



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:57 PM BST

PDB ID : 1B4M  
Title : NMR STRUCTURE OF APO CELLULAR RETINOL-BINDING PROTEIN II, 24 STRUCTURES  
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Deposited on : 1998-12-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

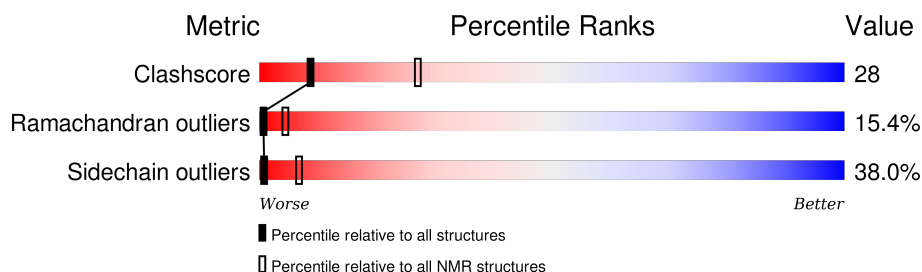
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	134	

## 2 Ensemble composition and analysis

This entry contains 24 models. Model 12 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:3-A:134 (132)	0.65	12

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	4, 6, 8, 11, 12, 15, 17, 21, 24
2	1, 2, 3, 5, 7, 10, 14, 18, 23
3	9, 19, 22
4	13, 20
Single-model clusters	16

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2168 atoms, of which 1073 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELLULAR RETINOL-BINDING PROTEIN II.

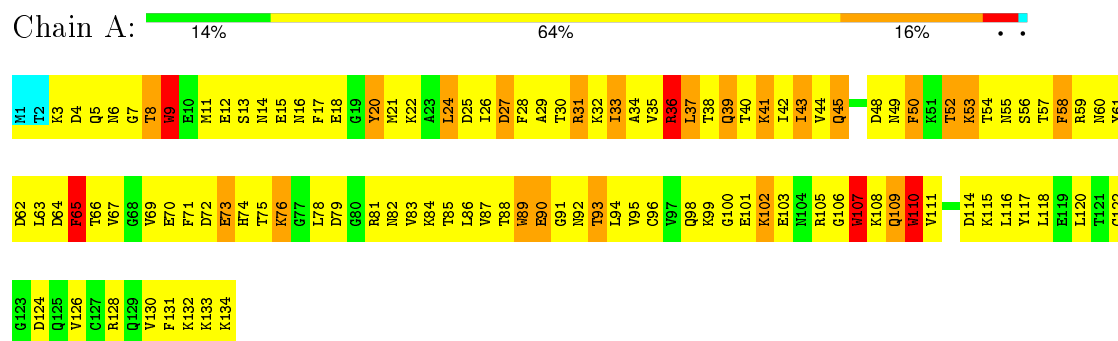
Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2168	686	1073	189	214	6	

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

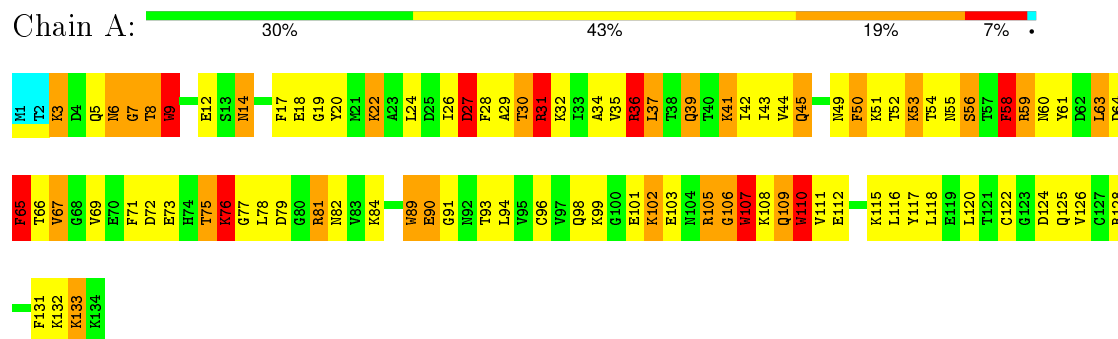


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

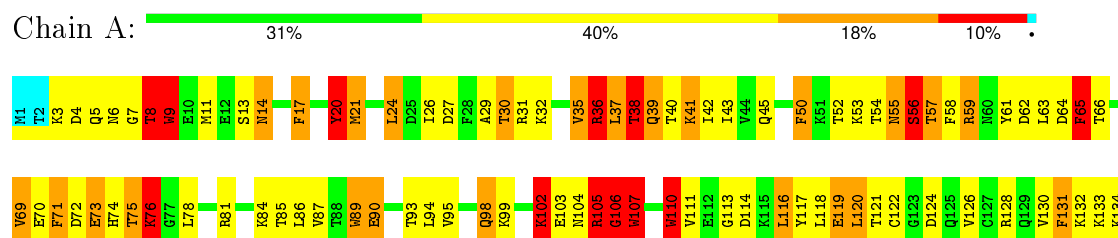
#### 4.2.1 Score per residue for model 1

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



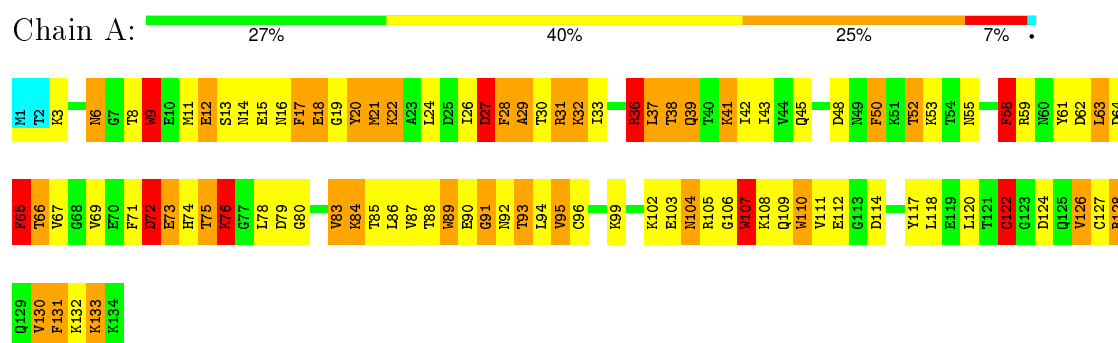
## 4.2.2 Score per residue for model 2

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



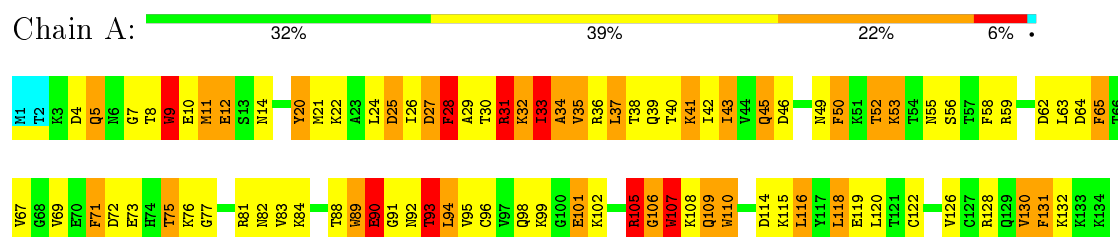
## 4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



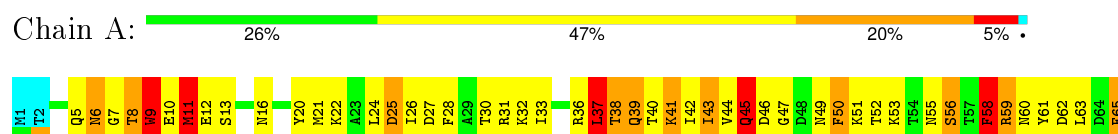
## 4.2.4 Score per residue for model 4

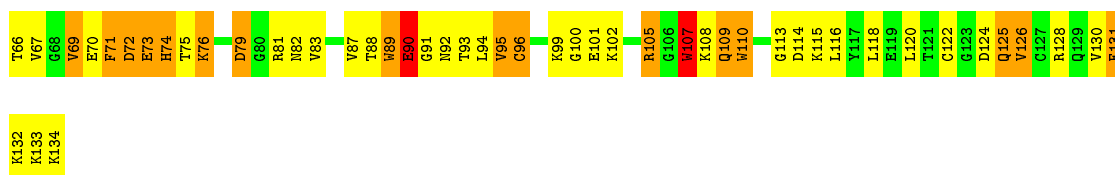
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



## 4.2.5 Score per residue for model 5

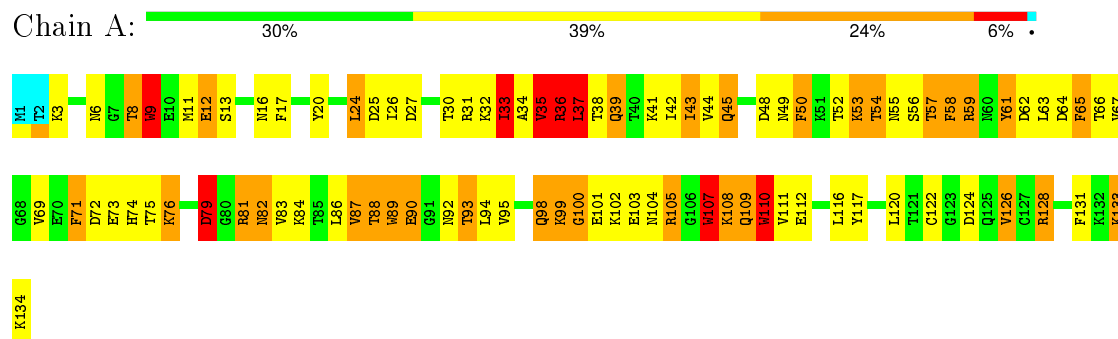
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II





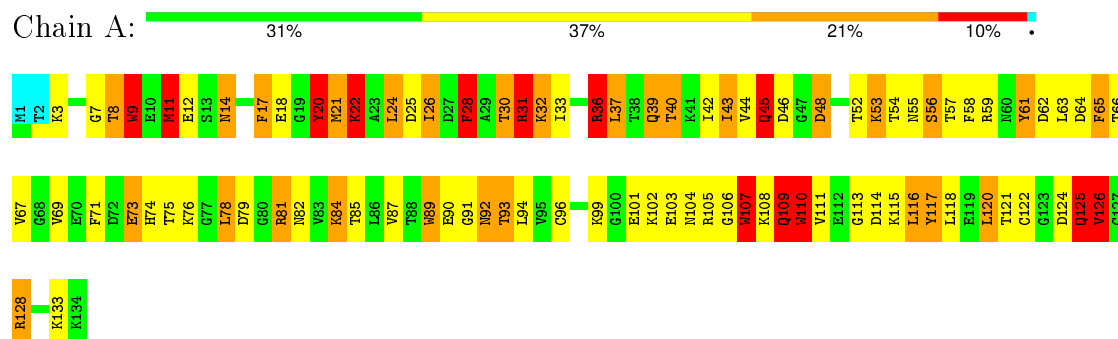
#### 4.2.6 Score per residue for model 6

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



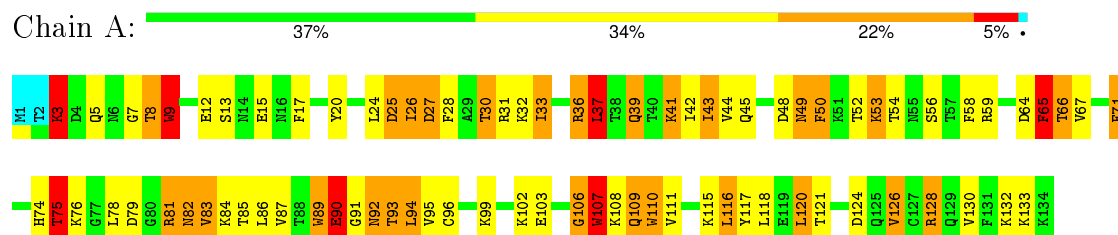
#### 4.2.7 Score per residue for model 7

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



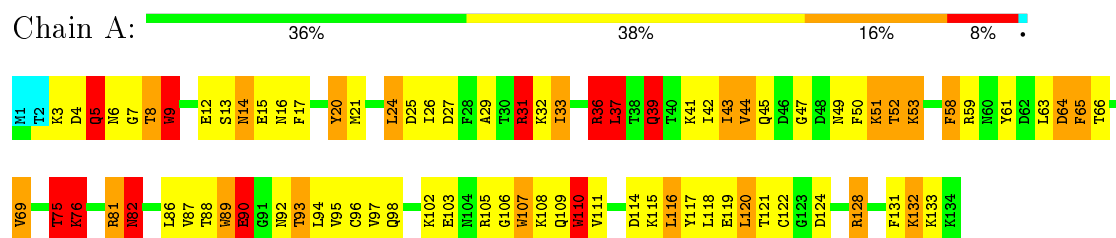
#### 4.2.8 Score per residue for model 8

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



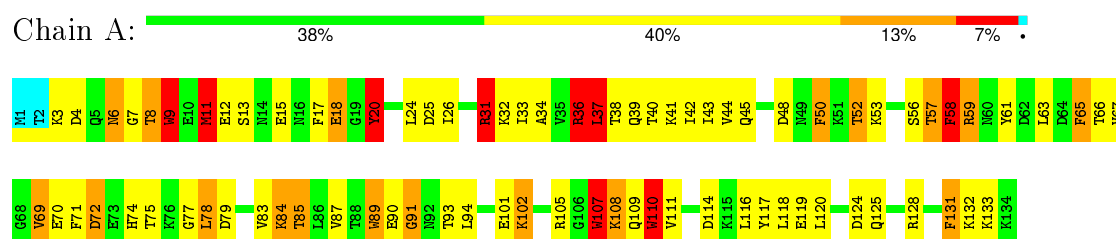
### 4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



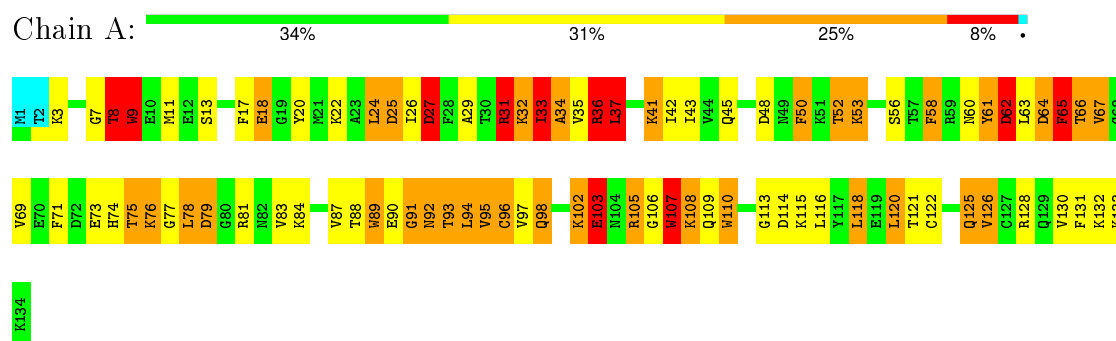
### 4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



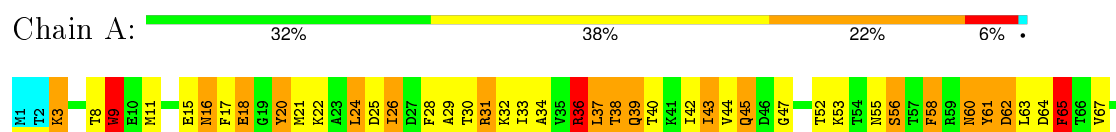
### 4.2.11 Score per residue for model 11

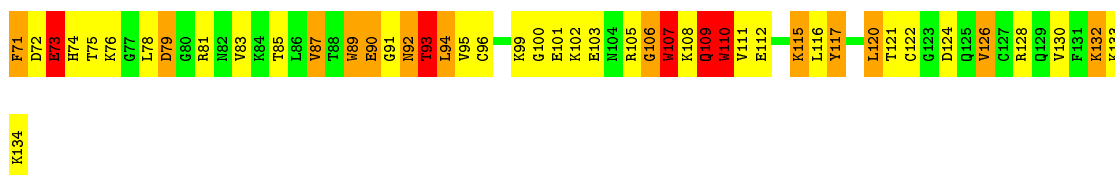
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

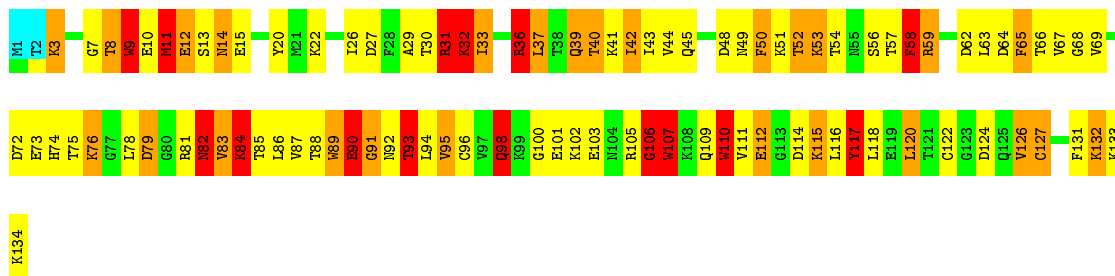




#### 4.2.13 Score per residue for model 13

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

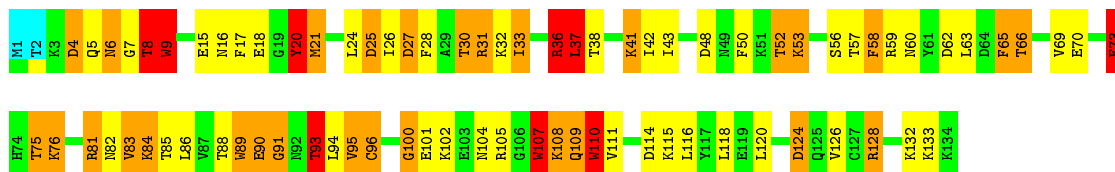
Chain A: 27% 41% 19% 11%



#### 4.2.14 Score per residue for model 14

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

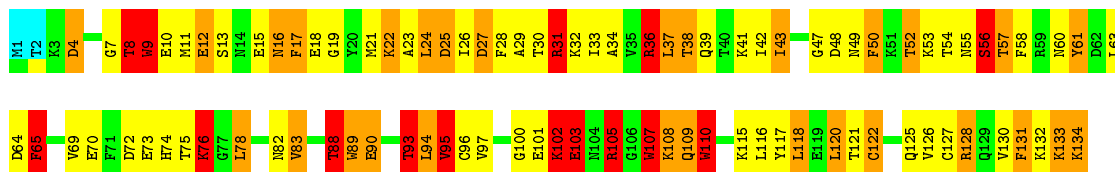
Chain A: 40% 31% 22% 7%



#### 4.2.15 Score per residue for model 15

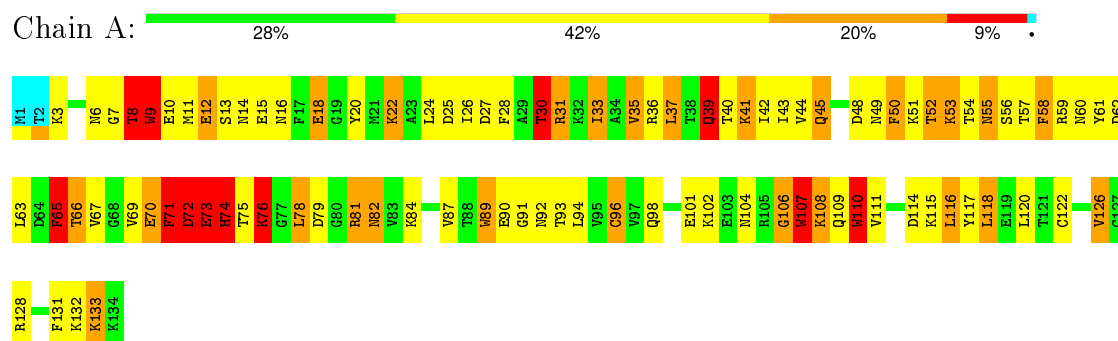
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 29% 37% 22% 11%



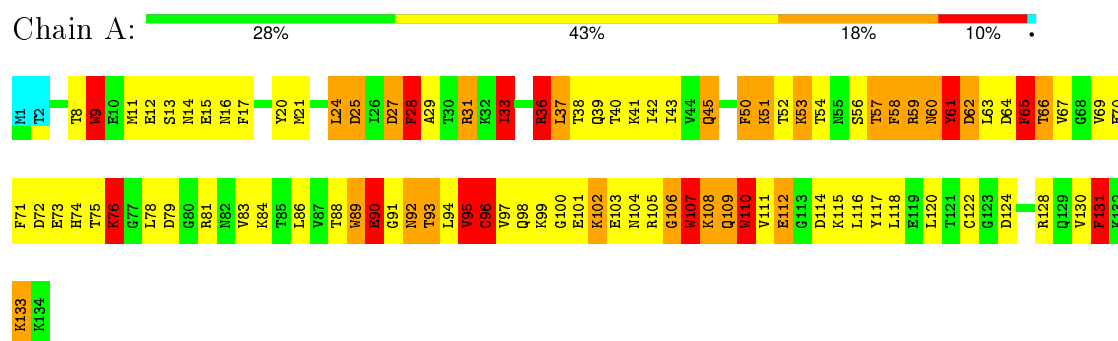
### 4.2.16 Score per residue for model 16

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



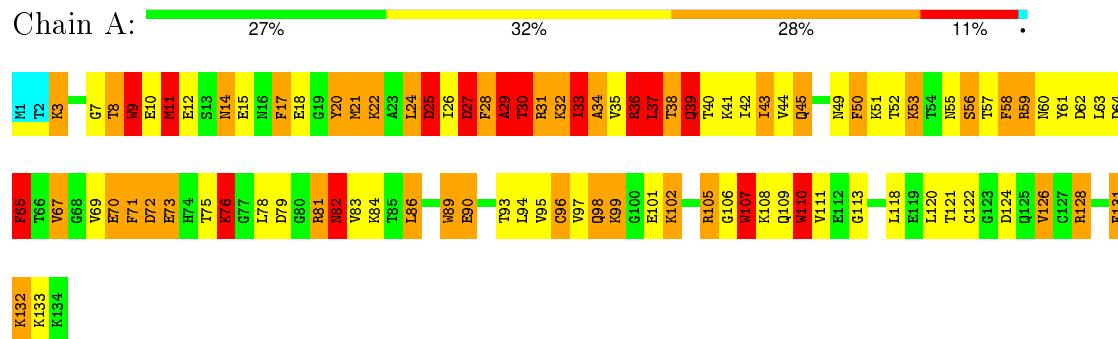
### 4.2.17 Score per residue for model 17

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



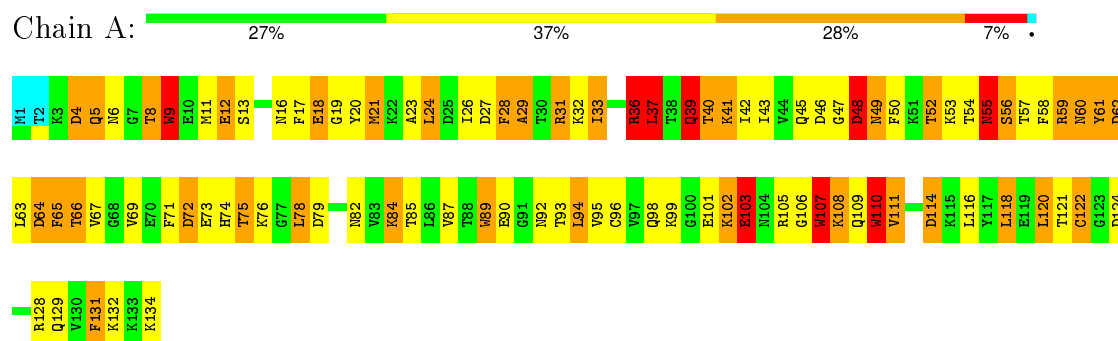
### 4.2.18 Score per residue for model 18

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



### 4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



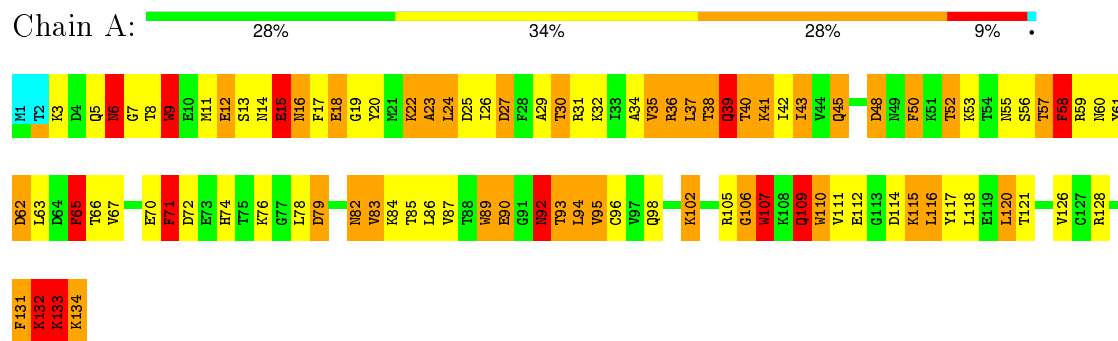
### 4.2.20 Score per residue for model 20

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



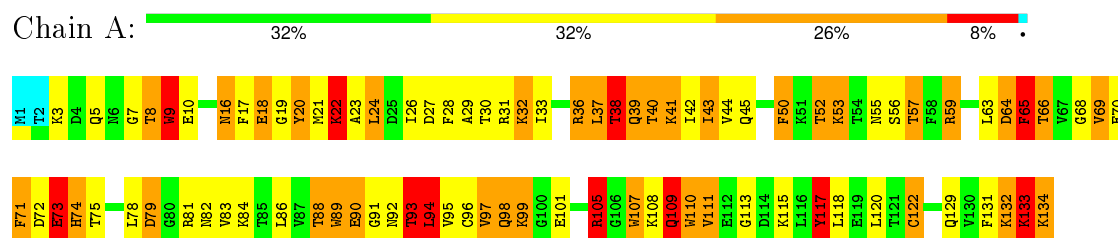
### 4.2.21 Score per residue for model 21

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



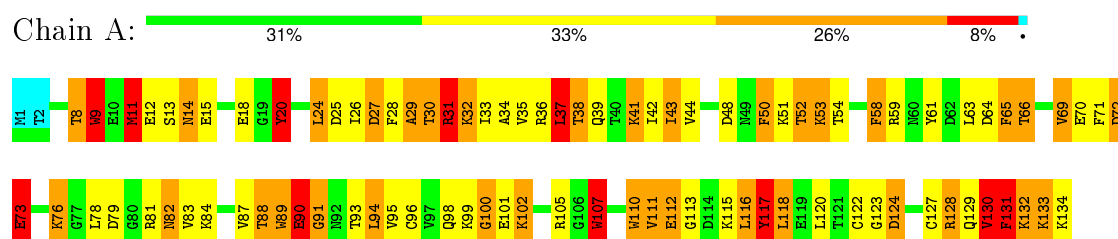
### 4.2.22 Score per residue for model 22

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



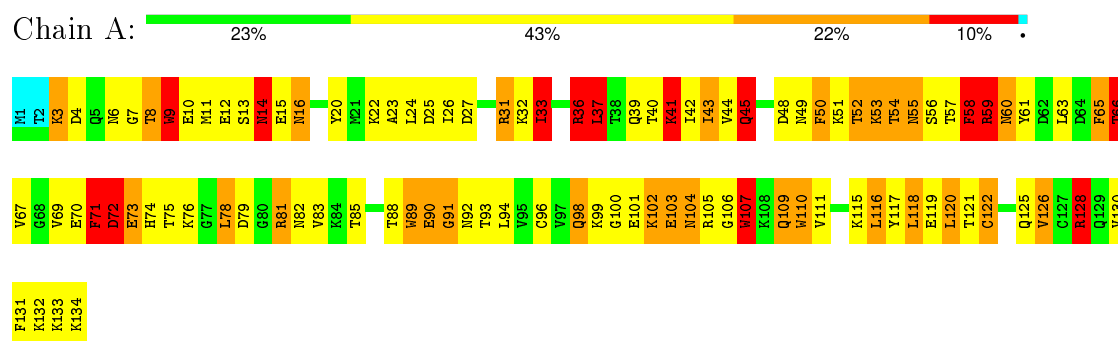
### 4.2.23 Score per residue for model 23

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



### 4.2.24 Score per residue for model 24

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *SIMULATED ANNEALING REFINEMENT*.

Of the 25 calculated structures, 24 were deposited, based on the following criterion: *FINAL PENALTY FUNCTION VALUES WITHIN 2 STANDARD DEVIATIONS FROM THE MEAN*.

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

Software name	Classification	Version
TINKER	refinement	
TINKER	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.07±0.01	6±1/1098 (0.6±0.1%)	2.28±0.05	48±4/1474 (3.3±0.2%)
All	All	1.07	145/26352 (0.6%)	2.29	1161/35376 (3.3%)

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	110	TRP	CD2-CE2	-7.11	1.32	1.41	13	22
1	A	110	TRP	CG-CD2	-6.83	1.32	1.43	23	18
1	A	107	TRP	CD2-CE2	-6.82	1.33	1.41	15	24
1	A	9	TRP	CD2-CE2	-6.75	1.33	1.41	2	17
1	A	89	TRP	CD2-CE2	-6.53	1.33	1.41	21	24
1	A	107	TRP	CG-CD2	-6.24	1.33	1.43	11	20
1	A	89	TRP	CG-CD2	-6.07	1.33	1.43	22	11
1	A	9	TRP	CG-CD2	-5.24	1.34	1.43	21	7
1	A	110	TRP	CD2-CE3	-5.15	1.32	1.40	4	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	ARG	NE-CZ-NH1	23.54	132.07	120.30	22	9
1	A	9	TRP	CD1-CG-CD2	-14.72	94.52	106.30	16	24
1	A	89	TRP	CD1-CG-CD2	14.71	118.07	106.30	7	24
1	A	89	TRP	CG-CD1-NE1	-14.30	95.80	110.10	24	24
1	A	128	ARG	NE-CZ-NH1	14.08	127.34	120.30	6	13
1	A	36	ARG	NE-CZ-NH2	14.01	127.31	120.30	6	11
1	A	31	ARG	NE-CZ-NH1	13.32	126.96	120.30	15	10
1	A	105	ARG	NE-CZ-NH2	-12.70	113.95	120.30	22	18
1	A	131	PHE	CB-CG-CD1	-12.64	111.95	120.80	23	9
1	A	59	ARG	NE-CZ-NH1	12.54	126.57	120.30	1	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	TYR	CB-CG-CD2	-12.11	113.73	121.00	21	10
1	A	65	PHE	CB-CG-CD2	-11.87	112.49	120.80	13	18
1	A	117	TYR	CB-CG-CD2	11.43	127.86	121.00	23	4
1	A	89	TRP	CD1-NE1-CE2	11.35	119.22	109.00	11	22
1	A	131	PHE	CB-CG-CD2	-11.33	112.87	120.80	21	13
1	A	9	TRP	CE2-CD2-CG	11.28	116.32	107.30	16	21
1	A	107	TRP	CD1-NE1-CE2	-11.15	98.97	109.00	11	22
1	A	58	PHE	CB-CG-CD1	-10.69	113.32	120.80	20	11
1	A	50	PHE	CB-CG-CD1	-10.66	113.33	120.80	21	8
1	A	65	PHE	CB-CG-CD1	-10.39	113.53	120.80	18	6
1	A	128	ARG	NE-CZ-NH2	10.11	125.35	120.30	16	6
1	A	9	TRP	CG-CD1-NE1	10.04	120.14	110.10	16	22
1	A	31	ARG	NE-CZ-NH2	-10.02	115.29	120.30	6	9
1	A	36	ARG	NE-CZ-NH1	9.95	125.27	120.30	4	10
1	A	50	PHE	CB-CG-CD2	-9.68	114.02	120.80	18	11
1	A	81	ARG	NE-CZ-NH2	-9.64	115.48	120.30	1	6
1	A	89	TRP	NE1-CE2-CZ2	9.56	140.92	130.40	11	24
1	A	61	TYR	CB-CG-CD1	-9.45	115.33	121.00	9	5
1	A	110	TRP	CD1-CG-CD2	9.16	113.63	106.30	13	18
1	A	37	LEU	O-C-N	9.15	137.34	122.70	22	17
1	A	28	PHE	CB-CG-CD1	-8.84	114.61	120.80	8	5
1	A	59	ARG	NE-CZ-NH2	8.84	124.72	120.30	9	10
1	A	107	TRP	NE1-CE2-CD2	8.84	116.14	107.30	14	17
1	A	91	GLY	O-C-N	8.54	136.37	122.70	14	17
1	A	14	ASN	O-C-N	8.53	136.34	122.70	21	5
1	A	28	PHE	CB-CG-CD2	8.52	126.76	120.80	8	4
1	A	58	PHE	CB-CG-CD2	-8.30	114.99	120.80	10	10
1	A	27	ASP	CB-CG-OD2	-8.22	110.90	118.30	23	11
1	A	9	TRP	CD1-NE1-CE2	-8.21	101.62	109.00	17	21
1	A	55	ASN	O-C-N	8.13	135.70	122.70	16	11
1	A	36	ARG	O-C-N	8.07	135.61	122.70	20	6
1	A	89	TRP	CA-CB-CG	-8.03	98.44	113.70	12	24
1	A	61	TYR	CG-CD2-CE2	-7.89	114.99	121.30	3	5
1	A	20	TYR	CB-CG-CD1	-7.86	116.28	121.00	9	6
1	A	117	TYR	CB-CG-CD1	7.85	125.71	121.00	20	7
1	A	73	GLU	OE1-CD-OE2	7.62	132.45	123.30	15	10
1	A	106	GLY	O-C-N	7.60	134.86	122.70	9	12
1	A	107	TRP	CE2-CD2-CG	-7.60	101.22	107.30	14	5
1	A	48	ASP	CB-CG-OD2	-7.57	111.49	118.30	6	2
1	A	71	PHE	CB-CG-CD1	7.52	126.06	120.80	21	2
1	A	72	ASP	CB-CG-OD2	-7.49	111.56	118.30	20	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	81	ARG	NE-CZ-NH1	7.49	124.05	120.30	6	5
1	A	64	ASP	CB-CG-OD1	-7.38	111.65	118.30	11	3
1	A	107	TRP	CA-CB-CG	-7.37	99.71	113.70	20	24
1	A	65	PHE	CD1-CG-CD2	7.36	127.87	118.30	4	11
1	A	22	LYS	O-C-N	7.35	134.46	122.70	24	10
1	A	7	GLY	O-C-N	7.34	134.44	122.70	13	17
1	A	61	TYR	CB-CG-CD2	-7.30	116.62	121.00	1	4
1	A	9	TRP	CG-CD2-CE3	-7.30	127.33	133.90	10	9
1	A	114	ASP	CB-CG-OD2	-7.29	111.74	118.30	5	3
1	A	104	ASN	O-C-N	7.26	134.31	122.70	24	5
1	A	48	ASP	CB-CG-OD1	-7.25	111.78	118.30	16	2
1	A	114	ASP	CB-CG-OD1	-7.20	111.82	118.30	9	8
1	A	107	TRP	CG-CD1-NE1	7.15	117.25	110.10	22	1
1	A	72	ASP	CB-CG-OD1	-7.12	111.89	118.30	10	3
1	A	21	MET	O-C-N	7.08	134.03	122.70	18	3
1	A	64	ASP	CB-CG-OD2	-7.05	111.95	118.30	3	13
1	A	114	ASP	O-C-N	6.93	133.79	122.70	20	7
1	A	8	THR	O-C-N	6.92	133.77	122.70	23	11
1	A	66	THR	O-C-N	6.90	133.74	122.70	20	2
1	A	83	VAL	O-C-N	6.86	133.68	122.70	21	5
1	A	27	ASP	CB-CG-OD1	-6.76	112.22	118.30	1	4
1	A	124	ASP	CB-CG-OD1	-6.75	112.22	118.30	5	3
1	A	24	LEU	O-C-N	6.74	133.48	122.70	21	3
1	A	39	GLN	O-C-N	6.71	133.44	122.70	9	10
1	A	70	GLU	O-C-N	6.70	133.42	122.70	2	3
1	A	5	GLN	O-C-N	6.69	133.40	122.70	9	7
1	A	71	PHE	CB-CG-CD2	6.66	125.46	120.80	11	1
1	A	61	TYR	CG-CD1-CE1	-6.65	115.98	121.30	24	2
1	A	90	GLU	OE1-CD-OE2	6.59	131.21	123.30	8	7
1	A	103	GLU	OE1-CD-OE2	6.59	131.21	123.30	3	2
1	A	29	ALA	O-C-N	6.57	133.21	122.70	2	7
1	A	11	MET	O-C-N	6.55	133.18	122.70	13	6
1	A	89	TRP	CB-CG-CD2	-6.51	118.14	126.60	12	21
1	A	105	ARG	O-C-N	6.50	134.26	123.20	17	10
1	A	110	TRP	CB-CG-CD2	-6.49	118.16	126.60	13	16
1	A	61	TYR	O-C-N	6.49	133.08	122.70	19	3
1	A	90	GLU	CA-C-O	6.45	133.64	120.10	4	11
1	A	77	GLY	O-C-N	6.42	132.98	122.70	11	4
1	A	75	THR	CA-CB-CG2	-6.40	103.44	112.40	20	7
1	A	89	TRP	CE3-CZ3-CH2	-6.36	114.20	121.20	20	23
1	A	62	ASP	CB-CG-OD1	6.36	124.03	118.30	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	VAL	O-C-N	6.36	132.87	122.70	18	6
1	A	101	GLU	OE1-CD-OE2	6.31	130.87	123.30	1	1
1	A	109	GLN	O-C-N	6.25	132.69	122.70	12	8
1	A	93	THR	O-C-N	6.24	132.68	122.70	12	4
1	A	32	LYS	O-C-N	6.23	132.67	122.70	12	4
1	A	65	PHE	CG-CD1-CE1	-6.22	113.95	120.80	23	4
1	A	79	ASP	CB-CG-OD2	-6.19	112.73	118.30	13	2
1	A	30	THR	O-C-N	6.19	132.60	122.70	18	6
1	A	117	TYR	CG-CD2-CE2	6.17	126.24	121.30	13	1
1	A	65	PHE	CG-CD2-CE2	-6.15	114.03	120.80	13	6
1	A	89	TRP	CG-CD2-CE3	-6.15	128.36	133.90	8	1
1	A	51	LYS	O-C-N	6.15	132.54	122.70	24	2
1	A	103	GLU	O-C-N	6.08	132.44	122.70	9	3
1	A	9	TRP	CB-CG-CD1	6.06	134.88	127.00	4	5
1	A	40	THR	O-C-N	6.05	132.37	122.70	18	2
1	A	18	GLU	O-C-N	6.04	133.47	123.20	22	3
1	A	64	ASP	OD1-CG-OD2	6.02	134.74	123.30	11	2
1	A	8	THR	CA-CB-CG2	-6.00	104.00	112.40	9	3
1	A	20	TYR	CG-CD2-CE2	-5.99	116.51	121.30	19	2
1	A	110	TRP	CE3-CZ3-CH2	-5.98	114.62	121.20	24	5
1	A	110	TRP	CE2-CD2-CE3	5.96	125.85	118.70	20	2
1	A	50	PHE	CD1-CG-CD2	5.94	126.02	118.30	21	6
1	A	107	TRP	CD1-CG-CD2	-5.92	101.56	106.30	22	5
1	A	56	SER	O-C-N	5.88	132.10	122.70	8	6
1	A	107	TRP	O-C-N	5.87	132.09	122.70	8	4
1	A	110	TRP	CE2-CD2-CG	-5.87	102.61	107.30	11	1
1	A	95	VAL	CB-CA-C	-5.86	100.27	111.40	11	12
1	A	49	ASN	O-C-N	5.85	132.06	122.70	1	5
1	A	110	TRP	CG-CD1-NE1	-5.82	104.28	110.10	13	3
1	A	110	TRP	CB-CG-CD1	-5.81	119.45	127.00	11	4
1	A	110	TRP	NE1-CE2-CD2	5.81	113.11	107.30	11	3
1	A	131	PHE	CG-CD1-CE1	-5.74	114.48	120.80	10	2
1	A	17	PHE	CB-CG-CD1	5.72	124.80	120.80	14	2
1	A	110	TRP	CD1-NE1-CE2	-5.71	103.86	109.00	11	3
1	A	130	VAL	CA-C-N	-5.69	104.68	117.20	17	1
1	A	41	LYS	O-C-N	5.69	131.81	122.70	24	1
1	A	96	CYS	CA-CB-SG	-5.69	103.76	114.00	4	2
1	A	131	PHE	CG-CD2-CE2	-5.67	114.57	120.80	19	1
1	A	117	TYR	O-C-N	5.64	131.73	122.70	24	2
1	A	4	ASP	CB-CG-OD2	-5.61	113.25	118.30	14	2
1	A	89	TRP	CE2-CD2-CE3	5.61	125.43	118.70	22	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	124	ASP	CB-CG-OD2	-5.60	113.26	118.30	23	2
1	A	42	ILE	O-C-N	5.59	131.65	122.70	13	1
1	A	50	PHE	CG-CD2-CE2	-5.57	114.68	120.80	11	2
1	A	110	TRP	CD2-CE2-CZ2	-5.55	115.63	122.30	8	2
1	A	130	VAL	CG1-CB-CG2	-5.55	102.02	110.90	8	2
1	A	61	TYR	CZ-CE2-CD2	5.54	124.78	119.80	3	1
1	A	20	TYR	CD1-CG-CD2	5.53	123.99	117.90	1	4
1	A	125	GLN	O-C-N	5.53	131.55	122.70	5	3
1	A	85	THR	O-C-N	5.50	131.50	122.70	10	2
1	A	44	VAL	CB-CA-C	-5.50	100.96	111.40	23	4
1	A	105	ARG	CA-C-N	-5.48	105.24	116.20	3	4
1	A	60	ASN	O-C-N	5.47	131.46	122.70	19	1
1	A	35	VAL	O-C-N	5.45	131.42	122.70	2	3
1	A	58	PHE	O-C-N	5.45	131.42	122.70	14	4
1	A	118	LEU	O-C-N	5.42	131.37	122.70	15	1
1	A	119	GLU	O-C-N	5.39	131.33	122.70	20	1
1	A	31	ARG	O-C-N	5.38	131.31	122.70	8	3
1	A	29	ALA	CA-C-N	-5.38	105.37	117.20	12	5
1	A	17	PHE	CG-CD1-CE1	-5.37	114.89	120.80	1	1
1	A	25	ASP	CB-CG-OD2	-5.37	113.47	118.30	18	1
1	A	89	TRP	CZ3-CH2-CZ2	5.36	128.03	121.60	8	16
1	A	27	ASP	O-C-N	5.36	131.28	122.70	3	1
1	A	88	THR	N-CA-CB	-5.35	100.13	110.30	22	3
1	A	89	TRP	NE1-CE2-CD2	-5.35	101.95	107.30	11	1
1	A	9	TRP	CB-CG-CD2	5.33	133.53	126.60	21	2
1	A	23	ALA	CA-C-N	-5.31	105.52	117.20	21	1
1	A	90	GLU	CA-C-N	-5.31	105.59	116.20	24	1
1	A	132	LYS	O-C-N	5.29	131.17	122.70	12	2
1	A	17	PHE	CB-CG-CD2	5.27	124.49	120.80	2	1
1	A	74	HIS	CA-CB-CG	-5.26	104.66	113.60	7	1
1	A	84	LYS	O-C-N	5.26	131.11	122.70	20	2
1	A	65	PHE	CA-C-O	5.24	131.11	120.10	8	1
1	A	25	ASP	CA-C-N	-5.24	105.67	117.20	12	1
1	A	94	LEU	CA-CB-CG	-5.24	103.24	115.30	22	1
1	A	79	ASP	CB-CG-OD1	-5.23	113.59	118.30	6	1
1	A	15	GLU	OE1-CD-OE2	5.23	129.57	123.30	13	1
1	A	130	VAL	CB-CA-C	-5.22	101.47	111.40	23	1
1	A	14	ASN	CA-CB-CG	-5.22	101.91	113.40	18	3
1	A	45	GLN	O-C-N	5.21	131.03	122.70	5	1
1	A	103	GLU	CA-C-N	-5.21	105.75	117.20	9	1
1	A	89	TRP	CD2-CE2-CZ2	-5.19	116.08	122.30	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	100	GLY	O-C-N	5.18	131.00	122.70	23	1
1	A	37	LEU	CA-CB-CG	-5.13	103.51	115.30	22	1
1	A	85	THR	CA-C-N	-5.10	105.97	117.20	20	3
1	A	107	TRP	NE1-CE2-CZ2	-5.06	124.84	130.40	12	1
1	A	59	ARG	O-C-N	5.05	130.78	122.70	24	1
1	A	23	ALA	O-C-N	5.05	130.78	122.70	21	2
1	A	34	ALA	CB-CA-C	-5.04	102.54	110.10	4	1
1	A	36	ARG	CA-C-N	-5.04	106.11	117.20	22	1
1	A	20	TYR	CZ-CE2-CD2	-5.03	115.27	119.80	22	1
1	A	15	GLU	O-C-N	-5.03	114.65	122.70	21	1
1	A	20	TYR	CG-CD1-CE1	-5.03	117.28	121.30	11	1
1	A	25	ASP	CB-CG-OD1	5.03	122.82	118.30	18	1
1	A	57	THR	O-C-N	5.02	130.72	122.70	15	1
1	A	73	GLU	N-CA-CB	-5.01	101.59	110.60	2	1

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1080	1055	1054	59±10
All	All	25920	25320	25296	1409

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:63:LEU:HD11	1:A:107:TRP:CZ2	1.01	1.91	7	6
1:A:37:LEU:HD11	1:A:58:PHE:CE1	1.00	1.91	19	3
1:A:24:LEU:HD11	1:A:79:ASP:HB2	0.98	1.34	20	1
1:A:37:LEU:HD21	1:A:58:PHE:CE2	0.97	1.93	9	2
1:A:65:PHE:CD1	1:A:87:VAL:HG21	0.92	2.00	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD21	1:A:107:TRP:CZ2	0.89	2.02	21	5
1:A:90:GLU:HB2	1:A:93:THR:HG23	0.89	1.45	4	3
1:A:36:ARG:C	1:A:37:LEU:HD13	0.86	1.90	17	1
1:A:67:VAL:HG21	1:A:89:TRP:CD1	0.84	2.07	8	8
1:A:67:VAL:HG11	1:A:89:TRP:CD1	0.84	2.08	17	4
1:A:41:LYS:CE	1:A:116:LEU:HD22	0.83	2.04	5	2
1:A:37:LEU:HD12	1:A:57:THR:CG2	0.82	2.05	24	2
1:A:24:LEU:HD11	1:A:79:ASP:CB	0.82	2.04	20	1
1:A:37:LEU:HD12	1:A:38:THR:N	0.81	1.90	21	6
1:A:37:LEU:HD11	1:A:58:PHE:CZ	0.81	2.11	8	3
1:A:36:ARG:C	1:A:37:LEU:HD23	0.81	1.96	24	10
1:A:94:LEU:HD21	1:A:109:GLN:CG	0.80	2.06	22	1
1:A:94:LEU:HD21	1:A:109:GLN:HG2	0.80	1.53	22	1
1:A:24:LEU:HD12	1:A:79:ASP:HB2	0.80	1.52	7	2
1:A:90:GLU:HG2	1:A:95:VAL:HG21	0.79	1.53	4	4
1:A:50:PHE:CD2	1:A:94:LEU:HD13	0.78	2.14	11	6
1:A:90:GLU:CB	1:A:93:THR:HG23	0.77	2.10	4	3
1:A:83:VAL:HG22	1:A:100:GLY:HA2	0.77	1.56	6	2
1:A:50:PHE:CD2	1:A:94:LEU:HD22	0.77	2.15	21	5
1:A:37:LEU:HD23	1:A:58:PHE:CD1	0.76	2.15	21	2
1:A:37:LEU:N	1:A:37:LEU:HD22	0.76	1.94	17	1
1:A:24:LEU:HD11	1:A:26:ILE:HB	0.75	1.59	3	7
1:A:37:LEU:N	1:A:37:LEU:HD23	0.74	1.97	9	4
1:A:23:ALA:HB2	1:A:125:GLN:HG3	0.74	1.60	24	1
1:A:63:LEU:HD21	1:A:65:PHE:CZ	0.73	2.19	13	1
1:A:37:LEU:HD11	1:A:58:PHE:HB3	0.73	1.59	24	5
1:A:67:VAL:HG21	1:A:89:TRP:NE1	0.73	1.99	12	5
1:A:9:TRP:CE3	1:A:116:LEU:HD22	0.73	2.18	8	1
1:A:37:LEU:HD23	1:A:37:LEU:N	0.72	1.97	14	5
1:A:37:LEU:HD12	1:A:37:LEU:C	0.71	2.06	4	6
1:A:118:LEU:HD12	1:A:131:PHE:CZ	0.70	2.21	18	1
1:A:67:VAL:HA	1:A:87:VAL:HG22	0.70	1.63	6	2
1:A:37:LEU:HD21	1:A:58:PHE:HB3	0.70	1.62	16	1
1:A:37:LEU:HD12	1:A:57:THR:OG1	0.70	1.85	7	1
1:A:109:GLN:HG2	1:A:116:LEU:HD13	0.70	1.64	10	1
1:A:14:ASN:HB2	1:A:130:VAL:HG12	0.69	1.65	23	1
1:A:9:TRP:CZ3	1:A:116:LEU:HD22	0.69	2.23	8	1
1:A:30:THR:HG23	1:A:34:ALA:O	0.68	1.89	18	1
1:A:36:ARG:HG3	1:A:37:LEU:N	0.68	2.03	19	3
1:A:83:VAL:HG11	1:A:98:GLN:HB3	0.68	1.64	22	1
1:A:37:LEU:O	1:A:37:LEU:HD12	0.68	1.89	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:TRP:CE3	1:A:89:TRP:HA	0.68	2.24	13	12
1:A:65:PHE:CE2	1:A:107:TRP:CH2	0.68	2.81	16	3
1:A:37:LEU:HD11	1:A:58:PHE:CD1	0.68	2.24	19	2
1:A:89:TRP:HA	1:A:89:TRP:CE3	0.67	2.24	2	12
1:A:120:LEU:HD12	1:A:121:THR:O	0.67	1.89	19	8
1:A:90:GLU:HB3	1:A:93:THR:HG22	0.67	1.64	12	5
1:A:24:LEU:HD13	1:A:79:ASP:HB2	0.67	1.67	6	4
1:A:109:GLN:HG2	1:A:118:LEU:HD22	0.67	1.66	1	1
1:A:65:PHE:CD2	1:A:87:VAL:HG21	0.67	2.24	19	4
1:A:37:LEU:H	1:A:37:LEU:HD22	0.67	1.48	17	1
1:A:24:LEU:N	1:A:24:LEU:HD23	0.67	2.04	19	2
1:A:37:LEU:HD13	1:A:37:LEU:C	0.67	2.09	18	1
1:A:9:TRP:CZ2	1:A:116:LEU:HD12	0.67	2.24	17	3
1:A:83:VAL:HG12	1:A:99:LYS:O	0.67	1.90	20	2
1:A:63:LEU:HD21	1:A:94:LEU:CD2	0.66	2.20	7	2
1:A:63:LEU:HD21	1:A:107:TRP:CE2	0.66	2.24	19	1
1:A:24:LEU:HD23	1:A:24:LEU:N	0.66	2.06	2	1
1:A:90:GLU:CG	1:A:95:VAL:HG21	0.66	2.21	4	3
1:A:37:LEU:HD23	1:A:58:PHE:CE2	0.66	2.25	4	3
1:A:37:LEU:HD23	1:A:58:PHE:CD2	0.66	2.26	12	4
1:A:50:PHE:CD1	1:A:65:PHE:CZ	0.65	2.83	19	1
1:A:9:TRP:CZ2	1:A:116:LEU:HD23	0.65	2.26	12	2
1:A:96:CYS:CB	1:A:107:TRP:CH2	0.65	2.79	11	6
1:A:24:LEU:HD12	1:A:78:LEU:O	0.65	1.92	22	2
1:A:90:GLU:N	1:A:93:THR:O	0.65	2.29	22	14
1:A:37:LEU:C	1:A:37:LEU:HD12	0.65	2.13	12	1
1:A:37:LEU:HD13	1:A:58:PHE:CZ	0.65	2.27	20	1
1:A:117:TYR:O	1:A:118:LEU:HD23	0.64	1.92	1	1
1:A:109:GLN:N	1:A:109:GLN:CD	0.64	2.51	15	1
1:A:67:VAL:HG13	1:A:88:THR:HA	0.64	1.70	11	3
1:A:8:THR:HG23	1:A:42:ILE:CG1	0.64	2.23	19	1
1:A:116:LEU:O	1:A:116:LEU:HD23	0.64	1.93	16	5
1:A:37:LEU:O	1:A:39:GLN:N	0.64	2.31	22	2
1:A:117:TYR:C	1:A:118:LEU:HD23	0.64	2.13	1	1
1:A:63:LEU:HD21	1:A:65:PHE:CE2	0.63	2.27	13	1
1:A:44:VAL:HG12	1:A:45:GLN:N	0.63	2.08	16	6
1:A:87:VAL:CG1	1:A:94:LEU:HD11	0.63	2.23	5	3
1:A:24:LEU:HD12	1:A:24:LEU:O	0.63	1.94	24	6
1:A:37:LEU:HD21	1:A:58:PHE:N	0.63	2.08	3	1
1:A:41:LYS:HE2	1:A:116:LEU:HD22	0.63	1.71	11	2
1:A:37:LEU:HD12	1:A:57:THR:HG23	0.62	1.69	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD13	1:A:58:PHE:CE2	0.62	2.28	20	1
1:A:85:THR:HG21	1:A:107:TRP:CZ3	0.62	2.29	21	1
1:A:116:LEU:HD12	1:A:116:LEU:O	0.62	1.93	10	1
1:A:43:ILE:HD11	1:A:50:PHE:CE2	0.62	2.29	8	1
1:A:50:PHE:CD1	1:A:94:LEU:HD13	0.62	2.30	10	1
1:A:37:LEU:HD23	1:A:58:PHE:CZ	0.62	2.30	4	1
1:A:107:TRP:NE1	1:A:109:GLN:NE2	0.62	2.47	15	5
1:A:65:PHE:CE1	1:A:87:VAL:HG21	0.61	2.30	10	2
1:A:65:PHE:CE2	1:A:107:TRP:CZ2	0.61	2.88	24	4
1:A:66:THR:HG22	1:A:69:VAL:HG23	0.61	1.72	14	4
1:A:52:THR:HG22	1:A:63:LEU:HB2	0.61	1.69	23	6
1:A:9:TRP:CH2	1:A:116:LEU:HD23	0.61	2.29	12	2
1:A:117:TYR:HB3	1:A:129:GLN:HB3	0.61	1.71	23	1
1:A:54:THR:HA	1:A:60:ASN:HB3	0.61	1.73	24	1
1:A:67:VAL:HG23	1:A:88:THR:HA	0.61	1.73	6	1
1:A:107:TRP:CD1	1:A:107:TRP:C	0.61	2.70	17	11
1:A:37:LEU:HD11	1:A:58:PHE:CD2	0.61	2.30	9	2
1:A:83:VAL:HG13	1:A:100:GLY:HA2	0.61	1.71	13	1
1:A:37:LEU:HD11	1:A:58:PHE:CG	0.61	2.31	9	2
1:A:50:PHE:CE1	1:A:94:LEU:HD22	0.60	2.31	15	3
1:A:28:PHE:N	1:A:28:PHE:CD1	0.60	2.69	4	2
1:A:73:GLU:CB	1:A:83:VAL:CA	0.60	2.79	14	1
1:A:34:ALA:HB1	1:A:58:PHE:CE2	0.60	2.31	10	1
1:A:24:LEU:HD22	1:A:105:ARG:NE	0.60	2.11	2	1
1:A:53:LYS:O	1:A:53:LYS:CE	0.60	2.49	24	1
1:A:63:LEU:HD11	1:A:107:TRP:HZ2	0.60	1.53	5	1
1:A:65:PHE:CE2	1:A:87:VAL:HG22	0.60	2.31	8	1
1:A:109:GLN:CG	1:A:118:LEU:HD22	0.60	2.26	1	1
1:A:24:LEU:C	1:A:24:LEU:HD12	0.60	2.17	3	2
1:A:94:LEU:HB3	1:A:109:GLN:CG	0.60	2.26	15	2
1:A:24:LEU:HD13	1:A:79:ASP:CB	0.60	2.27	6	3
1:A:129:GLN:O	1:A:130:VAL:HG13	0.60	1.97	23	1
1:A:133:LYS:C	1:A:133:LYS:HD3	0.59	2.17	22	1
1:A:13:SER:O	1:A:130:VAL:HG12	0.59	1.96	23	1
1:A:65:PHE:CG	1:A:87:VAL:HG21	0.59	2.32	13	2
1:A:133:LYS:HD2	1:A:133:LYS:N	0.59	2.13	22	1
1:A:43:ILE:CD1	1:A:50:PHE:CE1	0.59	2.85	6	3
1:A:33:ILE:HD12	1:A:33:ILE:N	0.59	2.12	23	3
1:A:89:TRP:CZ3	1:A:94:LEU:N	0.59	2.71	22	2
1:A:26:ILE:HD12	1:A:78:LEU:O	0.59	1.98	10	8
1:A:37:LEU:CD2	1:A:58:PHE:CE2	0.58	2.80	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:PHE:CD1	1:A:50:PHE:C	0.58	2.77	19	7
1:A:37:LEU:CD1	1:A:58:PHE:CE2	0.58	2.86	20	1
1:A:42:ILE:HD13	1:A:53:LYS:CD	0.58	2.28	14	1
1:A:39:GLN:CG	1:A:40:THR:N	0.58	2.66	22	5
1:A:37:LEU:HD12	1:A:57:THR:HG22	0.58	1.76	24	1
1:A:42:ILE:HD11	1:A:55:ASN:HB2	0.58	1.74	16	1
1:A:37:LEU:CD2	1:A:58:PHE:CD2	0.58	2.87	12	4
1:A:52:THR:HG22	1:A:63:LEU:CB	0.58	2.27	4	4
1:A:63:LEU:HD21	1:A:107:TRP:HZ2	0.58	1.58	15	3
1:A:9:TRP:CB	1:A:131:PHE:CD2	0.58	2.87	21	1
1:A:38:THR:HG22	1:A:39:GLN:N	0.58	2.13	2	1
1:A:37:LEU:C	1:A:37:LEU:CD1	0.58	2.71	18	3
1:A:31:ARG:O	1:A:33:ILE:HD12	0.58	1.98	15	1
1:A:120:LEU:HD12	1:A:121:THR:N	0.58	2.13	21	2
1:A:86:LEU:HD23	1:A:87:VAL:N	0.58	2.14	2	1
1:A:83:VAL:HG13	1:A:99:LYS:C	0.57	2.18	6	2
1:A:36:ARG:CG	1:A:37:LEU:N	0.57	2.67	20	3
1:A:17:PHE:CD1	1:A:18:GLU:N	0.57	2.72	22	1
1:A:9:TRP:N	1:A:9:TRP:CD1	0.57	2.72	14	7
1:A:41:LYS:NZ	1:A:116:LEU:HD21	0.57	2.14	4	1
1:A:37:LEU:HD23	1:A:58:PHE:CG	0.57	2.34	21	2
1:A:24:LEU:O	1:A:24:LEU:HD12	0.57	2.00	4	1
1:A:17:PHE:CZ	1:A:34:ALA:HB3	0.57	2.34	10	1
1:A:94:LEU:HD23	1:A:109:GLN:NE2	0.57	2.14	12	1
1:A:37:LEU:HD21	1:A:58:PHE:CB	0.57	2.29	16	1
1:A:14:ASN:N	1:A:14:ASN:ND2	0.57	2.52	7	1
1:A:23:ALA:HB1	1:A:122:CYS:O	0.57	2.00	19	3
1:A:9:TRP:CZ2	1:A:116:LEU:HD13	0.57	2.35	21	1
1:A:48:ASP:O	1:A:67:VAL:HG12	0.56	1.99	21	1
1:A:116:LEU:HD12	1:A:131:PHE:CG	0.56	2.35	23	1
1:A:17:PHE:CE2	1:A:35:VAL:HG22	0.56	2.35	18	1
1:A:9:TRP:CD1	1:A:9:TRP:N	0.56	2.74	15	13
1:A:54:THR:HA	1:A:60:ASN:CB	0.56	2.30	24	1
1:A:90:GLU:HB2	1:A:93:THR:HG22	0.56	1.76	23	2
1:A:8:THR:C	1:A:9:TRP:CD1	0.56	2.79	20	15
1:A:8:THR:HG22	1:A:134:LYS:HG2	0.56	1.77	23	1
1:A:21:MET:O	1:A:26:ILE:HG22	0.56	2.01	2	6
1:A:66:THR:O	1:A:69:VAL:HG23	0.56	2.01	24	2
1:A:90:GLU:CB	1:A:93:THR:HG22	0.56	2.31	23	6
1:A:37:LEU:HD11	1:A:58:PHE:CE2	0.56	2.36	9	1
1:A:45:GLN:CG	1:A:50:PHE:CD1	0.55	2.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TRP:CE3	1:A:133:LYS:HA	0.55	2.35	9	17
1:A:43:ILE:HD11	1:A:50:PHE:HE2	0.55	1.61	8	1
1:A:36:ARG:C	1:A:37:LEU:CD2	0.55	2.74	20	2
1:A:107:TRP:O	1:A:107:TRP:CD1	0.55	2.60	11	1
1:A:41:LYS:HA	1:A:55:ASN:CB	0.55	2.32	24	1
1:A:83:VAL:HG13	1:A:100:GLY:N	0.55	2.16	5	3
1:A:9:TRP:CH2	1:A:116:LEU:HD12	0.55	2.36	7	1
1:A:33:ILE:N	1:A:33:ILE:HD13	0.55	2.17	17	1
1:A:118:LEU:HB2	1:A:131:PHE:CE1	0.55	2.37	11	4
1:A:4:ASP:HA	1:A:111:VAL:HG21	0.55	1.79	19	1
1:A:34:ALA:HB1	1:A:58:PHE:CD2	0.55	2.36	10	1
1:A:37:LEU:HD12	1:A:58:PHE:CG	0.55	2.36	20	1
1:A:63:LEU:CD2	1:A:65:PHE:CZ	0.55	2.89	22	1
1:A:107:TRP:C	1:A:107:TRP:CD1	0.55	2.79	21	4
1:A:48:ASP:O	1:A:66:THR:HG23	0.55	2.02	11	1
1:A:45:GLN:HG3	1:A:50:PHE:CD1	0.55	2.37	13	1
1:A:96:CYS:CB	1:A:107:TRP:CZ2	0.55	2.90	20	1
1:A:37:LEU:CD2	1:A:57:THR:HG22	0.55	2.32	21	1
1:A:24:LEU:HD22	1:A:105:ARG:NH1	0.55	2.17	18	1
1:A:33:ILE:N	1:A:33:ILE:HD12	0.55	2.17	14	1
1:A:43:ILE:HD13	1:A:44:VAL:N	0.54	2.16	8	2
1:A:33:ILE:HD12	1:A:33:ILE:H	0.54	1.62	14	3
1:A:118:LEU:CB	1:A:131:PHE:CE1	0.54	2.91	11	3
1:A:50:PHE:C	1:A:50:PHE:CD1	0.54	2.77	22	7
1:A:50:PHE:CE2	1:A:94:LEU:HD22	0.54	2.37	21	7
1:A:37:LEU:CD2	1:A:37:LEU:N	0.54	2.64	17	4
1:A:37:LEU:CD1	1:A:58:PHE:CZ	0.54	2.90	20	1
1:A:95:VAL:HG13	1:A:108:LYS:NZ	0.54	2.17	6	1
1:A:38:THR:HA	1:A:56:SER:HB3	0.54	1.80	20	1
1:A:37:LEU:HD11	1:A:56:SER:CB	0.54	2.33	18	1
1:A:70:GLU:HG3	1:A:86:LEU:HD12	0.54	1.77	18	1
1:A:67:VAL:HG21	1:A:89:TRP:HE1	0.54	1.60	7	1
1:A:118:LEU:HD13	1:A:131:PHE:CZ	0.54	2.38	3	1
1:A:75:THR:HB	1:A:82:ASN:ND2	0.54	2.18	14	1
1:A:133:LYS:N	1:A:133:LYS:CD	0.54	2.70	22	1
1:A:118:LEU:HB2	1:A:131:PHE:CE2	0.54	2.38	23	1
1:A:26:ILE:CD1	1:A:78:LEU:HD12	0.53	2.33	23	1
1:A:38:THR:HG21	1:A:57:THR:HB	0.53	1.80	22	1
1:A:42:ILE:CG2	1:A:43:ILE:N	0.53	2.71	24	17
1:A:65:PHE:CG	1:A:66:THR:N	0.53	2.75	21	1
1:A:83:VAL:HG12	1:A:84:LYS:N	0.53	2.18	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:THR:HG23	1:A:34:ALA:C	0.53	2.23	18	1
1:A:27:ASP:O	1:A:28:PHE:CG	0.53	2.61	3	1
1:A:36:ARG:HD2	1:A:39:GLN:HB3	0.53	1.81	7	2
1:A:24:LEU:HD12	1:A:26:ILE:HB	0.53	1.79	18	1
1:A:9:TRP:HB2	1:A:131:PHE:CD1	0.53	2.37	23	1
1:A:37:LEU:CD2	1:A:58:PHE:CD1	0.53	2.91	18	1
1:A:104:ASN:O	1:A:121:THR:HG22	0.53	2.04	7	1
1:A:11:MET:HG3	1:A:131:PHE:CZ	0.53	2.39	5	1
1:A:93:THR:HG23	1:A:95:VAL:CG2	0.53	2.33	17	1
1:A:14:ASN:ND2	1:A:14:ASN:N	0.53	2.56	2	3
1:A:17:PHE:CD1	1:A:17:PHE:N	0.53	2.77	18	2
1:A:118:LEU:HB2	1:A:131:PHE:CZ	0.53	2.39	19	5
1:A:8:THR:HG23	1:A:42:ILE:HG12	0.53	1.81	19	1
1:A:42:ILE:HG22	1:A:43:ILE:N	0.52	2.19	15	19
1:A:34:ALA:HA	1:A:37:LEU:HD21	0.52	1.79	6	1
1:A:26:ILE:HD11	1:A:78:LEU:HA	0.52	1.81	12	1
1:A:102:LYS:CD	1:A:103:GLU:HG2	0.52	2.34	15	1
1:A:96:CYS:HB2	1:A:107:TRP:CH2	0.52	2.39	23	3
1:A:17:PHE:CZ	1:A:35:VAL:HG22	0.52	2.39	2	1
1:A:54:THR:CG2	1:A:55:ASN:N	0.52	2.73	24	1
1:A:131:PHE:N	1:A:131:PHE:CD1	0.52	2.77	1	2
1:A:50:PHE:CD1	1:A:51:LYS:N	0.52	2.77	23	2
1:A:52:THR:CG2	1:A:53:LYS:N	0.52	2.73	21	6
1:A:107:TRP:HE1	1:A:109:GLN:NE2	0.52	2.03	4	5
1:A:9:TRP:CG	1:A:131:PHE:CD2	0.52	2.97	21	1
1:A:37:LEU:HG	1:A:58:PHE:CE2	0.52	2.38	13	1
1:A:96:CYS:HB2	1:A:107:TRP:CZ3	0.52	2.40	11	3
1:A:11:MET:HG3	1:A:131:PHE:CE1	0.52	2.39	5	2
1:A:40:THR:CG2	1:A:41:LYS:N	0.52	2.72	16	3
1:A:37:LEU:CD2	1:A:58:PHE:CG	0.52	2.93	12	3
1:A:128:ARG:C	1:A:129:GLN:HG3	0.52	2.25	23	1
1:A:59:ARG:NH2	1:A:61:TYR:CE1	0.52	2.78	17	1
1:A:42:ILE:HD13	1:A:54:THR:HB	0.52	1.80	24	1
1:A:94:LEU:CD2	1:A:109:GLN:CG	0.52	2.87	22	1
1:A:37:LEU:HD21	1:A:57:THR:HG22	0.52	1.82	21	1
1:A:9:TRP:CZ2	1:A:116:LEU:CD1	0.52	2.93	21	1
1:A:26:ILE:CD1	1:A:78:LEU:HA	0.51	2.34	13	4
1:A:71:PHE:HB3	1:A:85:THR:HB	0.51	1.81	2	4
1:A:26:ILE:HD12	1:A:78:LEU:HD12	0.51	1.81	19	1
1:A:8:THR:HG23	1:A:40:THR:HG23	0.51	1.80	4	1
1:A:133:LYS:CG	1:A:134:LYS:N	0.51	2.73	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ARG:NH2	1:A:120:LEU:HD13	0.51	2.21	15	1
1:A:8:THR:CG2	1:A:40:THR:CG2	0.51	2.88	17	2
1:A:41:LYS:HE3	1:A:116:LEU:HD22	0.51	1.80	5	1
1:A:37:LEU:CD1	1:A:37:LEU:C	0.51	2.78	4	5
1:A:37:LEU:HD21	1:A:58:PHE:HE2	0.51	1.55	9	1
1:A:9:TRP:HB2	1:A:131:PHE:CD2	0.51	2.39	21	2
1:A:112:GLU:HG3	1:A:117:TYR:CZ	0.51	2.40	23	1
1:A:133:LYS:C	1:A:133:LYS:CD	0.51	2.76	22	1
1:A:65:PHE:CE1	1:A:87:VAL:CG2	0.51	2.93	5	1
1:A:117:TYR:CB	1:A:129:GLN:HB3	0.51	2.36	23	1
1:A:42:ILE:N	1:A:53:LYS:O	0.51	2.44	23	16
1:A:23:ALA:HB2	1:A:125:GLN:CG	0.51	2.34	24	1
1:A:41:LYS:HE3	1:A:118:LEU:HD11	0.51	1.82	3	1
1:A:73:GLU:CB	1:A:83:VAL:HA	0.51	2.36	14	1
1:A:14:ASN:ND2	1:A:15:GLU:N	0.51	2.57	23	1
1:A:50:PHE:HD2	1:A:94:LEU:HD13	0.51	1.66	24	1
1:A:74:HIS:ND1	1:A:74:HIS:N	0.51	2.57	10	1
1:A:43:ILE:HG12	1:A:50:PHE:CE1	0.51	2.40	13	1
1:A:37:LEU:HG	1:A:58:PHE:CZ	0.51	2.40	13	1
1:A:130:VAL:C	1:A:131:PHE:CD1	0.51	2.84	4	2
1:A:92:ASN:N	1:A:92:ASN:ND2	0.51	2.54	12	1
1:A:63:LEU:HD21	1:A:94:LEU:HD22	0.51	1.83	5	2
1:A:89:TRP:CE3	1:A:89:TRP:CA	0.51	2.94	22	12
1:A:65:PHE:CE2	1:A:87:VAL:CG2	0.51	2.93	21	2
1:A:20:TYR:C	1:A:20:TYR:CD1	0.51	2.84	20	3
1:A:18:GLU:HB2	1:A:31:ARG:CB	0.51	2.36	1	1
1:A:17:PHE:N	1:A:17:PHE:CD1	0.51	2.78	21	1
1:A:41:LYS:HD2	1:A:131:PHE:CZ	0.51	2.40	23	1
1:A:33:ILE:CG2	1:A:33:ILE:O	0.50	2.59	18	1
1:A:10:GLU:N	1:A:132:LYS:O	0.50	2.44	22	1
1:A:108:LYS:HG3	1:A:110:TRP:CH2	0.50	2.42	10	5
1:A:32:LYS:C	1:A:33:ILE:CG1	0.50	2.80	4	2
1:A:33:ILE:O	1:A:33:ILE:HG22	0.50	2.06	18	1
1:A:39:GLN:HG2	1:A:56:SER:N	0.50	2.20	21	1
1:A:63:LEU:CG	1:A:65:PHE:CE2	0.50	2.95	13	1
1:A:63:LEU:HG	1:A:65:PHE:CZ	0.50	2.42	1	6
1:A:86:LEU:HD21	1:A:88:THR:OG1	0.50	2.07	3	2
1:A:37:LEU:HB2	1:A:58:PHE:CE1	0.50	2.42	20	1
1:A:24:LEU:N	1:A:24:LEU:CD2	0.50	2.75	19	1
1:A:83:VAL:HG11	1:A:98:GLN:OE1	0.50	2.07	17	1
1:A:63:LEU:HG	1:A:65:PHE:CE2	0.50	2.42	22	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLU:CB	1:A:93:THR:CG2	0.50	2.90	8	3
1:A:90:GLU:CG	1:A:95:VAL:CG2	0.50	2.90	4	4
1:A:21:MET:CG	1:A:26:ILE:CG2	0.50	2.89	9	1
1:A:37:LEU:HD12	1:A:38:THR:H	0.50	1.64	21	1
1:A:9:TRP:CZ3	1:A:133:LYS:HB2	0.50	2.42	17	11
1:A:102:LYS:CD	1:A:103:GLU:N	0.50	2.75	24	5
1:A:118:LEU:O	1:A:118:LEU:HD23	0.50	2.06	15	1
1:A:87:VAL:HG13	1:A:96:CYS:SG	0.50	2.47	9	1
1:A:63:LEU:CD2	1:A:65:PHE:CE2	0.49	2.95	13	2
1:A:39:GLN:HG3	1:A:40:THR:N	0.49	2.21	19	3
1:A:10:GLU:O	1:A:12:GLU:N	0.49	2.45	13	5
1:A:82:ASN:ND2	1:A:82:ASN:N	0.49	2.59	6	1
1:A:11:MET:HE2	1:A:41:LYS:HB2	0.49	1.83	3	1
1:A:26:ILE:HD12	1:A:78:LEU:C	0.49	2.27	2	1
1:A:24:LEU:HD12	1:A:24:LEU:C	0.49	2.27	1	4
1:A:89:TRP:CZ3	1:A:93:THR:C	0.49	2.86	12	4
1:A:28:PHE:CD1	1:A:28:PHE:N	0.49	2.77	12	3
1:A:69:VAL:HG13	1:A:71:PHE:N	0.49	2.22	20	1
1:A:65:PHE:CD1	1:A:65:PHE:N	0.49	2.80	19	1
1:A:96:CYS:CB	1:A:107:TRP:CZ3	0.49	2.96	11	3
1:A:30:THR:HG22	1:A:30:THR:O	0.49	2.07	23	2
1:A:41:LYS:C	1:A:41:LYS:CD	0.49	2.80	21	4
1:A:58:PHE:N	1:A:58:PHE:CD1	0.49	2.80	20	1
1:A:11:MET:HE3	1:A:39:GLN:HG2	0.49	1.85	3	1
1:A:37:LEU:HD11	1:A:58:PHE:CB	0.49	2.34	10	1
1:A:8:THR:HG22	1:A:134:LYS:CG	0.49	2.38	23	1
1:A:65:PHE:CZ	1:A:107:TRP:CH2	0.49	3.00	24	2
1:A:96:CYS:HB2	1:A:107:TRP:CZ2	0.49	2.41	20	1
1:A:38:THR:O	1:A:38:THR:HG23	0.49	2.07	20	1
1:A:98:GLN:CB	1:A:105:ARG:HB2	0.49	2.37	20	2
1:A:65:PHE:CE2	1:A:87:VAL:HG21	0.49	2.42	21	1
1:A:69:VAL:HG12	1:A:71:PHE:N	0.49	2.21	2	1
1:A:65:PHE:CD2	1:A:87:VAL:CG2	0.49	2.95	8	1
1:A:41:LYS:HA	1:A:55:ASN:HB3	0.49	1.84	24	1
1:A:37:LEU:HD12	1:A:58:PHE:CD2	0.49	2.43	20	1
1:A:40:THR:O	1:A:40:THR:HG22	0.49	2.06	20	2
1:A:90:GLU:HB2	1:A:95:VAL:HG23	0.49	1.84	3	4
1:A:89:TRP:CA	1:A:89:TRP:CE3	0.49	2.96	9	6
1:A:107:TRP:HB2	1:A:120:LEU:CB	0.49	2.38	2	1
1:A:107:TRP:HB2	1:A:120:LEU:HB2	0.48	1.84	2	2
1:A:126:VAL:HG13	1:A:128:ARG:NH1	0.48	2.22	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:THR:CG2	1:A:82:ASN:ND2	0.48	2.76	14	1
1:A:41:LYS:CD	1:A:41:LYS:C	0.48	2.82	16	6
1:A:30:THR:O	1:A:33:ILE:HD12	0.48	2.08	16	1
1:A:50:PHE:CE2	1:A:94:LEU:HD13	0.48	2.42	11	3
1:A:26:ILE:O	1:A:26:ILE:HG23	0.48	2.07	8	2
1:A:20:TYR:OH	1:A:78:LEU:HD21	0.48	2.08	12	2
1:A:63:LEU:HG	1:A:65:PHE:CE1	0.48	2.44	19	1
1:A:26:ILE:CD1	1:A:78:LEU:C	0.48	2.82	12	1
1:A:37:LEU:HD21	1:A:58:PHE:H	0.48	1.67	3	1
1:A:65:PHE:CD2	1:A:87:VAL:HG11	0.48	2.43	11	1
1:A:65:PHE:CZ	1:A:87:VAL:CB	0.48	2.97	21	1
1:A:90:GLU:CB	1:A:93:THR:HG21	0.48	2.37	8	1
1:A:52:THR:HG23	1:A:53:LYS:N	0.48	2.24	9	2
1:A:126:VAL:O	1:A:126:VAL:HG13	0.48	2.09	18	3
1:A:43:ILE:HG13	1:A:50:PHE:CE1	0.48	2.43	2	3
1:A:131:PHE:CD1	1:A:131:PHE:N	0.48	2.82	11	1
1:A:54:THR:OG1	1:A:60:ASN:HB3	0.48	2.09	24	1
1:A:126:VAL:HG22	1:A:126:VAL:O	0.48	2.08	6	4
1:A:63:LEU:CD1	1:A:107:TRP:CZ2	0.48	2.89	5	2
1:A:65:PHE:CZ	1:A:87:VAL:HG11	0.48	2.44	21	1
1:A:83:VAL:CG1	1:A:100:GLY:HA2	0.48	2.39	13	1
1:A:98:GLN:HB2	1:A:106:GLY:N	0.48	2.24	13	3
1:A:39:GLN:HG2	1:A:40:THR:N	0.48	2.24	13	2
1:A:52:THR:O	1:A:63:LEU:N	0.48	2.46	3	3
1:A:9:TRP:CD1	1:A:41:LYS:CD	0.48	2.97	1	1
1:A:33:ILE:CD1	1:A:33:ILE:N	0.48	2.77	23	2
1:A:17:PHE:CD2	1:A:18:GLU:N	0.47	2.82	10	1
1:A:83:VAL:HG22	1:A:100:GLY:O	0.47	2.08	17	1
1:A:42:ILE:HD12	1:A:53:LYS:O	0.47	2.09	17	1
1:A:67:VAL:CG2	1:A:89:TRP:CD1	0.47	2.92	8	1
1:A:50:PHE:CD2	1:A:94:LEU:CD1	0.47	2.97	23	2
1:A:8:THR:HG22	1:A:42:ILE:HG23	0.47	1.85	9	1
1:A:19:GLY:HA2	1:A:22:LYS:CG	0.47	2.38	22	1
1:A:3:LYS:HB2	1:A:89:TRP:CH2	0.47	2.45	13	1
1:A:88:THR:HG23	1:A:95:VAL:HB	0.47	1.85	20	2
1:A:20:TYR:O	1:A:24:LEU:HD23	0.47	2.08	7	2
1:A:37:LEU:CD1	1:A:58:PHE:HB3	0.47	2.39	6	2
1:A:8:THR:CG2	1:A:40:THR:HG23	0.47	2.39	20	3
1:A:33:ILE:H	1:A:33:ILE:HD12	0.47	1.69	8	1
1:A:90:GLU:HB3	1:A:93:THR:HG23	0.47	1.85	15	1
1:A:66:THR:CG2	1:A:69:VAL:HG23	0.47	2.39	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LYS:HE3	1:A:131:PHE:CE2	0.47	2.44	21	1
1:A:9:TRP:CZ2	1:A:116:LEU:CD2	0.47	2.97	23	1
1:A:53:LYS:O	1:A:53:LYS:CD	0.47	2.63	24	1
1:A:75:THR:OG1	1:A:76:LYS:N	0.47	2.47	20	9
1:A:3:LYS:HB2	1:A:89:TRP:CZ3	0.47	2.45	7	2
1:A:109:GLN:CG	1:A:118:LEU:CD2	0.47	2.92	7	1
1:A:26:ILE:HG23	1:A:26:ILE:O	0.47	2.09	7	2
1:A:115:LYS:HG3	1:A:117:TYR:CD1	0.47	2.45	23	1
1:A:112:GLU:HB2	1:A:117:TYR:CD1	0.47	2.45	17	1
1:A:37:LEU:CG	1:A:58:PHE:CD2	0.47	2.98	13	2
1:A:63:LEU:HD11	1:A:107:TRP:CH2	0.47	2.43	6	2
1:A:9:TRP:CE3	1:A:133:LYS:CA	0.47	2.98	12	2
1:A:5:GLN:N	1:A:5:GLN:HE21	0.47	2.08	9	1
1:A:9:TRP:CD1	1:A:41:LYS:HE3	0.47	2.45	19	1
1:A:66:THR:CG2	1:A:69:VAL:HG21	0.47	2.40	5	1
1:A:16:ASN:OD1	1:A:19:GLY:N	0.47	2.48	15	2
1:A:26:ILE:CD1	1:A:79:ASP:N	0.47	2.78	12	1
1:A:21:MET:C	1:A:26:ILE:HG22	0.46	2.31	22	1
1:A:132:LYS:CD	1:A:132:LYS:C	0.46	2.81	18	1
1:A:83:VAL:HG13	1:A:100:GLY:H	0.46	1.68	5	1
1:A:98:GLN:HG3	1:A:105:ARG:CB	0.46	2.40	2	1
1:A:38:THR:CG2	1:A:39:GLN:N	0.46	2.78	2	1
1:A:92:ASN:O	1:A:93:THR:HB	0.46	2.10	12	5
1:A:66:THR:HB	1:A:69:VAL:HG23	0.46	1.87	11	1
1:A:94:LEU:O	1:A:109:GLN:NE2	0.46	2.48	21	1
1:A:88:THR:HG22	1:A:89:TRP:H	0.46	1.70	22	1
1:A:41:LYS:HD3	1:A:41:LYS:C	0.46	2.31	16	4
1:A:71:PHE:O	1:A:73:GLU:N	0.46	2.49	6	9
1:A:109:GLN:C	1:A:110:TRP:CG	0.46	2.87	14	4
1:A:26:ILE:HD11	1:A:78:LEU:CA	0.46	2.39	12	1
1:A:37:LEU:CG	1:A:58:PHE:CE2	0.46	2.98	13	1
1:A:17:PHE:CE1	1:A:35:VAL:HG13	0.46	2.46	18	1
1:A:8:THR:HG22	1:A:134:LYS:CE	0.46	2.41	23	1
1:A:42:ILE:HB	1:A:53:LYS:O	0.46	2.10	22	2
1:A:90:GLU:HB3	1:A:93:THR:HG21	0.46	1.87	8	1
1:A:81:ARG:CG	1:A:82:ASN:N	0.46	2.78	13	2
1:A:96:CYS:HB3	1:A:107:TRP:CH2	0.46	2.45	11	1
1:A:37:LEU:CB	1:A:58:PHE:CE1	0.46	2.98	20	1
1:A:37:LEU:HD23	1:A:58:PHE:CE1	0.46	2.45	21	2
1:A:73:GLU:HA	1:A:83:VAL:N	0.46	2.26	14	1
1:A:32:LYS:C	1:A:33:ILE:HD12	0.46	2.31	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:CE1	1:A:120:LEU:HD11	0.46	2.46	8	2
1:A:43:ILE:CG1	1:A:50:PHE:CE1	0.46	2.99	13	2
1:A:98:GLN:HG3	1:A:106:GLY:N	0.46	2.26	21	1
1:A:69:VAL:O	1:A:69:VAL:HG12	0.46	2.10	17	1
1:A:41:LYS:NZ	1:A:43:ILE:HD12	0.46	2.25	15	1
1:A:73:GLU:CB	1:A:83:VAL:N	0.46	2.79	14	1
1:A:98:GLN:HG2	1:A:106:GLY:N	0.46	2.25	2	1
1:A:9:TRP:CZ3	1:A:116:LEU:HG	0.46	2.45	23	1
1:A:66:THR:CG2	1:A:67:VAL:N	0.46	2.78	8	3
1:A:98:GLN:CD	1:A:105:ARG:HB3	0.46	2.31	18	1
1:A:37:LEU:HD21	1:A:58:PHE:CG	0.46	2.46	16	1
1:A:63:LEU:HD11	1:A:107:TRP:CE2	0.46	2.43	7	1
1:A:37:LEU:C	1:A:39:GLN:N	0.46	2.69	22	1
1:A:20:TYR:CD1	1:A:20:TYR:C	0.46	2.88	4	1
1:A:54:THR:CB	1:A:60:ASN:HB3	0.46	2.41	24	1
1:A:43:ILE:HD13	1:A:50:PHE:CE1	0.46	2.45	6	1
1:A:109:GLN:N	1:A:109:GLN:HE21	0.46	2.08	20	1
1:A:11:MET:CG	1:A:131:PHE:CE1	0.46	2.99	5	1
1:A:36:ARG:O	1:A:37:LEU:HD13	0.46	2.09	17	1
1:A:24:LEU:HD11	1:A:78:LEU:O	0.46	2.11	17	3
1:A:3:LYS:HG2	1:A:89:TRP:CZ3	0.46	2.45	20	1
1:A:73:GLU:HB3	1:A:83:VAL:CA	0.46	2.40	14	1
1:A:37:LEU:CD1	1:A:58:PHE:CE1	0.46	2.83	19	1
1:A:109:GLN:OE1	1:A:116:LEU:HD21	0.46	2.11	19	1
1:A:85:THR:O	1:A:85:THR:HG22	0.45	2.11	20	2
1:A:56:SER:HB2	1:A:58:PHE:CE1	0.45	2.46	11	2
1:A:41:LYS:HA	1:A:55:ASN:CA	0.45	2.41	24	1
1:A:109:GLN:HB2	1:A:116:LEU:HD12	0.45	1.87	12	1
1:A:44:VAL:N	1:A:51:LYS:O	0.45	2.48	9	1
1:A:21:MET:HG2	1:A:26:ILE:HG22	0.45	1.86	9	1
1:A:63:LEU:HD23	1:A:65:PHE:CZ	0.45	2.46	22	1
1:A:107:TRP:CD1	1:A:108:LYS:N	0.45	2.84	14	2
1:A:31:ARG:O	1:A:32:LYS:CB	0.45	2.64	13	1
1:A:126:VAL:HG13	1:A:126:VAL:O	0.45	2.12	21	3
1:A:107:TRP:CD1	1:A:109:GLN:NE2	0.45	2.84	14	4
1:A:106:GLY:O	1:A:121:THR:HG22	0.45	2.11	21	2
1:A:42:ILE:CD1	1:A:54:THR:HB	0.45	2.41	24	1
1:A:102:LYS:CD	1:A:103:GLU:CG	0.45	2.94	15	1
1:A:38:THR:O	1:A:38:THR:HG22	0.45	2.11	14	2
1:A:18:GLU:CG	1:A:19:GLY:N	0.45	2.79	15	1
1:A:98:GLN:CG	1:A:106:GLY:N	0.45	2.80	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:PHE:CE2	1:A:87:VAL:HB	0.45	2.46	21	1
1:A:130:VAL:HG23	1:A:131:PHE:N	0.45	2.26	23	1
1:A:107:TRP:CB	1:A:120:LEU:HB2	0.45	2.41	15	2
1:A:36:ARG:C	1:A:37:LEU:HD12	0.45	2.31	18	1
1:A:96:CYS:SG	1:A:107:TRP:CZ2	0.45	3.09	16	3
1:A:109:GLN:HG2	1:A:118:LEU:CD2	0.45	2.42	7	1
1:A:65:PHE:CD1	1:A:65:PHE:C	0.45	2.89	21	2
1:A:24:LEU:HD13	1:A:26:ILE:HD13	0.45	1.89	12	1
1:A:112:GLU:HG2	1:A:117:TYR:CD2	0.45	2.46	13	1
1:A:9:TRP:CZ3	1:A:133:LYS:HG3	0.45	2.47	18	2
1:A:52:THR:HB	1:A:63:LEU:HD23	0.45	1.87	23	2
1:A:21:MET:HG2	1:A:26:ILE:CG2	0.45	2.41	9	1
1:A:37:LEU:N	1:A:58:PHE:CE2	0.45	2.85	21	1
1:A:37:LEU:HG	1:A:58:PHE:CD1	0.45	2.47	6	2
1:A:65:PHE:CZ	1:A:87:VAL:HB	0.45	2.47	21	1
1:A:14:ASN:CB	1:A:130:VAL:HG12	0.45	2.41	23	1
1:A:109:GLN:OE1	1:A:118:LEU:HD22	0.45	2.10	8	1
1:A:81:ARG:O	1:A:82:ASN:ND2	0.45	2.50	8	1
1:A:28:PHE:O	1:A:29:ALA:HB3	0.45	2.12	15	1
1:A:43:ILE:CG2	1:A:43:ILE:O	0.45	2.64	18	1
1:A:11:MET:HB3	1:A:39:GLN:CD	0.45	2.31	7	1
1:A:15:GLU:HB3	1:A:128:ARG:C	0.45	2.32	21	1
1:A:15:GLU:HB2	1:A:128:ARG:HB3	0.45	1.89	23	1
1:A:31:ARG:HD3	1:A:32:LYS:N	0.44	2.27	13	1
1:A:85:THR:HG21	1:A:107:TRP:HZ3	0.44	1.70	21	1
1:A:8:THR:O	1:A:8:THR:HG23	0.44	2.13	23	1
1:A:94:LEU:CD2	1:A:109:GLN:HG3	0.44	2.41	22	1
1:A:120:LEU:HD11	1:A:122:CYS:SG	0.44	2.52	13	1
1:A:27:ASP:C	1:A:28:PHE:CD1	0.44	2.90	4	1
1:A:41:LYS:HA	1:A:55:ASN:HA	0.44	1.89	24	1
1:A:17:PHE:HZ	1:A:34:ALA:HB3	0.44	1.70	10	1
1:A:66:THR:HG23	1:A:67:VAL:N	0.44	2.27	8	1
1:A:116:LEU:HD23	1:A:116:LEU:O	0.44	2.12	8	1
1:A:8:THR:C	1:A:9:TRP:CG	0.44	2.90	1	1
1:A:64:ASP:C	1:A:65:PHE:CD1	0.44	2.91	18	1
1:A:63:LEU:O	1:A:65:PHE:N	0.44	2.51	11	2
1:A:98:GLN:NE2	1:A:105:ARG:HB3	0.44	2.27	4	1
1:A:83:VAL:HG22	1:A:100:GLY:CA	0.44	2.43	12	1
1:A:103:GLU:OE1	1:A:105:ARG:N	0.44	2.50	1	1
1:A:66:THR:HG22	1:A:69:VAL:HB	0.44	1.88	16	2
1:A:93:THR:HG23	1:A:95:VAL:HG23	0.44	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:VAL:O	1:A:126:VAL:HG22	0.44	2.13	13	1
1:A:48:ASP:O	1:A:67:VAL:HG23	0.44	2.11	13	2
1:A:34:ALA:O	1:A:36:ARG:N	0.44	2.50	23	3
1:A:63:LEU:HG	1:A:65:PHE:CD2	0.44	2.48	24	1
1:A:88:THR:CG2	1:A:89:TRP:N	0.44	2.80	15	2
1:A:66:THR:OG1	1:A:67:VAL:N	0.44	2.49	17	2
1:A:37:LEU:N	1:A:37:LEU:CD2	0.44	2.80	20	2
1:A:71:PHE:CB	1:A:85:THR:HB	0.44	2.42	3	2
1:A:39:GLN:CB	1:A:56:SER:HA	0.44	2.42	21	1
1:A:90:GLU:HB3	1:A:93:THR:CG2	0.44	2.43	8	1
1:A:102:LYS:HD3	1:A:103:GLU:N	0.44	2.28	2	2
1:A:21:MET:CA	1:A:26:ILE:HG22	0.44	2.43	15	1
1:A:7:GLY:N	1:A:43:ILE:HG22	0.44	2.28	9	1
1:A:37:LEU:HB3	1:A:58:PHE:CE2	0.44	2.47	21	1
1:A:37:LEU:CD1	1:A:58:PHE:CG	0.44	3.00	13	1
1:A:41:LYS:C	1:A:41:LYS:HD3	0.44	2.33	20	3
1:A:65:PHE:CE1	1:A:71:PHE:CD1	0.44	3.06	12	1
1:A:42:ILE:CD1	1:A:53:LYS:CD	0.44	2.95	14	1
1:A:75:THR:HG22	1:A:82:ASN:CB	0.44	2.42	14	1
1:A:65:PHE:CE1	1:A:94:LEU:HD21	0.44	2.48	8	1
1:A:93:THR:OG1	1:A:94:LEU:N	0.44	2.51	18	4
1:A:43:ILE:HG13	1:A:50:PHE:CZ	0.44	2.48	14	1
1:A:39:GLN:NE2	1:A:55:ASN:O	0.44	2.51	19	1
1:A:9:TRP:CZ2	1:A:116:LEU:HD21	0.44	2.48	23	1
1:A:37:LEU:CD1	1:A:58:PHE:CD2	0.43	3.01	13	2
1:A:109:GLN:O	1:A:110:TRP:CE3	0.43	2.71	8	3
1:A:34:ALA:HA	1:A:58:PHE:CE2	0.43	2.48	12	4
1:A:31:ARG:HG2	1:A:32:LYS:N	0.43	2.27	4	2
1:A:41:LYS:HE2	1:A:118:LEU:HD12	0.43	1.90	15	1
1:A:22:LYS:CE	1:A:22:LYS:HA	0.43	2.43	15	1
1:A:41:LYS:HE3	1:A:131:PHE:CZ	0.43	2.48	21	1
1:A:19:GLY:O	1:A:23:ALA:N	0.43	2.52	21	1
1:A:24:LEU:HD13	1:A:79:ASP:OD2	0.43	2.13	22	1
1:A:21:MET:HG3	1:A:26:ILE:CG2	0.43	2.43	7	1
1:A:126:VAL:O	1:A:126:VAL:HG12	0.43	2.13	14	1
1:A:109:GLN:HB3	1:A:116:LEU:CD2	0.43	2.44	13	1
1:A:15:GLU:HG3	1:A:16:ASN:N	0.43	2.27	24	2
1:A:57:THR:HG23	1:A:57:THR:O	0.43	2.14	6	2
1:A:17:PHE:CD2	1:A:35:VAL:HA	0.43	2.48	6	1
1:A:33:ILE:HG22	1:A:34:ALA:N	0.43	2.28	20	1
1:A:73:GLU:HB3	1:A:82:ASN:HA	0.43	1.91	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:O	1:A:58:PHE:CE1	0.43	2.71	16	1
1:A:39:GLN:CG	1:A:56:SER:HA	0.43	2.44	21	1
1:A:50:PHE:CE1	1:A:63:LEU:HD23	0.43	2.48	10	1
1:A:19:GLY:HA2	1:A:22:LYS:CB	0.43	2.43	1	2
1:A:65:PHE:CE1	1:A:87:VAL:HG11	0.43	2.49	13	1
1:A:31:ARG:HD3	1:A:31:ARG:C	0.43	2.33	13	1
1:A:42:ILE:O	1:A:53:LYS:N	0.43	2.52	10	4
1:A:90:GLU:HB2	1:A:95:VAL:CG2	0.43	2.44	11	1
1:A:8:THR:HG23	1:A:42:ILE:HG13	0.43	1.89	19	1
1:A:115:LYS:CG	1:A:117:TYR:CD1	0.43	3.02	23	1
1:A:9:TRP:HB2	1:A:131:PHE:CE1	0.43	2.48	23	1
1:A:108:LYS:HG3	1:A:110:TRP:CZ3	0.43	2.49	17	1
1:A:36:ARG:HG3	1:A:39:GLN:CB	0.43	2.43	8	1
1:A:56:SER:HB3	1:A:58:PHE:CD1	0.43	2.48	13	2
1:A:81:ARG:HA	1:A:81:ARG:NE	0.43	2.26	16	1
1:A:90:GLU:HG3	1:A:95:VAL:CG2	0.43	2.44	14	2
1:A:14:ASN:ND2	1:A:15:GLU:O	0.43	2.51	9	1
1:A:117:TYR:O	1:A:119:GLU:N	0.43	2.52	10	1
1:A:93:THR:OG1	1:A:109:GLN:O	0.43	2.37	8	1
1:A:70:GLU:O	1:A:72:ASP:N	0.43	2.52	16	2
1:A:98:GLN:HG3	1:A:105:ARG:C	0.43	2.34	1	1
1:A:11:MET:HE3	1:A:39:GLN:CG	0.43	2.44	3	1
1:A:8:THR:HG21	1:A:40:THR:CG2	0.43	2.44	19	1
1:A:41:LYS:HD2	1:A:131:PHE:CE1	0.43	2.49	23	1
1:A:28:PHE:O	1:A:29:ALA:HB2	0.43	2.14	18	1
1:A:75:THR:CB	1:A:82:ASN:ND2	0.43	2.81	14	1
1:A:9:TRP:HB2	1:A:131:PHE:CE2	0.43	2.49	10	2
1:A:110:TRP:C	1:A:111:VAL:HG23	0.42	2.35	20	2
1:A:126:VAL:HG12	1:A:126:VAL:O	0.42	2.14	16	1
1:A:30:THR:HG22	1:A:31:ARG:N	0.42	2.28	7	1
1:A:33:ILE:N	1:A:33:ILE:CD1	0.42	2.80	14	1
1:A:133:LYS:O	1:A:134:LYS:CB	0.42	2.67	22	1
1:A:73:GLU:HG2	1:A:83:VAL:CA	0.42	2.44	24	1
1:A:108:LYS:HD3	1:A:110:TRP:CZ3	0.42	2.49	6	1
1:A:15:GLU:O	1:A:17:PHE:N	0.42	2.52	3	2
1:A:6:ASN:OD1	1:A:6:ASN:N	0.42	2.52	21	1
1:A:105:ARG:CZ	1:A:105:ARG:HB3	0.42	2.43	22	1
1:A:37:LEU:HG	1:A:58:PHE:CD2	0.42	2.50	4	3
1:A:113:GLY:O	1:A:115:LYS:NZ	0.42	2.51	23	1
1:A:100:GLY:O	1:A:102:LYS:N	0.42	2.52	23	2
1:A:108:LYS:C	1:A:109:GLN:NE2	0.42	2.72	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLN:HG3	1:A:118:LEU:CD2	0.42	2.44	20	1
1:A:24:LEU:HD11	1:A:81:ARG:NH1	0.42	2.28	7	1
1:A:17:PHE:CD1	1:A:17:PHE:C	0.42	2.87	7	1
1:A:3:LYS:HE2	1:A:89:TRP:CE3	0.42	2.50	21	1
1:A:84:LYS:CA	1:A:84:LYS:HE2	0.42	2.44	10	1
1:A:130:VAL:HG23	1:A:131:PHE:H	0.42	1.73	23	1
1:A:9:TRP:CE2	1:A:116:LEU:HD21	0.42	2.50	23	1
1:A:97:VAL:O	1:A:99:LYS:N	0.42	2.52	22	2
1:A:11:MET:O	1:A:13:SER:N	0.42	2.53	13	1
1:A:11:MET:CE	1:A:14:ASN:ND2	0.42	2.82	18	1
1:A:81:ARG:HG3	1:A:82:ASN:N	0.42	2.30	9	1
1:A:111:VAL:HG22	1:A:116:LEU:HD12	0.42	1.91	19	1
1:A:3:LYS:HG2	1:A:89:TRP:CZ2	0.42	2.49	8	1
1:A:37:LEU:HD21	1:A:58:PHE:CD2	0.42	2.50	13	1
1:A:75:THR:OG1	1:A:81:ARG:N	0.42	2.51	4	1
1:A:52:THR:HB	1:A:63:LEU:HB3	0.42	1.92	19	4
1:A:9:TRP:CE3	1:A:133:LYS:CB	0.42	3.03	12	1
1:A:73:GLU:HB2	1:A:83:VAL:N	0.42	2.30	12	2
1:A:38:THR:HA	1:A:56:SER:CB	0.42	2.45	20	1
1:A:83:VAL:CG1	1:A:99:LYS:N	0.42	2.83	18	1
1:A:89:TRP:CE3	1:A:93:THR:O	0.42	2.73	19	2
1:A:82:ASN:C	1:A:83:VAL:CG2	0.42	2.87	23	1
1:A:45:GLN:HG2	1:A:50:PHE:CD1	0.42	2.50	22	1
1:A:26:ILE:CG2	1:A:27:ASP:N	0.42	2.82	11	1
1:A:104:ASN:O	1:A:122:CYS:N	0.42	2.53	24	2
1:A:24:LEU:HD13	1:A:79:ASP:CA	0.42	2.45	3	1
1:A:18:GLU:CG	1:A:31:ARG:HB2	0.42	2.44	23	1
1:A:21:MET:HB3	1:A:26:ILE:HG22	0.42	1.90	22	1
1:A:120:LEU:O	1:A:127:CYS:N	0.42	2.53	13	1
1:A:95:VAL:HG12	1:A:95:VAL:O	0.42	2.13	15	1
1:A:101:GLU:HG2	1:A:102:LYS:N	0.42	2.30	20	1
1:A:31:ARG:CG	1:A:32:LYS:N	0.42	2.83	20	1
1:A:18:GLU:OE1	1:A:19:GLY:N	0.42	2.52	3	1
1:A:63:LEU:CD2	1:A:94:LEU:HD22	0.42	2.44	7	1
1:A:85:THR:OG1	1:A:98:GLN:NE2	0.42	2.52	21	2
1:A:9:TRP:O	1:A:41:LYS:N	0.42	2.53	8	2
1:A:56:SER:HB3	1:A:58:PHE:CE1	0.42	2.50	13	2
1:A:102:LYS:HD3	1:A:103:GLU:HG2	0.42	1.91	15	1
1:A:3:LYS:HB3	1:A:89:TRP:CH2	0.42	2.49	10	1
1:A:83:VAL:HG11	1:A:98:GLN:HG2	0.42	1.92	11	1
1:A:104:ASN:O	1:A:121:THR:HB	0.42	2.14	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:THR:CG2	1:A:9:TRP:N	0.42	2.83	3	1
1:A:84:LYS:CB	1:A:99:LYS:HB2	0.42	2.45	7	1
1:A:83:VAL:CG1	1:A:84:LYS:N	0.42	2.82	14	1
1:A:90:GLU:HG3	1:A:95:VAL:HG21	0.42	1.92	14	1
1:A:86:LEU:C	1:A:86:LEU:HD23	0.42	2.35	2	1
1:A:88:THR:HG23	1:A:88:THR:O	0.42	2.14	17	1
1:A:132:LYS:C	1:A:132:LYS:CD	0.41	2.88	13	1
1:A:18:GLU:CB	1:A:31:ARG:HB3	0.41	2.45	11	1
1:A:3:LYS:O	1:A:45:GLN:NE2	0.41	2.53	12	1
1:A:40:THR:HG22	1:A:40:THR:O	0.41	2.15	19	1
1:A:129:GLN:O	1:A:130:VAL:CG1	0.41	2.68	23	1
1:A:60:ASN:N	1:A:60:ASN:ND2	0.41	2.67	17	1
1:A:71:PHE:O	1:A:85:THR:N	0.41	2.53	20	3
1:A:107:TRP:O	1:A:107:TRP:CD2	0.41	2.73	24	1
1:A:50:PHE:CG	1:A:50:PHE:O	0.41	2.72	24	1
1:A:109:GLN:HB2	1:A:116:LEU:CD1	0.41	2.44	12	1
1:A:18:GLU:O	1:A:22:LYS:N	0.41	2.53	21	3
1:A:37:LEU:O	1:A:57:THR:N	0.41	2.53	20	1
1:A:65:PHE:CE2	1:A:87:VAL:HG11	0.41	2.50	19	1
1:A:118:LEU:CB	1:A:131:PHE:CZ	0.41	3.03	19	1
1:A:85:THR:HG23	1:A:98:GLN:OE1	0.41	2.16	21	1
1:A:37:LEU:HB3	1:A:58:PHE:CZ	0.41	2.50	21	1
1:A:98:GLN:HG2	1:A:105:ARG:C	0.41	2.35	2	1
1:A:119:GLU:OE1	1:A:120:LEU:N	0.41	2.53	2	1
1:A:64:ASP:OD1	1:A:64:ASP:N	0.41	2.53	22	1
1:A:74:HIS:CE1	1:A:76:LYS:HE2	0.41	2.50	16	1
1:A:12:GLU:HG3	1:A:132:LYS:HG2	0.41	1.91	9	1
1:A:83:VAL:HG11	1:A:98:GLN:CG	0.41	2.45	11	1
1:A:59:ARG:HG3	1:A:60:ASN:N	0.41	2.30	24	1
1:A:16:ASN:N	1:A:16:ASN:OD1	0.41	2.54	12	2
1:A:110:TRP:CD1	1:A:117:TYR:HB2	0.41	2.51	15	1
1:A:83:VAL:HG13	1:A:99:LYS:N	0.41	2.30	18	1
1:A:112:GLU:CG	1:A:117:TYR:CE2	0.41	3.04	23	1
1:A:32:LYS:O	1:A:33:ILE:HG23	0.41	2.15	11	1
1:A:85:THR:HG22	1:A:85:THR:O	0.41	2.14	21	2
1:A:112:GLU:HB2	1:A:117:TYR:CE1	0.41	2.50	6	1
1:A:21:MET:HG2	1:A:26:ILE:HG21	0.41	1.92	15	1
1:A:102:LYS:HD3	1:A:103:GLU:CG	0.41	2.46	15	1
1:A:7:GLY:O	1:A:8:THR:HG23	0.41	2.15	1	1
1:A:116:LEU:HD12	1:A:131:PHE:CD2	0.41	2.51	23	1
1:A:50:PHE:C	1:A:51:LYS:HG3	0.41	2.35	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:THR:HG22	1:A:55:ASN:N	0.41	2.31	24	1
1:A:50:PHE:HE2	1:A:94:LEU:HD22	0.41	1.75	24	1
1:A:112:GLU:HB2	1:A:117:TYR:CD2	0.41	2.49	1	1
1:A:87:VAL:HG12	1:A:94:LEU:HD11	0.41	1.92	16	1
1:A:65:PHE:CD1	1:A:87:VAL:CG2	0.41	2.90	5	1
1:A:11:MET:HG3	1:A:130:VAL:HG21	0.41	1.92	23	1
1:A:121:THR:HG23	1:A:126:VAL:HG22	0.41	1.91	11	1
1:A:56:SER:HB2	1:A:58:PHE:CD1	0.41	2.50	6	1
1:A:56:SER:O	1:A:60:ASN:ND2	0.41	2.54	12	1
1:A:72:ASP:OD1	1:A:72:ASP:N	0.41	2.54	15	2
1:A:116:LEU:O	1:A:131:PHE:CG	0.41	2.73	16	1
1:A:42:ILE:CD1	1:A:53:LYS:HD2	0.41	2.45	14	1
1:A:33:ILE:O	1:A:37:LEU:HD22	0.41	2.15	6	1
1:A:36:ARG:HD2	1:A:39:GLN:CB	0.41	2.46	12	1
1:A:85:THR:HG23	1:A:96:CYS:SG	0.41	2.55	14	1
1:A:116:LEU:O	1:A:131:PHE:CD1	0.41	2.74	10	1
1:A:102:LYS:CD	1:A:102:LYS:C	0.41	2.89	17	1
1:A:39:GLN:NE2	1:A:54:THR:OG1	0.41	2.54	6	1
1:A:8:THR:O	1:A:134:LYS:N	0.41	2.54	15	1
1:A:26:ILE:HG23	1:A:27:ASP:N	0.41	2.31	1	1
1:A:36:ARG:O	1:A:37:LEU:CG	0.41	2.68	18	1
1:A:33:ILE:HD13	1:A:33:ILE:HA	0.41	1.55	18	1
1:A:24:LEU:C	1:A:24:LEU:CD1	0.41	2.88	3	1
1:A:6:ASN:ND2	1:A:44:VAL:O	0.41	2.54	16	1
1:A:73:GLU:O	1:A:74:HIS:ND1	0.41	2.54	16	1
1:A:52:THR:CG2	1:A:63:LEU:HD23	0.41	2.46	14	1
1:A:86:LEU:O	1:A:96:CYS:HA	0.41	2.16	14	2
1:A:18:GLU:HG3	1:A:19:GLY:N	0.41	2.30	19	1
1:A:20:TYR:CE1	1:A:24:LEU:HD21	0.41	2.51	2	1
1:A:39:GLN:CD	1:A:40:THR:N	0.41	2.74	2	1
1:A:14:ASN:HB2	1:A:130:VAL:CG1	0.41	2.42	23	1
1:A:50:PHE:CE2	1:A:94:LEU:CD2	0.41	3.04	13	1
1:A:26:ILE:HD13	1:A:78:LEU:C	0.41	2.36	15	1
1:A:36:ARG:O	1:A:37:LEU:HB3	0.41	2.16	20	1
1:A:32:LYS:HG2	1:A:33:ILE:N	0.41	2.31	18	1
1:A:65:PHE:C	1:A:65:PHE:CD1	0.41	2.94	3	1
1:A:52:THR:N	1:A:63:LEU:O	0.40	2.54	4	1
1:A:30:THR:O	1:A:33:ILE:N	0.40	2.54	18	1
1:A:63:LEU:CD2	1:A:107:TRP:CZ2	0.40	2.95	3	1
1:A:125:GLN:C	1:A:126:VAL:CG1	0.40	2.88	7	1
1:A:114:ASP:N	1:A:114:ASP:OD1	0.40	2.54	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:SER:OG	1:A:59:ARG:N	0.40	2.54	19	1
1:A:75:THR:C	1:A:76:LYS:CG	0.40	2.89	5	1
1:A:9:TRP:CZ3	1:A:115:LYS:HA	0.40	2.51	21	1
1:A:20:TYR:CD1	1:A:24:LEU:HD21	0.40	2.50	23	1
1:A:11:MET:O	1:A:12:GLU:CB	0.40	2.69	20	2
1:A:50:PHE:CD1	1:A:94:LEU:HD22	0.40	2.52	3	1
1:A:17:PHE:CG	1:A:18:GLU:N	0.40	2.85	7	1
1:A:98:GLN:CG	1:A:105:ARG:HB2	0.40	2.46	9	1
1:A:38:THR:HG22	1:A:38:THR:O	0.40	2.17	23	1
1:A:83:VAL:HG13	1:A:100:GLY:HA3	0.40	1.92	23	1
1:A:107:TRP:CD1	1:A:107:TRP:O	0.40	2.75	22	1
1:A:66:THR:HG22	1:A:69:VAL:CG2	0.40	2.45	22	1
1:A:45:GLN:HG3	1:A:50:PHE:CG	0.40	2.51	6	1
1:A:43:ILE:CD1	1:A:45:GLN:HB2	0.40	2.46	18	1
1:A:25:ASP:C	1:A:27:ASP:N	0.40	2.73	18	1
1:A:116:LEU:O	1:A:118:LEU:N	0.40	2.54	9	1
1:A:34:ALA:HA	1:A:37:LEU:CD2	0.40	2.46	10	1
1:A:71:PHE:N	1:A:85:THR:O	0.40	2.54	2	1
1:A:116:LEU:CD1	1:A:131:PHE:CD2	0.40	3.04	23	1
1:A:88:THR:N	1:A:95:VAL:O	0.40	2.54	23	1
1:A:132:LYS:O	1:A:134:LYS:N	0.40	2.54	23	1
1:A:73:GLU:HG3	1:A:82:ASN:CA	0.40	2.47	23	1
1:A:83:VAL:HG13	1:A:100:GLY:O	0.40	2.17	17	1
1:A:111:VAL:HG12	1:A:111:VAL:O	0.40	2.15	22	1
1:A:26:ILE:HD11	1:A:79:ASP:N	0.40	2.31	12	1
1:A:37:LEU:HD13	1:A:38:THR:N	0.40	2.31	18	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.40	2.53	18	1
1:A:83:VAL:O	1:A:85:THR:N	0.40	2.54	3	1
1:A:110:TRP:CD1	1:A:117:TYR:HB3	0.40	2.51	12	1
1:A:116:LEU:C	1:A:116:LEU:CD2	0.40	2.90	20	1
1:A:71:PHE:CE2	1:A:74:HIS:CD2	0.40	3.10	3	1
1:A:73:GLU:HB3	1:A:83:VAL:HA	0.40	1.93	14	1
1:A:132:LYS:CG	1:A:132:LYS:O	0.40	2.70	9	1
1:A:125:GLN:C	1:A:126:VAL:HG12	0.40	2.37	5	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/134 (98%)	78±4 (60±3%)	33±3 (25±3%)	20±3 (15±3%)	1	4
All	All	3144/3216 (98%)	1872 (60%)	788 (25%)	484 (15%)	1	4

All 85 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	111	VAL	20
1	A	36	ARG	17
1	A	25	ASP	15
1	A	126	VAL	15
1	A	12	GLU	14
1	A	76	LYS	13
1	A	72	ASP	13
1	A	45	GLN	12
1	A	38	THR	12
1	A	93	THR	12
1	A	106	GLY	12
1	A	11	MET	12
1	A	82	ASN	11
1	A	6	ASN	10
1	A	124	ASP	10
1	A	110	TRP	10
1	A	33	ILE	9
1	A	62	ASP	9
1	A	101	GLU	9
1	A	79	ASP	9
1	A	39	GLN	8
1	A	56	SER	8
1	A	29	ALA	8
1	A	16	ASN	8
1	A	27	ASP	8
1	A	71	PHE	8
1	A	31	ARG	7
1	A	91	GLY	7
1	A	133	LYS	7
1	A	113	GLY	7
1	A	102	LYS	7
1	A	40	THR	7
1	A	74	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	28	PHE	6
1	A	35	VAL	6
1	A	73	GLU	6
1	A	47	GLY	5
1	A	92	ASN	5
1	A	78	LEU	5
1	A	3	LYS	5
1	A	30	THR	5
1	A	70	GLU	5
1	A	8	THR	4
1	A	115	LYS	4
1	A	75	THR	4
1	A	37	LEU	4
1	A	81	ARG	4
1	A	32	LYS	4
1	A	57	THR	4
1	A	49	ASN	4
1	A	15	GLU	3
1	A	108	LYS	3
1	A	122	CYS	3
1	A	44	VAL	3
1	A	84	LYS	3
1	A	100	GLY	3
1	A	95	VAL	3
1	A	98	GLN	3
1	A	67	VAL	2
1	A	131	PHE	2
1	A	4	ASP	2
1	A	34	ALA	2
1	A	83	VAL	2
1	A	59	ARG	2
1	A	94	LEU	2
1	A	68	GLY	2
1	A	13	SER	2
1	A	64	ASP	2
1	A	9	TRP	2
1	A	125	GLN	2
1	A	10	GLU	1
1	A	58	PHE	1
1	A	103	GLU	1
1	A	80	GLY	1
1	A	14	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	117	TYR	1
1	A	129	GLN	1
1	A	123	GLY	1
1	A	54	THR	1
1	A	130	VAL	1
1	A	132	LYS	1
1	A	99	LYS	1
1	A	55	ASN	1
1	A	5	GLN	1
1	A	107	TRP	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/120 (98%)	73±4 (62±3%)	45±4 (38±3%)	1	7
All	All	2832/2880 (98%)	1756 (62%)	1076 (38%)	1	7

All 111 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	9	TRP	24
1	A	52	THR	24
1	A	120	LEU	24
1	A	31	ARG	22
1	A	102	LYS	21
1	A	53	LYS	21
1	A	76	LYS	21
1	A	110	TRP	20
1	A	41	LYS	20
1	A	107	TRP	20
1	A	132	LYS	20
1	A	33	ILE	18
1	A	66	THR	17
1	A	84	LYS	17
1	A	122	CYS	17

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Mol	Chain	Res	Type	Models (Total)
1	A	32	LYS	17
1	A	96	CYS	16
1	A	36	ARG	16
1	A	115	LYS	16
1	A	108	LYS	15
1	A	24	LEU	14
1	A	116	LEU	14
1	A	109	GLN	14
1	A	37	LEU	14
1	A	65	PHE	14
1	A	118	LEU	14
1	A	45	GLN	13
1	A	75	THR	13
1	A	43	ILE	13
1	A	30	THR	13
1	A	20	TYR	13
1	A	90	GLU	13
1	A	128	ARG	13
1	A	59	ARG	13
1	A	3	LYS	12
1	A	62	ASP	12
1	A	92	ASN	12
1	A	60	ASN	12
1	A	13	SER	12
1	A	48	ASP	11
1	A	54	THR	11
1	A	39	GLN	11
1	A	99	LYS	11
1	A	8	THR	11
1	A	81	ARG	11
1	A	82	ASN	11
1	A	74	HIS	10
1	A	57	THR	10
1	A	25	ASP	10
1	A	134	LYS	10
1	A	61	TYR	10
1	A	27	ASP	9
1	A	18	GLU	9
1	A	103	GLU	9
1	A	58	PHE	9
1	A	17	PHE	9
1	A	98	GLN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	94	LEU	9
1	A	6	ASN	8
1	A	69	VAL	8
1	A	101	GLU	8
1	A	21	MET	8
1	A	22	LYS	8
1	A	71	PHE	8
1	A	28	PHE	7
1	A	4	ASP	7
1	A	56	SER	7
1	A	14	ASN	7
1	A	130	VAL	7
1	A	49	ASN	7
1	A	93	THR	7
1	A	86	LEU	6
1	A	12	GLU	6
1	A	79	ASP	6
1	A	51	LYS	6
1	A	15	GLU	6
1	A	97	VAL	6
1	A	112	GLU	6
1	A	55	ASN	6
1	A	117	TYR	6
1	A	105	ARG	6
1	A	88	THR	5
1	A	83	VAL	5
1	A	16	ASN	5
1	A	119	GLU	5
1	A	73	GLU	5
1	A	5	GLN	5
1	A	11	MET	5
1	A	72	ASP	5
1	A	46	ASP	4
1	A	64	ASP	4
1	A	127	CYS	4
1	A	70	GLU	4
1	A	133	LYS	4
1	A	124	ASP	4
1	A	38	THR	4
1	A	63	LEU	3
1	A	125	GLN	3
1	A	26	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	121	THR	2
1	A	126	VAL	2
1	A	104	ASN	2
1	A	35	VAL	2
1	A	78	LEU	2
1	A	87	VAL	2
1	A	44	VAL	1
1	A	10	GLU	1
1	A	50	PHE	1
1	A	67	VAL	1
1	A	129	GLN	1
1	A	114	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided