



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:26 pm GMT

PDB ID : 1A7M
Title : LEUKAEMIA INHIBITORY FACTOR CHIMERA (MH35-LIF), NMR, 20
STRUCTURES
Authors : Hinds, M.G.; Maurer, T.; Zhang, J.-G.; Nicola, N.A.; Norton, R.S.
Deposited on : 1998-03-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

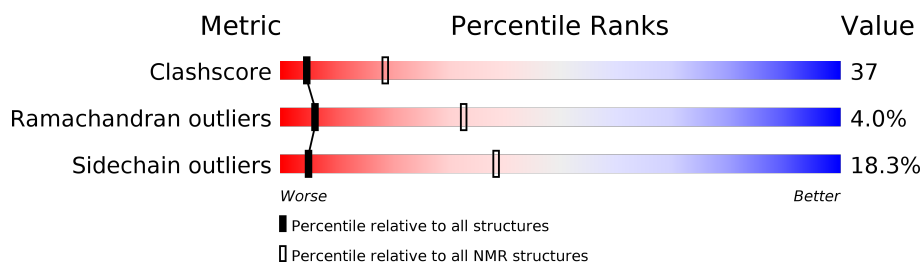
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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

Mol	Chain	Length	Quality of chain
1	A	180	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:24-A:60, A:67-A:71, A:76-A:132, A:153-A:180 (127)	0.36	1

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2803 atoms, of which 1413 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LEUKEMIA INHIBITORY FACTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	180	Total	C	H	N	O	S	0
			2803	882	1413	246	253	9	

There are 12 discrepancies between the modelled and reference sequences:

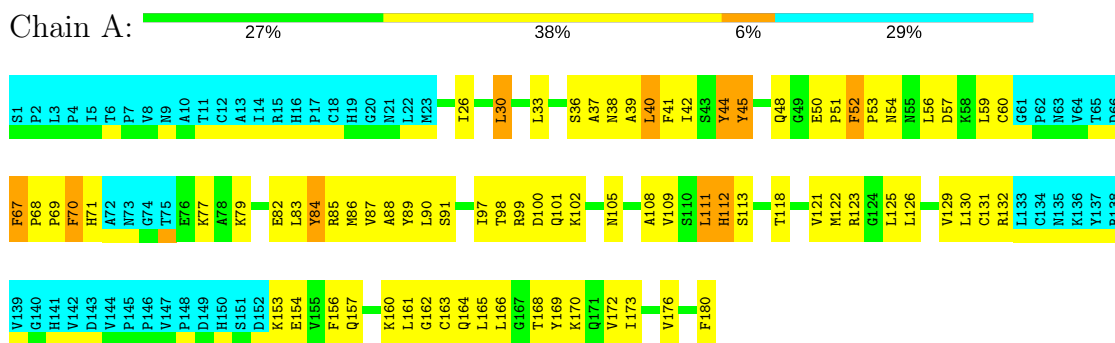
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	LEU	VAL	CONFLICT	UNP P09056
A	57	ASP	GLU	CONFLICT	UNP P09056
A	61	GLY	ALA	CONFLICT	UNP P09056
A	64	VAL	MET	CONFLICT	UNP P09056
A	69	PRO	SER	CONFLICT	UNP P09056
A	72	ALA	GLY	CONFLICT	UNP P09056
A	78	ALA	THR	CONFLICT	UNP P09056
A	107	SER	THR	CONFLICT	UNP P09056
A	112	HIS	GLN	CONFLICT	UNP P09056
A	113	SER	VAL	CONFLICT	UNP P09056
A	155	VAL	ALA	CONFLICT	UNP P09056
A	158	LYS	ARG	CONFLICT	UNP P09056

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: LEUKEMIA INHIBITORY FACTOR

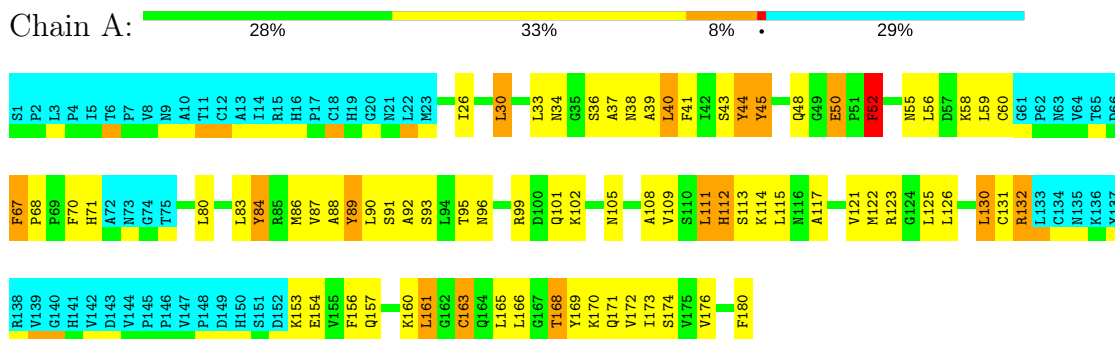


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

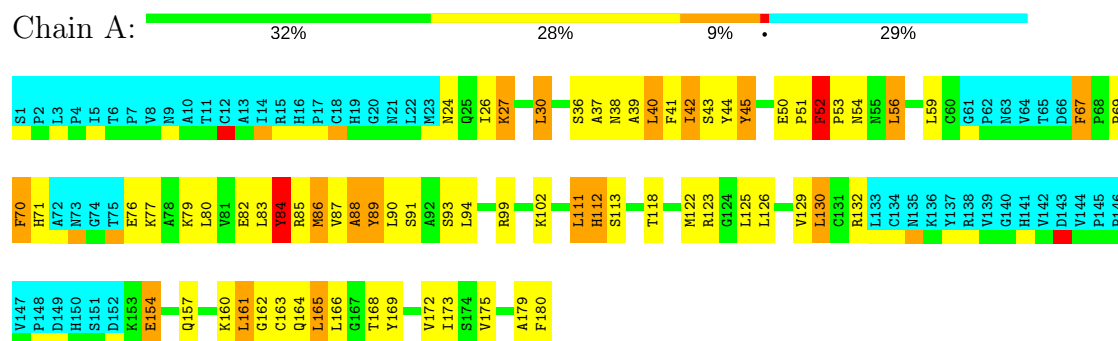
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



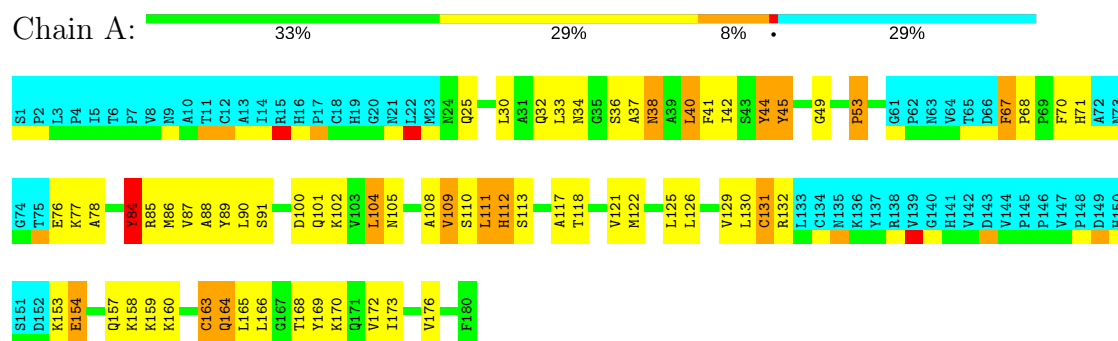
4.2.2 Score per residue for model 2

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



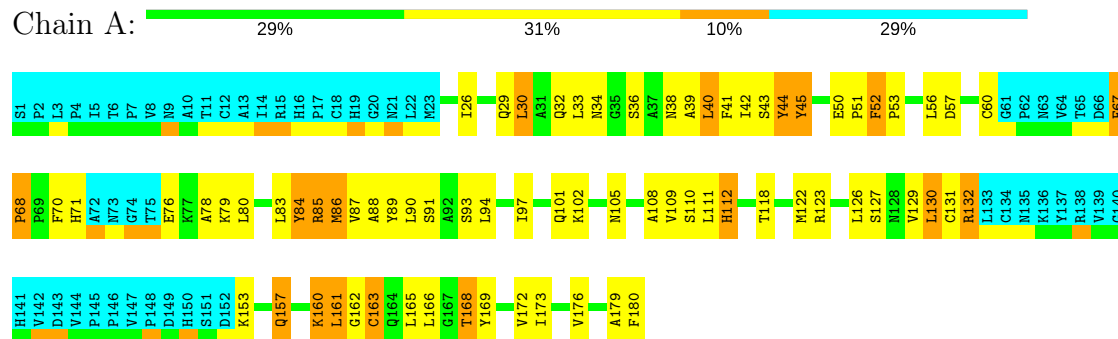
4.2.3 Score per residue for model 3

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



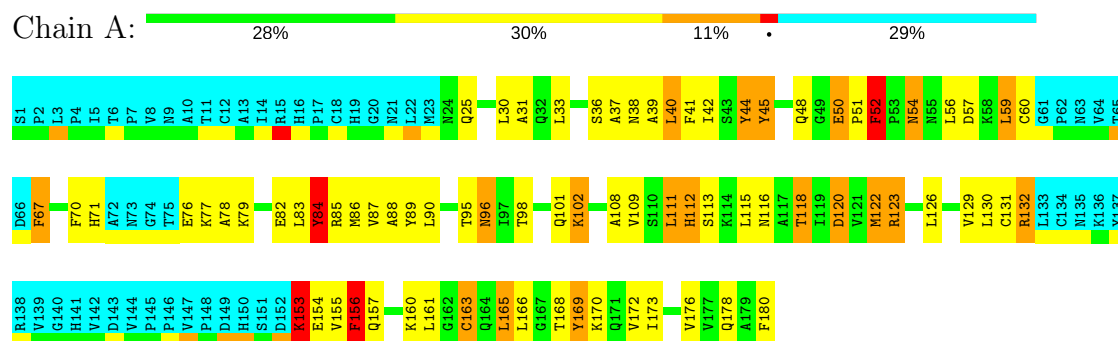
4.2.4 Score per residue for model 4

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.5 Score per residue for model 5

