Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 02:10 PM EST

PDB ID	:	1BF8
Title	:	PERIPLASMIC CHAPERONE FIMC, NMR, 20 STRUCTURES
Authors	:	Pellecchia, M.; Guntert, P.; Glockshuber, R.; Wuthrich, K.
Deposited on	:	1998-05-28

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:

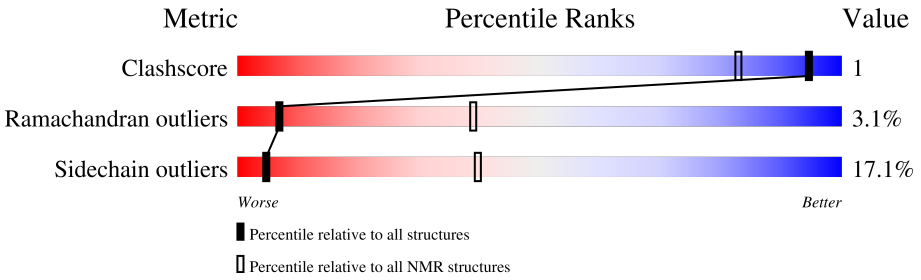
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	205	79% 15% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:2-A:92, A:106-A:205 (191)	0.78	11

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3234 atoms, of which 1636 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CHAPERONE PROTEIN FIMC.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	205	3234	1010	1636	276	306	6	0

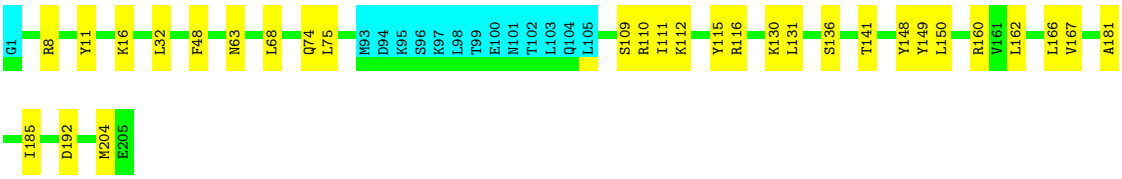
4 Residue-property plots (i)

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: CHAPERONE PROTEIN FIMC

Chain A: 79% 15% 7%



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

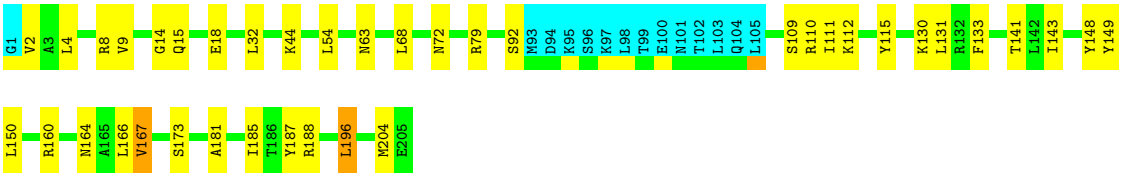
• Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 77% 16% 7%

4.2.2 Score per residue for model 2

• Molecule 1: CHAPERONE PROTEIN FIMC

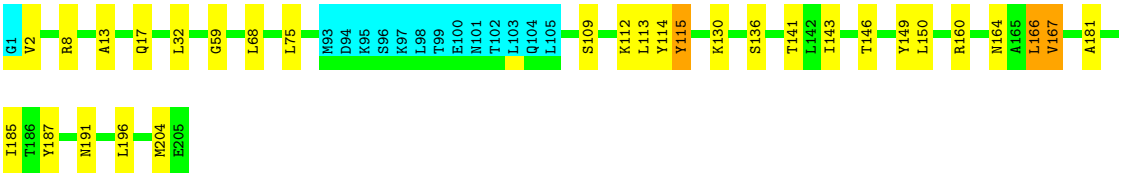
Chain A: 74% 18% • 7%



4.2.3 Score per residue for model 3

- Molecule 1: CHAPERONE PROTEIN FIMC

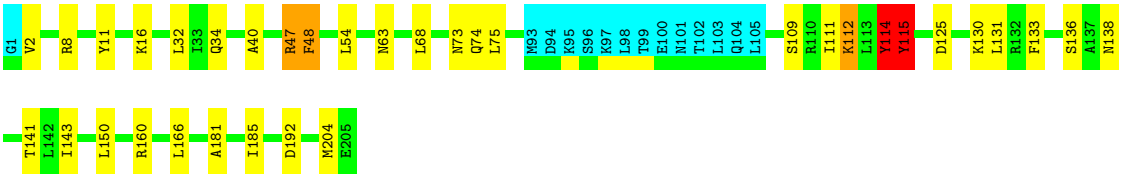
Chain A: 79% 13% • 7%



4.2.4 Score per residue for model 4

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 76% 15% •• 7%



4.2.5 Score per residue for model 5

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 76% 17% • 7%

4.2.6 Score per residue for model 6

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 75% 18% 7%

G1 L4 R8 A13 G14 Q15 K16 L32 I33 Q34 D41 K44 N63 L68 Q74 L75 R79 L82 M85 M93 D94 K95 S96 K97 L98 T99 E100 N101 T102 L103 Q104 L105 A106 R110 I111 K112 Y115 K130 L131 R132 F133 S136

T141 T146 Y149 L150 D180 A181 I185 T186 Y187 D192 Y193 K199 M204 E205

4.2.7 Score per residue for model 7

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 70% 21% • 7%

G1 R8 V9 I10 K16 T23 L32 I33 Q34 G46 R47 F48 F55 L68 T71 N72 N73 Q74 L75 P76 Q77 D78 R79 E80 N86 S92 M93 D94 K95 S96 K97 L98 T99 E100 N101 T102 L103 Q104 L105 S109 R110 I111 K112 L113 Y114 Y115 R116 L131

R132 F133 R134 R135 S136 A137 N138 S139 L140 T141 T146 P147 Y148 T153 R160 V161 L162 E163 N164 A165 L166 S173 R188 D192 Y193 M204 E205

4.2.8 Score per residue for model 8

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 74% 19% 7%

G1 R8 K16 N25 L32 I33 Q34 D41 R47 N63 R66 I67 L68 D69 A70 T71 N72 Q77 D78 R79 M93 D94 K95 S96 K97 L98 T99 E100 N101 T102 L103 Q104 L105 S109 R110 I111 K112 L113 Y114 Y115 L131 R132 F133 S136 T141 L142

I143 Y148 Y149 L150 R160 N164 A165 L166 V167 M170 S179 D180 A181 I185 R188 D192 K199 M204 E205

4.2.9 Score per residue for model 9

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 76% 16% 7%

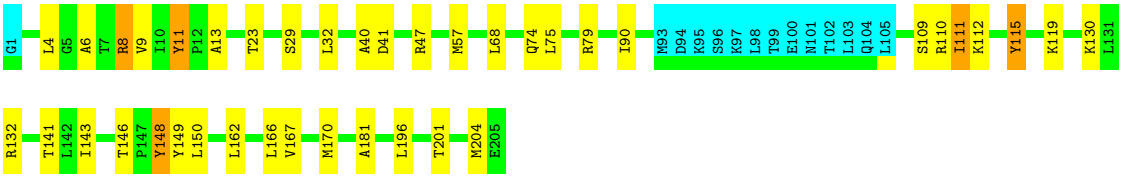
G1 R8 T30 Y31 L32 F48 L54 K58 N63 L68 N73 Q74 L75 P76 Q77 W84 M93 D94 K95 S96 K97 L98 T99 E100 N101 T102 L103 Q104 L105 S109 R110 I111 K112 R116 R135 S136 L140 T141 L150 R160 V161 L162 L166

S173 S179 D180 A181 N184 I185 T186 Y187 D192 K199 M204 E205

4.2.10 Score per residue for model 10

- Molecule 1: CHAPERONE PROTEIN FIMC

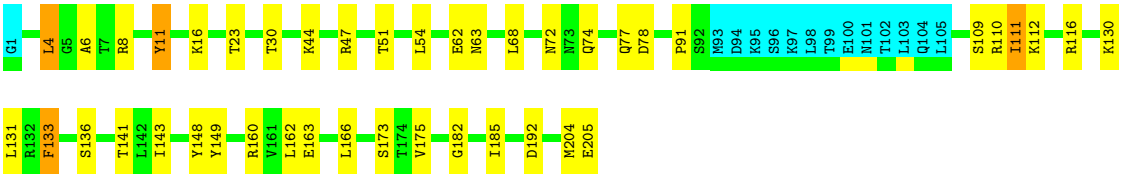
Chain A: 74% 17% • 7%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: CHAPERONE PROTEIN FIMC

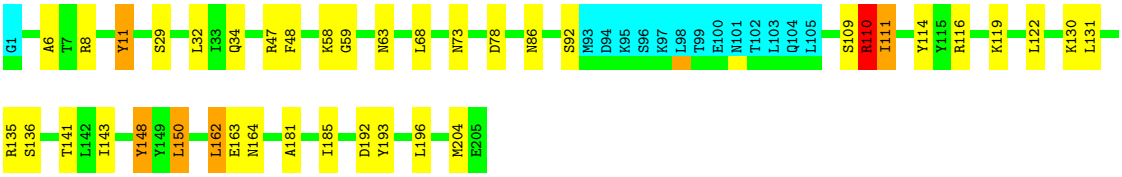
Chain A: 72% 19% • 7%



4.2.12 Score per residue for model 12

- Molecule 1: CHAPERONE PROTEIN FIMC

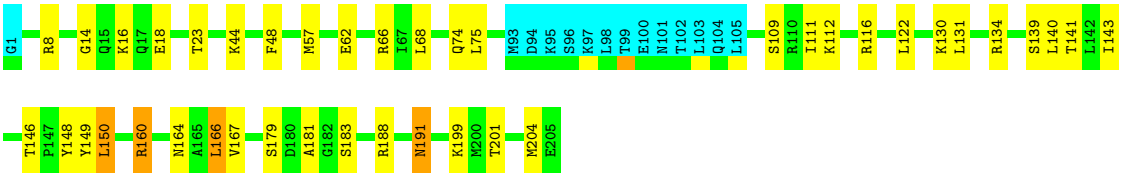
Chain A: 74% 17% • 7%



4.2.13 Score per residue for model 13

- Molecule 1: CHAPERONE PROTEIN FIMC

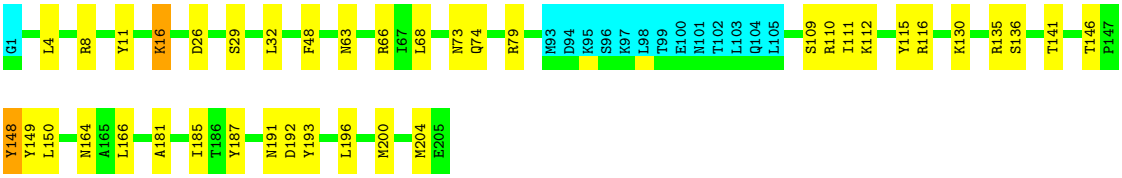
Chain A: 73% 18% • 7%



4.2.14 Score per residue for model 14

- Molecule 1: CHAPERONE PROTEIN FIMC

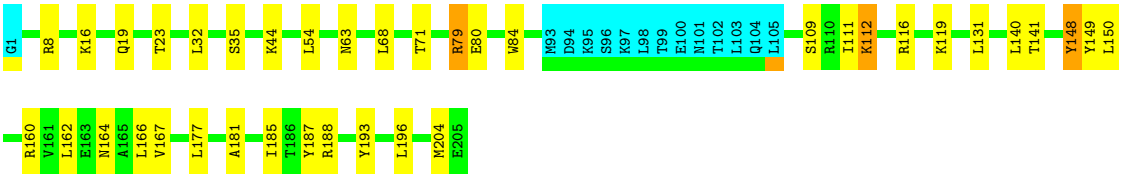
Chain A: 74% 18% • 7%



4.2.15 Score per residue for model 15

- Molecule 1: CHAPERONE PROTEIN FIMC

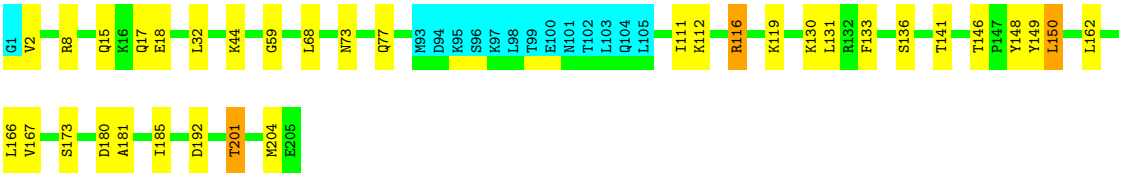
Chain A: 75% 17% • 7%



4.2.16 Score per residue for model 16

- Molecule 1: CHAPERONE PROTEIN FIMC

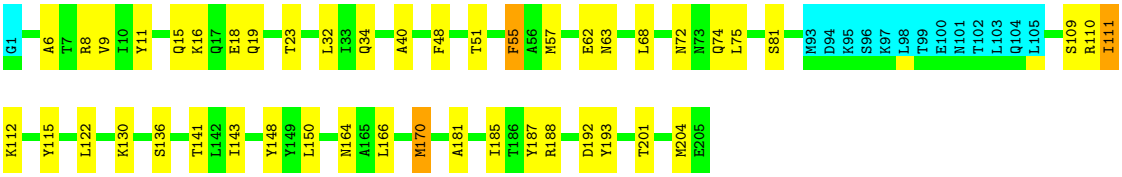
Chain A: 77% 15% • 7%



4.2.17 Score per residue for model 17

- Molecule 1: CHAPERONE PROTEIN FIMC

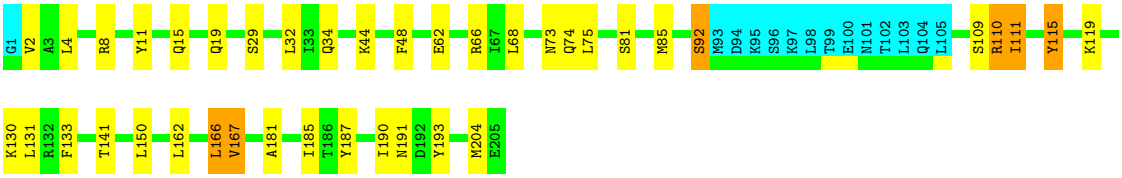
Chain A: 71% 21% • 7%



4.2.18 Score per residue for model 18

- Molecule 1: CHAPERONE PROTEIN FIMC

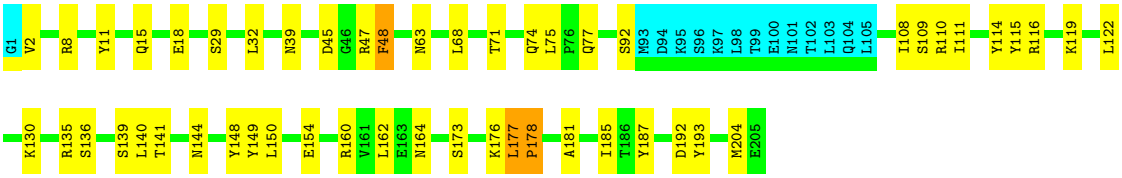
Chain A: 74% 17% • 7%



4.2.19 Score per residue for model 19

- Molecule 1: CHAPERONE PROTEIN FIMC

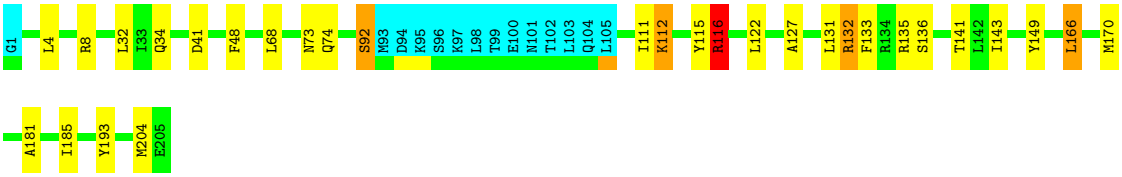
Chain A: 68% 23% • 7%



4.2.20 Score per residue for model 20

- Molecule 1: CHAPERONE PROTEIN FIMC

Chain A: 79% 12% • 7%



5 Refinement protocol and experimental data overview (i)

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

Of the 80 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
OPAL VERSION	refinement	2.6
DYANA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.59±0.00	0±0/1519 (0.0± 0.0%)	1.10±0.02	1±1/2067 (0.1± 0.1%)
All	All	0.59	0/30380 (0.0%)	1.10	26/41340 (0.1%)

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	2.4±1.6
All	All	0	47

There are no bond-length outliers.

All unique angle 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	11	TYR	CB-CG-CD2	-7.38	116.57	121.00	17	5
1	A	188	ARG	NE-CZ-NH2	-6.43	117.09	120.30	17	1
1	A	66	ARG	NE-CZ-NH2	-5.98	117.31	120.30	13	2
1	A	188	ARG	NE-CZ-NH1	5.88	123.24	120.30	17	1
1	A	148	TYR	CB-CG-CD1	-5.85	117.49	121.00	14	1
1	A	47	ARG	NE-CZ-NH2	-5.80	117.40	120.30	4	2
1	A	148	TYR	CB-CG-CD2	-5.56	117.66	121.00	15	1
1	A	116	ARG	NE-CZ-NH1	5.50	123.05	120.30	7	2
1	A	116	ARG	NE-CZ-NH2	-5.48	117.56	120.30	9	2
1	A	115	TYR	CB-CG-CD2	-5.42	117.75	121.00	20	3
1	A	132	ARG	NE-CZ-NH2	-5.39	117.60	120.30	20	3
1	A	160	ARG	NE-CZ-NH2	-5.38	117.61	120.30	11	1
1	A	187	TYR	CB-CG-CD1	-5.18	117.89	121.00	17	1
1	A	79	ARG	NE-CZ-NH2	-5.13	117.74	120.30	10	1

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	149	TYR	Sidechain	7
1	A	79	ARG	Sidechain	4
1	A	148	TYR	Sidechain	4
1	A	160	ARG	Sidechain	4
1	A	135	ARG	Sidechain	4
1	A	47	ARG	Sidechain	3
1	A	115	TYR	Sidechain	3
1	A	114	TYR	Sidechain	3
1	A	8	ARG	Sidechain	3
1	A	116	ARG	Sidechain	3
1	A	134	ARG	Sidechain	2
1	A	188	ARG	Sidechain	2
1	A	110	ARG	Sidechain	2
1	A	133	PHE	Sidechain	1
1	A	66	ARG	Sidechain	1
1	A	193	TYR	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	1490	1520	1520	3±2
All	All	29800	30400	30400	65

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:LEU:HD13	1:A:167:VAL:H	0.76	1.39	13	4
1:A:131:LEU:HD21	1:A:133:PHE:CE1	0.74	2.17	11	1
1:A:131:LEU:HD11	1:A:133:PHE:CZ	0.63	2.28	7	1
1:A:131:LEU:HD22	1:A:133:PHE:CE1	0.61	2.30	20	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HD13	1:A:150:LEU:HD13	0.60	1.71	13	2
1:A:112:LYS:HG3	1:A:166:LEU:HD11	0.58	1.75	20	1
1:A:82:LEU:HD11	1:A:112:LYS:HG3	0.55	1.79	6	1
1:A:162:LEU:HD21	1:A:175:VAL:HG21	0.55	1.77	11	1
1:A:131:LEU:HD22	1:A:150:LEU:HD11	0.53	1.81	12	2
1:A:166:LEU:HD13	1:A:167:VAL:N	0.51	2.20	2	3
1:A:112:LYS:HE2	1:A:114:TYR:CE2	0.51	2.40	5	2
1:A:6:ALA:O	1:A:111:ILE:HD11	0.50	2.06	11	4
1:A:131:LEU:HD13	1:A:150:LEU:CD1	0.50	2.36	13	1
1:A:162:LEU:HD23	1:A:163:GLU:H	0.50	1.66	12	2
1:A:162:LEU:HD23	1:A:163:GLU:N	0.49	2.22	11	1
1:A:131:LEU:HD22	1:A:133:PHE:CZ	0.48	2.44	4	2
1:A:112:LYS:HE2	1:A:114:TYR:CD2	0.48	2.44	7	1
1:A:84:TRP:CD2	1:A:112:LYS:HE2	0.48	2.44	15	1
1:A:150:LEU:H	1:A:167:VAL:HG21	0.47	1.69	8	1
1:A:122:LEU:HD22	1:A:148:TYR:CD2	0.47	2.45	12	1
1:A:153:THR:HG22	1:A:164:ASN:ND2	0.46	2.25	7	1
1:A:84:TRP:CE2	1:A:112:LYS:HE3	0.46	2.45	9	1
1:A:47:ARG:O	1:A:70:ALA:HB3	0.46	2.10	8	1
1:A:32:LEU:HD21	1:A:55:PHE:H	0.46	1.71	17	2
1:A:162:LEU:CD2	1:A:163:GLU:H	0.46	2.23	12	1
1:A:4:LEU:CD1	1:A:111:ILE:HD12	0.45	2.41	10	2
1:A:131:LEU:HD22	1:A:150:LEU:CD1	0.45	2.41	13	1
1:A:122:LEU:HD21	1:A:127:ALA:HB2	0.44	1.89	20	1
1:A:75:LEU:HD23	1:A:76:PRO:HD2	0.43	1.90	9	1
1:A:122:LEU:C	1:A:122:LEU:HD23	0.43	2.34	19	1
1:A:34:GLN:HE21	1:A:54:LEU:HD23	0.42	1.74	4	1
1:A:112:LYS:HE3	1:A:166:LEU:HD21	0.42	1.92	3	1
1:A:10:ILE:HG23	1:A:114:TYR:HB3	0.42	1.92	7	1
1:A:85:MET:HB3	1:A:111:ILE:HG22	0.42	1.90	18	1
1:A:75:LEU:HD21	1:A:115:TYR:CE2	0.41	2.50	7	1
1:A:48:PHE:CE1	1:A:115:TYR:CE2	0.41	3.08	4	2
1:A:113:LEU:HD23	1:A:113:LEU:C	0.41	2.36	3	1
1:A:131:LEU:HD23	1:A:132:ARG:N	0.41	2.30	20	1
1:A:84:TRP:CZ2	1:A:112:LYS:HE3	0.41	2.51	9	1
1:A:150:LEU:O	1:A:167:VAL:HG11	0.41	2.16	16	1
1:A:177:LEU:HD23	1:A:178:PRO:O	0.41	2.16	19	1
1:A:112:LYS:CG	1:A:166:LEU:HD11	0.41	2.46	20	1
1:A:131:LEU:HD23	1:A:132:ARG:H	0.41	1.76	20	1
1:A:133:PHE:CE1	1:A:187:TYR:CE2	0.40	3.09	2	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	190/205 (93%)	164±4 (86±2%)	20±3 (11±2%)	6±2 (3±1%)	7 39
All	All	3800/4100 (93%)	3277 (86%)	407 (11%)	116 (3%)	7 39

All 30 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	181	ALA	18
1	A	75	LEU	11
1	A	110	ARG	9
1	A	16	LYS	8
1	A	2	VAL	7
1	A	4	LEU	6
1	A	92	SER	5
1	A	74	GLN	5
1	A	40	ALA	4
1	A	72	ASN	4
1	A	199	LYS	4
1	A	196	LEU	3
1	A	13	ALA	3
1	A	17	GLN	3
1	A	59	GLY	3
1	A	15	GLN	3
1	A	106	ALA	2
1	A	138	ASN	2
1	A	14	GLY	2
1	A	179	SER	2
1	A	191	ASN	2
1	A	201	THR	2
1	A	46	GLY	1
1	A	182	GLY	1
1	A	71	THR	1
1	A	55	PHE	1
1	A	170	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	190	ILE	1
1	A	178	PRO	1
1	A	116	ARG	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	163/176 (93%)	135±4 (83±3%)	28±4 (17±3%)	5 40
All	All	3260/3520 (93%)	2703 (83%)	557 (17%)	5 40

All 98 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	68	LEU	20
1	A	141	THR	20
1	A	204	MET	20
1	A	8	ARG	18
1	A	111	ILE	18
1	A	185	ILE	17
1	A	32	LEU	16
1	A	150	LEU	16
1	A	166	LEU	16
1	A	109	SER	16
1	A	136	SER	15
1	A	112	LYS	14
1	A	130	LYS	13
1	A	48	PHE	12
1	A	63	ASN	11
1	A	192	ASP	11
1	A	115	TYR	10
1	A	148	TYR	10
1	A	143	ILE	10
1	A	164	ASN	9
1	A	73	ASN	9
1	A	162	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	44	LYS	8
1	A	187	TYR	8
1	A	193	TYR	8
1	A	146	THR	7
1	A	74	GLN	7
1	A	160	ARG	7
1	A	119	LYS	7
1	A	34	GLN	7
1	A	29	SER	6
1	A	167	VAL	6
1	A	18	GLU	6
1	A	149	TYR	6
1	A	173	SER	6
1	A	11	TYR	6
1	A	110	ARG	6
1	A	140	LEU	6
1	A	23	THR	6
1	A	77	GLN	6
1	A	116	ARG	6
1	A	170	MET	5
1	A	62	GLU	5
1	A	19	GLN	4
1	A	57	MET	4
1	A	54	LEU	4
1	A	196	LEU	4
1	A	114	TYR	4
1	A	79	ARG	4
1	A	201	THR	4
1	A	41	ASP	4
1	A	92	SER	4
1	A	86	ASN	3
1	A	9	VAL	3
1	A	15	GLN	3
1	A	188	ARG	3
1	A	191	ASN	3
1	A	16	LYS	3
1	A	47	ARG	3
1	A	125	ASP	2
1	A	25	ASN	2
1	A	184	ASN	2
1	A	180	ASP	2
1	A	71	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	80	GLU	2
1	A	30	THR	2
1	A	58	LYS	2
1	A	135	ARG	2
1	A	179	SER	2
1	A	51	THR	2
1	A	78	ASP	2
1	A	122	LEU	2
1	A	139	SER	2
1	A	177	LEU	2
1	A	81	SER	2
1	A	155	LEU	1
1	A	138	ASN	1
1	A	27	GLU	1
1	A	65	LEU	1
1	A	134	ARG	1
1	A	85	MET	1
1	A	66	ARG	1
1	A	75	LEU	1
1	A	90	ILE	1
1	A	205	GLU	1
1	A	183	SER	1
1	A	199	LYS	1
1	A	26	ASP	1
1	A	200	MET	1
1	A	35	SER	1
1	A	131	LEU	1
1	A	72	ASN	1
1	A	39	ASN	1
1	A	45	ASP	1
1	A	108	ILE	1
1	A	144	ASN	1
1	A	154	GLU	1
1	A	176	LYS	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