



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 04:01 AM UTC

PDB ID : 1DZC / pdb_00001dzc
Title : High resolution structure of acidic fibroblast growth factor. Mutant FGF-4-ALA-(24-154), 24 NMR structures
Authors : Lozano, R.M.; Pineda-Lucena, A.; Gonzalez, C.; Jimenez, M.A.; Cuevas, P.; Redondo-Horcajo, M.; Sanz, J.M.; Rico, M.; Gimenez-Gallego, G.
Deposited on : 2000-02-24

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

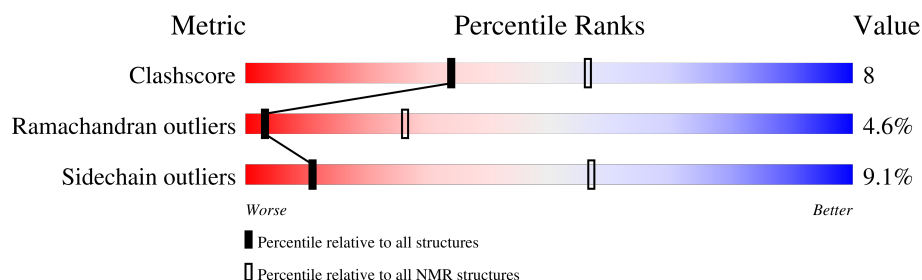
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	131	

2 Ensemble composition and analysis

This entry contains 24 models. Model 13 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:26-A:150 (125)	0.82	13

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 and 3 single-model clusters were found.

Cluster number	Models
1	6, 7, 8, 9, 10, 11, 13, 14, 22, 23, 24
2	1, 4, 12, 21
3	3, 5, 17
4	18, 19, 20
Single-model clusters	2; 15; 16

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1033 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FIBROBLAST GROWTH FACTOR 1.

Mol	Chain	Residues	Atoms					Trace
1	A	131	Total	C	N	O	S	0
			1033	648	180	201	4	

There are 3 discrepancies between the modelled and reference sequences:

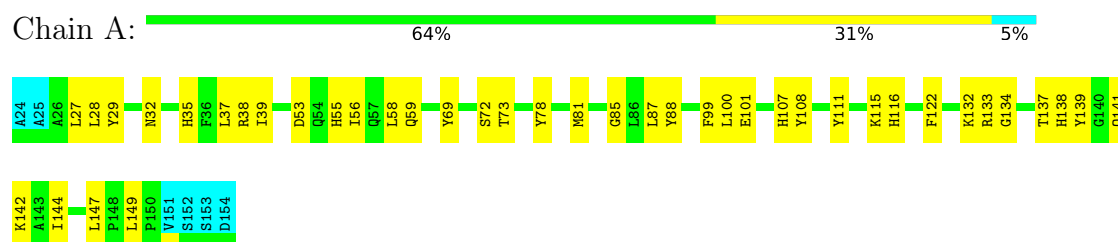
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	LYS	engineered mutation	UNP P05230
A	25	ALA	PRO	engineered mutation	UNP P05230
A	26	ALA	LYS	engineered mutation	UNP P05230

4 Residue-property plots

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: FIBROBLAST GROWTH FACTOR 1

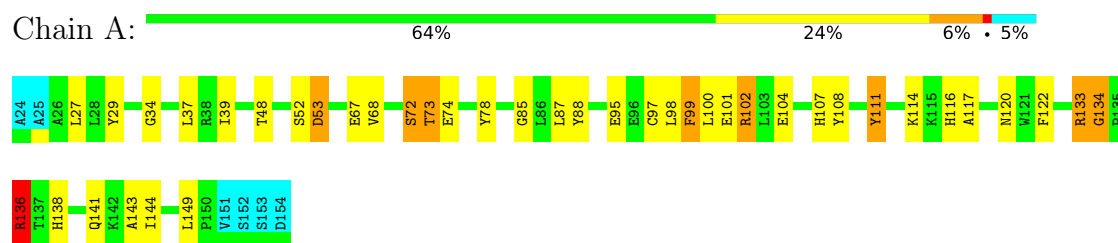


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

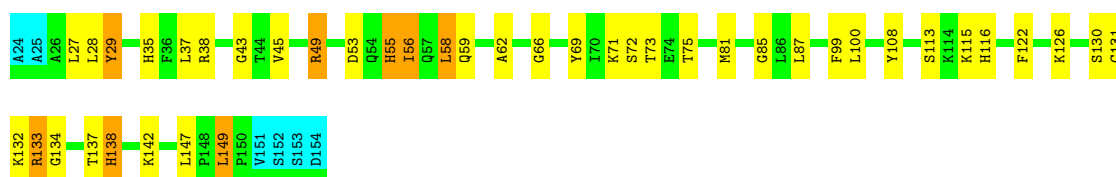
- Molecule 1: FIBROBLAST GROWTH FACTOR 1



4.2.2 Score per residue for model 2

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

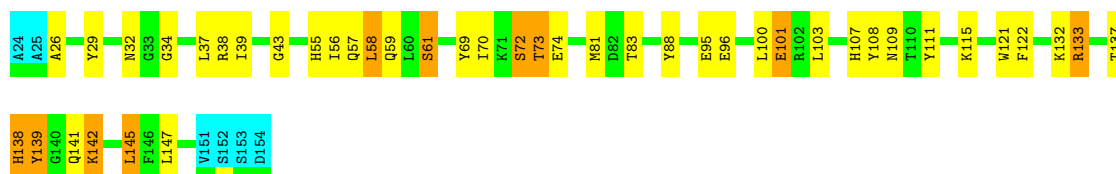




4.2.3 Score per residue for model 3

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

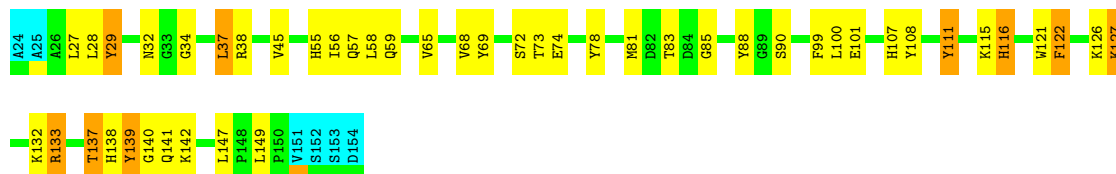
Chain A: 63% 25% 8% 5%



4.2.4 Score per residue for model 4

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

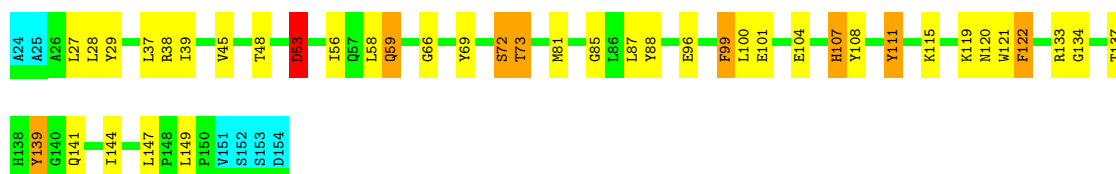
Chain A: 60% 29% 7% 5%



4.2.5 Score per residue for model 5

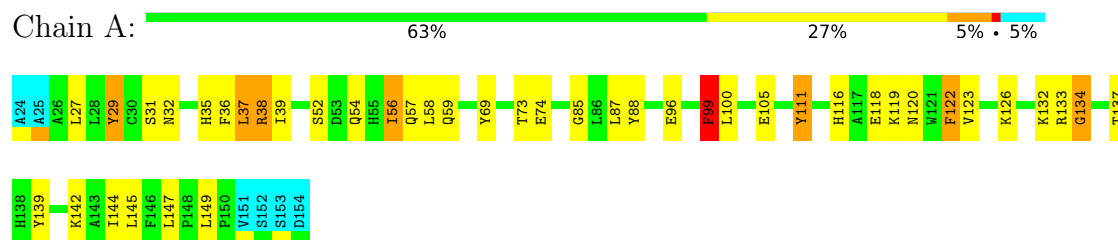
- Molecule 1: FIBROBLAST GROWTH FACTOR 1

Chain A: 64% 24% 6% 5%



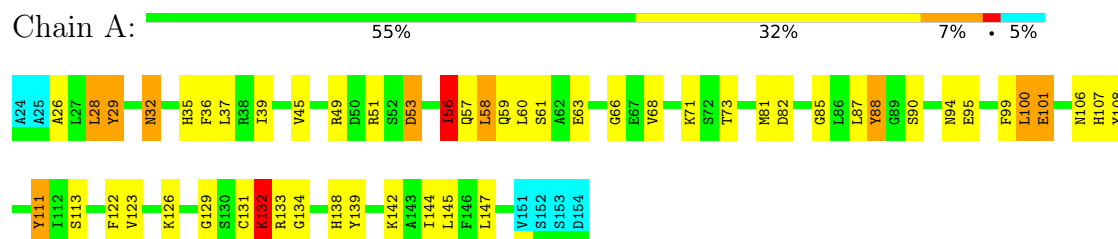
4.2.6 Score per residue for model 6

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



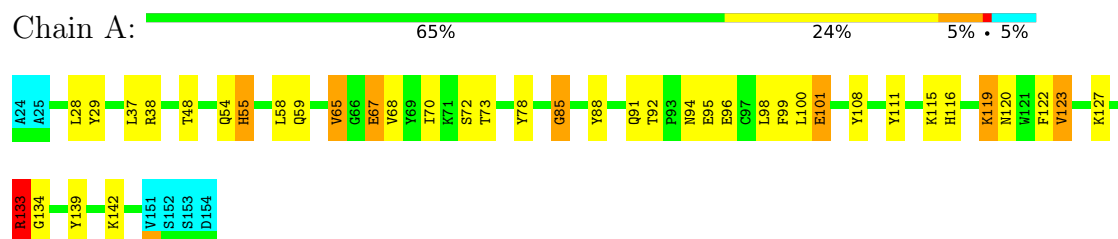
4.2.7 Score per residue for model 7

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



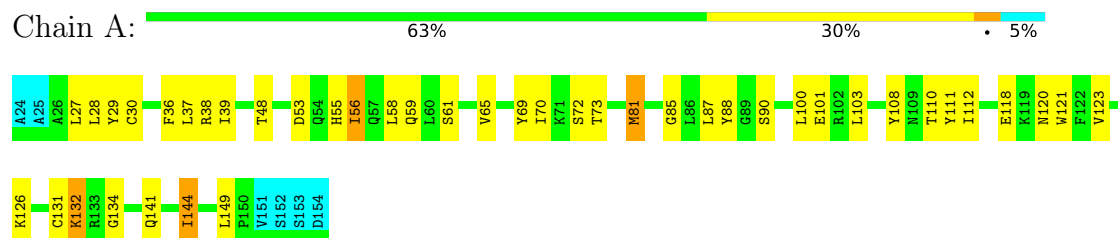
4.2.8 Score per residue for model 8

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



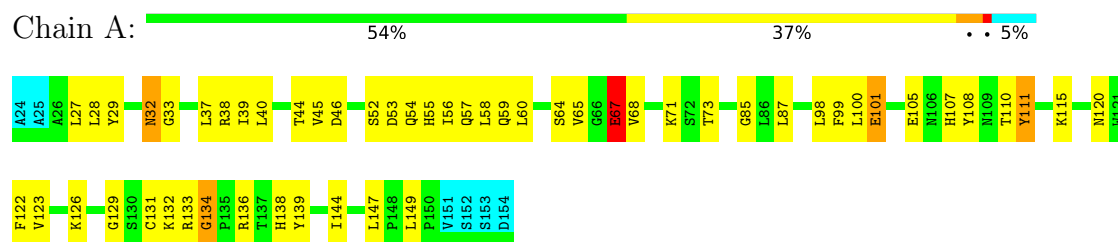
4.2.9 Score per residue for model 9

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



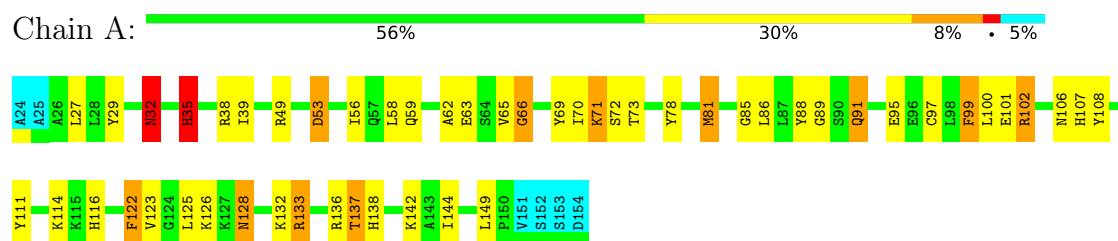
4.2.10 Score per residue for model 10

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



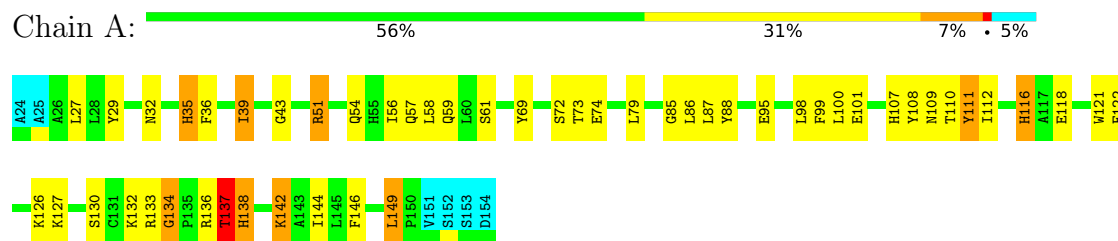
4.2.11 Score per residue for model 11

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



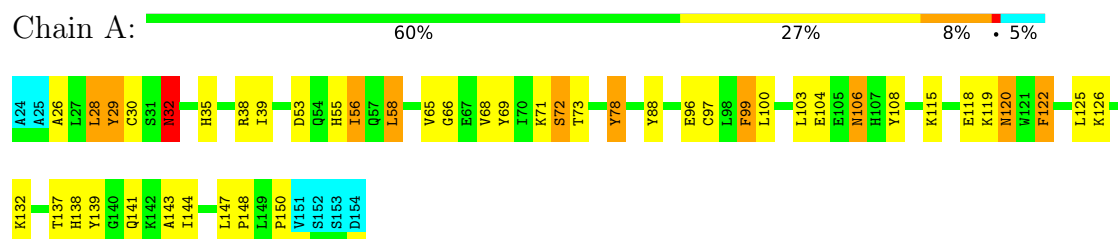
4.2.12 Score per residue for model 12

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



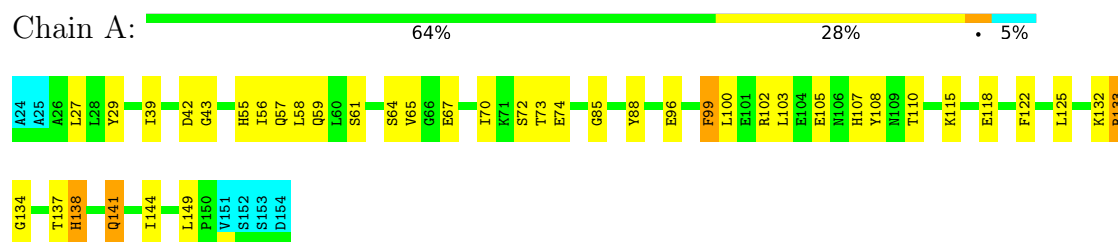
4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



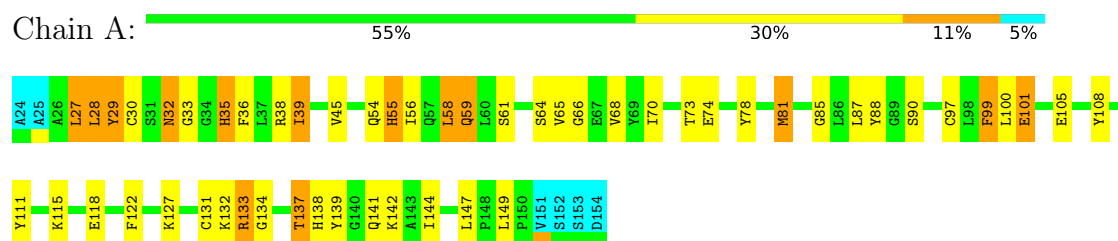
4.2.14 Score per residue for model 14

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



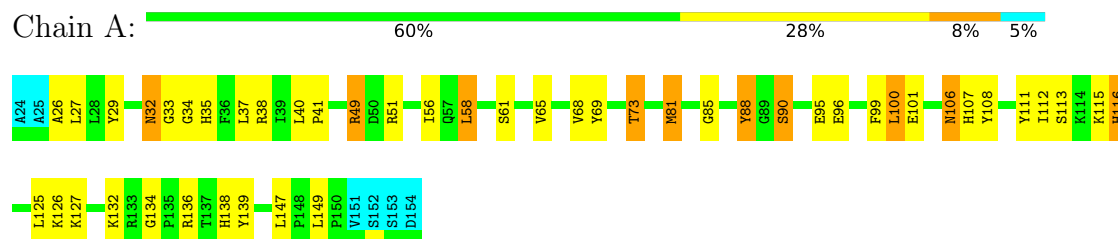
4.2.15 Score per residue for model 15

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



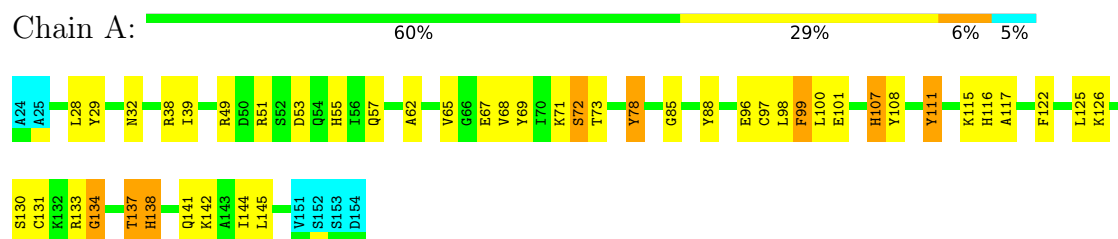
4.2.16 Score per residue for model 16

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



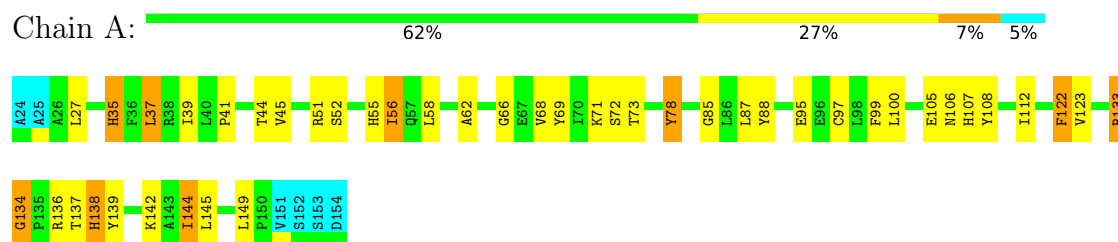
4.2.17 Score per residue for model 17

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



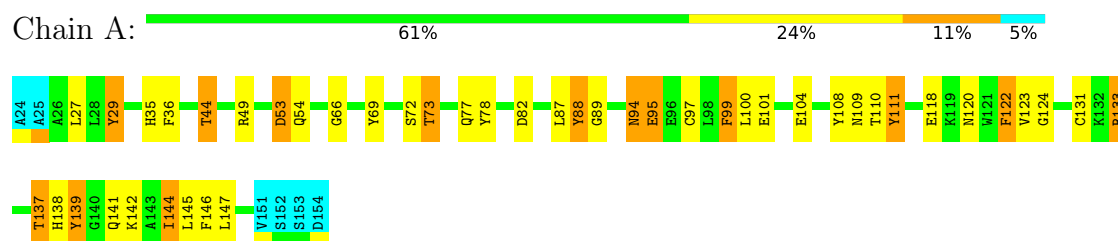
4.2.18 Score per residue for model 18

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



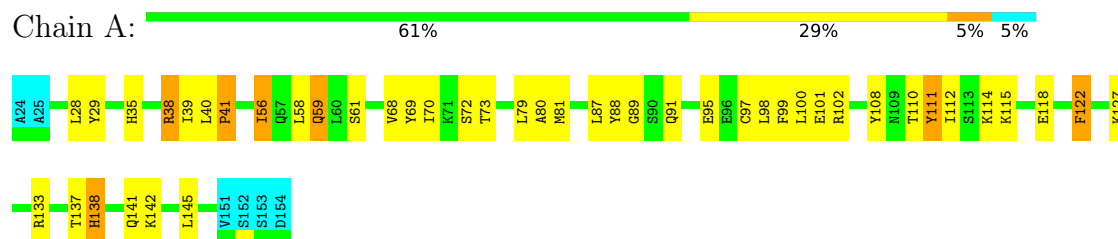
4.2.19 Score per residue for model 19

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



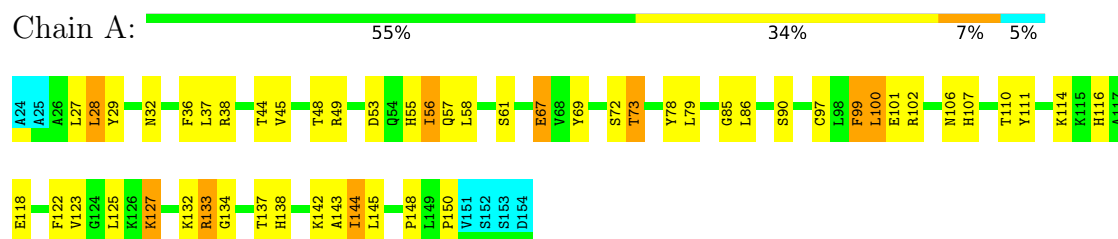
4.2.20 Score per residue for model 20

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



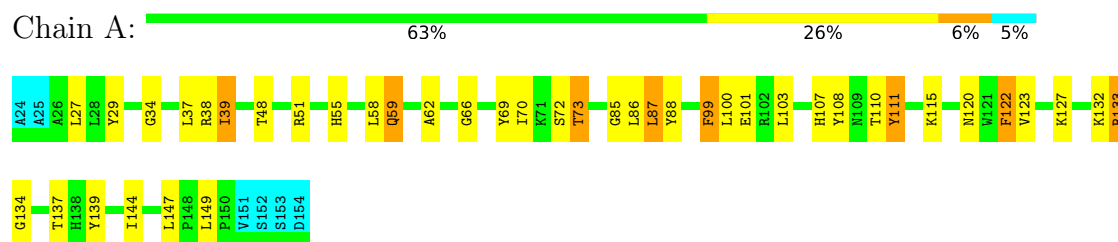
4.2.21 Score per residue for model 21

• Molecule 1: FIBROBLAST GROWTH FACTOR 1



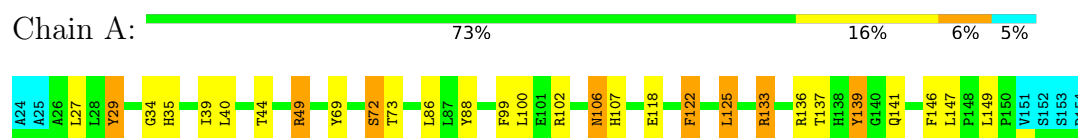
4.2.22 Score per residue for model 22

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



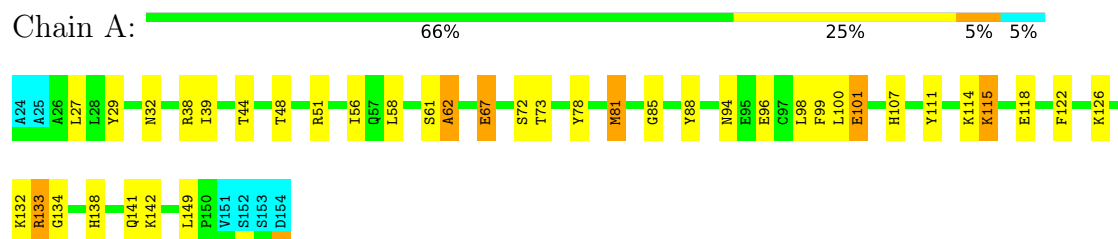
4.2.23 Score per residue for model 23

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



4.2.24 Score per residue for model 24

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS*.

Of the 24 calculated structures, 24 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
GROMOS	refinement	
GROMOS	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.97±0.02	1±1/1018 (0.1± 0.1%)	1.58±0.21	4±3/1376 (0.3± 0.2%)
All	All	0.97	15/24432 (0.1%)	1.59	98/33024 (0.3%)

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	9.6±2.2
All	All	0	231

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	91	GLN	CD-NE2	-9.46	1.13	1.33	11	1
1	A	116	HIS	CG-ND1	-5.83	1.31	1.38	6	2
1	A	35	HIS	CG-ND1	-5.41	1.32	1.38	23	4
1	A	55	HIS	CG-ND1	-5.33	1.32	1.38	8	2
1	A	107	HIS	CG-ND1	-5.32	1.32	1.38	16	2
1	A	138	HIS	CG-ND1	-5.17	1.32	1.38	13	3
1	A	138	HIS	CD2-NE2	-5.05	1.32	1.37	17	1

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLN	OE1-CD-NE2	-67.62	54.98	122.60	11	1
1	A	91	GLN	CG-CD-NE2	-19.39	87.32	116.40	11	1
1	A	32	ASN	CA-CB-CG	8.10	120.69	112.60	6	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLN	CG-CD-OE1	7.14	135.09	120.80	11	1
1	A	71	LYS	CG-CD-CE	-7.09	94.98	111.30	11	1
1	A	53	ASP	N-CA-C	6.93	121.49	113.38	5	1
1	A	116	HIS	CB-CG-CD2	-6.83	122.32	131.20	11	6
1	A	44	THR	N-CA-C	6.56	118.77	110.24	19	2
1	A	40	LEU	CA-C-N	6.53	128.00	119.84	20	2
1	A	40	LEU	C-N-CA	6.53	128.00	119.84	20	2
1	A	123	VAL	N-CA-C	6.38	117.81	109.58	8	3
1	A	35	HIS	CB-CG-CD2	-6.30	123.01	131.20	16	7
1	A	106	ASN	CA-CB-CG	6.28	118.88	112.60	13	2
1	A	90	SER	CA-C-N	6.22	128.61	120.28	15	2
1	A	90	SER	C-N-CA	6.22	128.61	120.28	15	2
1	A	133	ARG	N-CA-C	6.18	117.63	108.60	19	1
1	A	138	HIS	CB-CG-CD2	-5.98	123.43	131.20	13	9
1	A	107	HIS	CB-CG-CD2	-5.92	123.50	131.20	3	3
1	A	56	ILE	N-CA-C	5.81	114.72	106.53	12	2
1	A	114	LYS	CG-CD-CE	-5.81	97.94	111.30	11	1
1	A	102	ARG	NE-CZ-NH2	5.80	124.42	119.20	11	1
1	A	62	ALA	N-CA-C	5.73	118.89	110.30	24	2
1	A	95	GLU	N-CA-CB	-5.70	101.14	110.14	11	1
1	A	137	THR	N-CA-C	5.62	117.27	111.03	15	2
1	A	91	GLN	CB-CG-CD	5.61	122.13	112.60	11	1
1	A	127	LYS	N-CA-C	5.59	118.90	111.75	4	2
1	A	94	ASN	CA-C-N	5.58	128.52	120.38	8	2
1	A	94	ASN	C-N-CA	5.58	128.52	120.38	8	2
1	A	149	LEU	CB-CA-C	5.57	116.44	110.65	12	1
1	A	119	LYS	N-CA-CB	-5.49	101.52	110.42	5	3
1	A	125	LEU	N-CA-C	5.48	118.49	109.72	17	2
1	A	53	ASP	CA-CB-CG	5.45	118.05	112.60	11	1
1	A	99	PHE	CA-CB-CG	5.44	119.24	113.80	14	2
1	A	115	LYS	N-CA-CB	-5.33	101.49	110.49	24	1
1	A	26	ALA	N-CA-C	5.28	117.41	109.23	3	1
1	A	106	ASN	CA-C-N	5.26	131.58	121.54	11	1
1	A	106	ASN	C-N-CA	5.26	131.58	121.54	11	1
1	A	73	THR	CA-C-N	5.25	127.27	120.44	16	2
1	A	73	THR	C-N-CA	5.25	127.27	120.44	16	2
1	A	31	SER	CA-C-N	5.22	127.53	120.38	6	1
1	A	31	SER	C-N-CA	5.22	127.53	120.38	6	1
1	A	38	ARG	N-CA-C	5.20	116.78	108.41	6	2
1	A	138	HIS	N-CA-C	5.18	121.84	110.80	18	1
1	A	146	PHE	CA-CB-CG	5.13	118.93	113.80	23	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	SER	CA-C-N	5.12	131.32	121.54	4	1
1	A	72	SER	C-N-CA	5.12	131.32	121.54	4	1
1	A	149	LEU	N-CA-CB	-5.09	101.32	110.37	2	1
1	A	41	PRO	CA-N-CD	-5.07	104.91	112.00	20	1
1	A	28	LEU	N-CA-C	5.03	116.61	108.41	15	1
1	A	94	ASN	CA-CB-CG	-5.01	107.59	112.60	19	1
1	A	55	HIS	CB-CG-CD2	-5.00	124.70	131.20	14	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	88	TYR	Sidechain	21
1	A	122	PHE	Sidechain	21
1	A	29	TYR	Sidechain	20
1	A	108	TYR	Sidechain,Mainchain	20
1	A	69	TYR	Sidechain	17
1	A	72	SER	Mainchain	16
1	A	99	PHE	Sidechain	14
1	A	111	TYR	Sidechain	13
1	A	139	TYR	Sidechain	11
1	A	61	SER	Mainchain	10
1	A	78	TYR	Sidechain	6
1	A	102	ARG	Mainchain	5
1	A	132	LYS	Mainchain	5
1	A	56	ILE	Mainchain	4
1	A	32	ASN	Mainchain	3
1	A	65	VAL	Mainchain	3
1	A	90	SER	Mainchain	3
1	A	62	ALA	Mainchain	3
1	A	81	MET	Mainchain	3
1	A	131	CYS	Mainchain	3
1	A	53	ASP	Mainchain	2
1	A	133	ARG	Sidechain	2
1	A	138	HIS	Sidechain,Mainchain	2
1	A	119	LYS	Mainchain	2
1	A	38	ARG	Sidechain	2
1	A	103	LEU	Mainchain	2
1	A	117	ALA	Mainchain	1
1	A	136	ARG	Sidechain	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	HIS	Sidechain	1
1	A	118	GLU	Mainchain	1
1	A	82	ASP	Mainchain	1
1	A	129	GLY	Peptide	1
1	A	85	GLY	Mainchain	1
1	A	91	GLN	Sidechain	1
1	A	143	ALA	Mainchain	1
1	A	42	ASP	Mainchain	1
1	A	35	HIS	Sidechain	1
1	A	55	HIS	Sidechain	1
1	A	64	SER	Mainchain	1
1	A	127	LYS	Mainchain	1
1	A	36	PHE	Sidechain	1
1	A	54	GLN	Mainchain	1
1	A	49	ARG	Sidechain	1

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	995	0	971	16±4
All	All	23880	0	23304	385

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ARG:HB2	1:A:137:THR:HG21	0.88	1.44	21	1
1:A:85:GLY:HA3	1:A:134:GLY:H	0.77	1.39	10	12
1:A:87:LEU:HD21	1:A:133:ARG:HH11	0.76	1.41	6	2
1:A:27:LEU:HD21	1:A:36:PHE:HE2	0.74	1.43	15	1
1:A:27:LEU:HD21	1:A:53:ASP:HB3	0.72	1.62	1	2
1:A:38:ARG:HD2	1:A:55:HIS:HB2	0.71	1.62	17	9
1:A:96:GLU:HG3	1:A:115:LYS:HD2	0.71	1.62	5	4
1:A:28:LEU:H	1:A:56:ILE:HD11	0.70	1.46	13	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASN:HD22	1:A:143:ALA:HA	0.69	1.47	21	1
1:A:126:LYS:HB2	1:A:132:LYS:HB3	0.69	1.65	2	9
1:A:38:ARG:HD3	1:A:48:THR:HG21	0.65	1.67	9	3
1:A:67:GLU:HB3	1:A:98:LEU:HD22	0.65	1.67	17	1
1:A:85:GLY:HA2	1:A:133:ARG:HH11	0.65	1.50	4	2
1:A:39:ILE:HG21	1:A:72:SER:HB3	0.65	1.67	5	3
1:A:99:PHE:HB3	1:A:111:TYR:HB3	0.65	1.68	1	15
1:A:81:MET:HE2	1:A:133:ARG:HD3	0.64	1.66	20	1
1:A:102:ARG:NH2	1:A:120:ASN:HD21	0.63	1.92	1	1
1:A:124:GLY:HA2	1:A:146:PHE:HE1	0.63	1.53	19	1
1:A:142:LYS:HA	1:A:145:LEU:HD13	0.61	1.73	17	6
1:A:87:LEU:HD13	1:A:133:ARG:HH11	0.60	1.57	2	1
1:A:45:VAL:HG23	1:A:131:CYS:HB3	0.60	1.72	2	1
1:A:85:GLY:HA3	1:A:134:GLY:N	0.59	2.12	15	15
1:A:83:THR:HG21	1:A:115:LYS:HZ2	0.59	1.57	4	1
1:A:132:LYS:HG2	1:A:136:ARG:HE	0.59	1.58	12	1
1:A:67:GLU:H	1:A:100:LEU:HG	0.59	1.58	21	1
1:A:30:CYS:SG	1:A:32:ASN:HB2	0.59	2.38	15	2
1:A:85:GLY:HA2	1:A:133:ARG:NH1	0.59	2.13	4	1
1:A:81:MET:HE1	1:A:121:TRP:HB3	0.59	1.75	5	3
1:A:133:ARG:HB3	1:A:137:THR:HG21	0.58	1.73	14	2
1:A:99:PHE:HE1	1:A:133:ARG:HH12	0.58	1.41	7	1
1:A:101:GLU:HG2	1:A:111:TYR:HE1	0.58	1.59	8	7
1:A:29:TYR:HD2	1:A:147:LEU:HB3	0.58	1.59	16	10
1:A:110:THR:HG21	1:A:144:ILE:HD12	0.58	1.76	9	2
1:A:57:GLN:HB2	1:A:74:GLU:HB2	0.57	1.77	4	3
1:A:29:TYR:HB3	1:A:147:LEU:HB3	0.57	1.76	2	1
1:A:123:VAL:HA	1:A:133:ARG:HD2	0.57	1.75	8	1
1:A:49:ARG:CZ	1:A:49:ARG:H	0.56	2.12	23	3
1:A:127:LYS:H	1:A:127:LYS:HD3	0.56	1.59	8	1
1:A:139:TYR:HD1	1:A:144:ILE:HD11	0.56	1.61	7	3
1:A:87:LEU:HD11	1:A:133:ARG:NH1	0.56	2.15	12	2
1:A:142:LYS:H	1:A:142:LYS:HD2	0.56	1.61	12	2
1:A:38:ARG:HB3	1:A:56:ILE:HB	0.56	1.77	20	1
1:A:39:ILE:HG21	1:A:72:SER:OG	0.56	2.01	1	2
1:A:87:LEU:HD11	1:A:123:VAL:HG13	0.56	1.77	19	1
1:A:111:TYR:HB2	1:A:123:VAL:HG22	0.55	1.78	11	2
1:A:96:GLU:HG3	1:A:115:LYS:HD3	0.54	1.78	3	1
1:A:39:ILE:HG22	1:A:55:HIS:O	0.54	2.02	13	5
1:A:32:ASN:OD1	1:A:125:LEU:HB2	0.54	2.01	11	1
1:A:122:PHE:HB2	1:A:137:THR:O	0.54	2.03	22	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:HG21	1:A:72:SER:HB2	0.54	1.78	14	2
1:A:112:ILE:HD11	1:A:120:ASN:HA	0.54	1.79	9	1
1:A:137:THR:OG1	1:A:144:ILE:HG23	0.54	2.03	21	1
1:A:109:ASN:O	1:A:146:PHE:HB2	0.54	2.03	12	2
1:A:32:ASN:ND2	1:A:143:ALA:HA	0.53	2.17	21	1
1:A:28:LEU:HB2	1:A:58:LEU:HD11	0.53	1.81	2	1
1:A:126:LYS:HB3	1:A:130:SER:HB3	0.53	1.80	17	1
1:A:27:LEU:HD23	1:A:56:ILE:HG12	0.53	1.80	9	3
1:A:124:GLY:HA2	1:A:146:PHE:CE1	0.53	2.39	19	1
1:A:83:THR:HG21	1:A:115:LYS:NZ	0.53	2.18	4	1
1:A:87:LEU:HD13	1:A:133:ARG:HD3	0.53	1.81	1	1
1:A:96:GLU:HG2	1:A:115:LYS:HD3	0.52	1.81	13	2
1:A:110:THR:HG22	1:A:111:TYR:H	0.52	1.64	12	3
1:A:101:GLU:HG2	1:A:111:TYR:CE1	0.52	2.40	24	4
1:A:38:ARG:HE	1:A:48:THR:HG21	0.51	1.64	5	1
1:A:70:ILE:HD12	1:A:99:PHE:HD2	0.51	1.66	22	1
1:A:121:TRP:HB3	1:A:133:ARG:HH22	0.51	1.65	4	1
1:A:133:ARG:HA	1:A:137:THR:HG23	0.51	1.82	12	1
1:A:148:PRO:C	1:A:150:PRO:HD3	0.51	2.31	21	2
1:A:87:LEU:H	1:A:133:ARG:CZ	0.51	2.18	19	2
1:A:59:GLN:HB3	1:A:71:LYS:HB3	0.51	1.82	10	3
1:A:27:LEU:HB3	1:A:149:LEU:O	0.51	2.06	11	5
1:A:27:LEU:HD21	1:A:36:PHE:CE2	0.51	2.33	15	1
1:A:123:VAL:HA	1:A:133:ARG:HG2	0.51	1.81	22	1
1:A:138:HIS:CE1	1:A:141:GLN:HE22	0.51	2.24	20	4
1:A:60:LEU:HD23	1:A:68:VAL:HG21	0.51	1.81	7	2
1:A:67:GLU:HG3	1:A:114:LYS:HD2	0.50	1.83	24	1
1:A:101:GLU:HG2	1:A:111:TYR:CE2	0.50	2.41	3	1
1:A:87:LEU:HD12	1:A:131:CYS:SG	0.50	2.46	9	2
1:A:133:ARG:O	1:A:136:ARG:HG2	0.50	2.06	1	2
1:A:57:GLN:HB3	1:A:74:GLU:HB2	0.50	1.83	3	2
1:A:36:PHE:HB3	1:A:56:ILE:HD13	0.50	1.83	6	3
1:A:28:LEU:HB2	1:A:58:LEU:HD21	0.50	1.83	5	2
1:A:87:LEU:HD21	1:A:133:ARG:NH1	0.50	2.19	6	2
1:A:64:SER:HB3	1:A:67:GLU:HB3	0.50	1.83	14	1
1:A:27:LEU:HB2	1:A:149:LEU:O	0.50	2.07	1	8
1:A:95:GLU:HA	1:A:98:LEU:HD12	0.50	1.82	20	3
1:A:141:GLN:O	1:A:144:ILE:HG13	0.49	2.07	15	6
1:A:81:MET:HE3	1:A:113:SER:HB3	0.49	1.83	7	2
1:A:26:ALA:HB3	1:A:58:LEU:HG	0.49	1.83	16	2
1:A:40:LEU:HB2	1:A:44:THR:O	0.49	2.08	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:O	1:A:55:HIS:HB3	0.49	2.08	22	1
1:A:53:ASP:HA	1:A:56:ILE:HG23	0.49	1.85	5	4
1:A:37:LEU:O	1:A:56:ILE:HD13	0.48	2.08	5	4
1:A:59:GLN:HB2	1:A:73:THR:HG23	0.48	1.85	3	3
1:A:125:LEU:HB3	1:A:133:ARG:NH1	0.48	2.23	14	1
1:A:68:VAL:HG22	1:A:99:PHE:O	0.48	2.08	1	8
1:A:67:GLU:HG2	1:A:98:LEU:HD22	0.48	1.85	24	2
1:A:127:LYS:HD3	1:A:127:LYS:H	0.48	1.69	21	1
1:A:78:TYR:HB3	1:A:97:CYS:SG	0.48	2.49	18	8
1:A:53:ASP:H	1:A:56:ILE:HG23	0.47	1.67	7	1
1:A:62:ALA:HB2	1:A:68:VAL:HG12	0.47	1.85	18	2
1:A:116:HIS:HB2	1:A:121:TRP:HB2	0.47	1.86	12	1
1:A:123:VAL:HG12	1:A:133:ARG:NE	0.47	2.25	11	1
1:A:59:GLN:O	1:A:70:ILE:HA	0.47	2.10	20	7
1:A:37:LEU:O	1:A:56:ILE:HD12	0.47	2.10	9	2
1:A:39:ILE:HD12	1:A:45:VAL:HG22	0.47	1.87	7	2
1:A:80:ALA:HB2	1:A:97:CYS:SG	0.47	2.50	20	1
1:A:141:GLN:HB3	1:A:143:ALA:HB3	0.46	1.87	1	1
1:A:102:ARG:HH11	1:A:112:ILE:HD13	0.46	1.70	20	1
1:A:85:GLY:O	1:A:133:ARG:HG2	0.46	2.10	14	2
1:A:58:LEU:HA	1:A:72:SER:HA	0.46	1.88	3	2
1:A:91:GLN:HG3	1:A:92:THR:HG23	0.46	1.86	8	1
1:A:87:LEU:HD22	1:A:133:ARG:CZ	0.46	2.41	20	1
1:A:96:GLU:HG2	1:A:115:LYS:HD2	0.46	1.87	8	1
1:A:32:ASN:OD1	1:A:142:LYS:HG2	0.46	2.10	12	1
1:A:27:LEU:HD11	1:A:51:ARG:HE	0.46	1.70	18	1
1:A:54:GLN:HE21	1:A:55:HIS:CE1	0.46	2.28	15	1
1:A:88:TYR:CE2	1:A:90:SER:HB2	0.46	2.46	16	2
1:A:32:ASN:HB3	1:A:35:HIS:HE1	0.45	1.71	12	1
1:A:26:ALA:HB3	1:A:58:LEU:O	0.45	2.11	7	1
1:A:122:PHE:HB3	1:A:144:ILE:HG21	0.45	1.88	11	1
1:A:66:GLY:O	1:A:101:GLU:HG2	0.45	2.11	5	2
1:A:123:VAL:HG12	1:A:133:ARG:HE	0.45	1.72	11	1
1:A:56:ILE:HD11	1:A:58:LEU:HD23	0.45	1.89	4	1
1:A:35:HIS:HB2	1:A:125:LEU:HD13	0.45	1.88	13	1
1:A:38:ARG:HG3	1:A:48:THR:HG21	0.44	1.90	8	1
1:A:87:LEU:HD11	1:A:133:ARG:HG2	0.44	1.88	15	1
1:A:91:GLN:H	1:A:91:GLN:CD	0.44	2.20	20	1
1:A:99:PHE:HE1	1:A:133:ARG:NH1	0.44	2.10	7	1
1:A:126:LYS:HB2	1:A:132:LYS:HB2	0.44	1.90	7	1
1:A:125:LEU:HA	1:A:133:ARG:HH12	0.44	1.70	23	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:O	1:A:144:ILE:HA	0.44	2.13	7	1
1:A:81:MET:HE1	1:A:116:HIS:HB2	0.44	1.90	16	1
1:A:104:GLU:HB2	1:A:139:TYR:HE2	0.44	1.73	19	1
1:A:39:ILE:HD13	1:A:89:GLY:HA3	0.44	1.89	20	1
1:A:82:ASP:HB2	1:A:88:TYR:HE2	0.44	1.73	19	1
1:A:81:MET:HE2	1:A:113:SER:HB3	0.44	1.90	2	1
1:A:123:VAL:O	1:A:144:ILE:HG22	0.44	2.13	18	1
1:A:104:GLU:HB2	1:A:139:TYR:CE2	0.44	2.48	19	1
1:A:100:LEU:O	1:A:111:TYR:HA	0.44	2.12	7	1
1:A:27:LEU:HD12	1:A:56:ILE:HG13	0.44	1.88	24	1
1:A:133:ARG:HB2	1:A:137:THR:CG2	0.43	2.31	21	1
1:A:110:THR:HG21	1:A:144:ILE:HB	0.43	1.90	12	2
1:A:38:ARG:NH1	1:A:54:GLN:HB3	0.43	2.29	15	1
1:A:45:VAL:HG22	1:A:87:LEU:HB2	0.43	1.89	18	1
1:A:139:TYR:CD1	1:A:144:ILE:HD11	0.43	2.47	7	1
1:A:126:LYS:HD3	1:A:132:LYS:HD3	0.43	1.90	12	1
1:A:56:ILE:O	1:A:58:LEU:HD23	0.43	2.13	15	1
1:A:85:GLY:HA3	1:A:134:GLY:CA	0.43	2.44	7	2
1:A:77:GLN:HB3	1:A:89:GLY:HA3	0.43	1.91	19	1
1:A:27:LEU:HD22	1:A:36:PHE:CD2	0.43	2.49	12	1
1:A:100:LEU:HB3	1:A:112:ILE:HG23	0.42	1.92	16	1
1:A:37:LEU:HD21	1:A:79:LEU:HD21	0.42	1.90	21	1
1:A:142:LYS:HA	1:A:145:LEU:HB2	0.42	1.91	21	2
1:A:110:THR:HG22	1:A:144:ILE:O	0.42	2.15	21	1
1:A:45:VAL:CG2	1:A:87:LEU:HB2	0.42	2.45	2	1
1:A:102:ARG:CZ	1:A:120:ASN:HD21	0.42	2.27	1	1
1:A:38:ARG:HH12	1:A:54:GLN:HB2	0.42	1.75	6	1
1:A:132:LYS:HA	1:A:132:LYS:HE2	0.41	1.92	7	1
1:A:32:ASN:ND2	1:A:125:LEU:H	0.41	2.13	16	1
1:A:27:LEU:HB3	1:A:36:PHE:HE2	0.41	1.75	21	1
1:A:111:TYR:HB2	1:A:123:VAL:CG2	0.41	2.43	21	1
1:A:126:LYS:HB3	1:A:130:SER:HB2	0.41	1.92	12	2
1:A:139:TYR:HD1	1:A:140:GLY:N	0.41	2.13	4	1
1:A:67:GLU:HB2	1:A:98:LEU:HB3	0.41	1.92	8	1
1:A:38:ARG:HG3	1:A:48:THR:HB	0.41	1.93	21	1
1:A:27:LEU:HD23	1:A:27:LEU:C	0.41	2.41	15	1
1:A:103:LEU:HA	1:A:109:ASN:HA	0.41	1.91	3	1
1:A:27:LEU:HD23	1:A:56:ILE:HG13	0.41	1.93	10	1
1:A:110:THR:HG21	1:A:144:ILE:HD13	0.41	1.91	14	1
1:A:122:PHE:O	1:A:133:ARG:HB3	0.41	2.15	18	1
1:A:52:SER:C	1:A:54:GLN:H	0.41	2.24	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ARG:O	1:A:136:ARG:HG3	0.41	2.16	10	1
1:A:126:LYS:HB2	1:A:132:LYS:CB	0.41	2.46	16	1
1:A:45:VAL:HG21	1:A:87:LEU:HB2	0.40	1.92	5	1
1:A:35:HIS:CD2	1:A:125:LEU:HD13	0.40	2.51	11	1
1:A:57:GLN:HG3	1:A:73:THR:OG1	0.40	2.15	3	1
1:A:39:ILE:HD11	1:A:89:GLY:HA2	0.40	1.93	11	1
1:A:107:HIS:O	1:A:147:LEU:HD13	0.40	2.16	5	1
1:A:79:LEU:O	1:A:99:PHE:HE2	0.40	1.99	12	1
1:A:87:LEU:HD22	1:A:99:PHE:HZ	0.40	1.76	5	1
1:A:48:THR:HG21	1:A:52:SER:HB2	0.40	1.92	1	1
1:A:66:GLY:O	1:A:68:VAL:HG13	0.40	2.16	15	1
1:A:37:LEU:O	1:A:56:ILE:HG22	0.40	2.17	16	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	125/131 (95%)	95±4 (76±3%)	24±3 (20±2%)	6±2 (5±1%)	3	26
All	All	3000/3144 (95%)	2275 (76%)	586 (20%)	139 (5%)	3	26

All 36 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	73	THR	24
1	A	101	GLU	13
1	A	107	HIS	10
1	A	66	GLY	7
1	A	65	VAL	7
1	A	120	ASN	7
1	A	34	GLY	6
1	A	134	GLY	6
1	A	138	HIS	6
1	A	106	ASN	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	53	ASP	5
1	A	67	GLU	4
1	A	43	GLY	4
1	A	114	LYS	3
1	A	56	ILE	3
1	A	33	GLY	3
1	A	41	PRO	3
1	A	139	TYR	2
1	A	105	GLU	2
1	A	103	LEU	2
1	A	137	THR	2
1	A	104	GLU	1
1	A	83	THR	1
1	A	52	SER	1
1	A	131	CYS	1
1	A	132	LYS	1
1	A	133	ARG	1
1	A	64	SER	1
1	A	129	GLY	1
1	A	32	ASN	1
1	A	128	ASN	1
1	A	51	ARG	1
1	A	117	ALA	1
1	A	95	GLU	1
1	A	125	LEU	1
1	A	44	THR	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	108/112 (96%)	98±3 (91±3%)	10±3 (9±3%)	11	57
All	All	2592/2688 (96%)	2357 (91%)	235 (9%)	11	57

All 60 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	100	LEU	24
1	A	58	LEU	17
1	A	133	ARG	14
1	A	118	GLU	10
1	A	37	LEU	9
1	A	137	THR	9
1	A	142	LYS	8
1	A	49	ARG	7
1	A	28	LEU	7
1	A	59	GLN	7
1	A	95	GLU	6
1	A	81	MET	6
1	A	144	ILE	5
1	A	115	LYS	5
1	A	127	LYS	5
1	A	39	ILE	5
1	A	32	ASN	5
1	A	86	LEU	5
1	A	51	ARG	5
1	A	136	ARG	4
1	A	141	GLN	4
1	A	71	LYS	4
1	A	56	ILE	3
1	A	45	VAL	3
1	A	116	HIS	3
1	A	57	GLN	3
1	A	105	GLU	3
1	A	149	LEU	3
1	A	35	HIS	3
1	A	44	THR	3
1	A	74	GLU	2
1	A	147	LEU	2
1	A	104	GLU	2
1	A	63	GLU	2
1	A	94	ASN	2
1	A	132	LYS	2
1	A	54	GLN	2
1	A	67	GLU	2
1	A	112	ILE	2
1	A	106	ASN	2
1	A	75	THR	1
1	A	61	SER	1
1	A	145	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	139	TYR	1
1	A	96	GLU	1
1	A	53	ASP	1
1	A	138	HIS	1
1	A	30	CYS	1
1	A	123	VAL	1
1	A	46	ASP	1
1	A	65	VAL	1
1	A	128	ASN	1
1	A	120	ASN	1
1	A	27	LEU	1
1	A	107	HIS	1
1	A	52	SER	1
1	A	79	LEU	1
1	A	110	THR	1
1	A	87	LEU	1
1	A	40	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided