Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 06:55 PM EDT

PDB ID	:	1BW4
Title	:	THREE-DIMENSIONAL STRUCTURE IN SOLUTION OF BARWIN, A PROTEIN FROM BARLEY SEED
Authors	:	Poulsen, F.M.
Deposited on	:	1992-07-06

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 (i) 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 (i)) were used in the production of this report:

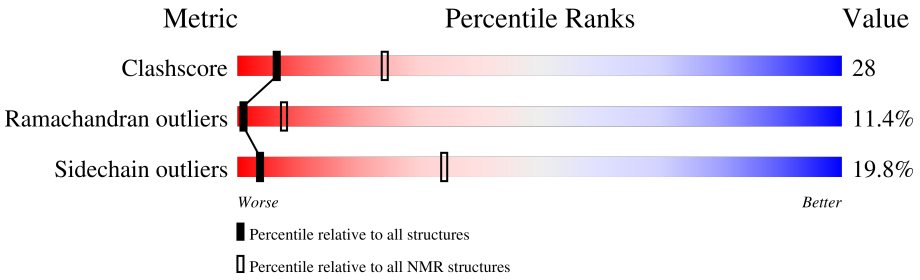
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	125	53% 30% 12% 5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:1-A:125 (125)	1.46	18

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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1863 atoms, of which 895 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BARWIN, BASIC BARLEY SEED PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	125	1863	603	895	175	184	6	0

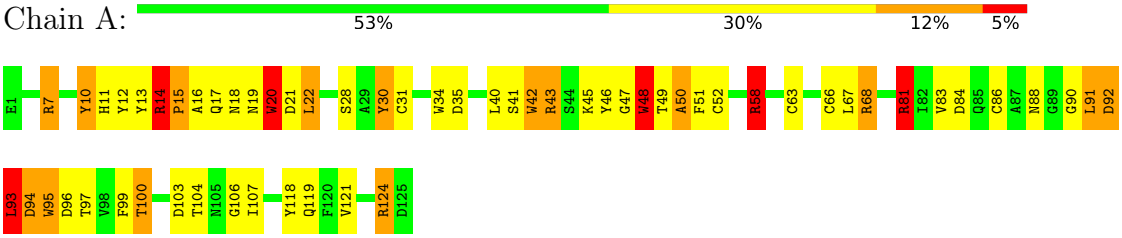
4 Residue-property plots

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: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A:



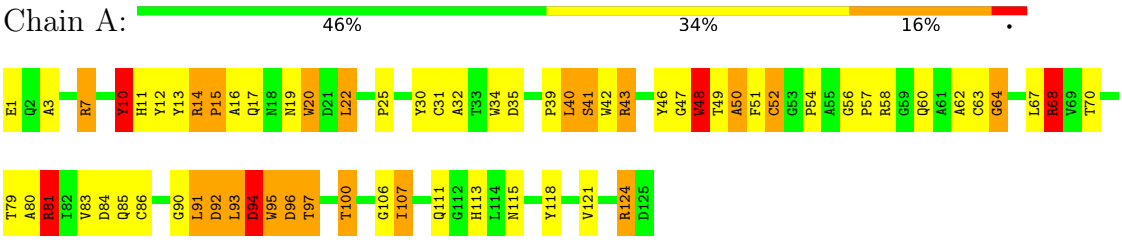
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

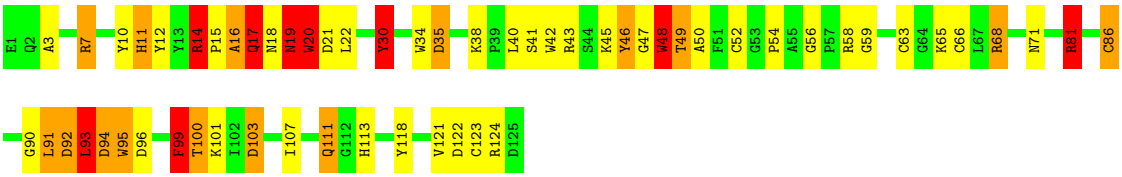
Chain A:



4.2.2 Score per residue for model 2

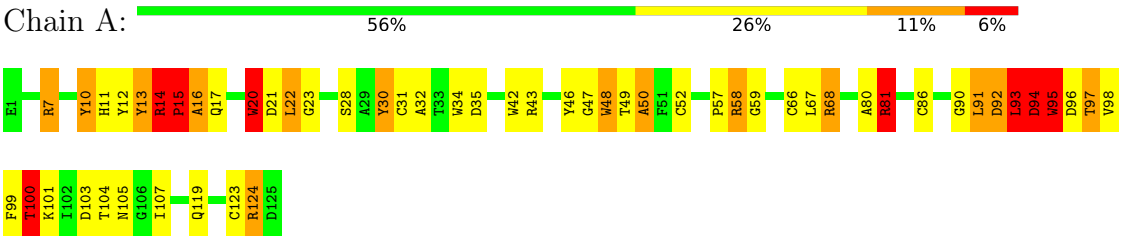
• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A:



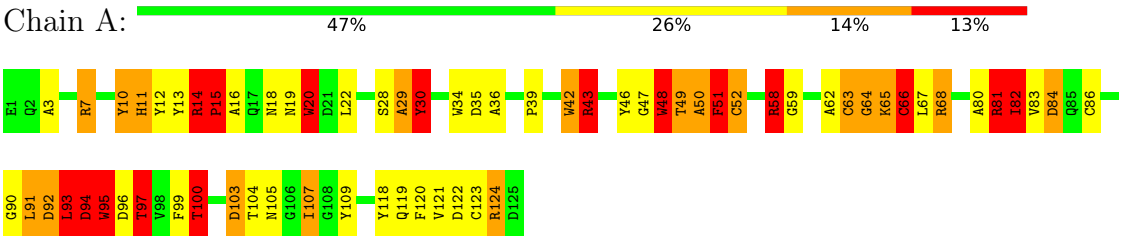
4.2.3 Score per residue for model 3

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



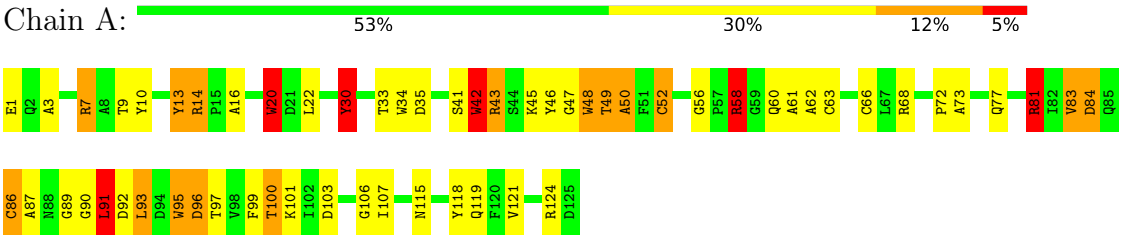
4.2.4 Score per residue for model 4

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



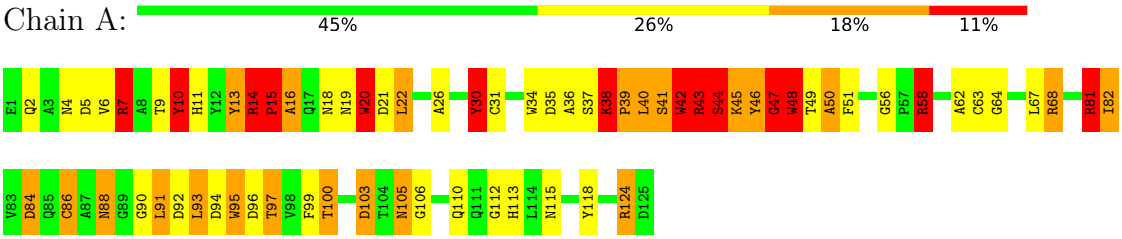
4.2.5 Score per residue for model 5

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



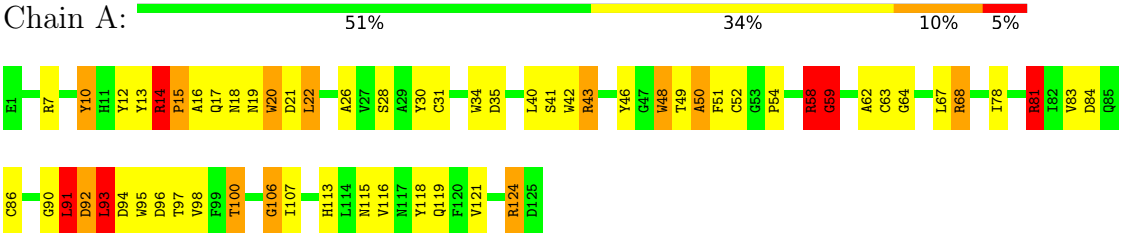
4.2.6 Score per residue for model 6

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



4.2.7 Score per residue for model 7

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

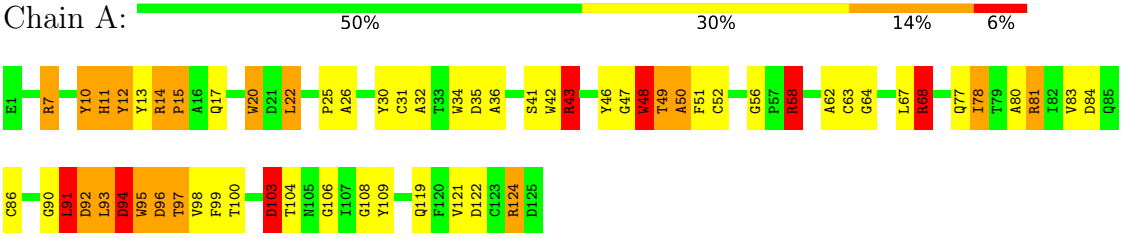


4.2.8 Score per residue for model 8

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

4.2.9 Score per residue for model 9

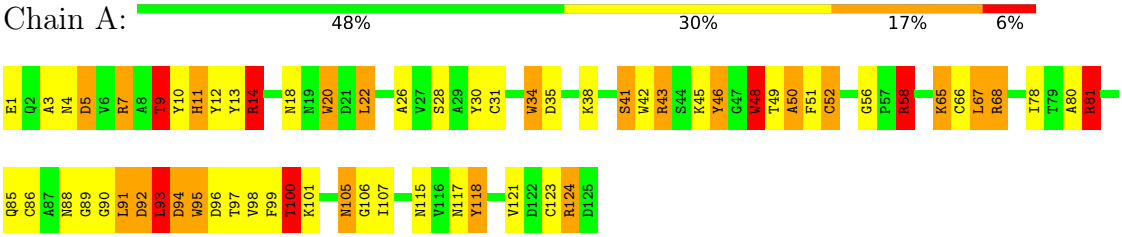
• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



4.2.10 Score per residue for model 10

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

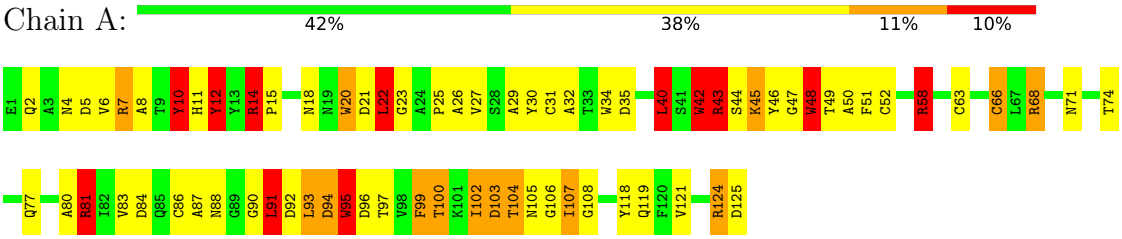
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

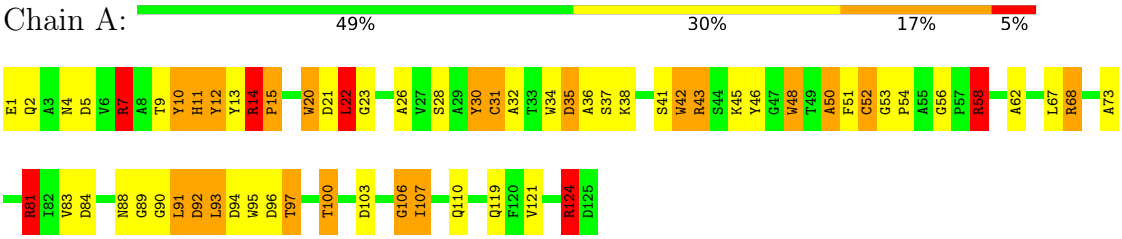
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

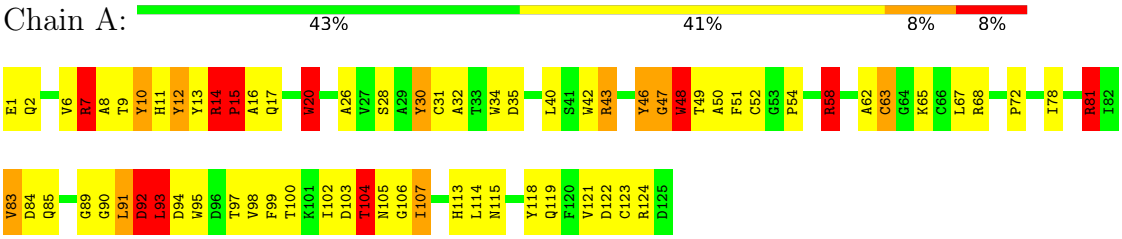
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

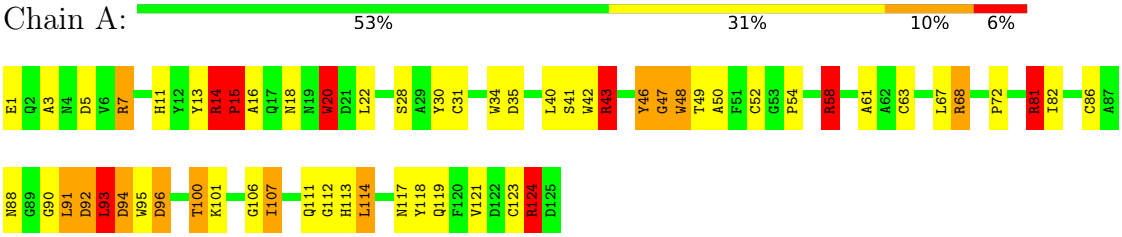
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

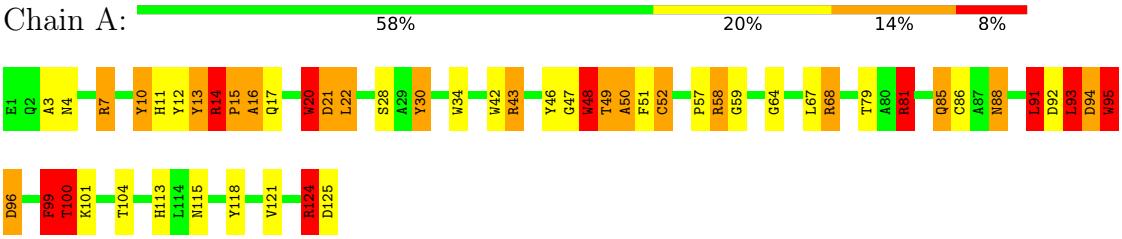
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

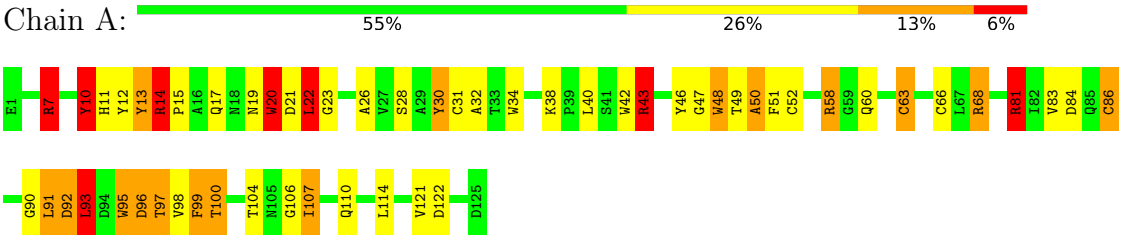
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

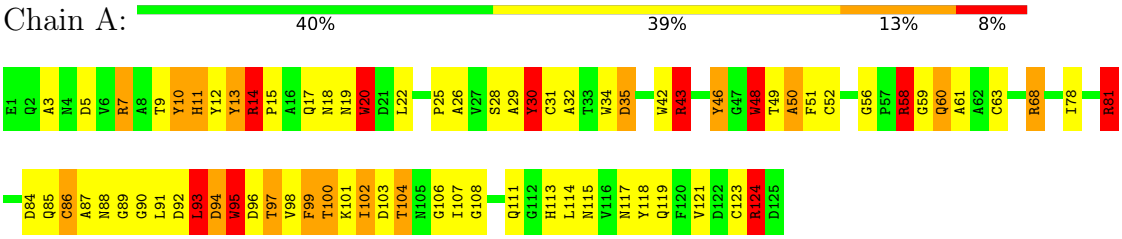
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

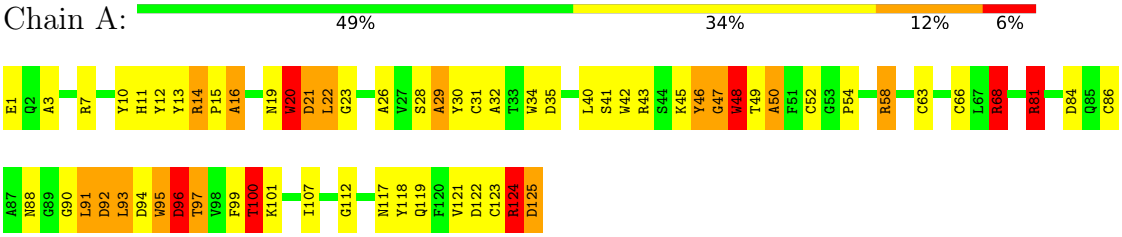
Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

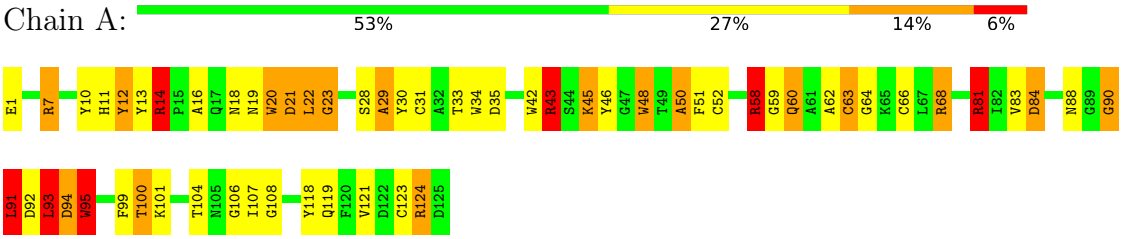
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

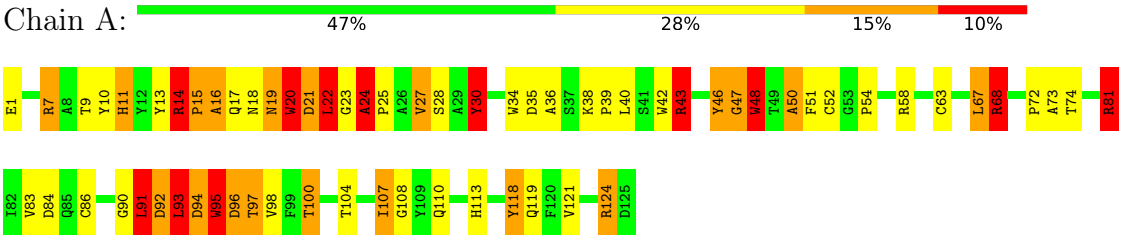
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A:



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided.

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	1.60±0.04	4±2/995 (0.4± 0.2%)	2.02±0.09	44±6/1358 (3.2± 0.5%)
All	All	1.60	85/19900 (0.4%)	2.02	882/27160 (3.2%)

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	7.0±0.4
All	All	0	140

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	42	TRP	CA-CB	-8.06	1.36	1.53	6	2
1	A	42	TRP	CG-CD2	-7.72	1.30	1.43	5	3
1	A	93	LEU	CA-CB	6.72	1.69	1.53	13	5
1	A	48	TRP	NE1-CE2	-6.71	1.28	1.37	15	7
1	A	48	TRP	CG-CD2	-6.63	1.32	1.43	11	14
1	A	64	GLY	CA-C	6.36	1.62	1.51	4	1
1	A	51	PHE	CA-CB	6.16	1.67	1.53	4	1
1	A	47	GLY	N-CA	6.14	1.55	1.46	6	1
1	A	48	TRP	CD2-CE3	-6.01	1.31	1.40	12	2
1	A	48	TRP	CD2-CE2	-5.85	1.34	1.41	15	3
1	A	81	ARG	CZ-NH1	-5.74	1.25	1.33	7	7
1	A	42	TRP	CG-CD1	-5.74	1.28	1.36	5	1
1	A	43	ARG	CZ-NH1	-5.63	1.25	1.33	9	1
1	A	15	PRO	CA-CB	-5.59	1.42	1.53	6	1
1	A	20	TRP	CG-CD2	-5.58	1.34	1.43	17	4
1	A	95	TRP	CG-CD2	-5.50	1.34	1.43	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	91	LEU	CA-CB	5.48	1.66	1.53	20	2
1	A	58	ARG	CZ-NH2	-5.45	1.25	1.33	4	1
1	A	81	ARG	CZ-NH2	-5.43	1.25	1.33	14	3
1	A	34	TRP	CG-CD2	-5.39	1.34	1.43	19	11
1	A	14	ARG	CZ-NH1	-5.35	1.26	1.33	11	1
1	A	20	TRP	CA-CB	5.30	1.65	1.53	7	1
1	A	20	TRP	NE1-CE2	-5.29	1.30	1.37	7	1
1	A	68	ARG	CZ-NH1	-5.24	1.26	1.33	1	1
1	A	81	ARG	NE-CZ	-5.22	1.26	1.33	12	1
1	A	124	ARG	CZ-NH1	-5.21	1.26	1.33	9	1
1	A	58	ARG	CZ-NH1	-5.16	1.26	1.33	12	1
1	A	108	GLY	N-CA	5.11	1.53	1.46	11	1
1	A	43	ARG	N-CA	5.07	1.56	1.46	6	1
1	A	50	ALA	N-CA	5.07	1.56	1.46	5	2
1	A	43	ARG	CZ-NH2	-5.01	1.26	1.33	4	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	43	ARG	NE-CZ-NH2	-17.28	111.66	120.30	12	8
1	A	81	ARG	NE-CZ-NH2	-16.85	111.88	120.30	17	10
1	A	42	TRP	CA-CB-CG	16.58	145.20	113.70	5	2
1	A	43	ARG	NE-CZ-NH1	15.52	128.06	120.30	12	8
1	A	42	TRP	NE1-CE2-CZ2	14.67	146.54	130.40	5	18
1	A	14	ARG	NE-CZ-NH2	-14.49	113.05	120.30	1	11
1	A	58	ARG	NE-CZ-NH1	-14.35	113.13	120.30	6	9
1	A	68	ARG	NE-CZ-NH2	-14.26	113.17	120.30	3	11
1	A	81	ARG	NE-CZ-NH1	14.10	127.35	120.30	17	10
1	A	42	TRP	CG-CD2-CE3	-13.67	121.60	133.90	5	3
1	A	20	TRP	NE1-CE2-CZ2	13.30	145.03	130.40	17	13
1	A	68	ARG	NE-CZ-NH1	-12.62	113.99	120.30	1	6
1	A	21	ASP	N-CA-C	-12.09	78.36	111.00	20	1
1	A	93	LEU	N-CA-C	-11.78	79.20	111.00	20	9
1	A	124	ARG	NE-CZ-NH1	-11.77	114.42	120.30	1	9
1	A	14	ARG	NE-CZ-NH1	-11.28	114.66	120.30	10	9
1	A	20	TRP	CD1-NE1-CE2	10.80	118.72	109.00	20	20
1	A	46	TYR	CB-CG-CD2	-10.71	114.57	121.00	20	1
1	A	58	ARG	NE-CZ-NH2	-10.67	114.97	120.30	4	7
1	A	48	TRP	CB-CG-CD1	-10.33	113.57	127.00	14	2
1	A	30	TYR	CB-CG-CD1	-10.32	114.81	121.00	8	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	42	TRP	CB-CG-CD2	-10.32	113.19	126.60	5	1
1	A	89	GLY	N-CA-C	10.28	138.80	113.10	8	2
1	A	48	TRP	CD1-NE1-CE2	10.24	118.21	109.00	4	20
1	A	81	ARG	N-CA-CB	-10.24	92.17	110.60	3	6
1	A	20	TRP	CB-CG-CD1	-10.00	113.99	127.00	19	8
1	A	42	TRP	CD1-NE1-CE2	9.98	117.99	109.00	18	20
1	A	13	TYR	O-C-N	9.90	138.55	122.70	15	3
1	A	48	TRP	CG-CD1-NE1	-9.80	100.30	110.10	11	19
1	A	66	CYS	N-CA-C	-9.80	84.53	111.00	4	1
1	A	84	ASP	CB-CG-OD2	-9.76	109.51	118.30	5	3
1	A	94	ASP	CB-CG-OD2	-9.46	109.78	118.30	7	8
1	A	20	TRP	CG-CD1-NE1	-9.38	100.72	110.10	20	18
1	A	95	TRP	CD1-NE1-CE2	9.32	117.39	109.00	1	20
1	A	92	ASP	CB-CG-OD2	-9.31	109.92	118.30	10	6
1	A	125	ASP	CB-CG-OD2	-9.19	110.03	118.30	18	4
1	A	43	ARG	CA-C-N	-9.18	97.01	117.20	6	1
1	A	48	TRP	CG-CD2-CE3	-9.16	125.65	133.90	12	4
1	A	34	TRP	CD1-NE1-CE2	9.12	117.21	109.00	19	20
1	A	20	TRP	NE1-CE2-CD2	-8.99	98.31	107.30	17	12
1	A	46	TYR	CB-CG-CD1	8.92	126.35	121.00	20	2
1	A	125	ASP	CB-CG-OD1	8.90	126.31	118.30	8	4
1	A	42	TRP	CA-C-N	-8.83	97.77	117.20	6	1
1	A	92	ASP	CB-CG-OD1	-8.77	110.41	118.30	8	5
1	A	30	TYR	CB-CG-CD2	8.70	126.22	121.00	5	7
1	A	103	ASP	CB-CG-OD2	-8.69	110.47	118.30	12	5
1	A	34	TRP	NE1-CE2-CZ2	8.66	139.93	130.40	19	20
1	A	94	ASP	CB-CG-OD1	-8.66	110.50	118.30	10	3
1	A	93	LEU	CB-CA-C	-8.62	93.82	110.20	20	3
1	A	48	TRP	NE1-CE2-CD2	-8.52	98.78	107.30	1	3
1	A	42	TRP	NE1-CE2-CD2	-8.52	98.78	107.30	5	16
1	A	65	LYS	N-CA-C	8.52	134.00	111.00	4	1
1	A	35	ASP	CB-CG-OD2	-8.37	110.76	118.30	18	10
1	A	48	TRP	NE1-CE2-CZ2	8.36	139.60	130.40	1	10
1	A	93	LEU	O-C-N	8.27	135.93	122.70	8	4
1	A	50	ALA	N-CA-CB	8.26	121.66	110.10	15	10
1	A	81	ARG	NH1-CZ-NH2	8.21	128.44	119.40	12	5
1	A	7	ARG	NE-CZ-NH1	-8.20	116.20	120.30	4	8
1	A	124	ARG	NE-CZ-NH2	-8.15	116.22	120.30	17	4
1	A	48	TRP	CE2-CD2-CG	8.14	113.81	107.30	12	2
1	A	42	TRP	CG-CD1-NE1	-8.08	102.02	110.10	18	20
1	A	34	TRP	CG-CD1-NE1	-8.00	102.10	110.10	16	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	7	ARG	NE-CZ-NH2	-7.92	116.34	120.30	5	11
1	A	20	TRP	CB-CG-CD2	7.91	136.89	126.60	19	5
1	A	50	ALA	N-CA-C	-7.86	89.78	111.00	10	11
1	A	100	THR	CA-CB-CG2	7.73	123.23	112.40	18	1
1	A	5	ASP	CB-CG-OD1	-7.72	111.35	118.30	14	1
1	A	24	ALA	N-CA-C	7.70	131.78	111.00	20	1
1	A	95	TRP	CG-CD1-NE1	-7.66	102.44	110.10	1	20
1	A	95	TRP	NE1-CE2-CZ2	7.63	138.79	130.40	2	14
1	A	48	TRP	CB-CG-CD2	7.62	136.51	126.60	14	2
1	A	95	TRP	CA-CB-CG	-7.60	99.26	113.70	1	11
1	A	22	LEU	CB-CG-CD1	-7.58	98.11	111.00	1	5
1	A	42	TRP	N-CA-CB	-7.58	96.95	110.60	5	1
1	A	81	ARG	CB-CA-C	7.56	125.52	110.40	3	4
1	A	92	ASP	N-CA-CB	-7.55	97.01	110.60	11	4
1	A	94	ASP	N-CA-C	7.51	131.28	111.00	13	1
1	A	96	ASP	CB-CG-OD2	-7.50	111.55	118.30	18	9
1	A	42	TRP	CE2-CD2-CE3	7.48	127.67	118.70	5	1
1	A	13	TYR	CB-CG-CD2	-7.46	116.52	121.00	18	2
1	A	20	TRP	CG-CD2-CE3	-7.43	127.22	133.90	18	4
1	A	96	ASP	CB-CG-OD1	7.38	124.94	118.30	18	1
1	A	48	TRP	CD1-CG-CD2	7.36	112.19	106.30	2	7
1	A	122	ASP	CB-CG-OD2	-7.36	111.68	118.30	13	5
1	A	40	LEU	CB-CG-CD1	-7.35	98.50	111.00	11	1
1	A	13	TYR	CB-CG-CD1	-7.34	116.59	121.00	17	3
1	A	41	SER	N-CA-C	-7.34	91.18	111.00	6	1
1	A	13	TYR	C-N-CA	7.26	139.85	121.70	15	2
1	A	42	TRP	CD1-CG-CD2	7.26	112.11	106.30	5	2
1	A	94	ASP	CA-CB-CG	-7.26	97.44	113.40	15	1
1	A	21	ASP	N-CA-CB	-7.23	97.59	110.60	15	1
1	A	20	TRP	CA-CB-CG	7.21	127.39	113.70	5	9
1	A	93	LEU	N-CA-CB	7.12	124.64	110.40	20	3
1	A	93	LEU	CB-CG-CD1	-7.10	98.93	111.00	8	3
1	A	49	THR	OG1-CB-CG2	-7.08	93.72	110.00	15	2
1	A	95	TRP	N-CA-C	-7.07	91.92	111.00	5	3
1	A	92	ASP	N-CA-C	7.06	130.06	111.00	8	11
1	A	100	THR	OG1-CB-CG2	-7.04	93.81	110.00	6	7
1	A	91	LEU	N-CA-C	7.03	129.99	111.00	5	5
1	A	59	GLY	N-CA-C	7.00	130.61	113.10	7	1
1	A	42	TRP	C-N-CA	6.97	139.13	121.70	6	1
1	A	94	ASP	CA-C-N	-6.96	101.88	117.20	15	5
1	A	44	SER	CA-C-O	-6.92	105.56	120.10	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	43	ARG	NH1-CZ-NH2	6.83	126.91	119.40	16	3
1	A	106	GLY	N-CA-C	6.75	129.96	113.10	7	2
1	A	43	ARG	O-C-N	6.69	133.40	122.70	6	1
1	A	58	ARG	NH1-CZ-NH2	6.68	126.75	119.40	5	4
1	A	82	ILE	CA-CB-CG1	6.66	123.66	111.00	4	1
1	A	29	ALA	N-CA-CB	-6.64	100.81	110.10	18	3
1	A	48	TRP	CH2-CZ2-CE2	6.61	124.00	117.40	8	1
1	A	13	TYR	N-CA-C	-6.59	93.21	111.00	15	1
1	A	12	TYR	CB-CG-CD2	-6.57	117.06	121.00	19	3
1	A	65	LYS	CB-CA-C	-6.52	97.35	110.40	4	1
1	A	20	TRP	CD1-CG-CD2	6.48	111.49	106.30	20	2
1	A	104	THR	OG1-CB-CG2	-6.47	95.13	110.00	17	4
1	A	48	TRP	N-CA-C	-6.45	93.58	111.00	11	1
1	A	42	TRP	O-C-N	6.40	132.94	122.70	6	1
1	A	1	GLU	OE1-CD-OE2	6.38	130.95	123.30	14	7
1	A	44	SER	CA-C-N	6.36	131.20	117.20	6	1
1	A	42	TRP	CD2-CE2-CZ2	-6.36	114.67	122.30	5	1
1	A	86	CYS	CA-CB-SG	6.34	125.41	114.00	15	2
1	A	63	CYS	CA-CB-SG	6.31	125.36	114.00	16	4
1	A	93	LEU	CA-CB-CG	6.27	129.71	115.30	13	1
1	A	14	ARG	NH1-CZ-NH2	6.25	126.28	119.40	14	4
1	A	52	CYS	CA-CB-SG	6.24	125.24	114.00	12	3
1	A	48	TRP	CB-CA-C	-6.23	97.94	110.40	12	2
1	A	34	TRP	NE1-CE2-CD2	-6.17	101.13	107.30	19	20
1	A	30	TYR	N-CA-C	6.15	127.61	111.00	4	4
1	A	102	ILE	CA-CB-CG1	6.13	122.66	111.00	11	3
1	A	94	ASP	N-CA-CB	-6.10	99.62	110.60	4	4
1	A	21	ASP	CA-CB-CG	-6.09	99.99	113.40	18	1
1	A	11	HIS	CA-CB-CG	-6.09	103.25	113.60	20	4
1	A	10	TYR	CB-CG-CD2	-6.06	117.36	121.00	17	6
1	A	124	ARG	NH1-CZ-NH2	5.96	125.95	119.40	1	2
1	A	34	TRP	CG-CD2-CE3	-5.94	128.56	133.90	7	5
1	A	123	CYS	CA-CB-SG	5.89	124.61	114.00	8	1
1	A	11	HIS	O-C-N	5.87	132.09	122.70	12	2
1	A	95	TRP	NE1-CE2-CD2	-5.85	101.45	107.30	11	4
1	A	44	SER	N-CA-CB	-5.84	101.74	110.50	6	1
1	A	58	ARG	N-CA-CB	-5.83	100.11	110.60	4	1
1	A	14	ARG	N-CA-C	5.82	126.72	111.00	15	1
1	A	48	TRP	CA-C-N	-5.79	104.47	117.20	10	1
1	A	103	ASP	CB-CG-OD1	-5.78	113.10	118.30	6	3
1	A	95	TRP	CG-CD2-CE3	-5.76	128.72	133.90	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	64	GLY	N-CA-C	5.72	127.41	113.10	4	1
1	A	13	TYR	CA-C-N	-5.72	104.61	117.20	15	1
1	A	49	THR	CA-C-N	-5.72	104.61	117.20	2	1
1	A	20	TRP	CE2-CD2-CG	5.72	111.88	107.30	18	2
1	A	42	TRP	CB-CG-CD1	5.71	134.43	127.00	5	2
1	A	49	THR	CA-CB-CG2	-5.68	104.45	112.40	4	1
1	A	49	THR	CA-CB-OG1	-5.66	97.11	109.00	16	1
1	A	49	THR	C-N-CA	-5.66	107.55	121.70	5	2
1	A	11	HIS	N-CA-C	-5.64	95.77	111.00	10	5
1	A	20	TRP	CH2-CZ2-CE2	5.63	123.03	117.40	15	4
1	A	50	ALA	CB-CA-C	-5.62	101.67	110.10	12	2
1	A	97	THR	CA-CB-OG1	5.62	120.79	109.00	6	1
1	A	65	LYS	CA-C-N	5.61	129.54	117.20	4	1
1	A	12	TYR	CB-CG-CD1	5.60	124.36	121.00	19	2
1	A	22	LEU	CB-CG-CD2	-5.59	101.49	111.00	12	1
1	A	31	CYS	N-CA-CB	-5.57	100.58	110.60	14	2
1	A	10	TYR	CB-CG-CD1	5.55	124.33	121.00	6	1
1	A	14	ARG	CG-CD-NE	-5.55	100.14	111.80	3	1
1	A	93	LEU	CA-C-N	-5.51	105.07	117.20	4	1
1	A	7	ARG	NH1-CZ-NH2	5.43	125.38	119.40	5	3
1	A	11	HIS	CA-C-N	-5.42	105.28	117.20	12	2
1	A	93	LEU	C-N-CA	5.41	135.23	121.70	15	3
1	A	31	CYS	CA-CB-SG	5.40	123.72	114.00	6	1
1	A	21	ASP	CB-CG-OD1	-5.40	113.44	118.30	18	1
1	A	99	PHE	CB-CG-CD2	5.39	124.57	120.80	15	1
1	A	79	THR	OG1-CB-CG2	-5.38	97.63	110.00	15	1
1	A	97	THR	OG1-CB-CG2	-5.37	97.66	110.00	20	3
1	A	66	CYS	N-CA-CB	-5.32	101.02	110.60	11	1
1	A	5	ASP	N-CA-CB	-5.31	101.05	110.60	12	1
1	A	95	TRP	N-CA-CB	-5.30	101.05	110.60	4	1
1	A	118	TYR	CB-CG-CD2	-5.30	117.82	121.00	10	1
1	A	68	ARG	NH1-CZ-NH2	5.27	125.20	119.40	1	2
1	A	43	ARG	N-CA-C	5.27	125.22	111.00	6	1
1	A	68	ARG	N-CA-C	-5.26	96.78	111.00	11	1
1	A	43	ARG	CA-CB-CG	-5.26	101.84	113.40	11	1
1	A	113	HIS	CA-CB-CG	-5.23	104.71	113.60	20	1
1	A	22	LEU	CA-C-N	-5.21	105.77	116.20	20	1
1	A	9	THR	N-CA-C	-5.21	96.94	111.00	10	1
1	A	48	TRP	N-CA-CB	5.21	119.97	110.60	12	1
1	A	94	ASP	CB-CA-C	5.17	120.75	110.40	11	1
1	A	84	ASP	CB-CG-OD1	-5.13	113.68	118.30	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	94	ASP	C-N-CA	5.12	134.50	121.70	19	1
1	A	68	ARG	CD-NE-CZ	-5.06	116.52	123.60	16	1
1	A	7	ARG	N-CA-C	-5.05	97.37	111.00	1	1
1	A	2	GLN	N-CA-CB	-5.03	101.54	110.60	6	1
1	A	13	TYR	CA-CB-CG	-5.01	103.87	113.40	17	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	7	ARG	Sidechain	20
1	A	14	ARG	Sidechain,Peptide	20
1	A	43	ARG	Sidechain	20
1	A	58	ARG	Sidechain	20
1	A	81	ARG	Sidechain	20
1	A	68	ARG	Sidechain	19
1	A	124	ARG	Sidechain	19

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	968	895	895	52±14
All	All	19360	17900	17900	1050

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PRO:HB2	1:A:48:TRP:CE3	0.97	1.94	7	1
1:A:65:LYS:H	1:A:82:ILE:HG23	0.93	1.23	4	1
1:A:20:TRP:CZ3	1:A:48:TRP:CD2	0.92	2.57	7	3
1:A:42:TRP:CE3	1:A:42:TRP:HA	0.86	2.03	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LYS:CA	1:A:82:ILE:HD13	0.82	2.04	4	1
1:A:15:PRO:HB2	1:A:48:TRP:CZ3	0.82	2.09	7	1
1:A:50:ALA:HB2	1:A:93:LEU:HD12	0.81	1.50	9	1
1:A:50:ALA:H	1:A:93:LEU:N	0.81	1.73	9	8
1:A:22:LEU:HD22	1:A:48:TRP:CH2	0.79	2.12	15	1
1:A:20:TRP:CD2	1:A:48:TRP:CZ3	0.79	2.70	1	3
1:A:22:LEU:HD22	1:A:48:TRP:CZ3	0.79	2.13	15	1
1:A:50:ALA:CB	1:A:93:LEU:HB3	0.78	2.09	16	14
1:A:81:ARG:HG2	1:A:123:CYS:SG	0.77	2.19	4	1
1:A:20:TRP:CE3	1:A:48:TRP:CE2	0.76	2.72	16	13
1:A:65:LYS:HA	1:A:82:ILE:HD13	0.76	1.55	4	1
1:A:50:ALA:HB2	1:A:93:LEU:CD1	0.76	2.10	9	3
1:A:50:ALA:O	1:A:92:ASP:HA	0.76	1.79	20	11
1:A:50:ALA:H	1:A:93:LEU:H	0.76	1.24	4	13
1:A:48:TRP:N	1:A:81:ARG:HB2	0.75	1.95	5	7
1:A:15:PRO:CB	1:A:48:TRP:CE3	0.75	2.69	7	3
1:A:40:LEU:O	1:A:43:ARG:HA	0.75	1.81	6	1
1:A:15:PRO:HB3	1:A:48:TRP:CE3	0.74	2.17	1	2
1:A:20:TRP:CZ3	1:A:48:TRP:CG	0.74	2.75	7	4
1:A:48:TRP:C	1:A:48:TRP:CD1	0.73	2.62	4	7
1:A:48:TRP:CG	1:A:48:TRP:O	0.73	2.40	15	1
1:A:13:TYR:HB3	1:A:93:LEU:HA	0.73	1.61	6	2
1:A:48:TRP:H	1:A:81:ARG:HB2	0.73	1.43	5	4
1:A:62:ALA:O	1:A:64:GLY:N	0.73	2.22	4	5
1:A:48:TRP:O	1:A:48:TRP:CD1	0.73	2.41	8	8
1:A:42:TRP:O	1:A:45:LYS:N	0.72	2.23	6	1
1:A:63:CYS:SG	1:A:83:VAL:O	0.70	2.50	5	1
1:A:44:SER:O	1:A:46:TYR:N	0.70	2.25	6	1
1:A:51:PHE:CZ	1:A:59:GLY:HA2	0.70	2.22	7	1
1:A:22:LEU:HD11	1:A:48:TRP:CZ2	0.69	2.22	1	1
1:A:22:LEU:CD2	1:A:48:TRP:CZ3	0.69	2.75	15	1
1:A:22:LEU:HD11	1:A:48:TRP:CH2	0.69	2.23	1	6
1:A:48:TRP:H	1:A:81:ARG:CB	0.69	2.00	16	6
1:A:20:TRP:O	1:A:22:LEU:N	0.69	2.25	15	2
1:A:49:THR:HG21	1:A:80:ALA:HB1	0.69	1.64	4	4
1:A:50:ALA:HB2	1:A:93:LEU:HB3	0.69	1.64	6	7
1:A:48:TRP:HE1	1:A:93:LEU:CD2	0.68	2.00	14	1
1:A:65:LYS:N	1:A:82:ILE:HG23	0.68	2.01	4	1
1:A:50:ALA:HB2	1:A:93:LEU:HD22	0.68	1.65	7	1
1:A:48:TRP:NE1	1:A:93:LEU:HD11	0.67	2.04	14	1
1:A:20:TRP:CE3	1:A:48:TRP:CZ2	0.67	2.83	19	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:TYR:HA	1:A:81:ARG:HB3	0.66	1.66	5	1
1:A:22:LEU:HD21	1:A:48:TRP:CH2	0.66	2.24	3	9
1:A:22:LEU:CD2	1:A:48:TRP:CH2	0.66	2.78	3	4
1:A:42:TRP:CE3	1:A:42:TRP:CA	0.66	2.77	11	2
1:A:46:TYR:CE2	1:A:123:CYS:SG	0.66	2.88	19	2
1:A:93:LEU:O	1:A:93:LEU:HG	0.65	1.91	5	7
1:A:48:TRP:N	1:A:81:ARG:CB	0.65	2.58	16	5
1:A:52:CYS:SG	1:A:91:LEU:N	0.65	2.68	4	1
1:A:11:HIS:HB3	1:A:90:GLY:N	0.65	2.06	10	4
1:A:66:CYS:N	1:A:82:ILE:CD1	0.65	2.60	4	1
1:A:42:TRP:CE3	1:A:45:LYS:HD2	0.65	2.26	11	1
1:A:15:PRO:CB	1:A:48:TRP:CZ3	0.65	2.80	7	3
1:A:20:TRP:HB3	1:A:48:TRP:CH2	0.65	2.27	16	6
1:A:41:SER:O	1:A:42:TRP:C	0.65	2.36	6	1
1:A:52:CYS:SG	1:A:88:ASN:ND2	0.64	2.70	15	1
1:A:40:LEU:O	1:A:41:SER:C	0.64	2.35	6	1
1:A:20:TRP:CE3	1:A:48:TRP:CE3	0.64	2.85	1	3
1:A:93:LEU:O	1:A:93:LEU:CG	0.64	2.46	5	3
1:A:20:TRP:CE3	1:A:48:TRP:CD2	0.63	2.87	7	4
1:A:31:CYS:SG	1:A:83:VAL:HG13	0.63	2.34	11	1
1:A:65:LYS:H	1:A:82:ILE:CG2	0.63	2.02	4	1
1:A:47:GLY:N	1:A:81:ARG:HB3	0.63	2.08	6	3
1:A:1:GLU:N	1:A:1:GLU:CD	0.62	2.52	18	1
1:A:48:TRP:N	1:A:97:THR:HG21	0.62	2.09	1	2
1:A:66:CYS:SG	1:A:81:ARG:HD2	0.62	2.35	2	3
1:A:62:ALA:O	1:A:82:ILE:HG21	0.62	1.95	4	1
1:A:66:CYS:N	1:A:82:ILE:HG12	0.62	2.08	4	1
1:A:15:PRO:HB3	1:A:94:ASP:O	0.62	1.94	6	2
1:A:48:TRP:CE2	1:A:93:LEU:HD21	0.62	2.30	7	1
1:A:22:LEU:CD1	1:A:48:TRP:CH2	0.62	2.83	11	4
1:A:50:ALA:N	1:A:93:LEU:HD22	0.62	2.09	3	6
1:A:41:SER:O	1:A:43:ARG:N	0.62	2.33	6	1
1:A:93:LEU:HD13	1:A:93:LEU:O	0.62	1.95	12	1
1:A:20:TRP:CH2	1:A:48:TRP:HB2	0.61	2.29	1	3
1:A:20:TRP:CB	1:A:48:TRP:CH2	0.61	2.83	14	4
1:A:11:HIS:H	1:A:91:LEU:N	0.61	1.93	8	2
1:A:20:TRP:CH2	1:A:48:TRP:CG	0.61	2.88	7	1
1:A:79:THR:O	1:A:81:ARG:NH1	0.61	2.32	1	1
1:A:50:ALA:N	1:A:93:LEU:HG	0.61	2.10	13	1
1:A:48:TRP:O	1:A:48:TRP:CG	0.61	2.54	13	6
1:A:48:TRP:CD1	1:A:48:TRP:C	0.61	2.72	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:HD12	1:A:93:LEU:O	0.61	1.95	13	1
1:A:20:TRP:CG	1:A:48:TRP:CZ2	0.61	2.89	8	5
1:A:20:TRP:CG	1:A:48:TRP:CZ3	0.60	2.90	1	3
1:A:50:ALA:N	1:A:93:LEU:H	0.60	1.93	4	11
1:A:47:GLY:O	1:A:48:TRP:CD1	0.60	2.55	2	4
1:A:66:CYS:SG	1:A:81:ARG:NH1	0.60	2.75	10	1
1:A:46:TYR:CD2	1:A:123:CYS:SG	0.60	2.95	19	2
1:A:50:ALA:HB3	1:A:93:LEU:N	0.60	2.12	4	2
1:A:10:TYR:O	1:A:10:TYR:CG	0.60	2.54	3	10
1:A:21:ASP:O	1:A:23:GLY:N	0.59	2.35	19	7
1:A:20:TRP:CD2	1:A:48:TRP:CZ2	0.59	2.90	8	5
1:A:13:TYR:CB	1:A:93:LEU:HA	0.59	2.26	6	2
1:A:11:HIS:CB	1:A:90:GLY:HA2	0.59	2.27	16	1
1:A:20:TRP:CZ3	1:A:48:TRP:CE2	0.59	2.90	7	1
1:A:20:TRP:CD2	1:A:48:TRP:CE3	0.59	2.91	1	3
1:A:95:TRP:O	1:A:95:TRP:CG	0.59	2.55	6	3
1:A:11:HIS:N	1:A:90:GLY:C	0.59	2.56	20	2
1:A:93:LEU:CG	1:A:93:LEU:O	0.59	2.49	3	7
1:A:86:CYS:SG	1:A:87:ALA:N	0.59	2.76	17	2
1:A:42:TRP:CZ2	1:A:45:LYS:HE2	0.58	2.33	11	1
1:A:52:CYS:H	1:A:91:LEU:CA	0.58	2.09	15	1
1:A:65:LYS:C	1:A:82:ILE:HG12	0.58	2.18	4	1
1:A:62:ALA:C	1:A:82:ILE:HG21	0.58	2.17	4	1
1:A:46:TYR:HB3	1:A:66:CYS:SG	0.58	2.38	5	1
1:A:48:TRP:NE1	1:A:93:LEU:HD21	0.58	2.14	7	2
1:A:42:TRP:CH2	1:A:45:LYS:HE2	0.58	2.33	11	1
1:A:48:TRP:O	1:A:93:LEU:CD2	0.58	2.51	11	2
1:A:46:TYR:CA	1:A:81:ARG:HB3	0.58	2.29	5	2
1:A:48:TRP:NE1	1:A:93:LEU:CD1	0.58	2.67	14	1
1:A:94:ASP:CG	1:A:95:TRP:H	0.57	2.02	19	3
1:A:13:TYR:HB3	1:A:93:LEU:HB2	0.57	1.74	12	3
1:A:42:TRP:C	1:A:44:SER:H	0.57	2.02	6	1
1:A:90:GLY:O	1:A:91:LEU:CB	0.57	2.52	10	2
1:A:81:ARG:HB3	1:A:81:ARG:NH1	0.57	2.14	17	1
1:A:50:ALA:N	1:A:93:LEU:CD2	0.57	2.67	3	6
1:A:30:TYR:HB3	1:A:63:CYS:SG	0.57	2.40	20	2
1:A:48:TRP:HE1	1:A:93:LEU:HD21	0.57	1.59	14	1
1:A:22:LEU:HD21	1:A:48:TRP:CZ2	0.57	2.34	14	3
1:A:52:CYS:N	1:A:86:CYS:SG	0.57	2.78	9	1
1:A:81:ARG:NH1	1:A:81:ARG:CG	0.57	2.68	15	2
1:A:20:TRP:CD1	1:A:43:ARG:HD2	0.56	2.36	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ALA:O	1:A:43:ARG:NH1	0.56	2.37	9	2
1:A:46:TYR:O	1:A:81:ARG:NH2	0.56	2.39	13	1
1:A:81:ARG:CB	1:A:81:ARG:HH11	0.56	2.13	15	2
1:A:12:TYR:CG	1:A:94:ASP:HB3	0.56	2.35	2	1
1:A:15:PRO:CB	1:A:94:ASP:O	0.56	2.53	6	1
1:A:50:ALA:N	1:A:93:LEU:HB3	0.56	2.15	16	6
1:A:48:TRP:CB	1:A:97:THR:HG21	0.56	2.30	7	1
1:A:15:PRO:CD	1:A:94:ASP:O	0.56	2.54	11	2
1:A:15:PRO:CB	1:A:48:TRP:HE3	0.56	2.14	1	2
1:A:94:ASP:O	1:A:97:THR:HG23	0.56	1.99	4	1
1:A:50:ALA:O	1:A:92:ASP:CA	0.56	2.53	20	3
1:A:46:TYR:O	1:A:47:GLY:C	0.56	2.44	6	3
1:A:46:TYR:C	1:A:81:ARG:HB3	0.56	2.20	19	3
1:A:50:ALA:H	1:A:93:LEU:HB3	0.56	1.60	10	4
1:A:58:ARG:NH2	1:A:84:ASP:HA	0.56	2.16	5	1
1:A:52:CYS:SG	1:A:89:GLY:HA3	0.56	2.41	10	2
1:A:44:SER:OG	1:A:81:ARG:NH1	0.56	2.39	6	1
1:A:16:ALA:N	1:A:20:TRP:HB3	0.55	2.17	18	4
1:A:65:LYS:HG2	1:A:67:LEU:CD1	0.55	2.32	4	1
1:A:81:ARG:NH1	1:A:81:ARG:HG2	0.55	2.17	15	2
1:A:44:SER:CB	1:A:81:ARG:NH1	0.55	2.69	6	1
1:A:42:TRP:CZ3	1:A:45:LYS:CB	0.55	2.89	11	1
1:A:46:TYR:O	1:A:48:TRP:N	0.55	2.39	14	1
1:A:48:TRP:N	1:A:81:ARG:HB3	0.55	2.16	13	2
1:A:93:LEU:O	1:A:93:LEU:HD23	0.55	2.02	7	9
1:A:20:TRP:CE3	1:A:43:ARG:CD	0.55	2.90	11	1
1:A:20:TRP:CE3	1:A:43:ARG:HD3	0.55	2.37	11	1
1:A:47:GLY:O	1:A:48:TRP:HB3	0.55	2.02	15	1
1:A:3:ALA:HB3	1:A:118:TYR:CZ	0.55	2.37	4	8
1:A:50:ALA:H	1:A:93:LEU:CB	0.55	2.15	10	4
1:A:62:ALA:HB1	1:A:82:ILE:HD12	0.54	1.79	4	1
1:A:15:PRO:HB2	1:A:20:TRP:CE3	0.54	2.36	13	1
1:A:20:TRP:HB2	1:A:48:TRP:CH2	0.54	2.38	17	5
1:A:81:ARG:CG	1:A:123:CYS:SG	0.54	2.95	4	1
1:A:48:TRP:CB	1:A:81:ARG:NH1	0.54	2.71	8	1
1:A:81:ARG:NH1	1:A:81:ARG:CB	0.54	2.70	17	1
1:A:81:ARG:N	1:A:81:ARG:HD3	0.54	2.18	1	1
1:A:20:TRP:CZ3	1:A:48:TRP:CD1	0.54	2.96	16	2
1:A:81:ARG:N	1:A:81:ARG:CD	0.54	2.71	1	1
1:A:99:PHE:O	1:A:101:LYS:N	0.54	2.40	15	5
1:A:65:LYS:C	1:A:82:ILE:CG1	0.54	2.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ALA:HA	1:A:84:ASP:OD1	0.54	2.03	5	1
1:A:42:TRP:CE3	1:A:45:LYS:HB3	0.54	2.38	11	1
1:A:20:TRP:CE3	1:A:48:TRP:CZ3	0.54	2.96	1	3
1:A:11:HIS:CB	1:A:90:GLY:HA3	0.54	2.33	6	1
1:A:40:LEU:O	1:A:43:ARG:CA	0.54	2.56	6	1
1:A:14:ARG:HD2	1:A:14:ARG:H	0.54	1.63	8	1
1:A:44:SER:HB2	1:A:81:ARG:NH1	0.53	2.19	6	1
1:A:84:ASP:CG	1:A:85:GLN:H	0.53	2.05	17	2
1:A:81:ARG:HH12	1:A:83:VAL:CG1	0.53	2.15	7	1
1:A:93:LEU:O	1:A:93:LEU:CD1	0.53	2.55	13	1
1:A:50:ALA:N	1:A:93:LEU:HD12	0.53	2.18	20	3
1:A:46:TYR:CG	1:A:66:CYS:SG	0.53	3.01	16	3
1:A:48:TRP:NE1	1:A:93:LEU:HD23	0.53	2.18	9	1
1:A:50:ALA:CB	1:A:84:ASP:HB3	0.53	2.33	12	1
1:A:48:TRP:HE1	1:A:93:LEU:CD1	0.53	2.17	14	1
1:A:15:PRO:CG	1:A:16:ALA:H	0.53	2.16	15	1
1:A:66:CYS:CB	1:A:121:VAL:O	0.53	2.57	4	1
1:A:50:ALA:O	1:A:92:ASP:CB	0.53	2.57	4	3
1:A:20:TRP:CH2	1:A:48:TRP:CD2	0.53	2.96	7	1
1:A:14:ARG:H	1:A:14:ARG:CD	0.53	2.16	8	1
1:A:107:ILE:HD12	1:A:107:ILE:H	0.53	1.63	4	1
1:A:48:TRP:NE1	1:A:83:VAL:HG11	0.53	2.19	1	1
1:A:63:CYS:C	1:A:82:ILE:CG2	0.53	2.77	4	1
1:A:81:ARG:CG	1:A:81:ARG:HH11	0.53	2.17	15	1
1:A:11:HIS:HB3	1:A:90:GLY:CA	0.53	2.33	1	4
1:A:49:THR:N	1:A:81:ARG:O	0.53	2.42	5	6
1:A:12:TYR:CB	1:A:92:ASP:O	0.53	2.57	7	1
1:A:46:TYR:CZ	1:A:123:CYS:SG	0.52	3.02	18	4
1:A:46:TYR:O	1:A:81:ARG:NH1	0.52	2.42	14	2
1:A:81:ARG:HA	1:A:123:CYS:SG	0.52	2.43	4	1
1:A:14:ARG:HB3	1:A:15:PRO:HA	0.52	1.80	6	1
1:A:81:ARG:NH1	1:A:123:CYS:SG	0.52	2.80	10	1
1:A:98:VAL:O	1:A:102:ILE:HG12	0.52	2.05	17	1
1:A:50:ALA:HB2	1:A:93:LEU:CG	0.52	2.35	13	4
1:A:96:ASP:O	1:A:98:VAL:N	0.52	2.43	9	4
1:A:20:TRP:HB2	1:A:48:TRP:CZ2	0.52	2.39	3	1
1:A:50:ALA:CA	1:A:93:LEU:HG	0.52	2.35	13	1
1:A:18:ASN:C	1:A:20:TRP:N	0.52	2.62	20	2
1:A:11:HIS:CB	1:A:91:LEU:H	0.52	2.16	8	1
1:A:11:HIS:CG	1:A:88:ASN:ND2	0.52	2.78	15	1
1:A:50:ALA:HB3	1:A:93:LEU:HB3	0.52	1.82	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ASN:ND2	1:A:106:GLY:N	0.52	2.58	10	1
1:A:48:TRP:CA	1:A:81:ARG:HB2	0.52	2.35	16	1
1:A:81:ARG:HD2	1:A:123:CYS:SG	0.52	2.44	2	1
1:A:48:TRP:H	1:A:81:ARG:C	0.52	2.08	16	4
1:A:42:TRP:C	1:A:42:TRP:CE3	0.52	2.83	6	1
1:A:49:THR:CG2	1:A:80:ALA:HB1	0.52	2.33	4	2
1:A:50:ALA:HB2	1:A:93:LEU:CB	0.52	2.34	6	2
1:A:94:ASP:O	1:A:95:TRP:CB	0.52	2.58	11	1
1:A:6:VAL:N	1:A:115:ASN:HD21	0.52	2.02	13	1
1:A:51:PHE:C	1:A:86:CYS:SG	0.52	2.88	16	1
1:A:42:TRP:CZ3	1:A:45:LYS:CG	0.52	2.92	11	1
1:A:47:GLY:O	1:A:81:ARG:HB2	0.52	2.05	20	1
1:A:48:TRP:N	1:A:81:ARG:O	0.51	2.44	19	2
1:A:66:CYS:N	1:A:82:ILE:CG1	0.51	2.73	4	1
1:A:47:GLY:N	1:A:81:ARG:CB	0.51	2.73	5	1
1:A:78:ILE:CG2	1:A:98:VAL:HG13	0.51	2.35	9	2
1:A:95:TRP:O	1:A:96:ASP:C	0.51	2.49	20	2
1:A:10:TYR:CD1	1:A:10:TYR:N	0.51	2.79	2	3
1:A:12:TYR:HB2	1:A:95:TRP:HA	0.51	1.82	11	1
1:A:15:PRO:HB3	1:A:48:TRP:HE3	0.51	1.62	12	1
1:A:47:GLY:O	1:A:81:ARG:N	0.51	2.44	20	1
1:A:39:PRO:O	1:A:41:SER:N	0.51	2.43	1	1
1:A:20:TRP:CD1	1:A:43:ARG:CD	0.51	2.94	4	1
1:A:20:TRP:CD2	1:A:43:ARG:HD3	0.51	2.41	11	1
1:A:66:CYS:SG	1:A:81:ARG:CD	0.51	2.99	11	1
1:A:83:VAL:HG13	1:A:84:ASP:N	0.51	2.21	1	2
1:A:50:ALA:HB2	1:A:93:LEU:HG	0.51	1.82	13	4
1:A:34:TRP:O	1:A:38:LYS:NZ	0.50	2.44	10	1
1:A:65:LYS:C	1:A:82:ILE:CD1	0.50	2.80	4	1
1:A:40:LEU:C	1:A:41:SER:O	0.50	2.42	6	1
1:A:49:THR:HG22	1:A:82:ILE:HA	0.50	1.83	6	1
1:A:90:GLY:O	1:A:91:LEU:HB2	0.50	2.06	11	3
1:A:14:ARG:HD2	1:A:95:TRP:CD2	0.50	2.40	19	1
1:A:51:PHE:O	1:A:52:CYS:SG	0.50	2.69	7	1
1:A:42:TRP:HA	1:A:42:TRP:HE3	0.50	1.62	11	1
1:A:49:THR:OG1	1:A:51:PHE:CE2	0.50	2.65	15	1
1:A:56:GLY:N	1:A:57:PRO:CD	0.50	2.75	1	1
1:A:24:ALA:CB	1:A:27:VAL:HB	0.50	2.36	20	1
1:A:10:TYR:CD2	1:A:99:PHE:CE2	0.50	3.00	2	1
1:A:47:GLY:N	1:A:81:ARG:HG3	0.50	2.21	4	1
1:A:50:ALA:N	1:A:93:LEU:HB2	0.50	2.22	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:HIS:HB3	1:A:90:GLY:HA2	0.50	1.84	18	2
1:A:111:GLN:N	1:A:111:GLN:NE2	0.50	2.60	2	1
1:A:30:TYR:HB2	1:A:85:GLN:OE1	0.50	2.06	8	1
1:A:49:THR:HA	1:A:93:LEU:HB2	0.50	1.82	9	1
1:A:48:TRP:O	1:A:49:THR:HG23	0.50	2.07	4	1
1:A:46:TYR:CD2	1:A:81:ARG:CG	0.50	2.94	6	1
1:A:47:GLY:H	1:A:81:ARG:HA	0.50	1.66	3	1
1:A:71:ASN:ND2	1:A:74:THR:OG1	0.50	2.44	11	1
1:A:20:TRP:O	1:A:43:ARG:NH2	0.50	2.45	14	1
1:A:48:TRP:H	1:A:81:ARG:CA	0.49	2.20	3	4
1:A:48:TRP:NE1	1:A:93:LEU:HD13	0.49	2.22	4	1
1:A:107:ILE:H	1:A:107:ILE:CD1	0.49	2.20	4	1
1:A:51:PHE:CD2	1:A:64:GLY:O	0.49	2.65	4	1
1:A:65:LYS:HG2	1:A:67:LEU:HD12	0.49	1.83	4	1
1:A:48:TRP:O	1:A:93:LEU:HD13	0.49	2.06	20	1
1:A:58:ARG:NH1	1:A:58:ARG:O	0.49	2.46	4	1
1:A:66:CYS:HA	1:A:80:ALA:O	0.49	2.07	4	2
1:A:48:TRP:H	1:A:81:ARG:HB3	0.49	1.67	8	1
1:A:15:PRO:HD2	1:A:94:ASP:O	0.49	2.06	11	1
1:A:15:PRO:HG2	1:A:93:LEU:CD1	0.49	2.37	17	1
1:A:65:LYS:N	1:A:65:LYS:HD2	0.49	2.22	10	1
1:A:16:ALA:O	1:A:19:ASN:N	0.49	2.45	18	3
1:A:15:PRO:O	1:A:17:GLN:N	0.49	2.46	8	4
1:A:42:TRP:CD2	1:A:45:LYS:HD2	0.49	2.43	11	1
1:A:11:HIS:HB3	1:A:90:GLY:HA3	0.49	1.84	2	3
1:A:92:ASP:C	1:A:93:LEU:O	0.49	2.47	9	1
1:A:37:SER:O	1:A:39:PRO:HD2	0.49	2.07	6	1
1:A:95:TRP:CE3	1:A:96:ASP:HB2	0.49	2.43	17	2
1:A:81:ARG:HH12	1:A:83:VAL:CG2	0.49	2.20	7	1
1:A:81:ARG:NH1	1:A:82:ILE:N	0.49	2.60	4	1
1:A:51:PHE:HB3	1:A:58:ARG:NH2	0.49	2.23	9	1
1:A:88:ASN:OD1	1:A:88:ASN:N	0.49	2.46	10	2
1:A:58:ARG:NH2	1:A:84:ASP:O	0.49	2.45	17	1
1:A:20:TRP:CB	1:A:48:TRP:CZ2	0.49	2.96	15	1
1:A:68:ARG:NH1	1:A:70:THR:OG1	0.48	2.45	1	1
1:A:42:TRP:HA	1:A:45:LYS:HB3	0.48	1.85	5	1
1:A:15:PRO:HG2	1:A:93:LEU:HD12	0.48	1.85	17	1
1:A:65:LYS:C	1:A:82:ILE:HD13	0.48	2.28	4	1
1:A:20:TRP:CE2	1:A:48:TRP:CE3	0.48	3.01	7	2
1:A:13:TYR:CG	1:A:93:LEU:HB2	0.48	2.43	15	1
1:A:12:TYR:CD1	1:A:12:TYR:N	0.48	2.81	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:O	1:A:97:THR:N	0.48	2.46	18	3
1:A:42:TRP:CZ2	1:A:45:LYS:CE	0.48	2.96	11	1
1:A:51:PHE:CE1	1:A:53:GLY:N	0.48	2.82	12	1
1:A:95:TRP:CD1	1:A:96:ASP:HB3	0.48	2.43	15	1
1:A:95:TRP:C	1:A:97:THR:H	0.48	2.12	18	2
1:A:49:THR:HA	1:A:93:LEU:HD23	0.48	1.84	17	1
1:A:47:GLY:CA	1:A:96:ASP:OD1	0.48	2.61	20	1
1:A:50:ALA:N	1:A:93:LEU:N	0.48	2.53	9	1
1:A:22:LEU:HD21	1:A:48:TRP:CZ3	0.48	2.43	20	1
1:A:20:TRP:CZ3	1:A:48:TRP:CE3	0.48	3.02	1	3
1:A:48:TRP:HE1	1:A:83:VAL:CB	0.48	2.21	12	1
1:A:14:ARG:N	1:A:15:PRO:CD	0.48	2.76	14	3
1:A:11:HIS:N	1:A:91:LEU:N	0.48	2.62	8	1
1:A:67:LEU:CD2	1:A:118:TYR:CD1	0.48	2.97	13	1
1:A:29:ALA:HB1	1:A:84:ASP:CG	0.48	2.29	18	4
1:A:38:LYS:HB2	1:A:45:LYS:CB	0.48	2.39	6	1
1:A:48:TRP:CD1	1:A:48:TRP:O	0.48	2.66	3	4
1:A:18:ASN:O	1:A:19:ASN:C	0.48	2.52	20	4
1:A:95:TRP:C	1:A:97:THR:N	0.48	2.66	5	2
1:A:46:TYR:CD2	1:A:81:ARG:HG2	0.48	2.44	6	1
1:A:48:TRP:CB	1:A:81:ARG:HH12	0.48	2.22	8	1
1:A:58:ARG:NE	1:A:59:GLY:N	0.47	2.62	4	1
1:A:94:ASP:CG	1:A:95:TRP:N	0.47	2.68	3	1
1:A:13:TYR:HB2	1:A:93:LEU:CA	0.47	2.39	15	1
1:A:48:TRP:C	1:A:48:TRP:HD1	0.47	2.10	4	1
1:A:16:ALA:HA	1:A:20:TRP:CB	0.47	2.39	20	1
1:A:67:LEU:HD23	1:A:120:PHE:HA	0.47	1.87	4	1
1:A:72:PRO:CG	1:A:117:ASN:ND2	0.47	2.78	8	1
1:A:66:CYS:SG	1:A:123:CYS:N	0.47	2.87	4	1
1:A:67:LEU:HD13	1:A:118:TYR:CD1	0.47	2.44	4	1
1:A:41:SER:C	1:A:43:ARG:N	0.47	2.63	6	1
1:A:12:TYR:HA	1:A:92:ASP:O	0.47	2.09	18	3
1:A:30:TYR:CB	1:A:85:GLN:OE1	0.47	2.62	8	1
1:A:42:TRP:CE3	1:A:45:LYS:CB	0.47	2.97	11	1
1:A:15:PRO:HG3	1:A:94:ASP:O	0.47	2.09	15	1
1:A:35:ASP:HB3	1:A:43:ARG:NH1	0.47	2.25	17	1
1:A:68:ARG:O	1:A:118:TYR:HA	0.47	2.10	18	1
1:A:14:ARG:O	1:A:95:TRP:HB2	0.47	2.10	2	1
1:A:50:ALA:CA	1:A:93:LEU:HD12	0.47	2.40	4	2
1:A:15:PRO:C	1:A:20:TRP:HB3	0.47	2.30	6	1
1:A:40:LEU:C	1:A:43:ARG:HA	0.47	2.29	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:GLU:CD	1:A:58:ARG:HH11	0.47	2.11	12	1
1:A:11:HIS:HB3	1:A:90:GLY:H	0.47	1.69	12	1
1:A:48:TRP:O	1:A:48:TRP:CD2	0.47	2.67	15	1
1:A:15:PRO:CB	1:A:93:LEU:HD23	0.47	2.39	20	1
1:A:52:CYS:H	1:A:91:LEU:HA	0.47	1.68	15	1
1:A:35:ASP:OD1	1:A:38:LYS:NZ	0.47	2.47	2	1
1:A:97:THR:O	1:A:101:LYS:CG	0.47	2.63	5	1
1:A:51:PHE:C	1:A:51:PHE:CD1	0.47	2.88	8	2
1:A:42:TRP:O	1:A:81:ARG:NH2	0.47	2.48	8	1
1:A:97:THR:OG1	1:A:98:VAL:N	0.47	2.48	13	2
1:A:83:VAL:CG1	1:A:84:ASP:N	0.47	2.78	1	1
1:A:51:PHE:CG	1:A:64:GLY:CA	0.46	2.98	4	1
1:A:9:THR:OG1	1:A:90:GLY:N	0.46	2.49	5	1
1:A:51:PHE:HZ	1:A:59:GLY:HA2	0.46	1.66	7	1
1:A:11:HIS:H	1:A:90:GLY:C	0.46	2.13	20	2
1:A:12:TYR:HB2	1:A:94:ASP:OD1	0.46	2.10	10	1
1:A:16:ALA:CA	1:A:20:TRP:HB3	0.46	2.40	20	1
1:A:31:CYS:O	1:A:32:ALA:C	0.46	2.54	11	10
1:A:38:LYS:HB3	1:A:41:SER:HB3	0.46	1.86	6	1
1:A:48:TRP:O	1:A:93:LEU:HD11	0.46	2.11	13	1
1:A:92:ASP:HB2	1:A:94:ASP:OD1	0.46	2.11	1	1
1:A:65:LYS:N	1:A:82:ILE:HD13	0.46	2.26	4	1
1:A:106:GLY:O	1:A:108:GLY:N	0.46	2.48	17	2
1:A:65:LYS:O	1:A:81:ARG:NH1	0.46	2.49	2	1
1:A:20:TRP:HB3	1:A:48:TRP:CZ2	0.46	2.45	14	6
1:A:96:ASP:C	1:A:98:VAL:N	0.46	2.68	9	1
1:A:10:TYR:O	1:A:10:TYR:CD1	0.46	2.69	3	1
1:A:93:LEU:O	1:A:93:LEU:CD2	0.46	2.63	3	6
1:A:16:ALA:HA	1:A:20:TRP:HB3	0.46	1.86	20	1
1:A:118:TYR:CD1	1:A:118:TYR:O	0.46	2.69	11	6
1:A:46:TYR:CA	1:A:81:ARG:HG2	0.46	2.41	6	1
1:A:66:CYS:O	1:A:121:VAL:O	0.46	2.34	4	1
1:A:6:VAL:O	1:A:8:ALA:N	0.46	2.49	11	2
1:A:40:LEU:O	1:A:43:ARG:HG3	0.46	2.11	11	1
1:A:22:LEU:HD23	1:A:93:LEU:HD21	0.46	1.86	20	1
1:A:20:TRP:CG	1:A:48:TRP:HZ2	0.46	2.29	8	1
1:A:15:PRO:CG	1:A:94:ASP:HB3	0.46	2.41	9	1
1:A:49:THR:HB	1:A:92:ASP:HB2	0.46	1.88	18	1
1:A:35:ASP:O	1:A:37:SER:N	0.46	2.48	6	2
1:A:38:LYS:CB	1:A:45:LYS:HB2	0.46	2.41	6	1
1:A:11:HIS:H	1:A:90:GLY:CA	0.46	2.24	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PRO:HB2	1:A:20:TRP:CG	0.46	2.46	11	1
1:A:117:ASN:ND2	1:A:117:ASN:N	0.46	2.63	18	1
1:A:44:SER:CB	1:A:81:ARG:HH12	0.46	2.23	6	1
1:A:18:ASN:ND2	1:A:21:ASP:HB3	0.46	2.26	7	1
1:A:94:ASP:O	1:A:97:THR:CG2	0.45	2.63	4	1
1:A:52:CYS:SG	1:A:89:GLY:N	0.45	2.89	12	1
1:A:50:ALA:CB	1:A:93:LEU:HG	0.45	2.41	13	1
1:A:47:GLY:O	1:A:81:ARG:NH1	0.45	2.49	11	1
1:A:48:TRP:O	1:A:93:LEU:HD23	0.45	2.11	15	3
1:A:111:GLN:HE21	1:A:113:HIS:CE1	0.45	2.30	1	1
1:A:85:GLN:OE1	1:A:85:GLN:N	0.45	2.49	8	1
1:A:72:PRO:HG2	1:A:117:ASN:ND2	0.45	2.25	14	1
1:A:106:GLY:O	1:A:107:ILE:C	0.45	2.55	13	7
1:A:48:TRP:HB3	1:A:97:THR:HG21	0.45	1.87	7	1
1:A:14:ARG:HG2	1:A:14:ARG:O	0.45	2.11	14	1
1:A:114:LEU:HD23	1:A:114:LEU:H	0.45	1.71	14	1
1:A:14:ARG:CD	1:A:14:ARG:N	0.45	2.80	8	1
1:A:14:ARG:NH1	1:A:27:VAL:HG22	0.45	2.26	11	1
1:A:38:LYS:CB	1:A:45:LYS:CB	0.45	2.95	6	1
1:A:103:ASP:O	1:A:105:ASN:N	0.45	2.49	4	1
1:A:68:ARG:NH2	1:A:77:GLN:OE1	0.45	2.49	9	1
1:A:41:SER:O	1:A:45:LYS:HB2	0.45	2.12	2	3
1:A:105:ASN:ND2	1:A:106:GLY:H	0.45	2.10	10	1
1:A:13:TYR:HB3	1:A:93:LEU:CB	0.45	2.39	12	1
1:A:51:PHE:O	1:A:86:CYS:SG	0.45	2.75	16	1
1:A:94:ASP:OD2	1:A:99:PHE:HB2	0.45	2.12	2	1
1:A:20:TRP:CH2	1:A:48:TRP:CB	0.45	2.99	7	2
1:A:50:ALA:HA	1:A:84:ASP:HB3	0.45	1.87	12	2
1:A:52:CYS:H	1:A:91:LEU:HB2	0.45	1.71	5	1
1:A:50:ALA:CB	1:A:84:ASP:HB2	0.45	2.41	7	1
1:A:58:ARG:NH2	1:A:67:LEU:HD12	0.45	2.27	10	1
1:A:43:ARG:CD	1:A:43:ARG:C	0.45	2.85	11	1
1:A:12:TYR:HB2	1:A:94:ASP:HB3	0.45	1.87	17	1
1:A:47:GLY:CA	1:A:81:ARG:NE	0.44	2.80	1	1
1:A:47:GLY:O	1:A:48:TRP:C	0.44	2.55	9	1
1:A:81:ARG:CZ	1:A:81:ARG:HB3	0.44	2.42	4	1
1:A:35:ASP:HB3	1:A:43:ARG:CZ	0.44	2.41	17	1
1:A:105:ASN:H	1:A:105:ASN:ND2	0.44	2.10	6	1
1:A:81:ARG:NE	1:A:83:VAL:CG2	0.44	2.81	12	1
1:A:45:LYS:NZ	1:A:125:ASP:OD2	0.44	2.44	18	1
1:A:51:PHE:O	1:A:85:GLN:HA	0.44	2.12	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:SER:O	1:A:45:LYS:CB	0.44	2.65	2	1
1:A:49:THR:O	1:A:83:VAL:HG12	0.44	2.13	4	1
1:A:35:ASP:O	1:A:43:ARG:HD3	0.44	2.11	7	1
1:A:81:ARG:HH12	1:A:83:VAL:HG11	0.44	1.71	7	1
1:A:51:PHE:N	1:A:84:ASP:O	0.44	2.50	11	2
1:A:47:GLY:CA	1:A:81:ARG:HG3	0.44	2.42	4	1
1:A:50:ALA:O	1:A:92:ASP:HB3	0.44	2.13	4	1
1:A:86:CYS:SG	1:A:88:ASN:O	0.44	2.76	6	1
1:A:105:ASN:OD1	1:A:107:ILE:HG12	0.44	2.13	11	1
1:A:91:LEU:H	1:A:91:LEU:HD23	0.44	1.72	15	1
1:A:12:TYR:CD1	1:A:95:TRP:O	0.44	2.71	3	1
1:A:59:GLY:O	1:A:60:GLN:C	0.44	2.56	19	2
1:A:11:HIS:O	1:A:92:ASP:O	0.44	2.35	20	1
1:A:51:PHE:CE2	1:A:58:ARG:HD3	0.44	2.48	10	1
1:A:58:ARG:HB3	1:A:62:ALA:HB2	0.44	1.90	12	1
1:A:93:LEU:O	1:A:93:LEU:HD22	0.44	2.13	12	1
1:A:81:ARG:NH1	1:A:83:VAL:CG2	0.44	2.80	7	1
1:A:118:TYR:C	1:A:119:GLN:NE2	0.44	2.71	7	1
1:A:15:PRO:CB	1:A:48:TRP:HE1	0.44	2.26	16	1
1:A:96:ASP:O	1:A:101:LYS:HE2	0.43	2.13	2	2
1:A:96:ASP:HA	1:A:100:THR:HG23	0.43	1.89	3	2
1:A:11:HIS:N	1:A:90:GLY:CA	0.43	2.81	4	1
1:A:16:ALA:HA	1:A:20:TRP:N	0.43	2.27	19	1
1:A:84:ASP:OD1	1:A:84:ASP:N	0.43	2.51	5	1
1:A:48:TRP:HE1	1:A:83:VAL:HG11	0.43	1.73	12	1
1:A:50:ALA:CB	1:A:93:LEU:CB	0.43	2.91	12	2
1:A:5:ASP:CG	1:A:117:ASN:HD21	0.43	2.16	17	1
1:A:16:ALA:O	1:A:17:GLN:C	0.43	2.57	2	1
1:A:10:TYR:OH	1:A:109:TYR:HA	0.43	2.14	8	1
1:A:3:ALA:HB3	1:A:118:TYR:CE1	0.43	2.48	14	2
1:A:96:ASP:HA	1:A:100:THR:CG2	0.43	2.44	4	1
1:A:85:GLN:N	1:A:85:GLN:CD	0.43	2.72	8	1
1:A:51:PHE:HA	1:A:91:LEU:O	0.43	2.13	9	2
1:A:81:ARG:HB3	1:A:81:ARG:CZ	0.43	2.43	17	1
1:A:16:ALA:HA	1:A:20:TRP:H	0.43	1.73	19	1
1:A:107:ILE:O	1:A:108:GLY:C	0.43	2.56	20	1
1:A:99:PHE:C	1:A:101:LYS:N	0.43	2.72	3	1
1:A:43:ARG:C	1:A:45:LYS:N	0.43	2.68	11	1
1:A:105:ASN:CG	1:A:106:GLY:N	0.43	2.72	13	1
1:A:66:CYS:SG	1:A:81:ARG:HA	0.43	2.53	18	1
1:A:91:LEU:HD23	1:A:91:LEU:O	0.43	2.13	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:OH	1:A:109:TYR:CD2	0.43	2.69	4	1
1:A:103:ASP:O	1:A:106:GLY:N	0.43	2.52	5	1
1:A:62:ALA:C	1:A:64:GLY:H	0.43	2.17	8	1
1:A:100:THR:OG1	1:A:101:LYS:N	0.43	2.52	18	1
1:A:67:LEU:CD2	1:A:120:PHE:HA	0.43	2.44	4	1
1:A:20:TRP:CD1	1:A:20:TRP:N	0.43	2.86	12	3
1:A:49:THR:CB	1:A:94:ASP:OD1	0.43	2.67	11	1
1:A:6:VAL:N	1:A:115:ASN:ND2	0.43	2.66	13	1
1:A:45:LYS:O	1:A:81:ARG:NE	0.43	2.51	19	1
1:A:10:TYR:CD1	1:A:112:GLY:O	0.43	2.72	6	1
1:A:22:LEU:CD2	1:A:93:LEU:HD21	0.43	2.44	8	1
1:A:9:THR:HG22	1:A:113:HIS:CB	0.43	2.44	13	1
1:A:83:VAL:HG11	1:A:93:LEU:HD11	0.43	1.90	13	1
1:A:20:TRP:CE2	1:A:43:ARG:NH1	0.43	2.86	11	1
1:A:84:ASP:CG	1:A:85:GLN:N	0.43	2.72	17	2
1:A:22:LEU:HD21	1:A:48:TRP:CE3	0.43	2.48	20	1
1:A:19:ASN:O	1:A:43:ARG:NH1	0.42	2.52	4	2
1:A:80:ALA:HB2	1:A:98:VAL:CG2	0.42	2.43	9	1
1:A:4:ASN:ND2	1:A:5:ASP:OD2	0.42	2.52	10	1
1:A:42:TRP:CE3	1:A:45:LYS:CD	0.42	3.02	11	1
1:A:49:THR:CA	1:A:93:LEU:HD23	0.42	2.44	17	1
1:A:91:LEU:O	1:A:91:LEU:CG	0.42	2.67	20	1
1:A:42:TRP:O	1:A:44:SER:C	0.42	2.57	6	1
1:A:15:PRO:CB	1:A:20:TRP:CE3	0.42	3.02	15	1
1:A:11:HIS:ND1	1:A:88:ASN:O	0.42	2.52	17	1
1:A:12:TYR:CB	1:A:94:ASP:HB3	0.42	2.44	17	1
1:A:58:ARG:NE	1:A:58:ARG:C	0.42	2.72	4	1
1:A:14:ARG:CB	1:A:15:PRO:HA	0.42	2.44	6	1
1:A:46:TYR:CB	1:A:81:ARG:HG2	0.42	2.44	6	1
1:A:2:GLN:HB3	1:A:119:GLN:HE22	0.42	1.74	12	1
1:A:56:GLY:O	1:A:58:ARG:NH1	0.42	2.52	9	1
1:A:48:TRP:O	1:A:93:LEU:CD1	0.42	2.68	13	1
1:A:93:LEU:HD22	1:A:93:LEU:O	0.42	2.15	14	1
1:A:22:LEU:CG	1:A:48:TRP:CH2	0.42	3.01	16	1
1:A:66:CYS:HB2	1:A:121:VAL:O	0.42	2.15	4	1
1:A:45:LYS:C	1:A:45:LYS:HD3	0.42	2.35	6	1
1:A:9:THR:OG1	1:A:90:GLY:HA2	0.42	2.14	8	1
1:A:96:ASP:C	1:A:100:THR:HG23	0.42	2.35	18	1
1:A:48:TRP:HA	1:A:81:ARG:CB	0.42	2.45	20	1
1:A:38:LYS:HB3	1:A:45:LYS:HB2	0.42	1.91	6	1
1:A:58:ARG:HG3	1:A:62:ALA:HB2	0.42	1.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:PRO:O	1:A:74:THR:N	0.42	2.53	20	2
1:A:51:PHE:CD1	1:A:64:GLY:HA2	0.42	2.50	4	1
1:A:107:ILE:HD12	1:A:107:ILE:N	0.42	2.27	4	1
1:A:48:TRP:O	1:A:93:LEU:HD22	0.42	2.14	9	1
1:A:48:TRP:H	1:A:97:THR:CB	0.42	2.27	12	1
1:A:84:ASP:N	1:A:84:ASP:OD1	0.42	2.53	6	1
1:A:106:GLY:C	1:A:108:GLY:N	0.42	2.73	9	1
1:A:95:TRP:O	1:A:100:THR:HG21	0.42	2.15	10	1
1:A:20:TRP:NE1	1:A:43:ARG:NH1	0.42	2.67	11	1
1:A:35:ASP:O	1:A:38:LYS:N	0.42	2.53	12	1
1:A:114:LEU:HG	1:A:115:ASN:H	0.42	1.75	13	1
1:A:95:TRP:CD1	1:A:99:PHE:HB3	0.42	2.50	4	1
1:A:46:TYR:CG	1:A:81:ARG:HG2	0.42	2.50	6	1
1:A:93:LEU:O	1:A:93:LEU:HD13	0.42	2.15	14	1
1:A:20:TRP:CZ3	1:A:48:TRP:NE1	0.41	2.88	9	2
1:A:5:ASP:N	1:A:117:ASN:OD1	0.41	2.53	10	1
1:A:38:LYS:NZ	1:A:42:TRP:CZ2	0.41	2.87	12	1
1:A:13:TYR:HB2	1:A:93:LEU:HA	0.41	1.92	15	1
1:A:18:ASN:O	1:A:20:TRP:N	0.41	2.53	2	1
1:A:51:PHE:HB3	1:A:64:GLY:HA3	0.41	1.92	4	1
1:A:43:ARG:O	1:A:44:SER:C	0.41	2.57	11	1
1:A:114:LEU:H	1:A:114:LEU:CD2	0.41	2.27	14	1
1:A:22:LEU:CD1	1:A:48:TRP:CZ3	0.41	3.04	15	1
1:A:67:LEU:HD21	1:A:118:TYR:CD1	0.41	2.50	20	1
1:A:5:ASP:O	1:A:7:ARG:NH2	0.41	2.53	6	1
1:A:11:HIS:HB2	1:A:90:GLY:CA	0.41	2.45	6	1
1:A:47:GLY:CA	1:A:81:ARG:HB3	0.41	2.45	6	1
1:A:11:HIS:CB	1:A:90:GLY:CA	0.41	2.99	19	1
1:A:22:LEU:HD11	1:A:48:TRP:CZ3	0.41	2.51	19	1
1:A:52:CYS:H	1:A:91:LEU:CB	0.41	2.28	20	1
1:A:42:TRP:CZ2	1:A:47:GLY:HA3	0.41	2.50	4	1
1:A:58:ARG:HH22	1:A:84:ASP:HA	0.41	1.76	5	1
1:A:6:VAL:O	1:A:115:ASN:ND2	0.41	2.53	6	1
1:A:12:TYR:CB	1:A:94:ASP:OD1	0.41	2.69	10	1
1:A:14:ARG:O	1:A:16:ALA:N	0.41	2.54	14	1
1:A:9:THR:OG1	1:A:89:GLY:C	0.41	2.59	17	1
1:A:29:ALA:HB1	1:A:84:ASP:HB2	0.41	1.91	17	1
1:A:12:TYR:CG	1:A:94:ASP:CB	0.41	3.03	2	1
1:A:51:PHE:HB2	1:A:65:LYS:HG3	0.41	1.93	4	1
1:A:65:LYS:HG2	1:A:67:LEU:CG	0.41	2.45	4	1
1:A:20:TRP:CZ2	1:A:48:TRP:CE3	0.41	3.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:CA	1:A:90:GLY:HA3	0.41	2.46	9	1
1:A:103:ASP:O	1:A:104:THR:C	0.41	2.59	9	1
1:A:49:THR:HA	1:A:93:LEU:HD12	0.41	1.93	13	1
1:A:15:PRO:HB3	1:A:48:TRP:CZ3	0.41	2.50	1	1
1:A:47:GLY:HA3	1:A:81:ARG:CZ	0.41	2.46	1	1
1:A:35:ASP:CG	1:A:83:VAL:HG23	0.41	2.35	4	1
1:A:31:CYS:O	1:A:35:ASP:N	0.41	2.54	7	1
1:A:82:ILE:O	1:A:85:GLN:NE2	0.41	2.54	8	1
1:A:96:ASP:O	1:A:99:PHE:N	0.41	2.54	9	2
1:A:48:TRP:HE1	1:A:83:VAL:CG1	0.41	2.29	12	1
1:A:85:GLN:O	1:A:85:GLN:NE2	0.41	2.54	15	1
1:A:11:HIS:CB	1:A:88:ASN:O	0.41	2.69	17	1
1:A:3:ALA:N	1:A:119:GLN:NE2	0.41	2.69	18	1
1:A:9:THR:C	1:A:91:LEU:H	0.41	2.20	20	1
1:A:96:ASP:O	1:A:101:LYS:CE	0.41	2.69	2	1
1:A:42:TRP:HA	1:A:45:LYS:CB	0.41	2.46	5	1
1:A:60:GLN:O	1:A:62:ALA:N	0.41	2.54	5	1
1:A:20:TRP:CD1	1:A:43:ARG:NH1	0.41	2.88	11	1
1:A:51:PHE:CE1	1:A:52:CYS:O	0.41	2.74	13	1
1:A:13:TYR:O	1:A:93:LEU:C	0.41	2.58	16	1
1:A:96:ASP:OD2	1:A:101:LYS:NZ	0.41	2.53	17	1
1:A:44:SER:HB2	1:A:81:ARG:CZ	0.40	2.45	6	1
1:A:95:TRP:O	1:A:95:TRP:CD2	0.40	2.74	6	1
1:A:17:GLN:HG3	1:A:18:ASN:N	0.40	2.31	7	1
1:A:96:ASP:O	1:A:97:THR:C	0.40	2.59	9	1
1:A:62:ALA:O	1:A:65:LYS:N	0.40	2.54	13	1
1:A:49:THR:OG1	1:A:92:ASP:HB2	0.40	2.16	14	1
1:A:93:LEU:HD23	1:A:93:LEU:O	0.40	2.16	17	1
1:A:114:LEU:HG	1:A:115:ASN:N	0.40	2.31	17	1
1:A:51:PHE:CD1	1:A:51:PHE:C	0.40	2.95	19	1
1:A:96:ASP:HA	1:A:100:THR:HG21	0.40	1.92	4	1
1:A:10:TYR:O	1:A:12:TYR:CD2	0.40	2.75	9	2
1:A:48:TRP:C	1:A:81:ARG:O	0.40	2.60	5	1
1:A:20:TRP:CZ3	1:A:95:TRP:HB2	0.40	2.52	6	1
1:A:48:TRP:CA	1:A:81:ARG:HB3	0.40	2.46	8	1
1:A:9:THR:O	1:A:90:GLY:O	0.40	2.39	10	1
1:A:15:PRO:CG	1:A:94:ASP:O	0.40	2.70	15	1
1:A:20:TRP:CE3	1:A:48:TRP:CH2	0.40	3.10	1	1
1:A:80:ALA:HA	1:A:81:ARG:CZ	0.40	2.45	1	1
1:A:22:LEU:CD2	1:A:93:LEU:HD11	0.40	2.46	6	1
1:A:91:LEU:HD23	1:A:91:LEU:N	0.40	2.31	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LYS:NZ	1:A:46:TYR:CD2	0.40	2.80	10	1
1:A:4:ASN:O	1:A:5:ASP:C	0.40	2.59	11	1
1:A:51:PHE:CE1	1:A:58:ARG:NE	0.40	2.87	13	1
1:A:71:ASN:OD1	1:A:71:ASN:C	0.40	2.59	2	1
1:A:43:ARG:HG3	1:A:48:TRP:CE3	0.40	2.51	4	1
1:A:20:TRP:C	1:A:22:LEU:H	0.40	2.20	11	1
1:A:48:TRP:H	1:A:97:THR:HG21	0.40	1.76	12	1
1:A:15:PRO:HG2	1:A:16:ALA:H	0.40	1.76	15	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	123/125 (98%)	79±5 (64±4%)	30±4 (25±3%)	14±3 (11±3%)	1	8
All	All	2460/2500 (98%)	1572 (64%)	608 (25%)	280 (11%)	1	8

All 61 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	91	LEU	16
1	A	107	ILE	16
1	A	28	SER	13
1	A	15	PRO	12
1	A	16	ALA	12
1	A	63	CYS	12
1	A	100	THR	12
1	A	22	LEU	10
1	A	26	ALA	10
1	A	14	ARG	9
1	A	41	SER	8
1	A	54	PRO	8
1	A	48	TRP	8
1	A	30	TYR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	56	GLY	6
1	A	95	TRP	6
1	A	97	THR	6
1	A	96	ASP	6
1	A	25	PRO	5
1	A	20	TRP	5
1	A	21	ASP	5
1	A	99	PHE	5
1	A	47	GLY	5
1	A	17	GLN	4
1	A	60	GLN	4
1	A	59	GLY	4
1	A	94	ASP	4
1	A	104	THR	4
1	A	73	ALA	4
1	A	64	GLY	3
1	A	36	ALA	3
1	A	39	PRO	3
1	A	61	ALA	3
1	A	72	PRO	3
1	A	19	ASN	2
1	A	40	LEU	2
1	A	113	HIS	2
1	A	57	PRO	2
1	A	43	ARG	2
1	A	83	VAL	2
1	A	45	LYS	2
1	A	82	ILE	2
1	A	33	THR	2
1	A	90	GLY	2
1	A	7	ARG	2
1	A	112	GLY	2
1	A	38	LYS	1
1	A	42	TRP	1
1	A	44	SER	1
1	A	46	TYR	1
1	A	106	GLY	1
1	A	109	TYR	1
1	A	87	ALA	1
1	A	102	ILE	1
1	A	89	GLY	1
1	A	103	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	111	GLN	1
1	A	124	ARG	1
1	A	23	GLY	1
1	A	24	ALA	1
1	A	27	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	97/97 (100%)	78±3 (80±3%)	19±3 (20±3%)	4 34
All	All	1940/1940 (100%)	1555 (80%)	385 (20%)	4 34

All 67 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	30	TYR	20
1	A	93	LEU	19
1	A	100	THR	18
1	A	121	VAL	17
1	A	91	LEU	16
1	A	46	TYR	15
1	A	10	TYR	14
1	A	86	CYS	14
1	A	52	CYS	13
1	A	20	TRP	12
1	A	58	ARG	12
1	A	48	TRP	11
1	A	67	LEU	11
1	A	13	TYR	10
1	A	81	ARG	10
1	A	119	GLN	10
1	A	40	LEU	9
1	A	12	TYR	7
1	A	99	PHE	7
1	A	115	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	14	ARG	6
1	A	88	ASN	6
1	A	35	ASP	5
1	A	97	THR	5
1	A	103	ASP	5
1	A	15	PRO	5
1	A	104	THR	5
1	A	18	ASN	5
1	A	124	ARG	5
1	A	94	ASP	4
1	A	17	GLN	4
1	A	110	GLN	4
1	A	113	HIS	4
1	A	78	ILE	4
1	A	19	ASN	3
1	A	105	ASN	3
1	A	42	TRP	3
1	A	4	ASN	3
1	A	7	ARG	3
1	A	9	THR	3
1	A	38	LYS	3
1	A	43	ARG	3
1	A	83	VAL	3
1	A	111	GLN	2
1	A	51	PHE	2
1	A	95	TRP	2
1	A	122	ASP	2
1	A	77	GLN	2
1	A	96	ASP	2
1	A	116	VAL	2
1	A	49	THR	2
1	A	92	ASP	2
1	A	31	CYS	2
1	A	85	GLN	2
1	A	2	GLN	2
1	A	22	LEU	2
1	A	114	LEU	2
1	A	84	ASP	2
1	A	118	TYR	2
1	A	66	CYS	1
1	A	82	ILE	1
1	A	33	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	5	ASP	1
1	A	65	LYS	1
1	A	45	LYS	1
1	A	1	GLU	1
1	A	68	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided