



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:18 PM BST

PDB ID : 1DZC
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
<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

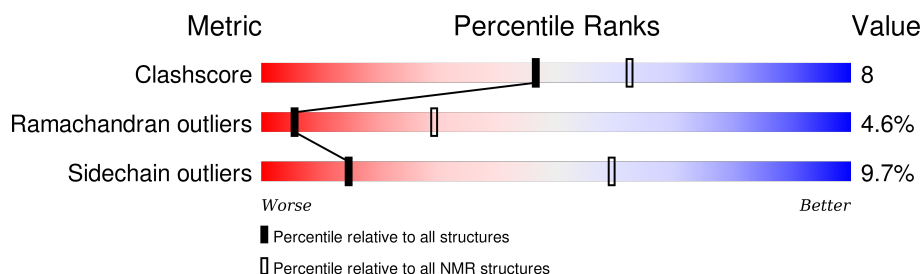
1 Overall quality at a glance

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	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)	0.47	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:

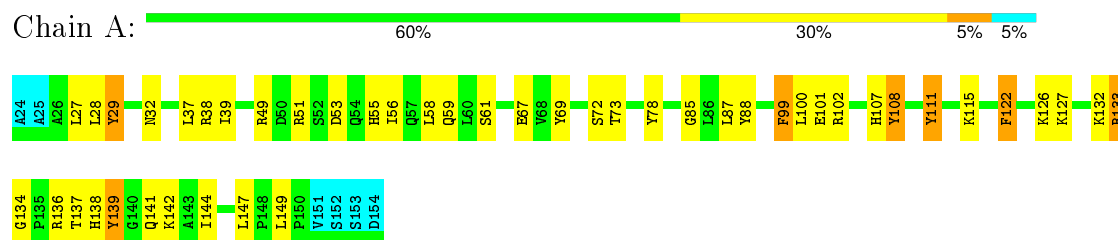
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	LYS	ENGINEERED MUTATION	UNP P05230
A	25	ALA	PRO	ENGINEERED MUTATION	UNP P05230
A	26	ALA	LYS	ENGINEERED MUTATION	UNP P05230

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: FIBROBLAST GROWTH FACTOR 1

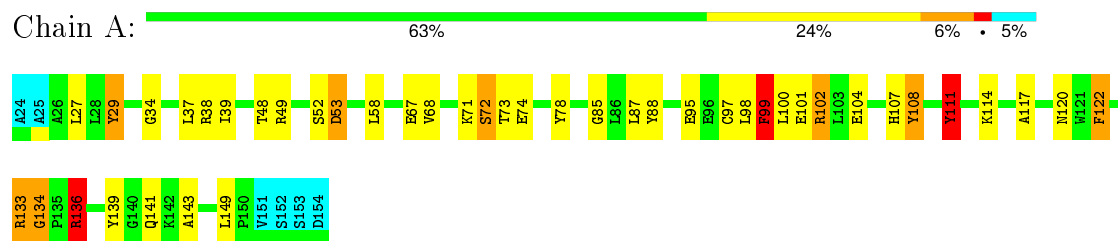


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

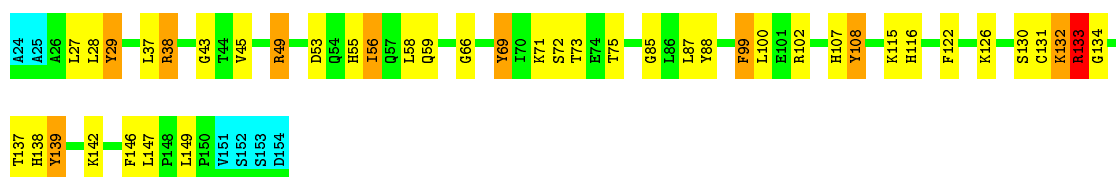
- Molecule 1: FIBROBLAST GROWTH FACTOR 1



4.2.2 Score per residue for model 2

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

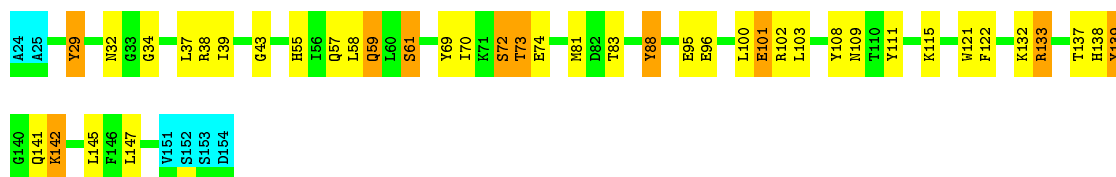




4.2.3 Score per residue for model 3

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

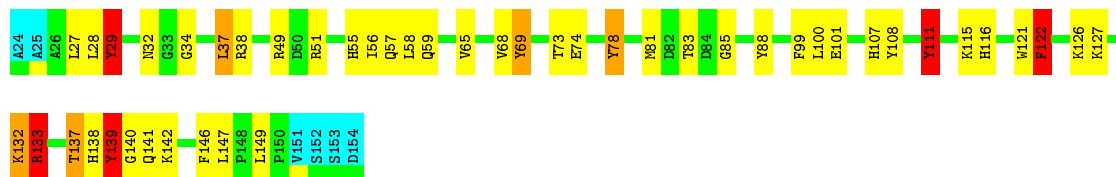
Chain A: 64% 24% 8% 5%



4.2.4 Score per residue for model 4

- Molecule 1: FIBROBLAST GROWTH FACTOR 1

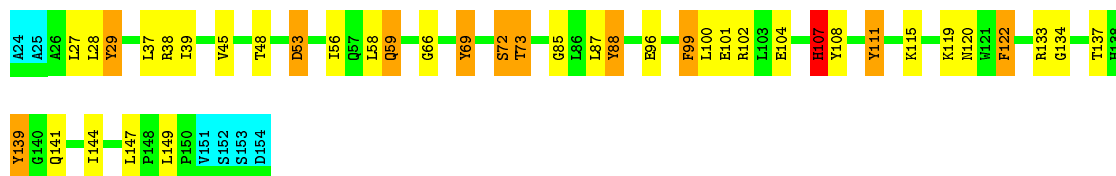
Chain A: 60% 28% 5%



4.2.5 Score per residue for model 5

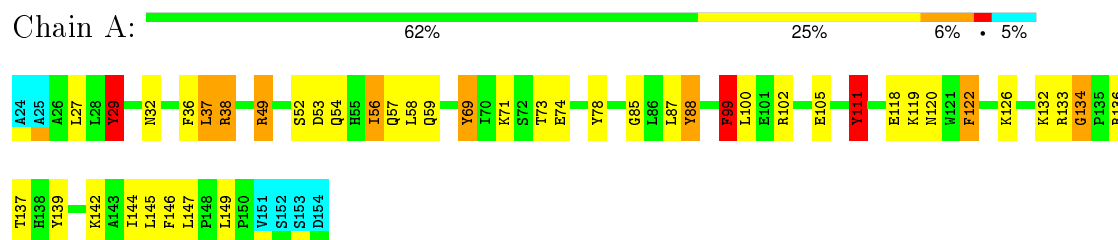
- Molecule 1: FIBROBLAST GROWTH FACTOR 1

Chain A: 65% 21% 8% 5%



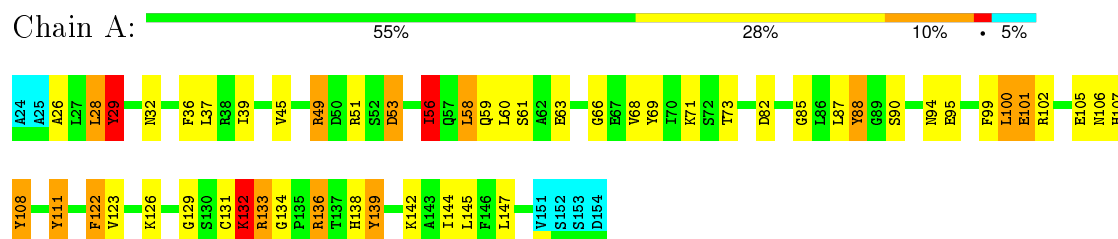
4.2.6 Score per residue for model 6

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



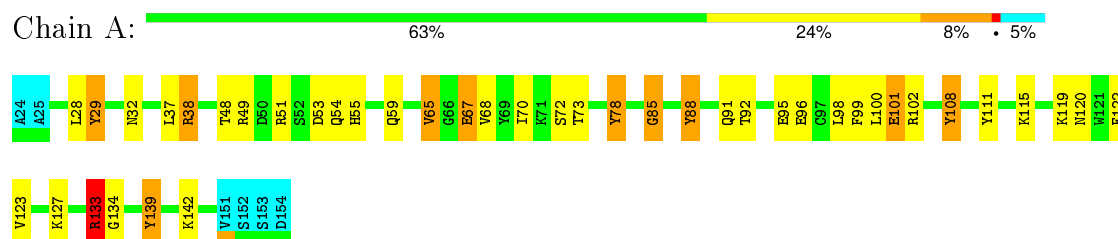
4.2.7 Score per residue for model 7

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



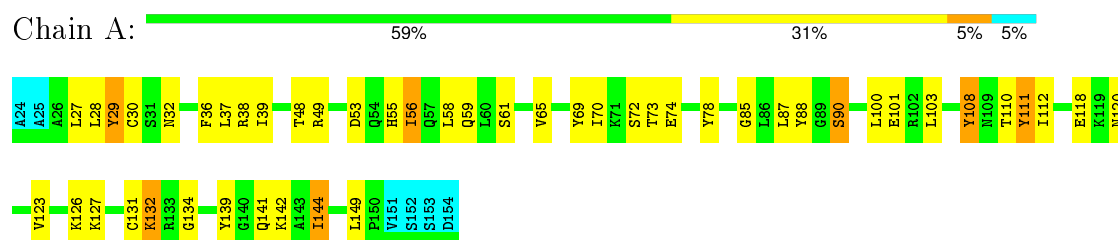
4.2.8 Score per residue for model 8

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



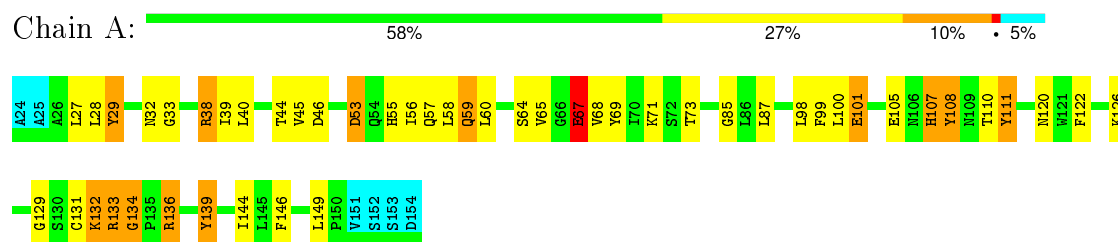
4.2.9 Score per residue for model 9

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



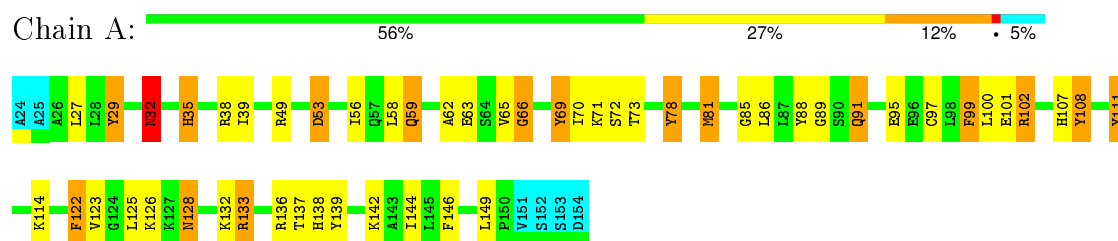
4.2.10 Score per residue for model 10

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



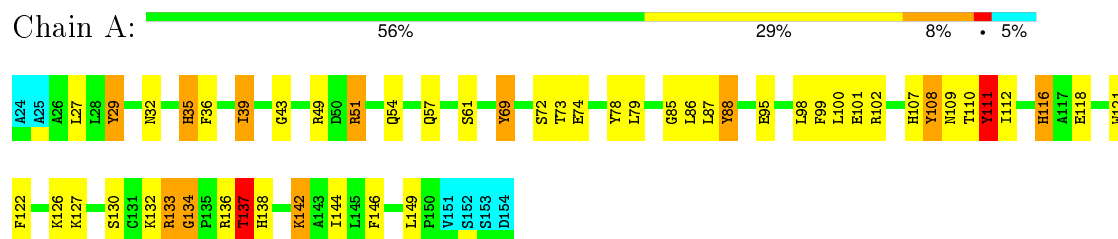
4.2.11 Score per residue for model 11

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



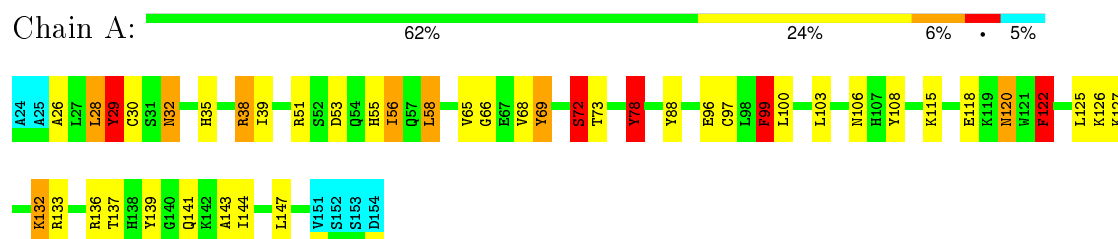
4.2.12 Score per residue for model 12

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



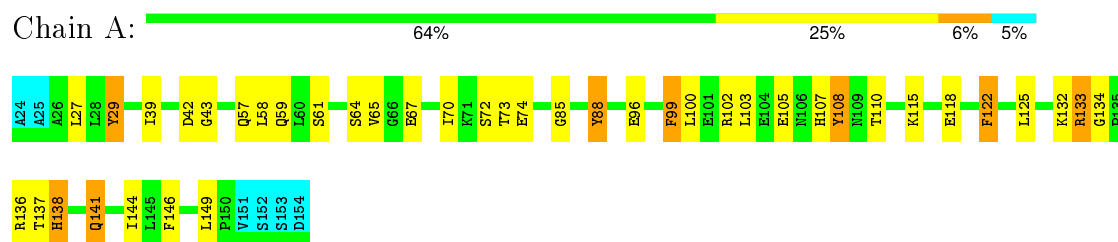
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



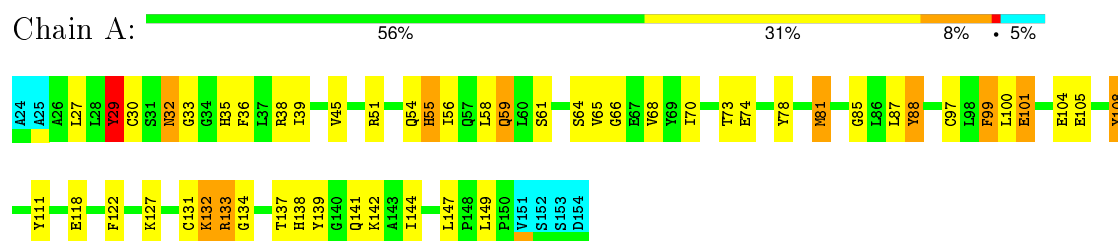
4.2.14 Score per residue for model 14

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



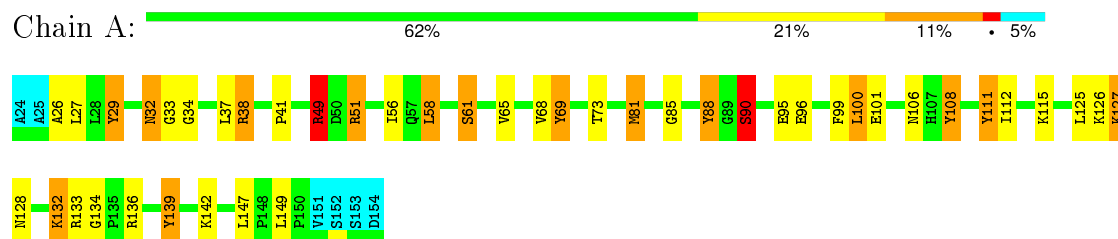
4.2.15 Score per residue for model 15

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



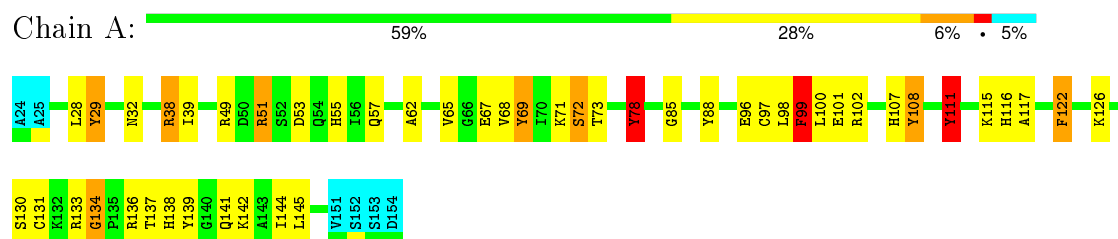
4.2.16 Score per residue for model 16

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



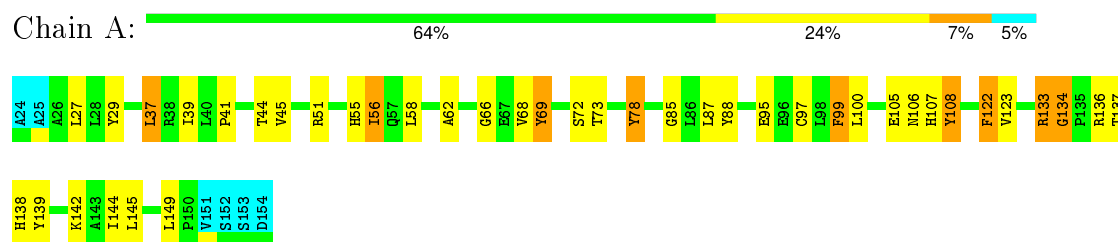
4.2.17 Score per residue for model 17

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



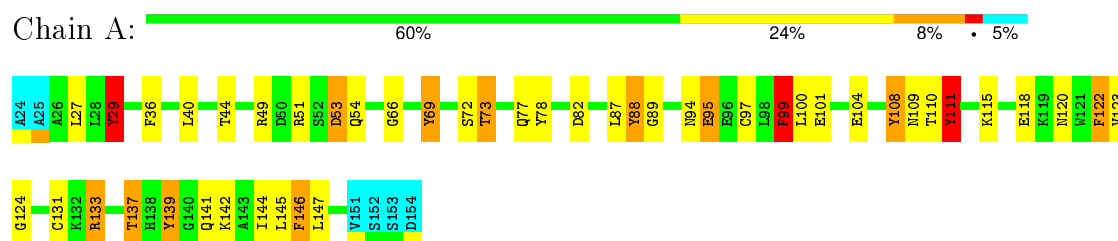
4.2.18 Score per residue for model 18

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



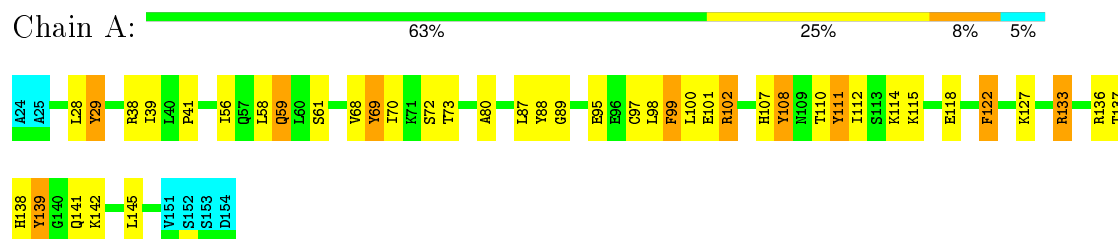
4.2.19 Score per residue for model 19

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



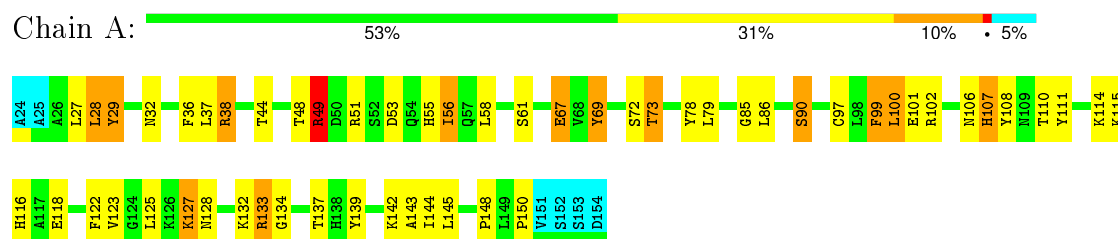
4.2.20 Score per residue for model 20

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



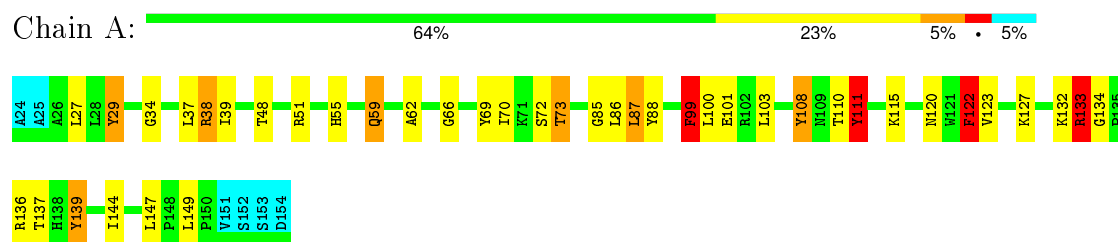
4.2.21 Score per residue for model 21

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



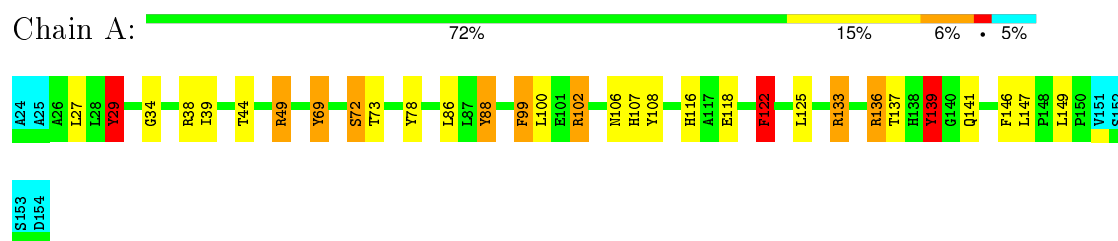
4.2.22 Score per residue for model 22

- Molecule 1: FIBROBLAST GROWTH FACTOR 1



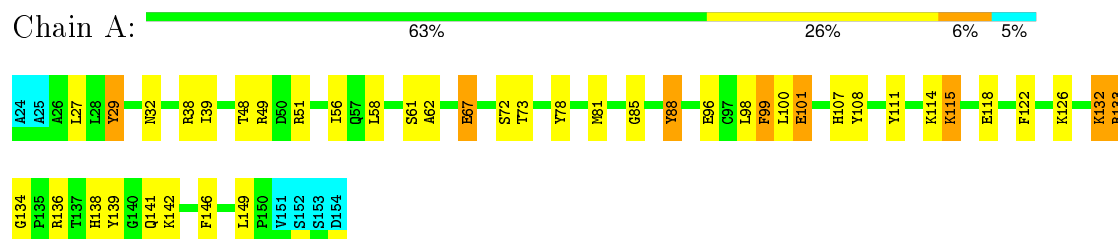
4.2.23 Score per residue for model 23

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

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	0.82±0.01	0±0/1018 (0.0±0.0%)	1.44±0.08	9±3/1376 (0.6±0.2%)
All	All	0.82	1/24432 (0.0%)	1.45	206/33024 (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	9.6±2.2
All	All	0	231

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	91	GLN	CD-NE2	-7.78	1.13	1.32	11	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	-29.10	54.98	121.90	11	1
1	A	91	GLN	CG-CD-NE2	-12.24	87.32	116.70	11	1
1	A	139	TYR	CB-CG-CD2	-10.32	114.81	121.00	2	14
1	A	29	TYR	CB-CG-CD2	-9.92	115.05	121.00	11	23
1	A	102	ARG	NE-CZ-NH1	8.85	124.72	120.30	17	10
1	A	108	TYR	CB-CG-CD1	-8.53	115.88	121.00	7	17
1	A	102	ARG	NE-CZ-NH2	8.25	124.42	120.30	11	3
1	A	136	ARG	NE-CZ-NH1	8.20	124.40	120.30	23	7
1	A	133	ARG	NE-CZ-NH1	7.97	124.29	120.30	2	8
1	A	146	PHE	CB-CG-CD2	-7.93	115.25	120.80	2	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	ARG	NE-CZ-NH1	7.81	124.20	120.30	12	6
1	A	99	PHE	CB-CG-CD2	-7.80	115.34	120.80	6	10
1	A	38	ARG	NE-CZ-NH2	-7.79	116.40	120.30	16	1
1	A	111	TYR	CB-CG-CD2	-7.58	116.45	121.00	17	10
1	A	38	ARG	NE-CZ-NH1	7.45	124.02	120.30	2	10
1	A	69	TYR	CB-CG-CD2	-7.28	116.63	121.00	11	6
1	A	69	TYR	CB-CG-CD1	-6.95	116.83	121.00	23	10
1	A	49	ARG	NE-CZ-NH2	6.79	123.70	120.30	1	1
1	A	91	GLN	CG-CD-OE1	6.74	135.09	121.60	11	1
1	A	51	ARG	NE-CZ-NH1	6.74	123.67	120.30	16	6
1	A	114	LYS	CD-CE-NZ	-6.67	96.37	111.70	11	1
1	A	122	PHE	CB-CG-CD2	-6.62	116.17	120.80	17	6
1	A	51	ARG	NE-CZ-NH2	-6.51	117.05	120.30	4	2
1	A	71	LYS	CD-CE-NZ	-6.27	97.28	111.70	11	1
1	A	108	TYR	CB-CG-CD2	-6.23	117.26	121.00	20	3
1	A	122	PHE	CB-CG-CD1	-6.23	116.44	120.80	7	1
1	A	139	TYR	CB-CG-CD1	-6.23	117.26	121.00	16	1
1	A	88	TYR	CB-CG-CD1	-6.21	117.27	121.00	3	3
1	A	88	TYR	CB-CG-CD2	-6.10	117.34	121.00	15	7
1	A	78	TYR	CB-CG-CD2	-5.98	117.41	121.00	4	6
1	A	61	SER	N-CA-CB	-5.83	101.75	110.50	16	1
1	A	78	TYR	CB-CG-CD1	-5.74	117.56	121.00	6	3
1	A	71	LYS	CG-CD-CE	-5.64	94.98	111.90	11	1
1	A	90	SER	CA-C-N	-5.43	105.26	117.20	9	3
1	A	136	ARG	NE-CZ-NH2	-5.33	117.64	120.30	6	4
1	A	95	GLU	N-CA-CB	-5.26	101.14	110.60	11	1
1	A	102	ARG	NH1-CZ-NH2	-5.25	113.62	119.40	12	1
1	A	99	PHE	CB-CG-CD1	-5.15	117.20	120.80	20	2
1	A	107	HIS	CA-C-N	-5.12	105.94	117.20	5	1
1	A	53	ASP	CB-CG-OD2	-5.09	113.72	118.30	11	1
1	A	133	ARG	NE-CZ-NH2	-5.06	117.77	120.30	7	1
1	A	115	LYS	N-CA-CB	-5.06	101.49	110.60	24	1
1	A	119	LYS	N-CA-CB	-5.04	101.52	110.60	5	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	122	PHE	Sidechain	21
1	A	88	TYR	Sidechain	21

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	108	TYR	Sidechain,Mainchain	20
1	A	29	TYR	Sidechain	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	132	LYS	Mainchain	5
1	A	102	ARG	Mainchain	5
1	A	56	ILE	Mainchain	4
1	A	131	CYS	Mainchain	3
1	A	65	VAL	Mainchain	3
1	A	90	SER	Mainchain	3
1	A	81	MET	Mainchain	3
1	A	32	ASN	Mainchain	3
1	A	62	ALA	Mainchain	3
1	A	53	ASP	Mainchain	2
1	A	38	ARG	Sidechain	2
1	A	103	LEU	Mainchain	2
1	A	119	LYS	Mainchain	2
1	A	138	HIS	Sidechain,Mainchain	2
1	A	133	ARG	Sidechain	2
1	A	117	ALA	Mainchain	1
1	A	127	LYS	Mainchain	1
1	A	143	ALA	Mainchain	1
1	A	55	HIS	Sidechain	1
1	A	49	ARG	Sidechain	1
1	A	42	ASP	Mainchain	1
1	A	129	GLY	Peptide	1
1	A	85	GLY	Mainchain	1
1	A	36	PHE	Sidechain	1
1	A	118	GLU	Mainchain	1
1	A	136	ARG	Sidechain	1
1	A	54	GLN	Mainchain	1
1	A	107	HIS	Sidechain	1
1	A	82	ASP	Mainchain	1
1	A	35	HIS	Sidechain	1
1	A	91	GLN	Sidechain	1
1	A	64	SER	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	995	0	971	16±4
All	All	23880	0	23304	374

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
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: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: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:99:PHE:HE1	1:A:133:ARG:HH12	0.58	1.41	7	1
1:A:133:ARG:HB3	1:A:137:THR:HG21	0.58	1.73	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:GLU:HG2	1:A:111:TYR:HE1	0.58	1.59	8	7
1:A:110:THR:HG21	1:A:144:ILE:HD12	0.58	1.76	9	2
1:A:29:TYR:HD2	1:A:147:LEU:HB3	0.58	1.59	16	10
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:81:MET:HE3	1:A:133:ARG:HH22	0.57	1.59	16	1
1:A:123:VAL:HA	1:A:133:ARG:HD2	0.57	1.75	8	1
1:A:49:ARG:H	1:A:49:ARG:CZ	0.56	2.12	23	2
1:A:127:LYS:H	1:A:127:LYS:HD3	0.56	1.59	8	2
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:39:ILE:HG22	1:A:55:HIS:O	0.54	2.02	13	5
1:A:96:GLU:HG3	1:A:115:LYS:HD3	0.54	1.78	3	1
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
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:126:LYS:HB3	1:A:130:SER:HB3	0.53	1.80	17	1
1:A:28:LEU:HB2	1:A:58:LEU:HD11	0.53	1.81	2	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:49:ARG:CZ	1:A:49:ARG:H	0.52	2.18	2	1
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:87:LEU:H	1:A:133:ARG:CZ	0.51	2.18	19	2
1:A:133:ARG:HA	1:A:137:THR:HG23	0.51	1.82	12	1
1:A:121:TRP:HB3	1:A:133:ARG:HH22	0.51	1.65	4	1
1:A:59:GLN:HB3	1:A:71:LYS:HB3	0.51	1.82	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HB3	1:A:149:LEU:O	0.51	2.06	11	5
1:A:123:VAL:HA	1:A:133:ARG:HG2	0.51	1.81	22	1
1:A:27:LEU:HD21	1:A:36:PHE:CE2	0.51	2.33	15	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:64:SER:HB3	1:A:67:GLU:HB3	0.50	1.83	14	1
1:A:87:LEU:HD21	1:A:133:ARG:NH1	0.50	2.19	6	2
1:A:28:LEU:HB2	1:A:58:LEU:HD21	0.50	1.83	5	2
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: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
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: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:39:ILE:HD12	1:A:45:VAL:HG22	0.47	1.87	7	2
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:80:ALA:HB2	1:A:97:CYS:SG	0.47	2.50	20	1
1:A:81:MET:HE3	1:A:121:TRP:HE3	0.47	1.69	3	1
1:A:141:GLN:HB3	1:A:143:ALA:HB3	0.46	1.87	1	1
1:A:148:PRO:C	1:A:150:PRO:HD3	0.46	2.31	21	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:27:LEU:HD11	1:A:51:ARG:HE	0.46	1.70	18	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: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:35:HIS:HB2	1:A:125:LEU:HD13	0.45	1.88	13	1
1:A:56:ILE:HD11	1:A:58:LEU:HD23	0.45	1.89	4	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: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
1:A:123:VAL:O	1:A:144:ILE:HA	0.44	2.13	7	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: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:27:LEU:HD12	1:A:56:ILE:HG13	0.44	1.88	24	1
1:A:100:LEU:O	1:A:111:TYR:HA	0.44	2.12	7	1
1:A:133:ARG:HB2	1:A:137:THR:CG2	0.43	2.31	21	1
1:A:45:VAL:HG22	1:A:87:LEU:HB2	0.43	1.89	18	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:HE2	1:A:132:LYS:HA	0.41	1.92	7	1
1:A:32:ASN:ND2	1:A:125:LEU:H	0.41	2.13	16	1
1:A:111:TYR:HB2	1:A:123:VAL:CG2	0.41	2.43	21	1
1:A:27:LEU:HB3	1:A:36:PHE:HE2	0.41	1.75	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:56:ILE:HG13	0.41	1.93	10	1
1:A:103:LEU:HA	1:A:109:ASN:HA	0.41	1.91	3	1
1:A:122:PHE:O	1:A:133:ARG:HB3	0.41	2.15	18	1
1:A:110:THR:HG21	1:A:144:ILE:HD13	0.41	1.91	14	1
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:37:LEU:O	1:A:56:ILE:HG22	0.40	2.17	16	1
1:A:66:GLY:O	1:A:68:VAL:HG13	0.40	2.16	15	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%)	5	29
All	All	3000/3144 (95%)	2275 (76%)	586 (20%)	139 (5%)	5	29

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	120	ASN	7
1	A	66	GLY	7
1	A	65	VAL	7
1	A	134	GLY	6
1	A	138	HIS	6
1	A	34	GLY	6
1	A	53	ASP	5
1	A	106	ASN	5
1	A	43	GLY	4
1	A	67	GLU	4
1	A	56	ILE	3
1	A	33	GLY	3
1	A	41	PRO	3
1	A	114	LYS	3
1	A	139	TYR	2
1	A	103	LEU	2
1	A	137	THR	2
1	A	105	GLU	2
1	A	95	GLU	1
1	A	128	ASN	1
1	A	131	CYS	1
1	A	52	SER	1
1	A	83	THR	1
1	A	125	LEU	1
1	A	133	ARG	1
1	A	32	ASN	1
1	A	132	LYS	1
1	A	129	GLY	1
1	A	104	GLU	1
1	A	64	SER	1
1	A	44	THR	1
1	A	117	ALA	1
1	A	51	ARG	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 (90±3%)	11±3 (10±3%)	15	59
All	All	2592/2688 (96%)	2340 (90%)	252 (10%)	15	59

All 58 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	133	ARG	15
1	A	49	ARG	12
1	A	58	LEU	12
1	A	118	GLU	10
1	A	32	ASN	10
1	A	142	LYS	10
1	A	59	GLN	9
1	A	127	LYS	9
1	A	132	LYS	9
1	A	37	LEU	8
1	A	137	THR	8
1	A	136	ARG	7
1	A	116	HIS	6
1	A	28	LEU	6
1	A	107	HIS	6
1	A	95	GLU	6
1	A	115	LYS	5
1	A	86	LEU	5
1	A	51	ARG	5
1	A	141	GLN	4
1	A	139	TYR	4
1	A	53	ASP	4
1	A	81	MET	4
1	A	105	GLU	4
1	A	128	ASN	3
1	A	149	LEU	3
1	A	71	LYS	3
1	A	44	THR	3
1	A	74	GLU	3
1	A	54	GLN	2
1	A	63	GLU	2
1	A	39	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	35	HIS	2
1	A	104	GLU	2
1	A	94	ASN	2
1	A	67	GLU	2
1	A	123	VAL	1
1	A	30	CYS	1
1	A	38	ARG	1
1	A	45	VAL	1
1	A	56	ILE	1
1	A	138	HIS	1
1	A	122	PHE	1
1	A	120	ASN	1
1	A	106	ASN	1
1	A	40	LEU	1
1	A	147	LEU	1
1	A	75	THR	1
1	A	72	SER	1
1	A	65	VAL	1
1	A	112	ILE	1
1	A	46	ASP	1
1	A	87	LEU	1
1	A	110	THR	1
1	A	57	GLN	1
1	A	61	SER	1
1	A	144	ILE	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