



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:38 PM UTC

PDB ID : 1A7M / pdb_00001a7m
Title : LEUKAEMIA INHIBITORY FACTOR CHIMERA (MH35-LIF), NMR, 20
STRUCTURES
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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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

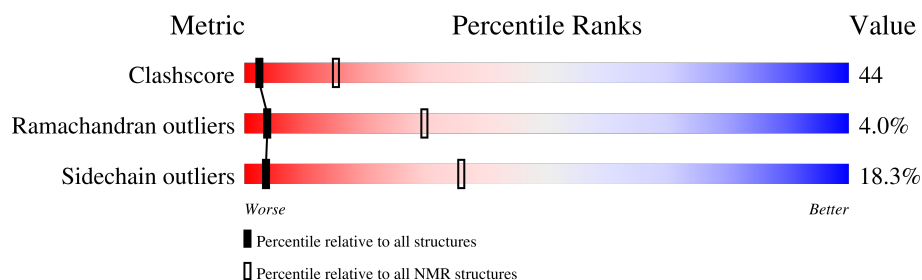
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

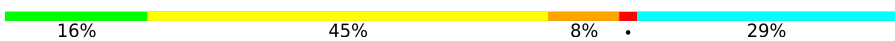
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	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)	0.62	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 4 clusters. No single-model clusters were found.

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

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:

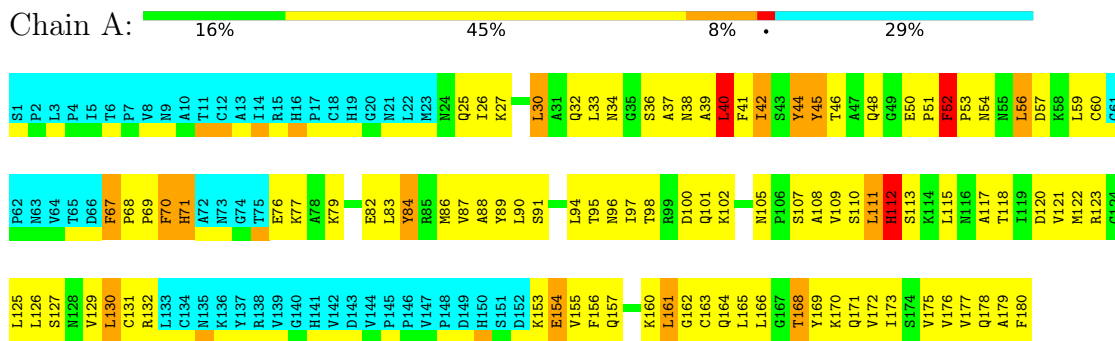
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	LEU	VAL	conflict	UNP P09056
A	57	ASP	GLU	conflict	UNP P09056
A	61	GLY	ALA	conflict	UNP P09056
A	64	VAL	MET	conflict	UNP P09056
A	69	PRO	SER	conflict	UNP P09056
A	72	ALA	GLY	conflict	UNP P09056
A	78	ALA	THR	conflict	UNP P09056
A	107	SER	THR	conflict	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, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: LEUKEMIA INHIBITORY FACTOR

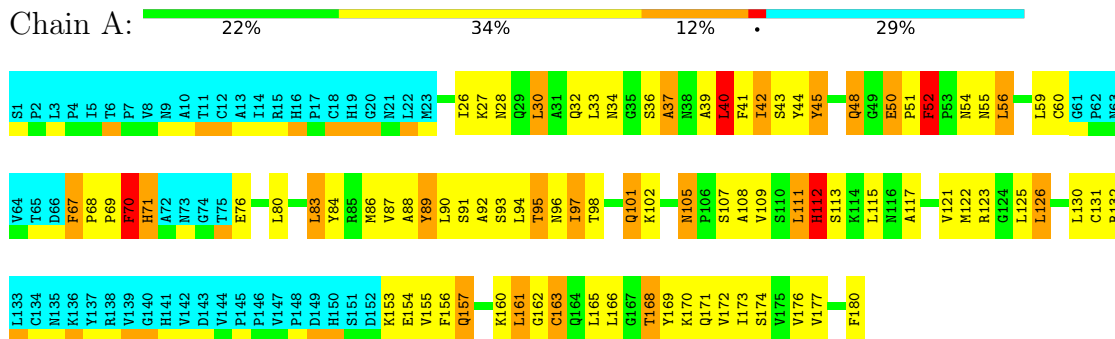


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



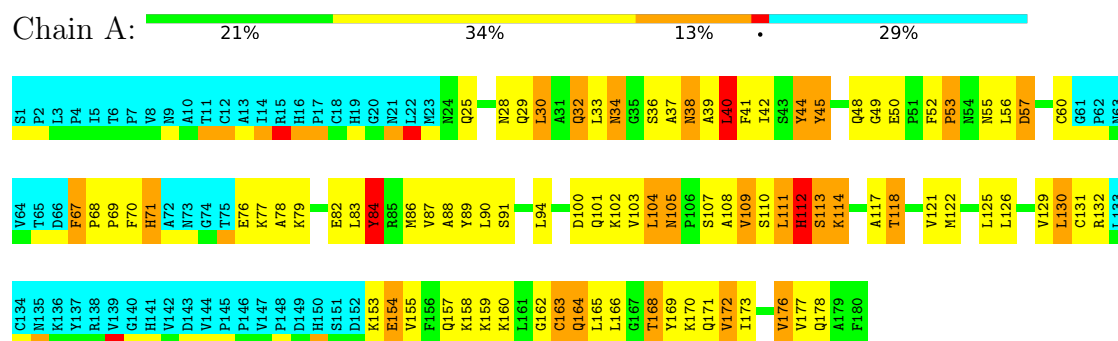
4.2.2 Score per residue for model 2

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



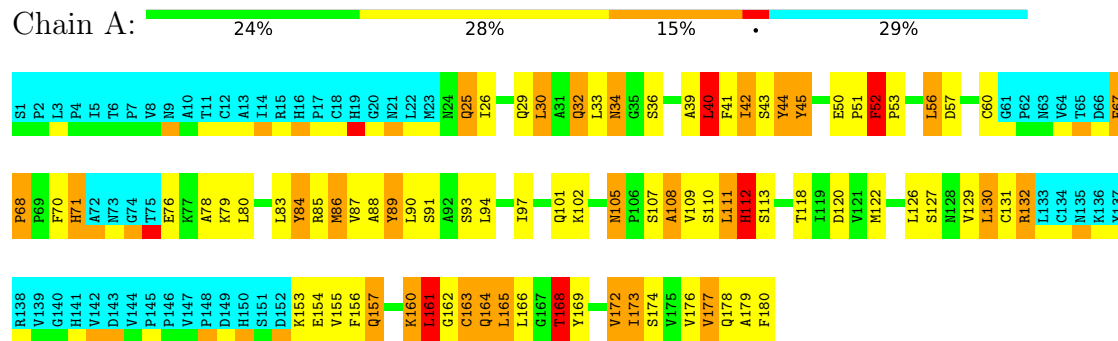
4.2.3 Score per residue for model 3

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.4 Score per residue for model 4

• Molecule 1: LEUKEMIA INHIBITORY FACTOR



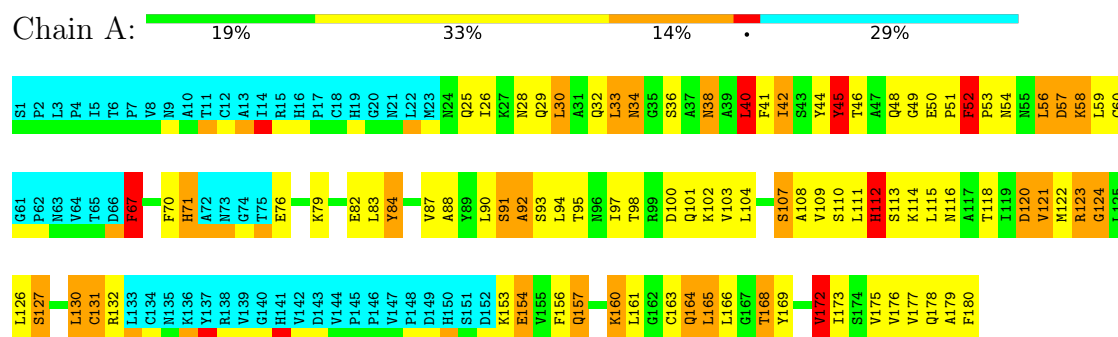
4.2.5 Score per residue for model 5

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



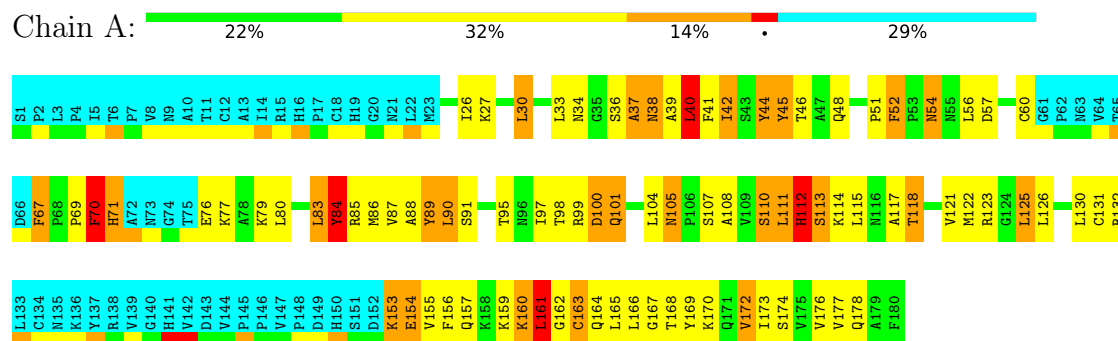
4.2.6 Score per residue for model 6

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



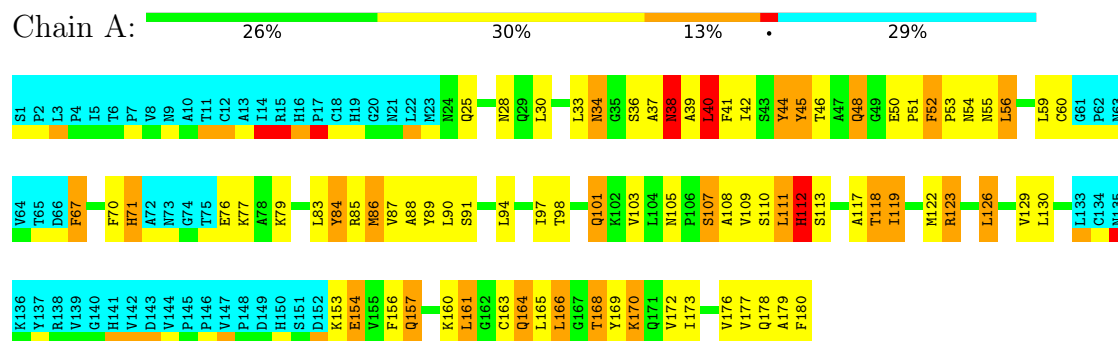
4.2.7 Score per residue for model 7

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



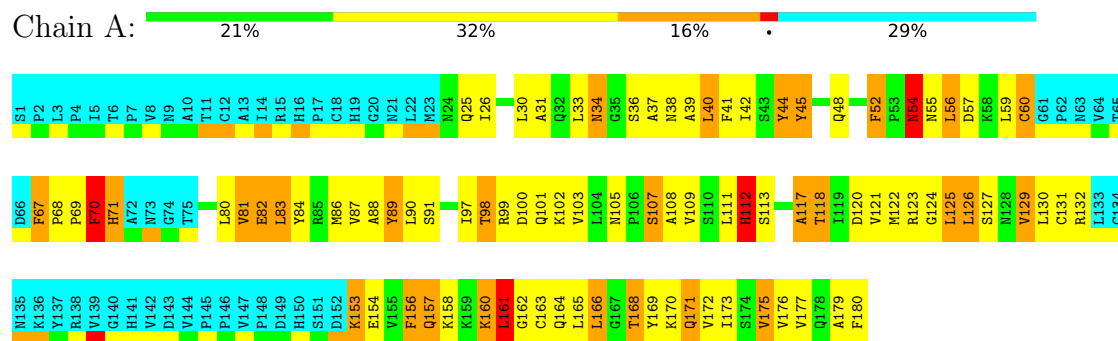
4.2.8 Score per residue for model 8

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



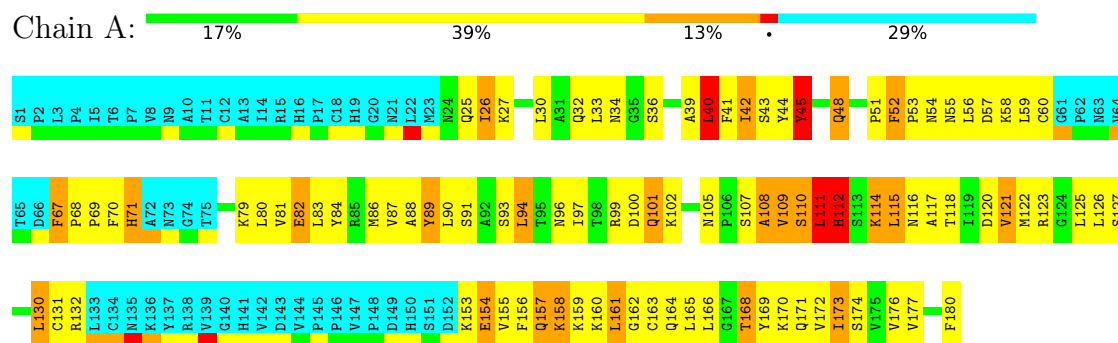
4.2.9 Score per residue for model 9

- Molecule 1: LEUKEMIA INHIBITORY FACTOR



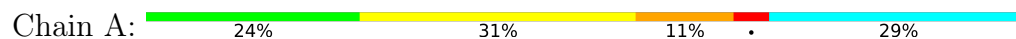
4.2.10 Score per residue for model 10

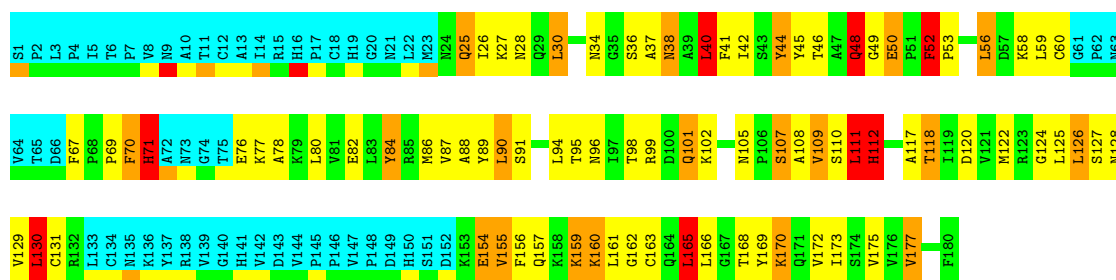
- Molecule 1: LEUKEMIA INHIBITORY FACTOR



4.2.11 Score per residue for model 11

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

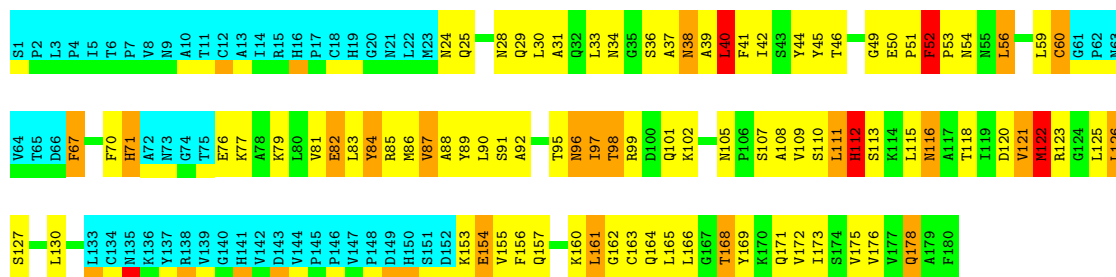




4.2.12 Score per residue for model 12

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

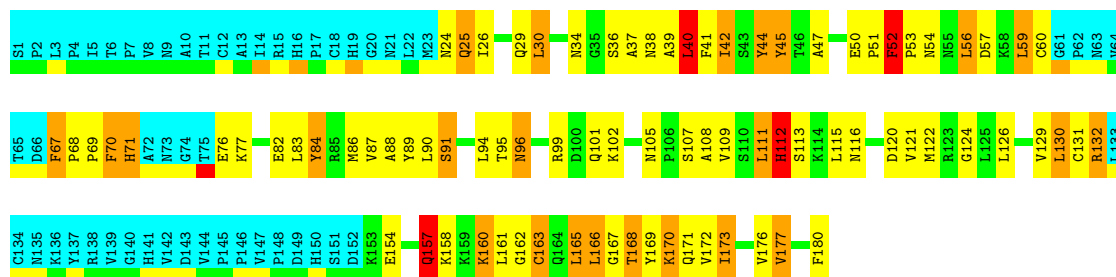
Chain A: 20% 38% 11% 29%



4.2.13 Score per residue for model 13

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

Chain A: 24% 31% 13% 29%

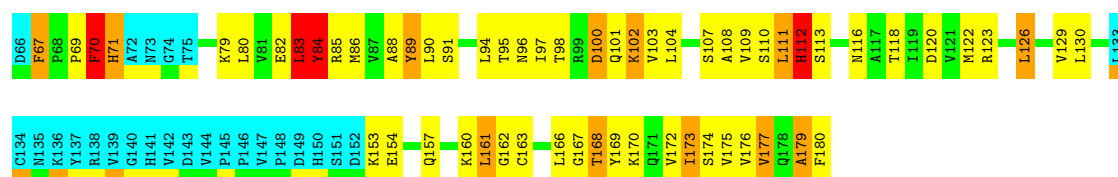


4.2.14 Score per residue for model 14

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

Chain A: 24% 32% 10% 29%

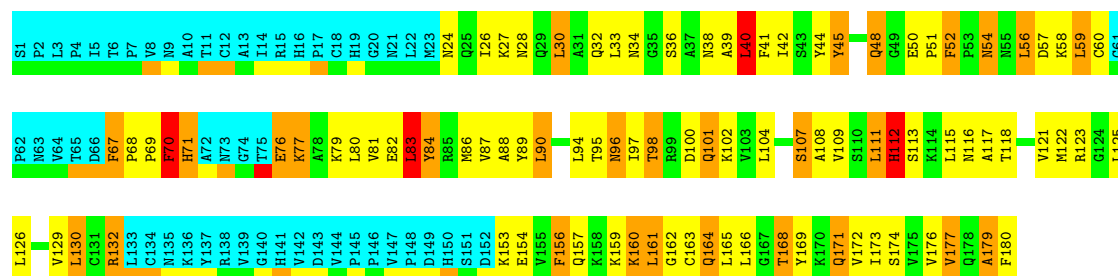




4.2.15 Score per residue for model 15

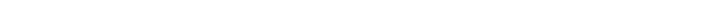
- Molecule 1: LEUKEMIA INHIBITORY FACTOR

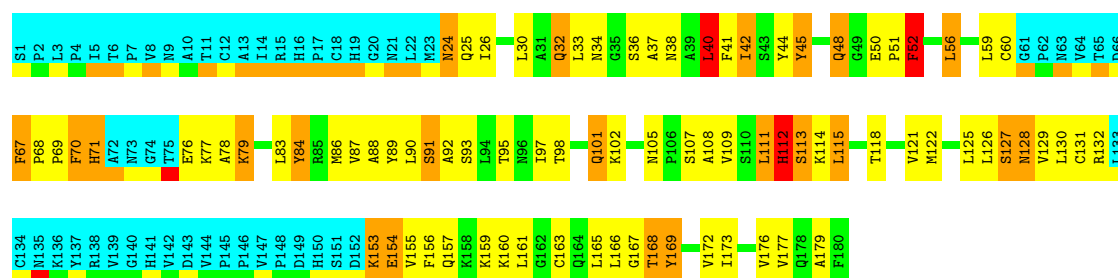
Chain A: 



4.2.16 Score per residue for model 16

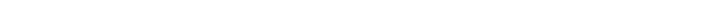
- Molecule 1: LEUKEMIA INHIBITORY FACTOR

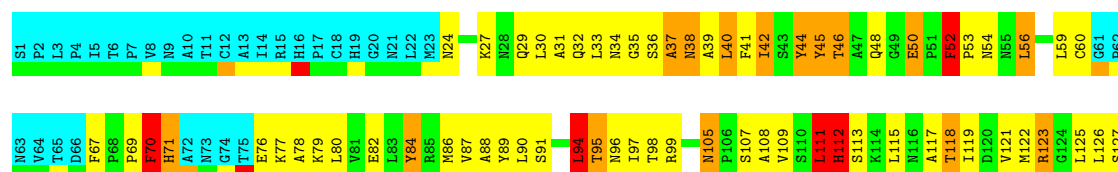
Chain A:  23% 33% 12% 1% 29%



4.2.17 Score per residue for model 17

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

Chain A: 

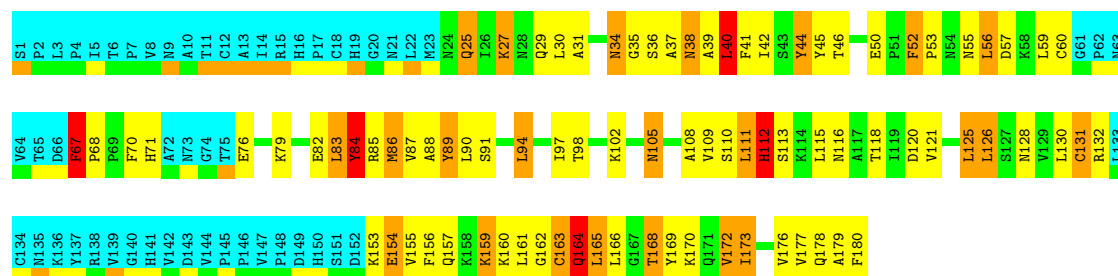




4.2.18 Score per residue for model 18

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

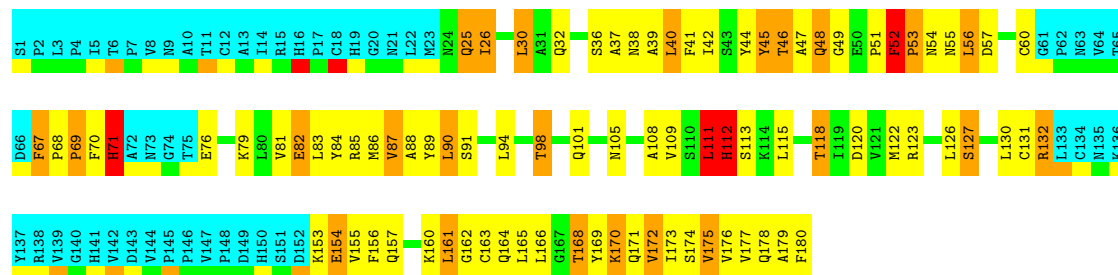
Chain A: 23% 32% 13% • 29%



4.2.19 Score per residue for model 19

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

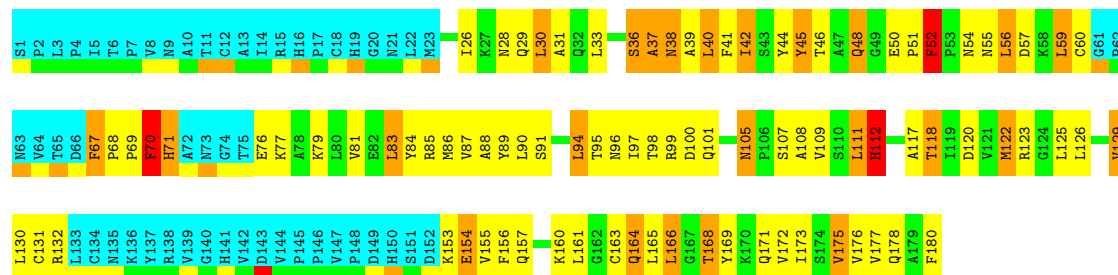
Chain A: 22% 33% 13% • 29%



4.2.20 Score per residue for model 20

- Molecule 1: LEUKEMIA INHIBITORY FACTOR

Chain A: 21% 35% 13% • 29%



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.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.81±0.02	6±1/1017 (0.6± 0.1%)	1.82±0.03	22±4/1373 (1.6± 0.3%)
All	All	1.81	118/20340 (0.6%)	1.82	430/27460 (1.6%)

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	0.1±0.3
All	All	0	2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	112	HIS	CG-ND1	-8.78	1.28	1.38	11	20
1	A	71	HIS	CG-ND1	-8.38	1.29	1.38	11	20
1	A	173	ILE	CA-CB	8.01	1.64	1.54	4	2
1	A	172	VAL	CA-CB	6.22	1.61	1.54	19	1
1	A	60	CYS	CA-CB	-6.07	1.44	1.53	9	1
1	A	45	TYR	CA-CB	5.93	1.62	1.53	6	2
1	A	42	ILE	CA-C	-5.71	1.46	1.52	13	2
1	A	168	THR	N-CA	5.69	1.53	1.46	2	2
1	A	52	PHE	N-CA	5.68	1.51	1.46	10	1
1	A	111	LEU	CA-CB	5.62	1.62	1.53	19	2
1	A	112	HIS	CD2-NE2	-5.57	1.31	1.37	11	19
1	A	68	PRO	CA-C	5.54	1.55	1.52	15	1
1	A	113	SER	N-CA	5.41	1.52	1.46	7	1
1	A	40	LEU	CA-CB	5.37	1.62	1.53	18	3
1	A	111	LEU	N-CA	5.37	1.52	1.46	10	3
1	A	97	ILE	CA-CB	5.34	1.60	1.54	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	105	ASN	N-CA	5.30	1.52	1.45	9	2
1	A	91	SER	N-CA	5.30	1.52	1.46	13	3
1	A	160	LYS	CA-CB	5.28	1.62	1.53	7	1
1	A	71	HIS	CD2-NE2	-5.24	1.32	1.37	15	18
1	A	34	ASN	N-CA	5.23	1.52	1.46	17	2
1	A	55	ASN	N-CA	5.22	1.51	1.46	8	1
1	A	164	GLN	N-CA	5.12	1.52	1.46	9	1
1	A	154	GLU	N-CA	5.12	1.52	1.46	17	2
1	A	123	ARG	N-CA	5.12	1.52	1.46	17	1
1	A	50	GLU	N-CA	5.12	1.49	1.46	18	1
1	A	24	ASN	N-CA	5.06	1.51	1.46	15	1
1	A	89	TYR	CA-CB	5.06	1.61	1.53	1	1
1	A	169	TYR	N-CA	5.04	1.52	1.46	16	1
1	A	42	ILE	CA-CB	5.02	1.59	1.54	1	1
1	A	99	ARG	CA-CB	5.00	1.61	1.53	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	49	GLY	N-CA-C	-13.62	99.01	111.95	6	6
1	A	37	ALA	N-CA-C	-10.18	100.01	111.71	1	4
1	A	25	GLN	N-CA-C	-9.82	96.53	111.56	14	14
1	A	70	PHE	CA-CB-CG	-9.66	104.14	113.80	9	7
1	A	164	GLN	N-CA-C	-9.55	100.87	111.28	6	6
1	A	76	GLU	N-CA-C	-9.54	100.58	110.97	20	5
1	A	107	SER	N-CA-C	-9.31	100.30	112.68	9	16
1	A	131	CYS	N-CA-C	-8.92	101.22	112.90	6	6
1	A	120	ASP	CA-CB-CG	-8.81	103.79	112.60	14	10
1	A	160	LYS	N-CA-C	8.76	122.74	112.93	13	1
1	A	52	PHE	CA-CB-CG	-8.25	105.55	113.80	9	9
1	A	67	PHE	N-CA-C	-8.17	99.76	110.39	18	2
1	A	56	LEU	N-CA-C	-8.15	102.40	111.28	17	16
1	A	40	LEU	N-CA-C	-8.08	101.17	111.02	10	14
1	A	71	HIS	CA-CB-CG	-8.01	105.79	113.80	9	7
1	A	67	PHE	CA-CB-CG	-7.97	105.83	113.80	9	3
1	A	87	VAL	N-CA-C	-7.70	103.73	110.74	19	2
1	A	82	GLU	N-CA-C	-7.58	103.01	111.28	3	4
1	A	168	THR	N-CA-C	-7.57	103.66	113.12	20	2
1	A	34	ASN	CA-CB-CG	-7.56	105.04	112.60	2	6
1	A	108	ALA	N-CA-C	-7.53	103.07	111.28	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	177	VAL	N-CA-C	-7.46	101.60	112.04	11	18
1	A	179	ALA	N-CA-C	-7.42	104.20	113.55	18	5
1	A	83	LEU	N-CA-C	-7.36	103.19	111.07	2	5
1	A	96	ASN	CA-CB-CG	-7.35	105.25	112.60	12	3
1	A	34	ASN	N-CA-C	-7.30	103.01	110.97	18	6
1	A	168	THR	CA-CB-OG1	-7.29	98.67	109.60	20	3
1	A	105	ASN	N-CA-C	7.27	122.20	109.48	5	9
1	A	94	LEU	N-CA-C	-7.26	103.29	111.14	10	4
1	A	175	VAL	N-CA-C	-7.16	106.10	112.12	19	4
1	A	121	VAL	N-CA-C	-7.15	102.11	111.05	16	4
1	A	95	THR	CA-CB-OG1	-7.05	99.03	109.60	16	7
1	A	123	ARG	N-CA-C	-6.86	103.83	111.71	6	4
1	A	27	LYS	N-CA-C	-6.70	103.91	111.14	14	3
1	A	127	SER	N-CA-C	-6.68	103.92	111.07	12	2
1	A	100	ASP	CA-CB-CG	-6.67	105.92	112.60	5	2
1	A	124	GLY	N-CA-C	-6.62	104.47	112.49	13	3
1	A	165	LEU	N-CA-C	-6.60	103.57	111.69	11	3
1	A	89	TYR	N-CA-C	-6.53	104.08	111.07	18	5
1	A	42	ILE	O-C-N	6.53	128.92	121.94	5	4
1	A	57	ASP	CA-CB-CG	-6.52	106.08	112.60	7	3
1	A	60	CYS	N-CA-CB	-6.36	102.74	111.65	12	1
1	A	171	GLN	OE1-CD-NE2	-6.34	116.26	122.60	9	3
1	A	24	ASN	OD1-CG-ND2	-6.33	116.27	122.60	15	4
1	A	105	ASN	OD1-CG-ND2	-6.32	116.28	122.60	2	5
1	A	159	LYS	N-CA-CB	-6.25	101.35	110.47	11	1
1	A	154	GLU	N-CA-C	6.23	121.09	111.56	18	2
1	A	172	VAL	N-CA-C	-6.22	104.68	110.53	6	4
1	A	103	VAL	N-CA-CB	-6.20	105.39	112.21	3	1
1	A	172	VAL	N-CA-CB	-6.19	101.60	110.52	4	4
1	A	110	SER	N-CA-C	-6.16	104.49	111.14	7	4
1	A	98	THR	CA-CB-OG1	-6.16	100.37	109.60	12	1
1	A	99	ARG	O-C-N	6.12	128.37	122.07	12	1
1	A	25	GLN	OE1-CD-NE2	-6.06	116.54	122.60	18	4
1	A	112	HIS	CE1-NE2-CD2	-6.04	102.97	109.00	9	20
1	A	127	SER	CA-CB-OG	-6.01	99.08	111.10	11	5
1	A	38	ASN	OD1-CG-ND2	-5.98	116.62	122.60	11	13
1	A	173	ILE	N-CA-C	-5.96	104.54	110.62	13	4
1	A	32	GLN	OE1-CD-NE2	-5.96	116.64	122.60	4	5
1	A	79	LYS	N-CA-C	-5.95	104.71	111.07	16	1
1	A	28	ASN	OD1-CG-ND2	-5.92	116.68	122.60	6	5
1	A	129	VAL	N-CA-C	-5.90	104.87	110.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	ASN	OD1-CG-ND2	-5.88	116.72	122.60	12	4
1	A	84	TYR	CA-CB-CG	-5.88	103.33	113.90	14	5
1	A	85	ARG	NE-CZ-NH1	-5.87	115.63	121.50	5	1
1	A	54	ASN	OD1-CG-ND2	-5.85	116.75	122.60	15	4
1	A	28	ASN	CA-CB-CG	-5.82	106.78	112.60	12	3
1	A	97	ILE	N-CA-C	-5.76	104.71	110.30	2	1
1	A	118	THR	OG1-CB-CG2	-5.76	97.78	109.30	5	1
1	A	29	GLN	OE1-CD-NE2	-5.72	116.88	122.60	17	2
1	A	164	GLN	OE1-CD-NE2	-5.71	116.89	122.60	2	4
1	A	50	GLU	N-CA-C	-5.71	101.82	110.50	3	2
1	A	157	GLN	OE1-CD-NE2	-5.70	116.90	122.60	1	4
1	A	164	GLN	CA-CB-CG	-5.70	102.70	114.10	18	1
1	A	154	GLU	N-CA-CB	-5.68	100.89	110.49	12	1
1	A	153	LYS	CA-C-O	-5.68	115.20	121.33	9	1
1	A	122	MET	N-CA-C	-5.67	105.02	111.14	20	2
1	A	178	GLN	N-CA-C	-5.66	105.69	112.59	4	2
1	A	55	ASN	OD1-CG-ND2	-5.61	116.99	122.60	20	1
1	A	81	VAL	CB-CA-C	-5.58	104.61	112.14	9	1
1	A	101	GLN	OE1-CD-NE2	-5.56	117.04	122.60	15	5
1	A	48	GLN	OE1-CD-NE2	-5.54	117.06	122.60	11	3
1	A	84	TYR	N-CA-CB	-5.51	101.17	110.49	6	1
1	A	60	CYS	N-CA-C	5.51	119.16	111.56	9	1
1	A	178	GLN	OE1-CD-NE2	-5.50	117.10	122.60	6	5
1	A	79	LYS	CA-C-O	5.48	126.77	120.90	3	1
1	A	40	LEU	CA-C-O	-5.46	115.06	121.07	1	1
1	A	165	LEU	CA-C-O	-5.46	115.27	121.00	8	1
1	A	24	ASN	CA-CB-CG	-5.46	107.14	112.60	17	1
1	A	176	VAL	N-CA-C	-5.43	105.08	111.00	17	1
1	A	121	VAL	N-CA-CB	-5.40	103.72	110.47	18	1
1	A	105	ASN	CA-C-N	5.39	125.00	119.56	9	1
1	A	105	ASN	C-N-CA	5.39	125.00	119.56	9	1
1	A	33	LEU	N-CA-C	-5.34	106.89	113.41	14	2
1	A	112	HIS	CA-C-O	-5.33	115.21	120.70	3	3
1	A	26	ILE	CA-CB-CG1	5.27	119.36	110.40	10	1
1	A	171	GLN	CG-CD-NE2	5.26	124.30	116.40	9	1
1	A	113	SER	CA-CB-OG	-5.25	100.59	111.10	3	3
1	A	117	ALA	N-CA-C	-5.25	105.25	110.97	9	1
1	A	96	ASN	O-C-N	5.22	127.52	122.09	12	1
1	A	96	ASN	OD1-CG-ND2	-5.21	117.39	122.60	11	2
1	A	116	ASN	CA-C-N	-5.21	113.78	120.65	14	1
1	A	116	ASN	C-N-CA	-5.21	113.78	120.65	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	ASN	N-CA-C	-5.19	105.63	111.28	15	1
1	A	168	THR	OG1-CB-CG2	-5.16	98.97	109.30	10	1
1	A	54	ASN	CA-CB-CG	-5.12	107.47	112.60	7	1
1	A	125	LEU	N-CA-C	-5.11	104.78	111.02	7	1
1	A	156	PHE	CA-CB-CG	-5.10	108.70	113.80	15	1
1	A	132	ARG	N-CA-C	-5.09	105.42	111.69	4	1
1	A	79	LYS	N-CA-CB	-5.09	102.64	110.12	7	1
1	A	71	HIS	CE1-NE2-CD2	-5.09	103.91	109.00	15	2
1	A	159	LYS	CA-C-O	5.07	125.68	119.64	18	1
1	A	165	LEU	CA-C-N	-5.07	113.70	120.54	6	1
1	A	165	LEU	C-N-CA	-5.07	113.70	120.54	6	1
1	A	164	GLN	CG-CD-NE2	5.06	123.98	116.40	4	1
1	A	130	LEU	N-CA-C	-5.05	105.05	111.11	11	1
1	A	107	SER	CA-CB-OG	-5.05	101.01	111.10	13	1
1	A	46	THR	N-CA-C	-5.05	105.69	111.14	19	1
1	A	119	ILE	N-CA-CB	-5.04	104.65	110.55	17	1
1	A	98	THR	OG1-CB-CG2	-5.04	99.21	109.30	19	1
1	A	114	LYS	N-CA-C	-5.04	105.79	111.28	3	1
1	A	35	GLY	N-CA-C	-5.03	106.69	112.83	17	1
1	A	92	ALA	N-CA-C	-5.03	105.49	110.97	6	1
1	A	44	TYR	CA-CB-CG	-5.01	104.88	113.90	7	1
1	A	88	ALA	N-CA-CB	-5.01	102.81	110.07	11	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 ⓘ

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	89±10
All	All	20000	20760	20760	1780

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 44.

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	8
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:44:TYR:CD1	1:A:44:TYR:C	0.64	2.75	3	6
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	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:76:GLU:H	1:A:76:GLU:CD	0.60	2.05	2	2
1:A:52:PHE:CE2	1:A:160:LYS:HG2	0.59	2.32	5	3
1:A:111:LEU:C	1:A:111:LEU:HD23	0.59	2.22	18	5
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:52:PHE:CZ	1:A:163:CYS:SG	0.58	2.97	20	5
1:A:157:GLN:HE21	1:A:157:GLN:N	0.58	1.96	6	1
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:45:TYR:C	1:A:45:TYR:CD1	0.57	2.82	11	7
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:111:LEU:C	1:A:111:LEU:HD12	0.57	2.25	3	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:50:GLU:HA	1:A:52:PHE:N	0.56	2.15	1	8
1:A:42:ILE:N	1:A:42:ILE:HD12	0.56	2.13	13	8
1:A:67:PHE:CZ	1:A:172:VAL:CG1	0.56	2.89	2	9
1:A:120:ASP:CG	1:A:123:ARG:NH2	0.56	2.64	5	1
1:A:153:LYS:HB2	1:A:156:PHE:HB2	0.56	1.78	6	2
1:A:45:TYR:HB2	1:A:163:CYS:SG	0.56	2.40	3	7
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	15
1:A:41:PHE:CE1	1:A:163:CYS:SG	0.56	2.98	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:88:ALA:HB2	1:A:126:LEU:HD21	0.55	1.78	6	10
1:A:70:PHE:CE2	1:A:82:GLU:HB2	0.55	2.36	6	2
1:A:40:LEU:HD12	1:A:166:LEU:HD11	0.55	1.79	12	8
1:A:83:LEU:HD22	1:A:180:PHE:CE2	0.55	2.37	8	6
1:A:86:MET:C	1:A:86:MET:SD	0.55	2.89	5	4
1:A:111:LEU:HD23	1:A:111:LEU:C	0.55	2.26	13	5
1:A:48:GLN:NE2	1:A:48:GLN:N	0.55	2.55	8	5
1:A:42:ILE:HA	1:A:45:TYR:CE2	0.55	2.37	20	6
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:68:PRO:CG	1:A:86:MET:SD	0.55	2.95	4	1
1:A:109:VAL:O	1:A:112:HIS:CD2	0.55	2.60	18	7
1:A:153:LYS:HB3	1:A:156:PHE:CD1	0.55	2.36	10	7
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:67:PHE:CD1	1:A:86:MET:HE2	0.55	2.37	10	1
1:A:168:THR:O	1:A:169:TYR:C	0.54	2.49	13	14
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:33:LEU:HD22	1:A:122:MET:HE3	0.54	1.78	1	2
1:A:52:PHE:HE1	1:A:163:CYS:SG	0.54	2.26	5	2
1:A:105:ASN:HB3	1:A:108:ALA:HB2	0.54	1.79	1	3
1:A:84:TYR:HA	1:A:126:LEU:CD2	0.54	2.32	18	4
1:A:154:GLU:H	1:A:154:GLU:CD	0.54	2.11	8	2
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:160:LYS:O	1:A:161:LEU:C	0.54	2.50	16	14
1:A:50:GLU:CD	1:A:50:GLU:H	0.54	2.11	5	2
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ALA:O	1:A:40:LEU:C	0.53	2.51	13	15
1:A:84:TYR:C	1:A:84:TYR:CD1	0.53	2.86	9	7
1:A:27:LYS:NZ	1:A:177:VAL:O	0.53	2.41	11	1
1:A:157:GLN:O	1:A:161:LEU:N	0.53	2.42	20	6
1:A:44:TYR:OH	1:A:163:CYS:N	0.53	2.41	18	10
1:A:57:ASP:CG	1:A:58:LYS:NZ	0.53	2.66	15	2
1:A:69:PRO:O	1:A:70:PHE:C	0.53	2.52	14	11
1:A:87:VAL:O	1:A:88:ALA:C	0.53	2.51	10	5
1:A:160:LYS:CG	1:A:163:CYS:SG	0.53	2.96	18	1
1:A:154:GLU:O	1:A:155:VAL:C	0.53	2.51	19	12
1:A:30:LEU:CD1	1:A:173:ILE:HG13	0.53	2.34	4	3
1:A:90:LEU:O	1:A:91:SER:C	0.53	2.51	4	14
1:A:101:GLN:CG	1:A:108:ALA:HB1	0.53	2.34	8	1
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:41:PHE:C	1:A:41:PHE:CD1	0.52	2.87	19	6
1:A:68:PRO:HG2	1:A:86:MET:SD	0.52	2.43	4	1
1:A:84:TYR:CE2	1:A:130:LEU:CD2	0.52	2.92	7	1
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:42:ILE:C	1:A:44:TYR:N	0.52	2.68	4	8
1:A:97:ILE:HA	1:A:101:GLN:OE1	0.52	2.05	4	1
1:A:48:GLN:N	1:A:48:GLN:CD	0.52	2.68	1	2
1:A:169:TYR:CD1	1:A:173:ILE:HG13	0.52	2.40	2	1
1:A:41:PHE:HE1	1:A:163:CYS:SG	0.52	2.28	5	7
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: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:84:TYR:CD2	1:A:130:LEU:HD23	0.51	2.40	1	3
1:A:112:HIS:ND1	1:A:113:SER:N	0.51	2.58	15	10
1:A:163:CYS:C	1:A:165:LEU:N	0.51	2.67	19	7
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:115:LEU:O	1:A:116:ASN:C	0.51	2.51	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:HIS:O	1:A:113:SER:C	0.51	2.53	12	15
1:A:160:LYS:C	1:A:162:GLY:N	0.51	2.68	2	9
1:A:166:LEU:HD13	1:A:169:TYR:CD2	0.51	2.40	14	4
1:A:86:MET:O	1:A:86:MET:HE2	0.51	2.05	8	1
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:NE	1:A:132:ARG:HA	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:56:LEU:HD12	1:A:56:LEU:C	0.50	2.31	11	15
1:A:118:THR:O	1:A:122:MET:CB	0.50	2.59	20	1
1:A:108:ALA:O	1:A:109:VAL:C	0.50	2.53	1	17
1:A:168:THR:O	1:A:171:GLN:N	0.50	2.43	13	5
1:A:33:LEU:N	1:A:33:LEU:HD22	0.50	2.21	5	1
1:A:155:VAL:O	1:A:159:LYS:NZ	0.50	2.45	18	1
1:A:56:LEU:O	1:A:60:CYS:N	0.50	2.44	5	13
1:A:83:LEU:O	1:A:84:TYR:C	0.50	2.54	1	4
1:A:89:TYR:CD1	1:A:89:TYR:C	0.50	2.89	2	8
1:A:89:TYR:C	1:A:89:TYR:CD1	0.50	2.89	9	1
1:A:172:VAL:O	1:A:175:VAL:HG12	0.50	2.07	17	2
1:A:33:LEU:N	1:A:33:LEU:CD2	0.50	2.75	5	1
1:A:129:VAL:O	1:A:130:LEU:C	0.50	2.52	13	1
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:109:VAL:HA	1:A:112:HIS:CD2	0.50	2.42	3	1
1:A:87:VAL:HG12	1:A:126:LEU:CD1	0.50	2.37	9	3
1:A:40:LEU:O	1:A:41:PHE:C	0.50	2.55	1	16
1:A:51:PRO:O	1:A:160:LYS:NZ	0.50	2.43	5	2
1:A:156:PHE:O	1:A:160:LYS:N	0.50	2.43	15	4
1:A:70:PHE:CD2	1:A:176:VAL:HG12	0.50	2.42	6	4
1:A:154:GLU:CD	1:A:155:VAL:N	0.50	2.70	12	1
1:A:26:ILE:HG13	1:A:180:PHE:CD1	0.49	2.42	6	5
1:A:42:ILE:N	1:A:42:ILE:CD1	0.49	2.75	5	1
1:A:162:GLY:O	1:A:166:LEU:N	0.49	2.45	12	5
1:A:165:LEU:O	1:A:166:LEU:C	0.49	2.54	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:99:ARG:CG	1:A:100:ASP:N	0.49	2.75	7	1
1:A:33:LEU:O	1:A:34:ASN:C	0.49	2.54	8	10
1:A:84:TYR:O	1:A:88:ALA:N	0.49	2.45	4	5
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:169:TYR:HA	1:A:172:VAL:CG2	0.49	2.38	14	3
1:A:122:MET:O	1:A:123:ARG:C	0.49	2.56	12	8
1:A:108:ALA:O	1:A:111:LEU:HG	0.49	2.08	6	3
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:99:ARG:O	1:A:100:ASP:C	0.49	2.55	10	2
1:A:105:ASN:OD1	1:A:159:LYS:NZ	0.49	2.46	3	1
1:A:36:SER:O	1:A:37:ALA:C	0.49	2.54	19	9
1:A:87:VAL:HG12	1:A:126:LEU:HD11	0.49	1.83	9	3
1:A:52:PHE:CZ	1:A:160:LYS:HB3	0.49	2.42	10	1
1:A:83:LEU:CD1	1:A:125:LEU:HD21	0.49	2.38	1	1
1:A:45:TYR:CB	1:A:163:CYS:SG	0.49	3.01	10	5
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:45:TYR:CE2	1:A:56:LEU:CD2	0.49	2.94	16	1
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:111:LEU:HG	1:A:112:HIS:N	0.48	2.22	19	2
1:A:95:THR:O	1:A:96:ASN:C	0.48	2.55	5	6
1:A:120:ASP:CG	1:A:123:ARG:HH21	0.48	2.16	5	1
1:A:108:ALA:O	1:A:111:LEU:N	0.48	2.46	9	6
1:A:84:TYR:CE1	1:A:126:LEU:HD13	0.48	2.43	12	1
1:A:69:PRO:O	1:A:85:ARG:NH2	0.48	2.46	19	1
1:A:97:ILE:O	1:A:98:THR:C	0.48	2.56	16	11
1:A:153:LYS:O	1:A:157:GLN:HB2	0.48	2.08	17	7
1:A:50:GLU:HA	1:A:52:PHE:H	0.48	1.69	12	5
1:A:87:VAL:CG1	1:A:122:MET:CG	0.48	2.91	20	1
1:A:33:LEU:O	1:A:37:ALA:N	0.48	2.47	20	3
1:A:40:LEU:HD22	1:A:44:TYR:CB	0.48	2.39	5	9
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:117:ALA:O	1:A:118:THR:C	0.48	2.57	10	6
1:A:112:HIS:ND1	1:A:112:HIS:C	0.48	2.71	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ASN:HB2	1:A:59:LEU:CD1	0.48	2.37	9	2
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:84:TYR:CE1	1:A:126:LEU:CB	0.48	2.97	3	1
1:A:96:ASN:OD1	1:A:99:ARG:NH1	0.48	2.47	17	1
1:A:56:LEU:HB2	1:A:60:CYS:SG	0.48	2.49	5	2
1:A:118:THR:HB	1:A:122:MET:HE3	0.48	1.85	9	1
1:A:166:LEU:HD13	1:A:169:TYR:CD1	0.48	2.43	20	3
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:86:MET:O	1:A:89:TYR:CE1	0.47	2.67	8	6
1:A:57:ASP:C	1:A:58:LYS:HE2	0.47	2.33	15	1
1:A:40:LEU:HD11	1:A:115:LEU:CD1	0.47	2.39	1	1
1:A:34:ASN:HA	1:A:173:ILE:CG2	0.47	2.40	13	3
1:A:41:PHE:CG	1:A:166:LEU:HB3	0.47	2.44	1	8
1:A:156:PHE:O	1:A:157:GLN:C	0.47	2.56	10	7
1:A:163:CYS:O	1:A:164:GLN:C	0.47	2.57	20	5
1:A:67:PHE:HB2	1:A:89:TYR:CZ	0.47	2.44	7	2
1:A:83:LEU:HD13	1:A:83:LEU:C	0.47	2.35	14	1
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:55:ASN:C	1:A:57:ASP:N	0.47	2.71	9	3
1:A:90:LEU:C	1:A:90:LEU:HD13	0.47	2.35	2	3
1:A:90:LEU:HG	1:A:94:LEU:CD1	0.47	2.40	6	1
1:A:172:VAL:HG23	1:A:173:ILE:N	0.47	2.25	9	5
1:A:52:PHE:CD2	1:A:160:LYS:HG2	0.47	2.44	13	1
1:A:94:LEU:CB	1:A:115:LEU:HD21	0.47	2.40	15	1
1:A:154:GLU:C	1:A:156:PHE:N	0.47	2.69	1	7
1:A:42:ILE:O	1:A:44:TYR:N	0.47	2.48	4	1
1:A:110:SER:O	1:A:111:LEU:C	0.47	2.58	6	6
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:33:LEU:CD2	1:A:122:MET:HE3	0.47	2.40	1	1
1:A:84:TYR:CE1	1:A:130:LEU:CD2	0.47	2.98	3	1
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:70:PHE:HA	1:A:82:GLU:CD	0.47	2.34	11	3
1:A:48:GLN:HE22	1:A:111:LEU:CD1	0.47	2.22	8	1
1:A:102:LYS:HG3	1:A:112:HIS:CD2	0.47	2.45	13	1
1:A:59:LEU:CD1	1:A:59:LEU:N	0.47	2.77	15	1
1:A:40:LEU:C	1:A:40:LEU:HD22	0.47	2.35	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:CD2	1:A:173:ILE:HG23	0.47	2.40	9	1
1:A:67:PHE:CD2	1:A:168:THR:CG2	0.47	2.98	17	2
1:A:154:GLU:O	1:A:157:GLN:N	0.46	2.48	9	9
1:A:76:GLU:CD	1:A:76:GLU:N	0.46	2.74	3	1
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:57:ASP:CG	1:A:58:LYS:N	0.46	2.73	10	1
1:A:165:LEU:O	1:A:169:TYR:N	0.46	2.47	1	2
1:A:70:PHE:CE2	1:A:82:GLU:HB3	0.46	2.46	5	2
1:A:52:PHE:CZ	1:A:160:LYS:HB2	0.46	2.45	11	2
1:A:41:PHE:CZ	1:A:56:LEU:HD13	0.46	2.46	18	3
1:A:52:PHE:CE2	1:A:59:LEU:HB3	0.46	2.46	13	1
1:A:50:GLU:O	1:A:159:LYS:NZ	0.46	2.48	16	1
1:A:160:LYS:O	1:A:162:GLY:N	0.46	2.48	14	6
1:A:173:ILE:C	1:A:175:VAL:H	0.46	2.18	19	4
1:A:56:LEU:HA	1:A:60:CYS:SG	0.46	2.50	7	2
1:A:71:HIS:O	1:A:71:HIS:ND1	0.46	2.48	6	1
1:A:33:LEU:CD2	1:A:121:VAL:HG21	0.46	2.40	15	2
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:41:PHE:CE2	1:A:56:LEU:HD13	0.46	2.46	18	2
1:A:87:VAL:HG13	1:A:122:MET:HE3	0.46	1.86	11	1
1:A:59:LEU:C	1:A:60:CYS:SG	0.46	2.98	12	1
1:A:27:LYS:NZ	1:A:180:PHE:OXT	0.46	2.47	17	1
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:96:ASN:CG	1:A:97:ILE:N	0.46	2.73	20	1
1:A:160:LYS:O	1:A:163:CYS:N	0.46	2.49	5	8
1:A:87:VAL:CB	1:A:126:LEU:HD11	0.46	2.41	10	5
1:A:87:VAL:CG2	1:A:122:MET:SD	0.46	3.04	6	1
1:A:90:LEU:C	1:A:90:LEU:HD23	0.46	2.35	13	1
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:44:TYR:CD2	1:A:111:LEU:HD11	0.46	2.45	18	2
1:A:67:PHE:CD2	1:A:89:TYR:OH	0.46	2.69	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ILE:HD12	1:A:97:ILE:N	0.46	2.25	16	1
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:86:MET:HA	1:A:89:TYR:CD2	0.45	2.46	13	3
1:A:48:GLN:O	1:A:159:LYS:NZ	0.45	2.49	3	1
1:A:84:TYR:CE1	1:A:126:LEU:HB3	0.45	2.47	3	1
1:A:30:LEU:O	1:A:31:ALA:C	0.45	2.58	18	6
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:67:PHE:CG	1:A:89:TYR:OH	0.45	2.70	20	3
1:A:59:LEU:HB3	1:A:160:LYS:CD	0.45	2.41	5	1
1:A:84:TYR:CD2	1:A:126:LEU:HD22	0.45	2.46	14	1
1:A:170:LYS:NZ	1:A:174:SER:OG	0.45	2.49	19	1
1:A:84:TYR:CD1	1:A:126:LEU:HG	0.45	2.47	3	1
1:A:176:VAL:C	1:A:178:GLN:N	0.45	2.73	5	4
1:A:111:LEU:C	1:A:111:LEU:CD2	0.45	2.90	18	2
1:A:67:PHE:CD1	1:A:168:THR:HB	0.45	2.46	15	1
1:A:112:HIS:O	1:A:115:LEU:N	0.45	2.49	19	3
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: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:43:SER:CB	1:A:114:LYS:NZ	0.45	2.80	10	1
1:A:69:PRO:O	1:A:71:HIS:N	0.45	2.49	17	2
1:A:60:CYS:SG	1:A:163:CYS:O	0.45	2.75	20	1
1:A:102:LYS:HB2	1:A:112:HIS:CD2	0.45	2.46	15	5
1:A:87:VAL:O	1:A:91:SER:N	0.45	2.49	8	5
1:A:45:TYR:CE2	1:A:53:PRO:HA	0.45	2.47	3	1
1:A:173:ILE:HA	1:A:176:VAL:CG2	0.45	2.41	18	2
1:A:118:THR:O	1:A:122:MET:CG	0.45	2.65	7	1
1:A:84:TYR:O	1:A:85:ARG:C	0.45	2.59	8	3
1:A:166:LEU:O	1:A:167:GLY:C	0.45	2.60	16	2
1:A:87:VAL:HG13	1:A:122:MET:CG	0.45	2.42	20	2
1:A:86:MET:O	1:A:90:LEU:HB2	0.45	2.11	18	1
1:A:52:PHE:C	1:A:54:ASN:H	0.45	2.20	15	7
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:81:VAL:O	1:A:82:GLU:C	0.45	2.60	10	1
1:A:27:LYS:HZ3	1:A:180:PHE:C	0.45	2.20	1	1
1:A:30:LEU:CD1	1:A:173:ILE:HG23	0.45	2.42	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:O	1:A:126:LEU:C	0.45	2.58	16	2
1:A:111:LEU:HD12	1:A:112:HIS:N	0.45	2.27	11	2
1:A:68:PRO:O	1:A:69:PRO:C	0.45	2.59	19	1
1:A:33:LEU:HD13	1:A:122:MET:HE2	0.45	1.88	15	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:101:GLN:HG3	1:A:108:ALA:HB1	0.44	1.88	8	1
1:A:111:LEU:CG	1:A:112:HIS:N	0.44	2.79	10	3
1:A:60:CYS:SG	1:A:163:CYS:C	0.44	3.01	19	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:107:SER:O	1:A:108:ALA:C	0.44	2.60	15	4
1:A:45:TYR:CD1	1:A:45:TYR:C	0.44	2.95	17	3
1:A:101:GLN:C	1:A:103:VAL:N	0.44	2.75	8	5
1:A:157:GLN:HE21	1:A:157:GLN:CA	0.44	2.25	6	1
1:A:60:CYS:HA	1:A:164:GLN:HA	0.44	1.88	12	2
1:A:131:CYS:O	1:A:132:ARG:C	0.44	2.61	10	1
1:A:68:PRO:O	1:A:70:PHE:N	0.44	2.50	13	2
1:A:67:PHE:CE2	1:A:168:THR:HB	0.44	2.47	16	1
1:A:44:TYR:HE1	1:A:163:CYS:CB	0.44	2.25	18	1
1:A:70:PHE:C	1:A:70:PHE:CD1	0.44	2.95	18	1
1:A:86:MET:O	1:A:90:LEU:CB	0.44	2.66	7	2
1:A:101:GLN:HG2	1:A:111:LEU:HD21	0.44	1.89	6	1
1:A:30:LEU:HD13	1:A:30:LEU:O	0.44	2.13	14	1
1:A:44:TYR:CD1	1:A:111:LEU:HD11	0.44	2.48	16	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:67:PHE:CE2	1:A:172:VAL:HG11	0.44	2.47	19	1
1:A:126:LEU:O	1:A:127:SER:C	0.44	2.61	4	4
1:A:34:ASN:O	1:A:37:ALA:HB3	0.44	2.12	18	2
1:A:76:GLU:HG3	1:A:77:LYS:N	0.44	2.28	15	1
1:A:68:PRO:O	1:A:85:ARG:NH2	0.44	2.51	19	1
1:A:52:PHE:C	1:A:54:ASN:N	0.44	2.76	10	4
1:A:30:LEU:HD12	1:A:177:VAL:CB	0.44	2.43	13	1
1:A:125:LEU:C	1:A:125:LEU:HD23	0.44	2.38	15	1
1:A:26:ILE:HD11	1:A:80:LEU:CD2	0.44	2.42	1	2
1:A:57:ASP:OD1	1:A:58:LYS:NZ	0.44	2.49	6	1
1:A:99:ARG:HG2	1:A:100:ASP:N	0.44	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LYS:NZ	1:A:156:PHE:CZ	0.44	2.86	7	1
1:A:125:LEU:O	1:A:128:ASN:N	0.44	2.50	16	1
1:A:174:SER:C	1:A:177:VAL:HG12	0.43	2.37	4	2
1:A:160:LYS:N	1:A:160:LYS:CD	0.43	2.80	13	1
1:A:48:GLN:CG	1:A:52:PHE:CD2	0.43	3.00	17	1
1:A:172:VAL:O	1:A:175:VAL:HB	0.43	2.13	2	1
1:A:153:LYS:O	1:A:157:GLN:HB3	0.43	2.13	8	1
1:A:156:PHE:O	1:A:159:LYS:N	0.43	2.51	10	1
1:A:158:LYS:HB2	1:A:158:LYS:NZ	0.43	2.27	10	1
1:A:48:GLN:CG	1:A:159:LYS:HB3	0.43	2.43	15	1
1:A:163:CYS:O	1:A:166:LEU:N	0.43	2.51	19	1
1:A:76:GLU:O	1:A:77:LYS:C	0.43	2.60	5	2
1:A:41:PHE:HB2	1:A:166:LEU:HD12	0.43	1.89	12	2
1:A:153:LYS:HB2	1:A:157:GLN:NE2	0.43	2.29	6	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:38:ASN:HD22	1:A:38:ASN:C	0.43	2.21	20	1
1:A:87:VAL:HG11	1:A:126:LEU:HD11	0.43	1.90	2	1
1:A:87:VAL:O	1:A:91:SER:CB	0.43	2.67	3	2
1:A:93:SER:OG	1:A:94:LEU:N	0.43	2.52	4	1
1:A:170:LYS:HD2	1:A:170:LYS:C	0.43	2.38	7	1
1:A:55:ASN:O	1:A:59:LEU:HG	0.43	2.13	1	1
1:A:45:TYR:O	1:A:46:THR:C	0.43	2.62	11	1
1:A:70:PHE:CD1	1:A:176:VAL:HG12	0.43	2.49	17	1
1:A:90:LEU:C	1:A:90:LEU:CD1	0.43	2.91	19	1
1:A:100:ASP:O	1:A:104:LEU:N	0.43	2.52	3	3
1:A:97:ILE:HD11	1:A:162:GLY:HA3	0.43	1.90	4	1
1:A:84:TYR:CZ	1:A:130:LEU:HD23	0.43	2.49	10	1
1:A:83:LEU:HG	1:A:180:PHE:CZ	0.43	2.48	18	2
1:A:47:ALA:HB3	1:A:111:LEU:CD2	0.43	2.44	19	1
1:A:33:LEU:O	1:A:36:SER:N	0.43	2.51	7	3
1:A:67:PHE:CD1	1:A:67:PHE:C	0.43	2.95	4	3
1:A:113:SER:OG	1:A:114:LYS:N	0.43	2.51	7	1
1:A:70:PHE:HA	1:A:82:GLU:HG2	0.43	1.91	9	1
1:A:70:PHE:CD2	1:A:82:GLU:HB2	0.43	2.49	10	2
1:A:97:ILE:HG23	1:A:101:GLN:CG	0.43	2.44	10	1
1:A:48:GLN:CD	1:A:101:GLN:HG3	0.43	2.39	1	1
1:A:129:VAL:O	1:A:132:ARG:HG2	0.43	2.14	3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:PRO:O	1:A:55:ASN:N	0.43	2.52	10	1
1:A:96:ASN:CG	1:A:97:ILE:H	0.43	2.21	20	1
1:A:33:LEU:HD12	1:A:33:LEU:N	0.43	2.27	1	1
1:A:45:TYR:CZ	1:A:56:LEU:CD2	0.43	3.02	20	2
1:A:87:VAL:CG1	1:A:122:MET:SD	0.43	3.07	20	1
1:A:48:GLN:HE22	1:A:101:GLN:NE2	0.42	2.12	9	1
1:A:160:LYS:HD3	1:A:160:LYS:C	0.42	2.39	9	1
1:A:157:GLN:NE2	1:A:158:LYS:N	0.42	2.67	13	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:42:ILE:C	1:A:44:TYR:H	0.42	2.23	13	2
1:A:92:ALA:O	1:A:93:SER:C	0.42	2.62	16	2
1:A:127:SER:O	1:A:131:CYS:N	0.42	2.52	6	1
1:A:86:MET:HE1	1:A:173:ILE:CD1	0.42	2.44	12	1
1:A:96:ASN:O	1:A:99:ARG:HG2	0.42	2.14	13	1
1:A:167:GLY:O	1:A:170:LYS:NZ	0.42	2.51	13	1
1:A:25:GLN:HE21	1:A:25:GLN:C	0.42	2.23	14	1
1:A:33:LEU:HD11	1:A:121:VAL:HG21	0.42	1.89	17	1
1:A:83:LEU:CG	1:A:84:TYR:N	0.42	2.83	2	1
1:A:26:ILE:CD1	1:A:80:LEU:HD22	0.42	2.45	4	1
1:A:44:TYR:CD2	1:A:44:TYR:C	0.42	2.95	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:33:LEU:HD22	1:A:33:LEU:N	0.42	2.29	14	1
1:A:85:ARG:CG	1:A:86:MET:N	0.42	2.83	19	1
1:A:59:LEU:HB2	1:A:160:LYS:HE2	0.42	1.91	20	1
1:A:45:TYR:CD1	1:A:46:THR:N	0.42	2.87	6	2
1:A:36:SER:C	1:A:38:ASN:N	0.42	2.74	17	3
1:A:60:CYS:O	1:A:167:GLY:HA3	0.42	2.13	7	1
1:A:67:PHE:CE1	1:A:86:MET:HE2	0.42	2.50	10	1
1:A:91:SER:O	1:A:92:ALA:C	0.42	2.62	12	1
1:A:87:VAL:O	1:A:91:SER:HB2	0.42	2.15	13	1
1:A:97:ILE:HG22	1:A:161:LEU:HB3	0.42	1.90	17	1
1:A:29:GLN:O	1:A:30:LEU:C	0.42	2.62	6	3
1:A:70:PHE:CD2	1:A:176:VAL:CG1	0.42	3.01	6	1
1:A:88:ALA:HB2	1:A:126:LEU:CD1	0.42	2.44	14	2
1:A:124:GLY:O	1:A:125:LEU:C	0.42	2.62	9	1
1:A:52:PHE:HB3	1:A:53:PRO:CD	0.42	2.45	12	1
1:A:169:TYR:CE1	1:A:173:ILE:HD13	0.42	2.49	14	1
1:A:55:ASN:O	1:A:56:LEU:C	0.42	2.59	1	2
1:A:132:ARG:NE	1:A:132:ARG:CA	0.42	2.82	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:GLY:O	1:A:168:THR:C	0.42	2.63	2	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:86:MET:HE1	1:A:173:ILE:HD11	0.42	1.90	9	1
1:A:100:ASP:OD1	1:A:158:LYS:NZ	0.42	2.52	9	1
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:56:LEU:CG	1:A:57:ASP:N	0.42	2.82	5	1
1:A:162:GLY:O	1:A:165:LEU:HB2	0.42	2.14	7	2
1:A:170:LYS:C	1:A:170:LYS:CD	0.42	2.93	7	1
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:34:ASN:O	1:A:35:GLY:C	0.42	2.62	18	1
1:A:118:THR:O	1:A:122:MET:HG3	0.42	2.14	19	1
1:A:120:ASP:O	1:A:123:ARG:HG3	0.42	2.15	6	1
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:115:LEU:HA	1:A:118:THR:OG1	0.42	2.15	10	1
1:A:155:VAL:CG2	1:A:156:PHE:N	0.42	2.83	11	1
1:A:26:ILE:HD12	1:A:180:PHE:CD1	0.42	2.49	14	2
1:A:48:GLN:CD	1:A:101:GLN:CG	0.42	2.93	1	1
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:52:PHE:HE1	1:A:60:CYS:SG	0.42	2.36	12	1
1:A:27:LYS:NZ	1:A:180:PHE:C	0.42	2.78	2	1
1:A:84:TYR:CZ	1:A:126:LEU:HB3	0.42	2.50	12	1
1:A:153:LYS:O	1:A:157:GLN:CG	0.42	2.68	18	1
1:A:50:GLU:HA	1:A:51:PRO:C	0.42	2.40	20	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: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:41:PHE:CD1	1:A:41:PHE:C	0.41	2.95	18	1
1:A:94:LEU:HG	1:A:115:LEU:HD11	0.41	1.92	19	1
1:A:94:LEU:O	1:A:97:ILE:HB	0.41	2.15	4	1
1:A:102:LYS:O	1:A:102:LYS:HD3	0.41	2.14	10	1
1:A:30:LEU:CD1	1:A:30:LEU:C	0.41	2.93	13	1
1:A:125:LEU:HD12	1:A:125:LEU:C	0.41	2.40	18	1
1:A:84:TYR:CE2	1:A:126:LEU:HD23	0.41	2.50	3	1
1:A:97:ILE:HD11	1:A:162:GLY:CA	0.41	2.46	12	1
1:A:56:LEU:HG	1:A:57:ASP:N	0.41	2.31	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:GLN:HB3	1:A:159:LYS:HB3	0.41	1.92	7	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: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:122:MET:SD	1:A:122:MET:C	0.41	3.04	12	1
1:A:83:LEU:HD13	1:A:84:TYR:N	0.41	2.30	14	1
1:A:83:LEU:HD12	1:A:83:LEU:C	0.41	2.40	2	1
1:A:26:ILE:CD1	1:A:80:LEU:CD2	0.41	2.98	4	1
1:A:33:LEU:HD11	1:A:121:VAL:HG11	0.41	1.91	12	1
1:A:101:GLN:NE2	1:A:101:GLN:HA	0.41	2.31	13	2
1:A:67:PHE:HE1	1:A:86:MET:SD	0.41	2.38	17	1
1:A:68:PRO:HD2	1:A:89:TYR:CE2	0.41	2.49	1	2
1:A:25:GLN:O	1:A:26:ILE:C	0.41	2.63	4	1
1:A:108:ALA:C	1:A:110:SER:N	0.41	2.79	6	1
1:A:83:LEU:O	1:A:87:VAL:HG23	0.41	2.16	9	1
1:A:80:LEU:O	1:A:81:VAL:C	0.41	2.63	15	1
1:A:30:LEU:HD11	1:A:173:ILE:HD12	0.41	1.92	18	1
1:A:67:PHE:O	1:A:69:PRO:CD	0.41	2.68	19	1
1:A:77:LYS:O	1:A:81:VAL:HB	0.41	2.16	20	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:83:LEU:O	1:A:86:MET:HB2	0.41	2.15	16	1
1:A:47:ALA:O	1:A:48:GLN:C	0.41	2.64	19	1
1:A:154:GLU:CD	1:A:155:VAL:H	0.41	2.23	20	1
1:A:83:LEU:CD2	1:A:86:MET:HE2	0.41	2.46	1	1
1:A:160:LYS:N	1:A:160:LYS:HD2	0.41	2.30	1	1
1:A:111:LEU:C	1:A:111:LEU:CD1	0.41	2.93	3	1
1:A:122:MET:SD	1:A:125:LEU:HD23	0.41	2.55	3	1
1:A:83:LEU:O	1:A:87:VAL:HG12	0.41	2.16	4	1
1:A:160:LYS:HB3	1:A:163:CYS:CB	0.41	2.46	5	1
1:A:67:PHE:CE1	1:A:172:VAL:HG11	0.41	2.51	6	1
1:A:98:THR:O	1:A:102:LYS:HB2	0.41	2.14	6	1
1:A:83:LEU:C	1:A:83:LEU:HD13	0.41	2.41	7	1
1:A:40:LEU:HD11	1:A:115:LEU:CD2	0.41	2.46	13	1
1:A:86:MET:O	1:A:89:TYR:CE2	0.41	2.74	15	1
1:A:94:LEU:O	1:A:95:THR:C	0.41	2.64	17	1
1:A:84:TYR:CZ	1:A:130:LEU:HG	0.41	2.51	1	1
1:A:84:TYR:O	1:A:87:VAL:N	0.41	2.53	8	1
1:A:90:LEU:CD2	1:A:165:LEU:HB3	0.41	2.46	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:56:LEU:C	1:A:56:LEU:HD12	0.40	2.41	13	1
1:A:97:ILE:O	1:A:101:GLN:N	0.40	2.55	4	1
1:A:99:ARG:HA	1:A:102:LYS:HB3	0.40	1.91	9	1
1:A:40:LEU:HD13	1:A:41:PHE:N	0.40	2.31	14	1
1:A:87:VAL:HG11	1:A:122:MET:SD	0.40	2.56	20	1
1:A:125:LEU:HD23	1:A:125:LEU:C	0.40	2.40	1	1
1:A:33:LEU:HD12	1:A:118:THR:HG22	0.40	1.93	5	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:60:CYS:O	1:A:164:GLN:CG	0.40	2.69	15	1
1:A:83:LEU:C	1:A:83:LEU:HD22	0.40	2.41	20	1
1:A:33:LEU:HD11	1:A:121:VAL:CG2	0.40	2.46	1	1
1:A:52:PHE:CD1	1:A:160:LYS:NZ	0.40	2.88	5	1
1:A:44:TYR:O	1:A:111:LEU:HD12	0.40	2.16	8	1
1:A:90:LEU:CD1	1:A:169:TYR:CD1	0.40	3.05	8	1
1:A:170:LYS:NZ	1:A:170:LYS:CB	0.40	2.85	11	1
1:A:57:ASP:CG	1:A:58:LYS:CE	0.40	2.95	15	1
1:A:172:VAL:O	1:A:173:ILE:C	0.40	2.65	17	1
1:A:27:LYS:C	1:A:27:LYS:CD	0.40	2.94	18	1
1:A:110:SER:OG	1:A:111:LEU:N	0.40	2.55	3	1
1:A:56:LEU:O	1:A:57:ASP:C	0.40	2.64	15	1
1:A:125:LEU:O	1:A:128:ASN:HB2	0.40	2.17	18	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	126/180 (70%)	98±4 (78±3%)	23±4 (18±3%)	5±2 (4±2%)	4	30
All	All	2520/3600 (70%)	1957 (78%)	463 (18%)	100 (4%)	4	30

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	70	PHE	11
1	A	51	PRO	11
1	A	53	PRO	9
1	A	161	LEU	9
1	A	154	GLU	8
1	A	50	GLU	3
1	A	109	VAL	3
1	A	43	SER	2
1	A	97	ILE	2
1	A	69	PRO	2
1	A	158	LYS	1
1	A	68	PRO	1
1	A	157	GLN	1
1	A	153	LYS	1
1	A	83	LEU	1
1	A	67	PHE	1
1	A	155	VAL	1
1	A	166	LEU	1
1	A	98	THR	1
1	A	24	ASN	1
1	A	129	VAL	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	112/158 (71%)	91±2 (82±2%)	21±2 (18±2%)	3	36
All	All	2240/3160 (71%)	1829 (82%)	411 (18%)	3	36

All 84 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	40	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	112	HIS	20
1	A	45	TYR	17
1	A	111	LEU	17
1	A	118	THR	16
1	A	30	LEU	14
1	A	67	PHE	13
1	A	130	LEU	13
1	A	168	THR	12
1	A	59	LEU	11
1	A	94	LEU	10
1	A	170	LYS	9
1	A	44	TYR	9
1	A	52	PHE	8
1	A	101	GLN	8
1	A	161	LEU	8
1	A	125	LEU	8
1	A	48	GLN	8
1	A	38	ASN	8
1	A	32	GLN	7
1	A	126	LEU	7
1	A	163	CYS	7
1	A	42	ILE	7
1	A	132	ARG	7
1	A	83	LEU	6
1	A	165	LEU	6
1	A	160	LYS	6
1	A	90	LEU	5
1	A	98	THR	5
1	A	154	GLU	5
1	A	174	SER	4
1	A	86	MET	4
1	A	105	ASN	4
1	A	164	GLN	4
1	A	114	LYS	4
1	A	29	GLN	4
1	A	153	LYS	4
1	A	157	GLN	4
1	A	115	LEU	4
1	A	25	GLN	4
1	A	50	GLU	3
1	A	71	HIS	3
1	A	27	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	56	LEU	3
1	A	107	SER	3
1	A	129	VAL	3
1	A	166	LEU	3
1	A	171	GLN	3
1	A	175	VAL	3
1	A	123	ARG	2
1	A	77	LYS	2
1	A	104	LEU	2
1	A	110	SER	2
1	A	76	GLU	2
1	A	96	ASN	2
1	A	102	LYS	2
1	A	122	MET	2
1	A	156	PHE	2
1	A	58	LYS	2
1	A	121	VAL	2
1	A	26	ILE	2
1	A	97	ILE	1
1	A	43	SER	1
1	A	93	SER	1
1	A	176	VAL	1
1	A	120	ASP	1
1	A	57	ASP	1
1	A	172	VAL	1
1	A	119	ILE	1
1	A	54	ASN	1
1	A	82	GLU	1
1	A	80	LEU	1
1	A	89	TYR	1
1	A	158	LYS	1
1	A	95	THR	1
1	A	24	ASN	1
1	A	100	ASP	1
1	A	173	ILE	1
1	A	128	ASN	1
1	A	46	THR	1
1	A	131	CYS	1
1	A	127	SER	1
1	A	178	GLN	1
1	A	36	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided