



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 11:29 PM UTC

PDB ID : 1B4M / pdb_00001b4m
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

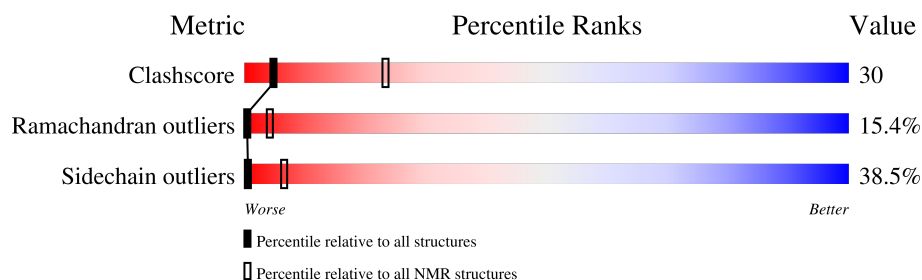
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

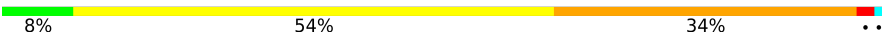
The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	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)	1.12	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

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.

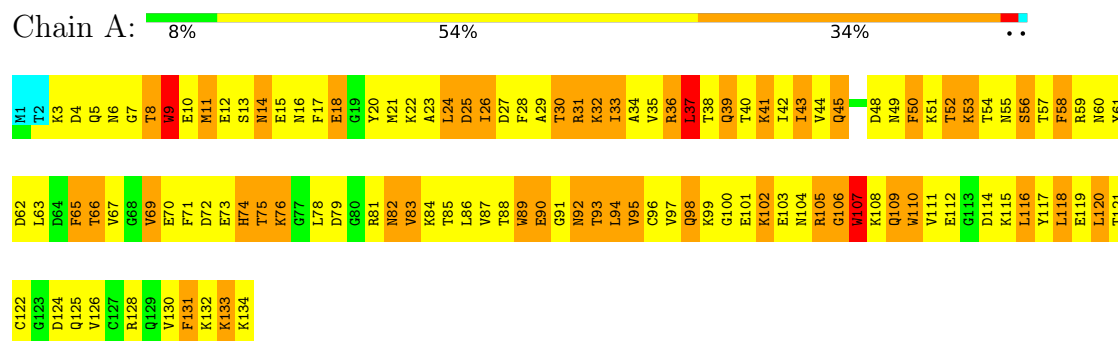
Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2168	686	1073	189	214	6	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: CELLULAR RETINOL-BINDING PROTEIN II

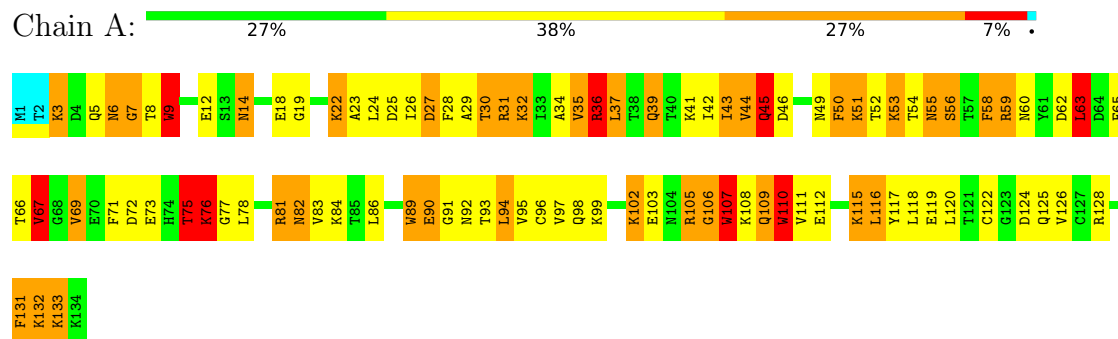


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

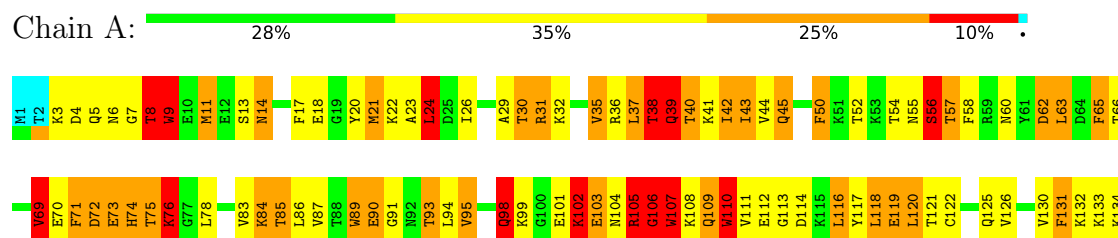
4.2.1 Score per residue for model 1

• Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



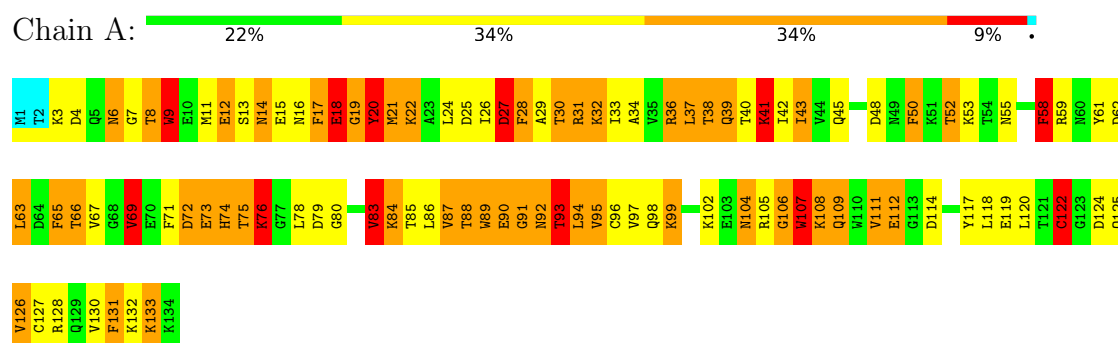
4.2.2 Score per residue for model 2

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



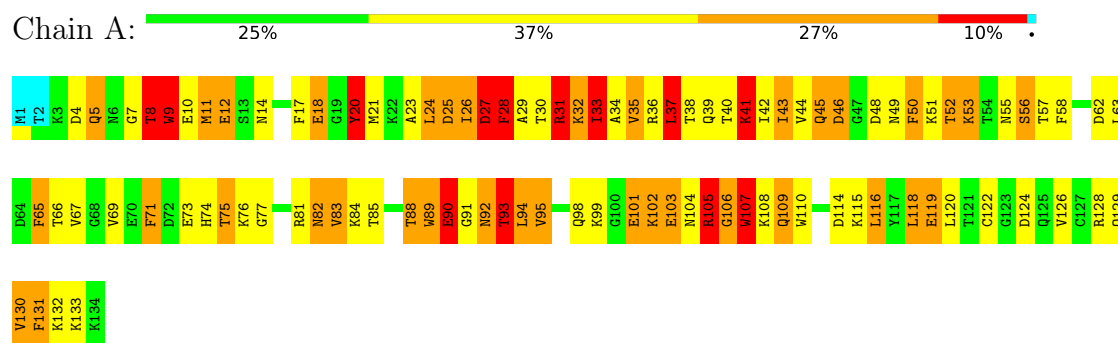
4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



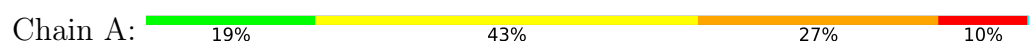
4.2.4 Score per residue for model 4

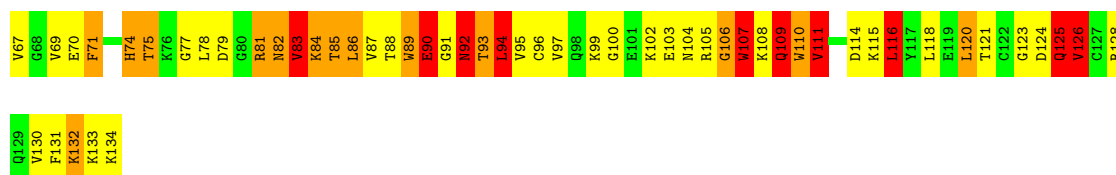
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.5 Score per residue for model 5

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

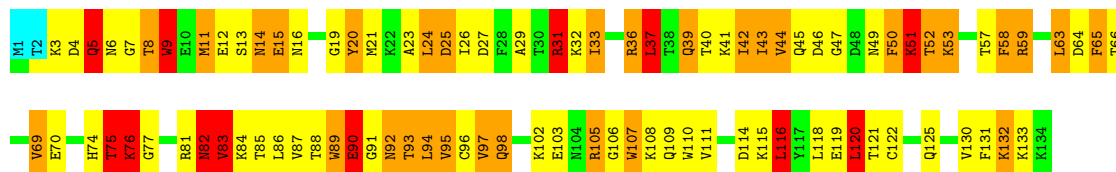




4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

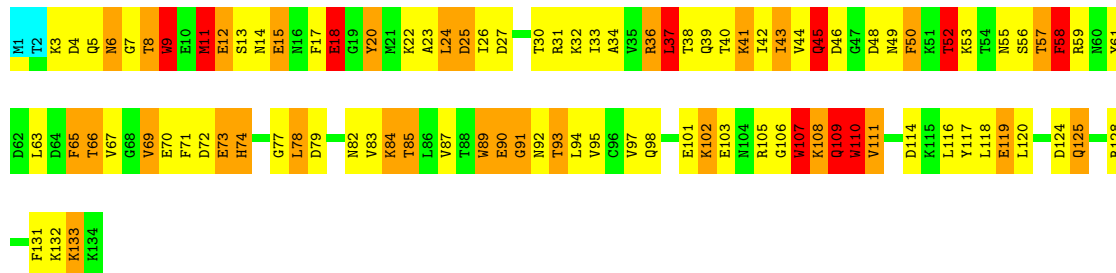
Chain A: 28% 38% 23% 9% .



4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

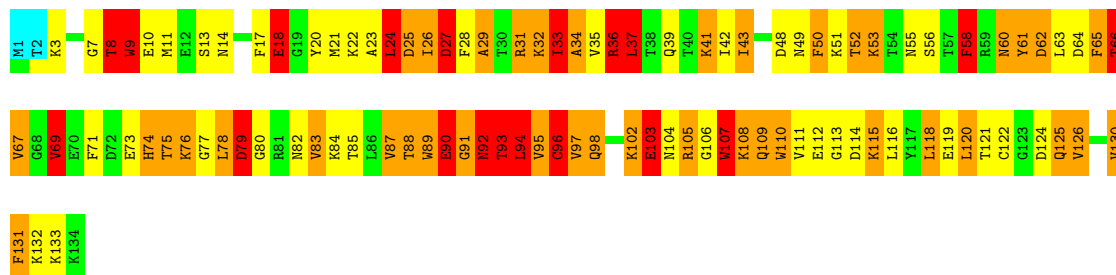
Chain A: 26% 43% 22% 7% .



4.2.11 Score per residue for model 11

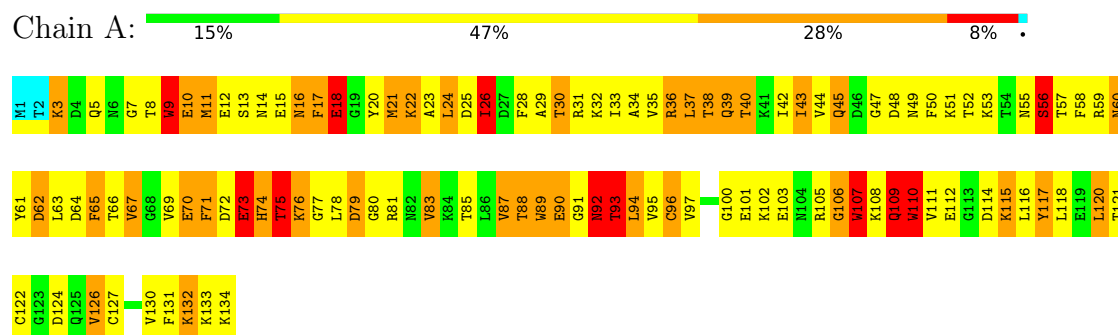
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 23% 31% 30% 14% .



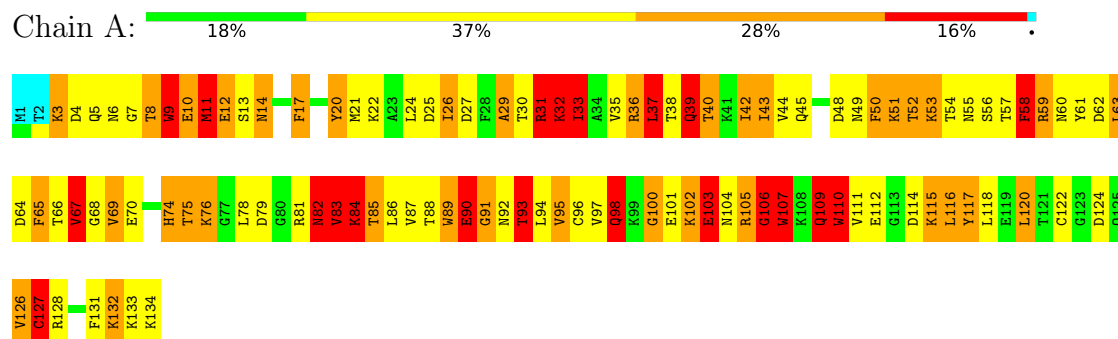
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



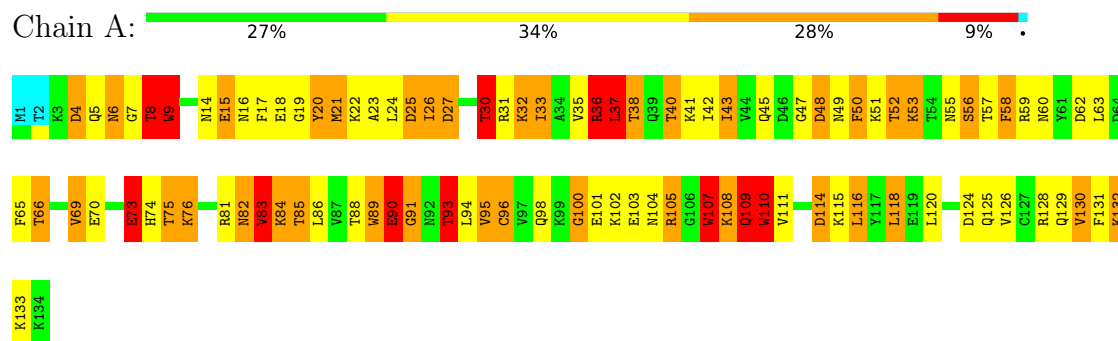
4.2.13 Score per residue for model 13

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



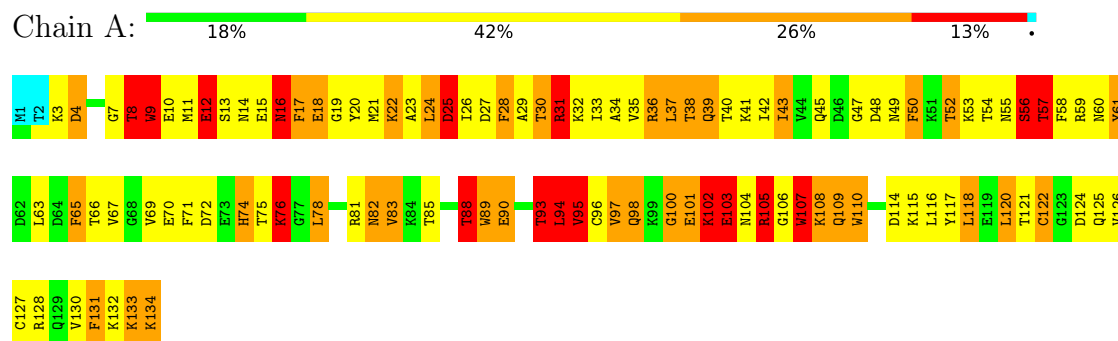
4.2.14 Score per residue for model 14

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



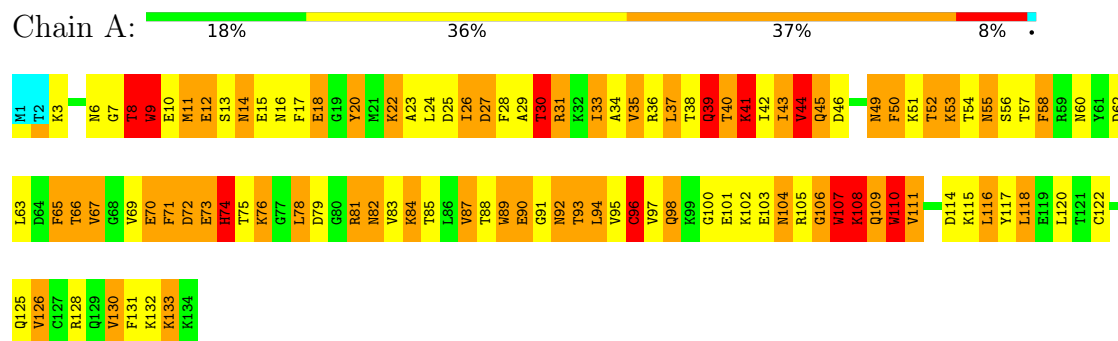
4.2.15 Score per residue for model 15

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



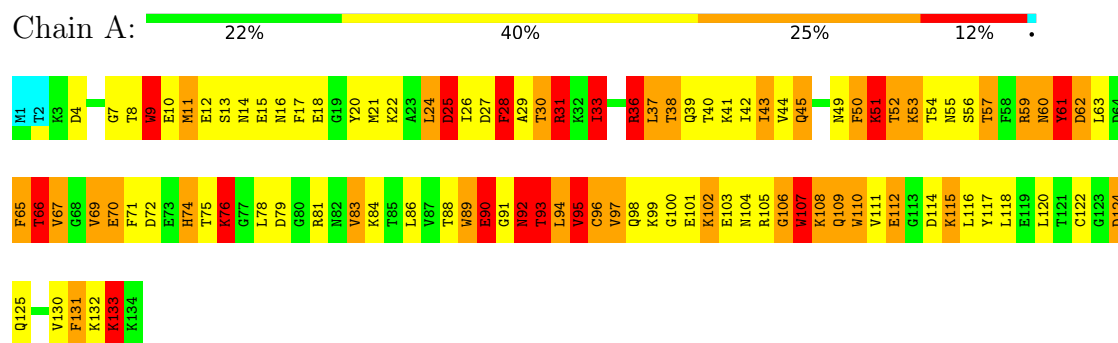
4.2.16 Score per residue for model 16

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.17 Score per residue for model 17

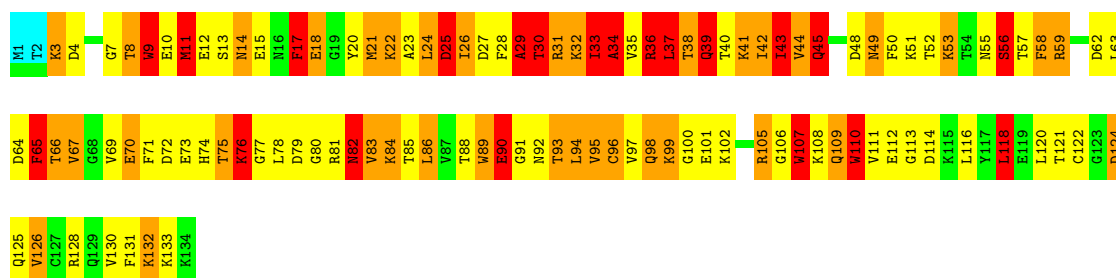
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.18 Score per residue for model 18

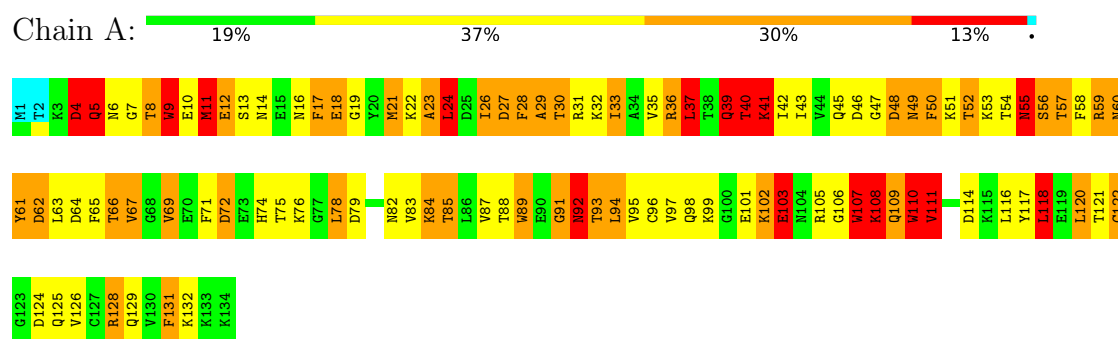
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II





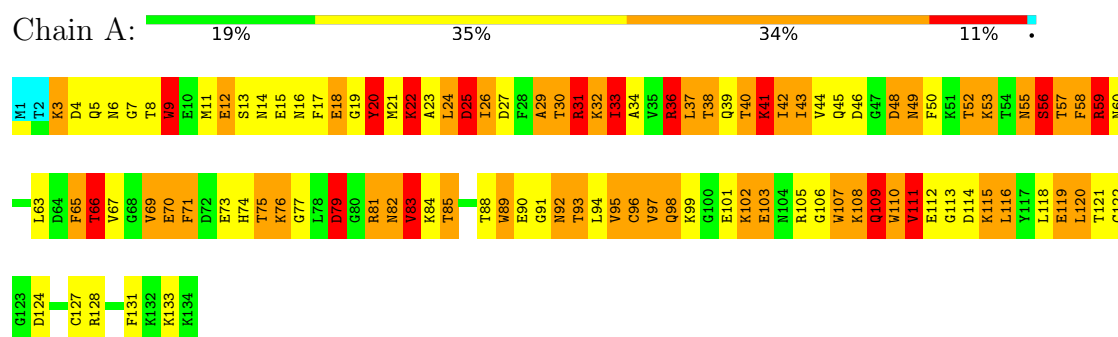
4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



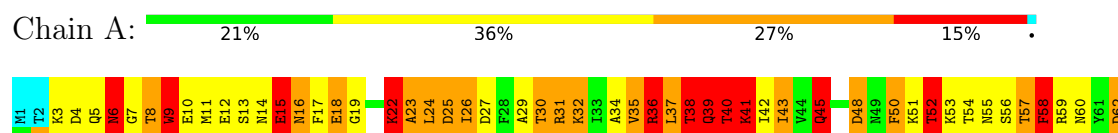
4.2.20 Score per residue for model 20

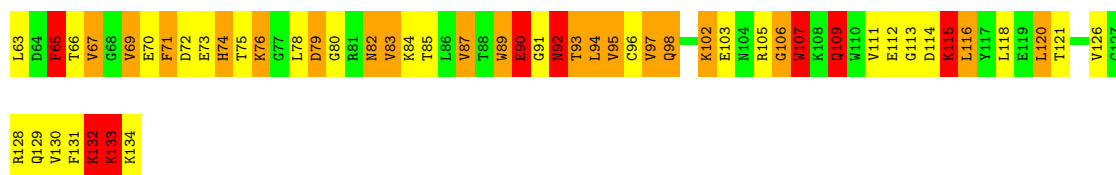
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.21 Score per residue for model 21

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

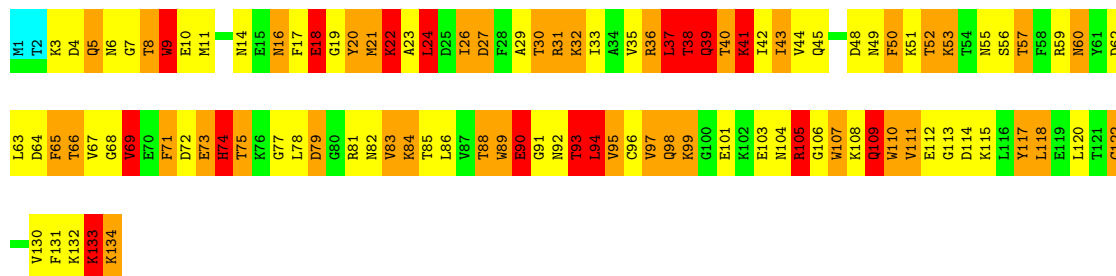




4.2.22 Score per residue for model 22

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

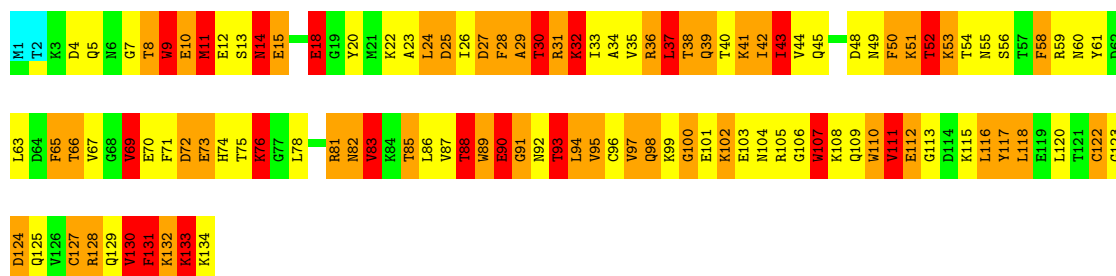
Chain A: 20% 37% 29% 12% .



4.2.23 Score per residue for model 23

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

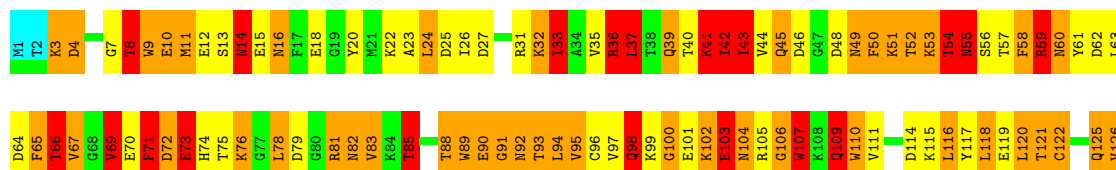
Chain A: 15% 37% 32% 15% .



4.2.24 Score per residue for model 24

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 17% 31% 36% 15% .



C127
R128
Q129
V130
F131
K132
K133
K134

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.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.28±0.02	1±1/1098 (0.1± 0.1%)	2.53±0.05	80±9/1474 (5.4± 0.6%)
All	All	1.28	32/26352 (0.1%)	2.53	1919/35376 (5.4%)

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	CG-CD2	-6.51	1.32	1.43	23	8
1	A	107	TRP	CG-CD2	-5.95	1.33	1.43	11	14
1	A	62	ASP	CA-C	-5.88	1.50	1.53	1	1
1	A	89	TRP	CG-CD2	-5.79	1.33	1.43	22	6
1	A	110	TRP	CD2-CE2	-5.02	1.32	1.41	13	2
1	A	9	TRP	CG-CD2	-5.01	1.34	1.43	21	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	VAL	O-C-N	12.99	132.87	121.96	18	22
1	A	90	GLU	CA-C-O	12.15	133.64	119.18	4	23
1	A	37	LEU	O-C-N	11.54	137.34	122.68	22	18
1	A	89	TRP	CG-CD1-NE1	-11.07	95.80	110.20	24	24
1	A	36	ARG	O-C-N	11.07	134.82	122.20	16	12
1	A	55	ASN	O-C-N	10.93	135.70	122.48	16	18
1	A	50	PHE	CA-CB-CG	-10.76	103.04	113.80	16	18
1	A	14	ASN	CA-CB-CG	-10.69	101.91	112.60	18	23
1	A	105	ARG	NE-CZ-NH1	10.57	132.07	121.50	22	4
1	A	91	GLY	O-C-N	10.52	136.37	122.70	14	21
1	A	21	MET	O-C-N	10.42	134.03	122.15	18	5
1	A	24	LEU	O-C-N	10.38	133.30	122.09	7	5
1	A	131	PHE	CA-CB-CG	-10.00	103.80	113.80	23	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	GLU	O-C-N	9.98	132.87	122.09	21	15
1	A	91	GLY	N-CA-C	-9.78	102.85	114.48	9	7
1	A	29	ALA	O-C-N	9.53	132.95	123.04	4	14
1	A	77	GLY	O-C-N	9.49	132.98	122.54	11	11
1	A	83	VAL	O-C-N	9.48	133.43	123.00	13	14
1	A	97	VAL	N-CA-C	9.35	119.72	106.53	7	15
1	A	106	GLY	O-C-N	9.35	134.86	122.70	9	20
1	A	61	TYR	O-C-N	9.32	132.92	122.11	12	11
1	A	104	ASN	O-C-N	9.28	134.31	122.71	24	10
1	A	66	THR	O-C-N	9.25	133.74	122.92	20	6
1	A	74	HIS	CA-CB-CG	-9.14	104.66	113.80	7	15
1	A	92	ASN	CA-CB-CG	-9.10	103.50	112.60	1	16
1	A	7	GLY	O-C-N	9.06	133.40	122.97	7	23
1	A	22	LYS	O-C-N	9.05	134.46	122.33	24	20
1	A	36	ARG	NE-CZ-NH2	9.01	127.31	119.20	6	1
1	A	65	PHE	CA-C-O	8.99	131.11	120.14	8	8
1	A	5	GLN	O-C-N	8.89	132.84	122.25	1	12
1	A	14	ASN	O-C-N	8.81	133.24	123.10	4	10
1	A	114	ASP	O-C-N	8.77	133.13	122.35	4	18
1	A	105	ARG	O-C-N	8.67	133.49	122.22	6	18
1	A	35	VAL	O-C-N	8.66	130.62	121.87	5	14
1	A	26	ILE	CA-C-O	8.65	128.47	119.91	22	13
1	A	8	THR	O-C-N	8.63	133.28	123.27	8	15
1	A	7	GLY	CA-C-O	-8.39	114.41	121.04	22	2
1	A	39	GLN	O-C-N	8.38	132.75	122.86	7	14
1	A	32	LYS	O-C-N	8.37	132.52	121.97	7	12
1	A	39	GLN	N-CA-C	8.34	118.96	108.45	22	2
1	A	93	THR	O-C-N	8.32	130.90	123.41	14	6
1	A	70	GLU	O-C-N	8.27	133.42	123.33	2	8
1	A	46	ASP	CA-CB-CG	-8.20	104.40	112.60	20	7
1	A	59	ARG	O-C-N	8.19	130.78	123.41	24	8
1	A	67	VAL	O-C-N	8.18	131.50	122.75	13	7
1	A	23	ALA	O-C-N	8.17	130.78	122.12	21	17
1	A	93	THR	N-CA-C	8.17	119.41	108.38	5	11
1	A	58	PHE	O-C-N	8.16	130.81	122.08	23	12
1	A	103	GLU	O-C-N	8.12	132.44	123.10	9	10
1	A	44	VAL	CB-CA-C	-8.10	101.52	111.32	13	9
1	A	30	THR	O-C-N	8.05	130.66	122.12	17	15
1	A	37	LEU	CA-C-O	-8.03	112.57	120.92	22	6
1	A	27	ASP	CA-CB-CG	-8.02	104.58	112.60	24	8
1	A	89	TRP	CA-CB-CG	-7.98	98.44	113.60	12	24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	ASP	CA-CB-CG	-7.97	104.63	112.60	13	14
1	A	11	MET	O-C-N	7.96	133.18	122.59	13	10
1	A	55	ASN	CA-CB-CG	-7.94	104.66	112.60	24	3
1	A	57	THR	N-CA-C	-7.81	102.80	112.88	19	3
1	A	5	GLN	OE1-CD-NE2	7.75	130.35	122.60	14	6
1	A	97	VAL	CA-C-O	7.74	128.63	120.51	10	7
1	A	56	SER	O-C-N	7.70	130.96	122.11	17	13
1	A	95	VAL	CB-CA-C	-7.66	100.27	111.68	11	21
1	A	9	TRP	CG-CD1-NE1	7.65	120.14	110.20	16	18
1	A	105	ARG	NE-CZ-NH2	7.65	126.08	119.20	21	7
1	A	42	ILE	O-C-N	7.63	131.65	123.02	13	5
1	A	34	ALA	CA-C-O	7.63	128.63	119.78	3	3
1	A	109	GLN	CA-C-O	-7.62	112.94	121.40	12	15
1	A	76	LYS	CA-C-O	7.61	128.01	119.41	21	5
1	A	9	TRP	CE2-CD2-CG	7.60	116.32	107.20	16	10
1	A	111	VAL	CA-C-O	7.55	130.22	120.78	8	10
1	A	117	TYR	O-C-N	7.52	131.73	122.86	24	3
1	A	10	GLU	O-C-N	7.51	129.90	122.09	12	3
1	A	81	ARG	CA-C-O	-7.51	115.49	119.77	23	1
1	A	109	GLN	O-C-N	7.45	132.69	122.78	12	17
1	A	92	ASN	CA-C-O	7.45	127.72	121.02	6	1
1	A	95	VAL	N-CA-C	7.43	118.59	109.30	8	5
1	A	107	TRP	O-C-N	7.41	131.85	123.19	12	16
1	A	132	LYS	O-C-N	7.40	131.17	123.62	12	6
1	A	83	VAL	N-CA-C	7.38	118.75	108.12	3	17
1	A	43	ILE	N-CA-CB	-7.38	102.69	110.95	18	11
1	A	95	VAL	N-CA-CB	-7.37	102.60	111.00	1	11
1	A	9	TRP	CD1-CG-CD2	-7.36	94.52	106.30	16	12
1	A	89	TRP	CD1-CG-CD2	7.36	118.07	106.30	7	23
1	A	125	GLN	OE1-CD-NE2	7.36	129.96	122.60	6	3
1	A	40	THR	O-C-N	7.35	132.37	122.82	18	9
1	A	24	LEU	N-CA-C	-7.32	103.00	112.23	8	7
1	A	107	TRP	CA-CB-CG	-7.31	99.71	113.60	20	24
1	A	41	LYS	O-C-N	7.31	131.81	122.89	24	3
1	A	17	PHE	CA-C-O	7.28	128.34	119.97	12	6
1	A	74	HIS	CB-CG-CD2	-7.26	121.76	131.20	11	8
1	A	75	THR	O-C-N	7.26	130.22	122.38	18	7
1	A	89	TRP	CA-C-O	-7.25	113.21	121.19	17	19
1	A	89	TRP	NE1-CE2-CZ2	7.21	140.92	130.10	11	19
1	A	69	VAL	CB-CA-C	-7.21	105.14	113.22	18	4
1	A	62	ASP	N-CA-C	7.19	115.65	108.75	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	100	GLY	O-C-N	7.19	131.00	123.81	23	5
1	A	25	ASP	CA-C-O	7.18	129.82	121.28	12	11
1	A	31	ARG	O-C-N	7.17	131.31	122.14	8	8
1	A	49	ASN	CA-C-O	-7.12	112.83	121.02	18	4
1	A	125	GLN	O-C-N	7.10	131.31	122.65	15	8
1	A	82	ASN	CA-CB-CG	-7.07	105.53	112.60	13	8
1	A	60	ASN	O-C-N	7.06	131.46	122.28	19	4
1	A	49	ASN	O-C-N	7.06	131.97	122.59	8	17
1	A	110	TRP	CE2-CD2-CE3	7.05	125.85	118.80	20	4
1	A	92	ASN	OD1-CG-ND2	7.04	129.65	122.60	23	4
1	A	104	ASN	CA-C-O	-7.04	113.55	122.63	24	5
1	A	38	THR	N-CA-CB	-7.00	103.39	111.79	14	3
1	A	11	MET	CA-C-N	7.00	130.59	120.38	18	6
1	A	11	MET	C-N-CA	7.00	130.59	120.38	18	6
1	A	97	VAL	N-CA-CB	-6.99	102.55	111.64	23	7
1	A	17	PHE	CA-CB-CG	-6.98	106.82	113.80	7	7
1	A	84	LYS	O-C-N	6.97	130.80	122.85	13	5
1	A	88	THR	N-CA-CB	-6.96	100.74	111.46	23	9
1	A	79	ASP	CA-CB-CG	-6.94	105.66	112.60	20	2
1	A	98	GLN	OE1-CD-NE2	6.94	129.54	122.60	21	2
1	A	109	GLN	CB-CG-CD	-6.92	100.84	112.60	3	12
1	A	51	LYS	O-C-N	6.89	132.54	122.97	24	5
1	A	4	ASP	CA-CB-CG	-6.88	105.72	112.60	18	15
1	A	31	ARG	CA-C-O	-6.87	114.22	121.98	22	10
1	A	51	LYS	N-CA-C	6.85	118.20	108.54	13	15
1	A	128	ARG	NE-CZ-NH2	6.84	125.35	119.20	16	2
1	A	60	ASN	CA-CB-CG	-6.83	105.77	112.60	11	3
1	A	69	VAL	CA-C-N	-6.79	112.85	122.63	20	9
1	A	69	VAL	C-N-CA	-6.79	112.85	122.63	20	9
1	A	39	GLN	CA-C-N	6.79	130.84	121.33	2	6
1	A	39	GLN	C-N-CA	6.79	130.84	121.33	2	6
1	A	104	ASN	N-CA-C	-6.79	99.44	109.62	24	2
1	A	110	TRP	CD2-CE2-CZ2	-6.77	115.63	122.40	8	3
1	A	108	LYS	N-CA-C	6.75	118.46	108.60	19	4
1	A	130	VAL	CA-C-O	6.75	128.12	120.90	16	3
1	A	11	MET	N-CA-CB	-6.74	101.80	111.84	23	2
1	A	107	TRP	NE1-CE2-CD2	6.72	116.14	107.40	14	9
1	A	52	THR	O-C-N	6.72	130.45	122.79	23	2
1	A	85	THR	O-C-N	6.70	131.50	123.33	10	6
1	A	27	ASP	CA-C-O	-6.66	114.25	121.44	3	1
1	A	118	LEU	O-C-N	6.65	131.37	122.26	15	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	89	TRP	CE2-CD2-CE3	6.63	125.43	118.80	22	22
1	A	130	VAL	CB-CA-C	-6.63	105.15	111.05	9	4
1	A	81	ARG	O-C-N	6.62	125.73	120.83	23	2
1	A	27	ASP	O-C-N	6.61	131.28	122.82	3	4
1	A	123	GLY	O-C-N	6.58	128.85	122.41	6	2
1	A	48	ASP	CA-CB-CG	-6.57	106.03	112.60	7	5
1	A	9	TRP	CG-CD2-CE3	-6.57	127.33	133.90	10	8
1	A	19	GLY	N-CA-C	-6.54	106.55	114.66	9	1
1	A	25	ASP	CA-CB-CG	-6.54	106.06	112.60	20	3
1	A	130	VAL	O-C-N	6.53	128.84	122.97	8	4
1	A	85	THR	N-CA-C	6.52	118.37	109.11	5	3
1	A	71	PHE	N-CA-C	6.52	119.22	109.25	11	4
1	A	74	HIS	ND1-CG-CD2	6.52	112.62	106.10	9	5
1	A	119	GLU	O-C-N	6.51	131.33	123.13	20	8
1	A	3	LYS	N-CA-C	6.49	119.32	111.40	20	2
1	A	37	LEU	N-CA-C	-6.49	104.05	112.68	13	2
1	A	20	TYR	CA-C-O	6.48	127.43	120.24	18	7
1	A	108	LYS	CA-C-O	6.45	128.30	121.33	7	3
1	A	11	MET	CA-C-O	-6.44	114.07	121.54	23	3
1	A	41	LYS	N-CA-C	-6.42	101.89	110.55	19	5
1	A	50	PHE	CA-C-O	-6.41	113.30	120.54	8	11
1	A	113	GLY	N-CA-C	6.36	117.52	111.67	21	1
1	A	96	CYS	O-C-N	6.35	129.75	123.46	11	2
1	A	45	GLN	O-C-N	6.35	131.03	122.59	5	7
1	A	82	ASN	O-C-N	6.35	130.20	122.20	14	1
1	A	44	VAL	O-C-N	6.33	126.66	121.85	17	1
1	A	89	TRP	CD2-CE2-CZ2	-6.32	116.08	122.40	6	13
1	A	39	GLN	OE1-CD-NE2	6.31	128.91	122.60	17	3
1	A	112	GLU	N-CA-C	6.31	119.01	108.73	11	6
1	A	131	PHE	N-CA-C	6.28	117.98	110.19	20	8
1	A	63	LEU	N-CA-C	6.28	118.45	110.61	7	2
1	A	125	GLN	N-CA-C	-6.26	105.47	113.23	8	2
1	A	85	THR	CA-CB-OG1	-6.25	100.23	109.60	5	7
1	A	18	GLU	N-CA-C	6.24	117.75	111.07	20	1
1	A	85	THR	CA-C-O	6.24	126.39	120.09	23	3
1	A	69	VAL	N-CA-C	-6.23	106.66	112.83	13	1
1	A	58	PHE	CA-C-N	-6.20	113.22	122.39	11	2
1	A	58	PHE	C-N-CA	-6.20	113.22	122.39	11	2
1	A	98	GLN	CA-C-N	-6.19	113.95	122.30	9	8
1	A	98	GLN	C-N-CA	-6.19	113.95	122.30	9	8
1	A	89	TRP	CB-CG-CD2	-6.18	118.14	126.80	12	21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	PHE	CD1-CG-CD2	6.18	127.87	118.60	4	4
1	A	64	ASP	CA-CB-CG	-6.17	106.42	112.60	24	3
1	A	110	TRP	CB-CG-CD2	-6.17	118.16	126.80	13	13
1	A	58	PHE	CA-CB-CG	-6.16	107.64	113.80	20	2
1	A	42	ILE	CA-C-O	6.16	125.70	120.22	18	1
1	A	66	THR	CA-C-N	-6.16	115.17	122.93	5	1
1	A	66	THR	C-N-CA	-6.16	115.17	122.93	5	1
1	A	41	LYS	CA-C-O	-6.16	113.67	120.38	21	4
1	A	24	LEU	CB-CA-C	-6.14	100.73	110.86	21	2
1	A	59	ARG	NE-CZ-NH2	6.13	124.72	119.20	9	2
1	A	85	THR	N-CA-CB	-6.13	103.06	110.53	22	7
1	A	73	GLU	CA-C-O	6.12	129.27	120.51	14	3
1	A	57	THR	O-C-N	6.12	130.72	122.59	15	3
1	A	98	GLN	CB-CA-C	-6.12	101.37	110.67	10	3
1	A	40	THR	CA-C-N	-6.10	114.58	123.00	21	6
1	A	40	THR	C-N-CA	-6.10	114.58	123.00	21	6
1	A	11	MET	N-CA-C	-6.08	103.27	111.54	23	1
1	A	44	VAL	CA-C-O	-6.07	115.54	120.70	17	1
1	A	50	PHE	O-C-N	6.07	129.68	122.46	21	5
1	A	94	LEU	O-C-N	6.06	130.66	122.59	4	2
1	A	104	ASN	CA-CB-CG	-6.06	106.54	112.60	16	8
1	A	42	ILE	N-CA-CB	-6.06	104.03	112.52	24	1
1	A	94	LEU	N-CA-C	6.03	118.63	111.33	17	8
1	A	124	ASP	O-C-N	6.03	130.61	122.59	23	5
1	A	39	GLN	CG-CD-NE2	-6.02	107.37	116.40	2	4
1	A	105	ARG	CA-C-O	6.00	126.38	119.35	10	1
1	A	118	LEU	CA-C-O	-5.99	113.55	120.49	22	1
1	A	33	ILE	CA-C-O	5.97	128.25	120.78	18	2
1	A	15	GLU	O-C-N	-5.97	114.65	122.59	21	1
1	A	103	GLU	N-CA-C	5.96	117.31	108.60	13	4
1	A	32	LYS	CA-C-N	-5.96	117.06	123.08	23	2
1	A	32	LYS	C-N-CA	-5.96	117.06	123.08	23	2
1	A	75	THR	CA-C-O	-5.96	114.16	120.71	18	2
1	A	5	GLN	CA-C-O	-5.95	113.51	120.53	10	6
1	A	132	LYS	CA-C-O	-5.95	112.72	119.98	24	2
1	A	125	GLN	CB-CG-CD	-5.95	102.49	112.60	16	4
1	A	77	GLY	N-CA-C	-5.93	106.84	114.85	9	2
1	A	5	GLN	CA-C-N	5.92	130.24	120.94	22	1
1	A	5	GLN	C-N-CA	5.92	130.24	120.94	22	1
1	A	100	GLY	CA-C-O	5.91	128.57	121.77	8	2
1	A	13	SER	O-C-N	5.90	129.82	123.56	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	124	ASP	CA-CB-CG	-5.89	106.71	112.60	17	1
1	A	25	ASP	N-CA-C	-5.88	103.81	111.74	12	1
1	A	116	LEU	CA-C-O	5.87	126.85	119.98	9	2
1	A	10	GLU	CB-CA-C	-5.87	103.83	111.40	13	2
1	A	109	GLN	OE1-CD-NE2	5.86	128.46	122.60	24	2
1	A	128	ARG	NE-CZ-NH1	5.84	127.34	121.50	6	2
1	A	128	ARG	CA-C-O	-5.83	114.52	120.71	1	1
1	A	115	LYS	O-C-N	5.83	128.66	123.41	21	6
1	A	71	PHE	CA-C-O	5.81	127.58	121.19	20	1
1	A	124	ASP	CA-C-N	-5.79	113.45	122.37	18	1
1	A	124	ASP	C-N-CA	-5.79	113.45	122.37	18	1
1	A	9	TRP	N-CA-C	5.79	117.85	108.41	22	5
1	A	127	CYS	CA-C-N	-5.79	114.17	122.67	23	2
1	A	127	CYS	C-N-CA	-5.79	114.17	122.67	23	2
1	A	105	ARG	CA-C-N	-5.78	116.07	121.62	15	1
1	A	105	ARG	C-N-CA	-5.78	116.07	121.62	15	1
1	A	43	ILE	CA-C-O	5.78	126.73	120.43	13	6
1	A	65	PHE	O-C-N	-5.78	116.83	123.42	8	1
1	A	91	GLY	CA-C-N	5.76	129.84	121.26	1	2
1	A	91	GLY	C-N-CA	5.76	129.84	121.26	1	2
1	A	115	LYS	CA-C-O	-5.75	115.02	121.40	1	2
1	A	40	THR	CB-CA-C	-5.75	104.30	111.43	2	2
1	A	131	PHE	CA-C-O	5.74	128.15	121.49	3	3
1	A	45	GLN	CA-CB-CG	-5.74	102.62	114.10	18	2
1	A	89	TRP	CD1-NE1-CE2	5.73	119.22	108.90	11	3
1	A	106	GLY	CA-C-N	5.72	131.97	122.54	9	2
1	A	106	GLY	C-N-CA	5.72	131.97	122.54	9	2
1	A	88	THR	O-C-N	-5.71	117.58	123.29	11	2
1	A	106	GLY	CA-C-O	-5.70	115.84	121.48	11	2
1	A	62	ASP	CA-CB-CG	-5.70	106.91	112.60	2	2
1	A	59	ARG	N-CA-C	5.69	117.93	108.99	1	3
1	A	95	VAL	CA-C-O	-5.69	114.28	120.71	2	2
1	A	83	VAL	N-CA-CB	-5.68	101.86	111.23	14	2
1	A	48	ASP	O-C-N	5.67	128.85	122.22	22	4
1	A	18	GLU	CA-C-O	-5.67	115.06	120.90	16	2
1	A	116	LEU	N-CA-C	5.66	117.60	107.80	1	3
1	A	20	TYR	N-CA-C	-5.66	104.73	111.69	20	3
1	A	8	THR	CA-C-O	-5.66	113.76	120.43	22	2
1	A	18	GLU	CB-CA-C	-5.65	102.01	110.88	20	4
1	A	129	GLN	CA-C-O	-5.64	115.57	121.55	14	1
1	A	42	ILE	CB-CA-C	-5.63	103.99	110.41	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	93	THR	CA-C-N	5.63	128.09	120.38	17	2
1	A	93	THR	C-N-CA	5.63	128.09	120.38	17	2
1	A	75	THR	CB-CA-C	-5.62	102.51	111.17	22	2
1	A	98	GLN	CA-C-O	5.60	126.75	120.92	20	1
1	A	63	LEU	CB-CA-C	-5.60	104.28	111.50	9	1
1	A	29	ALA	N-CA-C	-5.60	103.72	111.28	12	1
1	A	46	ASP	N-CA-CB	-5.60	105.07	111.79	6	2
1	A	35	VAL	CB-CA-C	-5.57	104.74	112.04	2	2
1	A	18	GLU	CB-CG-CD	-5.57	103.14	112.60	21	3
1	A	120	LEU	CA-C-O	5.55	126.24	120.30	20	2
1	A	89	TRP	CG-CD2-CE3	-5.54	128.36	133.90	8	1
1	A	110	TRP	N-CA-C	5.54	117.42	108.34	15	1
1	A	60	ASN	OD1-CG-ND2	5.53	128.13	122.60	20	1
1	A	107	TRP	CD1-NE1-CE2	-5.52	98.97	108.90	11	1
1	A	98	GLN	O-C-N	5.52	129.48	123.13	15	2
1	A	33	ILE	CB-CA-C	-5.52	104.92	111.65	13	1
1	A	114	ASP	N-CA-C	5.51	119.18	111.74	13	2
1	A	55	ASN	CA-C-N	5.50	128.51	120.71	20	1
1	A	55	ASN	C-N-CA	5.50	128.51	120.71	20	1
1	A	38	THR	CA-C-O	-5.49	114.10	120.31	13	1
1	A	122	CYS	O-C-N	5.49	129.90	122.59	23	1
1	A	111	VAL	N-CA-CB	-5.48	102.19	111.23	10	1
1	A	65	PHE	CA-CB-CG	-5.48	108.32	113.80	21	1
1	A	24	LEU	CA-C-O	5.48	125.70	119.18	24	1
1	A	69	VAL	N-CA-CB	-5.47	106.75	112.06	17	1
1	A	31	ARG	NE-CZ-NH1	5.46	126.96	121.50	15	1
1	A	52	THR	CA-C-O	-5.45	115.77	121.55	10	3
1	A	28	PHE	O-C-N	5.43	129.49	122.43	23	1
1	A	129	GLN	N-CA-C	5.43	117.53	110.53	4	1
1	A	84	LYS	CA-CB-CG	-5.43	103.25	114.10	22	3
1	A	107	TRP	CG-CD1-NE1	5.42	117.25	110.20	22	1
1	A	133	LYS	N-CA-C	5.41	118.19	108.17	4	1
1	A	55	ASN	N-CA-C	5.41	116.96	109.54	23	1
1	A	43	ILE	CA-C-N	-5.41	117.67	122.97	17	3
1	A	43	ILE	C-N-CA	-5.41	117.67	122.97	17	3
1	A	80	GLY	O-C-N	5.39	129.71	122.70	11	3
1	A	21	MET	N-CA-CB	-5.37	102.03	110.30	8	2
1	A	127	CYS	O-C-N	5.37	129.30	123.13	12	3
1	A	25	ASP	O-C-N	5.36	129.72	122.59	18	1
1	A	16	ASN	OD1-CG-ND2	-5.33	117.27	122.60	15	1
1	A	101	GLU	CB-CG-CD	-5.33	103.53	112.60	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	PHE	N-CA-C	5.33	117.10	108.41	9	2
1	A	54	THR	O-C-N	5.32	129.67	122.59	24	1
1	A	9	TRP	CB-CG-CD1	5.32	134.88	126.90	4	1
1	A	46	ASP	N-CA-C	5.31	116.85	107.61	9	2
1	A	62	ASP	O-C-N	5.31	129.65	122.59	22	2
1	A	89	TRP	CE3-CZ3-CH2	-5.31	114.20	121.10	20	6
1	A	21	MET	CA-C-N	5.30	127.82	120.29	12	3
1	A	21	MET	C-N-CA	5.30	127.82	120.29	12	3
1	A	94	LEU	CA-C-O	5.30	127.51	121.58	24	1
1	A	49	ASN	CA-C-N	5.28	130.52	122.65	17	1
1	A	49	ASN	C-N-CA	5.28	130.52	122.65	17	1
1	A	90	GLU	N-CA-CB	-5.27	102.69	110.49	17	1
1	A	73	GLU	N-CA-CB	-5.27	101.59	110.49	2	2
1	A	86	LEU	N-CA-C	5.26	116.87	108.41	8	2
1	A	15	GLU	CA-CB-CG	-5.26	103.59	114.10	14	3
1	A	64	ASP	N-CA-CB	-5.24	103.09	111.58	13	1
1	A	6	ASN	CA-CB-CG	-5.24	107.36	112.60	22	1
1	A	14	ASN	CB-CG-ND2	-5.24	108.53	116.40	23	1
1	A	67	VAL	N-CA-C	5.23	116.15	109.30	6	3
1	A	78	LEU	CB-CA-C	-5.23	103.02	111.28	5	1
1	A	88	THR	CA-C-O	5.21	126.89	121.31	24	4
1	A	9	TRP	CE2-CD2-CE3	-5.21	113.59	118.80	19	2
1	A	58	PHE	N-CA-CB	5.20	117.76	110.12	13	1
1	A	14	ASN	CA-C-N	-5.20	115.78	123.05	17	2
1	A	14	ASN	C-N-CA	-5.20	115.78	123.05	17	2
1	A	103	GLU	CB-CA-C	-5.19	100.73	109.50	9	3
1	A	10	GLU	CA-C-O	-5.19	115.38	120.98	24	1
1	A	36	ARG	NE-CZ-NH1	-5.18	116.32	121.50	6	1
1	A	34	ALA	CB-CA-C	-5.18	103.10	111.28	8	1
1	A	63	LEU	CA-C-O	-5.17	114.58	120.58	13	1
1	A	10	GLU	CA-CB-CG	-5.17	103.77	114.10	8	3
1	A	115	LYS	CA-C-N	-5.16	113.56	121.40	9	1
1	A	115	LYS	C-N-CA	-5.16	113.56	121.40	9	1
1	A	14	ASN	N-CA-C	5.16	117.05	108.02	10	3
1	A	96	CYS	CA-C-O	5.16	126.79	120.60	16	1
1	A	44	VAL	N-CA-C	5.15	116.32	111.48	16	1
1	A	131	PHE	CB-CG-CD1	-5.15	111.95	120.70	23	1
1	A	89	TRP	N-CA-C	-5.13	102.79	110.23	17	1
1	A	98	GLN	CG-CD-NE2	-5.13	108.71	116.40	2	1
1	A	63	LEU	CA-C-N	-5.12	113.96	122.92	13	2
1	A	63	LEU	C-N-CA	-5.12	113.96	122.92	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	133	LYS	CA-C-O	-5.12	115.38	120.96	17	1
1	A	39	GLN	CA-CB-CG	-5.11	103.89	114.10	18	1
1	A	71	PHE	CA-CB-CG	-5.11	108.69	113.80	20	1
1	A	67	VAL	N-CA-CB	-5.10	105.00	111.64	17	1
1	A	122	CYS	N-CA-CB	-5.09	103.71	111.66	5	1
1	A	15	GLU	CA-C-O	5.09	126.17	120.82	10	2
1	A	128	ARG	O-C-N	5.09	129.67	123.21	1	1
1	A	19	GLY	O-C-N	5.08	128.13	122.54	3	1
1	A	59	ARG	NE-CZ-NH1	5.07	126.57	121.50	1	2
1	A	133	LYS	CA-CB-CG	-5.04	104.02	114.10	23	1
1	A	127	CYS	CA-C-O	-5.04	116.21	121.55	13	1
1	A	74	HIS	CA-C-O	5.04	127.71	120.51	23	1
1	A	117	TYR	CA-C-N	-5.04	115.06	122.06	19	1
1	A	117	TYR	C-N-CA	-5.04	115.06	122.06	19	1
1	A	63	LEU	O-C-N	5.03	129.28	122.59	8	1
1	A	28	PHE	CA-C-O	-5.03	116.35	122.64	15	1
1	A	89	TRP	CZ3-CH2-CZ2	5.02	128.03	121.50	8	1
1	A	45	GLN	N-CA-C	5.02	118.98	107.48	10	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	64±11
All	All	25920	25320	25296	1536

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 30.

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:36:ARG:C	1:A:37:LEU:HD13	0.91	1.90	17	1
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:HD23	0.86	1.96	24	10
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: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:HD12	1:A:37:LEU:C	0.76	2.06	4	6
1:A:37:LEU:HD22	1:A:37:LEU:N	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:HD23	1:A:37:LEU:N	0.74	1.97	9	8
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:C	1:A:37:LEU:HD13	0.71	2.09	18	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLN:N	1:A:109:GLN:CD	0.69	2.51	15	1
1:A:117:TYR:C	1:A:118:LEU:HD23	0.68	2.13	1	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:37:LEU:HD12	1:A:37:LEU:O	0.68	1.89	16	2
1:A:83:VAL:HG11	1:A:98:GLN:HB3	0.68	1.64	22	1
1:A:89:TRP:HA	1:A:89:TRP:CE3	0.68	2.24	13	24
1:A:37:LEU:HD11	1:A:58:PHE:CD1	0.68	2.24	19	2
1:A:65:PHE:CE2	1:A:107:TRP:CH2	0.68	2.81	16	3
1:A:90:GLU:HB3	1:A:93:THR:HG22	0.67	1.64	12	5
1:A:120:LEU:HD12	1:A:121:THR:O	0.67	1.89	19	8
1:A:109:GLN:HG2	1:A:118:LEU:HD22	0.67	1.66	1	1
1:A:24:LEU:HD13	1:A:79:ASP:HB2	0.67	1.67	6	4
1:A:65:PHE:CD2	1:A:87:VAL:HG21	0.67	2.24	19	4
1:A:37:LEU:HD22	1:A:37:LEU:H	0.67	1.48	17	1
1:A:24:LEU:N	1:A:24:LEU:HD23	0.67	2.04	19	3
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:37:LEU:HD23	1:A:58:PHE:CE2	0.66	2.25	4	3
1:A:90:GLU:CG	1:A:95:VAL:HG21	0.66	2.21	4	3
1:A:107:TRP:C	1:A:107:TRP:CD1	0.66	2.70	17	6
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:21:MET:HE1	1:A:30:THR:CG2	0.65	2.22	14	1
1:A:90:GLU:N	1:A:93:THR:O	0.65	2.29	22	14
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:24:LEU:C	1:A:24:LEU:HD12	0.64	2.17	3	2
1:A:133:LYS:C	1:A:133:LYS:HD3	0.64	2.17	22	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:HD23	1:A:116:LEU:O	0.64	1.93	16	6
1:A:37:LEU:O	1:A:39:GLN:N	0.64	2.31	22	2
1:A:50:PHE:CD1	1:A:50:PHE:C	0.63	2.77	19	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	7
1:A:37:LEU:HD21	1:A:58:PHE:N	0.63	2.08	3	1
1:A:37:LEU:C	1:A:37:LEU:CD1	0.63	2.71	18	8
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
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:83:VAL:HG13	1:A:99:LYS:C	0.62	2.18	6	2
1:A:107:TRP:NE1	1:A:109:GLN:HE22	0.62	1.90	15	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:107:TRP:NE1	1:A:109:GLN:NE2	0.62	2.47	15	5
1:A:37:LEU:HD23	1:A:58:PHE:CZ	0.62	2.30	4	1
1:A:24:LEU:HD12	1:A:24:LEU:C	0.62	2.20	24	4
1:A:65:PHE:CE1	1:A:87:VAL:HG21	0.61	2.30	10	2
1:A:9:TRP:CH2	1:A:116:LEU:HD23	0.61	2.29	12	2
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:65:PHE:CE2	1:A:107:TRP:CZ2	0.61	2.88	24	4
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: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:8:THR:C	1:A:9:TRP:CD1	0.61	2.79	20	16
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:24:LEU:HD22	1:A:105:ARG:NE	0.60	2.11	2	1
1:A:34:ALA:HB1	1:A:58:PHE:CE2	0.60	2.31	10	1
1:A:73:GLU:CB	1:A:83:VAL:CA	0.60	2.79	14	1
1:A:63:LEU:HD11	1:A:107:TRP:HZ2	0.60	1.53	5	1
1:A:53:LYS:O	1:A:53:LYS:CE	0.60	2.49	24	1
1:A:109:GLN:CG	1:A:118:LEU:HD22	0.60	2.26	1	1
1:A:65:PHE:CE2	1:A:87:VAL:HG22	0.60	2.31	8	1
1:A:21:MET:HE1	1:A:30:THR:HG21	0.60	1.72	14	1
1:A:36:ARG:C	1:A:37:LEU:CD2	0.60	2.74	20	2
1:A:24:LEU:HD13	1:A:79:ASP:CB	0.60	2.27	6	3
1:A:94:LEU:HB3	1:A:109:GLN:CG	0.60	2.26	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:GLN:O	1:A:130:VAL:HG13	0.60	1.97	23	1
1:A:13:SER:O	1:A:130:VAL:HG12	0.59	1.96	23	1
1:A:11:MET:HE2	1:A:39:GLN:NE2	0.59	2.13	7	1
1:A:65:PHE:CG	1:A:87:VAL:HG21	0.59	2.32	13	2
1:A:43:ILE:CD1	1:A:50:PHE:CE1	0.59	2.85	6	3
1:A:133:LYS:HD2	1:A:133:LYS:N	0.59	2.13	22	1
1:A:50:PHE:C	1:A:50:PHE:CD1	0.59	2.77	22	11
1:A:33:ILE:HD12	1:A:33:ILE:N	0.59	2.12	23	4
1:A:26:ILE:HD12	1:A:78:LEU:O	0.59	1.98	10	8
1:A:89:TRP:CZ3	1:A:94:LEU:N	0.59	2.71	22	2
1:A:37:LEU:CD2	1:A:58:PHE:CE2	0.58	2.80	9	2
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:42:ILE:HD11	1:A:55:ASN:HB2	0.58	1.74	16	1
1:A:37:LEU:HD12	1:A:57:THR:HG22	0.58	1.76	24	1
1:A:37:LEU:CD2	1:A:58:PHE:CD2	0.58	2.87	12	4
1:A:38:THR:HG22	1:A:39:GLN:N	0.58	2.13	2	1
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:30:THR:HG23	1:A:34:ALA:C	0.58	2.23	18	1
1:A:9:TRP:CB	1:A:131:PHE:CD2	0.58	2.87	21	1
1:A:86:LEU:HD23	1:A:87:VAL:N	0.58	2.14	2	1
1:A:120:LEU:HD12	1:A:121:THR:N	0.58	2.13	21	2
1:A:31:ARG:O	1:A:33:ILE:HD12	0.58	1.98	15	1
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	10
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:17:PHE:CZ	1:A:34:ALA:HB3	0.57	2.34	10	1
1:A:14:ASN:N	1:A:14:ASN:ND2	0.57	2.52	7	2
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: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:107:TRP:CD1	1:A:107:TRP:C	0.56	2.77	13	12
1:A:17:PHE:CE2	1:A:35:VAL:HG22	0.56	2.35	18	1
1:A:128:ARG:C	1:A:129:GLN:HG3	0.56	2.25	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLU:HB2	1:A:93:THR:HG22	0.56	1.76	23	2
1:A:54:THR:HA	1:A:60:ASN:CB	0.56	2.30	24	1
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:37:LEU:N	1:A:37:LEU:HD23	0.56	2.14	20	1
1:A:133:LYS:C	1:A:133:LYS:CD	0.56	2.76	22	1
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
1:A:9:TRP:CE3	1:A:133:LYS:HA	0.55	2.35	9	17
1:A:20:TYR:C	1:A:20:TYR:CD1	0.55	2.84	20	3
1:A:43:ILE:HD11	1:A:50:PHE:HE2	0.55	1.61	8	1
1:A:107:TRP:O	1:A:107:TRP:CD1	0.55	2.60	11	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:41:LYS:HA	1:A:55:ASN:CB	0.55	2.32	24	1
1:A:118:LEU:HB2	1:A:131:PHE:CE1	0.55	2.37	11	4
1:A:34:ALA:HB1	1:A:58:PHE:CD2	0.55	2.36	10	1
1:A:4:ASP:HA	1:A:111:VAL:HG21	0.55	1.79	19	1
1:A:9:TRP:CD1	1:A:9:TRP:N	0.55	2.74	20	10
1:A:130:VAL:C	1:A:131:PHE:CD1	0.55	2.84	4	4
1:A:32:LYS:C	1:A:33:ILE:CG1	0.55	2.80	4	2
1:A:37:LEU:HD12	1:A:58:PHE:CG	0.55	2.36	20	1
1:A:48:ASP:O	1:A:66:THR:HG23	0.55	2.02	11	1
1:A:63:LEU:CD2	1:A:65:PHE:CZ	0.55	2.89	22	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: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	4
1:A:118:LEU:CB	1:A:131:PHE:CE1	0.54	2.91	11	3
1:A:50:PHE:CE2	1:A:94:LEU:HD22	0.54	2.37	21	7
1:A:26:ILE:HD12	1:A:78:LEU:C	0.54	2.27	2	2
1:A:37:LEU:N	1:A:37:LEU:CD2	0.54	2.64	17	6
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:THR:HA	1:A:56:SER:HB3	0.54	1.80	20	1
1:A:41:LYS:CD	1:A:41:LYS:C	0.54	2.80	21	12
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:89:TRP:CZ3	1:A:93:THR:C	0.53	2.86	12	14
1:A:26:ILE:CD1	1:A:78:LEU:HD12	0.53	2.33	23	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:38:THR:HG21	1:A:57:THR:HB	0.53	1.80	22	1
1:A:27:ASP:O	1:A:28:PHE:CG	0.53	2.61	3	1
1:A:83:VAL:HG12	1:A:84:LYS:N	0.53	2.18	14	2
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:11:MET:HG3	1:A:131:PHE:CZ	0.53	2.39	5	1
1:A:104:ASN:O	1:A:121:THR:HG22	0.53	2.04	7	1
1:A:93:THR:HG23	1:A:95:VAL:CG2	0.53	2.33	17	1
1:A:17:PHE:CD1	1:A:17:PHE:N	0.53	2.77	18	3
1:A:118:LEU:HB2	1:A:131:PHE:CZ	0.53	2.39	19	5
1:A:9:TRP:H	1:A:9:TRP:CD1	0.53	2.21	21	3
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:17:PHE:CZ	1:A:35:VAL:HG22	0.52	2.39	2	1
1:A:34:ALA:HA	1:A:37:LEU:HD21	0.52	1.79	6	1
1:A:96:CYS:HB2	1:A:107:TRP:CH2	0.52	2.39	23	3
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:131:PHE:N	1:A:131:PHE:CD1	0.52	2.77	1	3
1:A:26:ILE:CD1	1:A:78:LEU:C	0.52	2.82	12	1
1:A:54:THR:CG2	1:A:55:ASN:N	0.52	2.73	24	1
1:A:50:PHE:CD1	1:A:51:LYS:N	0.52	2.77	23	2
1:A:107:TRP:HE1	1:A:109:GLN:NE2	0.52	2.03	4	5
1:A:52:THR:CG2	1:A:53:LYS:N	0.52	2.73	21	6
1:A:9:TRP:CG	1:A:131:PHE:CD2	0.52	2.97	21	1
1:A:11:MET:HE2	1:A:39:GLN:HE21	0.52	1.63	7	1
1:A:37:LEU:HG	1:A:58:PHE:CE2	0.52	2.38	13	1
1:A:11:MET:HG3	1:A:131:PHE:CE1	0.52	2.39	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:CYS:HB2	1:A:107:TRP:CZ3	0.52	2.40	11	3
1:A:37:LEU:CD2	1:A:58:PHE:CG	0.52	2.93	12	3
1:A:40:THR:CG2	1:A:41:LYS:N	0.52	2.72	16	3
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:9:TRP:CZ2	1:A:116:LEU:CD1	0.52	2.93	21	1
1:A:37:LEU:HD21	1:A:57:THR:HG22	0.52	1.82	21	1
1:A:94:LEU:CD2	1:A:109:GLN:CG	0.52	2.87	22	1
1:A:71:PHE:HB3	1:A:85:THR:HB	0.51	1.81	2	4
1:A:26:ILE:CD1	1:A:78:LEU:HA	0.51	2.34	13	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:41:LYS:HE3	1:A:116:LEU:HD22	0.51	1.80	5	1
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: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:65:PHE:CE1	1:A:87:VAL:CG2	0.51	2.93	5	1
1:A:132:LYS:CD	1:A:132:LYS:C	0.51	2.81	18	2
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: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:23:ALA:HB2	1:A:125:GLN:CG	0.51	2.34	24	1
1:A:41:LYS:C	1:A:41:LYS:HD3	0.51	2.31	16	6
1:A:74:HIS:N	1:A:74:HIS:ND1	0.51	2.57	10	1
1:A:50:PHE:HD2	1:A:94:LEU:HD13	0.51	1.66	24	1
1:A:63:LEU:HD21	1:A:94:LEU:HD22	0.51	1.83	5	2
1:A:92:ASN:ND2	1:A:92:ASN:N	0.51	2.54	12	1
1:A:37:LEU:HG	1:A:58:PHE:CZ	0.51	2.40	13	1
1:A:43:ILE:HG12	1:A:50:PHE:CE1	0.51	2.40	13	1
1:A:89:TRP:CE3	1:A:89:TRP:CA	0.51	2.94	22	18
1:A:65:PHE:CE2	1:A:87:VAL:CG2	0.51	2.93	21	2
1:A:32:LYS:C	1:A:33:ILE:HD12	0.51	2.31	23	1
1:A:18:GLU:HB2	1:A:31:ARG:CB	0.51	2.36	1	1
1:A:41:LYS:HD2	1:A:131:PHE:CZ	0.51	2.40	23	1
1:A:98:GLN:CD	1:A:105:ARG:HB3	0.50	2.31	18	2
1:A:21:MET:C	1:A:26:ILE:HG22	0.50	2.31	22	1
1:A:10:GLU:N	1:A:132:LYS:O	0.50	2.44	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:C	1:A:39:GLN:N	0.50	2.69	22	1
1:A:108:LYS:HG3	1:A:110:TRP:CH2	0.50	2.42	10	5
1:A:41:LYS:HD3	1:A:41:LYS:C	0.50	2.32	4	7
1:A:33:ILE:HG22	1:A:33:ILE:O	0.50	2.06	18	1
1:A:39:GLN:HG2	1:A:56:SER:N	0.50	2.20	21	1
1:A:109:GLN:C	1:A:110:TRP:CG	0.50	2.86	18	9
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:83:VAL:HG11	1:A:98:GLN:OE1	0.50	2.07	17	1
1:A:24:LEU:N	1:A:24:LEU:CD2	0.50	2.75	19	1
1:A:37:LEU:HB2	1:A:58:PHE:CE1	0.50	2.42	20	1
1:A:63:LEU:HG	1:A:65:PHE:CE2	0.50	2.42	22	5
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:133:LYS:CG	1:A:134:LYS:N	0.50	2.73	21	3
1:A:65:PHE:CD1	1:A:65:PHE:C	0.50	2.89	21	2
1:A:36:ARG:C	1:A:37:LEU:HD12	0.50	2.31	18	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:87:VAL:HG13	1:A:96:CYS:SG	0.50	2.47	9	1
1:A:118:LEU:O	1:A:118:LEU:HD23	0.50	2.06	15	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:65:PHE:CD1	1:A:65:PHE:N	0.49	2.80	19	1
1:A:69:VAL:HG13	1:A:71:PHE:N	0.49	2.22	20	1
1:A:96:CYS:CB	1:A:107:TRP:CZ3	0.49	2.96	11	3
1:A:27:ASP:C	1:A:28:PHE:CD1	0.49	2.90	4	1
1:A:37:LEU:C	1:A:37:LEU:HD12	0.49	2.32	5	1
1:A:30:THR:HG22	1:A:30:THR:O	0.49	2.07	23	2
1:A:15:GLU:HB3	1:A:128:ARG:C	0.49	2.32	21	1
1:A:37:LEU:HD11	1:A:58:PHE:CB	0.49	2.34	10	1
1:A:58:PHE:N	1:A:58:PHE:CD1	0.49	2.80	20	1
1:A:8:THR:HG22	1:A:134:LYS:CG	0.49	2.38	23	1
1:A:8:THR:C	1:A:9:TRP:CG	0.49	2.90	1	3
1:A:11:MET:HB3	1:A:39:GLN:CD	0.49	2.31	7	2
1:A:65:PHE:CZ	1:A:107:TRP:CH2	0.49	3.00	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ASP:C	1:A:65:PHE:CD1	0.49	2.91	18	1
1:A:38:THR:O	1:A:38:THR:HG23	0.49	2.07	20	1
1:A:96:CYS:HB2	1:A:107:TRP:CZ2	0.49	2.41	20	1
1:A:69:VAL:HG12	1:A:71:PHE:N	0.49	2.21	2	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:65:PHE:CD2	1:A:87:VAL:CG2	0.49	2.95	8	1
1:A:37:LEU:HD12	1:A:58:PHE:CD2	0.49	2.43	20	1
1:A:41:LYS:HA	1:A:55:ASN:HB3	0.49	1.84	24	1
1:A:90:GLU:HB2	1:A:95:VAL:HG23	0.49	1.84	3	4
1:A:107:TRP:HB2	1:A:120:LEU:CB	0.49	2.38	2	1
1:A:40:THR:HG22	1:A:40:THR:O	0.49	2.06	20	2
1:A:107:TRP:HB2	1:A:120:LEU:HB2	0.48	1.84	2	2
1:A:75:THR:CG2	1:A:82:ASN:ND2	0.48	2.76	14	1
1:A:126:VAL:HG13	1:A:128:ARG:NH1	0.48	2.22	24	1
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:HG23	1:A:26:ILE:O	0.48	2.07	8	4
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: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:43:ILE:HG13	1:A:50:PHE:CE1	0.48	2.43	2	3
1:A:126:VAL:HG22	1:A:126:VAL:O	0.48	2.08	6	3
1:A:126:VAL:O	1:A:126:VAL:HG13	0.48	2.09	18	5
1:A:63:LEU:CD1	1:A:107:TRP:CZ2	0.48	2.89	5	2
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:33:ILE:O	1:A:33:ILE:CG2	0.48	2.59	18	1
1:A:65:PHE:CZ	1:A:87:VAL:HG11	0.48	2.44	21	1
1:A:54:THR:OG1	1:A:60:ASN:HB3	0.48	2.09	24	1
1:A:9:TRP:CD1	1:A:41:LYS:CD	0.48	2.97	1	1
1:A:98:GLN:HB2	1:A:106:GLY:N	0.48	2.24	13	3
1:A:52:THR:O	1:A:63:LEU:N	0.48	2.46	3	3
1:A:39:GLN:HG2	1:A:40:THR:N	0.48	2.24	13	2
1:A:83:VAL:CG1	1:A:100:GLY:HA2	0.48	2.39	13	1
1:A:33:ILE:N	1:A:33:ILE:CD1	0.48	2.77	23	3
1:A:17:PHE:CD2	1:A:18:GLU:N	0.47	2.82	10	1
1:A:31:ARG:C	1:A:31:ARG:HD3	0.47	2.33	13	1
1:A:42:ILE:HD12	1:A:53:LYS:O	0.47	2.09	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:VAL:HG22	1:A:100:GLY:O	0.47	2.08	17	1
1:A:14:ASN:ND2	1:A:14:ASN:N	0.47	2.61	24	1
1:A:98:GLN:HG3	1:A:105:ARG:C	0.47	2.34	1	1
1:A:50:PHE:CD2	1:A:94:LEU:CD1	0.47	2.97	23	2
1:A:67:VAL:CG2	1:A:89:TRP:CD1	0.47	2.92	8	1
1:A:8:THR:HG22	1:A:42:ILE:HG23	0.47	1.85	9	1
1:A:65:PHE:C	1:A:65:PHE:CD1	0.47	2.91	14	3
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:110:TRP:C	1:A:111:VAL:HG23	0.47	2.35	20	3
1:A:78:LEU:C	1:A:79:ASP:CG	0.47	2.82	11	1
1:A:3:LYS:HB2	1:A:89:TRP:CH2	0.47	2.45	13	1
1:A:19:GLY:HA2	1:A:22:LYS:CG	0.47	2.38	22	1
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:24:LEU:C	1:A:24:LEU:CD1	0.47	2.88	3	3
1:A:108:LYS:C	1:A:109:GLN:NE2	0.47	2.72	19	5
1:A:82:ASN:C	1:A:83:VAL:CG2	0.47	2.87	23	3
1:A:66:THR:CG2	1:A:69:VAL:HG23	0.47	2.39	14	2
1:A:90:GLU:HB3	1:A:93:THR:HG23	0.47	1.85	15	1
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: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:17:PHE:CD1	1:A:17:PHE:C	0.47	2.87	7	2
1:A:109:GLN:CG	1:A:118:LEU:CD2	0.47	2.92	7	1
1:A:112:GLU:HB2	1:A:117:TYR:CD1	0.47	2.45	17	1
1:A:115:LYS:HG3	1:A:117:TYR:CD1	0.47	2.45	23	1
1:A:53:LYS:O	1:A:53:LYS:CD	0.47	2.63	24	1
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:37:LEU:CG	1:A:58:PHE:CD2	0.47	2.98	13	2
1:A:66:THR:CG2	1:A:69:VAL:HG21	0.47	2.40	5	1
1:A:50:PHE:C	1:A:51:LYS:HG3	0.47	2.35	17	2
1:A:5:GLN:HE21	1:A:5:GLN:N	0.47	2.08	9	1
1:A:9:TRP:CD1	1:A:41:LYS:HE3	0.47	2.45	19	1
1:A:73:GLU:C	1:A:74:HIS:CG	0.47	2.92	10	1
1:A:26:ILE:CD1	1:A:79:ASP:N	0.47	2.78	12	1
1:A:16:ASN:OD1	1:A:19:GLY:N	0.47	2.48	15	2
1:A:38:THR:CG2	1:A:39:GLN:N	0.46	2.78	2	1
1:A:98:GLN:HG2	1:A:105:ARG:C	0.46	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:GLN:HG3	1:A:105:ARG:CB	0.46	2.40	2	1
1:A:83:VAL:HG13	1:A:100:GLY:H	0.46	1.68	5	1
1:A:86:LEU:HD23	1:A:86:LEU:C	0.46	2.35	2	1
1:A:28:PHE:CD1	1:A:28:PHE:N	0.46	2.83	17	3
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:71:PHE:O	1:A:73:GLU:N	0.46	2.49	6	9
1:A:26:ILE:HD11	1:A:78:LEU:CA	0.46	2.39	12	1
1:A:88:THR:HG22	1:A:89:TRP:H	0.46	1.70	22	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:90:GLU:HB3	1:A:93:THR:HG21	0.46	1.87	8	1
1:A:96:CYS:HB3	1:A:107:TRP:CH2	0.46	2.45	11	1
1:A:81:ARG:CG	1:A:82:ASN:N	0.46	2.78	13	2
1:A:73:GLU:HA	1:A:83:VAL:N	0.46	2.26	14	1
1:A:37:LEU:HD23	1:A:58:PHE:CE1	0.46	2.45	21	2
1:A:37:LEU:CB	1:A:58:PHE:CE1	0.46	2.98	20	1
1:A:42:ILE:HB	1:A:53:LYS:O	0.46	2.10	22	2
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:69:VAL:HG12	1:A:69:VAL:O	0.46	2.10	17	1
1:A:98:GLN:HG3	1:A:106:GLY:N	0.46	2.26	21	1
1:A:98:GLN:HG2	1:A:106:GLY:N	0.46	2.25	2	1
1:A:73:GLU:CB	1:A:83:VAL:N	0.46	2.79	14	1
1:A:41:LYS:NZ	1:A:43:ILE:HD12	0.46	2.25	15	1
1:A:9:TRP:CD1	1:A:9:TRP:H	0.46	2.29	23	1
1:A:9:TRP:CZ3	1:A:116:LEU:HG	0.46	2.45	23	1
1:A:41:LYS:C	1:A:41:LYS:CD	0.46	2.89	2	1
1:A:66:THR:CG2	1:A:67:VAL:N	0.46	2.78	8	3
1:A:63:LEU:HD11	1:A:107:TRP:CE2	0.46	2.43	7	1
1:A:37:LEU:HD21	1:A:58:PHE:CG	0.46	2.46	16	1
1:A:102:LYS:CD	1:A:102:LYS:C	0.46	2.89	17	3
1:A:11:MET:CG	1:A:131:PHE:CE1	0.46	2.99	5	1
1:A:43:ILE:HD13	1:A:50:PHE:CE1	0.46	2.45	6	1
1:A:36:ARG:O	1:A:37:LEU:HD13	0.46	2.09	17	1
1:A:109:GLN:HE21	1:A:109:GLN:N	0.46	2.08	20	1
1:A:54:THR:CB	1:A:60:ASN:HB3	0.46	2.41	24	1
1:A:24:LEU:HD11	1:A:78:LEU:O	0.46	2.11	17	3
1:A:73:GLU:HB3	1:A:83:VAL:CA	0.46	2.40	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:3:LYS:HG2	1:A:89:TRP:CZ3	0.46	2.45	20	1
1:A:107:TRP:CD1	1:A:109:GLN:HE22	0.45	2.29	14	2
1:A:56:SER:HB2	1:A:58:PHE:CE1	0.45	2.46	11	2
1:A:21:MET:HG2	1:A:26:ILE:HG22	0.45	1.86	9	1
1:A:44:VAL:N	1:A:51:LYS:O	0.45	2.48	9	1
1:A:109:GLN:HB2	1:A:116:LEU:HD12	0.45	1.87	12	1
1:A:85:THR:HG22	1:A:85:THR:O	0.45	2.11	20	2
1:A:41:LYS:HA	1:A:55:ASN:CA	0.45	2.41	24	1
1:A:106:GLY:O	1:A:121:THR:HG22	0.45	2.11	21	2
1:A:107:TRP:CD1	1:A:109:GLN:NE2	0.45	2.84	14	4
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:63:LEU:HD23	1:A:65:PHE:CZ	0.45	2.46	22	1
1:A:38:THR:HG22	1:A:38:THR:O	0.45	2.11	14	2
1:A:102:LYS:CD	1:A:103:GLU:CG	0.45	2.94	15	1
1:A:42:ILE:CD1	1:A:54:THR:HB	0.45	2.41	24	1
1:A:20:TYR:CD1	1:A:20:TYR:C	0.45	2.94	14	8
1:A:18:GLU:CG	1:A:19:GLY:N	0.45	2.79	15	1
1:A:26:ILE:HD13	1:A:78:LEU:C	0.45	2.36	15	1
1:A:65:PHE:CE2	1:A:87:VAL:HB	0.45	2.46	21	1
1:A:98:GLN:CG	1:A:106:GLY:N	0.45	2.80	21	1
1:A:130:VAL:HG23	1:A:131:PHE:N	0.45	2.26	23	1
1:A:39:GLN:CD	1:A:40:THR:N	0.45	2.74	2	1
1:A:107:TRP:CB	1:A:120:LEU:HB2	0.45	2.41	15	2
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:25:ASP:C	1:A:27:ASP:N	0.45	2.73	18	1
1:A:24:LEU:HD13	1:A:26:ILE:HD13	0.45	1.89	12	1
1:A:126:VAL:HG13	1:A:126:VAL:O	0.45	2.11	24	1
1:A:125:GLN:C	1:A:126:VAL:HG12	0.45	2.37	5	1
1:A:9:TRP:CZ3	1:A:133:LYS:HG3	0.45	2.47	18	2
1:A:21:MET:HG2	1:A:26:ILE:CG2	0.45	2.41	9	1
1:A:112:GLU:HG2	1:A:117:TYR:CD2	0.45	2.46	13	1
1:A:52:THR:HB	1:A:63:LEU:HD23	0.45	1.87	23	2
1:A:37:LEU:N	1:A:58:PHE:CE2	0.45	2.85	21	1
1:A:75:THR:C	1:A:76:LYS:CG	0.45	2.89	5	1
1:A:125:GLN:C	1:A:126:VAL:CG1	0.45	2.88	7	2
1:A:37:LEU:HG	1:A:58:PHE:CD1	0.45	2.47	6	2
1:A:116:LEU:CD2	1:A:116:LEU:C	0.45	2.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:81:ARG:O	1:A:82:ASN:ND2	0.45	2.50	8	1
1:A:109:GLN:OE1	1:A:118:LEU:HD22	0.45	2.10	8	1
1:A:28:PHE:O	1:A:29:ALA:HB3	0.45	2.12	15	1
1:A:73:GLU:HB3	1:A:83:VAL:C	0.45	2.37	14	1
1:A:43:ILE:O	1:A:43:ILE:CG2	0.45	2.64	18	1
1:A:83:VAL:CG1	1:A:98:GLN:C	0.45	2.90	22	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:HG23	1:A:8:THR:O	0.44	2.13	23	1
1:A:11:MET:HE2	1:A:131:PHE:CZ	0.44	2.46	9	1
1:A:17:PHE:HZ	1:A:34:ALA:HB3	0.44	1.70	10	1
1:A:75:THR:C	1:A:76:LYS:HG2	0.44	2.36	12	1
1:A:120:LEU:HD11	1:A:122:CYS:SG	0.44	2.52	13	1
1:A:94:LEU:CD2	1:A:109:GLN:HG3	0.44	2.41	22	1
1:A:41:LYS:HA	1:A:55:ASN:HA	0.44	1.89	24	1
1:A:66:THR:HG23	1:A:67:VAL:N	0.44	2.27	8	1
1:A:103:GLU:OE1	1:A:105:ARG:N	0.44	2.50	1	1
1:A:98:GLN:NE2	1:A:105:ARG:HB3	0.44	2.27	4	1
1:A:125:GLN:C	1:A:126:VAL:CG2	0.44	2.90	8	1
1:A:63:LEU:O	1:A:65:PHE:N	0.44	2.51	11	2
1:A:83:VAL:HG22	1:A:100:GLY:CA	0.44	2.43	12	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
1:A:19:GLY:C	1:A:22:LYS:HG3	0.44	2.38	22	1
1:A:34:ALA:O	1:A:36:ARG:N	0.44	2.50	23	3
1:A:48:ASP:O	1:A:67:VAL:HG23	0.44	2.11	13	2
1:A:126:VAL:O	1:A:126:VAL:HG22	0.44	2.13	13	2
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:63:LEU:HG	1:A:65:PHE:CD2	0.44	2.48	24	1
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:72:ASP:C	1:A:73:GLU:HG3	0.44	2.38	7	2
1:A:102:LYS:HD3	1:A:103:GLU:N	0.44	2.28	2	2
1:A:83:VAL:HG12	1:A:99:LYS:C	0.44	2.38	3	1
1:A:21:MET:HE3	1:A:78:LEU:HD11	0.44	1.89	8	1
1:A:90:GLU:HB3	1:A:93:THR:CG2	0.44	2.43	8	1
1:A:7:GLY:N	1:A:43:ILE:HG22	0.44	2.28	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:CA	1:A:26:ILE:HG22	0.44	2.43	15	1
1:A:37:LEU:HB3	1:A:58:PHE:CE2	0.44	2.47	21	1
1:A:27:ASP:C	1:A:28:PHE:CG	0.44	2.95	11	1
1:A:65:PHE:CE1	1:A:71:PHE:CD1	0.44	3.06	12	1
1:A:37:LEU:CD1	1:A:58:PHE:CG	0.44	3.00	13	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:94:LEU:HB3	1:A:109:GLN:CD	0.44	2.38	15	1
1:A:90:GLU:CD	1:A:95:VAL:HG21	0.44	2.37	24	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	3
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:18:GLU:CD	1:A:19:GLY:N	0.43	2.76	14	1
1:A:116:LEU:HD23	1:A:116:LEU:C	0.43	2.38	16	1
1:A:36:ARG:C	1:A:37:LEU:CD1	0.43	2.79	17	1
1:A:116:LEU:O	1:A:117:TYR:C	0.43	2.60	23	1
1:A:31:ARG:HG2	1:A:32:LYS:N	0.43	2.27	4	2
1:A:34:ALA:HA	1:A:58:PHE:CE2	0.43	2.48	12	4
1:A:11:MET:C	1:A:13:SER:N	0.43	2.75	5	2
1:A:109:GLN:O	1:A:110:TRP:CE3	0.43	2.71	8	3
1:A:22:LYS:CE	1:A:22:LYS:HA	0.43	2.43	15	1
1:A:41:LYS:HE2	1:A:118:LEU:HD12	0.43	1.90	15	1
1:A:19:GLY:O	1:A:23:ALA:N	0.43	2.52	21	1
1:A:41:LYS:HE3	1:A:131:PHE:CZ	0.43	2.48	21	1
1:A:21:MET:HG3	1:A:26:ILE:CG2	0.43	2.43	7	1
1:A:75:THR:CG2	1:A:82:ASN:CG	0.43	2.91	14	1
1:A:126:VAL:HG12	1:A:126:VAL:O	0.43	2.13	14	1
1:A:125:GLN:C	1:A:126:VAL:HG23	0.43	2.39	19	1
1:A:24:LEU:HD13	1:A:79:ASP:OD2	0.43	2.13	22	1
1:A:17:PHE:CD2	1:A:35:VAL:HA	0.43	2.48	6	1
1:A:57:THR:O	1:A:57:THR:HG23	0.43	2.14	6	2
1:A:50:PHE:CE1	1:A:63:LEU:HD23	0.43	2.48	10	1
1:A:109:GLN:HB3	1:A:116:LEU:CD2	0.43	2.44	13	1
1:A:35:VAL:O	1:A:58:PHE:CE1	0.43	2.71	16	1
1:A:73:GLU:HB3	1:A:82:ASN:HA	0.43	1.91	18	1
1:A:33:ILE:HG22	1:A:34:ALA:N	0.43	2.28	20	1
1:A:15:GLU:HG3	1:A:16:ASN:N	0.43	2.27	24	2
1:A:39:GLN:CG	1:A:56:SER:HA	0.43	2.44	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLY:HA2	1:A:22:LYS:CB	0.43	2.43	1	2
1:A:98:GLN:CG	1:A:105:ARG:C	0.43	2.91	2	1
1:A:17:PHE:C	1:A:17:PHE:CD1	0.43	2.96	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:65:PHE:CE1	1:A:87:VAL:HG11	0.43	2.49	13	1
1:A:108:LYS:HG3	1:A:110:TRP:CZ3	0.43	2.49	17	1
1:A:8:THR:HG23	1:A:42:ILE:HG13	0.43	1.89	19	1
1:A:9:TRP:HB2	1:A:131:PHE:CE1	0.43	2.48	23	1
1:A:115:LYS:CG	1:A:117:TYR:CD1	0.43	3.02	23	1
1:A:56:SER:HB3	1:A:58:PHE:CD1	0.43	2.48	13	2
1:A:90:GLU:HG3	1:A:95:VAL:CG2	0.43	2.44	14	2
1:A:36:ARG:HG3	1:A:39:GLN:CB	0.43	2.43	8	1
1:A:132:LYS:HD2	1:A:132:LYS:C	0.43	2.38	8	1
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:81:ARG:NE	1:A:81:ARG:HA	0.43	2.26	16	1
1:A:93:THR:OG1	1:A:109:GLN:O	0.43	2.37	8	1
1:A:103:GLU:CD	1:A:103:GLU:C	0.43	2.86	13	1
1:A:108:LYS:C	1:A:109:GLN:CD	0.43	2.86	15	1
1:A:70:GLU:O	1:A:72:ASP:N	0.43	2.52	16	2
1:A:8:THR:HG21	1:A:40:THR:CG2	0.43	2.44	19	1
1:A:18:GLU:CD	1:A:18:GLU:C	0.43	2.86	19	1
1:A:41:LYS:HD2	1:A:131:PHE:CE1	0.43	2.49	23	1
1:A:85:THR:O	1:A:85:THR:HG22	0.43	2.13	8	2
1:A:9:TRP:HB2	1:A:131:PHE:CE2	0.43	2.49	10	2
1:A:45:GLN:CD	1:A:50:PHE:CD2	0.43	2.97	10	1
1:A:75:THR:CB	1:A:82:ASN:ND2	0.43	2.81	14	1
1:A:28:PHE:O	1:A:29:ALA:HB2	0.43	2.14	18	1
1:A:5:GLN:CD	1:A:9:TRP:CH2	0.43	2.97	19	1
1:A:36:ARG:HG3	1:A:37:LEU:C	0.43	2.39	22	1
1:A:30:THR:HG22	1:A:31:ARG:N	0.42	2.28	7	1
1:A:102:LYS:HD3	1:A:102:LYS:C	0.42	2.39	13	1
1:A:35:VAL:C	1:A:37:LEU:N	0.42	2.74	16	1
1:A:126:VAL:O	1:A:126:VAL:HG12	0.42	2.14	16	1
1:A:15:GLU:O	1:A:17:PHE:N	0.42	2.52	3	2
1:A:79:ASP:CG	1:A:80:GLY:N	0.42	2.77	21	2
1:A:108:LYS:HD3	1:A:110:TRP:CZ3	0.42	2.49	6	1
1:A:6:ASN:OD1	1:A:6:ASN:N	0.42	2.52	21	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HG	1:A:58:PHE:CD2	0.42	2.50	4	3
1:A:24:LEU:C	1:A:25:ASP:CG	0.42	2.87	23	2
1:A:25:ASP:O	1:A:26:ILE:C	0.42	2.61	18	1
1:A:105:ARG:HB3	1:A:105:ARG:CZ	0.42	2.43	22	1
1:A:113:GLY:O	1:A:115:LYS:NZ	0.42	2.51	23	1
1:A:24:LEU:HD11	1:A:81:ARG:NH1	0.42	2.28	7	1
1:A:84:LYS:HE2	1:A:84:LYS:CA	0.42	2.44	10	1
1:A:109:GLN:HG3	1:A:118:LEU:CD2	0.42	2.44	20	1
1:A:3:LYS:HE2	1:A:89:TRP:CE3	0.42	2.50	21	1
1:A:9:TRP:CE2	1:A:116:LEU:HD21	0.42	2.50	23	1
1:A:100:GLY:O	1:A:102:LYS:N	0.42	2.52	23	2
1:A:130:VAL:HG23	1:A:131:PHE:H	0.42	1.73	23	1
1:A:11:MET:O	1:A:13:SER:N	0.42	2.53	13	1
1:A:97:VAL:O	1:A:99:LYS:N	0.42	2.52	22	2
1:A:11:MET:CE	1:A:14:ASN:ND2	0.42	2.82	18	1
1:A:111:VAL:HG22	1:A:116:LEU:HD12	0.42	1.91	19	1
1:A:75:THR:OG1	1:A:81:ARG:N	0.42	2.51	4	1
1:A:3:LYS:HG2	1:A:89:TRP:CZ2	0.42	2.49	8	1
1:A:120:LEU:HD12	1:A:120:LEU:C	0.42	2.40	9	2
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:37:LEU:HD21	1:A:58:PHE:CD2	0.42	2.50	13	1
1:A:52:THR:HB	1:A:63:LEU:HB3	0.42	1.92	19	4
1:A:30:THR:C	1:A:32:LYS:N	0.42	2.76	18	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:38:THR:HA	1:A:56:SER:CB	0.42	2.45	20	1
1:A:24:LEU:HD13	1:A:79:ASP:CA	0.42	2.45	3	1
1:A:104:ASN:O	1:A:122:CYS:N	0.42	2.53	24	2
1:A:73:GLU:CD	1:A:82:ASN:HB3	0.42	2.39	5	1
1:A:26:ILE:CG2	1:A:27:ASP:N	0.42	2.82	11	1
1:A:45:GLN:HG2	1:A:50:PHE:CD1	0.42	2.50	22	1
1:A:18:GLU:CG	1:A:31:ARG:HB2	0.42	2.44	23	1
1:A:85:THR:OG1	1:A:98:GLN:NE2	0.42	2.52	21	2
1:A:11:MET:HE3	1:A:39:GLN:CG	0.42	2.45	3	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:120:LEU:O	1:A:127:CYS:N	0.42	2.53	13	1
1:A:95:VAL:O	1:A:95:VAL:HG12	0.42	2.13	15	1
1:A:31:ARG:CG	1:A:32:LYS:N	0.42	2.83	20	1
1:A:101:GLU:HG2	1:A:102:LYS:N	0.42	2.30	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:HB3	1:A:26:ILE:HG22	0.42	1.90	22	1
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:43:ILE:HD13	1:A:43:ILE:C	0.42	2.38	8	1
1:A:3:LYS:HB3	1:A:89:TRP:CH2	0.42	2.49	10	1
1:A:102:LYS:HD3	1:A:103:GLU:HG2	0.42	1.91	15	1
1:A:81:ARG:C	1:A:82:ASN:CG	0.42	2.88	18	2
1:A:84:LYS:CB	1:A:99:LYS:HB2	0.42	2.45	7	1
1:A:107:TRP:C	1:A:108:LYS:HD2	0.42	2.40	17	2
1:A:83:VAL:HG11	1:A:98:GLN:HG2	0.42	1.92	11	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:88:THR:HG23	1:A:88:THR:O	0.42	2.14	17	1
1:A:104:ASN:O	1:A:121:THR:HB	0.42	2.14	24	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:60:ASN:ND2	1:A:60:ASN:N	0.41	2.67	17	1
1:A:40:THR:O	1:A:40:THR:HG22	0.41	2.15	19	1
1:A:74:HIS:C	1:A:75:THR:HG22	0.41	2.40	20	1
1:A:129:GLN:O	1:A:130:VAL:CG1	0.41	2.68	23	1
1:A:119:GLU:OE1	1:A:120:LEU:N	0.41	2.53	2	1
1:A:18:GLU:O	1:A:22:LYS:N	0.41	2.53	21	3
1:A:71:PHE:O	1:A:85:THR:N	0.41	2.53	20	3
1:A:109:GLN:HB2	1:A:116:LEU:CD1	0.41	2.44	12	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:37:LEU:O	1:A:57:THR:N	0.41	2.53	20	1
1:A:37:LEU:HB3	1:A:58:PHE:CZ	0.41	2.50	21	1
1:A:85:THR:HG23	1:A:98:GLN:OE1	0.41	2.16	21	1
1:A:50:PHE:O	1:A:50:PHE:CG	0.41	2.72	24	1
1:A:107:TRP:CD2	1:A:107:TRP:O	0.41	2.73	24	1
1:A:12:GLU:HG3	1:A:132:LYS:HG2	0.41	1.91	9	1
1:A:74:HIS:CE1	1:A:76:LYS:HE2	0.41	2.50	16	1
1:A:64:ASP:N	1:A:64:ASP:OD1	0.41	2.53	22	1
1:A:123:GLY:C	1:A:124:ASP:CG	0.41	2.89	6	1
1:A:83:VAL:HG11	1:A:98:GLN:CG	0.41	2.45	11	1
1:A:16:ASN:OD1	1:A:16:ASN:N	0.41	2.54	12	2
1:A:63:LEU:C	1:A:63:LEU:HD23	0.41	2.40	13	1
1:A:125:GLN:CD	1:A:125:GLN:N	0.41	2.78	14	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:GLU:CG	1:A:117:TYR:CE2	0.41	3.04	23	1
1:A:59:ARG:HG3	1:A:60:ASN:N	0.41	2.30	24	1
1:A:7:GLY:O	1:A:8:THR:HG23	0.41	2.15	1	1
1:A:101:GLU:CD	1:A:101:GLU:C	0.41	2.88	6	1
1:A:112:GLU:HB2	1:A:117:TYR:CE1	0.41	2.50	6	1
1:A:32:LYS:O	1:A:33:ILE:HG23	0.41	2.15	11	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:116:LEU:HD12	1:A:131:PHE:CD2	0.41	2.51	23	1
1:A:112:GLU:HB2	1:A:117:TYR:CD2	0.41	2.49	1	1
1:A:65:PHE:CD1	1:A:87:VAL:CG2	0.41	2.90	5	1
1:A:73:GLU:HB3	1:A:82:ASN:CG	0.41	2.40	7	1
1:A:87:VAL:HG12	1:A:94:LEU:HD11	0.41	1.92	16	1
1:A:11:MET:HG3	1:A:130:VAL:HG21	0.41	1.92	23	1
1:A:50:PHE:HE2	1:A:94:LEU:HD22	0.41	1.75	24	1
1:A:54:THR:HG22	1:A:55:ASN:N	0.41	2.31	24	1
1:A:72:ASP:OD1	1:A:72:ASP:N	0.41	2.54	15	2
1:A:56:SER:HB2	1:A:58:PHE:CD1	0.41	2.50	6	1
1:A:121:THR:HG23	1:A:126:VAL:HG22	0.41	1.91	11	1
1:A:56:SER:O	1:A:60:ASN:ND2	0.41	2.54	12	1
1:A:42:ILE:CD1	1:A:53:LYS:HD2	0.41	2.45	14	1
1:A:116:LEU:O	1:A:131:PHE:CG	0.41	2.73	16	1
1:A:33:ILE:O	1:A:37:LEU:HD22	0.41	2.15	6	1
1:A:116:LEU:O	1:A:131:PHE:CD1	0.41	2.74	10	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:26:ILE:HG23	1:A:27:ASP:N	0.41	2.31	1	1
1:A:81:ARG:C	1:A:82:ASN:ND2	0.41	2.79	1	1
1:A:20:TYR:CE1	1:A:24:LEU:HD21	0.41	2.51	2	1
1:A:39:GLN:NE2	1:A:54:THR:OG1	0.41	2.54	6	1
1:A:81:ARG:HG3	1:A:82:ASN:N	0.41	2.30	9	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:8:THR:O	1:A:134:LYS:N	0.41	2.54	15	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:33:ILE:HD13	1:A:33:ILE:HA	0.41	1.55	18	1
1:A:36:ARG:O	1:A:37:LEU:CG	0.41	2.68	18	1
1:A:18:GLU:HG3	1:A:19:GLY:N	0.41	2.30	19	1
1:A:14:ASN:HB2	1:A:130:VAL:CG1	0.41	2.42	23	1
1:A:73:GLU:HG2	1:A:82:ASN:CG	0.41	2.41	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TRP:NE1	1:A:41:LYS:HZ3	0.41	2.14	7	1
1:A:50:PHE:CE2	1:A:94:LEU:CD2	0.41	3.04	13	1
1:A:32:LYS:HG2	1:A:33:ILE:N	0.41	2.31	18	1
1:A:91:GLY:C	1:A:92:ASN:ND2	0.41	2.79	19	1
1:A:36:ARG:O	1:A:37:LEU:HB3	0.41	2.16	20	1
1:A:63:LEU:CD2	1:A:107:TRP:CZ2	0.40	2.95	3	1
1:A:52:THR:N	1:A:63:LEU:O	0.40	2.54	4	1
1:A:114:ASP:N	1:A:114:ASP:OD1	0.40	2.54	14	1
1:A:30:THR:O	1:A:33:ILE:N	0.40	2.54	18	1
1:A:56:SER:OG	1:A:59:ARG:N	0.40	2.54	19	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:50:PHE:CD1	1:A:94:LEU:HD22	0.40	2.52	3	1
1:A:11:MET:O	1:A:12:GLU:CB	0.40	2.69	20	2
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:11:MET:HE3	1:A:11:MET:HB2	0.40	1.87	19	1
1:A:65:PHE:CE2	1:A:66:THR:C	0.40	2.99	21	1
1:A:38:THR:O	1:A:38:THR:HG22	0.40	2.17	23	1
1:A:83:VAL:HG13	1:A:100:GLY:HA3	0.40	1.92	23	1
1:A:71:PHE:N	1:A:85:THR:O	0.40	2.54	2	1
1:A:34:ALA:C	1:A:36:ARG:N	0.40	2.79	6	1
1:A:45:GLN:HG3	1:A:50:PHE:CG	0.40	2.51	6	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:83:VAL:HG13	1:A:100:GLY:O	0.40	2.17	17	1
1:A:43:ILE:CD1	1:A:45:GLN:HB2	0.40	2.46	18	1
1:A:66:THR:HG22	1:A:69:VAL:CG2	0.40	2.45	22	1
1:A:107:TRP:CD1	1:A:107:TRP:O	0.40	2.75	22	1
1:A:73:GLU:HG3	1:A:82:ASN:CA	0.40	2.47	23	1
1:A:88:THR:N	1:A:95:VAL:O	0.40	2.54	23	1
1:A:116:LEU:CD1	1:A:131:PHE:CD2	0.40	3.04	23	1
1:A:132:LYS:O	1:A:134:LYS:N	0.40	2.54	23	1
1:A:83:VAL:O	1:A:85:THR:N	0.40	2.54	3	1
1:A:26:ILE:HD11	1:A:79:ASP:N	0.40	2.31	12	1
1:A:47:GLY:C	1:A:48:ASP:CG	0.40	2.87	14	1
1:A:118:LEU:CD1	1:A:118:LEU:C	0.40	2.94	14	1
1:A:64:ASP:OD1	1:A:64:ASP:N	0.40	2.53	18	1
1:A:15:GLU:CD	1:A:129:GLN:CG	0.40	2.95	21	1
1:A:111:VAL:O	1:A:111:VAL:HG12	0.40	2.15	22	1
1:A:71:PHE:CE2	1:A:74:HIS:CD2	0.40	3.10	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LYS:O	1:A:132:LYS:CG	0.40	2.70	9	1
1:A:110:TRP:CD1	1:A:117:TYR:HB3	0.40	2.51	12	1
1:A:73:GLU:HB3	1:A:83:VAL:HA	0.40	1.93	14	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	131/134 (98%)	78±4 (60±3%)	33±3 (25±3%)	20±3 (15±3%)	0	4
All	All	3144/3216 (98%)	1872 (60%)	788 (25%)	484 (15%)	0	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	126	VAL	15
1	A	25	ASP	15
1	A	12	GLU	14
1	A	72	ASP	13
1	A	76	LYS	13
1	A	45	GLN	12
1	A	93	THR	12
1	A	106	GLY	12
1	A	38	THR	12
1	A	11	MET	12
1	A	82	ASN	11
1	A	6	ASN	10
1	A	110	TRP	10
1	A	124	ASP	10
1	A	62	ASP	9
1	A	33	ILE	9
1	A	101	GLU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	79	ASP	9
1	A	27	ASP	8
1	A	39	GLN	8
1	A	56	SER	8
1	A	71	PHE	8
1	A	16	ASN	8
1	A	29	ALA	8
1	A	133	LYS	7
1	A	102	LYS	7
1	A	113	GLY	7
1	A	91	GLY	7
1	A	40	THR	7
1	A	74	HIS	7
1	A	31	ARG	7
1	A	28	PHE	6
1	A	35	VAL	6
1	A	73	GLU	6
1	A	3	LYS	5
1	A	30	THR	5
1	A	47	GLY	5
1	A	70	GLU	5
1	A	78	LEU	5
1	A	92	ASN	5
1	A	81	ARG	4
1	A	57	THR	4
1	A	32	LYS	4
1	A	75	THR	4
1	A	8	THR	4
1	A	49	ASN	4
1	A	115	LYS	4
1	A	37	LEU	4
1	A	122	CYS	3
1	A	84	LYS	3
1	A	98	GLN	3
1	A	100	GLY	3
1	A	44	VAL	3
1	A	108	LYS	3
1	A	15	GLU	3
1	A	95	VAL	3
1	A	4	ASP	2
1	A	83	VAL	2
1	A	13	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	94	LEU	2
1	A	64	ASP	2
1	A	125	GLN	2
1	A	34	ALA	2
1	A	67	VAL	2
1	A	9	TRP	2
1	A	59	ARG	2
1	A	68	GLY	2
1	A	131	PHE	2
1	A	80	GLY	1
1	A	10	GLU	1
1	A	99	LYS	1
1	A	107	TRP	1
1	A	5	GLN	1
1	A	129	GLN	1
1	A	58	PHE	1
1	A	132	LYS	1
1	A	117	TYR	1
1	A	14	ASN	1
1	A	123	GLY	1
1	A	130	VAL	1
1	A	54	THR	1
1	A	55	ASN	1
1	A	103	GLU	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±5 (62±4%)	45±5 (38±4%)	0 6
All	All	2832/2880 (98%)	1743 (62%)	1089 (38%)	0 6

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

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Mol	Chain	Res	Type	Models (Total)
1	A	52	THR	24
1	A	120	LEU	24
1	A	66	THR	22
1	A	53	LYS	20
1	A	102	LYS	20
1	A	107	TRP	20
1	A	31	ARG	19
1	A	132	LYS	19
1	A	76	LYS	18
1	A	33	ILE	18
1	A	37	LEU	17
1	A	84	LYS	17
1	A	122	CYS	17
1	A	32	LYS	16
1	A	96	CYS	16
1	A	109	GLN	16
1	A	118	LEU	16
1	A	30	THR	15
1	A	108	LYS	15
1	A	116	LEU	15
1	A	24	LEU	15
1	A	36	ARG	14
1	A	115	LYS	14
1	A	60	ASN	13
1	A	69	VAL	13
1	A	75	THR	13
1	A	90	GLU	13
1	A	8	THR	13
1	A	13	SER	13
1	A	41	LYS	13
1	A	128	ARG	13
1	A	43	ILE	13
1	A	54	THR	12
1	A	59	ARG	12
1	A	82	ASN	12
1	A	18	GLU	12
1	A	94	LEU	12
1	A	3	LYS	11
1	A	99	LYS	11
1	A	57	THR	11
1	A	62	ASP	11
1	A	65	PHE	11

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Mol	Chain	Res	Type	Models (Total)
1	A	45	GLN	11
1	A	48	ASP	11
1	A	92	ASN	11
1	A	97	VAL	11
1	A	74	HIS	10
1	A	98	GLN	10
1	A	39	GLN	10
1	A	25	ASP	10
1	A	103	GLU	10
1	A	21	MET	9
1	A	101	GLU	9
1	A	93	THR	9
1	A	6	ASN	8
1	A	12	GLU	8
1	A	56	SER	8
1	A	134	LYS	8
1	A	20	TYR	8
1	A	27	ASP	8
1	A	83	VAL	8
1	A	130	VAL	8
1	A	14	ASN	7
1	A	44	VAL	7
1	A	51	LYS	7
1	A	58	PHE	7
1	A	105	ARG	7
1	A	22	LYS	7
1	A	49	ASN	7
1	A	73	GLU	7
1	A	110	TRP	7
1	A	81	ARG	7
1	A	88	THR	7
1	A	17	PHE	7
1	A	86	LEU	6
1	A	38	THR	6
1	A	87	VAL	6
1	A	11	MET	6
1	A	28	PHE	6
1	A	61	TYR	6
1	A	26	ILE	6
1	A	85	THR	6
1	A	4	ASP	6
1	A	55	ASN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	125	GLN	5
1	A	112	GLU	5
1	A	117	TYR	5
1	A	5	GLN	5
1	A	71	PHE	5
1	A	79	ASP	5
1	A	15	GLU	5
1	A	133	LYS	5
1	A	10	GLU	5
1	A	70	GLU	5
1	A	63	LEU	4
1	A	67	VAL	4
1	A	119	GLU	4
1	A	127	CYS	4
1	A	72	ASP	4
1	A	121	THR	4
1	A	16	ASN	4
1	A	124	ASP	3
1	A	46	ASP	3
1	A	78	LEU	3
1	A	35	VAL	2
1	A	104	ASN	2
1	A	126	VAL	2
1	A	64	ASP	2
1	A	40	THR	2
1	A	42	ILE	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 oligosaccharides 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