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



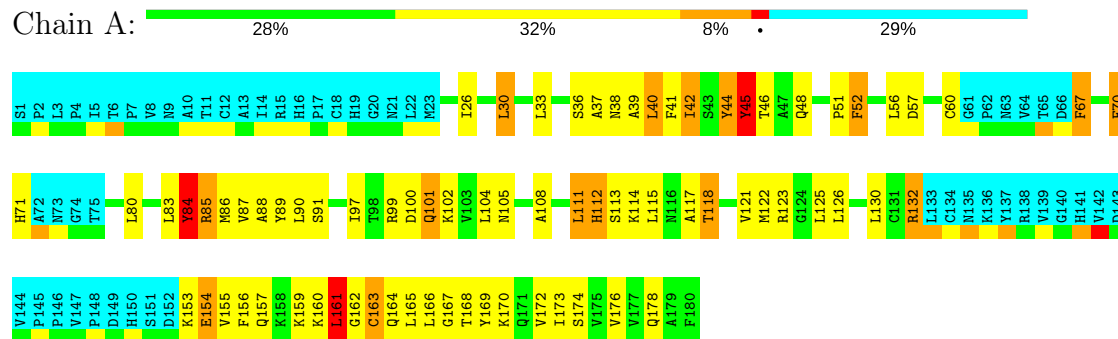
4.2.6 Score per residue for model 6

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.7 Score per residue for model 7

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.8 Score per residue for model 8

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



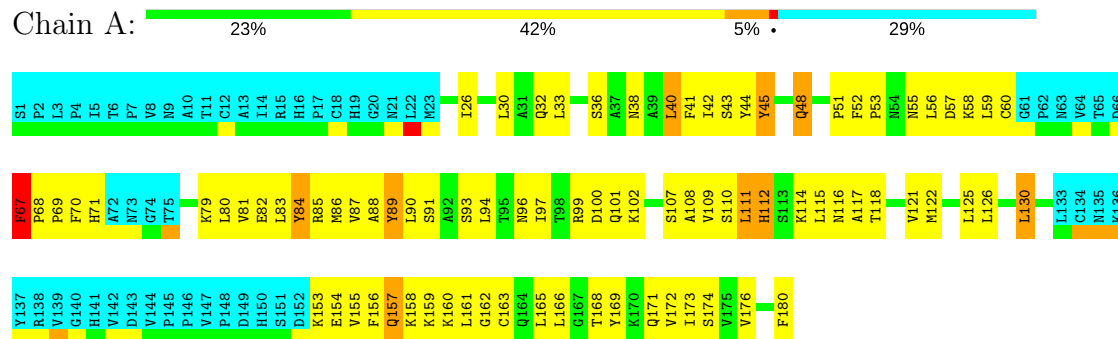
4.2.9 Score per residue for model 9

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



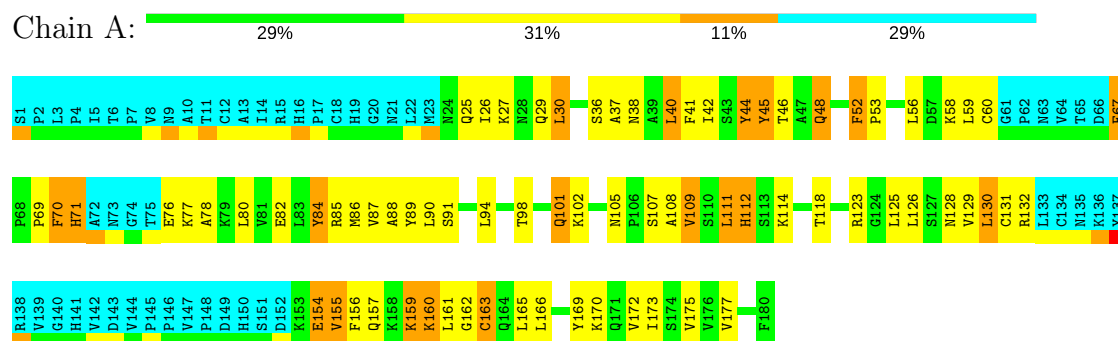
4.2.10 Score per residue for model 10

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



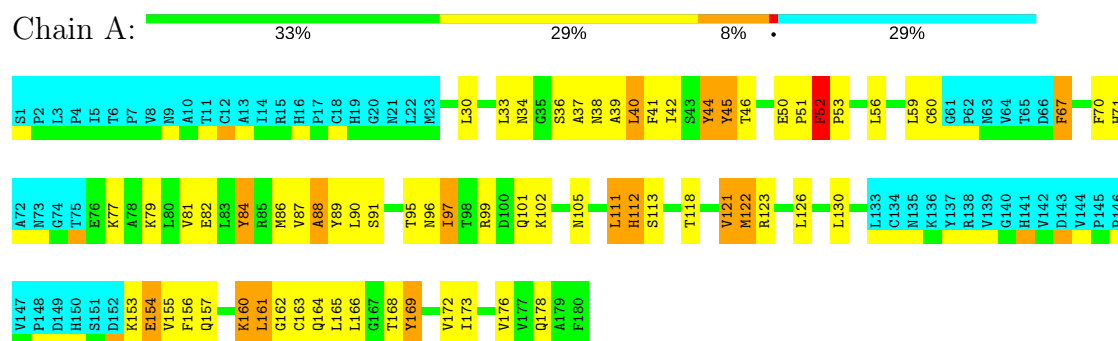
4.2.11 Score per residue for model 11

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



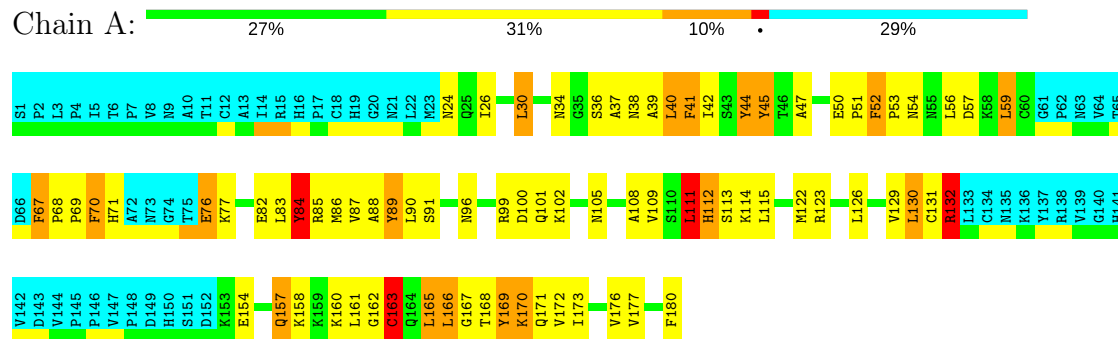
4.2.12 Score per residue for model 12

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



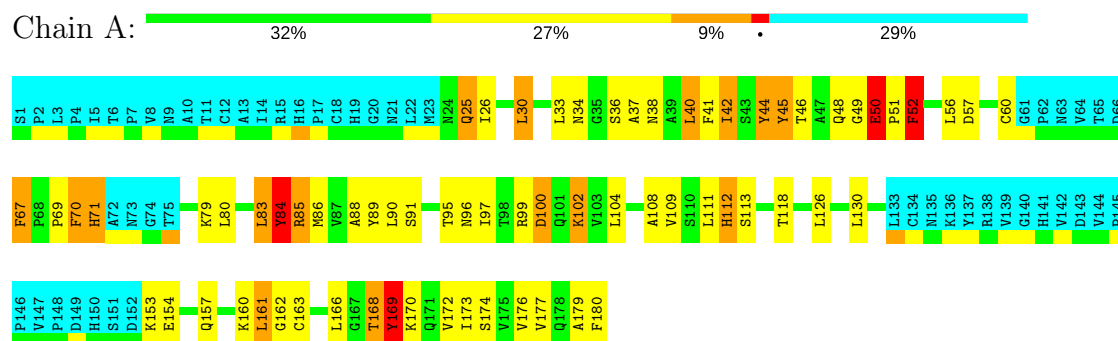
4.2.13 Score per residue for model 13

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



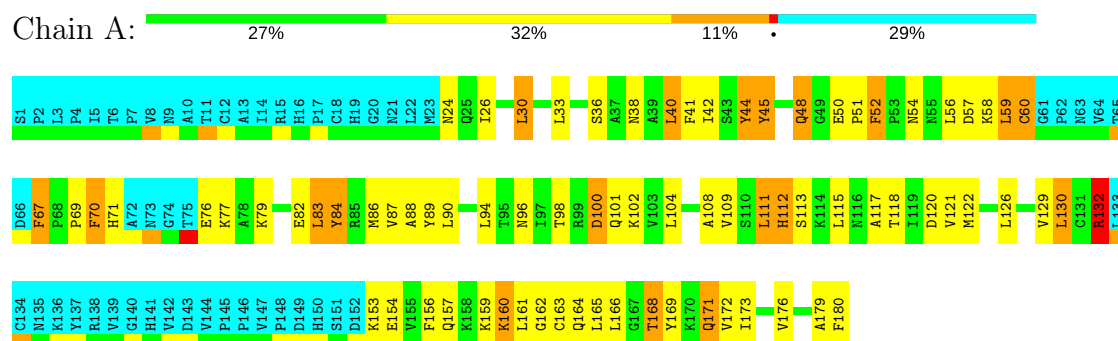
4.2.14 Score per residue for model 14

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



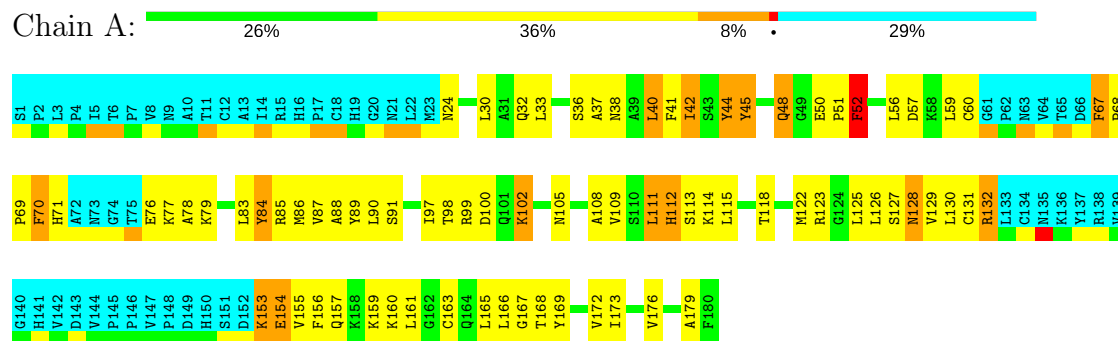
4.2.15 Score per residue for model 15

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



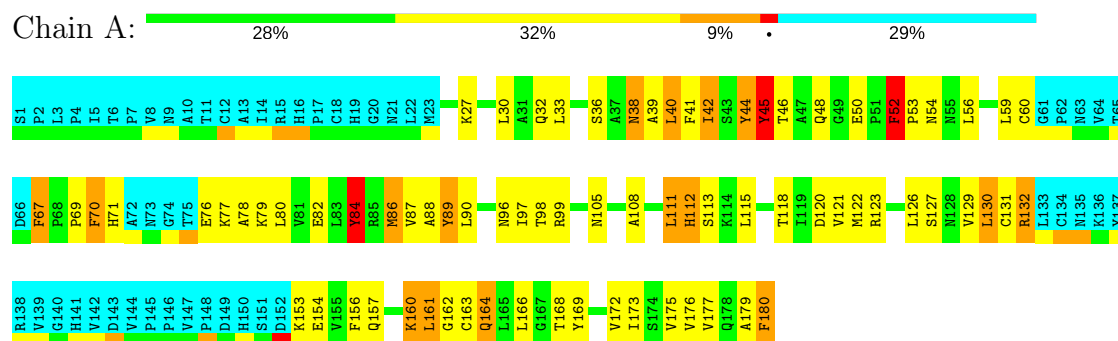
4.2.16 Score per residue for model 16

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



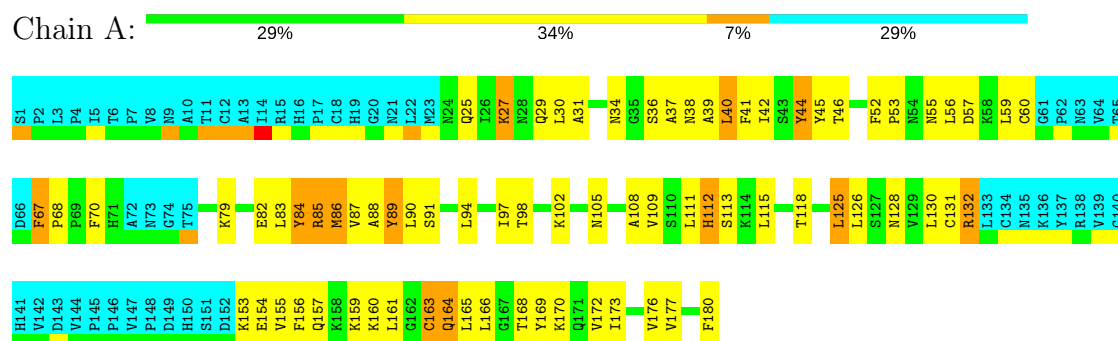
4.2.17 Score per residue for model 17

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



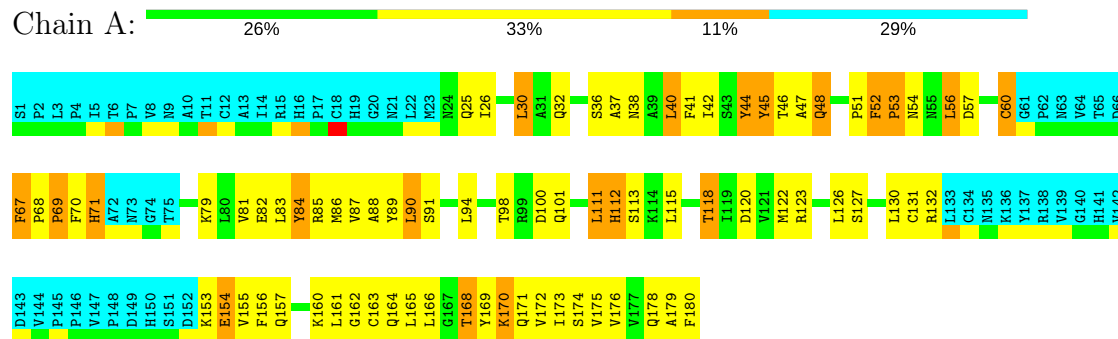
4.2.18 Score per residue for model 18

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



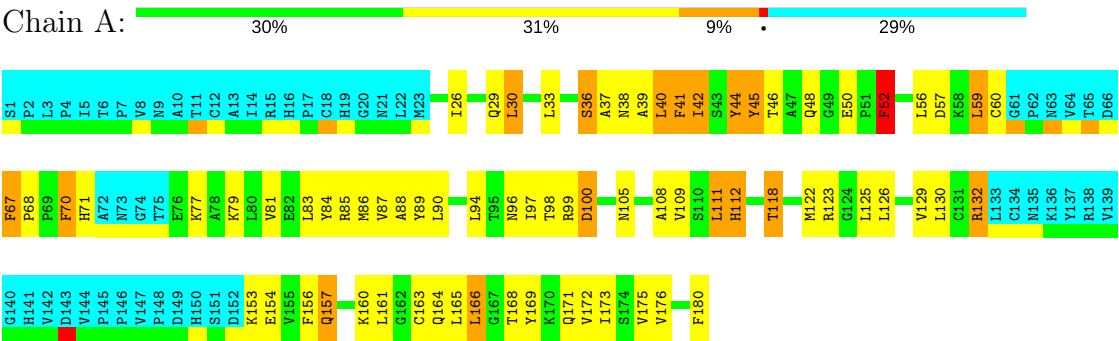
4.2.19 Score per residue for model 19

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.20 Score per residue for model 20

● Molecule 1: LEUKEMIA INHIBITORY FACTOR



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *DISTANCE GEOMETRY*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	
DYANA	structure solution	
X-PLOR	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	1.27±0.02	0±0/1017 (0.0±0.0%)	1.37±0.03	5±3/1373 (0.4±0.2%)
All	All	1.27	0/20340 (0.0%)	1.37	105/27460 (0.4%)

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	0.1±0.3
All	All	0	2

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	132	ARG	NE-CZ-NH2	-11.01	114.79	120.30	5	11
1	A	169	TYR	CB-CG-CD1	9.68	126.81	121.00	12	4
1	A	169	TYR	CB-CG-CD2	-9.39	115.37	121.00	12	4
1	A	85	ARG	NE-CZ-NH1	-9.34	115.63	120.30	5	1
1	A	85	ARG	NE-CZ-NH2	-9.16	115.72	120.30	18	10
1	A	123	ARG	NE-CZ-NH2	-8.63	115.98	120.30	5	10
1	A	52	PHE	CB-CG-CD2	-7.94	115.24	120.80	8	4
1	A	84	TYR	CB-CG-CD2	-7.46	116.52	121.00	1	9
1	A	99	ARG	NE-CZ-NH2	-7.11	116.75	120.30	14	6
1	A	52	PHE	CB-CG-CD1	6.97	125.68	120.80	8	5
1	A	45	TYR	CB-CG-CD1	6.82	125.09	121.00	7	1
1	A	57	ASP	CB-CG-OD2	-6.77	112.21	118.30	14	2
1	A	45	TYR	CB-CG-CD2	6.30	124.78	121.00	17	1
1	A	156	PHE	CB-CG-CD1	6.23	125.16	120.80	5	1
1	A	41	PHE	CB-CG-CD2	-5.85	116.71	120.80	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	131	CYS	CA-CB-SG	5.78	124.41	114.00	3	2
1	A	88	ALA	N-CA-CB	-5.75	102.06	110.10	2	3
1	A	100	ASP	CB-CG-OD2	-5.70	113.17	118.30	16	5
1	A	49	GLY	N-CA-C	-5.63	99.01	113.10	6	3
1	A	156	PHE	CB-CG-CD2	-5.52	116.94	120.80	5	1
1	A	120	ASP	CB-CG-OD2	-5.50	113.35	118.30	17	2
1	A	44	TYR	CB-CG-CD1	-5.41	117.75	121.00	7	1
1	A	154	GLU	N-CA-CB	-5.39	100.89	110.60	12	1
1	A	25	GLN	N-CA-C	-5.36	96.53	111.00	14	1
1	A	57	ASP	CB-CG-OD1	-5.36	113.48	118.30	4	3
1	A	76	GLU	OE1-CD-OE2	5.32	129.68	123.30	13	1
1	A	118	THR	OG1-CB-CG2	-5.31	97.78	110.00	5	1
1	A	84	TYR	CA-CB-CG	-5.30	103.33	113.40	14	3
1	A	111	LEU	CB-CG-CD2	5.26	119.94	111.00	13	1
1	A	84	TYR	N-CA-CB	-5.24	101.17	110.60	6	1
1	A	163	CYS	CA-CB-SG	5.18	123.33	114.00	11	2
1	A	84	TYR	CB-CG-CD1	5.17	124.10	121.00	1	1
1	A	159	LYS	N-CA-CB	-5.14	101.35	110.60	11	1
1	A	88	ALA	CB-CA-C	5.13	117.79	110.10	11	1
1	A	50	GLU	OE1-CD-OE2	5.00	129.30	123.30	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	68	PRO	Peptide	2

6.2 Too-close contacts [i](#)

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	1000	1038	1038	76±10
All	All	20000	20760	20760	1519

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:VAL:HG13	1:A:126:LEU:HD11	0.86	1.48	6	2
1:A:41:PHE:CZ	1:A:60:CYS:SG	0.85	2.69	19	3
1:A:41:PHE:CE1	1:A:60:CYS:SG	0.81	2.73	20	3
1:A:52:PHE:CD1	1:A:60:CYS:SG	0.81	2.73	9	3
1:A:160:LYS:HB2	1:A:163:CYS:SG	0.78	2.19	12	2
1:A:67:PHE:CZ	1:A:172:VAL:HG11	0.76	2.15	4	11
1:A:70:PHE:CE2	1:A:176:VAL:HG12	0.75	2.17	6	14
1:A:36:SER:HA	1:A:39:ALA:HB3	0.73	1.61	17	4
1:A:52:PHE:CE1	1:A:60:CYS:SG	0.72	2.82	12	4
1:A:44:TYR:CD1	1:A:45:TYR:N	0.71	2.59	18	3
1:A:160:LYS:HG3	1:A:163:CYS:SG	0.70	2.26	1	2
1:A:67:PHE:CE1	1:A:172:VAL:HG21	0.70	2.22	17	6
1:A:84:TYR:CE1	1:A:126:LEU:HD23	0.70	2.21	13	11
1:A:84:TYR:CZ	1:A:126:LEU:HD23	0.69	2.22	10	13
1:A:45:TYR:CE2	1:A:56:LEU:HD22	0.69	2.23	16	11
1:A:44:TYR:CD2	1:A:45:TYR:N	0.69	2.60	7	11
1:A:163:CYS:SG	1:A:164:GLN:N	0.68	2.67	12	2
1:A:84:TYR:CD2	1:A:126:LEU:HG	0.67	2.24	5	11
1:A:67:PHE:CZ	1:A:172:VAL:HG21	0.66	2.26	9	4
1:A:84:TYR:CE2	1:A:130:LEU:HD23	0.66	2.26	14	6
1:A:52:PHE:CE1	1:A:163:CYS:SG	0.65	2.90	5	3
1:A:160:LYS:CB	1:A:163:CYS:SG	0.65	2.84	18	2
1:A:42:ILE:CD1	1:A:42:ILE:N	0.65	2.60	2	4
1:A:102:LYS:HB3	1:A:112:HIS:CD2	0.65	2.27	2	6
1:A:67:PHE:CE2	1:A:172:VAL:HG21	0.64	2.27	15	2
1:A:87:VAL:CG1	1:A:126:LEU:HD11	0.64	2.22	17	13
1:A:153:LYS:HB2	1:A:156:PHE:CD2	0.63	2.29	5	1
1:A:83:LEU:HD22	1:A:180:PHE:CZ	0.63	2.29	2	3
1:A:160:LYS:HB3	1:A:163:CYS:SG	0.63	2.33	13	1
1:A:111:LEU:HD23	1:A:112:HIS:N	0.63	2.08	13	9
1:A:52:PHE:CZ	1:A:160:LYS:HG2	0.62	2.29	5	2
1:A:42:ILE:HD12	1:A:45:TYR:CE2	0.62	2.30	7	6
1:A:52:PHE:CD1	1:A:160:LYS:HE3	0.62	2.29	13	2
1:A:42:ILE:HA	1:A:45:TYR:CD2	0.62	2.29	20	3
1:A:84:TYR:CE1	1:A:130:LEU:HD23	0.61	2.31	3	1
1:A:42:ILE:HA	1:A:45:TYR:CE1	0.61	2.31	8	4
1:A:160:LYS:NZ	1:A:164:GLN:OE1	0.61	2.34	19	3
1:A:52:PHE:CE1	1:A:160:LYS:HE3	0.61	2.31	20	2
1:A:169:TYR:O	1:A:173:ILE:HB	0.61	1.96	12	7
1:A:44:TYR:HA	1:A:111:LEU:HD22	0.60	1.71	6	2
1:A:40:LEU:HD22	1:A:44:TYR:HB2	0.60	1.74	7	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:N	1:A:42:ILE:CD1	0.60	2.63	10	5
1:A:52:PHE:CE2	1:A:163:CYS:SG	0.60	2.95	16	4
1:A:41:PHE:CD1	1:A:166:LEU:HB3	0.60	2.31	1	14
1:A:84:TYR:CE2	1:A:126:LEU:HB3	0.60	2.31	18	12
1:A:102:LYS:CB	1:A:112:HIS:CD2	0.60	2.85	2	4
1:A:84:TYR:HA	1:A:126:LEU:HD22	0.60	1.73	18	5
1:A:42:ILE:HA	1:A:45:TYR:CD1	0.60	2.32	2	4
1:A:122:MET:SD	1:A:125:LEU:HD22	0.60	2.37	7	1
1:A:40:LEU:CD1	1:A:166:LEU:HD11	0.60	2.27	12	7
1:A:52:PHE:CE2	1:A:160:LYS:HG2	0.59	2.32	5	3
1:A:44:TYR:CD1	1:A:44:TYR:C	0.59	2.75	3	3
1:A:70:PHE:CD2	1:A:82:GLU:HB3	0.59	2.33	5	2
1:A:36:SER:O	1:A:40:LEU:N	0.58	2.36	5	20
1:A:173:ILE:HA	1:A:176:VAL:HG22	0.58	1.73	5	16
1:A:157:GLN:N	1:A:157:GLN:HE21	0.58	1.96	6	1
1:A:52:PHE:CZ	1:A:163:CYS:SG	0.58	2.97	20	5
1:A:112:HIS:CG	1:A:113:SER:N	0.58	2.70	14	6
1:A:94:LEU:HB3	1:A:119:ILE:HD11	0.58	1.75	8	1
1:A:122:MET:SD	1:A:123:ARG:N	0.57	2.77	12	2
1:A:45:TYR:HB2	1:A:52:PHE:CE1	0.57	2.34	12	3
1:A:127:SER:O	1:A:131:CYS:SG	0.57	2.62	16	2
1:A:105:ASN:HB2	1:A:108:ALA:HB2	0.57	1.76	17	4
1:A:170:LYS:HB3	1:A:170:LYS:NZ	0.57	2.15	11	2
1:A:79:LYS:NZ	1:A:179:ALA:O	0.57	2.38	2	6
1:A:89:TYR:CD1	1:A:90:LEU:N	0.56	2.73	8	10
1:A:101:GLN:HB3	1:A:108:ALA:HB1	0.56	1.77	11	2
1:A:153:LYS:HB2	1:A:156:PHE:HB2	0.56	1.78	6	2
1:A:50:GLU:HA	1:A:52:PHE:N	0.56	2.15	1	8
1:A:67:PHE:CZ	1:A:172:VAL:CG1	0.56	2.89	2	9
1:A:42:ILE:HD12	1:A:42:ILE:N	0.56	2.13	13	4
1:A:45:TYR:HB2	1:A:163:CYS:SG	0.56	2.40	3	7
1:A:44:TYR:C	1:A:44:TYR:CD1	0.56	2.78	17	2
1:A:33:LEU:HD21	1:A:121:VAL:CG2	0.56	2.31	10	2
1:A:44:TYR:CG	1:A:45:TYR:N	0.56	2.73	17	16
1:A:41:PHE:CE1	1:A:163:CYS:SG	0.56	2.98	20	3
1:A:87:VAL:CG1	1:A:126:LEU:CD1	0.56	2.83	20	12
1:A:89:TYR:CG	1:A:90:LEU:N	0.56	2.74	3	16
1:A:153:LYS:NZ	1:A:156:PHE:CE1	0.55	2.75	7	1
1:A:70:PHE:CE2	1:A:82:GLU:HB2	0.55	2.36	6	2
1:A:88:ALA:HB2	1:A:126:LEU:HD21	0.55	1.78	6	10
1:A:83:LEU:HD22	1:A:180:PHE:CE2	0.55	2.37	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD12	1:A:166:LEU:HD11	0.55	1.79	12	8
1:A:48:GLN:NE2	1:A:48:GLN:N	0.55	2.55	8	4
1:A:42:ILE:HA	1:A:45:TYR:CE2	0.55	2.37	20	6
1:A:76:GLU:H	1:A:76:GLU:CD	0.55	2.05	2	2
1:A:40:LEU:CD2	1:A:44:TYR:HB2	0.55	2.32	14	16
1:A:84:TYR:CE2	1:A:130:LEU:HG	0.55	2.36	9	1
1:A:153:LYS:HB3	1:A:156:PHE:CD1	0.55	2.36	10	7
1:A:109:VAL:O	1:A:112:HIS:CD2	0.55	2.60	18	7
1:A:68:PRO:CG	1:A:86:MET:SD	0.55	2.95	4	1
1:A:87:VAL:HG23	1:A:122:MET:SD	0.55	2.42	6	2
1:A:78:ALA:O	1:A:82:GLU:HB2	0.55	2.02	5	1
1:A:80:LEU:HB3	1:A:129:VAL:HG13	0.55	1.78	4	5
1:A:111:LEU:C	1:A:111:LEU:HD23	0.55	2.22	18	3
1:A:70:PHE:CZ	1:A:176:VAL:HG12	0.54	2.37	4	9
1:A:70:PHE:CZ	1:A:79:LYS:HA	0.54	2.37	10	9
1:A:105:ASN:HB3	1:A:108:ALA:HB2	0.54	1.79	1	3
1:A:52:PHE:HE1	1:A:163:CYS:SG	0.54	2.26	5	2
1:A:84:TYR:HA	1:A:126:LEU:CD2	0.54	2.32	18	4
1:A:41:PHE:CD2	1:A:42:ILE:CD1	0.54	2.90	16	3
1:A:45:TYR:HB2	1:A:52:PHE:CZ	0.54	2.38	5	2
1:A:37:ALA:HB1	1:A:170:LYS:HA	0.54	1.79	8	5
1:A:30:LEU:O	1:A:33:LEU:N	0.54	2.41	12	5
1:A:86:MET:O	1:A:89:TYR:CD1	0.54	2.61	7	1
1:A:48:GLN:N	1:A:48:GLN:HE21	0.54	2.01	8	1
1:A:90:LEU:CD2	1:A:169:TYR:CD1	0.54	2.91	17	1
1:A:42:ILE:N	1:A:42:ILE:HD12	0.54	2.17	10	4
1:A:44:TYR:O	1:A:48:GLN:NE2	0.54	2.40	1	1
1:A:153:LYS:CB	1:A:156:PHE:CD2	0.54	2.91	5	1
1:A:45:TYR:HB3	1:A:163:CYS:SG	0.54	2.43	7	1
1:A:30:LEU:HD11	1:A:173:ILE:CD1	0.53	2.33	14	1
1:A:44:TYR:OH	1:A:163:CYS:N	0.53	2.41	18	10
1:A:157:GLN:O	1:A:161:LEU:N	0.53	2.42	20	6
1:A:160:LYS:CG	1:A:163:CYS:SG	0.53	2.96	18	1
1:A:30:LEU:CD1	1:A:173:ILE:HG13	0.53	2.34	4	3
1:A:101:GLN:CG	1:A:108:ALA:HB1	0.53	2.34	8	1
1:A:45:TYR:C	1:A:45:TYR:CD1	0.53	2.82	11	2
1:A:41:PHE:CD1	1:A:166:LEU:CB	0.53	2.92	1	5
1:A:160:LYS:HA	1:A:163:CYS:HB2	0.52	1.80	9	3
1:A:111:LEU:HD23	1:A:111:LEU:C	0.52	2.25	14	4
1:A:84:TYR:CE2	1:A:130:LEU:CD2	0.52	2.92	7	1
1:A:68:PRO:HG2	1:A:86:MET:SD	0.52	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ALA:O	1:A:41:PHE:HB2	0.52	2.04	14	8
1:A:156:PHE:N	1:A:156:PHE:CD1	0.52	2.75	9	2
1:A:86:MET:O	1:A:89:TYR:CD2	0.52	2.63	20	2
1:A:87:VAL:HG13	1:A:126:LEU:CD1	0.52	2.30	4	2
1:A:111:LEU:HD12	1:A:111:LEU:C	0.52	2.25	3	2
1:A:97:ILE:HA	1:A:101:GLN:OE1	0.52	2.05	4	1
1:A:163:CYS:C	1:A:165:LEU:N	0.52	2.62	20	3
1:A:41:PHE:HE1	1:A:163:CYS:SG	0.52	2.28	5	7
1:A:169:TYR:CD1	1:A:173:ILE:HG13	0.52	2.40	2	1
1:A:85:ARG:HD2	1:A:86:MET:SD	0.52	2.45	4	1
1:A:87:VAL:CG1	1:A:122:MET:HB3	0.52	2.34	10	5
1:A:56:LEU:HD12	1:A:57:ASP:N	0.52	2.20	5	2
1:A:67:PHE:CZ	1:A:86:MET:SD	0.52	3.02	9	1
1:A:120:ASP:CG	1:A:123:ARG:NH2	0.52	2.64	5	1
1:A:70:PHE:HB2	1:A:86:MET:SD	0.51	2.45	16	1
1:A:120:ASP:HA	1:A:123:ARG:NH1	0.51	2.21	19	2
1:A:112:HIS:ND1	1:A:113:SER:N	0.51	2.58	15	10
1:A:84:TYR:CD2	1:A:130:LEU:HD23	0.51	2.40	1	3
1:A:27:LYS:NZ	1:A:177:VAL:O	0.51	2.41	11	2
1:A:30:LEU:HD12	1:A:177:VAL:HB	0.51	1.82	13	2
1:A:111:LEU:CD2	1:A:112:HIS:N	0.51	2.74	13	1
1:A:96:ASN:HD21	1:A:161:LEU:CD2	0.51	2.18	20	1
1:A:88:ALA:HB2	1:A:126:LEU:CD2	0.51	2.35	10	12
1:A:67:PHE:HD1	1:A:89:TYR:HH	0.51	1.48	2	1
1:A:166:LEU:HD13	1:A:169:TYR:CD2	0.51	2.40	14	4
1:A:41:PHE:HZ	1:A:60:CYS:SG	0.51	2.26	15	1
1:A:87:VAL:HB	1:A:126:LEU:HD11	0.51	1.83	7	5
1:A:169:TYR:O	1:A:173:ILE:CG1	0.51	2.58	5	3
1:A:52:PHE:CG	1:A:160:LYS:HE3	0.51	2.41	13	1
1:A:83:LEU:HG	1:A:180:PHE:CE2	0.51	2.41	18	3
1:A:52:PHE:O	1:A:56:LEU:N	0.51	2.44	17	6
1:A:132:ARG:HA	1:A:132:ARG:NE	0.50	2.21	1	1
1:A:87:VAL:HG13	1:A:122:MET:SD	0.50	2.46	15	5
1:A:102:LYS:CG	1:A:112:HIS:CD2	0.50	2.94	9	3
1:A:47:ALA:CB	1:A:111:LEU:HD23	0.50	2.36	19	1
1:A:108:ALA:HA	1:A:111:LEU:HD23	0.50	1.83	6	2
1:A:86:MET:C	1:A:86:MET:SD	0.50	2.89	5	2
1:A:118:THR:O	1:A:122:MET:CB	0.50	2.59	20	1
1:A:33:LEU:HD22	1:A:33:LEU:N	0.50	2.21	5	2
1:A:168:THR:O	1:A:171:GLN:N	0.50	2.43	13	5
1:A:155:VAL:O	1:A:159:LYS:NZ	0.50	2.45	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:O	1:A:60:CYS:N	0.50	2.44	5	13
1:A:172:VAL:O	1:A:175:VAL:HG12	0.50	2.07	17	2
1:A:157:GLN:HA	1:A:160:LYS:HG2	0.50	1.82	16	2
1:A:86:MET:SD	1:A:87:VAL:HG23	0.50	2.47	18	1
1:A:33:LEU:CD2	1:A:33:LEU:N	0.50	2.75	5	1
1:A:168:THR:O	1:A:169:TYR:C	0.50	2.49	13	7
1:A:87:VAL:HG12	1:A:126:LEU:CD1	0.50	2.37	9	3
1:A:109:VAL:HA	1:A:112:HIS:CD2	0.50	2.42	3	1
1:A:70:PHE:CD2	1:A:176:VAL:HG12	0.50	2.42	6	4
1:A:51:PRO:O	1:A:160:LYS:NZ	0.50	2.43	5	1
1:A:156:PHE:O	1:A:160:LYS:N	0.50	2.43	15	4
1:A:26:ILE:HG13	1:A:180:PHE:CD1	0.49	2.42	6	5
1:A:162:GLY:O	1:A:166:LEU:N	0.49	2.45	12	5
1:A:52:PHE:O	1:A:54:ASN:N	0.49	2.45	13	7
1:A:70:PHE:CD2	1:A:82:GLU:CG	0.49	2.95	13	1
1:A:40:LEU:O	1:A:44:TYR:N	0.49	2.45	6	14
1:A:154:GLU:H	1:A:154:GLU:CD	0.49	2.11	8	2
1:A:99:ARG:CG	1:A:100:ASP:N	0.49	2.75	7	1
1:A:84:TYR:O	1:A:88:ALA:N	0.49	2.45	4	5
1:A:169:TYR:HA	1:A:172:VAL:CG2	0.49	2.38	14	3
1:A:42:ILE:O	1:A:46:THR:HG23	0.49	2.07	17	9
1:A:84:TYR:HB2	1:A:129:VAL:HG11	0.49	1.83	9	4
1:A:108:ALA:O	1:A:111:LEU:HG	0.49	2.08	6	3
1:A:160:LYS:O	1:A:161:LEU:C	0.49	2.50	16	8
1:A:70:PHE:CE2	1:A:176:VAL:CG1	0.49	2.94	6	3
1:A:70:PHE:CG	1:A:176:VAL:HG12	0.49	2.43	17	2
1:A:105:ASN:OD1	1:A:159:LYS:NZ	0.49	2.46	3	1
1:A:52:PHE:CZ	1:A:160:LYS:HB3	0.49	2.42	10	1
1:A:87:VAL:HG12	1:A:126:LEU:HD11	0.49	1.83	9	3
1:A:45:TYR:CB	1:A:163:CYS:SG	0.49	3.01	10	5
1:A:84:TYR:CD1	1:A:84:TYR:C	0.49	2.86	9	4
1:A:83:LEU:CD1	1:A:125:LEU:HD21	0.49	2.38	1	1
1:A:45:TYR:CE2	1:A:56:LEU:CD2	0.49	2.94	16	1
1:A:165:LEU:N	1:A:165:LEU:CD2	0.49	2.75	5	2
1:A:52:PHE:HD1	1:A:60:CYS:SG	0.49	2.26	9	1
1:A:111:LEU:HG	1:A:112:HIS:N	0.48	2.22	19	2
1:A:26:ILE:O	1:A:30:LEU:HB2	0.48	2.07	1	7
1:A:79:LYS:HE2	1:A:179:ALA:HB1	0.48	1.83	4	2
1:A:39:ALA:O	1:A:40:LEU:C	0.48	2.51	13	10
1:A:108:ALA:O	1:A:111:LEU:N	0.48	2.46	9	6
1:A:69:PRO:O	1:A:85:ARG:NH2	0.48	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:TYR:CE1	1:A:126:LEU:HD13	0.48	2.43	12	1
1:A:57:ASP:CG	1:A:58:LYS:NZ	0.48	2.66	15	1
1:A:50:GLU:HA	1:A:52:PHE:H	0.48	1.69	12	5
1:A:153:LYS:O	1:A:157:GLN:HB2	0.48	2.08	17	7
1:A:50:GLU:CD	1:A:50:GLU:H	0.48	2.11	5	1
1:A:87:VAL:CG1	1:A:122:MET:CG	0.48	2.91	20	1
1:A:87:VAL:O	1:A:88:ALA:C	0.48	2.51	10	5
1:A:69:PRO:O	1:A:70:PHE:C	0.48	2.52	14	6
1:A:40:LEU:HD22	1:A:44:TYR:CB	0.48	2.39	5	9
1:A:33:LEU:O	1:A:37:ALA:N	0.48	2.47	20	3
1:A:44:TYR:CZ	1:A:48:GLN:OE1	0.48	2.66	10	3
1:A:48:GLN:NE2	1:A:111:LEU:CD1	0.48	2.76	20	2
1:A:154:GLU:O	1:A:155:VAL:C	0.48	2.51	19	5
1:A:55:ASN:HB2	1:A:59:LEU:CD1	0.48	2.37	9	2
1:A:90:LEU:O	1:A:91:SER:C	0.48	2.51	4	10
1:A:33:LEU:HD21	1:A:121:VAL:HG21	0.48	1.85	9	5
1:A:160:LYS:HA	1:A:163:CYS:CB	0.48	2.39	2	5
1:A:96:ASN:OD1	1:A:99:ARG:NH1	0.48	2.47	17	1
1:A:84:TYR:CE1	1:A:126:LEU:CB	0.48	2.97	3	1
1:A:166:LEU:HD13	1:A:169:TYR:CD1	0.48	2.43	20	3
1:A:56:LEU:HB2	1:A:60:CYS:SG	0.48	2.49	5	2
1:A:86:MET:O	1:A:89:TYR:CE1	0.47	2.67	8	6
1:A:84:TYR:CE2	1:A:126:LEU:CB	0.47	2.97	7	6
1:A:83:LEU:HD12	1:A:84:TYR:N	0.47	2.23	2	1
1:A:41:PHE:CD1	1:A:41:PHE:C	0.47	2.87	19	3
1:A:34:ASN:HA	1:A:173:ILE:CG2	0.47	2.40	13	3
1:A:40:LEU:HD11	1:A:115:LEU:CD1	0.47	2.39	1	1
1:A:41:PHE:CG	1:A:166:LEU:HB3	0.47	2.44	1	8
1:A:27:LYS:NZ	1:A:180:PHE:OXT	0.47	2.47	17	1
1:A:67:PHE:HB2	1:A:89:TYR:CZ	0.47	2.44	7	2
1:A:117:ALA:O	1:A:121:VAL:HG22	0.47	2.09	9	6
1:A:169:TYR:CE1	1:A:173:ILE:HG13	0.47	2.44	2	1
1:A:90:LEU:HG	1:A:94:LEU:CD1	0.47	2.40	6	1
1:A:42:ILE:C	1:A:44:TYR:N	0.47	2.68	4	6
1:A:48:GLN:N	1:A:48:GLN:CD	0.47	2.68	1	1
1:A:172:VAL:HG23	1:A:173:ILE:N	0.47	2.25	9	5
1:A:94:LEU:CB	1:A:115:LEU:HD21	0.47	2.40	15	1
1:A:52:PHE:CD2	1:A:160:LYS:HG2	0.47	2.44	13	1
1:A:70:PHE:CD2	1:A:82:GLU:CB	0.47	2.97	10	2
1:A:45:TYR:O	1:A:160:LYS:NZ	0.47	2.48	13	1
1:A:42:ILE:O	1:A:44:TYR:N	0.47	2.48	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CB	1:A:53:PRO:CD	0.47	2.92	6	3
1:A:94:LEU:CB	1:A:119:ILE:HD11	0.47	2.40	8	1
1:A:84:TYR:CE1	1:A:130:LEU:CD2	0.47	2.98	3	1
1:A:48:GLN:HE22	1:A:111:LEU:CD1	0.47	2.22	8	1
1:A:59:LEU:CD1	1:A:59:LEU:N	0.47	2.77	15	1
1:A:102:LYS:HG3	1:A:112:HIS:CD2	0.47	2.45	13	1
1:A:67:PHE:CD2	1:A:168:THR:CG2	0.47	2.98	17	2
1:A:30:LEU:CD2	1:A:173:ILE:HG23	0.47	2.40	9	1
1:A:154:GLU:O	1:A:157:GLN:N	0.46	2.48	9	9
1:A:33:LEU:CD1	1:A:118:THR:HG22	0.46	2.40	5	1
1:A:36:SER:O	1:A:39:ALA:N	0.46	2.48	13	2
1:A:41:PHE:CZ	1:A:56:LEU:HD13	0.46	2.46	18	3
1:A:165:LEU:O	1:A:169:TYR:N	0.46	2.47	1	2
1:A:50:GLU:O	1:A:159:LYS:NZ	0.46	2.48	16	1
1:A:52:PHE:CZ	1:A:160:LYS:HB2	0.46	2.45	11	2
1:A:27:LYS:HZ2	1:A:180:PHE:C	0.46	2.14	8	1
1:A:115:LEU:O	1:A:116:ASN:C	0.46	2.51	5	1
1:A:70:PHE:CE2	1:A:82:GLU:HB3	0.46	2.46	5	2
1:A:52:PHE:CE2	1:A:59:LEU:HB3	0.46	2.46	13	1
1:A:71:HIS:ND1	1:A:71:HIS:O	0.46	2.48	6	1
1:A:45:TYR:CD1	1:A:45:TYR:C	0.46	2.88	16	5
1:A:160:LYS:O	1:A:162:GLY:N	0.46	2.48	14	6
1:A:56:LEU:HA	1:A:60:CYS:SG	0.46	2.50	7	2
1:A:33:LEU:CD2	1:A:121:VAL:HG21	0.46	2.40	15	2
1:A:112:HIS:O	1:A:113:SER:C	0.46	2.53	12	11
1:A:30:LEU:HD11	1:A:173:ILE:HG23	0.46	1.87	1	2
1:A:87:VAL:HG11	1:A:126:LEU:CD1	0.46	2.40	2	5
1:A:102:LYS:NZ	1:A:112:HIS:CE1	0.46	2.82	5	1
1:A:168:THR:O	1:A:172:VAL:HG22	0.46	2.09	9	1
1:A:153:LYS:HB3	1:A:156:PHE:CD2	0.46	2.46	12	1
1:A:48:GLN:N	1:A:48:GLN:NE2	0.46	2.64	10	1
1:A:160:LYS:C	1:A:162:GLY:N	0.46	2.68	2	5
1:A:41:PHE:CE2	1:A:56:LEU:HD13	0.46	2.46	18	2
1:A:87:VAL:O	1:A:90:LEU:N	0.46	2.49	10	3
1:A:165:LEU:O	1:A:169:TYR:CB	0.46	2.63	19	8
1:A:165:LEU:N	1:A:165:LEU:HD22	0.46	2.25	7	1
1:A:67:PHE:CE2	1:A:86:MET:SD	0.46	3.08	9	1
1:A:52:PHE:CZ	1:A:60:CYS:SG	0.46	3.08	12	1
1:A:56:LEU:HD12	1:A:56:LEU:C	0.46	2.31	11	6
1:A:160:LYS:O	1:A:163:CYS:N	0.46	2.49	5	8
1:A:165:LEU:O	1:A:166:LEU:C	0.46	2.54	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:VAL:CG2	1:A:122:MET:SD	0.46	3.04	6	1
1:A:87:VAL:CB	1:A:126:LEU:HD11	0.46	2.41	10	5
1:A:173:ILE:CG2	1:A:174:SER:N	0.46	2.79	14	1
1:A:41:PHE:CE1	1:A:45:TYR:CD2	0.46	3.04	20	1
1:A:67:PHE:CD2	1:A:89:TYR:OH	0.46	2.69	11	3
1:A:97:ILE:N	1:A:97:ILE:HD12	0.46	2.25	16	1
1:A:44:TYR:CD2	1:A:111:LEU:HD11	0.46	2.45	18	2
1:A:118:THR:O	1:A:122:MET:HB2	0.46	2.11	20	1
1:A:34:ASN:HA	1:A:173:ILE:HG21	0.45	1.87	14	3
1:A:56:LEU:C	1:A:56:LEU:HD12	0.45	2.32	14	6
1:A:108:ALA:O	1:A:109:VAL:C	0.45	2.53	1	7
1:A:67:PHE:CG	1:A:89:TYR:OH	0.45	2.70	20	3
1:A:108:ALA:O	1:A:111:LEU:HB3	0.45	2.11	9	6
1:A:154:GLU:HG3	1:A:155:VAL:N	0.45	2.26	16	2
1:A:86:MET:HA	1:A:89:TYR:CD2	0.45	2.46	13	3
1:A:84:TYR:CE1	1:A:126:LEU:HB3	0.45	2.47	3	1
1:A:84:TYR:CD2	1:A:126:LEU:HD22	0.45	2.46	14	1
1:A:83:LEU:O	1:A:84:TYR:C	0.45	2.54	1	1
1:A:89:TYR:C	1:A:89:TYR:CD1	0.45	2.89	2	2
1:A:170:LYS:NZ	1:A:174:SER:OG	0.45	2.49	19	1
1:A:59:LEU:HB3	1:A:160:LYS:CD	0.45	2.41	5	1
1:A:112:HIS:O	1:A:115:LEU:N	0.45	2.49	19	3
1:A:84:TYR:CD1	1:A:126:LEU:HG	0.45	2.47	3	1
1:A:67:PHE:CD1	1:A:168:THR:HB	0.45	2.46	15	1
1:A:129:VAL:O	1:A:130:LEU:C	0.45	2.52	13	1
1:A:153:LYS:CB	1:A:156:PHE:HB2	0.45	2.42	9	3
1:A:48:GLN:OE1	1:A:159:LYS:HB3	0.45	2.12	11	1
1:A:30:LEU:HD11	1:A:173:ILE:HG13	0.45	1.89	13	1
1:A:43:SER:CB	1:A:114:LYS:NZ	0.45	2.80	10	1
1:A:40:LEU:O	1:A:41:PHE:C	0.45	2.55	14	10
1:A:86:MET:HA	1:A:89:TYR:CE2	0.45	2.46	1	4
1:A:82:GLU:O	1:A:86:MET:CB	0.45	2.64	2	1
1:A:69:PRO:O	1:A:71:HIS:N	0.45	2.49	17	2
1:A:154:GLU:CD	1:A:155:VAL:N	0.45	2.70	12	1
1:A:60:CYS:SG	1:A:163:CYS:O	0.45	2.75	20	1
1:A:87:VAL:O	1:A:91:SER:N	0.45	2.49	8	5
1:A:102:LYS:HB2	1:A:112:HIS:CD2	0.45	2.46	15	5
1:A:87:VAL:HG13	1:A:122:MET:CG	0.45	2.42	20	2
1:A:173:ILE:HA	1:A:176:VAL:CG2	0.45	2.41	18	2
1:A:86:MET:O	1:A:90:LEU:HB2	0.45	2.11	18	1
1:A:118:THR:O	1:A:122:MET:CG	0.45	2.65	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:TYR:CE2	1:A:53:PRO:HA	0.45	2.47	3	1
1:A:90:LEU:O	1:A:93:SER:N	0.45	2.50	10	2
1:A:30:LEU:CD2	1:A:176:VAL:HG23	0.45	2.41	12	2
1:A:30:LEU:CD1	1:A:173:ILE:HG23	0.45	2.42	2	3
1:A:111:LEU:HD12	1:A:112:HIS:N	0.45	2.27	11	2
1:A:176:VAL:HA	1:A:179:ALA:CB	0.45	2.42	16	1
1:A:67:PHE:CD2	1:A:168:THR:HB	0.44	2.47	14	3
1:A:155:VAL:HG23	1:A:156:PHE:N	0.44	2.27	11	1
1:A:47:ALA:HB3	1:A:111:LEU:HD12	0.44	1.89	13	1
1:A:70:PHE:HA	1:A:82:GLU:CG	0.44	2.42	13	1
1:A:111:LEU:CG	1:A:112:HIS:N	0.44	2.79	10	3
1:A:36:SER:O	1:A:37:ALA:C	0.44	2.54	19	7
1:A:101:GLN:HG3	1:A:108:ALA:HB1	0.44	1.88	8	1
1:A:33:LEU:O	1:A:34:ASN:C	0.44	2.54	8	4
1:A:122:MET:O	1:A:123:ARG:C	0.44	2.56	12	3
1:A:99:ARG:O	1:A:100:ASP:C	0.44	2.55	10	2
1:A:90:LEU:HD21	1:A:169:TYR:CD1	0.44	2.47	17	1
1:A:40:LEU:O	1:A:44:TYR:HB3	0.44	2.12	11	5
1:A:157:GLN:CA	1:A:157:GLN:HE21	0.44	2.25	6	1
1:A:89:TYR:CD1	1:A:89:TYR:C	0.44	2.90	1	1
1:A:67:PHE:CE2	1:A:168:THR:HB	0.44	2.47	16	1
1:A:60:CYS:HA	1:A:164:GLN:HA	0.44	1.88	12	2
1:A:44:TYR:HE1	1:A:163:CYS:CB	0.44	2.25	18	1
1:A:68:PRO:O	1:A:70:PHE:N	0.44	2.50	13	2
1:A:101:GLN:HG2	1:A:111:LEU:HD21	0.44	1.89	6	1
1:A:30:LEU:O	1:A:30:LEU:HD13	0.44	2.13	14	1
1:A:44:TYR:CD1	1:A:111:LEU:HD11	0.44	2.48	16	1
1:A:67:PHE:CE2	1:A:172:VAL:HG11	0.44	2.47	19	1
1:A:82:GLU:OE2	1:A:85:ARG:NH2	0.44	2.51	18	1
1:A:90:LEU:HG	1:A:94:LEU:HD13	0.44	1.88	18	1
1:A:86:MET:O	1:A:90:LEU:CB	0.44	2.66	7	2
1:A:68:PRO:O	1:A:85:ARG:NH2	0.44	2.51	19	1
1:A:34:ASN:O	1:A:37:ALA:HB3	0.44	2.12	18	2
1:A:120:ASP:CG	1:A:123:ARG:HH21	0.44	2.16	5	1
1:A:76:GLU:HG3	1:A:77:LYS:N	0.44	2.28	15	1
1:A:95:THR:O	1:A:96:ASN:C	0.44	2.55	5	4
1:A:30:LEU:HD12	1:A:177:VAL:CB	0.44	2.43	13	1
1:A:57:ASP:OD1	1:A:58:LYS:NZ	0.44	2.49	6	1
1:A:97:ILE:O	1:A:98:THR:C	0.44	2.56	16	6
1:A:26:ILE:HD11	1:A:80:LEU:CD2	0.44	2.42	1	2
1:A:125:LEU:O	1:A:128:ASN:N	0.44	2.50	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ARG:HG2	1:A:100:ASP:N	0.44	2.28	7	1
1:A:153:LYS:NZ	1:A:156:PHE:CZ	0.44	2.86	7	1
1:A:48:GLN:CG	1:A:52:PHE:CD2	0.43	3.00	17	1
1:A:160:LYS:N	1:A:160:LYS:CD	0.43	2.80	13	1
1:A:158:LYS:NZ	1:A:158:LYS:HB2	0.43	2.27	10	1
1:A:156:PHE:O	1:A:159:LYS:N	0.43	2.51	10	1
1:A:153:LYS:O	1:A:157:GLN:HB3	0.43	2.13	8	1
1:A:172:VAL:O	1:A:175:VAL:HB	0.43	2.13	2	1
1:A:163:CYS:O	1:A:166:LEU:N	0.43	2.51	19	1
1:A:48:GLN:CG	1:A:159:LYS:HB3	0.43	2.43	15	1
1:A:41:PHE:HB2	1:A:166:LEU:HD12	0.43	1.89	12	2
1:A:112:HIS:ND1	1:A:112:HIS:C	0.43	2.71	18	1
1:A:153:LYS:HB2	1:A:157:GLN:NE2	0.43	2.29	6	1
1:A:117:ALA:O	1:A:118:THR:C	0.43	2.57	10	1
1:A:48:GLN:NE2	1:A:101:GLN:OE1	0.43	2.52	11	1
1:A:76:GLU:CG	1:A:77:LYS:N	0.43	2.82	15	1
1:A:87:VAL:O	1:A:91:SER:CB	0.43	2.67	3	2
1:A:87:VAL:HG11	1:A:126:LEU:HD11	0.43	1.90	2	1
1:A:93:SER:OG	1:A:94:LEU:N	0.43	2.52	4	1
1:A:55:ASN:O	1:A:59:LEU:HG	0.43	2.13	1	1
1:A:70:PHE:CD1	1:A:176:VAL:HG12	0.43	2.49	17	1
1:A:100:ASP:O	1:A:104:LEU:N	0.43	2.52	3	3
1:A:84:TYR:CZ	1:A:130:LEU:HD23	0.43	2.49	10	1
1:A:47:ALA:HB3	1:A:111:LEU:CD2	0.43	2.44	19	1
1:A:83:LEU:HG	1:A:180:PHE:CZ	0.43	2.48	18	2
1:A:97:ILE:HD11	1:A:162:GLY:HA3	0.43	1.90	4	1
1:A:97:ILE:HG23	1:A:101:GLN:CG	0.43	2.44	10	1
1:A:70:PHE:CD2	1:A:82:GLU:HB2	0.43	2.49	10	2
1:A:33:LEU:O	1:A:36:SER:N	0.43	2.51	7	3
1:A:113:SER:OG	1:A:114:LYS:N	0.43	2.51	7	1
1:A:100:ASP:OD1	1:A:158:LYS:NZ	0.43	2.52	9	1
1:A:70:PHE:HA	1:A:82:GLU:HG2	0.43	1.91	9	1
1:A:57:ASP:C	1:A:58:LYS:HE2	0.43	2.33	15	1
1:A:51:PRO:O	1:A:55:ASN:N	0.43	2.52	10	1
1:A:83:LEU:HD23	1:A:176:VAL:HG21	0.43	1.89	5	1
1:A:95:THR:O	1:A:98:THR:HB	0.43	2.13	5	1
1:A:97:ILE:HD11	1:A:101:GLN:NE2	0.43	2.28	7	1
1:A:129:VAL:O	1:A:132:ARG:HG2	0.43	2.14	3	1
1:A:156:PHE:O	1:A:157:GLN:C	0.43	2.56	10	2
1:A:45:TYR:CZ	1:A:56:LEU:CD2	0.43	3.02	20	2
1:A:33:LEU:HD12	1:A:33:LEU:N	0.43	2.27	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ASN:C	1:A:57:ASP:N	0.43	2.71	9	2
1:A:87:VAL:CG1	1:A:122:MET:SD	0.43	3.07	20	1
1:A:163:CYS:O	1:A:164:GLN:C	0.43	2.57	20	1
1:A:83:LEU:C	1:A:83:LEU:HD13	0.42	2.35	14	1
1:A:56:LEU:CG	1:A:57:ASP:N	0.42	2.82	5	1
1:A:48:GLN:HE22	1:A:101:GLN:NE2	0.42	2.12	9	1
1:A:44:TYR:CE1	1:A:48:GLN:OE1	0.42	2.72	15	1
1:A:79:LYS:CE	1:A:179:ALA:O	0.42	2.67	15	1
1:A:157:GLN:NE2	1:A:158:LYS:N	0.42	2.67	13	1
1:A:127:SER:O	1:A:131:CYS:N	0.42	2.52	6	1
1:A:154:GLU:C	1:A:156:PHE:N	0.42	2.69	1	4
1:A:33:LEU:HD11	1:A:121:VAL:HG21	0.42	1.89	17	1
1:A:167:GLY:O	1:A:170:LYS:NZ	0.42	2.51	13	1
1:A:96:ASN:O	1:A:99:ARG:HG2	0.42	2.14	13	1
1:A:83:LEU:CG	1:A:84:TYR:N	0.42	2.83	2	1
1:A:90:LEU:C	1:A:90:LEU:HD13	0.42	2.35	2	1
1:A:85:ARG:CG	1:A:86:MET:N	0.42	2.83	19	1
1:A:67:PHE:HD2	1:A:89:TYR:HH	0.42	1.54	7	1
1:A:55:ASN:HB2	1:A:59:LEU:HD11	0.42	1.91	9	1
1:A:111:LEU:HD23	1:A:112:HIS:CA	0.42	2.44	13	1
1:A:59:LEU:HB2	1:A:160:LYS:HE2	0.42	1.91	20	1
1:A:26:ILE:CD1	1:A:80:LEU:HD22	0.42	2.45	4	1
1:A:45:TYR:CD1	1:A:46:THR:N	0.42	2.87	6	2
1:A:112:HIS:C	1:A:112:HIS:ND1	0.42	2.73	10	1
1:A:97:ILE:HG22	1:A:161:LEU:HB3	0.42	1.90	17	1
1:A:60:CYS:O	1:A:167:GLY:HA3	0.42	2.13	7	1
1:A:87:VAL:O	1:A:91:SER:HB2	0.42	2.15	13	1
1:A:101:GLN:C	1:A:103:VAL:N	0.42	2.72	6	1
1:A:110:SER:O	1:A:111:LEU:C	0.42	2.58	6	1
1:A:70:PHE:CD2	1:A:176:VAL:CG1	0.42	3.01	6	1
1:A:169:TYR:CE1	1:A:173:ILE:HD13	0.42	2.49	14	1
1:A:88:ALA:HB2	1:A:126:LEU:CD1	0.42	2.44	14	2
1:A:70:PHE:HA	1:A:82:GLU:CD	0.42	2.34	11	2
1:A:52:PHE:HB3	1:A:53:PRO:CD	0.42	2.45	12	1
1:A:132:ARG:NE	1:A:132:ARG:CA	0.42	2.82	1	1
1:A:38:ASN:O	1:A:42:ILE:HD13	0.42	2.15	8	2
1:A:44:TYR:CE2	1:A:163:CYS:N	0.42	2.88	3	2
1:A:129:VAL:HG12	1:A:130:LEU:N	0.42	2.29	15	1
1:A:169:TYR:O	1:A:173:ILE:CB	0.42	2.68	1	2
1:A:162:GLY:O	1:A:165:LEU:HB2	0.42	2.14	7	2
1:A:118:THR:O	1:A:122:MET:HG3	0.42	2.14	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LYS:O	1:A:157:GLN:CB	0.42	2.68	9	2
1:A:105:ASN:HB3	1:A:108:ALA:CB	0.42	2.44	13	1
1:A:40:LEU:C	1:A:40:LEU:HD22	0.42	2.35	20	2
1:A:120:ASP:O	1:A:123:ARG:HG3	0.42	2.15	6	1
1:A:115:LEU:HA	1:A:118:THR:OG1	0.42	2.15	10	1
1:A:26:ILE:HD12	1:A:180:PHE:CD1	0.42	2.49	14	2
1:A:155:VAL:CG2	1:A:156:PHE:N	0.42	2.83	11	1
1:A:173:ILE:C	1:A:175:VAL:H	0.42	2.18	19	2
1:A:90:LEU:HD13	1:A:91:SER:N	0.42	2.30	7	1
1:A:105:ASN:HB2	1:A:108:ALA:CB	0.42	2.44	20	2
1:A:101:GLN:CG	1:A:111:LEU:HD21	0.42	2.45	6	1
1:A:123:ARG:HD2	1:A:124:GLY:N	0.42	2.30	6	1
1:A:57:ASP:CG	1:A:58:LYS:N	0.42	2.73	10	1
1:A:30:LEU:O	1:A:31:ALA:C	0.42	2.58	5	2
1:A:111:LEU:C	1:A:111:LEU:HD12	0.42	2.35	17	1
1:A:52:PHE:HE1	1:A:60:CYS:SG	0.42	2.36	12	1
1:A:76:GLU:N	1:A:76:GLU:CD	0.42	2.74	3	1
1:A:153:LYS:O	1:A:157:GLN:CG	0.42	2.68	18	1
1:A:176:VAL:C	1:A:178:GLN:N	0.42	2.74	12	3
1:A:84:TYR:CZ	1:A:126:LEU:HB3	0.42	2.50	12	1
1:A:84:TYR:C	1:A:84:TYR:CD1	0.42	2.93	20	1
1:A:157:GLN:O	1:A:161:LEU:HB2	0.41	2.15	6	1
1:A:86:MET:HA	1:A:89:TYR:CE1	0.41	2.49	14	1
1:A:26:ILE:CG2	1:A:125:LEU:HG	0.41	2.45	1	1
1:A:92:ALA:O	1:A:96:ASN:ND2	0.41	2.53	1	1
1:A:94:LEU:HG	1:A:115:LEU:HD11	0.41	1.92	19	1
1:A:102:LYS:HD3	1:A:102:LYS:O	0.41	2.14	10	1
1:A:94:LEU:O	1:A:97:ILE:HB	0.41	2.15	4	1
1:A:56:LEU:HG	1:A:57:ASP:N	0.41	2.31	19	1
1:A:97:ILE:HD11	1:A:162:GLY:CA	0.41	2.46	12	1
1:A:59:LEU:C	1:A:60:CYS:SG	0.41	2.98	12	1
1:A:84:TYR:CE2	1:A:126:LEU:HD23	0.41	2.50	3	1
1:A:33:LEU:HD21	1:A:122:MET:HG3	0.41	1.92	16	1
1:A:68:PRO:HG2	1:A:86:MET:CG	0.41	2.46	16	1
1:A:48:GLN:HG3	1:A:52:PHE:CE2	0.41	2.49	17	1
1:A:48:GLN:HB3	1:A:159:LYS:HB3	0.41	1.92	7	1
1:A:29:GLN:O	1:A:32:GLN:N	0.41	2.54	6	1
1:A:96:ASN:ND2	1:A:161:LEU:HD13	0.41	2.31	10	1
1:A:83:LEU:HD13	1:A:84:TYR:N	0.41	2.30	14	1
1:A:96:ASN:CG	1:A:97:ILE:N	0.41	2.73	20	1
1:A:67:PHE:HE1	1:A:86:MET:SD	0.41	2.38	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD11	1:A:121:VAL:HG11	0.41	1.91	12	1
1:A:101:GLN:HA	1:A:101:GLN:NE2	0.41	2.31	13	2
1:A:90:LEU:HD23	1:A:90:LEU:C	0.41	2.35	13	1
1:A:26:ILE:CD1	1:A:80:LEU:CD2	0.41	2.98	4	1
1:A:68:PRO:HD2	1:A:89:TYR:CE2	0.41	2.49	1	2
1:A:67:PHE:O	1:A:69:PRO:CD	0.41	2.68	19	1
1:A:30:LEU:HD11	1:A:173:ILE:HD12	0.41	1.92	18	1
1:A:83:LEU:O	1:A:87:VAL:HG23	0.41	2.16	9	1
1:A:77:LYS:O	1:A:81:VAL:HB	0.41	2.16	20	1
1:A:83:LEU:O	1:A:86:MET:HB2	0.41	2.15	16	1
1:A:24:ASN:HA	1:A:27:LYS:HB3	0.41	1.93	2	1
1:A:102:LYS:HE2	1:A:112:HIS:NE2	0.41	2.29	4	1
1:A:98:THR:O	1:A:102:LYS:HB2	0.41	2.14	6	1
1:A:67:PHE:CE1	1:A:172:VAL:HG11	0.41	2.51	6	1
1:A:160:LYS:N	1:A:160:LYS:HD2	0.41	2.30	1	1
1:A:160:LYS:HB3	1:A:163:CYS:CB	0.41	2.46	5	1
1:A:122:MET:SD	1:A:125:LEU:HD23	0.41	2.55	3	1
1:A:86:MET:O	1:A:89:TYR:CE2	0.41	2.74	15	1
1:A:40:LEU:HD11	1:A:115:LEU:CD2	0.41	2.46	13	1
1:A:83:LEU:O	1:A:87:VAL:HG12	0.41	2.16	4	1
1:A:84:TYR:CZ	1:A:130:LEU:HG	0.41	2.51	1	1
1:A:90:LEU:CD2	1:A:165:LEU:HB3	0.41	2.46	11	1
1:A:84:TYR:O	1:A:87:VAL:N	0.41	2.53	8	1
1:A:68:PRO:O	1:A:69:PRO:C	0.41	2.59	19	1
1:A:160:LYS:HG2	1:A:164:GLN:HB2	0.41	1.93	17	1
1:A:176:VAL:CG2	1:A:177:VAL:N	0.41	2.83	17	1
1:A:154:GLU:OE2	1:A:158:LYS:NZ	0.40	2.53	10	1
1:A:40:LEU:HD13	1:A:41:PHE:N	0.40	2.31	14	1
1:A:125:LEU:O	1:A:126:LEU:C	0.40	2.58	16	1
1:A:36:SER:C	1:A:38:ASN:N	0.40	2.74	17	1
1:A:99:ARG:HA	1:A:102:LYS:HB3	0.40	1.91	9	1
1:A:87:VAL:HG11	1:A:122:MET:SD	0.40	2.56	20	1
1:A:97:ILE:O	1:A:101:GLN:N	0.40	2.55	4	1
1:A:29:GLN:NE2	1:A:121:VAL:CG2	0.40	2.84	6	1
1:A:112:HIS:ND1	1:A:116:ASN:OD1	0.40	2.54	10	1
1:A:100:ASP:O	1:A:104:LEU:HB2	0.40	2.15	14	1
1:A:33:LEU:HD12	1:A:118:THR:HG22	0.40	1.93	5	1
1:A:60:CYS:O	1:A:164:GLN:CG	0.40	2.69	15	1
1:A:33:LEU:HD11	1:A:121:VAL:CG2	0.40	2.46	1	1
1:A:170:LYS:CB	1:A:170:LYS:NZ	0.40	2.85	11	1
1:A:90:LEU:CD1	1:A:169:TYR:CD1	0.40	3.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:TYR:O	1:A:111:LEU:HD12	0.40	2.16	8	1
1:A:84:TYR:O	1:A:85:ARG:C	0.40	2.59	8	1
1:A:52:PHE:CD1	1:A:160:LYS:NZ	0.40	2.88	5	1
1:A:81:VAL:O	1:A:82:GLU:C	0.40	2.60	10	1
1:A:166:LEU:O	1:A:167:GLY:C	0.40	2.60	16	1
1:A:125:LEU:O	1:A:128:ASN:HB2	0.40	2.17	18	1
1:A:110:SER:OG	1:A:111:LEU:N	0.40	2.55	3	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	126/180 (70%)	98±4 (78±3%)	23±4 (18±3%)	5±2 (4±2%)	6	33
All	All	2520/3600 (70%)	1957 (78%)	463 (18%)	100 (4%)	6	33

All 23 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	52	PHE	16
1	A	84	TYR	13
1	A	51	PRO	11
1	A	70	PHE	11
1	A	161	LEU	9
1	A	53	PRO	9
1	A	154	GLU	8
1	A	50	GLU	3
1	A	109	VAL	3
1	A	97	ILE	2
1	A	69	PRO	2
1	A	43	SER	2
1	A	67	PHE	1
1	A	24	ASN	1
1	A	158	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	166	LEU	1
1	A	157	GLN	1
1	A	68	PRO	1
1	A	98	THR	1
1	A	153	LYS	1
1	A	83	LEU	1
1	A	155	VAL	1
1	A	129	VAL	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/158 (71%)	92±3 (82±2%)	21±3 (18±2%)	5	38
All	All	2240/3160 (71%)	1830 (82%)	410 (18%)	5	38

All 80 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	112	HIS	20
1	A	40	LEU	20
1	A	38	ASN	20
1	A	67	PHE	19
1	A	45	TYR	19
1	A	44	TYR	17
1	A	118	THR	16
1	A	111	LEU	15
1	A	30	LEU	14
1	A	130	LEU	13
1	A	59	LEU	11
1	A	168	THR	10
1	A	52	PHE	9
1	A	48	GLN	8
1	A	132	ARG	8
1	A	160	LYS	7
1	A	101	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	89	TYR	7
1	A	42	ILE	7
1	A	170	LYS	7
1	A	163	CYS	7
1	A	125	LEU	6
1	A	32	GLN	6
1	A	164	GLN	5
1	A	157	GLN	5
1	A	161	LEU	5
1	A	114	LYS	5
1	A	86	MET	5
1	A	25	GLN	5
1	A	165	LEU	4
1	A	71	HIS	4
1	A	29	GLN	4
1	A	154	GLU	4
1	A	94	LEU	4
1	A	83	LEU	4
1	A	54	ASN	4
1	A	102	LYS	4
1	A	107	SER	3
1	A	56	LEU	3
1	A	174	SER	3
1	A	166	LEU	3
1	A	98	THR	3
1	A	153	LYS	3
1	A	58	LYS	3
1	A	122	MET	3
1	A	123	ARG	3
1	A	171	GLN	3
1	A	115	LEU	2
1	A	110	SER	2
1	A	105	ASN	2
1	A	104	LEU	2
1	A	24	ASN	2
1	A	60	CYS	2
1	A	96	ASN	2
1	A	50	GLU	2
1	A	121	VAL	2
1	A	100	ASP	2
1	A	27	LYS	2
1	A	90	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	131	CYS	1
1	A	93	SER	1
1	A	57	ASP	1
1	A	85	ARG	1
1	A	175	VAL	1
1	A	41	PHE	1
1	A	128	ASN	1
1	A	126	LEU	1
1	A	119	ILE	1
1	A	82	GLU	1
1	A	127	SER	1
1	A	180	PHE	1
1	A	120	ASP	1
1	A	77	LYS	1
1	A	169	TYR	1
1	A	156	PHE	1
1	A	36	SER	1
1	A	76	GLU	1
1	A	80	LEU	1
1	A	178	GLN	1
1	A	43	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided