



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 1DZD / pdb_00001dzd
Title : High resolution structure of acidic fibroblast growth factor (27-154), 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

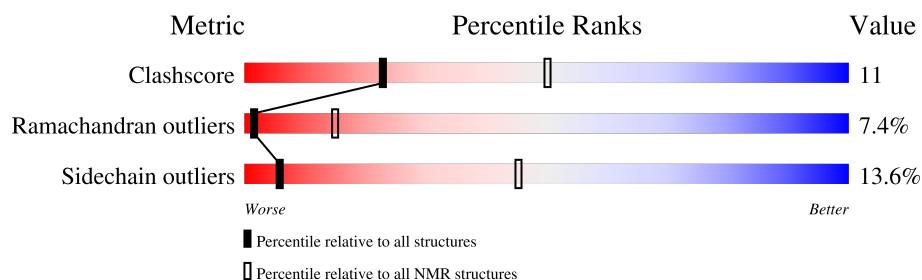
1 Overall quality at a glance

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	127	

2 Ensemble composition and analysis

This entry contains 24 models. Model 24 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:30-A:148 (119)	0.82	24

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

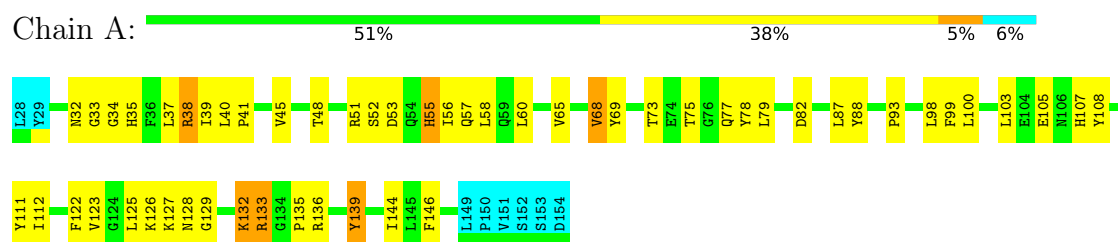
Mol	Chain	Residues	Atoms					Trace
1	A	127	Total	C	N	O	S	0
			1010	633	176	197	4	

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: ACIDIC FIBROBLAST GROWTH FACTOR

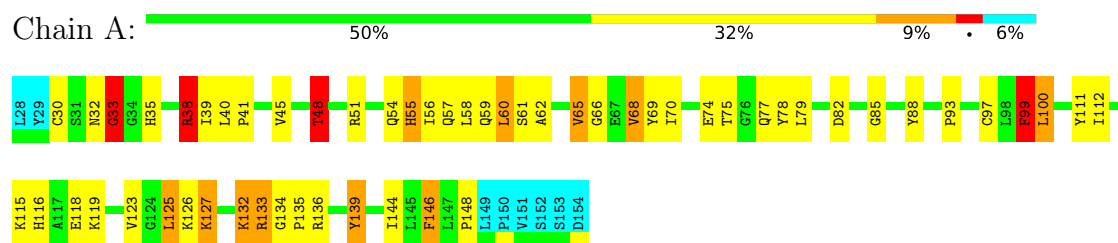


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

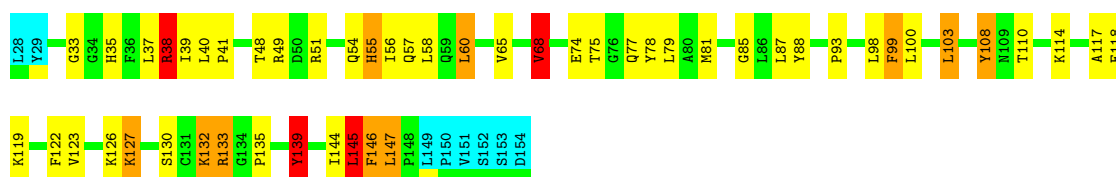
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.2 Score per residue for model 2

• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

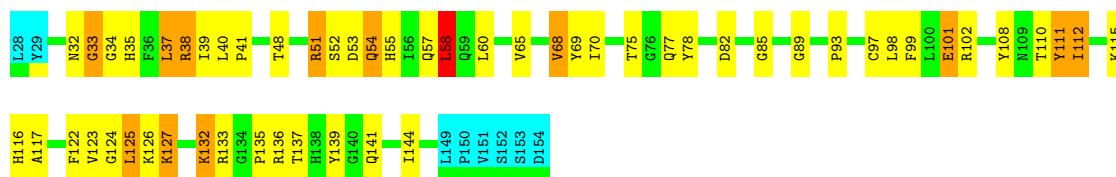




4.2.3 Score per residue for model 3

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

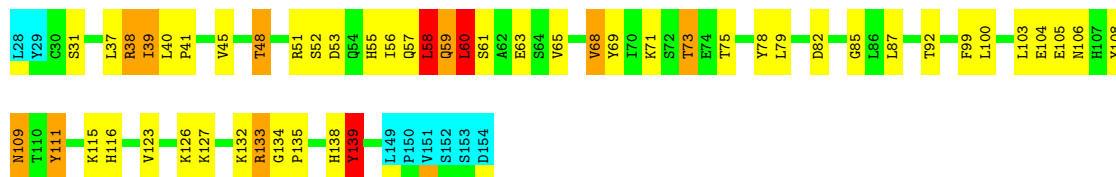
Chain A: 50% 33% 9% 6%



4.2.4 Score per residue for model 4

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

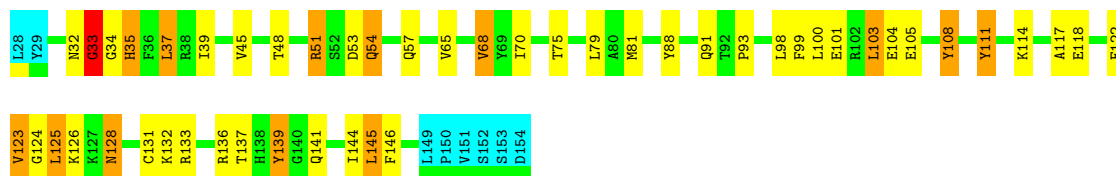
Chain A: 54% 31% 7% 6%



4.2.5 Score per residue for model 5

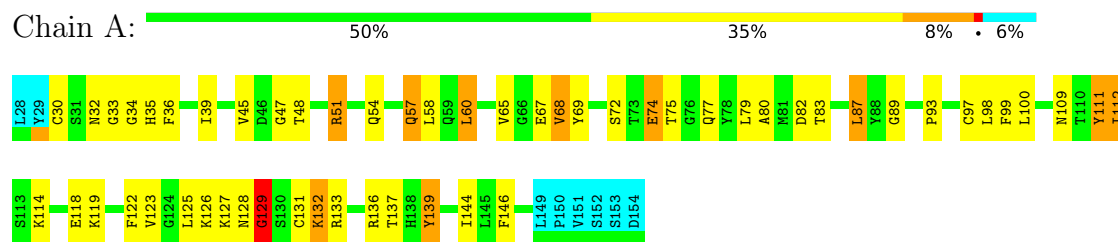
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 55% 28% 10% 6%



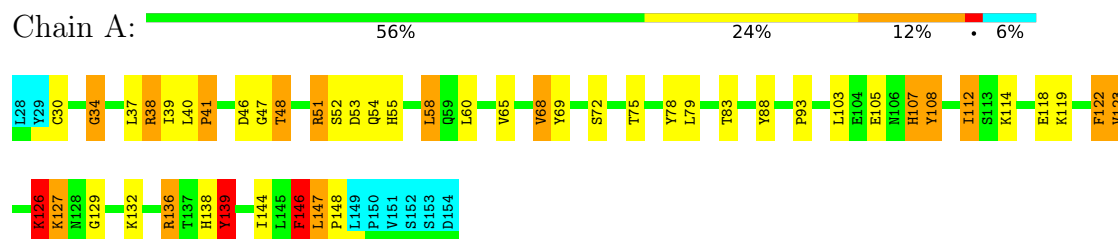
4.2.6 Score per residue for model 6

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



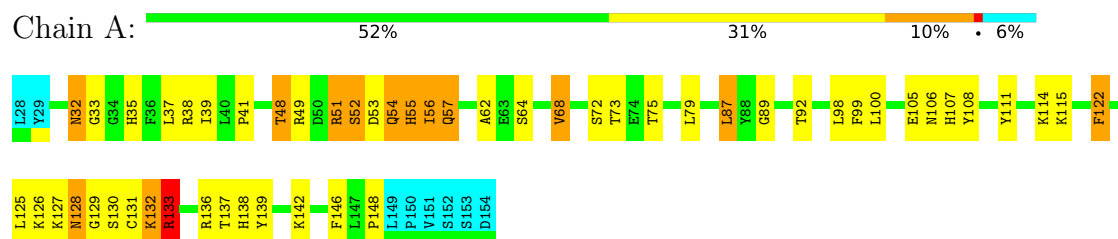
4.2.7 Score per residue for model 7

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



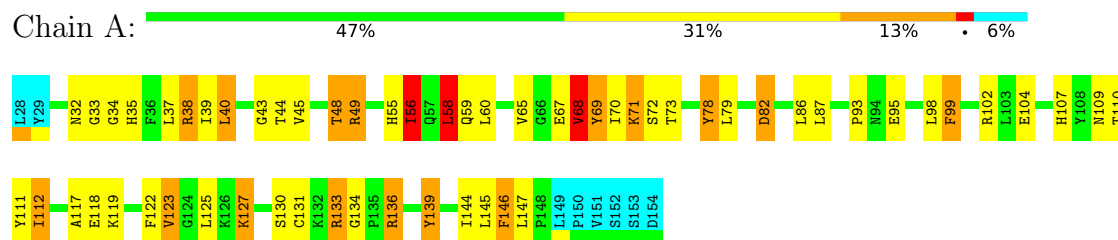
4.2.8 Score per residue for model 8

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



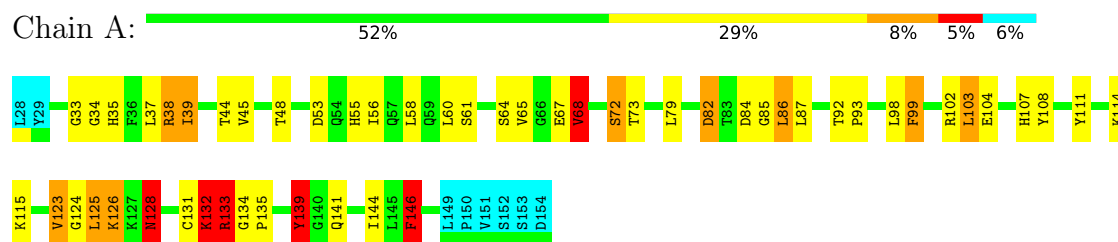
4.2.9 Score per residue for model 9

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



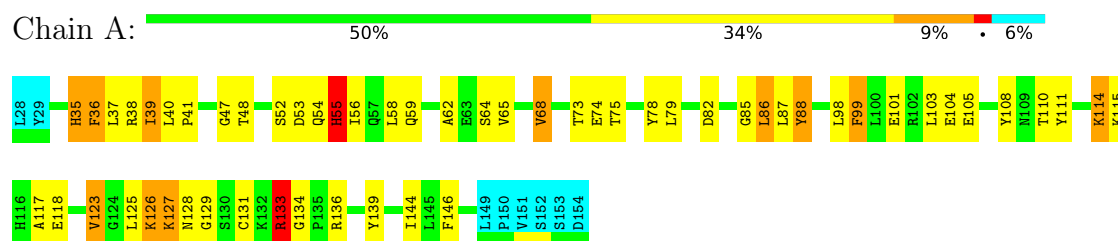
4.2.10 Score per residue for model 10

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



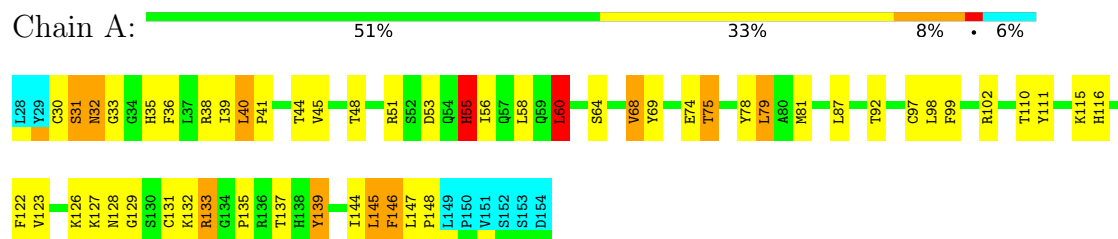
4.2.11 Score per residue for model 11

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



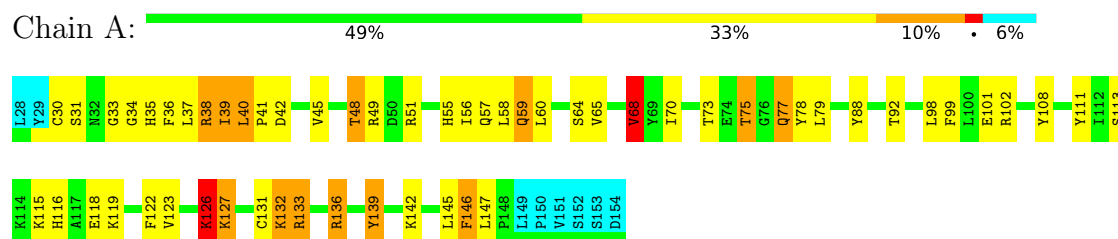
4.2.12 Score per residue for model 12

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



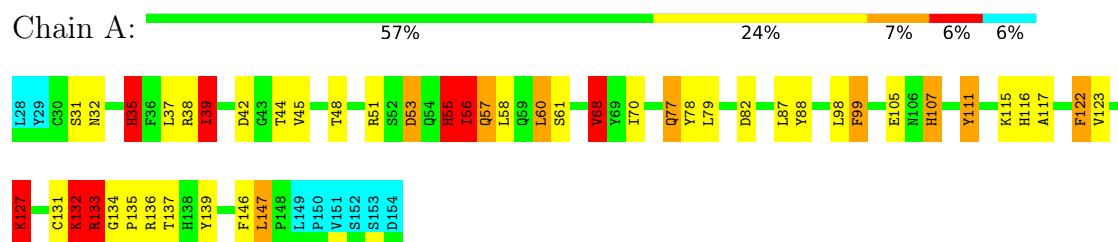
4.2.13 Score per residue for model 13

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



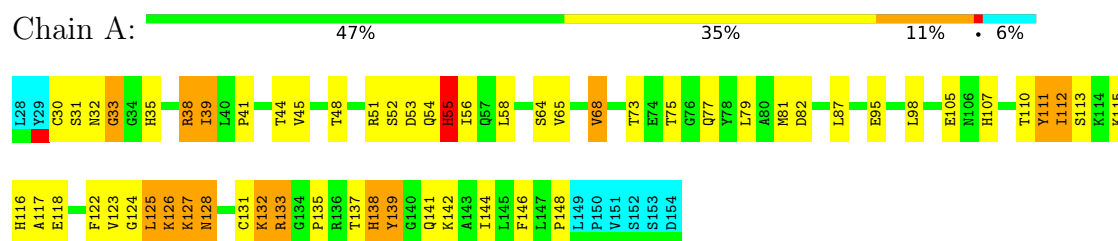
4.2.14 Score per residue for model 14

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



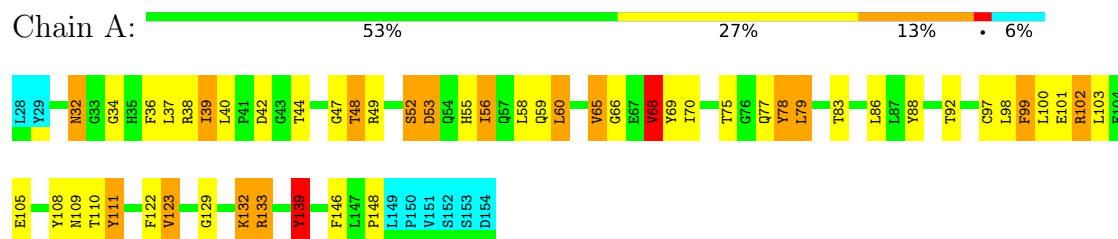
4.2.15 Score per residue for model 15

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



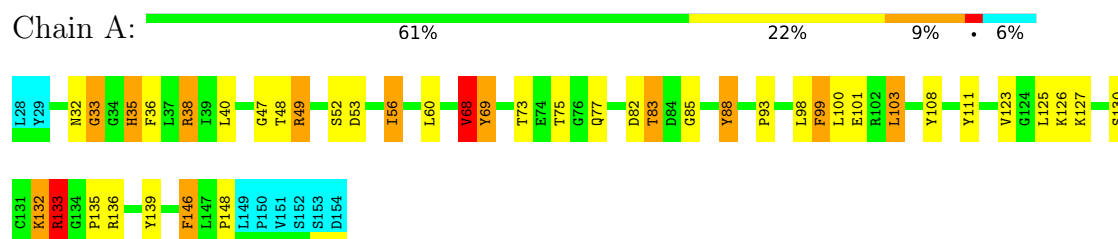
4.2.16 Score per residue for model 16

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



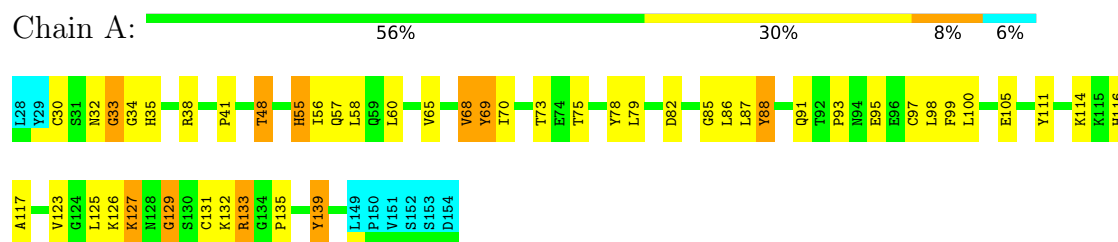
4.2.17 Score per residue for model 17

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



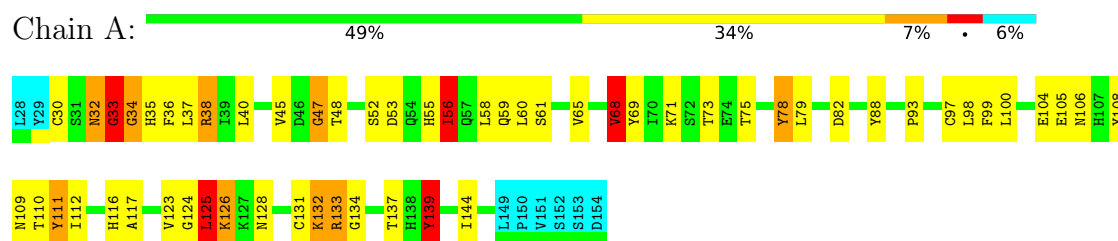
4.2.18 Score per residue for model 18

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



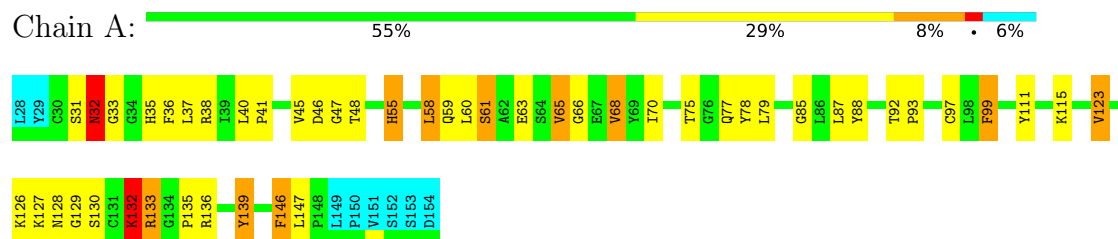
4.2.19 Score per residue for model 19

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



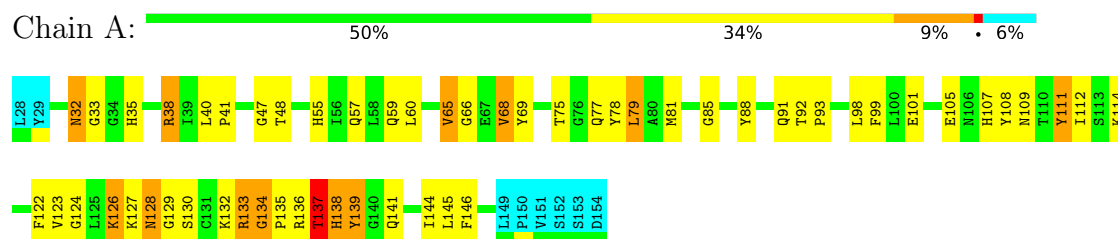
4.2.20 Score per residue for model 20

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



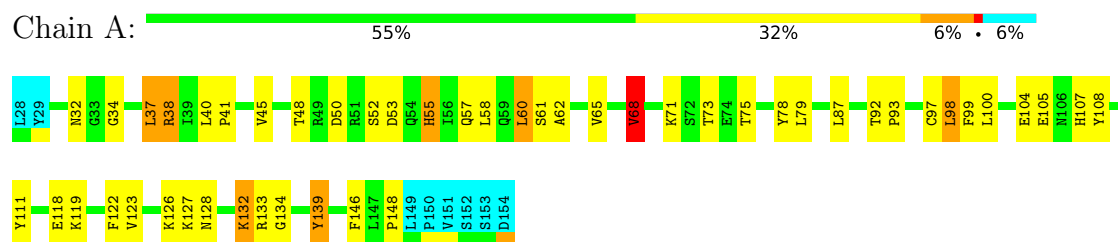
4.2.21 Score per residue for model 21

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



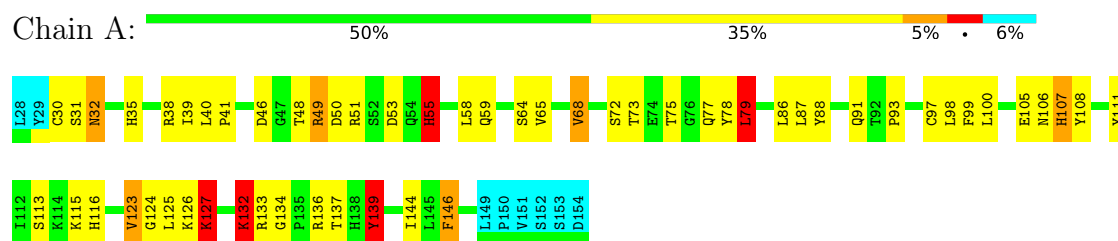
4.2.22 Score per residue for model 22

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



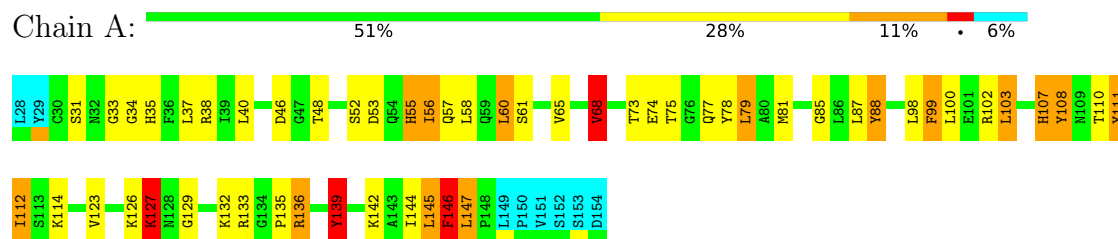
4.2.23 Score per residue for model 23

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



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	1.00±0.01	1±1/968 (0.1± 0.1%)	1.63±0.03	9±3/1306 (0.7± 0.2%)
All	All	1.00	13/23232 (0.1%)	1.63	214/31344 (0.7%)

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	8.5±1.8
All	All	0	205

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	116	HIS	CG-ND1	-5.66	1.32	1.38	19	6
1	A	35	HIS	CG-ND1	-5.43	1.32	1.38	19	3
1	A	107	HIS	CD2-NE2	-5.19	1.32	1.37	23	1
1	A	116	HIS	CD2-NE2	-5.17	1.32	1.37	18	1
1	A	55	HIS	CG-ND1	-5.14	1.32	1.38	24	1
1	A	107	HIS	CG-ND1	-5.05	1.32	1.38	10	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	56	ILE	N-CA-C	11.68	123.94	110.62	18	4
1	A	132	LYS	N-CA-C	10.12	124.94	108.34	8	11
1	A	49	ARG	NE-CZ-NH1	-10.06	111.44	121.50	17	1
1	A	133	ARG	N-CA-C	8.59	122.47	109.41	19	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	112	ILE	N-CA-CB	8.38	119.85	110.72	9	6
1	A	68	VAL	CA-CB-CG1	8.20	124.34	110.40	20	6
1	A	68	VAL	N-CA-C	8.13	119.82	108.12	21	14
1	A	146	PHE	N-CA-C	8.04	122.20	109.50	7	10
1	A	49	ARG	NE-CZ-NH2	7.83	126.25	119.20	17	1
1	A	74	GLU	CA-CB-CG	-7.73	98.64	114.10	6	1
1	A	49	ARG	CA-CB-CG	-7.67	98.77	114.10	17	1
1	A	68	VAL	CG1-CB-CG2	-7.57	94.15	110.80	2	9
1	A	68	VAL	CA-CB-CG2	7.50	123.16	110.40	17	6
1	A	102	ARG	N-CA-CB	-7.50	99.36	110.53	16	1
1	A	32	ASN	CA-CB-CG	7.46	120.06	112.60	8	10
1	A	93	PRO	N-CA-CB	7.36	107.04	102.92	5	2
1	A	99	PHE	N-CA-C	7.08	119.96	108.34	14	12
1	A	48	THR	N-CA-C	6.98	119.75	107.61	18	12
1	A	68	VAL	N-CA-CB	-6.78	103.36	111.90	1	5
1	A	35	HIS	CB-CG-CD2	-6.74	122.44	131.20	5	3
1	A	127	LYS	N-CA-C	6.71	125.10	110.80	13	9
1	A	38	ARG	CD-NE-CZ	6.62	133.66	124.40	2	2
1	A	60	LEU	N-CA-C	6.52	119.34	108.20	14	9
1	A	128	ASN	CA-CB-CG	6.11	118.71	112.60	22	5
1	A	32	ASN	N-CA-CB	-6.08	100.43	110.65	23	3
1	A	57	GLN	N-CA-CB	-6.00	102.10	110.38	3	1
1	A	130	SER	N-CA-C	5.98	118.27	110.43	20	1
1	A	38	ARG	N-CA-C	5.96	119.81	112.54	10	1
1	A	136	ARG	N-CA-CB	-5.94	102.57	111.25	7	2
1	A	53	ASP	CA-C-N	5.93	132.86	121.54	5	1
1	A	53	ASP	C-N-CA	5.93	132.86	121.54	5	1
1	A	126	LYS	CA-C-N	5.77	132.57	121.54	13	2
1	A	126	LYS	C-N-CA	5.77	132.57	121.54	13	2
1	A	114	LYS	CA-CB-CG	-5.75	102.61	114.10	10	1
1	A	33	GLY	CA-C-N	5.66	126.07	120.98	1	1
1	A	33	GLY	C-N-CA	5.66	126.07	120.98	1	1
1	A	33	GLY	N-CA-C	-5.53	100.08	113.18	5	4
1	A	40	LEU	CA-C-N	5.47	125.82	119.47	12	1
1	A	40	LEU	C-N-CA	5.47	125.82	119.47	12	1
1	A	82	ASP	CA-C-N	5.44	128.11	120.28	4	1
1	A	82	ASP	C-N-CA	5.44	128.11	120.28	4	1
1	A	107	HIS	CB-CG-CD2	-5.43	124.14	131.20	14	6
1	A	98	LEU	CD1-CG-CD2	-5.42	98.87	110.80	22	1
1	A	48	THR	N-CA-CB	5.40	116.40	110.35	8	1
1	A	34	GLY	N-CA-C	5.38	118.86	111.54	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	SER	CA-C-N	5.38	131.82	121.54	16	1
1	A	52	SER	C-N-CA	5.38	131.82	121.54	16	1
1	A	111	TYR	N-CA-C	5.37	116.20	107.23	15	2
1	A	58	LEU	N-CA-C	5.36	122.22	110.80	4	1
1	A	62	ALA	N-CA-C	5.36	117.47	109.59	8	3
1	A	137	THR	N-CA-C	5.32	117.89	107.57	12	3
1	A	138	HIS	CB-CG-CD2	-5.32	124.29	131.20	21	4
1	A	57	GLN	N-CA-C	5.30	119.67	111.56	4	1
1	A	71	LYS	N-CA-CB	-5.28	101.80	110.41	19	1
1	A	112	ILE	CB-CA-C	-5.26	104.31	111.15	1	2
1	A	32	ASN	CA-C-N	5.20	131.59	121.41	8	1
1	A	32	ASN	C-N-CA	5.20	131.59	121.41	8	1
1	A	125	LEU	CA-CB-CG	-5.19	98.15	116.30	19	1
1	A	82	ASP	CA-CB-CG	5.18	117.78	112.60	10	1
1	A	95	GLU	CB-CA-C	-5.17	101.89	110.68	15	1
1	A	55	HIS	CA-C-N	5.14	129.05	120.62	19	1
1	A	55	HIS	C-N-CA	5.14	129.05	120.62	19	1
1	A	54	GLN	N-CA-C	5.14	121.75	110.80	5	1
1	A	145	LEU	N-CA-C	5.13	117.77	107.41	2	1
1	A	106	ASN	N-CA-CB	-5.12	103.33	110.29	8	1
1	A	58	LEU	CB-CA-C	5.10	118.00	110.14	9	1
1	A	125	LEU	N-CA-C	5.07	117.24	109.07	19	1
1	A	53	ASP	N-CA-C	5.05	121.56	110.80	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	139	TYR	Sidechain,Mainchain	15
1	A	122	PHE	Sidechain	12
1	A	33	GLY	Mainchain,Peptide	11
1	A	78	TYR	Sidechain	11
1	A	108	TYR	Sidechain,Mainchain	11
1	A	88	TYR	Sidechain	10
1	A	146	PHE	Sidechain	10
1	A	55	HIS	Sidechain,Mainchain	9
1	A	117	ALA	Mainchain	9
1	A	52	SER	Mainchain	9
1	A	38	ARG	Sidechain	8
1	A	111	TYR	Sidechain	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	133	ARG	Mainchain,Sidechain	8
1	A	61	SER	Mainchain	7
1	A	69	TYR	Sidechain	6
1	A	31	SER	Mainchain	5
1	A	82	ASP	Mainchain	5
1	A	93	PRO	Mainchain	4
1	A	103	LEU	Mainchain	3
1	A	54	GLN	Mainchain	3
1	A	129	GLY	Mainchain	3
1	A	132	LYS	Peptide,Mainchain	3
1	A	107	HIS	Sidechain,Mainchain	3
1	A	130	SER	Mainchain	2
1	A	51	ARG	Sidechain	2
1	A	48	THR	Peptide	2
1	A	102	ARG	Mainchain	2
1	A	124	GLY	Mainchain	2
1	A	125	LEU	Mainchain	2
1	A	36	PHE	Sidechain	2
1	A	99	PHE	Sidechain	1
1	A	60	LEU	Mainchain	1
1	A	57	GLN	Peptide	1
1	A	41	PRO	Mainchain	1
1	A	126	LYS	Mainchain	1
1	A	136	ARG	Sidechain	1
1	A	43	GLY	Mainchain	1
1	A	71	LYS	Mainchain	1
1	A	85	GLY	Mainchain	1
1	A	40	LEU	Mainchain	1
1	A	32	ASN	Peptide	1
1	A	35	HIS	Sidechain	1
1	A	142	LYS	Mainchain	1
1	A	49	ARG	Sidechain	1
1	A	63	GLU	Mainchain	1
1	A	79	LEU	Mainchain	1
1	A	106	ASN	Mainchain	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	947	0	917	21±3
All	All	22728	0	22008	499

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:35:HIS:HB2	1:A:125:LEU:HD23	0.83	1.49	10	7
1:A:35:HIS:HB3	1:A:48:THR:H	0.80	1.36	5	16
1:A:38:ARG:HD2	1:A:55:HIS:HB2	0.79	1.54	12	4
1:A:99:PHE:HB3	1:A:111:TYR:HB3	0.78	1.53	20	14
1:A:126:LYS:HE3	1:A:128:ASN:HB2	0.74	1.58	6	8
1:A:78:TYR:HB3	1:A:97:CYS:SG	0.73	2.24	1	9
1:A:87:LEU:HD12	1:A:131:CYS:HB3	0.73	1.60	6	5
1:A:45:VAL:HG11	1:A:79:LEU:HD13	0.71	1.60	9	4
1:A:39:ILE:HG22	1:A:57:GLN:HB2	0.68	1.65	2	3
1:A:68:VAL:HG22	1:A:99:PHE:HB2	0.67	1.65	22	6
1:A:37:LEU:HB3	1:A:58:LEU:HD22	0.65	1.69	20	2
1:A:38:ARG:HD3	1:A:56:ILE:HG23	0.64	1.70	16	6
1:A:100:LEU:HD11	1:A:114:LYS:HE2	0.63	1.70	18	3
1:A:39:ILE:HG22	1:A:57:GLN:HB3	0.63	1.70	5	1
1:A:37:LEU:HD23	1:A:58:LEU:HD22	0.63	1.69	9	1
1:A:38:ARG:HH11	1:A:38:ARG:HB3	0.62	1.54	2	1
1:A:41:PRO:HD3	1:A:75:THR:HG21	0.62	1.70	12	2
1:A:79:LEU:HD21	1:A:123:VAL:HG21	0.62	1.72	9	6
1:A:104:GLU:HB2	1:A:108:TYR:HB2	0.61	1.71	19	5
1:A:59:GLN:HE21	1:A:73:THR:HG23	0.61	1.54	4	1
1:A:111:TYR:HD2	1:A:123:VAL:HG11	0.61	1.55	19	4
1:A:60:LEU:HD12	1:A:68:VAL:HG21	0.61	1.72	21	4
1:A:38:ARG:HH12	1:A:51:ARG:HA	0.61	1.55	7	2
1:A:48:THR:HG23	1:A:51:ARG:HG2	0.60	1.74	23	1
1:A:87:LEU:HD22	1:A:123:VAL:HG12	0.60	1.73	22	4
1:A:41:PRO:HD3	1:A:55:HIS:CG	0.60	2.32	21	11
1:A:68:VAL:O	1:A:98:LEU:HD12	0.59	1.97	22	5
1:A:38:ARG:HG2	1:A:40:LEU:HD22	0.59	1.74	1	12
1:A:45:VAL:HG11	1:A:79:LEU:CD1	0.59	2.27	13	11
1:A:39:ILE:HD11	1:A:89:GLY:HA2	0.59	1.73	6	3
1:A:133:ARG:H	1:A:133:ARG:NH1	0.59	1.93	10	5
1:A:107:HIS:HB3	1:A:147:LEU:HD21	0.58	1.73	7	2
1:A:68:VAL:HG12	1:A:99:PHE:O	0.58	1.99	11	3
1:A:69:TYR:CE1	1:A:93:PRO:HB2	0.58	2.33	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:A:79:LEU:HD11	0.58	1.76	16	1
1:A:133:ARG:HE	1:A:136:ARG:HD2	0.58	1.58	17	1
1:A:68:VAL:C	1:A:98:LEU:HD12	0.57	2.24	19	18
1:A:37:LEU:HB3	1:A:125:LEU:HD11	0.57	1.76	10	1
1:A:45:VAL:HG13	1:A:57:GLN:HE22	0.57	1.60	5	1
1:A:57:GLN:HG3	1:A:72:SER:HB2	0.57	1.75	6	2
1:A:37:LEU:HD21	1:A:79:LEU:HD22	0.57	1.77	4	5
1:A:124:GLY:HA3	1:A:137:THR:HG21	0.56	1.77	5	5
1:A:126:LYS:HG2	1:A:136:ARG:HH12	0.56	1.60	21	1
1:A:108:TYR:HB3	1:A:145:LEU:HB2	0.56	1.77	24	3
1:A:39:ILE:HG21	1:A:77:GLN:HB2	0.56	1.77	1	1
1:A:38:ARG:HH11	1:A:56:ILE:HG23	0.56	1.61	13	2
1:A:32:ASN:CG	1:A:33:GLY:H	0.56	2.08	6	3
1:A:123:VAL:HG23	1:A:146:PHE:CE2	0.56	2.36	15	1
1:A:133:ARG:HG2	1:A:134:GLY:H	0.55	1.59	11	2
1:A:85:GLY:HA3	1:A:135:PRO:HD3	0.55	1.79	18	9
1:A:101:GLU:HG2	1:A:111:TYR:HE1	0.54	1.62	3	4
1:A:38:ARG:HA	1:A:56:ILE:HA	0.54	1.78	12	7
1:A:123:VAL:HG23	1:A:146:PHE:HZ	0.54	1.63	7	3
1:A:87:LEU:HD11	1:A:131:CYS:HB3	0.54	1.79	8	1
1:A:32:ASN:HD22	1:A:127:LYS:HD3	0.54	1.63	3	1
1:A:110:THR:HG22	1:A:144:ILE:O	0.54	2.03	11	3
1:A:118:GLU:HG3	1:A:119:LYS:HE2	0.54	1.79	9	7
1:A:38:ARG:HG3	1:A:55:HIS:HB2	0.53	1.79	10	5
1:A:111:TYR:HB2	1:A:123:VAL:CG1	0.53	2.34	5	4
1:A:30:CYS:HB3	1:A:146:PHE:HD1	0.53	1.64	23	1
1:A:100:LEU:HD13	1:A:114:LYS:HE2	0.52	1.81	5	2
1:A:100:LEU:O	1:A:111:TYR:HA	0.52	2.04	1	5
1:A:87:LEU:H	1:A:87:LEU:CD2	0.52	2.17	8	1
1:A:141:GLN:O	1:A:144:ILE:HG12	0.52	2.05	10	2
1:A:98:LEU:HD23	1:A:99:PHE:N	0.52	2.20	9	1
1:A:65:VAL:HG13	1:A:66:GLY:H	0.51	1.64	21	3
1:A:70:ILE:HB	1:A:79:LEU:HB3	0.51	1.82	1	3
1:A:38:ARG:HB3	1:A:46:ASP:O	0.51	2.06	7	4
1:A:63:GLU:OE1	1:A:69:TYR:CE2	0.51	2.63	4	1
1:A:123:VAL:HG23	1:A:146:PHE:CZ	0.51	2.40	13	4
1:A:139:TYR:HA	1:A:144:ILE:HD11	0.51	1.81	12	9
1:A:125:LEU:HD13	1:A:146:PHE:HE2	0.51	1.64	5	1
1:A:125:LEU:HD13	1:A:146:PHE:HE1	0.51	1.65	1	1
1:A:37:LEU:HB2	1:A:58:LEU:HD22	0.51	1.83	7	1
1:A:30:CYS:SG	1:A:32:ASN:HB3	0.51	2.46	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD12	1:A:131:CYS:O	0.51	2.06	9	1
1:A:77:GLN:NE2	1:A:77:GLN:H	0.51	2.04	13	1
1:A:38:ARG:CG	1:A:55:HIS:HB2	0.50	2.36	10	4
1:A:39:ILE:O	1:A:55:HIS:HB3	0.50	2.06	4	1
1:A:79:LEU:HD21	1:A:123:VAL:HG11	0.50	1.84	13	3
1:A:58:LEU:HD22	1:A:70:ILE:HG21	0.50	1.82	3	2
1:A:123:VAL:HG13	1:A:146:PHE:HE2	0.50	1.66	17	1
1:A:63:GLU:OE1	1:A:69:TYR:HE2	0.50	1.90	4	1
1:A:60:LEU:HB2	1:A:68:VAL:CG2	0.50	2.37	6	3
1:A:41:PRO:HD3	1:A:55:HIS:CD2	0.49	2.43	15	2
1:A:125:LEU:HD13	1:A:146:PHE:CE2	0.49	2.42	6	1
1:A:81:MET:HE2	1:A:87:LEU:HD21	0.49	1.83	24	2
1:A:36:PHE:O	1:A:47:GLY:HA2	0.49	2.08	6	6
1:A:126:LYS:HE2	1:A:130:SER:H	0.49	1.68	8	1
1:A:133:ARG:O	1:A:135:PRO:HD2	0.49	2.08	12	4
1:A:61:SER:HB2	1:A:69:TYR:HB2	0.49	1.85	19	1
1:A:70:ILE:O	1:A:78:TYR:HA	0.49	2.08	9	1
1:A:144:ILE:HG13	1:A:145:LEU:HD12	0.49	1.85	9	1
1:A:67:GLU:HB3	1:A:98:LEU:HD21	0.49	1.85	9	1
1:A:125:LEU:HD11	1:A:131:CYS:SG	0.49	2.48	19	1
1:A:30:CYS:SG	1:A:34:GLY:HA2	0.49	2.48	7	1
1:A:37:LEU:O	1:A:45:VAL:HG13	0.49	2.08	13	1
1:A:59:GLN:HE22	1:A:71:LYS:HD3	0.48	1.68	4	1
1:A:102:ARG:HB2	1:A:110:THR:OG1	0.48	2.08	12	2
1:A:133:ARG:HG3	1:A:134:GLY:H	0.48	1.68	21	1
1:A:41:PRO:HA	1:A:77:GLN:HE22	0.48	1.69	20	1
1:A:87:LEU:HD21	1:A:123:VAL:HG12	0.48	1.85	14	3
1:A:31:SER:HB3	1:A:145:LEU:HB2	0.47	1.86	12	1
1:A:102:ARG:HB3	1:A:110:THR:O	0.47	2.09	16	1
1:A:56:ILE:HG13	1:A:57:GLN:OE1	0.47	2.10	24	1
1:A:57:GLN:O	1:A:70:ILE:HG22	0.47	2.10	5	1
1:A:38:ARG:HH11	1:A:56:ILE:CG2	0.47	2.22	13	2
1:A:49:ARG:HG3	1:A:129:GLY:HA3	0.47	1.86	16	1
1:A:79:LEU:HD23	1:A:99:PHE:CE2	0.47	2.44	23	1
1:A:111:TYR:O	1:A:122:PHE:HA	0.47	2.10	14	4
1:A:107:HIS:O	1:A:147:LEU:HB3	0.47	2.10	14	1
1:A:111:TYR:HB2	1:A:123:VAL:HG22	0.47	1.86	23	5
1:A:138:HIS:H	1:A:141:GLN:NE2	0.46	2.08	21	2
1:A:37:LEU:HD13	1:A:79:LEU:HD22	0.46	1.87	13	1
1:A:37:LEU:HD22	1:A:79:LEU:HD21	0.46	1.87	2	1
1:A:122:PHE:HB2	1:A:144:ILE:HG21	0.46	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ASN:HB3	1:A:111:TYR:CZ	0.46	2.45	4	4
1:A:70:ILE:HD12	1:A:79:LEU:HD23	0.46	1.86	14	1
1:A:99:PHE:CE2	1:A:123:VAL:HG13	0.46	2.45	14	1
1:A:51:ARG:HE	1:A:56:ILE:HG21	0.46	1.71	8	1
1:A:98:LEU:O	1:A:114:LYS:HB2	0.46	2.11	11	1
1:A:91:GLN:H	1:A:91:GLN:CD	0.46	2.19	5	2
1:A:77:GLN:NE2	1:A:91:GLN:HE21	0.46	2.09	21	1
1:A:104:GLU:OE2	1:A:145:LEU:HD22	0.46	2.11	5	1
1:A:125:LEU:HD13	1:A:146:PHE:CE1	0.46	2.46	1	2
1:A:30:CYS:C	1:A:32:ASN:H	0.45	2.18	1	1
1:A:127:LYS:HE3	1:A:136:ARG:HH12	0.45	1.70	3	1
1:A:51:ARG:H	1:A:51:ARG:CZ	0.45	2.24	5	2
1:A:39:ILE:HA	1:A:45:VAL:HG22	0.45	1.89	13	1
1:A:113:SER:HB3	1:A:116:HIS:HB2	0.45	1.88	23	3
1:A:38:ARG:HG2	1:A:40:LEU:HD12	0.45	1.88	13	1
1:A:60:LEU:H	1:A:60:LEU:HD23	0.45	1.71	17	1
1:A:51:ARG:HB3	1:A:56:ILE:HD13	0.45	1.87	13	1
1:A:79:LEU:O	1:A:99:PHE:HE2	0.45	1.94	5	2
1:A:37:LEU:HD23	1:A:131:CYS:SG	0.45	2.52	5	1
1:A:38:ARG:HE	1:A:40:LEU:HD11	0.45	1.71	9	1
1:A:39:ILE:HG21	1:A:77:GLN:O	0.45	2.12	16	1
1:A:38:ARG:NH1	1:A:48:THR:HG21	0.45	2.26	12	1
1:A:123:VAL:O	1:A:144:ILE:HG22	0.45	2.11	3	3
1:A:126:LYS:NZ	1:A:128:ASN:HB2	0.44	2.28	10	1
1:A:54:GLN:HG2	1:A:74:GLU:HB3	0.44	1.88	2	2
1:A:132:LYS:HG2	1:A:133:ARG:HH11	0.44	1.71	8	1
1:A:68:VAL:CG2	1:A:99:PHE:HB2	0.44	2.43	9	2
1:A:103:LEU:HD12	1:A:108:TYR:O	0.44	2.12	7	2
1:A:57:GLN:HE22	1:A:79:LEU:HD13	0.44	1.72	8	1
1:A:30:CYS:SG	1:A:125:LEU:HD13	0.44	2.52	19	1
1:A:32:ASN:ND2	1:A:33:GLY:H	0.44	2.10	18	2
1:A:33:GLY:HA3	1:A:127:LYS:HE2	0.44	1.88	12	1
1:A:102:ARG:HB2	1:A:110:THR:O	0.44	2.12	9	1
1:A:87:LEU:H	1:A:87:LEU:HD23	0.44	1.72	8	1
1:A:62:ALA:HA	1:A:68:VAL:HA	0.44	1.88	22	1
1:A:39:ILE:HD12	1:A:72:SER:HB3	0.44	1.88	23	1
1:A:39:ILE:HG22	1:A:77:GLN:HG3	0.44	1.90	23	1
1:A:49:ARG:NE	1:A:49:ARG:H	0.44	2.11	9	1
1:A:30:CYS:HB3	1:A:146:PHE:HB3	0.43	1.90	13	1
1:A:86:LEU:HB2	1:A:132:LYS:HB3	0.43	1.89	18	1
1:A:38:ARG:HB3	1:A:38:ARG:HH11	0.43	1.71	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:O	1:A:99:PHE:HE1	0.43	1.96	8	1
1:A:65:VAL:O	1:A:67:GLU:HG3	0.43	2.14	10	1
1:A:99:PHE:CE1	1:A:123:VAL:HG13	0.43	2.48	2	1
1:A:47:GLY:H	1:A:130:SER:HA	0.43	1.72	21	2
1:A:68:VAL:HG11	1:A:101:GLU:HG3	0.43	1.91	21	1
1:A:32:ASN:CG	1:A:125:LEU:HB3	0.43	2.39	3	1
1:A:101:GLU:HG2	1:A:111:TYR:CE1	0.43	2.47	3	1
1:A:59:GLN:HB3	1:A:71:LYS:O	0.43	2.14	9	1
1:A:108:TYR:HB3	1:A:145:LEU:HB3	0.43	1.89	13	1
1:A:86:LEU:HB2	1:A:132:LYS:HB2	0.42	1.90	23	1
1:A:67:GLU:HA	1:A:99:PHE:O	0.42	2.14	6	1
1:A:81:MET:HG2	1:A:116:HIS:CE1	0.42	2.49	12	1
1:A:133:ARG:HG2	1:A:134:GLY:N	0.42	2.28	11	2
1:A:59:GLN:HB2	1:A:73:THR:HB	0.42	1.91	13	1
1:A:39:ILE:HG22	1:A:77:GLN:HG2	0.42	1.90	14	1
1:A:126:LYS:HB2	1:A:132:LYS:HB2	0.42	1.92	20	1
1:A:49:ARG:HH21	1:A:50:ASP:HB2	0.42	1.73	23	1
1:A:37:LEU:HD23	1:A:58:LEU:HB2	0.42	1.91	4	1
1:A:39:ILE:HD13	1:A:72:SER:HB3	0.42	1.91	7	1
1:A:65:VAL:HG22	1:A:66:GLY:H	0.42	1.74	20	1
1:A:127:LYS:HE2	1:A:136:ARG:NH2	0.42	2.29	24	1
1:A:126:LYS:HB2	1:A:131:CYS:O	0.42	2.15	12	2
1:A:38:ARG:HB2	1:A:56:ILE:HG22	0.42	1.91	17	1
1:A:136:ARG:O	1:A:141:GLN:HG3	0.42	2.14	3	1
1:A:111:TYR:HB2	1:A:123:VAL:HG12	0.42	1.90	16	1
1:A:30:CYS:O	1:A:34:GLY:HA2	0.42	2.15	19	1
1:A:35:HIS:CD2	1:A:129:GLY:HA2	0.42	2.50	6	2
1:A:45:VAL:HG11	1:A:79:LEU:HD11	0.42	1.92	6	1
1:A:31:SER:O	1:A:142:LYS:HB3	0.42	2.15	24	2
1:A:68:VAL:HG23	1:A:70:ILE:HG13	0.42	1.91	16	1
1:A:133:ARG:HH21	1:A:136:ARG:NH1	0.42	2.12	1	1
1:A:85:GLY:C	1:A:86:LEU:HD23	0.42	2.40	11	1
1:A:38:ARG:CZ	1:A:52:SER:H	0.41	2.28	4	1
1:A:77:GLN:HB3	1:A:91:GLN:NE2	0.41	2.30	23	1
1:A:110:THR:HG21	1:A:139:TYR:CE1	0.41	2.50	2	1
1:A:58:LEU:HA	1:A:72:SER:HA	0.41	1.91	10	1
1:A:32:ASN:HB2	1:A:127:LYS:HE2	0.41	1.93	14	1
1:A:37:LEU:H	1:A:37:LEU:HD23	0.41	1.76	10	1
1:A:86:LEU:HD13	1:A:132:LYS:HB2	0.41	1.91	10	1
1:A:100:LEU:HD13	1:A:114:LYS:HD3	0.41	1.92	24	1
1:A:80:ALA:HB2	1:A:97:CYS:SG	0.41	2.55	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:HD13	1:A:72:SER:OG	0.41	2.15	10	1
1:A:32:ASN:CG	1:A:33:GLY:N	0.41	2.78	20	1
1:A:38:ARG:NH1	1:A:51:ARG:HA	0.41	2.31	4	1
1:A:103:LEU:HG	1:A:105:GLU:H	0.41	1.76	7	1
1:A:48:THR:HG23	1:A:51:ARG:HG3	0.41	1.93	12	1
1:A:60:LEU:HD21	1:A:148:PRO:HB3	0.41	1.92	12	1
1:A:98:LEU:HD12	1:A:98:LEU:HA	0.41	1.84	19	1
1:A:127:LYS:HE2	1:A:136:ARG:HH22	0.41	1.76	24	1
1:A:66:GLY:O	1:A:100:LEU:HA	0.40	2.16	1	1
1:A:45:VAL:HG12	1:A:131:CYS:SG	0.40	2.56	14	1
1:A:111:TYR:CD2	1:A:123:VAL:HG11	0.40	2.51	3	1
1:A:110:THR:HG23	1:A:145:LEU:HB3	0.40	1.93	24	1
1:A:38:ARG:NH1	1:A:52:SER:H	0.40	2.14	8	1
1:A:147:LEU:HD12	1:A:147:LEU:O	0.40	2.16	9	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	119/127 (94%)	86±4 (72±3%)	25±4 (21±3%)	9±3 (7±2%)	1	15
All	All	2856/3048 (94%)	2053 (72%)	592 (21%)	211 (7%)	1	15

