



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 04:55 PM UTC

PDB ID : 2KHZ / pdb_00002khz
Title : Solution Structure of RCL
Authors : Doddapaneni, K.; Mahler, B.; Yuan, C.; Wu, Z.
Deposited on : 2009-04-15

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

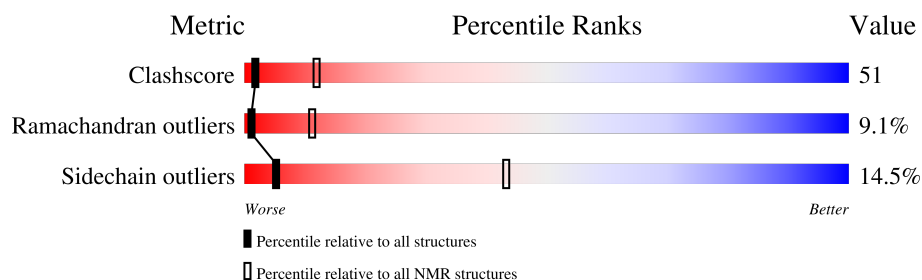
1 Overall quality at a glance

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	165	
1	B	165	

2 Ensemble composition and analysis

This entry contains 15 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:18, A:22-A:152, B:208-B:218, B:222-B:352 (284)	1.10	11

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 5, 9, 11
2	2, 10, 12, 15
3	3, 6, 8
Single-model clusters	4; 7; 13; 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4928 atoms, of which 2426 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called c-Myc-responsive protein Rcl.

Mol	Chain	Residues	Atoms						Trace
1	A	163	Total	C	H	N	O	S	0
			2464	782	1213	221	242	6	
1	B	163	Total	C	H	N	O	S	0
			2464	782	1213	221	242	6	

There are 4 discrepancies between the modelled and reference sequences:

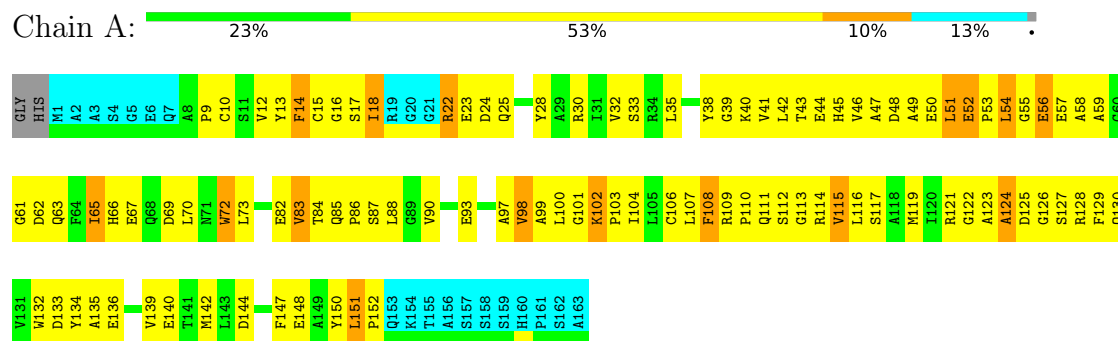
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O35820
A	0	HIS	-	expression tag	UNP O35820
B	199	GLY	-	expression tag	UNP O35820
B	200	HIS	-	expression tag	UNP O35820

4 Residue-property plots

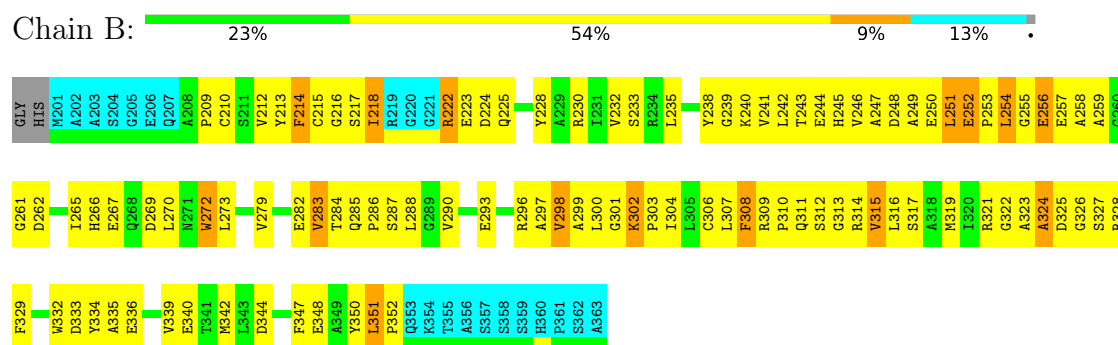
4.1 Average score per residue in the NMR ensemble

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: c-Myc-responsive protein Rcl



- Molecule 1: c-Myc-responsive protein Rcl

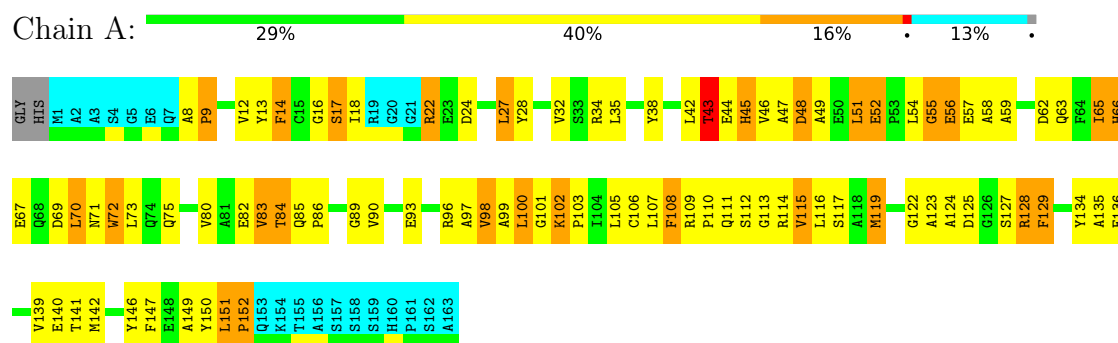


4.2 Scores per residue for each member of the ensemble

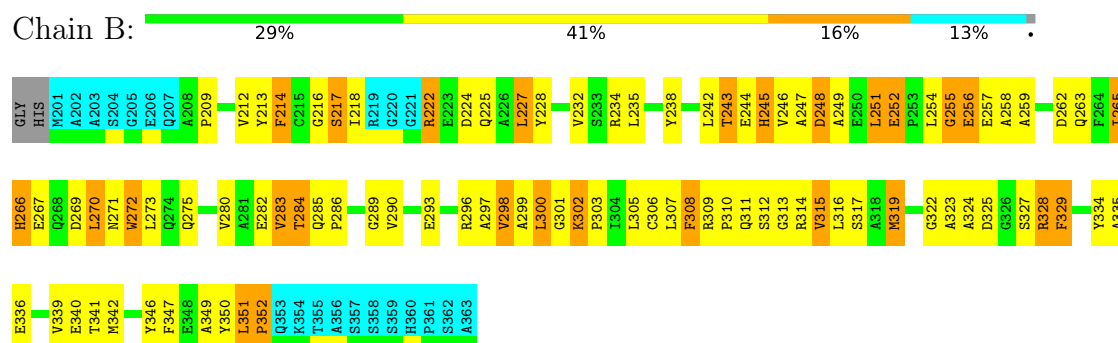
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: c-Myc-responsive protein Rcl

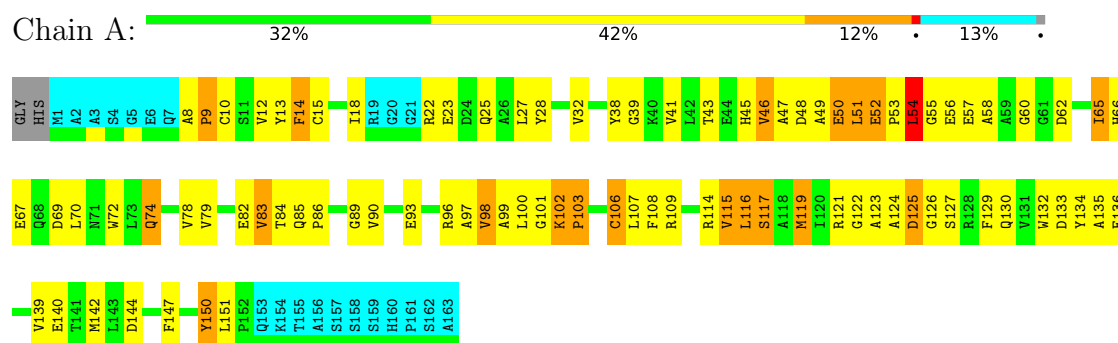


- Molecule 1: c-Myc-responsive protein Rcl

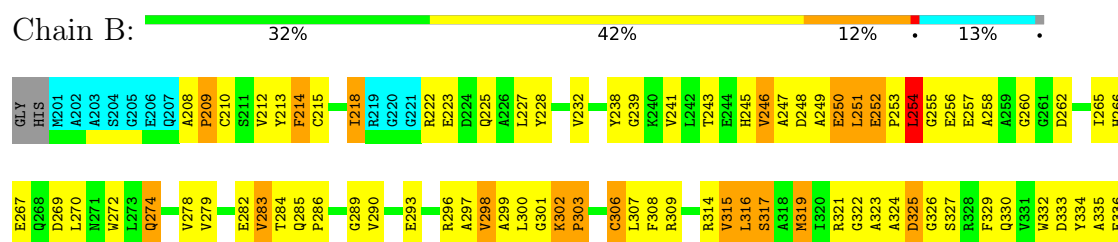


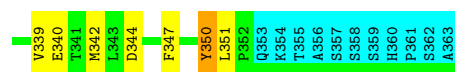
4.2.2 Score per residue for model 2

- Molecule 1: c-Myc-responsive protein Rcl



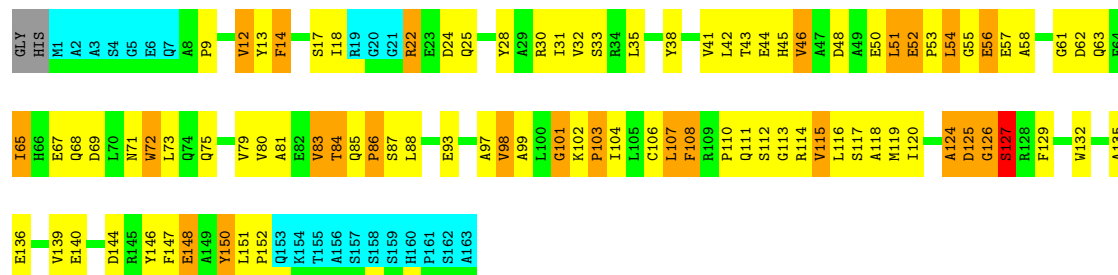
- Molecule 1: c-Myc-responsive protein Rcl



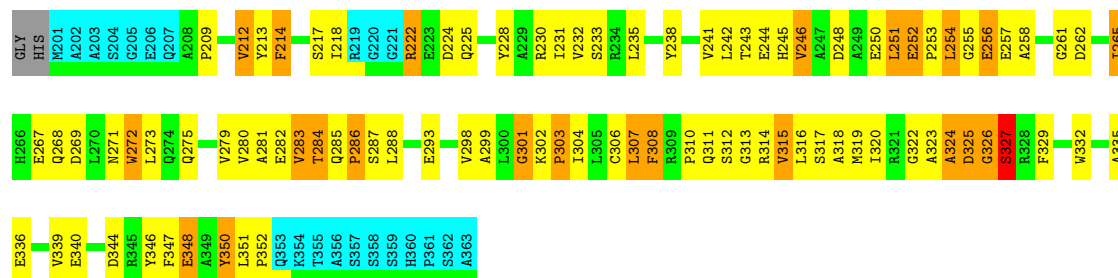


4.2.3 Score per residue for model 3

- Molecule 1: c-Myc-responsive protein Rcl

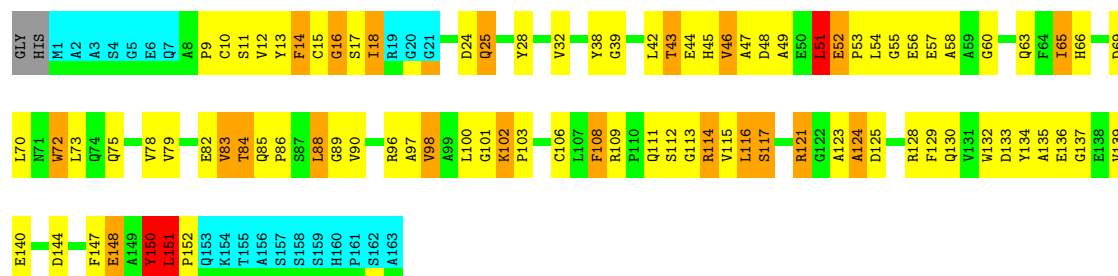


- Molecule 1: c-Myc-responsive protein Rcl

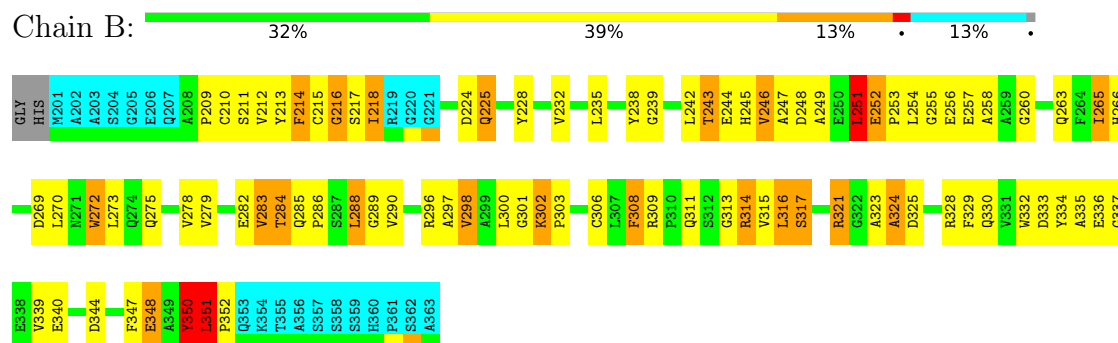


4.2.4 Score per residue for model 4

- Molecule 1: c-Myc-responsive protein Rcl



- Molecule 1: c-Myc-responsive protein Rcl

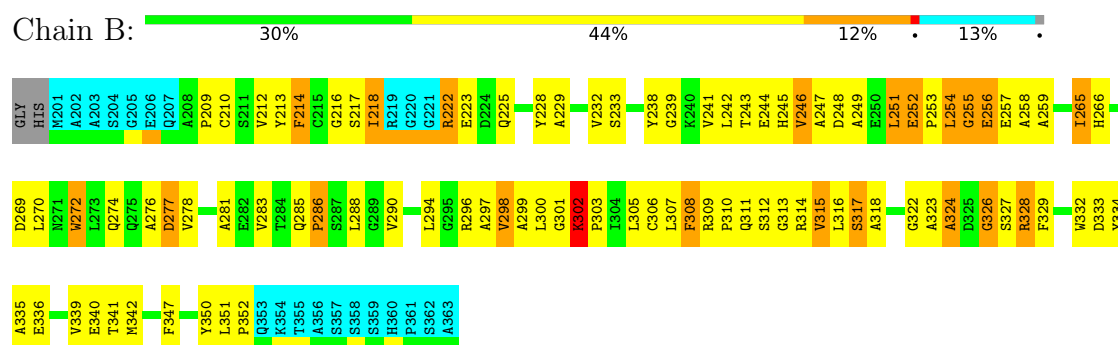


4.2.5 Score per residue for model 5

- Molecule 1: c-Myc-responsive protein Rcl

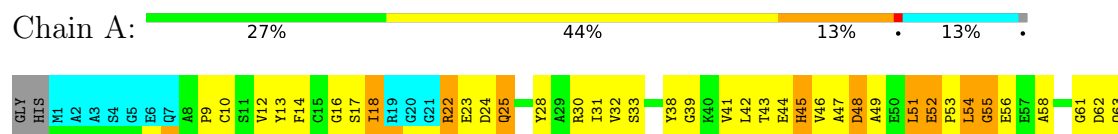


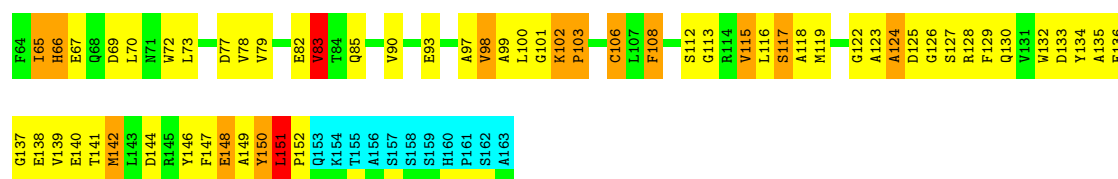
- Molecule 1: c-Myc-responsive protein Rcl



4.2.6 Score per residue for model 6

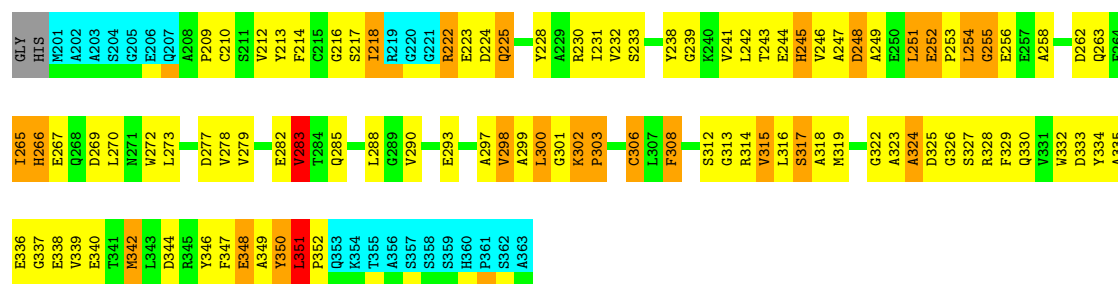
- Molecule 1: c-Myc-responsive protein Rcl





• Molecule 1: c-Myc-responsive protein Rcl

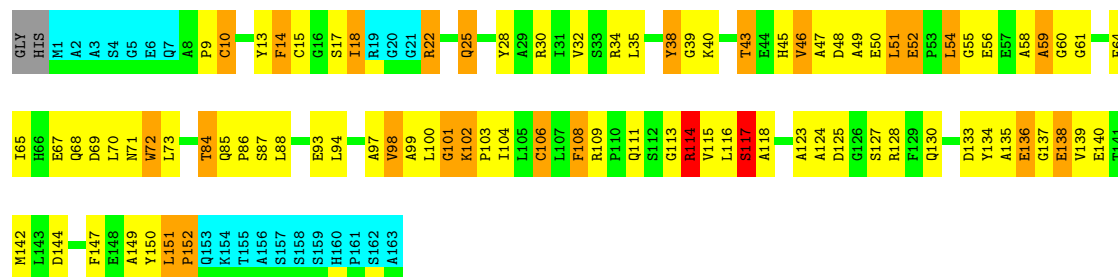
Chain B: 27% 44% 14% 13%



4.2.7 Score per residue for model 7

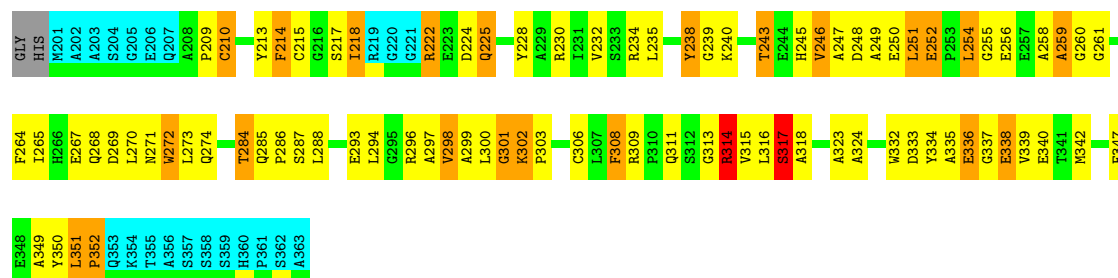
• Molecule 1: c-Myc-responsive protein Rcl

Chain A: 33% 38% 14% 13%



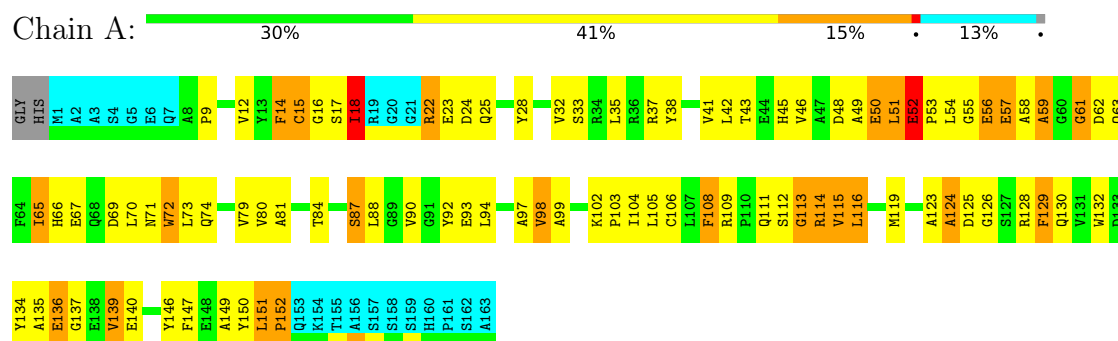
• Molecule 1: c-Myc-responsive protein Rcl

Chain B: 34% 38% 13% 13%

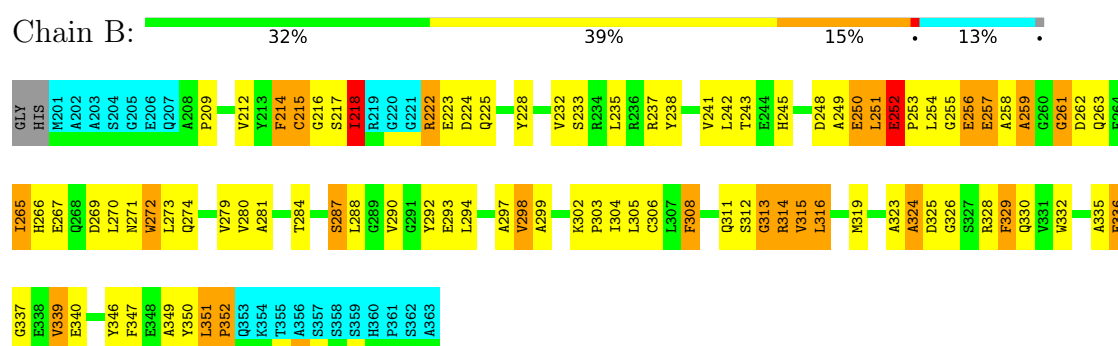


4.2.8 Score per residue for model 8

• Molecule 1: c-Myc-responsive protein Rcl

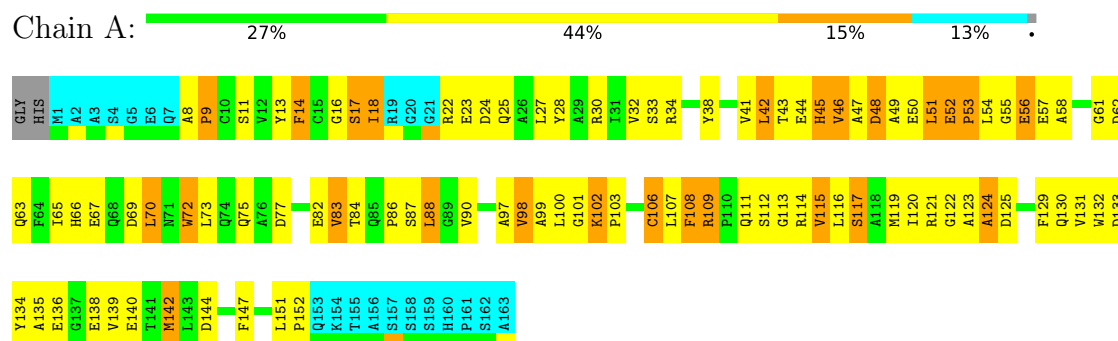


• Molecule 1: c-Myc-responsive protein Rcl

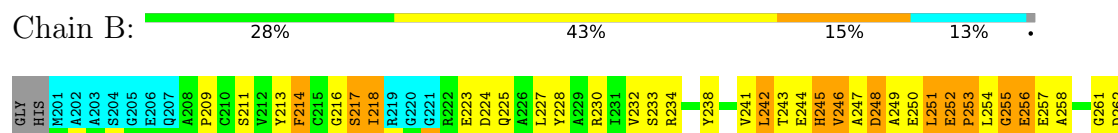


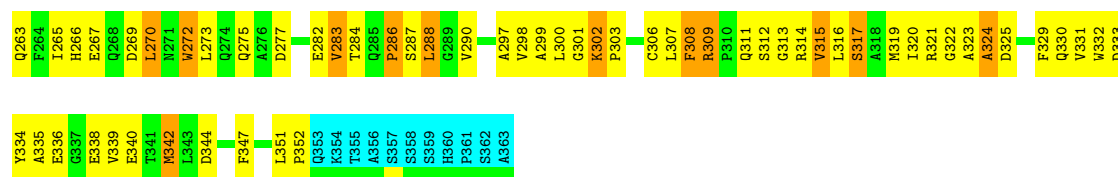
4.2.9 Score per residue for model 9

• Molecule 1: c-Myc-responsive protein Rcl



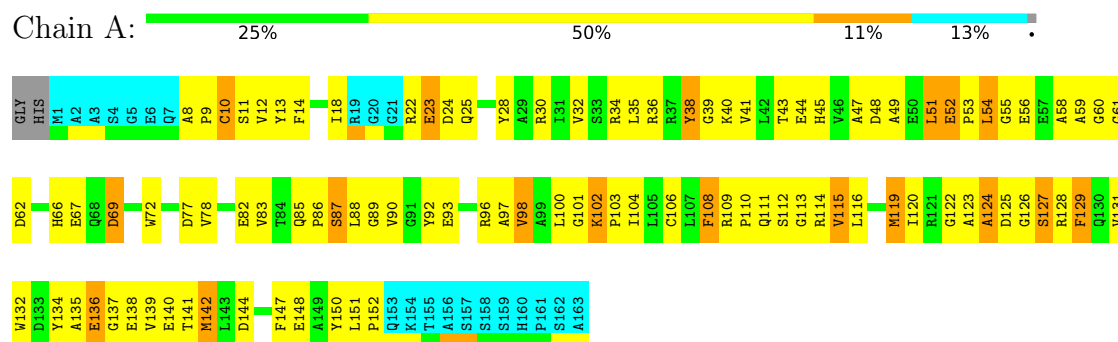
• Molecule 1: c-Myc-responsive protein Rcl



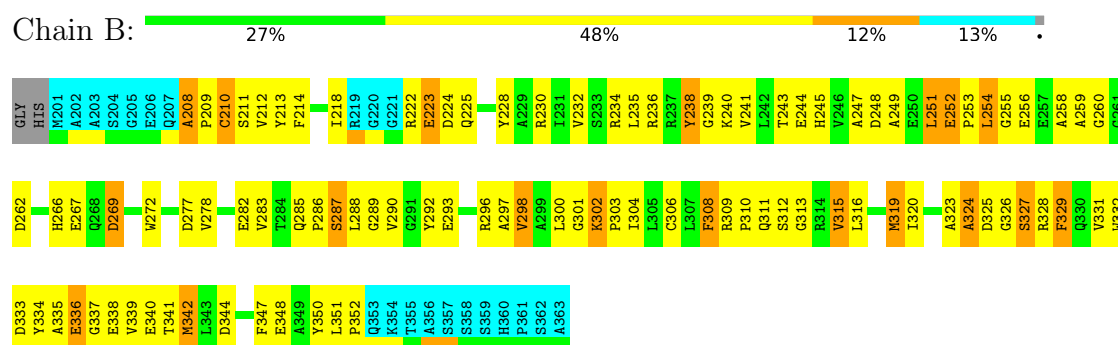


4.2.10 Score per residue for model 10

- Molecule 1: c-Myc-responsive protein Rcl

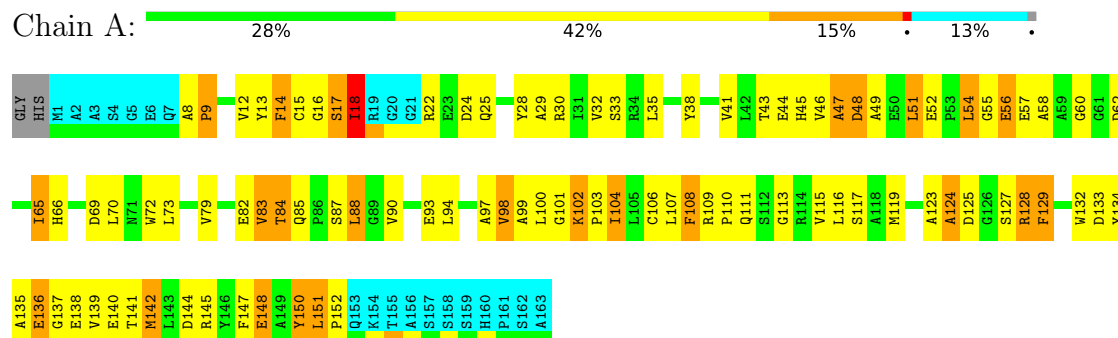


- Molecule 1: c-Myc-responsive protein Rcl

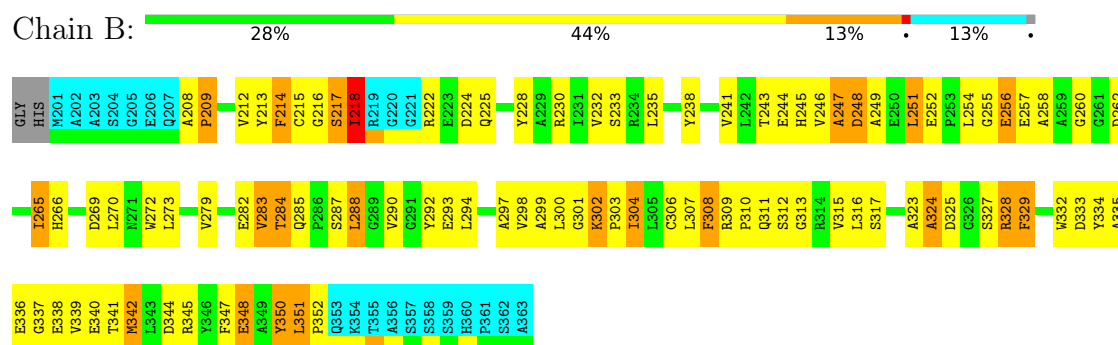


4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: c-Myc-responsive protein Rcl

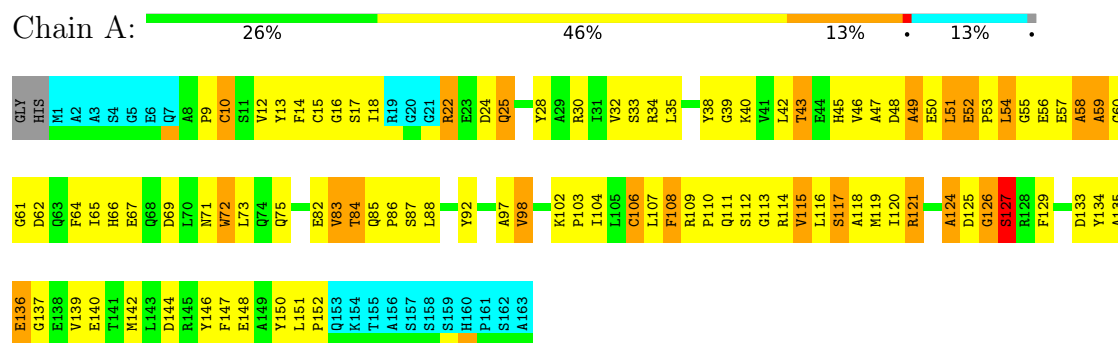


- Molecule 1: c-Myc-responsive protein Rcl



4.2.12 Score per residue for model 12

- Molecule 1: c-Myc-responsive protein Rcl



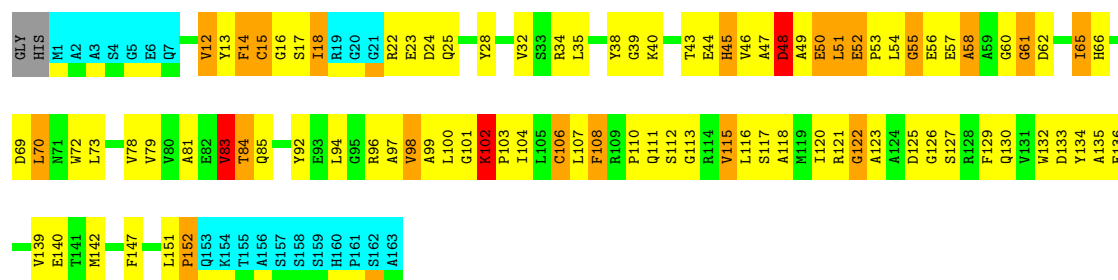
- Molecule 1: c-Myc-responsive protein Rcl



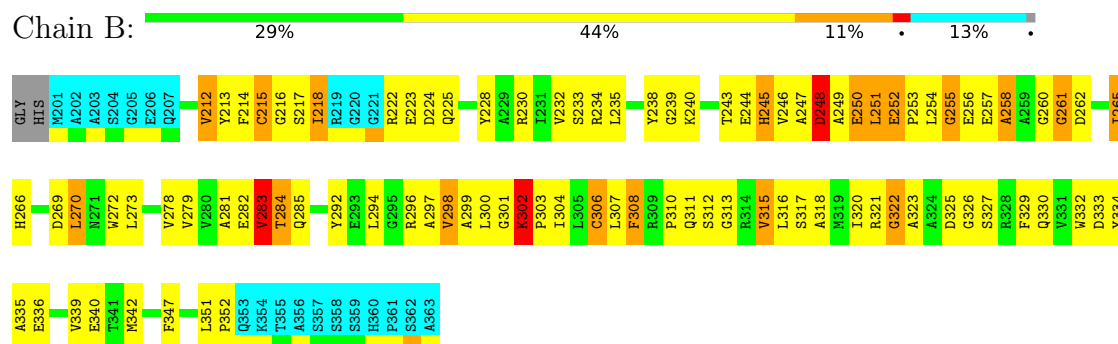
4.2.13 Score per residue for model 13

- Molecule 1: c-Myc-responsive protein Rcl



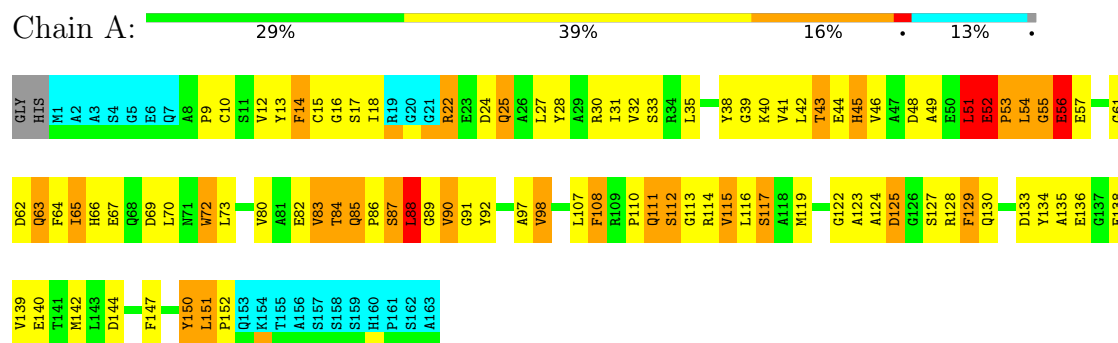


• Molecule 1: c-Myc-responsive protein Rcl

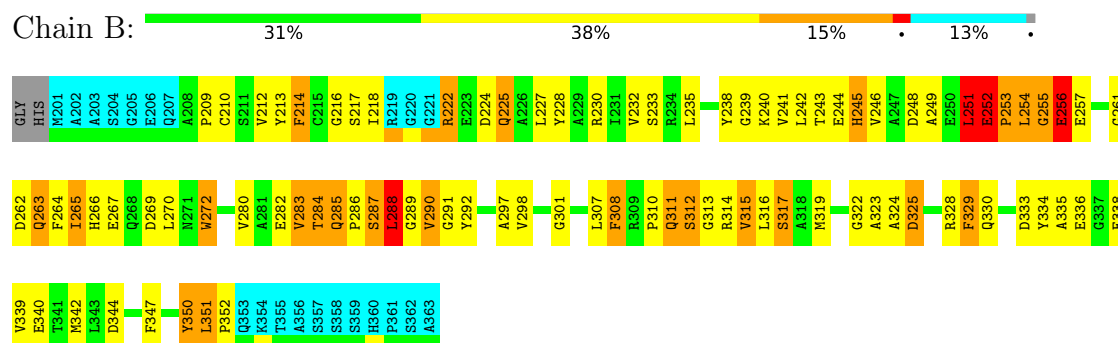


4.2.14 Score per residue for model 14

• Molecule 1: c-Myc-responsive protein Rcl

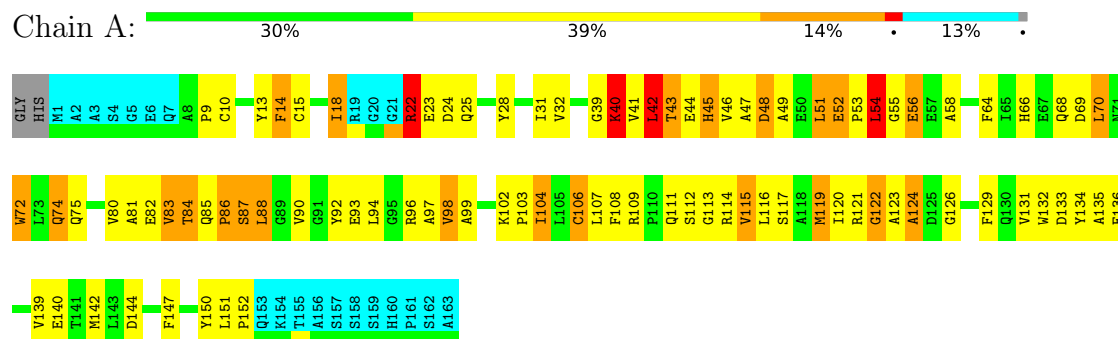


• Molecule 1: c-Myc-responsive protein Rcl

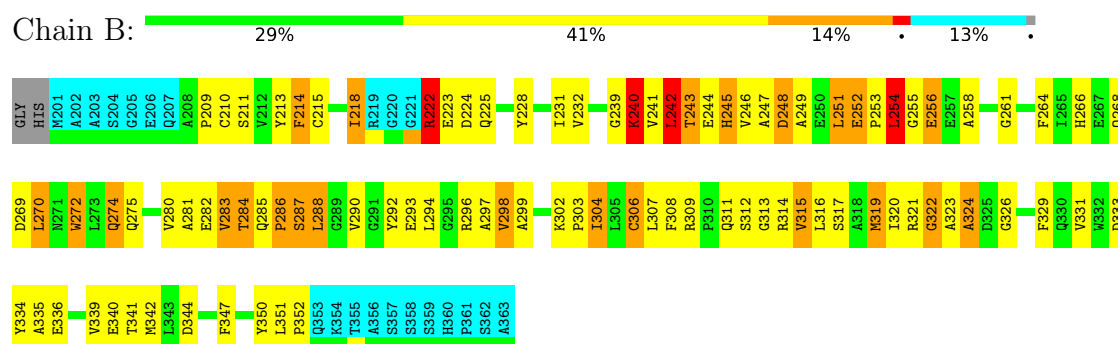


4.2.15 Score per residue for model 15

• Molecule 1: c-Myc-responsive protein Rcl



• Molecule 1: c-Myc-responsive protein Rcl



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	
TALOS	geometry optimization	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.47±0.01	0±0/1133 (0.0± 0.0%)	1.25±0.02	2±1/1538 (0.1± 0.1%)
1	B	1.47±0.01	0±0/1133 (0.0± 0.0%)	1.25±0.02	2±1/1538 (0.1± 0.1%)
All	All	1.47	6/33990 (0.0%)	1.25	57/46140 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	216	GLY	N-CA	5.41	1.50	1.45	13	3
1	A	16	GLY	N-CA	5.40	1.50	1.45	13	3

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	122	GLY	N-CA-C	-7.26	103.97	112.83	13	2
1	B	322	GLY	N-CA-C	-7.24	104.00	112.83	13	2
1	B	284	THR	N-CA-C	-6.63	105.48	113.97	14	1
1	A	84	THR	N-CA-C	-6.57	105.56	113.97	14	1
1	B	214	PHE	CA-CB-CG	-6.36	107.44	113.80	11	5
1	A	14	PHE	CA-CB-CG	-6.29	107.51	113.80	11	6
1	A	23	GLU	N-CA-C	-5.83	105.27	112.38	13	2
1	B	223	GLU	N-CA-C	-5.79	105.31	112.38	13	2
1	B	348	GLU	N-CA-C	-5.75	105.10	111.71	11	3
1	B	329	PHE	CA-CB-CG	-5.74	108.06	113.80	10	5
1	A	148	GLU	N-CA-C	-5.61	105.26	111.71	11	3
1	A	129	PHE	CA-CB-CG	-5.60	108.20	113.80	10	5
1	B	277	ASP	N-CA-C	-5.56	106.63	113.41	6	2
1	A	77	ASP	N-CA-C	-5.47	106.74	113.41	6	2
1	B	349	ALA	N-CA-C	-5.46	106.65	113.15	8	3
1	A	149	ALA	N-CA-C	-5.45	106.66	113.15	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	284	THR	CB-CA-C	-5.41	109.87	117.23	13	1
1	A	84	THR	CB-CA-C	-5.40	109.89	117.23	13	1
1	B	245	HIS	CA-CB-CG	-5.40	108.40	113.80	14	1
1	A	45	HIS	CA-CB-CG	-5.36	108.44	113.80	14	1
1	B	291	GLY	N-CA-C	-5.36	106.22	113.24	14	1
1	A	91	GLY	N-CA-C	-5.32	106.27	113.24	14	1
1	A	126	GLY	N-CA-C	-5.08	108.70	115.40	5	1
1	B	326	GLY	N-CA-C	-5.07	108.71	115.40	5	1
1	A	112	SER	N-CA-C	-5.03	107.00	114.64	4	1
1	B	312	SER	N-CA-C	-5.01	107.17	113.28	11	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1109	1080	1078	117±12
1	B	1109	1080	1078	116±11
All	All	33270	32400	32340	3370

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD23	1:A:116:LEU:H	1.05	1.04	8	2
1:A:51:LEU:H	1:A:51:LEU:HD13	1.05	1.08	5	2
1:A:51:LEU:HD13	1:A:51:LEU:H	1.04	1.05	15	6
1:B:251:LEU:HD13	1:B:251:LEU:H	1.04	1.07	5	7
1:B:316:LEU:HD23	1:B:316:LEU:H	1.02	1.04	8	2
1:A:135:ALA:O	1:A:137:GLY:O	0.96	1.84	7	1
1:B:335:ALA:O	1:B:337:GLY:O	0.96	1.83	7	1
1:B:251:LEU:HD22	1:B:251:LEU:H	0.95	1.20	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:H	1:A:51:LEU:HD22	0.93	1.20	3	3
1:A:51:LEU:HD22	1:A:51:LEU:H	0.90	1.22	11	2
1:B:248:ASP:O	1:B:251:LEU:HD22	0.88	1.69	13	3
1:A:51:LEU:HD13	1:A:51:LEU:N	0.88	1.84	10	8
1:A:48:ASP:O	1:A:51:LEU:HD22	0.88	1.68	13	3
1:B:347:PHE:CD1	1:B:351:LEU:HD12	0.87	2.04	5	8
1:B:251:LEU:HD13	1:B:251:LEU:N	0.87	1.84	10	7
1:A:147:PHE:CD1	1:A:151:LEU:HD12	0.87	2.05	5	8
1:B:248:ASP:O	1:B:250:GLU:N	0.86	2.09	12	1
1:A:48:ASP:O	1:A:50:GLU:N	0.85	2.09	12	1
1:A:25:GLN:NE2	1:A:49:ALA:HB3	0.85	1.86	12	2
1:A:85:GLN:N	1:A:86:PRO:CD	0.84	2.40	15	2
1:B:285:GLN:N	1:B:286:PRO:CD	0.84	2.41	15	2
1:A:116:LEU:HD23	1:A:116:LEU:N	0.84	1.88	8	2
1:B:225:GLN:NE2	1:B:249:ALA:HB3	0.83	1.87	12	2
1:A:51:LEU:H	1:A:51:LEU:CD1	0.83	1.87	15	7
1:B:251:LEU:H	1:B:251:LEU:CD1	0.83	1.87	15	7
1:B:316:LEU:HD23	1:B:316:LEU:N	0.83	1.88	8	2
1:B:287:SER:OG	1:B:290:VAL:HG23	0.83	1.74	8	3
1:A:116:LEU:H	1:A:116:LEU:CD2	0.82	1.85	8	3
1:B:350:TYR:CG	1:B:351:LEU:N	0.82	2.47	14	3
1:B:350:TYR:O	1:B:350:TYR:CG	0.82	2.32	6	3
1:A:150:TYR:O	1:A:150:TYR:CG	0.82	2.32	6	3
1:B:326:GLY:C	1:B:328:ARG:H	0.82	1.83	6	3
1:B:216:GLY:O	1:B:290:VAL:HG21	0.82	1.74	14	1
1:A:150:TYR:CG	1:A:151:LEU:N	0.81	2.47	14	3
1:B:316:LEU:H	1:B:316:LEU:CD2	0.81	1.85	8	3
1:B:228:TYR:O	1:B:232:VAL:HG23	0.81	1.76	4	14
1:B:335:ALA:O	1:B:336:GLU:C	0.81	2.23	7	11
1:A:16:GLY:O	1:A:90:VAL:HG21	0.81	1.75	14	1
1:A:87:SER:OG	1:A:90:VAL:HG23	0.81	1.75	8	2
1:B:326:GLY:O	1:B:328:ARG:N	0.80	2.15	6	2
1:A:28:TYR:O	1:A:32:VAL:HG23	0.80	1.77	4	14
1:A:48:ASP:O	1:A:51:LEU:HD21	0.80	1.76	4	6
1:A:111:GLN:O	1:A:113:GLY:N	0.79	2.16	14	1
1:A:126:GLY:O	1:A:128:ARG:N	0.79	2.15	6	2
1:B:212:VAL:HG11	1:B:235:LEU:HD22	0.79	1.55	12	7
1:B:311:GLN:O	1:B:313:GLY:N	0.79	2.15	14	1
1:A:12:VAL:HG11	1:A:35:LEU:HD22	0.78	1.54	11	7
1:B:251:LEU:N	1:B:251:LEU:HD22	0.78	1.93	4	6
1:A:127:SER:C	1:A:129:PHE:H	0.78	1.87	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:248:ASP:O	1:B:251:LEU:HD21	0.78	1.77	4	6
1:B:214:PHE:HA	1:B:280:VAL:O	0.78	1.79	8	3
1:B:251:LEU:H	1:B:251:LEU:CD2	0.78	1.90	11	5
1:A:135:ALA:O	1:A:137:GLY:N	0.77	2.18	7	7
1:B:306:CYS:SG	1:B:329:PHE:CZ	0.77	2.77	13	5
1:A:126:GLY:C	1:A:128:ARG:H	0.77	1.83	6	3
1:B:215:CYS:SG	1:B:281:ALA:HB2	0.77	2.19	13	2
1:B:251:LEU:HD22	1:B:251:LEU:N	0.77	1.94	11	2
1:A:66:HIS:ND1	1:B:319:MET:O	0.77	2.17	12	1
1:B:248:ASP:O	1:B:251:LEU:HD11	0.77	1.80	15	3
1:A:51:LEU:HD22	1:A:51:LEU:N	0.77	1.93	4	3
1:A:15:CYS:SG	1:A:81:ALA:HB2	0.77	2.20	13	2
1:A:14:PHE:HA	1:A:80:VAL:O	0.77	1.79	8	3
1:A:106:CYS:SG	1:A:129:PHE:CZ	0.77	2.78	13	5
1:A:48:ASP:O	1:A:51:LEU:HD11	0.76	1.79	15	3
1:A:135:ALA:O	1:A:136:GLU:C	0.76	2.24	7	11
1:A:25:GLN:HE22	1:A:47:ALA:H	0.76	1.24	11	1
1:B:248:ASP:C	1:B:251:LEU:HD11	0.76	2.06	5	5
1:B:335:ALA:O	1:B:337:GLY:N	0.76	2.17	7	7
1:A:49:ALA:O	1:A:54:LEU:HD21	0.76	1.81	10	3
1:A:48:ASP:C	1:A:51:LEU:HD11	0.75	2.06	5	5
1:B:249:ALA:O	1:B:254:LEU:HD21	0.75	1.81	10	3
1:A:54:LEU:HD12	1:A:54:LEU:N	0.75	1.96	6	6
1:B:300:LEU:C	1:B:300:LEU:HD13	0.75	2.06	1	2
1:A:25:GLN:NE2	1:A:50:GLU:N	0.75	2.34	8	2
1:A:119:MET:O	1:B:266:HIS:ND1	0.74	2.19	12	1
1:A:100:LEU:C	1:A:100:LEU:HD13	0.74	2.07	1	2
1:B:327:SER:C	1:B:329:PHE:H	0.74	1.87	2	4
1:B:225:GLN:NE2	1:B:250:GLU:N	0.74	2.35	8	2
1:B:254:LEU:O	1:B:255:GLY:O	0.73	2.06	6	2
1:B:225:GLN:HE22	1:B:247:ALA:H	0.73	1.24	11	1
1:A:147:PHE:CG	1:A:151:LEU:HD12	0.73	2.18	11	6
1:B:254:LEU:HD12	1:B:254:LEU:N	0.73	1.99	13	5
1:A:54:LEU:O	1:A:55:GLY:O	0.72	2.07	6	2
1:A:51:LEU:O	1:A:54:LEU:HD23	0.72	1.85	2	1
1:A:85:GLN:O	1:A:86:PRO:O	0.72	2.06	15	1
1:B:225:GLN:HE22	1:B:247:ALA:N	0.72	1.83	11	2
1:B:248:ASP:O	1:B:251:LEU:HG	0.72	1.83	12	1
1:B:225:GLN:NE2	1:B:247:ALA:H	0.72	1.83	11	1
1:B:251:LEU:N	1:B:251:LEU:HD13	0.72	1.98	4	2
1:A:25:GLN:NE2	1:A:47:ALA:H	0.72	1.82	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:GLN:O	1:B:286:PRO:O	0.72	2.06	15	1
1:B:323:ALA:O	1:B:324:ALA:HB2	0.72	1.85	10	1
1:A:48:ASP:O	1:A:51:LEU:HG	0.71	1.84	12	1
1:A:120:ILE:O	1:A:123:ALA:O	0.71	2.07	15	2
1:A:123:ALA:O	1:A:124:ALA:HB2	0.71	1.85	10	1
1:B:347:PHE:CG	1:B:351:LEU:HD12	0.71	2.18	11	6
1:B:235:LEU:O	1:B:238:TYR:O	0.71	2.09	7	4
1:A:25:GLN:HE22	1:A:47:ALA:N	0.71	1.83	11	2
1:B:320:ILE:O	1:B:323:ALA:O	0.71	2.06	15	2
1:A:35:LEU:O	1:A:38:TYR:O	0.71	2.09	7	4
1:A:46:VAL:O	1:A:48:ASP:N	0.71	2.24	13	3
1:B:313:GLY:O	1:B:314:ARG:O	0.71	2.09	7	1
1:B:213:TYR:OH	1:B:269:ASP:CG	0.71	2.34	1	3
1:A:113:GLY:O	1:A:114:ARG:O	0.70	2.09	7	1
1:A:22:ARG:CD	1:A:22:ARG:N	0.70	2.54	1	4
1:B:222:ARG:CD	1:B:222:ARG:N	0.70	2.54	1	3
1:B:222:ARG:NH2	1:B:255:GLY:H	0.70	1.84	11	1
1:A:13:TYR:OH	1:A:69:ASP:CG	0.70	2.34	1	3
1:B:251:LEU:O	1:B:254:LEU:HD23	0.70	1.85	2	1
1:B:243:THR:O	1:B:243:THR:HG22	0.70	1.87	13	1
1:A:49:ALA:O	1:A:54:LEU:HD11	0.70	1.87	12	4
1:B:225:GLN:NE2	1:B:246:VAL:O	0.70	2.25	3	6
1:A:119:MET:HE2	1:B:266:HIS:CE1	0.70	2.21	12	1
1:A:118:ALA:HB2	1:B:256:GLU:OE1	0.70	1.87	6	2
1:A:92:TYR:OH	1:B:298:VAL:HG21	0.70	1.86	12	1
1:B:251:LEU:CD1	1:B:251:LEU:N	0.70	2.55	9	2
1:A:116:LEU:HD22	1:A:131:VAL:HG11	0.70	1.63	9	2
1:A:22:ARG:NH2	1:A:55:GLY:H	0.70	1.84	11	1
1:B:246:VAL:O	1:B:248:ASP:N	0.70	2.23	13	3
1:B:249:ALA:O	1:B:254:LEU:HD11	0.70	1.86	12	4
1:A:43:THR:HG22	1:A:43:THR:O	0.70	1.86	13	1
1:A:66:HIS:CE1	1:B:319:MET:HE2	0.69	2.22	12	1
1:A:51:LEU:CD1	1:A:51:LEU:N	0.69	2.55	9	2
1:B:225:GLN:HE22	1:B:254:LEU:HD21	0.69	1.47	8	1
1:A:123:ALA:O	1:A:124:ALA:C	0.69	2.35	5	7
1:A:56:GLU:OE1	1:B:318:ALA:HB2	0.69	1.88	6	2
1:A:100:LEU:HD12	1:A:101:GLY:N	0.69	2.02	13	1
1:A:25:GLN:NE2	1:A:46:VAL:O	0.69	2.25	3	6
1:A:138:GLU:O	1:A:142:MET:SD	0.68	2.51	10	3
1:A:25:GLN:HE22	1:A:54:LEU:HD21	0.68	1.47	8	1
1:B:323:ALA:O	1:B:324:ALA:C	0.68	2.35	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:342:MET:SD	1:B:342:MET:N	0.68	2.67	11	3
1:A:88:LEU:C	1:A:90:VAL:H	0.68	1.96	14	2
1:B:218:ILE:HD13	1:B:218:ILE:N	0.68	2.04	11	2
1:B:316:LEU:HD22	1:B:331:VAL:HG11	0.68	1.64	9	2
1:A:55:GLY:O	1:A:57:GLU:N	0.68	2.26	11	7
1:A:43:THR:HG23	1:A:43:THR:O	0.68	1.88	3	2
1:B:300:LEU:HD12	1:B:301:GLY:N	0.68	2.02	13	1
1:A:18:ILE:HD13	1:A:18:ILE:N	0.68	2.03	11	2
1:A:98:VAL:HG21	1:B:292:TYR:OH	0.68	1.89	12	2
1:B:285:GLN:N	1:B:286:PRO:HD2	0.68	2.01	15	1
1:A:85:GLN:N	1:A:86:PRO:HD2	0.68	2.01	15	1
1:B:338:GLU:O	1:B:342:MET:SD	0.68	2.51	10	3
1:A:87:SER:O	1:B:288:LEU:HD23	0.67	1.88	12	2
1:B:255:GLY:O	1:B:257:GLU:N	0.67	2.27	11	7
1:B:243:THR:O	1:B:243:THR:HG23	0.67	1.88	3	2
1:A:142:MET:SD	1:A:142:MET:N	0.67	2.66	11	3
1:A:88:LEU:HD23	1:B:287:SER:O	0.67	1.88	12	2
1:B:216:GLY:O	1:B:217:SER:C	0.67	2.36	1	2
1:A:94:LEU:C	1:A:94:LEU:HD13	0.67	2.15	7	1
1:B:283:VAL:HG11	1:B:316:LEU:HD11	0.67	1.65	6	4
1:A:51:LEU:H	1:A:51:LEU:CD2	0.67	1.98	3	4
1:B:245:HIS:O	1:B:249:ALA:N	0.67	2.28	4	3
1:A:16:GLY:O	1:A:17:SER:C	0.67	2.37	1	2
1:A:83:VAL:HG11	1:A:116:LEU:HD11	0.67	1.65	6	3
1:B:225:GLN:NE2	1:B:249:ALA:C	0.67	2.53	8	2
1:A:45:HIS:O	1:A:49:ALA:N	0.66	2.27	4	3
1:A:124:ALA:HB3	1:A:129:PHE:CD1	0.66	2.26	12	2
1:A:87:SER:OG	1:A:88:LEU:N	0.66	2.27	15	2
1:A:97:ALA:O	1:A:101:GLY:O	0.66	2.11	10	2
1:B:225:GLN:HE21	1:B:250:GLU:N	0.66	1.88	9	2
1:A:47:ALA:O	1:A:48:ASP:C	0.66	2.38	12	2
1:B:294:LEU:C	1:B:294:LEU:HD13	0.66	2.15	7	1
1:A:94:LEU:HD22	1:A:106:CYS:SG	0.66	2.30	11	1
1:B:297:ALA:O	1:B:301:GLY:O	0.66	2.11	10	2
1:A:25:GLN:NE2	1:A:49:ALA:C	0.66	2.53	8	2
1:B:288:LEU:C	1:B:290:VAL:H	0.66	1.96	14	2
1:A:135:ALA:C	1:A:137:GLY:N	0.66	2.50	7	7
1:A:25:GLN:HE21	1:A:50:GLU:N	0.66	1.88	9	2
1:A:47:ALA:C	1:A:49:ALA:H	0.65	1.99	13	8
1:B:337:GLY:C	1:B:339:VAL:H	0.65	1.98	7	1
1:B:335:ALA:C	1:B:337:GLY:N	0.65	2.50	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:302:LYS:H	1:B:303:PRO:CD	0.65	2.05	2	1
1:B:294:LEU:HD22	1:B:306:CYS:SG	0.65	2.31	11	1
1:B:247:ALA:C	1:B:249:ALA:H	0.65	1.99	1	8
1:A:45:HIS:CG	1:A:46:VAL:N	0.65	2.65	3	2
1:A:66:HIS:CG	1:B:322:GLY:HA3	0.65	2.26	15	5
1:A:51:LEU:N	1:A:51:LEU:CD1	0.65	2.59	7	7
1:A:134:TYR:CD2	1:A:135:ALA:N	0.65	2.65	7	4
1:A:114:ARG:O	1:A:115:VAL:C	0.65	2.40	8	2
1:B:232:VAL:HG13	1:B:241:VAL:HG11	0.65	1.68	9	5
1:B:245:HIS:CG	1:B:246:VAL:N	0.65	2.64	3	2
1:B:324:ALA:HB3	1:B:329:PHE:CD1	0.65	2.26	12	2
1:A:102:LYS:H	1:A:103:PRO:CD	0.65	2.05	2	1
1:A:32:VAL:HG13	1:A:41:VAL:HG11	0.65	1.67	9	5
1:B:249:ALA:C	1:B:251:LEU:H	0.65	2.00	9	3
1:A:135:ALA:O	1:A:138:GLU:N	0.64	2.29	9	2
1:B:334:TYR:CD2	1:B:335:ALA:N	0.64	2.65	7	4
1:B:283:VAL:HG11	1:B:316:LEU:CD1	0.64	2.23	13	2
1:B:335:ALA:O	1:B:338:GLU:N	0.64	2.30	9	2
1:A:14:PHE:CG	1:A:14:PHE:O	0.64	2.51	8	3
1:B:326:GLY:O	1:B:327:SER:CB	0.64	2.46	10	3
1:A:122:GLY:HA3	1:B:266:HIS:CG	0.64	2.27	15	5
1:A:83:VAL:HG11	1:A:116:LEU:CD1	0.64	2.23	13	2
1:B:214:PHE:CG	1:B:214:PHE:O	0.64	2.51	8	2
1:A:126:GLY:O	1:A:127:SER:CB	0.64	2.45	10	3
1:A:150:TYR:C	1:A:150:TYR:CD1	0.64	2.76	3	1
1:B:326:GLY:C	1:B:328:ARG:N	0.64	2.53	6	3
1:A:124:ALA:O	1:A:129:PHE:CD2	0.63	2.51	10	1
1:B:350:TYR:C	1:B:350:TYR:CD1	0.63	2.77	3	1
1:A:137:GLY:C	1:A:139:VAL:H	0.63	1.98	7	1
1:B:272:TRP:CZ3	1:B:275:GLN:NE2	0.63	2.66	9	2
1:B:308:PHE:C	1:B:308:PHE:CD1	0.63	2.77	10	9
1:A:72:TRP:CZ3	1:A:75:GLN:NE2	0.63	2.66	9	2
1:A:51:LEU:N	1:A:51:LEU:CD2	0.63	2.62	14	3
1:A:69:ASP:CG	1:B:319:MET:HE1	0.63	2.18	1	1
1:B:324:ALA:O	1:B:325:ASP:CB	0.63	2.46	2	4
1:B:324:ALA:O	1:B:329:PHE:CD2	0.63	2.52	10	1
1:A:72:TRP:CD1	1:A:75:GLN:NE2	0.63	2.67	15	1
1:A:114:ARG:CD	1:A:114:ARG:N	0.63	2.61	4	1
1:B:314:ARG:N	1:B:314:ARG:CD	0.63	2.61	4	1
1:B:212:VAL:HA	1:B:278:VAL:O	0.63	1.93	13	4
1:B:248:ASP:C	1:B:251:LEU:HD21	0.63	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ALA:C	1:A:137:GLY:H	0.63	2.02	11	4
1:A:108:PHE:C	1:A:108:PHE:CD1	0.63	2.77	10	9
1:B:239:GLY:O	1:B:240:LYS:C	0.63	2.42	7	5
1:A:85:GLN:H	1:A:86:PRO:CD	0.63	2.06	15	2
1:B:266:HIS:ND1	1:B:267:GLU:N	0.63	2.47	9	4
1:A:124:ALA:O	1:A:125:ASP:CG	0.63	2.42	2	3
1:B:251:LEU:CD2	1:B:251:LEU:N	0.62	2.62	14	1
1:A:66:HIS:ND1	1:A:67:GLU:N	0.62	2.47	9	4
1:B:272:TRP:CD1	1:B:275:GLN:NE2	0.62	2.67	15	1
1:A:12:VAL:HA	1:A:78:VAL:O	0.62	1.94	13	4
1:B:324:ALA:O	1:B:325:ASP:CG	0.62	2.42	2	3
1:A:48:ASP:C	1:A:51:LEU:HD21	0.62	2.19	3	1
1:A:39:GLY:O	1:A:40:LYS:C	0.62	2.42	10	5
1:A:124:ALA:O	1:A:125:ASP:CB	0.62	2.46	2	4
1:A:54:LEU:N	1:A:54:LEU:CD1	0.62	2.62	6	3
1:B:254:LEU:N	1:B:254:LEU:CD1	0.62	2.62	6	3
1:B:252:GLU:H	1:B:253:PRO:CD	0.62	2.07	13	2
1:B:247:ALA:O	1:B:248:ASP:C	0.62	2.39	12	2
1:A:127:SER:O	1:A:128:ARG:CB	0.62	2.48	5	3
1:B:327:SER:O	1:B:328:ARG:HB2	0.62	1.95	5	3
1:A:49:ALA:C	1:A:51:LEU:H	0.62	2.00	9	3
1:A:119:MET:CA	1:B:266:HIS:ND1	0.62	2.63	12	1
1:B:327:SER:O	1:B:328:ARG:CB	0.62	2.48	5	3
1:B:335:ALA:C	1:B:337:GLY:H	0.62	2.01	4	4
1:A:52:GLU:H	1:A:53:PRO:CD	0.62	2.07	13	2
1:B:287:SER:OG	1:B:288:LEU:N	0.62	2.27	15	2
1:B:316:LEU:HD21	1:B:320:ILE:HG22	0.62	1.72	9	2
1:A:24:ASP:O	1:A:28:TYR:CG	0.61	2.53	1	10
1:A:127:SER:O	1:A:128:ARG:HB2	0.61	1.94	5	3
1:A:46:VAL:O	1:A:49:ALA:HB3	0.61	1.95	5	3
1:A:100:LEU:O	1:A:102:LYS:CE	0.61	2.48	10	3
1:B:309:ARG:NH1	1:B:311:GLN:NE2	0.61	2.48	4	3
1:B:285:GLN:H	1:B:286:PRO:CD	0.61	2.06	15	2
1:A:119:MET:HE1	1:B:269:ASP:CG	0.61	2.19	1	1
1:B:224:ASP:O	1:B:228:TYR:CG	0.61	2.53	1	11
1:A:18:ILE:CD1	1:A:18:ILE:H	0.61	2.08	11	1
1:B:254:LEU:HD12	1:B:254:LEU:H	0.61	1.56	14	1
1:A:92:TYR:CD2	1:B:319:MET:SD	0.61	2.94	15	1
1:B:327:SER:C	1:B:329:PHE:N	0.61	2.57	2	4
1:B:350:TYR:CD1	1:B:351:LEU:N	0.61	2.69	14	3
1:A:49:ALA:C	1:A:51:LEU:N	0.61	2.57	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLN:NE2	1:A:49:ALA:O	0.61	2.34	10	1
1:A:42:LEU:HD11	1:A:72:TRP:CD1	0.61	2.29	15	1
1:B:242:LEU:HD11	1:B:272:TRP:CD1	0.61	2.30	15	1
1:A:51:LEU:O	1:A:52:GLU:O	0.61	2.18	15	9
1:A:126:GLY:C	1:A:128:ARG:N	0.61	2.53	6	3
1:B:314:ARG:O	1:B:315:VAL:C	0.61	2.40	8	1
1:A:55:GLY:C	1:A:57:GLU:H	0.61	2.04	12	1
1:B:246:VAL:O	1:B:249:ALA:HB3	0.61	1.96	5	3
1:A:109:ARG:NH1	1:A:111:GLN:NE2	0.61	2.48	4	3
1:A:101:GLY:O	1:A:102:LYS:HB2	0.61	1.95	11	2
1:A:124:ALA:O	1:A:129:PHE:CE2	0.61	2.54	10	1
1:A:22:ARG:NH2	1:A:55:GLY:N	0.61	2.49	11	1
1:A:18:ILE:CD1	1:A:46:VAL:HG22	0.61	2.25	4	1
1:B:251:LEU:O	1:B:252:GLU:O	0.61	2.19	15	9
1:B:218:ILE:CD1	1:B:246:VAL:HG22	0.61	2.25	4	1
1:A:116:LEU:HD21	1:A:120:ILE:HG22	0.61	1.71	9	2
1:B:255:GLY:C	1:B:257:GLU:H	0.61	2.04	12	1
1:A:109:ARG:O	1:A:113:GLY:N	0.60	2.34	4	1
1:B:249:ALA:C	1:B:251:LEU:N	0.60	2.57	8	3
1:A:134:TYR:CD2	1:A:135:ALA:O	0.60	2.55	7	1
1:A:54:LEU:H	1:A:54:LEU:HD12	0.60	1.56	14	1
1:A:150:TYR:CD1	1:A:151:LEU:N	0.60	2.69	14	3
1:B:300:LEU:O	1:B:302:LYS:CE	0.60	2.48	10	3
1:B:323:ALA:O	1:B:325:ASP:N	0.60	2.34	8	3
1:B:247:ALA:C	1:B:249:ALA:N	0.60	2.54	12	9
1:A:83:VAL:O	1:A:114:ARG:NH1	0.60	2.35	2	1
1:B:301:GLY:O	1:B:302:LYS:C	0.60	2.44	13	1
1:A:119:MET:SD	1:B:292:TYR:CD2	0.60	2.95	15	1
1:B:287:SER:O	1:B:288:LEU:C	0.60	2.44	15	1
1:A:47:ALA:C	1:A:49:ALA:N	0.60	2.54	12	10
1:B:283:VAL:O	1:B:308:PHE:HA	0.60	1.96	15	4
1:A:123:ALA:O	1:A:125:ASP:N	0.60	2.35	8	3
1:B:218:ILE:H	1:B:218:ILE:CD1	0.60	2.09	11	2
1:B:309:ARG:O	1:B:313:GLY:N	0.60	2.35	4	1
1:B:301:GLY:O	1:B:302:LYS:HB2	0.60	1.96	11	2
1:A:66:HIS:ND1	1:B:319:MET:CA	0.60	2.65	12	1
1:B:256:GLU:C	1:B:258:ALA:H	0.60	2.04	15	2
1:B:272:TRP:CE3	1:B:275:GLN:NE2	0.60	2.70	9	2
1:A:101:GLY:O	1:A:102:LYS:C	0.60	2.44	13	1
1:B:323:ALA:O	1:B:329:PHE:CE1	0.60	2.55	13	2
1:A:127:SER:C	1:A:129:PHE:N	0.59	2.59	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:251:LEU:N	1:B:251:LEU:CD1	0.59	2.65	8	8
1:B:351:LEU:N	1:B:352:PRO:CD	0.59	2.65	10	4
1:A:83:VAL:O	1:A:108:PHE:HA	0.59	1.98	15	4
1:B:252:GLU:O	1:B:254:LEU:N	0.59	2.35	4	3
1:A:22:ARG:O	1:A:25:GLN:N	0.59	2.35	8	6
1:B:334:TYR:CD2	1:B:335:ALA:O	0.59	2.55	7	1
1:A:56:GLU:C	1:A:58:ALA:H	0.59	2.05	15	2
1:A:25:GLN:NE2	1:A:47:ALA:N	0.59	2.50	11	1
1:A:123:ALA:O	1:A:129:PHE:CE1	0.59	2.55	13	2
1:A:87:SER:O	1:A:88:LEU:C	0.59	2.44	15	1
1:B:222:ARG:O	1:B:225:GLN:N	0.59	2.35	8	5
1:A:151:LEU:N	1:A:152:PRO:CD	0.59	2.65	10	4
1:B:225:GLN:NE2	1:B:249:ALA:O	0.59	2.34	10	1
1:B:222:ARG:NH2	1:B:255:GLY:N	0.59	2.49	11	1
1:A:51:LEU:O	1:A:51:LEU:HD22	0.59	1.97	15	4
1:B:283:VAL:O	1:B:314:ARG:NH1	0.59	2.35	2	1
1:A:109:ARG:O	1:A:113:GLY:CA	0.59	2.50	4	1
1:A:100:LEU:HD23	1:A:100:LEU:O	0.59	1.98	6	1
1:B:222:ARG:NH2	1:B:285:GLN:NE2	0.59	2.50	10	1
1:B:251:LEU:O	1:B:251:LEU:HD22	0.59	1.97	15	4
1:A:13:TYR:CE2	1:A:43:THR:OG1	0.59	2.55	13	4
1:B:309:ARG:NH2	1:B:311:GLN:NE2	0.59	2.51	1	1
1:A:43:THR:HG23	1:A:69:ASP:OD1	0.59	1.98	13	1
1:A:119:MET:HE2	1:B:293:GLU:OE2	0.58	1.98	6	1
1:A:22:ARG:NH2	1:A:85:GLN:NE2	0.58	2.50	10	1
1:B:324:ALA:O	1:B:329:PHE:CE2	0.58	2.55	10	1
1:A:48:ASP:O	1:A:49:ALA:C	0.58	2.46	12	1
1:B:248:ASP:O	1:B:251:LEU:N	0.58	2.30	12	1
1:B:243:THR:HG23	1:B:269:ASP:OD1	0.58	1.99	13	1
1:A:47:ALA:O	1:A:49:ALA:N	0.58	2.36	12	7
1:A:100:LEU:HD13	1:A:100:LEU:O	0.58	1.97	1	2
1:A:109:ARG:NE	1:A:134:TYR:OH	0.58	2.35	2	2
1:A:72:TRP:CE3	1:A:75:GLN:NE2	0.58	2.70	9	2
1:A:49:ALA:O	1:A:51:LEU:N	0.58	2.36	13	3
1:A:48:ASP:O	1:A:51:LEU:N	0.58	2.30	12	1
1:B:214:PHE:CD2	1:B:232:VAL:HG22	0.58	2.33	4	10
1:B:350:TYR:O	1:B:351:LEU:C	0.58	2.47	14	6
1:B:216:GLY:O	1:B:217:SER:CB	0.58	2.52	9	1
1:B:242:LEU:CD1	1:B:272:TRP:CG	0.58	2.86	15	1
1:A:97:ALA:O	1:A:101:GLY:N	0.58	2.37	11	10
1:B:213:TYR:CE2	1:B:243:THR:OG1	0.58	2.57	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CD2	1:A:32:VAL:HG22	0.58	2.34	9	10
1:B:228:TYR:O	1:B:232:VAL:CG2	0.58	2.52	15	13
1:A:109:ARG:NH2	1:A:111:GLN:NE2	0.58	2.51	1	1
1:B:309:ARG:HH11	1:B:311:GLN:NE2	0.58	1.97	4	1
1:A:81:ALA:HB3	1:A:94:LEU:HD21	0.58	1.76	8	2
1:B:249:ALA:O	1:B:251:LEU:N	0.58	2.36	13	3
1:A:42:LEU:CD1	1:A:72:TRP:CG	0.58	2.86	15	1
1:B:329:PHE:C	1:B:329:PHE:CD1	0.58	2.82	4	8
1:A:63:GLN:CD	1:A:63:GLN:H	0.58	2.07	4	2
1:B:247:ALA:O	1:B:249:ALA:N	0.57	2.37	12	6
1:B:254:LEU:N	1:B:254:LEU:HD12	0.57	2.13	4	1
1:A:18:ILE:HD13	1:A:18:ILE:H	0.57	1.59	9	2
1:B:248:ASP:O	1:B:249:ALA:C	0.57	2.46	12	1
1:A:28:TYR:O	1:A:32:VAL:CG2	0.57	2.51	15	13
1:B:300:LEU:HD13	1:B:300:LEU:O	0.57	1.98	1	2
1:B:285:GLN:N	1:B:314:ARG:CZ	0.57	2.68	2	1
1:A:109:ARG:HH11	1:A:111:GLN:NE2	0.57	1.97	4	1
1:B:350:TYR:O	1:B:350:TYR:CD1	0.57	2.58	5	5
1:B:217:SER:CB	1:B:228:TYR:CE2	0.57	2.87	8	1
1:A:48:ASP:C	1:A:50:GLU:N	0.57	2.61	12	1
1:A:55:GLY:O	1:A:58:ALA:N	0.57	2.37	6	3
1:A:150:TYR:CD1	1:A:150:TYR:C	0.57	2.81	2	7
1:A:108:PHE:CD1	1:A:108:PHE:O	0.57	2.58	4	5
1:B:309:ARG:O	1:B:313:GLY:CA	0.57	2.51	4	1
1:A:17:SER:CB	1:A:28:TYR:CE2	0.57	2.87	8	1
1:A:16:GLY:O	1:A:17:SER:CB	0.57	2.51	9	1
1:A:25:GLN:NE2	1:A:47:ALA:O	0.57	2.37	12	1
1:B:309:ARG:NE	1:B:334:TYR:OH	0.57	2.37	2	2
1:B:263:GLN:CD	1:B:263:GLN:H	0.57	2.07	4	2
1:A:129:PHE:CD1	1:A:129:PHE:C	0.57	2.83	4	10
1:B:350:TYR:CD1	1:B:350:TYR:C	0.57	2.81	2	7
1:B:333:ASP:O	1:B:342:MET:HE2	0.57	1.99	6	1
1:A:18:ILE:CG2	1:A:54:LEU:HD22	0.57	2.29	7	1
1:B:218:ILE:CG2	1:B:254:LEU:HD22	0.57	2.30	7	1
1:B:218:ILE:HD13	1:B:218:ILE:H	0.57	1.59	9	2
1:A:99:ALA:CB	1:B:299:ALA:CB	0.57	2.83	5	11
1:A:45:HIS:CE1	1:A:65:ILE:HD11	0.57	2.34	2	2
1:B:309:ARG:CZ	1:B:311:GLN:NE2	0.57	2.68	9	3
1:A:51:LEU:N	1:A:51:LEU:HD22	0.57	2.15	2	4
1:B:308:PHE:CD1	1:B:308:PHE:O	0.57	2.58	4	5
1:A:48:ASP:O	1:A:51:LEU:CG	0.57	2.53	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LYS:CB	1:A:103:PRO:CD	0.57	2.83	9	7
1:A:150:TYR:O	1:A:151:LEU:C	0.57	2.47	14	6
1:B:302:LYS:CB	1:B:303:PRO:CD	0.57	2.83	9	7
1:A:85:GLN:N	1:A:114:ARG:CZ	0.57	2.67	2	1
1:A:24:ASP:O	1:A:28:TYR:CD1	0.57	2.58	10	6
1:B:251:LEU:N	1:B:251:LEU:HD12	0.57	2.14	12	3
1:B:258:ALA:O	1:B:260:GLY:N	0.57	2.38	12	2
1:B:217:SER:OG	1:B:289:GLY:N	0.57	2.38	1	1
1:A:127:SER:O	1:A:129:PHE:N	0.57	2.38	10	4
1:B:214:PHE:O	1:B:214:PHE:CG	0.57	2.55	9	4
1:A:13:TYR:CZ	1:A:44:GLU:OE2	0.57	2.57	4	1
1:A:89:GLY:N	1:B:317:SER:OG	0.57	2.38	4	1
1:B:347:PHE:O	1:B:351:LEU:N	0.57	2.38	5	3
1:A:58:ALA:O	1:A:60:GLY:N	0.57	2.38	12	2
1:B:248:ASP:O	1:B:251:LEU:CG	0.57	2.53	12	1
1:A:116:LEU:O	1:B:256:GLU:OE2	0.57	2.22	15	1
1:B:256:GLU:C	1:B:258:ALA:N	0.56	2.62	8	7
1:B:266:HIS:ND1	1:B:266:HIS:C	0.56	2.63	1	10
1:B:327:SER:O	1:B:329:PHE:N	0.56	2.37	10	4
1:B:320:ILE:O	1:B:323:ALA:C	0.56	2.48	15	2
1:A:17:SER:OG	1:A:89:GLY:N	0.56	2.38	1	1
1:B:255:GLY:O	1:B:258:ALA:N	0.56	2.37	6	3
1:A:52:GLU:N	1:A:53:PRO:CD	0.56	2.68	8	3
1:A:51:LEU:N	1:A:51:LEU:HD12	0.56	2.14	12	3
1:A:123:ALA:O	1:A:124:ALA:CB	0.56	2.49	10	1
1:B:324:ALA:O	1:B:331:VAL:HG23	0.56	2.00	10	1
1:A:46:VAL:HG12	1:A:47:ALA:N	0.56	2.15	11	2
1:A:110:PRO:O	1:A:113:GLY:N	0.56	2.39	11	5
1:B:252:GLU:N	1:B:253:PRO:CD	0.56	2.68	8	3
1:A:150:TYR:O	1:A:150:TYR:CD1	0.56	2.58	5	5
1:A:88:LEU:C	1:A:90:VAL:N	0.56	2.63	14	2
1:B:224:ASP:O	1:B:228:TYR:CD1	0.56	2.58	10	6
1:B:301:GLY:O	1:B:302:LYS:CB	0.56	2.53	6	2
1:A:15:CYS:SG	1:A:93:GLU:OE1	0.56	2.64	15	3
1:A:137:GLY:O	1:A:139:VAL:N	0.56	2.38	7	1
1:B:337:GLY:O	1:B:339:VAL:N	0.56	2.38	7	1
1:A:109:ARG:CZ	1:A:111:GLN:NE2	0.56	2.68	9	3
1:A:49:ALA:HB1	1:A:54:LEU:HD11	0.56	1.77	12	1
1:B:225:GLN:NE2	1:B:247:ALA:O	0.56	2.37	12	1
1:A:43:THR:OG1	1:A:72:TRP:CE3	0.56	2.57	4	1
1:A:82:GLU:OE1	1:A:134:TYR:OH	0.56	2.24	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ILE:O	1:A:123:ALA:C	0.56	2.49	15	2
1:A:14:PHE:O	1:A:14:PHE:CG	0.56	2.58	1	3
1:B:300:LEU:C	1:B:300:LEU:CD1	0.56	2.79	1	2
1:A:93:GLU:OE2	1:B:319:MET:HE2	0.56	2.00	6	1
1:B:300:LEU:O	1:B:300:LEU:HD23	0.56	1.99	6	1
1:B:281:ALA:HB3	1:B:294:LEU:HD21	0.56	1.76	8	2
1:A:66:HIS:ND1	1:A:66:HIS:C	0.56	2.63	1	10
1:B:297:ALA:O	1:B:301:GLY:N	0.56	2.38	11	11
1:B:242:LEU:O	1:B:243:THR:C	0.56	2.48	15	4
1:A:133:ASP:O	1:A:142:MET:HE2	0.56	2.00	6	1
1:A:137:GLY:C	1:A:139:VAL:N	0.56	2.63	7	1
1:B:313:GLY:O	1:B:314:ARG:NE	0.56	2.39	8	1
1:A:30:ARG:NE	1:A:34:ARG:HH22	0.56	1.98	12	2
1:B:230:ARG:NE	1:B:234:ARG:HH22	0.56	1.98	12	2
1:B:249:ALA:HB1	1:B:254:LEU:HD11	0.56	1.77	12	1
1:B:218:ILE:O	1:B:222:ARG:NE	0.56	2.39	13	1
1:B:266:HIS:NE2	1:B:270:LEU:CD1	0.56	2.69	13	1
1:B:255:GLY:O	1:B:256:GLU:C	0.56	2.48	6	6
1:A:55:GLY:O	1:A:56:GLU:C	0.56	2.47	6	4
1:B:264:PHE:CD1	1:B:268:GLN:OE1	0.56	2.59	15	2
1:A:124:ALA:O	1:A:131:VAL:HG23	0.56	2.01	10	1
1:B:248:ASP:C	1:B:250:GLU:N	0.56	2.61	12	1
1:A:52:GLU:O	1:A:54:LEU:N	0.56	2.34	4	3
1:A:45:HIS:CD2	1:A:69:ASP:CG	0.56	2.84	3	2
1:A:130:GLN:NE2	1:A:132:TRP:HE1	0.56	1.98	4	1
1:A:113:GLY:O	1:A:114:ARG:NE	0.56	2.38	8	1
1:A:117:SER:OG	1:B:289:GLY:N	0.56	2.39	4	1
1:A:17:SER:N	1:A:28:TYR:OH	0.56	2.38	7	3
1:A:24:ASP:OD1	1:A:28:TYR:CE1	0.56	2.59	8	1
1:A:18:ILE:O	1:A:22:ARG:NE	0.56	2.39	13	1
1:A:24:ASP:OD1	1:A:25:GLN:N	0.56	2.39	9	1
1:A:82:GLU:OE2	1:A:134:TYR:CZ	0.56	2.59	12	1
1:B:245:HIS:CE1	1:B:265:ILE:HD11	0.55	2.36	2	2
1:B:330:GLN:NE2	1:B:332:TRP:HE1	0.55	1.99	4	1
1:B:274:GLN:OE1	1:B:296:ARG:NH1	0.55	2.40	5	1
1:A:64:PHE:CD1	1:A:68:GLN:OE1	0.55	2.59	15	2
1:A:16:GLY:HA2	1:A:90:VAL:HG22	0.55	1.78	8	1
1:A:38:TYR:N	1:A:38:TYR:CD1	0.55	2.74	13	11
1:B:213:TYR:CB	1:B:279:VAL:HG22	0.55	2.31	6	3
1:B:217:SER:O	1:B:222:ARG:NH1	0.55	2.38	14	1
1:B:253:PRO:O	1:B:254:LEU:O	0.55	2.25	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:215:CYS:SG	1:B:293:GLU:OE1	0.55	2.64	15	3
1:B:217:SER:N	1:B:228:TYR:OH	0.55	2.38	7	2
1:B:222:ARG:CD	1:B:222:ARG:H	0.55	2.14	1	1
1:B:344:ASP:O	1:B:348:GLU:CG	0.55	2.55	12	5
1:B:253:PRO:C	1:B:254:LEU:HD22	0.55	2.26	8	2
1:A:17:SER:O	1:A:22:ARG:NH1	0.55	2.39	14	1
1:A:53:PRO:O	1:A:54:LEU:O	0.55	2.25	12	2
1:B:282:GLU:OE1	1:B:334:TYR:OH	0.55	2.24	4	1
1:B:234:ARG:NH2	1:B:340:GLU:OE1	0.55	2.40	7	1
1:A:56:GLU:OE2	1:B:316:LEU:O	0.55	2.24	15	2
1:B:232:VAL:HG13	1:B:241:VAL:HG21	0.55	1.77	15	1
1:B:246:VAL:HG12	1:B:247:ALA:N	0.55	2.16	11	2
1:B:245:HIS:CD2	1:B:269:ASP:CG	0.55	2.85	3	2
1:A:144:ASP:O	1:A:148:GLU:CG	0.55	2.55	12	5
1:A:101:GLY:O	1:A:102:LYS:CB	0.55	2.53	6	2
1:A:111:GLN:O	1:A:114:ARG:NH1	0.55	2.40	7	1
1:A:53:PRO:C	1:A:54:LEU:HD22	0.55	2.27	8	2
1:A:66:HIS:NE2	1:A:70:LEU:CD1	0.55	2.69	13	1
1:B:217:SER:OG	1:B:290:VAL:N	0.55	2.39	1	1
1:A:133:ASP:O	1:A:142:MET:SD	0.55	2.65	14	7
1:B:224:ASP:OD1	1:B:228:TYR:CE1	0.55	2.60	8	1
1:A:17:SER:OG	1:A:90:VAL:N	0.55	2.40	1	1
1:A:98:VAL:HG12	1:A:99:ALA:N	0.55	2.17	6	7
1:B:238:TYR:N	1:B:238:TYR:CD1	0.55	2.75	13	11
1:B:315:VAL:O	1:B:316:LEU:C	0.55	2.50	10	6
1:B:213:TYR:CE2	1:B:269:ASP:O	0.55	2.60	5	4
1:A:49:ALA:O	1:A:54:LEU:CD2	0.55	2.55	10	3
1:B:213:TYR:HB3	1:B:279:VAL:HG22	0.55	1.78	11	4
1:B:266:HIS:CE1	1:B:270:LEU:HG	0.55	2.36	13	2
1:A:56:GLU:C	1:A:58:ALA:N	0.55	2.63	8	6
1:B:256:GLU:O	1:B:258:ALA:N	0.55	2.39	8	5
1:A:42:LEU:O	1:A:43:THR:C	0.55	2.49	15	4
1:B:347:PHE:CD1	1:B:351:LEU:HD11	0.55	2.37	13	2
1:A:83:VAL:O	1:A:84:THR:OG1	0.55	2.23	1	2
1:A:72:TRP:CD1	1:A:75:GLN:CD	0.55	2.85	4	1
1:A:99:ALA:HB1	1:B:299:ALA:HB1	0.55	1.79	11	4
1:B:313:GLY:O	1:B:314:ARG:C	0.55	2.49	7	1
1:A:18:ILE:H	1:A:18:ILE:CD1	0.55	2.13	9	1
1:A:66:HIS:CE1	1:A:70:LEU:HG	0.55	2.37	13	2
1:B:244:GLU:O	1:B:246:VAL:N	0.55	2.40	9	2
1:B:301:GLY:O	1:B:303:PRO:N	0.55	2.40	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:242:LEU:HD11	1:B:272:TRP:CG	0.55	2.36	15	1
1:A:84:THR:C	1:A:114:ARG:CZ	0.54	2.80	2	1
1:B:213:TYR:CZ	1:B:244:GLU:OE2	0.54	2.60	4	2
1:A:146:TYR:O	1:A:149:ALA:HB3	0.54	2.03	6	1
1:B:311:GLN:O	1:B:314:ARG:NH1	0.54	2.40	7	1
1:B:216:GLY:HA2	1:B:290:VAL:HG22	0.54	1.79	8	1
1:A:34:ARG:NE	1:A:140:GLU:CD	0.54	2.65	13	1
1:B:215:CYS:SG	1:B:281:ALA:CB	0.54	2.94	13	1
1:A:13:TYR:CZ	1:A:44:GLU:OE1	0.54	2.60	15	1
1:B:214:PHE:CE2	1:B:232:VAL:CG2	0.54	2.90	9	4
1:A:13:TYR:HB3	1:A:79:VAL:HG22	0.54	1.78	11	3
1:A:108:PHE:CD1	1:A:108:PHE:C	0.54	2.85	13	3
1:B:308:PHE:CD1	1:B:308:PHE:C	0.54	2.85	13	3
1:B:234:ARG:NE	1:B:340:GLU:CD	0.54	2.65	13	1
1:A:32:VAL:HG13	1:A:41:VAL:HG21	0.54	1.78	15	1
1:A:115:VAL:O	1:A:116:LEU:C	0.54	2.49	10	7
1:B:234:ARG:NH2	1:B:238:TYR:OH	0.54	2.40	1	1
1:A:22:ARG:H	1:A:25:GLN:CB	0.54	2.15	2	1
1:B:333:ASP:O	1:B:342:MET:SD	0.54	2.65	14	7
1:A:13:TYR:CE2	1:A:69:ASP:O	0.54	2.60	5	4
1:A:147:PHE:O	1:A:151:LEU:N	0.54	2.33	12	4
1:B:346:TYR:O	1:B:349:ALA:HB3	0.54	2.03	6	1
1:B:309:ARG:NH1	1:B:334:TYR:OH	0.54	2.41	7	1
1:A:44:GLU:O	1:A:46:VAL:N	0.54	2.41	9	2
1:B:224:ASP:OD1	1:B:225:GLN:N	0.54	2.41	9	1
1:B:309:ARG:NH1	1:B:336:GLU:OE2	0.54	2.40	10	1
1:B:218:ILE:N	1:B:218:ILE:CD1	0.54	2.68	11	1
1:A:34:ARG:NH2	1:A:38:TYR:OH	0.54	2.40	1	1
1:A:97:ALA:O	1:A:101:GLY:CA	0.54	2.56	11	4
1:B:314:ARG:O	1:B:315:VAL:O	0.54	2.25	8	10
1:B:307:LEU:HD12	1:B:307:LEU:N	0.54	2.17	3	1
1:A:34:ARG:NH2	1:A:140:GLU:OE1	0.54	2.40	7	1
1:A:36:ARG:HH21	1:A:41:VAL:H	0.54	1.45	10	1
1:A:45:HIS:ND1	1:A:45:HIS:C	0.54	2.65	8	3
1:B:310:PRO:O	1:B:313:GLY:N	0.54	2.40	11	4
1:B:249:ALA:O	1:B:254:LEU:HD23	0.54	2.03	5	1
1:A:13:TYR:CB	1:A:79:VAL:HG22	0.54	2.33	11	3
1:B:333:ASP:O	1:B:342:MET:CE	0.54	2.56	7	3
1:A:56:GLU:O	1:A:58:ALA:N	0.54	2.40	8	4
1:B:284:THR:C	1:B:314:ARG:CZ	0.54	2.81	2	1
1:B:245:HIS:CD2	1:B:269:ASP:OD2	0.54	2.61	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:272:TRP:CD1	1:B:275:GLN:CD	0.54	2.86	4	1
1:A:38:TYR:CD2	1:A:147:PHE:CD2	0.54	2.96	9	2
1:B:225:GLN:HE21	1:B:246:VAL:C	0.54	2.11	5	1
1:B:248:ASP:N	1:B:248:ASP:OD1	0.54	2.40	9	1
1:B:225:GLN:NE2	1:B:247:ALA:N	0.54	2.50	11	1
1:B:282:GLU:OE2	1:B:334:TYR:CZ	0.54	2.61	12	1
1:A:42:LEU:HD11	1:A:72:TRP:CG	0.54	2.36	15	1
1:A:58:ALA:O	1:A:59:ALA:C	0.54	2.51	12	4
1:A:38:TYR:CD1	1:A:38:TYR:N	0.54	2.76	3	3
1:A:22:ARG:HE	1:A:54:LEU:CD1	0.54	2.15	5	1
1:A:74:GLN:OE1	1:A:96:ARG:NH1	0.54	2.41	5	1
1:A:109:ARG:NH1	1:A:136:GLU:OE2	0.54	2.40	10	2
1:B:244:GLU:CD	1:B:244:GLU:H	0.54	2.11	11	1
1:A:83:VAL:O	1:A:107:LEU:O	0.54	2.26	12	5
1:A:147:PHE:CD1	1:A:151:LEU:HD11	0.54	2.38	13	2
1:B:236:ARG:HH21	1:B:241:VAL:H	0.54	1.44	10	1
1:A:44:GLU:CD	1:A:44:GLU:H	0.54	2.10	11	1
1:A:49:ALA:C	1:A:54:LEU:HD11	0.54	2.27	12	1
1:A:41:VAL:O	1:A:43:THR:N	0.54	2.41	15	1
1:A:49:ALA:O	1:A:54:LEU:HD23	0.54	2.02	5	1
1:A:54:LEU:HD12	1:A:55:GLY:N	0.54	2.18	7	1
1:A:61:GLY:O	1:A:65:ILE:N	0.54	2.39	7	2
1:B:249:ALA:O	1:B:254:LEU:CD1	0.54	2.55	12	2
1:A:114:ARG:O	1:A:115:VAL:O	0.54	2.25	8	9
1:B:245:HIS:ND1	1:B:245:HIS:C	0.54	2.65	8	5
1:B:283:VAL:O	1:B:307:LEU:O	0.54	2.25	12	5
1:B:297:ALA:O	1:B:301:GLY:CA	0.54	2.55	11	4
1:B:213:TYR:OH	1:B:269:ASP:CB	0.54	2.56	2	6
1:B:282:GLU:O	1:B:290:VAL:HG11	0.54	2.03	9	4
1:B:238:TYR:CD1	1:B:238:TYR:N	0.54	2.76	3	3
1:A:14:PHE:CE2	1:A:32:VAL:CG2	0.54	2.90	9	2
1:B:320:ILE:O	1:B:323:ALA:HB3	0.54	2.03	13	2
1:B:249:ALA:C	1:B:254:LEU:HD11	0.54	2.28	12	1
1:A:120:ILE:O	1:A:123:ALA:N	0.54	2.41	15	2
1:B:254:LEU:CD2	1:B:254:LEU:N	0.53	2.71	1	1
1:A:15:CYS:SG	1:A:81:ALA:CB	0.53	2.95	13	1
1:A:70:LEU:N	1:A:70:LEU:CD2	0.53	2.71	2	4
1:B:298:VAL:HG12	1:B:299:ALA:N	0.53	2.18	6	7
1:B:339:VAL:CG1	1:B:340:GLU:N	0.53	2.72	12	15
1:A:82:GLU:O	1:A:90:VAL:HG11	0.53	2.02	9	4
1:B:325:ASP:OD2	1:B:328:ARG:NH1	0.53	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:LEU:HD12	1:A:107:LEU:N	0.53	2.19	3	1
1:B:222:ARG:HE	1:B:254:LEU:CD1	0.53	2.15	5	1
1:A:44:GLU:C	1:A:46:VAL:N	0.53	2.66	15	2
1:A:120:ILE:O	1:A:123:ALA:HB3	0.53	2.03	13	2
1:A:101:GLY:O	1:A:103:PRO:N	0.53	2.41	13	1
1:A:15:CYS:SG	1:A:93:GLU:CB	0.53	2.97	2	1
1:A:133:ASP:O	1:A:142:MET:CE	0.53	2.56	7	4
1:A:125:ASP:OD2	1:A:128:ARG:NH1	0.53	2.42	4	1
1:B:288:LEU:C	1:B:290:VAL:N	0.53	2.63	14	2
1:B:300:LEU:O	1:B:301:GLY:C	0.53	2.51	7	3
1:B:326:GLY:N	1:B:329:PHE:O	0.53	2.41	8	4
1:B:254:LEU:HD12	1:B:255:GLY:N	0.53	2.19	7	1
1:A:24:ASP:CG	1:A:28:TYR:CZ	0.53	2.87	8	1
1:A:56:GLU:HB2	1:B:315:VAL:HG21	0.53	1.79	14	1
1:A:13:TYR:HH	1:A:69:ASP:CG	0.53	2.11	1	1
1:A:54:LEU:CD2	1:A:54:LEU:N	0.53	2.72	1	1
1:B:350:TYR:O	1:B:352:PRO:N	0.53	2.42	14	4
1:A:43:THR:C	1:A:45:HIS:N	0.53	2.66	2	3
1:B:211:SER:OG	1:B:242:LEU:HD21	0.53	2.03	4	1
1:B:238:TYR:CD2	1:B:347:PHE:CD2	0.53	2.96	9	3
1:B:213:TYR:CZ	1:B:244:GLU:OE1	0.53	2.61	15	1
1:A:14:PHE:CD1	1:A:14:PHE:C	0.53	2.85	1	7
1:A:22:ARG:CD	1:A:22:ARG:H	0.53	2.14	1	1
1:A:112:SER:O	1:A:113:GLY:C	0.53	2.51	12	8
1:A:44:GLU:C	1:A:46:VAL:H	0.53	2.12	15	2
1:B:244:GLU:C	1:B:246:VAL:H	0.53	2.12	15	2
1:A:116:LEU:O	1:A:117:SER:CB	0.53	2.57	14	3
1:A:119:MET:SD	1:B:293:GLU:CG	0.53	2.97	8	1
1:A:48:ASP:N	1:A:48:ASP:OD1	0.53	2.41	9	1
1:B:230:ARG:NH2	1:B:340:GLU:OE2	0.53	2.42	11	1
1:A:49:ALA:O	1:A:54:LEU:CD1	0.53	2.57	13	2
1:A:80:VAL:HG22	1:A:105:LEU:HB3	0.53	1.80	8	2
1:B:312:SER:O	1:B:313:GLY:C	0.53	2.50	12	8
1:A:100:LEU:O	1:A:101:GLY:C	0.53	2.50	7	3
1:A:86:PRO:O	1:B:286:PRO:O	0.53	2.26	10	1
1:A:113:GLY:O	1:A:115:VAL:N	0.53	2.42	10	1
1:B:313:GLY:C	1:B:315:VAL:N	0.53	2.65	10	2
1:A:119:MET:O	1:B:266:HIS:CE1	0.53	2.62	12	1
1:A:84:THR:HG22	1:A:85:GLN:N	0.53	2.19	15	1
1:B:258:ALA:O	1:B:259:ALA:C	0.53	2.50	12	4
1:B:280:VAL:HG22	1:B:305:LEU:HB3	0.53	1.80	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:222:ARG:H	1:B:225:GLN:CB	0.53	2.16	2	1
1:B:222:ARG:CZ	1:B:285:GLN:HE22	0.53	2.17	6	1
1:A:113:GLY:O	1:A:114:ARG:C	0.53	2.50	7	1
1:B:224:ASP:CG	1:B:228:TYR:CZ	0.53	2.87	8	1
1:A:62:ASP:OD1	1:A:63:GLN:N	0.53	2.42	6	4
1:B:270:LEU:N	1:B:270:LEU:CD2	0.53	2.71	2	4
1:B:311:GLN:CG	1:B:312:SER:N	0.53	2.72	8	6
1:A:45:HIS:CD2	1:A:69:ASP:OD2	0.53	2.61	6	2
1:B:253:PRO:O	1:B:254:LEU:HD22	0.53	2.04	8	1
1:B:236:ARG:NH2	1:B:241:VAL:H	0.53	2.02	10	1
1:B:323:ALA:O	1:B:324:ALA:CB	0.53	2.50	10	1
1:A:129:PHE:C	1:A:129:PHE:CD1	0.53	2.86	14	1
1:A:69:ASP:C	1:A:69:ASP:OD1	0.53	2.52	10	2
1:B:215:CYS:SG	1:B:293:GLU:CB	0.53	2.97	2	1
1:A:125:ASP:C	1:A:125:ASP:OD1	0.53	2.52	3	2
1:B:214:PHE:C	1:B:214:PHE:CD1	0.53	2.87	3	1
1:B:302:LYS:O	1:B:304:ILE:CG1	0.53	2.57	3	4
1:A:100:LEU:C	1:A:100:LEU:CD1	0.52	2.83	2	2
1:A:111:GLN:CG	1:A:112:SER:N	0.52	2.71	8	6
1:A:139:VAL:CG1	1:A:140:GLU:N	0.52	2.71	12	15
1:A:114:ARG:NH1	1:A:114:ARG:HB2	0.52	2.19	2	1
1:A:11:SER:OG	1:A:42:LEU:HD21	0.52	2.04	4	1
1:A:22:ARG:CZ	1:A:85:GLN:HE22	0.52	2.17	6	1
1:B:244:GLU:C	1:B:246:VAL:N	0.52	2.66	15	2
1:B:320:ILE:O	1:B:323:ALA:N	0.52	2.41	15	2
1:A:72:TRP:NE1	1:A:75:GLN:NE2	0.52	2.57	15	1
1:B:241:VAL:O	1:B:243:THR:N	0.52	2.42	15	1
1:A:150:TYR:O	1:A:152:PRO:N	0.52	2.42	7	4
1:B:254:LEU:N	1:B:254:LEU:HD22	0.52	2.19	1	1
1:B:269:ASP:C	1:B:269:ASP:OD1	0.52	2.52	10	2
1:A:66:HIS:ND1	1:B:319:MET:C	0.52	2.67	12	1
1:A:121:ARG:NH2	1:A:125:ASP:OD2	0.52	2.41	12	1
1:A:13:TYR:OH	1:A:69:ASP:CB	0.52	2.56	2	6
1:A:45:HIS:O	1:A:46:VAL:C	0.52	2.53	15	6
1:A:148:GLU:N	1:A:148:GLU:OE1	0.52	2.42	3	1
1:A:126:GLY:N	1:A:129:PHE:O	0.52	2.41	8	5
1:A:109:ARG:NH1	1:A:134:TYR:OH	0.52	2.41	7	1
1:B:284:THR:HG22	1:B:313:GLY:N	0.52	2.20	7	1
1:A:34:ARG:NH1	1:A:139:VAL:CG1	0.52	2.72	9	1
1:A:36:ARG:NH2	1:A:41:VAL:H	0.52	2.02	10	1
1:B:214:PHE:O	1:B:243:THR:HG21	0.52	2.05	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:314:ARG:NH1	1:B:314:ARG:HB2	0.52	2.19	2	1
1:B:309:ARG:O	1:B:313:GLY:O	0.52	2.28	4	1
1:B:330:GLN:HE21	1:B:332:TRP:HE1	0.52	1.46	13	1
1:B:242:LEU:O	1:B:243:THR:O	0.52	2.27	15	1
1:B:217:SER:OG	1:B:285:GLN:NE2	0.52	2.43	6	1
1:B:347:PHE:CD1	1:B:351:LEU:CD1	0.52	2.93	13	11
1:A:130:GLN:CD	1:A:132:TRP:HE1	0.52	2.12	2	3
1:B:265:ILE:O	1:B:269:ASP:CG	0.52	2.53	13	10
1:B:280:VAL:HG12	1:B:281:ALA:N	0.52	2.20	3	2
1:A:56:GLU:CD	1:A:56:GLU:H	0.52	2.12	4	1
1:A:119:MET:C	1:B:266:HIS:ND1	0.52	2.68	12	1
1:B:321:ARG:O	1:B:322:GLY:C	0.52	2.51	13	2
1:A:85:GLN:N	1:A:114:ARG:NH2	0.52	2.57	2	1
1:B:234:ARG:NH1	1:B:339:VAL:CG1	0.52	2.73	9	1
1:A:130:GLN:HE21	1:A:132:TRP:HE1	0.52	1.46	13	1
1:B:243:THR:C	1:B:245:HIS:N	0.52	2.65	2	3
1:B:325:ASP:C	1:B:325:ASP:OD1	0.52	2.52	3	1
1:A:66:HIS:CE1	1:B:319:MET:O	0.52	2.63	12	1
1:A:147:PHE:CD1	1:A:151:LEU:CD1	0.52	2.93	10	10
1:A:113:GLY:C	1:A:115:VAL:H	0.52	2.13	10	3
1:B:261:GLY:O	1:B:265:ILE:N	0.52	2.40	7	2
1:B:321:ARG:NH2	1:B:325:ASP:OD2	0.52	2.42	12	1
1:A:118:ALA:HB2	1:B:256:GLU:HG3	0.52	1.82	13	1
1:A:42:LEU:O	1:A:44:GLU:N	0.52	2.43	3	4
1:A:80:VAL:HG12	1:A:81:ALA:N	0.52	2.20	3	2
1:A:118:ALA:N	1:B:256:GLU:OE2	0.52	2.43	3	3
1:A:78:VAL:HG12	1:A:79:VAL:N	0.52	2.19	4	1
1:A:30:ARG:NH2	1:A:140:GLU:OE2	0.52	2.42	11	1
1:B:272:TRP:NE1	1:B:275:GLN:NE2	0.52	2.57	15	1
1:B:284:THR:HG22	1:B:285:GLN:N	0.52	2.20	15	1
1:A:93:GLU:OE2	1:B:319:MET:SD	0.51	2.68	3	3
1:B:350:TYR:O	1:B:352:PRO:CD	0.51	2.58	7	4
1:A:84:THR:HG22	1:A:113:GLY:N	0.51	2.20	7	1
1:B:313:GLY:O	1:B:315:VAL:N	0.51	2.43	10	1
1:A:51:LEU:N	1:A:51:LEU:HD13	0.51	2.20	3	1
1:B:256:GLU:CD	1:B:256:GLU:H	0.51	2.12	4	1
1:B:251:LEU:O	1:B:251:LEU:CD2	0.51	2.59	15	2
1:A:119:MET:HA	1:B:266:HIS:ND1	0.51	2.19	12	1
1:A:92:TYR:CD1	1:A:92:TYR:C	0.51	2.88	14	2
1:A:42:LEU:CD1	1:A:42:LEU:C	0.51	2.84	15	1
1:B:213:TYR:CE1	1:B:244:GLU:OE2	0.51	2.63	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:262:ASP:OD1	1:B:263:GLN:N	0.51	2.42	6	4
1:A:86:PRO:N	1:A:114:ARG:HH21	0.51	2.04	2	1
1:A:133:ASP:OD1	1:A:134:TYR:N	0.51	2.44	4	1
1:B:278:VAL:HG12	1:B:279:VAL:N	0.51	2.19	4	1
1:B:351:LEU:N	1:B:352:PRO:HD3	0.51	2.20	10	3
1:A:123:ALA:HB3	1:A:129:PHE:CZ	0.51	2.40	9	1
1:A:56:GLU:HG3	1:B:318:ALA:HB2	0.51	1.82	13	1
1:A:65:ILE:O	1:A:69:ASP:CG	0.51	2.53	13	10
1:A:53:PRO:C	1:A:58:ALA:O	0.51	2.53	3	1
1:A:144:ASP:O	1:A:148:GLU:CD	0.51	2.54	3	1
1:A:108:PHE:CE2	1:A:113:GLY:O	0.51	2.64	4	1
1:A:109:ARG:O	1:A:113:GLY:O	0.51	2.29	4	1
1:A:17:SER:OG	1:A:85:GLN:NE2	0.51	2.42	6	1
1:B:323:ALA:HB3	1:B:329:PHE:CZ	0.51	2.40	9	1
1:A:115:VAL:HG21	1:B:256:GLU:HB2	0.51	1.82	14	1
1:A:150:TYR:O	1:A:152:PRO:CD	0.51	2.58	7	4
1:A:124:ALA:O	1:A:125:ASP:OD1	0.51	2.28	3	2
1:B:330:GLN:CD	1:B:332:TRP:HE1	0.51	2.13	2	3
1:A:119:MET:SD	1:B:293:GLU:OE2	0.51	2.69	3	3
1:A:151:LEU:N	1:A:152:PRO:HD2	0.51	2.21	4	3
1:A:116:LEU:HD21	1:A:120:ILE:CG2	0.51	2.34	9	2
1:B:323:ALA:O	1:B:325:ASP:CG	0.51	2.54	11	1
1:A:23:GLU:CD	1:A:23:GLU:H	0.51	2.14	15	2
1:B:248:ASP:C	1:B:251:LEU:CD2	0.51	2.83	3	1
1:B:344:ASP:O	1:B:348:GLU:CD	0.51	2.54	3	1
1:A:151:LEU:N	1:A:152:PRO:HD3	0.51	2.20	10	3
1:A:22:ARG:CG	1:A:22:ARG:HH11	0.51	2.19	7	1
1:A:125:ASP:HA	1:A:131:VAL:H	0.51	1.65	10	1
1:B:283:VAL:O	1:B:284:THR:OG1	0.51	2.24	1	2
1:B:253:PRO:C	1:B:258:ALA:O	0.51	2.54	3	1
1:B:243:THR:OG1	1:B:272:TRP:CE3	0.51	2.58	4	1
1:B:316:LEU:O	1:B:317:SER:CB	0.51	2.57	14	3
1:A:123:ALA:O	1:A:125:ASP:CG	0.51	2.54	11	1
1:B:225:GLN:CD	1:B:249:ALA:HB3	0.51	2.30	12	2
1:A:14:PHE:O	1:A:43:THR:HG21	0.51	2.06	14	1
1:B:222:ARG:N	1:B:222:ARG:CD	0.51	2.74	14	1
1:B:223:GLU:CD	1:B:223:GLU:H	0.51	2.14	15	2
1:A:102:LYS:O	1:A:104:ILE:CG1	0.51	2.58	3	5
1:B:267:GLU:CG	1:B:268:GLN:N	0.51	2.74	3	1
1:A:25:GLN:HE21	1:A:46:VAL:C	0.51	2.10	5	1
1:B:222:ARG:CG	1:B:222:ARG:HH11	0.51	2.19	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:SER:O	1:A:18:ILE:C	0.51	2.54	8	1
1:B:248:ASP:O	1:B:251:LEU:CD1	0.51	2.59	12	1
1:B:286:PRO:N	1:B:314:ARG:HH21	0.51	2.04	2	1
1:B:249:ALA:O	1:B:254:LEU:CD2	0.51	2.55	10	3
1:B:214:PHE:O	1:B:243:THR:CB	0.51	2.59	6	1
1:A:51:LEU:O	1:A:51:LEU:CD2	0.51	2.59	15	2
1:A:113:GLY:C	1:A:115:VAL:N	0.51	2.64	10	2
1:B:245:HIS:ND1	1:B:245:HIS:O	0.51	2.44	10	1
1:B:225:GLN:NE2	1:B:247:ALA:CA	0.51	2.74	13	1
1:B:328:ARG:O	1:B:330:GLN:NE2	0.51	2.44	14	1
1:A:42:LEU:O	1:A:43:THR:O	0.51	2.28	15	1
1:A:54:LEU:N	1:A:54:LEU:HD22	0.51	2.20	1	1
1:B:246:VAL:O	1:B:249:ALA:CB	0.51	2.59	9	5
1:B:255:GLY:C	1:B:257:GLU:N	0.51	2.69	12	2
1:B:213:TYR:OH	1:B:269:ASP:OD2	0.51	2.28	10	1
1:A:48:ASP:O	1:A:51:LEU:CD1	0.51	2.59	12	1
1:A:128:ARG:C	1:A:130:GLN:NE2	0.51	2.69	14	1
1:B:328:ARG:C	1:B:330:GLN:NE2	0.51	2.69	14	1
1:B:242:LEU:CD1	1:B:242:LEU:C	0.51	2.83	15	1
1:B:285:GLN:N	1:B:314:ARG:NH2	0.50	2.58	2	1
1:A:13:TYR:OH	1:A:69:ASP:O	0.50	2.29	5	6
1:A:25:GLN:CD	1:A:49:ALA:HB3	0.50	2.30	12	2
1:A:25:GLN:NE2	1:A:47:ALA:CA	0.50	2.74	13	1
1:A:116:LEU:O	1:A:117:SER:C	0.50	2.55	4	6
1:B:217:SER:CB	1:B:287:SER:OG	0.50	2.59	3	2
1:A:52:GLU:N	1:A:52:GLU:OE1	0.50	2.44	4	1
1:B:308:PHE:CE2	1:B:313:GLY:O	0.50	2.65	4	1
1:A:38:TYR:CE2	1:A:147:PHE:CD2	0.50	3.00	9	2
1:A:14:PHE:N	1:A:43:THR:OG1	0.50	2.44	6	1
1:B:253:PRO:O	1:B:258:ALA:O	0.50	2.30	6	1
1:A:25:GLN:HE21	1:A:49:ALA:HB3	0.50	1.66	8	1
1:B:316:LEU:HD23	1:B:321:ARG:HG2	0.50	1.82	9	1
1:A:13:TYR:CZ	1:A:43:THR:OG1	0.50	2.60	13	1
1:B:246:VAL:O	1:B:249:ALA:N	0.50	2.43	2	3
1:B:270:LEU:O	1:B:274:GLN:CG	0.50	2.60	15	2
1:B:324:ALA:O	1:B:325:ASP:OD1	0.50	2.28	3	2
1:A:45:HIS:NE2	1:A:69:ASP:OD2	0.50	2.44	6	1
1:B:251:LEU:H	1:B:251:LEU:HD13	0.50	1.66	8	1
1:A:66:HIS:ND1	1:B:319:MET:HA	0.50	2.21	12	1
1:A:48:ASP:C	1:A:51:LEU:CD2	0.50	2.84	3	1
1:B:232:VAL:HA	1:B:235:LEU:HD12	0.50	1.84	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:O	1:A:43:THR:CB	0.50	2.60	6	1
1:A:128:ARG:O	1:A:130:GLN:NE2	0.50	2.44	14	1
1:B:258:ALA:C	1:B:260:GLY:N	0.50	2.69	12	3
1:B:283:VAL:HB	1:B:316:LEU:HD11	0.50	1.84	4	1
1:B:333:ASP:OD1	1:B:334:TYR:N	0.50	2.44	4	1
1:B:351:LEU:N	1:B:352:PRO:HD2	0.50	2.22	4	2
1:B:213:TYR:OH	1:B:269:ASP:O	0.50	2.30	13	5
1:B:319:MET:SD	1:B:319:MET:N	0.50	2.85	9	2
1:B:244:GLU:O	1:B:245:HIS:C	0.50	2.53	13	4
1:A:49:ALA:HB1	1:A:54:LEU:CD1	0.50	2.37	12	1
1:A:13:TYR:CE1	1:A:44:GLU:OE2	0.50	2.65	15	1
1:A:56:GLU:O	1:A:57:GLU:C	0.50	2.55	3	6
1:B:238:TYR:N	1:B:238:TYR:HD1	0.50	2.04	8	7
1:B:242:LEU:C	1:B:244:GLU:H	0.50	2.15	1	2
1:A:102:LYS:N	1:A:103:PRO:CD	0.50	2.72	2	1
1:B:302:LYS:N	1:B:303:PRO:CD	0.50	2.72	2	1
1:A:17:SER:CB	1:A:87:SER:OG	0.50	2.59	3	2
1:A:67:GLU:CG	1:A:68:GLN:N	0.50	2.74	3	1
1:A:16:GLY:C	1:A:90:VAL:HG22	0.50	2.31	5	1
1:B:213:TYR:CE1	1:B:214:PHE:O	0.50	2.64	5	1
1:B:214:PHE:N	1:B:243:THR:OG1	0.50	2.45	6	1
1:A:119:MET:SD	1:B:289:GLY:O	0.50	2.70	14	1
1:B:348:GLU:N	1:B:348:GLU:OE1	0.50	2.45	3	1
1:A:53:PRO:O	1:A:54:LEU:HD22	0.50	2.06	8	1
1:B:245:HIS:NE2	1:B:265:ILE:CG1	0.50	2.75	14	1
1:B:214:PHE:CD1	1:B:214:PHE:C	0.50	2.85	1	5
1:B:282:GLU:CD	1:B:334:TYR:OH	0.50	2.55	4	3
1:B:238:TYR:CE2	1:B:347:PHE:CD2	0.50	3.00	9	2
1:B:313:GLY:C	1:B:315:VAL:H	0.50	2.14	10	3
1:B:312:SER:O	1:B:313:GLY:O	0.50	2.30	8	1
1:A:119:MET:SD	1:B:293:GLU:OE1	0.50	2.70	2	2
1:B:251:LEU:H	1:B:251:LEU:HD22	0.50	1.67	2	1
1:A:82:GLU:OE2	1:A:109:ARG:NH2	0.50	2.45	4	1
1:B:216:GLY:C	1:B:290:VAL:HG22	0.50	2.32	5	1
1:A:54:LEU:O	1:A:55:GLY:C	0.50	2.55	6	3
1:B:294:LEU:C	1:B:294:LEU:CD1	0.50	2.85	7	1
1:A:44:GLU:O	1:A:45:HIS:C	0.50	2.53	13	4
1:B:316:LEU:HD21	1:B:320:ILE:CG2	0.50	2.35	9	2
1:A:30:ARG:NE	1:A:34:ARG:NH2	0.50	2.60	12	2
1:A:121:ARG:O	1:A:122:GLY:C	0.50	2.50	13	2
1:B:316:LEU:O	1:B:317:SER:C	0.49	2.54	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:VAL:O	1:A:49:ALA:N	0.49	2.44	2	3
1:A:70:LEU:O	1:A:74:GLN:CG	0.49	2.60	15	2
1:A:56:GLU:OE2	1:B:318:ALA:N	0.49	2.45	7	3
1:A:83:VAL:HB	1:A:116:LEU:HD11	0.49	1.84	4	1
1:B:252:GLU:N	1:B:252:GLU:OE1	0.49	2.45	4	1
1:B:213:TYR:CE1	1:B:243:THR:CG2	0.49	2.95	6	1
1:B:217:SER:O	1:B:218:ILE:C	0.49	2.54	8	1
1:B:230:ARG:NE	1:B:234:ARG:NH2	0.49	2.59	12	2
1:B:213:TYR:CE2	1:B:273:LEU:N	0.49	2.80	11	2
1:A:43:THR:O	1:A:43:THR:CG2	0.49	2.58	13	2
1:A:88:LEU:HD12	1:B:320:ILE:HG13	0.49	1.84	3	1
1:B:213:TYR:CD2	1:B:273:LEU:HA	0.49	2.42	6	6
1:A:83:VAL:O	1:A:84:THR:C	0.49	2.55	9	2
1:A:112:SER:O	1:A:113:GLY:O	0.49	2.31	8	1
1:A:13:TYR:OH	1:A:69:ASP:OD2	0.49	2.30	10	1
1:A:25:GLN:HE22	1:A:47:ALA:CA	0.49	2.20	13	2
1:A:38:TYR:N	1:A:38:TYR:HD1	0.49	2.06	3	6
1:A:102:LYS:O	1:A:104:ILE:HG13	0.49	2.07	3	2
1:A:13:TYR:CE1	1:A:43:THR:CG2	0.49	2.95	6	1
1:A:119:MET:SD	1:A:119:MET:N	0.49	2.85	9	2
1:A:93:GLU:CG	1:B:319:MET:SD	0.49	3.00	8	1
1:A:13:TYR:CE2	1:A:73:LEU:N	0.49	2.80	11	2
1:A:66:HIS:NE2	1:A:70:LEU:HD11	0.49	2.21	13	1
1:B:292:TYR:C	1:B:292:TYR:CD1	0.49	2.88	14	1
1:B:298:VAL:CG1	1:B:299:ALA:N	0.49	2.75	6	4
1:B:339:VAL:HG13	1:B:340:GLU:N	0.49	2.21	9	8
1:A:93:GLU:OE1	1:B:319:MET:SD	0.49	2.70	2	2
1:B:222:ARG:CG	1:B:222:ARG:NH1	0.49	2.73	7	1
1:A:45:HIS:ND1	1:A:45:HIS:O	0.49	2.45	10	1
1:A:116:LEU:HD22	1:A:116:LEU:N	0.49	2.22	10	1
1:B:266:HIS:NE2	1:B:270:LEU:HD11	0.49	2.22	13	1
1:B:225:GLN:HE21	1:B:249:ALA:HB3	0.49	1.66	8	2
1:A:85:GLN:C	1:A:114:ARG:HH21	0.49	2.15	2	1
1:A:13:TYR:CE1	1:A:14:PHE:O	0.49	2.66	5	1
1:A:138:GLU:O	1:A:141:THR:N	0.49	2.46	11	2
1:B:222:ARG:O	1:B:225:GLN:CB	0.49	2.61	8	3
1:B:251:LEU:N	1:B:251:LEU:HD23	0.49	2.23	14	1
1:A:71:ASN:OD1	1:A:75:GLN:NE2	0.49	2.46	1	1
1:A:93:GLU:CD	1:B:319:MET:SD	0.49	2.96	1	1
1:A:58:ALA:C	1:A:60:GLY:N	0.49	2.70	13	3
1:B:245:HIS:O	1:B:246:VAL:C	0.49	2.53	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:322:GLY:O	1:B:323:ALA:C	0.49	2.56	2	4
1:B:245:HIS:NE2	1:B:269:ASP:OD2	0.49	2.45	6	1
1:B:274:GLN:O	1:B:302:LYS:NZ	0.49	2.41	8	1
1:A:116:LEU:HD23	1:A:121:ARG:HG2	0.49	1.83	9	1
1:A:123:ALA:HB3	1:A:129:PHE:CE1	0.49	2.42	9	1
1:B:285:GLN:C	1:B:314:ARG:HH21	0.49	2.16	2	1
1:B:217:SER:O	1:B:218:ILE:O	0.49	2.30	8	1
1:B:323:ALA:HB3	1:B:329:PHE:CE1	0.49	2.43	9	1
1:A:104:ILE:HD12	1:A:104:ILE:N	0.49	2.22	15	1
1:A:46:VAL:O	1:A:49:ALA:CB	0.49	2.60	9	5
1:A:48:ASP:OD1	1:A:48:ASP:C	0.49	2.56	6	1
1:B:255:GLY:O	1:B:256:GLU:O	0.49	2.31	8	3
1:B:338:GLU:O	1:B:341:THR:N	0.49	2.45	11	1
1:A:104:ILE:HD12	1:A:104:ILE:H	0.49	1.68	15	1
1:B:304:ILE:HD12	1:B:304:ILE:N	0.49	2.23	15	1
1:A:139:VAL:HG13	1:A:140:GLU:N	0.49	2.21	9	8
1:B:307:LEU:HB3	1:B:334:TYR:CD1	0.49	2.43	5	6
1:A:140:GLU:O	1:A:144:ASP:CG	0.49	2.56	15	5
1:B:256:GLU:O	1:B:257:GLU:C	0.49	2.56	3	4
1:B:280:VAL:HG12	1:B:281:ALA:H	0.49	1.67	3	1
1:B:254:LEU:O	1:B:255:GLY:C	0.49	2.55	6	3
1:A:98:VAL:CG1	1:A:99:ALA:N	0.49	2.74	6	3
1:A:13:TYR:CD2	1:A:73:LEU:HA	0.49	2.43	6	7
1:B:243:THR:OG1	1:B:272:TRP:CZ3	0.49	2.64	4	1
1:A:130:GLN:OE1	1:A:132:TRP:NE1	0.49	2.45	8	1
1:B:316:LEU:HD22	1:B:316:LEU:N	0.49	2.21	10	1
1:B:325:ASP:HA	1:B:331:VAL:H	0.49	1.66	10	1
1:A:51:LEU:N	1:A:51:LEU:HD23	0.49	2.22	14	1
1:B:265:ILE:O	1:B:269:ASP:OD1	0.48	2.30	2	1
1:A:82:GLU:CD	1:A:134:TYR:OH	0.48	2.55	4	3
1:B:263:GLN:CD	1:B:263:GLN:N	0.48	2.71	4	1
1:A:113:GLY:O	1:A:114:ARG:CZ	0.48	2.61	8	1
1:B:216:GLY:CA	1:B:290:VAL:HG22	0.48	2.38	8	1
1:B:302:LYS:O	1:B:303:PRO:C	0.48	2.56	12	7
1:B:329:PHE:CD1	1:B:329:PHE:C	0.48	2.91	3	3
1:A:63:GLN:CD	1:A:63:GLN:N	0.48	2.71	4	1
1:B:266:HIS:NE2	1:B:270:LEU:HG	0.48	2.23	9	2
1:A:22:ARG:O	1:A:25:GLN:CB	0.48	2.61	8	3
1:B:316:LEU:HD22	1:B:316:LEU:H	0.48	1.67	10	1
1:A:141:THR:CG2	1:A:145:ARG:NH1	0.48	2.76	11	1
1:B:225:GLN:HE22	1:B:247:ALA:CA	0.48	2.21	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:VAL:HA	1:A:35:LEU:HD12	0.48	1.84	12	1
1:A:116:LEU:N	1:A:116:LEU:HD23	0.48	2.24	2	1
1:A:80:VAL:HG12	1:A:81:ALA:H	0.48	1.67	3	1
1:B:261:GLY:O	1:B:262:ASP:C	0.48	2.57	8	5
1:B:302:LYS:O	1:B:304:ILE:HG13	0.48	2.09	8	2
1:A:94:LEU:C	1:A:94:LEU:CD1	0.48	2.85	7	1
1:A:55:GLY:O	1:A:56:GLU:O	0.48	2.31	8	3
1:B:249:ALA:HB1	1:B:254:LEU:CD1	0.48	2.37	12	1
1:A:42:LEU:C	1:A:44:GLU:H	0.48	2.15	1	2
1:B:217:SER:OG	1:B:289:GLY:CA	0.48	2.62	1	1
1:A:58:ALA:C	1:A:60:GLY:H	0.48	2.17	2	2
1:A:65:ILE:O	1:A:69:ASP:OD1	0.48	2.30	2	1
1:A:53:PRO:O	1:A:58:ALA:O	0.48	2.30	6	1
1:B:294:LEU:HD13	1:B:294:LEU:O	0.48	2.08	7	1
1:A:45:HIS:C	1:A:45:HIS:ND1	0.48	2.70	14	1
1:A:45:HIS:NE2	1:A:65:ILE:CG1	0.48	2.77	14	1
1:A:51:LEU:O	1:A:52:GLU:CB	0.48	2.62	14	1
1:A:43:THR:O	1:A:45:HIS:N	0.48	2.47	2	2
1:B:340:GLU:O	1:B:344:ASP:CG	0.48	2.57	15	4
1:A:61:GLY:O	1:A:62:ASP:C	0.48	2.55	12	7
1:A:94:LEU:HD13	1:A:94:LEU:O	0.48	2.08	7	1
1:B:214:PHE:CD2	1:B:214:PHE:O	0.48	2.67	9	2
1:B:251:LEU:O	1:B:252:GLU:CB	0.48	2.62	14	1
1:A:16:GLY:O	1:A:17:SER:O	0.48	2.32	1	1
1:A:17:SER:N	1:A:90:VAL:HG22	0.48	2.24	5	1
1:B:243:THR:OG1	1:B:246:VAL:HG23	0.48	2.09	7	1
1:A:74:GLN:O	1:A:102:LYS:NZ	0.48	2.41	8	1
1:A:102:LYS:O	1:A:104:ILE:HG12	0.48	2.08	11	1
1:A:34:ARG:NH2	1:A:140:GLU:CD	0.48	2.72	13	1
1:A:24:ASP:O	1:A:28:TYR:CD2	0.48	2.67	14	1
1:A:89:GLY:O	1:B:319:MET:SD	0.48	2.71	14	1
1:B:230:ARG:O	1:B:233:SER:OG	0.48	2.32	6	4
1:A:43:THR:OG1	1:A:72:TRP:CZ3	0.48	2.63	4	1
1:A:100:LEU:O	1:A:100:LEU:CD2	0.48	2.62	6	1
1:A:43:THR:OG1	1:A:46:VAL:HG23	0.48	2.09	7	1
1:B:213:TYR:CZ	1:B:243:THR:OG1	0.48	2.61	13	1
1:B:304:ILE:HD12	1:B:304:ILE:H	0.48	1.69	15	1
1:B:243:THR:O	1:B:245:HIS:N	0.48	2.46	2	2
1:A:101:GLY:O	1:A:102:LYS:CG	0.48	2.62	6	2
1:A:14:PHE:O	1:A:14:PHE:CD2	0.48	2.66	9	2
1:B:330:GLN:OE1	1:B:332:TRP:NE1	0.48	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:GLY:O	1:B:264:PHE:N	0.48	2.46	12	1
1:B:254:LEU:CD1	1:B:254:LEU:C	0.48	2.86	15	1
1:B:256:GLU:O	1:B:262:ASP:OD1	0.48	2.31	2	2
1:B:283:VAL:O	1:B:284:THR:C	0.48	2.54	9	2
1:A:102:LYS:CB	1:A:103:PRO:HD3	0.48	2.39	9	2
1:A:22:ARG:C	1:A:24:ASP:N	0.48	2.69	13	3
1:A:22:ARG:CG	1:A:22:ARG:NH1	0.48	2.73	7	1
1:A:68:GLN:N	1:A:68:GLN:CD	0.48	2.72	7	1
1:A:92:TYR:CE2	1:B:319:MET:SD	0.48	3.07	15	1
1:A:66:HIS:O	1:A:67:GLU:C	0.48	2.57	2	7
1:B:258:ALA:C	1:B:260:GLY:H	0.48	2.17	2	2
1:A:102:LYS:O	1:A:103:PRO:C	0.48	2.56	7	7
1:B:217:SER:OG	1:B:287:SER:OG	0.48	2.32	3	2
1:B:253:PRO:CB	1:B:258:ALA:O	0.48	2.62	3	1
1:A:53:PRO:O	1:A:58:ALA:CB	0.48	2.62	5	1
1:B:254:LEU:O	1:B:258:ALA:O	0.48	2.32	6	1
1:B:347:PHE:O	1:B:350:TYR:N	0.48	2.43	12	2
1:A:116:LEU:HD22	1:A:116:LEU:H	0.48	1.67	10	1
1:B:271:ASN:OD1	1:B:275:GLN:NE2	0.47	2.47	1	1
1:B:323:ALA:HB3	1:B:329:PHE:CE2	0.47	2.43	1	1
1:A:56:GLU:O	1:A:62:ASP:OD1	0.47	2.32	2	2
1:B:243:THR:C	1:B:245:HIS:H	0.47	2.17	10	2
1:A:53:PRO:CB	1:A:58:ALA:O	0.47	2.62	3	1
1:B:242:LEU:HD22	1:B:272:TRP:CD1	0.47	2.44	4	2
1:A:17:SER:O	1:A:18:ILE:O	0.47	2.31	8	1
1:B:302:LYS:O	1:B:304:ILE:HG12	0.47	2.08	11	1
1:A:17:SER:OG	1:A:89:GLY:CA	0.47	2.62	1	1
1:B:266:HIS:O	1:B:267:GLU:C	0.47	2.56	2	7
1:A:54:LEU:CD1	1:A:54:LEU:C	0.47	2.87	15	2
1:B:334:TYR:CB	1:B:342:MET:HE2	0.47	2.39	10	3
1:A:119:MET:HE2	1:B:266:HIS:ND1	0.47	2.24	12	1
1:B:264:PHE:CE1	1:B:268:GLN:OE1	0.47	2.67	15	1
1:B:242:LEU:O	1:B:244:GLU:N	0.47	2.43	3	4
1:B:308:PHE:O	1:B:333:ASP:HA	0.47	2.09	2	1
1:A:42:LEU:HD22	1:A:72:TRP:CD1	0.47	2.44	5	2
1:B:222:ARG:C	1:B:224:ASP:N	0.47	2.71	10	3
1:B:248:ASP:C	1:B:248:ASP:OD1	0.47	2.55	6	1
1:B:306:CYS:SG	1:B:329:PHE:CE1	0.47	3.05	15	1
1:B:316:LEU:N	1:B:316:LEU:HD23	0.47	2.24	2	1
1:B:252:GLU:OE1	1:B:252:GLU:CA	0.47	2.62	4	1
1:A:16:GLY:O	1:A:90:VAL:HG22	0.47	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:341:THR:CG2	1:B:345:ARG:NH1	0.47	2.78	11	1
1:A:120:ILE:CD1	1:B:292:TYR:CD1	0.47	2.97	12	2
1:A:107:LEU:HB3	1:A:134:TYR:CD1	0.47	2.44	1	6
1:A:108:PHE:O	1:A:133:ASP:HA	0.47	2.09	2	1
1:A:67:GLU:O	1:A:71:ASN:CG	0.47	2.57	3	1
1:A:120:ILE:HG13	1:B:288:LEU:HD12	0.47	1.85	3	1
1:B:267:GLU:O	1:B:271:ASN:CG	0.47	2.58	3	1
1:A:54:LEU:O	1:A:58:ALA:O	0.47	2.32	6	1
1:A:84:THR:O	1:A:85:GLN:C	0.47	2.58	11	3
1:B:259:ALA:O	1:B:260:GLY:C	0.47	2.57	7	2
1:B:292:TYR:CD1	1:B:292:TYR:C	0.47	2.92	13	1
1:B:301:GLY:O	1:B:302:LYS:CG	0.47	2.62	3	2
1:B:307:LEU:HA	1:B:332:TRP:O	0.47	2.09	13	2
1:B:217:SER:N	1:B:290:VAL:HG22	0.47	2.24	5	1
1:B:300:LEU:O	1:B:300:LEU:CD2	0.47	2.62	6	1
1:A:34:ARG:HE	1:A:140:GLU:CD	0.47	2.17	13	1
1:B:286:PRO:O	1:B:287:SER:CB	0.47	2.62	15	1
1:A:123:ALA:HB3	1:A:129:PHE:CE2	0.47	2.44	1	1
1:B:216:GLY:O	1:B:217:SER:O	0.47	2.32	1	1
1:B:222:ARG:NH1	1:B:224:ASP:OD2	0.47	2.48	1	1
1:A:100:LEU:O	1:A:102:LYS:CD	0.47	2.63	5	3
1:B:216:GLY:O	1:B:290:VAL:HG22	0.47	2.10	9	1
1:A:61:GLY:O	1:A:64:PHE:N	0.47	2.47	12	1
1:A:64:PHE:CD1	1:A:64:PHE:C	0.47	2.90	12	1
1:B:264:PHE:CD1	1:B:264:PHE:C	0.47	2.91	12	1
1:B:234:ARG:NH2	1:B:340:GLU:CD	0.47	2.73	13	1
1:A:86:PRO:O	1:A:87:SER:CB	0.47	2.63	15	1
1:A:119:MET:SD	1:B:292:TYR:CE2	0.47	3.08	15	1
1:A:24:ASP:OD2	1:A:85:GLN:NE2	0.47	2.47	1	1
1:A:107:LEU:HA	1:A:132:TRP:O	0.47	2.10	13	3
1:B:243:THR:O	1:B:243:THR:CG2	0.47	2.59	13	2
1:A:13:TYR:OH	1:A:69:ASP:CA	0.47	2.63	4	4
1:B:216:GLY:C	1:B:290:VAL:CG2	0.47	2.88	6	2
1:B:253:PRO:O	1:B:258:ALA:CB	0.47	2.62	5	1
1:A:116:LEU:HD22	1:A:131:VAL:CG1	0.47	2.39	9	1
1:A:52:GLU:OE1	1:A:52:GLU:CA	0.47	2.62	4	1
1:B:213:TYR:OH	1:B:269:ASP:HB3	0.47	2.10	4	3
1:B:334:TYR:CG	1:B:335:ALA:N	0.47	2.81	4	3
1:A:13:TYR:CZ	1:A:69:ASP:O	0.47	2.68	5	3
1:B:213:TYR:CZ	1:B:269:ASP:O	0.47	2.68	5	2
1:B:241:VAL:O	1:B:242:LEU:C	0.47	2.57	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:243:THR:O	1:B:244:GLU:C	0.47	2.58	6	2
1:B:249:ALA:C	1:B:251:LEU:HD12	0.47	2.35	12	1
1:A:106:CYS:SG	1:A:129:PHE:CE1	0.47	3.04	15	1
1:B:302:LYS:CB	1:B:303:PRO:HD3	0.47	2.39	9	3
1:A:10:CYS:O	1:A:39:GLY:CA	0.47	2.63	15	2
1:A:13:TYR:OH	1:A:69:ASP:HB3	0.47	2.10	4	3
1:A:55:GLY:C	1:A:57:GLU:N	0.47	2.70	4	2
1:B:213:TYR:C	1:B:213:TYR:CD1	0.47	2.92	5	1
1:B:337:GLY:C	1:B:339:VAL:N	0.47	2.63	7	1
1:B:313:GLY:O	1:B:314:ARG:CZ	0.47	2.62	8	1
1:A:64:PHE:CE1	1:A:68:GLN:OE1	0.47	2.68	15	1
1:A:66:HIS:NE2	1:A:70:LEU:HG	0.46	2.25	9	3
1:B:284:THR:C	1:B:314:ARG:NE	0.46	2.74	2	1
1:A:116:LEU:N	1:A:116:LEU:CD2	0.46	2.68	7	2
1:A:96:ARG:HE	1:A:96:ARG:HA	0.46	1.70	10	1
1:B:225:GLN:OE1	1:B:246:VAL:O	0.46	2.34	12	1
1:B:251:LEU:N	1:B:251:LEU:CD2	0.46	2.63	4	2
1:A:17:SER:OG	1:A:87:SER:OG	0.46	2.32	3	1
1:A:13:TYR:C	1:A:13:TYR:CD1	0.46	2.93	5	1
1:A:66:HIS:ND1	1:B:319:MET:HE2	0.46	2.25	12	1
1:B:213:TYR:HB3	1:B:279:VAL:HG13	0.46	1.88	11	4
1:A:16:GLY:C	1:A:90:VAL:CG2	0.46	2.88	6	2
1:A:134:TYR:CG	1:A:135:ALA:N	0.46	2.82	4	1
1:A:16:GLY:CA	1:A:90:VAL:HG22	0.46	2.39	8	1
1:A:88:LEU:O	1:A:92:TYR:N	0.46	2.42	8	2
1:A:56:GLU:O	1:A:62:ASP:OD2	0.46	2.33	10	1
1:B:256:GLU:O	1:B:262:ASP:OD2	0.46	2.33	10	1
1:B:296:ARG:HE	1:B:296:ARG:HA	0.46	1.70	10	1
1:B:213:TYR:OH	1:B:269:ASP:CA	0.46	2.64	4	4
1:A:41:VAL:O	1:A:42:LEU:C	0.46	2.57	9	2
1:A:134:TYR:CB	1:A:142:MET:HE2	0.46	2.40	10	3
1:B:268:GLN:N	1:B:268:GLN:CD	0.46	2.74	7	1
1:A:49:ALA:C	1:A:51:LEU:HD12	0.46	2.35	12	1
1:A:92:TYR:CD1	1:B:320:ILE:CD1	0.46	2.98	12	2
1:B:213:TYR:HH	1:B:269:ASP:CG	0.46	2.16	1	1
1:B:224:ASP:OD2	1:B:285:GLN:NE2	0.46	2.48	1	1
1:A:89:GLY:CA	1:B:317:SER:OG	0.46	2.64	2	2
1:B:210:CYS:O	1:B:239:GLY:CA	0.46	2.64	4	2
1:B:300:LEU:O	1:B:302:LYS:CD	0.46	2.63	5	3
1:A:28:TYR:OH	1:A:82:GLU:CD	0.46	2.59	11	1
1:B:214:PHE:CE1	1:B:282:GLU:OE2	0.46	2.69	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:PRO:O	1:A:111:GLN:C	0.46	2.58	11	6
1:B:210:CYS:O	1:B:239:GLY:HA3	0.46	2.11	2	5
1:B:325:ASP:OD1	1:B:325:ASP:C	0.46	2.58	10	2
1:A:109:ARG:CG	1:A:134:TYR:CE1	0.46	2.98	5	2
1:B:245:HIS:O	1:B:248:ASP:C	0.46	2.59	4	1
1:A:84:THR:O	1:A:114:ARG:CB	0.46	2.64	8	1
1:A:10:CYS:O	1:A:39:GLY:HA3	0.46	2.11	2	5
1:A:13:TYR:HB3	1:A:79:VAL:HG13	0.46	1.86	2	3
1:A:122:GLY:O	1:A:123:ALA:C	0.46	2.56	2	4
1:B:283:VAL:O	1:B:314:ARG:CZ	0.46	2.64	2	1
1:A:43:THR:O	1:A:44:GLU:C	0.46	2.58	6	2
1:A:139:VAL:O	1:A:142:MET:HG2	0.46	2.10	6	2
1:A:108:PHE:CG	1:A:116:LEU:HD21	0.46	2.46	10	1
1:A:82:GLU:CG	1:A:134:TYR:OH	0.46	2.64	14	1
1:A:75:GLN:O	1:A:75:GLN:CG	0.46	2.64	15	1
1:A:22:ARG:CZ	1:A:85:GLN:NE2	0.46	2.79	6	1
1:A:8:ALA:O	1:A:9:PRO:O	0.46	2.33	11	4
1:A:52:GLU:C	1:A:54:LEU:H	0.46	2.19	4	1
1:B:309:ARG:CG	1:B:334:TYR:CE1	0.46	2.98	5	2
1:A:45:HIS:O	1:A:48:ASP:OD1	0.46	2.33	6	1
1:A:123:ALA:HB2	1:B:292:TYR:OH	0.46	2.11	8	1
1:A:69:ASP:OD1	1:A:93:GLU:OE2	0.46	2.34	10	1
1:B:230:ARG:CZ	1:B:234:ARG:HH22	0.46	2.24	10	1
1:B:350:TYR:C	1:B:352:PRO:CD	0.46	2.88	12	2
1:A:25:GLN:OE1	1:A:46:VAL:O	0.46	2.33	12	1
1:A:121:ARG:HH12	1:A:125:ASP:CG	0.46	2.19	12	1
1:A:87:SER:H	1:B:288:LEU:CD2	0.46	2.24	3	1
1:A:45:HIS:O	1:A:48:ASP:C	0.46	2.58	4	1
1:A:49:ALA:O	1:A:54:LEU:CG	0.46	2.64	12	3
1:A:121:ARG:O	1:A:124:ALA:HB2	0.46	2.11	9	2
1:A:67:GLU:O	1:A:71:ASN:CB	0.46	2.64	7	3
1:B:308:PHE:CG	1:B:316:LEU:HD21	0.46	2.45	10	1
1:A:119:MET:SD	1:B:293:GLU:CD	0.45	2.99	1	1
1:A:47:ALA:O	1:A:50:GLU:CG	0.45	2.64	2	1
1:A:117:SER:OG	1:B:289:GLY:CA	0.45	2.64	2	2
1:A:54:LEU:C	1:A:54:LEU:HD13	0.45	2.36	3	1
1:B:316:LEU:HD22	1:B:331:VAL:CG1	0.45	2.40	9	1
1:A:150:TYR:C	1:A:152:PRO:CD	0.45	2.88	12	2
1:A:87:SER:O	1:A:88:LEU:CB	0.45	2.63	11	1
1:B:283:VAL:CG1	1:B:316:LEU:HD11	0.45	2.42	11	1
1:A:18:ILE:HD12	1:A:45:HIS:NE2	0.45	2.26	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ARG:HH11	1:B:298:VAL:CG1	0.45	2.24	15	1
1:A:108:PHE:CE1	1:A:109:ARG:O	0.45	2.69	5	3
1:B:249:ALA:O	1:B:254:LEU:CG	0.45	2.64	12	3
1:B:222:ARG:CZ	1:B:285:GLN:NE2	0.45	2.79	6	1
1:B:284:THR:O	1:B:314:ARG:CB	0.45	2.65	8	1
1:A:133:ASP:OD1	1:A:133:ASP:O	0.45	2.35	9	2
1:A:22:ARG:HH21	1:A:85:GLN:NE2	0.45	2.09	10	1
1:B:334:TYR:CD2	1:B:339:VAL:HG23	0.45	2.46	10	1
1:B:321:ARG:HH12	1:B:325:ASP:CG	0.45	2.19	12	1
1:B:282:GLU:CG	1:B:334:TYR:OH	0.45	2.64	14	1
1:B:285:GLN:H	1:B:286:PRO:HD3	0.45	1.71	15	1
1:A:62:ASP:CG	1:A:63:GLN:N	0.45	2.74	1	4
1:B:310:PRO:O	1:B:311:GLN:C	0.45	2.59	3	7
1:B:208:ALA:O	1:B:209:PRO:O	0.45	2.33	11	2
1:A:53:PRO:CA	1:A:58:ALA:O	0.45	2.64	3	1
1:A:18:ILE:HD13	1:A:46:VAL:HG22	0.45	1.88	4	1
1:B:218:ILE:HD13	1:B:246:VAL:HG22	0.45	1.88	4	1
1:B:282:GLU:OE2	1:B:309:ARG:NH2	0.45	2.46	4	1
1:A:81:ALA:CB	1:A:94:LEU:HD21	0.45	2.41	5	1
1:B:218:ILE:N	1:B:222:ARG:NH1	0.45	2.65	6	1
1:B:339:VAL:O	1:B:342:MET:HG2	0.45	2.11	10	2
1:A:100:LEU:O	1:A:101:GLY:O	0.45	2.34	7	1
1:B:269:ASP:OD1	1:B:293:GLU:OE2	0.45	2.35	10	1
1:B:228:TYR:OH	1:B:282:GLU:CD	0.45	2.60	11	1
1:B:224:ASP:O	1:B:228:TYR:CD2	0.45	2.69	14	1
1:B:254:LEU:C	1:B:254:LEU:HD12	0.45	2.36	15	1
1:A:43:THR:C	1:A:45:HIS:H	0.45	2.17	10	2
1:A:83:VAL:O	1:A:114:ARG:CZ	0.45	2.64	2	1
1:A:84:THR:C	1:A:114:ARG:NE	0.45	2.74	2	1
1:A:117:SER:CB	1:B:289:GLY:N	0.45	2.80	2	1
1:B:283:VAL:C	1:B:284:THR:HG1	0.45	2.17	3	1
1:A:30:ARG:O	1:A:33:SER:OG	0.45	2.32	6	2
1:B:342:MET:HE2	1:B:342:MET:N	0.45	2.27	9	1
1:B:218:ILE:HD12	1:B:245:HIS:NE2	0.45	2.27	13	1
1:A:14:PHE:CE1	1:A:82:GLU:OE2	0.45	2.69	15	1
1:B:285:GLN:O	1:B:286:PRO:C	0.45	2.60	4	5
1:B:346:TYR:CD1	1:B:346:TYR:C	0.45	2.94	12	4
1:A:89:GLY:N	1:B:317:SER:CB	0.45	2.80	2	1
1:A:88:LEU:C	1:A:88:LEU:CD2	0.45	2.88	4	1
1:B:321:ARG:O	1:B:324:ALA:HB2	0.45	2.11	9	2
1:B:287:SER:O	1:B:288:LEU:CB	0.45	2.63	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:HIS:O	1:A:49:ALA:HB2	0.45	2.11	12	1
1:A:49:ALA:O	1:A:50:GLU:C	0.45	2.58	13	1
1:B:253:PRO:CA	1:B:258:ALA:O	0.45	2.64	3	1
1:B:344:ASP:O	1:B:348:GLU:OE1	0.45	2.34	3	1
1:B:288:LEU:C	1:B:288:LEU:CD2	0.45	2.89	4	1
1:B:230:ARG:HH22	1:B:234:ARG:HH21	0.45	1.54	7	1
1:B:309:ARG:NH2	1:B:312:SER:OG	0.45	2.49	9	2
1:A:56:GLU:O	1:A:62:ASP:CG	0.45	2.60	10	1
1:A:87:SER:HB3	1:A:90:VAL:HG23	0.45	1.87	10	1
1:A:146:TYR:CD1	1:A:146:TYR:C	0.45	2.95	12	4
1:B:282:GLU:OE2	1:B:334:TYR:OH	0.45	2.35	10	4
1:A:142:MET:N	1:A:142:MET:HE2	0.45	2.26	9	1
1:B:328:ARG:CG	1:B:329:PHE:N	0.45	2.80	4	1
1:A:134:TYR:CD2	1:A:139:VAL:HG23	0.45	2.47	10	3
1:B:284:THR:O	1:B:285:GLN:C	0.45	2.57	7	3
1:B:287:SER:HB3	1:B:290:VAL:HG23	0.45	1.88	10	1
1:A:27:LEU:CD2	1:A:82:GLU:OE2	0.45	2.64	1	1
1:A:62:ASP:OD1	1:A:62:ASP:N	0.45	2.50	6	3
1:A:97:ALA:O	1:A:98:VAL:C	0.45	2.60	8	8
1:A:14:PHE:O	1:A:44:GLU:OE1	0.45	2.35	4	2
1:B:245:HIS:O	1:B:249:ALA:HB2	0.45	2.11	12	2
1:A:30:ARG:HH22	1:A:34:ARG:HH21	0.45	1.55	7	1
1:A:25:GLN:HE21	1:A:49:ALA:C	0.45	2.20	9	2
1:B:217:SER:O	1:B:224:ASP:OD2	0.45	2.35	9	1
1:A:125:ASP:C	1:A:127:SER:H	0.45	2.20	13	1
1:B:302:LYS:O	1:B:304:ILE:HD12	0.45	2.12	13	1
1:B:251:LEU:O	1:B:252:GLU:CG	0.45	2.65	14	1
1:A:22:ARG:NH1	1:A:24:ASP:CG	0.45	2.75	1	1
1:A:83:VAL:HG23	1:A:107:LEU:O	0.45	2.12	2	1
1:B:308:PHE:CE1	1:B:309:ARG:O	0.45	2.69	2	3
1:A:63:GLN:OE1	1:A:67:GLU:OE2	0.45	2.35	6	1
1:B:251:LEU:O	1:B:252:GLU:C	0.45	2.59	11	1
1:B:325:ASP:C	1:B:327:SER:H	0.45	2.20	13	1
1:B:218:ILE:CD1	1:B:246:VAL:HG13	0.45	2.42	15	1
1:A:83:VAL:O	1:A:114:ARG:NH2	0.44	2.50	2	1
1:B:262:ASP:OD1	1:B:262:ASP:N	0.44	2.49	2	3
1:B:230:ARG:O	1:B:233:SER:N	0.44	2.51	14	4
1:A:115:VAL:HG21	1:B:256:GLU:O	0.44	2.12	4	1
1:B:214:PHE:O	1:B:244:GLU:OE1	0.44	2.35	4	2
1:A:82:GLU:OE2	1:A:134:TYR:OH	0.44	2.35	10	3
1:B:211:SER:H	1:B:277:ASP:HB2	0.44	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:275:GLN:O	1:B:275:GLN:CG	0.44	2.64	15	1
1:B:281:ALA:CB	1:B:294:LEU:HD21	0.44	2.43	5	1
1:A:9:PRO:O	1:A:10:CYS:O	0.44	2.36	10	3
1:A:106:CYS:SG	1:A:130:GLN:O	0.44	2.70	7	2
1:B:288:LEU:O	1:B:292:TYR:N	0.44	2.43	8	2
1:B:249:ALA:O	1:B:250:GLU:C	0.44	2.58	13	1
1:A:54:LEU:C	1:A:54:LEU:CD1	0.44	2.90	3	2
1:B:242:LEU:HB3	1:B:272:TRP:CG	0.44	2.48	14	4
1:B:243:THR:O	1:B:246:VAL:CG1	0.44	2.66	3	1
1:A:18:ILE:N	1:A:22:ARG:NH1	0.44	2.66	6	1
1:A:59:ALA:O	1:A:60:GLY:C	0.44	2.57	7	2
1:A:14:PHE:CE1	1:A:46:VAL:HG21	0.44	2.47	13	1
1:B:234:ARG:HE	1:B:340:GLU:CD	0.44	2.19	13	1
1:B:294:LEU:HD23	1:B:304:ILE:CG2	0.44	2.43	15	1
1:B:247:ALA:O	1:B:250:GLU:CG	0.44	2.64	2	1
1:B:254:LEU:C	1:B:254:LEU:HD13	0.44	2.37	3	1
1:A:114:ARG:N	1:A:114:ARG:HD2	0.44	2.28	4	1
1:B:225:GLN:HE21	1:B:249:ALA:C	0.44	2.20	8	2
1:B:302:LYS:HB2	1:B:303:PRO:CD	0.44	2.42	9	1
1:B:333:ASP:OD1	1:B:333:ASP:O	0.44	2.34	9	3
1:B:256:GLU:O	1:B:262:ASP:CG	0.44	2.60	10	1
1:B:256:GLU:OE1	1:B:262:ASP:OD1	0.44	2.36	11	1
1:A:13:TYR:HH	1:A:69:ASP:C	0.44	2.19	13	1
1:A:56:GLU:O	1:B:315:VAL:HG21	0.44	2.13	4	1
1:B:245:HIS:O	1:B:248:ASP:OD1	0.44	2.35	6	1
1:A:13:TYR:CE1	1:A:44:GLU:OE1	0.44	2.71	9	1
1:A:52:GLU:O	1:A:53:PRO:C	0.44	2.60	14	2
1:A:102:LYS:O	1:A:104:ILE:HD12	0.44	2.12	13	1
1:A:22:ARG:NH1	1:A:24:ASP:OD2	0.44	2.50	1	1
1:B:262:ASP:CG	1:B:263:GLN:N	0.44	2.75	1	3
1:A:48:ASP:O	1:A:48:ASP:CG	0.44	2.61	2	1
1:A:51:LEU:C	1:A:52:GLU:O	0.44	2.61	6	2
1:A:117:SER:C	1:B:256:GLU:OE2	0.44	2.61	7	1
1:B:267:GLU:O	1:B:271:ASN:CB	0.44	2.64	7	3
1:A:102:LYS:HB2	1:A:103:PRO:CD	0.44	2.42	9	1
1:B:225:GLN:OE1	1:B:225:GLN:C	0.44	2.61	11	1
1:B:213:TYR:HH	1:B:269:ASP:C	0.44	2.19	13	1
1:A:51:LEU:O	1:A:52:GLU:CG	0.44	2.66	14	1
1:B:283:VAL:O	1:B:314:ARG:NH2	0.44	2.50	2	1
1:A:31:ILE:CG2	1:A:32:VAL:N	0.44	2.80	3	1
1:A:42:LEU:HB3	1:A:72:TRP:CG	0.44	2.47	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:O	1:A:46:VAL:CG1	0.44	2.66	3	1
1:A:88:LEU:CD2	1:B:287:SER:H	0.44	2.25	3	1
1:A:147:PHE:O	1:A:150:TYR:N	0.44	2.43	12	3
1:B:297:ALA:O	1:B:298:VAL:C	0.44	2.60	10	7
1:A:102:LYS:N	1:A:102:LYS:CD	0.44	2.80	7	1
1:A:17:SER:O	1:A:24:ASP:OD2	0.44	2.35	9	1
1:A:109:ARG:NH2	1:A:112:SER:OG	0.44	2.50	9	2
1:B:309:ARG:CZ	1:B:311:GLN:HE21	0.44	2.25	9	1
1:A:30:ARG:CZ	1:A:34:ARG:HH22	0.44	2.26	10	1
1:B:253:PRO:C	1:B:254:LEU:HD12	0.44	2.38	13	1
1:B:283:VAL:HG13	1:B:290:VAL:HG11	0.44	1.90	1	1
1:A:125:ASP:OD1	1:A:125:ASP:C	0.44	2.61	2	1
1:B:324:ALA:O	1:B:325:ASP:HB3	0.44	2.12	2	1
1:B:254:LEU:C	1:B:254:LEU:CD1	0.44	2.90	3	2
1:A:78:VAL:CG2	1:A:150:TYR:OH	0.44	2.66	4	1
1:B:300:LEU:O	1:B:301:GLY:O	0.44	2.35	7	1
1:A:59:ALA:CB	1:A:65:ILE:HD12	0.44	2.43	8	1
1:A:25:GLN:OE1	1:A:25:GLN:C	0.44	2.60	11	1
1:A:53:PRO:C	1:A:54:LEU:HD12	0.44	2.38	13	1
1:B:324:ALA:HB3	1:B:329:PHE:HD1	0.44	1.71	12	2
1:A:150:TYR:O	1:A:150:TYR:CD2	0.44	2.71	6	1
1:A:25:GLN:NE2	1:A:50:GLU:CA	0.44	2.80	8	2
1:A:18:ILE:CD1	1:A:46:VAL:HG13	0.44	2.43	15	1
1:A:72:TRP:O	1:A:75:GLN:N	0.43	2.51	1	2
1:B:222:ARG:NH1	1:B:224:ASP:CG	0.43	2.76	1	1
1:A:57:GLU:C	1:A:57:GLU:CD	0.43	2.86	2	1
1:B:229:ALA:O	1:B:233:SER:OG	0.43	2.34	5	1
1:A:92:TYR:OH	1:B:323:ALA:HB2	0.43	2.12	8	1
1:A:132:TRP:CD1	1:A:132:TRP:N	0.43	2.86	11	1
1:A:85:GLN:O	1:A:86:PRO:C	0.43	2.61	12	5
1:B:272:TRP:O	1:B:273:LEU:C	0.43	2.61	1	5
1:A:128:ARG:CG	1:A:129:PHE:N	0.43	2.80	4	1
1:A:147:PHE:O	1:A:151:LEU:HB2	0.43	2.14	15	2
1:B:305:LEU:HD11	1:B:332:TRP:CD2	0.43	2.47	5	1
1:A:14:PHE:CD2	1:A:32:VAL:CG2	0.43	3.02	6	3
1:A:127:SER:OG	1:A:128:ARG:N	0.43	2.51	7	2
1:B:230:ARG:CZ	1:B:234:ARG:NH2	0.43	2.82	10	1
1:A:51:LEU:O	1:A:52:GLU:C	0.43	2.60	11	1
1:A:56:GLU:OE1	1:A:62:ASP:OD1	0.43	2.36	11	1
1:A:83:VAL:CG1	1:A:116:LEU:HD11	0.43	2.42	11	1
1:A:86:PRO:O	1:A:87:SER:OG	0.43	2.35	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:C	1:A:102:LYS:H	0.43	2.21	13	1
1:B:225:GLN:NE2	1:B:249:ALA:CB	0.43	2.77	13	1
1:B:270:LEU:O	1:B:274:GLN:HG3	0.43	2.12	15	1
1:A:65:ILE:HG22	1:A:66:HIS:N	0.43	2.27	11	2
1:B:214:PHE:CD2	1:B:232:VAL:CG2	0.43	3.01	6	3
1:B:263:GLN:OE1	1:B:267:GLU:OE2	0.43	2.35	6	1
1:A:56:GLU:OE2	1:B:317:SER:C	0.43	2.61	7	1
1:A:117:SER:O	1:A:121:ARG:CG	0.43	2.66	9	1
1:B:316:LEU:O	1:B:317:SER:OG	0.43	2.37	14	2
1:B:246:VAL:CG1	1:B:247:ALA:N	0.43	2.82	11	1
1:A:54:LEU:C	1:A:54:LEU:HD12	0.43	2.37	15	1
1:B:227:LEU:CD2	1:B:282:GLU:OE2	0.43	2.67	1	1
1:B:231:ILE:CG2	1:B:232:VAL:N	0.43	2.80	3	1
1:A:18:ILE:HD11	1:A:46:VAL:HG22	0.43	1.88	4	1
1:A:100:LEU:O	1:A:102:LYS:HD3	0.43	2.13	4	1
1:B:278:VAL:CG2	1:B:350:TYR:OH	0.43	2.66	4	1
1:B:323:ALA:O	1:B:324:ALA:O	0.43	2.36	5	1
1:A:130:GLN:CB	1:A:132:TRP:HE1	0.43	2.26	6	2
1:B:330:GLN:CB	1:B:332:TRP:HE1	0.43	2.26	6	2
1:A:118:ALA:N	1:B:256:GLU:CD	0.43	2.77	7	1
1:B:213:TYR:OH	1:B:269:ASP:C	0.43	2.61	11	3
1:B:213:TYR:CE1	1:B:244:GLU:OE1	0.43	2.70	9	1
1:A:70:LEU:O	1:A:74:GLN:HG3	0.43	2.13	15	1
1:B:272:TRP:O	1:B:275:GLN:N	0.43	2.52	1	2
1:A:13:TYR:CZ	1:A:44:GLU:CD	0.43	2.96	4	1
1:B:314:ARG:N	1:B:314:ARG:HD2	0.43	2.27	4	1
1:B:211:SER:OG	1:B:277:ASP:CG	0.43	2.61	10	1
1:A:25:GLN:NE2	1:A:49:ALA:CB	0.43	2.78	13	1
1:B:214:PHE:CE1	1:B:246:VAL:HG21	0.43	2.48	13	1
1:B:213:TYR:CE1	1:B:244:GLU:CD	0.43	2.97	15	1
1:A:72:TRP:O	1:A:73:LEU:C	0.43	2.61	1	5
1:A:30:ARG:O	1:A:33:SER:N	0.43	2.51	12	3
1:B:347:PHE:O	1:B:351:LEU:HB2	0.43	2.13	15	2
1:B:231:ILE:CD1	1:B:282:GLU:OE1	0.43	2.67	6	1
1:A:56:GLU:CD	1:B:318:ALA:N	0.43	2.76	7	1
1:A:134:TYR:CD2	1:A:135:ALA:C	0.43	2.97	7	1
1:B:209:PRO:O	1:B:210:CYS:O	0.43	2.36	10	3
1:B:285:GLN:C	1:B:285:GLN:CD	0.43	2.87	7	1
1:A:11:SER:OG	1:A:77:ASP:CG	0.43	2.62	10	1
1:A:87:SER:O	1:A:88:LEU:HB2	0.43	2.13	11	1
1:A:92:TYR:HH	1:B:298:VAL:HG21	0.43	1.71	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:PHE:CE1	1:A:68:GLN:CD	0.43	2.97	15	1
1:A:144:ASP:O	1:A:148:GLU:OE1	0.43	2.36	3	1
1:B:332:TRP:CD1	1:B:332:TRP:N	0.43	2.85	11	4
1:B:252:GLU:O	1:B:253:PRO:C	0.43	2.60	14	4
1:A:110:PRO:C	1:A:113:GLY:H	0.43	2.22	11	1
1:A:138:GLU:O	1:A:139:VAL:C	0.43	2.61	11	1
1:B:287:SER:O	1:B:288:LEU:HB2	0.43	2.13	11	1
1:A:75:GLN:O	1:A:75:GLN:HG2	0.43	2.13	15	1
1:B:275:GLN:O	1:B:275:GLN:HG2	0.43	2.13	15	1
1:B:222:ARG:O	1:B:225:GLN:HB3	0.43	2.14	2	1
1:B:248:ASP:O	1:B:248:ASP:CG	0.43	2.61	2	1
1:A:13:TYR:CD1	1:A:14:PHE:N	0.43	2.86	4	1
1:B:246:VAL:O	1:B:247:ALA:C	0.43	2.62	4	1
1:A:105:LEU:HD11	1:A:132:TRP:CD2	0.43	2.48	5	1
1:A:133:ASP:OD1	1:A:133:ASP:C	0.43	2.60	7	2
1:A:11:SER:H	1:A:77:ASP:HB2	0.43	1.73	9	1
1:A:147:PHE:O	1:A:148:GLU:C	0.43	2.62	12	1
1:A:116:LEU:O	1:A:117:SER:OG	0.43	2.36	14	1
1:B:257:GLU:C	1:B:257:GLU:CD	0.43	2.86	2	1
1:B:344:ASP:CG	1:B:348:GLU:OE2	0.43	2.62	3	2
1:B:213:TYR:CD1	1:B:214:PHE:N	0.43	2.87	4	1
1:B:265:ILE:HG22	1:B:266:HIS:N	0.43	2.27	11	2
1:A:22:ARG:O	1:A:23:GLU:C	0.43	2.61	6	3
1:A:13:TYR:OH	1:A:69:ASP:C	0.43	2.62	11	3
1:A:18:ILE:HG22	1:A:54:LEU:HD22	0.43	1.90	7	1
1:A:102:LYS:CB	1:A:103:PRO:HD2	0.43	2.44	7	1
1:B:334:TYR:CD2	1:B:335:ALA:C	0.43	2.97	7	1
1:B:233:SER:C	1:B:237:ARG:NH1	0.43	2.76	8	1
1:B:317:SER:O	1:B:321:ARG:CG	0.43	2.66	9	1
1:B:310:PRO:C	1:B:313:GLY:H	0.43	2.22	11	1
1:A:88:LEU:HD22	1:A:88:LEU:HA	0.43	1.73	14	1
1:A:94:LEU:HD23	1:A:104:ILE:CG2	0.43	2.43	15	1
1:A:98:VAL:CG1	1:B:296:ARG:HH11	0.43	2.27	15	1
1:B:231:ILE:HD13	1:B:282:GLU:CD	0.43	2.39	15	1
1:A:124:ALA:HB3	1:A:129:PHE:HD1	0.43	1.72	3	1
1:A:77:ASP:O	1:A:77:ASP:OD1	0.43	2.36	5	1
1:B:214:PHE:O	1:B:243:THR:OG1	0.43	2.36	6	1
1:A:85:GLN:C	1:A:85:GLN:CD	0.43	2.86	7	1
1:B:213:TYR:CD1	1:B:213:TYR:C	0.43	2.97	10	1
1:A:48:ASP:O	1:A:48:ASP:OD1	0.43	2.37	14	1
1:B:330:GLN:N	1:B:330:GLN:CD	0.43	2.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:302:LYS:CB	1:B:303:PRO:HD2	0.42	2.44	7	1
1:B:333:ASP:OD1	1:B:333:ASP:C	0.42	2.59	7	2
1:B:225:GLN:NE2	1:B:250:GLU:CA	0.42	2.82	8	2
1:B:259:ALA:CB	1:B:265:ILE:HD12	0.42	2.43	8	1
1:B:222:ARG:HH21	1:B:285:GLN:NE2	0.42	2.11	10	1
1:B:347:PHE:O	1:B:348:GLU:C	0.42	2.62	12	1
1:A:124:ALA:O	1:A:125:ASP:HB3	0.42	2.12	2	1
1:B:279:VAL:O	1:B:303:PRO:O	0.42	2.38	3	2
1:B:277:ASP:O	1:B:277:ASP:OD1	0.42	2.37	5	1
1:A:69:ASP:N	1:A:69:ASP:OD1	0.42	2.52	7	1
1:A:46:VAL:CG1	1:A:47:ALA:N	0.42	2.81	11	1
1:A:41:VAL:O	1:A:44:GLU:CG	0.42	2.67	14	1
1:A:120:ILE:O	1:A:121:ARG:C	0.42	2.62	15	1
1:B:341:THR:O	1:B:342:MET:C	0.42	2.62	10	4
1:A:22:ARG:O	1:A:25:GLN:HB3	0.42	2.14	2	1
1:A:144:ASP:CG	1:A:148:GLU:OE2	0.42	2.63	3	2
1:A:123:ALA:O	1:A:124:ALA:O	0.42	2.37	5	1
1:B:222:ARG:O	1:B:223:GLU:C	0.42	2.61	10	3
1:A:44:GLU:O	1:A:46:VAL:O	0.42	2.38	13	1
1:B:297:ALA:C	1:B:304:ILE:HD11	0.42	2.39	13	1
1:B:248:ASP:O	1:B:248:ASP:OD1	0.42	2.36	14	1
1:B:274:GLN:NE2	1:B:296:ARG:NH2	0.42	2.67	15	1
1:A:57:GLU:CD	1:A:57:GLU:O	0.42	2.63	2	1
1:A:12:VAL:HG13	1:A:78:VAL:HG12	0.42	1.90	5	1
1:A:71:ASN:OD1	1:A:71:ASN:C	0.42	2.63	12	1
1:B:266:HIS:HE2	1:B:270:LEU:HD11	0.42	1.75	13	1
1:A:130:GLN:CD	1:A:130:GLN:N	0.42	2.77	14	1
1:B:285:GLN:NE2	1:B:286:PRO:O	0.42	2.53	7	1
1:A:97:ALA:HA	1:A:101:GLY:H	0.42	1.75	10	1
1:A:120:ILE:O	1:A:123:ALA:CA	0.42	2.68	13	1
1:A:13:TYR:CE1	1:A:44:GLU:CD	0.42	2.97	15	1
1:A:121:ARG:O	1:A:124:ALA:HB3	0.42	2.14	15	1
1:B:264:PHE:CE1	1:B:268:GLN:CD	0.42	2.98	15	1
1:A:42:LEU:C	1:A:44:GLU:N	0.42	2.77	1	2
1:A:132:TRP:N	1:A:132:TRP:CD1	0.42	2.88	4	4
1:A:29:ALA:O	1:A:33:SER:OG	0.42	2.32	5	2
1:A:33:SER:C	1:A:37:ARG:NH1	0.42	2.77	8	1
1:B:338:GLU:O	1:B:339:VAL:C	0.42	2.61	11	2
1:B:252:GLU:O	1:B:254:LEU:HD23	0.42	2.14	11	1
1:B:248:ASP:O	1:B:251:LEU:CD2	0.42	2.57	13	1
1:A:31:ILE:HG21	1:A:82:GLU:OE2	0.42	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:TYR:O	1:A:152:PRO:HD3	0.42	2.15	1	2
1:B:245:HIS:CD2	1:B:265:ILE:HG23	0.42	2.50	1	1
1:B:252:GLU:O	1:B:254:LEU:CD2	0.42	2.68	1	1
1:B:254:LEU:O	1:B:258:ALA:HB3	0.42	2.14	4	1
1:A:14:PHE:O	1:A:43:THR:OG1	0.42	2.38	6	1
1:A:101:GLY:C	1:A:102:LYS:CG	0.42	2.93	6	1
1:A:49:ALA:CB	1:A:54:LEU:HD11	0.42	2.45	12	1
1:A:51:LEU:CD1	1:A:51:LEU:H	0.42	2.27	12	1
1:B:242:LEU:C	1:B:244:GLU:N	0.42	2.77	1	1
1:A:127:SER:O	1:A:127:SER:OG	0.42	2.37	2	1
1:A:83:VAL:C	1:A:84:THR:OG1	0.42	2.63	3	1
1:A:98:VAL:CG1	1:B:296:ARG:NH1	0.42	2.83	4	1
1:B:300:LEU:O	1:B:302:LYS:HD3	0.42	2.14	4	1
1:B:350:TYR:O	1:B:350:TYR:CD2	0.42	2.71	6	2
1:A:14:PHE:CD2	1:A:14:PHE:O	0.42	2.73	7	1
1:A:45:HIS:C	1:A:45:HIS:HD1	0.42	2.23	10	1
1:A:97:ALA:C	1:A:104:ILE:HD11	0.42	2.39	13	1
1:B:300:LEU:C	1:B:302:LYS:H	0.42	2.21	13	1
1:B:218:ILE:HG23	1:B:225:GLN:OE1	0.42	2.15	2	1
1:A:17:SER:C	1:A:22:ARG:NH1	0.42	2.78	6	1
1:A:45:HIS:CD2	1:A:69:ASP:OD1	0.42	2.72	6	1
1:B:251:LEU:C	1:B:252:GLU:O	0.42	2.61	6	3
1:A:82:GLU:CD	1:A:82:GLU:C	0.42	2.88	11	1
1:B:248:ASP:C	1:B:250:GLU:H	0.42	2.22	12	1
1:B:244:GLU:O	1:B:246:VAL:O	0.42	2.38	13	1
1:B:320:ILE:O	1:B:323:ALA:CA	0.42	2.68	13	1
1:B:241:VAL:O	1:B:244:GLU:CG	0.42	2.68	14	1
1:B:284:THR:O	1:B:285:GLN:CB	0.42	2.68	14	1
1:B:222:ARG:NH1	1:B:254:LEU:HD11	0.42	2.30	15	1
1:A:48:ASP:OD2	1:A:48:ASP:O	0.42	2.38	3	1
1:B:245:HIS:CD2	1:B:269:ASP:OD1	0.42	2.73	6	1
1:B:269:ASP:N	1:B:269:ASP:OD1	0.42	2.52	7	1
1:A:109:ARG:CZ	1:A:111:GLN:HE21	0.42	2.28	9	1
1:B:296:ARG:NE	1:B:300:LEU:HD21	0.42	2.30	13	1
1:B:350:TYR:O	1:B:352:PRO:HD3	0.41	2.15	1	3
1:B:283:VAL:C	1:B:284:THR:OG1	0.41	2.63	3	1
1:B:283:VAL:O	1:B:284:THR:O	0.41	2.39	4	1
1:B:218:ILE:HG22	1:B:254:LEU:HD22	0.41	1.90	7	1
1:B:243:THR:OG1	1:B:246:VAL:CG2	0.41	2.68	7	1
1:B:217:SER:OG	1:B:287:SER:CB	0.41	2.68	12	1
1:B:283:VAL:CB	1:B:307:LEU:O	0.41	2.68	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:GLU:CG	1:A:57:GLU:H	0.41	2.27	14	1
1:A:123:ALA:O	1:A:125:ASP:OD1	0.41	2.38	1	2
1:B:214:PHE:CD2	1:B:243:THR:HG21	0.41	2.50	3	1
1:B:233:SER:O	1:B:237:ARG:NH1	0.41	2.53	8	1
1:A:96:ARG:NE	1:A:100:LEU:HD21	0.41	2.30	13	1
1:A:84:THR:O	1:A:85:GLN:CB	0.41	2.68	14	1
1:B:321:ARG:O	1:B:324:ALA:HB3	0.41	2.15	15	1
1:A:117:SER:C	1:A:119:MET:N	0.41	2.77	2	1
1:B:213:TYR:CZ	1:B:244:GLU:CD	0.41	2.98	4	1
1:B:217:SER:C	1:B:222:ARG:NH1	0.41	2.78	6	1
1:A:52:GLU:O	1:A:54:LEU:HD23	0.41	2.15	11	1
1:A:22:ARG:NH1	1:A:54:LEU:HD11	0.41	2.31	15	1
1:A:31:ILE:HD13	1:A:82:GLU:CD	0.41	2.40	15	1
1:B:222:ARG:NH1	1:B:222:ARG:CG	0.41	2.82	15	1
1:A:43:THR:OG1	1:A:46:VAL:CG2	0.41	2.68	7	2
1:A:45:HIS:CD2	1:A:65:ILE:HG23	0.41	2.50	1	1
1:A:22:ARG:H	1:A:25:GLN:HB2	0.41	1.75	2	1
1:A:122:GLY:C	1:B:266:HIS:CD2	0.41	2.98	6	1
1:B:255:GLY:C	1:B:256:GLU:O	0.41	2.63	8	1
1:A:87:SER:HB2	1:B:288:LEU:HD21	0.41	1.91	14	1
1:A:88:LEU:HD21	1:B:287:SER:CB	0.41	2.46	14	1
1:B:231:ILE:HG21	1:B:282:GLU:OE2	0.41	2.15	15	1
1:B:212:VAL:HG13	1:B:278:VAL:HG12	0.41	1.91	5	1
1:A:88:LEU:HD13	1:A:88:LEU:O	0.41	2.16	9	1
1:A:13:TYR:CD1	1:A:13:TYR:C	0.41	2.98	10	1
1:B:297:ALA:HA	1:B:301:GLY:H	0.41	1.75	10	1
1:A:18:ILE:N	1:A:18:ILE:CD1	0.41	2.68	11	1
1:A:52:GLU:O	1:A:54:LEU:CD2	0.41	2.69	1	1
1:B:323:ALA:O	1:B:325:ASP:OD1	0.41	2.38	9	2
1:A:86:PRO:HD3	1:A:114:ARG:HE	0.41	1.76	2	1
1:A:17:SER:N	1:A:90:VAL:CG2	0.41	2.83	5	1
1:A:54:LEU:HD12	1:A:54:LEU:O	0.41	2.16	5	1
1:B:334:TYR:HD2	1:B:335:ALA:O	0.41	1.96	7	1
1:B:282:GLU:CD	1:B:282:GLU:C	0.41	2.88	11	1
1:A:17:SER:OG	1:A:87:SER:CB	0.41	2.68	12	1
1:A:83:VAL:CB	1:A:107:LEU:O	0.41	2.69	12	1
1:A:66:HIS:HE2	1:A:70:LEU:HD11	0.41	1.74	13	1
1:A:55:GLY:C	1:A:56:GLU:O	0.41	2.64	15	1
1:A:85:GLN:H	1:A:86:PRO:HD3	0.41	1.71	15	1
1:A:133:ASP:O	1:A:142:MET:HE3	0.41	2.15	15	1
1:A:23:GLU:CD	1:A:23:GLU:N	0.41	2.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:TRP:CD1	1:A:75:GLN:OE1	0.41	2.74	4	1
1:B:252:GLU:C	1:B:254:LEU:H	0.41	2.19	4	1
1:A:31:ILE:CD1	1:A:82:GLU:OE1	0.41	2.69	6	1
1:A:25:GLN:HE21	1:A:49:ALA:CB	0.41	2.28	8	1
1:A:30:ARG:CZ	1:A:34:ARG:NH2	0.41	2.84	10	1
1:A:48:ASP:C	1:A:50:GLU:H	0.41	2.22	12	1
1:A:34:ARG:CZ	1:A:140:GLU:CD	0.41	2.94	13	1
1:B:234:ARG:CZ	1:B:340:GLU:CD	0.41	2.94	13	1
1:A:48:ASP:HA	1:A:51:LEU:HD11	0.41	1.92	2	1
1:A:79:VAL:O	1:A:103:PRO:O	0.41	2.39	8	2
1:B:218:ILE:HD11	1:B:246:VAL:HG22	0.41	1.89	4	1
1:B:332:TRP:N	1:B:332:TRP:CD1	0.41	2.88	4	2
1:A:85:GLN:NE2	1:A:86:PRO:O	0.41	2.53	7	1
1:B:214:PHE:O	1:B:214:PHE:CD2	0.41	2.72	8	1
1:B:225:GLN:HE21	1:B:249:ALA:CB	0.41	2.28	8	1
1:A:122:GLY:C	1:A:124:ALA:N	0.41	2.78	9	1
1:A:34:ARG:CZ	1:A:38:TYR:OH	0.41	2.69	1	1
1:B:257:GLU:O	1:B:258:ALA:C	0.41	2.63	1	1
1:B:248:ASP:OD2	1:B:248:ASP:O	0.41	2.38	3	1
1:A:46:VAL:O	1:A:47:ALA:C	0.41	2.62	4	1
1:A:78:VAL:C	1:A:79:VAL:HG23	0.41	2.41	4	1
1:B:211:SER:OG	1:B:242:LEU:CD2	0.41	2.68	4	1
1:B:213:TYR:CD2	1:B:273:LEU:CA	0.41	3.04	4	1
1:A:14:PHE:CD1	1:A:46:VAL:HG21	0.41	2.51	5	1
1:A:83:VAL:CG1	1:B:288:LEU:HD13	0.41	2.46	6	1
1:A:55:GLY:O	1:A:58:ALA:CB	0.41	2.69	7	1
1:B:264:PHE:O	1:B:268:GLN:OE1	0.41	2.39	7	1
1:A:41:VAL:O	1:A:41:VAL:HG12	0.41	2.16	9	1
1:A:22:ARG:HH21	1:A:85:GLN:CD	0.41	2.24	10	1
1:A:108:PHE:CD1	1:A:116:LEU:HD21	0.41	2.51	10	1
1:A:151:LEU:HD23	1:A:151:LEU:HA	0.41	1.75	11	1
1:A:87:SER:CB	1:B:288:LEU:HD21	0.41	2.46	14	1
1:A:88:LEU:HD21	1:B:287:SER:HB2	0.41	1.91	14	1
1:A:83:VAL:HG13	1:A:90:VAL:HG11	0.41	1.91	1	1
1:B:251:LEU:C	1:B:251:LEU:CD2	0.41	2.94	1	2
1:B:248:ASP:HA	1:B:251:LEU:HD11	0.41	1.92	2	1
1:A:96:ARG:NH1	1:B:298:VAL:CG1	0.41	2.83	4	1
1:A:87:SER:N	1:B:287:SER:O	0.41	2.54	11	1
1:A:30:ARG:O	1:A:31:ILE:C	0.41	2.64	14	1
1:B:251:LEU:HD23	1:B:251:LEU:C	0.41	2.41	14	1
1:B:254:LEU:H	1:B:254:LEU:CD1	0.41	2.27	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:256:GLU:CG	1:B:257:GLU:H	0.41	2.28	14	1
1:A:22:ARG:NH1	1:A:22:ARG:CG	0.41	2.82	15	1
1:A:141:THR:O	1:A:142:MET:C	0.40	2.63	1	2
1:B:307:LEU:N	1:B:307:LEU:CD1	0.40	2.83	3	1
1:A:13:TYR:CD2	1:A:73:LEU:CA	0.40	3.04	4	1
1:A:56:GLU:CD	1:A:56:GLU:N	0.40	2.79	4	1
1:B:217:SER:N	1:B:290:VAL:CG2	0.40	2.84	5	1
1:B:224:ASP:CG	1:B:228:TYR:CE1	0.40	2.99	8	1
1:B:347:PHE:O	1:B:352:PRO:CD	0.40	2.69	9	1
1:A:57:GLU:O	1:A:58:ALA:O	0.40	2.40	12	1
1:B:232:VAL:CG1	1:B:241:VAL:HG21	0.40	2.45	15	1
1:B:223:GLU:CD	1:B:223:GLU:N	0.40	2.79	2	1
1:B:317:SER:C	1:B:319:MET:N	0.40	2.77	2	1
1:B:282:GLU:C	1:B:283:VAL:CG2	0.40	2.94	3	1
1:A:54:LEU:O	1:A:58:ALA:HB3	0.40	2.16	4	1
1:A:125:ASP:OD2	1:A:127:SER:OG	0.40	2.39	7	1
1:A:109:ARG:NH1	1:A:136:GLU:CG	0.40	2.84	8	1
1:A:25:GLN:OE1	1:A:25:GLN:O	0.40	2.39	11	1
1:A:25:GLN:HE21	1:A:50:GLU:CG	0.40	2.29	12	1
1:A:151:LEU:HB2	1:A:152:PRO:CD	0.40	2.46	13	1
1:B:278:VAL:C	1:B:279:VAL:HG23	0.40	2.42	4	1
1:B:274:GLN:OE1	1:B:296:ARG:NH2	0.40	2.50	7	1
1:A:88:LEU:HD23	1:B:286:PRO:HA	0.40	1.94	9	1
1:B:288:LEU:HD13	1:B:288:LEU:O	0.40	2.16	9	1
1:B:308:PHE:CD1	1:B:316:LEU:HD21	0.40	2.51	10	1
1:B:251:LEU:CD1	1:B:251:LEU:H	0.40	2.27	12	1
1:B:246:VAL:C	1:B:248:ASP:N	0.40	2.79	13	1
1:A:110:PRO:CD	1:A:134:TYR:O	0.40	2.70	14	1
1:B:214:PHE:CD1	1:B:246:VAL:HG21	0.40	2.51	5	1
1:B:242:LEU:HD11	1:B:276:ALA:HA	0.40	1.93	5	1
1:B:255:GLY:O	1:B:258:ALA:CB	0.40	2.69	7	1
1:B:246:VAL:HG12	1:B:247:ALA:H	0.40	1.76	11	1
1:A:84:THR:O	1:A:114:ARG:CD	0.40	2.70	12	1
1:B:271:ASN:OD1	1:B:271:ASN:C	0.40	2.63	12	1
1:A:51:LEU:HD23	1:A:51:LEU:C	0.40	2.41	14	1
1:B:310:PRO:O	1:B:311:GLN:O	0.40	2.40	14	1
1:A:57:GLU:O	1:A:58:ALA:C	0.40	2.64	1	1
1:B:234:ARG:CZ	1:B:238:TYR:OH	0.40	2.70	1	1
1:B:283:VAL:HG23	1:B:307:LEU:O	0.40	2.15	2	1
1:A:11:SER:OG	1:A:42:LEU:CD2	0.40	2.69	4	1
1:A:109:ARG:HD3	1:A:134:TYR:CZ	0.40	2.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:HG21	1:A:150:TYR:OH	0.40	2.17	5	1
1:B:302:LYS:CD	1:B:302:LYS:N	0.40	2.81	7	1
1:A:24:ASP:CG	1:A:28:TYR:CE1	0.40	2.99	8	1
1:A:70:LEU:HD23	1:A:70:LEU:N	0.40	2.32	13	1
1:A:66:HIS:NE2	1:A:70:LEU:HD22	0.40	2.32	15	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	142/165 (86%)	111±3 (78±2%)	18±3 (13±2%)	13±2 (9±2%)	1	11
1	B	142/165 (86%)	111±2 (78±2%)	18±3 (13±2%)	13±2 (9±2%)	1	11
All	All	4260/4950 (86%)	3339 (78%)	535 (13%)	386 (9%)	1	11

All 102 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	52	GLU	13
1	A	115	VAL	13
1	B	252	GLU	13
1	B	315	VAL	13
1	A	9	PRO	11
1	A	124	ALA	11
1	B	209	PRO	11
1	B	324	ALA	11
1	A	56	GLU	8
1	A	102	LYS	8
1	B	256	GLU	8
1	B	302	LYS	8
1	A	151	LEU	7
1	A	152	PRO	7
1	B	351	LEU	7
1	B	352	PRO	7

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Mol	Chain	Res	Type	Models (Total)
1	A	136	GLU	7
1	B	336	GLU	7
1	A	84	THR	6
1	B	255	GLY	6
1	B	284	THR	6
1	A	55	GLY	5
1	A	46	VAL	5
1	A	54	LEU	5
1	B	246	VAL	5
1	B	254	LEU	5
1	A	43	THR	4
1	A	48	ASP	4
1	A	128	ARG	4
1	B	248	ASP	4
1	B	328	ARG	4
1	A	86	PRO	4
1	A	127	SER	4
1	B	286	PRO	4
1	B	327	SER	4
1	A	53	PRO	4
1	B	253	PRO	4
1	A	22	ARG	4
1	B	222	ARG	4
1	A	18	ILE	4
1	B	218	ILE	4
1	A	17	SER	3
1	B	217	SER	3
1	B	243	THR	3
1	A	103	PRO	3
1	A	125	ASP	3
1	A	126	GLY	3
1	B	303	PRO	3
1	B	325	ASP	3
1	B	326	GLY	3
1	A	51	LEU	3
1	B	251	LEU	3
1	A	10	CYS	3
1	A	59	ALA	3
1	A	117	SER	3
1	B	210	CYS	3
1	B	259	ALA	3
1	B	317	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	B	261	GLY	3
1	A	88	LEU	3
1	B	288	LEU	3
1	A	101	GLY	2
1	B	301	GLY	2
1	A	60	GLY	2
1	B	260	GLY	2
1	A	83	VAL	2
1	B	283	VAL	2
1	A	114	ARG	2
1	A	61	GLY	2
1	A	45	HIS	2
1	B	245	HIS	2
1	A	58	ALA	2
1	B	258	ALA	2
1	A	150	TYR	1
1	B	350	TYR	1
1	A	138	GLU	1
1	B	314	ARG	1
1	B	338	GLU	1
1	A	57	GLU	1
1	A	113	GLY	1
1	B	257	GLU	1
1	B	313	GLY	1
1	A	8	ALA	1
1	B	208	ALA	1
1	A	47	ALA	1
1	B	247	ALA	1
1	A	49	ALA	1
1	B	249	ALA	1
1	A	50	GLU	1
1	B	250	GLU	1
1	A	85	GLN	1
1	A	111	GLN	1
1	A	112	SER	1
1	B	285	GLN	1
1	B	311	GLN	1
1	B	312	SER	1
1	A	40	LYS	1
1	A	42	LEU	1
1	A	87	SER	1
1	B	240	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	B	242	LEU	1
1	B	287	SER	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	113/128 (88%)	97±3 (85±3%)	16±3 (15±3%)	5	43
1	B	113/128 (88%)	97±3 (86±3%)	16±3 (14±3%)	5	43
All	All	3390/3840 (88%)	2899 (86%)	491 (14%)	5	43

All 115 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	98	VAL	15
1	B	298	VAL	15
1	A	51	LEU	14
1	A	72	TRP	14
1	B	251	LEU	14
1	B	272	TRP	14
1	A	106	CYS	13
1	A	108	PHE	13
1	B	306	CYS	13
1	B	308	PHE	13
1	A	83	VAL	12
1	B	283	VAL	12
1	A	65	ILE	11
1	A	18	ILE	11
1	B	218	ILE	11
1	B	265	ILE	10
1	A	70	LEU	9
1	B	270	LEU	9
1	A	117	SER	9
1	B	317	SER	9
1	A	14	PHE	7
1	B	214	PHE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	54	LEU	7
1	A	22	ARG	6
1	B	222	ARG	6
1	A	150	TYR	6
1	B	254	LEU	6
1	B	350	TYR	6
1	A	15	CYS	5
1	A	25	GLN	5
1	B	225	GLN	5
1	A	27	LEU	4
1	A	43	THR	4
1	A	119	MET	4
1	B	227	LEU	4
1	B	243	THR	4
1	B	319	MET	4
1	A	50	GLU	4
1	B	250	GLU	4
1	A	102	LYS	4
1	B	215	CYS	4
1	B	302	LYS	4
1	A	142	MET	4
1	B	342	MET	4
1	A	45	HIS	3
1	B	245	HIS	3
1	B	300	LEU	3
1	A	116	LEU	3
1	A	121	ARG	3
1	B	316	LEU	3
1	B	321	ARG	3
1	A	12	VAL	3
1	B	212	VAL	3
1	A	52	GLU	3
1	A	88	LEU	3
1	A	114	ARG	3
1	B	252	GLU	3
1	B	288	LEU	3
1	B	314	ARG	3
1	A	48	ASP	3
1	B	248	ASP	3
1	A	87	SER	3
1	B	287	SER	3
1	A	42	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	242	LEU	3
1	A	104	ILE	3
1	B	304	ILE	3
1	A	66	HIS	2
1	A	96	ARG	2
1	A	100	LEU	2
1	B	266	HIS	2
1	B	296	ARG	2
1	A	74	GLN	2
1	B	274	GLN	2
1	A	127	SER	2
1	B	327	SER	2
1	A	151	LEU	2
1	B	351	LEU	2
1	A	38	TYR	2
1	B	238	TYR	2
1	A	40	LYS	2
1	B	240	LYS	2
1	A	46	VAL	1
1	A	107	LEU	1
1	A	148	GLU	1
1	B	246	VAL	1
1	B	307	LEU	1
1	B	348	GLU	1
1	A	17	SER	1
1	B	217	SER	1
1	A	41	VAL	1
1	B	241	VAL	1
1	A	138	GLU	1
1	B	338	GLU	1
1	A	139	VAL	1
1	B	339	VAL	1
1	A	109	ARG	1
1	B	309	ARG	1
1	A	69	ASP	1
1	B	269	ASP	1
1	A	84	THR	1
1	B	284	THR	1
1	A	56	GLU	1
1	A	63	GLN	1
1	A	64	PHE	1
1	A	90	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	112	SER	1
1	A	129	PHE	1
1	B	256	GLU	1
1	B	263	GLN	1
1	B	264	PHE	1
1	B	290	VAL	1
1	B	312	SER	1
1	B	329	PHE	1
1	B	211	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided