



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:29 PM BST

PDB ID : 1DZD
Title : HIGH RESOLUTION STRUCTURE OF ACIDIC FIBROBLAST GROWTH FACTOR (27-154), 24 NMR STRUCTURES
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Deposited on : 2000-02-24

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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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

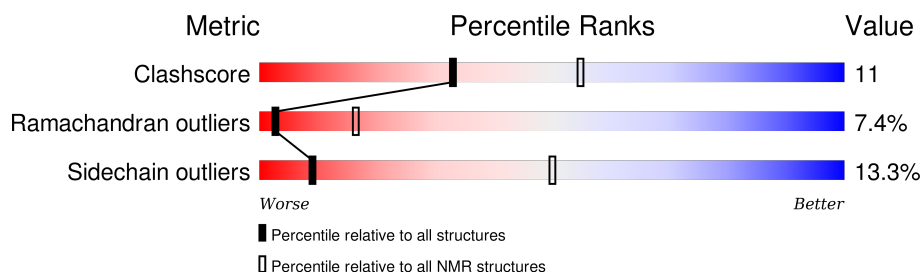
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	 49% 39% 6% • 6%

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)	0.48	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.

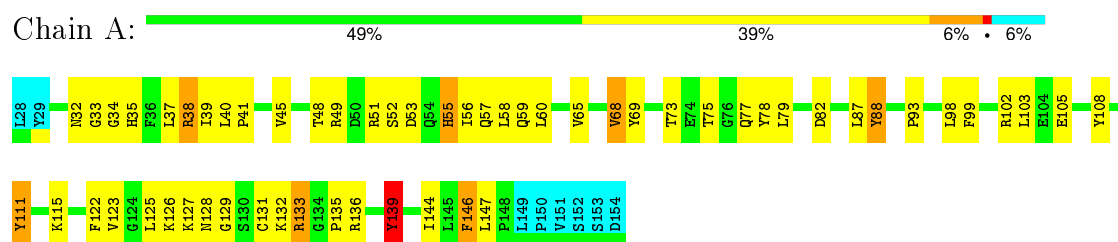
Mol	Chain	Residues	Atoms					Trace
1	A	127	Total	C	N	O	S	0
			1010	633	176	197	4	

4 Residue-property plots [i](#)

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: ACIDIC FIBROBLAST GROWTH FACTOR

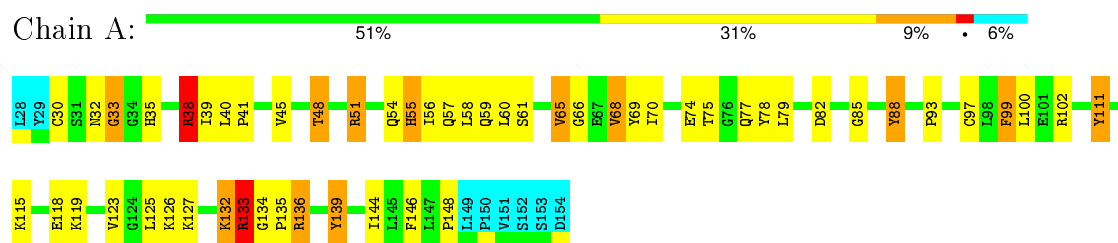


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

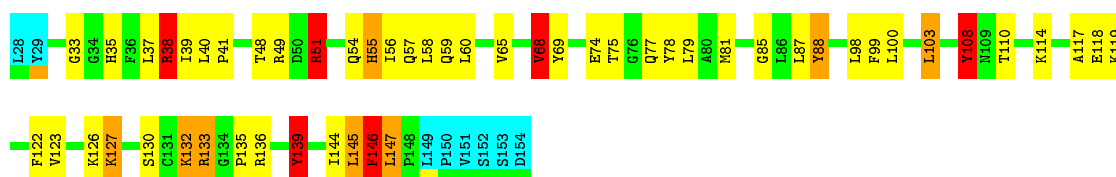
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.2 Score per residue for model 2

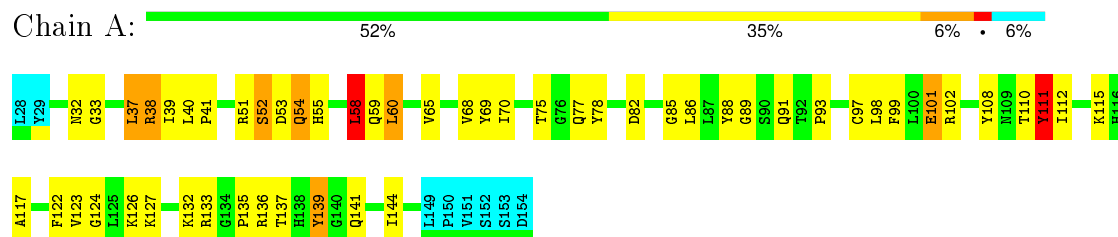
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR





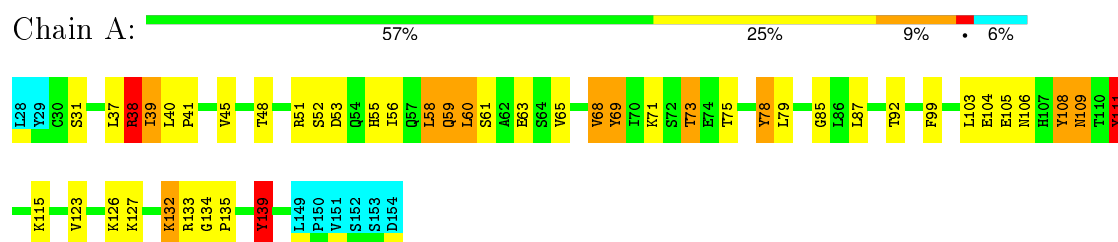
4.2.3 Score per residue for model 3

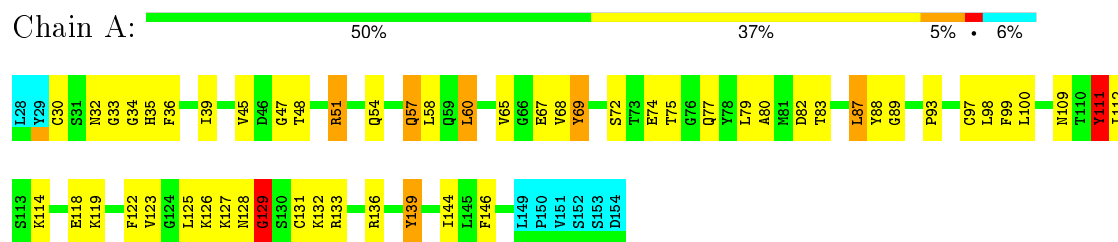
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.4 Score per residue for model 4

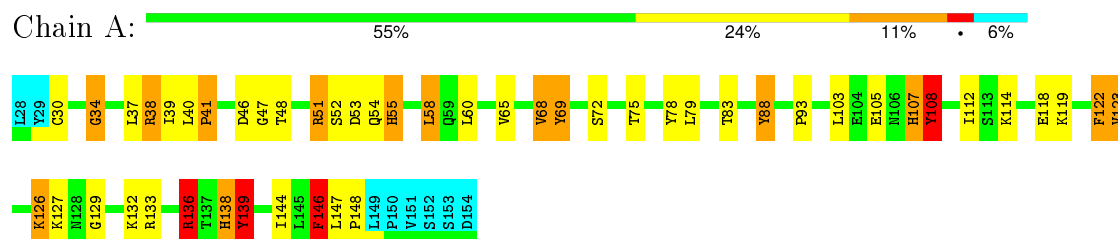
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR





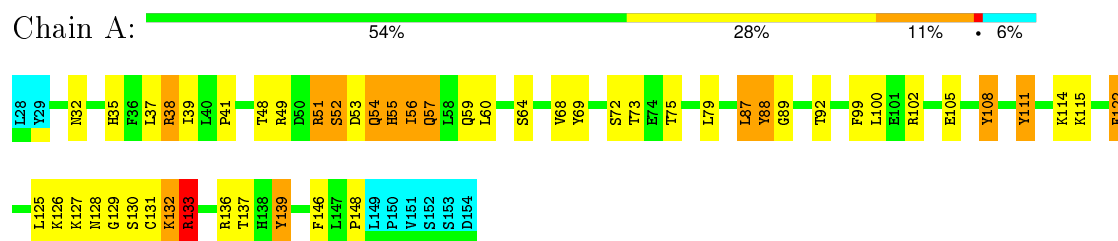
4.2.7 Score per residue for model 7

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



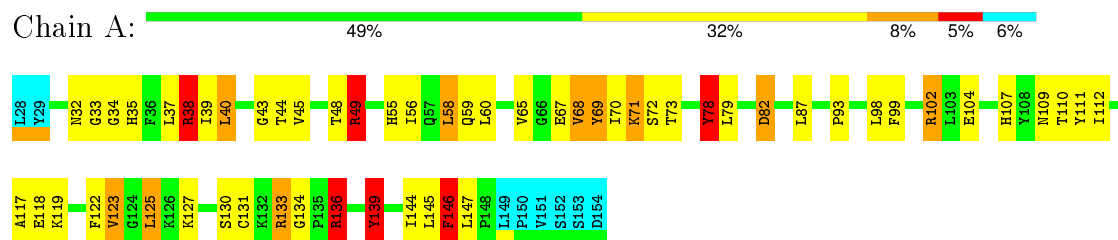
4.2.8 Score per residue for model 8

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



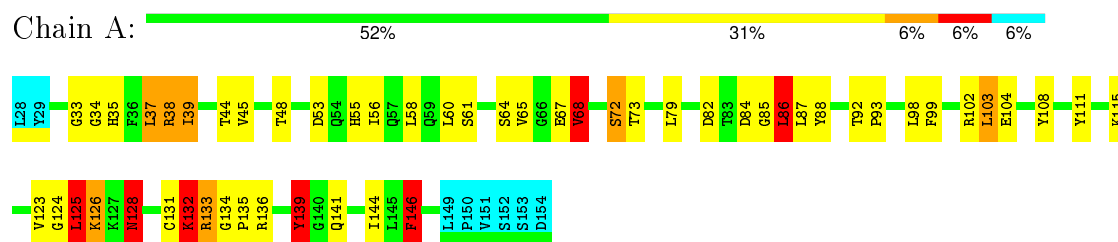
4.2.9 Score per residue for model 9

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



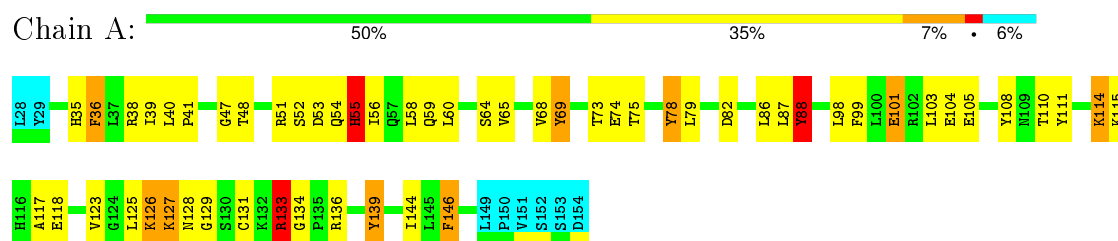
4.2.10 Score per residue for model 10

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



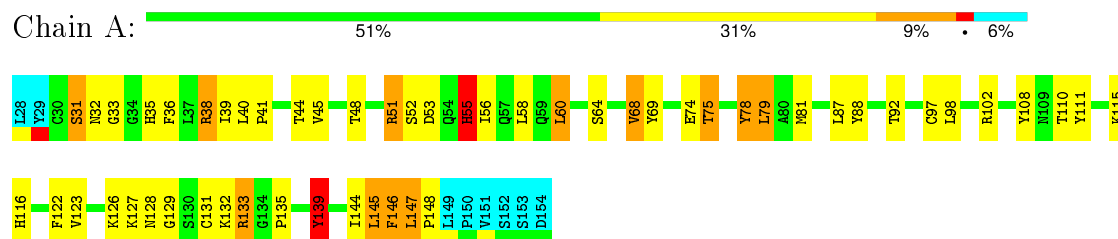
4.2.11 Score per residue for model 11

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



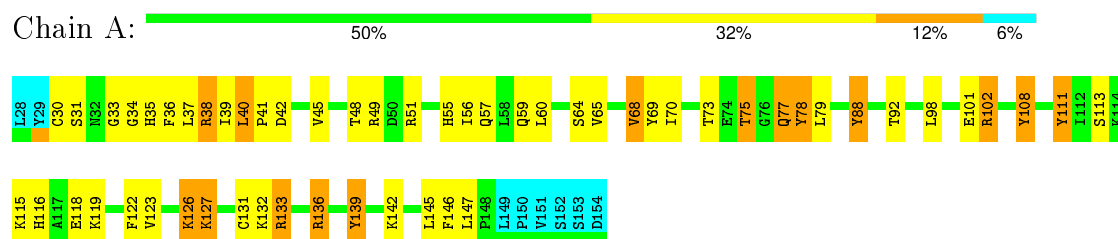
4.2.12 Score per residue for model 12

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



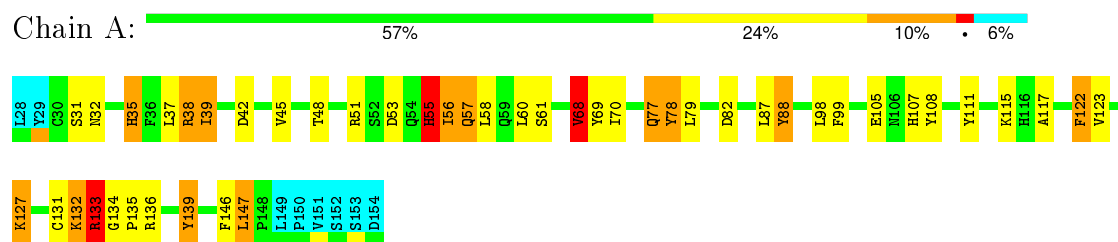
4.2.13 Score per residue for model 13

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



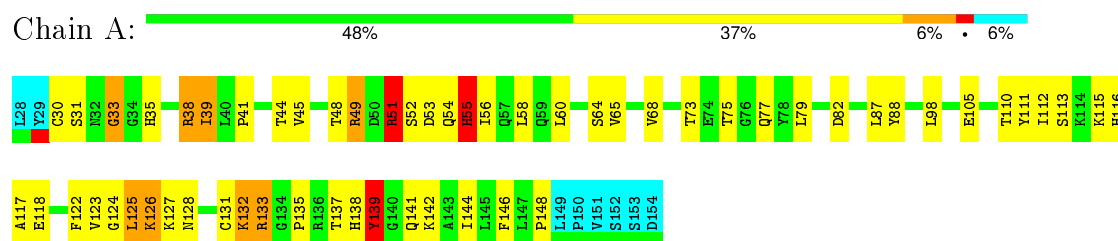
4.2.14 Score per residue for model 14

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



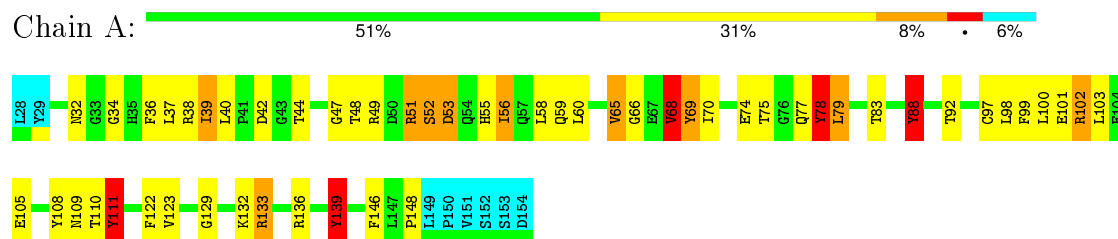
4.2.15 Score per residue for model 15

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



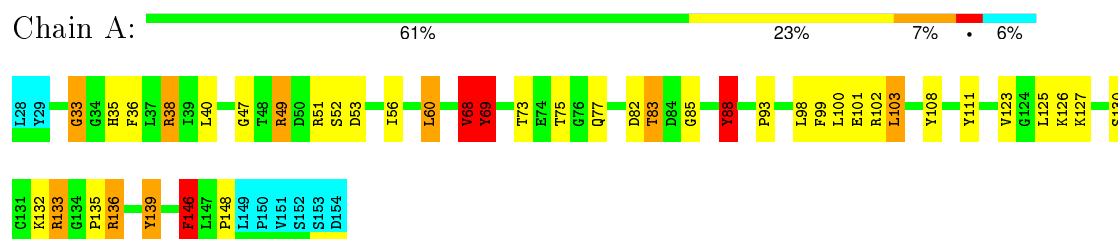
4.2.16 Score per residue for model 16

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



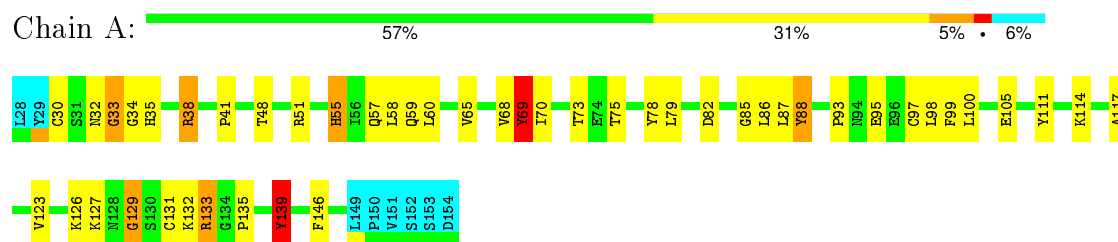
4.2.17 Score per residue for model 17

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



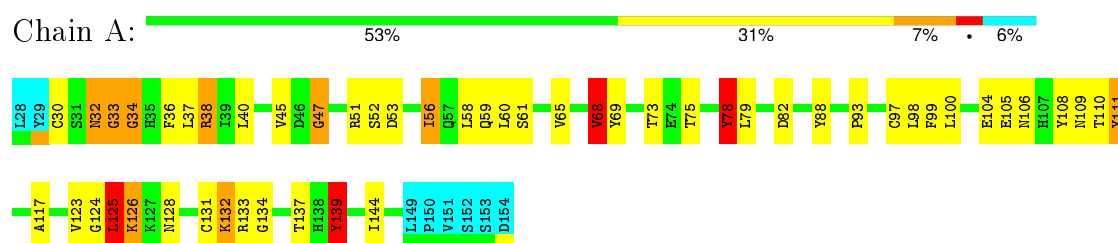
4.2.18 Score per residue for model 18

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



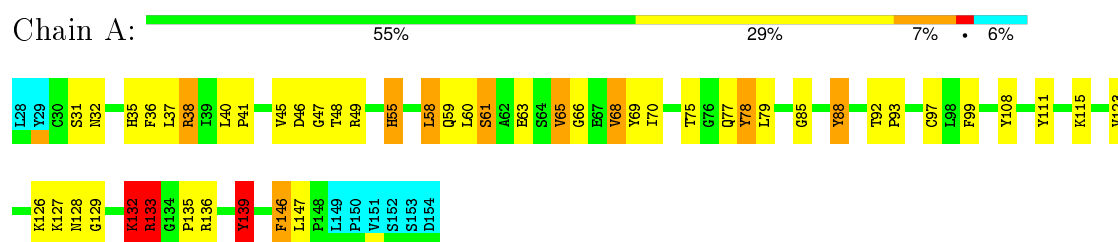
4.2.19 Score per residue for model 19

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



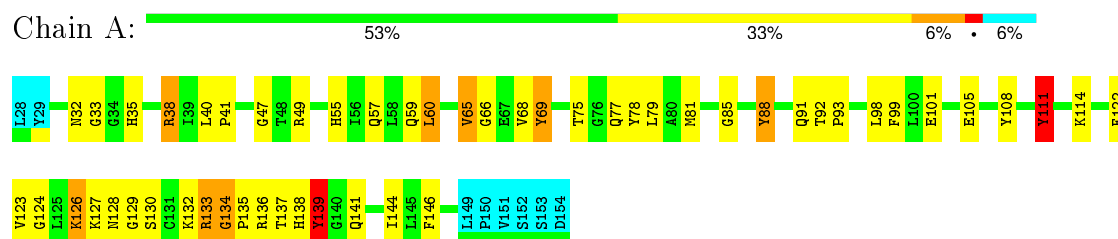
4.2.20 Score per residue for model 20

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



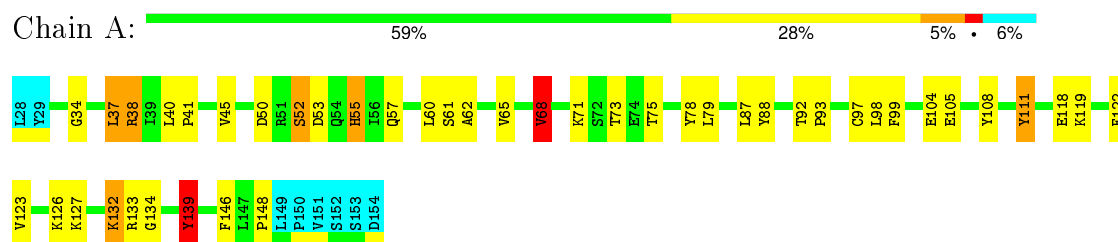
4.2.21 Score per residue for model 21

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



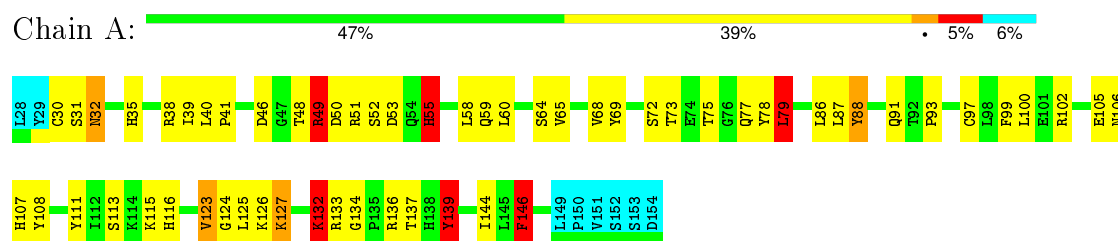
4.2.22 Score per residue for model 22

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



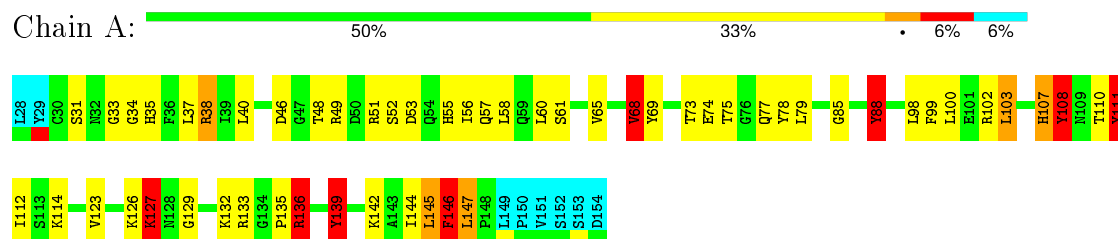
4.2.23 Score per residue for model 23

- 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	0.82±0.01	0±0/968 (0.0±0.0%)	1.46±0.04	8±3/1306 (0.6±0.2%)
All	All	0.82	0/23232 (0.0%)	1.46	203/31344 (0.6%)

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

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	ARG	NE-CZ-NH1	-17.71	111.44	120.30	17	8
1	A	49	ARG	NE-CZ-NH2	11.90	126.25	120.30	17	2
1	A	88	TYR	CB-CG-CD2	-11.44	114.13	121.00	20	19
1	A	68	VAL	CG1-CB-CG2	-10.47	94.15	110.90	2	9
1	A	136	ARG	NE-CZ-NH1	9.14	124.87	120.30	7	8
1	A	68	VAL	CA-CB-CG1	8.96	124.34	110.90	20	6
1	A	139	TYR	CB-CG-CD2	-8.96	115.62	121.00	7	17
1	A	38	ARG	NE-CZ-NH1	8.84	124.72	120.30	14	10
1	A	78	TYR	CB-CG-CD1	-8.56	115.86	121.00	20	5
1	A	108	TYR	CB-CG-CD2	-8.51	115.89	121.00	24	9
1	A	69	TYR	CB-CG-CD2	-8.38	115.97	121.00	4	15
1	A	68	VAL	CA-CB-CG2	8.17	123.16	110.90	17	6
1	A	133	ARG	NE-CZ-NH1	8.15	124.38	120.30	7	6
1	A	38	ARG	NE-CZ-NH2	-8.06	116.27	120.30	4	3
1	A	136	ARG	NE-CZ-NH2	-7.94	116.33	120.30	7	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	146	PHE	CB-CG-CD2	-7.92	115.25	120.80	23	9
1	A	125	LEU	CA-CB-CG	-7.46	98.15	115.30	19	4
1	A	111	TYR	CB-CG-CD1	-7.38	116.57	121.00	5	5
1	A	78	TYR	CB-CG-CD2	-7.22	116.67	121.00	9	4
1	A	38	ARG	CD-NE-CZ	7.19	133.66	123.60	2	2
1	A	102	ARG	NE-CZ-NH1	7.09	123.84	120.30	8	6
1	A	51	ARG	NE-CZ-NH1	7.00	123.80	120.30	2	7
1	A	111	TYR	CB-CG-CD2	-6.76	116.94	121.00	6	6
1	A	74	GLU	CA-CB-CG	-6.71	98.64	113.40	6	1
1	A	49	ARG	CA-CB-CG	-6.65	98.77	113.40	17	1
1	A	60	LEU	CB-CG-CD1	-6.45	100.04	111.00	17	9
1	A	102	ARG	N-CA-CB	-6.25	99.36	110.60	16	1
1	A	52	SER	CA-C-N	-5.86	104.30	117.20	16	5
1	A	49	ARG	NH1-CZ-NH2	-5.73	113.09	119.40	17	1
1	A	32	ASN	N-CA-CB	-5.68	100.38	110.60	9	2
1	A	108	TYR	CB-CG-CD1	-5.47	117.72	121.00	12	1
1	A	86	LEU	CB-CG-CD2	5.46	120.29	111.00	10	3
1	A	133	ARG	NE-CZ-NH2	-5.30	117.65	120.30	5	1
1	A	132	LYS	CA-C-N	-5.30	105.53	117.20	20	1
1	A	38	ARG	NH1-CZ-NH2	-5.26	113.61	119.40	2	1
1	A	127	LYS	N-CA-C	5.22	125.10	111.00	13	1
1	A	33	GLY	N-CA-C	-5.21	100.08	113.10	5	1
1	A	132	LYS	N-CA-C	5.16	124.94	111.00	8	1
1	A	136	ARG	N-CA-CB	-5.10	101.42	110.60	13	1
1	A	69	TYR	CB-CG-CD1	-5.08	117.95	121.00	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	Mainchain,Sidechain	15
1	A	122	PHE	Sidechain	12
1	A	108	TYR	Sidechain,Mainchain	11
1	A	33	GLY	Peptide,Mainchain	11
1	A	78	TYR	Sidechain	11
1	A	146	PHE	Sidechain	10
1	A	88	TYR	Sidechain	10
1	A	117	ALA	Mainchain	9
1	A	55	HIS	Sidechain,Mainchain	9
1	A	52	SER	Mainchain	9

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	133	ARG	Mainchain,Sidechain	8
1	A	38	ARG	Sidechain	8
1	A	111	TYR	Sidechain	8
1	A	61	SER	Mainchain	7
1	A	69	TYR	Sidechain	6
1	A	82	ASP	Mainchain	5
1	A	31	SER	Mainchain	5
1	A	93	PRO	Mainchain	4
1	A	103	LEU	Mainchain	3
1	A	54	GLN	Mainchain	3
1	A	132	LYS	Mainchain,Peptide	3
1	A	129	GLY	Mainchain	3
1	A	107	HIS	Sidechain,Mainchain	3
1	A	51	ARG	Sidechain	2
1	A	124	GLY	Mainchain	2
1	A	102	ARG	Mainchain	2
1	A	48	THR	Peptide	2
1	A	125	LEU	Mainchain	2
1	A	130	SER	Mainchain	2
1	A	36	PHE	Sidechain	2
1	A	32	ASN	Peptide	1
1	A	35	HIS	Sidechain	1
1	A	63	GLU	Mainchain	1
1	A	79	LEU	Mainchain	1
1	A	43	GLY	Mainchain	1
1	A	41	PRO	Mainchain	1
1	A	57	GLN	Peptide	1
1	A	71	LYS	Mainchain	1
1	A	106	ASN	Mainchain	1
1	A	142	LYS	Mainchain	1
1	A	126	LYS	Mainchain	1
1	A	99	PHE	Sidechain	1
1	A	49	ARG	Sidechain	1
1	A	40	LEU	Mainchain	1
1	A	60	LEU	Mainchain	1
1	A	136	ARG	Sidechain	1
1	A	85	GLY	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	20±4
All	All	22728	0	22008	490

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:41:PRO:HD3	1:A:75:THR:HG21	0.62	1.70	12	2
1:A:38:ARG:HB3	1:A:38:ARG:HH11	0.62	1.54	2	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:133:ARG:H	1:A:133:ARG:NH1	0.59	1.93	10	2
1:A:45:VAL:HG11	1:A:79:LEU:CD1	0.59	2.27	13	11
1:A:38:ARG:HG2	1:A:40:LEU:HD22	0.59	1.74	1	12
1:A:39:ILE:HD11	1:A:89:GLY:HA2	0.59	1.73	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:37:LEU:HB3	1:A:125:LEU:HD11	0.57	1.76	10	1
1:A:57:GLN:HG3	1:A:72:SER:HB2	0.57	1.75	6	2
1:A:45:VAL:HG13	1:A:57:GLN:HE22	0.57	1.60	5	1
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:38:ARG:HH11	1:A:56:ILE:HG23	0.56	1.61	13	2
1:A:39:ILE:HG21	1:A:77:GLN:HB2	0.56	1.77	1	1
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:38:ARG:HA	1:A:56:ILE:HA	0.54	1.78	12	7
1:A:101:GLU:HG2	1:A:111:TYR:HE1	0.54	1.62	3	4
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:68:VAL:C	1:A:98:LEU:HD12	0.53	2.24	19	16
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:70:ILE:HB	1:A:79:LEU:HB3	0.51	1.82	1	3
1:A:65:VAL:HG13	1:A:66:GLY:H	0.51	1.64	21	3
1:A:38:ARG:HB3	1:A:46:ASP:O	0.51	2.06	7	4
1:A:123:VAL:HG23	1:A:146:PHE:CZ	0.51	2.40	13	4
1:A:63:GLU:OE1	1:A:69:TYR:CE2	0.51	2.63	4	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:87:LEU:HD12	1:A:131:CYS:O	0.51	2.06	9	1
1:A:77:GLN:H	1:A:77:GLN:NE2	0.51	2.04	13	1
1:A:38:ARG:CG	1:A:55:HIS:HB2	0.50	2.36	10	4
1:A:32:ASN:CG	1:A:33:GLY:H	0.50	2.08	6	2
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:123:VAL:HG13	1:A:146:PHE:HE2	0.50	1.66	17	1
1:A:58:LEU:HD22	1:A:70:ILE:HG21	0.50	1.82	3	2
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: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: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: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:125:LEU:HD11	1:A:131:CYS:SG	0.49	2.48	19	1
1:A:67:GLU:HB3	1:A:98:LEU:HD21	0.49	1.85	9	1
1:A:37:LEU:O	1:A:45:VAL:HG13	0.49	2.08	13	1
1:A:30:CYS:SG	1:A:34:GLY:HA2	0.49	2.48	7	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:56:ILE:HG13	1:A:57:GLN:OE1	0.47	2.10	24	1
1:A:133:ARG:NH1	1:A:133:ARG:H	0.47	2.07	12	3
1:A:102:ARG:HB3	1:A:110:THR:O	0.47	2.09	16	1
1:A:38:ARG:HH11	1:A:56:ILE:CG2	0.47	2.22	13	2
1:A:57:GLN:O	1:A:70:ILE:HG22	0.47	2.10	5	1
1:A:79:LEU:HD23	1:A:99:PHE:CE2	0.47	2.44	23	1
1:A:49:ARG:HG3	1:A:129:GLY:HA3	0.47	1.86	16	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD13	1:A:79:LEU:HD22	0.46	1.87	13	1
1:A:122:PHE:HB2	1:A:144:ILE:HG21	0.46	1.88	7	1
1:A:37:LEU:HD22	1:A:79:LEU:HD21	0.46	1.87	2	1
1:A:99:PHE:CE2	1:A:123:VAL:HG13	0.46	2.45	14	1
1:A:70:ILE:HD12	1:A:79:LEU:HD23	0.46	1.86	14	1
1:A:109:ASN:HB3	1:A:111:TYR:CZ	0.46	2.45	4	4
1:A:98:LEU:O	1:A:114:LYS:HB2	0.46	2.11	11	1
1:A:51:ARG:HE	1:A:56:ILE:HG21	0.46	1.71	8	1
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:127:LYS:HE3	1:A:136:ARG:HH12	0.45	1.70	3	1
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:51:ARG:H	1:A:51:ARG:CZ	0.45	2.24	5	1
1:A:38:ARG:HG2	1:A:40:LEU:HD12	0.45	1.88	13	1
1:A:60:LEU:HD23	1:A:60:LEU:H	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:39:ILE:HG21	1:A:77:GLN:O	0.45	2.12	16	1
1:A:38:ARG:HE	1:A:40:LEU:HD11	0.45	1.71	9	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:30:CYS:SG	1:A:125:LEU:HD13	0.44	2.52	19	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ARG:CZ	1:A:51:ARG:H	0.43	2.27	2	1
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:47:GLY:H	1:A:130:SER:HA	0.43	1.72	21	2
1:A:99:PHE:CE1	1:A:123:VAL:HG13	0.43	2.48	2	1
1:A:68:VAL:HG11	1:A:101:GLU:HG3	0.43	1.91	21	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:59:GLN:HB2	1:A:73:THR:HB	0.42	1.91	13	1
1:A:133:ARG:HG2	1:A:134:GLY:N	0.42	2.28	11	2
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:127:LYS:HE2	1:A:136:ARG:NH2	0.42	2.29	24	1
1:A:37:LEU:HD23	1:A:58:LEU:HB2	0.42	1.91	4	1
1:A:65:VAL:HG22	1:A:66:GLY:H	0.42	1.74	20	1
1:A:39:ILE:HD13	1:A:72:SER:HB3	0.42	1.91	7	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:30:CYS:O	1:A:34:GLY:HA2	0.42	2.15	19	1
1:A:111:TYR:HB2	1:A:123:VAL:HG12	0.42	1.90	16	1
1:A:31:SER:O	1:A:142:LYS:HB3	0.42	2.15	24	2
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: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: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:91:GLN:CD	1:A:91:GLN:H	0.41	2.19	5	1
1:A:39:ILE:HD13	1:A:72:SER:OG	0.41	2.15	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ALA:HB2	1:A:97:CYS:SG	0.41	2.55	6	1
1:A:30:CYS:C	1:A:32:ASN:H	0.41	2.18	1	1
1:A:98:LEU:HA	1:A:98:LEU:HD12	0.41	1.84	19	1
1:A:127:LYS:HE2	1:A:136:ARG:HH22	0.41	1.76	24	1
1:A:38:ARG:NH1	1:A:51:ARG:HA	0.41	2.31	4	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:103:LEU:HG	1:A:105:GLU:H	0.41	1.76	7	1
1:A:45:VAL:HG12	1:A:131:CYS:SG	0.40	2.56	14	1
1:A:66:GLY:O	1:A:100:LEU:HA	0.40	2.16	1	1
1:A:110:THR:HG23	1:A:145:LEU:HB3	0.40	1.93	24	1
1:A:111:TYR:CD2	1:A:123:VAL:HG11	0.40	2.51	3	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%)	3	16
All	All	2856/3048 (94%)	2053 (72%)	592 (21%)	211 (7%)	3	16

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	139	TYR	7
1	A	134	GLY	7
1	A	129	GLY	7
1	A	64	SER	7
1	A	148	PRO	7
1	A	103	LEU	6
1	A	54	GLN	6
1	A	33	GLY	6
1	A	39	ILE	6
1	A	58	LEU	5
1	A	56	ILE	5
1	A	73	THR	4
1	A	37	LEU	3
1	A	51	ARG	3
1	A	133	ARG	3
1	A	47	GLY	2
1	A	123	VAL	2
1	A	72	SER	2
1	A	57	GLN	2
1	A	106	ASN	2
1	A	79	LEU	1
1	A	84	ASP	1
1	A	109	ASN	1
1	A	32	ASN	1
1	A	101	GLU	1
1	A	38	ARG	1
1	A	128	ASN	1
1	A	42	ASP	1
1	A	83	THR	1
1	A	126	LYS	1
1	A	138	HIS	1
1	A	93	PRO	1
1	A	74	GLU	1
1	A	88	TYR	1
1	A	50	ASP	1
1	A	114	LYS	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 (87±3%)	14±3 (13±3%)	9	50
All	All	2472/2664 (93%)	2142 (87%)	330 (13%)	9	50

All 62 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	24
1	A	75	THR	21
1	A	133	ARG	18
1	A	126	LYS	15
1	A	60	LEU	14
1	A	59	GLN	13
1	A	115	LYS	12
1	A	132	LYS	12
1	A	68	VAL	12
1	A	88	TYR	11
1	A	58	LEU	10
1	A	51	ARG	10
1	A	55	HIS	9
1	A	146	PHE	9
1	A	92	THR	9
1	A	73	THR	8
1	A	82	ASP	7
1	A	112	ILE	6
1	A	147	LEU	6
1	A	38	ARG	5
1	A	136	ARG	5
1	A	44	THR	5
1	A	49	ARG	5
1	A	79	LEU	4
1	A	37	LEU	4
1	A	32	ASN	4
1	A	40	LEU	4
1	A	57	GLN	4
1	A	83	THR	4
1	A	127	LYS	4
1	A	145	LEU	4
1	A	100	LEU	3
1	A	101	GLU	3
1	A	87	LEU	3
1	A	118	GLU	3
1	A	74	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ILE	3
1	A	104	GLU	2
1	A	114	LYS	2
1	A	81	MET	2
1	A	137	THR	2
1	A	42	ASP	2
1	A	125	LEU	2
1	A	128	ASN	2
1	A	123	VAL	2
1	A	48	THR	2
1	A	109	ASN	1
1	A	61	SER	1
1	A	103	LEU	1
1	A	71	LYS	1
1	A	91	GLN	1
1	A	31	SER	1
1	A	138	HIS	1
1	A	86	LEU	1
1	A	53	ASP	1
1	A	56	ILE	1
1	A	107	HIS	1
1	A	69	TYR	1
1	A	52	SER	1
1	A	95	GLU	1
1	A	102	ARG	1
1	A	36	PHE	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 carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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