Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 06:47 PM EDT

PDB ID	:	1BW3
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:

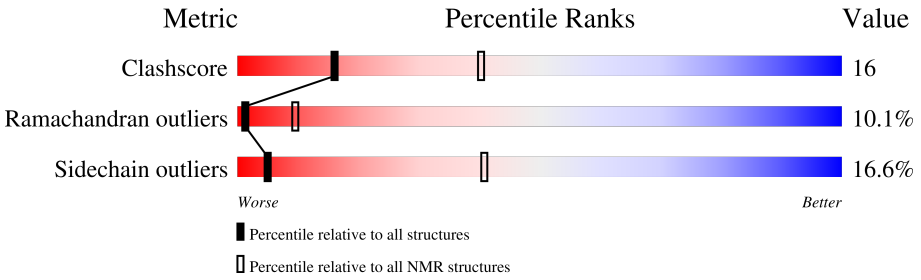
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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	55% 33% 8% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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)	1.57	6

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

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 (i)

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: 55% 33% 8% •

E1 R7 A8 T9 Y10 H11 Y12 Y13 R14 P15 A16 Q17 N18 N19 W20 D21 L22 S28 A29 Y30 C31 W34 D35 L40 S41 W42 R43 Y46 G47 W48 T49 A50 F51 R58 G59 L67 R68 R81 I82 V83 D84 Q85 C86 L91 D92 L93 D94 W95 D96 T97 V98

F99 T100 K101 I102 D103 T104 N105 G106 I107 G108 Y109 H113 Q119 F120 V121 D122 C123 R124 D125

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: 56% 34% 6% 5%

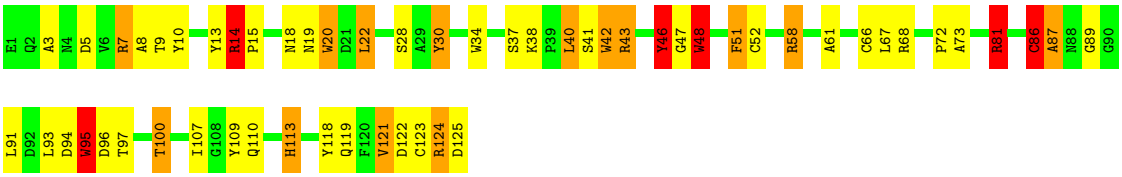
E1 Q2 A3 R7 A8 T9 Y13 R14 P15 A16 Q17 N18 N19 W20 D21 S28 A29 Y30 C31 W34 D35 A36 S37 K38 P39 L40 S41 W42 R43 Y46 G47 W48 F51 R58 A62 C63 L67 R68 R81 I82 V83 D84 Q85 C86 A87 N88 L91 D92 L93

D94 W95 D96 T97 V98 F99 T100 D103 Y109 H113 Y118 Q119 F120 V121 D122 C123 R124 D125

4.2.2 Score per residue for model 2

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

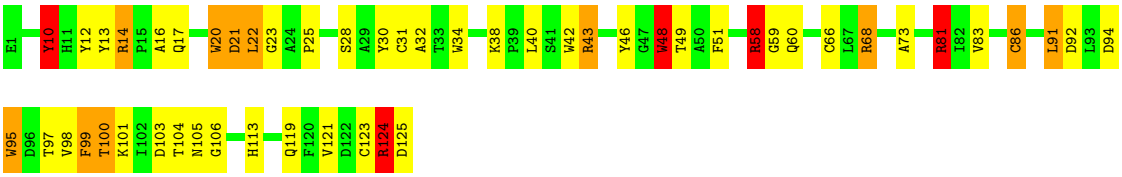
Chain A: 55% 29% 11% 5%



4.2.3 Score per residue for model 3

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

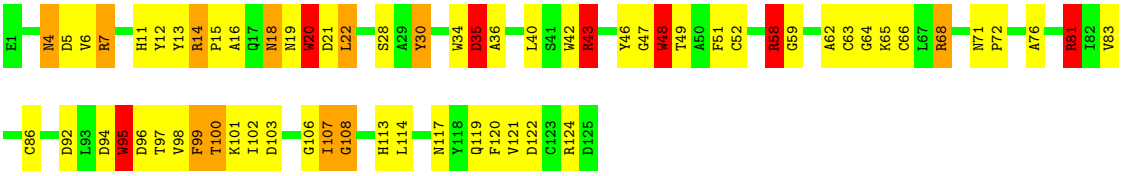
Chain A: 58% 29% 9% •



4.2.4 Score per residue for model 4

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

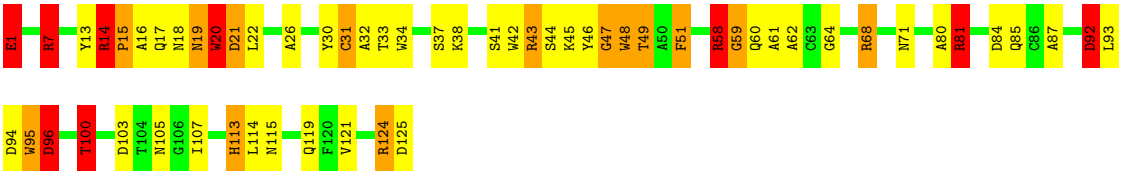
Chain A: 48% 38% 9% 6%



4.2.5 Score per residue for model 5

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 53% 29% 11% 7%



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 63% 26% 8% •

E1 N4 R7 Y12 Y13 R14 P15 N19 W20 D21 L22 A26 Y30 C31 W34 P39 L40 S41 W42 R43 W48 G53 G56 P57 R58 G59 Q60 L67 P72 R81 D84 N88 D92 L93 D94 W95 D96 T97 V98 F99 T100 K101

G106 H113 L114 N115 V116 N117 Y118 Q119 F120 V121 D122 C123 R124 D125

4.2.7 Score per residue for model 7

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 55% 30% 10% 5%

E1 Q2 A3 R7 A8 T9 Y10 H11 Y12 Y13 R14 P15 N18 N19 W20 D21 L22 G23 A24 Y30 C31 A32 T33 W34 D35 P39 L40 S41 W42 R43 Y46 G47 W48 F51 C52 G53 P54 R58 G59 Q60 A61 A62 C63 G64 K65 C66 L67 R68 Q77 R81 I82

V83 D84 G90 L91 D92 L93 D94 W95 D96 T97 V98 F99 T100 K101 H113 Y118 Q119 F120 V121 D122 C123 R124 D125

4.2.8 Score per residue for model 8

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 60% 25% 10% 6%

E1 R7 Y10 H11 Y12 Y13 R14 P15 N18 N19 W20 D21 L22 G23 S28 A29 Y30 C31 A32 T33 W34 D35 K38 P39 L40 S41 W42 R43 Y46 G47 W48 F51 C52 G53 R58 G59 Q60 A61 R68 R81 Q85 G90 L91 D92 L93 D94 W95 D96

T97 V98 F99 T100 K101 Y109 G112 H113 Q119 F120 V121 D122 C123 R124 D125

4.2.9 Score per residue for model 9

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 52% 36% 8% •

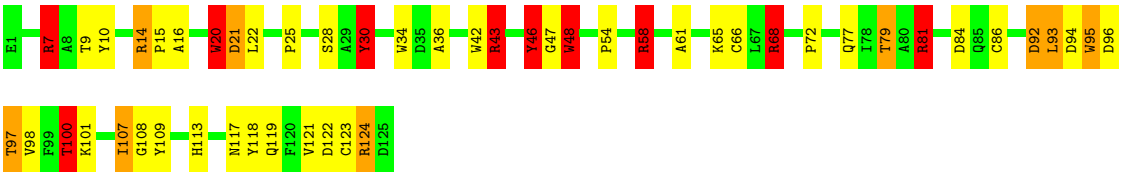
E1 N4 D5 V6 R7 A8 T9 Y10 H11 Y12 Y13 R14 P15 W20 D21 L22 S28 A29 Y30 C31 W34 D35 P39 W42 R43 S44 K45 Y46 G47 W48 T49 G56 P57 R58 G59 Q60 C63 G64 K65 C66 L67 R68 P72 Q77 R81 I82 V83 D84 Q85

C86 L91 D92 L93 D94 W95 D96 F99 T100 K101 I102 D103 T104 I107 Q110 H113 L114 N115 Y118 Q119 F120 V121 D122 C123 R124 D125

4.2.10 Score per residue for model 10

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

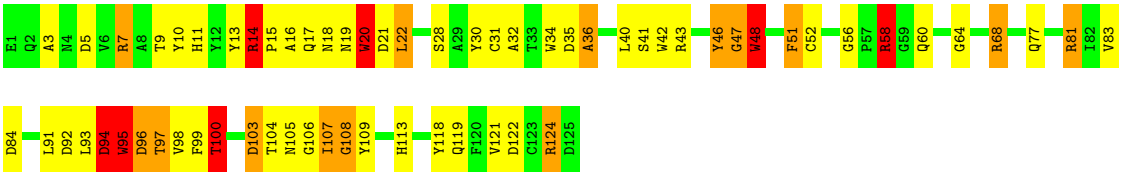
Chain A: 59% 26% 7% 8%



4.2.11 Score per residue for model 11

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

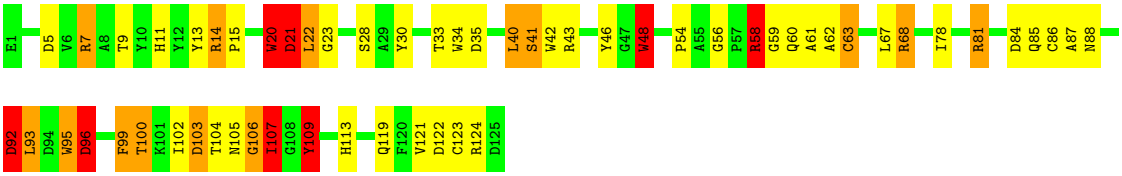
Chain A: 49% 34% 11% 6%



4.2.12 Score per residue for model 12

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

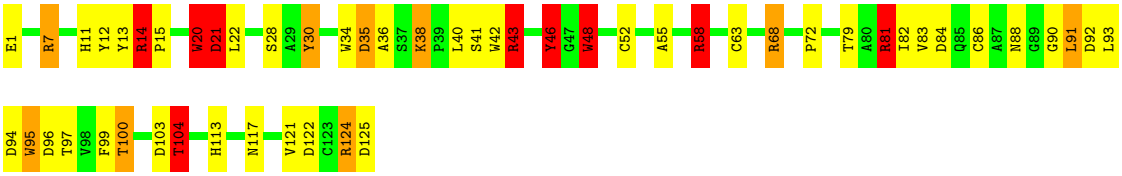
Chain A: 54% 29% 11% 6%



4.2.13 Score per residue for model 13

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

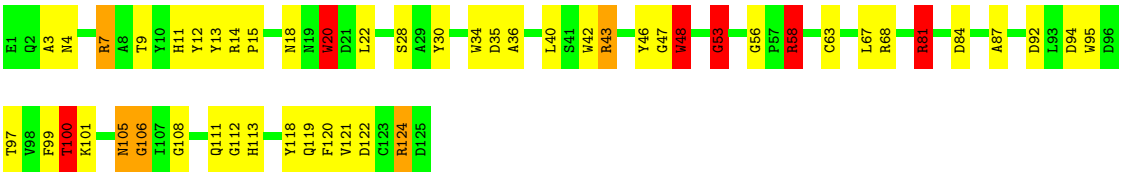
Chain A: 58% 28% 7% 7%



4.2.14 Score per residue for model 14

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

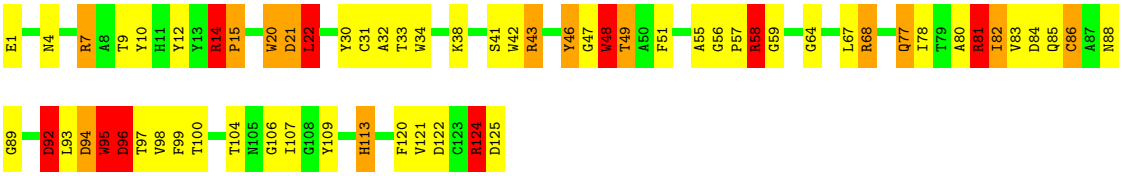
Chain A: 59% 32% • 5%



4.2.15 Score per residue for model 15

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

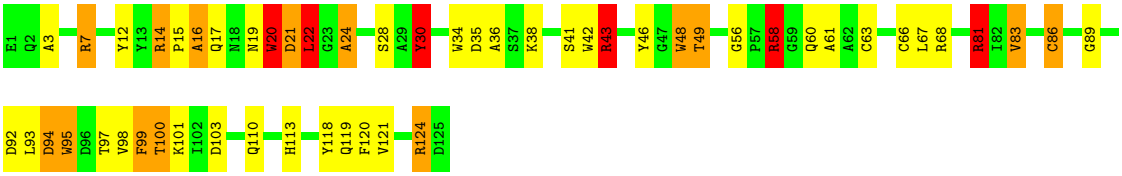
Chain A: 50% 33% 10% 7%



4.2.16 Score per residue for model 16

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

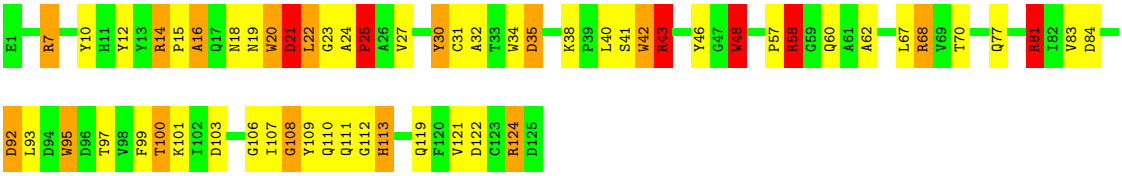
Chain A: 58% 26% 11% 5%



4.2.17 Score per residue for model 17

• Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

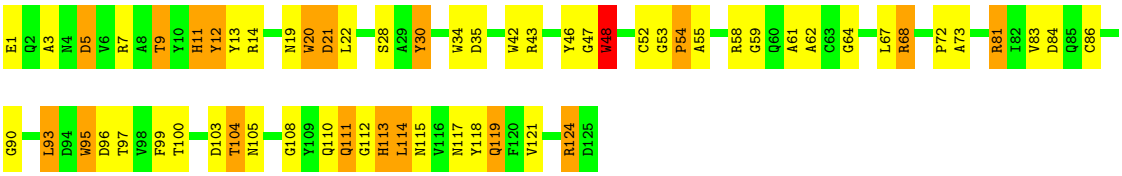
Chain A: 54% 30% 12% 5%



4.2.18 Score per residue for model 18

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

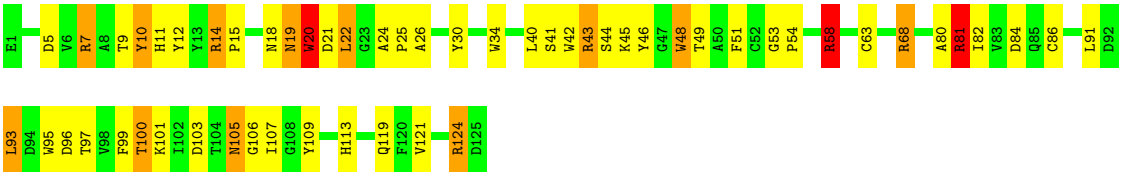
Chain A: 51% 34% 14% •



4.2.19 Score per residue for model 19

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

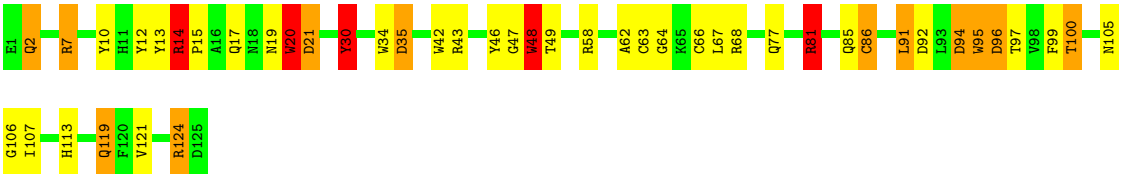
Chain A: 56% 32% 10% •



4.2.20 Score per residue for model 20

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 63% 23% 10% •



5 Refinement protocol and experimental data overview (i)

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	1.56±0.02	3±1/995 (0.3± 0.1%)	1.85±0.05	35±5/1358 (2.6± 0.3%)
All	All	1.56	54/19900 (0.3%)	1.85	699/27160 (2.6%)

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	6.6±0.7
All	All	0	132

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	48	TRP	CA-CB	7.92	1.71	1.53	5	1
1	A	48	TRP	CG-CD2	-7.40	1.31	1.43	4	9
1	A	20	TRP	CG-CD2	-6.45	1.32	1.43	15	3
1	A	81	ARG	CZ-NH1	-6.44	1.24	1.33	4	5
1	A	48	TRP	NE1-CE2	-6.24	1.29	1.37	6	8
1	A	43	ARG	CZ-NH2	-5.59	1.25	1.33	17	3
1	A	43	ARG	CZ-NH1	-5.57	1.25	1.33	4	2
1	A	34	TRP	CG-CD2	-5.57	1.34	1.43	6	12
1	A	95	TRP	CG-CD2	-5.38	1.34	1.43	14	3
1	A	47	GLY	N-CA	5.37	1.54	1.46	5	1
1	A	58	ARG	CZ-NH2	-5.25	1.26	1.33	10	1
1	A	42	TRP	CG-CD2	-5.20	1.34	1.43	13	1
1	A	48	TRP	CD2-CE2	-5.14	1.35	1.41	12	2
1	A	7	ARG	CZ-NH2	-5.08	1.26	1.33	10	1
1	A	124	ARG	CZ-NH2	-5.03	1.26	1.33	3	1
1	A	89	GLY	N-CA	5.03	1.53	1.46	2	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	81	ARG	NE-CZ-NH2	-21.50	109.55	120.30	9	8
1	A	81	ARG	NE-CZ-NH1	-19.65	110.47	120.30	4	12
1	A	58	ARG	NE-CZ-NH2	-17.36	111.62	120.30	10	8
1	A	68	ARG	NE-CZ-NH1	-16.81	111.89	120.30	5	8
1	A	10	TYR	CB-CG-CD2	-12.07	113.76	121.00	8	3
1	A	35	ASP	CB-CG-OD2	-11.66	107.81	118.30	18	9
1	A	14	ARG	NE-CZ-NH2	-11.48	114.56	120.30	13	6
1	A	10	TYR	CB-CG-CD1	11.08	127.65	121.00	8	2
1	A	43	ARG	NE-CZ-NH2	-11.03	114.79	120.30	7	9
1	A	7	ARG	NE-CZ-NH1	-10.72	114.94	120.30	5	12
1	A	89	GLY	N-CA-C	10.71	139.87	113.10	2	1
1	A	7	ARG	NE-CZ-NH2	-10.59	115.00	120.30	4	4
1	A	124	ARG	NE-CZ-NH2	-10.45	115.07	120.30	3	11
1	A	96	ASP	CB-CG-OD2	-10.38	108.96	118.30	13	6
1	A	14	ARG	NE-CZ-NH1	-10.15	115.22	120.30	10	11
1	A	95	TRP	CD1-NE1-CE2	9.92	117.93	109.00	18	20
1	A	58	ARG	NE-CZ-NH1	-9.78	115.41	120.30	16	5
1	A	42	TRP	CD1-NE1-CE2	9.72	117.75	109.00	17	20
1	A	92	ASP	CB-CG-OD2	-9.64	109.62	118.30	13	9
1	A	48	TRP	CD1-NE1-CE2	9.29	117.36	109.00	18	18
1	A	34	TRP	CD1-NE1-CE2	9.22	117.30	109.00	3	20
1	A	24	ALA	N-CA-C	9.20	135.85	111.00	17	1
1	A	58	ARG	NH1-CZ-NH2	9.11	129.42	119.40	10	2
1	A	20	TRP	CB-CG-CD1	-9.06	115.22	127.00	6	9
1	A	81	ARG	N-CA-CB	-8.96	94.48	110.60	16	4
1	A	48	TRP	CG-CD1-NE1	-8.93	101.17	110.10	20	20
1	A	43	ARG	NE-CZ-NH1	-8.91	115.84	120.30	19	3
1	A	20	TRP	CD1-NE1-CE2	8.87	116.98	109.00	13	20
1	A	20	TRP	NE1-CE2-CZ2	8.79	140.07	130.40	19	15
1	A	81	ARG	NH1-CZ-NH2	8.78	129.06	119.40	16	5
1	A	46	TYR	CB-CG-CD2	-8.78	115.73	121.00	15	4
1	A	42	TRP	NE1-CE2-CZ2	8.70	139.97	130.40	13	18
1	A	106	GLY	N-CA-C	8.58	134.54	113.10	12	1
1	A	68	ARG	NE-CZ-NH2	-8.42	116.09	120.30	18	7
1	A	103	ASP	CB-CG-OD2	-8.37	110.76	118.30	12	6
1	A	34	TRP	NE1-CE2-CZ2	8.35	139.58	130.40	8	20
1	A	95	TRP	CG-CD1-NE1	-8.31	101.79	110.10	18	20
1	A	84	ASP	CB-CG-OD2	-8.29	110.83	118.30	7	7
1	A	20	TRP	CG-CD1-NE1	-8.28	101.82	110.10	17	17
1	A	48	TRP	CB-CG-CD1	-8.22	116.31	127.00	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	53	GLY	N-CA-C	8.10	133.34	113.10	8	2
1	A	100	THR	OG1-CB-CG2	-8.05	91.49	110.00	4	15
1	A	30	TYR	CB-CG-CD1	-8.03	116.18	121.00	10	4
1	A	124	ARG	NE-CZ-NH1	-8.03	116.29	120.30	17	5
1	A	48	TRP	NE1-CE2-CZ2	8.01	139.21	130.40	4	5
1	A	122	ASP	CB-CG-OD2	-7.83	111.25	118.30	7	7
1	A	34	TRP	CG-CD1-NE1	-7.77	102.33	110.10	6	20
1	A	46	TYR	CB-CG-CD1	7.67	125.60	121.00	15	4
1	A	42	TRP	CG-CD1-NE1	-7.61	102.49	110.10	9	20
1	A	48	TRP	CG-CD2-CE3	7.59	140.73	133.90	6	4
1	A	95	TRP	NE1-CE2-CZ2	7.57	138.72	130.40	19	19
1	A	21	ASP	N-CA-C	-7.55	90.61	111.00	3	1
1	A	22	LEU	CB-CG-CD2	-7.55	98.17	111.00	15	1
1	A	92	ASP	CB-CG-OD1	-7.53	111.52	118.30	10	2
1	A	30	TYR	CB-CG-CD2	7.33	125.40	121.00	10	3
1	A	125	ASP	CB-CG-OD2	-7.33	111.71	118.30	7	4
1	A	20	TRP	NE1-CE2-CD2	-7.12	100.18	107.30	8	10
1	A	94	ASP	CB-CG-OD1	-7.07	111.93	118.30	10	3
1	A	20	TRP	CD1-CG-CD2	7.04	111.93	106.30	17	1
1	A	21	ASP	CB-CG-OD1	-6.98	112.02	118.30	18	2
1	A	20	TRP	CB-CG-CD2	6.92	135.59	126.60	6	4
1	A	21	ASP	N-CA-CB	-6.89	98.19	110.60	17	3
1	A	5	ASP	CB-CG-OD1	-6.76	112.21	118.30	18	5
1	A	10	TYR	N-CA-C	6.69	129.06	111.00	8	1
1	A	22	LEU	CB-CG-CD1	-6.67	99.65	111.00	8	2
1	A	48	TRP	CD1-CG-CD2	6.66	111.63	106.30	3	6
1	A	95	TRP	CA-CB-CG	-6.63	101.09	113.70	1	1
1	A	84	ASP	CB-CG-OD1	-6.59	112.36	118.30	14	1
1	A	35	ASP	CB-CG-OD1	-6.55	112.40	118.30	4	3
1	A	9	THR	OG1-CB-CG2	-6.50	95.06	110.00	18	6
1	A	94	ASP	CB-CG-OD2	-6.45	112.49	118.30	11	6
1	A	48	TRP	N-CA-C	6.45	128.42	111.00	15	2
1	A	34	TRP	CG-CD2-CE3	-6.36	128.18	133.90	2	7
1	A	68	ARG	NH1-CZ-NH2	6.36	126.39	119.40	5	5
1	A	109	TYR	CB-CG-CD2	-6.36	117.19	121.00	1	2
1	A	48	TRP	CA-CB-CG	-6.24	101.84	113.70	5	1
1	A	95	TRP	N-CA-C	-6.21	94.22	111.00	20	1
1	A	84	ASP	N-CA-CB	-6.16	99.52	110.60	7	3
1	A	1	GLU	OE1-CD-OE2	6.13	130.66	123.30	7	3
1	A	109	TYR	CB-CG-CD1	-6.12	117.33	121.00	15	3
1	A	7	ARG	NH1-CZ-NH2	6.10	126.11	119.40	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	34	TRP	NE1-CE2-CD2	-6.10	101.20	107.30	3	20
1	A	42	TRP	NE1-CE2-CD2	-6.06	101.24	107.30	18	17
1	A	124	ARG	NH1-CZ-NH2	6.05	126.06	119.40	11	3
1	A	48	TRP	NE1-CE2-CD2	-6.04	101.25	107.30	7	3
1	A	20	TRP	CA-CB-CG	5.97	125.05	113.70	1	3
1	A	20	TRP	CG-CD2-CE3	-5.96	128.53	133.90	15	2
1	A	21	ASP	CB-CG-OD2	-5.92	112.97	118.30	8	5
1	A	94	ASP	OD1-CG-OD2	5.91	134.53	123.30	5	1
1	A	30	TYR	N-CA-C	5.91	126.96	111.00	10	2
1	A	81	ARG	CB-CA-C	5.86	122.12	110.40	16	2
1	A	81	ARG	CD-NE-CZ	-5.82	115.46	123.60	19	1
1	A	104	THR	OG1-CB-CG2	-5.81	96.65	110.00	9	2
1	A	95	TRP	NE1-CE2-CD2	-5.73	101.57	107.30	12	15
1	A	14	ARG	NH1-CZ-NH2	5.73	125.70	119.40	3	3
1	A	20	TRP	CH2-CZ2-CE2	5.67	123.06	117.40	5	3
1	A	79	THR	OG1-CB-CG2	-5.67	96.97	110.00	10	1
1	A	97	THR	OG1-CB-CG2	-5.62	97.09	110.00	11	2
1	A	99	PHE	CB-CG-CD1	-5.59	116.89	120.80	13	2
1	A	42	TRP	CG-CD2-CE3	-5.58	128.88	133.90	13	1
1	A	86	CYS	CA-CB-SG	5.57	124.03	114.00	3	2
1	A	43	ARG	NH1-CZ-NH2	5.56	125.51	119.40	17	2
1	A	103	ASP	CB-CG-OD1	-5.55	113.30	118.30	16	3
1	A	96	ASP	CB-CG-OD1	5.51	123.26	118.30	13	2
1	A	107	ILE	CA-C-N	-5.47	105.26	116.20	12	1
1	A	94	ASP	N-CA-CB	-5.46	100.78	110.60	9	2
1	A	92	ASP	N-CA-CB	-5.42	100.84	110.60	13	1
1	A	31	CYS	CA-CB-SG	5.41	123.74	114.00	6	1
1	A	25	PRO	N-CA-C	-5.35	98.19	112.10	17	1
1	A	11	HIS	CA-CB-CG	-5.25	104.68	113.60	18	1
1	A	49	THR	OG1-CB-CG2	-5.18	98.08	110.00	16	1
1	A	48	TRP	CH2-CZ2-CE2	5.18	122.58	117.40	13	2
1	A	125	ASP	CB-CG-OD1	-5.18	113.64	118.30	15	1
1	A	103	ASP	N-CA-CB	-5.11	101.40	110.60	18	1
1	A	36	ALA	N-CA-C	5.10	124.77	111.00	11	1
1	A	63	CYS	N-CA-CB	-5.08	101.45	110.60	12	1
1	A	51	PHE	N-CA-C	-5.04	97.40	111.00	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	124	ARG	Sidechain	20
1	A	7	ARG	Sidechain	19
1	A	58	ARG	Sidechain	19
1	A	81	ARG	Sidechain	19
1	A	14	ARG	Sidechain	18
1	A	43	ARG	Sidechain	18
1	A	68	ARG	Sidechain	18
1	A	53	GLY	Peptide	1

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	30±9
All	All	19360	17900	17900	597

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:CYS:SG	1:A:81:ARG:NH1	0.84	2.50	3	1
1:A:47:GLY:C	1:A:48:TRP:CD1	0.78	2.57	5	2
1:A:48:TRP:CD1	1:A:48:TRP:N	0.77	2.49	5	6
1:A:22:LEU:CD2	1:A:48:TRP:CH2	0.77	2.68	10	4
1:A:48:TRP:H	1:A:81:ARG:CB	0.77	1.92	19	3
1:A:20:TRP:CZ3	1:A:48:TRP:NE1	0.74	2.55	7	5
1:A:48:TRP:O	1:A:48:TRP:CD1	0.70	2.44	19	5
1:A:66:CYS:SG	1:A:81:ARG:NH2	0.69	2.66	10	2
1:A:20:TRP:CE3	1:A:48:TRP:CE2	0.69	2.81	6	6
1:A:22:LEU:HD11	1:A:48:TRP:CZ3	0.67	2.25	11	5
1:A:81:ARG:CD	1:A:81:ARG:N	0.67	2.58	15	2
1:A:20:TRP:CE3	1:A:48:TRP:CZ2	0.66	2.82	12	10
1:A:48:TRP:H	1:A:81:ARG:CG	0.66	2.03	5	1
1:A:20:TRP:HB3	1:A:48:TRP:CZ2	0.66	2.26	6	6
1:A:48:TRP:CE3	1:A:93:LEU:HD21	0.66	2.26	12	2
1:A:20:TRP:HB3	1:A:48:TRP:CH2	0.66	2.25	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:CD2	1:A:48:TRP:CZ2	0.64	2.81	15	2
1:A:20:TRP:CZ3	1:A:48:TRP:CZ2	0.63	2.86	15	1
1:A:21:ASP:O	1:A:23:GLY:N	0.63	2.31	17	3
1:A:11:HIS:NE2	1:A:13:TYR:CE1	0.63	2.66	7	1
1:A:20:TRP:CH2	1:A:48:TRP:CE2	0.63	2.85	15	1
1:A:96:ASP:O	1:A:101:LYS:NZ	0.63	2.32	6	3
1:A:49:THR:HG21	1:A:80:ALA:HB1	0.63	1.71	19	1
1:A:31:CYS:SG	1:A:83:VAL:HG22	0.62	2.33	15	2
1:A:81:ARG:NH1	1:A:123:CYS:SG	0.61	2.73	3	3
1:A:22:LEU:HD21	1:A:48:TRP:CH2	0.61	2.31	8	7
1:A:11:HIS:CD2	1:A:13:TYR:CD1	0.61	2.89	7	1
1:A:47:GLY:N	1:A:81:ARG:NE	0.61	2.49	15	1
1:A:20:TRP:O	1:A:22:LEU:N	0.60	2.34	17	7
1:A:13:TYR:CD1	1:A:13:TYR:O	0.60	2.55	7	1
1:A:22:LEU:HD21	1:A:48:TRP:CE3	0.60	2.32	18	1
1:A:107:ILE:CD1	1:A:107:ILE:H	0.60	2.09	12	3
1:A:48:TRP:N	1:A:81:ARG:CB	0.59	2.66	9	3
1:A:22:LEU:HD21	1:A:48:TRP:CZ3	0.59	2.33	18	2
1:A:20:TRP:CD2	1:A:48:TRP:CZ2	0.59	2.91	16	6
1:A:48:TRP:H	1:A:81:ARG:HB2	0.58	1.58	19	1
1:A:86:CYS:SG	1:A:89:GLY:N	0.57	2.77	16	1
1:A:47:GLY:CA	1:A:81:ARG:HG3	0.57	2.29	5	1
1:A:68:ARG:NH2	1:A:79:THR:OG1	0.56	2.38	10	1
1:A:48:TRP:HB3	1:A:81:ARG:CZ	0.56	2.30	14	1
1:A:14:ARG:N	1:A:15:PRO:CD	0.56	2.68	15	1
1:A:46:TYR:CG	1:A:66:CYS:SG	0.56	2.99	9	2
1:A:48:TRP:N	1:A:81:ARG:CG	0.56	2.69	5	1
1:A:105:ASN:ND2	1:A:105:ASN:H	0.56	1.98	14	1
1:A:20:TRP:CZ3	1:A:94:ASP:HB2	0.56	2.35	13	2
1:A:20:TRP:CH2	1:A:43:ARG:O	0.56	2.59	3	1
1:A:20:TRP:CH2	1:A:48:TRP:CZ2	0.56	2.94	15	1
1:A:13:TYR:CD1	1:A:13:TYR:N	0.56	2.74	12	2
1:A:66:CYS:SG	1:A:81:ARG:HA	0.56	2.40	20	1
1:A:35:ASP:O	1:A:43:ARG:NH1	0.56	2.38	4	2
1:A:20:TRP:CZ3	1:A:48:TRP:CD1	0.55	2.95	8	1
1:A:58:ARG:HG2	1:A:59:GLY:N	0.55	2.16	15	1
1:A:47:GLY:N	1:A:81:ARG:HB3	0.55	2.16	9	1
1:A:48:TRP:CZ2	1:A:93:LEU:HG	0.55	2.36	10	1
1:A:107:ILE:HD12	1:A:107:ILE:H	0.55	1.62	4	1
1:A:48:TRP:CE3	1:A:93:LEU:HD11	0.55	2.36	12	1
1:A:11:HIS:CD2	1:A:12:TYR:H	0.55	2.20	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:N	1:A:81:ARG:HG3	0.54	2.17	5	1
1:A:22:LEU:HD22	1:A:48:TRP:CH2	0.54	2.36	10	1
1:A:48:TRP:O	1:A:49:THR:HG23	0.54	2.02	19	1
1:A:95:TRP:O	1:A:95:TRP:CG	0.54	2.60	17	4
1:A:19:ASN:O	1:A:19:ASN:ND2	0.54	2.41	16	1
1:A:95:TRP:O	1:A:96:ASP:C	0.54	2.46	5	1
1:A:48:TRP:H	1:A:81:ARG:NE	0.54	2.00	5	1
1:A:13:TYR:O	1:A:14:ARG:CB	0.54	2.56	7	1
1:A:20:TRP:CG	1:A:48:TRP:CZ2	0.54	2.96	4	7
1:A:11:HIS:CG	1:A:12:TYR:H	0.54	2.20	18	4
1:A:49:THR:CG2	1:A:80:ALA:HB1	0.54	2.32	5	2
1:A:48:TRP:O	1:A:93:LEU:CD2	0.54	2.56	10	1
1:A:48:TRP:H	1:A:81:ARG:C	0.53	2.07	16	2
1:A:48:TRP:CE2	1:A:93:LEU:HG	0.53	2.38	10	1
1:A:47:GLY:CA	1:A:81:ARG:HE	0.53	2.17	15	1
1:A:48:TRP:O	1:A:93:LEU:HD23	0.53	2.02	10	2
1:A:48:TRP:HB3	1:A:81:ARG:NH2	0.53	2.18	14	3
1:A:66:CYS:SG	1:A:81:ARG:HG2	0.53	2.43	4	1
1:A:15:PRO:O	1:A:17:GLN:N	0.53	2.42	5	3
1:A:13:TYR:O	1:A:13:TYR:CG	0.53	2.62	7	1
1:A:18:ASN:N	1:A:21:ASP:HB2	0.53	2.18	17	1
1:A:48:TRP:H	1:A:81:ARG:CD	0.53	2.17	5	1
1:A:22:LEU:HD11	1:A:48:TRP:CH2	0.53	2.38	12	3
1:A:11:HIS:CG	1:A:12:TYR:N	0.53	2.77	13	4
1:A:81:ARG:NE	1:A:81:ARG:H	0.53	2.01	15	1
1:A:22:LEU:CD2	1:A:48:TRP:CZ3	0.52	2.92	18	2
1:A:13:TYR:N	1:A:13:TYR:CD1	0.52	2.77	20	1
1:A:80:ALA:HA	1:A:81:ARG:CZ	0.52	2.34	15	1
1:A:99:PHE:O	1:A:101:LYS:N	0.52	2.43	8	3
1:A:107:ILE:H	1:A:107:ILE:HD12	0.52	1.64	12	3
1:A:48:TRP:N	1:A:81:ARG:HB2	0.52	2.19	19	2
1:A:117:ASN:ND2	1:A:117:ASN:N	0.52	2.57	4	2
1:A:48:TRP:CE3	1:A:93:LEU:CB	0.52	2.92	6	2
1:A:38:LYS:O	1:A:43:ARG:CZ	0.52	2.58	16	3
1:A:51:PHE:CG	1:A:51:PHE:O	0.52	2.62	11	2
1:A:51:PHE:CE2	1:A:56:GLY:HA3	0.52	2.40	15	1
1:A:48:TRP:NE1	1:A:93:LEU:HD22	0.52	2.19	17	1
1:A:13:TYR:O	1:A:14:ARG:HB2	0.51	2.04	7	2
1:A:105:ASN:ND2	1:A:106:GLY:H	0.51	2.03	14	1
1:A:49:THR:N	1:A:81:ARG:O	0.51	2.44	4	3
1:A:35:ASP:CG	1:A:43:ARG:NH2	0.51	2.63	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ARG:NH1	1:A:77:GLN:OE1	0.51	2.43	10	2
1:A:3:ALA:HB3	1:A:118:TYR:CZ	0.51	2.41	11	6
1:A:86:CYS:SG	1:A:89:GLY:CA	0.51	2.99	16	1
1:A:107:ILE:H	1:A:107:ILE:CD1	0.51	2.19	4	1
1:A:81:ARG:N	1:A:81:ARG:HD3	0.51	2.21	8	2
1:A:51:PHE:O	1:A:51:PHE:CD1	0.50	2.64	1	1
1:A:7:ARG:O	1:A:7:ARG:CG	0.50	2.59	5	1
1:A:19:ASN:OD1	1:A:43:ARG:NH1	0.50	2.44	1	2
1:A:100:THR:OG1	1:A:101:LYS:NZ	0.50	2.44	10	1
1:A:18:ASN:H	1:A:21:ASP:HB2	0.50	1.65	17	1
1:A:51:PHE:CE2	1:A:53:GLY:HA2	0.50	2.42	8	1
1:A:56:GLY:CA	1:A:120:PHE:CZ	0.50	2.94	15	2
1:A:31:CYS:SG	1:A:63:CYS:O	0.50	2.69	1	1
1:A:36:ALA:O	1:A:43:ARG:NH2	0.50	2.45	1	2
1:A:10:TYR:O	1:A:10:TYR:CD1	0.50	2.64	3	1
1:A:107:ILE:O	1:A:109:TYR:N	0.50	2.45	11	1
1:A:1:GLU:N	1:A:55:ALA:O	0.50	2.34	15	3
1:A:76:ALA:HB2	1:A:103:ASP:HB2	0.50	1.83	4	1
1:A:72:PRO:HG2	1:A:117:ASN:ND2	0.50	2.22	6	3
1:A:76:ALA:CB	1:A:103:ASP:HB2	0.50	2.36	4	1
1:A:20:TRP:CD1	1:A:43:ARG:HD2	0.50	2.42	13	1
1:A:94:ASP:CG	1:A:95:TRP:N	0.50	2.65	11	1
1:A:95:TRP:CE3	1:A:96:ASP:HB3	0.50	2.42	18	2
1:A:46:TYR:HB3	1:A:66:CYS:SG	0.49	2.47	9	2
1:A:22:LEU:HD23	1:A:48:TRP:CZ2	0.49	2.42	15	1
1:A:46:TYR:CA	1:A:81:ARG:HG2	0.49	2.37	19	1
1:A:15:PRO:HG3	1:A:48:TRP:CE3	0.49	2.42	8	1
1:A:72:PRO:HD3	1:A:117:ASN:ND2	0.49	2.22	13	1
1:A:15:PRO:HA	1:A:21:ASP:N	0.49	2.23	15	1
1:A:46:TYR:O	1:A:81:ARG:NH2	0.49	2.46	1	1
1:A:86:CYS:SG	1:A:86:CYS:O	0.49	2.69	2	1
1:A:88:ASN:OD1	1:A:89:GLY:N	0.49	2.46	15	1
1:A:47:GLY:O	1:A:81:ARG:N	0.49	2.45	2	3
1:A:94:ASP:O	1:A:96:ASP:N	0.49	2.46	15	1
1:A:35:ASP:CB	1:A:43:ARG:HH21	0.49	2.21	17	1
1:A:18:ASN:C	1:A:20:TRP:N	0.49	2.64	19	2
1:A:49:THR:CG2	1:A:81:ARG:C	0.49	2.81	15	1
1:A:48:TRP:O	1:A:92:ASP:HA	0.49	2.08	7	4
1:A:20:TRP:CZ3	1:A:43:ARG:O	0.49	2.65	8	1
1:A:48:TRP:O	1:A:93:LEU:HD22	0.49	2.07	13	2
1:A:48:TRP:CG	1:A:48:TRP:O	0.49	2.65	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TRP:CE3	1:A:93:LEU:HB3	0.49	2.43	6	1
1:A:20:TRP:CD1	1:A:20:TRP:N	0.49	2.81	8	1
1:A:53:GLY:O	1:A:58:ARG:NH2	0.49	2.45	19	1
1:A:48:TRP:O	1:A:48:TRP:CG	0.48	2.66	13	2
1:A:48:TRP:NE1	1:A:93:LEU:CD2	0.48	2.76	13	2
1:A:96:ASP:O	1:A:101:LYS:HE2	0.48	2.08	9	1
1:A:96:ASP:O	1:A:101:LYS:CE	0.48	2.61	8	2
1:A:95:TRP:CG	1:A:95:TRP:O	0.48	2.66	20	1
1:A:94:ASP:O	1:A:95:TRP:CB	0.48	2.61	4	1
1:A:48:TRP:O	1:A:49:THR:CG2	0.48	2.61	19	1
1:A:97:THR:OG1	1:A:98:VAL:N	0.48	2.47	1	7
1:A:59:GLY:O	1:A:61:ALA:N	0.48	2.47	5	1
1:A:30:TYR:CZ	1:A:61:ALA:HB2	0.48	2.43	7	1
1:A:3:ALA:HB3	1:A:118:TYR:CE1	0.48	2.44	14	4
1:A:11:HIS:CE1	1:A:88:ASN:OD1	0.48	2.67	12	1
1:A:105:ASN:HD22	1:A:106:GLY:N	0.48	2.06	19	1
1:A:20:TRP:CZ3	1:A:48:TRP:CE2	0.48	3.01	15	2
1:A:58:ARG:HH11	1:A:82:ILE:CD1	0.48	2.21	13	1
1:A:25:PRO:HD2	1:A:27:VAL:HG23	0.48	1.86	17	1
1:A:85:GLN:HG2	1:A:86:CYS:N	0.48	2.24	20	1
1:A:81:ARG:HH11	1:A:81:ARG:HB2	0.48	1.67	8	1
1:A:58:ARG:NH1	1:A:120:PHE:CG	0.47	2.82	1	1
1:A:58:ARG:NH1	1:A:59:GLY:O	0.47	2.46	12	1
1:A:76:ALA:HB2	1:A:103:ASP:CB	0.47	2.38	4	1
1:A:47:GLY:H	1:A:81:ARG:HA	0.47	1.69	9	1
1:A:85:GLN:HG2	1:A:86:CYS:SG	0.47	2.49	15	1
1:A:38:LYS:O	1:A:43:ARG:NH1	0.47	2.48	2	1
1:A:47:GLY:O	1:A:48:TRP:CB	0.47	2.62	4	2
1:A:94:ASP:OD1	1:A:94:ASP:N	0.47	2.47	20	1
1:A:96:ASP:O	1:A:101:LYS:HE3	0.47	2.09	4	1
1:A:97:THR:O	1:A:101:LYS:NZ	0.47	2.44	14	1
1:A:114:LEU:HG	1:A:115:ASN:N	0.47	2.24	5	1
1:A:20:TRP:CE3	1:A:48:TRP:CD2	0.47	3.02	6	1
1:A:48:TRP:H	1:A:81:ARG:CA	0.47	2.21	16	1
1:A:18:ASN:H	1:A:21:ASP:CB	0.47	2.21	17	1
1:A:40:LEU:H	1:A:40:LEU:CD2	0.47	2.23	17	1
1:A:95:TRP:O	1:A:95:TRP:CD1	0.47	2.68	17	1
1:A:51:PHE:CD2	1:A:84:ASP:O	0.47	2.67	1	2
1:A:35:ASP:C	1:A:43:ARG:NH1	0.47	2.68	4	1
1:A:22:LEU:HD21	1:A:48:TRP:CZ2	0.47	2.44	8	2
1:A:65:LYS:NZ	1:A:122:ASP:OD1	0.47	2.47	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ASP:N	1:A:92:ASP:OD1	0.47	2.48	20	1
1:A:93:LEU:CD2	1:A:93:LEU:N	0.47	2.77	10	1
1:A:47:GLY:O	1:A:48:TRP:HB3	0.46	2.10	4	1
1:A:60:GLN:O	1:A:62:ALA:N	0.46	2.48	12	1
1:A:122:ASP:OD2	1:A:124:ARG:NH1	0.46	2.48	13	1
1:A:16:ALA:O	1:A:19:ASN:N	0.46	2.49	11	4
1:A:81:ARG:HH11	1:A:81:ARG:CA	0.46	2.23	4	1
1:A:48:TRP:CE3	1:A:93:LEU:HB2	0.46	2.45	15	2
1:A:96:ASP:HA	1:A:100:THR:CG2	0.46	2.40	10	1
1:A:2:GLN:HG2	1:A:119:GLN:NE2	0.46	2.26	20	1
1:A:103:ASP:O	1:A:104:THR:C	0.46	2.53	11	1
1:A:49:THR:HG23	1:A:82:ILE:HA	0.46	1.87	15	1
1:A:10:TYR:CD1	1:A:10:TYR:N	0.46	2.84	17	1
1:A:49:THR:OG1	1:A:81:ARG:N	0.46	2.49	19	1
1:A:40:LEU:O	1:A:41:SER:C	0.46	2.53	12	5
1:A:48:TRP:N	1:A:81:ARG:HG3	0.46	2.25	5	1
1:A:107:ILE:HD12	1:A:107:ILE:N	0.46	2.25	9	1
1:A:15:PRO:HB3	1:A:22:LEU:CB	0.46	2.41	15	1
1:A:46:TYR:HA	1:A:81:ARG:CG	0.46	2.41	16	1
1:A:20:TRP:HB2	1:A:48:TRP:CZ2	0.46	2.45	19	1
1:A:48:TRP:O	1:A:93:LEU:N	0.46	2.48	6	2
1:A:45:LYS:O	1:A:81:ARG:NE	0.46	2.48	9	1
1:A:96:ASP:CB	1:A:99:PHE:HB3	0.46	2.41	15	1
1:A:9:THR:OG1	1:A:10:TYR:N	0.46	2.49	10	3
1:A:81:ARG:CD	1:A:81:ARG:H	0.45	2.23	5	1
1:A:11:HIS:NE2	1:A:13:TYR:CD1	0.45	2.84	7	1
1:A:10:TYR:HA	1:A:12:TYR:CE1	0.45	2.46	8	1
1:A:48:TRP:NE1	1:A:93:LEU:HD23	0.45	2.26	13	1
1:A:19:ASN:ND2	1:A:43:ARG:HH22	0.45	2.09	8	1
1:A:45:LYS:HE3	1:A:125:ASP:CG	0.45	2.31	9	1
1:A:48:TRP:CH2	1:A:93:LEU:CD1	0.45	2.99	10	1
1:A:84:ASP:CG	1:A:85:GLN:H	0.45	2.14	1	2
1:A:46:TYR:O	1:A:47:GLY:C	0.45	2.54	2	2
1:A:62:ALA:O	1:A:64:GLY:N	0.45	2.50	20	2
1:A:53:GLY:N	1:A:54:PRO:CD	0.45	2.80	7	3
1:A:96:ASP:HB3	1:A:99:PHE:HB3	0.45	1.87	12	2
1:A:42:TRP:CZ3	1:A:81:ARG:NE	0.45	2.85	17	1
1:A:58:ARG:NH2	1:A:120:PHE:CZ	0.45	2.85	4	1
1:A:48:TRP:O	1:A:93:LEU:HD13	0.45	2.11	11	1
1:A:15:PRO:HB3	1:A:22:LEU:CA	0.45	2.41	15	1
1:A:47:GLY:O	1:A:81:ARG:HB2	0.45	2.12	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ASN:O	1:A:20:TRP:HB2	0.45	2.12	16	4
1:A:20:TRP:CE3	1:A:48:TRP:HZ2	0.45	2.30	2	2
1:A:31:CYS:O	1:A:32:ALA:C	0.45	2.55	17	5
1:A:12:TYR:CD1	1:A:12:TYR:N	0.45	2.85	6	2
1:A:59:GLY:O	1:A:60:GLN:C	0.45	2.55	3	3
1:A:38:LYS:HB2	1:A:43:ARG:NE	0.45	2.26	17	1
1:A:20:TRP:C	1:A:22:LEU:N	0.44	2.67	3	2
1:A:94:ASP:HB3	1:A:97:THR:CG2	0.44	2.41	16	1
1:A:112:GLY:O	1:A:113:HIS:C	0.44	2.55	17	1
1:A:10:TYR:C	1:A:10:TYR:CD1	0.44	2.90	2	1
1:A:71:ASN:HD22	1:A:102:ILE:CD1	0.44	2.24	4	1
1:A:20:TRP:CE3	1:A:48:TRP:NE1	0.44	2.86	8	2
1:A:38:LYS:O	1:A:43:ARG:NE	0.44	2.50	8	1
1:A:48:TRP:O	1:A:81:ARG:NH2	0.44	2.50	15	1
1:A:58:ARG:HG3	1:A:62:ALA:HB2	0.44	1.90	1	1
1:A:9:THR:OG1	1:A:90:GLY:N	0.44	2.50	18	1
1:A:51:PHE:O	1:A:85:GLN:NE2	0.44	2.50	8	1
1:A:105:ASN:N	1:A:105:ASN:HD22	0.44	2.11	14	1
1:A:51:PHE:CD1	1:A:58:ARG:CZ	0.44	3.00	7	1
1:A:107:ILE:C	1:A:109:TYR:H	0.44	2.16	10	2
1:A:88:ASN:OD1	1:A:88:ASN:N	0.44	2.51	1	1
1:A:94:ASP:O	1:A:95:TRP:C	0.44	2.56	2	2
1:A:46:TYR:CG	1:A:81:ARG:NH2	0.44	2.86	10	1
1:A:44:SER:OG	1:A:45:LYS:N	0.44	2.50	19	2
1:A:108:GLY:O	1:A:112:GLY:N	0.44	2.51	14	1
1:A:93:LEU:H	1:A:93:LEU:HD23	0.44	1.73	18	1
1:A:51:PHE:HB3	1:A:82:ILE:CG2	0.44	2.43	1	1
1:A:20:TRP:HB2	1:A:43:ARG:NH1	0.44	2.28	7	2
1:A:96:ASP:HA	1:A:100:THR:HG23	0.44	1.89	11	2
1:A:22:LEU:CD2	1:A:48:TRP:CE2	0.44	3.01	15	1
1:A:5:ASP:CG	1:A:115:ASN:HD21	0.44	2.17	18	1
1:A:46:TYR:HB3	1:A:81:ARG:HB3	0.43	1.90	5	1
1:A:121:VAL:HG13	1:A:122:ASP:N	0.43	2.29	2	2
1:A:37:SER:O	1:A:43:ARG:NH2	0.43	2.51	5	1
1:A:5:ASP:C	1:A:115:ASN:ND2	0.43	2.72	9	1
1:A:16:ALA:HA	1:A:20:TRP:N	0.43	2.29	17	1
1:A:10:TYR:HB3	1:A:12:TYR:CE2	0.43	2.48	8	1
1:A:83:VAL:CG1	1:A:84:ASP:N	0.43	2.82	9	1
1:A:105:ASN:ND2	1:A:105:ASN:N	0.43	2.63	14	1
1:A:111:GLN:O	1:A:113:HIS:N	0.43	2.51	18	1
1:A:18:ASN:O	1:A:19:ASN:C	0.43	2.56	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ARG:N	1:A:15:PRO:HD2	0.43	2.28	15	1
1:A:20:TRP:CG	1:A:48:TRP:HZ2	0.43	2.31	20	2
1:A:86:CYS:O	1:A:87:ALA:C	0.43	2.57	2	1
1:A:91:LEU:HD23	1:A:91:LEU:N	0.43	2.28	3	1
1:A:58:ARG:HG3	1:A:62:ALA:CB	0.43	2.43	5	1
1:A:114:LEU:HD23	1:A:114:LEU:H	0.43	1.74	18	1
1:A:13:TYR:CZ	1:A:14:ARG:NH2	0.43	2.84	2	1
1:A:42:TRP:HE1	1:A:125:ASP:CG	0.43	2.16	2	1
1:A:48:TRP:CE2	1:A:93:LEU:HD22	0.43	2.49	16	1
1:A:97:THR:O	1:A:101:LYS:HG3	0.43	2.13	17	1
1:A:62:ALA:C	1:A:64:GLY:H	0.43	2.17	18	1
1:A:106:GLY:O	1:A:108:GLY:N	0.43	2.52	17	2
1:A:45:LYS:O	1:A:46:TYR:CD1	0.43	2.71	9	1
1:A:105:ASN:H	1:A:105:ASN:HD22	0.43	1.56	14	1
1:A:21:ASP:O	1:A:24:ALA:N	0.43	2.52	16	1
1:A:94:ASP:HB3	1:A:97:THR:HG23	0.43	1.89	20	1
1:A:22:LEU:HD11	1:A:48:TRP:CZ2	0.43	2.49	8	1
1:A:46:TYR:CE2	1:A:79:THR:HB	0.43	2.48	13	1
1:A:48:TRP:O	1:A:92:ASP:HB3	0.43	2.14	15	1
1:A:18:ASN:O	1:A:20:TRP:N	0.43	2.51	19	2
1:A:51:PHE:O	1:A:52:CYS:SG	0.43	2.77	11	1
1:A:19:ASN:O	1:A:21:ASP:N	0.43	2.52	1	2
1:A:38:LYS:O	1:A:43:ARG:CD	0.43	2.67	3	1
1:A:1:GLU:OE1	1:A:1:GLU:N	0.43	2.48	5	1
1:A:48:TRP:H	1:A:98:VAL:CG2	0.43	2.27	8	1
1:A:107:ILE:CD1	1:A:107:ILE:N	0.43	2.82	9	1
1:A:20:TRP:NE1	1:A:43:ARG:CB	0.43	2.82	17	1
1:A:31:CYS:HB2	1:A:83:VAL:HG23	0.42	1.90	3	2
1:A:22:LEU:CB	1:A:32:ALA:HB2	0.42	2.44	11	1
1:A:13:TYR:CD2	1:A:14:ARG:N	0.42	2.87	12	1
1:A:3:ALA:HB2	1:A:55:ALA:HB2	0.42	1.91	18	1
1:A:13:TYR:C	1:A:14:ARG:HD3	0.42	2.34	2	1
1:A:9:THR:HG22	1:A:113:HIS:HB3	0.42	1.90	15	1
1:A:35:ASP:OD1	1:A:43:ARG:NH2	0.42	2.52	17	1
1:A:106:GLY:HA3	1:A:114:LEU:HD22	0.42	1.89	4	1
1:A:61:ALA:O	1:A:65:LYS:NZ	0.42	2.53	10	1
1:A:93:LEU:HD22	1:A:93:LEU:H	0.42	1.74	12	1
1:A:48:TRP:CD1	1:A:93:LEU:HD22	0.42	2.49	2	1
1:A:14:ARG:NH1	1:A:48:TRP:CH2	0.42	2.87	7	1
1:A:59:GLY:C	1:A:61:ALA:N	0.42	2.71	7	1
1:A:81:ARG:HB2	1:A:81:ARG:NH1	0.42	2.29	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TRP:CE3	1:A:83:VAL:HG11	0.42	2.49	13	1
1:A:38:LYS:O	1:A:43:ARG:HD3	0.42	2.15	3	1
1:A:49:THR:CG2	1:A:98:VAL:HG21	0.42	2.44	3	1
1:A:118:TYR:CD1	1:A:118:TYR:C	0.42	2.92	9	1
1:A:107:ILE:C	1:A:109:TYR:N	0.42	2.73	12	1
1:A:81:ARG:N	1:A:81:ARG:NE	0.42	2.67	15	1
1:A:3:ALA:CB	1:A:118:TYR:CZ	0.42	3.03	16	1
1:A:48:TRP:CD1	1:A:93:LEU:HB3	0.42	2.50	19	1
1:A:12:TYR:CD1	1:A:92:ASP:O	0.42	2.72	8	1
1:A:90:GLY:O	1:A:91:LEU:CB	0.42	2.68	13	2
1:A:19:ASN:HD21	1:A:43:ARG:NH1	0.42	2.11	16	1
1:A:37:SER:OG	1:A:38:LYS:N	0.42	2.53	2	1
1:A:35:ASP:O	1:A:36:ALA:C	0.42	2.57	4	1
1:A:16:ALA:N	1:A:20:TRP:HB3	0.42	2.30	1	1
1:A:49:THR:HG23	1:A:81:ARG:O	0.42	2.15	5	1
1:A:46:TYR:CE2	1:A:123:CYS:SG	0.42	3.13	12	1
1:A:48:TRP:CZ3	1:A:93:LEU:HD11	0.42	2.50	18	1
1:A:81:ARG:HH11	1:A:81:ARG:CB	0.41	2.27	4	1
1:A:47:GLY:O	1:A:93:LEU:HD22	0.41	2.15	5	1
1:A:54:PRO:O	1:A:58:ARG:NH2	0.41	2.53	10	1
1:A:20:TRP:CH2	1:A:48:TRP:NE1	0.41	2.88	15	1
1:A:93:LEU:HD23	1:A:93:LEU:N	0.41	2.30	18	1
1:A:81:ARG:N	1:A:81:ARG:CD	0.41	2.83	8	1
1:A:20:TRP:CB	1:A:48:TRP:CH2	0.41	3.03	16	1
1:A:10:TYR:OH	1:A:111:GLN:N	0.41	2.52	17	1
1:A:4:ASN:O	1:A:6:VAL:HG23	0.41	2.15	4	1
1:A:117:ASN:N	1:A:117:ASN:HD22	0.41	2.13	4	1
1:A:48:TRP:HA	1:A:93:LEU:HD13	0.41	1.92	5	1
1:A:81:ARG:HD3	1:A:81:ARG:H	0.41	1.73	8	1
1:A:35:ASP:OD1	1:A:38:LYS:NZ	0.41	2.53	13	1
1:A:15:PRO:CG	1:A:48:TRP:CH2	0.41	3.04	15	1
1:A:35:ASP:CG	1:A:43:ARG:HH21	0.41	2.18	17	1
1:A:58:ARG:O	1:A:62:ALA:CB	0.41	2.68	17	1
1:A:47:GLY:O	1:A:81:ARG:NH2	0.41	2.52	20	1
1:A:105:ASN:ND2	1:A:105:ASN:O	0.41	2.53	11	1
1:A:36:ALA:C	1:A:43:ARG:HH12	0.41	2.19	13	1
1:A:58:ARG:NH1	1:A:82:ILE:CD1	0.41	2.83	13	1
1:A:70:THR:OG1	1:A:77:GLN:HB3	0.41	2.14	17	1
1:A:2:GLN:NE2	1:A:2:GLN:O	0.41	2.53	20	1
1:A:46:TYR:C	1:A:81:ARG:HB3	0.41	2.35	16	2
1:A:10:TYR:OH	1:A:109:TYR:HA	0.41	2.14	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TRP:CG	1:A:48:TRP:CH2	0.41	3.08	16	1
1:A:95:TRP:C	1:A:97:THR:H	0.41	2.17	16	1
1:A:15:PRO:C	1:A:17:GLN:N	0.41	2.73	5	1
1:A:18:ASN:O	1:A:19:ASN:CB	0.41	2.68	5	1
1:A:11:HIS:O	1:A:95:TRP:CD1	0.41	2.74	9	1
1:A:13:TYR:HB2	1:A:94:ASP:O	0.41	2.16	9	1
1:A:106:GLY:C	1:A:108:GLY:H	0.41	2.19	11	1
1:A:59:GLY:H	1:A:62:ALA:HB2	0.41	1.75	4	1
1:A:15:PRO:HB3	1:A:48:TRP:CH2	0.41	2.51	7	1
1:A:58:ARG:HG2	1:A:62:ALA:CB	0.41	2.45	7	1
1:A:77:GLN:NE2	1:A:78:ILE:N	0.41	2.69	15	1
1:A:21:ASP:C	1:A:23:GLY:N	0.41	2.74	8	1
1:A:118:TYR:CD1	1:A:118:TYR:O	0.41	2.73	11	1
1:A:95:TRP:CE3	1:A:95:TRP:O	0.41	2.74	15	1
1:A:8:ALA:O	1:A:113:HIS:HA	0.41	2.16	2	1
1:A:72:PRO:CD	1:A:117:ASN:ND2	0.41	2.84	4	1
1:A:7:ARG:HB2	1:A:113:HIS:CE1	0.41	2.51	5	1
1:A:13:TYR:O	1:A:14:ARG:HD3	0.41	2.16	5	1
1:A:31:CYS:SG	1:A:83:VAL:HG13	0.41	2.56	11	1
1:A:47:GLY:O	1:A:81:ARG:CB	0.41	2.68	18	1
1:A:24:ALA:O	1:A:25:PRO:C	0.41	2.59	19	1
1:A:42:TRP:CH2	1:A:81:ARG:NE	0.41	2.89	1	1
1:A:58:ARG:NH1	1:A:58:ARG:O	0.41	2.54	14	1
1:A:31:CYS:O	1:A:33:THR:N	0.41	2.54	15	1
1:A:80:ALA:C	1:A:81:ARG:HD3	0.41	2.36	15	1
1:A:92:ASP:O	1:A:93:LEU:HD12	0.41	2.15	17	1
1:A:110:GLN:O	1:A:111:GLN:HB2	0.41	2.15	17	1
1:A:105:ASN:OD1	1:A:106:GLY:N	0.41	2.54	20	1
1:A:51:PHE:CD1	1:A:52:CYS:N	0.40	2.89	2	1
1:A:96:ASP:O	1:A:98:VAL:N	0.40	2.55	15	1
1:A:48:TRP:N	1:A:81:ARG:HB3	0.40	2.31	16	1
1:A:99:PHE:CD1	1:A:99:PHE:O	0.40	2.74	17	1
1:A:21:ASP:O	1:A:22:LEU:C	0.40	2.60	5	1
1:A:46:TYR:CD1	1:A:66:CYS:SG	0.40	3.14	16	1
1:A:76:ALA:CB	1:A:103:ASP:CB	0.40	3.00	4	1
1:A:46:TYR:HA	1:A:81:ARG:HG2	0.40	1.91	9	2
1:A:118:TYR:C	1:A:119:GLN:NE2	0.40	2.74	10	2
1:A:58:ARG:O	1:A:59:GLY:C	0.40	2.60	5	1
1:A:91:LEU:O	1:A:92:ASP:C	0.40	2.60	7	1
1:A:72:PRO:CD	1:A:117:ASN:HD22	0.40	2.29	10	1
1:A:110:GLN:O	1:A:111:GLN:CB	0.40	2.70	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:THR:HB	1:A:91:LEU:O	0.40	2.16	20	1
1:A:56:GLY:HA3	1:A:120:PHE:CZ	0.40	2.52	14	1
1:A:118:TYR:O	1:A:119:GLN:NE2	0.40	2.55	18	1
1:A:17:GLN:C	1:A:19:ASN:H	0.40	2.19	20	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%)	80±3 (65±3%)	31±5 (25±4%)	12±3 (10±2%)	1 9
All	All	2460/2500 (98%)	1595 (65%)	616 (25%)	249 (10%)	1 9

All 53 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	15	PRO	15
1	A	28	SER	13
1	A	21	ASP	12
1	A	20	TRP	11
1	A	99	PHE	11
1	A	95	TRP	9
1	A	107	ILE	9
1	A	41	SER	8
1	A	30	TYR	7
1	A	63	CYS	7
1	A	14	ARG	7
1	A	16	ALA	6
1	A	22	LEU	6
1	A	100	THR	6
1	A	104	THR	6
1	A	61	ALA	5
1	A	97	THR	5
1	A	106	GLY	5

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Mol	Chain	Res	Type	Models (Total)
1	A	83	VAL	5
1	A	108	GLY	5
1	A	19	ASN	5
1	A	60	GLN	5
1	A	91	LEU	5
1	A	39	PRO	4
1	A	87	ALA	4
1	A	96	ASP	4
1	A	48	TRP	4
1	A	64	GLY	4
1	A	56	GLY	4
1	A	92	ASP	4
1	A	73	ALA	3
1	A	110	GLN	3
1	A	25	PRO	3
1	A	26	ALA	3
1	A	59	GLY	3
1	A	54	PRO	3
1	A	47	GLY	3
1	A	109	TYR	3
1	A	36	ALA	3
1	A	72	PRO	2
1	A	33	THR	2
1	A	53	GLY	2
1	A	24	ALA	2
1	A	112	GLY	2
1	A	57	PRO	2
1	A	82	ILE	2
1	A	93	LEU	1
1	A	38	LYS	1
1	A	90	GLY	1
1	A	102	ILE	1
1	A	103	ASP	1
1	A	32	ALA	1
1	A	111	GLN	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%)	81±3 (83±3%)	16±3 (17±3%)	5 41
All	All	1940/1940 (100%)	1618 (83%)	322 (17%)	5 41

All 60 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	113	HIS	20
1	A	121	VAL	20
1	A	100	THR	19
1	A	58	ARG	16
1	A	119	GLN	16
1	A	46	TYR	14
1	A	48	TRP	14
1	A	86	CYS	13
1	A	67	LEU	12
1	A	13	TYR	9
1	A	14	ARG	8
1	A	92	ASP	8
1	A	12	TYR	7
1	A	81	ARG	7
1	A	18	ASN	6
1	A	40	LEU	6
1	A	105	ASN	6
1	A	4	ASN	5
1	A	20	TRP	4
1	A	91	LEU	4
1	A	22	LEU	4
1	A	51	PHE	4
1	A	10	TYR	4
1	A	77	GLN	4
1	A	94	ASP	4
1	A	93	LEU	4
1	A	31	CYS	3
1	A	38	LYS	3
1	A	122	ASP	3
1	A	124	ARG	3
1	A	35	ASP	3
1	A	52	CYS	3
1	A	19	ASN	3
1	A	7	ARG	3
1	A	97	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	104	THR	3
1	A	2	GLN	2
1	A	103	ASP	2
1	A	17	GLN	2
1	A	65	LYS	2
1	A	99	PHE	2
1	A	1	GLU	2
1	A	49	THR	2
1	A	88	ASN	2
1	A	83	VAL	2
1	A	43	ARG	2
1	A	96	ASP	2
1	A	5	ASP	1
1	A	71	ASN	1
1	A	85	GLN	1
1	A	115	ASN	1
1	A	11	HIS	1
1	A	84	ASP	1
1	A	9	THR	1
1	A	63	CYS	1
1	A	78	ILE	1
1	A	21	ASP	1
1	A	111	GLN	1
1	A	114	LEU	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 monosaccharides 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 (i)

No chemical shift data were provided