



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 03:28 AM UTC

PDB ID : 2WC2 / pdb_00002wc2
Title : Nmr structure of catabolite activator protein in the unliganded state
Authors : Popovych, N.; Tzeng, S.R.; Kalodimos, C.G.
Deposited on : 2009-03-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

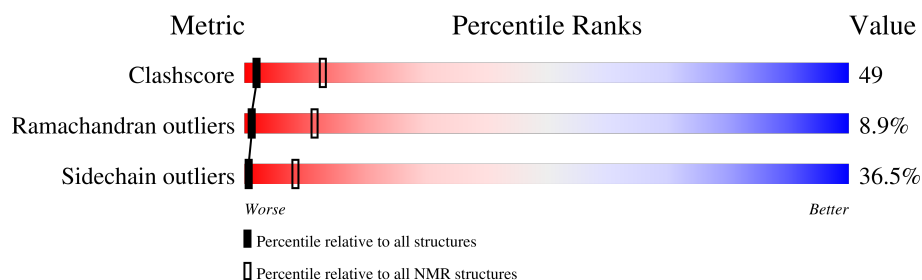
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

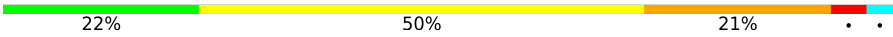
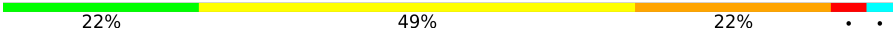
The overall completeness of chemical shifts assignment was not calculated.

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	209	
1	B	209	

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:8-A:209, B:8-B:209 (404)	1.10	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6704 atoms, of which 3404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CATABOLITE GENE ACTIVATOR.

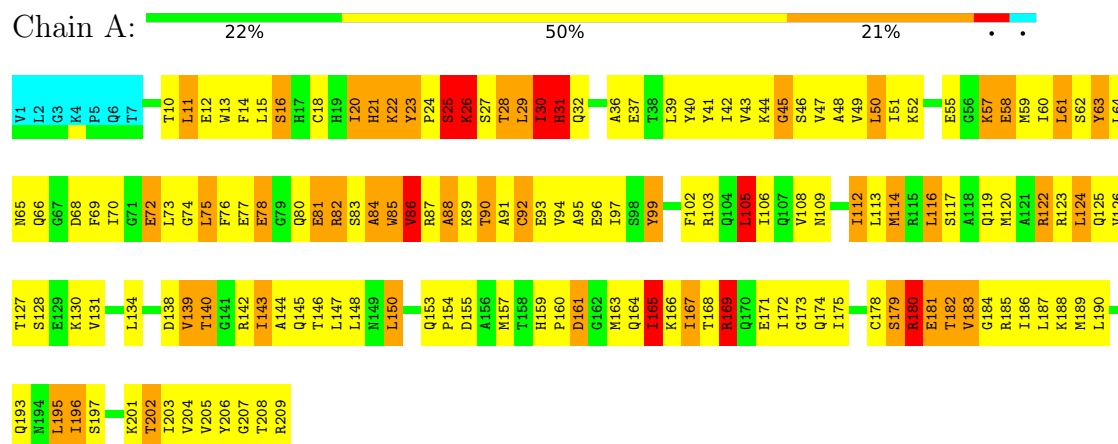
Mol	Chain	Residues	Atoms						Trace
1	A	209	Total	C	H	N	O	S	0
			3352	1044	1702	290	307	9	
1	B	209	Total	C	H	N	O	S	0
			3352	1044	1702	290	307	9	

4 Residue-property plots

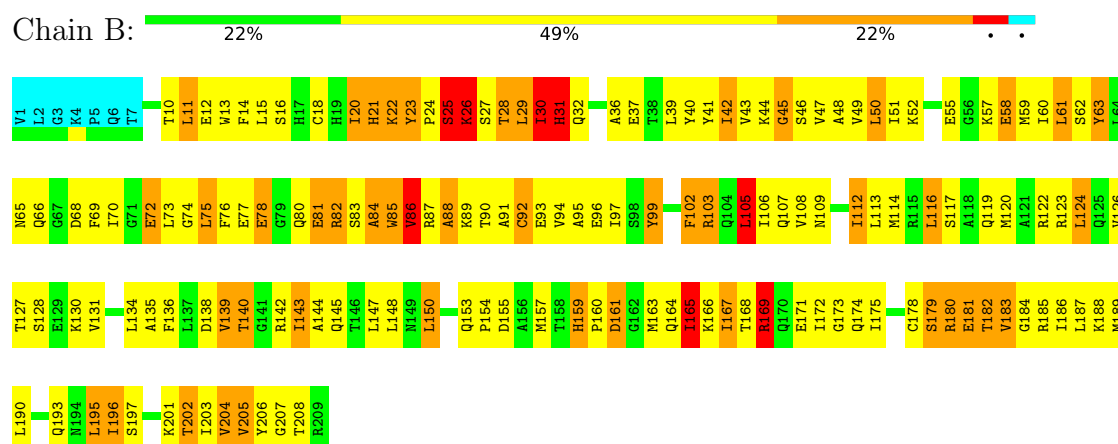
4.1 Average score per residue in the NMR ensemble

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: CATABOLITE GENE ACTIVATOR



• Molecule 1: CATABOLITE GENE ACTIVATOR

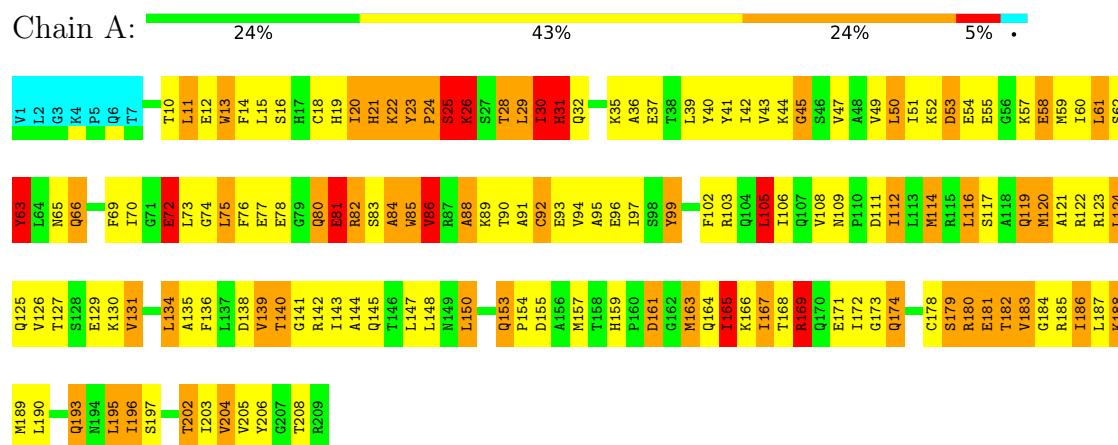


4.2 Scores per residue for each member of the ensemble

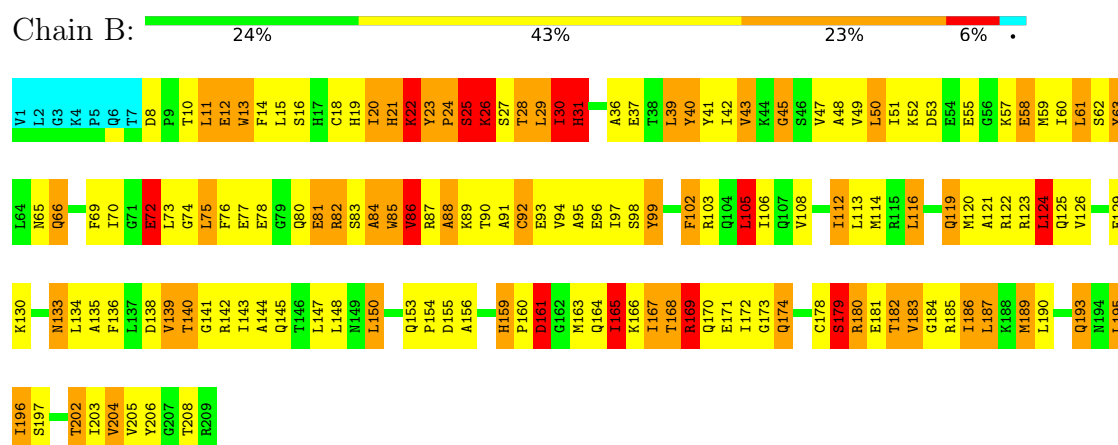
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CATABOLITE GENE ACTIVATOR



• Molecule 1: CATABOLITE GENE ACTIVATOR



4.2.2 Score per residue for model 2

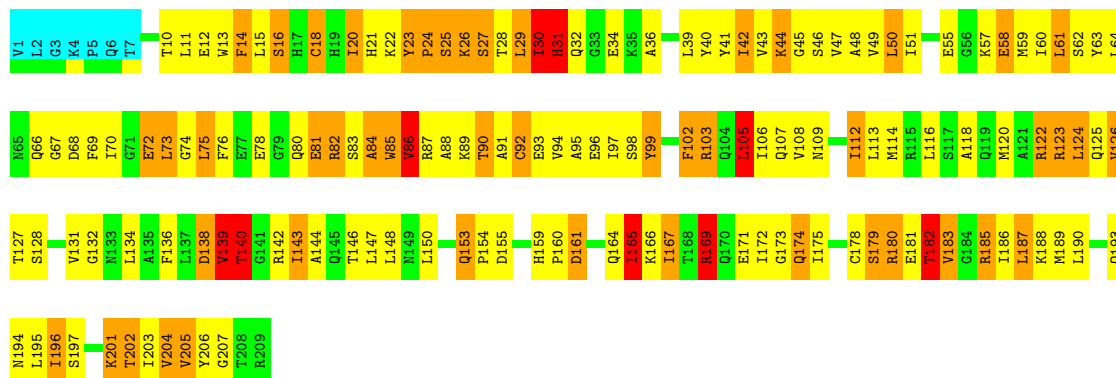
• Molecule 1: CATABOLITE GENE ACTIVATOR





• Molecule 1: CATABOLITE GENE ACTIVATOR

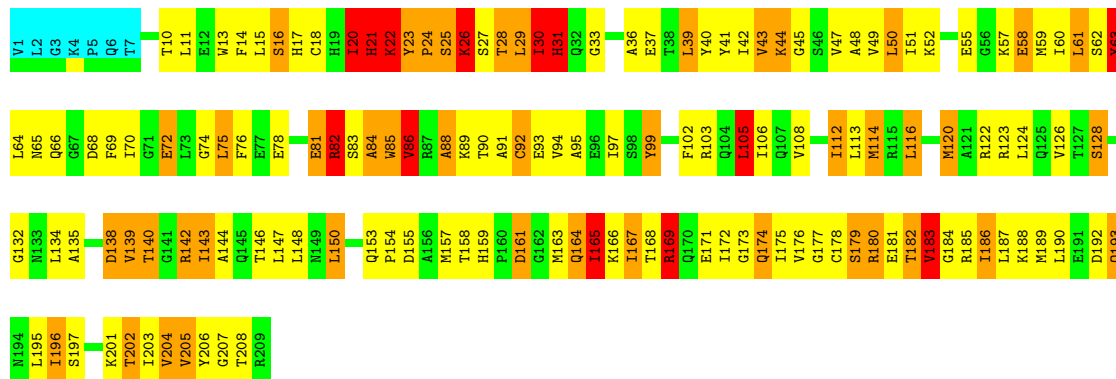
Chain B: 25% 44% 23% • •



4.2.3 Score per residue for model 3 (medoid)

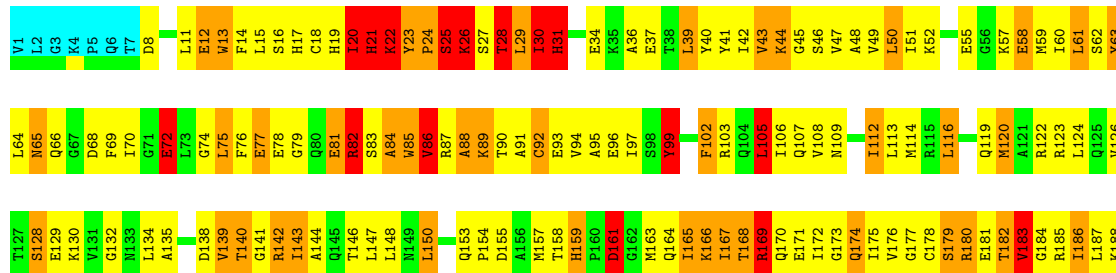
• Molecule 1: CATABOLITE GENE ACTIVATOR

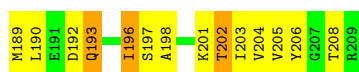
Chain A: 27% 43% 21% 6% •



• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 21% 47% 21% 8% •

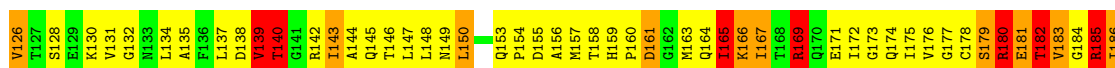
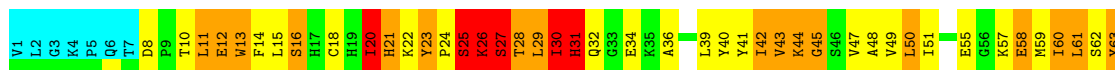




4.2.4 Score per residue for model 4

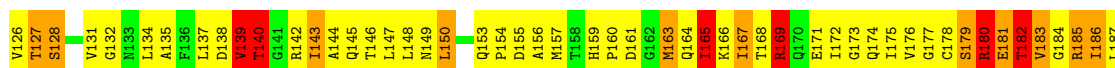
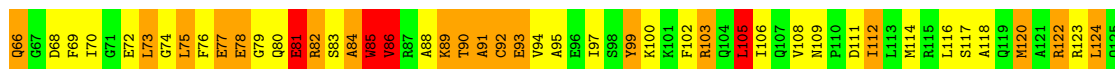
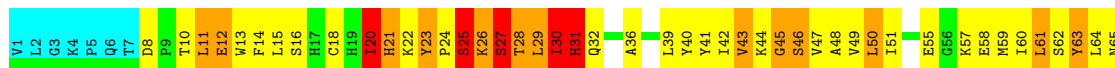
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 22% 44% 23% 7%



- Molecule 1: CATABOLITE GENE ACTIVATOR

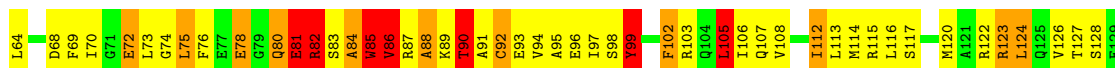
Chain B: 21% 47% 22% 7%

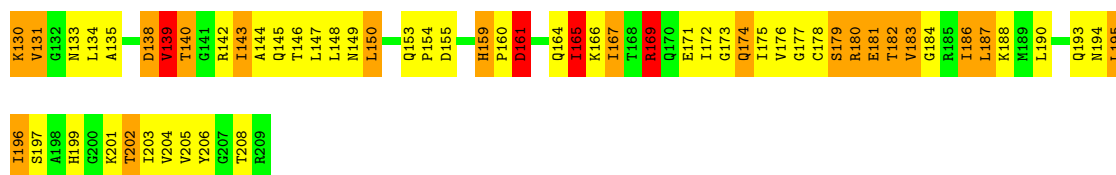


4.2.5 Score per residue for model 5

- Molecule 1: CATABOLITE GENE ACTIVATOR

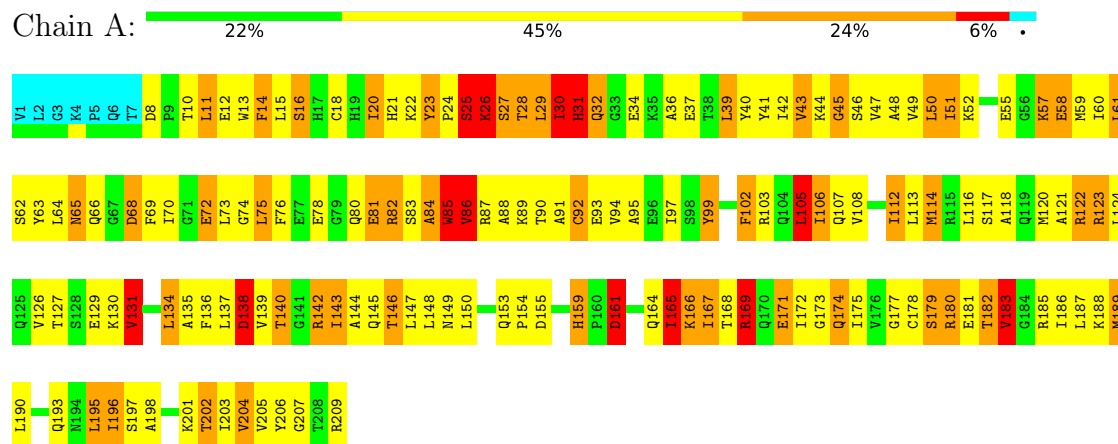
Chain A: 23% 44% 22% 8%



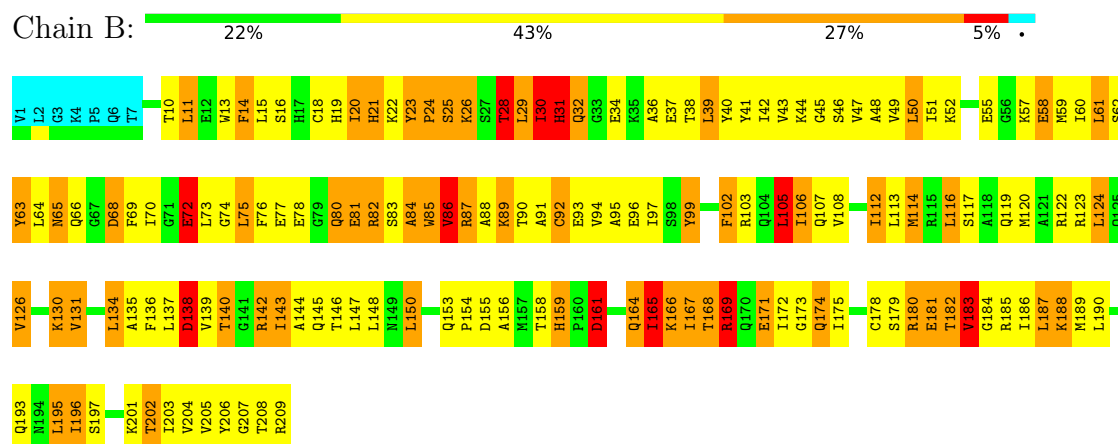


4.2.7 Score per residue for model 7

• Molecule 1: CATABOLITE GENE ACTIVATOR

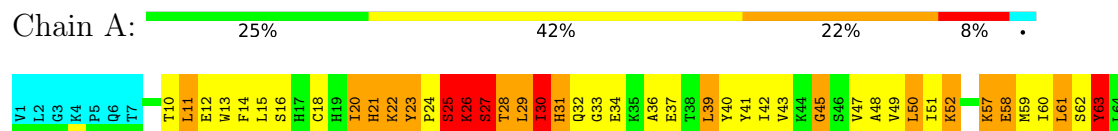


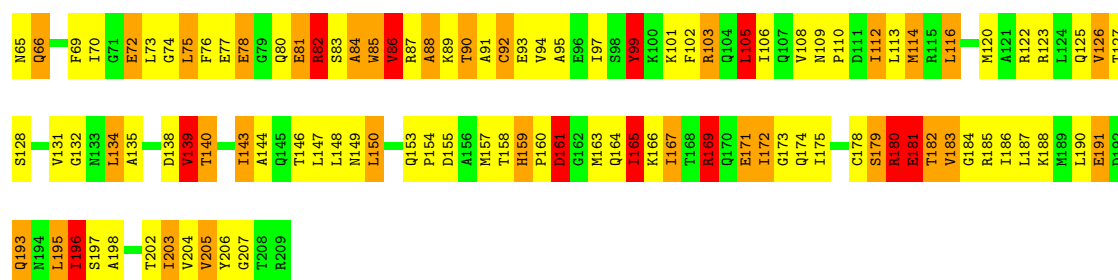
• Molecule 1: CATABOLITE GENE ACTIVATOR



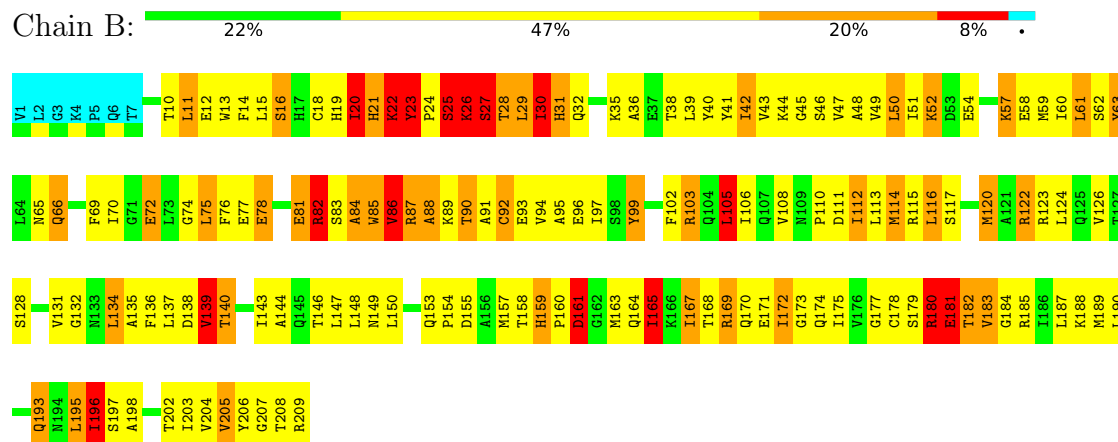
4.2.8 Score per residue for model 8

• Molecule 1: CATABOLITE GENE ACTIVATOR



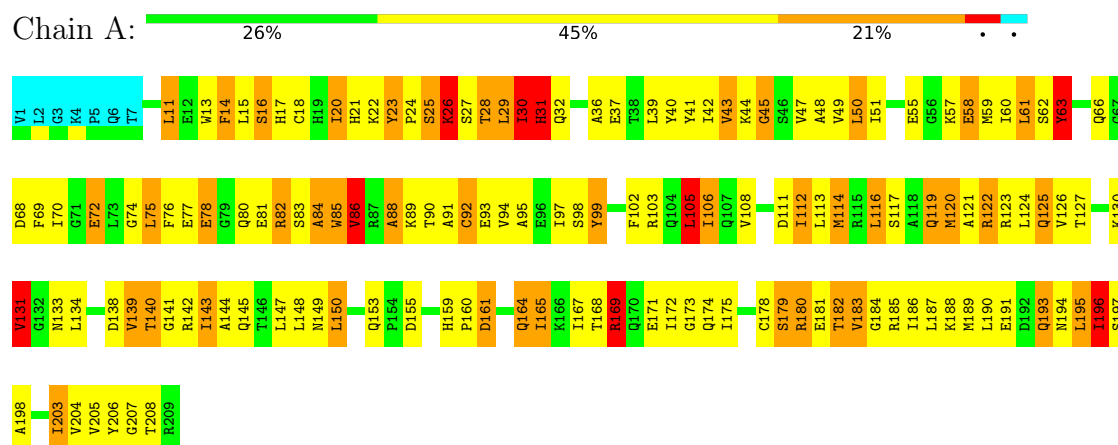


• Molecule 1: CATABOLITE GENE ACTIVATOR

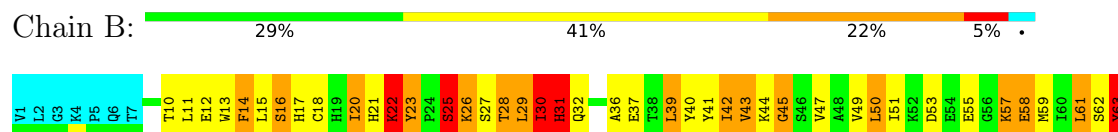


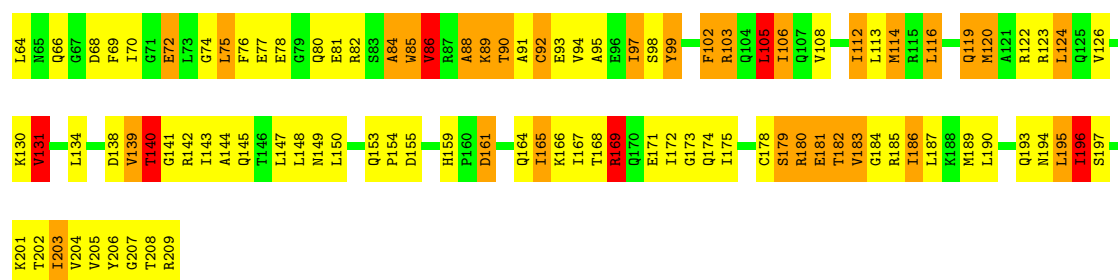
4.2.9 Score per residue for model 9

• Molecule 1: CATABOLITE GENE ACTIVATOR



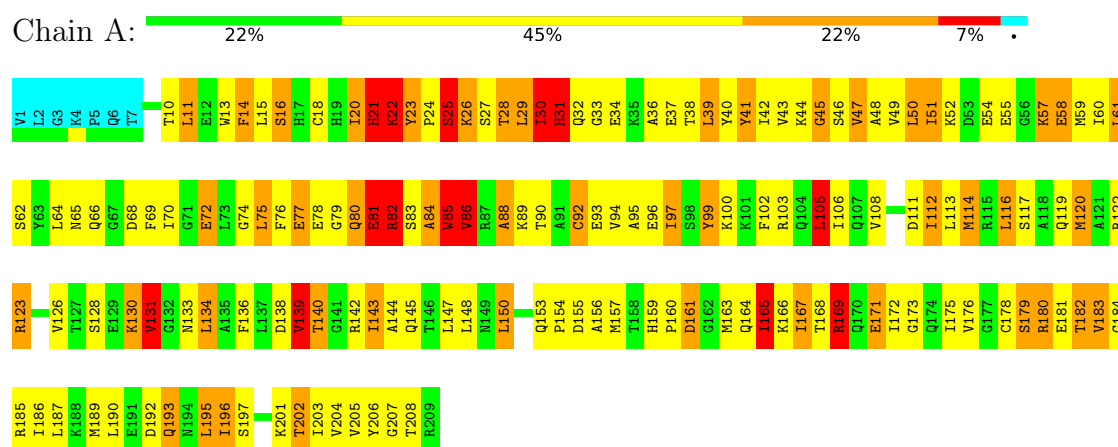
• Molecule 1: CATABOLITE GENE ACTIVATOR



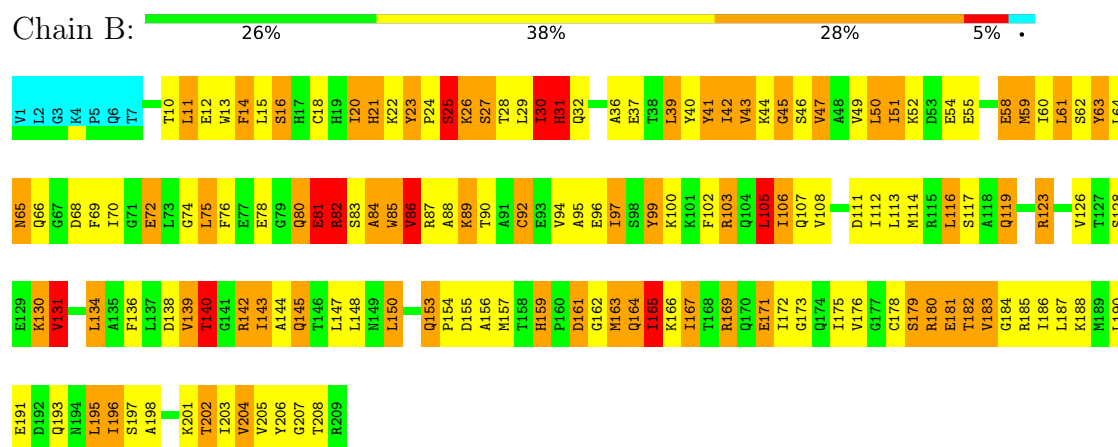


4.2.10 Score per residue for model 10

- Molecule 1: CATABOLITE GENE ACTIVATOR



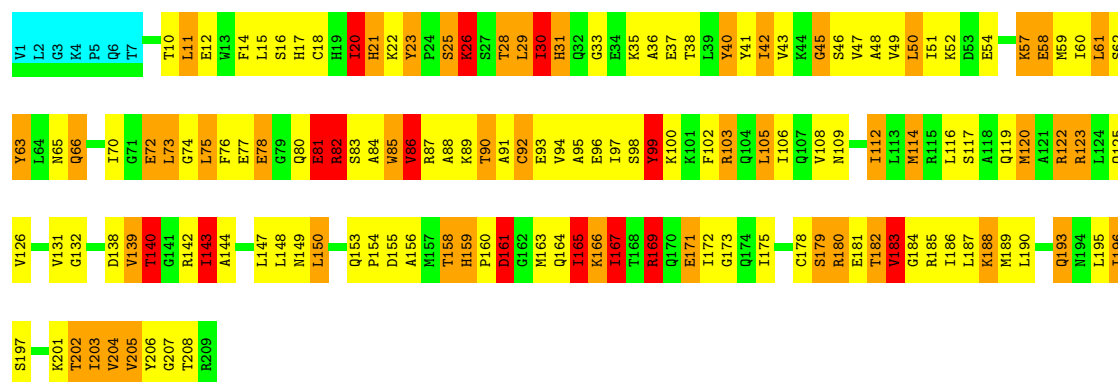
- Molecule 1: CATABOLITE GENE ACTIVATOR



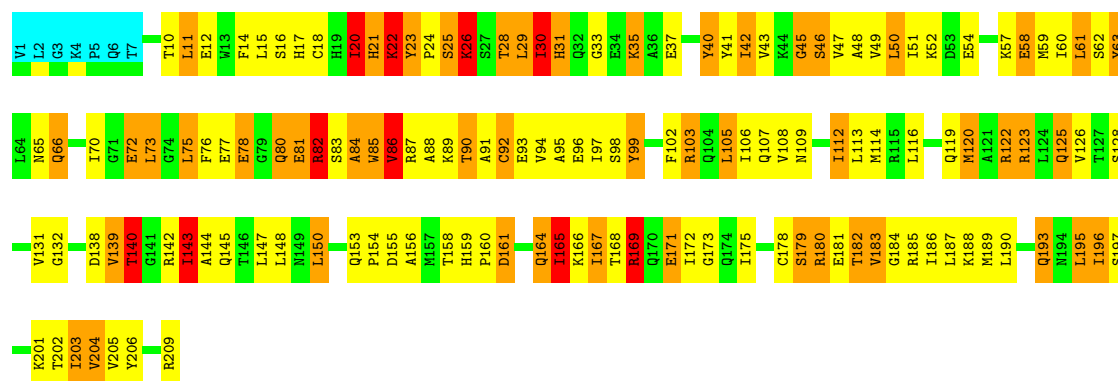
4.2.11 Score per residue for model 11

- Molecule 1: CATABOLITE GENE ACTIVATOR



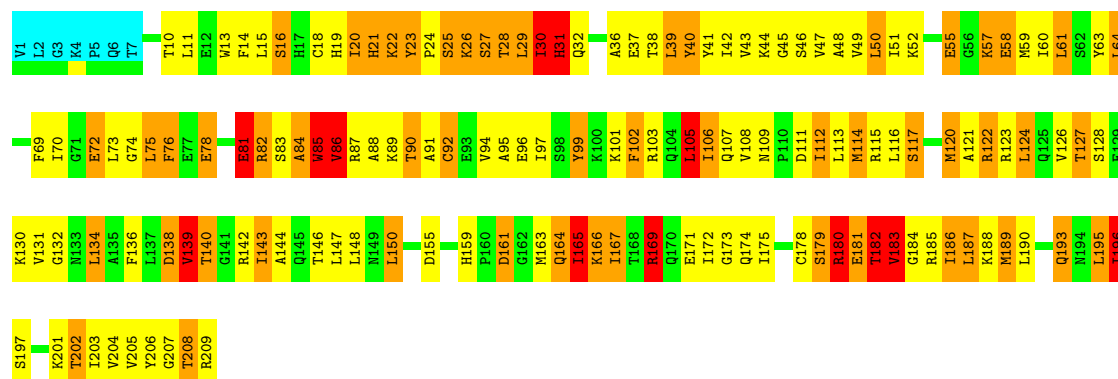
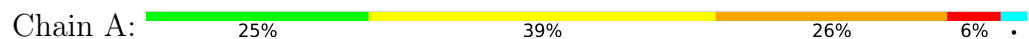


- Molecule 1: CATABOLITE GENE ACTIVATOR

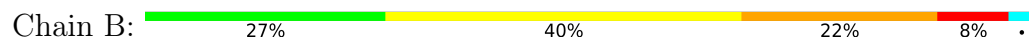


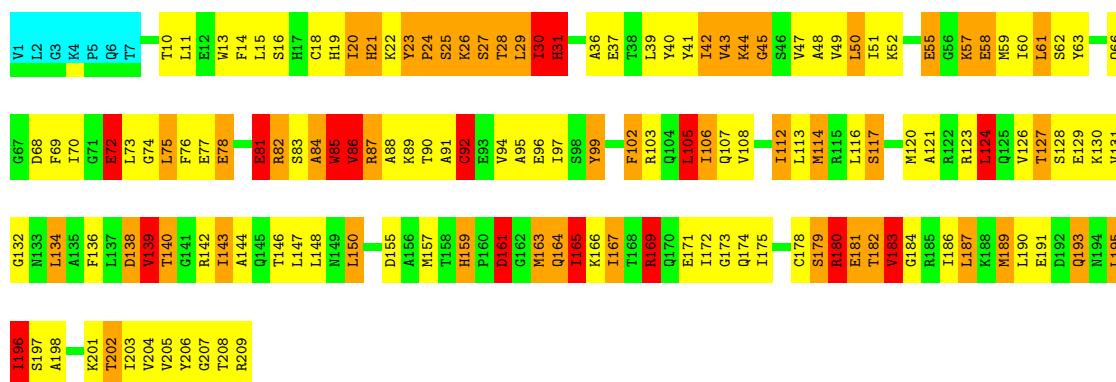
4.2.12 Score per residue for model 12

- Molecule 1: CATABOLITE GENE ACTIVATOR



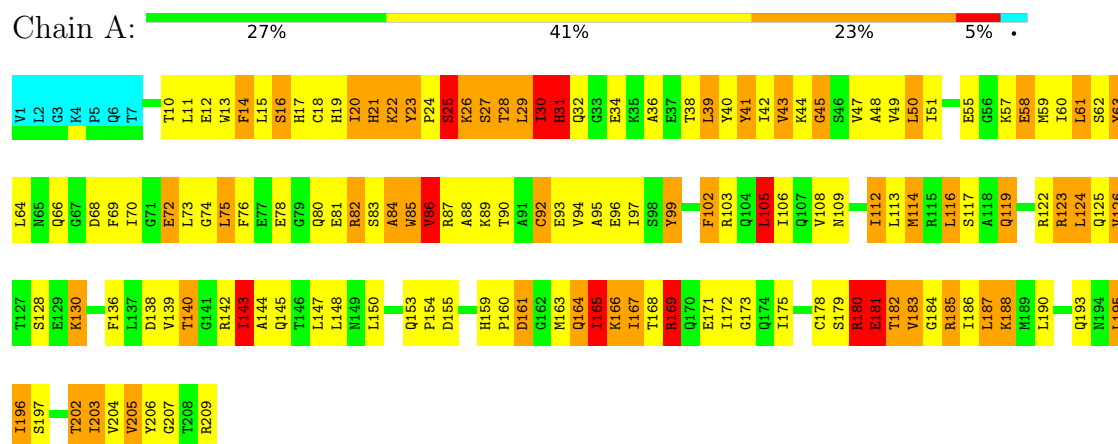
- Molecule 1: CATABOLITE GENE ACTIVATOR



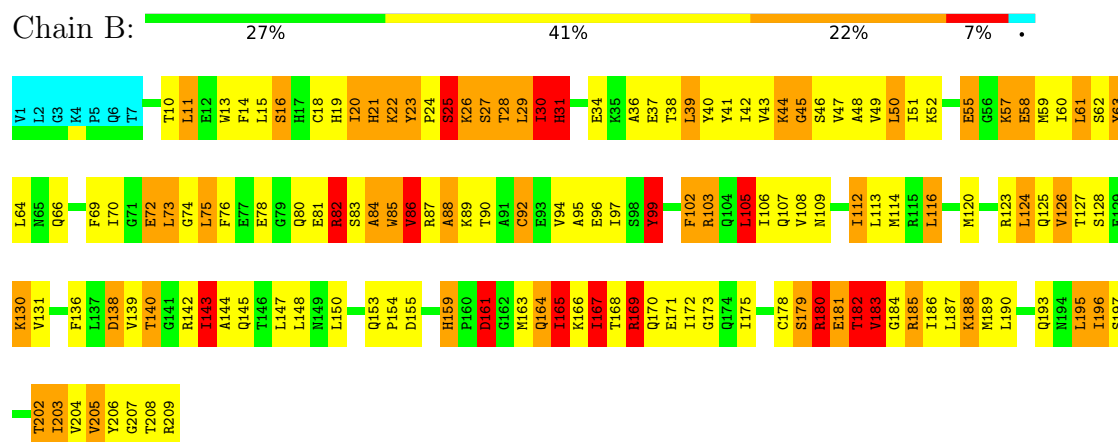


4.2.13 Score per residue for model 13

- Molecule 1: CATABOLITE GENE ACTIVATOR

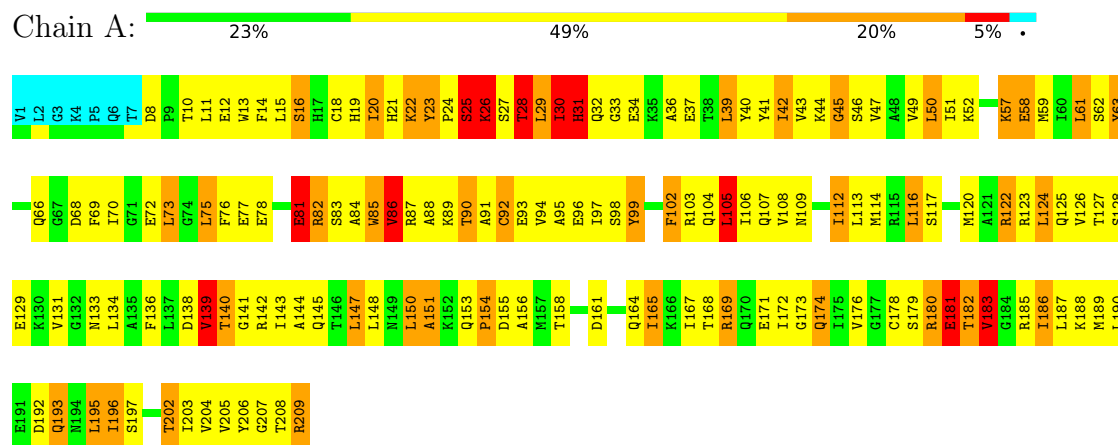


- Molecule 1: CATABOLITE GENE ACTIVATOR

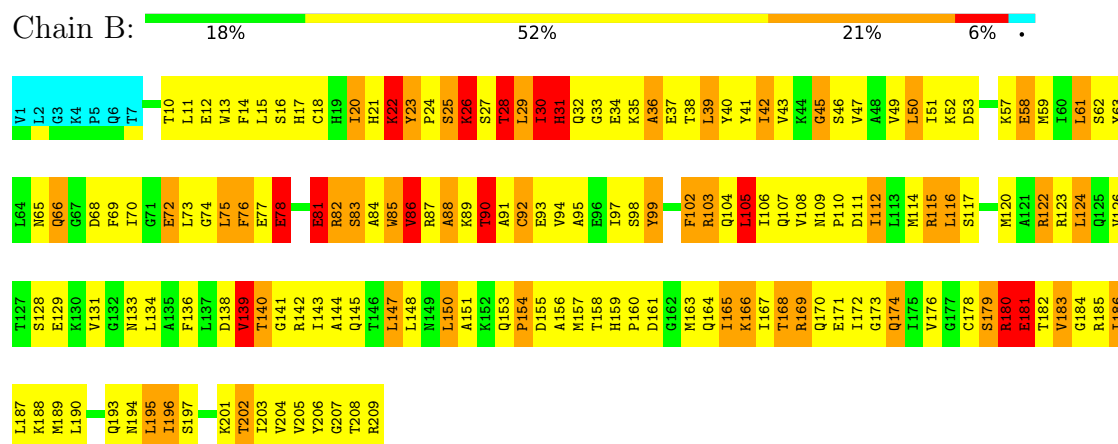


4.2.14 Score per residue for model 14

- Molecule 1: CATABOLITE GENE ACTIVATOR

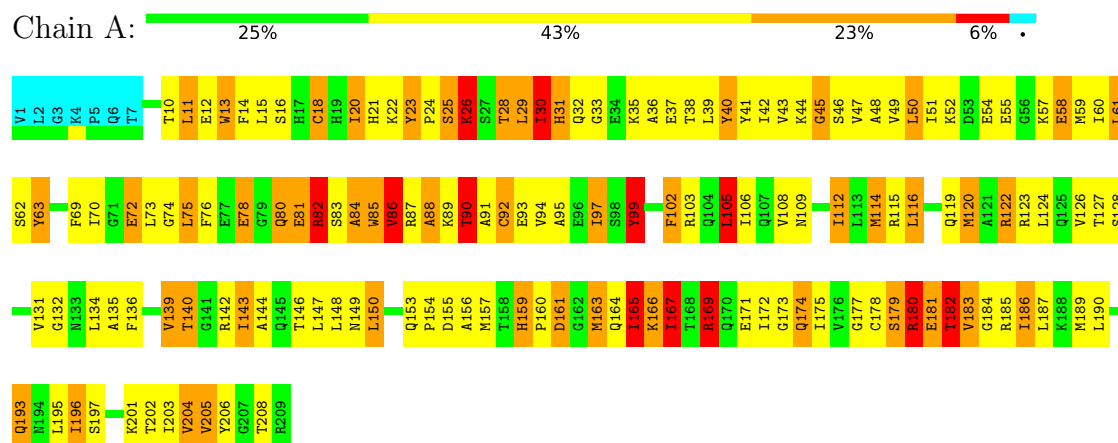


• Molecule 1: CATABOLITE GENE ACTIVATOR

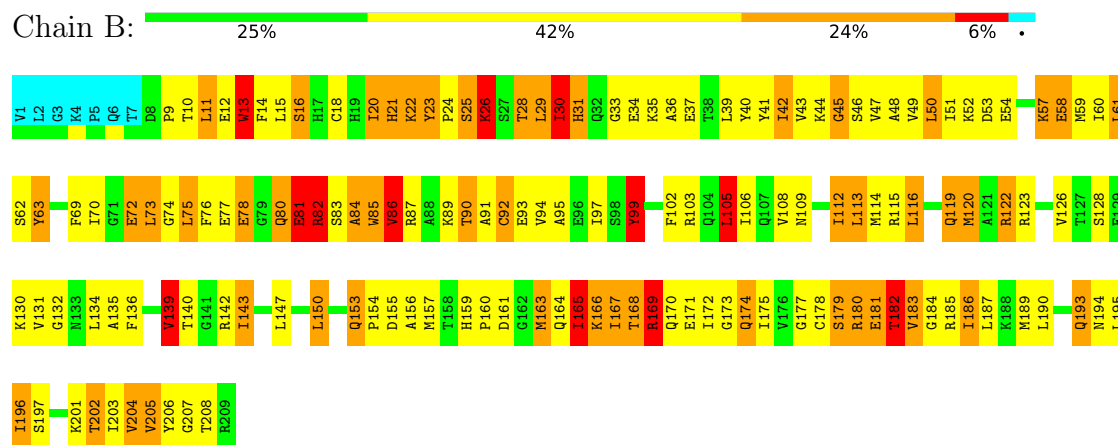


4.2.15 Score per residue for model 15

• Molecule 1: CATABOLITE GENE ACTIVATOR

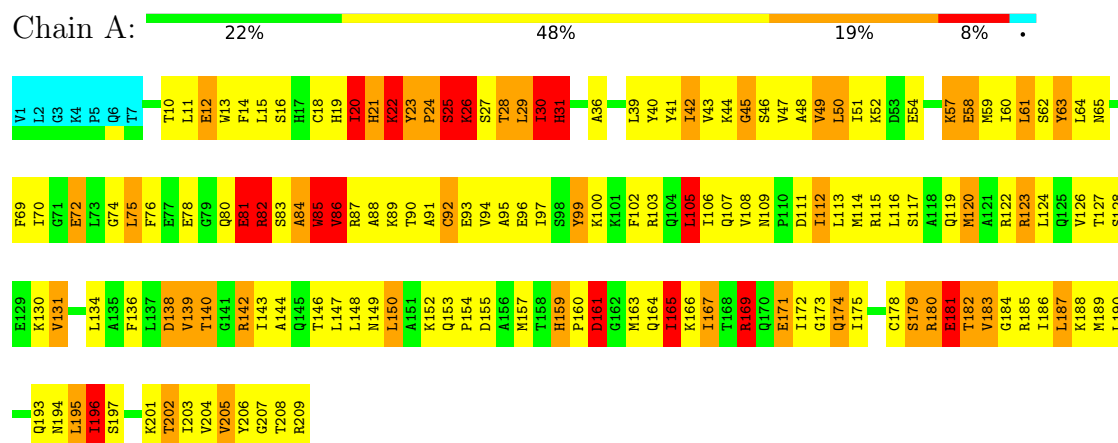


• Molecule 1: CATABOLITE GENE ACTIVATOR

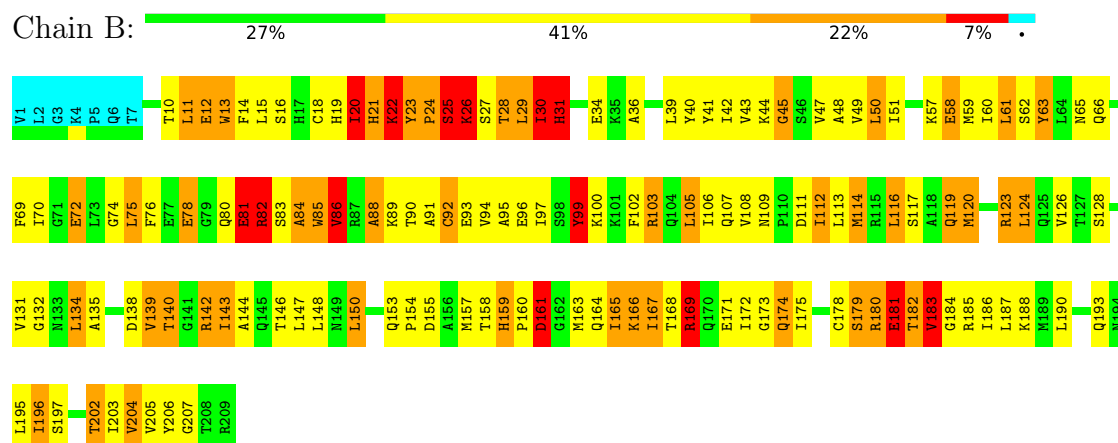


4.2.16 Score per residue for model 16

- Molecule 1: CATABOLITE GENE ACTIVATOR

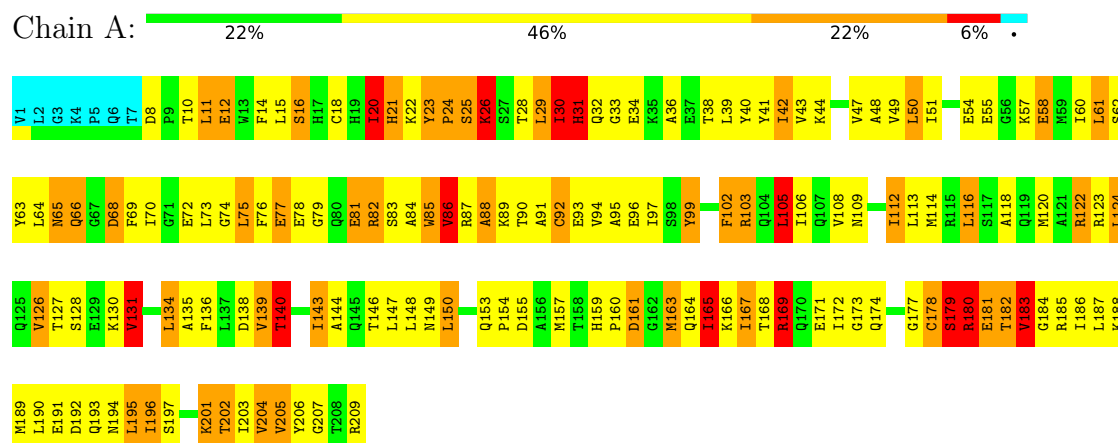


- Molecule 1: CATABOLITE GENE ACTIVATOR

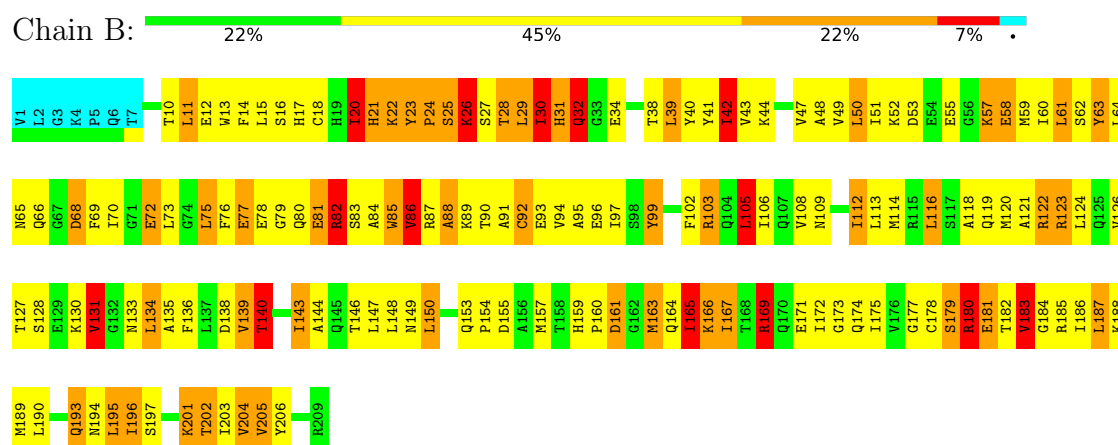


4.2.17 Score per residue for model 17

• Molecule 1: CATABOLITE GENE ACTIVATOR



• Molecule 1: CATABOLITE GENE ACTIVATOR



4.2.18 Score per residue for model 18

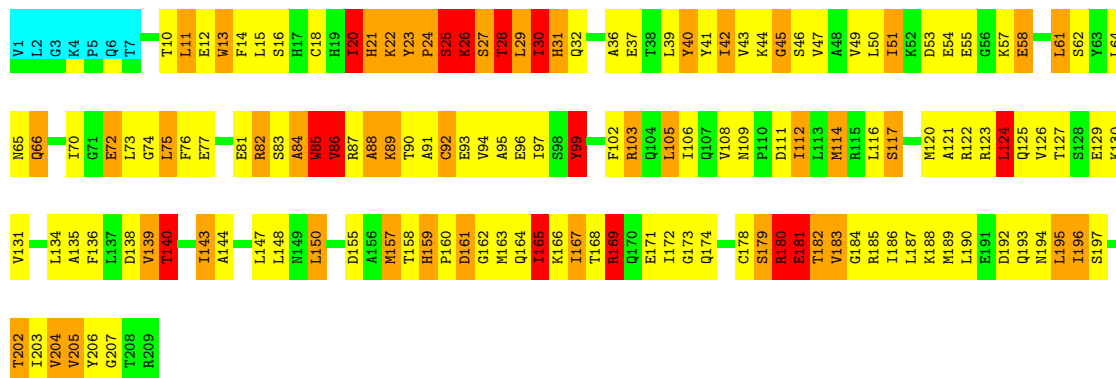
• Molecule 1: CATABOLITE GENE ACTIVATOR





• Molecule 1: CATABOLITE GENE ACTIVATOR

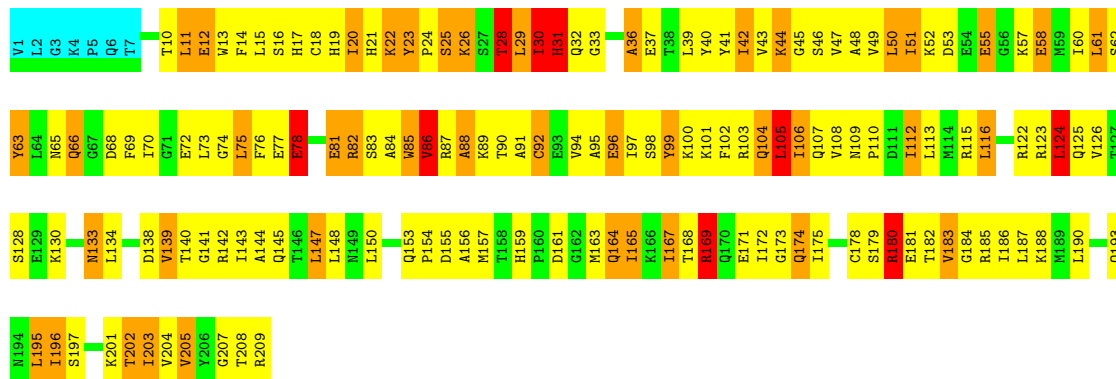
Chain B: 27% 43% 21% 7%



4.2.19 Score per residue for model 19

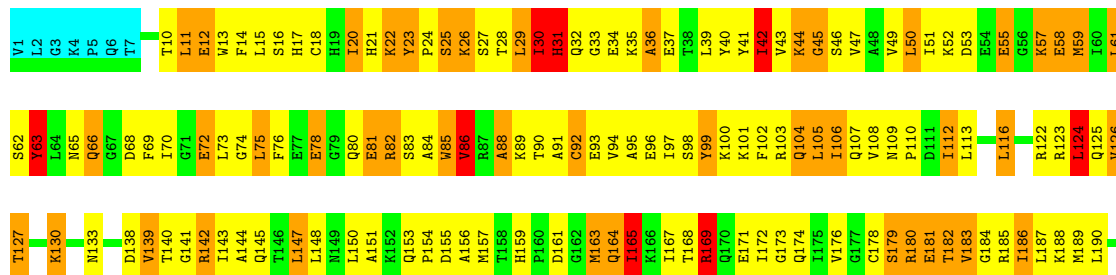
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 23% 49% 21%



• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 23% 46% 24%

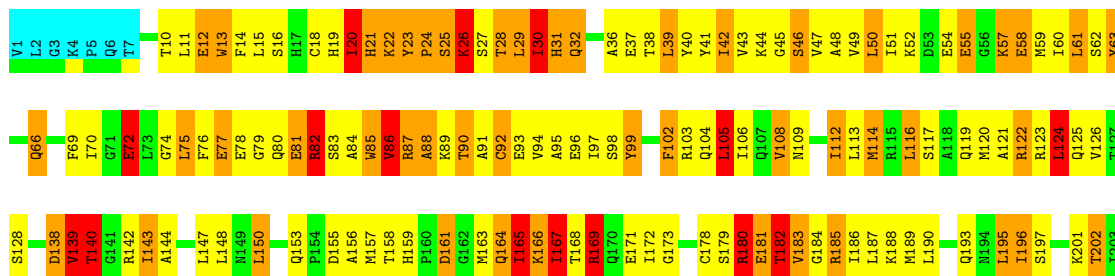




4.2.20 Score per residue for model 20

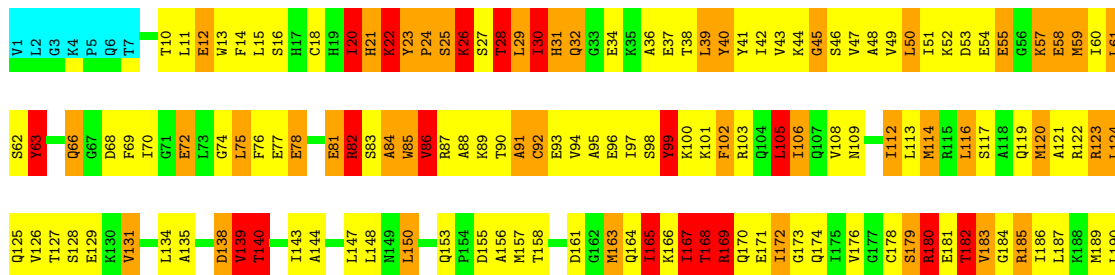
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 25% 41% 23% 7% .



- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 23% 44% 22% 9% .



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
HADDOCK-CNS	refinement	
NMRView	structure solution	
ARIA	structure solution	
HADDOCK	structure solution	
CNS	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	0.93±0.03	2±1/1624 (0.1± 0.1%)	1.39±0.02	21±2/2186 (1.0± 0.1%)
1	B	0.92±0.02	1±1/1624 (0.1± 0.1%)	1.39±0.03	22±3/2186 (1.0± 0.1%)
All	All	0.92	68/64960 (0.1%)	1.39	868/87438 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.6
1	B	0.0±0.0	0.7±0.7
All	All	0	28

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	26	LYS	C-O	-7.44	1.14	1.24	5	16
1	B	26	LYS	C-O	-6.79	1.15	1.24	12	14
1	A	20	ILE	N-CA	6.57	1.53	1.46	4	6
1	B	20	ILE	N-CA	6.40	1.53	1.46	20	7
1	A	27	SER	C-N	-6.09	1.25	1.33	8	3
1	B	21	HIS	C-N	5.87	1.38	1.33	3	1
1	B	27	SER	C-N	-5.84	1.26	1.33	8	3
1	A	66	GLN	C-N	-5.82	1.25	1.33	17	1
1	A	21	HIS	C-N	5.73	1.37	1.33	3	3
1	B	139	VAL	CA-C	5.62	1.59	1.52	12	2
1	B	63	TYR	C-O	-5.59	1.16	1.23	7	1
1	A	31	HIS	CA-C	5.42	1.60	1.52	17	2
1	B	139	VAL	N-CA	5.41	1.53	1.46	8	1
1	A	25	SER	C-N	-5.35	1.26	1.33	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	97	ILE	C-N	-5.16	1.26	1.33	15	1
1	A	27	SER	N-CA	-5.11	1.40	1.46	5	1
1	A	139	VAL	CA-C	5.11	1.59	1.52	20	1
1	A	139	VAL	N-CA	5.05	1.52	1.46	8	1
1	A	183	VAL	C-N	-5.02	1.27	1.33	12	1
1	A	166	LYS	C-N	-5.01	1.27	1.33	4	1
1	A	186	ILE	C-N	-5.00	1.27	1.33	4	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	205	VAL	N-CA-C	-13.15	87.91	107.37	11	19
1	B	138	ASP	N-CA-C	11.64	125.97	112.93	12	5
1	B	205	VAL	N-CA-C	-11.61	90.37	106.85	4	20
1	A	180	ARG	N-CA-C	-11.51	99.28	113.20	17	3
1	A	13	TRP	N-CA-C	-11.22	101.83	114.62	20	18
1	A	138	ASP	N-CA-C	10.85	125.08	112.93	12	5
1	A	171	GLU	N-CA-C	-10.79	99.60	111.36	7	20
1	B	182	THR	N-CA-C	-10.61	99.68	111.14	11	18
1	B	180	ARG	N-CA-C	-10.58	100.39	113.20	14	2
1	B	171	GLU	N-CA-C	-10.52	99.89	111.36	5	20
1	A	182	THR	N-CA-C	-10.17	100.15	111.14	5	17
1	A	105	LEU	N-CA-C	-10.02	99.37	111.69	19	20
1	B	105	LEU	N-CA-C	-9.76	99.69	111.69	17	20
1	B	86	VAL	N-CA-C	9.02	121.89	108.46	18	20
1	B	22	LYS	CA-C-O	9.01	123.17	117.94	18	11
1	A	185	ARG	N-CA-C	-8.87	101.19	111.03	8	16
1	B	185	ARG	N-CA-C	-8.86	101.57	111.14	11	15
1	A	22	LYS	CA-C-O	8.81	123.05	117.94	16	8
1	A	86	VAL	N-CA-C	8.77	122.35	108.85	10	20
1	A	189	MET	N-CA-C	-8.23	102.50	112.54	12	2
1	A	169	ARG	N-CA-C	-7.90	103.53	113.01	12	20
1	B	45	GLY	N-CA-C	-7.85	102.83	112.33	12	14
1	B	169	ARG	N-CA-C	-7.56	103.32	112.54	12	20
1	B	165	ILE	N-CA-C	-7.48	98.48	108.06	19	1
1	B	150	LEU	N-CA-C	-7.48	103.42	112.54	7	19
1	A	25	SER	N-CA-C	7.47	121.03	110.50	7	6
1	A	150	LEU	N-CA-C	-7.41	103.50	112.54	7	19
1	A	28	THR	N-CA-C	-7.35	98.64	110.32	5	14
1	A	88	ALA	N-CA-C	7.21	119.62	110.24	4	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	SER	N-CA-C	-7.12	104.47	113.02	17	19
1	B	28	THR	N-CA-C	-6.94	99.29	110.32	20	15
1	A	66	GLN	CA-C-O	-6.92	113.97	121.44	17	1
1	A	30	ILE	N-CA-CB	6.89	122.60	111.23	20	1
1	A	24	PRO	N-CA-C	-6.86	100.71	111.34	3	8
1	B	16	SER	N-CA-C	-6.85	104.80	113.02	9	18
1	A	91	ALA	N-CA-C	-6.79	99.61	109.59	19	3
1	B	91	ALA	N-CA-C	-6.79	99.61	109.59	19	5
1	A	45	GLY	N-CA-C	-6.75	102.93	110.96	8	15
1	B	24	PRO	N-CA-C	-6.74	100.89	111.34	20	8
1	B	205	VAL	CB-CA-C	6.71	119.77	111.25	2	8
1	B	186	ILE	N-CA-C	6.61	117.36	110.62	4	4
1	A	99	TYR	N-CA-C	-6.56	105.38	113.19	15	5
1	A	168	THR	N-CA-C	-6.56	102.07	110.53	14	5
1	B	168	THR	N-CA-C	-6.50	101.16	110.59	14	8
1	A	205	VAL	CB-CA-C	6.50	119.18	111.32	16	6
1	B	13	TRP	N-CA-C	-6.49	105.52	113.50	20	19
1	B	183	VAL	N-CA-C	-6.48	102.97	112.04	7	6
1	B	99	TYR	N-CA-C	-6.48	105.48	113.19	18	4
1	A	183	VAL	N-CA-C	-6.37	103.12	112.04	7	8
1	B	88	ALA	N-CA-C	6.35	118.50	110.24	17	10
1	A	186	ILE	N-CA-C	6.35	117.09	110.62	15	2
1	A	25	SER	CA-C-N	6.33	133.64	121.54	12	13
1	A	25	SER	C-N-CA	6.33	133.64	121.54	12	13
1	A	137	LEU	CA-C-N	6.30	133.72	122.31	7	1
1	A	137	LEU	C-N-CA	6.30	133.72	122.31	7	1
1	B	43	VAL	CA-C-O	6.28	124.43	118.90	9	8
1	B	22	LYS	N-CA-C	6.28	113.93	108.78	8	5
1	B	25	SER	N-CA-C	6.28	119.02	110.55	17	6
1	A	127	THR	N-CA-C	-6.17	105.23	112.89	7	5
1	A	181	GLU	N-CA-C	6.17	120.99	111.56	8	8
1	A	43	VAL	CA-C-O	6.05	124.23	118.90	3	5
1	B	72	GLU	N-CA-C	-6.04	104.78	111.36	12	8
1	B	100	LYS	N-CA-C	-6.04	104.62	111.14	4	2
1	B	25	SER	CA-C-N	5.99	132.98	121.54	6	11
1	B	25	SER	C-N-CA	5.99	132.98	121.54	6	11
1	A	63	TYR	O-C-N	5.97	129.81	123.42	19	6
1	B	63	TYR	O-C-N	5.96	129.95	123.10	19	3
1	A	12	GLU	N-CA-C	-5.95	105.98	113.18	7	15
1	A	28	THR	CA-C-O	5.95	127.45	120.43	4	1
1	B	181	GLU	N-CA-C	5.92	120.56	112.68	4	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	143	ILE	N-CA-C	5.90	121.61	109.34	4	14
1	A	22	LYS	N-CA-C	5.89	113.61	108.78	10	2
1	A	54	GLU	N-CA-C	-5.88	105.87	113.16	20	6
1	A	143	ILE	N-CA-C	5.87	121.54	109.34	11	13
1	B	12	GLU	N-CA-C	-5.84	106.11	113.18	8	13
1	B	124	LEU	N-CA-C	-5.79	104.97	111.28	1	8
1	B	137	LEU	CA-C-N	5.79	133.83	122.61	7	1
1	B	137	LEU	C-N-CA	5.79	133.83	122.61	7	1
1	B	28	THR	CA-C-O	5.75	126.80	120.31	4	1
1	A	126	VAL	N-CA-C	-5.71	106.90	111.81	17	2
1	B	187	LEU	CB-CA-C	5.67	120.21	110.79	12	2
1	B	127	THR	N-CA-C	-5.65	106.35	113.18	4	5
1	A	182	THR	CA-C-O	5.60	125.30	119.14	14	1
1	B	128	SER	N-CA-C	-5.60	106.62	113.50	4	2
1	A	124	LEU	N-CA-C	-5.59	105.19	112.23	19	5
1	B	85	TRP	CA-C-N	-5.57	113.83	122.69	4	3
1	B	85	TRP	C-N-CA	-5.57	113.83	122.69	4	3
1	B	28	THR	O-C-N	5.56	128.97	123.46	13	1
1	B	189	MET	N-CA-C	-5.55	105.32	111.71	12	1
1	A	28	THR	O-C-N	5.55	128.96	123.46	13	2
1	A	85	TRP	CA-C-N	-5.51	115.28	122.94	12	5
1	A	85	TRP	C-N-CA	-5.51	115.28	122.94	12	5
1	B	54	GLU	N-CA-C	-5.50	106.34	113.16	15	3
1	A	47	VAL	N-CA-C	5.47	115.49	108.82	10	1
1	B	88	ALA	CA-C-O	-5.45	115.76	120.88	13	2
1	A	31	HIS	N-CA-CB	-5.42	101.33	110.49	7	2
1	B	20	ILE	CB-CA-C	-5.40	104.76	111.08	3	1
1	A	32	GLN	N-CA-C	-5.39	106.18	114.16	9	1
1	A	100	LYS	N-CA-C	-5.38	105.49	111.36	4	2
1	A	24	PRO	CA-C-O	5.36	127.78	121.56	5	1
1	A	72	GLU	N-CA-C	-5.33	105.56	111.36	13	5
1	A	30	ILE	CA-CB-CG1	5.32	119.44	110.40	20	1
1	B	87	ARG	N-CA-C	-5.31	100.37	108.76	12	2
1	A	196	ILE	N-CA-CB	5.29	119.96	111.23	16	1
1	B	28	THR	CA-C-N	-5.29	111.44	121.54	10	1
1	B	28	THR	C-N-CA	-5.29	111.44	121.54	10	1
1	A	20	ILE	CB-CA-C	-5.28	104.28	111.15	3	1
1	A	90	THR	CA-C-O	-5.28	115.00	120.70	5	2
1	A	63	TYR	N-CA-C	-5.26	102.68	110.46	6	1
1	B	143	ILE	CB-CA-C	-5.25	102.68	111.29	4	1
1	B	31	HIS	N-CA-CB	-5.24	101.64	110.49	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	165	ILE	O-C-N	-5.23	118.17	123.19	19	1
1	A	78	GLU	N-CA-C	-5.23	104.68	111.74	18	1
1	B	172	ILE	CA-C-O	-5.22	114.98	120.57	20	2
1	A	43	VAL	O-C-N	5.21	127.41	122.20	5	1
1	A	64	LEU	N-CA-CB	5.19	120.03	111.62	12	1
1	B	47	VAL	N-CA-C	5.19	115.15	108.82	10	1
1	B	90	THR	CA-C-O	-5.18	115.11	120.70	14	1
1	B	24	PRO	CA-C-O	5.15	127.95	121.67	12	2
1	B	165	ILE	CA-C-O	-5.13	116.13	120.96	19	1
1	A	31	HIS	CA-CB-CG	5.13	118.93	113.80	19	1
1	A	143	ILE	CB-CA-C	-5.12	102.89	111.29	11	1
1	B	24	PRO	CA-C-N	5.11	128.97	120.94	7	1
1	B	24	PRO	C-N-CA	5.11	128.97	120.94	7	1
1	A	172	ILE	CA-C-O	-5.11	115.10	120.57	6	2
1	B	43	VAL	O-C-N	5.10	127.23	122.23	10	1
1	B	89	LYS	N-CA-C	-5.08	106.17	112.93	10	1
1	A	179	SER	CA-C-O	5.07	127.76	120.51	17	1
1	B	24	PRO	O-C-N	5.05	129.27	123.06	12	1
1	A	151	ALA	N-CA-C	-5.04	107.12	113.28	14	1
1	A	138	ASP	CA-CB-CG	-5.04	107.56	112.60	16	1
1	B	133	ASN	N-CA-C	-5.02	106.33	112.90	17	1
1	B	23	TYR	N-CA-C	5.00	113.89	108.14	8	1
1	B	63	TYR	CA-C-O	5.00	126.58	121.23	20	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	31	HIS	Mainchain	13
1	B	31	HIS	Mainchain	11
1	B	179	SER	Mainchain	1
1	A	138	ASP	Mainchain	1
1	B	138	ASP	Mainchain	1
1	B	92	CYS	Mainchain	1

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	1599	1642	1636	161±12
1	B	1599	1642	1636	162±12
All	All	63960	65680	65440	6322

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 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:O	1:A:66:GLN:CG	1.08	2.02	17	2
1:A:43:VAL:O	1:A:66:GLN:HG3	1.06	1.47	17	3
1:B:43:VAL:O	1:B:66:GLN:CG	1.01	2.08	17	2
1:B:18:CYS:SG	1:B:95:ALA:HB1	0.97	2.00	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG12	0.97	1.32	13	3
1:B:169:ARG:HB3	1:B:187:LEU:HD12	0.96	1.37	20	19
1:A:18:CYS:SG	1:A:95:ALA:HB1	0.96	2.01	18	20
1:B:44:LYS:HA	1:B:66:GLN:HG3	0.94	1.39	17	6
1:A:169:ARG:HB3	1:A:187:LEU:HD12	0.93	1.39	15	20
1:A:153:GLN:OE1	1:A:155:ASP:OD2	0.93	1.87	14	1
1:B:43:VAL:O	1:B:66:GLN:HG3	0.92	1.62	17	2
1:B:153:GLN:OE1	1:B:155:ASP:OD2	0.90	1.89	14	1
1:A:49:VAL:HB	1:A:62:SER:O	0.90	1.65	16	4
1:B:173:GLY:HA2	1:B:178:CYS:O	0.89	1.66	17	19
1:B:49:VAL:HB	1:B:62:SER:O	0.88	1.68	6	3
1:B:51:ILE:O	1:B:58:GLU:HA	0.87	1.68	20	20
1:A:42:ILE:HD11	1:A:46:SER:HA	0.87	1.47	11	8
1:A:135:ALA:HB3	1:B:135:ALA:HB3	0.87	1.45	3	7
1:A:15:LEU:HA	1:A:18:CYS:SG	0.86	2.10	20	20
1:B:22:LYS:HB3	1:B:92:CYS:O	0.86	1.70	12	19
1:A:70:ILE:HG23	1:A:86:VAL:HG21	0.85	1.46	10	15
1:B:40:TYR:O	1:B:70:ILE:HB	0.85	1.71	2	20
1:B:45:GLY:H	1:B:66:GLN:HG2	0.84	1.29	8	8
1:B:42:ILE:HD11	1:B:46:SER:HA	0.84	1.48	11	10
1:A:40:TYR:O	1:A:70:ILE:HB	0.84	1.73	12	20
1:A:45:GLY:H	1:A:66:GLN:HG2	0.84	1.33	19	7
1:A:15:LEU:HB3	1:A:20:ILE:HD11	0.84	1.50	1	14
1:A:190:LEU:HD22	1:A:196:ILE:CG1	0.84	2.03	16	16
1:A:124:LEU:HD21	1:B:124:LEU:HD21	0.83	1.48	18	1
1:A:173:GLY:HA2	1:A:178:CYS:O	0.83	1.72	17	19
1:A:42:ILE:HA	1:A:94:VAL:HG12	0.83	1.50	6	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ILE:O	1:A:58:GLU:HA	0.83	1.74	14	20
1:B:72:GLU:HB3	1:B:116:LEU:HD11	0.82	1.49	7	16
1:B:44:LYS:HA	1:B:66:GLN:CG	0.82	2.05	17	1
1:B:18:CYS:HA	1:B:97:ILE:HG21	0.82	1.51	11	20
1:A:187:LEU:HD22	1:A:190:LEU:HD11	0.81	1.51	13	14
1:B:42:ILE:HA	1:B:94:VAL:HG12	0.81	1.51	11	18
1:B:42:ILE:HD12	1:B:47:VAL:HG13	0.81	1.50	14	10
1:A:41:TYR:HB3	1:A:95:ALA:HB3	0.81	1.52	8	16
1:B:193:GLN:HA	1:B:196:ILE:O	0.81	1.74	8	20
1:B:147:LEU:HD22	1:B:167:ILE:HD13	0.81	1.52	11	5
1:B:41:TYR:HB3	1:B:95:ALA:HB3	0.81	1.52	13	16
1:A:143:ILE:HG12	1:A:183:VAL:HG22	0.80	1.52	20	4
1:A:44:LYS:HA	1:A:66:GLN:HG3	0.80	1.51	17	5
1:A:18:CYS:HA	1:A:97:ILE:HG21	0.80	1.54	8	20
1:B:15:LEU:HB3	1:B:20:ILE:HD11	0.80	1.52	20	11
1:B:164:GLN:HB3	1:B:204:VAL:HG23	0.80	1.51	18	12
1:B:47:VAL:HB	1:B:87:ARG:O	0.80	1.77	15	6
1:B:22:LYS:HG2	1:B:23:TYR:CD1	0.80	2.12	12	19
1:B:37:GLU:HA	1:B:99:TYR:CE2	0.79	2.12	15	14
1:A:20:ILE:HD13	1:A:95:ALA:HB2	0.79	1.52	18	10
1:B:45:GLY:N	1:B:66:GLN:HG2	0.79	1.93	11	8
1:B:196:ILE:HG22	1:B:197:SER:H	0.79	1.38	11	14
1:B:15:LEU:HD22	1:B:20:ILE:HD11	0.78	1.55	17	5
1:B:22:LYS:HG3	1:B:94:VAL:HG22	0.78	1.54	1	17
1:B:20:ILE:HD13	1:B:95:ALA:HB2	0.78	1.55	18	9
1:B:75:LEU:HB2	1:B:99:TYR:CD2	0.78	2.14	17	18
1:A:20:ILE:HG13	1:A:43:VAL:HG21	0.78	1.55	2	1
1:B:146:THR:HG21	1:B:175:ILE:HG21	0.77	1.55	6	9
1:A:59:MET:HE3	1:A:174:GLN:HB3	0.77	1.57	4	1
1:B:43:VAL:O	1:B:66:GLN:HG2	0.77	1.77	17	1
1:A:196:ILE:HG22	1:A:197:SER:H	0.77	1.38	2	13
1:B:44:LYS:CA	1:B:66:GLN:HG3	0.77	2.09	17	1
1:A:51:ILE:HG21	1:B:128:SER:HB3	0.77	1.57	15	9
1:A:128:SER:HB3	1:B:51:ILE:HG21	0.77	1.57	15	11
1:A:193:GLN:HA	1:A:196:ILE:O	0.77	1.80	1	19
1:A:26:LYS:H	1:A:88:ALA:HB3	0.76	1.40	6	7
1:A:48:ALA:HB1	1:A:60:ILE:HD12	0.76	1.55	8	6
1:B:15:LEU:HA	1:B:18:CYS:SG	0.76	2.20	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG13	0.76	1.56	8	11
1:B:49:VAL:HA	1:B:85:TRP:O	0.76	1.81	4	7
1:A:44:LYS:HG2	1:A:66:GLN:NE2	0.76	1.96	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:LYS:HG2	1:B:23:TYR:CE1	0.76	2.15	12	18
1:A:22:LYS:C	1:A:23:TYR:HD1	0.75	1.89	19	15
1:B:26:LYS:H	1:B:88:ALA:HB3	0.75	1.42	10	8
1:A:47:VAL:HB	1:A:87:ARG:O	0.75	1.81	12	4
1:A:72:GLU:HB3	1:A:116:LEU:HD11	0.75	1.56	3	15
1:A:75:LEU:HB2	1:A:99:TYR:CD2	0.75	2.17	2	19
1:B:167:ILE:HD11	1:B:203:ILE:HD12	0.74	1.59	9	2
1:B:172:ILE:HG13	1:B:187:LEU:HD11	0.74	1.59	19	7
1:A:49:VAL:HA	1:A:85:TRP:O	0.74	1.82	7	9
1:B:22:LYS:C	1:B:23:TYR:HD1	0.74	1.90	20	15
1:A:147:LEU:HA	1:A:150:LEU:HD12	0.74	1.58	16	13
1:A:77:GLU:HA	1:B:121:ALA:HB1	0.74	1.58	18	3
1:A:164:GLN:HB3	1:A:204:VAL:HG23	0.74	1.57	5	10
1:B:139:VAL:HG23	1:B:176:VAL:HG11	0.74	1.60	20	4
1:A:22:LYS:HG2	1:A:23:TYR:CD1	0.74	2.18	6	18
1:B:53:ASP:HB3	1:B:55:GLU:OE2	0.73	1.83	19	1
1:A:123:ARG:O	1:A:126:VAL:HG12	0.73	1.83	14	16
1:B:49:VAL:HG12	1:B:61:LEU:HD11	0.73	1.59	19	17
1:A:106:ILE:HD13	1:A:113:LEU:HD13	0.73	1.60	3	11
1:B:47:VAL:HG22	1:B:64:LEU:HD12	0.73	1.60	6	8
1:B:14:PHE:CD2	1:B:105:LEU:HD21	0.73	2.17	2	13
1:A:37:GLU:HA	1:A:99:TYR:CE2	0.73	2.17	1	14
1:A:45:GLY:N	1:A:66:GLN:HG2	0.73	1.98	11	6
1:A:14:PHE:CD2	1:A:105:LEU:HD21	0.73	2.19	7	12
1:A:11:LEU:O	1:A:15:LEU:HG	0.73	1.83	2	20
1:A:42:ILE:HD12	1:A:47:VAL:HG13	0.73	1.60	14	11
1:A:43:VAL:O	1:A:66:GLN:HG2	0.73	1.82	17	1
1:B:20:ILE:HG12	1:B:43:VAL:HG21	0.72	1.61	4	3
1:B:155:ASP:HB3	1:B:165:ILE:CG2	0.72	2.15	9	7
1:B:14:PHE:HD2	1:B:105:LEU:HD21	0.72	1.44	15	4
1:A:123:ARG:HA	1:A:126:VAL:HG12	0.72	1.61	3	5
1:B:75:LEU:HG	1:B:76:PHE:N	0.72	1.98	6	18
1:B:138:ASP:O	1:B:142:ARG:HB2	0.72	1.85	13	8
1:B:99:TYR:O	1:B:103:ARG:HB3	0.71	1.84	14	16
1:A:138:ASP:O	1:A:142:ARG:HB2	0.71	1.85	13	8
1:B:44:LYS:HE2	1:B:66:GLN:OE1	0.71	1.85	19	2
1:A:24:PRO:HA	1:A:91:ALA:HB2	0.71	1.60	5	12
1:B:11:LEU:O	1:B:15:LEU:HG	0.71	1.84	9	20
1:B:36:ALA:HB3	1:B:74:GLY:HA3	0.71	1.61	4	16
1:B:169:ARG:CB	1:B:187:LEU:HD12	0.71	2.15	11	18
1:A:75:LEU:HG	1:A:76:PHE:N	0.71	1.99	6	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PHE:CZ	1:B:121:ALA:HB2	0.71	2.20	12	1
1:B:31:HIS:CE1	1:B:50:LEU:HG	0.71	2.21	8	15
1:B:28:THR:HG23	1:B:86:VAL:O	0.71	1.86	19	1
1:A:190:LEU:HD13	1:A:196:ILE:HD11	0.71	1.62	13	2
1:A:172:ILE:HG13	1:A:187:LEU:HD11	0.71	1.63	9	7
1:B:155:ASP:HB3	1:B:165:ILE:HG22	0.71	1.63	6	20
1:A:44:LYS:HA	1:A:66:GLN:CG	0.70	2.16	17	2
1:B:84:ALA:O	1:B:85:TRP:HB2	0.70	1.87	9	20
1:B:190:LEU:HD22	1:B:196:ILE:CG1	0.70	2.16	12	16
1:A:76:PHE:CD1	1:A:120:MET:HE1	0.70	2.22	14	1
1:A:22:LYS:HB3	1:A:92:CYS:O	0.70	1.86	14	19
1:A:29:LEU:N	1:A:29:LEU:HD23	0.70	2.01	17	15
1:B:29:LEU:HD23	1:B:29:LEU:N	0.70	2.01	17	17
1:B:69:PHE:CD1	1:B:116:LEU:HD12	0.70	2.22	6	8
1:A:20:ILE:HD13	1:A:43:VAL:HG21	0.70	1.62	15	2
1:B:179:SER:C	1:B:181:GLU:H	0.70	1.93	19	20
1:A:141:GLY:O	1:A:145:GLN:HB2	0.70	1.87	1	4
1:B:48:ALA:HB1	1:B:60:ILE:HD12	0.69	1.63	8	4
1:B:46:SER:O	1:B:89:LYS:HB3	0.69	1.87	18	9
1:B:157:MET:O	1:B:163:MET:HA	0.69	1.87	8	12
1:A:169:ARG:CB	1:A:187:LEU:HD12	0.69	2.17	13	17
1:B:187:LEU:HD22	1:B:190:LEU:HD11	0.69	1.62	9	13
1:A:144:ALA:O	1:A:148:LEU:HG	0.69	1.87	19	20
1:B:144:ALA:O	1:B:148:LEU:HG	0.69	1.88	1	19
1:A:179:SER:C	1:A:181:GLU:H	0.69	1.94	8	19
1:A:47:VAL:HG22	1:A:64:LEU:HD12	0.69	1.62	6	10
1:B:72:GLU:HB2	1:B:120:MET:SD	0.69	2.28	12	7
1:A:36:ALA:HB3	1:A:74:GLY:HA3	0.69	1.63	10	18
1:A:22:LYS:HD2	1:A:92:CYS:SG	0.69	2.28	12	9
1:A:69:PHE:CD1	1:A:116:LEU:HD12	0.68	2.24	6	5
1:A:72:GLU:HA	1:A:75:LEU:HD23	0.68	1.65	1	4
1:A:172:ILE:HG22	1:A:183:VAL:HG21	0.68	1.66	10	20
1:A:31:HIS:CD2	1:A:31:HIS:O	0.68	2.46	12	13
1:B:44:LYS:HD2	1:B:66:GLN:CD	0.68	2.14	20	1
1:A:186:ILE:O	1:A:189:MET:HG2	0.68	1.89	11	14
1:A:46:SER:O	1:A:89:LYS:HB3	0.68	1.88	18	10
1:B:11:LEU:HD11	1:B:41:TYR:CE2	0.68	2.24	13	9
1:A:76:PHE:CZ	1:B:117:SER:HB3	0.68	2.24	14	1
1:A:116:LEU:HG	1:A:120:MET:HE1	0.68	1.64	18	1
1:A:106:ILE:HG22	1:A:112:ILE:CG2	0.67	2.20	3	16
1:A:164:GLN:HA	1:A:203:ILE:O	0.67	1.89	9	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:ARG:HD2	1:B:77:GLU:OE2	0.67	1.89	7	4
1:B:141:GLY:O	1:B:145:GLN:HB2	0.67	1.89	1	4
1:A:103:ARG:O	1:A:106:ILE:HG12	0.67	1.89	19	1
1:A:84:ALA:O	1:A:85:TRP:HB2	0.67	1.88	17	20
1:B:187:LEU:HD23	1:B:190:LEU:HD12	0.67	1.64	10	1
1:A:147:LEU:HD22	1:A:167:ILE:HD13	0.67	1.67	11	5
1:A:18:CYS:HA	1:A:97:ILE:CG2	0.67	2.20	14	20
1:B:28:THR:CA	1:B:29:LEU:HD23	0.67	2.20	4	16
1:A:53:ASP:HB3	1:A:55:GLU:OE2	0.67	1.90	19	1
1:A:22:LYS:HG3	1:A:94:VAL:HG22	0.67	1.64	1	18
1:A:106:ILE:HG22	1:A:112:ILE:HG22	0.67	1.65	3	7
1:A:157:MET:O	1:A:163:MET:HA	0.67	1.88	8	11
1:B:29:LEU:C	1:B:30:ILE:HG13	0.67	2.15	1	19
1:B:172:ILE:HG22	1:B:183:VAL:HG21	0.67	1.65	20	20
1:A:29:LEU:O	1:A:30:ILE:HG13	0.67	1.90	20	3
1:A:155:ASP:HB3	1:A:165:ILE:HG22	0.66	1.66	10	20
1:A:103:ARG:O	1:A:107:GLN:HB3	0.66	1.90	14	1
1:A:28:THR:HA	1:A:29:LEU:HD23	0.66	1.66	16	9
1:B:29:LEU:CB	1:B:86:VAL:HB	0.66	2.20	10	2
1:B:44:LYS:HD3	1:B:66:GLN:NE2	0.66	2.05	12	1
1:A:186:ILE:HG22	1:A:187:LEU:HD23	0.66	1.67	16	14
1:A:33:GLY:N	1:A:82:ARG:HD3	0.66	2.05	17	5
1:A:117:SER:HA	1:A:120:MET:SD	0.66	2.31	12	1
1:A:69:PHE:CG	1:A:116:LEU:HD12	0.66	2.25	17	15
1:A:121:ALA:HB2	1:B:76:PHE:CZ	0.66	2.26	12	1
1:B:31:HIS:O	1:B:31:HIS:CD2	0.66	2.49	12	17
1:B:24:PRO:HA	1:B:91:ALA:CB	0.66	2.21	3	8
1:A:22:LYS:HG2	1:A:23:TYR:CE1	0.66	2.26	9	18
1:A:11:LEU:HD12	1:A:15:LEU:HG	0.66	1.67	5	3
1:A:171:GLU:HA	1:A:174:GLN:NE2	0.66	2.06	7	1
1:B:44:LYS:HG2	1:B:66:GLN:NE2	0.66	2.05	17	2
1:A:124:LEU:O	1:A:128:SER:HB2	0.66	1.91	14	1
1:B:186:ILE:O	1:B:190:LEU:HG	0.66	1.91	10	13
1:A:29:LEU:C	1:A:30:ILE:HG13	0.65	2.15	2	19
1:A:41:TYR:HB2	1:A:95:ALA:HB3	0.65	1.68	7	1
1:B:123:ARG:O	1:B:126:VAL:HG12	0.65	1.90	9	16
1:B:196:ILE:HG22	1:B:204:VAL:O	0.65	1.91	4	10
1:B:143:ILE:HG12	1:B:183:VAL:HG22	0.65	1.68	10	5
1:A:11:LEU:HD21	1:A:41:TYR:CE2	0.65	2.26	19	6
1:A:196:ILE:HG22	1:A:204:VAL:O	0.65	1.92	15	4
1:A:197:SER:O	1:A:204:VAL:HB	0.65	1.91	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:CG	1:A:66:GLN:NE2	0.65	2.59	17	1
1:A:28:THR:CA	1:A:29:LEU:HD23	0.65	2.22	4	16
1:A:47:VAL:HA	1:A:89:LYS:H	0.65	1.51	14	6
1:B:164:GLN:HA	1:B:203:ILE:O	0.65	1.90	9	15
1:B:143:ILE:O	1:B:147:LEU:HG	0.65	1.91	5	18
1:A:29:LEU:HD23	1:A:29:LEU:N	0.65	2.05	16	2
1:B:44:LYS:HA	1:B:66:GLN:CD	0.65	2.16	17	1
1:B:103:ARG:O	1:B:106:ILE:HG12	0.65	1.91	19	1
1:A:30:ILE:HD12	1:A:86:VAL:HG21	0.65	1.69	2	3
1:B:186:ILE:HG22	1:B:187:LEU:HD23	0.65	1.68	16	10
1:A:77:GLU:OE2	1:B:122:ARG:HD2	0.65	1.92	9	1
1:B:42:ILE:HD11	1:B:47:VAL:HG13	0.65	1.69	9	1
1:A:31:HIS:CE1	1:A:50:LEU:HG	0.65	2.26	8	15
1:A:39:LEU:HD13	1:A:102:PHE:CZ	0.65	2.27	20	2
1:B:11:LEU:HD21	1:B:41:TYR:CE2	0.65	2.26	2	8
1:A:14:PHE:HD2	1:A:105:LEU:HD21	0.65	1.50	1	5
1:B:18:CYS:HA	1:B:97:ILE:CG2	0.65	2.23	2	20
1:A:144:ALA:HB2	1:A:195:LEU:HD21	0.65	1.66	13	6
1:B:103:ARG:O	1:B:107:GLN:HB3	0.64	1.92	14	3
1:B:44:LYS:CG	1:B:66:GLN:NE2	0.64	2.60	17	1
1:A:20:ILE:O	1:A:21:HIS:HB2	0.64	1.91	20	14
1:A:24:PRO:HA	1:A:91:ALA:CB	0.64	2.22	20	10
1:B:23:TYR:CD1	1:B:23:TYR:N	0.64	2.64	1	19
1:B:24:PRO:HA	1:B:91:ALA:HB2	0.64	1.68	3	12
1:B:47:VAL:HA	1:B:89:LYS:H	0.64	1.52	9	7
1:B:76:PHE:CD1	1:B:120:MET:HE1	0.64	2.27	14	1
1:B:116:LEU:HG	1:B:120:MET:HE1	0.64	1.67	18	1
1:B:20:ILE:O	1:B:21:HIS:HB2	0.64	1.93	1	15
1:A:187:LEU:HD22	1:A:190:LEU:CD1	0.64	2.23	13	16
1:B:20:ILE:HG23	1:B:43:VAL:HG21	0.64	1.68	2	6
1:B:190:LEU:HD13	1:B:196:ILE:HD11	0.64	1.69	9	3
1:B:69:PHE:CG	1:B:116:LEU:HD12	0.64	2.28	13	16
1:A:30:ILE:HD12	1:A:86:VAL:CG2	0.64	2.22	2	8
1:A:69:PHE:CE2	1:A:116:LEU:HA	0.64	2.28	16	7
1:A:166:LYS:HB3	1:A:202:THR:HG22	0.64	1.67	5	1
1:B:31:HIS:CE1	1:B:58:GLU:HB3	0.64	2.27	8	3
1:A:179:SER:HB3	1:A:181:GLU:OE2	0.64	1.93	14	1
1:A:42:ILE:HD11	1:A:47:VAL:HG13	0.64	1.70	12	3
1:A:146:THR:HG21	1:A:175:ILE:HG21	0.64	1.67	6	9
1:A:150:LEU:HD13	1:A:167:ILE:HG12	0.63	1.68	4	8
1:B:47:VAL:O	1:B:63:TYR:HB3	0.63	1.93	9	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:197:SER:HB2	1:B:206:TYR:CE1	0.63	2.28	17	13
1:A:48:ALA:HB1	1:A:60:ILE:HD13	0.63	1.69	16	9
1:B:106:ILE:HD13	1:B:113:LEU:HD13	0.63	1.70	7	11
1:B:123:ARG:HA	1:B:126:VAL:HG12	0.63	1.70	14	5
1:A:20:ILE:HG12	1:A:43:VAL:HG21	0.63	1.69	10	1
1:A:190:LEU:HD13	1:A:196:ILE:HD12	0.63	1.69	14	15
1:B:23:TYR:N	1:B:23:TYR:HD1	0.63	1.91	1	1
1:B:49:VAL:HG22	1:B:85:TRP:O	0.63	1.93	13	17
1:A:18:CYS:CB	1:A:97:ILE:HG12	0.63	2.24	14	12
1:A:22:LYS:C	1:A:23:TYR:CD1	0.63	2.77	2	19
1:A:23:TYR:N	1:A:23:TYR:CD1	0.63	2.67	3	6
1:B:48:ALA:HB1	1:B:60:ILE:HD13	0.63	1.70	15	11
1:B:182:THR:O	1:B:185:ARG:HB2	0.63	1.94	5	5
1:B:70:ILE:HG23	1:B:86:VAL:HG21	0.63	1.68	15	12
1:A:143:ILE:O	1:A:147:LEU:HG	0.63	1.93	18	17
1:B:134:LEU:HD22	1:B:174:GLN:O	0.63	1.94	1	12
1:A:44:LYS:CA	1:A:66:GLN:HG3	0.63	2.23	17	3
1:B:69:PHE:CE2	1:B:116:LEU:HA	0.63	2.28	13	6
1:A:11:LEU:HD11	1:A:41:TYR:CE2	0.63	2.28	11	11
1:A:44:LYS:O	1:A:92:CYS:HB3	0.63	1.94	16	5
1:A:82:ARG:HG2	1:A:83:SER:N	0.63	2.09	17	17
1:A:187:LEU:HA	1:A:190:LEU:HG	0.63	1.68	8	19
1:B:41:TYR:HB2	1:B:95:ALA:HB3	0.63	1.70	7	1
1:A:28:THR:C	1:A:29:LEU:HD23	0.63	2.19	12	17
1:B:42:ILE:HD11	1:B:46:SER:CA	0.63	2.24	18	8
1:B:20:ILE:CG1	1:B:43:VAL:HG21	0.62	2.24	4	4
1:A:87:ARG:HD3	1:A:88:ALA:O	0.62	1.94	11	1
1:A:49:VAL:HG22	1:A:85:TRP:O	0.62	1.94	6	15
1:B:82:ARG:HG2	1:B:83:SER:N	0.62	2.08	12	13
1:A:99:TYR:O	1:A:103:ARG:HB3	0.62	1.94	2	17
1:B:187:LEU:HA	1:B:190:LEU:HG	0.62	1.69	9	19
1:B:59:MET:HE2	1:B:174:GLN:HB3	0.62	1.71	4	1
1:A:47:VAL:O	1:A:63:TYR:HB3	0.62	1.94	9	14
1:B:103:ARG:O	1:B:106:ILE:HG13	0.62	1.95	18	6
1:B:61:LEU:HD12	1:B:62:SER:N	0.62	2.10	19	1
1:A:72:GLU:HB2	1:A:120:MET:SD	0.62	2.35	1	8
1:B:166:LYS:HG2	1:B:202:THR:HG22	0.62	1.70	9	1
1:B:33:GLY:N	1:B:82:ARG:HD3	0.62	2.10	11	2
1:A:155:ASP:HB3	1:A:165:ILE:CG2	0.62	2.24	9	9
1:A:134:LEU:HD22	1:A:174:GLN:O	0.62	1.94	16	11
1:B:31:HIS:CG	1:B:31:HIS:O	0.62	2.53	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:180:ARG:HA	1:B:183:VAL:HG12	0.62	1.72	8	7
1:B:30:ILE:HD12	1:B:86:VAL:CG2	0.61	2.25	1	11
1:B:190:LEU:HD22	1:B:196:ILE:HG13	0.61	1.73	17	13
1:A:197:SER:HB2	1:A:206:TYR:CE1	0.61	2.30	17	13
1:A:60:ILE:HB	1:A:174:GLN:CD	0.61	2.19	3	5
1:B:39:LEU:HD11	1:B:41:TYR:CE1	0.61	2.31	7	1
1:A:42:ILE:CA	1:A:94:VAL:HG12	0.61	2.23	20	15
1:A:49:VAL:HG12	1:A:61:LEU:HD11	0.61	1.72	10	15
1:A:29:LEU:CB	1:A:86:VAL:HB	0.61	2.25	6	1
1:B:190:LEU:HD13	1:B:196:ILE:CD1	0.61	2.26	13	3
1:B:22:LYS:C	1:B:23:TYR:CD1	0.61	2.78	5	19
1:B:186:ILE:O	1:B:189:MET:HG2	0.61	1.94	11	12
1:A:42:ILE:HD11	1:A:46:SER:CA	0.61	2.25	20	7
1:A:117:SER:HB3	1:B:76:PHE:CZ	0.61	2.30	14	1
1:B:11:LEU:HD12	1:B:15:LEU:HG	0.61	1.72	5	4
1:B:87:ARG:HD3	1:B:88:ALA:O	0.61	1.96	11	1
1:B:49:VAL:CG1	1:B:61:LEU:HD11	0.61	2.26	19	1
1:A:103:ARG:HA	1:A:106:ILE:CG1	0.61	2.26	17	17
1:A:31:HIS:O	1:A:31:HIS:CG	0.61	2.54	2	14
1:B:52:LYS:HA	1:B:57:LYS:O	0.61	1.96	7	9
1:B:147:LEU:CD2	1:B:203:ILE:HG21	0.61	2.26	19	1
1:B:25:SER:O	1:B:26:LYS:HG3	0.61	1.96	10	2
1:A:134:LEU:O	1:A:177:GLY:HA3	0.61	1.96	4	5
1:B:42:ILE:CA	1:B:94:VAL:HG12	0.60	2.26	20	16
1:B:150:LEU:HD13	1:B:167:ILE:HG12	0.60	1.73	3	10
1:B:190:LEU:HD13	1:B:196:ILE:HD12	0.60	1.73	20	15
1:B:147:LEU:HD22	1:B:167:ILE:CD1	0.60	2.26	11	4
1:B:166:LYS:HG3	1:B:202:THR:HG23	0.60	1.73	15	1
1:A:49:VAL:HG12	1:A:61:LEU:CD1	0.60	2.27	10	20
1:A:117:SER:HB2	1:B:76:PHE:CE1	0.60	2.31	4	3
1:A:147:LEU:HD22	1:A:167:ILE:CD1	0.60	2.26	7	5
1:B:59:MET:HE3	1:B:174:GLN:HB2	0.60	1.73	3	2
1:A:77:GLU:HG3	1:A:79:GLY:N	0.60	2.11	20	4
1:B:59:MET:HE3	1:B:175:ILE:HA	0.60	1.70	10	1
1:A:43:VAL:C	1:A:66:GLN:HG3	0.60	2.19	17	1
1:A:31:HIS:CG	1:A:31:HIS:O	0.60	2.55	15	4
1:A:131:VAL:HG12	1:B:131:VAL:HG12	0.60	1.73	9	4
1:A:20:ILE:HA	1:A:94:VAL:O	0.60	1.97	12	14
1:B:49:VAL:HG12	1:B:61:LEU:CD1	0.60	2.27	9	19
1:B:20:ILE:HD13	1:B:43:VAL:HG21	0.60	1.72	20	2
1:B:103:ARG:HA	1:B:106:ILE:CG1	0.60	2.26	18	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ILE:CD1	1:A:186:ILE:HD13	0.60	2.27	1	3
1:B:150:LEU:HB3	1:B:165:ILE:HG21	0.60	1.73	11	4
1:A:196:ILE:HG22	1:A:197:SER:N	0.60	2.11	19	12
1:B:28:THR:HA	1:B:29:LEU:HD23	0.60	1.72	1	7
1:B:50:LEU:CB	1:B:60:ILE:HA	0.60	2.26	10	12
1:A:23:TYR:CD1	1:A:23:TYR:N	0.60	2.70	17	12
1:B:147:LEU:HA	1:B:150:LEU:HD12	0.60	1.74	5	12
1:A:44:LYS:HE2	1:A:66:GLN:OE1	0.60	1.95	19	1
1:A:19:HIS:HB3	1:A:96:GLU:O	0.60	1.97	1	7
1:B:41:TYR:O	1:B:43:VAL:HG23	0.60	1.97	11	11
1:B:42:ILE:HD11	1:B:64:LEU:HD12	0.60	1.72	10	2
1:A:48:ALA:CB	1:A:60:ILE:HD12	0.60	2.27	3	4
1:A:41:TYR:CB	1:A:95:ALA:HB3	0.60	2.26	7	6
1:B:89:LYS:CE	1:B:155:ASP:OD1	0.60	2.50	10	1
1:A:37:GLU:HA	1:A:99:TYR:CZ	0.60	2.31	11	4
1:B:28:THR:HA	1:B:87:ARG:HA	0.60	1.71	15	4
1:A:143:ILE:HD13	1:A:186:ILE:HG21	0.59	1.72	8	2
1:A:173:GLY:CA	1:A:178:CYS:O	0.59	2.50	14	3
1:A:180:ARG:O	1:A:184:GLY:HA3	0.59	1.97	19	14
1:B:196:ILE:HG22	1:B:209:ARG:OXT	0.59	1.96	9	1
1:B:44:LYS:O	1:B:92:CYS:HB3	0.59	1.96	16	6
1:B:159:HIS:CE1	1:B:161:ASP:HB3	0.59	2.33	18	5
1:A:51:ILE:HD12	1:A:61:LEU:HB3	0.59	1.74	7	1
1:A:63:TYR:O	1:A:64:LEU:HD23	0.59	1.97	12	1
1:A:63:TYR:CD2	1:A:89:LYS:HD2	0.59	2.32	18	2
1:B:28:THR:C	1:B:29:LEU:HD23	0.59	2.22	12	15
1:A:28:THR:HA	1:A:87:ARG:HA	0.59	1.73	11	4
1:B:179:SER:HB2	1:B:181:GLU:OE2	0.59	1.98	14	1
1:A:53:ASP:HB2	1:A:57:LYS:HG2	0.59	1.74	1	2
1:B:31:HIS:CE1	1:B:58:GLU:HB2	0.59	2.32	1	5
1:B:106:ILE:HG22	1:B:112:ILE:CG2	0.59	2.27	17	14
1:A:122:ARG:NH2	1:B:78:GLU:HB3	0.59	2.13	19	6
1:A:31:HIS:CE1	1:A:58:GLU:HB3	0.59	2.31	8	4
1:A:103:ARG:O	1:A:106:ILE:HG13	0.59	1.97	1	9
1:B:196:ILE:HG22	1:B:197:SER:N	0.59	2.12	19	10
1:A:76:PHE:CE2	1:A:120:MET:HG3	0.59	2.33	12	1
1:B:197:SER:HG	1:B:206:TYR:HE1	0.59	1.41	19	1
1:B:27:SER:O	1:B:88:ALA:N	0.59	2.32	13	3
1:A:195:LEU:O	1:A:209:ARG:HB3	0.59	1.98	20	1
1:B:134:LEU:O	1:B:177:GLY:HA3	0.59	1.97	4	6
1:B:180:ARG:O	1:B:184:GLY:HA3	0.59	1.98	12	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PRO:HA	1:A:91:ALA:CA	0.59	2.28	12	10
1:A:77:GLU:OE2	1:B:122:ARG:HA	0.59	1.97	9	1
1:B:50:LEU:HB3	1:B:60:ILE:HG22	0.59	1.75	10	1
1:B:22:LYS:HD2	1:B:92:CYS:SG	0.58	2.38	15	13
1:B:47:VAL:HA	1:B:89:LYS:N	0.58	2.12	12	15
1:B:102:PHE:CE1	1:B:106:ILE:HG21	0.58	2.33	12	9
1:A:182:THR:O	1:A:185:ARG:HB2	0.58	1.97	4	6
1:A:27:SER:O	1:A:88:ALA:N	0.58	2.34	13	3
1:A:102:PHE:CE1	1:A:106:ILE:HG21	0.58	2.32	12	9
1:B:169:ARG:CB	1:B:187:LEU:HD13	0.58	2.28	10	1
1:B:51:ILE:HD12	1:B:61:LEU:HB3	0.58	1.72	18	1
1:A:23:TYR:HD1	1:A:23:TYR:N	0.58	1.96	3	7
1:B:42:ILE:HG21	1:B:45:GLY:O	0.58	1.98	2	1
1:B:196:ILE:HG13	1:B:197:SER:N	0.58	2.14	13	1
1:B:99:TYR:HA	1:B:102:PHE:HB3	0.58	1.76	20	14
1:B:43:VAL:C	1:B:66:GLN:HG3	0.58	2.23	17	1
1:B:179:SER:C	1:B:181:GLU:N	0.58	2.61	14	19
1:B:69:PHE:CG	1:B:116:LEU:HD13	0.58	2.34	2	1
1:B:172:ILE:CG2	1:B:183:VAL:HG21	0.58	2.28	14	8
1:A:11:LEU:HD11	1:A:41:TYR:HE2	0.58	1.59	5	4
1:A:123:ARG:CA	1:A:126:VAL:HG12	0.58	2.28	3	2
1:A:31:HIS:O	1:A:31:HIS:CD2	0.58	2.56	10	4
1:B:31:HIS:O	1:B:31:HIS:CG	0.58	2.56	12	11
1:A:102:PHE:CE2	1:A:106:ILE:HG23	0.58	2.33	3	1
1:A:72:GLU:CB	1:A:116:LEU:HD11	0.58	2.28	7	5
1:A:20:ILE:CG1	1:A:43:VAL:HG21	0.58	2.29	2	1
1:B:139:VAL:HA	1:B:176:VAL:CG1	0.58	2.29	3	1
1:A:30:ILE:HG22	1:A:34:GLU:HB2	0.58	1.74	10	3
1:A:143:ILE:HG21	1:A:187:LEU:HD21	0.58	1.75	10	4
1:A:123:ARG:HA	1:A:126:VAL:CG1	0.57	2.29	14	2
1:A:41:TYR:O	1:A:43:VAL:HG23	0.57	1.98	11	9
1:A:70:ILE:HD13	1:A:86:VAL:HG11	0.57	1.76	13	14
1:A:186:ILE:O	1:A:190:LEU:HG	0.57	2.00	17	13
1:B:70:ILE:HD13	1:B:86:VAL:HG11	0.57	1.76	20	14
1:A:52:LYS:HA	1:A:57:LYS:O	0.57	1.98	7	12
1:B:60:ILE:HB	1:B:174:GLN:CD	0.57	2.25	7	5
1:B:28:THR:HA	1:B:29:LEU:HD22	0.57	1.77	13	1
1:A:72:GLU:CB	1:A:120:MET:HE1	0.57	2.29	4	1
1:A:117:SER:HB2	1:B:76:PHE:CZ	0.57	2.34	4	5
1:B:117:SER:HA	1:B:120:MET:CE	0.57	2.29	4	1
1:B:61:LEU:HD22	1:B:62:SER:HB2	0.57	1.75	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD22	1:A:20:ILE:HD11	0.57	1.76	17	3
1:B:169:ARG:CG	1:B:187:LEU:HD12	0.57	2.30	2	2
1:B:190:LEU:CD1	1:B:196:ILE:HD12	0.57	2.29	18	12
1:B:174:GLN:HG2	1:B:175:ILE:N	0.57	2.14	6	3
1:A:28:THR:HB	1:A:87:ARG:HA	0.57	1.76	2	4
1:B:138:ASP:CG	1:B:138:ASP:O	0.57	2.48	12	2
1:B:104:GLN:O	1:B:107:GLN:HG2	0.57	2.00	19	1
1:A:138:ASP:CG	1:A:138:ASP:O	0.57	2.48	20	1
1:A:53:ASP:HB2	1:A:57:LYS:CG	0.56	2.30	1	1
1:B:187:LEU:HD22	1:B:190:LEU:CD1	0.56	2.30	1	15
1:A:41:TYR:O	1:A:43:VAL:HG13	0.56	2.00	19	4
1:B:169:ARG:HB3	1:B:187:LEU:HD13	0.56	1.75	10	1
1:A:23:TYR:N	1:A:23:TYR:HD1	0.56	1.98	16	1
1:A:172:ILE:CG2	1:A:183:VAL:HG21	0.56	2.30	14	8
1:B:197:SER:HB3	1:B:206:TYR:CE1	0.56	2.35	15	6
1:A:22:LYS:H	1:A:93:GLU:HA	0.56	1.59	17	17
1:B:166:LYS:HA	1:B:201:LYS:O	0.56	2.01	10	6
1:B:167:ILE:CD1	1:B:203:ILE:HD12	0.56	2.30	10	10
1:B:11:LEU:HD11	1:B:41:TYR:HE2	0.56	1.61	5	1
1:B:114:MET:HA	1:B:117:SER:OG	0.56	2.00	7	7
1:B:144:ALA:HB2	1:B:195:LEU:HD21	0.56	1.77	9	5
1:B:190:LEU:HD22	1:B:196:ILE:HG12	0.56	1.77	13	3
1:B:18:CYS:CB	1:B:97:ILE:HG12	0.56	2.31	6	16
1:A:14:PHE:CD1	1:A:14:PHE:C	0.56	2.83	10	8
1:B:37:GLU:HA	1:B:99:TYR:CZ	0.56	2.36	11	3
1:A:44:LYS:HA	1:A:66:GLN:CD	0.56	2.24	17	1
1:B:119:GLN:O	1:B:123:ARG:HD3	0.56	2.00	7	9
1:A:113:LEU:HD12	1:A:116:LEU:HD23	0.56	1.76	2	1
1:A:59:MET:HE3	1:A:174:GLN:HB2	0.56	1.76	6	2
1:B:39:LEU:HD11	1:B:41:TYR:HE1	0.56	1.61	7	1
1:A:147:LEU:CD2	1:A:203:ILE:HG21	0.56	2.30	19	2
1:B:23:TYR:HD1	1:B:23:TYR:N	0.56	1.98	3	6
1:A:49:VAL:N	1:A:62:SER:O	0.56	2.39	14	13
1:A:118:ALA:O	1:A:122:ARG:HB2	0.56	2.01	2	4
1:B:173:GLY:CA	1:B:178:CYS:O	0.56	2.54	14	3
1:B:65:ASN:O	1:B:68:ASP:HB2	0.56	2.01	7	4
1:B:20:ILE:HG13	1:B:95:ALA:HB2	0.56	1.76	4	1
1:B:42:ILE:HG22	1:B:68:ASP:H	0.56	1.59	12	2
1:A:89:LYS:CE	1:A:155:ASP:OD1	0.56	2.53	10	1
1:B:109:ASN:CG	1:B:112:ILE:HG13	0.56	2.25	14	2
1:B:22:LYS:CG	1:B:94:VAL:HG22	0.56	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:VAL:N	1:B:62:SER:O	0.56	2.39	14	14
1:B:149:ASN:O	1:B:153:GLN:HG3	0.56	2.00	8	2
1:B:53:ASP:HB2	1:B:57:LYS:CG	0.56	2.31	1	1
1:B:167:ILE:HD12	1:B:203:ILE:HD12	0.56	1.76	11	2
1:A:187:LEU:CD2	1:A:190:LEU:HD11	0.56	2.31	8	4
1:B:197:SER:O	1:B:204:VAL:HB	0.56	2.01	9	3
1:B:166:LYS:HG2	1:B:202:THR:HG23	0.56	1.77	13	1
1:A:22:LYS:HB3	1:A:92:CYS:C	0.55	2.26	2	9
1:A:149:ASN:O	1:A:153:GLN:HG3	0.55	2.01	8	2
1:B:63:TYR:CD2	1:B:89:LYS:HD2	0.55	2.35	8	2
1:A:29:LEU:HD12	1:A:40:TYR:CD1	0.55	2.36	10	1
1:B:183:VAL:HG13	1:B:187:LEU:HD12	0.55	1.77	10	1
1:B:20:ILE:HA	1:B:94:VAL:O	0.55	2.01	1	16
1:B:167:ILE:HD11	1:B:203:ILE:CD1	0.55	2.29	9	1
1:B:53:ASP:OD1	1:B:57:LYS:HB3	0.55	2.02	14	1
1:A:169:ARG:HB2	1:A:180:ARG:HB3	0.55	1.78	2	14
1:A:179:SER:C	1:A:181:GLU:N	0.55	2.65	13	19
1:B:18:CYS:HB3	1:B:97:ILE:HG12	0.55	1.78	14	14
1:B:169:ARG:HB2	1:B:180:ARG:HB3	0.55	1.78	7	11
1:A:51:ILE:HA	1:A:84:ALA:HB1	0.55	1.76	15	3
1:B:14:PHE:CD1	1:B:14:PHE:C	0.55	2.85	7	8
1:A:60:ILE:O	1:A:174:GLN:HG3	0.55	2.01	3	3
1:B:198:ALA:HB2	1:B:203:ILE:HG12	0.55	1.78	12	4
1:B:180:ARG:O	1:B:184:GLY:CA	0.55	2.55	13	16
1:A:11:LEU:C	1:A:13:TRP:H	0.55	2.10	20	1
1:B:45:GLY:HA3	1:B:92:CYS:CB	0.55	2.31	16	5
1:A:8:ASP:O	1:A:12:GLU:HB2	0.55	2.01	4	1
1:A:29:LEU:HD12	1:A:70:ILE:HG21	0.55	1.78	11	8
1:A:47:VAL:HA	1:A:89:LYS:N	0.55	2.16	17	14
1:B:190:LEU:CD2	1:B:195:LEU:HB3	0.55	2.31	13	10
1:A:50:LEU:HB2	1:A:59:MET:C	0.55	2.27	15	15
1:B:29:LEU:O	1:B:30:ILE:HG13	0.55	2.01	6	5
1:A:114:MET:HA	1:A:117:SER:OG	0.55	2.02	12	6
1:B:41:TYR:CB	1:B:95:ALA:HB3	0.55	2.31	15	8
1:A:121:ALA:HB1	1:B:77:GLU:HA	0.55	1.76	18	4
1:B:124:LEU:HA	1:B:128:SER:HB2	0.55	1.79	14	1
1:B:50:LEU:HB2	1:B:59:MET:C	0.55	2.27	20	19
1:B:143:ILE:HG23	1:B:172:ILE:HG21	0.55	1.77	16	13
1:A:171:GLU:O	1:A:175:ILE:HG13	0.55	2.02	10	4
1:B:143:ILE:HD13	1:B:186:ILE:HG12	0.55	1.79	10	2
1:B:76:PHE:CG	1:B:120:MET:HE3	0.55	2.36	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PHE:HD2	1:A:120:MET:SD	0.55	2.25	16	7
1:A:164:GLN:HB3	1:A:204:VAL:CG2	0.55	2.32	20	7
1:B:189:MET:SD	1:B:195:LEU:HD13	0.55	2.42	7	3
1:B:11:LEU:O	1:B:14:PHE:HB3	0.54	2.02	7	5
1:B:143:ILE:HD12	1:B:143:ILE:H	0.54	1.62	10	1
1:A:24:PRO:HA	1:A:91:ALA:HA	0.54	1.78	12	7
1:A:42:ILE:CD1	1:A:47:VAL:HG13	0.54	2.32	8	6
1:A:139:VAL:HG23	1:A:176:VAL:HG11	0.54	1.78	14	3
1:B:20:ILE:HD13	1:B:95:ALA:CB	0.54	2.32	13	6
1:A:39:LEU:HB2	1:A:75:LEU:HD22	0.54	1.78	13	1
1:A:99:TYR:HA	1:A:102:PHE:HB3	0.54	1.79	20	11
1:A:20:ILE:HD13	1:A:95:ALA:CB	0.54	2.31	16	8
1:A:159:HIS:CE1	1:A:161:ASP:HB3	0.54	2.37	18	4
1:A:42:ILE:HD13	1:A:46:SER:HA	0.54	1.79	2	1
1:A:105:LEU:HG	1:A:106:ILE:N	0.54	2.17	14	8
1:A:72:GLU:CG	1:A:120:MET:HE2	0.54	2.33	14	1
1:A:52:LYS:O	1:B:129:GLU:HA	0.54	2.03	6	3
1:B:14:PHE:CD2	1:B:102:PHE:CE2	0.54	2.95	8	8
1:B:80:GLN:O	1:B:81:GLU:HB2	0.54	2.03	7	7
1:A:28:THR:HA	1:A:29:LEU:HD22	0.54	1.79	10	2
1:A:61:LEU:HD13	1:A:62:SER:N	0.54	2.18	14	8
1:B:72:GLU:O	1:B:76:PHE:HB3	0.54	2.03	4	4
1:A:164:GLN:C	1:A:165:ILE:HG13	0.54	2.28	12	12
1:B:22:LYS:HB3	1:B:92:CYS:C	0.54	2.28	14	11
1:A:20:ILE:HG23	1:A:43:VAL:HG21	0.54	1.80	6	9
1:B:8:ASP:O	1:B:12:GLU:HB2	0.54	2.03	3	2
1:A:142:ARG:O	1:A:145:GLN:HB3	0.54	2.03	5	4
1:B:105:LEU:HG	1:B:106:ILE:N	0.54	2.17	14	7
1:B:132:GLY:HA2	1:B:135:ALA:HB3	0.54	1.79	5	1
1:A:81:GLU:O	1:A:82:ARG:HD2	0.54	2.02	14	1
1:B:151:ALA:HA	1:B:156:ALA:HB2	0.54	1.78	19	2
1:B:208:THR:O	1:B:209:ARG:HB2	0.54	2.01	14	1
1:B:150:LEU:CD1	1:B:167:ILE:HG12	0.54	2.33	15	4
1:A:138:ASP:OD2	1:A:142:ARG:HD3	0.54	2.03	11	1
1:A:186:ILE:HA	1:A:189:MET:HE3	0.54	1.79	14	1
1:B:19:HIS:HB3	1:B:96:GLU:O	0.54	2.02	1	9
1:B:113:LEU:HD12	1:B:116:LEU:HD23	0.54	1.78	2	1
1:B:39:LEU:HD22	1:B:102:PHE:CD1	0.54	2.38	13	7
1:A:195:LEU:O	1:A:209:ARG:HG3	0.54	2.02	12	4
1:B:134:LEU:HD13	1:B:174:GLN:O	0.54	2.03	7	1
1:B:29:LEU:HB3	1:B:40:TYR:CZ	0.54	2.38	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:ARG:O	1:A:184:GLY:CA	0.53	2.56	10	17
1:A:197:SER:CB	1:A:206:TYR:CE1	0.53	2.91	1	17
1:B:41:TYR:O	1:B:94:VAL:HA	0.53	2.02	11	7
1:A:41:TYR:CD1	1:A:41:TYR:C	0.53	2.85	13	7
1:B:197:SER:CB	1:B:206:TYR:CE1	0.53	2.91	1	16
1:B:22:LYS:H	1:B:93:GLU:HA	0.53	1.62	17	17
1:B:45:GLY:HA3	1:B:92:CYS:HB3	0.53	1.80	10	15
1:B:123:ARG:HA	1:B:126:VAL:CG1	0.53	2.34	14	2
1:A:166:LYS:C	1:A:167:ILE:HG13	0.53	2.28	15	2
1:B:77:GLU:HG3	1:B:79:GLY:N	0.53	2.19	5	5
1:A:11:LEU:O	1:A:14:PHE:HB3	0.53	2.03	7	3
1:B:72:GLU:CB	1:B:116:LEU:HD11	0.53	2.33	18	4
1:A:167:ILE:HD11	1:A:203:ILE:CD1	0.53	2.33	9	1
1:B:20:ILE:HG13	1:B:43:VAL:HG21	0.53	1.79	15	1
1:B:24:PRO:HA	1:B:91:ALA:CA	0.53	2.33	20	9
1:A:183:VAL:O	1:A:187:LEU:HG	0.53	2.04	4	3
1:A:76:PHE:CG	1:A:120:MET:HE3	0.53	2.38	18	1
1:A:18:CYS:HB3	1:A:97:ILE:HG12	0.53	1.80	17	14
1:A:129:GLU:HA	1:B:52:LYS:O	0.53	2.03	6	2
1:A:190:LEU:CD1	1:A:196:ILE:HD12	0.53	2.34	11	14
1:B:156:ALA:HA	1:B:164:GLN:O	0.53	2.02	20	4
1:A:29:LEU:HD23	1:A:86:VAL:HB	0.53	1.79	13	1
1:A:45:GLY:HA3	1:A:92:CYS:HB3	0.53	1.81	10	15
1:B:24:PRO:HA	1:B:91:ALA:HA	0.53	1.80	12	9
1:B:49:VAL:HG13	1:B:85:TRP:HA	0.53	1.80	19	5
1:B:99:TYR:CD1	1:B:99:TYR:C	0.53	2.86	20	14
1:B:164:GLN:HG3	1:B:202:THR:HG22	0.53	1.81	19	2
1:B:143:ILE:HG21	1:B:187:LEU:HD21	0.53	1.79	20	4
1:A:174:GLN:HG2	1:A:175:ILE:N	0.53	2.18	6	1
1:A:80:GLN:O	1:A:81:GLU:HB2	0.53	2.03	5	8
1:A:143:ILE:HG23	1:A:172:ILE:HG21	0.53	1.80	4	14
1:A:180:ARG:HA	1:A:183:VAL:HG12	0.53	1.80	20	6
1:A:198:ALA:HB2	1:A:203:ILE:HG12	0.53	1.80	8	3
1:B:171:GLU:HB3	1:B:175:ILE:HD12	0.53	1.79	7	1
1:A:106:ILE:HG22	1:A:112:ILE:HG21	0.53	1.81	7	7
1:A:31:HIS:HA	1:A:82:ARG:HG3	0.53	1.80	17	6
1:B:42:ILE:HG12	1:B:42:ILE:O	0.53	2.02	5	1
1:A:134:LEU:HB3	1:A:175:ILE:O	0.53	2.04	9	1
1:A:41:TYR:O	1:A:94:VAL:HA	0.53	2.03	11	6
1:A:45:GLY:HA3	1:A:92:CYS:CB	0.53	2.34	16	7
1:B:42:ILE:O	1:B:67:GLY:HA2	0.53	2.03	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:TYR:O	1:B:43:VAL:HG13	0.53	2.04	5	3
1:B:32:GLN:H	1:B:82:ARG:HG3	0.53	1.64	6	2
1:A:29:LEU:HD22	1:A:29:LEU:N	0.53	2.19	10	2
1:B:123:ARG:HD3	1:B:123:ARG:N	0.53	2.19	20	1
1:A:119:GLN:O	1:A:123:ARG:HD3	0.52	2.05	2	8
1:B:183:VAL:HG13	1:B:187:LEU:CD1	0.52	2.34	10	1
1:B:126:VAL:O	1:B:130:LYS:HB2	0.52	2.04	13	1
1:B:11:LEU:HD11	1:B:41:TYR:OH	0.52	2.04	19	1
1:A:99:TYR:CD1	1:A:99:TYR:C	0.52	2.87	3	14
1:A:48:ALA:HB1	1:A:60:ILE:HG21	0.52	1.81	4	1
1:B:23:TYR:O	1:B:91:ALA:HA	0.52	2.05	1	8
1:B:164:GLN:C	1:B:165:ILE:HG13	0.52	2.29	12	14
1:B:165:ILE:O	1:B:165:ILE:HD12	0.52	2.04	20	2
1:B:22:LYS:CB	1:B:92:CYS:O	0.52	2.51	12	1
1:A:196:ILE:CD1	1:A:203:ILE:HG23	0.52	2.35	13	1
1:B:139:VAL:HG22	1:B:143:ILE:HD11	0.52	1.81	20	1
1:A:39:LEU:HD11	1:A:41:TYR:CE1	0.52	2.39	7	1
1:A:73:LEU:HD23	1:A:120:MET:SD	0.52	2.44	11	1
1:A:100:LYS:O	1:A:103:ARG:HG2	0.52	2.04	19	1
1:A:22:LYS:N	1:A:93:GLU:HA	0.52	2.19	2	10
1:B:30:ILE:O	1:B:86:VAL:HG23	0.52	2.05	2	1
1:A:29:LEU:CD1	1:A:70:ILE:HG21	0.52	2.34	19	6
1:B:20:ILE:HD12	1:B:43:VAL:HG21	0.52	1.81	9	2
1:A:121:ALA:CB	1:B:77:GLU:HA	0.52	2.35	18	1
1:B:23:TYR:CB	1:B:24:PRO:HD2	0.52	2.34	10	7
1:B:25:SER:HB3	1:B:90:THR:N	0.52	2.20	4	2
1:B:106:ILE:HG22	1:B:112:ILE:HG22	0.52	1.80	17	6
1:B:32:GLN:N	1:B:82:ARG:HG3	0.52	2.19	17	3
1:A:29:LEU:N	1:A:29:LEU:CD2	0.52	2.73	18	15
1:B:76:PHE:HD2	1:B:120:MET:SD	0.52	2.28	11	6
1:B:76:PHE:CD2	1:B:120:MET:SD	0.52	3.03	12	3
1:A:166:LYS:HG3	1:A:201:LYS:HB3	0.52	1.82	4	1
1:B:76:PHE:HB3	1:B:120:MET:HE1	0.52	1.80	5	1
1:B:134:LEU:HD22	1:B:176:VAL:HA	0.52	1.80	10	1
1:B:196:ILE:CD1	1:B:203:ILE:HG23	0.52	2.34	13	1
1:A:124:LEU:HA	1:A:128:SER:HB2	0.52	1.82	14	1
1:B:173:GLY:HA3	1:B:178:CYS:O	0.52	2.05	14	1
1:A:49:VAL:HG13	1:A:85:TRP:HA	0.52	1.81	19	5
1:A:138:ASP:O	1:A:140:THR:N	0.52	2.43	8	10
1:A:23:TYR:HD2	1:A:27:SER:CB	0.52	2.17	14	5
1:A:65:ASN:O	1:A:68:ASP:HB2	0.52	2.05	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD21	1:A:41:TYR:CE2	0.52	2.40	10	2
1:A:142:ARG:O	1:A:145:GLN:HB2	0.52	2.04	13	1
1:A:124:LEU:HG	1:B:124:LEU:HD23	0.52	1.81	20	1
1:B:138:ASP:O	1:B:140:THR:N	0.51	2.44	10	11
1:A:135:ALA:HA	1:B:135:ALA:HA	0.51	1.83	5	1
1:B:48:ALA:O	1:B:87:ARG:HB3	0.51	2.05	15	2
1:B:102:PHE:CE2	1:B:106:ILE:HG23	0.51	2.40	17	2
1:A:61:LEU:C	1:A:61:LEU:HD22	0.51	2.30	12	17
1:B:29:LEU:N	1:B:29:LEU:CD2	0.51	2.72	1	12
1:A:162:GLY:HA3	1:A:204:VAL:CG2	0.51	2.35	2	1
1:A:197:SER:HB3	1:A:206:TYR:CE1	0.51	2.40	13	3
1:A:178:CYS:SG	1:A:183:VAL:HB	0.51	2.44	17	1
1:A:14:PHE:CD2	1:A:102:PHE:CE2	0.51	2.97	3	7
1:A:96:GLU:O	1:A:96:GLU:HG3	0.51	2.05	17	4
1:B:36:ALA:CB	1:B:74:GLY:HA3	0.51	2.34	7	10
1:A:51:ILE:HD12	1:B:128:SER:HA	0.51	1.81	4	1
1:A:42:ILE:HG12	1:A:42:ILE:O	0.51	2.05	5	1
1:B:61:LEU:HD22	1:B:61:LEU:C	0.51	2.31	5	2
1:B:50:LEU:HB2	1:B:59:MET:O	0.51	2.05	11	6
1:A:47:VAL:HA	1:A:89:LYS:CB	0.51	2.35	12	4
1:B:22:LYS:NZ	1:B:29:LEU:HD11	0.51	2.21	13	1
1:A:33:GLY:HA2	1:A:82:ARG:HB3	0.51	1.82	19	2
1:B:179:SER:O	1:B:181:GLU:N	0.51	2.32	1	10
1:A:36:ALA:CB	1:A:74:GLY:HA3	0.51	2.35	7	12
1:B:51:ILE:HA	1:B:84:ALA:HB1	0.51	1.81	2	5
1:B:103:ARG:C	1:B:106:ILE:HG13	0.51	2.31	18	4
1:B:47:VAL:HA	1:B:89:LYS:CB	0.51	2.35	12	3
1:B:193:GLN:HG2	1:B:197:SER:OG	0.51	2.05	19	1
1:B:61:LEU:C	1:B:61:LEU:HD22	0.51	2.30	12	16
1:B:106:ILE:HG22	1:B:112:ILE:HG21	0.51	1.82	2	8
1:B:30:ILE:HD12	1:B:86:VAL:HG23	0.51	1.81	4	4
1:A:165:ILE:HD12	1:A:165:ILE:O	0.51	2.05	20	2
1:A:50:LEU:CB	1:A:60:ILE:HA	0.51	2.36	15	9
1:B:183:VAL:O	1:B:187:LEU:HG	0.51	2.05	4	4
1:B:63:TYR:OH	1:B:175:ILE:HD11	0.51	2.05	13	1
1:A:109:ASN:CG	1:A:112:ILE:HG13	0.51	2.29	14	1
1:B:139:VAL:CG2	1:B:183:VAL:HG23	0.51	2.36	20	2
1:A:114:MET:HE2	1:B:113:LEU:HD21	0.51	1.82	1	1
1:B:25:SER:O	1:B:26:LYS:CB	0.51	2.59	19	15
1:B:47:VAL:CG2	1:B:64:LEU:HD12	0.51	2.35	6	3
1:B:146:THR:O	1:B:149:ASN:HB3	0.51	2.06	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:167:ILE:HG13	1:B:203:ILE:HD12	0.51	1.81	14	1
1:B:187:LEU:N	1:B:187:LEU:HD23	0.51	2.20	1	4
1:B:30:ILE:HG22	1:B:34:GLU:HB2	0.51	1.83	13	2
1:A:72:GLU:HB2	1:A:120:MET:CE	0.51	2.36	5	2
1:A:47:VAL:CG2	1:A:64:LEU:HD12	0.51	2.35	6	1
1:A:22:LYS:HE2	1:A:27:SER:OG	0.51	2.06	10	1
1:B:14:PHE:CE1	1:B:41:TYR:CD2	0.51	2.99	17	3
1:A:208:THR:O	1:A:209:ARG:HB2	0.51	2.05	19	2
1:A:11:LEU:HD11	1:A:41:TYR:OH	0.51	2.06	19	1
1:A:153:GLN:HB3	1:A:154:PRO:HD2	0.51	1.83	15	15
1:B:45:GLY:HA3	1:B:92:CYS:HA	0.51	1.83	20	8
1:A:78:GLU:HB3	1:B:122:ARG:NH2	0.51	2.21	19	4
1:A:102:PHE:CZ	1:A:106:ILE:HG21	0.51	2.41	15	7
1:A:109:ASN:OD1	1:A:112:ILE:HG13	0.51	2.06	19	2
1:B:31:HIS:HA	1:B:82:ARG:HG3	0.51	1.83	15	5
1:A:139:VAL:CG2	1:A:183:VAL:HG23	0.51	2.36	4	4
1:A:61:LEU:HD22	1:A:62:SER:HB2	0.51	1.81	10	6
1:B:82:ARG:CG	1:B:83:SER:N	0.50	2.73	12	17
1:B:164:GLN:HB3	1:B:204:VAL:CG2	0.50	2.36	1	6
1:B:14:PHE:CD1	1:B:15:LEU:HD23	0.50	2.42	19	6
1:B:166:LYS:CA	1:B:202:THR:HA	0.50	2.36	4	7
1:B:29:LEU:HB2	1:B:86:VAL:HB	0.50	1.83	10	2
1:A:169:ARG:HG3	1:A:180:ARG:HB3	0.50	1.83	20	1
1:A:150:LEU:CD1	1:A:167:ILE:HG12	0.50	2.35	4	7
1:B:60:ILE:HG21	1:B:63:TYR:CE2	0.50	2.41	1	9
1:A:60:ILE:HD11	1:A:87:ARG:NH1	0.50	2.21	2	1
1:A:166:LYS:O	1:A:166:LYS:HD3	0.50	2.06	7	1
1:B:29:LEU:HD22	1:B:29:LEU:N	0.50	2.20	13	1
1:A:82:ARG:CG	1:A:83:SER:N	0.50	2.74	5	18
1:B:123:ARG:CA	1:B:126:VAL:HG12	0.50	2.36	3	4
1:A:205:VAL:HG12	1:A:209:ARG:OXT	0.50	2.07	5	2
1:A:191:GLU:HG2	1:A:198:ALA:O	0.50	2.06	9	1
1:A:166:LYS:HG2	1:A:202:THR:HG23	0.50	1.83	20	2
1:A:29:LEU:HB3	1:A:40:TYR:CZ	0.50	2.41	13	1
1:A:106:ILE:CD1	1:A:113:LEU:HD22	0.50	2.36	19	1
1:B:121:ALA:O	1:B:124:LEU:HB2	0.50	2.06	18	3
1:B:90:THR:O	1:B:91:ALA:C	0.50	2.55	11	5
1:B:73:LEU:HD23	1:B:120:MET:SD	0.50	2.46	11	1
1:A:77:GLU:HA	1:B:121:ALA:CB	0.50	2.34	18	1
1:A:103:ARG:HA	1:A:106:ILE:HG12	0.50	1.83	4	7
1:B:18:CYS:HB3	1:B:97:ILE:CD1	0.50	2.37	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:PHE:CD1	1:A:116:LEU:HD13	0.50	2.41	2	1
1:B:60:ILE:O	1:B:174:GLN:HG3	0.50	2.07	15	4
1:A:146:THR:HG21	1:A:175:ILE:HG23	0.50	1.84	7	1
1:B:143:ILE:HG12	1:B:183:VAL:CG2	0.50	2.36	11	1
1:B:72:GLU:HA	1:B:75:LEU:HD23	0.50	1.82	8	6
1:A:23:TYR:CB	1:A:24:PRO:HD2	0.50	2.36	10	7
1:B:42:ILE:CD1	1:B:46:SER:HA	0.50	2.35	4	3
1:B:146:THR:HG21	1:B:175:ILE:HG23	0.50	1.81	7	1
1:A:11:LEU:HD23	1:A:14:PHE:HB3	0.50	1.84	9	4
1:A:166:LYS:HB3	1:A:202:THR:HA	0.50	1.82	20	2
1:A:164:GLN:HB2	1:A:202:THR:HG22	0.50	1.84	12	1
1:B:81:GLU:O	1:B:82:ARG:HD2	0.50	2.06	14	1
1:A:75:LEU:CB	1:A:99:TYR:CD2	0.50	2.95	11	9
1:A:196:ILE:CG2	1:A:197:SER:H	0.50	2.17	18	7
1:A:46:SER:HB2	1:A:64:LEU:C	0.50	2.32	12	1
1:A:42:ILE:HG12	1:A:94:VAL:HG12	0.50	1.84	2	1
1:B:187:LEU:CD2	1:B:190:LEU:HD11	0.50	2.35	9	4
1:A:129:GLU:O	1:A:130:LYS:HG2	0.50	2.07	6	1
1:B:23:TYR:CD2	1:B:27:SER:HB3	0.50	2.42	6	2
1:A:187:LEU:HA	1:A:190:LEU:CG	0.50	2.37	8	1
1:B:11:LEU:HD23	1:B:14:PHE:HB3	0.50	1.84	19	2
1:A:143:ILE:H	1:A:143:ILE:HD12	0.50	1.64	10	1
1:A:124:LEU:HG	1:B:124:LEU:CD2	0.50	2.37	20	3
1:A:104:GLN:O	1:A:107:GLN:HG2	0.50	2.06	19	1
1:B:33:GLY:HA2	1:B:82:ARG:HB3	0.50	1.83	19	1
1:A:123:ARG:C	1:A:126:VAL:HG12	0.50	2.30	14	2
1:A:42:ILE:CD1	1:A:46:SER:HA	0.50	2.36	5	3
1:B:50:LEU:HB3	1:B:60:ILE:HA	0.50	1.83	10	2
1:A:89:LYS:HE2	1:A:155:ASP:OD1	0.50	2.07	10	1
1:B:55:GLU:OE1	1:B:57:LYS:HB2	0.50	2.06	20	3
1:A:186:ILE:HA	1:A:189:MET:HG2	0.50	1.84	17	1
1:B:166:LYS:HA	1:B:202:THR:HA	0.49	1.84	6	13
1:A:169:ARG:HB2	1:A:180:ARG:CB	0.49	2.37	11	7
1:B:103:ARG:HA	1:B:106:ILE:HG12	0.49	1.83	4	7
1:A:11:LEU:HD12	1:A:15:LEU:CG	0.49	2.38	4	2
1:A:196:ILE:HG12	1:A:209:ARG:OXT	0.49	2.07	7	2
1:B:171:GLU:O	1:B:175:ILE:HG13	0.49	2.07	10	2
1:A:50:LEU:HB2	1:A:59:MET:O	0.49	2.08	11	5
1:B:196:ILE:CG2	1:B:197:SER:H	0.49	2.16	6	6
1:B:47:VAL:HG21	1:B:86:VAL:HG12	0.49	1.83	2	2
1:A:31:HIS:CE1	1:A:58:GLU:HB2	0.49	2.42	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:SER:HB3	1:B:51:ILE:CG2	0.49	2.35	5	5
1:B:109:ASN:OD1	1:B:112:ILE:HG13	0.49	2.07	19	2
1:A:60:ILE:HG21	1:A:63:TYR:CE2	0.49	2.43	16	4
1:B:61:LEU:HD13	1:B:62:SER:N	0.49	2.22	15	6
1:B:50:LEU:HA	1:B:61:LEU:HD12	0.49	1.84	11	1
1:B:147:LEU:O	1:B:150:LEU:HB2	0.49	2.07	20	3
1:A:185:ARG:O	1:A:189:MET:HE3	0.49	2.07	20	1
1:A:25:SER:O	1:A:26:LYS:CB	0.49	2.60	19	17
1:A:164:GLN:HG3	1:A:202:THR:HG22	0.49	1.83	14	3
1:A:166:LYS:HA	1:A:202:THR:HA	0.49	1.83	12	11
1:B:102:PHE:CZ	1:B:106:ILE:HG21	0.49	2.43	9	7
1:A:138:ASP:O	1:A:138:ASP:CG	0.49	2.54	6	4
1:B:29:LEU:HD12	1:B:70:ILE:HG21	0.49	1.84	11	10
1:B:143:ILE:HD12	1:B:186:ILE:HB	0.49	1.84	18	2
1:A:24:PRO:CA	1:A:91:ALA:HB2	0.49	2.34	5	1
1:B:50:LEU:HB3	1:B:60:ILE:HD13	0.49	1.84	17	3
1:B:42:ILE:CD1	1:B:47:VAL:HG13	0.49	2.37	13	5
1:B:23:TYR:HD2	1:B:27:SER:CB	0.49	2.20	14	3
1:A:144:ALA:HB2	1:A:195:LEU:CD2	0.49	2.37	18	4
1:A:120:MET:O	1:A:123:ARG:HB2	0.49	2.07	16	2
1:A:50:LEU:HB3	1:A:60:ILE:HD13	0.49	1.84	6	3
1:A:49:VAL:CA	1:A:85:TRP:O	0.49	2.59	16	2
1:A:41:TYR:HD1	1:A:68:ASP:O	0.49	1.91	10	2
1:B:169:ARG:HG3	1:B:180:ARG:HB2	0.49	1.85	10	1
1:A:190:LEU:HD13	1:A:196:ILE:CD1	0.49	2.37	13	2
1:B:103:ARG:HA	1:B:106:ILE:HG13	0.49	1.85	13	9
1:B:64:LEU:HB3	1:B:68:ASP:CB	0.49	2.37	2	2
1:A:146:THR:HG21	1:A:175:ILE:CG2	0.49	2.37	7	1
1:A:117:SER:HB3	1:B:76:PHE:CE2	0.49	2.43	14	1
1:B:22:LYS:NZ	1:B:88:ALA:HB2	0.49	2.23	18	2
1:B:101:LYS:O	1:B:104:GLN:HG2	0.49	2.08	19	1
1:A:135:ALA:HB1	1:B:135:ALA:HB1	0.49	1.84	1	2
1:B:75:LEU:CB	1:B:99:TYR:CD2	0.49	2.95	6	11
1:B:138:ASP:O	1:B:142:ARG:CB	0.49	2.60	7	1
1:B:143:ILE:CD1	1:B:183:VAL:HA	0.49	2.37	18	1
1:A:40:TYR:HB2	1:A:70:ILE:HB	0.49	1.83	20	1
1:A:90:THR:O	1:A:91:ALA:C	0.49	2.56	11	7
1:A:135:ALA:CB	1:B:135:ALA:HB3	0.49	2.36	6	2
1:A:41:TYR:CE1	1:A:69:PHE:HD1	0.49	2.26	7	1
1:A:14:PHE:O	1:A:17:HIS:HB2	0.49	2.08	9	1
1:A:69:PHE:CG	1:A:116:LEU:HD13	0.48	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:ILE:HG22	1:A:171:GLU:HG3	0.48	1.84	8	1
1:B:22:LYS:CG	1:B:23:TYR:CD1	0.48	2.96	16	1
1:A:184:GLY:O	1:A:188:LYS:HB2	0.48	2.08	6	5
1:B:22:LYS:N	1:B:93:GLU:HA	0.48	2.23	2	11
1:A:81:GLU:O	1:A:82:ARG:HD3	0.48	2.09	2	3
1:A:32:GLN:N	1:A:82:ARG:HG3	0.48	2.23	6	3
1:A:59:MET:HE3	1:A:175:ILE:HA	0.48	1.85	10	1
1:B:15:LEU:HD21	1:B:41:TYR:HE2	0.48	1.68	10	1
1:A:37:GLU:O	1:A:99:TYR:CD1	0.48	2.66	19	1
1:A:14:PHE:CD1	1:A:15:LEU:HD23	0.48	2.43	19	7
1:A:102:PHE:CE2	1:A:106:ILE:CG2	0.48	2.96	3	4
1:B:41:TYR:CD1	1:B:41:TYR:C	0.48	2.91	6	6
1:A:157:MET:O	1:A:163:MET:HB3	0.48	2.08	3	1
1:B:143:ILE:CG2	1:B:187:LEU:HD21	0.48	2.38	5	4
1:A:47:VAL:CG1	1:A:88:ALA:HA	0.48	2.38	12	1
1:B:180:ARG:HD2	1:B:181:GLU:OE2	0.48	2.07	12	1
1:B:31:HIS:HB2	1:B:84:ALA:HA	0.48	1.84	14	1
1:A:54:GLU:HB2	1:B:133:ASN:OD1	0.48	2.07	1	1
1:A:39:LEU:HD22	1:A:102:PHE:CD1	0.48	2.43	20	6
1:A:51:ILE:HG21	1:B:128:SER:HB2	0.48	1.85	3	1
1:B:140:THR:O	1:B:142:ARG:N	0.48	2.46	3	1
1:B:11:LEU:HD23	1:B:14:PHE:CG	0.48	2.44	9	1
1:A:33:GLY:N	1:A:82:ARG:HD2	0.48	2.24	10	1
1:B:18:CYS:HA	1:B:97:ILE:HG23	0.48	1.84	10	1
1:B:143:ILE:HD13	1:B:186:ILE:CG1	0.48	2.38	20	1
1:B:143:ILE:HD13	1:B:186:ILE:HG13	0.48	1.85	1	1
1:A:121:ALA:O	1:A:124:LEU:HB2	0.48	2.07	18	2
1:B:156:ALA:HA	1:B:165:ILE:HG23	0.48	1.84	20	2
1:B:169:ARG:CA	1:B:187:LEU:HD12	0.48	2.38	11	1
1:B:143:ILE:HD13	1:B:183:VAL:HA	0.48	1.85	18	2
1:A:130:LYS:HG3	1:A:133:ASN:OD1	0.48	2.08	19	1
1:B:99:TYR:C	1:B:99:TYR:HD1	0.48	2.17	5	9
1:A:18:CYS:HA	1:A:97:ILE:HG23	0.48	1.84	10	3
1:A:34:GLU:OE2	1:A:82:ARG:HB2	0.48	2.08	17	5
1:A:103:ARG:HA	1:A:106:ILE:HG13	0.48	1.84	13	8
1:A:103:ARG:O	1:A:107:GLN:HG2	0.48	2.09	18	1
1:A:23:TYR:O	1:A:91:ALA:HA	0.48	2.08	5	7
1:A:99:TYR:C	1:A:99:TYR:HD1	0.48	2.17	3	10
1:B:39:LEU:HG	1:B:40:TYR:N	0.48	2.24	3	3
1:B:118:ALA:O	1:B:122:ARG:HB2	0.48	2.08	2	4
1:B:187:LEU:HD23	1:B:187:LEU:N	0.48	2.24	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:ALA:CB	1:B:60:ILE:HD12	0.48	2.37	8	3
1:A:156:ALA:HA	1:A:165:ILE:HG23	0.48	1.85	20	4
1:A:166:LYS:HB3	1:A:202:THR:HG23	0.48	1.86	10	1
1:A:124:LEU:HA	1:A:128:SER:CB	0.48	2.38	14	1
1:A:147:LEU:CD2	1:A:167:ILE:HD11	0.48	2.39	19	2
1:A:169:ARG:HG3	1:A:180:ARG:CB	0.48	2.39	20	1
1:A:190:LEU:CD2	1:A:195:LEU:HB3	0.48	2.39	14	6
1:A:122:ARG:CZ	1:B:78:GLU:HB3	0.48	2.38	20	3
1:A:143:ILE:CG2	1:A:187:LEU:HD21	0.48	2.38	8	2
1:B:72:GLU:HG3	1:B:120:MET:HE2	0.48	1.86	14	1
1:B:77:GLU:O	1:B:78:GLU:HB2	0.48	2.09	14	1
1:A:124:LEU:HG	1:B:124:LEU:HG	0.48	1.86	13	4
1:B:96:GLU:HG3	1:B:96:GLU:O	0.48	2.09	17	2
1:A:109:ASN:CB	1:A:112:ILE:HG13	0.48	2.39	11	2
1:B:106:ILE:HD13	1:B:113:LEU:HD22	0.48	1.85	15	3
1:A:173:GLY:HA3	1:A:178:CYS:O	0.48	2.09	14	1
1:A:42:ILE:HB	1:A:68:ASP:O	0.47	2.09	2	1
1:A:166:LYS:HA	1:A:201:LYS:O	0.47	2.10	10	4
1:A:11:LEU:HD23	1:A:14:PHE:CG	0.47	2.44	14	4
1:B:143:ILE:CG1	1:B:183:VAL:HG22	0.47	2.38	10	1
1:A:47:VAL:C	1:A:89:LYS:HB2	0.47	2.34	14	3
1:A:54:GLU:OE1	1:B:130:LYS:HE3	0.47	2.09	15	1
1:B:51:ILE:CD1	1:B:61:LEU:HB3	0.47	2.39	18	1
1:A:45:GLY:HA3	1:A:92:CYS:HA	0.47	1.85	20	6
1:A:147:LEU:O	1:A:150:LEU:HB2	0.47	2.09	20	4
1:B:33:GLY:H	1:B:82:ARG:HB2	0.47	1.68	14	1
1:B:143:ILE:HD12	1:B:186:ILE:CB	0.47	2.39	18	2
1:B:8:ASP:O	1:B:12:GLU:HG2	0.47	2.09	1	1
1:B:14:PHE:CE1	1:B:41:TYR:HD2	0.47	2.27	2	1
1:B:28:THR:HB	1:B:87:ARG:HA	0.47	1.86	7	4
1:A:23:TYR:CD2	1:A:27:SER:HB3	0.47	2.44	6	1
1:A:51:ILE:HD13	1:A:51:ILE:H	0.47	1.69	7	1
1:B:69:PHE:CB	1:B:116:LEU:HD12	0.47	2.39	9	3
1:B:138:ASP:OD2	1:B:142:ARG:HD3	0.47	2.09	11	1
1:A:109:ASN:HB2	1:A:112:ILE:HG13	0.47	1.86	13	11
1:A:27:SER:N	1:A:88:ALA:HB3	0.47	2.25	14	4
1:B:166:LYS:HB3	1:B:202:THR:HG23	0.47	1.87	5	1
1:B:134:LEU:HB3	1:B:175:ILE:O	0.47	2.09	9	1
1:A:76:PHE:CE1	1:B:117:SER:HB2	0.47	2.45	10	1
1:B:75:LEU:CB	1:B:99:TYR:HD2	0.47	2.22	20	2
1:B:33:GLY:HA2	1:B:82:ARG:CB	0.47	2.39	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:PHE:O	1:B:106:ILE:HG23	0.47	2.08	19	1
1:B:153:GLN:HB3	1:B:154:PRO:HD2	0.47	1.85	17	15
1:A:123:ARG:HD3	1:A:123:ARG:N	0.47	2.23	7	1
1:A:153:GLN:C	1:A:155:ASP:H	0.47	2.16	8	1
1:A:190:LEU:HD23	1:A:195:LEU:HB3	0.47	1.85	19	2
1:B:147:LEU:HD21	1:B:203:ILE:HG21	0.47	1.86	14	1
1:A:103:ARG:C	1:A:106:ILE:HG13	0.47	2.34	18	4
1:A:179:SER:O	1:A:181:GLU:N	0.47	2.48	13	8
1:B:169:ARG:HB2	1:B:180:ARG:CB	0.47	2.39	11	5
1:A:27:SER:H	1:A:88:ALA:HB3	0.47	1.70	14	3
1:A:14:PHE:CE1	1:A:41:TYR:HD2	0.47	2.27	2	3
1:B:69:PHE:CD1	1:B:116:LEU:HD13	0.47	2.45	2	1
1:A:76:PHE:CD2	1:A:120:MET:SD	0.47	3.08	16	5
1:A:157:MET:O	1:A:163:MET:CA	0.47	2.63	8	1
1:A:150:LEU:HB3	1:A:165:ILE:HG21	0.47	1.86	9	3
1:A:64:LEU:HD13	1:A:68:ASP:HB3	0.47	1.84	10	1
1:B:122:ARG:O	1:B:125:GLN:HG2	0.47	2.08	11	1
1:A:46:SER:HB2	1:A:64:LEU:O	0.47	2.09	12	1
1:A:141:GLY:O	1:A:145:GLN:CB	0.47	2.63	14	1
1:B:147:LEU:CD2	1:B:167:ILE:HD11	0.47	2.40	14	1
1:A:20:ILE:HD12	1:A:43:VAL:HG21	0.47	1.86	11	3
1:A:22:LYS:NZ	1:A:88:ALA:HB2	0.47	2.25	9	3
1:A:167:ILE:HD11	1:A:203:ILE:HD12	0.47	1.86	9	1
1:A:164:GLN:OE1	1:A:202:THR:HB	0.47	2.10	19	1
1:A:60:ILE:HB	1:A:174:GLN:NE2	0.47	2.25	3	2
1:A:180:ARG:HD2	1:A:181:GLU:OE1	0.47	2.10	4	3
1:B:153:GLN:C	1:B:155:ASP:H	0.47	2.17	8	1
1:A:14:PHE:CE1	1:A:41:TYR:CD2	0.47	3.03	1	6
1:B:45:GLY:HA3	1:B:92:CYS:CA	0.47	2.39	16	3
1:B:60:ILE:HB	1:B:174:GLN:NE2	0.47	2.25	6	4
1:B:157:MET:O	1:B:163:MET:HB3	0.47	2.09	3	1
1:B:47:VAL:HB	1:B:88:ALA:HA	0.47	1.85	5	2
1:B:130:LYS:HA	1:B:133:ASN:OD1	0.47	2.09	5	3
1:A:128:SER:O	1:B:51:ILE:HG13	0.47	2.10	10	1
1:B:33:GLY:N	1:B:82:ARG:HB2	0.47	2.25	14	1
1:B:124:LEU:O	1:B:128:SER:HB2	0.47	2.10	14	1
1:B:166:LYS:C	1:B:167:ILE:HG13	0.47	2.35	20	1
1:A:51:ILE:CG2	1:B:128:SER:HB3	0.46	2.38	5	4
1:A:11:LEU:HD13	1:A:41:TYR:OH	0.46	2.11	10	3
1:B:109:ASN:CB	1:B:112:ILE:HG13	0.46	2.40	11	3
1:A:77:GLU:OE1	1:B:122:ARG:HD2	0.46	2.10	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ILE:CD1	1:A:183:VAL:HG22	0.46	2.41	16	2
1:B:102:PHE:CE2	1:B:106:ILE:HG22	0.46	2.45	19	1
1:B:76:PHE:CE2	1:B:116:LEU:HG	0.46	2.45	2	1
1:A:166:LYS:CA	1:A:202:THR:HA	0.46	2.40	4	4
1:B:178:CYS:SG	1:B:182:THR:HB	0.46	2.50	5	1
1:B:64:LEU:HA	1:B:123:ARG:NH2	0.46	2.24	17	2
1:B:102:PHE:CE2	1:B:106:ILE:CG2	0.46	2.99	15	3
1:B:23:TYR:HB3	1:B:24:PRO:HD2	0.46	1.86	13	1
1:B:99:TYR:HD1	1:B:100:LYS:N	0.46	2.08	20	1
1:A:25:SER:HB3	1:A:90:THR:N	0.46	2.24	19	2
1:B:41:TYR:CE1	1:B:69:PHE:HD1	0.46	2.29	7	1
1:A:143:ILE:HG23	1:A:172:ILE:CG2	0.46	2.40	8	1
1:A:28:THR:CA	1:A:29:LEU:HD22	0.46	2.40	10	1
1:B:25:SER:O	1:B:26:LYS:CG	0.46	2.63	10	1
1:A:72:GLU:O	1:A:76:PHE:HB3	0.46	2.10	12	1
1:A:76:PHE:CE1	1:A:113:LEU:HD21	0.46	2.45	17	1
1:A:39:LEU:HD22	1:A:102:PHE:CE1	0.46	2.45	20	1
1:B:22:LYS:HG3	1:B:94:VAL:CG2	0.46	2.39	19	2
1:B:30:ILE:HD12	1:B:86:VAL:HG21	0.46	1.86	1	1
1:A:32:GLN:HA	1:A:32:GLN:OE1	0.46	2.09	4	1
1:B:142:ARG:O	1:B:145:GLN:HB3	0.46	2.10	4	4
1:A:18:CYS:HB3	1:A:97:ILE:CD1	0.46	2.41	13	5
1:A:76:PHE:HB3	1:A:120:MET:HE1	0.46	1.87	5	1
1:B:186:ILE:HA	1:B:189:MET:HE3	0.46	1.88	7	2
1:A:72:GLU:HG3	1:A:120:MET:HE2	0.46	1.86	14	1
1:A:167:ILE:CD1	1:A:203:ILE:HD12	0.46	2.40	6	6
1:A:64:LEU:HA	1:A:123:ARG:NH2	0.46	2.26	10	3
1:A:133:ASN:HD21	1:A:142:ARG:NH2	0.46	2.09	2	1
1:B:123:ARG:C	1:B:126:VAL:HG12	0.46	2.35	14	3
1:A:8:ASP:CG	1:A:115:ARG:HH12	0.46	2.19	5	1
1:A:14:PHE:CE2	1:A:102:PHE:CE1	0.46	3.04	10	2
1:A:15:LEU:HD22	1:A:20:ILE:CD1	0.46	2.40	11	2
1:A:96:GLU:O	1:A:97:ILE:HG23	0.46	2.11	11	2
1:A:155:ASP:CB	1:A:165:ILE:HG22	0.46	2.41	15	2
1:A:28:THR:CB	1:A:87:ARG:HA	0.46	2.41	17	2
1:A:76:PHE:CE2	1:A:120:MET:HE3	0.46	2.45	2	1
1:B:196:ILE:CG2	1:B:197:SER:N	0.46	2.78	19	3
1:B:27:SER:N	1:B:88:ALA:HB3	0.46	2.26	9	5
1:B:50:LEU:HD23	1:B:50:LEU:O	0.46	2.11	5	1
1:A:78:GLU:HB3	1:B:122:ARG:CZ	0.46	2.40	9	1
1:B:187:LEU:HA	1:B:190:LEU:CG	0.46	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:96:GLU:O	1:B:96:GLU:HG3	0.46	2.11	10	1
1:A:34:GLU:O	1:A:82:ARG:HA	0.46	2.11	14	1
1:B:44:LYS:CE	1:B:66:GLN:OE1	0.46	2.59	19	1
1:A:41:TYR:CE2	1:A:69:PHE:CE1	0.46	3.04	16	4
1:B:109:ASN:HB2	1:B:112:ILE:HG13	0.46	1.87	18	9
1:A:184:GLY:O	1:A:185:ARG:C	0.46	2.59	15	2
1:A:122:ARG:HA	1:B:77:GLU:OE2	0.46	2.11	8	1
1:A:61:LEU:HD22	1:A:61:LEU:C	0.46	2.36	19	3
1:B:143:ILE:O	1:B:147:LEU:HD12	0.46	2.11	19	1
1:A:70:ILE:CG2	1:A:86:VAL:HG21	0.46	2.32	10	1
1:B:96:GLU:O	1:B:97:ILE:HG23	0.46	2.11	11	2
1:A:146:THR:O	1:A:149:ASN:HB2	0.46	2.11	16	1
1:B:155:ASP:CB	1:B:165:ILE:HG22	0.46	2.41	20	1
1:A:127:THR:O	1:A:131:VAL:HG23	0.46	2.11	6	2
1:A:64:LEU:HB3	1:A:68:ASP:CB	0.46	2.41	2	2
1:A:113:LEU:HD21	1:B:114:MET:HG2	0.46	1.88	9	1
1:A:76:PHE:CE2	1:A:116:LEU:HG	0.46	2.46	2	1
1:B:60:ILE:HD11	1:B:87:ARG:NH1	0.46	2.26	2	1
1:A:76:PHE:HD2	1:A:120:MET:CE	0.46	2.24	7	1
1:B:29:LEU:CD1	1:B:70:ILE:HG21	0.46	2.41	9	3
1:A:30:ILE:O	1:A:86:VAL:HG23	0.45	2.11	2	1
1:B:140:THR:C	1:B:142:ARG:N	0.45	2.74	3	1
1:B:150:LEU:HD13	1:B:165:ILE:HD13	0.45	1.88	5	1
1:A:187:LEU:N	1:A:187:LEU:HD23	0.45	2.26	13	3
1:A:139:VAL:HG21	1:A:183:VAL:HG23	0.45	1.88	10	1
1:A:128:SER:HB3	1:B:128:SER:HB3	0.45	1.87	14	1
1:A:53:ASP:CB	1:A:57:LYS:HG2	0.45	2.42	19	2
1:B:138:ASP:O	1:B:138:ASP:CG	0.45	2.59	4	2
1:B:184:GLY:O	1:B:188:LYS:HB2	0.45	2.11	13	2
1:A:11:LEU:HD21	1:A:41:TYR:CZ	0.45	2.46	16	2
1:B:47:VAL:HA	1:B:89:LYS:HB3	0.45	1.87	18	1
1:A:31:HIS:CE1	1:A:58:GLU:CB	0.45	3.00	20	5
1:A:114:MET:HG2	1:B:113:LEU:HD21	0.45	1.88	9	2
1:A:125:GLN:O	1:A:125:GLN:HG3	0.45	2.10	9	1
1:B:117:SER:HA	1:B:120:MET:SD	0.45	2.51	4	1
1:B:193:GLN:CA	1:B:196:ILE:O	0.45	2.59	12	1
1:B:147:LEU:HD13	1:B:203:ILE:HG21	0.45	1.87	18	1
1:B:76:PHE:CE2	1:B:120:MET:SD	0.45	3.10	4	1
1:A:147:LEU:HD22	1:A:167:ILE:HD11	0.45	1.89	13	1
1:A:169:ARG:CG	1:A:187:LEU:HD12	0.45	2.42	5	3
1:A:124:LEU:CD2	1:B:124:LEU:HG	0.45	2.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:GLN:CB	1:A:204:VAL:HG23	0.45	2.42	4	1
1:B:209:ARG:HG3	1:B:209:ARG:OXT	0.45	2.12	8	1
1:A:97:ILE:HD12	1:A:102:PHE:HB2	0.45	1.89	10	2
1:B:142:ARG:O	1:B:145:GLN:HB2	0.45	2.12	13	1
1:A:124:LEU:CA	1:A:128:SER:HB2	0.45	2.42	14	1
1:B:33:GLY:CA	1:B:82:ARG:HB2	0.45	2.41	14	1
1:A:150:LEU:C	1:A:152:LYS:N	0.45	2.73	16	1
1:B:185:ARG:O	1:B:189:MET:HE3	0.45	2.11	20	1
1:B:53:ASP:CB	1:B:57:LYS:HG2	0.45	2.41	1	1
1:B:184:GLY:O	1:B:185:ARG:C	0.45	2.59	15	3
1:A:47:VAL:HB	1:A:88:ALA:HA	0.45	1.87	5	2
1:A:131:VAL:HG12	1:A:132:GLY:N	0.45	2.26	6	1
1:B:27:SER:H	1:B:88:ALA:HB3	0.45	1.70	14	2
1:A:81:GLU:O	1:A:83:SER:N	0.45	2.50	11	2
1:A:187:LEU:HD23	1:A:187:LEU:N	0.45	2.26	16	8
1:A:119:GLN:OE1	1:A:119:GLN:HA	0.45	2.12	6	1
1:B:138:ASP:OD2	1:B:138:ASP:C	0.45	2.60	6	1
1:A:103:ARG:O	1:A:107:GLN:HB2	0.45	2.12	12	2
1:B:14:PHE:CE2	1:B:102:PHE:CE1	0.45	3.05	10	1
1:A:14:PHE:HD1	1:A:15:LEU:HD23	0.45	1.72	14	3
1:A:48:ALA:CB	1:A:60:ILE:HD13	0.45	2.40	15	2
1:A:180:ARG:NH1	1:A:181:GLU:HA	0.45	2.27	17	1
1:B:40:TYR:N	1:B:40:TYR:CD2	0.45	2.84	20	2
1:A:47:VAL:HG21	1:A:86:VAL:HG12	0.45	1.89	17	2
1:B:195:LEU:O	1:B:209:ARG:HG3	0.45	2.12	7	3
1:B:39:LEU:HD13	1:B:102:PHE:CZ	0.45	2.46	9	1
1:B:15:LEU:HD21	1:B:41:TYR:CE2	0.45	2.46	10	1
1:A:23:TYR:HB3	1:A:24:PRO:HD2	0.45	1.87	13	1
1:B:39:LEU:HB2	1:B:75:LEU:HD22	0.45	1.89	13	1
1:B:144:ALA:HB2	1:B:195:LEU:CD2	0.45	2.42	18	2
1:A:196:ILE:CG2	1:A:197:SER:N	0.45	2.80	19	2
1:A:11:LEU:O	1:A:15:LEU:N	0.45	2.50	5	8
1:B:139:VAL:HG23	1:B:176:VAL:CG1	0.45	2.42	5	1
1:A:51:ILE:HG21	1:B:128:SER:CB	0.45	2.41	10	1
1:B:47:VAL:HG21	1:B:70:ILE:HD11	0.45	1.88	12	1
1:A:63:TYR:OH	1:A:175:ILE:HD11	0.45	2.12	13	1
1:A:190:LEU:CD1	1:A:203:ILE:HD13	0.44	2.42	14	2
1:B:157:MET:O	1:B:163:MET:CA	0.44	2.62	8	1
1:A:143:ILE:CG1	1:A:183:VAL:HG22	0.44	2.38	10	1
1:B:20:ILE:HG21	1:B:43:VAL:HG21	0.44	1.89	10	1
1:A:124:LEU:C	1:A:128:SER:HB2	0.44	2.36	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:LEU:HD21	1:A:174:GLN:O	0.44	2.12	14	2
1:A:20:ILE:CD1	1:A:95:ALA:HB2	0.44	2.40	16	1
1:B:190:LEU:CD1	1:B:203:ILE:HD13	0.44	2.41	16	1
1:B:27:SER:O	1:B:88:ALA:HB2	0.44	2.12	18	1
1:B:14:PHE:HD1	1:B:15:LEU:HD23	0.44	1.72	20	3
1:A:172:ILE:HB	1:A:183:VAL:HG11	0.44	1.88	3	1
1:A:143:ILE:HD12	1:A:186:ILE:HB	0.44	1.89	4	2
1:A:32:GLN:O	1:A:34:GLU:HG3	0.44	2.12	7	2
1:B:106:ILE:HD12	1:B:113:LEU:HB2	0.44	1.87	5	2
1:A:135:ALA:HB3	1:B:135:ALA:CB	0.44	2.40	6	1
1:B:41:TYR:CE2	1:B:69:PHE:CE1	0.44	3.04	17	3
1:B:120:MET:O	1:B:123:ARG:HB2	0.44	2.11	11	1
1:A:31:HIS:HB2	1:A:84:ALA:HA	0.44	1.87	14	1
1:A:147:LEU:HD21	1:A:203:ILE:HG21	0.44	1.89	14	1
1:A:49:VAL:CB	1:A:62:SER:O	0.44	2.54	16	1
1:A:52:LYS:O	1:B:129:GLU:HG2	0.44	2.12	18	1
1:B:51:ILE:HD13	1:B:51:ILE:H	0.44	1.72	18	1
1:A:102:PHE:CE2	1:A:106:ILE:HG22	0.44	2.47	19	1
1:A:76:PHE:CZ	1:B:117:SER:HB2	0.44	2.46	7	4
1:A:196:ILE:HD12	1:A:203:ILE:HG23	0.44	1.88	13	2
1:A:103:ARG:C	1:A:106:ILE:HG12	0.44	2.38	19	1
1:A:85:TRP:C	1:A:86:VAL:HG22	0.44	2.38	20	1
1:A:20:ILE:O	1:A:21:HIS:CB	0.44	2.65	16	7
1:B:189:MET:CG	1:B:195:LEU:HB2	0.44	2.42	1	1
1:A:23:TYR:CD2	1:A:27:SER:CB	0.44	3.00	2	2
1:A:114:MET:HE3	1:B:113:LEU:HD21	0.44	1.88	3	1
1:A:128:SER:HA	1:B:51:ILE:HD12	0.44	1.90	4	1
1:A:143:ILE:HD13	1:A:183:VAL:HG22	0.44	1.90	13	2
1:B:103:ARG:O	1:B:107:GLN:HB2	0.44	2.13	12	4
1:B:72:GLU:HB2	1:B:120:MET:CE	0.44	2.43	7	3
1:A:47:VAL:HG21	1:A:70:ILE:HD11	0.44	1.90	7	1
1:A:143:ILE:CD1	1:A:186:ILE:HG13	0.44	2.41	10	1
1:B:42:ILE:HD11	1:B:64:LEU:CD1	0.44	2.43	10	1
1:A:104:GLN:O	1:A:108:VAL:HB	0.44	2.13	20	1
1:A:204:VAL:O	1:A:204:VAL:HG12	0.44	2.12	20	1
1:A:128:SER:HB2	1:B:51:ILE:HG21	0.44	1.90	3	1
1:A:149:ASN:O	1:A:153:GLN:HG2	0.44	2.12	4	1
1:A:166:LYS:HB3	1:A:202:THR:CG2	0.44	2.40	5	1
1:B:20:ILE:CD1	1:B:43:VAL:HG21	0.44	2.43	11	1
1:B:106:ILE:HB	1:B:113:LEU:HB2	0.44	1.89	15	1
1:B:159:HIS:O	1:B:161:ASP:N	0.44	2.49	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:82:ARG:C	1:B:84:ALA:H	0.44	2.21	7	3
1:B:39:LEU:O	1:B:96:GLU:HA	0.44	2.13	20	3
1:B:76:PHE:HD2	1:B:120:MET:CE	0.44	2.25	7	1
1:A:110:PRO:HB3	1:B:110:PRO:HB3	0.44	1.90	19	2
1:B:11:LEU:HD21	1:B:41:TYR:CZ	0.44	2.47	20	2
1:A:195:LEU:HA	1:A:209:ARG:NH2	0.44	2.27	16	1
1:A:189:MET:SD	1:A:195:LEU:HD13	0.44	2.53	18	1
1:A:51:ILE:HG23	1:A:61:LEU:CD1	0.44	2.42	7	1
1:A:134:LEU:HD13	1:A:174:GLN:O	0.44	2.12	7	1
1:B:53:ASP:CG	1:B:54:GLU:H	0.44	2.21	18	1
1:B:11:LEU:O	1:B:15:LEU:N	0.44	2.48	11	5
1:A:138:ASP:O	1:A:142:ARG:CB	0.44	2.65	7	1
1:A:15:LEU:HA	1:A:18:CYS:HG	0.44	1.72	11	1
1:B:169:ARG:HA	1:B:187:LEU:HD12	0.44	1.88	11	1
1:A:40:TYR:CD2	1:A:40:TYR:N	0.44	2.85	12	1
1:A:47:VAL:H	1:A:64:LEU:HB2	0.44	1.72	12	1
1:B:169:ARG:HG3	1:B:180:ARG:CB	0.44	2.43	15	1
1:B:169:ARG:HD3	1:B:180:ARG:HB3	0.44	1.90	17	1
1:A:105:LEU:HD11	1:A:112:ILE:HD12	0.44	1.89	19	1
1:B:100:LYS:O	1:B:103:ARG:HG2	0.44	2.13	19	1
1:B:106:ILE:HD12	1:B:113:LEU:HD22	0.44	1.88	19	1
1:A:40:TYR:O	1:A:70:ILE:N	0.44	2.51	20	1
1:A:30:ILE:HD12	1:A:86:VAL:HG23	0.43	1.90	4	4
1:A:82:ARG:C	1:A:84:ALA:H	0.43	2.21	11	5
1:A:191:GLU:O	1:A:191:GLU:HG2	0.43	2.13	17	2
1:B:159:HIS:HD2	1:B:162:GLY:O	0.43	1.96	18	2
1:A:143:ILE:HG12	1:A:183:VAL:CG2	0.43	2.40	11	1
1:A:113:LEU:O	1:A:116:LEU:HB3	0.43	2.12	12	1
1:B:111:ASP:O	1:B:115:ARG:HB3	0.43	2.13	14	1
1:B:9:PRO:O	1:B:13:TRP:HB2	0.43	2.13	15	1
1:B:166:LYS:HB2	1:B:202:THR:HA	0.43	1.90	18	1
1:B:106:ILE:CD1	1:B:113:LEU:HD22	0.43	2.44	19	1
1:B:156:ALA:HB1	1:B:163:MET:SD	0.43	2.52	5	1
1:B:196:ILE:HG12	1:B:209:ARG:OXT	0.43	2.12	7	1
1:A:55:GLU:OE1	1:A:57:LYS:HB2	0.43	2.13	20	2
1:A:18:CYS:SG	1:A:19:HIS:N	0.43	2.92	19	1
1:A:42:ILE:HG12	1:A:94:VAL:CG1	0.43	2.42	2	1
1:B:46:SER:O	1:B:90:THR:HG23	0.43	2.14	2	1
1:A:139:VAL:HA	1:A:176:VAL:CG1	0.43	2.43	3	1
1:A:146:THR:O	1:A:149:ASN:HB3	0.43	2.13	6	3
1:B:138:ASP:C	1:B:140:THR:N	0.43	2.75	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ILE:HD12	1:A:186:ILE:CB	0.43	2.43	18	1
1:B:142:ARG:HB3	1:B:176:VAL:HG13	0.43	1.90	19	1
1:B:23:TYR:CD2	1:B:27:SER:CB	0.43	3.01	2	1
1:B:138:ASP:O	1:B:139:VAL:C	0.43	2.61	2	4
1:B:34:GLU:OE2	1:B:82:ARG:HB2	0.43	2.13	3	3
1:B:11:LEU:HD13	1:B:41:TYR:OH	0.43	2.13	9	1
1:A:76:PHE:CD2	1:A:120:MET:HE2	0.43	2.49	12	1
1:A:126:VAL:O	1:A:130:LYS:HB2	0.43	2.14	13	1
1:A:30:ILE:HG21	1:A:36:ALA:HA	0.43	1.90	14	1
1:A:151:ALA:HA	1:A:156:ALA:HB2	0.43	1.90	14	1
1:A:143:ILE:HD13	1:A:183:VAL:HA	0.43	1.90	17	2
1:B:155:ASP:O	1:B:156:ALA:C	0.43	2.60	4	4
1:B:180:ARG:HD2	1:B:181:GLU:OE1	0.43	2.14	7	2
1:B:25:SER:O	1:B:26:LYS:HB2	0.43	2.14	11	2
1:B:35:LYS:HA	1:B:81:GLU:HA	0.43	1.89	19	3
1:B:153:GLN:CB	1:B:154:PRO:HD2	0.43	2.44	3	2
1:A:132:GLY:HA2	1:A:135:ALA:HB3	0.43	1.89	5	1
1:A:11:LEU:HA	1:A:14:PHE:HB3	0.43	1.90	6	3
1:A:190:LEU:O	1:A:197:SER:HA	0.43	2.12	19	2
1:A:69:PHE:CB	1:A:116:LEU:HD12	0.43	2.44	9	3
1:A:187:LEU:O	1:A:190:LEU:HG	0.43	2.13	9	1
1:B:27:SER:O	1:B:29:LEU:CD2	0.43	2.65	18	2
1:A:127:THR:O	1:A:127:THR:HG22	0.43	2.14	14	1
1:B:159:HIS:CG	1:B:160:PRO:HD2	0.43	2.49	14	1
1:B:48:ALA:CB	1:B:60:ILE:HD13	0.43	2.42	15	1
1:B:53:ASP:HB2	1:B:57:LYS:HB2	0.43	1.91	15	1
1:A:143:ILE:HD12	1:A:186:ILE:HD13	0.43	1.90	17	1
1:B:76:PHE:CE2	1:B:120:MET:HE3	0.43	2.49	2	1
1:A:33:GLY:H	1:A:82:ARG:HB2	0.43	1.73	14	1
1:A:156:ALA:HA	1:A:164:GLN:O	0.43	2.13	19	1
1:B:53:ASP:HB2	1:B:57:LYS:HG2	0.43	1.89	1	1
1:B:143:ILE:HD13	1:B:183:VAL:HG22	0.43	1.90	7	2
1:B:47:VAL:C	1:B:89:LYS:HB2	0.43	2.38	5	2
1:B:32:GLN:O	1:B:34:GLU:HG3	0.43	2.14	7	1
1:B:22:LYS:HB2	1:B:94:VAL:HG22	0.43	1.89	12	1
1:B:18:CYS:HB3	1:B:97:ILE:CG1	0.43	2.42	14	3
1:B:49:VAL:HG13	1:B:85:TRP:O	0.43	2.14	15	1
1:A:130:LYS:O	1:A:130:LYS:HG2	0.43	2.14	19	1
1:B:166:LYS:CB	1:B:202:THR:HA	0.43	2.43	20	1
1:A:30:ILE:CG2	1:A:34:GLU:HB2	0.43	2.44	2	1
1:B:23:TYR:CD2	1:B:27:SER:HB2	0.43	2.49	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:137:LEU:HG	1:B:178:CYS:SG	0.43	2.53	4	1
1:A:158:THR:HA	1:A:163:MET:HB3	0.43	1.91	5	2
1:A:50:LEU:HA	1:A:61:LEU:HD12	0.43	1.91	11	2
1:A:47:VAL:HG12	1:A:88:ALA:HA	0.43	1.91	12	1
1:A:196:ILE:HG22	1:A:209:ARG:O	0.43	2.13	13	1
1:B:30:ILE:CG2	1:B:34:GLU:HB2	0.43	2.43	17	2
1:A:147:LEU:CG	1:A:167:ILE:HD11	0.43	2.44	14	1
1:A:169:ARG:HB3	1:A:187:LEU:CD1	0.43	2.40	16	1
1:B:178:CYS:SG	1:B:183:VAL:HB	0.43	2.54	17	1
1:A:39:LEU:HG	1:A:40:TYR:N	0.43	2.27	3	3
1:B:11:LEU:HA	1:B:14:PHE:HB3	0.43	1.91	20	2
1:B:41:TYR:C	1:B:41:TYR:HD1	0.43	2.22	6	1
1:A:153:GLN:C	1:A:155:ASP:N	0.43	2.77	8	1
1:B:14:PHE:O	1:B:17:HIS:HB2	0.43	2.13	9	1
1:A:33:GLY:HA2	1:A:82:ARG:NH1	0.43	2.29	11	1
1:A:49:VAL:HB	1:A:62:SER:C	0.43	2.39	14	1
1:B:20:ILE:O	1:B:21:HIS:CB	0.43	2.67	15	1
1:A:139:VAL:HG22	1:A:143:ILE:HD11	0.43	1.91	20	1
1:B:70:ILE:CD1	1:B:86:VAL:HG11	0.42	2.44	5	1
1:A:32:GLN:OE1	1:A:32:GLN:HA	0.42	2.14	6	1
1:A:137:LEU:HG	1:A:178:CYS:SG	0.42	2.54	6	1
1:A:159:HIS:O	1:A:161:ASP:N	0.42	2.51	16	4
1:B:34:GLU:O	1:B:82:ARG:HA	0.42	2.14	14	1
1:B:51:ILE:HD12	1:B:61:LEU:CB	0.42	2.43	18	1
1:A:138:ASP:O	1:A:139:VAL:C	0.42	2.62	20	3
1:A:155:ASP:O	1:A:156:ALA:C	0.42	2.62	4	2
1:B:31:HIS:CA	1:B:82:ARG:HG3	0.42	2.44	8	1
1:A:114:MET:O	1:A:117:SER:HB2	0.42	2.14	14	1
1:A:113:LEU:HD21	1:B:114:MET:HE2	0.42	1.91	18	2
1:A:8:ASP:CG	1:A:11:LEU:HB2	0.42	2.39	4	1
1:A:25:SER:O	1:A:26:LYS:HG3	0.42	2.13	6	1
1:A:102:PHE:CD2	1:A:103:ARG:N	0.42	2.87	17	2
1:A:190:LEU:CD2	1:A:196:ILE:HG12	0.42	2.23	13	1
1:B:114:MET:O	1:B:117:SER:HB2	0.42	2.13	14	1
1:B:44:LYS:HD3	1:B:66:GLN:HB3	0.42	1.91	18	1
1:A:52:LYS:HG3	1:A:58:GLU:HB3	0.42	1.90	1	1
1:B:172:ILE:O	1:B:173:GLY:C	0.42	2.59	8	5
1:B:168:THR:HB	1:B:170:GLN:OE1	0.42	2.14	15	4
1:A:20:ILE:HG23	1:A:43:VAL:CG2	0.42	2.45	7	2
1:B:41:TYR:O	1:B:95:ALA:N	0.42	2.49	14	2
1:A:31:HIS:CA	1:A:82:ARG:HG3	0.42	2.45	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:CB	1:A:94:VAL:HG12	0.42	2.45	5	1
1:A:114:MET:CE	1:B:113:LEU:HD21	0.42	2.44	15	2
1:B:42:ILE:O	1:B:42:ILE:HG23	0.42	2.14	8	2
1:B:60:ILE:HD11	1:B:87:ARG:HD3	0.42	1.91	8	1
1:A:11:LEU:HD22	1:A:41:TYR:HE2	0.42	1.74	13	2
1:A:150:LEU:HD13	1:A:165:ILE:HD13	0.42	1.92	14	2
1:B:117:SER:HA	1:B:120:MET:HE2	0.42	1.91	12	1
1:B:169:ARG:HA	1:B:172:ILE:HG12	0.42	1.92	15	1
1:A:166:LYS:CB	1:A:202:THR:HA	0.42	2.45	16	2
1:A:122:ARG:O	1:A:125:GLN:HG2	0.42	2.14	18	1
1:A:18:CYS:HB2	1:A:97:ILE:HG12	0.42	1.90	19	1
1:A:48:ALA:HB1	1:A:60:ILE:HG23	0.42	1.90	19	1
1:B:37:GLU:O	1:B:99:TYR:CD1	0.42	2.72	19	1
1:A:99:TYR:HA	1:A:102:PHE:CD2	0.42	2.50	20	1
1:A:121:ALA:HA	1:A:124:LEU:HB2	0.42	1.91	4	1
1:A:41:TYR:C	1:A:41:TYR:HD1	0.42	2.21	6	1
1:B:35:LYS:HB3	1:B:37:GLU:CD	0.42	2.40	6	1
1:B:81:GLU:O	1:B:83:SER:N	0.42	2.52	10	3
1:B:143:ILE:CD1	1:B:186:ILE:HD13	0.42	2.44	11	1
1:A:75:LEU:CG	1:A:76:PHE:N	0.42	2.81	14	1
1:A:172:ILE:O	1:A:176:VAL:HG23	0.42	2.14	14	1
1:B:143:ILE:HD12	1:B:186:ILE:HD12	0.42	1.91	14	1
1:A:196:ILE:HD12	1:A:203:ILE:CG2	0.42	2.45	16	1
1:A:169:ARG:HD3	1:A:180:ARG:HB3	0.42	1.92	17	2
1:B:185:ARG:C	1:B:189:MET:HE3	0.42	2.39	20	1
1:B:14:PHE:HE2	1:B:102:PHE:CE1	0.42	2.32	10	2
1:B:21:HIS:HA	1:B:93:GLU:OE1	0.42	2.14	5	1
1:B:167:ILE:HD12	1:B:167:ILE:O	0.42	2.14	9	1
1:B:179:SER:HB3	1:B:180:ARG:H	0.42	1.46	14	1
1:A:76:PHE:CD2	1:A:120:MET:HE1	0.42	2.49	17	1
1:B:76:PHE:CD2	1:B:120:MET:HE2	0.42	2.50	17	1
1:A:159:HIS:C	1:A:161:ASP:H	0.42	2.21	18	1
1:B:59:MET:HB3	1:B:174:GLN:HG2	0.42	1.91	20	1
1:B:31:HIS:CE1	1:B:58:GLU:CB	0.42	3.03	2	4
1:B:81:GLU:O	1:B:82:ARG:HD3	0.42	2.15	12	4
1:B:77:GLU:O	1:B:78:GLU:CB	0.42	2.68	4	2
1:B:139:VAL:HG21	1:B:178:CYS:SG	0.42	2.55	5	1
1:B:76:PHE:CD1	1:B:113:LEU:HD11	0.42	2.50	6	1
1:A:14:PHE:CE2	1:A:102:PHE:CD1	0.42	3.08	7	2
1:A:51:ILE:CD1	1:A:61:LEU:HB3	0.42	2.45	7	1
1:B:41:TYR:HD1	1:B:68:ASP:O	0.42	1.98	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:TYR:CD1	1:A:68:ASP:O	0.42	2.73	13	1
1:B:189:MET:SD	1:B:195:LEU:HB2	0.42	2.55	13	1
1:A:147:LEU:HG	1:A:167:ILE:HD11	0.42	1.90	14	1
1:A:25:SER:HB3	1:A:89:LYS:C	0.42	2.40	15	1
1:A:42:ILE:HD11	1:A:64:LEU:CD1	0.42	2.44	17	1
1:A:57:LYS:O	1:A:57:LYS:HG3	0.42	2.14	19	1
1:B:143:ILE:CD1	1:B:186:ILE:HG13	0.42	2.45	1	1
1:B:172:ILE:HG22	1:B:183:VAL:CG2	0.42	2.44	10	1
1:B:166:LYS:O	1:B:167:ILE:HG23	0.42	2.15	13	1
1:B:190:LEU:HD22	1:B:196:ILE:CB	0.42	2.45	16	1
1:A:116:LEU:CG	1:A:120:MET:HE1	0.42	2.41	18	1
1:A:39:LEU:O	1:A:96:GLU:HA	0.42	2.15	20	1
1:A:22:LYS:HB2	1:A:94:VAL:N	0.42	2.30	2	2
1:A:129:GLU:O	1:A:130:LYS:HG3	0.42	2.15	7	1
1:B:14:PHE:CE2	1:B:102:PHE:CD1	0.42	3.08	7	1
1:B:147:LEU:HD22	1:B:167:ILE:HD11	0.42	1.92	13	1
1:A:40:TYR:HB2	1:A:70:ILE:CG2	0.42	2.45	16	1
1:B:143:ILE:CD1	1:B:183:VAL:HG22	0.42	2.45	16	1
1:B:42:ILE:HD11	1:B:64:LEU:CB	0.42	2.45	17	1
1:B:119:GLN:OE1	1:B:119:GLN:HA	0.42	2.14	20	1
1:A:120:MET:HE3	1:A:120:MET:HB2	0.41	1.64	16	3
1:A:172:ILE:O	1:A:173:GLY:C	0.41	2.62	12	7
1:A:73:LEU:HD21	1:B:124:LEU:CD1	0.41	2.45	2	1
1:B:22:LYS:HB2	1:B:94:VAL:N	0.41	2.30	2	1
1:A:125:GLN:HE21	1:B:77:GLU:CD	0.41	2.23	9	1
1:B:15:LEU:HB3	1:B:20:ILE:CD1	0.41	2.45	15	1
1:B:120:MET:HE3	1:B:120:MET:HB2	0.41	1.77	20	1
1:B:25:SER:HB3	1:B:90:THR:CA	0.41	2.44	9	2
1:A:41:TYR:C	1:A:41:TYR:CD1	0.41	2.98	5	1
1:B:153:GLN:C	1:B:155:ASP:N	0.41	2.76	8	1
1:A:196:ILE:HG21	1:A:203:ILE:HG23	0.41	1.91	11	1
1:A:180:ARG:HD2	1:A:181:GLU:OE2	0.41	2.15	12	1
1:B:169:ARG:HD2	1:B:170:GLN:N	0.41	2.31	14	1
1:A:124:LEU:CD1	1:B:73:LEU:HD21	0.41	2.45	4	2
1:A:50:LEU:HD23	1:A:50:LEU:O	0.41	2.15	5	1
1:B:113:LEU:O	1:B:113:LEU:HG	0.41	2.14	5	1
1:B:205:VAL:HG12	1:B:209:ARG:O	0.41	2.15	5	1
1:A:73:LEU:HA	1:A:77:GLU:HB2	0.41	1.92	8	1
1:A:134:LEU:HD22	1:A:176:VAL:HA	0.41	1.92	10	1
1:B:103:ARG:O	1:B:107:GLN:HG3	0.41	2.15	13	2
1:A:77:GLU:O	1:A:78:GLU:CB	0.41	2.68	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:196:ILE:HG21	1:B:203:ILE:HG23	0.41	1.92	11	1
1:A:11:LEU:HD23	1:A:14:PHE:CB	0.41	2.45	13	2
1:A:85:TRP:CZ2	1:A:123:ARG:HG2	0.41	2.51	16	1
1:A:159:HIS:HD2	1:A:162:GLY:O	0.41	1.98	18	1
1:A:72:GLU:HG2	1:A:116:LEU:HD11	0.41	1.91	4	1
1:A:41:TYR:HB3	1:A:95:ALA:CB	0.41	2.37	8	1
1:A:15:LEU:HD21	1:A:41:TYR:HE2	0.41	1.74	10	1
1:B:40:TYR:CD2	1:B:40:TYR:N	0.41	2.89	12	1
1:A:45:GLY:HA3	1:A:92:CYS:CA	0.41	2.46	18	1
1:A:106:ILE:HD12	1:A:113:LEU:HD22	0.41	1.90	19	1
1:A:185:ARG:C	1:A:189:MET:HE3	0.41	2.40	20	1
1:B:127:THR:O	1:B:131:VAL:HG22	0.41	2.15	6	1
1:A:14:PHE:HE2	1:A:97:ILE:HD11	0.41	1.75	8	1
1:A:14:PHE:HE2	1:A:102:PHE:CE1	0.41	2.34	13	2
1:B:23:TYR:CB	1:B:24:PRO:CD	0.41	2.99	10	1
1:B:52:LYS:HG2	1:B:58:GLU:HB3	0.41	1.91	10	1
1:B:164:GLN:CB	1:B:204:VAL:HG23	0.41	2.41	10	1
1:B:134:LEU:HD21	1:B:174:GLN:O	0.41	2.15	14	1
1:B:31:HIS:O	1:B:32:GLN:HB2	0.41	2.14	17	1
1:B:147:LEU:HD22	1:B:196:ILE:HD13	0.41	1.91	19	1
1:B:73:LEU:HG	1:B:85:TRP:CD2	0.41	2.51	2	2
1:B:149:ASN:O	1:B:153:GLN:HG2	0.41	2.16	4	1
1:A:8:ASP:O	1:A:12:GLU:HG3	0.41	2.15	5	1
1:A:198:ALA:CB	1:A:203:ILE:HG12	0.41	2.46	8	1
1:B:15:LEU:HD22	1:B:20:ILE:CD1	0.41	2.46	11	1
1:B:47:VAL:CG1	1:B:88:ALA:HA	0.41	2.46	12	1
1:A:72:GLU:HG2	1:A:73:LEU:N	0.41	2.31	14	1
1:B:190:LEU:HD23	1:B:195:LEU:HB3	0.41	1.91	14	1
1:A:53:ASP:CG	1:A:54:GLU:H	0.41	2.23	18	1
1:A:102:PHE:O	1:A:106:ILE:HG23	0.41	2.15	19	2
1:B:180:ARG:HA	1:B:183:VAL:CG1	0.41	2.45	1	1
1:B:166:LYS:HB3	1:B:202:THR:HA	0.41	1.92	16	2
1:A:189:MET:SD	1:A:195:LEU:HB2	0.41	2.56	6	1
1:A:41:TYR:CE1	1:A:69:PHE:CD1	0.41	3.08	7	1
1:A:70:ILE:CD1	1:A:86:VAL:HG11	0.41	2.46	20	3
1:A:138:ASP:C	1:A:140:THR:N	0.41	2.78	10	1
1:A:82:ARG:NE	1:A:83:SER:H	0.41	2.13	11	1
1:A:27:SER:O	1:A:29:LEU:CD2	0.41	2.69	16	2
1:B:42:ILE:HG22	1:B:68:ASP:N	0.41	2.29	12	1
1:B:196:ILE:CG1	1:B:197:SER:N	0.41	2.79	13	1
1:B:42:ILE:CG2	1:B:94:VAL:HG12	0.41	2.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD13	1:A:203:ILE:HG21	0.41	1.92	18	1
1:B:103:ARG:C	1:B:106:ILE:HG12	0.41	2.40	19	1
1:A:75:LEU:HB3	1:A:99:TYR:CD2	0.41	2.51	20	1
1:B:139:VAL:HG21	1:B:183:VAL:HG23	0.41	1.91	20	1
1:B:172:ILE:HB	1:B:183:VAL:HG11	0.41	1.92	3	1
1:A:50:LEU:HB3	1:A:60:ILE:HA	0.41	1.93	6	1
1:B:113:LEU:O	1:B:116:LEU:HB3	0.41	2.15	12	1
1:A:196:ILE:HG13	1:A:197:SER:N	0.41	2.30	13	1
1:A:179:SER:O	1:A:183:VAL:HB	0.41	2.16	16	1
1:A:169:ARG:HA	1:A:172:ILE:CG1	0.41	2.46	17	1
1:B:205:VAL:O	1:B:205:VAL:HG23	0.41	2.16	19	1
1:B:127:THR:HG22	1:B:131:VAL:HG13	0.41	1.92	20	1
1:B:183:VAL:HG13	1:B:187:LEU:HG	0.41	1.92	1	1
1:A:45:GLY:C	1:A:92:CYS:HB3	0.41	2.41	2	1
1:A:61:LEU:HD22	1:A:62:SER:HB3	0.41	1.92	2	1
1:A:164:GLN:HB3	1:A:204:VAL:HB	0.41	1.93	2	1
1:B:23:TYR:CE2	1:B:27:SER:HB2	0.41	2.51	2	1
1:B:186:ILE:HA	1:B:189:MET:HG2	0.41	1.93	4	3
1:A:167:ILE:HD12	1:A:167:ILE:O	0.41	2.15	10	2
1:A:77:GLU:O	1:A:78:GLU:HB2	0.41	2.15	6	1
1:A:59:MET:CE	1:A:175:ILE:HA	0.41	2.46	10	1
1:B:186:ILE:HG23	1:B:195:LEU:HD13	0.41	1.92	12	1
1:A:22:LYS:HE2	1:A:88:ALA:HB2	0.41	1.93	13	1
1:B:102:PHE:CD2	1:B:103:ARG:N	0.41	2.89	13	3
1:A:25:SER:O	1:A:26:LYS:HB2	0.41	2.15	15	2
1:B:170:GLN:O	1:B:174:GLN:HB2	0.41	2.16	14	1
1:B:179:SER:OG	1:B:181:GLU:HB2	0.41	2.15	17	1
1:A:138:ASP:OD1	1:A:142:ARG:HD3	0.41	2.16	18	1
1:A:124:LEU:HB2	1:B:124:LEU:HG	0.41	1.92	19	1
1:A:23:TYR:CD2	1:A:27:SER:HB2	0.41	2.51	2	3
1:B:198:ALA:CB	1:B:203:ILE:HG12	0.41	2.46	8	1
1:A:114:MET:HE2	1:B:76:PHE:CE1	0.41	2.50	13	1
1:A:42:ILE:HG23	1:A:42:ILE:O	0.41	2.16	15	1
1:B:73:LEU:HD13	1:B:77:GLU:HB2	0.41	1.93	15	1
1:B:166:LYS:CG	1:B:202:THR:HG23	0.41	2.44	15	1
1:A:18:CYS:CA	1:A:97:ILE:CG2	0.41	2.98	16	2
1:B:35:LYS:HA	1:B:81:GLU:CA	0.41	2.46	19	1
1:B:44:LYS:CD	1:B:66:GLN:CD	0.41	2.90	20	1
1:A:78:GLU:HB3	1:B:122:ARG:NH1	0.40	2.31	2	1
1:A:14:PHE:HE2	1:A:102:PHE:CD1	0.40	2.34	7	1
1:A:73:LEU:HD13	1:A:77:GLU:HG3	0.40	1.93	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:198:ALA:HA	1:B:203:ILE:HA	0.40	1.91	10	1
1:B:182:THR:O	1:B:186:ILE:HD12	0.40	2.16	13	1
1:B:76:PHE:CD1	1:B:76:PHE:C	0.40	3.00	14	1
1:B:147:LEU:HD21	1:B:167:ILE:HD11	0.40	1.93	14	1
1:A:76:PHE:CD2	1:A:120:MET:HE3	0.40	2.51	18	1
1:A:124:LEU:CD2	1:B:124:LEU:HD21	0.40	2.33	18	1
1:B:186:ILE:O	1:B:189:MET:HB2	0.40	2.16	19	1
1:B:169:ARG:HG3	1:B:180:ARG:HB3	0.40	1.92	20	1
1:A:42:ILE:O	1:A:67:GLY:HA2	0.40	2.16	2	1
1:B:32:GLN:OE1	1:B:32:GLN:HA	0.40	2.16	4	1
1:A:83:SER:O	1:A:84:ALA:HB3	0.40	2.16	6	2
1:B:14:PHE:HE2	1:B:102:PHE:CD1	0.40	2.33	7	1
1:B:53:ASP:HB2	1:B:57:LYS:HB3	0.40	1.94	9	1
1:B:59:MET:O	1:B:59:MET:HG2	0.40	2.16	10	1
1:A:31:HIS:HE2	1:A:58:GLU:HB2	0.40	1.76	11	1
1:B:153:GLN:HB2	1:B:154:PRO:HD2	0.40	1.92	14	1
1:A:169:ARG:HA	1:A:172:ILE:HG12	0.40	1.92	17	1
1:B:11:LEU:HD21	1:B:41:TYR:OH	0.40	2.16	17	1
1:A:205:VAL:HG23	1:A:205:VAL:O	0.40	2.15	19	1
1:B:14:PHE:CE2	1:B:97:ILE:HD11	0.40	2.52	19	1
1:B:34:GLU:O	1:B:82:ARG:N	0.40	2.54	20	1
1:B:83:SER:O	1:B:84:ALA:HB3	0.40	2.16	4	1
1:A:34:GLU:O	1:A:82:ARG:N	0.40	2.53	5	1
1:B:147:LEU:HD12	1:B:196:ILE:CD1	0.40	2.47	6	1
1:A:42:ILE:O	1:A:42:ILE:HG23	0.40	2.16	8	1
1:B:72:GLU:CB	1:B:120:MET:SD	0.40	3.07	12	1
1:B:158:THR:HA	1:B:163:MET:HB3	0.40	1.93	18	1
1:B:73:LEU:HG	1:B:85:TRP:CE3	0.40	2.51	2	1
1:B:129:GLU:O	1:B:130:LYS:HG3	0.40	2.15	3	1
1:A:189:MET:CG	1:A:195:LEU:HB2	0.40	2.46	5	1
1:B:42:ILE:CB	1:B:94:VAL:HG12	0.40	2.47	5	1
1:A:171:GLU:HB3	1:A:175:ILE:HD12	0.40	1.92	7	1
1:B:187:LEU:HD23	1:B:203:ILE:HD11	0.40	1.92	10	1
1:B:31:HIS:NE2	1:B:58:GLU:HB2	0.40	2.32	11	1
1:A:18:CYS:HB3	1:A:97:ILE:CG1	0.40	2.46	13	1
1:B:110:PRO:O	1:B:114:MET:HB2	0.40	2.17	14	1
1:B:172:ILE:HG21	1:B:183:VAL:CG2	0.40	2.46	14	1
1:B:179:SER:O	1:B:183:VAL:HB	0.40	2.16	18	1
1:B:143:ILE:HG23	1:B:172:ILE:CG2	0.40	2.46	1	1
1:A:49:VAL:O	1:A:61:LEU:HD13	0.40	2.15	4	1
1:B:25:SER:HB3	1:B:89:LYS:C	0.40	2.42	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:TYR:CZ	1:A:69:PHE:CE1	0.40	3.09	7	1
1:B:72:GLU:OE2	1:B:72:GLU:N	0.40	2.53	10	1
1:A:124:LEU:HD23	1:B:124:LEU:HD23	0.40	1.91	12	1
1:A:147:LEU:HD21	1:A:167:ILE:HD11	0.40	1.93	14	1
1:A:153:GLN:HB2	1:A:154:PRO:HD2	0.40	1.93	14	1
1:B:141:GLY:O	1:B:145:GLN:CB	0.40	2.67	14	1
1:A:72:GLU:OE2	1:A:72:GLU:N	0.40	2.54	17	1
1:B:53:ASP:N	1:B:57:LYS:O	0.40	2.54	17	1
1:A:143:ILE:CD1	1:A:183:VAL:HA	0.40	2.46	18	1
1:B:49:VAL:HG13	1:B:85:TRP:CA	0.40	2.46	19	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	201/209 (96%)	157±4 (78±2%)	26±4 (13±2%)	18±2 (9±1%)	1	12
1	B	201/209 (96%)	158±3 (79±2%)	25±3 (13±2%)	18±2 (9±1%)	1	11
All	All	8040/8360 (96%)	6296 (78%)	1032 (13%)	712 (9%)	1	11

All 81 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	21	HIS	20
1	A	26	LYS	20
1	A	30	ILE	20
1	A	31	HIS	20
1	A	81	GLU	20
1	A	85	TRP	20
1	A	161	ASP	20
1	A	196	ILE	20
1	B	21	HIS	20
1	B	26	LYS	20
1	B	30	ILE	20

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Mol	Chain	Res	Type	Models (Total)
1	B	31	HIS	20
1	B	81	GLU	20
1	B	85	TRP	20
1	B	161	ASP	20
1	A	78	GLU	19
1	B	78	GLU	19
1	B	196	ILE	19
1	B	180	ARG	18
1	A	165	ILE	17
1	A	180	ARG	17
1	B	84	ALA	17
1	B	139	VAL	17
1	A	139	VAL	16
1	A	207	GLY	16
1	A	84	ALA	15
1	B	165	ILE	15
1	B	140	THR	15
1	A	140	THR	14
1	B	207	GLY	14
1	A	160	PRO	13
1	B	66	GLN	11
1	B	160	PRO	11
1	B	82	ARG	10
1	A	66	GLN	9
1	B	132	GLY	8
1	A	82	ARG	8
1	A	132	GLY	7
1	B	42	ILE	7
1	A	131	VAL	5
1	A	143	ILE	4
1	A	32	GLN	4
1	B	32	GLN	4
1	B	131	VAL	4
1	A	42	ILE	4
1	A	201	LYS	3
1	B	143	ILE	3
1	B	130	LYS	3
1	A	167	ILE	3
1	B	128	SER	2
1	B	185	ARG	2
1	A	88	ALA	2
1	B	88	ALA	2

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Mol	Chain	Res	Type	Models (Total)
1	A	130	LYS	2
1	B	167	ILE	2
1	A	181	GLU	2
1	B	36	ALA	2
1	B	99	TYR	2
1	B	135	ALA	2
1	A	179	SER	2
1	A	45	GLY	1
1	A	128	SER	1
1	A	138	ASP	1
1	B	141	GLY	1
1	A	185	ARG	1
1	A	28	THR	1
1	B	28	THR	1
1	B	201	LYS	1
1	B	137	LEU	1
1	A	136	PHE	1
1	B	136	PHE	1
1	A	208	THR	1
1	B	208	THR	1
1	A	154	PRO	1
1	B	154	PRO	1
1	B	181	GLU	1
1	B	179	SER	1
1	A	133	ASN	1
1	A	36	ALA	1
1	A	83	SER	1
1	B	53	ASP	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	174/180 (97%)	110±4 (64±2%)	64±4 (36±2%)	1	8
1	B	174/180 (97%)	110±3 (63±2%)	64±3 (37±2%)	1	8
All	All	6960/7200 (97%)	4417 (63%)	2543 (37%)	1	8

All 274 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	20	ILE	20
1	A	23	TYR	20
1	A	25	SER	20
1	A	30	ILE	20
1	A	50	LEU	20
1	A	58	GLU	20
1	A	61	LEU	20
1	A	75	LEU	20
1	A	82	ARG	20
1	A	86	VAL	20
1	A	92	CYS	20
1	A	99	TYR	20
1	A	105	LEU	20
1	A	108	VAL	20
1	A	139	VAL	20
1	A	140	THR	20
1	A	165	ILE	20
1	A	182	THR	20
1	A	183	VAL	20
1	A	195	LEU	20
1	B	20	ILE	20
1	B	23	TYR	20
1	B	25	SER	20
1	B	30	ILE	20
1	B	50	LEU	20
1	B	61	LEU	20
1	B	75	LEU	20
1	B	82	ARG	20
1	B	86	VAL	20
1	B	92	CYS	20
1	B	99	TYR	20
1	B	105	LEU	20
1	B	108	VAL	20
1	B	112	ILE	20
1	B	139	VAL	20
1	B	165	ILE	20
1	B	182	THR	20
1	B	183	VAL	20
1	A	10	THR	19
1	A	29	LEU	19
1	A	39	LEU	19

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Mol	Chain	Res	Type	Models (Total)
1	A	90	THR	19
1	A	112	ILE	19
1	A	169	ARG	19
1	B	10	THR	19
1	B	39	LEU	19
1	B	90	THR	19
1	B	140	THR	19
1	B	202	THR	19
1	A	114	MET	18
1	A	167	ILE	18
1	A	202	THR	18
1	B	29	LEU	18
1	B	58	GLU	18
1	B	114	MET	18
1	B	159	HIS	18
1	B	167	ILE	18
1	B	195	LEU	18
1	A	72	GLU	17
1	A	122	ARG	17
1	A	159	HIS	17
1	A	188	LYS	17
1	B	63	TYR	17
1	B	72	GLU	17
1	B	169	ARG	17
1	A	57	LYS	17
1	B	124	LEU	16
1	B	179	SER	16
1	B	57	LYS	16
1	A	63	TYR	15
1	A	161	ASP	15
1	B	116	LEU	15
1	B	131	VAL	15
1	B	188	LYS	15
1	A	73	LEU	14
1	A	124	LEU	14
1	A	131	VAL	14
1	B	55	GLU	14
1	B	73	LEU	14
1	B	161	ASP	14
1	A	11	LEU	13
1	A	65	ASN	13
1	B	11	LEU	13

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Mol	Chain	Res	Type	Models (Total)
1	A	55	GLU	12
1	A	81	GLU	12
1	A	116	LEU	12
1	A	179	SER	12
1	A	204	VAL	12
1	A	208	THR	12
1	B	22	LYS	12
1	B	27	SER	12
1	B	80	GLN	12
1	B	81	GLU	12
1	B	122	ARG	12
1	B	204	VAL	12
1	A	16	SER	12
1	A	180	ARG	12
1	B	103	ARG	12
1	A	80	GLN	11
1	B	65	ASN	11
1	B	102	PHE	11
1	B	208	THR	11
1	A	123	ARG	11
1	B	123	ARG	11
1	A	32	GLN	10
1	A	125	GLN	10
1	A	130	LYS	10
1	A	142	ARG	10
1	A	193	GLN	10
1	B	130	LYS	10
1	B	136	PHE	10
1	B	163	MET	10
1	B	168	THR	10
1	A	44	LYS	10
1	B	16	SER	10
1	A	22	LYS	10
1	A	136	PHE	9
1	B	120	MET	9
1	B	142	ARG	9
1	B	174	GLN	9
1	A	27	SER	9
1	A	102	PHE	9
1	A	166	LYS	9
1	A	201	LYS	9
1	B	126	VAL	9

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Mol	Chain	Res	Type	Models (Total)
1	B	180	ARG	9
1	A	181	GLU	9
1	A	120	MET	8
1	A	134	LEU	8
1	A	174	GLN	8
1	B	87	ARG	8
1	A	31	HIS	8
1	A	126	VAL	8
1	B	32	GLN	8
1	B	201	LYS	8
1	B	205	VAL	8
1	A	164	GLN	8
1	B	158	THR	8
1	B	166	LYS	8
1	B	68	ASP	8
1	B	134	LEU	8
1	A	168	THR	7
1	B	98	SER	7
1	B	125	GLN	7
1	B	193	GLN	7
1	A	28	THR	7
1	A	87	ARG	7
1	A	98	SER	7
1	A	103	ARG	7
1	B	31	HIS	7
1	B	42	ILE	7
1	B	44	LYS	7
1	B	194	ASN	7
1	A	158	THR	7
1	B	28	THR	7
1	A	68	ASP	7
1	A	133	ASN	7
1	B	106	ILE	7
1	A	38	THR	7
1	A	111	ASP	6
1	A	163	MET	6
1	B	119	GLN	6
1	B	127	THR	6
1	A	205	VAL	6
1	A	77	GLU	6
1	B	38	THR	6
1	B	164	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	B	181	GLU	6
1	A	13	TRP	5
1	A	119	GLN	5
1	A	186	ILE	5
1	B	13	TRP	5
1	B	40	TYR	5
1	B	186	ILE	5
1	A	52	LYS	5
1	B	12	GLU	5
1	B	14	PHE	5
1	A	192	ASP	5
1	B	17	HIS	5
1	B	77	GLU	5
1	B	89	LYS	5
1	B	111	ASP	5
1	A	14	PHE	5
1	A	127	THR	5
1	A	203	ILE	5
1	B	187	LEU	4
1	A	12	GLU	4
1	A	101	LYS	4
1	A	117	SER	4
1	A	194	ASN	4
1	B	153	GLN	4
1	A	17	HIS	4
1	B	52	LYS	4
1	A	42	ILE	4
1	B	191	GLU	4
1	A	78	GLU	4
1	A	106	ILE	4
1	A	196	ILE	4
1	B	203	ILE	4
1	A	40	TYR	4
1	A	115	ARG	4
1	A	35	LYS	3
1	A	153	GLN	3
1	B	133	ASN	3
1	B	192	ASP	3
1	B	145	GLN	3
1	A	8	ASP	3
1	A	51	ILE	3
1	B	35	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	B	115	ARG	3
1	B	196	ILE	3
1	B	59	MET	3
1	A	187	LEU	3
1	B	78	GLU	3
1	B	170	GLN	2
1	B	189	MET	2
1	A	18	CYS	2
1	B	107	GLN	2
1	A	137	LEU	2
1	A	185	ARG	2
1	B	46	SER	2
1	A	107	GLN	2
1	A	93	GLU	2
1	A	145	GLN	2
1	A	149	ASN	2
1	A	143	ILE	2
1	B	97	ILE	2
1	A	41	TYR	2
1	A	100	LYS	2
1	B	51	ILE	2
1	B	54	GLU	2
1	B	117	SER	2
1	B	129	GLU	2
1	B	138	ASP	2
1	A	104	GLN	2
1	A	147	LEU	2
1	B	83	SER	2
1	B	104	GLN	2
1	B	147	LEU	2
1	A	53	ASP	1
1	B	18	CYS	1
1	A	60	ILE	1
1	A	89	LYS	1
1	B	93	GLU	1
1	B	8	ASP	1
1	B	53	ASP	1
1	A	37	GLU	1
1	B	37	GLU	1
1	B	199	HIS	1
1	A	43	VAL	1
1	A	146	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	191	GLU	1
1	A	54	GLU	1
1	A	97	ILE	1
1	B	41	TYR	1
1	B	100	LYS	1
1	B	209	ARG	1
1	A	76	PHE	1
1	B	185	ARG	1
1	A	129	GLU	1
1	A	209	ARG	1
1	B	76	PHE	1
1	B	113	LEU	1
1	A	49	VAL	1
1	A	178	CYS	1
1	A	157	MET	1
1	B	96	GLU	1
1	B	157	MET	1
1	A	96	GLU	1
1	A	138	ASP	1
1	A	175	ILE	1
1	B	34	GLU	1
1	A	46	SER	1
1	B	101	LYS	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 [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