



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 PM UTC

PDB ID : 1EI1 / pdb_00001ei1
Title : NMR STRUCTURE OF HOLO CELLULAR RETINOL-BINDING PROTEIN II
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Deposited on : 2000-02-25

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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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

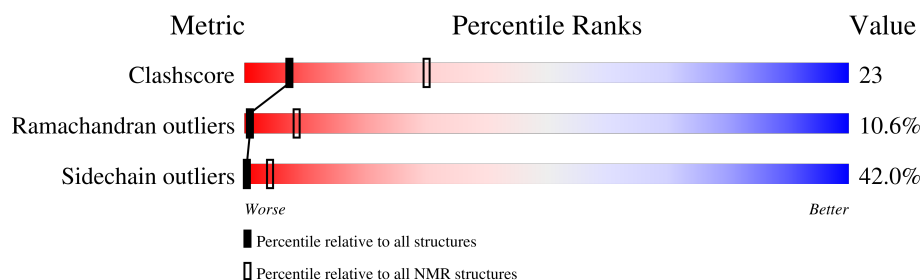
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

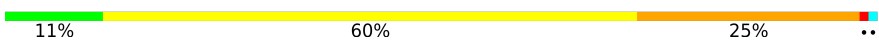
The overall completeness of chemical shifts assignment was not calculated.

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 25 models. Model 2 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)	0.85	2

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 5, 6, 7, 8, 9, 10, 14, 16, 18, 21, 23
2	1, 4, 11, 12, 13, 15, 17, 19, 20, 22, 24
Single-model clusters	25

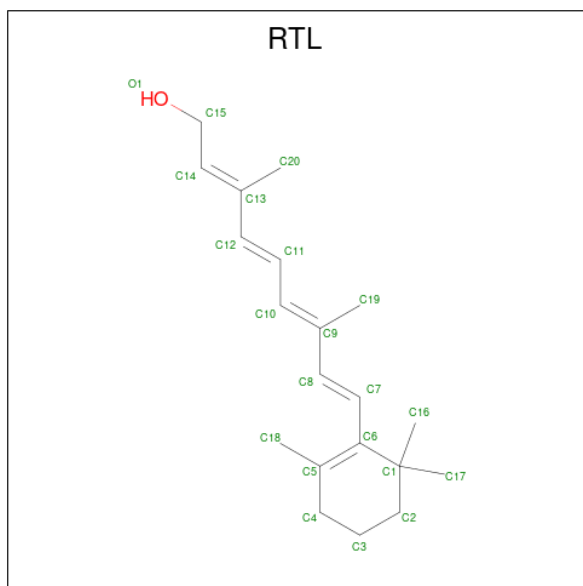
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2219 atoms, of which 1103 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	

- Molecule 2 is RETINOL (CCD ID: RTL) (formula: $C_{20}H_{30}O$).



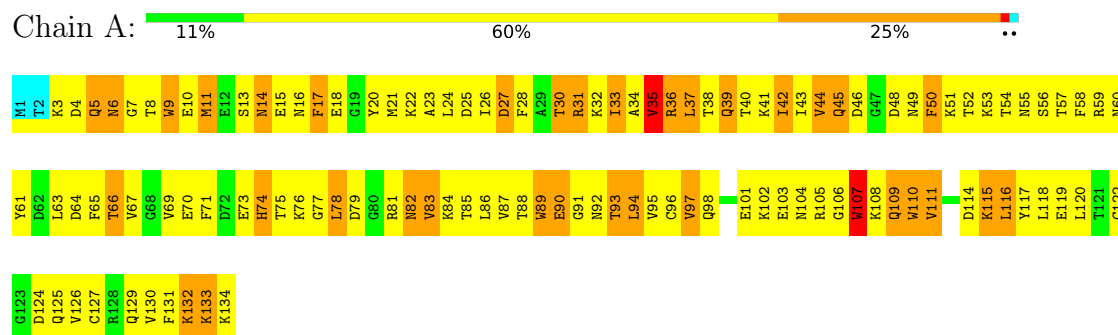
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			51	20	30	1

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

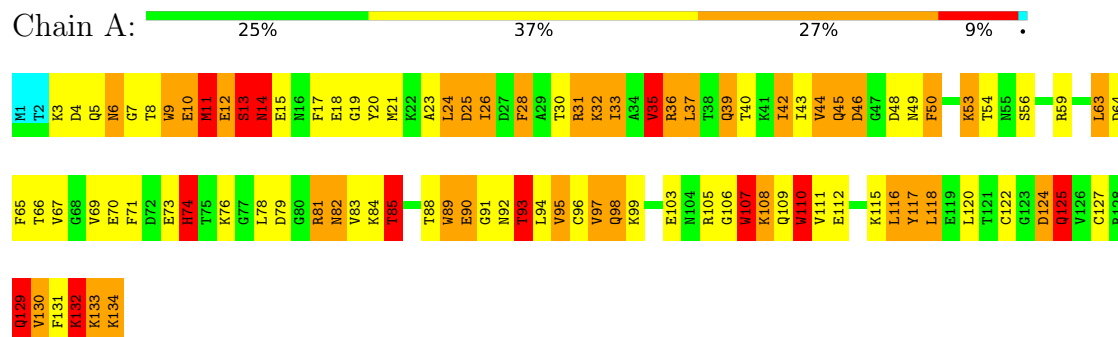


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

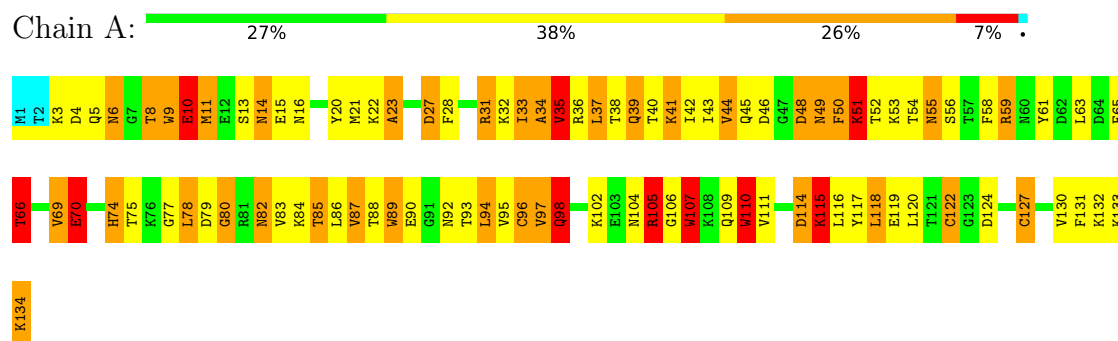
4.2.1 Score per residue for model 1

• Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



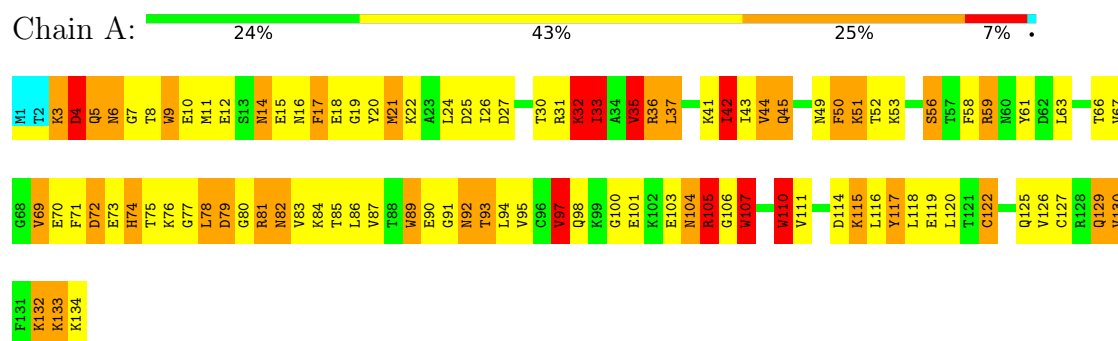
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



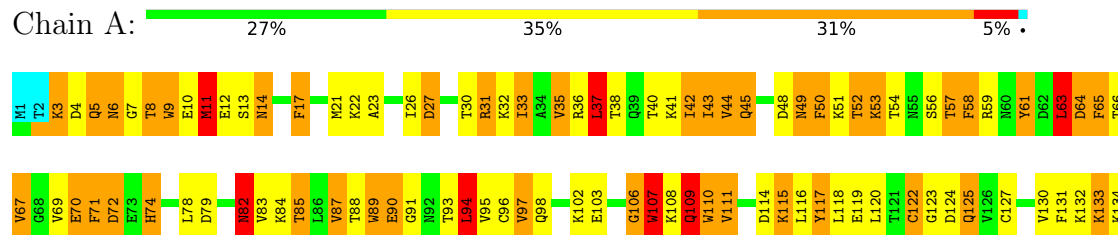
4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



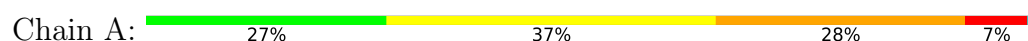
4.2.4 Score per residue for model 4

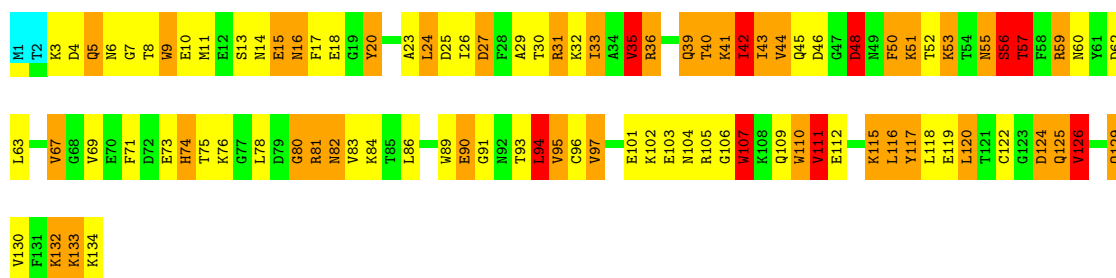
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.5 Score per residue for model 5

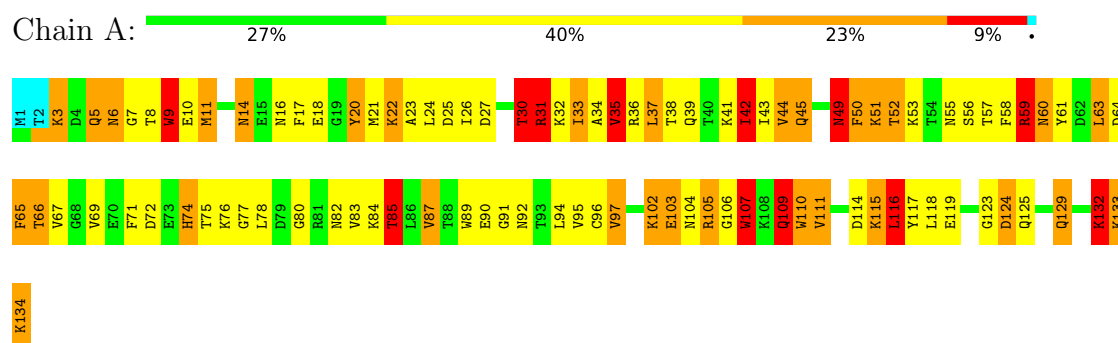
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II





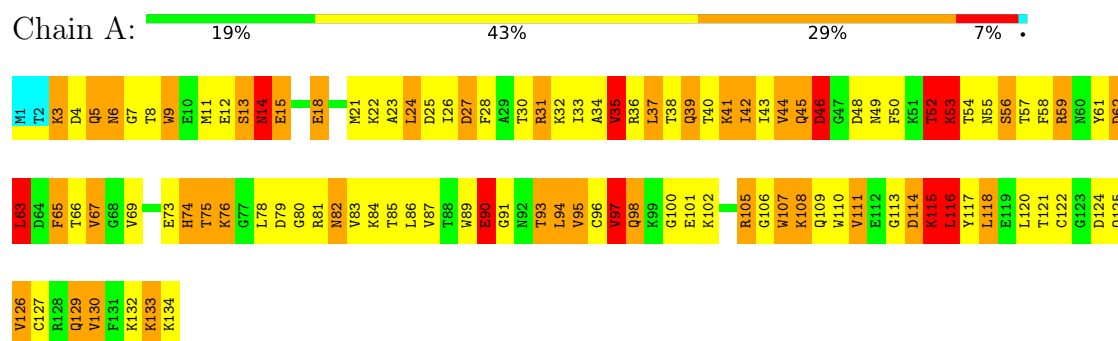
4.2.6 Score per residue for model 6

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



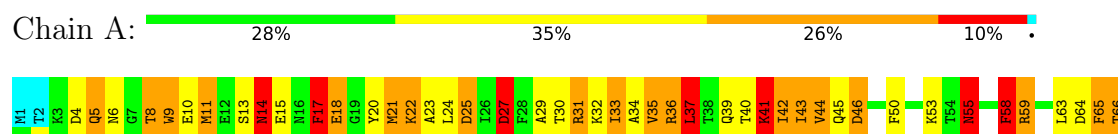
4.2.7 Score per residue for model 7

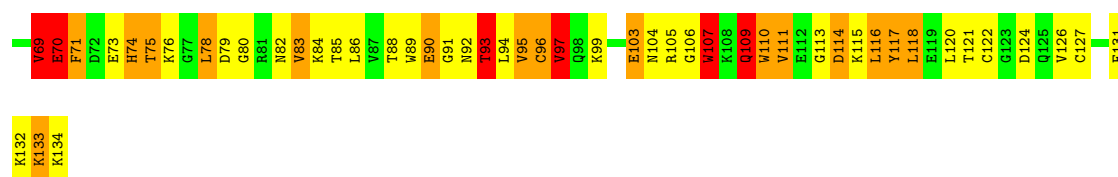
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.8 Score per residue for model 8

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

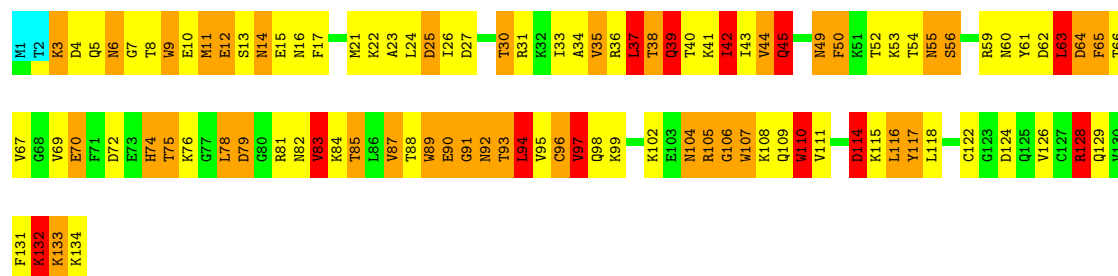




4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

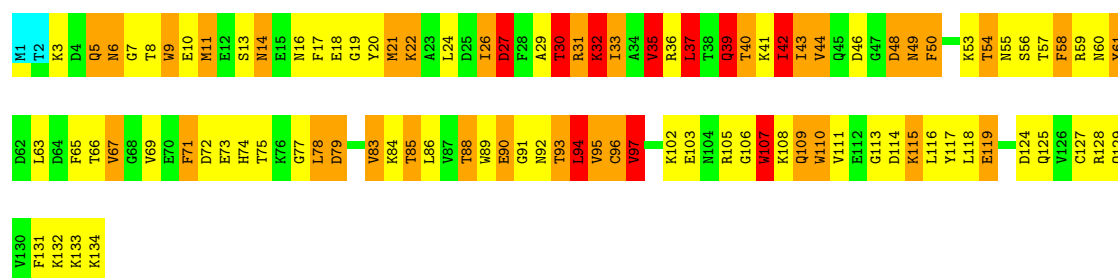
Chain A: 22% 40% 28% 9% .



4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

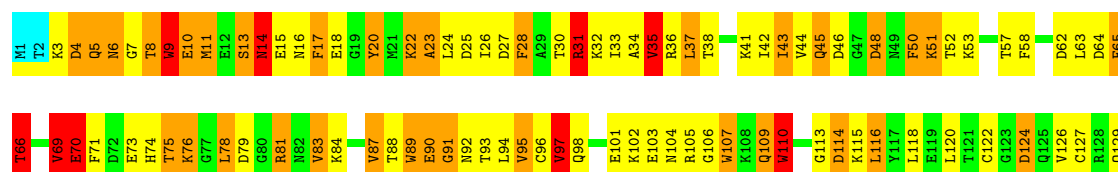
Chain A: 25% 41% 25% 7% .



4.2.11 Score per residue for model 11

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 25% 40% 26% 7% .

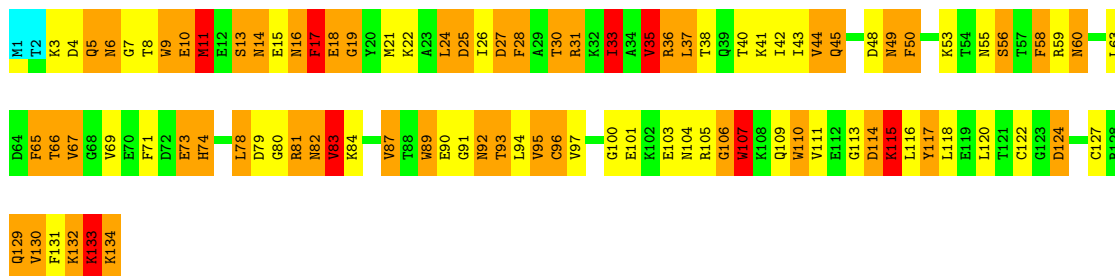


V130
F131
K132
K133
K134

4.2.12 Score per residue for model 12

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

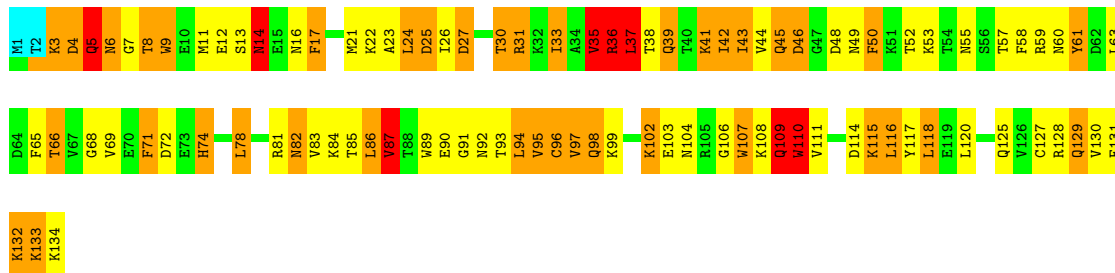
Chain A: 27% 31% 35% 6%



4.2.13 Score per residue for model 13

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

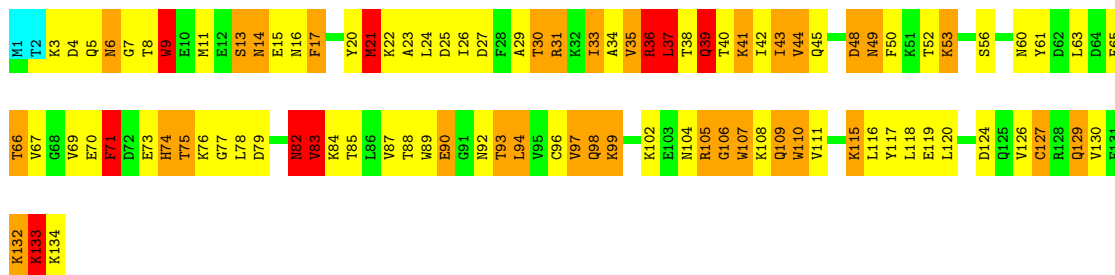
Chain A: 27% 37% 29% 6%



4.2.14 Score per residue for model 14

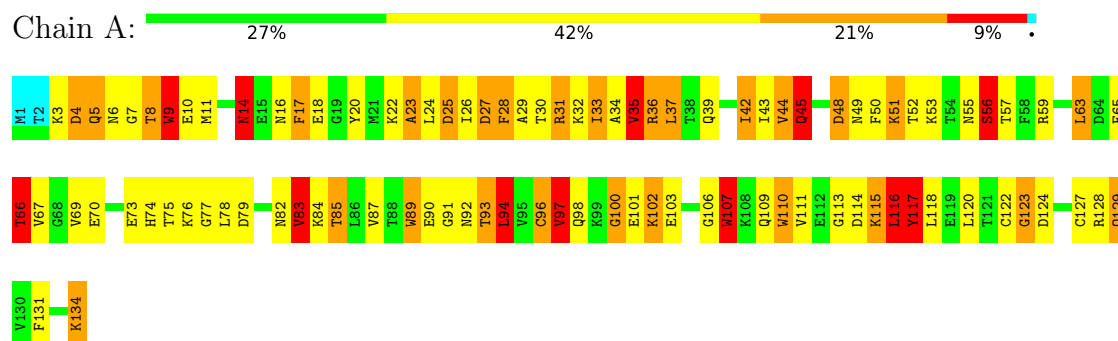
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 26% 42% 24% 7%



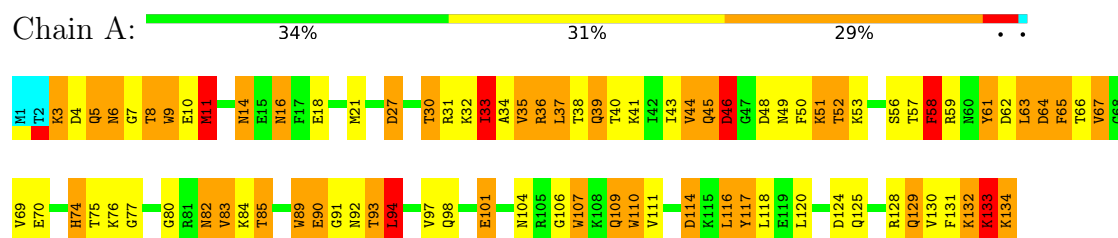
4.2.15 Score per residue for model 15

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



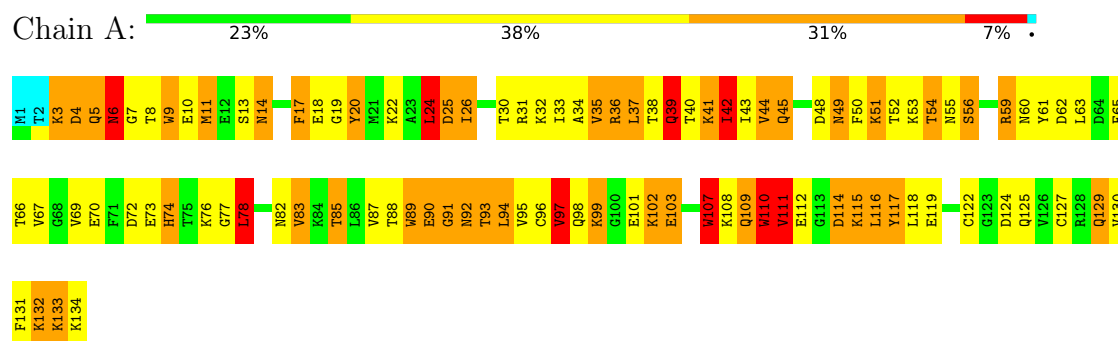
4.2.16 Score per residue for model 16

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



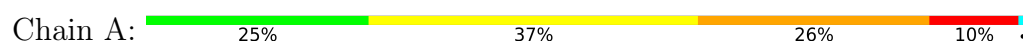
4.2.17 Score per residue for model 17

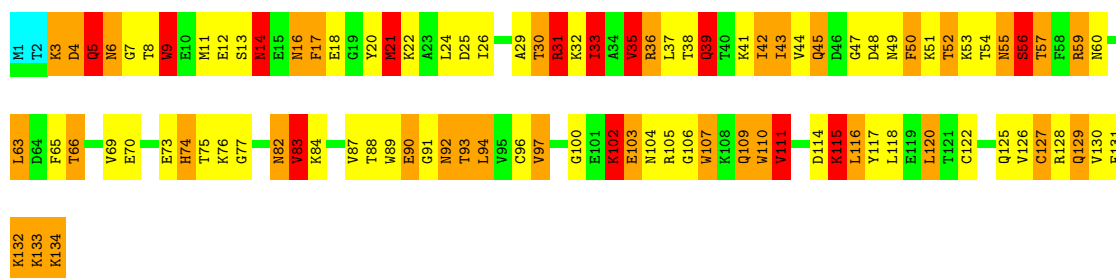
- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II



4.2.18 Score per residue for model 18

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

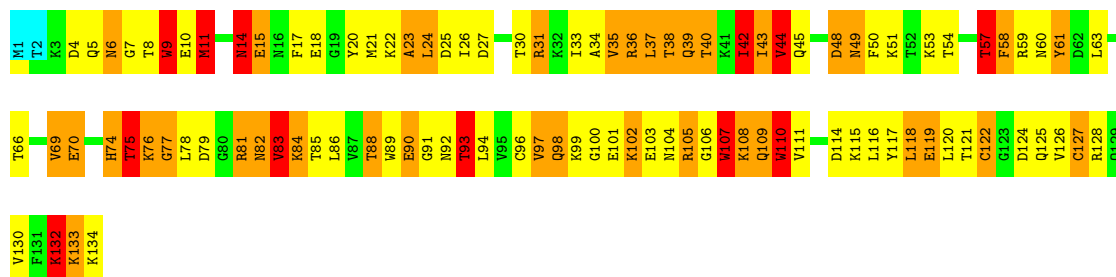




4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

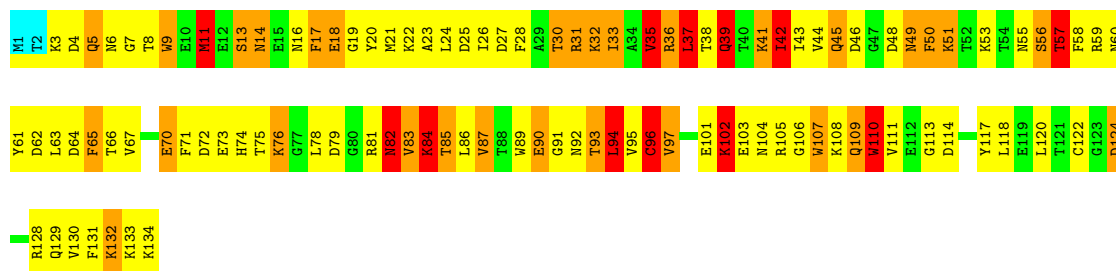
Chain A: 22% 40% 28% 9%



4.2.20 Score per residue for model 20

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

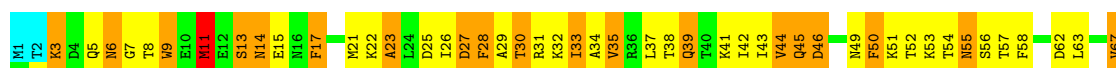
Chain A: 19% 48% 22% 9%

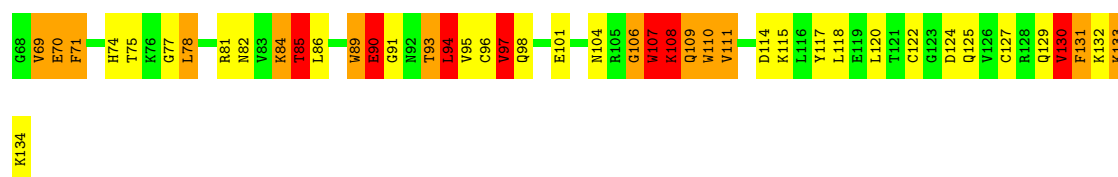


4.2.21 Score per residue for model 21

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 31% 38% 24% 6%

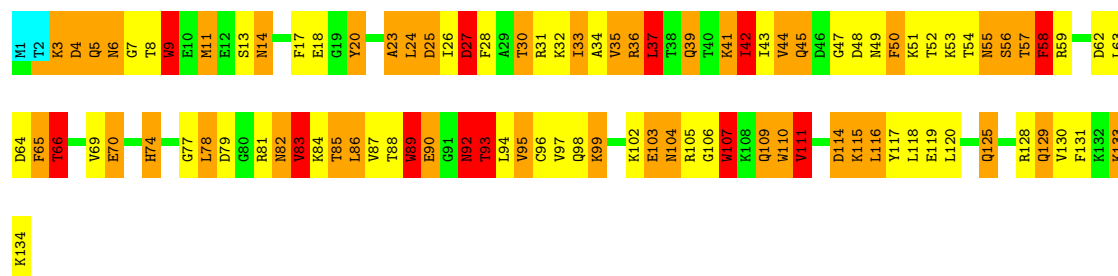




4.2.22 Score per residue for model 22

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

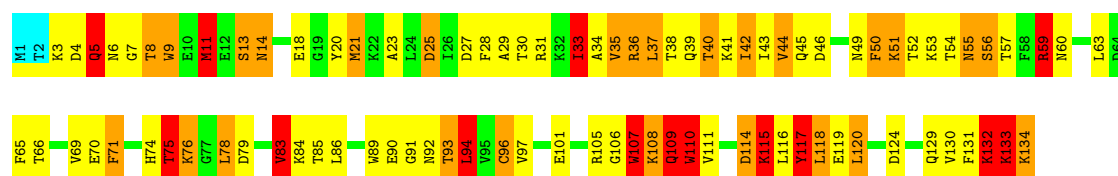
Chain A: 25% 33% 31% 9%



4.2.23 Score per residue for model 23

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 31% 37% 19% 10%



4.2.24 Score per residue for model 24

- Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

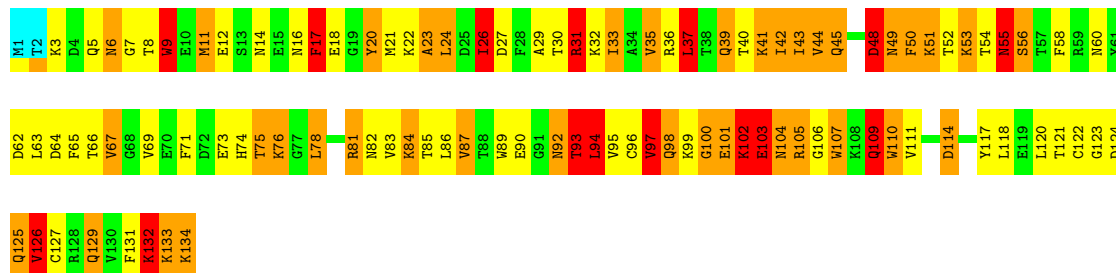
Chain A: 20% 44% 25% 10%



4.2.25 Score per residue for model 25

● Molecule 1: CELLULAR RETINOL-BINDING PROTEIN II

Chain A: 22% 37% 28% 11% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry & simulated annealing*.

Of the 30 calculated structures, 25 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	structure solution	3.3
Tinker	refinement	3.3

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: RTL

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	1.26±0.02	2±1/1098 (0.2± 0.1%)	2.42±0.05	66±7/1474 (4.5± 0.5%)
All	All	1.26	56/27450 (0.2%)	2.42	1649/36850 (4.5%)

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	-6.27	1.32	1.43	7	22
1	A	89	TRP	CG-CD2	-6.27	1.32	1.43	8	24
1	A	107	TRP	CG-CD2	-5.85	1.33	1.43	10	10

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	106	GLY	O-C-N	14.34	133.96	123.35	9	23
1	A	7	GLY	O-C-N	13.03	135.63	123.65	1	23
1	A	90	GLU	CA-C-O	12.31	132.32	119.51	25	24
1	A	132	LYS	O-C-N	11.65	134.21	123.26	25	15
1	A	30	THR	O-C-N	11.09	133.95	122.08	13	19
1	A	5	GLN	O-C-N	10.44	133.30	122.03	21	17
1	A	89	TRP	CG-CD1-NE1	-10.31	96.80	110.20	12	25
1	A	14	ASN	CA-CB-CG	-10.06	102.54	112.60	15	21
1	A	20	TYR	CA-C-O	9.53	130.51	120.70	19	4
1	A	124	ASP	O-C-N	9.45	132.14	122.12	19	16
1	A	69	VAL	O-C-N	9.39	134.16	122.32	1	20
1	A	114	ASP	O-C-N	9.31	134.88	122.41	11	17
1	A	37	LEU	O-C-N	9.29	133.82	122.86	14	18
1	A	83	VAL	O-C-N	9.24	133.21	122.95	16	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	GLN	O-C-N	9.22	133.56	122.68	18	13
1	A	110	TRP	CD2-CE2-CZ2	-9.21	113.19	122.40	12	16
1	A	21	MET	O-C-N	8.87	132.27	122.15	1	11
1	A	91	GLY	O-C-N	8.78	134.11	122.70	20	17
1	A	110	TRP	CE2-CD2-CE3	8.68	127.48	118.80	12	14
1	A	103	GLU	O-C-N	8.68	134.13	122.59	18	11
1	A	56	SER	O-C-N	8.63	131.35	122.03	23	16
1	A	74	HIS	CA-CB-CG	-8.59	105.21	113.80	6	14
1	A	50	PHE	CA-CB-CG	-8.59	105.21	113.80	6	22
1	A	43	ILE	N-CA-CB	-8.57	102.30	112.07	8	3
1	A	23	ALA	O-C-N	8.44	132.65	122.27	14	15
1	A	14	ASN	O-C-N	8.37	132.79	123.25	12	17
1	A	111	VAL	CA-C-O	8.27	131.12	120.78	8	9
1	A	130	VAL	O-C-N	8.23	130.38	122.97	1	4
1	A	89	TRP	O-C-N	8.04	133.11	122.82	7	14
1	A	111	VAL	N-CA-C	8.00	119.29	109.30	13	10
1	A	25	ASP	CA-C-O	7.95	131.87	120.51	6	13
1	A	126	VAL	N-CA-C	7.94	119.30	107.15	9	9
1	A	132	LYS	CA-C-O	-7.93	112.97	121.14	2	18
1	A	101	GLU	CA-C-O	7.93	127.43	119.97	12	3
1	A	89	TRP	CD1-CG-CD2	7.92	118.97	106.30	11	7
1	A	13	SER	O-C-N	7.92	131.27	123.04	24	6
1	A	105	ARG	O-C-N	7.90	131.01	122.64	8	13
1	A	11	MET	O-C-N	7.86	132.88	122.82	20	17
1	A	4	ASP	CA-CB-CG	-7.86	104.74	112.60	23	10
1	A	17	PHE	CA-C-O	7.86	128.54	119.35	20	9
1	A	59	ARG	O-C-N	7.81	129.44	121.79	7	6
1	A	65	PHE	CA-C-O	7.79	130.12	120.54	12	11
1	A	92	ASN	OD1-CG-ND2	7.78	130.38	122.60	10	7
1	A	11	MET	CA-C-O	-7.72	112.54	120.96	6	7
1	A	63	LEU	O-C-N	7.71	130.82	122.34	4	3
1	A	46	ASP	CA-CB-CG	-7.69	104.91	112.60	1	9
1	A	97	VAL	CA-C-O	7.68	130.38	120.78	1	9
1	A	105	ARG	NE-CZ-NH2	7.65	126.08	119.20	22	3
1	A	45	GLN	N-CA-C	7.65	118.66	107.88	13	13
1	A	77	GLY	O-C-N	7.59	129.54	122.17	17	12
1	A	69	VAL	N-CA-CB	-7.59	105.06	112.65	21	3
1	A	106	GLY	CA-C-O	-7.58	114.62	120.76	9	3
1	A	92	ASN	CA-CB-CG	-7.56	105.04	112.60	13	11
1	A	85	THR	O-C-N	7.47	131.69	123.10	1	5
1	A	7	GLY	CA-C-O	-7.46	114.31	121.62	15	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	THR	O-C-N	7.46	131.70	123.13	19	7
1	A	105	ARG	CA-C-N	-7.42	117.06	122.18	6	9
1	A	105	ARG	C-N-CA	-7.42	117.06	122.18	6	9
1	A	92	ASN	CA-C-O	7.40	127.59	119.15	25	3
1	A	22	LYS	O-C-N	7.40	132.25	122.33	8	12
1	A	107	TRP	O-C-N	7.40	131.85	123.27	1	3
1	A	51	LYS	O-C-N	7.40	131.69	123.33	17	7
1	A	55	ASN	O-C-N	7.40	130.91	122.55	22	10
1	A	18	GLU	O-C-N	7.37	131.33	122.27	23	9
1	A	130	VAL	CB-CA-C	-7.36	101.96	111.53	19	4
1	A	109	GLN	CA-C-O	-7.32	113.95	122.37	20	8
1	A	4	ASP	N-CA-C	-7.30	102.37	110.91	12	3
1	A	45	GLN	O-C-N	7.28	131.47	123.10	7	13
1	A	27	ASP	CA-CB-CG	-7.26	105.34	112.60	10	5
1	A	74	HIS	CB-CG-CD2	-7.21	121.82	131.20	2	10
1	A	128	ARG	NE-CZ-NH2	7.11	125.60	119.20	18	3
1	A	36	ARG	NE-CZ-NH1	7.10	128.60	121.50	16	6
1	A	5	GLN	OE1-CD-NE2	7.09	129.69	122.60	24	5
1	A	133	LYS	N-CA-C	7.09	118.86	108.86	3	9
1	A	9	TRP	CE2-CD2-CG	7.09	115.70	107.20	25	1
1	A	89	TRP	NE1-CE2-CZ2	7.07	140.71	130.10	12	15
1	A	59	ARG	NE-CZ-NH2	7.07	125.56	119.20	7	3
1	A	66	THR	CA-C-N	-7.05	113.66	122.48	22	8
1	A	66	THR	C-N-CA	-7.05	113.66	122.48	22	8
1	A	5	GLN	CA-C-O	-7.05	113.64	120.90	25	8
1	A	49	ASN	O-C-N	7.04	131.95	122.59	6	8
1	A	61	TYR	O-C-N	7.04	131.44	123.42	20	8
1	A	78	LEU	CA-C-O	7.03	127.94	119.78	8	1
1	A	114	ASP	CA-CB-CG	-7.00	105.60	112.60	13	8
1	A	89	TRP	CG-CD2-CE3	-7.00	126.90	133.90	9	11
1	A	50	PHE	N-CA-C	6.93	117.65	107.88	24	6
1	A	83	VAL	N-CA-C	6.92	116.98	108.53	11	7
1	A	89	TRP	CA-C-O	-6.89	114.00	121.44	18	14
1	A	49	ASN	CA-C-O	-6.89	114.08	121.38	24	3
1	A	112	GLU	CA-C-O	6.88	126.97	119.40	5	3
1	A	39	GLN	OE1-CD-NE2	6.86	129.46	122.60	8	5
1	A	5	GLN	N-CA-C	-6.85	102.49	111.74	15	8
1	A	88	THR	N-CA-CB	-6.85	101.93	110.98	22	3
1	A	57	THR	O-C-N	6.83	133.61	122.20	22	5
1	A	36	ARG	NE-CZ-NH2	6.83	125.35	119.20	7	9
1	A	108	LYS	CB-CA-C	-6.79	102.44	111.74	17	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	ILE	CB-CA-C	-6.78	103.15	112.24	12	8
1	A	76	LYS	CA-C-O	6.77	127.68	119.49	11	3
1	A	82	ASN	CA-CB-CG	-6.76	105.84	112.60	14	5
1	A	48	ASP	O-C-N	6.75	129.10	121.88	24	6
1	A	21	MET	CA-C-N	6.75	130.00	120.28	7	3
1	A	21	MET	C-N-CA	6.75	130.00	120.28	7	3
1	A	109	GLN	CB-CG-CD	-6.75	101.13	112.60	6	12
1	A	9	TRP	CG-CD2-CE3	-6.74	127.16	133.90	11	4
1	A	79	ASP	CA-CB-CG	-6.73	105.87	112.60	23	8
1	A	60	ASN	O-C-N	6.73	131.06	123.19	12	7
1	A	126	VAL	CB-CA-C	-6.72	103.20	111.88	9	2
1	A	40	THR	O-C-N	6.72	131.19	122.93	7	7
1	A	98	GLN	CB-CA-C	-6.71	96.51	110.40	25	1
1	A	17	PHE	CA-CB-CG	-6.70	107.10	113.80	20	1
1	A	125	GLN	O-C-N	6.69	131.49	122.59	24	5
1	A	32	LYS	O-C-N	6.69	130.49	122.27	10	7
1	A	105	ARG	NE-CZ-NH1	6.69	128.19	121.50	19	6
1	A	89	TRP	CE2-CD2-CE3	6.67	125.47	118.80	18	8
1	A	98	GLN	OE1-CD-NE2	6.66	129.26	122.60	25	5
1	A	19	GLY	N-CA-C	-6.65	106.42	114.66	17	6
1	A	102	LYS	O-C-N	6.65	131.43	122.59	25	4
1	A	104	ASN	CA-C-O	-6.64	111.02	120.51	25	2
1	A	111	VAL	N-CA-CB	-6.62	103.54	110.95	1	3
1	A	53	LYS	O-C-N	6.61	130.88	123.48	24	6
1	A	98	GLN	O-C-N	6.59	130.76	122.65	25	3
1	A	26	ILE	CA-C-O	6.58	129.84	121.15	1	4
1	A	35	VAL	O-C-N	6.58	128.34	121.89	1	7
1	A	64	ASP	CA-CB-CG	-6.57	106.03	112.60	25	5
1	A	82	ASN	OD1-CG-ND2	6.53	129.13	122.60	1	1
1	A	110	TRP	CD1-CG-CD2	6.52	116.72	106.30	2	7
1	A	75	THR	O-C-N	6.51	130.53	122.20	11	4
1	A	87	VAL	O-C-N	6.50	130.16	122.36	13	1
1	A	18	GLU	N-CA-C	6.49	118.02	111.07	19	8
1	A	35	VAL	N-CA-C	6.48	116.64	110.42	15	9
1	A	126	VAL	N-CA-CB	-6.47	101.59	112.47	5	1
1	A	16	ASN	CA-CB-CG	-6.47	106.13	112.60	20	7
1	A	30	THR	CA-C-N	6.47	129.59	120.28	21	3
1	A	30	THR	C-N-CA	6.47	129.59	120.28	21	3
1	A	93	THR	O-C-N	6.46	131.95	122.97	19	6
1	A	118	LEU	CA-C-O	-6.46	114.52	121.56	19	7
1	A	90	GLU	N-CA-C	6.45	118.03	110.41	23	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	THR	CA-C-O	6.45	128.95	120.11	19	2
1	A	122	CYS	O-C-N	6.45	130.75	122.81	4	3
1	A	34	ALA	CA-C-O	6.44	127.38	119.97	23	12
1	A	103	GLU	CB-CA-C	-6.44	101.34	111.51	15	3
1	A	124	ASP	CA-CB-CG	-6.44	106.16	112.60	10	3
1	A	131	PHE	CA-CB-CG	-6.43	107.37	113.80	15	1
1	A	71	PHE	CB-CA-C	-6.43	102.71	110.94	13	3
1	A	115	LYS	O-C-N	6.42	131.13	122.59	23	6
1	A	73	GLU	CA-C-O	6.42	129.76	121.67	1	2
1	A	82	ASN	O-C-N	6.38	131.54	123.12	22	6
1	A	89	TRP	CA-CB-CG	-6.38	101.48	113.60	19	12
1	A	35	VAL	CB-CA-C	-6.36	103.55	112.14	11	9
1	A	110	TRP	CG-CD1-NE1	-6.35	101.94	110.20	3	5
1	A	100	GLY	O-C-N	6.35	130.95	122.70	7	5
1	A	43	ILE	O-C-N	6.34	129.15	122.62	15	2
1	A	121	THR	N-CA-C	-6.31	105.53	112.72	7	2
1	A	36	ARG	O-C-N	6.30	129.64	122.20	3	5
1	A	98	GLN	CG-CD-NE2	-6.30	106.95	116.40	25	1
1	A	48	ASP	CA-CB-CG	-6.29	106.31	112.60	16	4
1	A	96	CYS	O-C-N	6.26	131.16	123.21	23	5
1	A	93	THR	CA-C-N	6.25	131.08	121.83	8	1
1	A	93	THR	C-N-CA	6.25	131.08	121.83	8	1
1	A	65	PHE	CA-CB-CG	-6.22	107.58	113.80	6	2
1	A	109	GLN	CA-C-N	-6.22	112.61	121.50	24	2
1	A	109	GLN	C-N-CA	-6.22	112.61	121.50	24	2
1	A	55	ASN	CA-C-N	6.21	128.61	120.28	20	1
1	A	55	ASN	C-N-CA	6.21	128.61	120.28	20	1
1	A	71	PHE	N-CA-C	6.21	118.30	107.49	13	15
1	A	55	ASN	CA-CB-CG	-6.21	106.39	112.60	18	4
1	A	3	LYS	N-CA-C	6.21	117.31	108.74	5	3
1	A	43	ILE	CB-CA-C	-6.21	102.92	111.49	24	8
1	A	117	TYR	CA-C-N	-6.21	112.72	121.72	3	8
1	A	117	TYR	C-N-CA	-6.21	112.72	121.72	3	8
1	A	12	GLU	CA-C-O	6.18	127.45	119.98	18	2
1	A	55	ASN	CA-C-O	-6.16	115.17	122.13	22	1
1	A	25	ASP	CA-CB-CG	-6.16	106.44	112.60	5	3
1	A	93	THR	CA-C-O	-6.15	113.91	121.78	19	4
1	A	128	ARG	CA-C-N	-6.14	112.72	121.50	19	2
1	A	128	ARG	C-N-CA	-6.14	112.72	121.50	19	2
1	A	24	LEU	CA-C-O	6.14	127.08	120.63	17	1
1	A	116	LEU	O-C-N	6.12	130.98	123.21	24	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLY	CA-C-N	6.10	130.80	122.07	4	1
1	A	91	GLY	C-N-CA	6.10	130.80	122.07	4	1
1	A	9	TRP	N-CA-C	6.10	117.67	108.46	18	1
1	A	130	VAL	CA-C-O	6.07	126.40	120.27	4	8
1	A	24	LEU	CB-CA-C	-6.07	103.47	111.42	11	2
1	A	110	TRP	CE2-CD2-CG	-6.06	99.93	107.20	12	2
1	A	62	ASP	CA-CB-CG	-6.06	106.54	112.60	20	4
1	A	66	THR	CA-C-O	-6.01	115.14	121.99	11	1
1	A	14	ASN	CA-C-N	-6.00	112.65	120.44	23	4
1	A	14	ASN	C-N-CA	-6.00	112.65	120.44	23	4
1	A	67	VAL	O-C-N	5.96	130.03	122.57	7	3
1	A	58	PHE	O-C-N	5.96	128.44	122.12	8	2
1	A	8	THR	O-C-N	5.95	130.18	123.27	2	5
1	A	109	GLN	O-C-N	5.91	130.49	122.57	16	1
1	A	9	TRP	CG-CD1-NE1	5.88	117.85	110.20	14	2
1	A	104	ASN	CA-CB-CG	-5.86	106.74	112.60	21	3
1	A	125	GLN	OE1-CD-NE2	5.86	128.46	122.60	18	3
1	A	60	ASN	CA-CB-CG	-5.86	106.74	112.60	10	6
1	A	85	THR	CA-CB-OG1	-5.85	100.83	109.60	13	4
1	A	50	PHE	CA-C-O	-5.83	113.96	120.54	21	2
1	A	95	VAL	O-C-N	5.82	129.84	122.57	24	4
1	A	58	PHE	N-CA-C	5.81	117.61	111.28	10	1
1	A	107	TRP	N-CA-C	5.80	118.23	109.23	1	4
1	A	37	LEU	CA-C-O	-5.79	114.36	121.02	23	5
1	A	119	GLU	O-C-N	5.79	130.08	123.31	17	3
1	A	123	GLY	O-C-N	5.79	130.22	122.70	15	1
1	A	116	LEU	CA-C-N	-5.78	115.29	123.03	5	4
1	A	116	LEU	C-N-CA	-5.78	115.29	123.03	5	4
1	A	125	GLN	CB-CG-CD	-5.77	102.78	112.60	17	5
1	A	129	GLN	CA-C-O	-5.77	115.52	121.87	1	1
1	A	57	THR	N-CA-C	-5.77	104.68	110.97	24	2
1	A	85	THR	N-CA-C	5.77	118.93	109.76	25	6
1	A	107	TRP	CA-CB-CG	-5.77	102.64	113.60	5	3
1	A	91	GLY	N-CA-C	-5.75	107.45	114.92	18	1
1	A	65	PHE	O-C-N	-5.74	117.23	123.26	16	2
1	A	30	THR	N-CA-C	5.72	117.98	111.11	10	7
1	A	109	GLN	CB-CA-C	-5.71	101.23	110.77	21	3
1	A	117	TYR	O-C-N	5.71	130.65	123.23	4	1
1	A	65	PHE	CD1-CG-CD2	5.69	127.13	118.60	4	3
1	A	39	GLN	CG-CD-NE2	-5.69	107.87	116.40	9	3
1	A	28	PHE	N-CA-C	5.68	118.41	111.82	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	HIS	ND1-CG-CD2	5.67	111.77	106.10	18	4
1	A	89	TRP	CD2-CE2-CZ2	-5.67	116.73	122.40	10	6
1	A	30	THR	CA-C-O	-5.66	114.88	120.82	17	3
1	A	13	SER	CB-CA-C	-5.64	100.60	111.78	20	6
1	A	18	GLU	CB-CA-C	-5.64	101.27	110.85	7	5
1	A	59	ARG	CD-NE-CZ	-5.62	116.53	124.40	8	2
1	A	95	VAL	CB-CA-C	-5.62	102.24	111.51	3	1
1	A	16	ASN	O-C-N	5.61	130.05	122.59	16	3
1	A	127	CYS	CA-C-O	-5.61	114.64	120.70	18	1
1	A	39	GLN	CA-C-N	5.59	130.89	123.00	24	2
1	A	39	GLN	C-N-CA	5.59	130.89	123.00	24	2
1	A	12	GLU	O-C-N	5.59	128.49	121.95	13	1
1	A	127	CYS	O-C-N	5.59	128.99	122.84	14	1
1	A	49	ASN	OD1-CG-ND2	-5.58	117.03	122.60	9	3
1	A	67	VAL	N-CA-C	5.55	115.32	106.88	14	6
1	A	122	CYS	N-CA-CB	-5.55	102.18	110.17	9	1
1	A	109	GLN	OE1-CD-NE2	5.55	128.15	122.60	20	1
1	A	95	VAL	CA-C-O	-5.54	114.80	121.28	3	1
1	A	108	LYS	CA-C-O	5.54	128.43	120.51	13	1
1	A	21	MET	N-CA-CB	-5.52	101.72	110.22	14	4
1	A	16	ASN	OD1-CG-ND2	-5.52	117.08	122.60	10	1
1	A	89	TRP	NE1-CE2-CD2	-5.51	100.23	107.40	20	3
1	A	15	GLU	CA-CB-CG	-5.51	103.08	114.10	1	4
1	A	33	ILE	CA-C-O	5.50	126.20	120.25	3	1
1	A	52	THR	O-C-N	5.50	130.01	123.24	6	2
1	A	101	GLU	N-CA-C	-5.50	105.30	112.23	11	1
1	A	95	VAL	N-CA-CB	-5.49	102.17	111.23	9	1
1	A	104	ASN	N-CA-CB	-5.49	101.21	110.49	25	1
1	A	70	GLU	O-C-N	5.48	129.88	122.59	21	3
1	A	74	HIS	CA-C-O	5.46	127.13	120.25	8	2
1	A	9	TRP	CD1-CG-CD2	-5.46	97.56	106.30	25	1
1	A	85	THR	N-CA-CB	-5.46	102.87	111.05	21	2
1	A	31	ARG	O-C-N	5.45	129.47	122.39	4	3
1	A	52	THR	N-CA-CB	-5.45	102.22	111.69	24	3
1	A	18	GLU	CA-C-N	-5.45	113.48	120.34	5	1
1	A	18	GLU	C-N-CA	-5.45	113.48	120.34	5	1
1	A	6	ASN	CA-C-N	-5.43	117.98	122.16	19	1
1	A	6	ASN	C-N-CA	-5.43	117.98	122.16	19	1
1	A	105	ARG	N-CA-CB	5.42	116.42	110.35	10	1
1	A	80	GLY	O-C-N	5.41	129.74	122.70	2	2
1	A	45	GLN	CA-C-O	5.41	127.24	121.45	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	ILE	CA-C-N	5.41	127.87	120.35	15	1
1	A	42	ILE	C-N-CA	5.41	127.87	120.35	15	1
1	A	84	LYS	CA-C-N	5.41	128.39	120.71	20	1
1	A	84	LYS	C-N-CA	5.41	128.39	120.71	20	1
1	A	94	LEU	O-C-N	5.40	129.77	122.59	16	1
1	A	107	TRP	CE2-CD2-CG	5.39	113.67	107.20	8	1
1	A	128	ARG	O-C-N	5.38	129.62	123.48	9	4
1	A	107	TRP	CD1-NE1-CE2	-5.36	99.26	108.90	12	2
1	A	39	GLN	N-CA-C	5.36	117.64	110.35	21	3
1	A	117	TYR	CA-C-O	5.35	126.39	120.71	12	1
1	A	18	GLU	CB-CG-CD	-5.35	103.51	112.60	12	3
1	A	48	ASP	CA-C-N	5.35	129.84	121.76	7	1
1	A	48	ASP	C-N-CA	5.35	129.84	121.76	7	1
1	A	23	ALA	CA-C-N	5.34	129.21	122.16	6	1
1	A	23	ALA	C-N-CA	5.34	129.21	122.16	6	1
1	A	49	ASN	N-CA-CB	-5.33	105.40	111.79	15	1
1	A	50	PHE	CD1-CG-CD2	5.33	126.59	118.60	6	1
1	A	14	ASN	CA-C-O	-5.31	115.56	121.51	14	2
1	A	127	CYS	CA-C-N	-5.31	115.61	123.05	10	1
1	A	127	CYS	C-N-CA	-5.31	115.61	123.05	10	1
1	A	45	GLN	CA-CB-CG	-5.31	103.48	114.10	5	3
1	A	124	ASP	CA-C-O	-5.31	115.92	121.55	1	1
1	A	42	ILE	O-C-N	5.31	129.21	122.57	6	1
1	A	92	ASN	N-CA-C	-5.30	106.49	113.17	1	2
1	A	133	LYS	N-CA-CB	-5.30	103.19	111.56	17	2
1	A	106	GLY	CA-C-N	5.29	130.88	122.94	6	2
1	A	106	GLY	C-N-CA	5.29	130.88	122.94	6	2
1	A	38	THR	O-C-N	5.29	129.14	122.37	7	1
1	A	25	ASP	N-CA-CB	-5.29	103.68	111.71	20	1
1	A	15	GLU	CB-CG-CD	-5.26	103.65	112.60	19	1
1	A	62	ASP	O-C-N	5.26	129.56	123.30	16	1
1	A	89	TRP	CB-CG-CD1	-5.26	119.01	126.90	11	1
1	A	110	TRP	CG-CD2-CE3	-5.26	128.64	133.90	15	1
1	A	39	GLN	CA-CB-CG	-5.25	103.61	114.10	14	1
1	A	86	LEU	CA-C-O	5.24	127.29	120.11	13	1
1	A	122	CYS	N-CA-C	5.24	117.47	110.35	15	1
1	A	110	TRP	CE3-CZ3-CH2	-5.23	114.30	121.10	18	1
1	A	87	VAL	CA-C-O	5.23	126.02	120.48	2	1
1	A	51	LYS	N-CA-C	5.22	117.01	108.55	5	2
1	A	83	VAL	N-CA-CB	-5.21	106.33	112.32	11	1
1	A	107	TRP	NE1-CE2-CD2	5.21	114.17	107.40	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	VAL	CA-C-N	-5.18	114.38	122.51	4	2
1	A	67	VAL	C-N-CA	-5.18	114.38	122.51	4	2
1	A	90	GLU	N-CA-CB	-5.18	105.57	111.79	23	1
1	A	110	TRP	CB-CG-CD2	-5.18	119.55	126.80	3	1
1	A	133	LYS	O-C-N	5.18	129.48	122.59	23	1
1	A	10	GLU	CA-CB-CG	-5.18	103.75	114.10	12	1
1	A	131	PHE	N-CA-C	5.17	117.83	109.40	21	1
1	A	108	LYS	CA-CB-CG	-5.16	103.78	114.10	21	1
1	A	41	LYS	CA-C-N	-5.16	114.08	122.33	18	1
1	A	41	LYS	C-N-CA	-5.16	114.08	122.33	18	1
1	A	112	GLU	CB-CG-CD	-5.15	103.84	112.60	5	1
1	A	29	ALA	O-C-N	5.15	128.61	122.27	5	1
1	A	76	LYS	CA-CB-CG	-5.13	103.83	114.10	3	1
1	A	58	PHE	CB-CG-CD1	5.12	129.41	120.70	22	1
1	A	120	LEU	O-C-N	5.11	129.04	123.27	18	1
1	A	9	TRP	CB-CG-CD2	5.11	133.95	126.80	25	1
1	A	31	ARG	CA-C-O	-5.10	113.77	119.79	11	1
1	A	97	VAL	N-CA-CB	-5.10	102.52	111.39	9	1
1	A	124	ASP	CB-CA-C	-5.09	102.88	110.88	11	1
1	A	73	GLU	N-CA-CB	-5.09	102.31	110.46	14	2
1	A	59	ARG	N-CA-C	5.09	115.72	107.32	15	1
1	A	74	HIS	N-CA-C	5.09	115.06	107.88	24	1
1	A	86	LEU	N-CA-C	5.09	116.46	107.61	22	1
1	A	46	ASP	N-CA-C	5.08	116.40	110.41	5	1
1	A	13	SER	CA-C-O	5.08	126.78	121.25	20	1
1	A	102	LYS	N-CA-C	5.08	121.61	110.80	25	1
1	A	41	LYS	CA-C-O	-5.07	115.31	120.99	16	2
1	A	100	GLY	CA-C-O	5.07	129.39	120.57	25	1
1	A	31	ARG	NE-CZ-NH2	5.06	123.75	119.20	18	1
1	A	111	VAL	CB-CA-C	-5.05	105.17	111.08	1	1
1	A	89	TRP	CD1-NE1-CE2	5.04	117.98	108.90	12	2
1	A	89	TRP	CA-C-N	-5.04	113.37	122.54	13	1
1	A	89	TRP	C-N-CA	-5.04	113.37	122.54	13	1
1	A	107	TRP	CG-CD2-CE3	-5.03	128.87	133.90	6	1
1	A	10	GLU	CA-C-N	5.03	127.99	120.90	2	1
1	A	10	GLU	C-N-CA	5.03	127.99	120.90	2	1
1	A	94	LEU	CA-C-O	5.03	126.35	121.67	25	1
1	A	48	ASP	CA-C-O	-5.02	115.43	121.40	13	1
1	A	38	THR	CA-C-O	-5.01	115.21	120.92	19	1
1	A	14	ASN	CB-CA-C	-5.01	102.93	110.24	17	1
1	A	40	THR	CA-C-O	-5.00	116.11	121.56	14	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	49±9
2	A	21	30	30	5±3
All	All	27525	27125	27100	1267

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:CD2	1:A:35:VAL:HG22	0.93	1.99	25	5
1:A:26:ILE:HG21	1:A:30:THR:HG21	0.90	1.40	9	2
1:A:109:GLN:CG	1:A:118:LEU:HD13	0.89	1.96	20	7
1:A:109:GLN:HG2	1:A:118:LEU:HD13	0.89	1.44	20	7
1:A:37:LEU:HD22	1:A:38:THR:N	0.83	1.88	2	1
1:A:26:ILE:CG1	1:A:30:THR:HG21	0.82	2.04	21	3
1:A:9:TRP:CZ2	1:A:43:ILE:HD12	0.81	2.11	8	19
1:A:33:ILE:HD12	1:A:58:PHE:CD1	0.81	2.10	20	1
1:A:107:TRP:HB3	1:A:118:LEU:HD11	0.80	1.54	13	12
1:A:101:GLU:C	1:A:102:LYS:HG2	0.80	2.01	25	1
1:A:107:TRP:CB	1:A:118:LEU:HD11	0.79	2.07	13	24
1:A:107:TRP:HB2	1:A:118:LEU:HD11	0.79	1.54	12	18
1:A:33:ILE:HD13	1:A:58:PHE:CD1	0.77	2.15	19	3
1:A:10:GLU:HG2	1:A:40:THR:HG23	0.77	1.54	10	2
1:A:37:LEU:HD13	1:A:37:LEU:O	0.76	1.80	2	1
1:A:9:TRP:CE3	1:A:116:LEU:HD11	0.75	2.16	16	3
1:A:34:ALA:HA	1:A:57:THR:HG23	0.75	1.59	22	1
1:A:34:ALA:HB2	2:A:135:RTL:H31	0.73	1.60	8	1
1:A:37:LEU:HD12	1:A:37:LEU:C	0.72	2.09	19	2
1:A:11:MET:HE2	1:A:39:GLN:NE2	0.72	1.99	21	1
1:A:105:ARG:NH2	2:A:135:RTL:H193	0.72	2.00	9	3
1:A:20:TYR:OH	2:A:135:RTL:H192	0.72	1.83	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:TYR:CD2	1:A:78:LEU:HD13	0.71	2.20	2	1
1:A:109:GLN:HG3	1:A:118:LEU:HD13	0.71	1.60	16	5
1:A:37:LEU:HD12	1:A:39:GLN:CG	0.71	2.16	6	1
1:A:78:LEU:HD21	2:A:135:RTL:H172	0.71	1.60	17	4
1:A:26:ILE:HG12	1:A:30:THR:HG21	0.71	1.61	15	3
1:A:118:LEU:HD23	1:A:131:PHE:CE1	0.71	2.21	21	5
1:A:24:LEU:HD11	1:A:78:LEU:O	0.70	1.85	10	1
1:A:56:SER:CB	2:A:135:RTL:H162	0.70	2.16	20	2
2:A:135:RTL:C8	2:A:135:RTL:H161	0.69	2.16	7	15
2:A:135:RTL:H171	2:A:135:RTL:C8	0.69	2.16	10	2
1:A:31:ARG:O	1:A:35:VAL:HG23	0.69	1.87	25	14
1:A:87:VAL:HG22	1:A:94:LEU:O	0.69	1.87	20	2
1:A:93:THR:HG23	1:A:110:TRP:CB	0.69	2.18	12	14
1:A:29:ALA:O	1:A:33:ILE:HD12	0.68	1.89	10	1
1:A:29:ALA:O	1:A:33:ILE:HD13	0.68	1.89	15	5
1:A:33:ILE:CG2	1:A:37:LEU:HD23	0.67	2.20	19	1
1:A:42:ILE:C	1:A:42:ILE:HD13	0.67	2.14	13	1
1:A:26:ILE:CG2	1:A:30:THR:HG21	0.67	2.17	9	1
1:A:26:ILE:HG13	1:A:30:THR:HG21	0.67	1.66	21	3
1:A:56:SER:HB3	2:A:135:RTL:H162	0.67	1.67	20	2
1:A:8:THR:OG1	1:A:42:ILE:HD12	0.66	1.90	18	10
1:A:37:LEU:HD13	1:A:37:LEU:C	0.66	2.15	2	1
1:A:9:TRP:N	1:A:9:TRP:CD1	0.66	2.64	14	23
1:A:17:PHE:CD1	1:A:35:VAL:HG22	0.66	2.26	19	7
1:A:20:TYR:OH	2:A:135:RTL:H193	0.66	1.90	18	5
1:A:121:THR:HG22	1:A:126:VAL:HG13	0.66	1.67	8	1
1:A:24:LEU:N	1:A:24:LEU:HD23	0.65	2.06	7	3
1:A:24:LEU:HD12	1:A:26:ILE:HB	0.65	1.68	7	1
1:A:24:LEU:HD12	1:A:81:ARG:CZ	0.65	2.21	20	1
1:A:8:THR:C	1:A:9:TRP:CG	0.65	2.74	15	25
1:A:86:LEU:C	1:A:86:LEU:HD23	0.65	2.15	5	3
1:A:33:ILE:N	1:A:33:ILE:HD13	0.65	2.06	3	4
1:A:99:LYS:C	1:A:102:LYS:HD3	0.65	2.17	25	1
1:A:5:GLN:OE1	1:A:94:LEU:HD22	0.65	1.92	4	1
1:A:24:LEU:HD12	1:A:26:ILE:HG12	0.65	1.68	25	1
1:A:37:LEU:HD12	1:A:39:GLN:HG3	0.64	1.69	6	1
1:A:44:VAL:HG12	1:A:51:LYS:O	0.64	1.92	16	1
1:A:107:TRP:CD2	2:A:135:RTL:H201	0.64	2.28	6	6
1:A:120:LEU:HD22	1:A:122:CYS:SG	0.64	2.33	1	2
1:A:75:THR:HG21	1:A:81:ARG:CZ	0.63	2.23	19	1
1:A:87:VAL:HG23	1:A:96:CYS:SG	0.63	2.33	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ASP:O	1:A:66:THR:HG22	0.63	1.92	22	3
1:A:9:TRP:CE3	1:A:116:LEU:HD12	0.63	2.28	9	1
1:A:109:GLN:CD	1:A:118:LEU:HD13	0.63	2.19	17	2
1:A:26:ILE:CD1	1:A:78:LEU:HD23	0.62	2.23	11	2
1:A:11:MET:HE3	1:A:39:GLN:OE1	0.62	1.94	14	1
1:A:43:ILE:HD11	1:A:109:GLN:OE1	0.62	1.95	9	1
1:A:24:LEU:HD12	1:A:26:ILE:CG1	0.62	2.25	25	1
1:A:59:ARG:O	2:A:135:RTL:H173	0.62	1.94	17	4
1:A:93:THR:HG23	1:A:110:TRP:HB3	0.62	1.68	15	10
1:A:67:VAL:HG11	1:A:89:TRP:HD1	0.62	1.54	3	1
2:A:135:RTL:C8	2:A:135:RTL:C17	0.62	2.77	10	10
1:A:118:LEU:HD23	1:A:129:GLN:HG3	0.62	1.70	1	1
1:A:78:LEU:HD21	2:A:135:RTL:H42	0.62	1.71	21	3
1:A:107:TRP:CE2	2:A:135:RTL:H203	0.62	2.30	22	4
1:A:109:GLN:HG2	1:A:116:LEU:HD11	0.61	1.73	11	1
1:A:75:THR:HG21	1:A:81:ARG:NE	0.61	2.10	19	1
1:A:109:GLN:HB2	1:A:118:LEU:HD13	0.60	1.72	14	3
1:A:59:ARG:HB3	2:A:135:RTL:H172	0.60	1.72	6	1
1:A:54:THR:HG21	2:A:135:RTL:H10	0.60	1.72	2	2
1:A:67:VAL:HG11	1:A:89:TRP:CD1	0.60	2.31	3	5
1:A:96:CYS:C	1:A:97:VAL:HG22	0.60	2.22	8	13
1:A:14:ASN:ND2	1:A:14:ASN:H	0.60	1.93	1	2
1:A:9:TRP:CD1	1:A:41:LYS:HD2	0.60	2.31	17	3
1:A:65:PHE:CD2	1:A:85:THR:CG2	0.59	2.85	17	7
1:A:83:VAL:HG21	1:A:98:GLN:NE2	0.59	2.12	17	1
1:A:109:GLN:NE2	1:A:118:LEU:HD13	0.59	2.12	17	1
1:A:26:ILE:HG21	1:A:30:THR:OG1	0.59	1.97	6	2
1:A:33:ILE:CD1	1:A:58:PHE:CD1	0.59	2.85	24	3
1:A:11:MET:HE3	1:A:39:GLN:HB3	0.59	1.73	22	1
1:A:9:TRP:CD1	1:A:41:LYS:HE2	0.59	2.32	12	4
1:A:39:GLN:NE2	1:A:40:THR:H	0.59	1.95	9	1
1:A:109:GLN:CB	1:A:116:LEU:HD21	0.59	2.26	8	1
1:A:93:THR:HG23	1:A:110:TRP:HB2	0.59	1.74	12	2
1:A:116:LEU:H	1:A:116:LEU:HD22	0.59	1.58	22	1
1:A:110:TRP:C	1:A:111:VAL:HG23	0.59	2.23	5	4
1:A:33:ILE:CD1	1:A:58:PHE:CE1	0.59	2.85	24	2
1:A:20:TYR:CE2	2:A:135:RTL:H181	0.58	2.33	1	3
1:A:23:ALA:HB1	1:A:122:CYS:SG	0.58	2.38	11	1
1:A:125:GLN:C	1:A:126:VAL:HG23	0.58	2.22	25	2
1:A:10:GLU:CG	1:A:40:THR:HG23	0.58	2.28	10	1
1:A:34:ALA:CA	1:A:57:THR:HG23	0.58	2.27	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LYS:C	1:A:42:ILE:HG22	0.58	2.23	25	5
1:A:9:TRP:HZ2	1:A:43:ILE:HD12	0.58	1.59	19	11
1:A:29:ALA:C	1:A:33:ILE:HD12	0.58	2.24	10	1
1:A:87:VAL:HG23	1:A:96:CYS:CB	0.57	2.29	13	1
1:A:65:PHE:CG	1:A:85:THR:CG2	0.57	2.87	17	1
1:A:110:TRP:CH2	1:A:117:TYR:HB2	0.57	2.34	2	16
1:A:98:GLN:HG2	1:A:99:LYS:N	0.57	2.15	25	1
1:A:14:ASN:ND2	1:A:129:GLN:NE2	0.57	2.52	14	1
1:A:107:TRP:CD2	2:A:135:RTL:C20	0.57	2.88	23	7
1:A:106:GLY:O	1:A:120:LEU:HD13	0.57	2.00	12	3
1:A:87:VAL:HG23	1:A:96:CYS:N	0.57	2.15	12	1
1:A:11:MET:HE3	1:A:39:GLN:CD	0.56	2.25	19	1
1:A:120:LEU:HD12	1:A:122:CYS:SG	0.56	2.40	4	2
1:A:101:GLU:HB3	1:A:105:ARG:HB2	0.56	1.78	25	1
1:A:65:PHE:CD2	1:A:85:THR:HG22	0.56	2.36	14	3
1:A:23:ALA:C	1:A:24:LEU:HD23	0.56	2.25	24	2
1:A:11:MET:HE3	1:A:39:GLN:CB	0.56	2.30	22	1
2:A:135:RTL:C8	2:A:135:RTL:C16	0.56	2.84	17	11
1:A:20:TYR:CE1	1:A:120:LEU:HD12	0.56	2.36	23	2
1:A:94:LEU:HD11	1:A:109:GLN:HB2	0.56	1.76	20	1
1:A:65:PHE:CE1	1:A:87:VAL:CG2	0.56	2.89	24	1
1:A:116:LEU:HD23	1:A:117:TYR:N	0.56	2.15	1	1
1:A:125:GLN:CG	1:A:126:VAL:N	0.56	2.68	5	1
1:A:133:LYS:O	1:A:134:LYS:HB3	0.56	2.00	23	1
1:A:83:VAL:HG12	1:A:99:LYS:O	0.56	2.01	14	2
1:A:109:GLN:HG2	1:A:118:LEU:HD22	0.56	1.77	19	1
1:A:83:VAL:HG21	1:A:98:GLN:OE1	0.56	2.01	19	1
1:A:24:LEU:CD1	1:A:81:ARG:CZ	0.55	2.84	20	1
1:A:61:TYR:CD2	1:A:78:LEU:CD1	0.55	2.90	10	1
1:A:9:TRP:CD1	1:A:9:TRP:N	0.55	2.74	11	1
1:A:24:LEU:HD12	1:A:81:ARG:NE	0.55	2.15	20	1
1:A:23:ALA:CB	1:A:101:GLU:HB2	0.55	2.32	25	1
1:A:118:LEU:HD23	1:A:129:GLN:HG2	0.55	1.78	9	4
1:A:61:TYR:CE2	1:A:63:LEU:CD2	0.55	2.89	7	3
1:A:43:ILE:HG22	1:A:44:VAL:N	0.55	2.16	16	20
1:A:11:MET:CG	1:A:131:PHE:CZ	0.55	2.90	22	5
1:A:20:TYR:CZ	1:A:120:LEU:CD1	0.55	2.89	11	1
1:A:83:VAL:HG12	1:A:100:GLY:HA3	0.55	1.79	15	1
1:A:107:TRP:N	1:A:107:TRP:CD1	0.55	2.75	9	4
1:A:37:LEU:C	1:A:37:LEU:CD1	0.55	2.77	19	2
1:A:20:TYR:HE2	2:A:135:RTL:H181	0.54	1.61	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:GLU:HG2	1:A:86:LEU:HD12	0.54	1.78	2	2
1:A:17:PHE:CG	1:A:35:VAL:CG2	0.54	2.90	14	3
1:A:96:CYS:CB	1:A:107:TRP:CH2	0.54	2.90	22	2
1:A:9:TRP:CD1	1:A:41:LYS:CE	0.54	2.91	12	1
1:A:70:GLU:CG	1:A:86:LEU:HD12	0.54	2.32	19	1
1:A:118:LEU:HG	1:A:129:GLN:HB3	0.54	1.77	25	2
1:A:67:VAL:HG22	1:A:87:VAL:CG1	0.54	2.32	25	1
1:A:37:LEU:CD1	1:A:39:GLN:HG2	0.54	2.33	24	1
1:A:48:ASP:O	1:A:67:VAL:HG23	0.54	2.03	5	1
1:A:107:TRP:CG	2:A:135:RTL:C20	0.54	2.91	18	3
1:A:78:LEU:HD21	2:A:135:RTL:C17	0.54	2.33	17	1
1:A:70:GLU:HB3	1:A:86:LEU:HD12	0.54	1.79	23	1
1:A:48:ASP:O	1:A:66:THR:HG23	0.54	2.03	25	1
1:A:120:LEU:HD13	1:A:122:CYS:SG	0.54	2.43	19	2
1:A:95:VAL:HG22	1:A:108:LYS:HG2	0.54	1.80	4	2
1:A:94:LEU:O	1:A:94:LEU:HD12	0.54	2.03	14	4
1:A:50:PHE:C	1:A:50:PHE:CD1	0.53	2.86	13	12
1:A:109:GLN:NE2	1:A:131:PHE:CD2	0.53	2.77	16	1
1:A:8:THR:CG2	1:A:133:LYS:CE	0.53	2.86	2	1
1:A:14:ASN:N	1:A:14:ASN:ND2	0.53	2.56	13	2
1:A:45:GLN:CB	1:A:50:PHE:CD1	0.53	2.92	21	1
1:A:37:LEU:HD13	1:A:39:GLN:HG2	0.53	1.79	24	1
1:A:107:TRP:CE3	2:A:135:RTL:H201	0.53	2.39	14	4
1:A:65:PHE:CE2	1:A:85:THR:HG23	0.53	2.39	1	1
1:A:34:ALA:CB	1:A:57:THR:CG2	0.53	2.87	22	1
1:A:65:PHE:CE2	1:A:85:THR:CG2	0.53	2.92	16	2
1:A:129:GLN:HG2	1:A:131:PHE:CE1	0.53	2.38	9	3
1:A:107:TRP:HB3	1:A:120:LEU:HD21	0.53	1.81	14	1
1:A:93:THR:O	1:A:94:LEU:HD23	0.53	2.04	16	2
1:A:54:THR:HG21	2:A:135:RTL:C10	0.53	2.34	17	1
1:A:118:LEU:HG	1:A:129:GLN:HB2	0.53	1.79	23	1
1:A:28:PHE:C	1:A:28:PHE:CD1	0.52	2.86	1	2
1:A:94:LEU:HD12	1:A:96:CYS:SG	0.52	2.44	9	1
1:A:50:PHE:CD1	1:A:50:PHE:C	0.52	2.88	23	3
1:A:87:VAL:HG23	1:A:96:CYS:CA	0.52	2.35	12	1
1:A:129:GLN:N	1:A:129:GLN:OE1	0.52	2.43	23	2
1:A:107:TRP:CD1	1:A:107:TRP:N	0.52	2.75	6	15
1:A:65:PHE:CE2	1:A:85:THR:HG22	0.52	2.39	15	3
1:A:33:ILE:O	1:A:37:LEU:HD23	0.52	2.04	7	4
1:A:102:LYS:C	1:A:103:GLU:CG	0.52	2.83	25	1
1:A:17:PHE:CG	1:A:35:VAL:HG22	0.52	2.40	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:GLN:CB	1:A:50:PHE:CB	0.52	2.87	22	1
1:A:110:TRP:CH2	1:A:117:TYR:HB3	0.52	2.40	8	2
1:A:98:GLN:CG	1:A:99:LYS:N	0.52	2.71	25	1
1:A:5:GLN:OE1	1:A:43:ILE:HD13	0.51	2.05	17	2
1:A:17:PHE:CG	1:A:35:VAL:HG23	0.51	2.40	14	1
1:A:116:LEU:HD13	1:A:116:LEU:N	0.51	2.20	22	2
1:A:37:LEU:HD22	1:A:37:LEU:C	0.51	2.30	2	1
1:A:11:MET:HG3	1:A:131:PHE:CZ	0.51	2.40	4	3
1:A:20:TYR:C	1:A:20:TYR:CD1	0.51	2.88	18	1
1:A:23:ALA:HB1	1:A:101:GLU:HB2	0.51	1.81	25	1
1:A:32:LYS:HG3	1:A:33:ILE:HD13	0.51	1.81	3	1
1:A:96:CYS:O	1:A:97:VAL:HG13	0.51	2.05	8	2
1:A:52:THR:HG23	1:A:63:LEU:CB	0.51	2.36	18	2
1:A:74:HIS:CD2	1:A:76:LYS:HG3	0.51	2.40	7	2
1:A:41:LYS:NZ	2:A:135:RTL:C15	0.51	2.74	20	1
1:A:11:MET:HE3	1:A:39:GLN:NE2	0.51	2.20	19	2
1:A:107:TRP:CD2	2:A:135:RTL:H203	0.51	2.41	23	3
1:A:111:VAL:HG22	1:A:116:LEU:HD11	0.51	1.83	6	1
1:A:20:TYR:CE1	1:A:120:LEU:CD1	0.51	2.94	8	1
1:A:132:LYS:O	1:A:133:LYS:HB2	0.51	2.06	12	2
1:A:92:ASN:ND2	1:A:92:ASN:N	0.51	2.57	22	2
1:A:42:ILE:C	1:A:42:ILE:CD1	0.51	2.84	13	1
1:A:8:THR:C	1:A:9:TRP:CD1	0.50	2.89	22	5
1:A:14:ASN:ND2	1:A:129:GLN:HE21	0.50	2.04	14	1
1:A:74:HIS:CD2	1:A:74:HIS:C	0.50	2.89	23	2
1:A:20:TYR:CZ	1:A:120:LEU:HD11	0.50	2.41	11	1
1:A:93:THR:O	1:A:95:VAL:HG23	0.50	2.06	7	1
1:A:82:ASN:O	1:A:83:VAL:HG13	0.50	2.06	14	1
1:A:44:VAL:HG13	1:A:44:VAL:O	0.50	2.06	7	13
1:A:105:ARG:CZ	1:A:105:ARG:HB2	0.50	2.36	19	1
1:A:110:TRP:C	1:A:110:TRP:CD1	0.50	2.90	25	3
1:A:11:MET:CG	1:A:131:PHE:CE1	0.50	2.95	8	5
1:A:45:GLN:HG3	1:A:50:PHE:CB	0.50	2.36	9	1
1:A:33:ILE:HG22	1:A:34:ALA:N	0.50	2.21	15	1
1:A:83:VAL:HG21	1:A:98:GLN:HE21	0.50	1.64	17	1
1:A:107:TRP:CG	2:A:135:RTL:H201	0.50	2.41	18	2
1:A:16:ASN:HB2	1:A:127:CYS:CB	0.50	2.37	14	1
1:A:99:LYS:HA	1:A:103:GLU:HA	0.50	1.84	22	2
1:A:11:MET:HG2	1:A:131:PHE:CE1	0.49	2.42	17	8
1:A:45:GLN:HG2	1:A:50:PHE:CB	0.49	2.37	2	1
1:A:118:LEU:CG	1:A:129:GLN:HB3	0.49	2.37	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TRP:CD1	1:A:41:LYS:CD	0.49	2.94	13	2
1:A:9:TRP:HB2	1:A:131:PHE:CD2	0.49	2.41	22	6
1:A:11:MET:HE1	1:A:41:LYS:HB2	0.49	1.85	2	1
1:A:102:LYS:N	1:A:102:LYS:CD	0.49	2.75	19	1
1:A:107:TRP:CZ3	2:A:135:RTL:C15	0.49	2.96	1	1
1:A:33:ILE:HG21	1:A:58:PHE:HB2	0.49	1.83	10	2
1:A:109:GLN:CG	1:A:116:LEU:CD1	0.49	2.91	18	1
1:A:50:PHE:CE1	1:A:67:VAL:CG2	0.49	2.95	21	1
1:A:83:VAL:C	1:A:84:LYS:HG2	0.49	2.33	4	1
1:A:67:VAL:CG1	1:A:89:TRP:CD1	0.49	2.95	12	2
1:A:50:PHE:CD1	1:A:50:PHE:N	0.49	2.79	21	1
1:A:31:ARG:CD	1:A:32:LYS:N	0.49	2.76	1	1
1:A:8:THR:CG2	1:A:133:LYS:HE2	0.49	2.38	2	1
1:A:16:ASN:CB	1:A:127:CYS:HB3	0.49	2.37	14	2
1:A:63:LEU:O	1:A:63:LEU:HD13	0.49	2.08	9	1
1:A:35:VAL:HG12	1:A:36:ARG:N	0.49	2.21	18	3
1:A:11:MET:HG3	1:A:131:PHE:CE1	0.49	2.43	20	1
1:A:52:THR:CG2	1:A:63:LEU:CB	0.48	2.91	24	1
1:A:65:PHE:CD1	1:A:66:THR:N	0.48	2.81	2	3
1:A:110:TRP:CH2	1:A:117:TYR:CB	0.48	2.96	12	7
1:A:106:GLY:C	1:A:107:TRP:CD1	0.48	2.91	21	1
1:A:34:ALA:HA	1:A:37:LEU:HD12	0.48	1.83	2	1
1:A:83:VAL:C	1:A:84:LYS:CG	0.48	2.83	4	1
1:A:20:TYR:CE2	1:A:120:LEU:HD11	0.48	2.43	5	1
1:A:61:TYR:CD1	1:A:78:LEU:HD11	0.48	2.43	13	1
1:A:83:VAL:HG21	1:A:98:GLN:CD	0.48	2.34	22	1
1:A:14:ASN:ND2	1:A:14:ASN:N	0.48	2.60	1	3
1:A:12:GLU:O	1:A:38:THR:HG22	0.48	2.08	4	1
1:A:109:GLN:HB2	1:A:116:LEU:HD21	0.48	1.85	6	1
1:A:6:ASN:OD1	1:A:44:VAL:HG23	0.48	2.09	10	1
1:A:48:ASP:O	1:A:67:VAL:N	0.48	2.47	17	2
1:A:98:GLN:HB3	1:A:105:ARG:HD3	0.48	1.85	25	1
1:A:99:LYS:CA	1:A:102:LYS:HB3	0.48	2.39	25	1
1:A:133:LYS:CG	1:A:134:LYS:N	0.48	2.76	23	5
1:A:24:LEU:O	1:A:26:ILE:N	0.48	2.47	12	4
1:A:87:VAL:HG23	1:A:95:VAL:C	0.48	2.34	12	1
1:A:45:GLN:CB	1:A:50:PHE:HB3	0.48	2.37	1	4
1:A:26:ILE:CG1	1:A:79:ASP:HB2	0.48	2.39	10	1
1:A:39:GLN:HB3	1:A:56:SER:HA	0.48	1.85	5	2
1:A:11:MET:N	1:A:39:GLN:O	0.47	2.46	24	8
1:A:67:VAL:HG11	1:A:89:TRP:NE1	0.47	2.24	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:GLN:HB2	1:A:50:PHE:CD1	0.47	2.44	21	1
1:A:33:ILE:HG13	1:A:58:PHE:CD2	0.47	2.44	22	1
1:A:75:THR:HG23	1:A:83:VAL:HG21	0.47	1.86	23	1
1:A:15:GLU:O	1:A:17:PHE:N	0.47	2.48	5	1
1:A:24:LEU:N	1:A:24:LEU:CD2	0.47	2.76	7	2
1:A:118:LEU:HB3	1:A:129:GLN:HB3	0.47	1.87	16	3
1:A:17:PHE:CB	1:A:35:VAL:HG22	0.47	2.38	8	1
1:A:109:GLN:HE21	1:A:118:LEU:HD22	0.47	1.68	9	2
1:A:8:THR:HA	1:A:42:ILE:HB	0.47	1.86	13	1
1:A:96:CYS:HB3	1:A:107:TRP:CH2	0.47	2.45	22	1
1:A:17:PHE:CD1	1:A:35:VAL:CG2	0.47	2.97	9	3
1:A:23:ALA:HB3	1:A:24:LEU:HD23	0.47	1.86	19	4
1:A:65:PHE:CG	1:A:66:THR:N	0.47	2.82	7	1
1:A:87:VAL:CG1	1:A:88:THR:N	0.47	2.76	11	3
1:A:105:ARG:HH22	2:A:135:RTL:H193	0.47	1.69	14	1
1:A:82:ASN:ND2	1:A:82:ASN:C	0.47	2.73	20	1
1:A:50:PHE:CZ	1:A:67:VAL:CG2	0.47	2.97	21	1
1:A:67:VAL:HG13	1:A:87:VAL:HG12	0.47	1.86	3	2
1:A:44:VAL:CG1	1:A:51:LYS:HD2	0.47	2.38	15	1
1:A:45:GLN:CG	1:A:46:ASP:N	0.47	2.77	16	1
1:A:109:GLN:HG2	1:A:118:LEU:CD1	0.47	2.38	17	1
1:A:33:ILE:HG13	1:A:58:PHE:CE1	0.47	2.44	4	2
1:A:41:LYS:CD	1:A:42:ILE:N	0.47	2.77	20	1
1:A:107:TRP:CE3	2:A:135:RTL:C20	0.47	2.98	14	1
1:A:23:ALA:CB	1:A:24:LEU:HD23	0.47	2.39	13	1
1:A:116:LEU:HD23	1:A:131:PHE:HB3	0.47	1.87	22	1
1:A:9:TRP:CE3	1:A:133:LYS:HB2	0.47	2.45	14	2
1:A:31:ARG:NH2	2:A:135:RTL:H182	0.47	2.24	14	1
1:A:57:THR:HB	2:A:135:RTL:H21	0.47	1.86	22	1
1:A:5:GLN:NE2	1:A:5:GLN:HA	0.46	2.25	7	2
1:A:15:GLU:N	1:A:128:ARG:O	0.46	2.48	9	1
1:A:3:LYS:HD2	1:A:89:TRP:CZ3	0.46	2.45	11	1
1:A:86:LEU:HD23	1:A:86:LEU:O	0.46	2.10	3	2
1:A:16:ASN:C	1:A:17:PHE:CG	0.46	2.91	5	1
1:A:39:GLN:CG	1:A:56:SER:HA	0.46	2.40	9	1
1:A:49:ASN:ND2	1:A:49:ASN:N	0.46	2.63	19	1
1:A:11:MET:HG2	1:A:131:PHE:CD1	0.46	2.45	20	1
1:A:3:LYS:HD3	1:A:89:TRP:CZ3	0.46	2.44	2	2
1:A:97:VAL:HG23	1:A:106:GLY:N	0.46	2.25	9	1
1:A:69:VAL:HG12	1:A:69:VAL:O	0.46	2.10	11	2
1:A:83:VAL:C	1:A:84:LYS:CD	0.46	2.88	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD23	1:A:129:GLN:CG	0.46	2.38	1	2
1:A:96:CYS:C	1:A:97:VAL:CG2	0.46	2.89	13	5
1:A:98:GLN:HE22	1:A:105:ARG:NH1	0.46	2.08	2	1
1:A:134:LYS:CD	1:A:134:LYS:N	0.46	2.78	2	7
1:A:21:MET:HG3	1:A:31:ARG:HG3	0.46	1.87	14	1
1:A:5:GLN:CD	1:A:94:LEU:HD22	0.46	2.35	5	2
1:A:26:ILE:HG22	1:A:27:ASP:N	0.46	2.26	6	2
1:A:99:LYS:CD	1:A:99:LYS:N	0.46	2.79	17	1
1:A:45:GLN:HG2	1:A:50:PHE:HB3	0.46	1.86	2	1
1:A:3:LYS:HE2	1:A:92:ASN:CA	0.46	2.41	18	1
1:A:120:LEU:HG	1:A:129:GLN:CD	0.46	2.35	23	1
1:A:45:GLN:CG	1:A:50:PHE:CB	0.46	2.93	25	2
1:A:33:ILE:N	1:A:33:ILE:CD1	0.46	2.79	3	1
1:A:110:TRP:O	1:A:110:TRP:CG	0.46	2.69	12	2
1:A:71:PHE:C	1:A:71:PHE:CD1	0.46	2.92	10	1
1:A:9:TRP:CD1	1:A:41:LYS:HE3	0.46	2.46	22	1
1:A:53:LYS:N	1:A:53:LYS:CD	0.46	2.79	5	1
1:A:20:TYR:CE2	2:A:135:RTL:H7	0.46	2.45	6	1
2:A:135:RTL:C17	2:A:135:RTL:H8	0.46	2.40	10	2
1:A:31:ARG:HH22	2:A:135:RTL:H182	0.46	1.71	14	1
1:A:130:VAL:HG12	1:A:130:VAL:O	0.46	2.11	23	1
1:A:30:THR:HG22	1:A:31:ARG:N	0.46	2.24	24	1
1:A:26:ILE:HD12	1:A:78:LEU:O	0.45	2.11	5	1
1:A:109:GLN:NE2	1:A:118:LEU:HD22	0.45	2.27	9	1
1:A:33:ILE:HG12	1:A:58:PHE:CZ	0.45	2.46	16	2
1:A:57:THR:HG22	1:A:58:PHE:N	0.45	2.26	19	1
1:A:23:ALA:HB2	1:A:122:CYS:O	0.45	2.11	21	1
1:A:116:LEU:HD11	1:A:133:LYS:HB3	0.45	1.88	22	1
1:A:13:SER:HB3	1:A:130:VAL:N	0.45	2.26	23	1
1:A:107:TRP:HB2	1:A:118:LEU:CD1	0.45	2.41	1	2
1:A:118:LEU:O	1:A:129:GLN:N	0.45	2.49	25	12
1:A:26:ILE:HG13	1:A:79:ASP:HB2	0.45	1.88	10	1
1:A:67:VAL:HG11	1:A:89:TRP:HE1	0.45	1.71	12	1
1:A:37:LEU:HD12	1:A:57:THR:H	0.45	1.71	22	1
1:A:39:GLN:HG3	1:A:56:SER:HA	0.45	1.88	24	1
1:A:31:ARG:C	1:A:31:ARG:HD3	0.45	2.36	8	1
1:A:83:VAL:HG11	1:A:98:GLN:NE2	0.45	2.26	9	1
1:A:39:GLN:NE2	2:A:135:RTL:H161	0.45	2.27	20	1
1:A:75:THR:CB	1:A:81:ARG:NH2	0.45	2.79	20	1
1:A:40:THR:O	1:A:55:ASN:N	0.45	2.50	2	3
1:A:41:LYS:NZ	2:A:135:RTL:C14	0.45	2.79	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:C	1:A:86:LEU:CD2	0.45	2.89	5	2
1:A:120:LEU:HD12	1:A:129:GLN:NE2	0.45	2.26	7	1
1:A:78:LEU:HD21	2:A:135:RTL:H32	0.45	1.88	9	1
1:A:120:LEU:O	1:A:121:THR:HG23	0.45	2.11	24	1
1:A:81:ARG:NE	1:A:81:ARG:CA	0.45	2.79	11	1
1:A:50:PHE:CE2	1:A:67:VAL:HG22	0.45	2.47	20	2
1:A:6:ASN:ND2	1:A:45:GLN:N	0.45	2.64	17	1
1:A:40:THR:CG2	1:A:41:LYS:N	0.45	2.80	5	1
1:A:80:GLY:C	1:A:81:ARG:CG	0.45	2.89	5	1
1:A:75:THR:CB	1:A:80:GLY:HA3	0.45	2.41	7	1
1:A:13:SER:O	1:A:130:VAL:N	0.45	2.49	1	4
1:A:134:LYS:N	1:A:134:LYS:HD2	0.45	2.25	12	2
1:A:33:ILE:HG22	1:A:37:LEU:HD23	0.45	1.88	19	2
1:A:98:GLN:C	1:A:99:LYS:CD	0.45	2.90	17	1
1:A:65:PHE:CD1	1:A:71:PHE:HB3	0.45	2.47	4	2
1:A:83:VAL:HG11	1:A:98:GLN:CD	0.45	2.37	15	2
1:A:31:ARG:HD3	1:A:32:LYS:N	0.45	2.27	6	4
1:A:132:LYS:O	1:A:133:LYS:CB	0.45	2.65	9	5
1:A:39:GLN:NE2	1:A:55:ASN:C	0.45	2.75	24	2
1:A:45:GLN:CG	1:A:50:PHE:HB3	0.45	2.41	9	1
1:A:109:GLN:NE2	1:A:131:PHE:CE2	0.45	2.85	2	1
1:A:5:GLN:CD	1:A:94:LEU:CD2	0.45	2.90	5	1
1:A:12:GLU:HA	1:A:38:THR:HG22	0.45	1.88	9	1
1:A:39:GLN:CD	1:A:56:SER:HA	0.45	2.37	9	1
1:A:107:TRP:CZ3	2:A:135:RTL:H151	0.45	2.47	11	1
1:A:17:PHE:CE1	1:A:35:VAL:HA	0.45	2.46	17	1
1:A:98:GLN:HB3	1:A:105:ARG:CD	0.45	2.42	25	1
1:A:9:TRP:O	1:A:11:MET:N	0.44	2.50	11	2
1:A:26:ILE:O	1:A:27:ASP:CB	0.44	2.64	24	6
1:A:63:LEU:HD13	1:A:73:GLU:OE2	0.44	2.12	15	1
1:A:9:TRP:CE3	1:A:116:LEU:CD1	0.44	2.97	16	1
1:A:109:GLN:HG3	1:A:118:LEU:HD22	0.44	1.89	16	1
1:A:56:SER:O	1:A:57:THR:HG23	0.44	2.13	5	1
1:A:39:GLN:CD	1:A:54:THR:CG2	0.44	2.90	10	1
1:A:116:LEU:CD2	1:A:131:PHE:HB3	0.44	2.41	22	1
1:A:110:TRP:CZ3	1:A:117:TYR:O	0.44	2.69	23	1
1:A:109:GLN:HG2	1:A:116:LEU:CD1	0.44	2.43	18	1
1:A:118:LEU:HG	1:A:129:GLN:CB	0.44	2.41	20	1
1:A:118:LEU:CG	1:A:129:GLN:HB2	0.44	2.41	23	1
1:A:31:ARG:CD	1:A:31:ARG:N	0.44	2.81	14	1
1:A:13:SER:HB2	1:A:130:VAL:CG2	0.44	2.43	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:PHE:CE1	1:A:67:VAL:HA	0.44	2.48	24	1
1:A:80:GLY:C	1:A:81:ARG:HG2	0.44	2.36	5	1
1:A:132:LYS:HG2	1:A:133:LYS:N	0.44	2.28	6	2
1:A:87:VAL:HG13	1:A:94:LEU:O	0.44	2.13	7	1
1:A:24:LEU:HD12	1:A:26:ILE:CD1	0.44	2.43	17	1
1:A:41:LYS:HZ2	1:A:42:ILE:N	0.44	2.10	22	1
1:A:118:LEU:HB3	1:A:129:GLN:CB	0.44	2.42	23	1
1:A:24:LEU:HD12	1:A:26:ILE:HD11	0.44	1.90	1	1
1:A:6:ASN:ND2	1:A:45:GLN:HB2	0.44	2.27	15	1
1:A:3:LYS:N	1:A:3:LYS:CD	0.44	2.78	16	1
1:A:61:TYR:OH	1:A:75:THR:HG22	0.44	2.12	19	1
1:A:84:LYS:CD	1:A:84:LYS:N	0.44	2.80	21	1
1:A:85:THR:HG23	1:A:86:LEU:N	0.44	2.27	21	1
1:A:27:ASP:CG	1:A:28:PHE:N	0.44	2.75	2	2
1:A:125:GLN:HG2	1:A:126:VAL:N	0.44	2.28	5	1
1:A:114:ASP:CG	1:A:115:LYS:N	0.44	2.75	8	1
1:A:78:LEU:HD21	2:A:135:RTL:C3	0.44	2.43	9	1
1:A:24:LEU:HD12	1:A:26:ILE:HG13	0.44	1.89	17	1
1:A:83:VAL:HA	1:A:84:LYS:HE3	0.44	1.88	19	1
1:A:120:LEU:N	1:A:129:GLN:OE1	0.44	2.51	23	1
1:A:32:LYS:CE	1:A:36:ARG:NE	0.44	2.81	1	1
1:A:69:VAL:C	1:A:70:GLU:CG	0.44	2.91	8	1
1:A:96:CYS:HB2	1:A:107:TRP:CZ2	0.44	2.47	9	1
1:A:109:GLN:HB3	1:A:118:LEU:HD13	0.44	1.89	10	1
1:A:65:PHE:CE1	1:A:71:PHE:CB	0.44	3.01	13	1
1:A:8:THR:O	1:A:134:LYS:HA	0.44	2.13	15	1
1:A:8:THR:O	1:A:9:TRP:CG	0.44	2.70	15	1
1:A:36:ARG:CD	1:A:37:LEU:HD23	0.44	2.43	14	1
1:A:14:ASN:O	1:A:17:PHE:CE1	0.44	2.71	17	2
1:A:26:ILE:HG13	1:A:30:THR:CG2	0.44	2.39	21	1
1:A:8:THR:HB	1:A:133:LYS:CE	0.43	2.42	2	1
1:A:45:GLN:HB3	1:A:50:PHE:HB3	0.43	1.89	4	1
1:A:20:TYR:OH	1:A:120:LEU:HD11	0.43	2.13	11	1
1:A:28:PHE:CD1	1:A:29:ALA:N	0.43	2.85	21	1
1:A:37:LEU:CD1	1:A:39:GLN:CG	0.43	2.95	24	1
1:A:37:LEU:HD13	1:A:39:GLN:CG	0.43	2.43	24	1
1:A:9:TRP:HA	1:A:133:LYS:CB	0.43	2.43	21	3
1:A:17:PHE:CB	1:A:35:VAL:CG2	0.43	2.96	4	1
1:A:11:MET:HE3	1:A:131:PHE:HZ	0.43	1.73	17	1
1:A:11:MET:HG2	1:A:131:PHE:CZ	0.43	2.49	18	3
1:A:95:VAL:HG22	1:A:108:LYS:HD3	0.43	1.90	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD23	1:A:37:LEU:O	0.43	2.14	9	1
1:A:58:PHE:CD1	1:A:58:PHE:C	0.43	2.96	22	1
1:A:61:TYR:CD1	1:A:78:LEU:HD13	0.43	2.49	4	1
1:A:61:TYR:CG	1:A:78:LEU:CD1	0.43	3.01	10	1
1:A:20:TYR:CE2	1:A:24:LEU:HD22	0.43	2.49	20	1
1:A:65:PHE:CE1	1:A:87:VAL:HG21	0.43	2.48	24	1
1:A:23:ALA:HB2	1:A:122:CYS:SG	0.43	2.53	2	1
1:A:65:PHE:CD1	1:A:71:PHE:HB2	0.43	2.49	8	1
1:A:68:GLY:N	1:A:87:VAL:HG12	0.43	2.28	13	1
1:A:5:GLN:HG3	1:A:43:ILE:HG21	0.43	1.90	23	1
1:A:51:LYS:CD	1:A:51:LYS:C	0.43	2.91	2	1
1:A:44:VAL:O	1:A:44:VAL:HG13	0.43	2.13	8	5
1:A:13:SER:C	1:A:14:ASN:ND2	0.43	2.76	14	1
1:A:14:ASN:O	1:A:17:PHE:CZ	0.43	2.71	17	1
1:A:3:LYS:HE3	1:A:89:TRP:CH2	0.43	2.48	21	1
1:A:80:GLY:C	1:A:81:ARG:HG3	0.43	2.38	3	1
1:A:16:ASN:CB	1:A:127:CYS:CB	0.43	2.97	14	1
1:A:98:GLN:C	1:A:99:LYS:HD3	0.43	2.39	14	2
1:A:51:LYS:C	1:A:51:LYS:CD	0.43	2.92	21	1
1:A:41:LYS:C	1:A:41:LYS:HD3	0.43	2.39	25	1
1:A:28:PHE:CD1	1:A:28:PHE:N	0.43	2.86	11	2
1:A:30:THR:HG22	2:A:135:RTL:C4	0.43	2.44	15	1
1:A:23:ALA:HB1	1:A:105:ARG:NH1	0.43	2.29	19	1
1:A:118:LEU:HD12	1:A:119:GLU:H	0.43	1.74	19	1
1:A:63:LEU:O	1:A:64:ASP:C	0.43	2.62	4	2
1:A:65:PHE:CE2	1:A:87:VAL:HB	0.43	2.49	11	1
1:A:12:GLU:OE2	1:A:130:VAL:HG11	0.42	2.13	1	1
1:A:59:ARG:CB	2:A:135:RTL:H22	0.42	2.44	3	1
1:A:8:THR:CG2	1:A:9:TRP:N	0.42	2.82	5	3
1:A:65:PHE:CE1	1:A:70:GLU:HA	0.42	2.48	9	1
1:A:129:GLN:HG3	1:A:130:VAL:N	0.42	2.29	11	1
1:A:116:LEU:CD2	1:A:131:PHE:CB	0.42	2.97	13	1
1:A:51:LYS:HD3	1:A:51:LYS:C	0.42	2.39	19	1
1:A:99:LYS:HA	1:A:102:LYS:HB3	0.42	1.90	25	1
1:A:3:LYS:HD2	1:A:89:TRP:CH2	0.42	2.48	4	1
1:A:87:VAL:HG23	1:A:96:CYS:HB2	0.42	1.90	6	1
1:A:75:THR:HB	1:A:80:GLY:HA3	0.42	1.91	7	2
1:A:17:PHE:HB3	1:A:35:VAL:CG2	0.42	2.44	11	1
1:A:17:PHE:CD1	1:A:35:VAL:HA	0.42	2.49	17	1
1:A:57:THR:CG2	1:A:58:PHE:N	0.42	2.82	20	1
1:A:65:PHE:CD1	1:A:65:PHE:C	0.42	2.96	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG22	1:A:44:VAL:O	0.42	2.14	25	1
1:A:113:GLY:O	1:A:115:LYS:N	0.42	2.52	10	2
1:A:6:ASN:ND2	1:A:45:GLN:CB	0.42	2.83	15	1
1:A:30:THR:HG23	1:A:58:PHE:CE2	0.42	2.49	20	1
1:A:98:GLN:CB	1:A:105:ARG:HD3	0.42	2.45	25	1
1:A:24:LEU:O	1:A:24:LEU:HG	0.42	2.14	14	1
1:A:44:VAL:HG12	1:A:51:LYS:HD2	0.42	1.90	15	1
1:A:59:ARG:HB2	2:A:135:RTL:C2	0.42	2.44	16	2
1:A:14:ASN:HB3	1:A:129:GLN:NE2	0.42	2.29	18	1
1:A:107:TRP:CE3	2:A:135:RTL:H152	0.42	2.50	19	1
1:A:94:LEU:HD21	1:A:109:GLN:HB2	0.42	1.91	20	1
1:A:69:VAL:O	1:A:69:VAL:HG12	0.42	2.15	21	2
1:A:26:ILE:HD11	1:A:78:LEU:HD23	0.42	1.91	25	1
1:A:75:THR:OG1	1:A:81:ARG:N	0.42	2.53	11	3
1:A:97:VAL:HG23	1:A:106:GLY:CA	0.42	2.44	9	1
1:A:3:LYS:HE3	1:A:93:THR:N	0.42	2.30	12	1
1:A:6:ASN:ND2	1:A:45:GLN:H	0.42	2.12	17	1
1:A:101:GLU:HG2	1:A:123:GLY:N	0.42	2.30	25	1
1:A:133:LYS:HG3	1:A:134:LYS:CD	0.42	2.45	6	1
1:A:41:LYS:NZ	1:A:52:THR:OG1	0.42	2.53	7	1
1:A:16:ASN:C	1:A:18:GLU:N	0.42	2.77	18	2
1:A:81:ARG:NH1	1:A:102:LYS:NZ	0.42	2.68	20	1
1:A:116:LEU:HD23	1:A:116:LEU:C	0.42	2.39	1	1
1:A:8:THR:HB	1:A:133:LYS:HE3	0.42	1.90	2	1
1:A:3:LYS:HD3	1:A:89:TRP:CH2	0.42	2.50	17	1
1:A:102:LYS:O	1:A:104:ASN:N	0.42	2.52	22	1
1:A:21:MET:HE1	1:A:30:THR:HB	0.42	1.91	24	1
1:A:91:GLY:C	1:A:92:ASN:CG	0.42	2.88	24	1
1:A:107:TRP:CZ3	2:A:135:RTL:H152	0.42	2.50	1	1
1:A:67:VAL:O	1:A:67:VAL:HG12	0.42	2.15	6	1
1:A:30:THR:HG22	1:A:31:ARG:NH1	0.42	2.30	14	1
1:A:83:VAL:HA	1:A:84:LYS:CE	0.42	2.45	19	1
1:A:102:LYS:N	1:A:102:LYS:HD3	0.42	2.29	19	1
1:A:24:LEU:CD1	1:A:81:ARG:NH2	0.42	2.83	20	1
1:A:52:THR:CG2	1:A:63:LEU:HB3	0.42	2.45	24	1
1:A:31:ARG:CD	1:A:31:ARG:C	0.42	2.92	1	1
1:A:33:ILE:O	1:A:37:LEU:HD12	0.42	2.15	2	1
1:A:8:THR:O	1:A:9:TRP:CD2	0.42	2.73	15	1
1:A:14:ASN:ND2	1:A:20:TYR:OH	0.42	2.53	15	1
1:A:61:TYR:HB2	1:A:78:LEU:HD11	0.42	1.91	17	1
1:A:95:VAL:HG22	1:A:108:LYS:HE2	0.42	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:CE2	1:A:120:LEU:CD1	0.42	3.02	2	1
1:A:116:LEU:HD23	1:A:118:LEU:N	0.42	2.30	8	1
1:A:110:TRP:CD1	1:A:110:TRP:C	0.42	2.98	11	2
1:A:65:PHE:CD1	1:A:85:THR:HG22	0.42	2.50	17	1
1:A:49:ASN:O	1:A:49:ASN:ND2	0.41	2.53	4	1
1:A:109:GLN:NE2	2:A:135:RTL:O1	0.41	2.53	11	2
1:A:67:VAL:HG22	1:A:87:VAL:HG11	0.41	1.92	25	1
1:A:95:VAL:O	1:A:95:VAL:HG12	0.41	2.13	5	2
1:A:52:THR:OG1	1:A:53:LYS:N	0.41	2.52	7	1
1:A:61:TYR:CE2	1:A:63:LEU:HD23	0.41	2.48	7	1
1:A:14:ASN:N	1:A:14:ASN:HD22	0.41	2.12	12	1
1:A:24:LEU:HB3	1:A:81:ARG:NH1	0.41	2.30	12	1
1:A:36:ARG:HG2	1:A:37:LEU:N	0.41	2.30	19	3
1:A:21:MET:HG3	1:A:31:ARG:CG	0.41	2.45	14	1
1:A:122:CYS:C	1:A:124:ASP:N	0.41	2.78	24	1
1:A:26:ILE:CD1	1:A:79:ASP:HB3	0.41	2.45	1	1
1:A:39:GLN:HB2	1:A:55:ASN:C	0.41	2.40	5	1
1:A:109:GLN:CB	1:A:118:LEU:HD13	0.41	2.45	10	2
1:A:23:ALA:O	1:A:102:LYS:NZ	0.41	2.53	15	1
1:A:102:LYS:N	1:A:102:LYS:HD2	0.41	2.31	17	2
1:A:34:ALA:CB	1:A:57:THR:HG23	0.41	2.45	22	1
1:A:100:GLY:O	1:A:105:ARG:CD	0.41	2.69	25	1
1:A:40:THR:HG22	1:A:41:LYS:N	0.41	2.31	2	1
1:A:116:LEU:HD12	1:A:116:LEU:C	0.41	2.40	11	1
1:A:5:GLN:OE1	1:A:43:ILE:HG21	0.41	2.16	18	1
1:A:11:MET:O	1:A:38:THR:HG22	0.41	2.15	19	1
1:A:70:GLU:HG3	1:A:86:LEU:HD12	0.41	1.91	19	1
1:A:93:THR:C	1:A:94:LEU:HD23	0.41	2.40	21	1
1:A:20:TYR:CE2	1:A:129:GLN:NE2	0.41	2.89	22	1
1:A:39:GLN:HB2	1:A:56:SER:HA	0.41	1.90	15	1
1:A:120:LEU:HD23	1:A:129:GLN:HB2	0.41	1.92	18	1
1:A:65:PHE:CZ	1:A:85:THR:HG22	0.41	2.50	20	1
1:A:122:CYS:O	1:A:124:ASP:N	0.41	2.52	24	1
1:A:84:LYS:N	1:A:84:LYS:HD3	0.41	2.30	25	1
1:A:61:TYR:HB2	2:A:135:RTL:H171	0.41	1.92	2	1
1:A:81:ARG:NE	1:A:81:ARG:HA	0.41	2.30	11	1
1:A:26:ILE:HG23	1:A:30:THR:HB	0.41	1.91	22	2
1:A:65:PHE:CE1	1:A:85:THR:HG22	0.41	2.51	6	2
1:A:15:GLU:C	1:A:17:PHE:N	0.41	2.77	12	1
1:A:73:GLU:CB	1:A:83:VAL:HG22	0.41	2.46	12	1
1:A:89:TRP:CE3	1:A:93:THR:O	0.41	2.73	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:THR:O	1:A:77:GLY:N	0.41	2.54	19	2
1:A:41:LYS:C	1:A:42:ILE:CG2	0.41	2.94	17	1
1:A:118:LEU:HD23	1:A:129:GLN:HB3	0.41	1.93	18	1
1:A:50:PHE:CZ	1:A:67:VAL:HG22	0.41	2.50	21	1
1:A:107:TRP:HB3	1:A:120:LEU:CD2	0.41	2.46	24	1
2:A:135:RTL:H8	2:A:135:RTL:H171	0.41	1.93	3	1
1:A:83:VAL:HG11	1:A:98:GLN:OE1	0.41	2.15	4	1
1:A:41:LYS:CD	2:A:135:RTL:H14	0.41	2.46	8	1
1:A:9:TRP:CE3	1:A:116:LEU:HD23	0.41	2.51	11	1
1:A:31:ARG:N	1:A:31:ARG:HD2	0.41	2.31	14	1
1:A:71:PHE:CD1	1:A:71:PHE:C	0.41	2.96	14	1
1:A:87:VAL:C	1:A:88:THR:HG23	0.41	2.41	18	1
1:A:26:ILE:HD13	1:A:30:THR:HG21	0.41	1.92	20	1
1:A:56:SER:HB2	2:A:135:RTL:H162	0.41	1.89	20	1
1:A:39:GLN:HG3	1:A:56:SER:CA	0.41	2.46	24	1
1:A:72:ASP:OD1	1:A:72:ASP:N	0.41	2.54	3	1
1:A:43:ILE:CG2	1:A:44:VAL:N	0.41	2.84	10	2
1:A:86:LEU:HD23	1:A:86:LEU:C	0.41	2.40	13	1
1:A:65:PHE:CG	1:A:85:THR:HG22	0.41	2.51	17	1
1:A:24:LEU:C	1:A:25:ASP:CG	0.41	2.89	18	1
1:A:56:SER:O	1:A:57:THR:CB	0.41	2.68	18	1
1:A:120:LEU:N	1:A:127:CYS:O	0.41	2.54	19	1
1:A:11:MET:HG2	1:A:131:PHE:CE2	0.41	2.51	22	1
1:A:45:GLN:HB3	1:A:50:PHE:CB	0.41	2.45	22	1
1:A:124:ASP:C	1:A:125:GLN:CG	0.41	2.92	1	1
1:A:8:THR:HG22	1:A:9:TRP:N	0.41	2.30	10	3
1:A:65:PHE:CD1	1:A:71:PHE:CB	0.41	3.04	13	1
1:A:48:ASP:OD2	1:A:49:ASN:ND2	0.41	2.54	14	1
1:A:32:LYS:HG2	1:A:33:ILE:HD13	0.41	1.92	22	1
1:A:90:GLU:N	1:A:93:THR:O	0.40	2.54	7	1
1:A:16:ASN:O	1:A:19:GLY:N	0.40	2.54	12	1
1:A:17:PHE:N	1:A:17:PHE:CD1	0.40	2.89	12	1
2:A:135:RTL:C8	2:A:135:RTL:H172	0.40	2.46	13	1
1:A:30:THR:CG2	2:A:135:RTL:C4	0.40	2.98	15	1
1:A:116:LEU:HG	1:A:131:PHE:CB	0.40	2.46	17	1
1:A:21:MET:O	1:A:25:ASP:N	0.40	2.54	18	1
1:A:18:GLU:HG3	1:A:19:GLY:N	0.40	2.31	1	1
1:A:27:ASP:OD2	1:A:29:ALA:HB3	0.40	2.16	8	1
1:A:79:ASP:OD2	1:A:81:ARG:NE	0.40	2.54	11	1
1:A:116:LEU:CD2	1:A:131:PHE:HB2	0.40	2.46	13	1
1:A:83:VAL:HG11	1:A:102:LYS:NZ	0.40	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:LYS:O	1:A:110:TRP:N	0.40	2.54	19	1
1:A:9:TRP:HA	1:A:133:LYS:HB3	0.40	1.93	21	1
1:A:45:GLN:CB	1:A:50:PHE:HB2	0.40	2.46	22	1
1:A:75:THR:O	1:A:80:GLY:N	0.40	2.54	24	1
1:A:18:GLU:OE1	1:A:31:ARG:NH1	0.40	2.55	7	1
1:A:45:GLN:HG2	1:A:46:ASP:N	0.40	2.30	7	1
1:A:9:TRP:CE2	1:A:43:ILE:HD12	0.40	2.50	8	1
1:A:37:LEU:HD22	1:A:37:LEU:HA	0.40	1.63	8	1
1:A:86:LEU:HD23	1:A:88:THR:HG23	0.40	1.93	8	1
1:A:81:ARG:CZ	1:A:81:ARG:HB2	0.40	2.45	12	1
1:A:30:THR:CG2	2:A:135:RTL:H42	0.40	2.46	15	1
1:A:43:ILE:HG22	1:A:44:VAL:H	0.40	1.76	22	1
1:A:118:LEU:CB	1:A:129:GLN:HB2	0.40	2.47	23	1
1:A:79:ASP:OD1	1:A:81:ARG:N	0.40	2.54	1	1
1:A:33:ILE:HG13	1:A:58:PHE:CD1	0.40	2.51	3	1
1:A:66:THR:HG22	1:A:69:VAL:CG2	0.40	2.47	3	1
1:A:39:GLN:CD	1:A:56:SER:N	0.40	2.80	9	1
1:A:16:ASN:O	1:A:18:GLU:N	0.40	2.55	12	1
1:A:3:LYS:HE3	1:A:89:TRP:CZ3	0.40	2.52	22	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%)	86±4 (66±3%)	31±4 (24±3%)	14±3 (11±2%)	1	8
All	All	3275/3350 (98%)	2157 (66%)	771 (24%)	347 (11%)	1	8

All 64 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	6	ASN	22
1	A	44	VAL	20
1	A	94	LEU	16

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Mol	Chain	Res	Type	Models (Total)
1	A	115	LYS	15
1	A	95	VAL	14
1	A	27	ASP	14
1	A	104	ASN	14
1	A	111	VAL	14
1	A	133	LYS	13
1	A	42	ILE	12
1	A	82	ASN	11
1	A	25	ASP	10
1	A	70	GLU	9
1	A	97	VAL	9
1	A	39	GLN	9
1	A	76	LYS	9
1	A	101	GLU	8
1	A	10	GLU	7
1	A	49	ASN	7
1	A	3	LYS	6
1	A	4	ASP	6
1	A	114	ASP	5
1	A	91	GLY	5
1	A	57	THR	5
1	A	103	GLU	5
1	A	113	GLY	5
1	A	80	GLY	4
1	A	81	ARG	4
1	A	122	CYS	4
1	A	123	GLY	4
1	A	48	ASP	4
1	A	64	ASP	3
1	A	72	ASP	3
1	A	124	ASP	3
1	A	16	ASN	3
1	A	126	VAL	3
1	A	5	GLN	3
1	A	13	SER	2
1	A	132	LYS	2
1	A	79	ASP	2
1	A	56	SER	2
1	A	15	GLU	2
1	A	92	ASN	2
1	A	17	PHE	2
1	A	45	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	78	LEU	2
1	A	9	TRP	2
1	A	47	GLY	2
1	A	102	LYS	2
1	A	73	GLU	1
1	A	125	GLN	1
1	A	40	THR	1
1	A	130	VAL	1
1	A	59	ARG	1
1	A	62	ASP	1
1	A	63	LEU	1
1	A	100	GLY	1
1	A	109	GLN	1
1	A	24	LEU	1
1	A	90	GLU	1
1	A	89	TRP	1
1	A	93	THR	1
1	A	14	ASN	1
1	A	11	MET	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%)	68±4 (58±3%)	50±4 (42±3%)	0	4
All	All	2950/3000 (98%)	1710 (58%)	1240 (42%)	0	4

All 113 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	25
1	A	31	ARG	25
1	A	53	LYS	25
1	A	63	LEU	25
1	A	107	TRP	25
1	A	37	LEU	24

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Mol	Chain	Res	Type	Models (Total)
1	A	93	THR	24
1	A	97	VAL	24
1	A	35	VAL	23
1	A	42	ILE	23
1	A	84	LYS	23
1	A	134	LYS	23
1	A	94	LEU	22
1	A	36	ARG	21
1	A	78	LEU	21
1	A	33	ILE	20
1	A	6	ASN	19
1	A	14	ASN	19
1	A	74	HIS	19
1	A	66	THR	18
1	A	115	LYS	18
1	A	41	LYS	18
1	A	116	LEU	18
1	A	90	GLU	17
1	A	52	THR	17
1	A	102	LYS	17
1	A	82	ASN	16
1	A	127	CYS	16
1	A	129	GLN	16
1	A	3	LYS	15
1	A	132	LYS	15
1	A	51	LYS	15
1	A	75	THR	15
1	A	11	MET	14
1	A	49	ASN	14
1	A	59	ARG	14
1	A	83	VAL	14
1	A	24	LEU	13
1	A	85	THR	13
1	A	58	PHE	13
1	A	133	LYS	13
1	A	38	THR	13
1	A	54	THR	12
1	A	56	SER	12
1	A	55	ASN	12
1	A	70	GLU	12
1	A	87	VAL	12
1	A	4	ASP	11

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Mol	Chain	Res	Type	Models (Total)
1	A	5	GLN	11
1	A	13	SER	11
1	A	32	LYS	11
1	A	110	TRP	11
1	A	22	LYS	11
1	A	10	GLU	10
1	A	17	PHE	10
1	A	27	ASP	10
1	A	57	THR	10
1	A	120	LEU	10
1	A	46	ASP	9
1	A	98	GLN	9
1	A	119	GLU	9
1	A	21	MET	9
1	A	45	GLN	9
1	A	117	TYR	9
1	A	114	ASP	9
1	A	28	PHE	8
1	A	81	ARG	8
1	A	48	ASP	8
1	A	92	ASN	8
1	A	73	GLU	8
1	A	76	LYS	8
1	A	99	LYS	7
1	A	39	GLN	7
1	A	122	CYS	7
1	A	109	GLN	7
1	A	96	CYS	7
1	A	125	GLN	6
1	A	15	GLU	6
1	A	72	ASP	6
1	A	79	ASP	6
1	A	124	ASP	6
1	A	30	THR	6
1	A	12	GLU	5
1	A	105	ARG	5
1	A	130	VAL	5
1	A	40	THR	5
1	A	103	GLU	5
1	A	62	ASP	5
1	A	20	TYR	5
1	A	128	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	26	ILE	5
1	A	88	THR	4
1	A	108	LYS	4
1	A	69	VAL	4
1	A	50	PHE	4
1	A	71	PHE	4
1	A	64	ASP	4
1	A	111	VAL	3
1	A	25	ASP	3
1	A	86	LEU	3
1	A	101	GLU	3
1	A	44	VAL	3
1	A	8	THR	3
1	A	104	ASN	2
1	A	60	ASN	2
1	A	18	GLU	2
1	A	16	ASN	1
1	A	126	VAL	1
1	A	67	VAL	1
1	A	61	TYR	1
1	A	95	VAL	1
1	A	65	PHE	1
1	A	121	THR	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	RTL	A	135	-	21,21,21	1.90±0.16	2±0 (9±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	RTL	A	135	-	28,28,28	2.38±0.13	10±1 (34±4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RTL	A	135	-	-	0±0,14,31,31	0±0,1,1,1

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
2	A	135	RTL	C1-C6	9.05	1.42	1.53	10	25
2	A	135	RTL	C4-C5	4.92	1.41	1.51	10	25

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

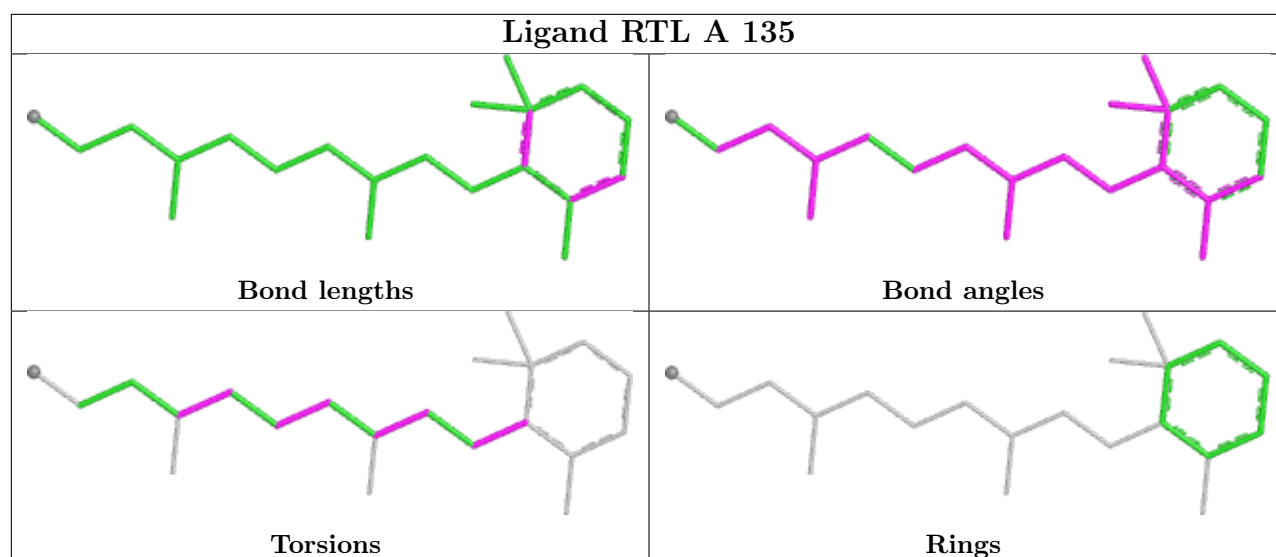
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	135	RTL	C17-C1-C16	6.71	89.42	108.63	16	25
2	A	135	RTL	C11-C10-C9	6.63	117.98	127.28	1	25
2	A	135	RTL	C4-C5-C6	5.70	115.00	122.70	14	22
2	A	135	RTL	C2-C1-C6	5.45	118.35	110.44	19	5
2	A	135	RTL	C15-C14-C13	5.11	118.32	126.61	20	11
2	A	135	RTL	C20-C13-C12	4.71	110.90	118.09	15	24
2	A	135	RTL	C17-C1-C6	4.52	117.33	110.24	15	20
2	A	135	RTL	C18-C5-C6	4.35	129.23	124.48	20	19
2	A	135	RTL	C19-C9-C8	4.26	111.59	118.09	8	17
2	A	135	RTL	C16-C1-C6	3.75	116.13	110.24	5	14
2	A	135	RTL	C7-C8-C9	3.27	121.40	126.23	15	6
2	A	135	RTL	C8-C7-C6	3.10	118.72	127.00	2	17
2	A	135	RTL	C3-C4-C5	2.87	119.17	114.06	15	9
2	A	135	RTL	C19-C9-C10	2.84	127.42	122.82	7	10
2	A	135	RTL	C1-C6-C5	2.83	118.76	122.64	15	1
2	A	135	RTL	C12-C13-C14	2.82	122.42	118.49	20	3
2	A	135	RTL	C20-C13-C14	2.49	128.04	123.73	9	6
2	A	135	RTL	C8-C9-C10	2.45	122.87	119.01	8	1
2	A	135	RTL	C2-C3-C4	2.33	116.39	111.28	9	3

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided