Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 05:43 PM EDT

PDB ID	:	2K60
Title	:	NMR structure of calcium-loaded STIM1 EF-SAM
Authors	:	Stathopulos, P.B.; Ikura, M.
Deposited on	:	2008-07-02

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

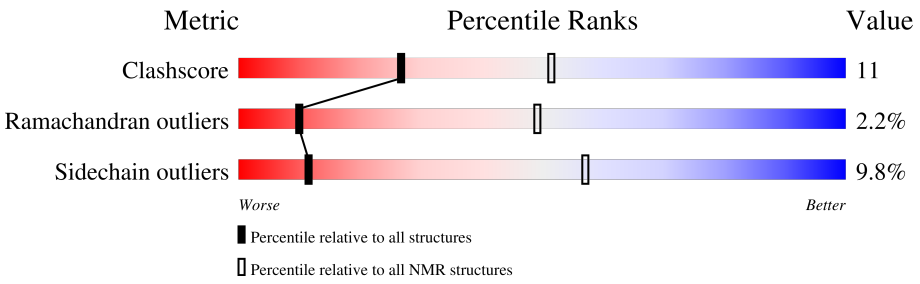
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (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	150	64% 25% • 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 20 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:65-A:201 (137)	0.63	20

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2396 atoms, of which 1174 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (Stromal interaction molecule 1).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2395	767	1174	206	243	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q13586
A	-4	SER	-	expression tag	UNP Q13586
A	-3	HIS	-	expression tag	UNP Q13586
A	-2	MET	-	expression tag	UNP Q13586
A	-1	ALA	-	expression tag	UNP Q13586
A	0	SER	-	expression tag	UNP Q13586

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	1	1	1

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: PROTEIN (Stromal interaction molecule 1)

Chain A: 64% 25% • 9%

G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 N70 I71 H72 K73 D76 D77 D78 V83 E87 S88 D89 L92 R93 L96 N97 P101 K104 H105 H109 L114 I115 E118 D119 L120 W121 K122 L141 Y144 L147 P148 Q149 E152

T153 F154 R155 K156 L157 Q158 L159 S160 A163 R166 L167 T170 N171 R184 Q188 L192 L195 G201

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: PROTEIN (Stromal interaction molecule 1)

Chain A: 59% 29% • 9%

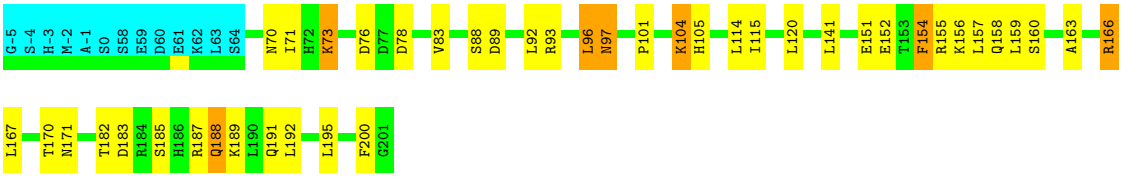
G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 V68 I71 H72 K73 L74 D78 D82 V83 D84 V85 E86 E87 L92 L96 N97 Y98 H99 D100 P101 K104 H105 S106 H109 G110 E111 D112 K113 L114 I115 S116 V117 E118 K122 V134 V137

L141 V145 E146 L147 P148 Q149 F154 R155 K156 L157 S160 A163 R166 T170 N171 T175 L179 K180 R184 S185 H186 R187 Q188 L192 L195 L199 F200 G201

4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN (Stromal interaction molecule 1)

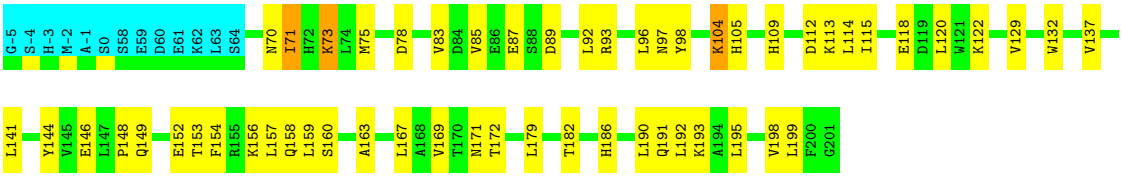
Chain A: 63% 24% 5% 9%



4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

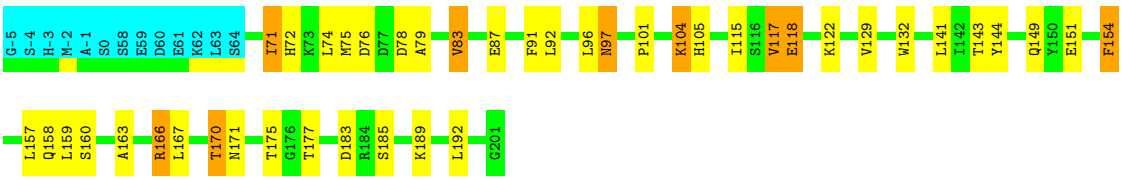
Chain A: 55% 35% • 9%



4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 63% 23% 6% 9%



4.2.5 Score per residue for model 5

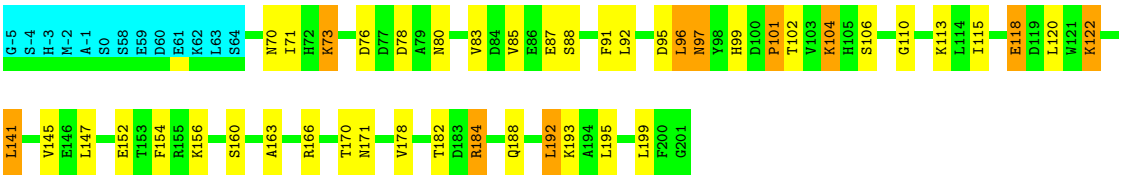
- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 65% 22% • 9%

4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

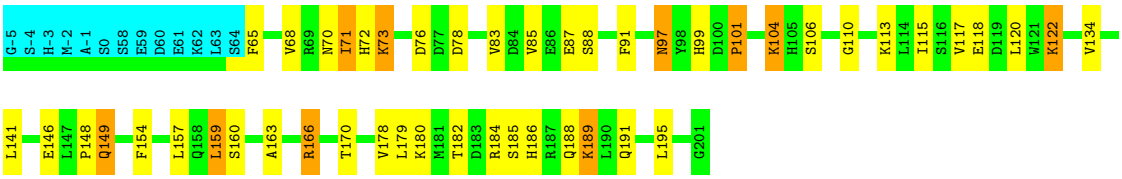
Chain A: 61% 23% 7% 9%



4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

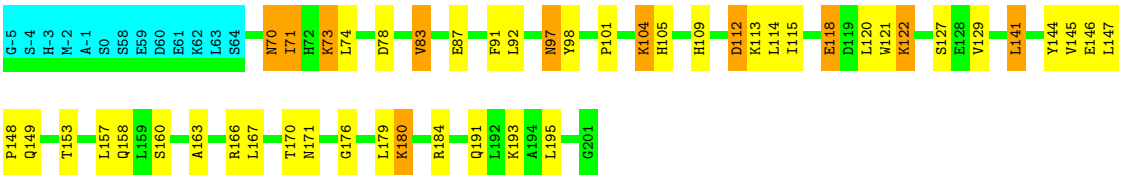
Chain A: 59% 25% 7% 9%



4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

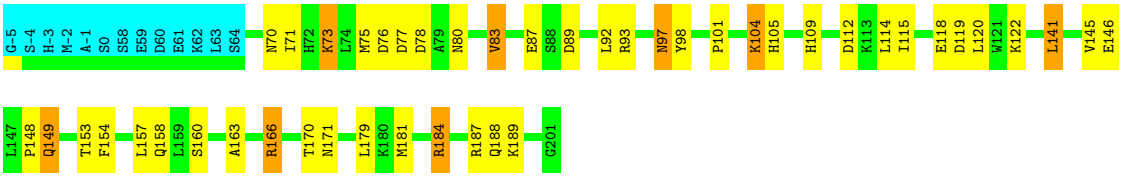
Chain A: 59% 25% 7% 9%



4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 61% 25% 5% 9%



4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 61% 27% • 9%

G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 F65 E66 R69 N70 I71 M75 D76 D77 D78 A79 V83 D84 V85 E86 E87 S88 D89 L92 R93 L96 N97 P101 K104 H105 H109 D112 K113 V134 V138 L141 Y144 V145 E146 L147

P148 Q149 Y150 E151 E152 T153 F154 R155 K156 L159 S160 A163 R166 V178 T182 S185 Q188 K189 L192 K193 A194 L195 L199 F200 G201

4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 57% 31% • 9%

G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 V68 I71 H72 K73 L74 M75 D76 D77 D78 V83 E87 S88 D89 L92 R93 L96 N97 P101 K104 H105 H109 D112 I115 E118 D119 L120 W121 K122 V134 V137 L141

V145 E146 L147 P148 Q149 Y150 E151 E152 T153 K156 L157 Q158 L159 S160 A163 R166 L167 T170 N171 T172 K180 M181 T182 D183 R184 R187 Q188 K189 L190 Q191 L192 L195 G201

4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 62% 24% 5% 9%

G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 N70 I71 H72 K73 L74 M75 D76 D77 D78 V83 E87 F91 L92 R93 E94 D95 L96 N97 Y98 P101 K104 H105 L114 I115 L120 V129 V134 L141 V145 E146 L147 E152 T153 F154

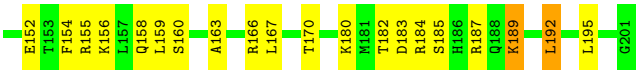
R155 K156 L157 Q158 L159 S160 A163 M164 P165 R166 N171 V178 L179 K180 D183 R187 Q188 L192 L195 L199 F200 G201

4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 59% 25% 8% 9%

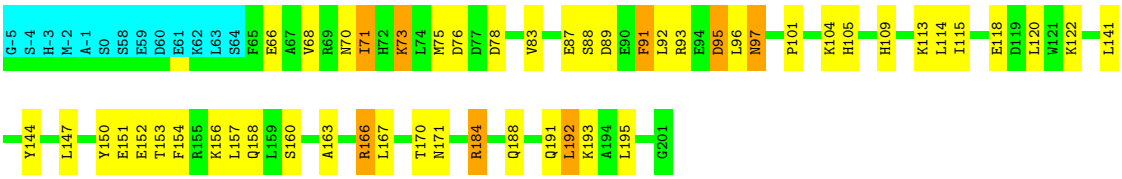
G-5 S-4 H-3 M-2 A-1 S0 S58 E59 D60 E61 K62 L63 S64 V68 I71 H72 K73 L74 M75 D76 A79 V83 E87 S88 D89 R93 E94 D95 L96 N97 Y98 H99 D100 P101 K104 H109 D112 I115 E118 D119 L120 W121 K122 V134 L141 L147



4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN (Stromal interaction molecule 1)

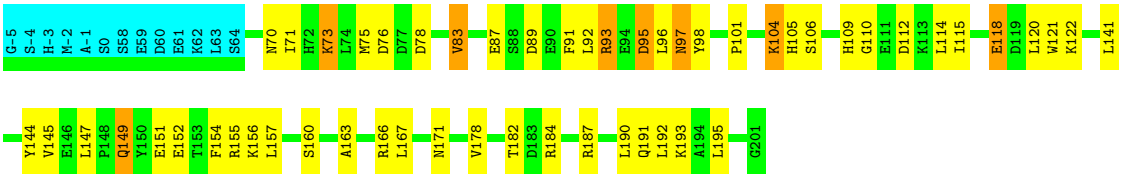
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN (Stromal interaction molecule 1)

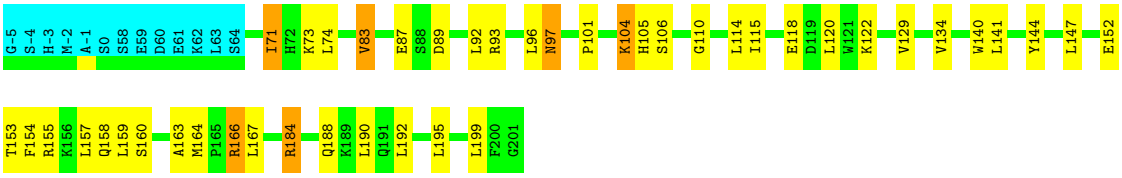
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (Stromal interaction molecule 1)

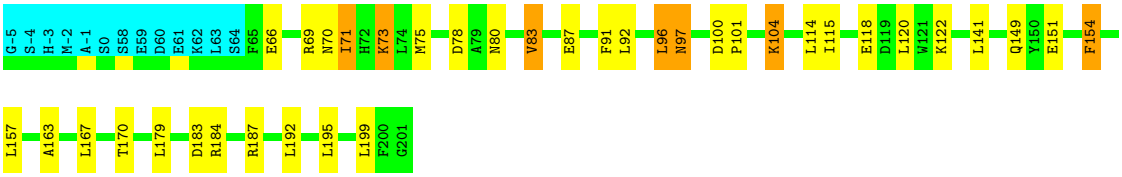
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN (Stromal interaction molecule 1)

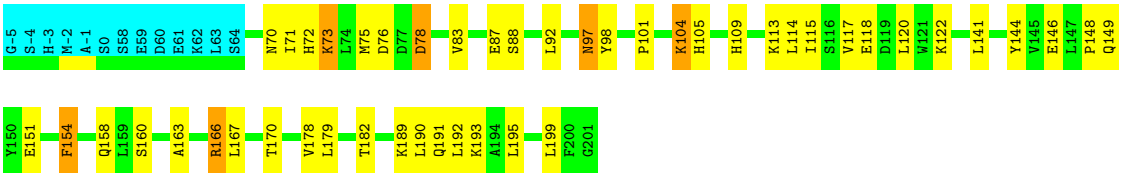
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 60% 27% • 9%



4.2.19 Score per residue for model 19

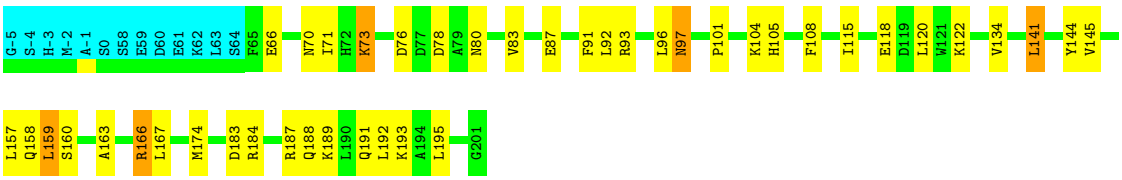
- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 67% 21% • 9%

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: PROTEIN (Stromal interaction molecule 1)

Chain A: 63% 25% • 9%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, simulated annealing.*

Of the 250 calculated structures, 20 were deposited, based on the following criterion: *20 structures for lowest energy.*

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

Software name	Classification	Version
CNS	refinement	v1.1
CYANA	structure solution	v2.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.79±0.02	1±0/1152 (0.1± 0.0%)	0.74±0.01	1±0/1563 (0.0± 0.0%)
All	All	0.79	19/23040 (0.1%)	0.74	14/31260 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	GLU	CD-OE1	-6.52	1.18	1.25	12	11
1	A	87	GLU	CD-OE2	-6.04	1.19	1.25	4	8

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	87	GLU	OE1-CD-OE2	-6.33	115.71	123.30	19	14

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	93	ARG	Sidechain	2
1	A	184	ARG	Sidechain	1

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	1127	1088	1088	24±4
2	A	1	0	0	1±1
All	All	22560	21760	21760	489

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ASP:O	1:A:93:ARG:HG3	0.70	1.87	5	11
1:A:76:ASP:OD1	2:A:686:CA:CA	0.67	1.72	10	2
1:A:96:LEU:HA	1:A:192:LEU:HD13	0.67	1.67	11	11
1:A:78:ASP:OD1	2:A:686:CA:CA	0.62	1.77	15	9
1:A:184:ARG:O	1:A:188:GLN:HG2	0.62	1.95	7	7
1:A:76:ASP:HB2	1:A:83:VAL:HG12	0.61	1.73	10	7
1:A:83:VAL:O	1:A:114:LEU:HA	0.60	1.96	12	10
1:A:70:ASN:O	1:A:73:LYS:HG3	0.59	1.97	15	13
1:A:115:ILE:HG22	1:A:120:LEU:HD11	0.58	1.76	5	16
1:A:93:ARG:HG2	1:A:101:PRO:HD3	0.58	1.75	13	7
1:A:160:SER:H	1:A:163:ALA:HB3	0.58	1.59	7	19
1:A:76:ASP:HB2	1:A:83:VAL:HG22	0.57	1.77	7	8
1:A:163:ALA:HA	1:A:166:ARG:HG3	0.57	1.76	9	11
1:A:109:HIS:CD2	1:A:112:ASP:HB3	0.57	2.35	3	4
1:A:167:LEU:HD13	1:A:190:LEU:HD12	0.56	1.76	11	5
1:A:118:GLU:O	1:A:122:LYS:HD3	0.56	2.00	9	17
1:A:151:GLU:HA	1:A:154:PHE:CE2	0.56	2.35	14	7
1:A:152:GLU:O	1:A:156:LYS:HG2	0.56	2.01	15	10
1:A:144:TYR:O	1:A:193:LYS:HE2	0.56	2.01	3	3
1:A:97:ASN:OD1	1:A:101:PRO:HA	0.55	2.01	7	18
1:A:112:ASP:OD1	1:A:114:LEU:HG	0.54	2.02	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:MET:SD	1:A:92:LEU:HD13	0.54	2.43	10	8
1:A:188:GLN:O	1:A:192:LEU:HB2	0.53	2.03	12	3
1:A:183:ASP:O	1:A:187:ARG:HG2	0.53	2.03	17	6
1:A:163:ALA:HA	1:A:166:ARG:CG	0.53	2.34	16	11
1:A:149:GLN:O	1:A:149:GLN:HG3	0.53	2.03	3	6
1:A:129:VAL:HA	1:A:132:TRP:CE3	0.53	2.39	3	2
1:A:71:ILE:O	1:A:74:LEU:HB2	0.52	2.04	4	7
1:A:104:LYS:HA	1:A:104:LYS:HE2	0.52	1.82	15	10
1:A:70:ASN:ND2	1:A:169:VAL:HG21	0.51	2.19	3	1
1:A:191:GLN:O	1:A:195:LEU:HB3	0.51	2.05	7	8
1:A:129:VAL:HG13	1:A:164:MET:SD	0.51	2.45	16	2
1:A:109:HIS:CD2	1:A:113:LYS:HB2	0.51	2.41	14	2
1:A:104:LYS:HE2	1:A:104:LYS:O	0.51	2.06	10	8
1:A:104:LYS:CE	1:A:200:PHE:HB2	0.51	2.35	2	1
1:A:144:TYR:HB3	1:A:193:LYS:HG2	0.50	1.83	18	5
1:A:91:PHE:O	1:A:95:ASP:HB2	0.50	2.07	15	4
1:A:145:VAL:HG12	1:A:147:LEU:HD23	0.50	1.81	11	2
1:A:152:GLU:O	1:A:155:ARG:HG2	0.50	2.06	13	3
1:A:171:ASN:ND2	1:A:180:LYS:HG3	0.50	2.22	8	1
1:A:185:SER:O	1:A:189:LYS:HD3	0.50	2.07	7	2
1:A:145:VAL:HG13	1:A:189:LYS:HB3	0.50	1.83	20	1
1:A:85:VAL:HG12	1:A:113:LYS:HB2	0.50	1.84	10	4
1:A:75:MET:O	1:A:88:SER:HA	0.50	2.07	19	1
1:A:83:VAL:CG1	1:A:88:SER:HB3	0.49	2.37	18	6
1:A:147:LEU:HD12	1:A:149:GLN:OE1	0.49	2.08	11	1
1:A:71:ILE:HG22	1:A:195:LEU:HD13	0.49	1.83	17	5
1:A:134:VAL:HA	1:A:159:LEU:O	0.49	2.07	12	6
1:A:104:LYS:HA	1:A:104:LYS:CE	0.49	2.37	15	9
1:A:95:ASP:O	1:A:192:LEU:HD22	0.49	2.08	14	4
1:A:171:ASN:ND2	1:A:183:ASP:HB2	0.49	2.23	12	1
1:A:85:VAL:CG1	1:A:113:LYS:HA	0.49	2.37	5	1
1:A:141:LEU:O	1:A:145:VAL:HB	0.49	2.08	5	8
1:A:195:LEU:O	1:A:199:LEU:HG	0.48	2.08	17	7
1:A:78:ASP:OD2	1:A:80:ASN:HB3	0.48	2.09	9	4
1:A:92:LEU:HD12	1:A:96:LEU:HD11	0.48	1.84	2	2
1:A:85:VAL:CG1	1:A:113:LYS:HB2	0.48	2.39	7	2
1:A:92:LEU:HD23	1:A:105:HIS:CD2	0.48	2.44	10	15
1:A:153:THR:HB	1:A:179:LEU:HD11	0.48	1.86	9	1
1:A:149:GLN:HG3	1:A:149:GLN:O	0.48	2.09	19	1
1:A:112:ASP:O	1:A:113:LYS:HG3	0.47	2.09	8	1
1:A:106:SER:O	1:A:110:GLY:HA2	0.47	2.10	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:HIS:HB3	1:A:112:ASP:O	0.47	2.08	3	5
1:A:141:LEU:O	1:A:145:VAL:HG12	0.47	2.10	9	1
1:A:185:SER:O	1:A:189:LYS:HG2	0.47	2.09	2	3
1:A:74:LEU:O	1:A:91:PHE:HB3	0.47	2.10	4	1
1:A:150:TYR:HA	1:A:153:THR:HG22	0.47	1.86	14	3
1:A:104:LYS:HE3	1:A:200:PHE:HB2	0.47	1.87	2	1
1:A:115:ILE:CG2	1:A:120:LEU:HD11	0.47	2.39	15	9
1:A:163:ALA:O	1:A:167:LEU:HG	0.46	2.10	11	8
1:A:93:ARG:CG	1:A:101:PRO:HD3	0.46	2.40	13	1
1:A:118:GLU:O	1:A:121:TRP:HB3	0.46	2.11	13	3
1:A:66:GLU:O	1:A:70:ASN:HB2	0.46	2.10	14	2
1:A:156:LYS:HA	1:A:156:LYS:HE2	0.46	1.88	1	1
1:A:153:THR:O	1:A:157:LEU:HG	0.46	2.11	3	2
1:A:188:GLN:HE21	1:A:188:GLN:HA	0.46	1.71	2	2
1:A:118:GLU:HG3	1:A:119:ASP:N	0.45	2.26	9	1
1:A:72:HIS:CG	1:A:117:VAL:HG12	0.45	2.47	4	1
1:A:151:GLU:HA	1:A:154:PHE:CD2	0.45	2.47	18	4
1:A:68:VAL:HA	1:A:71:ILE:CD1	0.45	2.42	14	1
1:A:66:GLU:O	1:A:69:ARG:HG2	0.45	2.11	10	2
1:A:68:VAL:HA	1:A:71:ILE:HD12	0.44	1.88	11	3
1:A:167:LEU:HB2	1:A:174:MET:SD	0.44	2.52	20	1
1:A:65:PHE:HA	1:A:68:VAL:HG22	0.44	1.89	7	1
1:A:71:ILE:CG2	1:A:195:LEU:HD13	0.44	2.43	17	5
1:A:144:TYR:O	1:A:193:LYS:HE3	0.44	2.12	14	2
1:A:108:PHE:CE2	1:A:115:ILE:HA	0.43	2.48	20	1
1:A:180:LYS:HG3	1:A:181:MET:O	0.43	2.13	11	1
1:A:93:ARG:HG2	1:A:101:PRO:CD	0.43	2.43	11	1
1:A:76:ASP:OD2	1:A:79:ALA:HA	0.43	2.13	10	1
1:A:163:ALA:HA	1:A:166:ARG:HB3	0.43	1.89	15	1
1:A:146:GLU:O	1:A:148:PRO:HD3	0.43	2.13	9	6
1:A:151:GLU:O	1:A:155:ARG:HG2	0.43	2.13	15	1
1:A:72:HIS:O	1:A:75:MET:HE3	0.43	2.14	18	1
1:A:193:LYS:N	1:A:193:LYS:HD2	0.43	2.28	6	1
1:A:171:ASN:O	1:A:175:THR:HG22	0.43	2.13	1	2
1:A:73:LYS:HD2	1:A:73:LYS:C	0.43	2.34	6	1
1:A:140:TRP:O	1:A:144:TYR:HB2	0.43	2.13	16	1
1:A:171:ASN:HB2	1:A:186:HIS:HD1	0.42	1.74	3	1
1:A:96:LEU:HA	1:A:192:LEU:CD1	0.42	2.44	4	1
1:A:109:HIS:ND1	1:A:113:LYS:HB2	0.42	2.29	8	1
1:A:134:VAL:O	1:A:137:VAL:HG12	0.42	2.15	11	2
1:A:188:GLN:HA	1:A:188:GLN:OE1	0.42	2.14	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:HG	1:A:186:HIS:NE2	0.42	2.30	1	1
1:A:104:LYS:NZ	1:A:199:LEU:HB3	0.42	2.30	10	1
1:A:72:HIS:CG	1:A:117:VAL:HG22	0.42	2.50	1	1
1:A:104:LYS:HE2	1:A:104:LYS:C	0.42	2.35	10	1
1:A:92:LEU:HD12	1:A:96:LEU:HD21	0.41	1.91	4	1
1:A:138:VAL:HA	1:A:141:LEU:HD23	0.41	1.92	10	1
1:A:83:VAL:HG12	1:A:115:ILE:HB	0.41	1.93	1	1
1:A:195:LEU:HA	1:A:198:VAL:HG12	0.41	1.93	3	1
1:A:143:THR:HG23	1:A:144:TYR:CD2	0.41	2.51	4	1
1:A:83:VAL:HG22	1:A:115:ILE:HG12	0.41	1.91	4	1
1:A:72:HIS:HB2	1:A:117:VAL:HG12	0.41	1.90	7	2
1:A:104:LYS:HE2	1:A:104:LYS:HA	0.41	1.93	9	2
1:A:184:ARG:CZ	1:A:188:GLN:HG3	0.41	2.46	14	1
1:A:171:ASN:HB3	1:A:187:ARG:HB3	0.41	1.92	15	2
1:A:180:LYS:HB3	1:A:186:HIS:CD2	0.41	2.51	7	1
1:A:82:ASP:HA	1:A:115:ILE:O	0.40	2.17	1	1
1:A:179:LEU:HD23	1:A:186:HIS:NE2	0.40	2.31	3	1
1:A:163:ALA:HA	1:A:166:ARG:HG2	0.40	1.92	12	1
1:A:153:THR:HB	1:A:179:LEU:HD13	0.40	1.93	8	1
1:A:93:ARG:HG2	1:A:101:PRO:HG3	0.40	1.93	20	1
1:A:137:VAL:HG11	1:A:159:LEU:C	0.40	2.37	3	1
1:A:127:SER:OG	1:A:129:VAL:HG23	0.40	2.16	8	1
1:A:149:GLN:HG2	1:A:179:LEU:HD12	0.40	1.92	8	1
1:A:68:VAL:HG22	1:A:72:HIS:NE2	0.40	2.31	13	1
1:A:92:LEU:CD1	1:A:96:LEU:HD21	0.40	2.46	15	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	136/150 (91%)	118±2 (87±1%)	15±2 (11±2%)	3±2 (2±1%)	10	49
All	All	2720/3000 (91%)	2363 (87%)	297 (11%)	60 (2%)	10	49

All 15 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	170	THR	12
1	A	158	GLN	11
1	A	98	TYR	6
1	A	178	VAL	6
1	A	91	PHE	5
1	A	99	HIS	4
1	A	101	PRO	4
1	A	180	LYS	2
1	A	79	ALA	2
1	A	102	THR	2
1	A	179	LEU	2
1	A	177	THR	1
1	A	112	ASP	1
1	A	176	GLY	1
1	A	76	ASP	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	126/137 (92%)	114±2 (90±2%)	12±2 (10±2%)	11 57
All	All	2520/2740 (92%)	2273 (90%)	247 (10%)	11 57

All 35 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	71	ILE	20
1	A	97	ASN	20
1	A	104	LYS	20
1	A	141	LEU	20
1	A	73	LYS	18
1	A	166	ARG	15
1	A	157	LEU	14
1	A	154	PHE	13
1	A	147	LEU	10
1	A	83	VAL	10
1	A	182	THR	9

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Mol	Chain	Res	Type	Models (Total)
1	A	184	ARG	8
1	A	149	GLN	8
1	A	96	LEU	7
1	A	159	LEU	7
1	A	192	LEU	7
1	A	78	ASP	5
1	A	171	ASN	4
1	A	118	GLU	4
1	A	122	LYS	4
1	A	189	LYS	4
1	A	95	ASP	3
1	A	188	GLN	2
1	A	172	THR	2
1	A	70	ASN	2
1	A	180	LYS	2
1	A	117	VAL	1
1	A	183	ASP	1
1	A	156	LYS	1
1	A	181	MET	1
1	A	68	VAL	1
1	A	109	HIS	1
1	A	119	ASP	1
1	A	100	ASP	1
1	A	179	LEU	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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