



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:15 pm GMT

PDB ID : 1V6F
Title : Solution Structure of Glia Maturation Factor-beta from Mus Musculus
Authors : Goroncy, A.K.; Kigawa, T.; Koshiba, S.; Tomizawa, T.; Kobayashi, N.; Tochio, N.; Inoue, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-11-29

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

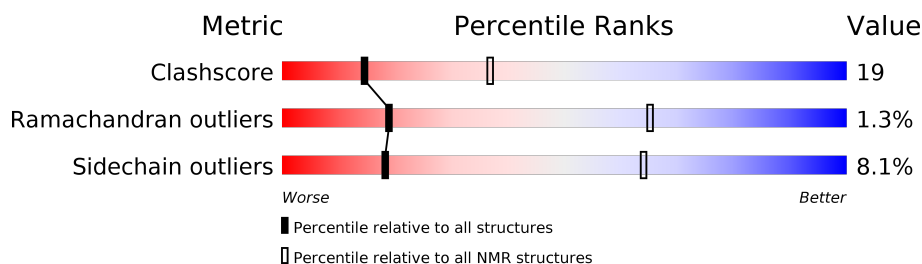
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	151	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:14-A:43, A:48-A:81, A:89-A:145 (121)	0.17	1

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2391 atoms, of which 1188 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called glia maturation factor, beta.

Mol	Chain	Residues	Atoms						Trace
1	A	151	Total	C	H	N	O	S	0
			2391	754	1188	203	240	6	

There are 13 discrepancies between the modelled and reference sequences:

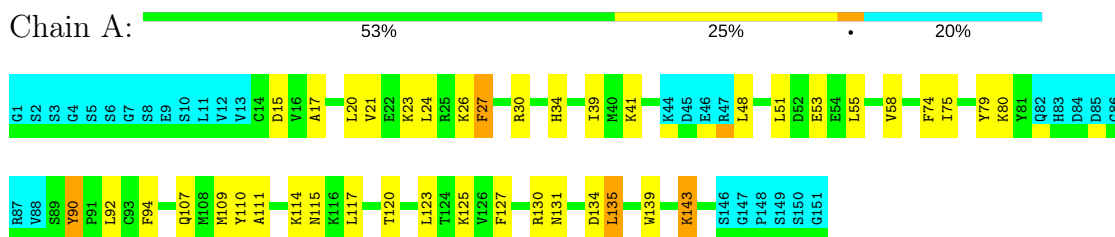
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	GB 12851526
A	2	SER	-	CLONING ARTIFACT	GB 12851526
A	3	SER	-	CLONING ARTIFACT	GB 12851526
A	4	GLY	-	CLONING ARTIFACT	GB 12851526
A	5	SER	-	CLONING ARTIFACT	GB 12851526
A	6	SER	-	CLONING ARTIFACT	GB 12851526
A	7	GLY	-	CLONING ARTIFACT	GB 12851526
A	146	SER	-	CLONING ARTIFACT	GB 12851526
A	147	GLY	-	CLONING ARTIFACT	GB 12851526
A	148	PRO	-	CLONING ARTIFACT	GB 12851526
A	149	SER	-	CLONING ARTIFACT	GB 12851526
A	150	SER	-	CLONING ARTIFACT	GB 12851526
A	151	GLY	-	CLONING ARTIFACT	GB 12851526

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: glia maturation factor, beta

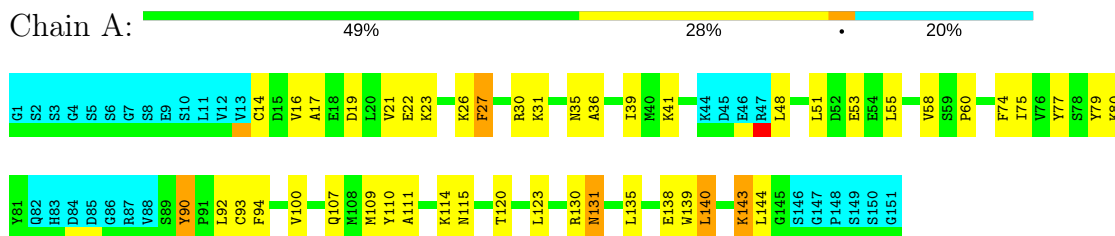


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

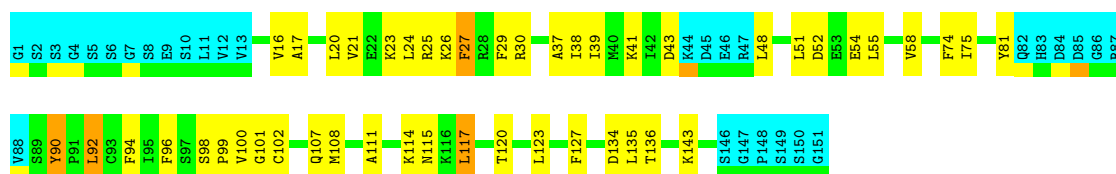
- Molecule 1: glia maturation factor, beta



4.2.2 Score per residue for model 2

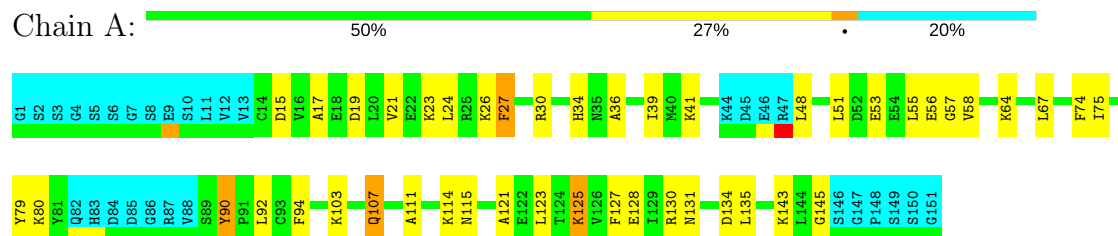
- Molecule 1: glia maturation factor, beta





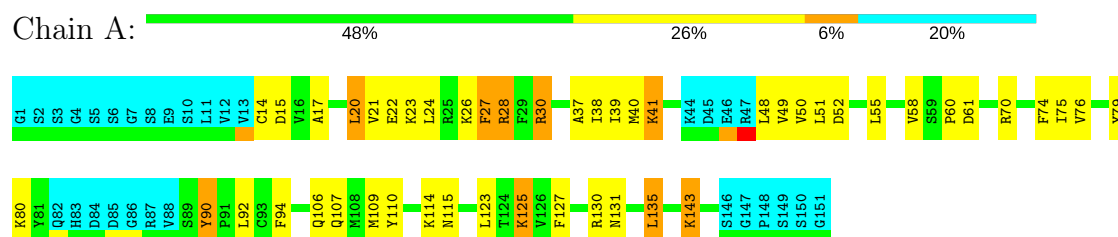
4.2.3 Score per residue for model 3

- Molecule 1: glia maturation factor, beta



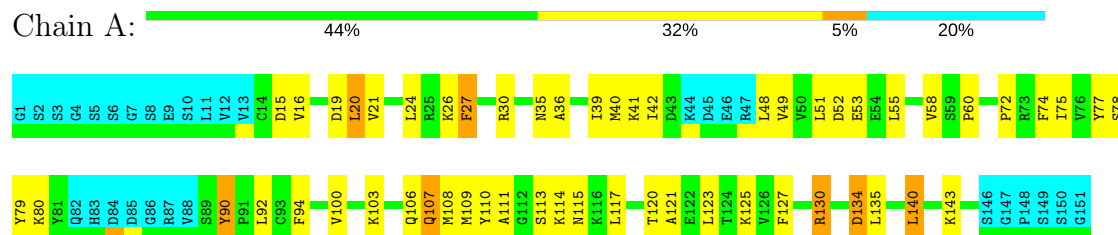
4.2.4 Score per residue for model 4

- Molecule 1: glia maturation factor, beta



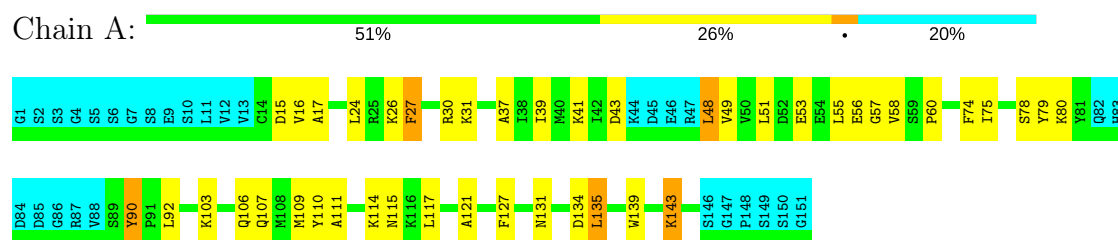
4.2.5 Score per residue for model 5

- Molecule 1: glia maturation factor, beta



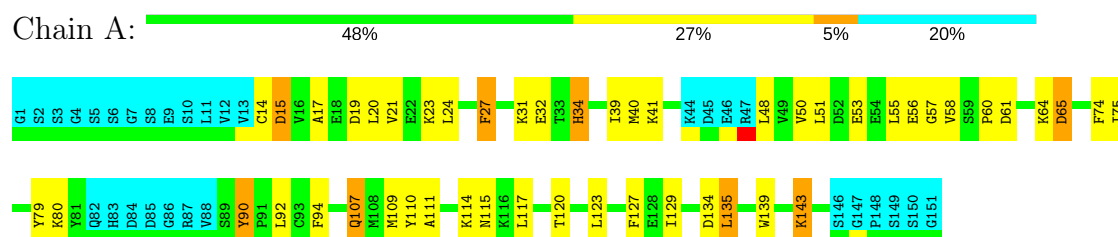
4.2.6 Score per residue for model 6

- Molecule 1: glia maturation factor, beta



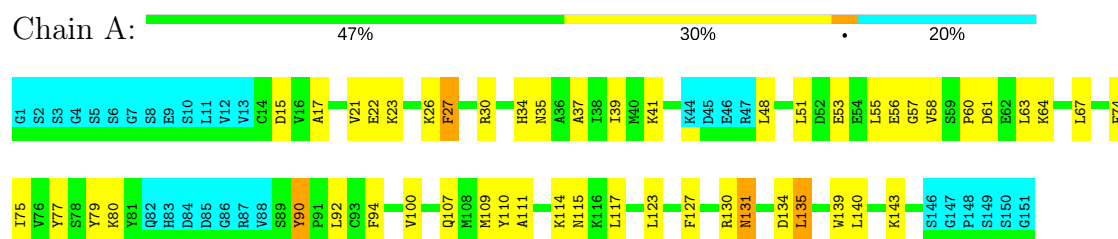
4.2.7 Score per residue for model 7

- Molecule 1: glia maturation factor, beta



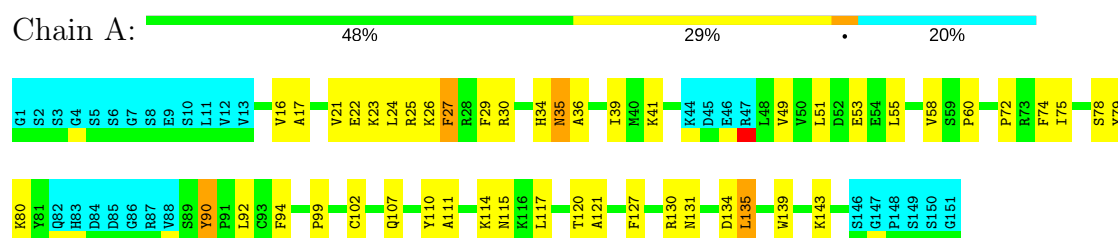
4.2.8 Score per residue for model 8

- Molecule 1: glia maturation factor, beta



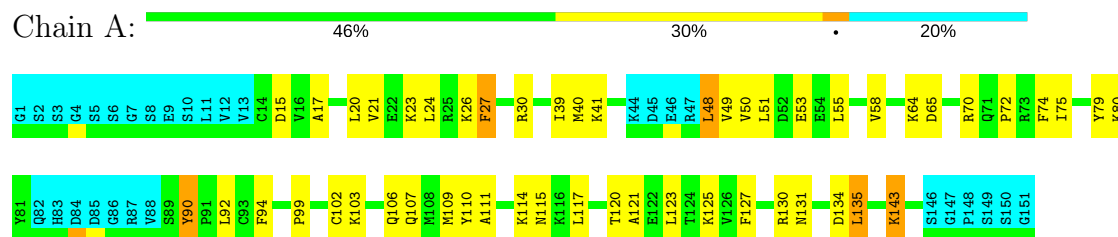
4.2.9 Score per residue for model 9

- Molecule 1: glia maturation factor, beta



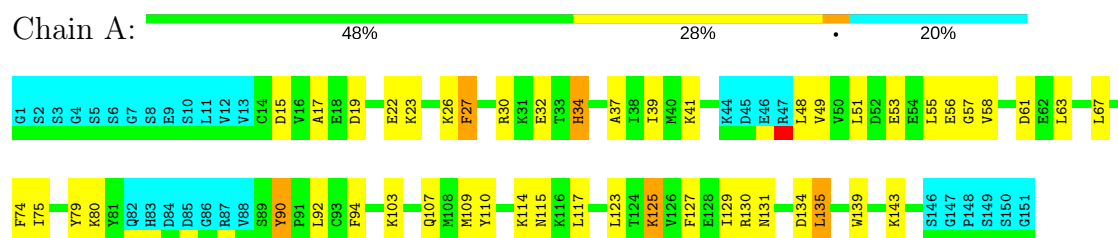
4.2.10 Score per residue for model 10

- Molecule 1: glia maturation factor, beta



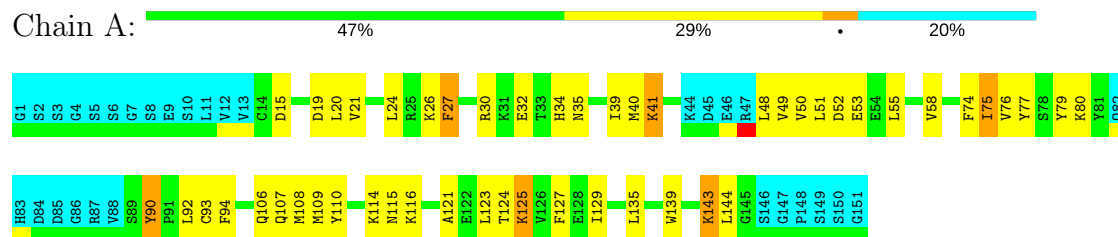
4.2.11 Score per residue for model 11

- Molecule 1: glia maturation factor, beta



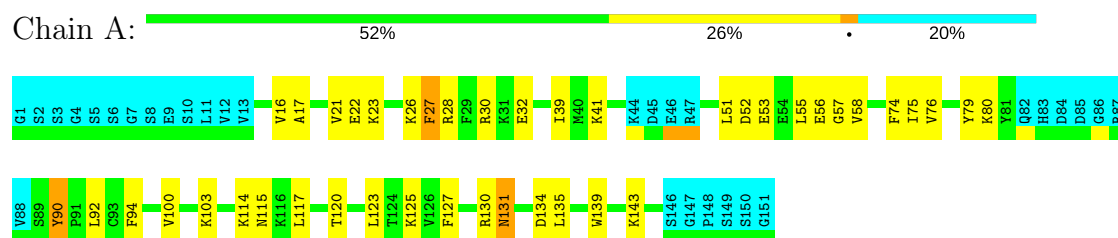
4.2.12 Score per residue for model 12

- Molecule 1: glia maturation factor, beta



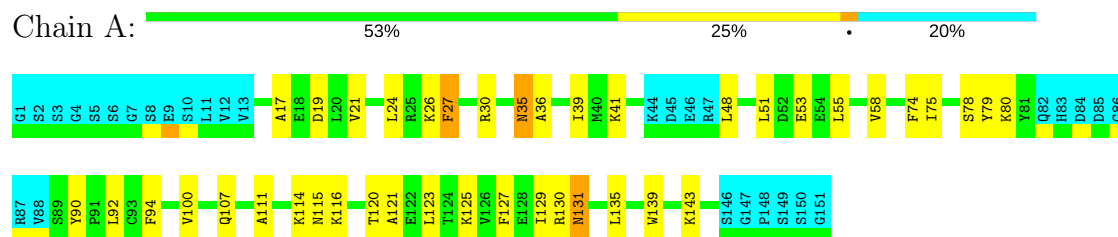
4.2.13 Score per residue for model 13

- Molecule 1: glia maturation factor, beta



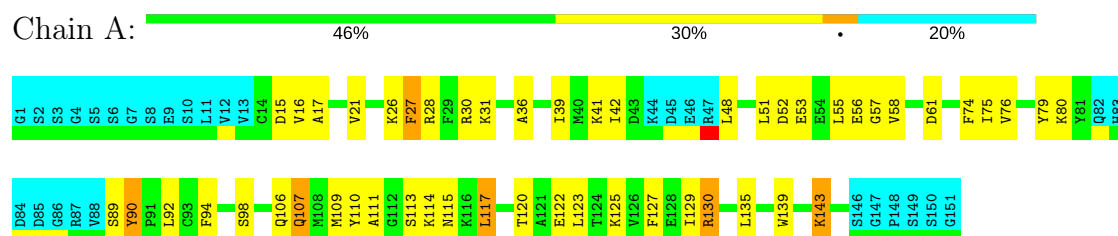
4.2.14 Score per residue for model 14

- Molecule 1: glia maturation factor, beta



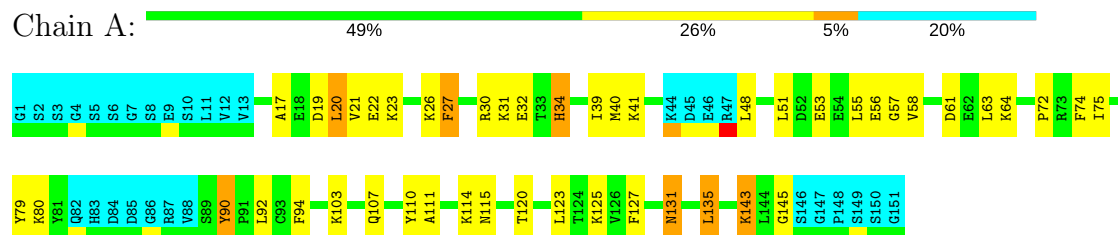
4.2.15 Score per residue for model 15

- Molecule 1: glia maturation factor, beta



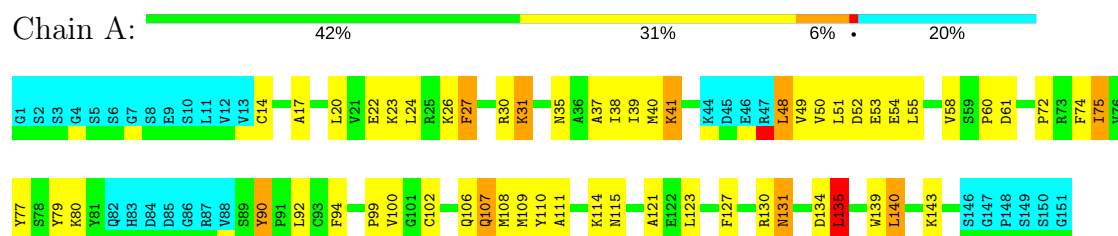
4.2.16 Score per residue for model 16

- Molecule 1: glia maturation factor, beta



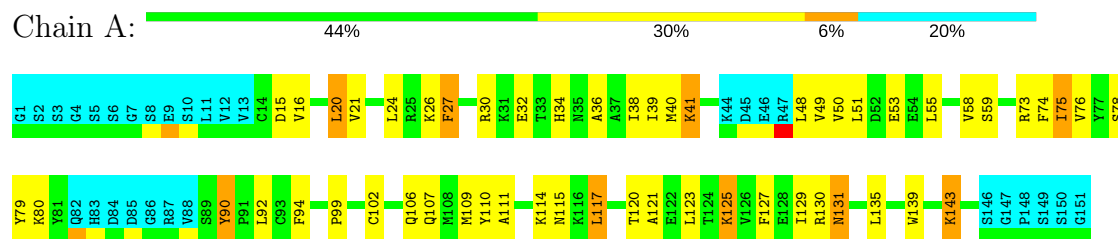
4.2.17 Score per residue for model 17

- Molecule 1: glia maturation factor, beta



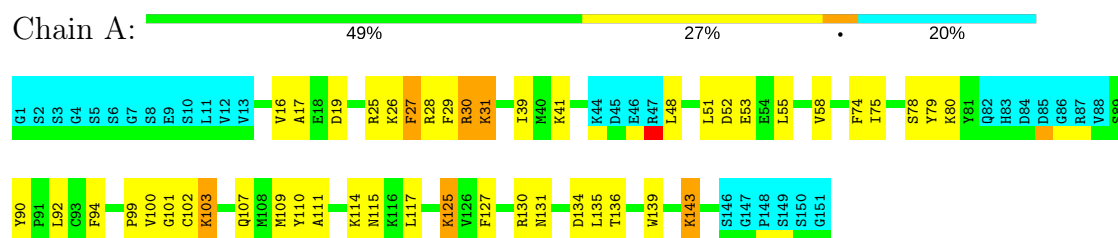
4.2.18 Score per residue for model 18

- Molecule 1: glia maturation factor, beta



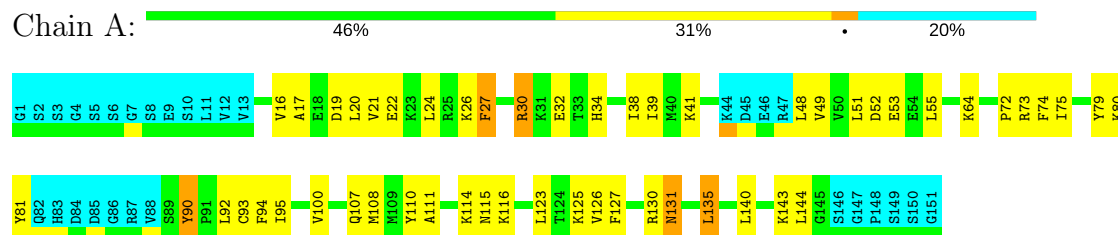
4.2.19 Score per residue for model 19

- Molecule 1: glia maturation factor, beta



4.2.20 Score per residue for model 20

- Molecule 1: glia maturation factor, beta



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 100 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	refinement	2.0.17

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	997	1001	1000	38±7
All	All	19940	20020	20000	766

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CD1	1:A:92:LEU:HD11	0.93	1.99	15	16
1:A:39:ILE:HD12	1:A:53:GLU:CG	0.92	1.95	12	16
1:A:27:PHE:CD1	1:A:92:LEU:HD21	0.91	2.01	19	4
1:A:27:PHE:CG	1:A:92:LEU:HD21	0.87	2.04	9	4
1:A:23:LYS:HD2	1:A:51:LEU:HD23	0.86	1.45	2	1
1:A:23:LYS:CD	1:A:51:LEU:HD23	0.82	2.04	2	1
1:A:39:ILE:HD12	1:A:53:GLU:HG3	0.81	1.53	15	14
1:A:74:PHE:C	1:A:75:ILE:HD12	0.79	1.98	5	20
1:A:60:PRO:HB3	1:A:140:LEU:HD23	0.76	1.56	5	3
1:A:39:ILE:HD12	1:A:53:GLU:CD	0.73	2.02	20	8
1:A:75:ILE:N	1:A:75:ILE:HD12	0.73	1.98	17	11
1:A:94:PHE:HB2	1:A:123:LEU:HD13	0.73	1.61	5	16
1:A:51:LEU:HD13	1:A:51:LEU:C	0.72	2.04	6	5
1:A:100:VAL:HG13	1:A:130:ARG:O	0.71	1.85	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD11	1:A:40:MET:HG2	0.71	1.63	16	7
1:A:64:LYS:HB3	1:A:135:LEU:HD23	0.71	1.62	20	3
1:A:16:VAL:HG21	1:A:120:THR:HG21	0.69	1.64	15	2
1:A:51:LEU:C	1:A:51:LEU:HD13	0.69	2.07	1	11
1:A:109:MET:CE	1:A:110:TYR:CE2	0.69	2.76	15	8
1:A:74:PHE:CD2	1:A:117:LEU:CD1	0.68	2.76	6	2
1:A:53:GLU:OE1	1:A:55:LEU:HD21	0.68	1.88	17	3
1:A:75:ILE:HD12	1:A:75:ILE:N	0.68	2.03	12	9
1:A:60:PRO:O	1:A:135:LEU:HD22	0.68	1.87	8	6
1:A:37:ALA:HB3	1:A:55:LEU:HB2	0.67	1.66	11	4
1:A:109:MET:CE	1:A:110:TYR:CE1	0.66	2.79	18	5
1:A:24:LEU:HD13	1:A:121:ALA:HB2	0.66	1.66	10	9
1:A:27:PHE:CE1	1:A:92:LEU:HD11	0.65	2.26	15	15
1:A:17:ALA:HB2	1:A:48:LEU:HD23	0.65	1.67	14	5
1:A:100:VAL:HG23	1:A:130:ARG:O	0.65	1.92	8	5
1:A:51:LEU:HD21	1:A:54:GLU:HG3	0.64	1.68	2	1
1:A:55:LEU:HB3	1:A:58:VAL:HG11	0.63	1.70	17	17
1:A:38:ILE:HG23	1:A:51:LEU:CD2	0.63	2.24	18	2
1:A:74:PHE:CD2	1:A:117:LEU:HD11	0.62	2.28	6	4
1:A:41:LYS:HE3	1:A:50:VAL:HG23	0.62	1.71	17	1
1:A:17:ALA:O	1:A:21:VAL:HG23	0.61	1.95	4	9
1:A:60:PRO:CB	1:A:140:LEU:HD23	0.61	2.25	1	3
1:A:79:TYR:CE2	1:A:80:LYS:O	0.61	2.53	9	2
1:A:27:PHE:CG	1:A:92:LEU:CD2	0.60	2.84	9	4
1:A:90:TYR:CD1	1:A:90:TYR:N	0.60	2.69	17	9
1:A:21:VAL:HG13	1:A:120:THR:CG2	0.60	2.26	18	7
1:A:74:PHE:CD2	1:A:117:LEU:CD2	0.60	2.84	2	4
1:A:41:LYS:HZ3	1:A:50:VAL:HG23	0.60	1.56	12	1
1:A:134:ASP:OD1	1:A:139:TRP:CD1	0.60	2.55	19	5
1:A:41:LYS:HD3	1:A:50:VAL:HG23	0.59	1.74	18	2
1:A:38:ILE:HG23	1:A:51:LEU:HD23	0.59	1.72	4	1
1:A:130:ARG:CZ	1:A:131:ASN:ND2	0.59	2.66	17	1
1:A:55:LEU:HD12	1:A:58:VAL:HG11	0.58	1.72	11	2
1:A:25:ARG:O	1:A:29:PHE:CD2	0.58	2.56	19	3
1:A:74:PHE:CE2	1:A:117:LEU:HD11	0.58	2.32	6	1
1:A:38:ILE:HG23	1:A:51:LEU:HD13	0.58	1.74	2	1
1:A:130:ARG:NE	1:A:131:ASN:ND2	0.57	2.52	10	6
1:A:109:MET:CE	1:A:110:TYR:CZ	0.56	2.89	19	3
1:A:109:MET:HE2	1:A:110:TYR:CE1	0.56	2.36	4	4
1:A:107:GLN:O	1:A:111:ALA:HB2	0.56	2.01	20	15
1:A:37:ALA:HB3	1:A:55:LEU:HD12	0.56	1.76	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:HD12	1:A:110:TYR:CD1	0.55	2.36	15	2
1:A:16:VAL:HG12	1:A:117:LEU:HD22	0.55	1.78	19	2
1:A:96:PHE:CZ	1:A:98:SER:OG	0.55	2.60	2	1
1:A:27:PHE:CE1	1:A:36:ALA:HB3	0.55	2.37	18	2
1:A:30:ARG:NH2	1:A:36:ALA:HB2	0.55	2.17	1	4
1:A:130:ARG:NE	1:A:131:ASN:HD21	0.55	2.00	18	2
1:A:64:LYS:CB	1:A:135:LEU:HD23	0.55	2.31	10	2
1:A:15:ASP:HB2	1:A:48:LEU:HD11	0.54	1.78	12	6
1:A:24:LEU:HD11	1:A:40:MET:SD	0.54	2.43	7	1
1:A:39:ILE:O	1:A:51:LEU:HD12	0.54	2.01	2	1
1:A:27:PHE:CE1	1:A:78:SER:HB2	0.54	2.38	14	4
1:A:90:TYR:N	1:A:90:TYR:CD1	0.54	2.74	4	11
1:A:131:ASN:N	1:A:131:ASN:OD1	0.54	2.41	20	3
1:A:31:LYS:CD	1:A:31:LYS:O	0.53	2.57	17	1
1:A:63:LEU:HD21	1:A:75:ILE:HG21	0.53	1.80	16	2
1:A:20:LEU:CD2	1:A:49:VAL:HG12	0.53	2.33	20	1
1:A:93:CYS:SG	1:A:144:LEU:HD21	0.53	2.44	20	3
1:A:129:ILE:CG2	1:A:139:TRP:CZ2	0.53	2.92	15	6
1:A:78:SER:OG	1:A:92:LEU:HD22	0.53	2.04	6	2
1:A:20:LEU:CD2	1:A:20:LEU:C	0.53	2.76	18	2
1:A:16:VAL:HG21	1:A:120:THR:CG2	0.53	2.32	15	1
1:A:131:ASN:OD1	1:A:131:ASN:N	0.52	2.41	13	4
1:A:107:GLN:O	1:A:111:ALA:CB	0.52	2.58	15	15
1:A:75:ILE:N	1:A:75:ILE:CD1	0.52	2.70	17	7
1:A:55:LEU:CD1	1:A:63:LEU:CD1	0.52	2.88	8	1
1:A:53:GLU:OE2	1:A:55:LEU:HD21	0.52	2.05	18	1
1:A:20:LEU:CD1	1:A:49:VAL:HG12	0.52	2.34	5	3
1:A:94:PHE:CD1	1:A:126:VAL:HG23	0.52	2.39	20	1
1:A:79:TYR:CG	1:A:80:LYS:N	0.52	2.78	5	19
1:A:74:PHE:C	1:A:75:ILE:CD1	0.52	2.77	5	15
1:A:109:MET:HE2	1:A:110:TYR:CE2	0.52	2.40	10	4
1:A:51:LEU:CD1	1:A:51:LEU:C	0.52	2.77	3	8
1:A:38:ILE:HG23	1:A:51:LEU:HD21	0.51	1.83	18	1
1:A:17:ALA:CB	1:A:49:VAL:O	0.51	2.59	4	3
1:A:127:PHE:CE2	1:A:143:LYS:HB2	0.50	2.41	17	4
1:A:51:LEU:C	1:A:51:LEU:CD1	0.50	2.78	20	4
1:A:64:LYS:HA	1:A:67:LEU:HD12	0.50	1.82	3	2
1:A:139:TRP:CZ2	1:A:143:LYS:HE3	0.50	2.41	1	2
1:A:75:ILE:CD1	1:A:75:ILE:N	0.50	2.75	5	5
1:A:16:VAL:HG12	1:A:117:LEU:CD2	0.50	2.37	19	1
1:A:31:LYS:O	1:A:31:LYS:CD	0.50	2.59	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LYS:O	1:A:30:ARG:N	0.50	2.44	6	19
1:A:15:ASP:CB	1:A:48:LEU:HD11	0.50	2.36	12	4
1:A:39:ILE:O	1:A:51:LEU:CD1	0.50	2.60	2	1
1:A:27:PHE:CE2	1:A:76:VAL:O	0.49	2.65	12	4
1:A:106:GLN:O	1:A:109:MET:N	0.49	2.45	15	7
1:A:21:VAL:O	1:A:24:LEU:N	0.49	2.45	20	5
1:A:127:PHE:CD1	1:A:143:LYS:HB3	0.49	2.42	20	17
1:A:21:VAL:HG13	1:A:120:THR:HG23	0.49	1.85	1	2
1:A:30:ARG:NH2	1:A:32:GLU:CD	0.49	2.66	13	1
1:A:51:LEU:HD12	1:A:52:ASP:N	0.49	2.22	2	1
1:A:20:LEU:HD21	1:A:40:MET:HG2	0.49	1.84	12	2
1:A:16:VAL:O	1:A:16:VAL:HG23	0.49	2.08	20	2
1:A:51:LEU:HD22	1:A:52:ASP:N	0.49	2.23	19	1
1:A:72:PRO:HG2	1:A:110:TYR:CD2	0.49	2.43	17	6
1:A:40:MET:HE2	1:A:76:VAL:HG23	0.49	1.84	4	2
1:A:39:ILE:O	1:A:51:LEU:CD2	0.48	2.61	19	1
1:A:106:GLN:OE1	1:A:109:MET:CE	0.48	2.61	10	1
1:A:110:TYR:O	1:A:114:LYS:N	0.48	2.45	15	1
1:A:109:MET:HE1	1:A:110:TYR:CE2	0.48	2.42	8	1
1:A:41:LYS:CD	1:A:41:LYS:N	0.48	2.77	4	2
1:A:114:LYS:O	1:A:115:ASN:C	0.48	2.52	15	20
1:A:99:PRO:O	1:A:102:CYS:N	0.48	2.47	19	5
1:A:31:LYS:CG	1:A:31:LYS:O	0.48	2.61	17	1
1:A:20:LEU:HD12	1:A:50:VAL:CA	0.47	2.40	10	3
1:A:129:ILE:HG22	1:A:139:TRP:CZ2	0.47	2.44	15	2
1:A:51:LEU:HD13	1:A:52:ASP:N	0.47	2.23	17	5
1:A:55:LEU:HD12	1:A:63:LEU:CD1	0.47	2.39	8	1
1:A:27:PHE:CZ	1:A:36:ALA:HB3	0.47	2.44	18	3
1:A:17:ALA:HB2	1:A:48:LEU:HD12	0.47	1.85	17	3
1:A:20:LEU:HD11	1:A:40:MET:CG	0.47	2.40	18	4
1:A:41:LYS:NZ	1:A:50:VAL:HG23	0.47	2.23	12	1
1:A:127:PHE:CE1	1:A:143:LYS:HB3	0.47	2.45	16	2
1:A:125:LYS:HB3	1:A:127:PHE:CZ	0.47	2.45	18	10
1:A:48:LEU:HD13	1:A:49:VAL:N	0.47	2.24	6	3
1:A:95:ILE:HG21	1:A:135:LEU:HD13	0.47	1.87	20	1
1:A:21:VAL:HG22	1:A:120:THR:HG21	0.47	1.87	2	2
1:A:41:LYS:NZ	1:A:51:LEU:C	0.47	2.68	12	1
1:A:127:PHE:CG	1:A:143:LYS:HB3	0.46	2.45	17	1
1:A:51:LEU:HD13	1:A:53:GLU:N	0.46	2.25	18	1
1:A:22:GLU:CG	1:A:23:LYS:N	0.46	2.78	17	8
1:A:32:GLU:HB3	1:A:34:HIS:CE1	0.46	2.46	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HG21	1:A:120:THR:OG1	0.46	2.11	2	2
1:A:134:ASP:OD2	1:A:139:TRP:CD1	0.46	2.69	13	1
1:A:78:SER:OG	1:A:92:LEU:CD1	0.46	2.64	14	1
1:A:100:VAL:CG2	1:A:130:ARG:O	0.45	2.65	17	3
1:A:41:LYS:HD2	1:A:41:LYS:N	0.45	2.26	4	2
1:A:35:ASN:N	1:A:35:ASN:OD1	0.45	2.49	14	1
1:A:38:ILE:HD11	1:A:54:GLU:OE2	0.45	2.11	17	1
1:A:35:ASN:OD1	1:A:35:ASN:N	0.45	2.50	9	1
1:A:39:ILE:O	1:A:51:LEU:HD22	0.45	2.12	18	3
1:A:30:ARG:NH2	1:A:32:GLU:OE1	0.45	2.50	12	1
1:A:134:ASP:O	1:A:136:THR:N	0.45	2.50	2	2
1:A:56:GLU:O	1:A:57:GLY:C	0.44	2.56	6	8
1:A:16:VAL:HG22	1:A:116:LYS:HE2	0.44	1.90	20	1
1:A:79:TYR:CD2	1:A:80:LYS:N	0.44	2.85	18	2
1:A:41:LYS:HZ2	1:A:52:ASP:N	0.44	2.10	12	1
1:A:130:ARG:NH2	1:A:134:ASP:OD1	0.44	2.51	5	1
1:A:35:ASN:ND2	1:A:77:TYR:OH	0.44	2.50	17	5
1:A:32:GLU:OE1	1:A:34:HIS:NE2	0.44	2.51	12	1
1:A:138:GLU:CD	1:A:138:GLU:C	0.44	2.77	1	1
1:A:17:ALA:N	1:A:48:LEU:CD1	0.44	2.81	6	3
1:A:74:PHE:CD2	1:A:117:LEU:HD21	0.43	2.48	2	3
1:A:60:PRO:O	1:A:135:LEU:CD2	0.43	2.63	8	1
1:A:94:PHE:CZ	1:A:114:LYS:HG3	0.43	2.49	8	2
1:A:23:LYS:CD	1:A:51:LEU:HG	0.43	2.44	7	3
1:A:64:LYS:HG2	1:A:65:ASP:N	0.43	2.29	7	1
1:A:99:PRO:O	1:A:101:GLY:N	0.43	2.50	19	2
1:A:94:PHE:CE1	1:A:114:LYS:HG3	0.43	2.49	20	4
1:A:16:VAL:CG1	1:A:117:LEU:CD2	0.43	2.97	19	1
1:A:94:PHE:HB3	1:A:126:VAL:CB	0.43	2.43	20	1
1:A:17:ALA:N	1:A:48:LEU:HD11	0.43	2.28	6	1
1:A:143:LYS:N	1:A:143:LYS:HD2	0.42	2.29	17	1
1:A:28:ARG:NE	1:A:28:ARG:HA	0.42	2.29	4	1
1:A:39:ILE:CD1	1:A:53:GLU:CD	0.42	2.84	20	1
1:A:15:ASP:HB2	1:A:48:LEU:CD2	0.42	2.45	10	2
1:A:20:LEU:HD13	1:A:51:LEU:HB2	0.42	1.90	2	1
1:A:20:LEU:HD22	1:A:50:VAL:C	0.42	2.35	7	1
1:A:15:ASP:HB2	1:A:48:LEU:CD1	0.42	2.44	12	4
1:A:16:VAL:CG1	1:A:117:LEU:HD22	0.42	2.44	5	2
1:A:17:ALA:HB2	1:A:49:VAL:O	0.42	2.13	4	1
1:A:16:VAL:CG1	1:A:117:LEU:HD12	0.42	2.44	18	1
1:A:64:LYS:CA	1:A:135:LEU:HD23	0.42	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:CD1	1:A:117:LEU:N	0.42	2.82	15	1
1:A:27:PHE:CZ	1:A:76:VAL:O	0.42	2.73	12	1
1:A:37:ALA:HB3	1:A:55:LEU:CB	0.42	2.40	11	1
1:A:92:LEU:HB3	1:A:123:LEU:HD23	0.42	1.90	8	2
1:A:41:LYS:HE2	1:A:52:ASP:CB	0.42	2.45	4	1
1:A:94:PHE:C	1:A:94:PHE:CD1	0.42	2.92	11	4
1:A:79:TYR:HB2	1:A:140:LEU:HD21	0.42	1.92	20	1
1:A:79:TYR:CD1	1:A:140:LEU:HD23	0.42	2.49	8	1
1:A:27:PHE:HB3	1:A:92:LEU:CD2	0.41	2.45	19	2
1:A:27:PHE:CE1	1:A:78:SER:CB	0.41	3.02	9	2
1:A:27:PHE:HD2	1:A:38:ILE:HD12	0.41	1.75	20	1
1:A:16:VAL:HG23	1:A:16:VAL:O	0.41	2.14	6	1
1:A:103:LYS:NZ	1:A:103:LYS:CB	0.41	2.83	19	1
1:A:41:LYS:CE	1:A:52:ASP:HA	0.41	2.45	4	1
1:A:26:LYS:O	1:A:27:PHE:C	0.41	2.58	9	1
1:A:28:ARG:NH1	1:A:122:GLU:O	0.41	2.53	15	1
1:A:39:ILE:HD12	1:A:53:GLU:OE2	0.41	2.15	15	1
1:A:20:LEU:HD23	1:A:20:LEU:O	0.41	2.15	4	1
1:A:74:PHE:CZ	1:A:110:TYR:HB3	0.41	2.50	12	1
1:A:27:PHE:CB	1:A:92:LEU:HD21	0.41	2.46	19	1
1:A:67:LEU:CD2	1:A:75:ILE:HG12	0.41	2.45	11	2
1:A:21:VAL:O	1:A:22:GLU:C	0.41	2.59	20	1
1:A:143:LYS:HD2	1:A:143:LYS:N	0.41	2.30	5	1
1:A:41:LYS:CD	1:A:50:VAL:HG23	0.41	2.45	18	1
1:A:130:ARG:CD	1:A:131:ASN:ND2	0.41	2.84	10	1
1:A:89:SER:C	1:A:90:TYR:CD1	0.41	2.95	15	1
1:A:99:PRO:C	1:A:101:GLY:N	0.40	2.74	19	1
1:A:98:SER:O	1:A:130:ARG:O	0.40	2.40	15	1
1:A:63:LEU:HD21	1:A:75:ILE:CG2	0.40	2.46	16	1
1:A:130:ARG:O	1:A:131:ASN:OD1	0.40	2.39	9	2
1:A:99:PRO:O	1:A:102:CYS:SG	0.40	2.80	17	1
1:A:49:VAL:HG21	1:A:117:LEU:HD11	0.40	1.93	18	1
1:A:94:PHE:CD1	1:A:94:PHE:C	0.40	2.95	4	1
1:A:55:LEU:N	1:A:55:LEU:CD2	0.40	2.84	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	121/151 (80%)	107±2 (88±2%)	13±2 (11±2%)	2±1 (1±1%)	19	65
All	All	2420/3020 (80%)	2133 (88%)	256 (11%)	31 (1%)	19	65

All 5 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	135	LEU	20
1	A	34	HIS	6
1	A	145	GLY	2
1	A	100	VAL	2
1	A	43	ASP	1

6.3.2 Protein sidechains ⓘ

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	112/136 (82%)	103±2 (92±2%)	9±2 (8±2%)	18	64
All	All	2240/2720 (82%)	2059 (92%)	181 (8%)	18	64

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	27	PHE	20
1	A	41	LYS	20
1	A	90	TYR	18
1	A	143	LYS	12
1	A	19	ASP	10
1	A	125	LYS	9
1	A	131	ASN	9
1	A	107	GLN	8
1	A	103	LYS	8
1	A	61	ASP	7
1	A	31	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	134	ASP	5
1	A	20	LEU	4
1	A	108	MET	4
1	A	28	ARG	3
1	A	48	LEU	3
1	A	117	LEU	3
1	A	30	ARG	3
1	A	140	LEU	3
1	A	75	ILE	3
1	A	15	ASP	3
1	A	116	LYS	2
1	A	70	ARG	2
1	A	65	ASP	2
1	A	35	ASN	2
1	A	130	ARG	2
1	A	73	ARG	2
1	A	113	SER	2
1	A	135	LEU	2
1	A	59	SER	1
1	A	92	LEU	1
1	A	128	GLU	1
1	A	124	THR	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 carbohydrates 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

No chemical shift data were provided