2.53	19	1
1:A:78:GLN:NE2	1:A:120:GLN:O	0.42	2.52	9	1
1:A:76:PRO:HG2	1:A:120:GLN:NE2	0.42	2.30	19	1
1:A:104:ALA:HB1	1:A:108:VAL:HG22	0.42	1.92	11	1
1:A:153:ILE:HD12	1:A:153:ILE:N	0.42	2.30	19	1
1:A:169:ILE:HG22	1:A:170:ASP:N	0.42	2.30	7	7
1:A:157:TRP:HB2	1:A:159:VAL:HG12	0.42	1.92	7	1
1:A:70:GLU:O	1:A:70:GLU:OE2	0.42	2.38	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:ASP:O	1:A:114:ALA:HB2	0.42	2.14	14	1
1:A:96:TYR:CE1	1:A:108:VAL:HG11	0.42	2.50	15	1
1:A:127:ILE:HD12	1:A:127:ILE:H	0.42	1.75	15	1
1:A:107:ASN:C	1:A:109:SER:N	0.41	2.74	4	2
1:A:118:LEU:O	1:A:119:ALA:C	0.41	2.58	5	1
1:A:159:VAL:CG1	1:A:160:LYS:N	0.41	2.84	9	1
1:A:97:GLN:CD	1:A:162:THR:CG2	0.41	2.88	20	1
1:A:77:PRO:HB2	1:A:89:THR:CG2	0.41	2.46	1	6
1:A:71:HIS:HB2	1:A:96:TYR:CD2	0.41	2.50	2	1
1:A:82:CYS:SG	1:A:130:MET:O	0.41	2.78	6	1
1:A:77:PRO:CB	1:A:90:VAL:O	0.41	2.68	9	1
1:A:99:ILE:CD1	1:A:159:VAL:HA	0.41	2.45	15	1
1:A:73:ILE:HD11	1:A:111:PHE:CE2	0.41	2.51	11	1
1:A:133:ASP:C	1:A:135:THR:N	0.41	2.74	18	1
1:A:100:ASP:OD1	1:A:102:VAL:CG2	0.41	2.67	1	2
1:A:123:LEU:CB	1:A:127:ILE:HD13	0.41	2.36	17	1
1:A:153:ILE:HG22	1:A:153:ILE:O	0.41	2.15	8	1
1:A:100:ASP:CG	1:A:102:VAL:HG22	0.41	2.36	11	1
1:A:116:VAL:HG23	1:A:117:LYS:N	0.41	2.29	4	1
1:A:81:ILE:O	1:A:82:CYS:O	0.41	2.39	7	2
1:A:73:ILE:HD11	1:A:96:TYR:CD2	0.41	2.51	13	1
1:A:90:VAL:HG21	1:A:127:ILE:HG12	0.41	1.92	14	1
1:A:163:ARG:CZ	1:A:163:ARG:HB3	0.41	2.46	14	1
1:A:97:GLN:HG2	1:A:162:THR:CG2	0.41	2.46	18	1
1:A:134:GLU:C	1:A:136:LEU:N	0.41	2.74	19	1
1:A:93:VAL:CG2	1:A:165:GLU:HB2	0.41	2.46	20	1
1:A:115:ILE:C	1:A:117:LYS:N	0.41	2.74	20	1
1:A:136:LEU:HD12	1:A:137:SER:N	0.41	2.31	1	1
1:A:87:VAL:O	1:A:87:VAL:CG1	0.41	2.69	2	1
1:A:78:GLN:OE1	1:A:80:VAL:CG1	0.41	2.68	11	1
1:A:145:ARG:O	1:A:146:LEU:C	0.40	2.60	10	1
1:A:139:ARG:CZ	1:A:139:ARG:CB	0.40	2.99	16	1
1:A:156:ARG:CZ	1:A:156:ARG:CB	0.40	2.99	16	1
1:A:141:ILE:H	1:A:141:ILE:HD12	0.40	1.77	5	1
1:A:139:ARG:C	1:A:139:ARG:CD	0.40	2.90	12	1
1:A:151:ASP:OD1	1:A:151:ASP:O	0.40	2.40	15	1
1:A:111:PHE:CE2	1:A:115:ILE:CG1	0.40	3.04	17	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	104/113 (92%)	84±3 (81±3%)	17±3 (16±3%)	4±1 (3±1%)	6 36
All	All	2080/2260 (92%)	1679 (81%)	331 (16%)	70 (3%)	6 36

All 10 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	132	LEU	20
1	A	82	CYS	19
1	A	98	VAL	6
1	A	105	VAL	6
1	A	108	VAL	4
1	A	138	GLY	4
1	A	168	ARG	3
1	A	135	THR	3
1	A	69	ARG	3
1	A	102	VAL	2

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	95/103 (92%)	86±2 (91±3%)	9±2 (9±3%)	13 60
All	All	1900/2060 (92%)	1729 (91%)	171 (9%)	13 60

All 33 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	130	MET	19
1	A	111	PHE	17
1	A	74	ASP	15
1	A	160	LYS	14
1	A	151	ASP	13
1	A	70	GLU	10
1	A	162	THR	10
1	A	110	ASP	7
1	A	91	ASP	7
1	A	148	GLU	5
1	A	133	ASP	5
1	A	156	ARG	4
1	A	85	ASN	4
1	A	152	LYS	4
1	A	164	VAL	3
1	A	145	ARG	3
1	A	84	ASP	3
1	A	69	ARG	3
1	A	163	ARG	3
1	A	155	ASP	3
1	A	135	THR	2
1	A	168	ARG	2
1	A	117	LYS	2
1	A	140	ASP	2
1	A	136	LEU	2
1	A	143	ASN	2
1	A	150	LEU	1
1	A	82	CYS	1
1	A	107	ASN	1
1	A	139	ARG	1
1	A	99	ILE	1
1	A	159	VAL	1
1	A	93	VAL	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