All 44 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	65	VAL	19
1	A	127	LYS	18
1	A	53	ASP	15
1	A	132	LYS	13
1	A	105	GLU	12
1	A	34	GLY	10
1	A	77	GLN	8
1	A	136	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	A	134	GLY	7
1	A	139	TYR	7
1	A	148	PRO	7
1	A	129	GLY	7
1	A	64	SER	7
1	A	33	GLY	6
1	A	103	LEU	6
1	A	54	GLN	6
1	A	39	ILE	6
1	A	56	ILE	5
1	A	58	LEU	5
1	A	73	THR	4
1	A	51	ARG	3
1	A	37	LEU	3
1	A	133	ARG	3
1	A	106	ASN	2
1	A	47	GLY	2
1	A	123	VAL	2
1	A	72	SER	2
1	A	57	GLN	2
1	A	101	GLU	1
1	A	138	HIS	1
1	A	109	ASN	1
1	A	84	ASP	1
1	A	128	ASN	1
1	A	74	GLU	1
1	A	114	LYS	1
1	A	79	LEU	1
1	A	126	LYS	1
1	A	42	ASP	1
1	A	38	ARG	1
1	A	83	THR	1
1	A	88	TYR	1
1	A	32	ASN	1
1	A	50	ASP	1
1	A	93	PRO	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	103/111 (93%)	89±3 (86±3%)	14±3 (14±3%)	6	45
All	All	2472/2664 (93%)	2136 (86%)	336 (14%)	6	45

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	139	TYR	23
1	A	75	THR	21
1	A	133	ARG	17
1	A	126	LYS	15
1	A	60	LEU	14
1	A	68	VAL	14
1	A	115	LYS	12
1	A	58	LEU	12
1	A	59	GLN	9
1	A	132	LYS	9
1	A	92	THR	9
1	A	88	TYR	8
1	A	73	THR	8
1	A	55	HIS	8
1	A	82	ASP	7
1	A	112	ILE	7
1	A	100	LEU	6
1	A	147	LEU	6
1	A	39	ILE	6
1	A	123	VAL	6
1	A	79	LEU	6
1	A	44	THR	6
1	A	125	LEU	5
1	A	49	ARG	5
1	A	145	LEU	5
1	A	51	ARG	5
1	A	38	ARG	4
1	A	127	LYS	4
1	A	37	LEU	4
1	A	83	THR	4
1	A	87	LEU	4
1	A	137	THR	4
1	A	146	PHE	4
1	A	32	ASN	4
1	A	57	GLN	4
1	A	40	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ILE	4
1	A	86	LEU	4
1	A	81	MET	3
1	A	118	GLU	3
1	A	74	GLU	3
1	A	136	ARG	3
1	A	48	THR	2
1	A	101	GLU	2
1	A	109	ASN	2
1	A	103	LEU	2
1	A	114	LYS	2
1	A	95	GLU	2
1	A	104	GLU	2
1	A	128	ASN	2
1	A	42	ASP	2
1	A	142	LYS	1
1	A	36	PHE	1
1	A	30	CYS	1
1	A	102	ARG	1
1	A	31	SER	1
1	A	52	SER	1
1	A	53	ASP	1
1	A	61	SER	1
1	A	71	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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