



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 06:16 AM UTC

PDB ID : 5T1O / pdb_00005t1o
BMRB ID : 30159
Title : Solution-state NMR and SAXS structural ensemble of NPr (1-85) in complex with EIN-Ntr (170-424)
Authors : Strickland, M.; Stanley, A.M.; Wang, G.; Schwieters, C.D.; Buchanan, S.; Peterkofsky, A.; Tjandra, N.
Deposited on : 2016-08-19

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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

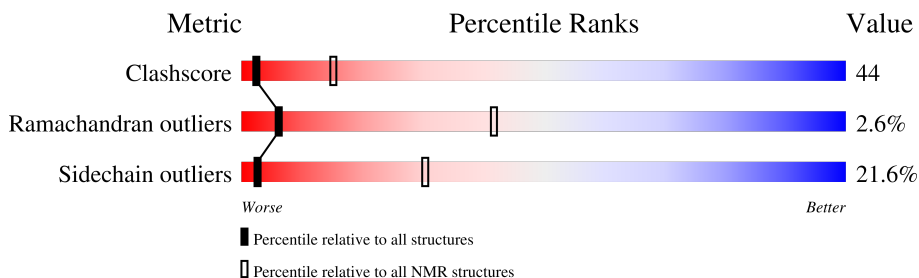
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 29%.

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	85	
2	B	256	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:1-A:85, B:170-B:187, B:202-B:311, B:322-B:397 (289)	0.86	8

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5287 atoms, of which 2646 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phosphocarrier protein NPr.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1298	402	653	108	130	5	

- Molecule 2 is a protein called Phosphoenolpyruvate-protein phosphotransferase PtsP.

Mol	Chain	Residues	Atoms						Trace
2	B	255	Total	C	H	N	O	S	0
			3989	1256	1993	354	383	3	

There are 2 discrepancies between the modelled and reference sequences:

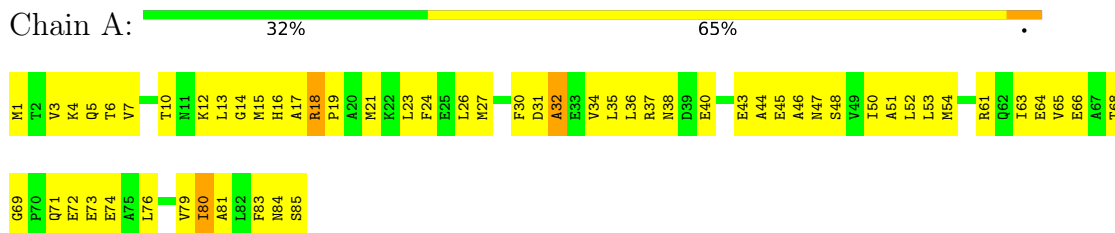
Chain	Residue	Modelled	Actual	Comment	Reference
B	169	GLY	-	expression tag	UNP P37177
B	356	GLN	HIS	engineered mutation	UNP P37177

4 Residue-property plots

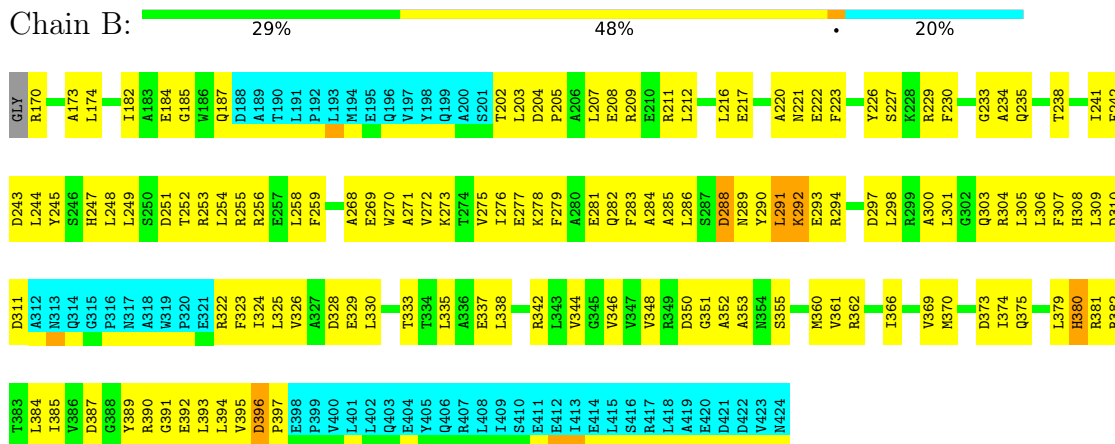
4.1 Average score per residue in the NMR ensemble

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: Phosphocarrier protein NPr



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



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: Phosphocarrier protein NPr



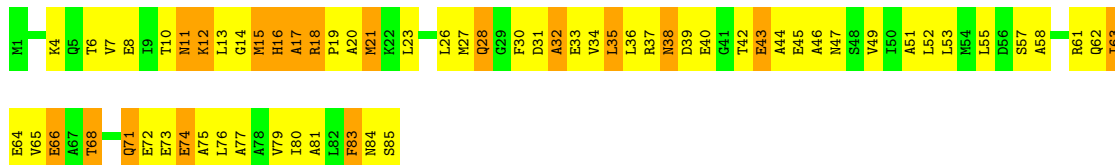
- Molecule 1: Phosphocarrier protein NPr



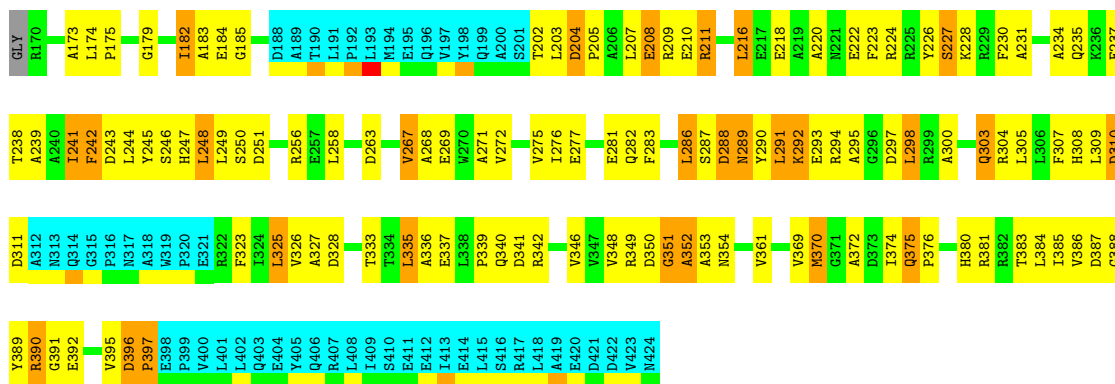


4.2.3 Score per residue for model 3

- Molecule 1: Phosphocarrier protein NPr

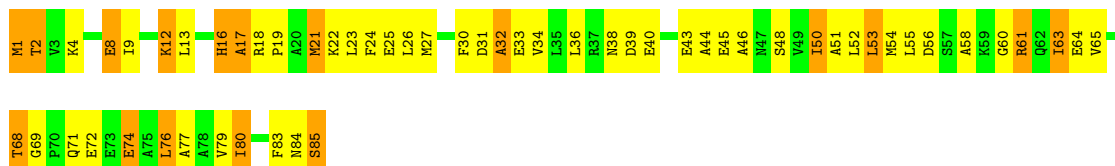


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



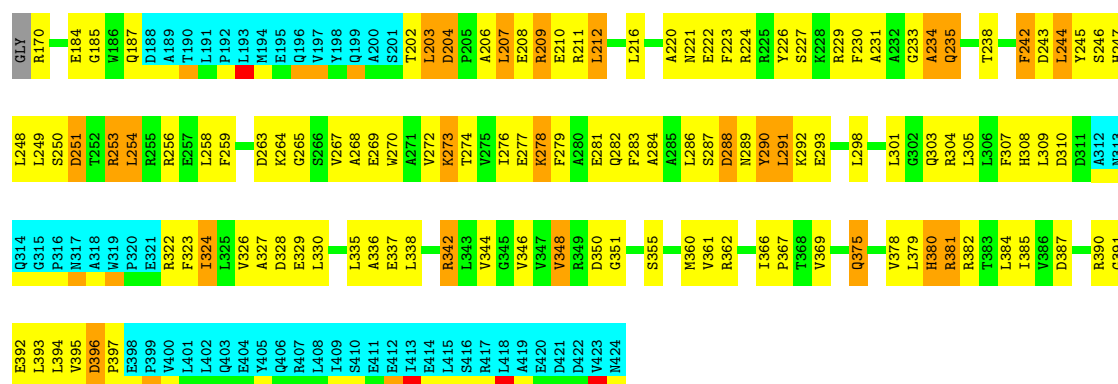
4.2.4 Score per residue for model 4

- Molecule 1: Phosphocarrier protein NPr



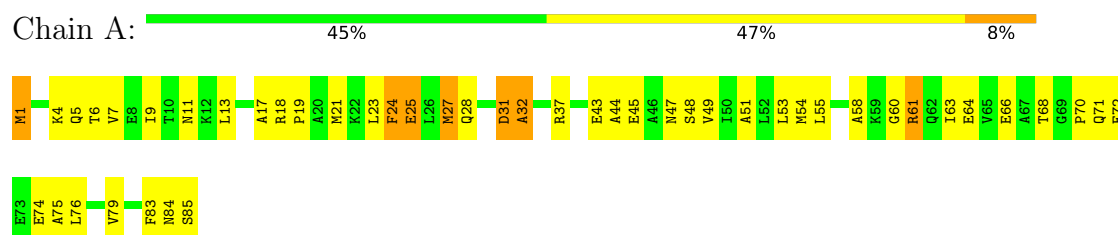
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



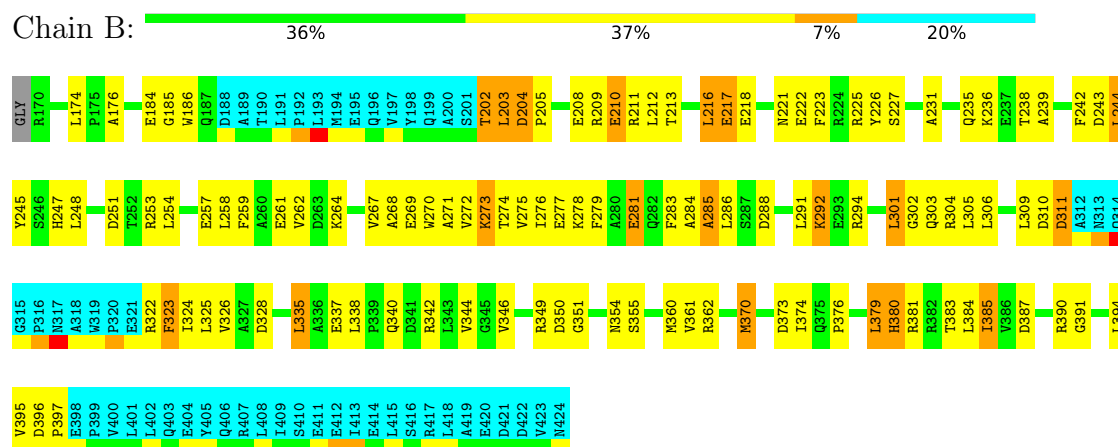


4.2.5 Score per residue for model 5

- Molecule 1: Phosphocarrier protein NPr

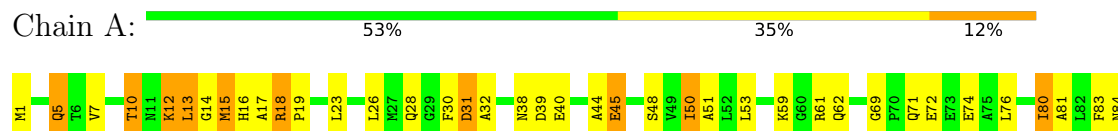


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



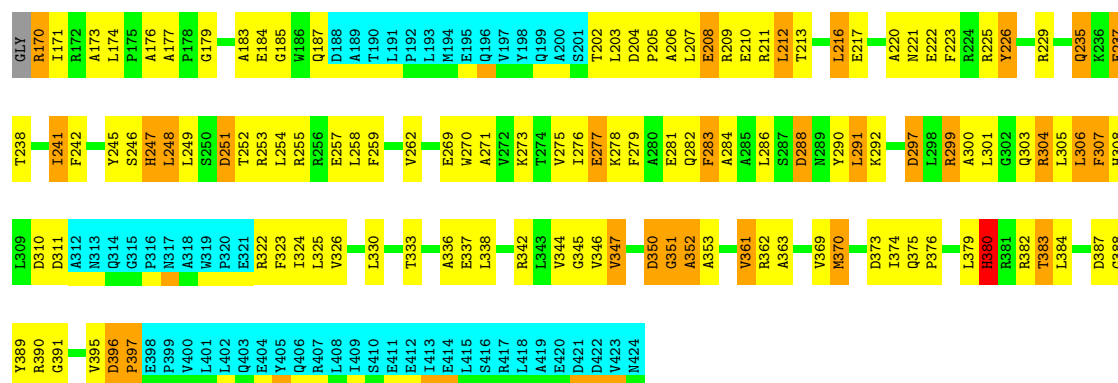
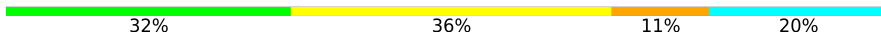
4.2.6 Score per residue for model 6

- Molecule 1: Phosphocarrier protein NPr



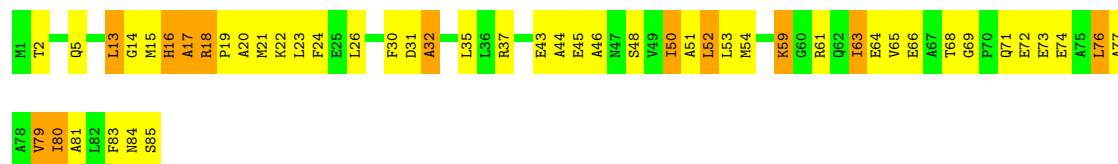
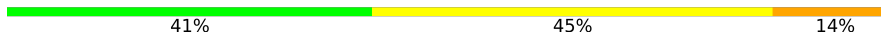
S85

- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

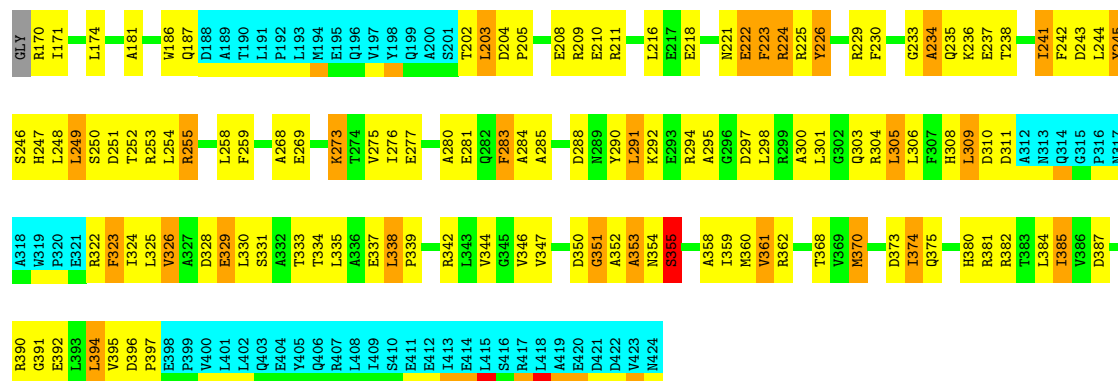
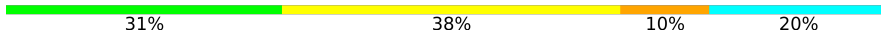
Chain B: 

4.2.7 Score per residue for model 7

- Molecule 1: Phosphocarrier protein NPr

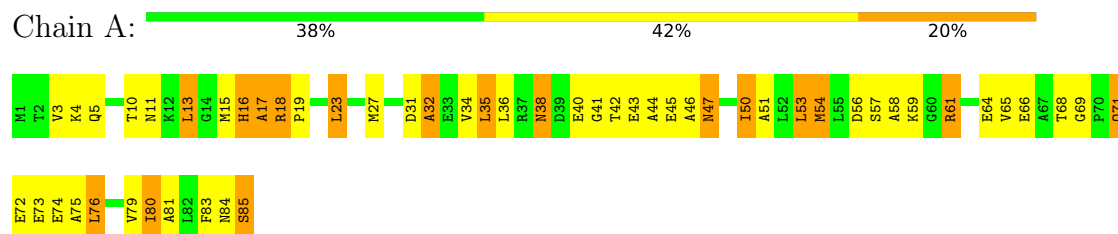
Chain A: 

- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

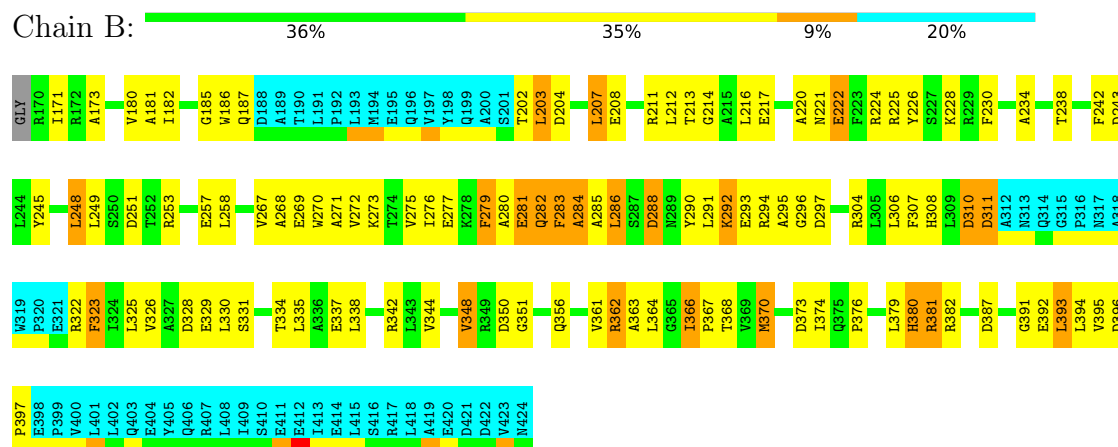
Chain B: 

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Phosphocarrier protein NPR

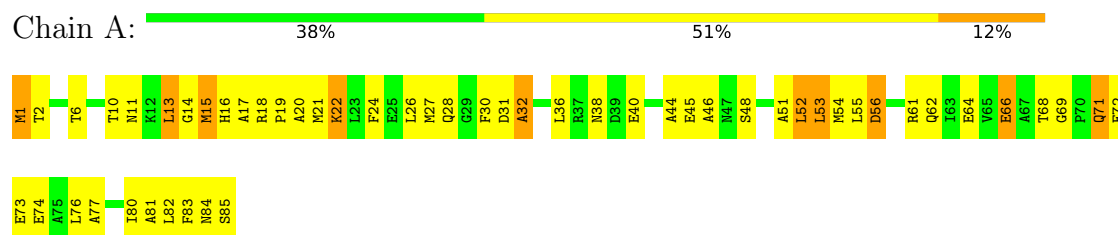


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

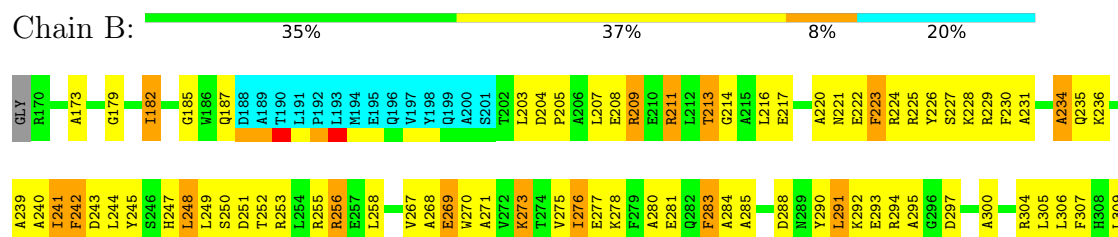


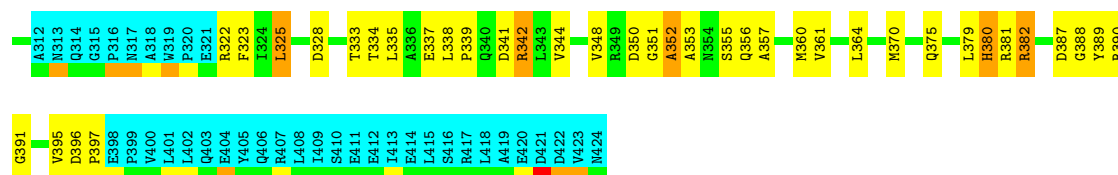
4.2.9 Score per residue for model 9

- Molecule 1: Phosphocarrier protein NPR



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

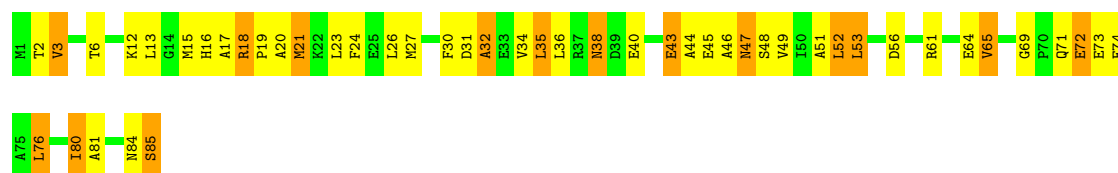




4.2.10 Score per residue for model 10

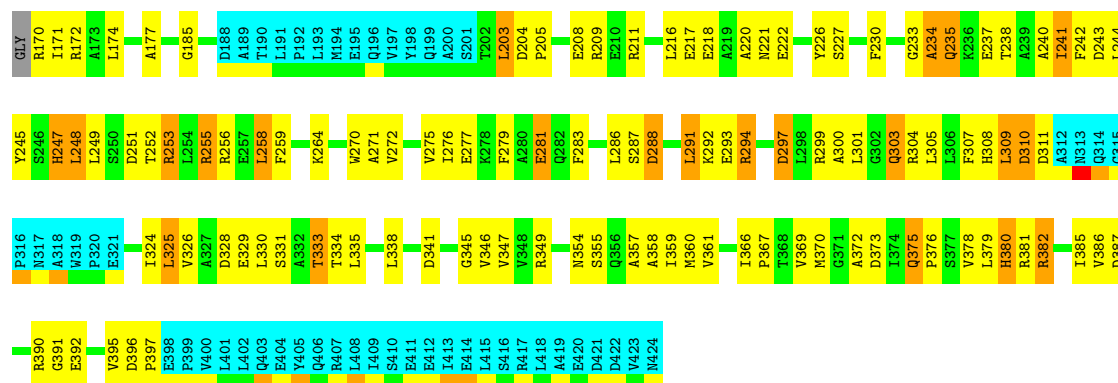
- Molecule 1: Phosphocarrier protein NPr

Chain A: 44% 39% 18%



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

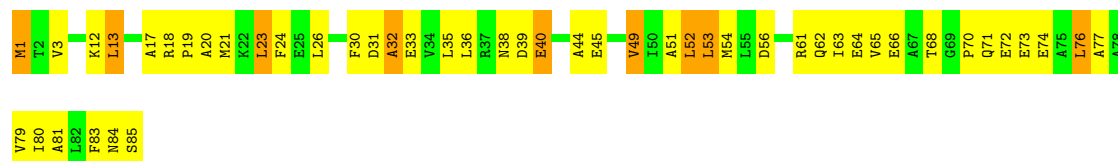
Chain B: 34% 37% 9% 20%



4.2.11 Score per residue for model 11

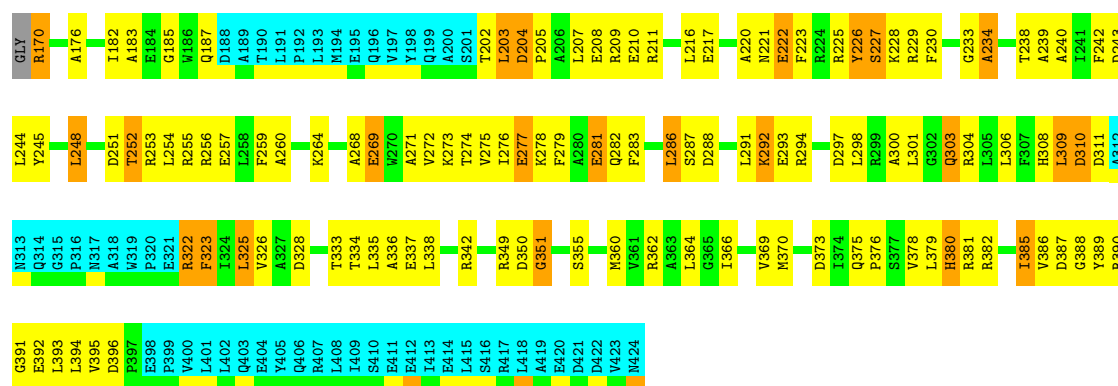
- Molecule 1: Phosphocarrier protein NPr

Chain A: 42% 47% 11%



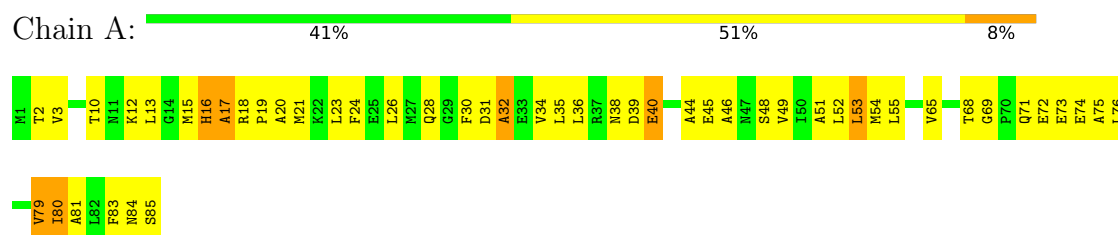
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 32% 38% 9% 20%

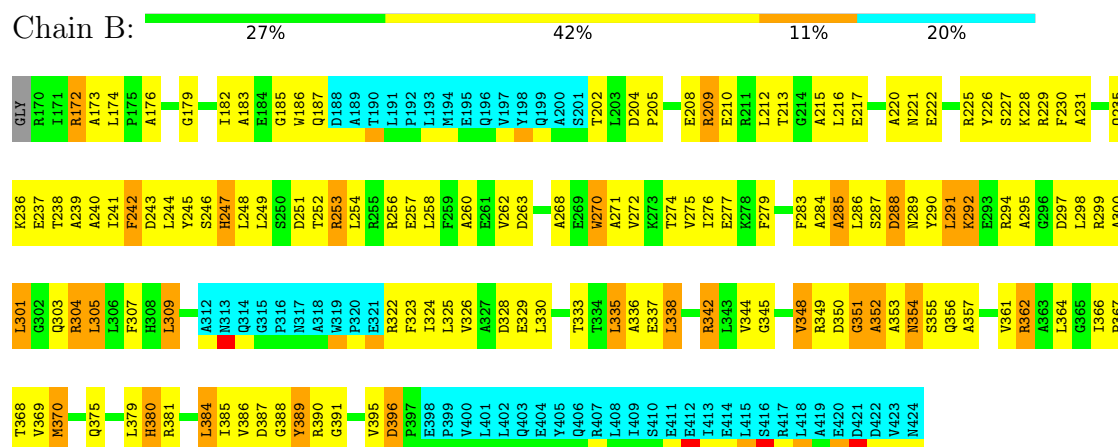


4.2.12 Score per residue for model 12

- Molecule 1: Phosphocarrier protein NPr

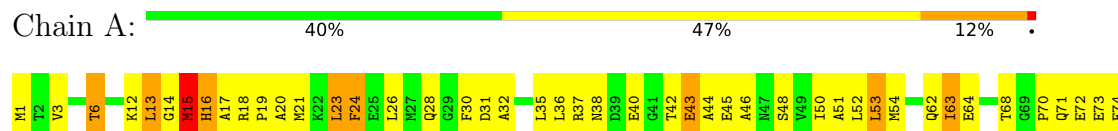


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



4.2.13 Score per residue for model 13

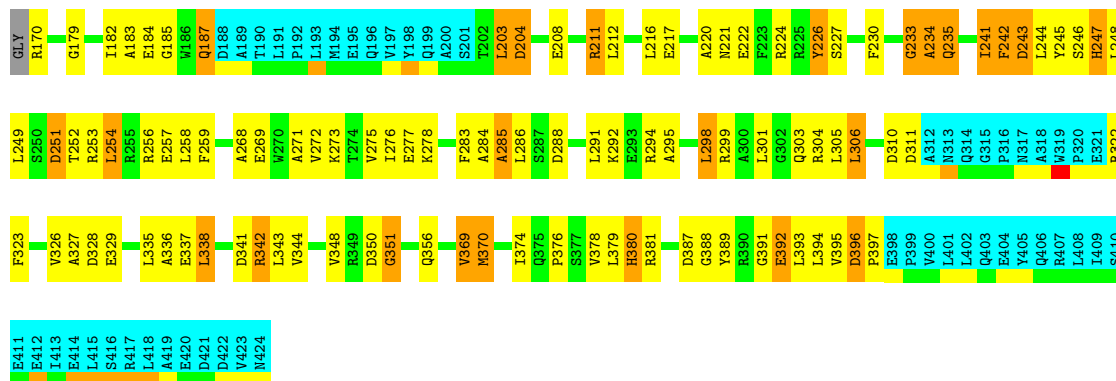
- Molecule 1: Phosphocarrier protein NPr





• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

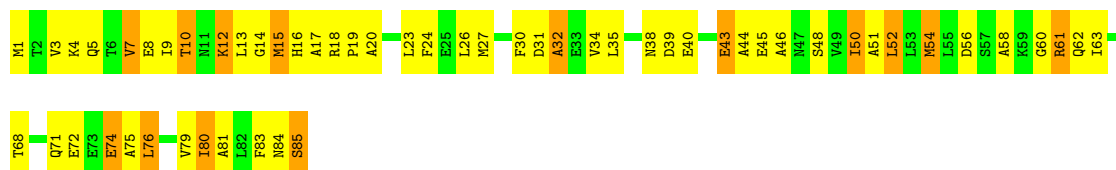
Chain B: 39% 31% 10% 20%



4.2.14 Score per residue for model 14

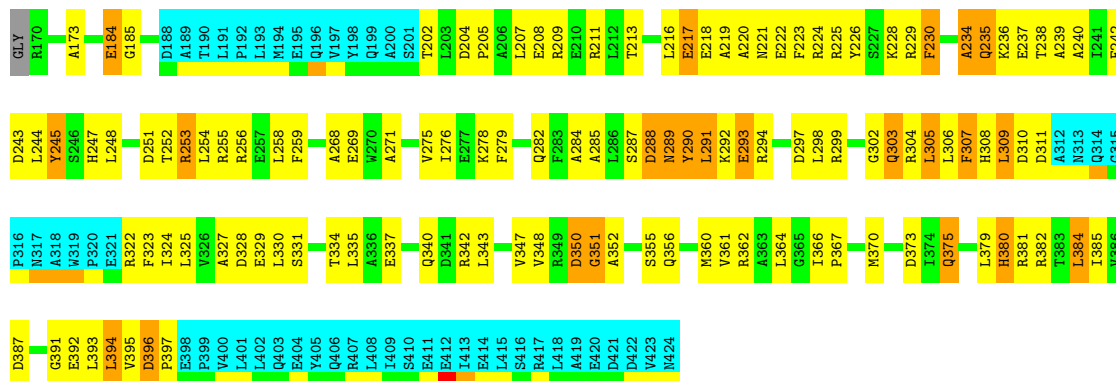
• Molecule 1: Phosphocarrier protein NPr

Chain A: 34% 49% 16%



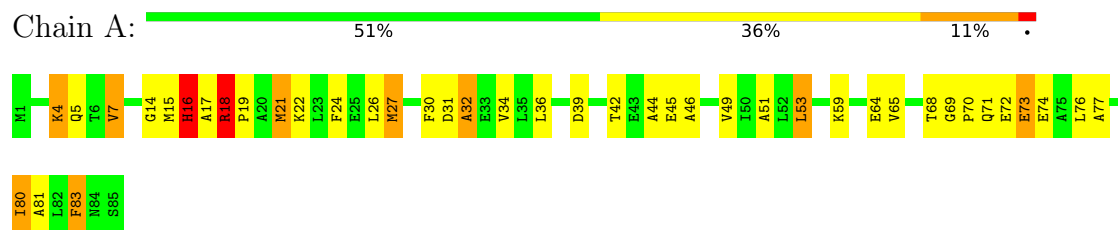
• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 32% 39% 9% 20%

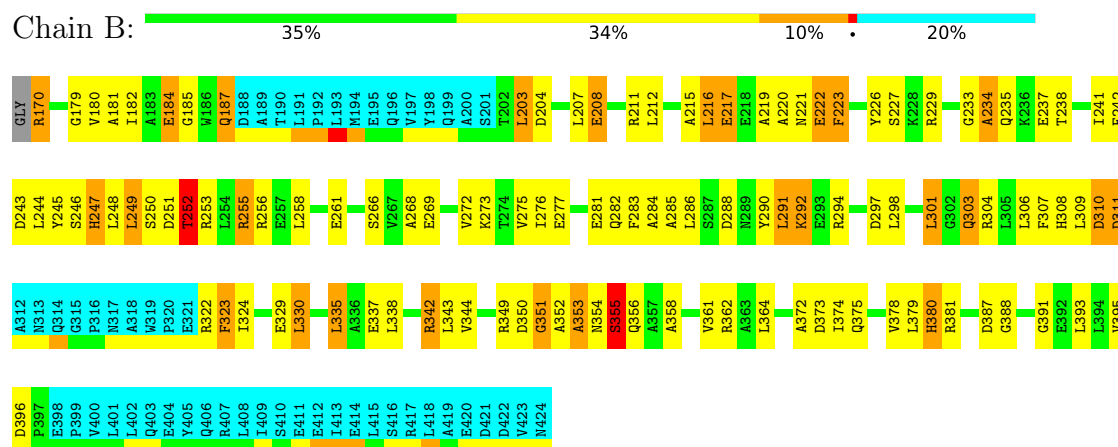


4.2.15 Score per residue for model 15

- Molecule 1: Phosphocarrier protein NPr

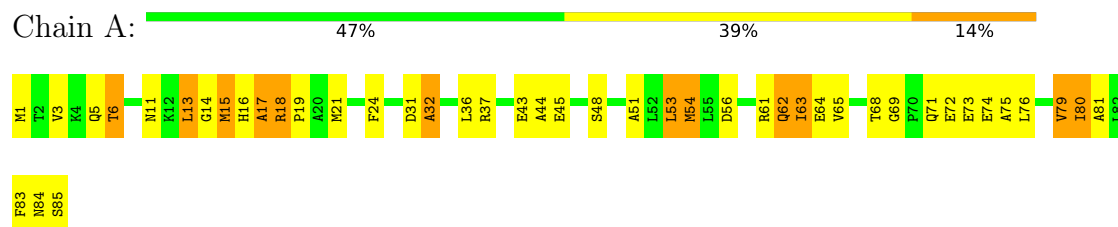


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

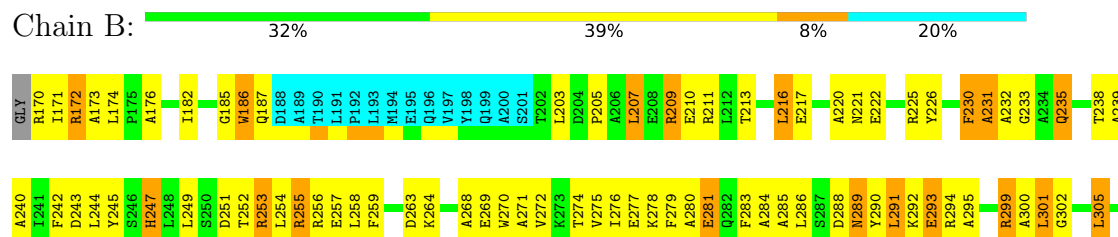


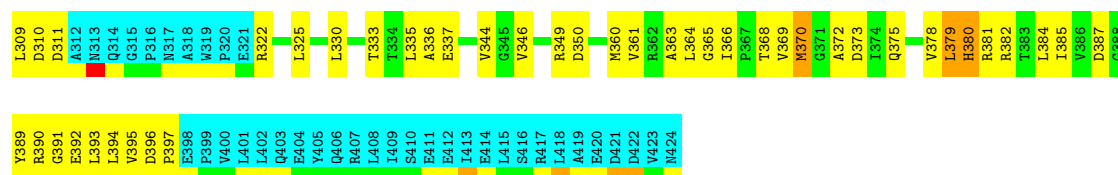
4.2.16 Score per residue for model 16

- Molecule 1: Phosphocarrier protein NPr



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

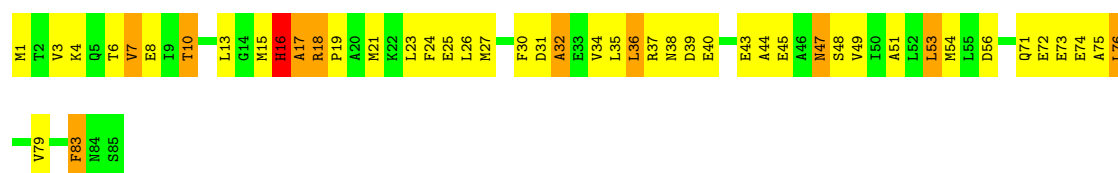




4.2.17 Score per residue for model 17

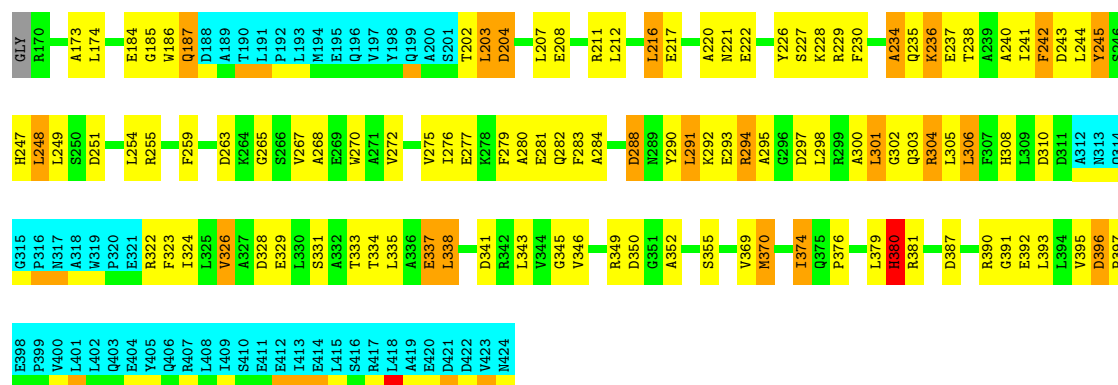
- Molecule 1: Phosphocarrier protein NPr

Chain A: 45% 42% 12%



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

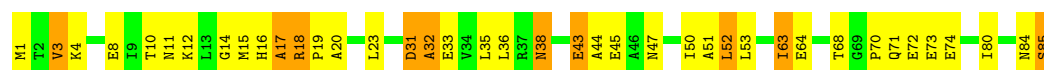
Chain B: 37% 34% 8% 20%



4.2.18 Score per residue for model 18

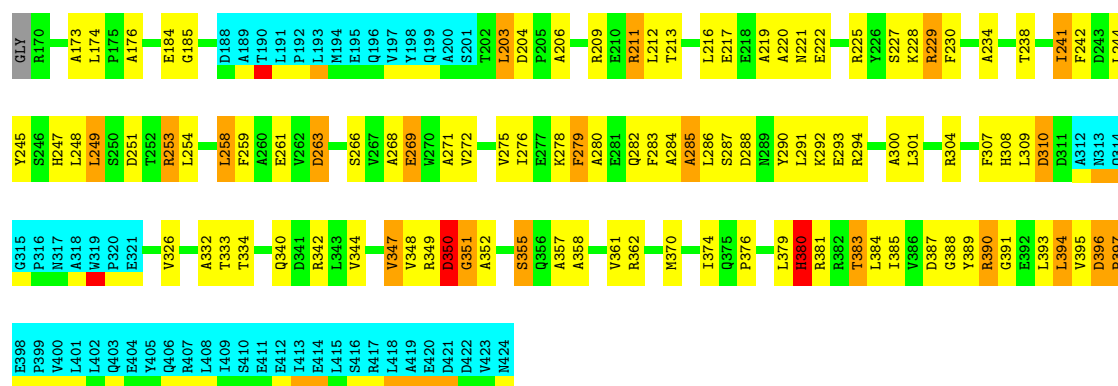
- Molecule 1: Phosphocarrier protein NPr

Chain A: 53% 35% 12%



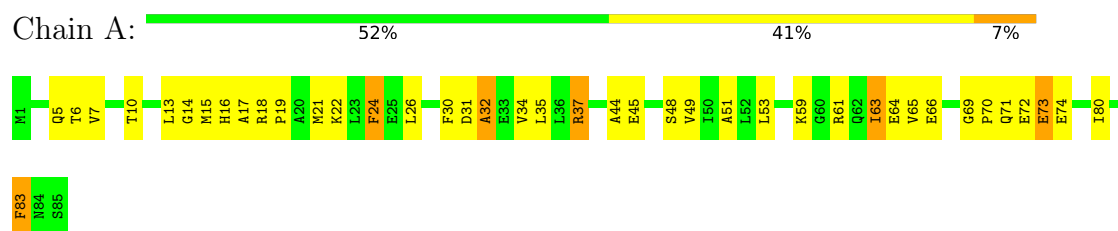
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 39% 32% 8% 20%

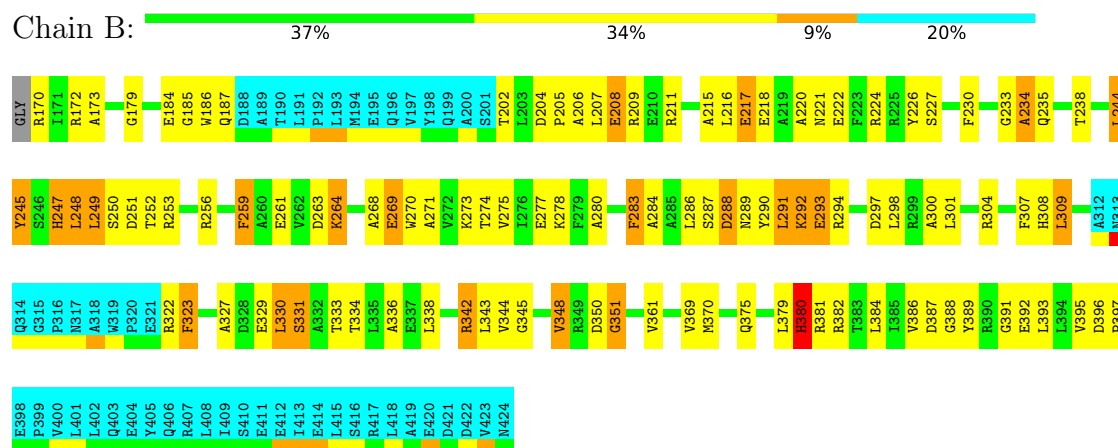


4.2.19 Score per residue for model 19

- Molecule 1: Phosphocarrier protein NPr

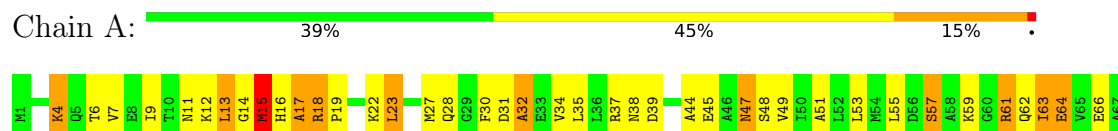


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



4.2.20 Score per residue for model 20

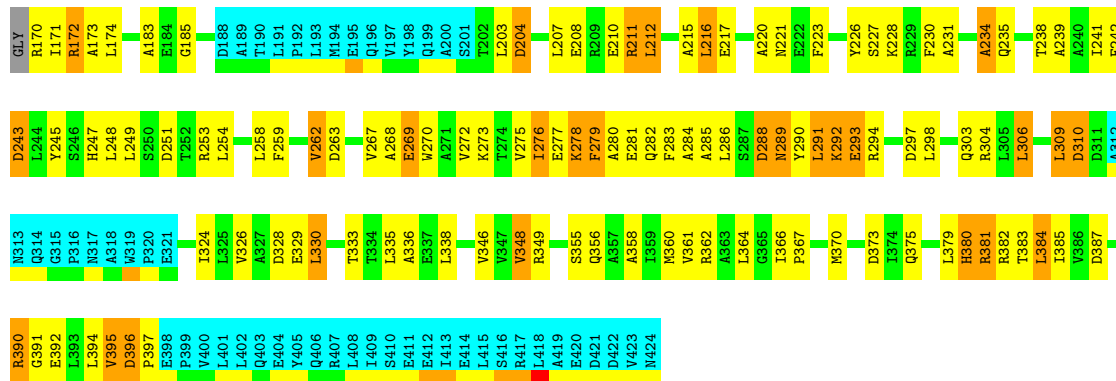
- Molecule 1: Phosphocarrier protein NPr





● Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 35% 34% 11% 20%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *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	refinement	2.37.7
ANALYSIS	structure solution	2.4.2
TopSpin	structure solution	3.0
Gaussian	structure solution	9
NMRPipe	structure solution	8.2
TALOS-N	structure solution	4.12

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1391
Number of shifts mapped to atoms	1391
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	29%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	645	653	653	68±16
2	B	1587	1608	1607	131±13
All	All	44640	45220	45200	3908

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 43.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:HA	1:A:19:PRO:CD	1.27	1.56	18	1
1:A:15:MET:CA	1:A:19:PRO:HG2	1.27	1.60	18	1
1:A:10:THR:O	1:A:11:ASN:OD1	1.24	1.55	8	3
1:A:53:LEU:HD22	1:A:53:LEU:O	1.23	1.32	16	2
1:A:15:MET:HA	1:A:19:PRO:CG	1.20	1.67	18	1
2:B:338:LEU:O	2:B:338:LEU:HD22	1.13	1.42	7	1
1:A:15:MET:CA	1:A:19:PRO:CG	1.12	2.26	18	1
1:A:20:ALA:CB	1:A:52:LEU:HD21	1.11	1.74	18	1
1:A:10:THR:C	1:A:11:ASN:OD1	1.11	1.94	3	1
1:A:9:ILE:HG22	1:A:61:ARG:O	1.11	1.44	5	3
1:A:53:LEU:HD13	1:A:54:MET:N	1.11	1.59	16	2
1:A:76:LEU:O	1:A:80:ILE:HG23	1.11	1.46	11	3
1:A:15:MET:O	1:A:17:ALA:N	1.09	1.86	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:395:VAL:O	2:B:397:PRO:CD	1.08	2.00	18	2
1:A:18:ARG:H	1:A:19:PRO:HD2	1.08	1.04	20	3
1:A:10:THR:O	1:A:11:ASN:CG	1.06	1.98	3	3
1:A:15:MET:CA	1:A:19:PRO:CD	1.06	2.33	18	1
2:B:203:LEU:HD13	2:B:203:LEU:N	1.05	1.61	17	2
2:B:393:LEU:HD22	2:B:393:LEU:N	1.05	1.65	8	1
2:B:395:VAL:O	2:B:397:PRO:HD3	1.05	1.48	18	1
1:A:14:GLY:O	1:A:19:PRO:CG	1.04	2.05	18	4
1:A:17:ALA:HB3	1:A:18:ARG:HH11	1.04	1.11	17	2
2:B:338:LEU:HD22	2:B:338:LEU:C	1.03	1.78	7	1
1:A:3:VAL:HG21	1:A:72:GLU:OE1	1.03	1.53	1	1
2:B:244:LEU:C	2:B:244:LEU:HD13	1.03	1.78	19	1
1:A:9:ILE:HG21	1:A:58:ALA:O	1.02	1.54	14	3
2:B:330:LEU:HD23	2:B:330:LEU:H	1.02	1.10	14	2
1:A:15:MET:HB3	1:A:19:PRO:CB	1.02	1.85	18	1
2:B:233:GLY:O	2:B:234:ALA:O	1.02	1.77	10	9
1:A:15:MET:CA	1:A:19:PRO:HD2	1.01	1.84	18	1
2:B:286:LEU:HD12	2:B:288:ASP:OD1	1.00	1.56	2	1
1:A:53:LEU:HD13	1:A:53:LEU:C	1.00	1.81	16	2
1:A:53:LEU:O	2:B:291:LEU:HD21	1.00	1.55	18	1
1:A:74:GLU:OE1	1:A:75:ALA:N	1.00	1.94	12	1
2:B:384:LEU:O	2:B:384:LEU:HD22	1.00	1.56	20	1
2:B:395:VAL:C	2:B:397:PRO:HD3	0.99	1.83	3	15
1:A:71:GLN:O	1:A:74:GLU:HG3	0.99	1.56	12	1
1:A:16:HIS:O	1:A:19:PRO:HD2	0.99	1.57	7	1
1:A:15:MET:HB3	1:A:19:PRO:HB2	0.99	1.35	18	1
1:A:37:ARG:O	1:A:63:ILE:HG23	0.98	1.58	5	3
2:B:176:ALA:HB2	2:B:370:MET:SD	0.98	1.97	16	3
1:A:34:VAL:C	1:A:35:LEU:HD22	0.98	1.84	12	3
2:B:173:ALA:HB1	2:B:370:MET:O	0.97	1.59	18	11
2:B:286:LEU:HD23	2:B:287:SER:N	0.97	1.73	4	1
1:A:14:GLY:O	1:A:19:PRO:HG3	0.96	1.58	18	2
2:B:395:VAL:O	2:B:397:PRO:N	0.96	1.98	18	13
2:B:248:LEU:HD23	2:B:249:LEU:N	0.96	1.75	10	3
1:A:15:MET:HB3	1:A:19:PRO:CG	0.96	1.91	18	1
2:B:244:LEU:HD12	2:B:245:TYR:N	0.95	1.76	17	1
2:B:203:LEU:H	2:B:203:LEU:HD23	0.95	1.14	11	1
1:A:71:GLN:HB3	1:A:74:GLU:HG2	0.95	1.38	12	1
2:B:392:GLU:C	2:B:393:LEU:HD13	0.94	1.85	8	1
2:B:204:ASP:O	2:B:208:GLU:HB2	0.94	1.61	5	8
2:B:251:ASP:O	2:B:253:ARG:N	0.94	2.00	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:251:ASP:OD1	2:B:251:ASP:O	0.94	1.84	17	10
2:B:204:ASP:O	2:B:208:GLU:CB	0.94	2.16	13	9
1:A:15:MET:CB	1:A:19:PRO:CG	0.93	2.45	18	1
1:A:26:LEU:O	1:A:30:PHE:CD2	0.93	2.21	10	8
1:A:53:LEU:HB2	2:B:291:LEU:HD13	0.93	1.40	16	1
1:A:75:ALA:O	1:A:79:VAL:HG13	0.92	1.64	16	3
2:B:182:ILE:HD13	2:B:182:ILE:H	0.92	1.21	3	1
2:B:244:LEU:HD23	2:B:244:LEU:C	0.92	1.90	5	5
1:A:18:ARG:H	1:A:19:PRO:CD	0.91	1.78	20	3
2:B:203:LEU:HD22	2:B:203:LEU:H	0.91	1.25	17	2
1:A:53:LEU:HD23	1:A:54:MET:N	0.91	1.81	9	2
1:A:74:GLU:CD	1:A:75:ALA:N	0.91	2.27	12	1
1:A:15:MET:SD	1:A:19:PRO:HD3	0.91	2.05	20	1
1:A:72:GLU:CD	1:A:73:GLU:N	0.91	2.29	1	8
1:A:13:LEU:HD13	1:A:13:LEU:H	0.91	1.26	1	2
2:B:242:PHE:CG	2:B:243:ASP:N	0.90	2.39	12	6
2:B:395:VAL:O	2:B:396:ASP:OD1	0.90	1.89	8	2
2:B:351:GLY:O	2:B:352:ALA:O	0.90	1.89	9	3
2:B:244:LEU:HD23	2:B:244:LEU:O	0.90	1.65	15	3
2:B:286:LEU:HD21	2:B:288:ASP:O	0.90	1.67	11	1
1:A:13:LEU:N	1:A:13:LEU:HD22	0.90	1.80	16	2
2:B:184:GLU:O	2:B:324:ILE:HG22	0.90	1.66	4	1
2:B:203:LEU:N	2:B:203:LEU:CD1	0.90	2.30	8	2
2:B:286:LEU:HD12	2:B:288:ASP:OD2	0.90	1.67	3	1
1:A:50:ILE:O	1:A:53:LEU:HG	0.89	1.64	7	2
2:B:322:ARG:O	2:B:323:PHE:CG	0.89	2.25	6	6
2:B:350:ASP:O	2:B:352:ALA:N	0.89	2.05	3	4
1:A:14:GLY:C	1:A:19:PRO:HG2	0.89	1.91	18	1
2:B:248:LEU:C	2:B:248:LEU:HD13	0.89	1.91	3	2
2:B:216:LEU:HD23	2:B:217:GLU:N	0.89	1.83	17	1
2:B:394:LEU:N	2:B:394:LEU:HD22	0.88	1.83	7	2
2:B:286:LEU:O	2:B:286:LEU:HD23	0.88	1.68	11	1
2:B:380:HIS:CD2	2:B:381:ARG:H	0.88	1.86	16	2
2:B:217:GLU:O	2:B:221:ASN:HB3	0.88	1.67	2	1
1:A:53:LEU:HD22	1:A:53:LEU:C	0.88	1.91	16	2
1:A:13:LEU:HD13	1:A:13:LEU:N	0.88	1.84	1	1
1:A:5:GLN:OE1	1:A:76:LEU:HD21	0.88	1.68	15	2
1:A:30:PHE:CD1	1:A:30:PHE:O	0.88	2.27	14	8
1:A:53:LEU:C	1:A:53:LEU:HD12	0.87	1.94	11	3
1:A:71:GLN:HB3	1:A:74:GLU:CG	0.87	1.99	12	1
1:A:15:MET:HA	1:A:19:PRO:HD2	0.87	1.38	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HA	1:A:83:PHE:CZ	0.87	2.04	5	1
2:B:251:ASP:C	2:B:253:ARG:H	0.87	1.78	11	15
2:B:380:HIS:ND1	2:B:381:ARG:N	0.87	2.23	10	2
1:A:15:MET:HE1	1:A:19:PRO:CG	0.86	1.99	20	1
2:B:241:ILE:HG23	2:B:242:PHE:N	0.86	1.84	10	1
1:A:15:MET:N	1:A:19:PRO:HG2	0.86	1.84	18	1
1:A:74:GLU:CD	1:A:75:ALA:H	0.86	1.77	12	1
1:A:77:ALA:O	1:A:80:ILE:HG13	0.86	1.71	4	2
2:B:361:VAL:O	2:B:366:ILE:HG22	0.86	1.71	16	1
2:B:291:LEU:HD13	2:B:292:LYS:N	0.86	1.84	12	1
1:A:10:THR:C	1:A:11:ASN:CG	0.86	2.41	3	2
1:A:20:ALA:HB2	1:A:52:LEU:HD21	0.86	1.44	18	1
1:A:18:ARG:N	1:A:19:PRO:HD2	0.86	1.86	20	12
2:B:393:LEU:HD22	2:B:393:LEU:H	0.86	1.19	8	1
1:A:76:LEU:O	1:A:79:VAL:HG22	0.85	1.71	16	3
1:A:23:LEU:HD11	1:A:79:VAL:HG22	0.85	1.49	5	2
1:A:13:LEU:N	1:A:13:LEU:HD13	0.85	1.86	16	1
1:A:15:MET:CB	1:A:19:PRO:HG2	0.85	1.98	18	1
1:A:13:LEU:HD23	1:A:13:LEU:H	0.85	1.31	4	3
2:B:286:LEU:HB2	2:B:291:LEU:HD21	0.85	1.47	20	1
2:B:379:LEU:O	2:B:381:ARG:N	0.85	2.10	16	15
2:B:248:LEU:O	2:B:251:ASP:OD2	0.85	1.94	7	7
2:B:357:ALA:O	2:B:361:VAL:HG23	0.85	1.71	10	3
2:B:271:ALA:O	2:B:275:VAL:HG22	0.85	1.72	9	4
1:A:53:LEU:HD11	2:B:286:LEU:HD22	0.85	1.47	8	1
1:A:30:PHE:HB2	1:A:71:GLN:CD	0.84	1.97	3	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.84	1.88	19	3
2:B:279:PHE:O	2:B:283:PHE:CD2	0.84	2.30	17	1
2:B:366:ILE:HG13	2:B:367:PRO:HD2	0.84	1.48	10	2
2:B:322:ARG:O	2:B:323:PHE:CD2	0.84	2.31	6	1
1:A:17:ALA:HB3	1:A:18:ARG:NH1	0.84	1.87	17	1
1:A:62:GLN:C	1:A:63:ILE:HD13	0.84	1.98	20	1
1:A:76:LEU:O	1:A:79:VAL:HG12	0.83	1.73	4	4
2:B:242:PHE:CD1	2:B:242:PHE:C	0.83	2.55	4	4
1:A:34:VAL:O	1:A:35:LEU:HD13	0.83	1.73	19	3
1:A:71:GLN:O	1:A:74:GLU:CG	0.83	2.25	12	1
2:B:279:PHE:O	2:B:283:PHE:CE2	0.83	2.31	17	1
2:B:395:VAL:C	2:B:396:ASP:OD1	0.83	2.22	8	4
2:B:251:ASP:O	2:B:251:ASP:OD1	0.83	1.97	19	2
2:B:207:LEU:O	2:B:211:ARG:HB3	0.82	1.74	8	1
2:B:290:TYR:O	2:B:293:GLU:OE2	0.82	1.97	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:272:VAL:O	2:B:276:ILE:HG23	0.82	1.75	20	6
2:B:249:LEU:HD13	2:B:249:LEU:C	0.82	1.99	17	1
2:B:344:VAL:HG13	2:B:345:GLY:N	0.82	1.88	1	1
2:B:301:LEU:HD12	2:B:301:LEU:O	0.82	1.74	2	4
2:B:290:TYR:O	2:B:293:GLU:CD	0.82	2.22	14	1
2:B:286:LEU:CB	2:B:291:LEU:HD21	0.82	2.02	20	1
2:B:344:VAL:HG13	2:B:345:GLY:H	0.82	1.34	1	1
2:B:216:LEU:C	2:B:216:LEU:HD12	0.82	2.00	5	1
2:B:280:ALA:O	2:B:284:ALA:CB	0.82	2.28	17	5
1:A:56:ASP:OD2	2:B:291:LEU:HD11	0.82	1.74	9	1
1:A:15:MET:CE	1:A:19:PRO:CD	0.82	2.57	20	1
2:B:241:ILE:O	2:B:244:LEU:HG	0.82	1.75	17	1
1:A:36:LEU:N	1:A:36:LEU:HD22	0.81	1.90	10	2
2:B:322:ARG:C	2:B:323:PHE:CD1	0.81	2.59	17	2
2:B:322:ARG:O	2:B:323:PHE:CD1	0.81	2.33	17	10
1:A:21:MET:SD	1:A:21:MET:N	0.81	2.53	10	3
2:B:223:PHE:CD1	2:B:224:ARG:N	0.81	2.49	4	1
2:B:212:LEU:C	2:B:212:LEU:HD13	0.81	2.00	17	2
2:B:338:LEU:HD13	2:B:342:ARG:NH1	0.81	1.90	12	1
2:B:338:LEU:O	2:B:338:LEU:CD2	0.81	2.29	7	1
2:B:338:LEU:C	2:B:338:LEU:CD2	0.81	2.54	7	1
1:A:18:ARG:N	1:A:18:ARG:HE	0.81	1.74	16	3
2:B:350:ASP:O	2:B:351:GLY:O	0.81	1.99	14	4
1:A:9:ILE:HG12	1:A:63:ILE:HD11	0.81	1.53	20	1
1:A:72:GLU:CD	1:A:73:GLU:H	0.80	1.83	1	4
2:B:271:ALA:O	2:B:275:VAL:HG12	0.80	1.76	13	1
2:B:384:LEU:N	2:B:384:LEU:CD1	0.80	2.43	20	1
2:B:385:ILE:N	2:B:385:ILE:HD12	0.80	1.92	1	3
2:B:280:ALA:O	2:B:284:ALA:HB2	0.80	1.77	19	3
1:A:53:LEU:HD12	1:A:53:LEU:O	0.80	1.77	11	1
1:A:20:ALA:CB	1:A:52:LEU:CD2	0.80	2.60	18	1
2:B:275:VAL:HG23	2:B:276:ILE:N	0.80	1.92	16	5
1:A:30:PHE:CD1	1:A:30:PHE:C	0.80	2.60	14	8
1:A:20:ALA:HB1	1:A:52:LEU:HD21	0.80	1.51	18	1
1:A:38:ASN:ND2	1:A:42:THR:H	0.79	1.74	8	1
2:B:393:LEU:N	2:B:393:LEU:CD2	0.79	2.40	8	1
2:B:361:VAL:HA	2:B:364:LEU:HD21	0.79	1.53	16	1
2:B:255:ARG:N	2:B:255:ARG:HE	0.79	1.75	17	1
2:B:257:GLU:OE2	2:B:279:PHE:CE1	0.79	2.35	5	2
2:B:330:LEU:H	2:B:330:LEU:CD2	0.79	1.90	14	2
2:B:253:ARG:O	2:B:256:ARG:HG3	0.79	1.77	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:258:LEU:HD21	2:B:272:VAL:HG23	0.79	1.55	1	1
2:B:241:ILE:CG2	2:B:242:PHE:N	0.79	2.45	10	3
2:B:203:LEU:N	2:B:203:LEU:HD23	0.79	1.93	4	2
1:A:15:MET:CB	1:A:19:PRO:HD2	0.79	2.08	18	1
1:A:77:ALA:O	1:A:80:ILE:HG12	0.79	1.78	9	2
2:B:244:LEU:O	2:B:244:LEU:HD22	0.79	1.76	19	1
2:B:341:ASP:OD1	2:B:342:ARG:N	0.79	2.16	9	4
1:A:14:GLY:O	1:A:19:PRO:HG2	0.79	1.75	18	4
2:B:288:ASP:O	2:B:292:LYS:CB	0.79	2.31	17	6
2:B:244:LEU:C	2:B:244:LEU:CD1	0.79	2.54	19	1
1:A:63:ILE:HD13	1:A:63:ILE:O	0.78	1.77	7	2
2:B:338:LEU:HD13	2:B:338:LEU:H	0.78	1.36	7	1
2:B:379:LEU:HD22	2:B:379:LEU:N	0.78	1.93	5	3
2:B:226:TYR:CE2	2:B:336:ALA:O	0.78	2.37	19	5
1:A:53:LEU:HD23	2:B:291:LEU:HB3	0.78	1.56	8	1
2:B:354:ASN:O	2:B:355:SER:O	0.78	2.01	15	2
2:B:182:ILE:HD13	2:B:182:ILE:N	0.78	1.91	3	2
1:A:15:MET:CB	1:A:19:PRO:CD	0.78	2.61	18	1
1:A:72:GLU:OE1	1:A:73:GLU:N	0.78	2.17	1	6
2:B:185:GLY:O	2:B:380:HIS:O	0.78	2.02	6	19
2:B:286:LEU:HD23	2:B:286:LEU:C	0.77	2.04	11	2
1:A:31:ASP:O	1:A:70:PRO:HD2	0.77	1.78	13	5
1:A:30:PHE:CD1	1:A:74:GLU:OE1	0.77	2.37	12	1
1:A:15:MET:SD	1:A:15:MET:N	0.77	2.58	20	1
2:B:170:ARG:C	2:B:171:ILE:HD12	0.77	2.04	6	2
1:A:13:LEU:HD22	1:A:13:LEU:H	0.77	1.36	16	1
2:B:395:VAL:C	2:B:397:PRO:CD	0.77	2.57	3	12
1:A:53:LEU:C	1:A:53:LEU:CD1	0.77	2.56	8	5
1:A:53:LEU:HD13	2:B:291:LEU:HD13	0.77	1.54	7	1
2:B:258:LEU:HD12	2:B:258:LEU:C	0.77	2.05	18	1
2:B:288:ASP:HB2	2:B:291:LEU:HD22	0.77	1.57	18	1
1:A:10:THR:HG22	1:A:10:THR:O	0.77	1.76	19	1
1:A:53:LEU:HG	2:B:291:LEU:HD22	0.77	1.57	16	1
2:B:303:GLN:HG3	2:B:304:ARG:N	0.77	1.95	14	3
1:A:23:LEU:HD11	1:A:79:VAL:HG23	0.76	1.56	12	1
1:A:63:ILE:HD13	1:A:63:ILE:N	0.76	1.96	20	1
2:B:393:LEU:HD12	2:B:393:LEU:O	0.76	1.79	16	1
2:B:382:ARG:HH22	2:B:396:ASP:CG	0.76	1.89	6	1
2:B:248:LEU:C	2:B:248:LEU:HD23	0.76	2.05	6	4
2:B:338:LEU:N	2:B:338:LEU:HD22	0.76	1.93	8	2
2:B:384:LEU:HD13	2:B:384:LEU:H	0.76	1.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:MET:HA	1:A:30:PHE:CZ	0.76	2.16	3	8
2:B:184:GLU:O	2:B:324:ILE:CG2	0.76	2.33	4	1
2:B:248:LEU:O	2:B:251:ASP:CG	0.76	2.29	20	9
2:B:248:LEU:HD12	2:B:248:LEU:O	0.76	1.79	8	1
2:B:380:HIS:CG	2:B:381:ARG:H	0.76	1.98	16	2
1:A:35:LEU:HD21	1:A:37:ARG:NE	0.76	1.96	13	1
1:A:23:LEU:HD21	1:A:79:VAL:HG22	0.76	1.56	1	1
2:B:275:VAL:HG23	2:B:276:ILE:H	0.76	1.40	6	3
2:B:304:ARG:O	2:B:308:HIS:ND1	0.76	2.19	14	3
2:B:291:LEU:HG	2:B:292:LYS:N	0.76	1.95	19	2
1:A:14:GLY:C	1:A:15:MET:SD	0.76	2.68	20	1
1:A:69:GLY:O	1:A:72:GLU:HG3	0.75	1.81	1	2
2:B:223:PHE:CD1	2:B:223:PHE:C	0.75	2.64	4	2
1:A:5:GLN:C	1:A:5:GLN:NE2	0.75	2.44	6	1
1:A:53:LEU:O	1:A:53:LEU:CD2	0.75	2.25	16	2
1:A:53:LEU:CG	2:B:291:LEU:HD22	0.75	2.11	16	1
2:B:203:LEU:O	2:B:204:ASP:OD1	0.75	2.05	5	6
1:A:72:GLU:N	1:A:72:GLU:OE1	0.75	2.19	11	4
1:A:9:ILE:HG23	1:A:9:ILE:O	0.75	1.81	14	3
2:B:254:LEU:O	2:B:258:LEU:HD12	0.75	1.79	13	2
1:A:34:VAL:O	1:A:35:LEU:HD12	0.75	1.81	20	4
2:B:230:PHE:CE2	2:B:239:ALA:HB2	0.75	2.16	16	1
2:B:288:ASP:O	2:B:292:LYS:N	0.75	2.18	17	6
2:B:384:LEU:HD22	2:B:384:LEU:C	0.75	2.06	20	1
1:A:18:ARG:N	1:A:19:PRO:CD	0.74	2.50	10	17
1:A:18:ARG:N	1:A:19:PRO:HD3	0.74	1.97	6	1
2:B:291:LEU:C	2:B:291:LEU:HD12	0.74	2.07	20	2
1:A:13:LEU:H	1:A:13:LEU:CD2	0.74	1.92	16	4
2:B:216:LEU:O	2:B:220:ALA:N	0.74	2.20	6	18
2:B:241:ILE:CG2	2:B:242:PHE:H	0.74	1.94	10	1
2:B:291:LEU:HD13	2:B:291:LEU:C	0.74	2.07	12	1
1:A:16:HIS:O	1:A:17:ALA:HB2	0.74	1.83	18	5
2:B:332:ALA:N	2:B:357:ALA:HB2	0.74	1.97	18	2
2:B:286:LEU:CD2	2:B:288:ASP:N	0.74	2.50	4	1
2:B:374:ILE:O	2:B:376:PRO:HD3	0.74	1.82	5	4
1:A:5:GLN:CD	1:A:5:GLN:O	0.74	2.30	14	1
2:B:258:LEU:HD13	2:B:258:LEU:C	0.74	2.08	5	1
2:B:379:LEU:O	2:B:380:HIS:C	0.74	2.30	6	16
1:A:80:ILE:O	1:A:84:ASN:OD1	0.74	2.06	11	2
2:B:378:VAL:O	2:B:380:HIS:CD2	0.74	2.40	10	1
2:B:364:LEU:HD11	2:B:366:ILE:CG2	0.74	2.12	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ILE:HD13	1:A:63:ILE:C	0.74	2.08	7	2
2:B:204:ASP:O	2:B:208:GLU:HB3	0.74	1.82	13	1
1:A:16:HIS:O	1:A:17:ALA:CB	0.74	2.36	18	5
2:B:343:LEU:HD11	2:B:345:GLY:O	0.74	1.82	17	1
1:A:15:MET:HE1	1:A:19:PRO:HG3	0.74	1.59	20	1
2:B:288:ASP:CG	2:B:291:LEU:HD23	0.74	2.07	20	1
2:B:352:ALA:O	2:B:353:ALA:HB3	0.74	1.83	15	5
1:A:30:PHE:CD1	1:A:71:GLN:NE2	0.74	2.56	3	1
2:B:301:LEU:O	2:B:301:LEU:HD13	0.74	1.82	6	1
1:A:17:ALA:C	1:A:19:PRO:HD2	0.74	2.07	10	3
2:B:289:ASN:HD22	2:B:290:TYR:N	0.74	1.80	20	1
2:B:233:GLY:O	2:B:234:ALA:C	0.73	2.30	10	8
1:A:19:PRO:O	1:A:23:LEU:HD13	0.73	1.82	17	3
1:A:15:MET:O	1:A:16:HIS:C	0.73	2.30	12	5
1:A:83:PHE:O	1:A:83:PHE:CD1	0.73	2.41	17	3
2:B:204:ASP:O	2:B:208:GLU:HG2	0.73	1.81	7	6
2:B:216:LEU:HG	2:B:217:GLU:N	0.73	1.97	5	1
2:B:330:LEU:HD23	2:B:330:LEU:N	0.73	1.93	14	2
1:A:16:HIS:O	1:A:21:MET:SD	0.73	2.46	15	1
1:A:15:MET:CE	1:A:19:PRO:CG	0.73	2.66	20	1
2:B:208:GLU:OE1	2:B:268:ALA:N	0.73	2.21	20	1
1:A:49:VAL:O	1:A:53:LEU:HD12	0.73	1.82	17	2
2:B:395:VAL:O	2:B:396:ASP:C	0.73	2.30	3	20
2:B:174:LEU:O	2:B:370:MET:SD	0.73	2.47	12	1
2:B:354:ASN:O	2:B:358:ALA:HB3	0.73	1.84	15	2
1:A:36:LEU:C	1:A:37:ARG:HG2	0.72	2.09	1	1
2:B:387:ASP:O	2:B:391:GLY:N	0.72	2.21	19	20
1:A:18:ARG:CB	1:A:19:PRO:HD3	0.72	2.14	2	7
1:A:30:PHE:HE1	1:A:32:ALA:O	0.72	1.67	17	8
1:A:15:MET:SD	1:A:19:PRO:CD	0.72	2.76	20	1
2:B:275:VAL:HG13	2:B:276:ILE:N	0.72	1.99	17	4
1:A:26:LEU:C	1:A:30:PHE:CD2	0.72	2.67	10	8
2:B:301:LEU:C	2:B:301:LEU:HD12	0.72	2.10	16	2
2:B:392:GLU:N	2:B:392:GLU:OE1	0.72	2.22	8	1
2:B:249:LEU:HD23	2:B:250:SER:N	0.72	1.98	19	2
2:B:251:ASP:OD1	2:B:253:ARG:N	0.72	2.23	6	3
1:A:16:HIS:C	1:A:19:PRO:HD2	0.72	2.09	7	1
2:B:301:LEU:HD12	2:B:301:LEU:C	0.72	2.09	17	2
2:B:184:GLU:CB	2:B:323:PHE:CE2	0.72	2.73	4	2
1:A:10:THR:O	1:A:10:THR:OG1	0.72	2.03	14	5
2:B:384:LEU:C	2:B:385:ILE:HD13	0.72	2.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:174:LEU:N	2:B:174:LEU:HD22	0.72	1.99	7	4
1:A:36:LEU:N	1:A:36:LEU:HD12	0.72	1.99	8	3
2:B:247:HIS:O	2:B:251:ASP:HB3	0.71	1.84	4	4
2:B:202:THR:C	2:B:203:LEU:HD13	0.71	2.10	17	2
2:B:249:LEU:HG	2:B:250:SER:N	0.71	1.99	7	2
2:B:290:TYR:O	2:B:293:GLU:OE1	0.71	2.07	14	1
2:B:379:LEU:O	2:B:380:HIS:O	0.71	2.09	11	2
2:B:289:ASN:ND2	2:B:290:TYR:H	0.71	1.82	20	2
2:B:203:LEU:HD23	2:B:203:LEU:N	0.71	1.95	11	2
2:B:204:ASP:OD1	2:B:208:GLU:OE2	0.71	2.07	15	2
1:A:26:LEU:HD12	1:A:30:PHE:CE1	0.71	2.21	7	2
2:B:384:LEU:O	2:B:384:LEU:CD2	0.71	2.38	20	1
2:B:379:LEU:HD22	2:B:379:LEU:H	0.71	1.46	9	2
2:B:203:LEU:HD13	2:B:203:LEU:H	0.71	1.43	8	2
2:B:339:PRO:HB2	2:B:341:ASP:OD1	0.71	1.85	1	3
1:A:69:GLY:O	1:A:72:GLU:HB3	0.71	1.86	9	7
1:A:53:LEU:CD1	1:A:53:LEU:N	0.71	2.54	15	2
2:B:380:HIS:CG	2:B:380:HIS:O	0.71	2.44	7	1
1:A:53:LEU:C	1:A:53:LEU:CD2	0.71	2.60	16	4
2:B:325:LEU:HD13	2:B:325:LEU:C	0.71	2.10	12	3
2:B:249:LEU:HD12	2:B:301:LEU:HD11	0.70	1.63	19	1
2:B:248:LEU:HD23	2:B:248:LEU:C	0.70	2.11	10	2
1:A:13:LEU:N	1:A:13:LEU:CD2	0.70	2.52	1	3
2:B:242:PHE:CD2	2:B:243:ASP:N	0.70	2.58	12	2
2:B:300:ALA:CB	2:B:333:THR:HG21	0.70	2.16	11	2
1:A:5:GLN:OE1	1:A:80:ILE:HD12	0.70	1.86	7	2
1:A:13:LEU:H	1:A:13:LEU:CD1	0.70	1.85	1	2
1:A:9:ILE:HG23	1:A:60:GLY:H	0.70	1.46	14	3
1:A:31:ASP:O	1:A:32:ALA:HB2	0.70	1.86	10	20
2:B:251:ASP:OD1	2:B:254:LEU:N	0.70	2.23	6	3
2:B:299:ARG:HG3	2:B:300:ALA:N	0.70	2.01	6	1
2:B:272:VAL:O	2:B:276:ILE:CG2	0.70	2.40	18	3
2:B:242:PHE:C	2:B:242:PHE:CD1	0.70	2.70	13	1
1:A:75:ALA:O	1:A:79:VAL:HG23	0.70	1.86	1	5
2:B:244:LEU:HD13	2:B:245:TYR:N	0.70	2.00	19	1
2:B:288:ASP:N	2:B:288:ASP:OD1	0.70	2.25	20	1
1:A:76:LEU:C	1:A:76:LEU:HD23	0.70	2.11	15	2
1:A:71:GLN:HG2	1:A:74:GLU:HB2	0.69	1.62	3	1
2:B:258:LEU:HD21	2:B:275:VAL:HG21	0.69	1.64	3	1
2:B:184:GLU:HB2	2:B:323:PHE:CE2	0.69	2.22	4	2
2:B:174:LEU:HD12	2:B:174:LEU:N	0.69	2.02	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:289:ASN:ND2	2:B:290:TYR:N	0.69	2.40	20	2
1:A:83:PHE:CD1	1:A:83:PHE:O	0.69	2.45	19	1
2:B:294:ARG:HH11	2:B:297:ASP:CG	0.69	1.96	2	1
2:B:338:LEU:H	2:B:338:LEU:CD1	0.69	2.00	7	1
2:B:307:PHE:CD1	2:B:307:PHE:C	0.69	2.71	14	1
2:B:335:LEU:C	2:B:335:LEU:HD23	0.69	2.13	17	1
1:A:12:LYS:O	1:A:12:LYS:CD	0.69	2.41	14	3
2:B:222:GLU:O	2:B:226:TYR:CD1	0.69	2.46	17	6
1:A:16:HIS:O	1:A:17:ALA:HB3	0.69	1.88	2	4
2:B:204:ASP:O	2:B:208:GLU:CG	0.69	2.41	10	7
2:B:338:LEU:HB2	2:B:342:ARG:NE	0.69	2.03	12	1
2:B:172:ARG:HE	2:B:172:ARG:N	0.69	1.86	16	1
2:B:330:LEU:HD23	2:B:348:VAL:HG22	0.69	1.64	20	1
1:A:32:ALA:HB1	1:A:68:THR:O	0.69	1.87	13	12
1:A:15:MET:O	1:A:16:HIS:O	0.69	2.11	7	1
1:A:15:MET:C	1:A:17:ALA:N	0.69	2.49	15	1
2:B:288:ASP:O	2:B:292:LYS:HB3	0.69	1.88	2	6
2:B:270:TRP:CZ2	2:B:274:THR:OG1	0.69	2.45	5	1
1:A:5:GLN:C	1:A:5:GLN:HE21	0.68	1.97	6	1
1:A:64:GLU:O	1:A:66:GLU:OE1	0.68	2.11	8	1
1:A:5:GLN:CD	1:A:5:GLN:C	0.68	2.62	14	1
1:A:14:GLY:O	1:A:15:MET:SD	0.68	2.51	16	1
2:B:230:PHE:O	2:B:234:ALA:N	0.68	2.26	17	10
2:B:240:ALA:O	2:B:243:ASP:OD1	0.68	2.11	14	1
1:A:34:VAL:C	1:A:35:LEU:HD12	0.68	2.14	17	3
2:B:244:LEU:C	2:B:244:LEU:CD2	0.68	2.64	5	3
2:B:384:LEU:CD1	2:B:384:LEU:H	0.68	1.99	20	1
1:A:26:LEU:C	1:A:30:PHE:CE2	0.68	2.72	3	8
1:A:10:THR:O	1:A:10:THR:HG22	0.68	1.88	18	2
2:B:378:VAL:O	2:B:380:HIS:ND1	0.68	2.25	16	1
2:B:350:ASP:O	2:B:351:GLY:C	0.68	2.37	1	7
2:B:251:ASP:O	2:B:251:ASP:CG	0.68	2.35	4	2
1:A:16:HIS:O	1:A:18:ARG:N	0.68	2.26	7	4
2:B:394:LEU:N	2:B:394:LEU:CD2	0.68	2.57	7	1
1:A:14:GLY:O	1:A:15:MET:CB	0.68	2.42	3	4
1:A:76:LEU:O	1:A:76:LEU:HD13	0.68	1.89	8	2
2:B:300:ALA:CB	2:B:333:THR:OG1	0.68	2.42	18	4
1:A:18:ARG:N	1:A:18:ARG:NE	0.68	2.41	16	3
1:A:50:ILE:HD12	2:B:283:PHE:CE1	0.68	2.24	18	1
2:B:227:SER:OG	2:B:242:PHE:HB2	0.68	1.88	3	2
2:B:275:VAL:HG13	2:B:276:ILE:H	0.68	1.49	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:344:VAL:CG1	2:B:345:GLY:H	0.68	2.01	1	1
1:A:12:LYS:O	1:A:12:LYS:CG	0.68	2.40	12	5
1:A:13:LEU:N	1:A:13:LEU:HD12	0.68	2.04	9	1
1:A:64:GLU:CD	1:A:64:GLU:O	0.68	2.37	10	1
1:A:76:LEU:HD12	1:A:76:LEU:O	0.68	1.89	10	1
1:A:9:ILE:CG2	1:A:61:ARG:O	0.67	2.36	5	2
2:B:374:ILE:HD13	2:B:374:ILE:N	0.67	2.04	7	1
1:A:71:GLN:O	1:A:74:GLU:CD	0.67	2.37	12	1
1:A:20:ALA:HB1	1:A:52:LEU:CD2	0.67	2.18	18	3
2:B:279:PHE:CD2	2:B:282:GLN:NE2	0.67	2.62	4	3
2:B:275:VAL:CG2	2:B:276:ILE:N	0.67	2.57	16	3
2:B:307:PHE:CD1	2:B:307:PHE:O	0.67	2.48	14	1
2:B:323:PHE:CE2	2:B:342:ARG:NE	0.67	2.62	3	1
2:B:249:LEU:HD13	2:B:249:LEU:O	0.67	1.88	17	1
1:A:70:PRO:O	1:A:73:GLU:OE2	0.67	2.11	15	2
2:B:251:ASP:OD1	2:B:251:ASP:C	0.67	2.36	4	8
1:A:13:LEU:H	1:A:13:LEU:HD22	0.67	1.45	1	1
2:B:344:VAL:CG1	2:B:345:GLY:N	0.67	2.58	1	1
2:B:207:LEU:O	2:B:211:ARG:CB	0.67	2.41	8	5
1:A:11:ASN:O	1:A:11:ASN:ND2	0.67	2.28	18	2
2:B:251:ASP:C	2:B:253:ARG:N	0.67	2.45	11	17
1:A:35:LEU:HD21	1:A:37:ARG:HE	0.67	1.49	13	1
2:B:230:PHE:CD2	2:B:239:ALA:HB2	0.67	2.24	16	1
2:B:384:LEU:O	2:B:384:LEU:HD13	0.67	1.90	20	1
1:A:13:LEU:O	1:A:83:PHE:CD1	0.67	2.48	11	8
2:B:366:ILE:CG2	2:B:367:PRO:HD2	0.67	2.20	4	3
2:B:395:VAL:O	2:B:395:VAL:HG13	0.67	1.89	8	4
2:B:242:PHE:CZ	2:B:336:ALA:HB2	0.67	2.25	20	2
2:B:286:LEU:C	2:B:286:LEU:CD2	0.67	2.67	11	1
1:A:38:ASN:ND2	1:A:54:MET:SD	0.66	2.68	17	2
2:B:272:VAL:O	2:B:276:ILE:CG1	0.66	2.43	18	4
2:B:288:ASP:O	2:B:292:LYS:HB2	0.66	1.90	8	3
1:A:24:PHE:CZ	2:B:247:HIS:CE1	0.66	2.83	10	2
2:B:226:TYR:OH	2:B:336:ALA:O	0.66	2.09	6	1
2:B:272:VAL:O	2:B:276:ILE:HG12	0.66	1.90	16	6
2:B:238:THR:O	2:B:241:ILE:CG1	0.66	2.43	17	3
1:A:63:ILE:HD11	1:A:65:VAL:HG23	0.66	1.64	7	1
2:B:244:LEU:CD1	2:B:245:TYR:N	0.66	2.57	17	1
2:B:352:ALA:O	2:B:353:ALA:CB	0.66	2.43	2	5
1:A:53:LEU:HD12	1:A:54:MET:N	0.66	2.05	7	1
1:A:17:ALA:CB	1:A:18:ARG:HH11	0.66	1.97	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:230:PHE:O	2:B:234:ALA:HB3	0.66	1.89	18	1
2:B:172:ARG:N	2:B:172:ARG:NE	0.66	2.43	2	2
1:A:71:GLN:OE1	1:A:75:ALA:N	0.66	2.28	3	1
2:B:283:PHE:CE2	2:B:298:LEU:CD1	0.66	2.79	3	1
2:B:258:LEU:HD23	2:B:259:PHE:N	0.66	2.05	7	1
1:A:38:ASN:N	1:A:38:ASN:HD22	0.66	1.88	10	2
2:B:223:PHE:CD1	2:B:304:ARG:NH1	0.66	2.63	5	1
2:B:389:TYR:CD1	2:B:389:TYR:C	0.66	2.74	12	1
2:B:352:ALA:HB3	2:B:355:SER:OG	0.66	1.90	18	2
1:A:53:LEU:HD13	1:A:54:MET:CA	0.66	2.21	16	2
1:A:23:LEU:HD22	1:A:34:VAL:HG11	0.66	1.68	10	1
2:B:385:ILE:HG23	2:B:385:ILE:O	0.66	1.89	10	2
2:B:380:HIS:CD2	2:B:381:ARG:N	0.66	2.63	16	1
2:B:284:ALA:O	2:B:286:LEU:O	0.66	2.14	12	5
2:B:249:LEU:HD11	2:B:301:LEU:HD11	0.66	1.68	6	1
2:B:280:ALA:O	2:B:284:ALA:HB3	0.66	1.91	9	5
2:B:211:ARG:NE	2:B:309:LEU:CD1	0.66	2.58	14	1
2:B:286:LEU:HD22	2:B:288:ASP:O	0.66	1.90	4	1
1:A:47:ASN:C	1:A:47:ASN:HD22	0.66	1.98	8	1
2:B:283:PHE:O	2:B:291:LEU:HD11	0.66	1.91	12	2
2:B:227:SER:CB	2:B:242:PHE:CB	0.65	2.73	4	5
1:A:80:ILE:C	1:A:80:ILE:HD12	0.65	2.15	3	1
1:A:13:LEU:HD13	1:A:13:LEU:O	0.65	1.91	8	1
1:A:16:HIS:C	1:A:18:ARG:H	0.65	1.99	8	4
2:B:337:GLU:C	2:B:338:LEU:HD22	0.65	2.17	8	2
2:B:385:ILE:HG22	2:B:385:ILE:O	0.65	1.92	2	1
1:A:13:LEU:HD23	1:A:13:LEU:C	0.65	2.16	5	1
2:B:230:PHE:CD2	2:B:238:THR:HG21	0.65	2.26	11	3
2:B:304:ARG:O	2:B:308:HIS:CD2	0.65	2.49	2	7
2:B:186:TRP:CD1	2:B:186:TRP:C	0.65	2.74	16	2
2:B:182:ILE:N	2:B:182:ILE:CD1	0.65	2.60	3	2
1:A:9:ILE:CG2	1:A:58:ALA:O	0.65	2.39	14	3
1:A:23:LEU:HD21	1:A:79:VAL:HG12	0.65	1.68	8	1
2:B:338:LEU:N	2:B:338:LEU:CD2	0.65	2.60	8	2
2:B:227:SER:HB3	2:B:242:PHE:CD2	0.65	2.26	9	1
2:B:384:LEU:HD13	2:B:385:ILE:N	0.65	2.06	14	2
2:B:204:ASP:N	2:B:205:PRO:HD3	0.65	2.07	2	5
2:B:277:GLU:O	2:B:281:GLU:OE1	0.65	2.15	15	8
2:B:227:SER:CB	2:B:242:PHE:HB2	0.65	2.22	4	4
1:A:24:PHE:O	1:A:28:GLN:OE1	0.65	2.14	13	2
1:A:9:ILE:CG1	1:A:63:ILE:HD11	0.65	2.21	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:278:LYS:O	2:B:281:GLU:CD	0.65	2.39	20	1
2:B:353:ALA:HB1	2:B:362:ARG:NH1	0.65	2.07	12	2
1:A:16:HIS:NE2	2:B:290:TYR:CE2	0.65	2.64	9	2
2:B:254:LEU:O	2:B:254:LEU:HD23	0.65	1.90	18	1
2:B:207:LEU:O	2:B:211:ARG:HB2	0.65	1.91	19	5
2:B:301:LEU:HG	2:B:302:GLY:N	0.65	2.07	5	4
2:B:375:GLN:O	2:B:378:VAL:HG22	0.65	1.92	16	2
2:B:273:LYS:O	2:B:277:GLU:HB2	0.65	1.92	6	3
2:B:338:LEU:CD1	2:B:338:LEU:N	0.65	2.60	7	1
1:A:38:ASN:HD21	1:A:58:ALA:HB2	0.65	1.51	3	1
1:A:4:LYS:N	1:A:4:LYS:CD	0.65	2.60	15	1
2:B:288:ASP:O	2:B:291:LEU:HD23	0.65	1.92	19	1
1:A:18:ARG:CB	1:A:19:PRO:CD	0.64	2.75	2	5
2:B:283:PHE:N	2:B:283:PHE:CD2	0.64	2.62	8	2
2:B:227:SER:OG	2:B:242:PHE:HB3	0.64	1.92	5	1
1:A:15:MET:O	1:A:19:PRO:HD2	0.64	1.91	15	1
1:A:13:LEU:HD12	1:A:13:LEU:O	0.64	1.91	17	1
1:A:20:ALA:HB1	1:A:52:LEU:HD11	0.64	1.67	18	1
2:B:392:GLU:C	2:B:393:LEU:HD23	0.64	2.16	1	2
2:B:241:ILE:HG13	2:B:242:PHE:H	0.64	1.51	12	3
1:A:21:MET:C	1:A:21:MET:SD	0.64	2.80	4	5
2:B:211:ARG:NH2	2:B:269:GLU:OE2	0.64	2.30	6	3
1:A:8:GLU:O	1:A:8:GLU:CD	0.64	2.40	17	1
2:B:301:LEU:C	2:B:301:LEU:CD1	0.64	2.71	17	5
2:B:283:PHE:CD1	2:B:283:PHE:N	0.64	2.60	18	4
2:B:215:ALA:HB1	2:B:309:LEU:HD22	0.64	1.69	12	1
2:B:211:ARG:NH1	2:B:269:GLU:OE2	0.64	2.30	7	3
2:B:249:LEU:HD12	2:B:250:SER:N	0.64	2.06	1	1
2:B:326:VAL:HG13	2:B:326:VAL:O	0.64	1.92	20	3
2:B:375:GLN:CD	2:B:375:GLN:H	0.64	2.00	3	7
2:B:275:VAL:CG2	2:B:276:ILE:H	0.64	2.06	6	2
2:B:174:LEU:N	2:B:174:LEU:CD2	0.64	2.59	7	4
2:B:259:PHE:O	2:B:262:VAL:HG22	0.64	1.93	2	3
2:B:366:ILE:HG23	2:B:367:PRO:HD2	0.64	1.70	4	4
2:B:349:ARG:HH11	2:B:374:ILE:N	0.64	1.90	5	1
1:A:53:LEU:HB2	2:B:291:LEU:CD1	0.64	2.21	16	1
1:A:16:HIS:O	1:A:16:HIS:ND1	0.64	2.31	3	1
1:A:49:VAL:O	1:A:53:LEU:HD13	0.64	1.93	5	3
2:B:259:PHE:CD1	2:B:259:PHE:N	0.64	2.64	11	1
2:B:286:LEU:N	2:B:286:LEU:HD12	0.64	2.06	5	1
1:A:17:ALA:O	1:A:18:ARG:HB2	0.64	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:227:SER:CB	2:B:242:PHE:CG	0.64	2.81	12	1
2:B:340:GLN:CD	2:B:340:GLN:O	0.64	2.41	14	1
2:B:248:LEU:C	2:B:248:LEU:CD1	0.63	2.66	3	4
1:A:1:MET:SD	1:A:1:MET:N	0.63	2.70	9	3
2:B:396:ASP:CG	2:B:396:ASP:O	0.63	2.42	6	1
2:B:338:LEU:CD2	2:B:339:PRO:O	0.63	2.46	7	1
1:A:38:ASN:ND2	1:A:38:ASN:C	0.63	2.54	8	1
1:A:72:GLU:C	1:A:72:GLU:OE1	0.63	2.41	8	3
2:B:306:LEU:O	2:B:310:ASP:OD2	0.63	2.15	11	1
1:A:35:LEU:N	1:A:35:LEU:CD2	0.63	2.61	19	3
2:B:238:THR:O	2:B:241:ILE:HG12	0.63	1.94	17	3
2:B:384:LEU:N	2:B:384:LEU:HD13	0.63	2.01	20	1
2:B:248:LEU:HD12	2:B:248:LEU:C	0.63	2.18	8	2
2:B:205:PRO:O	2:B:209:ARG:N	0.63	2.31	10	5
2:B:243:ASP:OD1	2:B:244:LEU:N	0.63	2.31	14	1
1:A:13:LEU:CD1	1:A:19:PRO:HG2	0.63	2.23	14	1
2:B:245:TYR:OH	2:B:297:ASP:CG	0.63	2.41	11	3
2:B:267:VAL:O	2:B:271:ALA:CB	0.63	2.46	5	2
1:A:21:MET:HG3	1:A:22:LYS:N	0.63	2.07	4	1
2:B:244:LEU:HD23	2:B:245:TYR:N	0.63	2.09	5	1
1:A:13:LEU:CD1	1:A:13:LEU:H	0.63	2.06	9	1
2:B:380:HIS:CG	2:B:381:ARG:N	0.63	2.63	16	1
1:A:15:MET:HG2	1:A:16:HIS:N	0.63	2.07	20	1
1:A:30:PHE:CE1	1:A:32:ALA:O	0.63	2.51	17	8
1:A:23:LEU:HD22	1:A:34:VAL:HG21	0.63	1.69	20	1
2:B:223:PHE:CZ	2:B:304:ARG:NH1	0.63	2.67	3	2
2:B:325:LEU:C	2:B:325:LEU:HD23	0.63	2.19	8	1
2:B:183:ALA:O	2:B:384:LEU:CD1	0.63	2.47	20	1
1:A:63:ILE:HG13	1:A:64:GLU:N	0.63	2.08	13	3
1:A:5:GLN:NE2	1:A:5:GLN:O	0.63	2.31	6	1
1:A:47:ASN:CG	1:A:47:ASN:O	0.63	2.42	20	2
2:B:288:ASP:CB	2:B:291:LEU:HD23	0.63	2.24	20	1
1:A:84:ASN:O	1:A:85:SER:HB2	0.62	1.94	6	4
2:B:301:LEU:HD13	2:B:301:LEU:C	0.62	2.19	6	1
1:A:56:ASP:OD1	2:B:288:ASP:OD2	0.62	2.16	9	1
2:B:172:ARG:N	2:B:172:ARG:HE	0.62	1.90	2	1
1:A:30:PHE:CB	1:A:71:GLN:CD	0.62	2.72	3	1
1:A:3:VAL:O	1:A:3:VAL:CG1	0.62	2.47	10	3
2:B:204:ASP:N	2:B:205:PRO:CD	0.62	2.63	2	5
2:B:361:VAL:CG1	2:B:362:ARG:N	0.62	2.62	6	3
2:B:223:PHE:CG	2:B:224:ARG:N	0.62	2.67	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:382:ARG:NH2	2:B:396:ASP:CG	0.62	2.56	6	1
2:B:203:LEU:H	2:B:203:LEU:CD2	0.62	2.01	8	4
2:B:291:LEU:C	2:B:291:LEU:HD22	0.62	2.18	12	1
2:B:252:THR:OG1	2:B:253:ARG:NH1	0.62	2.30	16	1
1:A:38:ASN:N	1:A:38:ASN:OD1	0.62	2.30	18	1
1:A:77:ALA:HA	1:A:80:ILE:HG12	0.62	1.70	4	1
2:B:286:LEU:N	2:B:286:LEU:CD1	0.62	2.63	5	1
2:B:353:ALA:HB1	2:B:362:ARG:HH12	0.62	1.54	6	1
1:A:63:ILE:C	1:A:63:ILE:CD1	0.62	2.70	7	2
2:B:392:GLU:O	2:B:393:LEU:HD13	0.62	1.93	8	1
1:A:18:ARG:HB2	1:A:19:PRO:HD3	0.62	1.71	11	4
2:B:242:PHE:O	2:B:245:TYR:N	0.62	2.32	10	10
1:A:13:LEU:N	1:A:13:LEU:HD23	0.62	2.10	7	1
2:B:222:GLU:HG3	2:B:226:TYR:CE1	0.62	2.30	12	1
1:A:9:ILE:O	1:A:9:ILE:CG2	0.62	2.48	14	3
2:B:279:PHE:CD2	2:B:280:ALA:N	0.62	2.68	18	1
2:B:291:LEU:O	2:B:294:ARG:N	0.62	2.32	14	10
2:B:349:ARG:NE	2:B:372:ALA:O	0.62	2.32	10	2
2:B:226:TYR:CE1	2:B:304:ARG:NH1	0.62	2.68	11	1
1:A:24:PHE:CZ	1:A:46:ALA:O	0.62	2.52	15	4
2:B:247:HIS:ND1	2:B:247:HIS:C	0.62	2.55	10	3
2:B:375:GLN:CD	2:B:375:GLN:N	0.62	2.58	10	9
2:B:231:ALA:CB	2:B:239:ALA:HB2	0.62	2.25	12	2
1:A:13:LEU:HD23	1:A:13:LEU:N	0.62	2.06	4	1
1:A:24:PHE:CE1	1:A:46:ALA:O	0.62	2.52	15	2
1:A:53:LEU:CB	2:B:291:LEU:HD13	0.62	2.23	16	1
1:A:13:LEU:HD12	1:A:13:LEU:C	0.62	2.20	17	1
2:B:203:LEU:H	2:B:203:LEU:HD12	0.61	1.55	1	1
1:A:71:GLN:HG2	1:A:74:GLU:CB	0.61	2.24	3	1
2:B:227:SER:OG	2:B:242:PHE:CB	0.61	2.48	5	3
1:A:20:ALA:CB	1:A:52:LEU:HD11	0.61	2.25	14	5
2:B:203:LEU:HD12	2:B:265:GLY:O	0.61	1.95	17	1
1:A:77:ALA:HA	1:A:80:ILE:CG1	0.61	2.25	4	1
2:B:225:ARG:O	2:B:229:ARG:HG2	0.61	1.94	7	1
1:A:38:ASN:N	1:A:38:ASN:ND2	0.61	2.46	10	2
1:A:49:VAL:O	1:A:53:LEU:HG	0.61	1.95	12	2
1:A:71:GLN:CB	1:A:74:GLU:CG	0.61	2.78	12	1
2:B:301:LEU:C	2:B:301:LEU:HD23	0.61	2.20	18	2
2:B:230:PHE:O	2:B:234:ALA:CB	0.61	2.48	18	1
1:A:33:GLU:OE1	1:A:35:LEU:HD13	0.61	1.95	3	1
2:B:222:GLU:OE2	2:B:226:TYR:CD2	0.61	2.52	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:300:ALA:HB1	2:B:333:THR:HG21	0.61	1.71	17	2
2:B:306:LEU:O	2:B:310:ASP:OD1	0.61	2.17	6	4
2:B:366:ILE:HG13	2:B:367:PRO:CD	0.61	2.23	10	2
2:B:215:ALA:CB	2:B:309:LEU:HD22	0.61	2.25	20	3
2:B:330:LEU:HD13	2:B:348:VAL:HG22	0.61	1.72	2	1
2:B:383:THR:O	2:B:384:LEU:HD12	0.61	1.94	5	1
2:B:211:ARG:NH2	2:B:269:GLU:CD	0.61	2.59	6	1
1:A:35:LEU:C	1:A:36:LEU:HD23	0.61	2.19	2	2
2:B:286:LEU:HD13	2:B:292:LYS:N	0.61	2.10	4	1
2:B:283:PHE:CD2	2:B:283:PHE:N	0.61	2.64	6	1
2:B:289:ASN:CG	2:B:290:TYR:N	0.61	2.58	12	3
2:B:249:LEU:C	2:B:249:LEU:CD1	0.61	2.72	17	1
2:B:203:LEU:HD23	2:B:203:LEU:O	0.61	1.95	18	1
2:B:286:LEU:CD2	2:B:288:ASP:H	0.61	2.08	4	1
2:B:223:PHE:CD1	2:B:246:SER:OG	0.61	2.47	7	1
2:B:374:ILE:HD13	2:B:374:ILE:O	0.61	1.96	17	1
1:A:36:LEU:N	1:A:36:LEU:CD2	0.61	2.63	10	4
1:A:36:LEU:CD2	1:A:46:ALA:HB2	0.61	2.26	3	2
2:B:222:GLU:OE2	2:B:226:TYR:CD1	0.61	2.54	13	2
1:A:38:ASN:ND2	1:A:41:GLY:N	0.61	2.48	8	1
1:A:27:MET:CE	1:A:32:ALA:O	0.61	2.48	15	1
2:B:335:LEU:C	2:B:337:GLU:H	0.61	2.03	3	12
1:A:53:LEU:HD23	2:B:291:LEU:CB	0.61	2.24	8	1
2:B:291:LEU:C	2:B:291:LEU:CD1	0.61	2.72	20	3
2:B:384:LEU:HD13	2:B:384:LEU:C	0.61	2.21	14	1
2:B:273:LYS:O	2:B:276:ILE:HG13	0.61	1.95	20	1
2:B:205:PRO:O	2:B:209:ARG:CB	0.61	2.49	14	8
2:B:269:GLU:CD	2:B:269:GLU:H	0.61	2.04	9	3
2:B:275:VAL:CG1	2:B:276:ILE:N	0.61	2.63	17	4
2:B:385:ILE:HG23	2:B:394:LEU:HB2	0.61	1.72	5	1
2:B:251:ASP:OD1	2:B:253:ARG:CB	0.61	2.48	6	1
1:A:71:GLN:O	1:A:74:GLU:OE2	0.61	2.19	12	1
2:B:309:LEU:HD12	2:B:309:LEU:O	0.61	1.94	14	1
2:B:283:PHE:C	2:B:283:PHE:CD1	0.61	2.79	19	1
2:B:183:ALA:O	2:B:384:LEU:HD13	0.61	1.96	20	1
2:B:203:LEU:HD13	2:B:265:GLY:HA2	0.61	1.71	4	1
2:B:253:ARG:HE	2:B:254:LEU:N	0.61	1.94	5	2
2:B:274:THR:O	2:B:278:LYS:N	0.61	2.31	11	3
1:A:62:GLN:NE2	1:A:63:ILE:O	0.61	2.34	16	1
2:B:226:TYR:CD2	2:B:336:ALA:O	0.60	2.54	13	2
2:B:227:SER:HB3	2:B:242:PHE:HB2	0.60	1.72	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PHE:CE2	2:B:247:HIS:NE2	0.60	2.68	16	3
2:B:258:LEU:C	2:B:258:LEU:CD1	0.60	2.72	18	2
1:A:56:ASP:CG	2:B:288:ASP:OD2	0.60	2.44	9	2
2:B:173:ALA:CB	2:B:370:MET:O	0.60	2.46	18	2
2:B:331:SER:OG	2:B:334:THR:OG1	0.60	2.18	17	1
2:B:325:LEU:HD13	2:B:326:VAL:N	0.60	2.11	11	4
1:A:83:PHE:CD1	1:A:83:PHE:C	0.60	2.77	17	4
2:B:271:ALA:O	2:B:275:VAL:HG13	0.60	1.95	6	1
2:B:244:LEU:HD23	2:B:294:ARG:NH2	0.60	2.11	7	1
2:B:288:ASP:HB3	2:B:291:LEU:HD21	0.60	1.73	7	1
1:A:3:VAL:HG21	1:A:72:GLU:OE2	0.60	1.96	12	3
2:B:213:THR:CG2	2:B:214:GLY:N	0.60	2.63	9	2
1:A:7:VAL:HG23	1:A:83:PHE:CZ	0.60	2.31	15	2
2:B:219:ALA:O	2:B:222:GLU:HG3	0.60	1.96	15	1
2:B:258:LEU:HG	2:B:259:PHE:N	0.60	2.11	18	1
1:A:53:LEU:HG	2:B:291:LEU:HD12	0.60	1.73	3	1
1:A:71:GLN:HE22	1:A:75:ALA:HB2	0.60	1.56	3	1
2:B:241:ILE:HG22	2:B:242:PHE:N	0.60	2.11	9	7
2:B:279:PHE:CD1	2:B:279:PHE:C	0.60	2.79	20	1
1:A:31:ASP:O	1:A:32:ALA:CB	0.60	2.49	10	16
1:A:13:LEU:HD23	1:A:13:LEU:O	0.60	1.96	5	1
2:B:286:LEU:HD23	2:B:292:LYS:N	0.60	2.11	10	1
1:A:35:LEU:O	1:A:66:GLU:OE1	0.60	2.20	11	1
1:A:23:LEU:HD12	1:A:34:VAL:HG11	0.60	1.73	8	2
2:B:286:LEU:CD1	2:B:288:ASP:OD2	0.60	2.49	3	1
2:B:221:ASN:O	2:B:225:ARG:NE	0.60	2.34	6	1
2:B:224:ARG:NE	2:B:246:SER:OG	0.60	2.34	13	1
1:A:36:LEU:HD23	1:A:36:LEU:N	0.60	2.12	2	2
1:A:53:LEU:CD1	2:B:283:PHE:O	0.60	2.50	9	1
1:A:27:MET:HA	1:A:30:PHE:CE2	0.60	2.32	10	7
2:B:338:LEU:CD1	2:B:342:ARG:NH1	0.60	2.64	12	1
2:B:184:GLU:O	2:B:324:ILE:HG12	0.60	1.97	6	2
2:B:213:THR:O	2:B:217:GLU:OE1	0.60	2.19	12	2
2:B:290:TYR:OH	2:B:294:ARG:NH1	0.60	2.35	19	2
1:A:49:VAL:HG13	2:B:248:LEU:HD21	0.60	1.72	11	1
2:B:358:ALA:HB1	2:B:362:ARG:HH11	0.60	1.57	18	1
2:B:179:GLY:O	2:B:388:GLY:N	0.60	2.35	1	8
2:B:327:ALA:O	2:B:348:VAL:HA	0.60	1.97	1	5
2:B:172:ARG:HE	2:B:172:ARG:CA	0.60	2.08	2	2
1:A:54:MET:O	1:A:54:MET:SD	0.60	2.59	7	2
2:B:226:TYR:CD1	2:B:304:ARG:NH1	0.60	2.70	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:286:LEU:CB	2:B:291:LEU:CD2	0.60	2.80	20	1
2:B:231:ALA:HB2	2:B:239:ALA:HB2	0.59	1.72	12	4
2:B:257:GLU:OE2	2:B:279:PHE:CZ	0.59	2.55	8	4
2:B:385:ILE:HG13	2:B:385:ILE:O	0.59	1.95	11	1
1:A:36:LEU:CD1	1:A:46:ALA:HB2	0.59	2.27	8	5
2:B:174:LEU:N	2:B:370:MET:O	0.59	2.35	6	11
2:B:216:LEU:HD12	2:B:216:LEU:O	0.59	1.97	5	1
2:B:216:LEU:CG	2:B:217:GLU:N	0.59	2.65	5	1
2:B:278:LYS:O	2:B:281:GLU:OE2	0.59	2.20	20	1
1:A:2:THR:HG23	1:A:68:THR:HG23	0.59	1.74	4	1
2:B:328:ASP:OD1	2:B:328:ASP:N	0.59	2.36	7	2
1:A:28:GLN:N	1:A:28:GLN:HE21	0.59	1.95	1	1
1:A:37:ARG:HH11	1:A:66:GLU:CD	0.59	2.06	5	1
1:A:15:MET:SD	1:A:18:ARG:HD2	0.59	2.38	7	1
2:B:218:GLU:O	2:B:222:GLU:CB	0.59	2.51	2	2
1:A:2:THR:CG2	1:A:68:THR:OG1	0.59	2.51	4	1
1:A:13:LEU:O	1:A:83:PHE:CD2	0.59	2.55	16	2
2:B:284:ALA:HB2	2:B:295:ALA:CB	0.59	2.28	8	1
2:B:322:ARG:O	2:B:323:PHE:HD1	0.59	1.79	8	1
2:B:366:ILE:CG1	2:B:367:PRO:HD2	0.59	2.24	10	2
2:B:208:GLU:CD	2:B:268:ALA:H	0.59	2.05	20	1
2:B:241:ILE:HG13	2:B:242:PHE:N	0.59	2.13	15	3
1:A:3:VAL:HG13	1:A:3:VAL:O	0.59	1.98	14	2
1:A:36:LEU:HD21	1:A:46:ALA:HB2	0.59	1.74	3	2
1:A:6:THR:OG1	1:A:62:GLN:NE2	0.59	2.36	13	2
2:B:304:ARG:NH2	2:B:337:GLU:OE1	0.59	2.36	17	1
2:B:284:ALA:O	2:B:286:LEU:N	0.59	2.35	13	5
2:B:378:VAL:HG12	2:B:378:VAL:O	0.59	1.97	15	3
2:B:211:ARG:NH2	2:B:269:GLU:OE1	0.59	2.36	6	3
2:B:237:GLU:OE1	2:B:238:THR:N	0.59	2.36	6	1
2:B:256:ARG:NH1	2:B:259:PHE:CD2	0.59	2.71	10	1
2:B:255:ARG:N	2:B:255:ARG:NE	0.59	2.51	17	1
1:A:5:GLN:NE2	1:A:6:THR:O	0.59	2.35	2	2
2:B:273:LYS:O	2:B:277:GLU:CG	0.59	2.51	13	1
1:A:62:GLN:NE2	1:A:64:GLU:OE1	0.59	2.35	20	1
2:B:385:ILE:HD12	2:B:385:ILE:H	0.58	1.57	1	1
2:B:383:THR:HG22	2:B:385:ILE:CD1	0.58	2.28	2	1
2:B:223:PHE:O	2:B:227:SER:OG	0.58	2.21	3	1
1:A:24:PHE:N	1:A:24:PHE:CD2	0.58	2.68	7	1
2:B:250:SER:O	2:B:255:ARG:NH2	0.58	2.36	9	1
2:B:369:VAL:O	2:B:370:MET:SD	0.58	2.61	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:184:GLU:H	2:B:184:GLU:CD	0.58	2.06	15	1
2:B:384:LEU:HD12	2:B:394:LEU:O	0.58	1.98	18	2
1:A:36:LEU:HD12	1:A:65:VAL:HG22	0.58	1.75	3	1
2:B:235:GLN:O	2:B:238:THR:OG1	0.58	2.21	7	4
2:B:270:TRP:CE2	2:B:274:THR:OG1	0.58	2.56	5	1
2:B:212:LEU:HG	2:B:213:THR:N	0.58	2.13	18	1
1:A:77:ALA:O	1:A:80:ILE:CG1	0.58	2.48	4	1
2:B:286:LEU:CD2	2:B:286:LEU:C	0.58	2.76	4	1
1:A:37:ARG:O	1:A:63:ILE:CG2	0.58	2.46	5	1
2:B:328:ASP:OD1	2:B:329:GLU:N	0.58	2.37	12	6
2:B:271:ALA:O	2:B:275:VAL:HG23	0.58	1.99	2	5
2:B:344:VAL:HG12	2:B:344:VAL:O	0.58	1.97	13	6
2:B:184:GLU:O	2:B:324:ILE:CG1	0.58	2.51	6	2
2:B:249:LEU:HD23	2:B:249:LEU:C	0.58	2.24	19	1
2:B:237:GLU:CG	2:B:238:THR:N	0.58	2.65	17	1
1:A:15:MET:CE	1:A:19:PRO:HG3	0.58	2.24	20	1
1:A:8:GLU:CD	1:A:8:GLU:H	0.58	2.06	1	2
2:B:291:LEU:CG	2:B:292:LYS:N	0.58	2.65	19	4
2:B:375:GLN:H	2:B:375:GLN:CD	0.58	2.06	6	2
2:B:222:GLU:O	2:B:226:TYR:HB2	0.58	1.99	12	3
2:B:259:PHE:CD2	2:B:259:PHE:N	0.58	2.69	13	3
2:B:364:LEU:HD11	2:B:366:ILE:HG22	0.58	1.75	16	1
2:B:247:HIS:C	2:B:247:HIS:ND1	0.58	2.60	19	1
2:B:396:ASP:OD1	2:B:396:ASP:N	0.58	2.34	12	3
1:A:71:GLN:OE1	1:A:74:GLU:HB3	0.58	1.98	3	1
1:A:18:ARG:O	1:A:22:LYS:CG	0.58	2.52	7	1
2:B:281:GLU:O	2:B:285:ALA:HB2	0.58	1.99	16	3
1:A:38:ASN:ND2	1:A:40:GLU:N	0.58	2.52	8	1
2:B:351:GLY:C	2:B:352:ALA:O	0.58	2.47	9	2
2:B:253:ARG:C	2:B:253:ARG:HE	0.58	2.06	18	1
2:B:222:GLU:OE2	2:B:304:ARG:NH1	0.58	2.37	2	10
2:B:283:PHE:CD2	2:B:284:ALA:N	0.58	2.72	7	2
1:A:16:HIS:C	1:A:18:ARG:N	0.58	2.62	8	2
2:B:235:GLN:NE2	2:B:238:THR:HG23	0.58	2.13	10	1
2:B:291:LEU:HD22	2:B:291:LEU:O	0.58	1.99	12	1
1:A:62:GLN:CD	1:A:63:ILE:N	0.58	2.61	16	1
2:B:393:LEU:O	2:B:393:LEU:CD1	0.58	2.52	16	1
1:A:19:PRO:O	1:A:23:LEU:HD23	0.58	1.99	13	3
2:B:251:ASP:OD1	2:B:253:ARG:CA	0.58	2.52	6	1
1:A:20:ALA:HB2	1:A:52:LEU:HD11	0.58	1.75	14	5
2:B:290:TYR:C	2:B:293:GLU:CD	0.58	2.72	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:249:LEU:O	2:B:255:ARG:NH2	0.58	2.37	16	1
2:B:209:ARG:CG	2:B:210:GLU:N	0.58	2.67	12	2
1:A:53:LEU:CD1	1:A:54:MET:N	0.58	2.52	16	2
2:B:290:TYR:CD2	2:B:291:LEU:CD2	0.58	2.86	8	1
2:B:223:PHE:CE2	2:B:242:PHE:CE2	0.58	2.92	9	1
2:B:373:ASP:C	2:B:374:ILE:HD13	0.57	2.24	7	1
1:A:53:LEU:HD23	1:A:53:LEU:C	0.57	2.24	9	2
2:B:268:ALA:O	2:B:272:VAL:HG22	0.57	1.99	3	6
2:B:290:TYR:C	2:B:291:LEU:HD12	0.57	2.24	2	1
1:A:13:LEU:HD12	1:A:13:LEU:H	0.57	1.56	9	1
2:B:292:LYS:CD	2:B:292:LYS:C	0.57	2.77	2	1
1:A:28:GLN:N	1:A:28:GLN:OE1	0.57	2.36	3	1
1:A:63:ILE:CG2	1:A:64:GLU:N	0.57	2.67	19	3
2:B:204:ASP:HB2	2:B:208:GLU:HG2	0.57	1.75	8	2
1:A:24:PHE:O	1:A:28:GLN:CD	0.57	2.47	13	1
1:A:43:GLU:CD	1:A:43:GLU:N	0.57	2.63	1	3
2:B:384:LEU:O	2:B:385:ILE:HD13	0.57	1.99	7	1
2:B:291:LEU:CD1	2:B:292:LYS:N	0.57	2.65	12	2
2:B:222:GLU:CD	2:B:304:ARG:HH11	0.57	2.07	7	3
2:B:384:LEU:C	2:B:384:LEU:CD1	0.57	2.78	14	1
1:A:47:ASN:O	1:A:47:ASN:CG	0.57	2.47	17	1
2:B:292:LYS:HG3	2:B:293:GLU:N	0.57	2.13	2	2
2:B:375:GLN:N	2:B:375:GLN:OE1	0.57	2.38	4	3
2:B:217:GLU:O	2:B:221:ASN:ND2	0.57	2.38	12	11
1:A:26:LEU:HD22	1:A:30:PHE:CE1	0.57	2.34	11	4
2:B:364:LEU:HD12	2:B:365:GLY:N	0.57	2.14	16	1
2:B:286:LEU:CB	2:B:291:LEU:HD22	0.57	2.30	19	1
2:B:330:LEU:HD13	2:B:348:VAL:CG2	0.57	2.29	2	1
2:B:273:LYS:CD	2:B:273:LYS:C	0.57	2.78	7	2
1:A:24:PHE:CZ	2:B:247:HIS:NE2	0.57	2.73	16	3
2:B:385:ILE:C	2:B:385:ILE:HD12	0.57	2.24	11	1
2:B:227:SER:OG	2:B:242:PHE:CD1	0.57	2.57	12	1
2:B:288:ASP:O	2:B:291:LEU:CD2	0.57	2.53	19	1
2:B:330:LEU:HD23	2:B:348:VAL:CG2	0.57	2.29	20	1
2:B:248:LEU:HD13	2:B:249:LEU:N	0.57	2.14	3	2
2:B:253:ARG:C	2:B:253:ARG:NE	0.57	2.63	18	2
1:A:56:ASP:OD2	2:B:291:LEU:HD22	0.57	2.00	11	1
2:B:288:ASP:HB2	2:B:291:LEU:HD23	0.57	1.76	20	1
1:A:13:LEU:N	1:A:13:LEU:CD1	0.57	2.67	9	3
2:B:396:ASP:N	2:B:397:PRO:CD	0.57	2.68	20	13
1:A:2:THR:HG23	1:A:68:THR:CG2	0.57	2.29	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:376:PRO:HA	2:B:379:LEU:HD23	0.57	1.76	5	1
1:A:14:GLY:O	1:A:15:MET:C	0.57	2.47	6	2
1:A:16:HIS:NE2	2:B:290:TYR:CD2	0.57	2.72	9	1
2:B:184:GLU:CD	2:B:184:GLU:N	0.57	2.61	14	3
1:A:77:ALA:C	1:A:80:ILE:HG13	0.56	2.24	4	1
2:B:176:ALA:O	2:B:362:ARG:NH2	0.56	2.38	11	2
2:B:379:LEU:HD13	2:B:384:LEU:HD22	0.56	1.75	6	1
2:B:245:TYR:O	2:B:248:LEU:N	0.56	2.34	7	4
2:B:258:LEU:HD11	2:B:275:VAL:HG21	0.56	1.76	9	1
1:A:43:GLU:H	1:A:43:GLU:CD	0.56	2.07	13	1
2:B:246:SER:O	2:B:249:LEU:HD23	0.56	2.00	15	1
2:B:289:ASN:CG	2:B:290:TYR:H	0.56	2.08	12	1
1:A:18:ARG:HE	1:A:18:ARG:H	0.56	1.42	16	1
2:B:208:GLU:CD	2:B:208:GLU:N	0.56	2.63	2	1
2:B:202:THR:O	2:B:204:ASP:OD2	0.56	2.24	5	1
2:B:251:ASP:OD2	2:B:253:ARG:HB2	0.56	2.00	6	1
2:B:374:ILE:N	2:B:374:ILE:CD1	0.56	2.67	7	1
1:A:53:LEU:HD11	2:B:286:LEU:HG	0.56	1.76	16	1
1:A:12:LYS:O	1:A:12:LYS:HD3	0.56	2.00	14	1
2:B:293:GLU:OE1	2:B:294:ARG:N	0.56	2.34	14	1
1:A:53:LEU:N	1:A:53:LEU:HD13	0.56	2.15	15	1
2:B:230:PHE:CE2	2:B:238:THR:HG21	0.56	2.36	19	1
1:A:8:GLU:N	1:A:8:GLU:CD	0.56	2.64	4	1
1:A:72:GLU:OE1	1:A:72:GLU:C	0.56	2.49	13	1
2:B:364:LEU:CD1	2:B:366:ILE:HB	0.56	2.31	16	1
2:B:249:LEU:HG	2:B:301:LEU:HD11	0.56	1.77	18	1
1:A:69:GLY:O	1:A:72:GLU:CG	0.56	2.52	1	4
2:B:361:VAL:HA	2:B:364:LEU:CD2	0.56	2.29	16	1
1:A:63:ILE:CG1	1:A:64:GLU:N	0.56	2.67	13	2
2:B:306:LEU:O	2:B:306:LEU:HD23	0.56	2.01	11	2
2:B:302:GLY:O	2:B:306:LEU:HD12	0.56	2.01	14	1
2:B:286:LEU:HD13	2:B:291:LEU:HD13	0.56	1.78	15	1
1:A:31:ASP:N	1:A:71:GLN:OE1	0.56	2.37	20	1
2:B:291:LEU:O	2:B:292:LYS:C	0.56	2.49	14	16
1:A:18:ARG:HB3	1:A:19:PRO:HD3	0.56	1.78	2	1
2:B:213:THR:HG23	2:B:214:GLY:N	0.56	2.15	8	1
2:B:222:GLU:HG2	2:B:226:TYR:CE1	0.56	2.35	9	1
2:B:203:LEU:O	2:B:203:LEU:CD2	0.56	2.54	18	1
2:B:290:TYR:O	2:B:293:GLU:HG3	0.56	2.01	19	1
2:B:284:ALA:O	2:B:285:ALA:C	0.56	2.48	12	8
1:A:49:VAL:HG21	2:B:248:LEU:HD23	0.56	1.76	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:HIS:CG	1:A:17:ALA:N	0.56	2.70	13	2
2:B:222:GLU:O	2:B:226:TYR:CG	0.56	2.59	15	4
2:B:247:HIS:O	2:B:251:ASP:HB2	0.56	2.01	3	1
1:A:18:ARG:O	1:A:22:LYS:HG2	0.56	2.02	7	1
2:B:268:ALA:O	2:B:271:ALA:N	0.56	2.38	9	1
2:B:209:ARG:HG2	2:B:210:GLU:N	0.56	2.15	12	1
2:B:333:THR:HG23	2:B:334:THR:N	0.55	2.16	9	4
1:A:43:GLU:CD	1:A:43:GLU:H	0.55	2.09	3	2
2:B:248:LEU:C	2:B:248:LEU:CD2	0.55	2.74	6	4
1:A:24:PHE:CE1	2:B:247:HIS:NE2	0.55	2.74	10	1
1:A:38:ASN:OD1	1:A:54:MET:SD	0.55	2.64	12	1
2:B:244:LEU:HD13	2:B:244:LEU:O	0.55	2.01	19	1
1:A:79:VAL:CG1	1:A:80:ILE:N	0.55	2.70	11	6
1:A:71:GLN:CD	1:A:71:GLN:O	0.55	2.48	3	1
2:B:396:ASP:O	2:B:397:PRO:O	0.55	2.24	3	1
2:B:220:ALA:O	2:B:223:PHE:CE2	0.55	2.59	4	1
2:B:291:LEU:HD12	2:B:292:LYS:N	0.55	2.16	5	1
2:B:393:LEU:N	2:B:393:LEU:HD13	0.55	2.13	8	1
2:B:293:GLU:C	2:B:293:GLU:OE1	0.55	2.49	16	1
2:B:276:ILE:C	2:B:276:ILE:HD12	0.55	2.26	18	1
1:A:37:ARG:NE	1:A:43:GLU:OE2	0.55	2.39	7	1
2:B:361:VAL:HG11	2:B:368:THR:OG1	0.55	2.01	8	2
2:B:223:PHE:CE2	2:B:242:PHE:CZ	0.55	2.95	9	1
1:A:20:ALA:HB1	1:A:52:LEU:CD1	0.55	2.30	18	1
2:B:349:ARG:NH2	2:B:374:ILE:O	0.55	2.39	18	1
1:A:72:GLU:CG	1:A:73:GLU:N	0.55	2.69	3	7
2:B:382:ARG:NH1	2:B:383:THR:O	0.55	2.39	6	1
2:B:187:GLN:OE1	2:B:326:VAL:O	0.55	2.25	7	1
2:B:209:ARG:NH2	2:B:259:PHE:CZ	0.55	2.75	7	1
2:B:325:LEU:C	2:B:325:LEU:CD1	0.55	2.79	12	3
1:A:5:GLN:C	1:A:5:GLN:OE1	0.55	2.49	14	1
1:A:3:VAL:HG12	1:A:3:VAL:O	0.55	2.02	2	1
2:B:379:LEU:N	2:B:379:LEU:CD2	0.55	2.67	9	3
2:B:279:PHE:O	2:B:283:PHE:CE1	0.55	2.60	8	2
1:A:63:ILE:HG12	1:A:64:GLU:N	0.55	2.15	7	2
1:A:38:ASN:HD21	1:A:40:GLU:CA	0.55	2.15	8	1
1:A:5:GLN:CD	1:A:76:LEU:HD21	0.55	2.25	15	1
2:B:204:ASP:N	2:B:204:ASP:OD1	0.55	2.38	9	3
2:B:360:MET:CG	2:B:361:VAL:N	0.55	2.70	1	1
2:B:237:GLU:O	2:B:241:ILE:HD13	0.55	2.01	3	1
2:B:294:ARG:O	2:B:297:ASP:N	0.55	2.39	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:346:VAL:HG13	2:B:368:THR:HG23	0.55	1.79	7	1
2:B:213:THR:O	2:B:217:GLU:OE2	0.55	2.24	16	1
2:B:283:PHE:CD1	2:B:284:ALA:N	0.55	2.74	17	1
2:B:220:ALA:O	2:B:223:PHE:CD2	0.55	2.59	4	1
2:B:360:MET:O	2:B:364:LEU:HD13	0.55	2.01	20	2
2:B:211:ARG:CZ	2:B:309:LEU:HD21	0.55	2.32	11	1
1:A:74:GLU:OE1	1:A:74:GLU:C	0.55	2.48	12	1
2:B:344:VAL:O	2:B:366:ILE:HG23	0.55	2.01	1	1
2:B:222:GLU:CD	2:B:222:GLU:C	0.55	2.75	9	1
2:B:299:ARG:NH1	2:B:303:GLN:N	0.55	2.55	12	1
2:B:217:GLU:C	2:B:217:GLU:CD	0.55	2.74	14	2
2:B:221:ASN:O	2:B:225:ARG:CG	0.55	2.55	14	1
2:B:364:LEU:HD11	2:B:366:ILE:CB	0.55	2.31	16	1
1:A:44:ALA:CA	1:A:51:ALA:HB1	0.55	2.32	19	20
1:A:53:LEU:O	2:B:286:LEU:HD13	0.55	2.02	1	1
2:B:286:LEU:O	2:B:292:LYS:HD2	0.55	2.01	1	1
2:B:390:ARG:NH1	2:B:392:GLU:OE2	0.55	2.40	1	1
2:B:392:GLU:O	2:B:393:LEU:HD23	0.55	2.02	1	2
1:A:30:PHE:HB2	1:A:71:GLN:CG	0.55	2.32	3	1
2:B:283:PHE:C	2:B:285:ALA:H	0.55	2.10	8	1
2:B:187:GLN:O	2:B:187:GLN:NE2	0.55	2.39	15	3
1:A:37:ARG:O	1:A:63:ILE:HG22	0.55	2.01	20	1
2:B:333:THR:CG2	2:B:334:THR:N	0.55	2.70	2	4
2:B:203:LEU:N	2:B:203:LEU:HD22	0.55	2.05	17	2
2:B:212:LEU:CG	2:B:213:THR:N	0.55	2.70	18	1
2:B:279:PHE:CD2	2:B:279:PHE:C	0.55	2.83	18	1
1:A:84:ASN:O	1:A:84:ASN:OD1	0.54	2.26	3	1
2:B:338:LEU:N	2:B:338:LEU:HD23	0.54	2.16	13	1
2:B:231:ALA:HB2	2:B:239:ALA:CB	0.54	2.32	20	1
2:B:246:SER:O	2:B:250:SER:OG	0.54	2.23	3	2
2:B:203:LEU:C	2:B:204:ASP:OD1	0.54	2.51	13	2
1:A:40:GLU:OE2	1:A:61:ARG:NH2	0.54	2.39	6	2
2:B:245:TYR:CZ	2:B:297:ASP:CB	0.54	2.90	9	1
1:A:18:ARG:HA	1:A:18:ARG:NE	0.54	2.16	1	1
2:B:242:PHE:O	2:B:243:ASP:C	0.54	2.50	10	14
2:B:268:ALA:O	2:B:269:GLU:C	0.54	2.50	8	11
2:B:307:PHE:O	2:B:310:ASP:OD1	0.54	2.26	8	3
1:A:50:ILE:HA	1:A:53:LEU:HD23	0.54	1.79	4	2
2:B:279:PHE:CD2	2:B:282:GLN:OE1	0.54	2.59	17	1
2:B:258:LEU:CG	2:B:259:PHE:N	0.54	2.71	18	1
2:B:203:LEU:H	2:B:203:LEU:CD1	0.54	2.13	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:251:ASP:CG	2:B:253:ARG:H	0.54	2.09	6	1
2:B:288:ASP:OD1	2:B:288:ASP:N	0.54	2.37	12	1
1:A:21:MET:CG	1:A:22:LYS:N	0.54	2.71	4	1
2:B:187:GLN:CD	2:B:187:GLN:N	0.54	2.65	4	2
2:B:222:GLU:N	2:B:225:ARG:HH11	0.54	2.00	6	1
1:A:38:ASN:ND2	1:A:38:ASN:O	0.54	2.41	8	1
2:B:256:ARG:NE	2:B:256:ARG:CA	0.54	2.68	9	1
2:B:251:ASP:OD2	2:B:253:ARG:NH2	0.54	2.41	12	2
2:B:330:LEU:HD12	2:B:330:LEU:O	0.54	2.01	15	1
1:A:23:LEU:HD23	1:A:23:LEU:C	0.54	2.28	18	1
2:B:276:ILE:O	2:B:280:ALA:HB2	0.54	2.02	18	1
1:A:15:MET:SD	1:A:19:PRO:HG3	0.54	2.42	20	1
1:A:39:ASP:OD1	1:A:40:GLU:N	0.54	2.40	11	4
2:B:245:TYR:CD1	2:B:245:TYR:C	0.54	2.86	5	1
2:B:379:LEU:H	2:B:379:LEU:CD2	0.54	2.14	9	2
2:B:245:TYR:OH	2:B:297:ASP:OD2	0.54	2.24	11	2
2:B:346:VAL:HG23	2:B:368:THR:HG23	0.54	1.77	16	1
2:B:235:GLN:HG2	2:B:236:LYS:H	0.54	1.62	2	2
1:A:7:VAL:HB	1:A:83:PHE:CE2	0.54	2.38	19	2
2:B:203:LEU:N	2:B:203:LEU:CD2	0.54	2.60	4	2
2:B:211:ARG:HH12	2:B:269:GLU:CD	0.54	2.10	5	3
2:B:235:GLN:NE2	2:B:238:THR:H	0.54	2.01	6	1
2:B:211:ARG:HG3	2:B:212:LEU:N	0.54	2.17	8	1
1:A:56:ASP:CG	2:B:291:LEU:HD11	0.54	2.26	9	1
2:B:242:PHE:CD1	2:B:242:PHE:N	0.54	2.75	11	1
2:B:282:GLN:CG	2:B:283:PHE:N	0.54	2.71	11	1
2:B:222:GLU:OE2	2:B:226:TYR:CE1	0.54	2.60	13	1
2:B:393:LEU:C	2:B:393:LEU:HD23	0.54	2.28	17	1
1:A:61:ARG:NH2	1:A:62:GLN:H	0.54	2.00	20	1
1:A:11:ASN:OD1	1:A:11:ASN:N	0.54	2.41	3	1
2:B:331:SER:O	2:B:334:THR:OG1	0.54	2.25	2	3
2:B:212:LEU:C	2:B:212:LEU:CD1	0.54	2.74	17	2
2:B:172:ARG:N	2:B:172:ARG:CD	0.54	2.71	2	1
2:B:221:ASN:OD1	2:B:224:ARG:NH1	0.54	2.41	8	2
2:B:215:ALA:HB2	2:B:309:LEU:HD12	0.54	1.80	15	1
2:B:235:GLN:HE21	2:B:237:GLU:CD	0.54	2.11	17	1
2:B:172:ARG:CD	2:B:172:ARG:H	0.53	2.16	20	3
2:B:218:GLU:O	2:B:222:GLU:HB3	0.53	2.03	2	1
1:A:32:ALA:CB	1:A:68:THR:O	0.53	2.57	11	6
2:B:258:LEU:HD23	2:B:258:LEU:C	0.53	2.28	7	1
2:B:291:LEU:O	2:B:294:ARG:HB2	0.53	2.03	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:212:LEU:HG	2:B:213:THR:H	0.53	1.62	18	1
2:B:303:GLN:HG2	2:B:304:ARG:N	0.53	2.18	3	2
2:B:223:PHE:CZ	2:B:242:PHE:CZ	0.53	2.97	9	1
1:A:23:LEU:HD21	1:A:79:VAL:HG23	0.53	1.79	13	2
1:A:73:GLU:CG	1:A:74:GLU:N	0.53	2.70	9	3
2:B:172:ARG:CZ	2:B:392:GLU:OE2	0.53	2.56	10	1
1:A:14:GLY:O	1:A:15:MET:HB2	0.53	2.03	13	2
2:B:245:TYR:O	2:B:248:LEU:HB2	0.53	2.02	14	1
2:B:288:ASP:O	2:B:291:LEU:CG	0.53	2.56	19	1
1:A:48:SER:OG	2:B:253:ARG:NE	0.53	2.42	2	1
2:B:350:ASP:OD1	2:B:351:GLY:N	0.53	2.41	2	3
2:B:291:LEU:HG	2:B:292:LYS:H	0.53	1.62	19	2
2:B:241:ILE:HG23	2:B:242:PHE:H	0.53	1.48	10	1
1:A:30:PHE:CG	1:A:74:GLU:CD	0.53	2.86	12	1
2:B:290:TYR:OH	2:B:294:ARG:NH2	0.53	2.39	12	1
2:B:309:LEU:CD1	2:B:309:LEU:O	0.53	2.56	14	1
2:B:338:LEU:CB	2:B:342:ARG:HE	0.53	2.17	12	1
1:A:56:ASP:OD2	2:B:291:LEU:HD23	0.53	2.02	4	1
2:B:329:GLU:OE2	2:B:330:LEU:O	0.53	2.27	8	2
2:B:395:VAL:HG22	2:B:396:ASP:OD1	0.53	2.02	8	3
2:B:211:ARG:CB	2:B:211:ARG:HH21	0.53	2.16	9	1
2:B:326:VAL:HG22	2:B:347:VAL:CG2	0.53	2.33	10	1
1:A:74:GLU:OE1	1:A:75:ALA:CA	0.53	2.56	12	1
1:A:53:LEU:CB	2:B:291:LEU:HD22	0.53	2.33	16	1
2:B:261:GLU:O	2:B:264:LYS:CG	0.53	2.57	19	1
2:B:286:LEU:CD2	2:B:287:SER:N	0.53	2.64	4	1
1:A:13:LEU:CD2	1:A:13:LEU:H	0.53	2.15	7	1
2:B:288:ASP:HB3	2:B:291:LEU:HD11	0.53	1.81	14	2
1:A:19:PRO:O	1:A:23:LEU:CD1	0.53	2.57	17	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.53	2.62	20	1
2:B:273:LYS:CG	2:B:274:THR:N	0.53	2.71	4	1
2:B:349:ARG:HH11	2:B:373:ASP:C	0.53	2.12	5	2
2:B:184:GLU:HB2	2:B:323:PHE:CD2	0.53	2.38	17	1
1:A:23:LEU:HD11	1:A:79:VAL:CG2	0.53	2.34	2	2
1:A:71:GLN:O	1:A:72:GLU:C	0.53	2.50	3	20
2:B:247:HIS:O	2:B:247:HIS:ND1	0.53	2.42	3	1
2:B:183:ALA:HB3	2:B:324:ILE:HG23	0.53	1.80	6	1
1:A:56:ASP:C	2:B:288:ASP:OD2	0.53	2.52	14	1
2:B:244:LEU:HD12	2:B:244:LEU:C	0.53	2.29	17	1
2:B:288:ASP:OD2	2:B:291:LEU:HD23	0.53	2.04	20	2
2:B:276:ILE:HG13	2:B:277:GLU:N	0.53	2.19	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:SD	2:B:240:ALA:O	0.53	2.67	16	1
2:B:383:THR:OG1	2:B:396:ASP:HB3	0.53	2.03	18	1
2:B:204:ASP:O	2:B:208:GLU:N	0.52	2.38	3	2
2:B:207:LEU:O	2:B:211:ARG:CG	0.52	2.57	8	5
2:B:211:ARG:NH1	2:B:269:GLU:OE1	0.52	2.39	3	1
2:B:322:ARG:C	2:B:323:PHE:CG	0.52	2.87	6	2
2:B:361:VAL:HG12	2:B:362:ARG:N	0.52	2.18	6	2
2:B:364:LEU:HD23	2:B:366:ILE:HD12	0.52	1.81	11	1
1:A:4:LYS:CD	1:A:4:LYS:H	0.52	2.17	15	1
2:B:216:LEU:O	2:B:220:ALA:CB	0.52	2.57	15	1
2:B:244:LEU:O	2:B:248:LEU:N	0.52	2.42	17	1
2:B:340:GLN:CD	2:B:340:GLN:H	0.52	2.12	18	1
2:B:208:GLU:OE2	2:B:268:ALA:HB2	0.52	2.04	20	1
2:B:351:GLY:O	2:B:352:ALA:C	0.52	2.50	9	3
2:B:323:PHE:CD1	2:B:324:ILE:N	0.52	2.77	5	1
2:B:277:GLU:O	2:B:281:GLU:CD	0.52	2.52	6	2
1:A:38:ASN:HD22	1:A:42:THR:H	0.52	1.42	8	1
2:B:259:PHE:O	2:B:259:PHE:CD1	0.52	2.62	19	2
2:B:250:SER:O	2:B:255:ARG:NE	0.52	2.42	15	1
2:B:221:ASN:C	2:B:225:ARG:HE	0.52	2.12	8	3
1:A:28:GLN:HE22	2:B:247:HIS:CE1	0.52	2.22	9	1
2:B:204:ASP:OD1	2:B:208:GLU:HG2	0.52	2.04	20	2
1:A:1:MET:C	1:A:1:MET:SD	0.52	2.91	11	1
1:A:8:GLU:OE1	1:A:62:GLN:OE1	0.52	2.26	14	1
2:B:305:LEU:O	2:B:309:LEU:HD12	0.52	2.03	16	1
2:B:283:PHE:N	2:B:283:PHE:CD1	0.52	2.75	13	1
2:B:221:ASN:OD1	2:B:224:ARG:CZ	0.52	2.58	14	1
2:B:212:LEU:HD11	2:B:255:ARG:NH2	0.52	2.19	17	1
1:A:53:LEU:HD13	2:B:283:PHE:CD1	0.52	2.40	19	1
2:B:283:PHE:CD2	2:B:298:LEU:HD13	0.52	2.40	3	1
1:A:27:MET:HG3	1:A:28:GLN:N	0.52	2.19	5	1
2:B:253:ARG:HE	2:B:253:ARG:C	0.52	2.12	5	1
1:A:14:GLY:O	1:A:15:MET:O	0.52	2.28	6	1
1:A:3:VAL:O	1:A:3:VAL:HG13	0.52	2.04	10	1
2:B:335:LEU:HD23	2:B:335:LEU:O	0.52	2.04	13	1
1:A:15:MET:C	1:A:19:PRO:HD2	0.52	2.29	15	1
2:B:291:LEU:N	2:B:291:LEU:CD1	0.52	2.71	18	1
1:A:80:ILE:CG2	1:A:81:ALA:N	0.52	2.73	15	8
2:B:239:ALA:O	2:B:243:ASP:CB	0.52	2.58	9	3
2:B:233:GLY:C	2:B:234:ALA:O	0.52	2.53	4	3
2:B:270:TRP:O	2:B:273:LYS:HG3	0.52	2.03	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:277:GLU:O	2:B:281:GLU:OE2	0.52	2.28	5	2
1:A:38:ASN:OD1	1:A:40:GLU:CB	0.52	2.58	8	1
2:B:394:LEU:CD2	2:B:394:LEU:N	0.52	2.72	16	1
2:B:253:ARG:O	2:B:256:ARG:CG	0.52	2.55	1	1
2:B:297:ASP:OD2	2:B:356:GLN:NE2	0.52	2.42	1	1
1:A:25:GLU:N	1:A:25:GLU:CD	0.52	2.68	5	2
2:B:187:GLN:CD	2:B:187:GLN:H	0.52	2.13	4	1
2:B:171:ILE:O	2:B:392:GLU:CD	0.52	2.53	7	1
2:B:171:ILE:C	2:B:392:GLU:OE2	0.52	2.52	7	1
2:B:381:ARG:C	2:B:382:ARG:HG2	0.52	2.28	7	1
2:B:286:LEU:HD23	2:B:288:ASP:OD1	0.52	2.04	8	1
2:B:187:GLN:NE2	2:B:187:GLN:C	0.52	2.68	15	2
2:B:364:LEU:HD11	2:B:366:ILE:HB	0.52	1.82	16	1
2:B:258:LEU:HA	2:B:275:VAL:HG11	0.52	1.80	18	1
2:B:392:GLU:C	2:B:392:GLU:CD	0.52	2.74	8	1
2:B:283:PHE:N	2:B:283:PHE:HD1	0.52	2.01	18	2
2:B:227:SER:OG	2:B:242:PHE:CG	0.52	2.59	2	2
2:B:245:TYR:N	2:B:245:TYR:CD1	0.52	2.77	20	2
1:A:43:GLU:OE1	1:A:45:GLU:N	0.52	2.42	17	2
2:B:243:ASP:O	2:B:247:HIS:CD2	0.52	2.63	17	1
1:A:2:THR:HG22	1:A:68:THR:OG1	0.52	2.05	1	3
1:A:8:GLU:CD	1:A:8:GLU:N	0.52	2.67	1	1
1:A:12:LYS:CG	1:A:14:GLY:O	0.52	2.58	1	1
1:A:80:ILE:O	1:A:84:ASN:ND2	0.52	2.43	14	3
2:B:249:LEU:HB3	2:B:301:LEU:HD21	0.52	1.82	1	1
2:B:286:LEU:HD23	2:B:292:LYS:CA	0.52	2.35	1	1
2:B:347:VAL:HG22	2:B:369:VAL:HG23	0.52	1.82	1	1
1:A:57:SER:O	1:A:61:ARG:CZ	0.52	2.58	3	1
1:A:38:ASN:HD21	1:A:55:LEU:HD12	0.52	1.65	4	2
2:B:275:VAL:CG1	2:B:276:ILE:H	0.52	2.17	17	3
2:B:218:GLU:CD	2:B:218:GLU:O	0.52	2.53	10	2
2:B:248:LEU:HG	2:B:249:LEU:N	0.52	2.19	8	1
2:B:255:ARG:NH1	2:B:258:LEU:CD1	0.52	2.73	10	1
1:A:26:LEU:HG	1:A:30:PHE:HD1	0.52	1.65	12	1
2:B:205:PRO:O	2:B:209:ARG:HB2	0.52	2.04	16	2
2:B:186:TRP:CH2	2:B:381:ARG:NH1	0.52	2.78	17	1
2:B:258:LEU:CD1	2:B:275:VAL:HG11	0.51	2.35	1	1
2:B:284:ALA:C	2:B:286:LEU:N	0.51	2.68	13	5
1:A:64:GLU:C	1:A:66:GLU:OE2	0.51	2.53	3	1
2:B:382:ARG:HH12	2:B:396:ASP:CB	0.51	2.17	6	1
2:B:222:GLU:OE1	2:B:304:ARG:NE	0.51	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:217:GLU:HG2	2:B:221:ASN:ND2	0.51	2.20	15	3
2:B:340:GLN:CD	2:B:340:GLN:N	0.51	2.68	18	1
2:B:217:GLU:O	2:B:221:ASN:HB2	0.51	2.03	10	10
2:B:248:LEU:CD1	2:B:253:ARG:NH2	0.51	2.73	11	1
2:B:270:TRP:CD1	2:B:270:TRP:N	0.51	2.75	1	1
1:A:10:THR:O	1:A:11:ASN:ND2	0.51	2.41	3	1
2:B:246:SER:O	2:B:250:SER:CB	0.51	2.58	3	2
2:B:184:GLU:HB3	2:B:323:PHE:CE2	0.51	2.39	4	1
2:B:394:LEU:HB3	2:B:397:PRO:HG3	0.51	1.83	4	3
1:A:13:LEU:O	1:A:13:LEU:CD2	0.51	2.57	5	1
1:A:35:LEU:C	1:A:36:LEU:HD12	0.51	2.31	18	3
1:A:15:MET:C	1:A:17:ALA:H	0.51	2.10	15	1
2:B:269:GLU:N	2:B:269:GLU:OE1	0.51	2.44	9	5
2:B:273:LYS:CD	2:B:274:THR:N	0.51	2.73	4	1
2:B:323:PHE:CD1	2:B:323:PHE:C	0.51	2.86	5	1
2:B:205:PRO:O	2:B:209:ARG:NE	0.51	2.42	6	1
2:B:276:ILE:CG2	2:B:277:GLU:N	0.51	2.73	6	2
2:B:185:GLY:C	2:B:380:HIS:O	0.51	2.52	3	1
2:B:258:LEU:CD2	2:B:275:VAL:HG21	0.51	2.36	15	3
2:B:329:GLU:CD	2:B:329:GLU:O	0.51	2.54	4	1
1:A:38:ASN:HD21	1:A:40:GLU:C	0.51	2.13	8	1
1:A:47:ASN:C	1:A:47:ASN:ND2	0.51	2.68	8	1
2:B:393:LEU:HD12	2:B:393:LEU:C	0.51	2.30	16	1
1:A:37:ARG:O	1:A:63:ILE:HD12	0.51	2.06	2	1
1:A:38:ASN:CG	1:A:40:GLU:H	0.51	2.14	8	1
1:A:69:GLY:O	1:A:72:GLU:OE1	0.51	2.29	9	1
2:B:249:LEU:HD11	2:B:305:LEU:HD11	0.51	1.82	9	1
1:A:2:THR:CG2	1:A:3:VAL:N	0.51	2.73	10	1
1:A:53:LEU:HB3	2:B:286:LEU:HD22	0.51	1.82	10	1
2:B:396:ASP:O	2:B:396:ASP:CG	0.51	2.51	18	2
2:B:335:LEU:C	2:B:337:GLU:N	0.51	2.69	3	6
2:B:294:ARG:O	2:B:295:ALA:C	0.51	2.54	3	7
2:B:223:PHE:CE1	2:B:304:ARG:NH1	0.51	2.79	3	1
1:A:2:THR:HG23	1:A:68:THR:OG1	0.51	2.06	4	1
2:B:181:ALA:HB1	2:B:344:VAL:O	0.51	2.06	7	1
2:B:286:LEU:HG	2:B:287:SER:N	0.51	2.21	10	2
2:B:174:LEU:N	2:B:174:LEU:CD1	0.51	2.73	12	1
2:B:304:ARG:CZ	2:B:337:GLU:OE1	0.51	2.59	17	1
2:B:283:PHE:CE2	2:B:298:LEU:HD13	0.51	2.40	3	1
2:B:245:TYR:CZ	2:B:297:ASP:HB3	0.51	2.40	12	3
1:A:4:LYS:O	1:A:5:GLN:CG	0.51	2.59	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:288:ASP:N	2:B:291:LEU:HD23	0.51	2.21	19	1
2:B:226:TYR:CZ	2:B:336:ALA:O	0.51	2.63	19	4
1:A:27:MET:SD	1:A:27:MET:C	0.51	2.93	5	1
2:B:379:LEU:O	2:B:382:ARG:N	0.51	2.32	9	3
1:A:47:ASN:O	1:A:47:ASN:ND2	0.51	2.43	17	1
2:B:254:LEU:HD23	2:B:254:LEU:C	0.51	2.31	18	1
1:A:84:ASN:O	1:A:85:SER:CB	0.51	2.59	7	15
1:A:80:ILE:CG1	1:A:81:ALA:N	0.51	2.74	9	3
2:B:175:PRO:HB3	2:B:388:GLY:O	0.51	2.06	3	1
2:B:245:TYR:OH	2:B:297:ASP:HB2	0.51	2.07	6	3
1:A:16:HIS:O	1:A:19:PRO:CD	0.51	2.48	7	1
1:A:17:ALA:O	1:A:21:MET:N	0.51	2.35	7	1
1:A:79:VAL:CG2	1:A:80:ILE:N	0.51	2.73	8	3
1:A:17:ALA:O	1:A:20:ALA:N	0.51	2.44	9	1
1:A:76:LEU:HD12	1:A:76:LEU:C	0.51	2.31	10	1
2:B:238:THR:O	2:B:241:ILE:HG22	0.51	2.06	10	1
2:B:338:LEU:HD13	2:B:342:ARG:HH11	0.51	1.64	12	1
2:B:253:ARG:NH1	2:B:279:PHE:CE2	0.50	2.79	1	1
2:B:390:ARG:O	2:B:391:GLY:C	0.50	2.54	2	7
2:B:242:PHE:CD1	2:B:243:ASP:N	0.50	2.77	3	2
1:A:13:LEU:HA	1:A:83:PHE:CE2	0.50	2.40	5	1
2:B:202:THR:HG23	2:B:202:THR:O	0.50	2.06	11	1
2:B:386:VAL:HG22	2:B:393:LEU:HD12	0.50	1.81	11	1
1:A:7:VAL:CG2	1:A:83:PHE:CE2	0.50	2.94	15	1
2:B:211:ARG:NH2	2:B:268:ALA:HB3	0.50	2.21	20	1
1:A:44:ALA:HA	1:A:51:ALA:HB1	0.50	1.84	11	20
2:B:173:ALA:O	2:B:391:GLY:O	0.50	2.29	9	5
2:B:342:ARG:C	2:B:342:ARG:CD	0.50	2.84	2	1
2:B:338:LEU:O	2:B:338:LEU:HD13	0.50	2.06	7	1
2:B:222:GLU:OE2	2:B:223:PHE:N	0.50	2.44	15	1
1:A:53:LEU:O	2:B:288:ASP:OD2	0.50	2.29	12	2
1:A:54:MET:SD	1:A:54:MET:C	0.50	2.94	4	3
2:B:310:ASP:OD1	2:B:310:ASP:N	0.50	2.43	5	1
1:A:58:ALA:HB2	1:A:61:ARG:HH11	0.50	1.67	8	1
2:B:297:ASP:CG	2:B:356:GLN:NE2	0.50	2.70	14	1
2:B:293:GLU:HG3	2:B:294:ARG:N	0.50	2.21	16	1
1:A:23:LEU:HD23	1:A:23:LEU:O	0.50	2.06	18	1
1:A:15:MET:HE3	1:A:19:PRO:CD	0.50	2.35	20	1
1:A:71:GLN:NE2	1:A:71:GLN:C	0.50	2.69	3	1
1:A:38:ASN:HD21	1:A:40:GLU:CB	0.50	2.19	8	1
1:A:76:LEU:HD13	1:A:76:LEU:C	0.50	2.32	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:294:ARG:NH1	2:B:297:ASP:OD2	0.50	2.42	2	1
2:B:182:ILE:HG22	2:B:385:ILE:HG23	0.50	1.83	3	1
1:A:53:LEU:HB2	2:B:286:LEU:HD12	0.50	1.82	4	1
1:A:5:GLN:CD	1:A:80:ILE:HD11	0.50	2.31	6	1
1:A:17:ALA:C	1:A:19:PRO:CD	0.50	2.82	9	1
2:B:350:ASP:N	2:B:350:ASP:OD1	0.50	2.43	11	1
2:B:186:TRP:CZ3	2:B:381:ARG:NH1	0.50	2.79	17	1
2:B:245:TYR:OH	2:B:297:ASP:O	0.50	2.30	17	1
1:A:16:HIS:ND1	1:A:17:ALA:N	0.50	2.60	4	2
2:B:224:ARG:O	2:B:228:LYS:HB2	0.50	2.06	3	2
2:B:352:ALA:C	2:B:354:ASN:H	0.50	2.14	3	1
2:B:203:LEU:HD12	2:B:204:ASP:N	0.50	2.22	6	1
2:B:326:VAL:HG22	2:B:347:VAL:CG1	0.50	2.37	18	1
2:B:185:GLY:CA	2:B:380:HIS:O	0.50	2.59	3	1
2:B:208:GLU:OE1	2:B:268:ALA:HB2	0.50	2.06	7	2
1:A:25:GLU:N	1:A:25:GLU:OE1	0.50	2.45	5	1
2:B:213:THR:OG1	2:B:255:ARG:CZ	0.50	2.60	6	2
2:B:235:GLN:NE2	2:B:238:THR:OG1	0.50	2.44	6	1
2:B:279:PHE:O	2:B:283:PHE:CD1	0.50	2.65	6	4
1:A:17:ALA:O	1:A:18:ARG:C	0.50	2.52	9	3
1:A:64:GLU:CD	1:A:64:GLU:C	0.50	2.79	10	1
2:B:385:ILE:O	2:B:385:ILE:CG2	0.50	2.59	10	1
2:B:287:SER:O	2:B:288:ASP:C	0.50	2.55	18	4
2:B:238:THR:HG22	2:B:360:MET:SD	0.50	2.46	14	1
2:B:216:LEU:O	2:B:220:ALA:HB3	0.50	2.07	15	1
2:B:254:LEU:HD23	2:B:255:ARG:HH22	0.50	1.66	16	1
2:B:255:ARG:NE	2:B:255:ARG:CA	0.50	2.73	17	1
1:A:15:MET:C	1:A:16:HIS:O	0.50	2.55	7	1
2:B:248:LEU:HD23	2:B:249:LEU:CA	0.50	2.35	10	2
1:A:62:GLN:OE1	1:A:63:ILE:N	0.50	2.45	16	1
2:B:172:ARG:H	2:B:172:ARG:HD3	0.50	1.65	20	1
2:B:270:TRP:CE3	2:B:274:THR:OG1	0.50	2.64	2	1
2:B:307:PHE:O	2:B:310:ASP:CG	0.50	2.55	15	2
1:A:84:ASN:C	1:A:85:SER:OG	0.50	2.53	14	2
2:B:247:HIS:ND1	2:B:247:HIS:O	0.50	2.44	10	2
2:B:211:ARG:HH21	2:B:211:ARG:CG	0.50	2.20	9	1
2:B:225:ARG:HE	2:B:229:ARG:HH12	0.50	1.50	14	1
2:B:349:ARG:CD	2:B:372:ALA:O	0.50	2.59	15	1
2:B:276:ILE:O	2:B:279:PHE:CD2	0.50	2.65	20	1
1:A:64:GLU:O	1:A:66:GLU:OE2	0.49	2.29	9	2
2:B:288:ASP:OD2	2:B:290:TYR:CB	0.49	2.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ALA:O	1:A:80:ILE:HG22	0.49	2.07	15	2
2:B:258:LEU:HD23	2:B:275:VAL:HG21	0.49	1.84	15	4
2:B:304:ARG:HH22	2:B:336:ALA:C	0.49	2.15	11	1
2:B:338:LEU:CB	2:B:342:ARG:NE	0.49	2.75	12	1
1:A:27:MET:N	1:A:30:PHE:CE2	0.49	2.80	1	8
2:B:256:ARG:CD	2:B:257:GLU:N	0.49	2.75	1	1
2:B:335:LEU:HG	2:B:360:MET:HE1	0.49	1.83	5	1
2:B:251:ASP:OD1	2:B:253:ARG:HB3	0.49	2.07	6	1
1:A:53:LEU:N	1:A:53:LEU:HD23	0.49	2.22	10	2
1:A:53:LEU:HD22	2:B:291:LEU:HD12	0.49	1.83	10	1
1:A:27:MET:CE	1:A:34:VAL:HG23	0.49	2.37	15	1
1:A:15:MET:HB3	1:A:19:PRO:CD	0.49	2.31	18	1
2:B:184:GLU:N	2:B:184:GLU:OE1	0.49	2.46	4	2
1:A:71:GLN:O	1:A:71:GLN:CG	0.49	2.60	3	1
1:A:50:ILE:HD12	2:B:282:GLN:OE1	0.49	2.07	14	1
2:B:259:PHE:CD1	2:B:259:PHE:C	0.49	2.87	19	1
2:B:292:LYS:CG	2:B:293:GLU:N	0.49	2.75	2	1
2:B:395:VAL:O	2:B:395:VAL:HG23	0.49	2.08	5	3
2:B:369:VAL:C	2:B:370:MET:SD	0.49	2.95	6	3
1:A:38:ASN:OD1	1:A:40:GLU:HB2	0.49	2.06	8	1
2:B:362:ARG:HG2	2:B:363:ALA:N	0.49	2.23	8	1
2:B:325:LEU:CD1	2:B:342:ARG:HH11	0.49	2.21	9	1
2:B:354:ASN:O	2:B:355:SER:C	0.49	2.55	15	1
2:B:182:ILE:O	2:B:182:ILE:HG23	0.49	2.05	8	2
2:B:286:LEU:CD1	2:B:288:ASP:OD1	0.49	2.48	2	1
1:A:36:LEU:HD11	1:A:46:ALA:HB2	0.49	1.82	8	3
1:A:13:LEU:C	1:A:13:LEU:CD2	0.49	2.84	5	1
2:B:216:LEU:C	2:B:216:LEU:CD1	0.49	2.65	5	1
2:B:245:TYR:OH	2:B:297:ASP:CB	0.49	2.60	6	2
2:B:342:ARG:HA	2:B:342:ARG:HE	0.49	1.67	6	1
2:B:373:ASP:OD1	2:B:374:ILE:HD13	0.49	2.07	7	1
2:B:217:GLU:O	2:B:221:ASN:CG	0.49	2.55	18	5
2:B:294:ARG:O	2:B:297:ASP:HB2	0.49	2.06	10	1
1:A:57:SER:HB3	2:B:288:ASP:OD2	0.49	2.08	20	1
2:B:283:PHE:CE2	2:B:298:LEU:HD11	0.49	2.42	3	1
2:B:308:HIS:C	2:B:310:ASP:N	0.49	2.68	8	3
2:B:203:LEU:HD13	2:B:265:GLY:CA	0.49	2.36	4	1
2:B:288:ASP:HB3	2:B:291:LEU:CD2	0.49	2.38	5	2
2:B:382:ARG:HH12	2:B:396:ASP:CG	0.49	2.16	6	1
2:B:252:THR:HG22	2:B:255:ARG:NH1	0.49	2.22	9	1
1:A:69:GLY:O	1:A:72:GLU:CD	0.49	2.56	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:172:ARG:NH2	2:B:392:GLU:OE2	0.49	2.46	10	1
2:B:211:ARG:CZ	2:B:309:LEU:HD11	0.49	2.38	14	1
2:B:230:PHE:C	2:B:232:ALA:N	0.49	2.70	16	1
1:A:4:LYS:HD3	1:A:4:LYS:N	0.49	2.23	20	1
1:A:15:MET:CE	1:A:15:MET:N	0.49	2.75	20	1
2:B:281:GLU:N	2:B:281:GLU:OE2	0.49	2.46	2	1
2:B:203:LEU:C	2:B:204:ASP:CG	0.49	2.79	17	3
2:B:208:GLU:OE1	2:B:268:ALA:CB	0.49	2.60	17	3
2:B:338:LEU:HD22	2:B:339:PRO:O	0.49	2.06	7	1
1:A:38:ASN:HD21	1:A:41:GLY:N	0.49	2.06	8	1
1:A:16:HIS:C	1:A:16:HIS:CD2	0.49	2.91	12	1
2:B:249:LEU:HD21	2:B:301:LEU:HD21	0.49	1.84	13	1
1:A:18:ARG:NE	1:A:18:ARG:CA	0.49	2.76	10	2
1:A:52:LEU:O	1:A:56:ASP:OD1	0.49	2.31	4	1
1:A:13:LEU:O	1:A:13:LEU:CG	0.49	2.61	5	1
1:A:31:ASP:N	1:A:31:ASP:OD1	0.49	2.46	5	1
2:B:171:ILE:O	2:B:392:GLU:OE1	0.49	2.31	10	2
1:A:38:ASN:HD21	1:A:40:GLU:HB3	0.49	1.67	8	1
1:A:43:GLU:OE1	1:A:45:GLU:CG	0.49	2.61	8	1
2:B:395:VAL:O	2:B:395:VAL:CG1	0.49	2.60	8	4
2:B:235:GLN:HG3	2:B:238:THR:OG1	0.49	2.08	10	1
1:A:7:VAL:HG23	1:A:83:PHE:CE2	0.49	2.42	15	1
2:B:261:GLU:C	2:B:266:SER:OG	0.49	2.55	18	2
2:B:230:PHE:O	2:B:232:ALA:N	0.49	2.46	16	1
1:A:49:VAL:HG11	2:B:248:LEU:HD12	0.49	1.84	20	1
2:B:245:TYR:O	2:B:248:LEU:HB3	0.49	2.07	10	4
2:B:338:LEU:HD13	2:B:338:LEU:N	0.49	2.06	7	1
2:B:385:ILE:C	2:B:385:ILE:CD1	0.49	2.84	11	1
1:A:13:LEU:H	1:A:13:LEU:HD23	0.49	1.67	13	2
2:B:273:LYS:HG3	2:B:274:THR:N	0.49	2.23	4	1
1:A:76:LEU:C	1:A:76:LEU:CD1	0.49	2.86	8	2
1:A:56:ASP:OD1	2:B:288:ASP:CG	0.49	2.55	9	1
2:B:328:ASP:O	2:B:350:ASP:OD1	0.49	2.31	13	2
2:B:244:LEU:C	2:B:244:LEU:HD22	0.49	2.27	19	1
1:A:15:MET:N	1:A:15:MET:HE2	0.49	2.23	20	1
1:A:3:VAL:CG2	1:A:72:GLU:HB2	0.48	2.37	1	1
1:A:71:GLN:O	1:A:74:GLU:N	0.48	2.46	7	19
2:B:268:ALA:HA	2:B:271:ALA:HB3	0.48	1.83	8	6
2:B:202:THR:HG23	2:B:204:ASP:OD1	0.48	2.08	3	1
2:B:396:ASP:N	2:B:397:PRO:HD3	0.48	2.21	3	6
2:B:305:LEU:O	2:B:309:LEU:HD23	0.48	2.08	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:290:TYR:CD1	2:B:290:TYR:O	0.48	2.66	8	1
2:B:227:SER:HB3	2:B:242:PHE:CB	0.48	2.38	9	2
2:B:230:PHE:O	2:B:233:GLY:N	0.48	2.45	16	2
2:B:256:ARG:O	2:B:260:ALA:HB2	0.48	2.07	12	1
1:A:12:LYS:C	1:A:14:GLY:H	0.48	2.16	18	4
2:B:385:ILE:N	2:B:385:ILE:CD1	0.48	2.65	1	1
1:A:6:THR:HG23	1:A:62:GLN:CD	0.48	2.33	3	1
1:A:15:MET:SD	1:A:19:PRO:CG	0.48	3.01	20	1
1:A:16:HIS:CG	2:B:291:LEU:HD11	0.48	2.44	2	1
1:A:1:MET:SD	1:A:1:MET:C	0.48	2.96	4	1
2:B:187:GLN:C	2:B:187:GLN:HE21	0.48	2.16	13	2
1:A:7:VAL:O	1:A:7:VAL:HG22	0.48	2.09	17	2
2:B:249:LEU:HD23	2:B:250:SER:H	0.48	1.68	15	1
2:B:322:ARG:O	2:B:322:ARG:CG	0.48	2.61	17	1
2:B:357:ALA:O	2:B:361:VAL:HG22	0.48	2.08	9	1
2:B:384:LEU:HD12	2:B:386:VAL:HG13	0.48	1.84	12	1
2:B:244:LEU:O	2:B:247:HIS:ND1	0.48	2.44	13	1
1:A:5:GLN:O	1:A:65:VAL:HG22	0.48	2.09	19	2
1:A:15:MET:HB3	1:A:19:PRO:HD3	0.48	1.84	19	1
1:A:65:VAL:C	1:A:66:GLU:OE2	0.48	2.57	3	1
2:B:385:ILE:CD1	2:B:397:PRO:HD2	0.48	2.38	4	1
2:B:177:ALA:O	2:B:388:GLY:HA3	0.48	2.08	6	1
2:B:238:THR:O	2:B:242:PHE:CD1	0.48	2.66	10	1
2:B:273:LYS:O	2:B:277:GLU:CB	0.48	2.62	13	1
2:B:240:ALA:C	2:B:243:ASP:OD1	0.48	2.56	14	1
2:B:244:LEU:HD13	2:B:294:ARG:HH22	0.48	1.68	17	1
2:B:203:LEU:O	2:B:203:LEU:CG	0.48	2.57	18	1
2:B:249:LEU:C	2:B:249:LEU:CD2	0.48	2.86	19	1
2:B:331:SER:HG	2:B:334:THR:CB	0.48	2.20	19	1
2:B:208:GLU:N	2:B:208:GLU:OE1	0.48	2.46	6	2
2:B:209:ARG:CG	2:B:259:PHE:CD1	0.48	2.97	4	1
1:A:37:ARG:NH1	1:A:66:GLU:CD	0.48	2.71	5	1
2:B:186:TRP:CE3	2:B:187:GLN:O	0.48	2.66	8	1
2:B:330:LEU:CD2	2:B:330:LEU:N	0.48	2.69	10	1
2:B:186:TRP:CD1	2:B:186:TRP:O	0.48	2.67	16	1
2:B:361:VAL:HG13	2:B:362:ARG:N	0.48	2.23	1	1
2:B:382:ARG:NH2	2:B:396:ASP:OD2	0.48	2.47	19	5
2:B:291:LEU:HD13	2:B:292:LYS:CA	0.48	2.38	12	1
2:B:281:GLU:N	2:B:281:GLU:CD	0.48	2.72	2	2
1:A:79:VAL:HG13	1:A:80:ILE:N	0.48	2.23	4	2
2:B:244:LEU:CD2	2:B:294:ARG:HH11	0.48	2.20	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:241:ILE:HG22	2:B:242:PHE:H	0.48	1.68	9	1
1:A:21:MET:HB3	2:B:244:LEU:HD13	0.48	1.85	10	1
2:B:325:LEU:HB3	2:B:346:VAL:HG13	0.48	1.85	10	1
2:B:345:GLY:C	2:B:346:VAL:HG23	0.48	2.34	10	1
2:B:343:LEU:CD1	2:B:345:GLY:O	0.48	2.59	17	1
1:A:8:GLU:OE1	1:A:8:GLU:N	0.48	2.45	18	1
1:A:10:THR:O	1:A:10:THR:CG2	0.48	2.50	19	2
2:B:360:MET:SD	2:B:364:LEU:HD22	0.48	2.49	20	1
2:B:208:GLU:N	2:B:208:GLU:CD	0.48	2.70	6	1
1:A:24:PHE:CE2	2:B:247:HIS:CE1	0.48	3.01	10	2
1:A:62:GLN:N	1:A:62:GLN:CD	0.48	2.71	11	1
2:B:326:VAL:HG12	2:B:376:PRO:HG3	0.48	1.84	11	1
2:B:244:LEU:O	2:B:244:LEU:HD23	0.48	2.09	13	1
2:B:184:GLU:OE1	2:B:381:ARG:O	0.48	2.32	18	1
2:B:252:THR:O	2:B:256:ARG:CG	0.48	2.62	19	1
2:B:291:LEU:HD12	2:B:291:LEU:O	0.48	2.07	20	1
1:A:28:GLN:HE21	1:A:28:GLN:CA	0.48	2.22	1	1
2:B:258:LEU:HD12	2:B:275:VAL:HG11	0.48	1.86	1	1
2:B:269:GLU:N	2:B:269:GLU:CD	0.48	2.71	1	2
1:A:14:GLY:O	1:A:15:MET:HB3	0.48	2.09	7	3
1:A:50:ILE:HD12	2:B:283:PHE:CE2	0.48	2.44	6	1
2:B:251:ASP:OD2	2:B:253:ARG:CB	0.48	2.61	6	1
2:B:222:GLU:OE2	2:B:304:ARG:CZ	0.48	2.62	8	1
2:B:222:GLU:OE1	2:B:304:ARG:NH1	0.48	2.47	19	2
2:B:308:HIS:N	2:B:308:HIS:ND1	0.48	2.61	11	1
2:B:253:ARG:CZ	2:B:253:ARG:CB	0.48	2.91	12	1
2:B:305:LEU:HD23	2:B:305:LEU:O	0.48	2.08	14	1
2:B:384:LEU:C	2:B:384:LEU:CD2	0.48	2.79	20	1
1:A:16:HIS:CE1	2:B:291:LEU:HD11	0.47	2.44	2	1
1:A:36:LEU:O	1:A:43:GLU:OE1	0.47	2.32	2	1
2:B:284:ALA:O	2:B:292:LYS:NZ	0.47	2.45	9	4
2:B:212:LEU:HD13	2:B:212:LEU:O	0.47	2.08	17	2
2:B:350:ASP:OD1	2:B:350:ASP:O	0.47	2.32	5	2
1:A:83:PHE:N	1:A:83:PHE:CD2	0.47	2.77	8	1
2:B:211:ARG:CG	2:B:211:ARG:NH2	0.47	2.75	9	1
1:A:15:MET:O	1:A:18:ARG:N	0.47	2.47	15	1
2:B:212:LEU:HD12	2:B:212:LEU:C	0.47	2.34	18	1
2:B:286:LEU:HB2	2:B:291:LEU:CD2	0.47	2.28	20	1
2:B:293:GLU:OE2	2:B:356:GLN:CD	0.47	2.57	20	1
2:B:291:LEU:O	2:B:293:GLU:N	0.47	2.48	2	2
2:B:244:LEU:HD12	2:B:244:LEU:O	0.47	2.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:340:GLN:O	2:B:340:GLN:CG	0.47	2.62	5	1
1:A:6:THR:CG2	1:A:62:GLN:CD	0.47	2.87	9	1
1:A:62:GLN:CD	1:A:62:GLN:N	0.47	2.69	14	1
2:B:375:GLN:OE1	2:B:375:GLN:N	0.47	2.45	19	1
1:A:43:GLU:N	1:A:43:GLU:OE1	0.47	2.47	3	1
1:A:80:ILE:HD12	1:A:81:ALA:N	0.47	2.24	3	1
2:B:340:GLN:O	2:B:340:GLN:CD	0.47	2.57	5	1
2:B:222:GLU:O	2:B:226:TYR:CB	0.47	2.62	12	2
1:A:79:VAL:HG22	1:A:83:PHE:CZ	0.47	2.43	11	1
2:B:236:LYS:O	2:B:240:ALA:N	0.47	2.39	17	2
1:A:56:ASP:O	2:B:288:ASP:OD2	0.47	2.32	14	1
2:B:349:ARG:HE	2:B:373:ASP:C	0.47	2.17	15	1
2:B:235:GLN:OE1	2:B:363:ALA:HB3	0.47	2.09	16	1
2:B:251:ASP:OD1	2:B:253:ARG:CZ	0.47	2.62	16	1
1:A:80:ILE:HG22	1:A:81:ALA:N	0.47	2.24	16	9
2:B:387:ASP:OD1	2:B:387:ASP:C	0.47	2.57	5	10
1:A:71:GLN:CG	1:A:74:GLU:CB	0.47	2.91	3	1
1:A:80:ILE:C	1:A:80:ILE:CD1	0.47	2.84	3	1
2:B:349:ARG:CB	2:B:372:ALA:O	0.47	2.63	3	2
1:A:76:LEU:O	1:A:80:ILE:CG2	0.47	2.41	9	2
1:A:5:GLN:OE1	1:A:7:VAL:HG23	0.47	2.09	14	1
1:A:38:ASN:HA	1:A:63:ILE:HG22	0.47	1.86	14	2
2:B:230:PHE:CE2	2:B:239:ALA:CB	0.47	2.95	16	1
1:A:15:MET:HE3	1:A:19:PRO:HD2	0.47	1.84	20	1
2:B:293:GLU:O	2:B:294:ARG:C	0.47	2.58	17	5
2:B:293:GLU:O	2:B:295:ALA:N	0.47	2.48	2	3
1:A:53:LEU:HG	1:A:54:MET:N	0.47	2.22	11	2
2:B:226:TYR:O	2:B:229:ARG:CG	0.47	2.63	12	2
2:B:247:HIS:HA	2:B:250:SER:OG	0.47	2.09	7	2
2:B:221:ASN:OD1	2:B:224:ARG:NH2	0.47	2.48	14	1
2:B:180:VAL:HG22	2:B:181:ALA:N	0.47	2.25	15	1
1:A:49:VAL:CG2	2:B:248:LEU:HD11	0.47	2.39	19	1
2:B:186:TRP:CG	2:B:342:ARG:HH12	0.47	2.28	19	1
1:A:45:GLU:CD	1:A:47:ASN:HD21	0.47	2.17	2	1
2:B:223:PHE:CZ	2:B:304:ARG:CZ	0.47	2.97	20	2
2:B:374:ILE:HG23	2:B:374:ILE:O	0.47	2.08	3	1
2:B:376:PRO:O	2:B:380:HIS:ND1	0.47	2.48	3	1
2:B:239:ALA:O	2:B:243:ASP:CG	0.47	2.58	14	2
2:B:288:ASP:OD2	2:B:291:LEU:HB2	0.47	2.10	12	1
2:B:267:VAL:O	2:B:268:ALA:C	0.47	2.57	20	1
2:B:384:LEU:O	2:B:384:LEU:CD1	0.47	2.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLU:OE1	1:A:43:GLU:CA	0.47	2.60	1	1
2:B:170:ARG:N	2:B:393:LEU:O	0.47	2.47	19	4
1:A:47:ASN:OD1	1:A:47:ASN:C	0.47	2.57	3	2
2:B:328:ASP:N	2:B:328:ASP:OD1	0.47	2.43	9	4
2:B:227:SER:O	2:B:228:LYS:C	0.47	2.57	3	2
2:B:335:LEU:O	2:B:337:GLU:N	0.47	2.48	3	1
2:B:245:TYR:CD1	2:B:245:TYR:O	0.47	2.68	5	1
2:B:393:LEU:H	2:B:393:LEU:CD2	0.47	2.05	8	1
1:A:71:GLN:C	1:A:74:GLU:HG3	0.47	2.31	12	1
2:B:176:ALA:CB	2:B:370:MET:SD	0.47	2.92	12	1
2:B:245:TYR:HA	2:B:248:LEU:HD22	0.47	1.86	14	1
1:A:11:ASN:CG	1:A:11:ASN:O	0.47	2.57	16	1
1:A:13:LEU:C	1:A:13:LEU:CD1	0.47	2.87	17	1
2:B:244:LEU:HD12	2:B:245:TYR:CA	0.47	2.39	17	1
1:A:30:PHE:HA	1:A:71:GLN:OE1	0.47	2.10	20	1
2:B:335:LEU:HD21	2:B:343:LEU:CD1	0.47	2.40	2	1
2:B:303:GLN:CG	2:B:304:ARG:N	0.47	2.76	3	2
2:B:349:ARG:HB2	2:B:372:ALA:O	0.47	2.09	3	2
2:B:272:VAL:HG23	2:B:273:LYS:N	0.47	2.25	4	1
1:A:63:ILE:HG22	1:A:64:GLU:N	0.47	2.23	5	2
2:B:281:GLU:OE1	2:B:281:GLU:N	0.47	2.48	10	2
2:B:291:LEU:C	2:B:293:GLU:OE1	0.47	2.58	14	1
2:B:203:LEU:HD23	2:B:203:LEU:H	0.47	1.60	15	2
2:B:248:LEU:O	2:B:248:LEU:HD23	0.47	2.10	15	1
1:A:16:HIS:O	1:A:16:HIS:CG	0.47	2.67	19	1
2:B:383:THR:O	2:B:396:ASP:OD1	0.47	2.33	20	1
1:A:79:VAL:HG12	1:A:80:ILE:N	0.47	2.25	2	2
2:B:253:ARG:C	2:B:253:ARG:CD	0.47	2.88	5	2
1:A:50:ILE:HG12	1:A:51:ALA:N	0.47	2.25	8	2
1:A:79:VAL:HG23	1:A:80:ILE:N	0.47	2.24	8	3
2:B:235:GLN:NE2	2:B:237:GLU:OE1	0.47	2.48	15	2
2:B:211:ARG:HH22	2:B:269:GLU:CD	0.47	2.18	13	1
2:B:343:LEU:C	2:B:343:LEU:HD23	0.47	2.35	13	1
2:B:366:ILE:HG23	2:B:366:ILE:O	0.47	2.10	16	1
2:B:288:ASP:O	2:B:291:LEU:HG	0.47	2.09	20	2
1:A:53:LEU:HD13	2:B:286:LEU:HB2	0.47	1.87	11	1
2:B:350:ASP:C	2:B:350:ASP:OD1	0.47	2.58	12	1
2:B:353:ALA:O	2:B:354:ASN:C	0.47	2.58	12	1
1:A:83:PHE:CD2	1:A:83:PHE:N	0.47	2.82	16	1
2:B:293:GLU:CG	2:B:294:ARG:N	0.47	2.78	16	1
2:B:225:ARG:C	2:B:229:ARG:NH2	0.47	2.74	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:MET:HE1	1:A:61:ARG:HH12	0.46	1.69	1	1
2:B:272:VAL:O	2:B:276:ILE:HD13	0.46	2.10	1	2
2:B:251:ASP:OD1	2:B:253:ARG:HB2	0.46	2.10	4	1
2:B:381:ARG:H	2:B:381:ARG:HD3	0.46	1.70	4	1
1:A:12:LYS:O	1:A:12:LYS:HG3	0.46	2.10	12	2
1:A:40:GLU:OE2	1:A:61:ARG:CZ	0.46	2.63	6	1
1:A:76:LEU:C	1:A:76:LEU:CD2	0.46	2.89	14	3
2:B:226:TYR:CE1	2:B:229:ARG:NH1	0.46	2.83	6	1
2:B:235:GLN:CD	2:B:238:THR:OG1	0.46	2.58	6	1
1:A:18:ARG:O	1:A:22:LYS:HB2	0.46	2.10	9	2
2:B:257:GLU:OE1	2:B:279:PHE:CE1	0.46	2.68	11	2
2:B:299:ARG:HD2	2:B:299:ARG:O	0.46	2.10	14	1
2:B:335:LEU:HD21	2:B:343:LEU:HD22	0.46	1.87	15	1
1:A:38:ASN:HA	1:A:63:ILE:CG2	0.46	2.40	20	1
1:A:12:LYS:C	1:A:14:GLY:N	0.46	2.73	18	4
2:B:249:LEU:HD21	2:B:301:LEU:HD13	0.46	1.86	2	1
2:B:271:ALA:O	2:B:275:VAL:CG2	0.46	2.63	11	4
2:B:245:TYR:OH	2:B:301:LEU:HD13	0.46	2.10	4	1
2:B:270:TRP:O	2:B:274:THR:OG1	0.46	2.32	4	1
1:A:6:THR:HG23	1:A:6:THR:O	0.46	2.11	5	1
1:A:7:VAL:HG23	1:A:7:VAL:O	0.46	2.11	5	1
2:B:283:PHE:C	2:B:285:ALA:N	0.46	2.71	8	1
1:A:24:PHE:O	1:A:28:GLN:NE2	0.46	2.49	13	1
2:B:355:SER:O	2:B:356:GLN:C	0.46	2.58	15	1
2:B:259:PHE:CE2	2:B:263:ASP:OD2	0.46	2.68	16	1
1:A:36:LEU:HD12	1:A:36:LEU:N	0.46	2.25	18	1
2:B:340:GLN:O	2:B:343:LEU:O	0.46	2.33	1	1
2:B:227:SER:CB	2:B:242:PHE:HB3	0.46	2.41	3	2
1:A:53:LEU:HB2	2:B:291:LEU:HD22	0.46	1.87	16	2
2:B:330:LEU:HD21	2:B:348:VAL:CG1	0.46	2.41	8	1
2:B:289:ASN:O	2:B:291:LEU:N	0.46	2.49	14	1
2:B:182:ILE:O	2:B:322:ARG:NH2	0.46	2.49	16	1
2:B:335:LEU:C	2:B:335:LEU:CD2	0.46	2.85	17	1
1:A:15:MET:HE2	1:A:15:MET:H	0.46	1.71	20	1
1:A:37:ARG:H	1:A:63:ILE:HD12	0.46	1.71	2	1
2:B:324:ILE:CG2	2:B:325:LEU:N	0.46	2.76	7	2
2:B:361:VAL:HG23	2:B:362:ARG:N	0.46	2.25	4	4
2:B:186:TRP:O	2:B:326:VAL:CG2	0.46	2.63	7	1
2:B:276:ILE:HG22	2:B:277:GLU:N	0.46	2.25	9	1
2:B:243:ASP:OD1	2:B:243:ASP:C	0.46	2.58	13	1
2:B:273:LYS:O	2:B:277:GLU:HG2	0.46	2.09	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:343:LEU:HD23	2:B:344:VAL:N	0.46	2.26	1	1
2:B:288:ASP:OD2	2:B:290:TYR:HB2	0.46	2.10	4	1
2:B:359:ILE:CG2	2:B:360:MET:N	0.46	2.78	7	1
2:B:349:ARG:NH2	2:B:376:PRO:HD3	0.46	2.25	10	1
2:B:386:VAL:HG22	2:B:393:LEU:CD1	0.46	2.41	11	1
2:B:297:ASP:OD1	2:B:356:GLN:NE2	0.46	2.49	14	1
1:A:27:MET:CA	1:A:30:PHE:CE2	0.46	2.99	10	3
1:A:30:PHE:CG	1:A:71:GLN:CD	0.46	2.93	3	1
1:A:18:ARG:O	1:A:21:MET:HG3	0.46	2.11	4	1
2:B:251:ASP:CG	2:B:253:ARG:CB	0.46	2.88	6	1
2:B:293:GLU:HA	2:B:293:GLU:OE1	0.46	2.11	11	1
2:B:184:GLU:N	2:B:184:GLU:CD	0.46	2.74	13	1
2:B:244:LEU:O	2:B:248:LEU:HG	0.46	2.11	4	1
2:B:392:GLU:O	2:B:392:GLU:CD	0.46	2.59	8	1
2:B:245:TYR:CZ	2:B:297:ASP:HB2	0.46	2.45	9	1
2:B:293:GLU:C	2:B:293:GLU:CD	0.46	2.84	9	2
2:B:262:VAL:CG2	2:B:263:ASP:N	0.46	2.78	20	1
2:B:256:ARG:O	2:B:260:ALA:CB	0.46	2.64	12	1
2:B:394:LEU:HD22	2:B:397:PRO:HB3	0.46	1.86	13	1
2:B:279:PHE:CE2	2:B:298:LEU:HB3	0.46	2.46	20	1
2:B:297:ASP:OD2	2:B:333:THR:HG23	0.46	2.10	20	1
2:B:235:GLN:HG2	2:B:236:LYS:N	0.46	2.26	2	2
2:B:288:ASP:CB	2:B:291:LEU:HD21	0.46	2.39	7	1
2:B:355:SER:OG	2:B:358:ALA:CB	0.46	2.64	10	1
2:B:297:ASP:CG	2:B:356:GLN:HE22	0.46	2.19	14	1
2:B:171:ILE:HD12	2:B:393:LEU:HD11	0.46	1.87	16	1
2:B:325:LEU:HD23	2:B:326:VAL:N	0.46	2.26	8	3
2:B:329:GLU:O	2:B:329:GLU:OE1	0.46	2.33	7	1
1:A:14:GLY:C	1:A:16:HIS:H	0.46	2.19	9	1
1:A:65:VAL:HG23	1:A:65:VAL:O	0.46	2.11	10	1
2:B:338:LEU:HD23	2:B:338:LEU:H	0.46	1.71	13	1
1:A:15:MET:HG2	1:A:16:HIS:H	0.46	1.69	20	1
2:B:388:GLY:O	2:B:389:TYR:C	0.45	2.59	3	3
2:B:379:LEU:HA	2:B:382:ARG:HB2	0.45	1.89	4	1
2:B:376:PRO:HA	2:B:379:LEU:HD12	0.45	1.88	8	1
2:B:210:GLU:CG	2:B:211:ARG:N	0.45	2.79	16	1
2:B:343:LEU:HD23	2:B:345:GLY:H	0.45	1.71	19	1
2:B:172:ARG:CD	2:B:172:ARG:N	0.45	2.79	20	1
2:B:294:ARG:NH1	2:B:297:ASP:CG	0.45	2.72	2	1
2:B:268:ALA:O	2:B:272:VAL:N	0.45	2.38	5	1
1:A:65:VAL:O	1:A:65:VAL:CG2	0.45	2.64	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:248:LEU:CD2	2:B:253:ARG:HH11	0.45	2.23	12	1
2:B:301:LEU:HD23	2:B:301:LEU:O	0.45	2.11	13	1
2:B:288:ASP:CB	2:B:291:LEU:HD11	0.45	2.42	14	1
2:B:283:PHE:CE1	2:B:298:LEU:HD12	0.45	2.46	15	1
2:B:182:ILE:O	2:B:183:ALA:HB2	0.45	2.10	13	4
2:B:286:LEU:CD1	2:B:291:LEU:HB3	0.45	2.41	4	1
2:B:310:ASP:O	2:B:311:ASP:C	0.45	2.59	5	3
1:A:36:LEU:N	1:A:36:LEU:CD1	0.45	2.72	8	3
2:B:224:ARG:CZ	2:B:225:ARG:HH22	0.45	2.24	9	1
2:B:244:LEU:O	2:B:248:LEU:HD13	0.45	2.12	14	1
2:B:289:ASN:C	2:B:291:LEU:N	0.45	2.72	14	1
2:B:394:LEU:HD12	2:B:397:PRO:HG3	0.45	1.89	5	1
2:B:212:LEU:HB3	2:B:255:ARG:NH2	0.45	2.27	6	1
2:B:394:LEU:HD23	2:B:397:PRO:HG3	0.45	1.87	8	1
2:B:256:ARG:NH2	2:B:260:ALA:CB	0.45	2.79	11	1
1:A:71:GLN:HB2	1:A:74:GLU:OE2	0.45	2.11	12	1
2:B:300:ALA:HB1	2:B:333:THR:OG1	0.45	2.10	12	1
2:B:187:GLN:H	2:B:187:GLN:CD	0.45	2.19	19	1
2:B:247:HIS:O	2:B:251:ASP:N	0.45	2.50	14	3
2:B:342:ARG:CD	2:B:342:ARG:C	0.45	2.90	4	1
1:A:50:ILE:O	1:A:53:LEU:CG	0.45	2.52	7	1
2:B:177:ALA:CB	2:B:366:ILE:O	0.45	2.64	10	1
2:B:378:VAL:O	2:B:380:HIS:CE1	0.45	2.69	11	1
1:A:6:THR:N	1:A:64:GLU:OE2	0.45	2.50	13	1
2:B:290:TYR:C	2:B:293:GLU:OE1	0.45	2.59	14	1
1:A:18:ARG:HA	1:A:18:ARG:HE	0.45	1.72	1	1
2:B:249:LEU:HD21	2:B:301:LEU:HD22	0.45	1.87	2	1
2:B:384:LEU:C	2:B:385:ILE:HD12	0.45	2.36	2	1
2:B:394:LEU:HD22	2:B:394:LEU:H	0.45	1.62	7	1
1:A:15:MET:HE3	1:A:18:ARG:HG2	0.45	1.89	9	1
1:A:21:MET:CB	2:B:244:LEU:HD13	0.45	2.42	10	1
2:B:235:GLN:NE2	2:B:237:GLU:CG	0.45	2.79	14	1
2:B:203:LEU:O	2:B:203:LEU:HG	0.45	2.11	18	1
2:B:244:LEU:HD23	2:B:294:ARG:HH11	0.45	1.72	18	1
2:B:247:HIS:CG	2:B:248:LEU:N	0.45	2.83	19	1
2:B:171:ILE:HD13	2:B:373:ASP:OD1	0.45	2.12	20	1
2:B:286:LEU:HB3	2:B:291:LEU:HD21	0.45	1.83	20	1
2:B:184:GLU:HB2	2:B:323:PHE:CZ	0.45	2.46	4	1
2:B:288:ASP:OD2	2:B:291:LEU:N	0.45	2.45	5	1
1:A:53:LEU:HA	2:B:291:LEU:HD13	0.45	1.89	9	1
1:A:61:ARG:C	1:A:62:GLN:NE2	0.45	2.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:235:GLN:N	2:B:235:GLN:OE1	0.45	2.49	13	1
2:B:276:ILE:HD13	2:B:302:GLY:HA2	0.45	1.89	14	1
2:B:289:ASN:O	2:B:290:TYR:C	0.45	2.60	14	1
1:A:5:GLN:N	1:A:64:GLU:OE2	0.45	2.50	15	1
2:B:293:GLU:C	2:B:295:ALA:N	0.45	2.70	2	4
1:A:45:GLU:CD	1:A:47:ASN:OD1	0.45	2.60	2	1
1:A:80:ILE:HG13	1:A:81:ALA:N	0.45	2.27	11	3
2:B:205:PRO:O	2:B:209:ARG:HB3	0.45	2.12	7	2
1:A:53:LEU:HD13	2:B:291:LEU:HD12	0.45	1.86	6	1
2:B:171:ILE:HD12	2:B:171:ILE:N	0.45	2.27	6	2
1:A:43:GLU:CD	1:A:43:GLU:O	0.45	2.59	8	2
2:B:227:SER:HB3	2:B:242:PHE:CG	0.45	2.46	9	1
1:A:40:GLU:OE2	1:A:40:GLU:N	0.45	2.49	12	1
2:B:395:VAL:HG12	2:B:396:ASP:CG	0.45	2.37	13	1
1:A:18:ARG:HE	1:A:18:ARG:CA	0.45	2.24	17	1
2:B:244:LEU:O	2:B:244:LEU:CD2	0.45	2.60	19	1
2:B:245:TYR:CE2	2:B:249:LEU:HD12	0.45	2.46	4	1
2:B:373:ASP:OD1	2:B:373:ASP:N	0.45	2.46	8	1
2:B:225:ARG:O	2:B:229:ARG:HG3	0.45	2.12	11	1
1:A:26:LEU:HG	1:A:30:PHE:CD1	0.45	2.46	12	1
1:A:30:PHE:CG	1:A:74:GLU:OE1	0.45	2.69	12	1
2:B:217:GLU:HG3	2:B:218:GLU:N	0.45	2.27	14	1
1:A:36:LEU:HD22	1:A:65:VAL:HG22	0.45	1.88	15	1
2:B:250:SER:O	2:B:255:ARG:NH1	0.45	2.50	15	1
2:B:216:LEU:HD23	2:B:216:LEU:C	0.45	2.36	17	1
2:B:354:ASN:OD1	2:B:355:SER:N	0.45	2.50	5	1
2:B:385:ILE:HG23	2:B:394:LEU:CB	0.45	2.42	5	1
2:B:256:ARG:CG	2:B:257:GLU:N	0.45	2.79	12	2
1:A:4:LYS:N	1:A:4:LYS:HD2	0.45	2.26	15	1
1:A:18:ARG:NH1	1:A:21:MET:CE	0.45	2.80	16	1
1:A:48:SER:OG	2:B:253:ARG:CZ	0.44	2.65	2	1
2:B:235:GLN:HG3	2:B:237:GLU:H	0.44	1.72	3	1
2:B:206:ALA:O	2:B:210:GLU:HB2	0.44	2.13	6	2
2:B:270:TRP:O	2:B:274:THR:CB	0.44	2.66	4	1
2:B:205:PRO:O	2:B:209:ARG:CG	0.44	2.66	6	1
1:A:30:PHE:HA	1:A:71:GLN:NE2	0.44	2.27	7	1
2:B:272:VAL:O	2:B:276:ILE:HG22	0.44	2.12	11	1
2:B:350:ASP:CG	2:B:351:GLY:H	0.44	2.20	11	1
1:A:76:LEU:CD2	1:A:76:LEU:O	0.44	2.65	14	1
2:B:342:ARG:O	2:B:344:VAL:HG23	0.44	2.13	15	1
2:B:230:PHE:O	2:B:231:ALA:C	0.44	2.61	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:349:ARG:CZ	2:B:374:ILE:O	0.44	2.65	17	1
1:A:3:VAL:O	1:A:3:VAL:HG12	0.44	2.12	18	1
1:A:9:ILE:HD12	1:A:13:LEU:HA	0.44	1.89	20	1
2:B:216:LEU:CD1	2:B:255:ARG:NH2	0.44	2.80	10	1
2:B:256:ARG:CZ	2:B:259:PHE:CD2	0.44	3.01	10	1
2:B:309:LEU:O	2:B:309:LEU:CG	0.44	2.62	14	1
2:B:355:SER:O	2:B:358:ALA:N	0.44	2.50	15	1
1:A:49:VAL:HG23	2:B:248:LEU:HD11	0.44	1.89	19	1
2:B:272:VAL:CG1	2:B:273:LYS:N	0.44	2.80	1	1
2:B:212:LEU:HD21	2:B:258:LEU:CB	0.44	2.42	4	1
1:A:72:GLU:HG2	1:A:73:GLU:N	0.44	2.26	10	1
2:B:259:PHE:N	2:B:259:PHE:HD1	0.44	2.06	11	1
2:B:245:TYR:CE1	2:B:297:ASP:HB3	0.44	2.48	19	2
1:A:36:LEU:O	1:A:43:GLU:OE2	0.44	2.35	17	1
2:B:288:ASP:CB	2:B:291:LEU:HD22	0.44	2.37	18	1
1:A:2:THR:HG22	1:A:3:VAL:N	0.44	2.27	10	2
2:B:231:ALA:C	2:B:233:GLY:N	0.44	2.76	4	1
1:A:84:ASN:O	1:A:85:SER:HB3	0.44	2.12	9	1
2:B:338:LEU:HD12	2:B:342:ARG:NH2	0.44	2.28	9	1
2:B:279:PHE:O	2:B:282:GLN:HG2	0.44	2.12	11	1
2:B:297:ASP:O	2:B:301:LEU:HD12	0.44	2.13	12	1
2:B:392:GLU:HG2	2:B:393:LEU:N	0.44	2.28	17	2
1:A:59:LYS:CG	1:A:59:LYS:O	0.44	2.65	20	1
2:B:248:LEU:O	2:B:248:LEU:HD22	0.44	2.13	3	1
1:A:12:LYS:O	1:A:12:LYS:HG2	0.44	2.13	12	2
2:B:308:HIS:O	2:B:310:ASP:N	0.44	2.51	8	2
1:A:35:LEU:C	1:A:36:LEU:HD22	0.44	2.37	10	1
2:B:349:ARG:CG	2:B:350:ASP:N	0.44	2.79	16	1
2:B:324:ILE:C	2:B:324:ILE:HD12	0.44	2.36	20	1
2:B:267:VAL:O	2:B:271:ALA:N	0.44	2.40	5	2
1:A:33:GLU:OE2	1:A:34:VAL:N	0.44	2.50	4	1
2:B:270:TRP:CH2	2:B:274:THR:OG1	0.44	2.66	5	1
2:B:207:LEU:O	2:B:211:ARG:N	0.44	2.43	15	2
2:B:209:ARG:HH22	2:B:256:ARG:HH22	0.44	1.56	9	1
2:B:256:ARG:HE	2:B:256:ARG:HA	0.44	1.71	14	2
2:B:273:LYS:O	2:B:276:ILE:HG12	0.44	2.13	15	1
1:A:18:ARG:NE	1:A:18:ARG:H	0.44	2.08	16	1
2:B:218:GLU:CD	2:B:308:HIS:HD1	0.44	2.20	19	1
1:A:44:ALA:O	1:A:45:GLU:C	0.44	2.61	12	20
1:A:23:LEU:HD23	1:A:46:ALA:HB1	0.44	1.88	7	1
2:B:331:SER:HB3	2:B:333:THR:HG22	0.44	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:240:ALA:O	2:B:244:LEU:HD12	0.44	2.13	10	1
1:A:49:VAL:HG21	2:B:248:LEU:CD1	0.44	2.43	15	1
2:B:374:ILE:O	2:B:374:ILE:HG23	0.44	2.12	15	1
2:B:346:VAL:CG2	2:B:368:THR:HG23	0.44	2.42	16	1
2:B:301:LEU:HD12	2:B:305:LEU:HD23	0.44	1.88	17	1
1:A:55:LEU:HD23	1:A:55:LEU:O	0.44	2.12	20	1
2:B:360:MET:HG2	2:B:361:VAL:N	0.44	2.27	1	1
2:B:396:ASP:N	2:B:396:ASP:OD1	0.44	2.50	4	1
2:B:223:PHE:CZ	2:B:301:LEU:CD2	0.44	3.00	6	1
2:B:248:LEU:O	2:B:251:ASP:HB3	0.44	2.13	6	2
1:A:65:VAL:HG11	1:A:79:VAL:HG11	0.44	1.89	12	3
2:B:374:ILE:HG21	2:B:379:LEU:HD21	0.44	1.90	8	1
1:A:18:ARG:NH1	2:B:240:ALA:CB	0.44	2.81	9	2
2:B:342:ARG:HG3	2:B:343:LEU:N	0.44	2.28	15	2
1:A:18:ARG:NH1	1:A:21:MET:HE1	0.44	2.28	16	1
2:B:216:LEU:CD2	2:B:217:GLU:N	0.44	2.71	17	1
2:B:301:LEU:C	2:B:301:LEU:CD2	0.44	2.91	18	1
2:B:348:VAL:HG22	2:B:349:ARG:N	0.44	2.28	18	1
2:B:329:GLU:C	2:B:329:GLU:OE1	0.44	2.61	1	1
2:B:288:ASP:O	2:B:291:LEU:HB3	0.44	2.13	12	2
2:B:218:GLU:CD	2:B:218:GLU:C	0.44	2.86	10	2
2:B:325:LEU:C	2:B:325:LEU:CD2	0.44	2.90	8	1
2:B:205:PRO:O	2:B:206:ALA:C	0.44	2.61	19	1
2:B:270:TRP:CD2	2:B:274:THR:OG1	0.44	2.70	19	1
2:B:270:TRP:O	2:B:274:THR:HG23	0.43	2.12	1	1
1:A:17:ALA:O	1:A:18:ARG:CZ	0.43	2.66	2	1
2:B:218:GLU:O	2:B:222:GLU:HB2	0.43	2.13	3	2
1:A:20:ALA:O	1:A:24:PHE:CZ	0.43	2.71	7	1
2:B:187:GLN:CD	2:B:187:GLN:O	0.43	2.61	12	1
1:A:27:MET:HE2	1:A:32:ALA:O	0.43	2.13	15	1
2:B:237:GLU:HG2	2:B:238:THR:N	0.43	2.28	17	1
1:A:30:PHE:C	1:A:30:PHE:HD1	0.43	2.18	3	3
2:B:382:ARG:NH1	2:B:396:ASP:OD1	0.43	2.52	6	1
1:A:26:LEU:HD12	1:A:30:PHE:CD1	0.43	2.48	7	1
2:B:171:ILE:C	2:B:392:GLU:CD	0.43	2.86	7	1
1:A:4:LYS:C	1:A:5:GLN:CG	0.43	2.91	8	1
2:B:308:HIS:C	2:B:310:ASP:H	0.43	2.21	8	1
1:A:30:PHE:HB3	1:A:74:GLU:OE2	0.43	2.13	12	1
2:B:208:GLU:HG3	2:B:268:ALA:HB2	0.43	1.88	19	1
2:B:326:VAL:O	2:B:326:VAL:CG1	0.43	2.64	20	2
2:B:342:ARG:CD	2:B:342:ARG:O	0.43	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLU:OE1	1:A:43:GLU:N	0.43	2.51	4	1
2:B:229:ARG:CG	2:B:230:PHE:N	0.43	2.80	9	1
2:B:345:GLY:C	2:B:346:VAL:CG2	0.43	2.91	10	1
1:A:36:LEU:O	1:A:37:ARG:HG2	0.43	2.13	13	1
2:B:219:ALA:HB2	2:B:308:HIS:ND1	0.43	2.28	14	2
2:B:292:LYS:HG2	2:B:293:GLU:N	0.43	2.28	1	2
2:B:227:SER:O	2:B:230:PHE:N	0.43	2.51	4	1
1:A:21:MET:SD	2:B:244:LEU:HD12	0.43	2.53	5	1
2:B:277:GLU:OE2	2:B:281:GLU:OE2	0.43	2.36	8	1
2:B:291:LEU:O	2:B:294:ARG:CB	0.43	2.67	8	1
1:A:27:MET:HE1	1:A:32:ALA:O	0.43	2.12	15	1
2:B:299:ARG:HG2	2:B:300:ALA:N	0.43	2.28	16	1
1:A:8:GLU:CD	1:A:8:GLU:C	0.43	2.87	17	1
2:B:288:ASP:O	2:B:288:ASP:OD1	0.43	2.37	17	1
2:B:223:PHE:CE2	2:B:304:ARG:NH1	0.43	2.87	20	1
2:B:173:ALA:HB2	2:B:393:LEU:HD11	0.43	1.90	19	2
2:B:203:LEU:HD12	2:B:203:LEU:N	0.43	2.26	1	1
2:B:217:GLU:N	2:B:217:GLU:CD	0.43	2.75	1	1
1:A:27:MET:C	1:A:28:GLN:OE1	0.43	2.62	3	1
2:B:184:GLU:OE1	2:B:381:ARG:CG	0.43	2.66	3	1
2:B:323:PHE:C	2:B:342:ARG:NH1	0.43	2.77	4	1
2:B:221:ASN:O	2:B:225:ARG:HD3	0.43	2.13	7	2
2:B:375:GLN:OE1	2:B:375:GLN:CA	0.43	2.67	14	1
1:A:6:THR:HG23	1:A:62:GLN:OE1	0.43	2.14	3	1
2:B:216:LEU:HD22	2:B:255:ARG:CZ	0.43	2.44	7	1
2:B:258:LEU:C	2:B:258:LEU:CD2	0.43	2.92	7	1
2:B:281:GLU:O	2:B:285:ALA:N	0.43	2.52	7	1
2:B:350:ASP:OD1	2:B:350:ASP:C	0.43	2.60	7	1
2:B:212:LEU:CD1	2:B:258:LEU:HD13	0.43	2.43	15	1
1:A:15:MET:CE	1:A:20:ALA:HB2	0.43	2.43	18	1
2:B:278:LYS:O	2:B:282:GLN:CG	0.43	2.66	18	1
2:B:286:LEU:N	2:B:286:LEU:CD2	0.43	2.82	18	1
2:B:209:ARG:HG3	2:B:210:GLU:N	0.43	2.28	6	1
2:B:283:PHE:O	2:B:284:ALA:C	0.43	2.62	6	1
2:B:382:ARG:NH1	2:B:396:ASP:CG	0.43	2.77	6	1
2:B:359:ILE:HG23	2:B:360:MET:N	0.43	2.28	7	1
2:B:222:GLU:HG2	2:B:226:TYR:CD1	0.43	2.49	9	1
2:B:249:LEU:CD1	2:B:305:LEU:HD11	0.43	2.44	9	1
2:B:353:ALA:C	2:B:355:SER:N	0.43	2.76	12	1
1:A:45:GLU:OE2	1:A:47:ASN:OD1	0.43	2.37	17	1
2:B:384:LEU:N	2:B:384:LEU:HD12	0.43	2.25	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ASN:ND2	1:A:55:LEU:HD23	0.43	2.28	3	1
2:B:171:ILE:O	2:B:393:LEU:HD22	0.43	2.14	8	1
2:B:286:LEU:O	2:B:292:LYS:NZ	0.43	2.51	8	1
1:A:56:ASP:CG	2:B:288:ASP:CG	0.43	2.86	10	1
1:A:3:VAL:O	1:A:76:LEU:HD12	0.43	2.14	11	2
2:B:236:LYS:O	2:B:237:GLU:C	0.43	2.61	14	3
2:B:238:THR:O	2:B:241:ILE:HG13	0.43	2.13	17	2
2:B:395:VAL:HG12	2:B:396:ASP:OD1	0.43	2.13	13	1
1:A:73:GLU:HG2	1:A:74:GLU:H	0.43	1.74	19	1
2:B:210:GLU:C	2:B:210:GLU:CD	0.43	2.86	20	2
2:B:273:LYS:HG3	2:B:274:THR:H	0.43	1.74	4	1
1:A:14:GLY:C	1:A:16:HIS:N	0.43	2.77	9	1
1:A:15:MET:O	1:A:16:HIS:CB	0.43	2.67	9	1
2:B:256:ARG:NE	2:B:256:ARG:HA	0.43	2.29	9	1
2:B:305:LEU:O	2:B:309:LEU:HB2	0.43	2.14	9	1
2:B:248:LEU:HD12	2:B:253:ARG:HH22	0.43	1.72	11	1
1:A:20:ALA:HB1	1:A:52:LEU:HD22	0.43	1.90	13	1
1:A:39:ASP:OD1	1:A:39:ASP:O	0.43	2.37	20	1
2:B:325:LEU:O	2:B:346:VAL:HG23	0.43	2.14	1	1
2:B:384:LEU:HD11	2:B:393:LEU:HD11	0.43	1.90	2	2
2:B:362:ARG:CG	2:B:363:ALA:N	0.43	2.81	6	1
2:B:186:TRP:O	2:B:326:VAL:HG22	0.43	2.14	7	1
2:B:329:GLU:O	2:B:329:GLU:CD	0.43	2.62	7	1
2:B:203:LEU:CD1	2:B:203:LEU:H	0.43	2.03	8	1
2:B:349:ARG:NH1	2:B:375:GLN:OE1	0.43	2.51	11	2
1:A:35:LEU:CD2	1:A:37:ARG:HE	0.43	2.22	13	1
2:B:219:ALA:HA	2:B:222:GLU:HG2	0.43	1.90	15	1
2:B:283:PHE:O	2:B:291:LEU:HD21	0.43	2.14	15	1
2:B:286:LEU:HB2	2:B:291:LEU:HD22	0.43	1.91	15	1
2:B:301:LEU:HD13	2:B:301:LEU:O	0.43	2.14	15	1
2:B:349:ARG:HE	2:B:374:ILE:N	0.43	2.12	15	1
1:A:69:GLY:O	1:A:72:GLU:HG2	0.43	2.14	16	1
1:A:71:GLN:NE2	1:A:74:GLU:HG3	0.43	2.28	18	1
2:B:343:LEU:HD23	2:B:343:LEU:C	0.43	2.39	19	1
2:B:390:ARG:O	2:B:390:ARG:HG3	0.43	2.14	20	1
1:A:22:LYS:O	1:A:26:LEU:HD23	0.42	2.14	4	1
2:B:347:VAL:O	2:B:347:VAL:HG22	0.42	2.13	6	1
2:B:293:GLU:O	2:B:296:GLY:N	0.42	2.51	8	1
2:B:273:LYS:HZ2	2:B:273:LYS:HB2	0.42	1.73	9	1
2:B:387:ASP:O	2:B:388:GLY:C	0.42	2.62	11	1
1:A:35:LEU:HD21	1:A:37:ARG:CZ	0.42	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:299:ARG:HD2	2:B:299:ARG:C	0.42	2.38	13	1
2:B:249:LEU:CG	2:B:250:SER:N	0.42	2.81	15	1
1:A:56:ASP:OD2	2:B:291:LEU:CG	0.42	2.67	17	1
2:B:324:ILE:CD1	2:B:326:VAL:HG13	0.42	2.44	17	1
2:B:186:TRP:CD1	2:B:342:ARG:HH12	0.42	2.32	19	1
2:B:238:THR:OG1	2:B:360:MET:SD	0.42	2.70	2	1
1:A:8:GLU:O	1:A:83:PHE:CE1	0.42	2.72	3	1
1:A:26:LEU:HB3	1:A:30:PHE:CE2	0.42	2.49	9	2
2:B:288:ASP:OD1	2:B:291:LEU:N	0.42	2.47	4	1
2:B:243:ASP:C	2:B:243:ASP:OD1	0.42	2.61	5	1
2:B:348:VAL:CG2	2:B:350:ASP:O	0.42	2.68	8	1
2:B:355:SER:OG	2:B:358:ALA:HB2	0.42	2.14	10	2
2:B:245:TYR:CZ	2:B:294:ARG:NE	0.42	2.86	12	1
1:A:35:LEU:HD12	1:A:36:LEU:N	0.42	2.29	13	1
2:B:176:ALA:O	2:B:362:ARG:HD3	0.42	2.14	18	1
1:A:23:LEU:HD13	1:A:79:VAL:HG23	0.42	1.91	7	1
2:B:288:ASP:HB3	2:B:291:LEU:CG	0.42	2.44	7	2
2:B:245:TYR:CE2	2:B:294:ARG:NH2	0.42	2.87	9	1
2:B:283:PHE:HB3	2:B:295:ALA:HB2	0.42	1.91	12	1
2:B:322:ARG:O	2:B:323:PHE:HB3	0.42	2.13	12	1
1:A:56:ASP:OD2	2:B:288:ASP:OD2	0.42	2.36	16	1
2:B:209:ARG:O	2:B:212:LEU:HG	0.42	2.15	18	1
2:B:263:ASP:O	2:B:263:ASP:CG	0.42	2.61	18	1
2:B:222:GLU:CD	2:B:304:ARG:NH1	0.42	2.77	19	1
1:A:72:GLU:CD	1:A:72:GLU:C	0.42	2.87	1	1
2:B:350:ASP:C	2:B:352:ALA:N	0.42	2.76	3	2
2:B:258:LEU:CD1	2:B:272:VAL:HG12	0.42	2.45	2	1
1:A:5:GLN:HE22	1:A:80:ILE:HB	0.42	1.75	15	2
2:B:245:TYR:O	2:B:246:SER:C	0.42	2.62	12	1
2:B:289:ASN:OD1	2:B:290:TYR:N	0.42	2.42	12	1
2:B:348:VAL:HG22	2:B:370:MET:SD	0.42	2.54	13	1
2:B:303:GLN:CD	2:B:303:GLN:C	0.42	2.87	14	1
1:A:17:ALA:C	1:A:21:MET:SD	0.42	3.02	15	1
2:B:290:TYR:OH	2:B:294:ARG:CZ	0.42	2.66	18	1
2:B:281:GLU:HG2	2:B:282:GLN:N	0.42	2.29	20	1
2:B:345:GLY:C	2:B:346:VAL:HG12	0.42	2.38	1	1
2:B:282:GLN:C	2:B:282:GLN:CD	0.42	2.87	3	1
1:A:23:LEU:CD1	1:A:79:VAL:HG22	0.42	2.35	5	1
2:B:237:GLU:CD	2:B:237:GLU:C	0.42	2.87	10	1
2:B:237:GLU:O	2:B:241:ILE:N	0.42	2.45	10	1
2:B:286:LEU:HD11	2:B:288:ASP:HB3	0.42	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:268:ALA:O	2:B:272:VAL:HG13	0.42	2.13	12	1
2:B:299:ARG:HH11	2:B:303:GLN:N	0.42	2.13	12	1
1:A:40:GLU:CD	1:A:40:GLU:H	0.42	2.22	13	1
1:A:20:ALA:CB	1:A:52:LEU:CD1	0.42	2.98	14	1
1:A:84:ASN:O	1:A:85:SER:OG	0.42	2.37	14	1
2:B:268:ALA:O	2:B:272:VAL:HG23	0.42	2.14	18	1
2:B:208:GLU:O	2:B:212:LEU:HB2	0.42	2.15	8	1
1:A:43:GLU:OE1	1:A:45:GLU:OE1	0.42	2.37	10	1
2:B:300:ALA:HB3	2:B:333:THR:HG21	0.42	1.90	10	1
2:B:186:TRP:CB	2:B:323:PHE:CD1	0.42	3.03	12	1
2:B:216:LEU:HD11	2:B:249:LEU:O	0.42	2.13	12	1
2:B:324:ILE:HG23	2:B:345:GLY:C	0.42	2.40	12	1
2:B:295:ALA:O	2:B:298:LEU:HB2	0.42	2.15	13	1
2:B:283:PHE:CZ	2:B:298:LEU:HD12	0.42	2.49	15	1
2:B:279:PHE:CD2	2:B:283:PHE:CZ	0.42	3.07	16	1
1:A:66:GLU:C	1:A:66:GLU:CD	0.42	2.86	20	1
1:A:6:THR:O	1:A:6:THR:HG23	0.42	2.14	1	2
2:B:209:ARG:O	2:B:209:ARG:NE	0.42	2.53	4	1
2:B:210:GLU:OE1	2:B:210:GLU:O	0.42	2.38	5	1
1:A:59:LYS:O	1:A:59:LYS:CG	0.42	2.67	7	1
2:B:293:GLU:CD	2:B:356:GLN:HE21	0.42	2.21	8	1
2:B:213:THR:HG22	2:B:214:GLY:N	0.42	2.30	9	1
1:A:53:LEU:HD13	2:B:291:LEU:HD23	0.42	1.92	12	1
2:B:353:ALA:O	2:B:355:SER:N	0.42	2.53	12	1
2:B:299:ARG:C	2:B:299:ARG:CD	0.42	2.92	13	1
1:A:26:LEU:O	1:A:30:PHE:CG	0.42	2.72	14	1
2:B:242:PHE:N	2:B:242:PHE:CD1	0.42	2.85	16	1
2:B:283:PHE:CD1	2:B:283:PHE:C	0.42	2.97	17	1
1:A:24:PHE:CD1	2:B:247:HIS:CE1	0.42	3.08	19	1
2:B:258:LEU:HD13	2:B:259:PHE:N	0.42	2.30	5	1
2:B:203:LEU:HD12	2:B:204:ASP:H	0.42	1.74	6	1
2:B:208:GLU:HG2	2:B:262:VAL:HG21	0.42	1.90	12	1
2:B:326:VAL:O	2:B:376:PRO:HB3	0.42	2.14	13	1
2:B:374:ILE:O	2:B:374:ILE:CG2	0.42	2.66	15	1
2:B:228:LYS:H	2:B:228:LYS:HD2	0.42	1.73	20	1
2:B:330:LEU:HD11	2:B:346:VAL:HG11	0.42	1.90	6	1
1:A:4:LYS:C	1:A:5:GLN:HG3	0.42	2.39	8	1
2:B:350:ASP:OD2	2:B:351:GLY:N	0.42	2.52	8	1
2:B:242:PHE:CE2	2:B:336:ALA:HB2	0.42	2.50	11	1
2:B:269:GLU:OE1	2:B:269:GLU:CA	0.42	2.64	16	1
2:B:281:GLU:O	2:B:285:ALA:CB	0.42	2.67	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:349:ARG:C	2:B:350:ASP:CG	0.42	2.88	18	1
2:B:279:PHE:CZ	2:B:298:LEU:CB	0.42	3.03	20	1
2:B:203:LEU:CD1	2:B:203:LEU:N	0.42	2.82	1	1
2:B:248:LEU:CD1	2:B:253:ARG:HH22	0.42	2.27	11	2
2:B:329:GLU:CD	2:B:331:SER:HG	0.42	2.23	1	1
1:A:17:ALA:O	1:A:21:MET:CB	0.42	2.68	7	1
2:B:392:GLU:OE1	2:B:392:GLU:CA	0.42	2.62	8	1
1:A:16:HIS:CD2	2:B:290:TYR:CE2	0.42	3.08	9	1
2:B:392:GLU:OE1	2:B:392:GLU:C	0.42	2.63	13	1
2:B:209:ARG:NE	2:B:255:ARG:NH1	0.42	2.68	14	1
1:A:62:GLN:CD	1:A:62:GLN:C	0.42	2.87	16	1
2:B:393:LEU:C	2:B:393:LEU:CD2	0.42	2.93	17	1
2:B:228:LYS:HD2	2:B:228:LYS:N	0.42	2.30	20	1
1:A:27:MET:C	1:A:28:GLN:HE21	0.41	2.22	1	1
2:B:291:LEU:C	2:B:293:GLU:N	0.41	2.77	3	2
2:B:287:SER:O	2:B:289:ASN:N	0.41	2.54	3	1
2:B:208:GLU:CD	2:B:268:ALA:HB2	0.41	2.40	5	1
2:B:303:GLN:C	2:B:303:GLN:CD	0.41	2.87	5	1
2:B:269:GLU:CD	2:B:269:GLU:N	0.41	2.78	7	2
2:B:282:GLN:HB3	2:B:283:PHE:CE2	0.41	2.50	8	1
1:A:53:LEU:N	1:A:53:LEU:CD2	0.41	2.83	10	1
1:A:31:ASP:C	1:A:31:ASP:OD1	0.41	2.63	11	1
2:B:326:VAL:CG1	2:B:376:PRO:HG3	0.41	2.45	11	1
2:B:288:ASP:HB3	2:B:291:LEU:CD1	0.41	2.44	14	1
1:A:38:ASN:ND2	1:A:63:ILE:CG2	0.41	2.83	20	1
1:A:40:GLU:O	1:A:40:GLU:HG2	0.41	2.15	4	1
1:A:66:GLU:CD	1:A:66:GLU:N	0.41	2.78	8	1
1:A:49:VAL:CG1	2:B:248:LEU:HD21	0.41	2.45	11	1
2:B:281:GLU:N	2:B:281:GLU:OE1	0.41	2.53	11	1
1:A:49:VAL:HG21	2:B:248:LEU:HD11	0.41	1.90	15	1
1:A:36:LEU:C	1:A:37:ARG:HG3	0.41	2.40	16	1
2:B:217:GLU:OE2	2:B:221:ASN:ND2	0.41	2.53	17	1
2:B:288:ASP:O	2:B:288:ASP:CG	0.41	2.63	17	1
2:B:348:VAL:HG22	2:B:350:ASP:H	0.41	1.75	18	1
2:B:335:LEU:HD13	2:B:335:LEU:O	0.41	2.15	2	1
2:B:282:GLN:CD	2:B:282:GLN:O	0.41	2.64	3	1
1:A:53:LEU:CG	1:A:54:MET:N	0.41	2.83	4	2
2:B:245:TYR:O	2:B:248:LEU:CB	0.41	2.68	7	1
1:A:72:GLU:C	1:A:72:GLU:CD	0.41	2.89	8	1
2:B:217:GLU:O	2:B:221:ASN:CB	0.41	2.69	10	2
2:B:170:ARG:N	2:B:394:LEU:HD23	0.41	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:CB	1:A:69:GLY:HA3	0.41	2.45	15	1
2:B:238:THR:CG2	2:B:360:MET:SD	0.41	3.08	16	1
2:B:288:ASP:OD1	2:B:292:LYS:HB2	0.41	2.15	17	1
2:B:293:GLU:OE2	2:B:356:GLN:NE2	0.41	2.54	20	1
1:A:28:GLN:N	1:A:28:GLN:NE2	0.41	2.64	1	1
1:A:5:GLN:OE1	1:A:6:THR:O	0.41	2.38	2	1
2:B:204:ASP:OD2	2:B:207:LEU:HD12	0.41	2.15	3	1
1:A:39:ASP:OD2	1:A:62:GLN:OE1	0.41	2.38	6	1
2:B:342:ARG:HA	2:B:342:ARG:NE	0.41	2.29	6	1
2:B:237:GLU:O	2:B:238:THR:C	0.41	2.62	7	1
2:B:345:GLY:O	2:B:346:VAL:CG2	0.41	2.68	10	1
1:A:83:PHE:CD1	1:A:83:PHE:N	0.41	2.88	14	2
2:B:299:ARG:NE	2:B:299:ARG:O	0.41	2.54	12	1
1:A:3:VAL:HB	1:A:72:GLU:OE1	0.41	2.16	13	1
2:B:211:ARG:NE	2:B:309:LEU:HD12	0.41	2.28	14	1
2:B:325:LEU:HD22	2:B:335:LEU:HD21	0.41	1.92	16	1
2:B:290:TYR:O	2:B:293:GLU:HG2	0.41	2.15	18	1
1:A:15:MET:CG	1:A:16:HIS:H	0.41	2.27	20	1
2:B:291:LEU:O	2:B:294:ARG:CG	0.41	2.68	1	2
2:B:208:GLU:HB3	2:B:262:VAL:HG11	0.41	1.93	2	1
2:B:342:ARG:C	2:B:342:ARG:NE	0.41	2.78	2	1
2:B:385:ILE:HD12	2:B:385:ILE:N	0.41	2.30	2	1
1:A:71:GLN:CG	1:A:74:GLU:HB3	0.41	2.44	3	1
1:A:80:ILE:CD1	1:A:81:ALA:N	0.41	2.84	3	1
2:B:209:ARG:HG2	2:B:259:PHE:CD1	0.41	2.49	4	1
2:B:278:LYS:NZ	2:B:278:LYS:CB	0.41	2.83	4	1
2:B:262:VAL:C	2:B:264:LYS:N	0.41	2.77	5	1
1:A:64:GLU:N	1:A:64:GLU:OE1	0.41	2.53	7	1
2:B:223:PHE:CD2	2:B:242:PHE:CE2	0.41	3.09	9	1
1:A:40:GLU:CD	1:A:61:ARG:NH2	0.41	2.78	10	1
2:B:255:ARG:HG2	2:B:259:PHE:CE2	0.41	2.51	11	1
2:B:276:ILE:HG23	2:B:277:GLU:N	0.41	2.31	11	1
1:A:49:VAL:O	1:A:53:LEU:CG	0.41	2.67	12	1
2:B:344:VAL:O	2:B:344:VAL:HG12	0.41	2.16	15	1
2:B:279:PHE:O	2:B:283:PHE:CG	0.41	2.73	16	1
1:A:16:HIS:ND1	2:B:290:TYR:CZ	0.41	2.89	17	1
2:B:288:ASP:OD1	2:B:290:TYR:N	0.41	2.54	19	1
1:A:9:ILE:HG12	1:A:63:ILE:CD1	0.41	2.35	20	1
1:A:53:LEU:N	1:A:53:LEU:HD12	0.41	2.30	5	1
1:A:13:LEU:O	1:A:83:PHE:CG	0.41	2.73	6	2
1:A:16:HIS:ND1	1:A:17:ALA:HB2	0.41	2.31	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:276:ILE:CG1	2:B:277:GLU:N	0.41	2.83	8	2
1:A:70:PRO:HG2	1:A:71:GLN:NE2	0.41	2.31	11	1
1:A:38:ASN:OD1	1:A:42:THR:OG1	0.41	2.38	13	1
2:B:185:GLY:O	2:B:381:ARG:HA	0.41	2.15	13	1
2:B:295:ALA:O	2:B:298:LEU:N	0.41	2.51	13	1
2:B:344:VAL:O	2:B:344:VAL:CG1	0.41	2.69	13	1
1:A:21:MET:HE2	2:B:244:LEU:HD12	0.41	1.91	15	1
2:B:258:LEU:HD23	2:B:275:VAL:CG2	0.41	2.44	15	1
2:B:272:VAL:HG13	2:B:273:LYS:N	0.41	2.29	1	1
2:B:328:ASP:O	2:B:351:GLY:N	0.41	2.50	5	1
2:B:324:ILE:HG22	2:B:345:GLY:HA3	0.41	1.92	6	1
2:B:350:ASP:CG	2:B:351:GLY:N	0.41	2.79	8	1
2:B:204:ASP:CG	2:B:208:GLU:HG2	0.41	2.40	9	1
2:B:209:ARG:NE	2:B:255:ARG:HH12	0.41	2.14	14	1
1:A:5:GLN:HG2	1:A:5:GLN:O	0.41	2.14	15	1
1:A:14:GLY:C	1:A:15:MET:CG	0.41	2.92	15	1
2:B:222:GLU:HG3	2:B:223:PHE:N	0.41	2.29	15	1
1:A:43:GLU:OE1	1:A:43:GLU:C	0.41	2.63	2	1
1:A:73:GLU:HG3	1:A:74:GLU:N	0.41	2.30	9	1
1:A:53:LEU:HD21	2:B:286:LEU:HG	0.41	1.91	13	1
2:B:347:VAL:O	2:B:347:VAL:HG13	0.41	2.15	14	1
2:B:222:GLU:OE2	2:B:223:PHE:CA	0.41	2.68	15	1
1:A:17:ALA:CB	1:A:18:ARG:NH1	0.41	2.73	17	1
2:B:292:LYS:C	2:B:294:ARG:N	0.41	2.78	1	1
2:B:341:ASP:OD1	2:B:342:ARG:HG2	0.41	2.16	1	1
1:A:43:GLU:C	1:A:43:GLU:CD	0.41	2.89	2	1
2:B:254:LEU:HD13	2:B:254:LEU:O	0.41	2.15	2	1
1:A:30:PHE:CG	1:A:71:GLN:NE2	0.41	2.87	3	1
1:A:36:LEU:CD1	1:A:65:VAL:HG13	0.41	2.46	3	1
1:A:38:ASN:HD21	1:A:58:ALA:CB	0.41	2.25	3	1
1:A:38:ASN:ND2	1:A:58:ALA:HB2	0.41	2.27	3	1
2:B:352:ALA:C	2:B:354:ASN:N	0.41	2.79	3	1
1:A:77:ALA:CA	1:A:80:ILE:CG1	0.41	2.97	4	1
2:B:342:ARG:O	2:B:342:ARG:HG2	0.41	2.16	4	1
2:B:203:LEU:HD13	2:B:262:VAL:O	0.41	2.15	6	1
1:A:20:ALA:O	1:A:24:PHE:CE2	0.41	2.74	7	1
1:A:74:GLU:N	1:A:74:GLU:CD	0.41	2.79	7	2
2:B:226:TYR:CD1	2:B:229:ARG:NH1	0.41	2.89	15	2
1:A:35:LEU:O	1:A:66:GLU:CD	0.41	2.63	8	1
1:A:79:VAL:O	1:A:83:PHE:CG	0.41	2.74	8	1
1:A:45:GLU:HB3	1:A:47:ASN:HD22	0.41	1.76	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:348:VAL:HG23	2:B:349:ARG:N	0.41	2.30	12	1
2:B:389:TYR:CG	2:B:390:ARG:N	0.41	2.86	12	1
2:B:235:GLN:OE1	2:B:235:GLN:O	0.41	2.37	13	1
2:B:235:GLN:OE1	2:B:235:GLN:C	0.41	2.63	13	1
2:B:204:ASP:OD1	2:B:208:GLU:CD	0.41	2.63	15	1
1:A:37:ARG:O	1:A:64:GLU:OE1	0.41	2.38	16	1
2:B:245:TYR:OH	2:B:301:LEU:CB	0.41	2.69	16	1
1:A:76:LEU:HD23	1:A:76:LEU:O	0.41	2.15	17	1
2:B:216:LEU:HD12	2:B:249:LEU:CD1	0.41	2.46	17	1
2:B:330:LEU:HD12	2:B:330:LEU:H	0.41	1.76	19	1
1:A:15:MET:CG	1:A:16:HIS:N	0.41	2.72	20	1
2:B:245:TYR:OH	2:B:294:ARG:NE	0.41	2.54	20	1
2:B:387:ASP:OD2	2:B:390:ARG:CZ	0.41	2.69	6	1
2:B:209:ARG:HD2	2:B:259:PHE:CE2	0.41	2.51	7	1
1:A:66:GLU:OE1	1:A:66:GLU:N	0.41	2.54	8	1
2:B:211:ARG:HH21	2:B:211:ARG:HB3	0.41	1.75	9	1
2:B:348:VAL:O	2:B:370:MET:HA	0.41	2.16	9	1
2:B:243:ASP:CG	2:B:244:LEU:N	0.41	2.79	14	1
2:B:384:LEU:HD22	2:B:394:LEU:O	0.41	2.16	14	1
1:A:21:MET:HE2	2:B:244:LEU:CD1	0.41	2.45	15	1
2:B:364:LEU:HD12	2:B:364:LEU:C	0.41	2.41	16	1
2:B:237:GLU:HG2	2:B:238:THR:H	0.41	1.76	17	1
1:A:31:ASP:H	1:A:71:GLN:CD	0.41	2.23	19	1
2:B:273:LYS:O	2:B:277:GLU:OE1	0.41	2.39	19	1
2:B:208:GLU:OE2	2:B:267:VAL:HG12	0.40	2.16	3	1
2:B:270:TRP:CE3	2:B:270:TRP:O	0.40	2.74	5	1
1:A:38:ASN:ND2	1:A:41:GLY:H	0.40	2.10	8	1
2:B:235:GLN:HE21	2:B:238:THR:HG23	0.40	1.76	10	1
2:B:326:VAL:HG11	2:B:379:LEU:HD12	0.40	1.94	12	1
2:B:330:LEU:O	2:B:330:LEU:HG	0.40	2.15	14	1
2:B:252:THR:O	2:B:256:ARG:HB2	0.40	2.16	15	1
2:B:216:LEU:HD11	2:B:255:ARG:NE	0.40	2.32	16	1
2:B:332:ALA:H	2:B:357:ALA:HB2	0.40	1.75	18	1
1:A:7:VAL:HG13	1:A:7:VAL:O	0.40	2.15	20	1
2:B:279:PHE:O	2:B:280:ALA:C	0.40	2.64	20	1
1:A:53:LEU:CD1	2:B:291:LEU:HD13	0.40	2.39	7	1
2:B:392:GLU:C	2:B:393:LEU:CD1	0.40	2.76	8	1
2:B:393:LEU:N	2:B:393:LEU:CD1	0.40	2.75	8	1
2:B:204:ASP:OD1	2:B:208:GLU:CG	0.40	2.69	11	1
2:B:282:GLN:HG2	2:B:283:PHE:N	0.40	2.30	11	1
2:B:349:ARG:NH1	2:B:373:ASP:C	0.40	2.80	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:174:LEU:HD12	2:B:174:LEU:H	0.40	1.71	12	1
1:A:53:LEU:HD13	1:A:53:LEU:H	0.40	1.76	15	1
2:B:202:THR:O	2:B:267:VAL:HG22	0.40	2.17	17	1
2:B:204:ASP:C	2:B:206:ALA:N	0.40	2.79	18	1
2:B:244:LEU:HD23	2:B:294:ARG:NH1	0.40	2.31	18	1
1:A:16:HIS:ND1	2:B:291:LEU:HD11	0.40	2.31	2	1
2:B:326:VAL:CG1	2:B:347:VAL:HG13	0.40	2.46	2	1
1:A:38:ASN:ND2	1:A:55:LEU:HD12	0.40	2.32	4	1
1:A:13:LEU:O	1:A:13:LEU:HG	0.40	2.17	5	1
2:B:235:GLN:OE1	2:B:235:GLN:N	0.40	2.54	5	1
1:A:38:ASN:ND2	1:A:40:GLU:CA	0.40	2.84	8	1
2:B:292:LYS:NZ	2:B:292:LYS:HB2	0.40	2.31	11	1
2:B:352:ALA:HB3	2:B:355:SER:HB3	0.40	1.93	14	1
2:B:241:ILE:CG1	2:B:242:PHE:N	0.40	2.84	15	1
1:A:41:GLY:O	1:A:43:GLU:OE2	0.40	2.40	1	1
1:A:49:VAL:O	1:A:53:LEU:CD1	0.40	2.69	3	1
2:B:382:ARG:HH12	2:B:396:ASP:HB3	0.40	1.75	6	1
2:B:356:GLN:CG	2:B:357:ALA:N	0.40	2.84	9	1
2:B:245:TYR:CD2	2:B:294:ARG:NH1	0.40	2.89	12	1
2:B:270:TRP:O	2:B:274:THR:N	0.40	2.37	12	1
2:B:221:ASN:O	2:B:225:ARG:HG3	0.40	2.16	14	1
2:B:373:ASP:OD1	2:B:373:ASP:C	0.40	2.64	14	1
2:B:385:ILE:O	2:B:385:ILE:HG13	0.40	2.16	14	1
2:B:207:LEU:O	2:B:211:ARG:HG3	0.40	2.17	15	1
2:B:279:PHE:CE2	2:B:282:GLN:OE1	0.40	2.74	17	1
2:B:251:ASP:OD2	2:B:253:ARG:NH1	0.40	2.54	19	1
2:B:329:GLU:C	2:B:329:GLU:CD	0.40	2.90	19	1
2:B:248:LEU:HD23	2:B:249:LEU:HD23	0.40	1.93	20	1
1:A:5:GLN:NE2	1:A:76:LEU:HG	0.40	2.32	7	1
2:B:180:VAL:HG12	2:B:181:ALA:N	0.40	2.31	8	1
2:B:283:PHE:CE2	2:B:294:ARG:NH1	0.40	2.89	11	1
2:B:358:ALA:O	2:B:361:VAL:CG2	0.40	2.70	15	1
2:B:358:ALA:HB1	2:B:362:ARG:NH1	0.40	2.31	15	1
2:B:378:VAL:O	2:B:378:VAL:CG1	0.40	2.69	15	1
2:B:212:LEU:HD21	2:B:272:VAL:CG2	0.40	2.47	20	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	83/85 (98%)	73±1 (88±1%)	8±1 (9±1%)	2±1 (3±1%)	5	39
2	B	203/256 (79%)	181±4 (89±2%)	17±4 (8±2%)	5±2 (2±1%)	7	44
All	All	5720/6820 (84%)	5078 (89%)	496 (9%)	146 (3%)	6	42

All 27 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	32	ALA	18
2	B	380	HIS	18
2	B	234	ALA	13
2	B	351	GLY	12
1	A	17	ALA	11
2	B	311	ASP	9
1	A	16	HIS	9
2	B	353	ALA	5
1	A	18	ARG	5
1	A	15	MET	5
2	B	252	THR	5
2	B	288	ASP	4
2	B	352	ALA	4
2	B	396	ASP	4
2	B	285	ALA	4
2	B	336	ALA	3
2	B	397	PRO	3
2	B	350	ASP	2
2	B	233	GLY	2
2	B	294	ARG	2
2	B	355	SER	2
2	B	292	LYS	1
2	B	237	GLU	1
2	B	284	ALA	1
2	B	309	LEU	1
2	B	290	TYR	1

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Mol	Chain	Res	Type	Models (Total)
2	B	231	ALA	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	68/68 (100%)	53±3 (78±4%)	15±3 (22±4%)	2	29
2	B	160/205 (78%)	126±5 (79±3%)	34±5 (21±3%)	3	30
All	All	4560/5460 (84%)	3573 (78%)	987 (22%)	3	30

All 197 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)
2	B	291	LEU	15
1	A	80	ILE	14
2	B	203	LEU	14
1	A	48	SER	14
2	B	309	LEU	13
1	A	13	LEU	12
1	A	63	ILE	11
2	B	305	LEU	11
2	B	342	ARG	11
2	B	303	GLN	11
2	B	338	LEU	11
2	B	226	TYR	10
2	B	235	GLN	10
2	B	292	LYS	10
2	B	369	VAL	10
2	B	370	MET	10
1	A	1	MET	10
1	A	53	LEU	10
1	A	23	LEU	9
2	B	306	LEU	9
2	B	325	LEU	9
2	B	301	LEU	9
2	B	335	LEU	9

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Mol	Chain	Res	Type	Models (Total)
2	B	298	LEU	9
1	A	43	GLU	8
2	B	247	HIS	8
1	A	18	ARG	8
2	B	254	LEU	8
2	B	278	LYS	8
1	A	4	LYS	8
2	B	248	LEU	8
1	A	61	ARG	8
1	A	76	LEU	8
2	B	288	ASP	8
1	A	15	MET	7
1	A	47	ASN	7
2	B	212	LEU	7
2	B	346	VAL	7
2	B	389	TYR	7
2	B	242	PHE	7
2	B	330	LEU	7
2	B	355	SER	7
1	A	12	LYS	7
2	B	204	ASP	7
2	B	216	LEU	7
2	B	241	ILE	7
2	B	310	ASP	7
2	B	202	THR	7
2	B	170	ARG	7
1	A	10	THR	6
2	B	187	GLN	6
2	B	207	LEU	6
2	B	228	LYS	6
2	B	238	THR	6
2	B	245	TYR	6
2	B	329	GLU	6
2	B	364	LEU	6
2	B	264	LYS	6
2	B	269	GLU	6
2	B	270	TRP	6
2	B	281	GLU	6
2	B	348	VAL	6
2	B	396	ASP	6
1	A	21	MET	6
1	A	38	ASN	6

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Mol	Chain	Res	Type	Models (Total)
2	B	211	ARG	6
2	B	227	SER	6
2	B	263	ASP	6
2	B	384	LEU	6
2	B	390	ARG	6
2	B	392	GLU	6
1	A	50	ILE	6
1	A	85	SER	6
2	B	222	GLU	6
2	B	253	ARG	6
2	B	273	LYS	6
2	B	283	PHE	6
2	B	293	GLU	6
1	A	24	PHE	6
2	B	323	PHE	6
1	A	52	LEU	6
1	A	27	MET	5
1	A	66	GLU	5
2	B	375	GLN	5
2	B	380	HIS	5
1	A	79	VAL	5
2	B	172	ARG	5
2	B	208	GLU	5
2	B	249	LEU	5
2	B	255	ARG	5
2	B	326	VAL	5
2	B	289	ASN	5
2	B	361	VAL	5
2	B	244	LEU	5
1	A	59	LYS	5
2	B	223	PHE	5
2	B	252	THR	5
1	A	6	THR	5
1	A	28	GLN	4
1	A	65	VAL	4
2	B	256	ARG	4
2	B	356	GLN	4
2	B	373	ASP	4
2	B	381	ARG	4
2	B	386	VAL	4
2	B	393	LEU	4
1	A	16	HIS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ASP	4
2	B	236	LYS	4
2	B	304	ARG	4
2	B	347	VAL	4
1	A	35	LEU	4
1	A	83	PHE	4
2	B	267	VAL	4
2	B	209	ARG	4
2	B	324	ILE	4
1	A	54	MET	4
2	B	217	GLU	4
2	B	344	VAL	4
1	A	7	VAL	4
2	B	258	LEU	4
2	B	307	PHE	4
2	B	350	ASP	4
2	B	279	PHE	4
2	B	382	ARG	4
1	A	73	GLU	4
1	A	5	GLN	3
1	A	8	GLU	3
1	A	37	ARG	3
2	B	276	ILE	3
2	B	322	ARG	3
2	B	366	ILE	3
1	A	3	VAL	3
1	A	55	LEU	3
2	B	337	GLU	3
1	A	68	THR	3
1	A	71	GLN	3
1	A	74	GLU	3
2	B	182	ILE	3
2	B	286	LEU	3
2	B	383	THR	3
2	B	229	ARG	3
2	B	251	ASP	3
2	B	360	MET	3
1	A	31	ASP	3
2	B	210	GLU	3
2	B	385	ILE	3
2	B	277	GLU	3
2	B	299	ARG	3

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Mol	Chain	Res	Type	Models (Total)
2	B	374	ILE	3
2	B	394	LEU	3
2	B	362	ARG	3
1	A	22	LYS	3
2	B	186	TRP	2
2	B	343	LEU	2
1	A	36	LEU	2
1	A	82	LEU	2
2	B	262	VAL	2
2	B	395	VAL	2
1	A	11	ASN	2
1	A	42	THR	2
1	A	2	THR	2
2	B	290	TYR	2
1	A	25	GLU	2
2	B	379	LEU	2
2	B	297	ASP	2
2	B	224	ARG	2
1	A	56	ASP	2
1	A	57	SER	2
2	B	282	GLN	2
2	B	331	SER	2
2	B	333	THR	2
2	B	341	ASP	2
2	B	354	ASN	2
1	A	33	GLU	2
1	A	40	GLU	2
1	A	64	GLU	2
2	B	243	ASP	2
2	B	184	GLU	2
2	B	230	PHE	2
2	B	340	GLN	1
2	B	221	ASN	1
2	B	225	ARG	1
2	B	261	GLU	1
1	A	45	GLU	1
2	B	246	SER	1
2	B	257	GLU	1
2	B	334	THR	1
2	B	213	THR	1
1	A	72	GLU	1
2	B	294	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	328	ASP	1
2	B	359	ILE	1
1	A	49	VAL	1
2	B	311	ASP	1
1	A	62	GLN	1
2	B	259	PHE	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

The completeness of assignment taking into account all chemical shift lists is 29% for the well-defined parts and 30% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *NPr_EIN_Complex.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	197
Number of shifts mapped to atoms	197
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	51	0.61 ± 0.35	None needed (imprecise)
$^{13}\text{C}_\beta$	42	0.70 ± 0.08	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	52	0.18 ± 0.49	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 5%, i.e. 197 atoms were assigned a chemical shift out of a possible 3966. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	155/1445 (11%)	52/587 (9%)	51/578 (9%)	52/280 (19%)
Sidechain	42/2323 (2%)	0/1518 (0%)	42/708 (6%)	0/97 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/198 (0%)	0/99 (0%)	0/93 (0%)	0/6 (0%)
Overall	197/3966 (5%)	52/2204 (2%)	93/1379 (7%)	52/383 (14%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 197 atoms were assigned a chemical shift out of a possible 4656. 0 out of 68 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	155/1693 (9%)	52/686 (8%)	51/680 (8%)	52/327 (16%)
Sidechain	42/2735 (2%)	0/1784 (0%)	42/840 (5%)	0/111 (0%)
Aromatic	0/228 (0%)	0/113 (0%)	0/108 (0%)	0/7 (0%)
Overall	197/4656 (4%)	52/2583 (2%)	93/1628 (6%)	52/445 (12%)

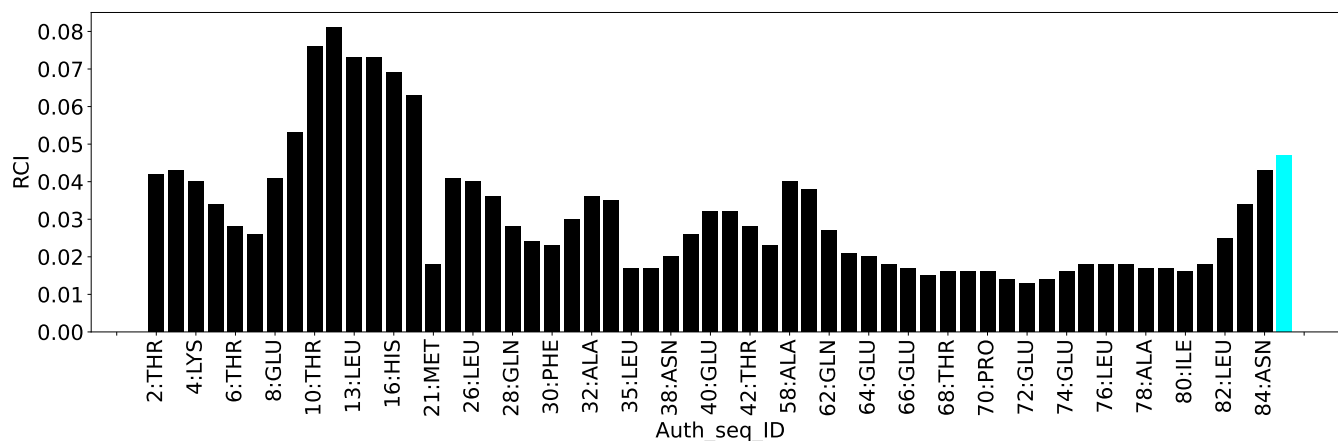
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *EIN_NPr_Complex.str*

7.2.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1194
Number of shifts mapped to atoms	1194
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	249	0.13 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	229	1.10 ± 0.09	Should be checked
$^{13}\text{C}'$	250	-0.23 ± 0.09	None needed (< 0.5 ppm)
^{15}N	232	0.69 ± 0.17	Should be applied

7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 24%, i.e. 962 atoms were assigned a chemical shift out of a possible 3966. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	778/1445 (54%)	188/587 (32%)	402/578 (70%)	188/280 (67%)
Sidechain	182/2323 (8%)	0/1518 (0%)	182/708 (26%)	0/97 (0%)
Aromatic	2/198 (1%)	1/99 (1%)	0/93 (0%)	1/6 (17%)
Overall	962/3966 (24%)	189/2204 (9%)	584/1379 (42%)	189/383 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 26%, i.e. 1194 atoms were assigned a chemical shift out of a possible 4656. 0 out of 68 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	963/1693 (57%)	232/686 (34%)	499/680 (73%)	232/327 (71%)
Sidechain	229/2735 (8%)	0/1784 (0%)	229/840 (27%)	0/111 (0%)
Aromatic	2/228 (1%)	1/113 (1%)	0/108 (0%)	1/7 (14%)
Overall	1194/4656 (26%)	233/2583 (9%)	728/1628 (45%)	233/445 (52%)

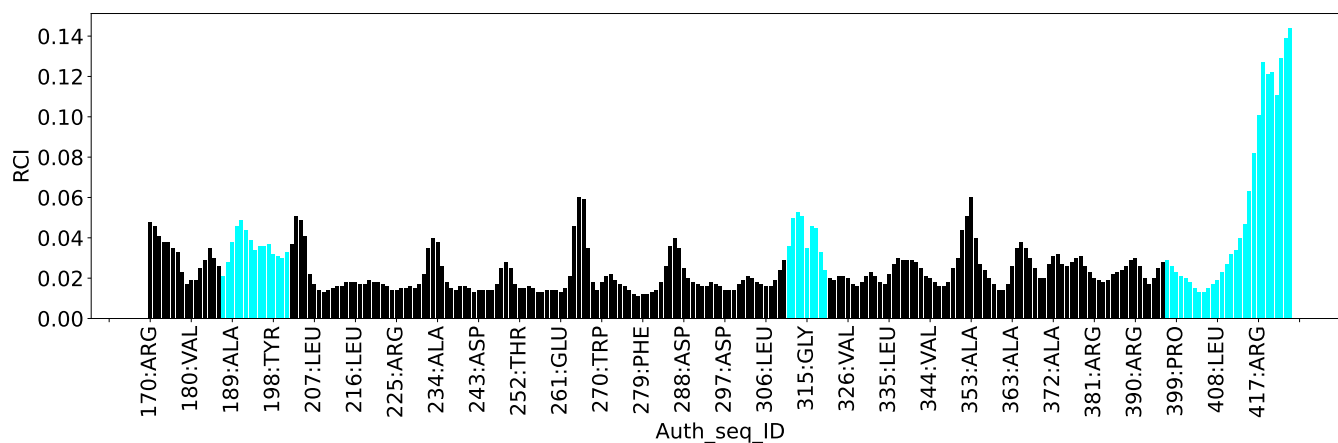
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	988
Intra-residue ($ i-j =0$)	10
Sequential ($ i-j =1$)	314
Medium range ($ i-j >1$ and $ i-j <5$)	211
Long range ($ i-j \geq 5$)	84
Inter-chain	45
Hydrogen bond restraints	324
Disulfide bond restraints	0
Total dihedral-angle restraints	451
Number of unmapped restraints	0
Number of restraints per residue	4.2
Number of long range restraints per residue ¹	0.6

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	54.0	0.2
0.2-0.5 (Medium)	65.5	0.5
>0.5 (Large)	25.4	8.67

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	28.8	9.94
10.0-20.0 (Medium)	6.0	19.65
>20.0 (Large)	0.7	29.11

9 Distance violation analysis ⓘ

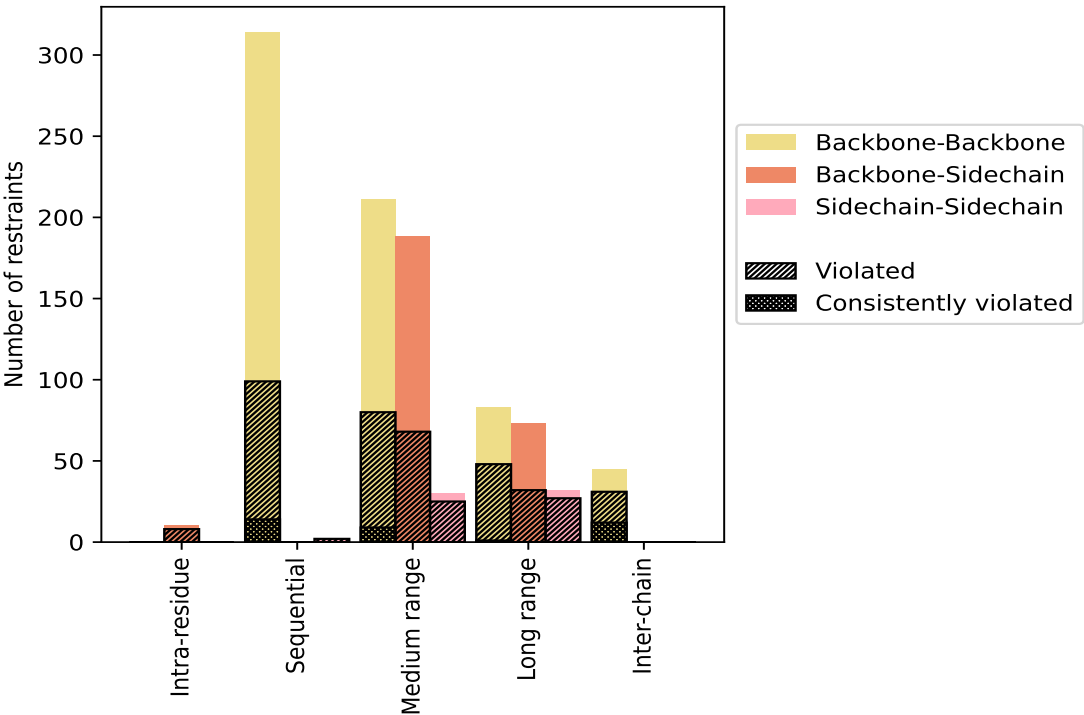
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	10	1.0	8	80.0	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	10	1.0	8	80.0	0.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	314	31.8	99	31.5	10.0	14	4.5	1.4
Backbone-Backbone	314	31.8	99	31.5	10.0	14	4.5	1.4
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	211	21.4	80	37.9	8.1	9	4.3	0.9
Backbone-Backbone	211	21.4	80	37.9	8.1	9	4.3	0.9
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	84	8.5	49	58.3	5.0	1	1.2	0.1
Backbone-Backbone	83	8.4	48	57.8	4.9	1	1.2	0.1
Backbone-Sidechain	1	0.1	1	100.0	0.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	45	4.6	31	68.9	3.1	12	26.7	1.2
Backbone-Backbone	45	4.6	31	68.9	3.1	12	26.7	1.2
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	324	32.8	153	47.2	15.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	988	100.0	420	42.5	42.5	36	3.6	3.6
Backbone-Backbone	653	66.1	258	39.5	26.1	36	5.5	3.6
Backbone-Sidechain	271	27.4	108	39.9	10.9	0	0.0	0.0
Sidechain-Sidechain	64	6.5	54	84.4	5.5	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	40	50	36	21	147	0.54	7.39	0.95	0.25
2	2	35	52	33	21	143	0.58	6.73	0.99	0.26
3	1	39	54	32	21	147	0.56	5.42	1.02	0.25
4	3	43	56	40	20	162	0.51	7.81	0.96	0.23
5	2	41	46	35	20	144	0.51	5.97	0.91	0.24
6	0	44	50	33	21	148	0.61	7.83	1.05	0.26
7	2	41	55	26	24	148	0.56	7.95	1.02	0.24
8	1	46	57	30	23	157	0.52	6.62	0.91	0.24
9	1	44	48	32	23	148	0.63	8.67	1.2	0.24
10	2	47	60	27	21	157	0.56	6.41	1.01	0.25

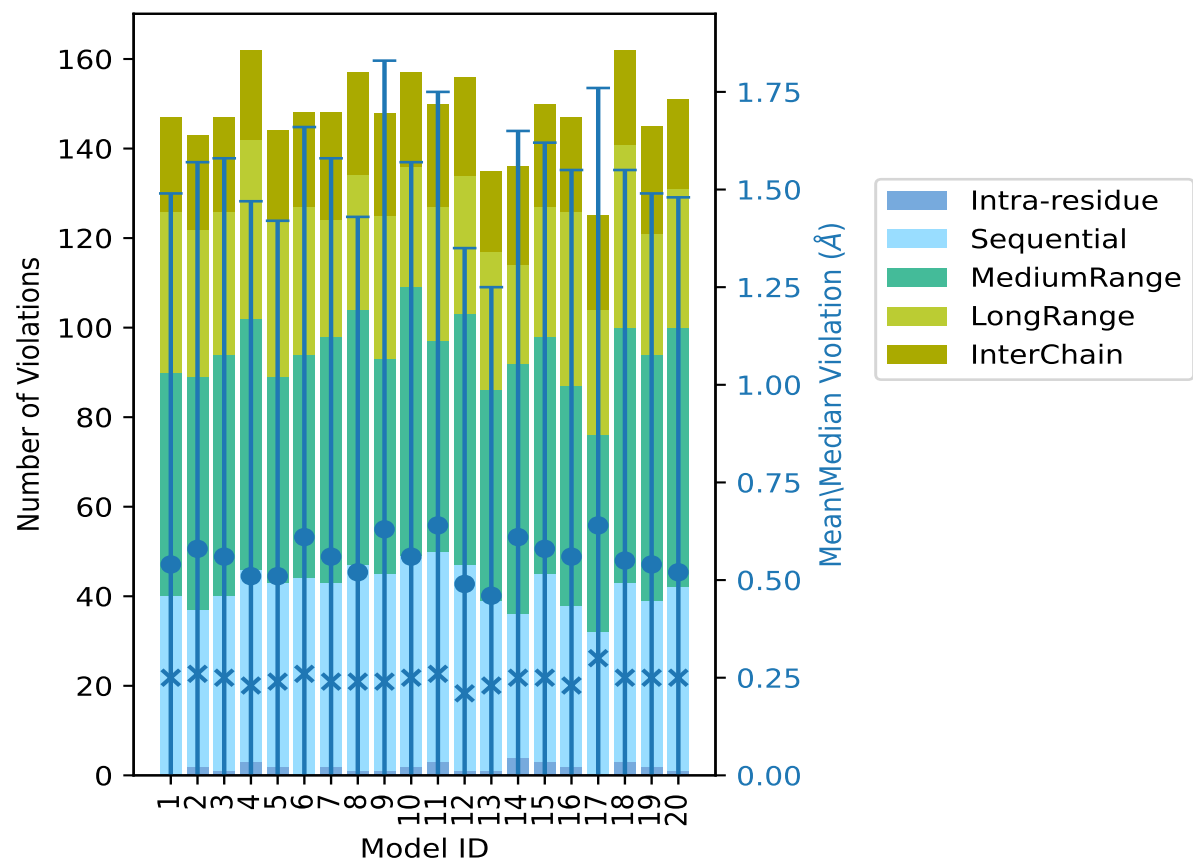
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	47	47	30	23	150	0.64	7.81	1.11	0.26
12	1	46	56	31	22	156	0.49	6.07	0.86	0.21
13	1	38	47	31	18	135	0.46	6.04	0.79	0.23
14	4	32	56	22	22	136	0.61	6.21	1.04	0.25
15	3	42	53	29	23	150	0.58	7.02	1.04	0.25
16	2	36	49	39	21	147	0.56	6.76	0.99	0.23
17	0	32	44	28	21	125	0.64	8.14	1.12	0.3
18	3	40	57	41	21	162	0.55	8.11	1.0	0.25
19	2	37	55	27	24	145	0.54	6.74	0.95	0.25
20	1	41	58	31	20	151	0.52	7.41	0.96	0.25

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

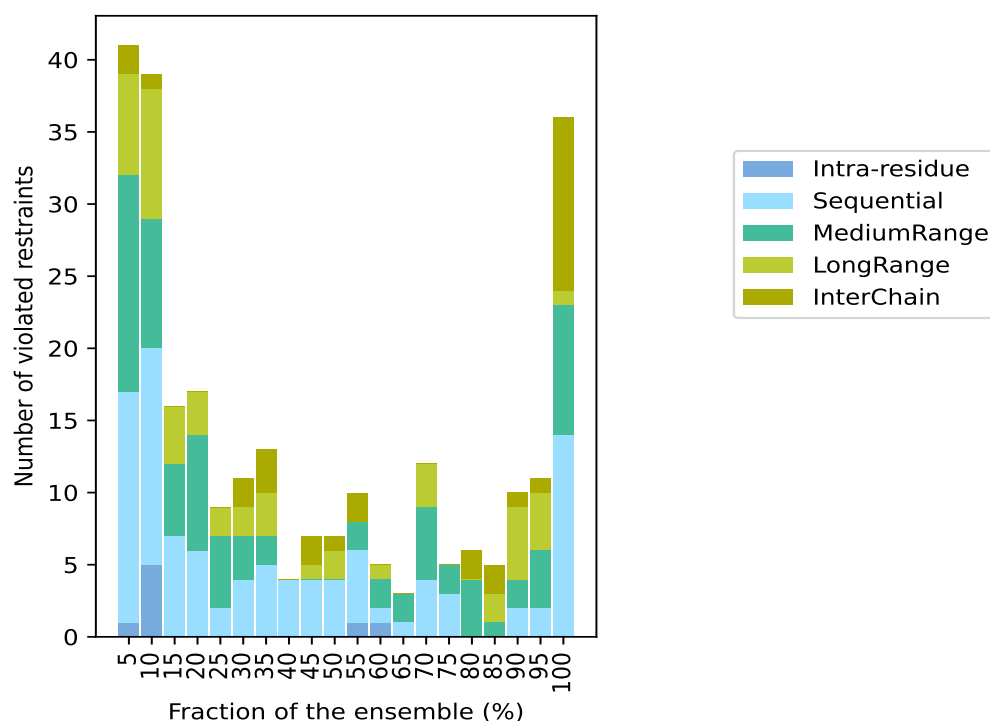
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 397(IR:2, SQ:215, MR:131, LR:35, IC:14) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	16	15	7	2	41	1	5.0
5	15	9	9	1	39	2	10.0
0	7	5	4	0	16	3	15.0
0	6	8	3	0	17	4	20.0
0	2	5	2	0	9	5	25.0
0	4	3	2	2	11	6	30.0
0	5	2	3	3	13	7	35.0
0	4	0	0	0	4	8	40.0
0	4	0	1	2	7	9	45.0
0	4	0	2	1	7	10	50.0
1	5	2	0	2	10	11	55.0
1	1	2	1	0	5	12	60.0
0	1	2	0	0	3	13	65.0
0	4	5	3	0	12	14	70.0
0	3	2	0	0	5	15	75.0
0	0	4	0	2	6	16	80.0
0	0	1	2	2	5	17	85.0
0	2	2	5	1	10	18	90.0
0	2	4	4	1	11	19	95.0
0	14	9	1	12	36	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

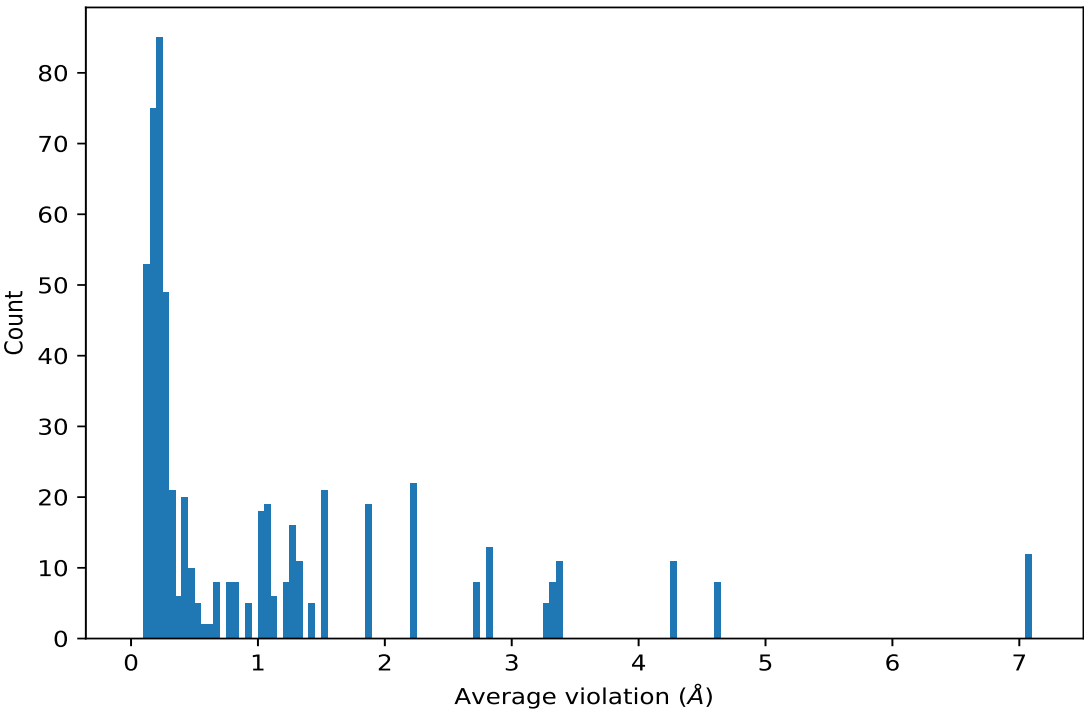
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:H	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:HH12	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH12	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH22	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH21	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HD2	1:61:A:ARG:HH11	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:H	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:HH11	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:HH11	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HE1	1:61:A:ARG:H	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HD2	1:61:A:ARG:HH12	20	7.06	0.87	6.89
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:HH12	20	7.06	0.87	6.89
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	20	4.62	0.51	4.44
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG2	20	4.62	0.51	4.44
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	20	4.62	0.51	4.44
(1,14)	1:47:A:ASN:O	2:257:B:GLU:H	20	4.62	0.51	4.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,14)	1:47:A:ASN:HD22	2:257:B:GLU:H	20	4.62	0.51	4.44
(1,14)	1:53:A:LEU:HD22	2:257:B:GLU:OE2	20	4.62	0.51	4.44
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HB2	20	4.62	0.51	4.44
(1,14)	1:47:A:ASN:HD22	2:257:B:GLU:HG2	20	4.62	0.51	4.44
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH11	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD21	2:255:B:ARG:H	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:H	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:OD1	2:255:B:ARG:H	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH22	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:O	2:255:B:ARG:HE	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD21	2:255:B:ARG:HG2	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HD3	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH12	20	4.25	0.61	4.44
(1,12)	1:47:A:ASN:OD1	2:255:B:ARG:HH22	20	4.25	0.61	4.44
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:OD1	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HH	1:11:A:ASN:HB3	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HB3	1:11:A:ASN:O	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HD1	1:11:A:ASN:O	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HD1	1:11:A:ASN:HD22	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HD2	1:11:A:ASN:O	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HE1	1:11:A:ASN:O	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:H	1:11:A:ASN:HD22	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HE1	1:11:A:ASN:HD22	20	3.39	1.15	3.62
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:HD22	20	3.39	1.15	3.62
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	20	3.34	0.79	3.36
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	20	3.34	0.79	3.36
(1,8)	1:47:A:ASN:HA	2:250:B:SER:HG	20	3.34	0.79	3.36
(1,8)	1:47:A:ASN:O	2:250:B:SER:HG	20	3.34	0.79	3.36
(1,8)	1:21:A:MET:HE2	2:250:B:SER:HG	20	3.34	0.79	3.36
(1,8)	1:47:A:ASN:HD21	2:250:B:SER:O	20	3.34	0.79	3.36
(1,8)	1:47:A:ASN:OD1	2:250:B:SER:O	20	3.34	0.79	3.36
(1,8)	1:21:A:MET:HE1	2:250:B:SER:HG	20	3.34	0.79	3.36
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	20	3.3	1.23	3.18
(1,41)	2:290:B:TYR:HB2	1:54:A:MET:N	20	3.3	1.23	3.18
(1,41)	2:279:B:PHE:HE2	1:54:A:MET:HE1	20	3.3	1.23	3.18
(1,41)	2:279:B:PHE:HD2	1:54:A:MET:H	20	3.3	1.23	3.18
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	20	3.3	1.23	3.18
(1,13)	1:47:A:ASN:HD21	2:256:B:ARG:HG2	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HH22	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB2	20	2.82	1.35	2.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB3	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HB3	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:OD1	2:256:B:ARG:HG3	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:OD1	2:256:B:ARG:HB3	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH12	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HD3	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH22	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HH11	20	2.82	1.35	2.77
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HG3	20	2.82	1.35	2.77
(1,16)	1:53:A:LEU:HD11	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HD13	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HD22	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HD23	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HD21	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HD12	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:53:A:LEU:HG	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,16)	1:54:A:MET:HE2	2:281:B:GLU:O	20	2.71	0.71	2.86
(1,1)	1:16:A:HIS:HD2	2:356:B:GLN:HA	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB3	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HD2	2:356:B:GLN:HB3	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:OE1	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:OE1	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HB3	2:356:B:GLN:OE1	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HG2	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HE21	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HB3	2:356:B:GLN:HB3	20	2.2	0.99	2.42
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HA	1:16:A:HIS:HD2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HD2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HE1	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HE2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HB3	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HG2	1:16:A:HIS:HE2	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HE21	1:16:A:HIS:HE1	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HB3	20	2.2	0.99	2.42
(1,2)	2:356:B:GLN:HB2	1:16:A:HIS:HE2	20	2.2	0.99	2.42
(1,43)	2:290:B:TYR:H	1:57:A:SER:HA	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HD1	1:57:A:SER:HA	20	1.85	0.7	1.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HB2	1:57:A:SER:N	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:H	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HD2	1:57:A:SER:N	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:H	1:57:A:SER:HG	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HD1	1:57:A:SER:N	20	1.85	0.7	1.8
(1,43)	2:290:B:TYR:HD2	1:57:A:SER:H	20	1.85	0.7	1.8
(1,15)	1:53:A:LEU:HD12	2:279:B:PHE:HD2	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD13	2:279:B:PHE:O	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD12	2:279:B:PHE:O	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:HD2	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HG	2:279:B:PHE:O	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD11	2:279:B:PHE:O	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD11	2:279:B:PHE:HD2	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:HE2	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD21	2:279:B:PHE:HD2	20	1.3	0.6	1.27
(1,15)	1:53:A:LEU:HD23	2:279:B:PHE:HE1	20	1.3	0.6	1.27
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	20	0.55	0.08	0.54
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	20	0.52	0.09	0.5
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	20	0.52	0.09	0.5
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	20	0.47	0.03	0.46
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	20	0.47	0.03	0.46
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	20	0.4	0.09	0.36
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	20	0.39	0.07	0.4
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	20	0.39	0.15	0.38
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	20	0.35	0.05	0.36
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	20	0.35	0.06	0.36
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	20	0.35	0.04	0.33
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	20	0.33	0.09	0.34
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	20	0.33	0.05	0.32
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	20	0.32	0.06	0.32
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	20	0.32	0.08	0.32
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	20	0.3	0.09	0.26
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	20	0.29	0.1	0.3
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	20	0.29	0.07	0.3
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	20	0.29	0.06	0.28
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	20	0.28	0.06	0.29
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	20	0.22	0.06	0.22
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	20	0.22	0.03	0.22
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	20	0.21	0.04	0.21
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	20	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,31)	2:290:B:TYR:HE2	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:HD2	1:15:A:MET:HE1	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:HH	1:15:A:MET:HE3	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:HH	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:HD2	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:244:B:LEU:HD12	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:244:B:LEU:HD23	1:15:A:MET:HB2	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:HB2	1:15:A:MET:O	19	1.88	1.3	1.6
(1,31)	2:290:B:TYR:OH	1:15:A:MET:HE2	19	1.88	1.3	1.6
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	19	0.4	0.1	0.39
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	19	0.4	0.1	0.39
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	19	0.38	0.14	0.37
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	19	0.35	0.16	0.31
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	19	0.31	0.1	0.31
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	19	0.3	0.13	0.28
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	19	0.25	0.07	0.24
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	19	0.21	0.06	0.23
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	19	0.17	0.05	0.15
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	19	0.17	0.05	0.15
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	19	0.17	0.05	0.15
(1,20)	1:57:A:SER:HB3	2:285:B:ALA:O	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB3	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HE2	2:285:B:ALA:HB2	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB2	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD21	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD12	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD13	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:O	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD13	2:285:B:ALA:HB2	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:HB2	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HG2	2:285:B:ALA:HB3	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB1	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HG	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:53:A:LEU:HD22	2:285:B:ALA:H	18	1.25	0.6	1.25
(1,20)	1:54:A:MET:HE2	2:285:B:ALA:HB1	18	1.25	0.6	1.25
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	18	0.41	0.16	0.42
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	18	0.28	0.12	0.24
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	18	0.28	0.12	0.23
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	18	0.27	0.07	0.27
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	18	0.26	0.08	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	18	0.26	0.07	0.25
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	18	0.24	0.06	0.25
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	18	0.21	0.06	0.2
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	18	0.2	0.05	0.19
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	18	0.18	0.07	0.16
(1,27)	1:53:A:LEU:HD21	2:293:B:GLU:N	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:N	17	1.53	0.72	1.5
(1,27)	1:16:A:HIS:HD2	2:293:B:GLU:OE2	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HB2	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD12	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:56:A:ASP:OD2	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:16:A:HIS:HE2	2:293:B:GLU:HB3	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD13	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:OE1	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HG	2:293:B:GLU:H	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:HG2	17	1.53	0.72	1.5
(1,27)	1:53:A:LEU:HD22	2:293:B:GLU:N	17	1.53	0.72	1.5
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD22	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD11	2:248:B:LEU:HD12	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD13	2:248:B:LEU:HD22	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HA	2:248:B:LEU:HD22	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD11	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD23	2:248:B:LEU:HD12	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HE2	2:248:B:LEU:H	17	1.02	0.66	0.7
(1,7)	1:47:A:ASN:O	2:248:B:LEU:HD11	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HE1	2:248:B:LEU:HB2	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HG2	2:248:B:LEU:HD22	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD23	2:248:B:LEU:HG	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HE3	2:248:B:LEU:HB2	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD11	2:248:B:LEU:HD22	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD22	2:248:B:LEU:HD13	17	1.02	0.66	0.7
(1,7)	1:47:A:ASN:O	2:248:B:LEU:HA	17	1.02	0.66	0.7
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD12	17	1.02	0.66	0.7
(1,7)	1:21:A:MET:HA	2:248:B:LEU:HD11	17	1.02	0.66	0.7
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	17	0.33	0.13	0.31
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	17	0.23	0.08	0.23
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	17	0.23	0.09	0.22
(1,35)	2:244:B:LEU:HD11	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:HA	16	1.08	0.41	1.08
(1,35)	2:243:B:ASP:OD1	1:22:A:LYS:N	16	1.08	0.41	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,35)	2:244:B:LEU:HG	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,35)	2:247:B:HIS:HD2	1:22:A:LYS:HA	16	1.08	0.41	1.08
(1,35)	2:244:B:LEU:HG	1:22:A:LYS:H	16	1.08	0.41	1.08
(1,35)	2:244:B:LEU:HD13	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,35)	2:243:B:ASP:OD1	1:22:A:LYS:HA	16	1.08	0.41	1.08
(1,35)	2:244:B:LEU:HD12	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,35)	2:244:B:LEU:HD23	1:22:A:LYS:N	16	1.08	0.41	1.08
(1,19)	1:53:A:LEU:HD11	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD13	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD22	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD23	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HG	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD12	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD21	2:284:B:ALA:N	16	0.77	0.47	0.66
(1,19)	1:53:A:LEU:HD21	2:284:B:ALA:HA	16	0.77	0.47	0.66
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	16	0.36	0.11	0.37
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	16	0.3	0.22	0.26
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	16	0.24	0.07	0.23
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	16	0.2	0.1	0.16
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	16	0.18	0.05	0.16
(2,49)	2:201:B:SER:H	2:202:B:THR:H	15	0.31	0.14	0.25
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	15	0.27	0.14	0.19
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	15	0.25	0.11	0.23
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	15	0.24	0.07	0.24
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	15	0.2	0.06	0.18
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	15	0.2	0.06	0.18
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	15	0.18	0.06	0.16
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	14	0.27	0.07	0.27
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	14	0.27	0.07	0.27
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	14	0.23	0.1	0.2
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	14	0.23	0.06	0.24
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	14	0.23	0.06	0.24
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	14	0.23	0.09	0.22
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	14	0.22	0.08	0.2
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	14	0.21	0.06	0.18
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	14	0.19	0.06	0.2
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	14	0.18	0.07	0.16
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	14	0.16	0.04	0.16
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	14	0.15	0.04	0.15
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	14	0.15	0.04	0.15
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	14	0.15	0.04	0.14
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	14	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	13	0.54	0.62	0.27
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	13	0.54	0.62	0.27
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	13	0.25	0.1	0.25
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	13	0.24	0.04	0.24
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	13	0.23	0.07	0.21
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	13	0.22	0.08	0.21
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	13	0.14	0.03	0.14
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	12	0.27	0.16	0.22
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	12	0.26	0.11	0.26
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	12	0.25	0.09	0.25
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	12	0.23	0.1	0.2
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	12	0.19	0.08	0.17
(1,44)	2:290:B:TYR:HB2	1:59:A:LYS:HD2	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE3	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ1	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:HB3	1:59:A:LYS:HZ3	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ2	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HD3	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE2	11	1.21	0.69	1.29
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ3	11	1.21	0.69	1.29
(1,10)	1:47:A:ASN:HB2	2:252:B:THR:HG23	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HB2	2:252:B:THR:HG1	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:H	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:HG21	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:OG1	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:OD1	2:252:B:THR:HG1	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HD22	2:252:B:THR:HG1	11	1.09	0.52	1.29
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:HG1	11	1.09	0.52	1.29
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	11	0.64	0.63	0.32
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	11	0.42	0.24	0.38
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	11	0.28	0.12	0.25
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	11	0.24	0.09	0.26
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	11	0.24	0.06	0.23
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	11	0.23	0.05	0.22
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	11	0.2	0.06	0.19
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	11	0.18	0.05	0.2
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	11	0.18	0.05	0.18
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	11	0.16	0.03	0.15
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	11	0.15	0.03	0.15
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	11	0.13	0.03	0.11
(1,40)	2:244:B:LEU:HD23	1:53:A:LEU:HD22	10	0.81	0.55	0.61
(1,40)	2:244:B:LEU:HD21	1:53:A:LEU:HD21	10	0.81	0.55	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,40)	2:279:B:PHE:O	1:53:A:LEU:HD22	10	0.81	0.55	0.61
(1,40)	2:290:B:TYR:HD2	1:53:A:LEU:HD21	10	0.81	0.55	0.61
(1,40)	2:290:B:TYR:HD2	1:53:A:LEU:HA	10	0.81	0.55	0.61
(1,40)	2:248:B:LEU:HD13	1:53:A:LEU:HD11	10	0.81	0.55	0.61
(1,40)	2:290:B:TYR:HB2	1:53:A:LEU:HA	10	0.81	0.55	0.61
(1,40)	2:248:B:LEU:HD12	1:53:A:LEU:HD12	10	0.81	0.55	0.61
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	10	0.33	0.12	0.29
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	10	0.3	0.12	0.3
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	10	0.28	0.11	0.3
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	10	0.23	0.1	0.24
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	10	0.22	0.07	0.22
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	10	0.21	0.09	0.19
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	10	0.2	0.07	0.2
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	10	0.2	0.07	0.2
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	10	0.18	0.04	0.19
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	10	0.16	0.03	0.15
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	10	0.16	0.03	0.16
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	10	0.16	0.03	0.16
(1,29)	1:53:A:LEU:HB2	2:295:B:ALA:H	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD21	2:295:B:ALA:HA	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HG	2:295:B:ALA:H	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD12	2:295:B:ALA:H	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD22	2:295:B:ALA:HB2	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD23	2:295:B:ALA:H	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD22	2:295:B:ALA:HA	9	1.5	0.93	1.7
(1,29)	1:53:A:LEU:HD13	2:295:B:ALA:H	9	1.5	0.93	1.7
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	9	0.64	0.61	0.26
(1,26)	1:53:A:LEU:HD21	2:292:B:LYS:N	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HD23	2:292:B:LYS:N	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HB2	2:292:B:LYS:H	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HB3	2:292:B:LYS:N	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HG	2:292:B:LYS:H	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HD22	2:292:B:LYS:H	9	0.46	0.24	0.4
(1,26)	1:53:A:LEU:HD22	2:292:B:LYS:N	9	0.46	0.24	0.4
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	9	0.18	0.1	0.15
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	9	0.18	0.05	0.18
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	9	0.16	0.04	0.15
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	9	0.14	0.02	0.16
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	9	0.14	0.02	0.16
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	8	0.44	0.52	0.2
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	8	0.44	0.52	0.2
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	8	0.41	0.09	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	8	0.35	0.13	0.32
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	8	0.27	0.12	0.22
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	8	0.23	0.07	0.22
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	8	0.22	0.06	0.23
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	8	0.21	0.07	0.22
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	8	0.19	0.07	0.18
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	8	0.18	0.07	0.16
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	8	0.18	0.05	0.15
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	8	0.14	0.03	0.14
(1,36)	2:247:B:HIS:HB3	1:47:A:ASN:HA	7	0.93	0.64	1.03
(1,36)	2:247:B:HIS:HE2	1:47:A:ASN:OD1	7	0.93	0.64	1.03
(1,36)	2:248:B:LEU:HA	1:47:A:ASN:O	7	0.93	0.64	1.03
(1,36)	2:248:B:LEU:HD11	1:47:A:ASN:O	7	0.93	0.64	1.03
(1,36)	2:247:B:HIS:HE1	1:47:A:ASN:HA	7	0.93	0.64	1.03
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:HA	7	0.68	0.52	0.52
(1,3)	1:18:A:ARG:HH11	2:241:B:ILE:H	7	0.68	0.52	0.52
(1,3)	1:16:A:HIS:HE1	2:241:B:ILE:HD11	7	0.68	0.52	0.52
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:N	7	0.68	0.52	0.52
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:O	7	0.68	0.52	0.52
(1,3)	1:16:A:HIS:O	2:241:B:ILE:HD13	7	0.68	0.52	0.52
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	7	0.68	0.63	0.33
(1,37)	2:247:B:HIS:HE2	1:48:A:SER:HA	7	0.42	0.2	0.44
(1,37)	2:247:B:HIS:HD2	1:48:A:SER:HA	7	0.42	0.2	0.44
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:HB3	7	0.42	0.2	0.44
(1,37)	2:279:B:PHE:HZ	1:48:A:SER:HG	7	0.42	0.2	0.44
(1,37)	2:247:B:HIS:HE1	1:48:A:SER:HA	7	0.42	0.2	0.44
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:HG	7	0.42	0.2	0.44
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:OG	7	0.42	0.2	0.44
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	7	0.38	0.16	0.35
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	7	0.33	0.15	0.29
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	7	0.21	0.08	0.18
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	7	0.21	0.08	0.18
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	7	0.19	0.07	0.15
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	7	0.19	0.07	0.15
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	7	0.18	0.07	0.17
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	7	0.18	0.07	0.17
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	7	0.18	0.05	0.21
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	7	0.17	0.05	0.18
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	7	0.17	0.05	0.16
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	7	0.17	0.07	0.14
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	7	0.13	0.02	0.13
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	7	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,17)	1:53:A:LEU:HD22	2:282:B:GLN:O	6	1.41	0.66	1.7
(1,17)	1:53:A:LEU:HD11	2:282:B:GLN:O	6	1.41	0.66	1.7
(1,17)	1:53:A:LEU:HD13	2:282:B:GLN:O	6	1.41	0.66	1.7
(1,17)	1:53:A:LEU:HB2	2:282:B:GLN:HG2	6	1.41	0.66	1.7
(1,17)	1:54:A:MET:HE3	2:282:B:GLN:O	6	1.41	0.66	1.7
(1,33)	2:241:B:ILE:H	1:18:A:ARG:HH12	6	1.11	0.44	1.26
(1,33)	2:241:B:ILE:H	1:18:A:ARG:HH11	6	1.11	0.44	1.26
(1,33)	2:290:B:TYR:OH	1:18:A:ARG:N	6	1.11	0.44	1.26
(1,33)	2:244:B:LEU:HD23	1:18:A:ARG:H	6	1.11	0.44	1.26
(1,33)	2:244:B:LEU:HB2	1:18:A:ARG:HA	6	1.11	0.44	1.26
(1,33)	2:244:B:LEU:HD13	1:18:A:ARG:HA	6	1.11	0.44	1.26
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	6	0.38	0.07	0.37
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	6	0.32	0.21	0.22
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	6	0.3	0.21	0.21
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	6	0.3	0.15	0.29
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	6	0.3	0.07	0.3
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	6	0.27	0.09	0.28
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	6	0.23	0.11	0.19
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	6	0.23	0.07	0.2
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	6	0.23	0.07	0.2
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	6	0.23	0.07	0.2
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	6	0.21	0.06	0.21
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	6	0.2	0.07	0.19
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	6	0.18	0.05	0.16
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	6	0.18	0.06	0.16
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	6	0.18	0.07	0.14
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	6	0.18	0.03	0.19
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	6	0.16	0.03	0.18
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	6	0.15	0.05	0.14
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	6	0.15	0.05	0.14
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	5	1.04	0.71	0.96
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	5	0.48	0.26	0.47
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	5	0.4	0.07	0.39
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	5	0.31	0.21	0.24
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	5	0.29	0.14	0.28
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	5	0.28	0.1	0.22
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	5	0.26	0.1	0.21
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	5	0.23	0.08	0.24
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	5	0.22	0.07	0.24
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	5	0.22	0.17	0.13
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	5	0.22	0.17	0.13
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	5	0.22	0.05	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	5	0.21	0.11	0.13
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	5	0.18	0.04	0.16
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	5	0.17	0.06	0.13
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	5	0.15	0.02	0.15
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	5	0.15	0.04	0.14
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	5	0.15	0.04	0.14
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	5	0.14	0.03	0.14
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	5	0.14	0.03	0.14
(2,350)	2:314:B:GLN:H	2:315:B:GLY:H	4	0.35	0.16	0.36
(2,500)	2:379:B:LEU:H	2:380:B:HIS:H	4	0.33	0.09	0.34
(2,502)	2:380:B:HIS:H	2:378:B:VAL:H	4	0.3	0.09	0.31
(2,560)	2:396:B:ASP:H	2:383:B:THR:H	4	0.28	0.11	0.26
(3,52)	2:217:B:GLU:O	2:221:B:ASN:H	4	0.26	0.13	0.23
(3,222)	2:335:B:LEU:O	2:338:B:LEU:H	4	0.24	0.02	0.24
(3,147)	2:269:B:GLU:O	2:273:B:LYS:N	4	0.23	0.05	0.24
(2,225)	2:414:B:GLU:H	2:413:B:ILE:H	4	0.21	0.06	0.22
(2,607)	2:413:B:ILE:H	2:414:B:GLU:H	4	0.21	0.06	0.22
(2,168)	2:253:B:ARG:H	2:256:B:ARG:H	4	0.2	0.03	0.22
(3,229)	2:342:B:ARG:O	2:323:B:PHE:N	4	0.2	0.06	0.19
(2,526)	2:385:B:ILE:H	2:394:B:LEU:H	4	0.2	0.02	0.2
(2,423)	2:345:B:GLY:H	2:325:B:LEU:H	4	0.2	0.09	0.18
(2,444)	2:358:B:ALA:H	2:357:B:ALA:H	4	0.2	0.06	0.2
(3,8)	2:177:B:ALA:O	2:368:B:THR:H	4	0.2	0.05	0.2
(2,118)	2:227:B:SER:H	2:229:B:ARG:H	4	0.19	0.08	0.16
(2,446)	2:359:B:ILE:H	2:361:B:VAL:H	4	0.18	0.09	0.14
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH21	4	0.18	0.04	0.18
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH22	4	0.18	0.04	0.18
(3,21)	2:194:B:MET:O	2:273:B:LYS:NZ	4	0.16	0.02	0.16
(3,53)	2:218:B:GLU:O	2:222:B:GLU:N	4	0.16	0.04	0.15
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE21	4	0.16	0.05	0.15
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE22	4	0.16	0.05	0.15
(2,56)	2:207:B:LEU:H	2:209:B:ARG:H	4	0.15	0.03	0.15
(2,579)	2:404:B:GLU:H	2:402:B:LEU:H	4	0.15	0.03	0.14
(2,184)	2:259:B:PHE:H	2:256:B:ARG:H	4	0.14	0.02	0.14
(2,586)	2:405:B:TYR:H	2:402:B:LEU:H	4	0.13	0.04	0.12
(3,271)	2:370:B:MET:O	2:174:B:LEU:N	4	0.13	0.01	0.12
(2,465)	2:366:B:ILE:H	2:365:B:GLY:H	4	0.11	0.01	0.11
(3,185)	2:297:B:ASP:OD1	2:356:B:GLN:NE2	3	0.66	0.48	0.49
(2,348)	2:314:B:GLN:H	2:313:B:ASN:H	3	0.57	0.28	0.62
(2,48)	2:198:B:TYR:H	2:270:B:TRP:HE1	3	0.34	0.18	0.36
(2,351)	2:315:B:GLY:H	2:314:B:GLN:H	3	0.33	0.1	0.29
(3,282)	2:384:B:LEU:O	2:183:B:ALA:H	3	0.29	0.05	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,36)	2:188:B:ASP:H	2:326:B:VAL:H	3	0.29	0.07	0.32
(3,28)	2:206:B:ALA:O	2:210:B:GLU:H	3	0.28	0.12	0.33
(2,563)	2:400:B:VAL:H	2:402:B:LEU:H	3	0.26	0.21	0.12
(3,168)	2:280:B:ALA:O	2:284:B:ALA:H	3	0.26	0.08	0.23
(3,107)	2:251:B:ASP:O	2:253:B:ARG:N	3	0.26	0.17	0.16
(2,608)	2:413:B:ILE:H	2:411:B:GLU:H	3	0.26	0.12	0.22
(2,283)	2:286:B:LEU:H	2:283:B:PHE:H	3	0.25	0.09	0.19
(2,576)	2:403:B:GLN:H	2:400:B:VAL:H	3	0.23	0.16	0.14
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ1	3	0.22	0.1	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ2	3	0.22	0.1	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ3	3	0.22	0.1	0.15
(3,236)	2:347:B:VAL:O	2:327:B:ALA:H	3	0.22	0.05	0.23
(3,109)	2:251:B:ASP:OD1	2:253:B:ARG:N	3	0.21	0.04	0.21
(2,432)	2:349:B:ARG:H	2:327:B:ALA:H	3	0.21	0.1	0.15
(2,433)	2:349:B:ARG:H	2:350:B:ASP:H	3	0.2	0.05	0.2
(3,309)	2:403:B:GLN:O	2:407:B:ARG:N	3	0.2	0.07	0.25
(2,42)	2:194:B:MET:H	2:193:B:LEU:H	3	0.2	0.05	0.19
(3,281)	2:384:B:LEU:O	2:183:B:ALA:N	3	0.2	0.09	0.19
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ1	3	0.18	0.04	0.18
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ2	3	0.18	0.04	0.18
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ3	3	0.18	0.04	0.18
(2,38)	2:190:B:THR:H	2:189:B:ALA:H	3	0.18	0.07	0.15
(2,448)	2:361:B:VAL:H	2:360:B:MET:H	3	0.17	0.03	0.16
(2,450)	2:360:B:MET:H	2:361:B:VAL:H	3	0.17	0.03	0.16
(3,211)	2:327:B:ALA:O	2:349:B:ARG:N	3	0.17	0.05	0.13
(3,102)	2:246:B:SER:O	2:250:B:SER:HG	3	0.16	0.04	0.17
(3,23)	2:204:B:ASP:O	2:208:B:GLU:N	3	0.14	0.02	0.12
(2,356)	2:323:B:PHE:H	2:344:B:VAL:H	3	0.13	0.02	0.12
(3,206)	2:323:B:PHE:O	2:344:B:VAL:H	3	0.13	0.01	0.14
(3,225)	2:337:B:GLU:OE2	2:303:B:GLN:NE2	3	0.13	0.01	0.13
(2,185)	2:259:B:PHE:H	2:261:B:GLU:H	3	0.12	0.02	0.11
(3,49)	2:217:B:GLU:O	2:221:B:ASN:ND2	3	0.11	0.01	0.1
(4,3)	2:281:B:GLU:OE1	2:281:B:GLU:N	2	0.5	0.06	0.5
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ1	2	0.43	0.16	0.43
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ2	2	0.43	0.16	0.43
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ3	2	0.43	0.16	0.43
(3,302)	2:399:B:PRO:O	2:403:B:GLN:H	2	0.42	0.26	0.42
(2,489)	2:375:B:GLN:H	2:378:B:VAL:H	2	0.31	0.04	0.31
(3,278)	2:379:B:LEU:O	2:382:B:ARG:H	2	0.3	0.16	0.3
(2,29)	2:185:B:GLY:H	2:383:B:THR:H	2	0.28	0.17	0.28
(3,93)	2:244:B:LEU:O	2:248:B:LEU:N	2	0.27	0.08	0.27
(2,437)	2:350:B:ASP:H	2:351:B:GLY:H	2	0.26	0.14	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,241)	2:352:B:ALA:O	2:355:B:SER:OG	2	0.26	0.04	0.26
(3,324)	2:407:B:ARG:O	2:411:B:GLU:H	2	0.26	0.12	0.26
(3,101)	2:246:B:SER:O	2:250:B:SER:OG	2	0.24	0.03	0.24
(2,218)	2:270:B:TRP:H	2:273:B:LYS:H	2	0.22	0.1	0.22
(2,513)	2:382:B:ARG:H	2:185:B:GLY:H	2	0.22	0.12	0.22
(3,127)	2:257:B:GLU:OE1	2:278:B:LYS:NZ	2	0.22	0.02	0.22
(3,260)	2:361:B:VAL:O	2:366:B:ILE:H	2	0.22	0.06	0.22
(2,453)	2:362:B:ARG:H	2:360:B:MET:H	2	0.22	0.04	0.22
(2,501)	2:380:B:HIS:H	2:379:B:LEU:H	2	0.22	0.01	0.22
(4,6)	2:328:B:ASP:OD1	2:328:B:ASP:H	2	0.21	0.05	0.21
(1,6)	1:21:A:MET:HG2	2:247:B:HIS:HB2	2	0.2	0.06	0.2
(1,6)	1:47:A:ASN:OD1	2:247:B:HIS:HE2	2	0.2	0.06	0.2
(3,105)	2:247:B:HIS:O	2:250:B:SER:OG	2	0.2	0.03	0.2
(2,139)	2:240:B:ALA:H	2:241:B:ILE:H	2	0.2	0.04	0.2
(2,604)	2:411:B:GLU:H	2:412:B:GLU:H	2	0.2	0.07	0.2
(2,28)	2:184:B:GLU:H	2:384:B:LEU:H	2	0.19	0.0	0.19
(2,519)	2:384:B:LEU:H	2:184:B:GLU:H	2	0.19	0.0	0.19
(3,27)	2:206:B:ALA:O	2:210:B:GLU:N	2	0.19	0.05	0.19
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH11	2	0.19	0.07	0.19
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH12	2	0.19	0.07	0.19
(2,6)	2:173:B:ALA:H	2:392:B:GLU:H	2	0.18	0.08	0.18
(3,172)	2:283:B:PHE:O	2:286:B:LEU:H	2	0.18	0.04	0.18
(3,258)	2:361:B:VAL:O	2:365:B:GLY:H	2	0.18	0.04	0.18
(3,7)	2:177:B:ALA:O	2:368:B:THR:N	2	0.18	0.01	0.18
(2,220)	2:270:B:TRP:H	2:272:B:VAL:H	2	0.18	0.03	0.18
(3,136)	2:261:B:GLU:O	2:266:B:SER:H	2	0.18	0.04	0.18
(3,190)	2:299:B:ARG:O	2:303:B:GLN:H	2	0.18	0.03	0.18
(3,273)	2:373:B:ASP:O	2:349:B:ARG:NH1	2	0.18	0.04	0.18
(3,145)	2:269:B:GLU:OE2	2:211:B:ARG:NH1	2	0.17	0.03	0.17
(2,107)	2:222:B:GLU:H	2:223:B:PHE:H	2	0.17	0.04	0.17
(2,584)	2:405:B:TYR:H	2:408:B:LEU:H	2	0.16	0.0	0.16
(3,243)	2:353:B:ALA:O	2:362:B:ARG:NH1	2	0.16	0.04	0.16
(2,18)	2:181:B:ALA:H	2:386:B:VAL:H	2	0.16	0.02	0.16
(2,128)	2:230:B:PHE:H	2:229:B:ARG:H	2	0.16	0.04	0.16
(2,528)	2:386:B:VAL:H	2:181:B:ALA:H	2	0.16	0.02	0.16
(2,602)	2:411:B:GLU:H	2:409:B:ILE:H	2	0.16	0.01	0.16
(3,149)	2:270:B:TRP:O	2:274:B:THR:OG1	2	0.15	0.03	0.15
(2,297)	2:294:B:ARG:H	2:292:B:LYS:H	2	0.15	0.0	0.15
(2,275)	2:284:B:ALA:H	2:285:B:ALA:H	2	0.14	0.02	0.14
(2,278)	2:285:B:ALA:H	2:284:B:ALA:H	2	0.14	0.02	0.14
(3,63)	2:222:B:GLU:OE1	2:308:B:HIS:NE2	2	0.14	0.0	0.14
(3,139)	2:267:B:VAL:O	2:271:B:ALA:N	2	0.14	0.04	0.14

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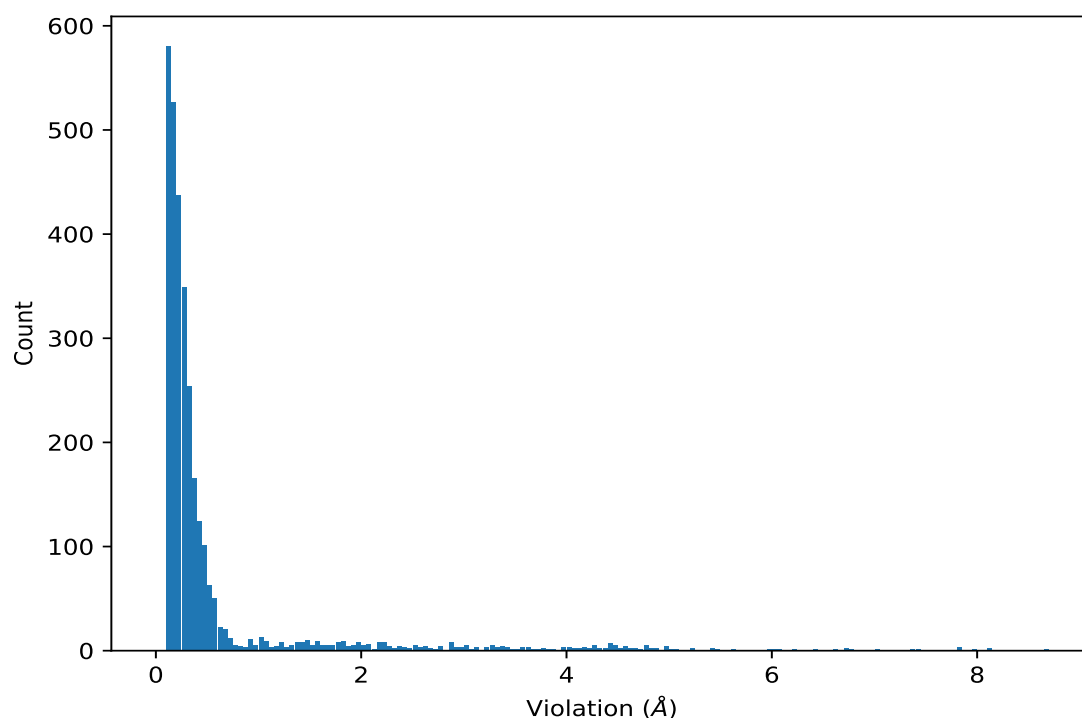
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,362)	2:324:B:ILE:H	2:184:B:GLU:H	2	0.14	0.02	0.14
(2,436)	2:350:B:ASP:H	2:349:B:ARG:H	2	0.14	0.04	0.14
(2,267)	2:282:B:GLN:H	2:281:B:GLU:H	2	0.13	0.02	0.13
(2,410)	2:341:B:ASP:H	2:342:B:ARG:H	2	0.13	0.02	0.13
(3,18)	2:186:B:TRP:O	2:326:B:VAL:H	2	0.13	0.01	0.13
(3,240)	2:348:B:VAL:O	2:372:B:ALA:H	2	0.13	0.02	0.13
(2,399)	2:337:B:GLU:H	2:335:B:LEU:H	2	0.12	0.02	0.12
(2,422)	2:345:B:GLY:H	2:323:B:PHE:H	2	0.12	0.02	0.12
(2,490)	2:375:B:GLN:H	2:374:B:ILE:H	2	0.12	0.02	0.12
(4,5)	2:328:B:ASP:OD1	2:328:B:ASP:N	2	0.12	0.02	0.12
(2,243)	2:275:B:VAL:H	2:277:B:GLU:H	2	0.12	0.01	0.12
(2,323)	2:304:B:ARG:H	2:303:B:GLN:H	2	0.12	0.0	0.12
(4,2)	2:269:B:GLU:OE1	2:269:B:GLU:H	2	0.12	0.01	0.12
(4,9)	2:375:B:GLN:OE1	2:375:B:GLN:N	2	0.12	0.0	0.12
(2,407)	2:340:B:GLN:H	2:341:B:ASP:H	2	0.12	0.02	0.12
(2,470)	2:369:B:VAL:H	2:368:B:THR:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:H	9	8.67
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:H	17	8.14
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:H	18	8.11
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:H	7	7.95
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH21	6	7.83
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:H	4	7.81
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:HH11	11	7.81
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:H	20	7.41
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:H	1	7.39
(1,45)	2:290:B:TYR:HB3	1:61:A:ARG:HH12	15	7.02
(1,45)	2:290:B:TYR:HE1	1:61:A:ARG:H	16	6.76
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH22	19	6.74
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:HH12	2	6.73
(1,45)	2:290:B:TYR:HD2	1:61:A:ARG:HH11	8	6.62
(1,45)	2:290:B:TYR:HB2	1:61:A:ARG:HH11	10	6.41
(1,45)	2:290:B:TYR:HD2	1:61:A:ARG:HH12	14	6.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH22	12	6.07
(1,45)	2:290:B:TYR:HE1	1:61:A:ARG:H	13	6.04
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH22	5	5.97
(1,14)	1:47:A:ASN:O	2:257:B:GLU:H	5	5.6
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HB2	10	5.47
(1,45)	2:290:B:TYR:H	1:61:A:ARG:HH12	3	5.42
(1,14)	1:53:A:LEU:HD22	2:257:B:GLU:OE2	7	5.41
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	3	5.24
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	11	5.21
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG2	18	5.06
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB2	3	5.0
(1,41)	2:279:B:PHE:HD2	1:54:A:MET:H	4	4.99
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	2	4.98
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB3	14	4.97
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	20	4.96
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	9	4.88
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	4	4.87
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG2	2	4.84
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	16	4.81
(1,12)	1:47:A:ASN:OD1	2:255:B:ARG:H	12	4.79
(1,8)	1:47:A:ASN:HD21	2:250:B:SER:O	9	4.77
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	19	4.76
(1,31)	2:290:B:TYR:HB2	1:15:A:MET:O	19	4.75
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	11	4.75
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	1	4.74
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB2	9	4.69
(1,12)	1:47:A:ASN:O	2:255:B:ARG:HE	15	4.66
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	6	4.64
(1,41)	2:290:B:TYR:HB2	1:54:A:MET:N	2	4.61
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	15	4.59
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	10	4.59
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	15	4.57
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	14	4.57
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	8	4.54
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	9	4.5
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	17	4.48
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	7	4.47
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH11	11	4.47
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:O	7	4.46
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	8	4.46
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HB3	5	4.44
(1,12)	1:47:A:ASN:OD1	2:255:B:ARG:HH22	20	4.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	6	4.41
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	4	4.41
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	15	4.41
(1,14)	1:47:A:ASN:HD22	2:257:B:GLU:H	6	4.4
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	16	4.4
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	9	4.35
(1,12)	1:47:A:ASN:O	2:255:B:ARG:H	3	4.35
(1,41)	2:290:B:TYR:HB2	1:54:A:MET:N	10	4.34
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	13	4.3
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	14	4.27
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	16	4.27
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	11	4.26
(1,12)	1:47:A:ASN:HD21	2:255:B:ARG:H	5	4.26
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	10	4.25
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	14	4.23
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HD3	18	4.2
(1,41)	2:279:B:PHE:HE2	1:54:A:MET:HE1	3	4.19
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	1	4.17
(1,12)	1:47:A:ASN:HD21	2:255:B:ARG:HG2	17	4.17
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	8	4.14
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	20	4.11
(1,30)	2:290:B:TYR:HD2	1:11:A:ASN:O	17	4.07
(1,14)	1:47:A:ASN:HD22	2:257:B:GLU:HG2	17	4.06
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:HD22	18	4.04
(1,30)	2:290:B:TYR:HB3	1:11:A:ASN:O	3	4.02
(1,14)	1:47:A:ASN:O	2:257:B:GLU:HG3	19	4.0
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	9	3.97
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	9	3.97
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	9	3.95
(1,8)	1:47:A:ASN:O	2:250:B:SER:HG	7	3.87
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	2	3.82
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	18	3.78
(1,14)	1:47:A:ASN:O	2:257:B:GLU:OE2	12	3.75
(1,8)	1:47:A:ASN:O	2:250:B:SER:O	3	3.7
(1,13)	1:47:A:ASN:OD1	2:256:B:ARG:HG3	20	3.67
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:OD1	14	3.62
(1,16)	1:53:A:LEU:HD22	2:281:B:GLU:O	5	3.62
(1,30)	2:290:B:TYR:H	1:11:A:ASN:HD22	12	3.61
(1,43)	2:290:B:TYR:H	1:57:A:SER:HG	11	3.58
(1,13)	1:47:A:ASN:OD1	2:256:B:ARG:HG3	10	3.56
(1,8)	1:47:A:ASN:HA	2:250:B:SER:HG	4	3.56
(1,16)	1:53:A:LEU:HD11	2:281:B:GLU:O	19	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:47:A:ASN:OD1	2:256:B:ARG:HB3	11	3.49
(1,16)	1:53:A:LEU:HD22	2:281:B:GLU:O	17	3.44
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HB3	16	3.4
(1,1)	1:16:A:HIS:HB3	2:356:B:GLN:HB3	16	3.4
(1,30)	2:290:B:TYR:HD2	1:11:A:ASN:O	8	3.37
(1,8)	1:47:A:ASN:HD21	2:250:B:SER:O	17	3.36
(1,16)	1:53:A:LEU:HD21	2:281:B:GLU:O	14	3.35
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	1	3.35
(1,16)	1:53:A:LEU:HD23	2:281:B:GLU:O	15	3.33
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HB3	6	3.32
(1,16)	1:53:A:LEU:HD11	2:281:B:GLU:O	6	3.3
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH11	1	3.28
(1,27)	1:53:A:LEU:HB2	2:293:B:GLU:H	11	3.26
(1,8)	1:21:A:MET:HE2	2:250:B:SER:HG	14	3.26
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HB3	10	3.26
(1,1)	1:16:A:HIS:HB3	2:356:B:GLN:OE1	10	3.26
(1,16)	1:53:A:LEU:HD13	2:281:B:GLU:O	12	3.24
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	15	3.23
(1,16)	1:53:A:LEU:HD21	2:281:B:GLU:O	18	3.23
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH22	13	3.14
(1,41)	2:290:B:TYR:HB2	1:54:A:MET:N	16	3.13
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:H	6	3.11
(1,41)	2:290:B:TYR:HB2	1:54:A:MET:N	13	3.08
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	3	3.04
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	3	3.04
(1,2)	2:356:B:GLN:HE21	1:16:A:HIS:HE1	15	3.02
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HE21	15	3.02
(1,16)	1:53:A:LEU:HD22	2:281:B:GLU:O	3	3.0
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HD3	13	2.96
(1,30)	2:290:B:TYR:HD1	1:11:A:ASN:O	4	2.95
(1,8)	1:21:A:MET:HE2	2:250:B:SER:HG	8	2.95
(1,12)	1:47:A:ASN:HD22	2:255:B:ARG:HH12	19	2.9
(1,2)	2:356:B:GLN:HA	1:16:A:HIS:HD2	1	2.9
(1,1)	1:16:A:HIS:HD2	2:356:B:GLN:HA	1	2.9
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	12	2.89
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	19	2.89
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	17	2.88
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	17	2.88
(1,16)	1:53:A:LEU:HD12	2:281:B:GLU:O	8	2.87
(1,16)	1:53:A:LEU:HG	2:281:B:GLU:O	16	2.86
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE2	18	2.86
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB3	18	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	2:290:B:TYR:H	1:57:A:SER:HA	4	2.76
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	6	2.76
(1,29)	1:53:A:LEU:HD21	2:295:B:ALA:HA	7	2.76
(1,31)	2:290:B:TYR:HD2	1:15:A:MET:O	10	2.75
(1,30)	2:290:B:TYR:HH	1:11:A:ASN:HB3	2	2.72
(1,30)	2:290:B:TYR:HE1	1:11:A:ASN:O	10	2.68
(1,16)	1:53:A:LEU:HD13	2:281:B:GLU:O	2	2.67
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:HD22	20	2.64
(1,15)	1:53:A:LEU:HG	2:279:B:PHE:O	16	2.64
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HE2	6	2.63
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:OE1	6	2.63
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	9	2.58
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HG3	19	2.58
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	11	2.57
(1,27)	1:53:A:LEU:HB2	2:293:B:GLU:H	7	2.53
(1,16)	1:53:A:LEU:HD13	2:281:B:GLU:O	10	2.53
(1,15)	1:53:A:LEU:HG	2:279:B:PHE:O	8	2.5
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HD2	11	2.5
(1,1)	1:16:A:HIS:HD2	2:356:B:GLN:HB3	11	2.5
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	15	2.46
(1,16)	1:54:A:MET:HE2	2:281:B:GLU:O	20	2.45
(1,43)	2:290:B:TYR:H	1:57:A:SER:HA	17	2.44
(1,13)	1:47:A:ASN:HD21	2:256:B:ARG:HG2	1	2.41
(1,16)	1:53:A:LEU:HD11	2:281:B:GLU:O	1	2.4
(1,29)	1:53:A:LEU:HD12	2:295:B:ALA:H	9	2.37
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	5	2.37
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE2	14	2.35
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB3	14	2.35
(1,43)	2:290:B:TYR:H	1:57:A:SER:HA	1	2.32
(1,31)	2:244:B:LEU:HD23	1:15:A:MET:HB2	18	2.3
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ2	11	2.27
(1,7)	1:47:A:ASN:O	2:248:B:LEU:HA	16	2.27
(1,16)	1:53:A:LEU:HD22	2:281:B:GLU:O	11	2.26
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	18	2.25
(1,20)	1:53:A:LEU:HD13	2:285:B:ALA:HB2	12	2.24
(1,8)	1:47:A:ASN:HD22	2:250:B:SER:O	6	2.24
(1,31)	2:290:B:TYR:OH	1:15:A:MET:HE2	20	2.23
(1,29)	1:53:A:LEU:HB2	2:295:B:ALA:H	16	2.23
(1,29)	1:53:A:LEU:HD22	2:295:B:ALA:HB2	11	2.22
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:H	6	2.22
(1,8)	1:21:A:MET:HE1	2:250:B:SER:HG	18	2.22
(1,30)	2:290:B:TYR:HB2	1:11:A:ASN:OD1	1	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:53:A:LEU:HG	2:293:B:GLU:H	15	2.19
(1,2)	2:356:B:GLN:HG2	1:16:A:HIS:HE2	12	2.19
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HG2	12	2.19
(1,41)	2:290:B:TYR:HB3	1:54:A:MET:N	5	2.18
(1,7)	1:21:A:MET:HA	2:248:B:LEU:HD22	4	2.17
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE3	9	2.15
(1,40)	2:279:B:PHE:O	1:53:A:LEU:HD22	11	2.15
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	11	2.15
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	14	2.12
(1,36)	2:248:B:LEU:HA	1:47:A:ASN:O	8	2.09
(1,43)	2:290:B:TYR:HD2	1:57:A:SER:N	8	2.08
(1,31)	2:290:B:TYR:HD2	1:15:A:MET:HE1	2	2.06
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:H	16	2.06
(1,17)	1:53:A:LEU:HB2	2:282:B:GLN:HG2	17	2.05
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HH22	2	2.05
(1,31)	2:244:B:LEU:HD12	1:15:A:MET:O	12	2.04
(1,43)	2:290:B:TYR:H	1:57:A:SER:HA	3	2.02
(1,30)	2:290:B:TYR:HD1	1:11:A:ASN:HD22	5	2.02
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	20	2.01
(1,17)	1:53:A:LEU:HD11	2:282:B:GLN:O	6	2.0
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HE1	7	1.99
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:OE1	7	1.99
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:HA	5	1.97
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	20	1.96
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	20	1.96
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	20	1.96
(1,27)	1:53:A:LEU:HD12	2:293:B:GLU:H	9	1.96
(1,8)	1:47:A:ASN:OD1	2:250:B:SER:O	13	1.96
(1,16)	1:53:A:LEU:HD21	2:281:B:GLU:O	7	1.94
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HD3	12	1.93
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	7	1.91
(1,31)	2:290:B:TYR:HE2	1:15:A:MET:O	13	1.9
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	7	1.9
(1,43)	2:290:B:TYR:HD1	1:57:A:SER:HA	2	1.88
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:H	19	1.88
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	6	1.86
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH22	16	1.85
(1,17)	1:53:A:LEU:HD11	2:282:B:GLN:O	19	1.83
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	6	1.81
(1,43)	2:290:B:TYR:HB2	1:57:A:SER:N	10	1.81
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	19	1.8
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	2	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	2	1.8
(1,20)	1:54:A:MET:HE2	2:285:B:ALA:HB2	3	1.8
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:OG1	9	1.8
(1,3)	1:16:A:HIS:O	2:241:B:ILE:HD13	18	1.8
(1,43)	2:290:B:TYR:HB2	1:57:A:SER:N	6	1.79
(1,19)	1:53:A:LEU:HD23	2:284:B:ALA:N	20	1.79
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	8	1.79
(1,16)	1:53:A:LEU:HD11	2:281:B:GLU:O	13	1.78
(1,7)	1:21:A:MET:HE2	2:248:B:LEU:H	8	1.76
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	15	1.75
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	15	1.75
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	2	1.75
(1,7)	1:53:A:LEU:HD23	2:248:B:LEU:HG	12	1.73
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	14	1.7
(1,43)	2:290:B:TYR:HD1	1:57:A:SER:N	16	1.7
(1,29)	1:53:A:LEU:HB2	2:295:B:ALA:H	4	1.7
(1,20)	1:54:A:MET:HG2	2:285:B:ALA:HB3	14	1.7
(1,27)	1:16:A:HIS:HE2	2:293:B:GLU:HB3	12	1.69
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:H	15	1.68
(1,7)	1:21:A:MET:HE3	2:248:B:LEU:HB2	13	1.68
(1,20)	1:53:A:LEU:HD22	2:285:B:ALA:H	17	1.66
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	3	1.65
(1,35)	2:244:B:LEU:HD12	1:22:A:LYS:N	18	1.64
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	18	1.64
(1,33)	2:290:B:TYR:OH	1:18:A:ARG:N	14	1.6
(1,31)	2:290:B:TYR:HH	1:15:A:MET:O	15	1.6
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB3	2	1.6
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	12	1.58
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	18	1.58
(1,19)	1:53:A:LEU:HD23	2:284:B:ALA:N	15	1.58
(1,4)	1:18:A:ARG:HH22	2:243:B:ASP:HB3	10	1.57
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	12	1.56
(1,17)	1:53:A:LEU:HD22	2:282:B:GLN:O	5	1.56
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:H	4	1.56
(1,20)	1:53:A:LEU:HD13	2:285:B:ALA:H	10	1.55
(1,15)	1:53:A:LEU:HD12	2:279:B:PHE:O	13	1.55
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	2	1.54
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:H	6	1.54
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	4	1.52
(1,27)	1:56:A:ASP:OD2	2:293:B:GLU:H	10	1.5
(1,27)	1:53:A:LEU:HD22	2:293:B:GLU:N	20	1.5
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	2	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE2	15	1.49
(1,33)	2:244:B:LEU:HD23	1:18:A:ARG:H	18	1.49
(1,16)	1:53:A:LEU:HD13	2:281:B:GLU:O	9	1.48
(1,20)	1:57:A:SER:HB3	2:285:B:ALA:O	1	1.47
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HD3	19	1.45
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:HA	15	1.45
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:HG2	18	1.45
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE2	2	1.45
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB3	2	1.45
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	2	1.44
(1,31)	2:290:B:TYR:HE2	1:15:A:MET:O	1	1.43
(1,36)	2:247:B:HIS:HB3	1:47:A:ASN:HA	17	1.42
(1,33)	2:244:B:LEU:HD13	1:18:A:ARG:HA	20	1.42
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	17	1.42
(1,43)	2:290:B:TYR:HD2	1:57:A:SER:H	14	1.41
(1,30)	2:290:B:TYR:HE1	1:11:A:ASN:O	13	1.41
(1,15)	1:53:A:LEU:HD11	2:279:B:PHE:O	9	1.4
(1,40)	2:290:B:TYR:HD2	1:53:A:LEU:HD21	8	1.38
(1,35)	2:244:B:LEU:HD13	1:22:A:LYS:N	14	1.38
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	19	1.38
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	19	1.38
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	5	1.37
(1,15)	1:53:A:LEU:HD11	2:279:B:PHE:O	19	1.37
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:H	7	1.36
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:HG21	7	1.35
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	7	1.34
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH11	15	1.34
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:HG1	14	1.34
(3,185)	2:297:B:ASP:OD1	2:356:B:GLN:NE2	15	1.31
(1,27)	1:53:A:LEU:HD21	2:293:B:GLU:N	5	1.31
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE3	17	1.29
(1,10)	1:47:A:ASN:HB3	2:252:B:THR:OG1	16	1.29
(1,7)	1:53:A:LEU:HD13	2:248:B:LEU:HD22	3	1.26
(1,29)	1:53:A:LEU:HG	2:295:B:ALA:H	8	1.24
(1,27)	1:16:A:HIS:HD2	2:293:B:GLU:OE2	4	1.24
(1,19)	1:53:A:LEU:HD13	2:284:B:ALA:N	12	1.23
(1,35)	2:243:B:ASP:OD1	1:22:A:LYS:N	6	1.21
(1,35)	2:244:B:LEU:HD11	1:22:A:LYS:N	7	1.21
(1,19)	1:53:A:LEU:HD22	2:284:B:ALA:N	11	1.21
(1,2)	2:356:B:GLN:OE1	1:16:A:HIS:HE1	5	1.2
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:OE1	5	1.2
(1,15)	1:53:A:LEU:HD12	2:279:B:PHE:O	6	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD22	1	1.18
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:H	8	1.15
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:OE1	14	1.15
(1,35)	2:244:B:LEU:HD11	1:22:A:LYS:N	1	1.13
(1,7)	1:53:A:LEU:HD23	2:248:B:LEU:HD12	7	1.12
(1,33)	2:241:B:ILE:H	1:18:A:ARG:HH12	2	1.1
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	16	1.09
(1,36)	2:247:B:HIS:HB3	1:47:A:ASN:HA	4	1.08
(1,35)	2:244:B:LEU:HD13	1:22:A:LYS:N	20	1.08
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HD2	4	1.08
(1,1)	1:16:A:HIS:HD2	2:356:B:GLN:HB3	4	1.08
(1,35)	2:244:B:LEU:HD11	1:22:A:LYS:N	8	1.07
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	6	1.06
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	6	1.06
(1,41)	2:290:B:TYR:HD2	1:54:A:MET:N	19	1.05
(1,35)	2:244:B:LEU:HG	1:22:A:LYS:H	12	1.04
(1,36)	2:248:B:LEU:HD11	1:47:A:ASN:O	11	1.03
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB2	5	1.03
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB1	18	1.03
(1,16)	1:53:A:LEU:HD23	2:281:B:GLU:O	4	1.03
(1,15)	1:53:A:LEU:HD13	2:279:B:PHE:O	2	1.03
(1,43)	2:290:B:TYR:HD1	1:57:A:SER:N	13	1.02
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:N	14	1.02
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HE3	3	1.01
(1,35)	2:247:B:HIS:HD2	1:22:A:LYS:HA	11	1.01
(1,19)	1:53:A:LEU:HD22	2:284:B:ALA:N	5	1.01
(1,15)	1:53:A:LEU:HD21	2:279:B:PHE:HD2	15	1.0
(1,10)	1:47:A:ASN:HB2	2:252:B:THR:HG1	8	1.0
(1,15)	1:53:A:LEU:HD13	2:279:B:PHE:O	10	0.99
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:H	19	0.98
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	6	0.96
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	8	0.95
(1,19)	1:53:A:LEU:HG	2:284:B:ALA:N	16	0.95
(1,40)	2:290:B:TYR:HD2	1:53:A:LEU:HA	9	0.94
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	20	0.92
(1,40)	2:279:B:PHE:O	1:53:A:LEU:HD22	4	0.92
(1,20)	1:53:A:LEU:HD12	2:285:B:ALA:H	8	0.92
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:O	4	0.92
(1,10)	1:47:A:ASN:OD1	2:252:B:THR:HG1	10	0.92
(1,15)	1:53:A:LEU:HD12	2:279:B:PHE:HD2	1	0.91
(1,31)	2:290:B:TYR:HH	1:15:A:MET:O	17	0.9
(1,27)	1:53:A:LEU:HD13	2:293:B:GLU:H	13	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	2:356:B:GLN:HB3	1:16:A:HIS:HE1	8	0.9
(1,1)	1:16:A:HIS:HE1	2:356:B:GLN:HB3	8	0.9
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	7	0.89
(2,348)	2:314:B:GLN:H	2:313:B:ASN:H	12	0.89
(1,31)	2:290:B:TYR:HE2	1:15:A:MET:O	4	0.87
(1,26)	1:53:A:LEU:HB2	2:292:B:LYS:H	11	0.84
(1,20)	1:53:A:LEU:HG	2:285:B:ALA:H	16	0.84
(1,35)	2:243:B:ASP:OD1	1:22:A:LYS:HA	16	0.83
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	1	0.81
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	14	0.79
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	14	0.79
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:O	11	0.79
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	18	0.76
(1,19)	1:53:A:LEU:HD11	2:284:B:ALA:N	1	0.76
(1,44)	2:290:B:TYR:HB2	1:59:A:LYS:HD2	1	0.74
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	5	0.74
(1,29)	1:53:A:LEU:HD22	2:295:B:ALA:HA	15	0.74
(1,30)	2:290:B:TYR:HE1	1:11:A:ASN:HD22	16	0.73
(1,26)	1:53:A:LEU:HB3	2:292:B:LYS:N	12	0.73
(1,15)	1:53:A:LEU:HD11	2:279:B:PHE:HD2	12	0.73
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	8	0.72
(2,49)	2:201:B:SER:H	2:202:B:THR:H	1	0.7
(1,31)	2:290:B:TYR:HH	1:15:A:MET:O	9	0.7
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD11	6	0.7
(1,2)	2:356:B:GLN:HG2	1:16:A:HIS:HE2	13	0.7
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HG2	13	0.7
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	2	0.69
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:HB3	7	0.69
(1,19)	1:53:A:LEU:HD21	2:284:B:ALA:N	14	0.69
(3,302)	2:399:B:PRO:O	2:403:B:GLN:H	18	0.68
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	9	0.68
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	9	0.68
(1,31)	2:290:B:TYR:OH	1:15:A:MET:O	16	0.68
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	7	0.67
(1,37)	2:247:B:HIS:HD2	1:48:A:SER:HA	5	0.67
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	5	0.66
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	11	0.66
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	11	0.66
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	11	0.66
(1,35)	2:244:B:LEU:HG	1:22:A:LYS:N	9	0.66
(1,26)	1:53:A:LEU:HG	2:292:B:LYS:H	15	0.66
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:HE2	14	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	7	0.65
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	10	0.65
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	4	0.65
(1,43)	2:290:B:TYR:HB3	1:57:A:SER:N	5	0.65
(1,13)	1:47:A:ASN:O	2:256:B:ARG:HH12	12	0.65
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	2	0.64
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	6	0.64
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	16	0.64
(1,15)	1:53:A:LEU:HD23	2:279:B:PHE:HE1	20	0.64
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	11	0.63
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	19	0.63
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	4	0.63
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	7	0.63
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	10	0.63
(2,348)	2:314:B:GLN:H	2:313:B:ASN:H	17	0.62
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	13	0.62
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	6	0.62
(1,40)	2:248:B:LEU:HD13	1:53:A:LEU:HD11	10	0.62
(1,19)	1:53:A:LEU:HD13	2:284:B:ALA:N	2	0.62
(3,301)	2:399:B:PRO:O	2:403:B:GLN:N	18	0.61
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	5	0.61
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	3	0.61
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	17	0.61
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	1	0.61
(1,35)	2:244:B:LEU:HD23	1:22:A:LYS:N	19	0.61
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	13	0.6
(1,40)	2:244:B:LEU:HD23	1:53:A:LEU:HD22	1	0.6
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:N	3	0.6
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	19	0.59
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	19	0.59
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ1	8	0.59
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ2	8	0.59
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ3	8	0.59
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	18	0.59
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	10	0.59
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	6	0.59
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	6	0.59
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	8	0.58
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	4	0.58
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	11	0.58
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	17	0.58
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	19	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	11	0.58
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	17	0.58
(1,26)	1:53:A:LEU:HD23	2:292:B:LYS:N	6	0.58
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	3	0.57
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	20	0.57
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	11	0.57
(2,350)	2:314:B:GLN:H	2:315:B:GLY:H	2	0.57
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	4	0.57
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	6	0.57
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	20	0.57
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	4	0.57
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	8	0.57
(1,20)	1:54:A:MET:HE3	2:285:B:ALA:HB1	15	0.57
(1,19)	1:53:A:LEU:HD22	2:284:B:ALA:N	3	0.57
(1,17)	1:54:A:MET:HE3	2:282:B:GLN:O	18	0.57
(4,3)	2:281:B:GLU:OE1	2:281:B:GLU:N	14	0.56
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	1	0.56
(2,563)	2:400:B:VAL:H	2:402:B:LEU:H	18	0.56
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	3	0.56
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	13	0.56
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	19	0.56
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	19	0.56
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	1	0.56
(1,7)	1:21:A:MET:HG2	2:248:B:LEU:HD22	11	0.56
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	14	0.55
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	18	0.55
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	7	0.55
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	7	0.55
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	16	0.55
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	9	0.55
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	16	0.55
(2,48)	2:198:B:TYR:H	2:270:B:TRP:HE1	6	0.55
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	11	0.55
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	17	0.55
(1,33)	2:244:B:LEU:HB2	1:18:A:ARG:HA	19	0.55
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:HA	15	0.55
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	9	0.54
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	14	0.54
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	16	0.54
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	17	0.54
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	5	0.54
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	14	0.54
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	15	0.54
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	13	0.54
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	7	0.53
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	17	0.53
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	15	0.53
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	10	0.53
(1,19)	1:53:A:LEU:HG	2:284:B:ALA:N	8	0.53
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	10	0.52
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	10	0.52
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	7	0.52
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	14	0.52
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	4	0.52
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	17	0.52
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	15	0.52
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	6	0.52
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	9	0.52
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	7	0.52
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	7	0.52
(2,49)	2:201:B:SER:H	2:202:B:THR:H	19	0.52
(1,33)	2:241:B:ILE:H	1:18:A:ARG:HH11	3	0.52
(1,20)	1:53:A:LEU:HD11	2:285:B:ALA:HB2	13	0.52
(1,3)	1:18:A:ARG:HH11	2:241:B:ILE:H	3	0.52
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	18	0.51
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	10	0.51
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	20	0.51
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	17	0.51
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	3	0.51
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	9	0.51
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	1	0.51
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	7	0.51
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	7	0.51
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	1	0.51
(1,36)	2:248:B:LEU:HD11	1:47:A:ASN:O	9	0.51
(1,28)	1:53:A:LEU:HB2	2:294:B:ARG:HD3	9	0.51
(1,7)	1:47:A:ASN:O	2:248:B:LEU:HD11	9	0.51
(3,107)	2:251:B:ASP:O	2:253:B:ARG:N	11	0.5
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	4	0.5
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	7	0.5
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	20	0.5
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	7	0.5
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	1	0.5
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	6	0.5
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	12	0.5
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	18	0.5
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	1	0.5
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	6	0.5
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	12	0.5
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	18	0.5
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	11	0.5
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	18	0.5
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	7	0.5
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	12	0.5
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	20	0.5
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ1	7	0.5
(1,10)	1:47:A:ASN:HB2	2:252:B:THR:HG1	3	0.5
(3,185)	2:297:B:ASP:OD1	2:356:B:GLN:NE2	19	0.49
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	2	0.49
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	10	0.49
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	18	0.49
(2,460)	2:364:B:LEU:H	2:366:B:ILE:H	16	0.49
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	1	0.49
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	12	0.49
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	3	0.49
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	10	0.49
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	17	0.49
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	3	0.49
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	10	0.49
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	17	0.49
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	1	0.49
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	8	0.49
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	1	0.49
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	1	0.49
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	10	0.49
(1,19)	1:53:A:LEU:HD11	2:284:B:ALA:N	19	0.49
(1,7)	1:21:A:MET:HA	2:248:B:LEU:HD11	19	0.49
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	10	0.48
(3,146)	2:269:B:GLU:OE2	2:211:B:ARG:HH11	3	0.48
(3,146)	2:269:B:GLU:OE2	2:211:B:ARG:HH12	3	0.48
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	12	0.48
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	19	0.48
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	6	0.48
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	1	0.48
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	7	0.48
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	2	0.48
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	13	0.48
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	20	0.48
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	15	0.48
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	15	0.48
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	7	0.48
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	10	0.48
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	13	0.48
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	20	0.48
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	5	0.48
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	9	0.48
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	4	0.48
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	3	0.47
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	6	0.47
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	7	0.47
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	14	0.47
(3,52)	2:217:B:GLU:O	2:221:B:ASN:H	3	0.47
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	4	0.47
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	11	0.47
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	2	0.47
(2,351)	2:315:B:GLY:H	2:314:B:GLN:H	2	0.47
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	2	0.47
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	2	0.47
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	2	0.47
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	11	0.47
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	14	0.47
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	2	0.47
(1,37)	2:279:B:PHE:HZ	1:48:A:SER:HG	8	0.47
(1,31)	2:290:B:TYR:HE2	1:15:A:MET:O	11	0.47
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	13	0.46
(3,278)	2:379:B:LEU:O	2:382:B:ARG:H	4	0.46
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	8	0.46
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	3	0.46
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	11	0.46
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	16	0.46
(2,576)	2:403:B:GLN:H	2:400:B:VAL:H	18	0.46
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	17	0.46
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	8	0.46
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	2	0.46
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	4	0.46
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	5	0.46
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	19	0.46
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	20	0.46
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	4	0.46
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	5	0.46
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	19	0.46
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	20	0.46
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	9	0.46
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	11	0.46
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	9	0.46
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	5	0.46
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	3	0.46
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	8	0.46
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	13	0.46
(1,7)	1:21:A:MET:HE1	2:248:B:LEU:HB2	10	0.46
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:HA	2	0.46
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	8	0.45
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	4	0.45
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	8	0.45
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	15	0.45
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	18	0.45
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	15	0.45
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	9	0.45
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	9	0.45
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	1	0.45
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	15	0.45
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	18	0.45
(2,29)	2:185:B:GLY:H	2:383:B:THR:H	11	0.45
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	8	0.45
(1,40)	2:248:B:LEU:HD12	1:53:A:LEU:HD12	17	0.45
(1,7)	1:53:A:LEU:HD12	2:248:B:LEU:HD12	17	0.45
(4,3)	2:281:B:GLU:OE1	2:281:B:GLU:N	19	0.44
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	16	0.44
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	19	0.44
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	18	0.44
(2,560)	2:396:B:ASP:H	2:383:B:THR:H	17	0.44
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	1	0.44
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	17	0.44
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	16	0.44
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	8	0.44
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	16	0.44
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	11	0.44
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	16	0.44
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	19	0.44
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	19	0.44
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	20	0.44
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	12	0.44
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	8	0.44
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	14	0.44
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	12	0.44
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	4	0.44
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	16	0.44
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	17	0.44
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	9	0.44
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:HG	17	0.44
(1,17)	1:53:A:LEU:HD13	2:282:B:GLN:O	12	0.44
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	12	0.43
(3,164)	2:276:B:ILE:O	2:280:B:ALA:H	18	0.43
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	11	0.43
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	11	0.43
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	13	0.43
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	3	0.43
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	11	0.43
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	16	0.43
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	18	0.43
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	4	0.43
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	3	0.43
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	6	0.43
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	18	0.43
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	17	0.43
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	18	0.43
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	2	0.43
(1,40)	2:290:B:TYR:HB2	1:53:A:LEU:HA	13	0.43
(1,13)	1:47:A:ASN:HD22	2:256:B:ARG:HH11	17	0.43
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	9	0.42
(2,608)	2:413:B:ILE:H	2:411:B:GLU:H	20	0.42
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	6	0.42
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	10	0.42
(2,500)	2:379:B:LEU:H	2:380:B:HIS:H	15	0.42
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	17	0.42
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	13	0.42
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	3	0.42
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	17	0.42
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	19	0.42
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	13	0.42
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	14	0.42
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	13	0.42
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	14	0.42
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	19	0.42
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	4	0.42
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	19	0.42
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	1	0.42
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	20	0.42
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	3	0.42
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	8	0.42
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	9	0.42
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	4	0.42
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	10	0.42
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	17	0.41
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	10	0.41
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	9	0.41
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	9	0.41
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	9	0.41
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	10	0.41
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	3	0.41
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	11	0.41
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	9	0.41
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	8	0.41
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	13	0.41
(2,502)	2:380:B:HIS:H	2:378:B:VAL:H	3	0.41
(2,500)	2:379:B:LEU:H	2:380:B:HIS:H	8	0.41
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	11	0.41
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	16	0.41
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	16	0.41
(2,337)	2:310:B:ASP:H	2:308:B:HIS:H	10	0.41
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	20	0.41
(2,210)	2:266:B:SER:H	2:265:B:GLY:H	8	0.41
(2,208)	2:265:B:GLY:H	2:266:B:SER:H	8	0.41
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	1	0.41
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	17	0.41
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	3	0.41
(2,111)	2:308:B:HIS:H	2:310:B:ASP:H	10	0.41
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	6	0.41
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	13	0.41
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	13	0.4
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	8	0.4
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	19	0.4
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	20	0.4
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	1	0.4
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	18	0.4
(3,28)	2:206:B:ALA:O	2:210:B:GLU:H	20	0.4
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	10	0.4
(2,437)	2:350:B:ASP:H	2:351:B:GLY:H	4	0.4
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	17	0.4
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	5	0.4
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	16	0.4
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	5	0.4
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	4	0.4
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	6	0.4
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	16	0.4
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	19	0.4
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	17	0.4
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	1	0.4
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	2	0.4
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	7	0.4
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	7	0.4
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	16	0.4
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	20	0.4
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	11	0.4
(1,26)	1:53:A:LEU:HD22	2:292:B:LYS:H	19	0.4
(1,19)	1:53:A:LEU:HD11	2:284:B:ALA:N	6	0.4
(1,7)	1:53:A:LEU:HD11	2:248:B:LEU:HD12	2	0.4
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	4	0.39
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	5	0.39
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	2	0.39
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	2	0.39
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	5	0.39
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	18	0.39
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	1	0.39
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	6	0.39
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	17	0.39
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	11	0.39
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	10	0.39
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	11	0.39
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	4	0.39
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	7	0.39
(2,350)	2:314:B:GLN:H	2:315:B:GLY:H	6	0.39
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	5	0.39
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	19	0.39
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	7	0.39
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	17	0.39
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	18	0.39
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	12	0.39
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	20	0.39
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	10	0.39
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	18	0.39
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	5	0.39
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	4	0.39
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	6	0.39
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	9	0.39
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	4	0.39
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	4	0.39
(2,49)	2:201:B:SER:H	2:202:B:THR:H	4	0.39
(2,49)	2:201:B:SER:H	2:202:B:THR:H	10	0.39
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	14	0.39
(3,324)	2:407:B:ARG:O	2:411:B:GLU:H	20	0.38
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	17	0.38
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	4	0.38
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	8	0.38
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	6	0.38
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	7	0.38
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	7	0.38
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	12	0.38
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	18	0.38
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	17	0.38
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	4	0.38
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	4	0.38
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	6	0.38
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	16	0.38
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	15	0.38
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	17	0.38
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	6	0.38
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	5	0.38
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	1	0.38
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	12	0.38
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	13	0.38
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	16	0.38
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	8	0.38
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	12	0.38
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	19	0.38
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	4	0.38
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	6	0.38
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	15	0.38
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	7	0.38
(1,27)	1:53:A:LEU:HD21	2:293:B:GLU:N	1	0.38
(1,10)	1:47:A:ASN:HB2	2:252:B:THR:HG23	2	0.38
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	5	0.37
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	9	0.37
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	9	0.37
(3,168)	2:280:B:ALA:O	2:284:B:ALA:H	18	0.37
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	4	0.37
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	2	0.37
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	9	0.37
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	18	0.37
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	13	0.37
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	4	0.37
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	8	0.37
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	12	0.37
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	1	0.37
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	5	0.37
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	12	0.37
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	18	0.37
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	13	0.37
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	17	0.37
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	12	0.37
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	14	0.37
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	18	0.37
(2,283)	2:286:B:LEU:H	2:283:B:PHE:H	9	0.37
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	5	0.37
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	7	0.37
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	3	0.37
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	2	0.37
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	14	0.37
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	18	0.37
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	16	0.37
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	11	0.37
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	14	0.37
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	11	0.37
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	11	0.37
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	12	0.37
(1,44)	2:290:B:TYR:HB3	1:59:A:LYS:HZ3	8	0.37
(1,40)	2:244:B:LEU:HD21	1:53:A:LEU:HD21	2	0.37
(1,7)	1:53:A:LEU:HD11	2:248:B:LEU:HD22	14	0.37
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	20	0.36
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ1	5	0.36
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ2	5	0.36
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ3	5	0.36
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	2	0.36
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	10	0.36
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	20	0.36
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	20	0.36
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	20	0.36
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	1	0.36
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	9	0.36
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	15	0.36
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	18	0.36
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	2	0.36
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	1	0.36
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	8	0.36
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	18	0.36
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	5	0.36
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	2	0.36
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	7	0.36
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	16	0.36
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	13	0.36
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	14	0.36
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	12	0.36
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	19	0.36
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	8	0.36
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	10	0.36
(2,48)	2:198:B:TYR:H	2:270:B:TRP:HE1	5	0.36
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	15	0.36
(1,31)	2:290:B:TYR:HH	1:15:A:MET:HE3	3	0.36
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	11	0.35
(3,282)	2:384:B:LEU:O	2:183:B:ALA:H	20	0.35
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	14	0.35
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,93)	2:244:B:LEU:O	2:248:B:LEU:N	10	0.35
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	3	0.35
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	9	0.35
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	10	0.35
(2,432)	2:349:B:ARG:H	2:327:B:ALA:H	3	0.35
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	3	0.35
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	19	0.35
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	12	0.35
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	15	0.35
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	1	0.35
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	20	0.35
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	9	0.35
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	13	0.35
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	17	0.35
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	15	0.35
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	5	0.35
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	8	0.35
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	11	0.35
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	10	0.35
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	11	0.35
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	13	0.35
(2,49)	2:201:B:SER:H	2:202:B:THR:H	9	0.35
(2,36)	2:188:B:ASP:H	2:326:B:VAL:H	2	0.35
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	20	0.35
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	8	0.35
(1,37)	2:247:B:HIS:HE1	1:48:A:SER:HA	10	0.35
(1,2)	2:356:B:GLN:HB2	1:16:A:HIS:HE2	20	0.35
(1,1)	1:16:A:HIS:HE2	2:356:B:GLN:HB2	20	0.35
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	3	0.34
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	3	0.34
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	8	0.34
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	17	0.34
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	17	0.34
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	17	0.34
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	14	0.34
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	1	0.34
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	2	0.34
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	20	0.34
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	9	0.34
(2,513)	2:382:B:ARG:H	2:185:B:GLY:H	4	0.34
(2,489)	2:375:B:GLN:H	2:378:B:VAL:H	3	0.34
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	17	0.34
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	3	0.34
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	7	0.34
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	14	0.34
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	1	0.34
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	9	0.34
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	16	0.34
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	9	0.34
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	11	0.34
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	7	0.34
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	7	0.34
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	16	0.34
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	12	0.34
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	10	0.34
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	4	0.34
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	8	0.34
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	12	0.34
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	14	0.34
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	17	0.34
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	15	0.34
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	9	0.34
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	16	0.34
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	18	0.34
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	9	0.34
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	14	0.34
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	15	0.34
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	5	0.34
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	15	0.34
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	10	0.34
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	11	0.34
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	12	0.34
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	18	0.34
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	12	0.34
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	20	0.34
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	5	0.34
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	18	0.34
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	3	0.34
(1,20)	1:54:A:MET:HE2	2:285:B:ALA:HB1	20	0.34
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	11	0.33
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	8	0.33
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	13	0.33
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	3	0.33
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	8	0.33
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	15	0.33
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	14	0.33
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	5	0.33
(3,28)	2:206:B:ALA:O	2:210:B:GLU:H	9	0.33
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	15	0.33
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	2	0.33
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	1	0.33
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	17	0.33
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	14	0.33
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	19	0.33
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	2	0.33
(2,502)	2:380:B:HIS:H	2:378:B:VAL:H	1	0.33
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	18	0.33
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	20	0.33
(2,446)	2:359:B:ILE:H	2:361:B:VAL:H	13	0.33
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	20	0.33
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	5	0.33
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	5	0.33
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	18	0.33
(2,350)	2:314:B:GLN:H	2:315:B:GLY:H	11	0.33
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	2	0.33
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	7	0.33
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	19	0.33
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	4	0.33
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	11	0.33
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	15	0.33
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	7	0.33
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	6	0.33
(2,118)	2:227:B:SER:H	2:229:B:ARG:H	7	0.33
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	2	0.33
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	19	0.33
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	1	0.33
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	19	0.33
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	17	0.33
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	18	0.33
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	18	0.33
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	11	0.33
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	2	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	1	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	10	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	13	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	14	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	16	0.33
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	19	0.33
(1,35)	2:243:B:ASP:OD2	1:22:A:LYS:HA	13	0.33
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	15	0.32
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	7	0.32
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	10	0.32
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	16	0.32
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	16	0.32
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	16	0.32
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	20	0.32
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	20	0.32
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	17	0.32
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	9	0.32
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	20	0.32
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	18	0.32
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	18	0.32
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	13	0.32
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	1	0.32
(2,606)	2:412:B:GLU:H	2:411:B:GLU:H	18	0.32
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	8	0.32
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	5	0.32
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	6	0.32
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	10	0.32
(2,560)	2:396:B:ASP:H	2:383:B:THR:H	6	0.32
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	2	0.32
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	20	0.32
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	7	0.32
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	17	0.32
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	10	0.32
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	14	0.32
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	9	0.32
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	6	0.32
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	18	0.32
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	14	0.32
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	19	0.32
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	4	0.32
(2,218)	2:270:B:TRP:H	2:273:B:LYS:H	9	0.32
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	2	0.32
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	15	0.32
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	1	0.32
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	10	0.32
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	4	0.32
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	7	0.32
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	14	0.32
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	15	0.32
(2,36)	2:188:B:ASP:H	2:326:B:VAL:H	16	0.32
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	17	0.32
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	20	0.32
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	3	0.32
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	6	0.32
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	12	0.32
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	20	0.32
(1,20)	1:53:A:LEU:HD21	2:285:B:ALA:H	7	0.32
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	2	0.31
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	15	0.31
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	11	0.31
(3,281)	2:384:B:LEU:O	2:183:B:ALA:N	20	0.31
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	1	0.31
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	6	0.31
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	6	0.31
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	7	0.31
(3,50)	2:217:B:GLU:O	2:221:B:ASN:HD21	2	0.31
(3,50)	2:217:B:GLU:O	2:221:B:ASN:HD22	2	0.31
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	14	0.31
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	19	0.31
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	19	0.31
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	20	0.31
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	11	0.31
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	7	0.31
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	12	0.31
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	19	0.31
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	17	0.31
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	18	0.31
(2,423)	2:345:B:GLY:H	2:325:B:LEU:H	16	0.31
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	6	0.31
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	12	0.31
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	14	0.31
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	17	0.31
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	13	0.31
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	3	0.31
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	5	0.31
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	9	0.31
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	9	0.31
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	10	0.31
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	11	0.31
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	4	0.31
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	5	0.31
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	11	0.31
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	17	0.31
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	3	0.31
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	12	0.31
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	14	0.31
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	20	0.31
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	9	0.31
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	11	0.31
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	8	0.31
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	18	0.31
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	13	0.31
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	3	0.31
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	4	0.31
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	20	0.31
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	11	0.31
(1,3)	1:21:A:MET:HG2	2:241:B:ILE:O	17	0.31
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	11	0.3
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	17	0.3
(3,282)	2:384:B:LEU:O	2:183:B:ALA:H	18	0.3
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	4	0.3
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	4	0.3
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	20	0.3
(3,241)	2:352:B:ALA:O	2:355:B:SER:OG	9	0.3
(3,229)	2:342:B:ARG:O	2:323:B:PHE:N	7	0.3
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	10	0.3
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	10	0.3
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	13	0.3
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	7	0.3
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	16	0.3
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	14	0.3
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	19	0.3
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	20	0.3
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	6	0.3
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	2	0.3
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	2	0.3
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	3	0.3
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	3	0.3
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	1	0.3
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	20	0.3
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	2	0.3
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	6	0.3
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	13	0.3
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	6	0.3
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	13	0.3
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	11	0.3
(2,291)	2:292:B:LYS:H	2:290:B:TYR:H	6	0.3
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	8	0.3
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	15	0.3
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	4	0.3
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	8	0.3
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	15	0.3
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	3	0.3
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	16	0.3
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	18	0.3
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	2	0.3
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	6	0.3
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	1	0.3
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	19	0.3
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	1	0.3
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	7	0.3
(2,20)	2:181:B:ALA:H	2:180:B:VAL:H	9	0.3
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	5	0.3
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	16	0.3
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	5	0.29
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	14	0.29
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	18	0.29
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	18	0.29
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	2	0.29
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	1	0.29
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	1	0.29
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	15	0.29
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	15	0.29
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	6	0.29
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	5	0.29
(3,147)	2:269:B:GLU:O	2:273:B:LYS:N	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	4	0.29
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	15	0.29
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	10	0.29
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	11	0.29
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	7	0.29
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	5	0.29
(3,71)	2:223:B:PHE:O	2:227:B:SER:OG	3	0.29
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	2	0.29
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	20	0.29
(2,607)	2:413:B:ILE:H	2:414:B:GLU:H	19	0.29
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	4	0.29
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	5	0.29
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	20	0.29
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	19	0.29
(2,502)	2:380:B:HIS:H	2:378:B:VAL:H	8	0.29
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	20	0.29
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	3	0.29
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	13	0.29
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	15	0.29
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	11	0.29
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	12	0.29
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	5	0.29
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	18	0.29
(2,351)	2:315:B:GLY:H	2:314:B:GLN:H	6	0.29
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	15	0.29
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	3	0.29
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	12	0.29
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	12	0.29
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	17	0.29
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	20	0.29
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	6	0.29
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	12	0.29
(2,225)	2:414:B:GLU:H	2:413:B:ILE:H	19	0.29
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	20	0.29
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	20	0.29
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	10	0.29
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	18	0.29
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	4	0.29
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	6	0.29
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	19	0.29
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	12	0.29
(2,154)	2:245:B:TYR:H	2:244:B:LEU:H	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	8	0.29
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	15	0.29
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	13	0.29
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	20	0.29
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	3	0.29
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	1	0.29
(2,55)	2:207:B:LEU:H	2:206:B:ALA:H	8	0.29
(2,53)	2:206:B:ALA:H	2:207:B:LEU:H	8	0.29
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	7	0.29
(2,49)	2:201:B:SER:H	2:202:B:THR:H	6	0.29
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	15	0.29
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	19	0.29
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	8	0.29
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	13	0.29
(1,26)	1:53:A:LEU:HD21	2:292:B:LYS:N	18	0.29
(1,19)	1:53:A:LEU:HD12	2:284:B:ALA:N	10	0.29
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	16	0.28
(3,280)	2:382:B:ARG:O	2:185:B:GLY:H	11	0.28
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	2	0.28
(3,236)	2:347:B:VAL:O	2:327:B:ALA:H	1	0.28
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	15	0.28
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	6	0.28
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	6	0.28
(3,222)	2:335:B:LEU:O	2:338:B:LEU:H	12	0.28
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	16	0.28
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	18	0.28
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	18	0.28
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	2	0.28
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	7	0.28
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	3	0.28
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	8	0.28
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	9	0.28
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	9	0.28
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	14	0.28
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	14	0.28
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	17	0.28
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	12	0.28
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	10	0.28
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	14	0.28
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	19	0.28
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	16	0.28
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	1	0.28
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	11	0.28
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	5	0.28
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	15	0.28
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	14	0.28
(2,500)	2:379:B:LEU:H	2:380:B:HIS:H	1	0.28
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	7	0.28
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	12	0.28
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	17	0.28
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	6	0.28
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	15	0.28
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	3	0.28
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	18	0.28
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	18	0.28
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	19	0.28
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	19	0.28
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	2	0.28
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	20	0.28
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	2	0.28
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	20	0.28
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	1	0.28
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	5	0.28
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	2	0.28
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	15	0.28
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	10	0.28
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	16	0.28
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	3	0.28
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	5	0.28
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	16	0.28
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	9	0.28
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	12	0.28
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	6	0.28
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	14	0.28
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	20	0.27
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	15	0.27
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	19	0.27
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	18	0.27
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	18	0.27
(3,262)	2:366:B:ILE:O	2:368:B:THR:HG1	12	0.27
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	4	0.27
(3,260)	2:361:B:VAL:O	2:366:B:ILE:H	10	0.27
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	5	0.27
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ1	19	0.27
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ2	19	0.27
(3,174)	2:284:B:ALA:O	2:292:B:LYS:HZ3	19	0.27
(3,109)	2:251:B:ASP:OD1	2:253:B:ARG:N	6	0.27
(3,101)	2:246:B:SER:O	2:250:B:SER:OG	3	0.27
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	9	0.27
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	13	0.27
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	4	0.27
(3,52)	2:217:B:GLU:O	2:221:B:ASN:H	20	0.27
(3,51)	2:217:B:GLU:O	2:221:B:ASN:N	3	0.27
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	10	0.27
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	10	0.27
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	5	0.27
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	5	0.27
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	5	0.27
(3,8)	2:177:B:ALA:O	2:368:B:THR:H	16	0.27
(2,604)	2:411:B:GLU:H	2:412:B:GLU:H	7	0.27
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	13	0.27
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	6	0.27
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	18	0.27
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	15	0.27
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	9	0.27
(2,489)	2:375:B:GLN:H	2:378:B:VAL:H	16	0.27
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	10	0.27
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	3	0.27
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	15	0.27
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	10	0.27
(2,444)	2:358:B:ALA:H	2:357:B:ALA:H	1	0.27
(2,433)	2:349:B:ARG:H	2:350:B:ASP:H	3	0.27
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	16	0.27
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	10	0.27
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	2	0.27
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	15	0.27
(2,406)	2:172:B:ARG:H	2:173:B:ALA:H	15	0.27
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	11	0.27
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	9	0.27
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	16	0.27
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	3	0.27
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	8	0.27
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	9	0.27
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	15	0.27
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	6	0.27
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	16	0.27
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	3	0.27
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	4	0.27
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	13	0.27
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	6	0.27
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	1	0.27
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	7	0.27
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	9	0.27
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	18	0.27
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	11	0.27
(2,49)	2:201:B:SER:H	2:202:B:THR:H	11	0.27
(2,42)	2:194:B:MET:H	2:193:B:LEU:H	8	0.27
(2,38)	2:190:B:THR:H	2:189:B:ALA:H	14	0.27
(2,6)	2:173:B:ALA:H	2:392:B:GLU:H	10	0.27
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	17	0.27
(1,15)	1:53:A:LEU:HD22	2:279:B:PHE:HD2	7	0.27
(4,10)	2:375:B:GLN:OE1	2:375:B:GLN:H	10	0.26
(4,6)	2:328:B:ASP:OD1	2:328:B:ASP:H	18	0.26
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	11	0.26
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH11	8	0.26
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH12	8	0.26
(3,311)	2:404:B:GLU:OE2	2:407:B:ARG:NH1	8	0.26
(3,309)	2:403:B:GLN:O	2:407:B:ARG:N	10	0.26
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	12	0.26
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	1	0.26
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	8	0.26
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	8	0.26
(3,203)	2:313:B:ASN:O	2:314:B:GLN:NE2	18	0.26
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	9	0.26
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	14	0.26
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	17	0.26
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	1	0.26
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	9	0.26
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	13	0.26
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	8	0.26
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	2	0.26
(2,562)	2:400:B:VAL:H	2:403:B:GLN:H	18	0.26
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	13	0.26
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	6	0.26
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	3	0.26
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	19	0.26
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	4	0.26
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	10	0.26
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	1	0.26
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	10	0.26
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	8	0.26
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	10	0.26
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	10	0.26
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	7	0.26
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	14	0.26
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	19	0.26
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	14	0.26
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	14	0.26
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	6	0.26
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	11	0.26
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	2	0.26
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	13	0.26
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	18	0.26
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	10	0.26
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	13	0.26
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	10	0.26
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	14	0.26
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	16	0.26
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	4	0.26
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	4	0.26
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	13	0.26
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	13	0.26
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	17	0.26
(2,134)	2:232:B:ALA:H	2:233:B:GLY:H	2	0.26
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	17	0.26
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	20	0.26
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	20	0.26
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	20	0.26
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	3	0.26
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	19	0.26
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	6	0.26
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	15	0.26
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	11	0.26
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	12	0.26
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	18	0.26
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	2:247:B:HIS:HE1	1:47:A:ASN:HA	19	0.26
(1,26)	1:53:A:LEU:HB2	2:292:B:LYS:H	7	0.26
(1,6)	1:21:A:MET:HG2	2:247:B:HIS:HB2	9	0.26
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	18	0.25
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	3	0.25
(3,309)	2:403:B:GLN:O	2:407:B:ARG:N	17	0.25
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	20	0.25
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	10	0.25
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	4	0.25
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	12	0.25
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	12	0.25
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	15	0.25
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	15	0.25
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	4	0.25
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	4	0.25
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	18	0.25
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	18	0.25
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	1	0.25
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	19	0.25
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	6	0.25
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	4	0.25
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	4	0.25
(3,180)	2:291:B:LEU:O	2:294:B:ARG:H	2	0.25
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	6	0.25
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	15	0.25
(3,147)	2:269:B:GLU:O	2:273:B:LYS:N	4	0.25
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	19	0.25
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	5	0.25
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	13	0.25
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	12	0.25
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	20	0.25
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	19	0.25
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	6	0.25
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	5	0.25
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	15	0.25
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	19	0.25
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	10	0.25
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	16	0.25
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	5	0.25
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	1	0.25
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	8	0.25
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	8	0.25
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	14	0.25
(2,453)	2:362:B:ARG:H	2:360:B:MET:H	12	0.25
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	8	0.25
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	14	0.25
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	19	0.25
(2,423)	2:345:B:GLY:H	2:325:B:LEU:H	1	0.25
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	1	0.25
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	14	0.25
(2,375)	2:327:B:ALA:H	2:349:B:ARG:H	3	0.25
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	10	0.25
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	16	0.25
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	7	0.25
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	8	0.25
(2,280)	2:285:B:ALA:H	2:282:B:GLN:H	8	0.25
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	9	0.25
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	2	0.25
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	10	0.25
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	6	0.25
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	20	0.25
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	6	0.25
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	6	0.25
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	2	0.25
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	3	0.25
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	4	0.25
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	4	0.25
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	11	0.25
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	18	0.25
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	1	0.25
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	17	0.25
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	19	0.25
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	11	0.25
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	5	0.25
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	15	0.25
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	20	0.25
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	7	0.25
(2,49)	2:201:B:SER:H	2:202:B:THR:H	5	0.25
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	18	0.25
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	5	0.25
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	20	0.25
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	3	0.25
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	2:290:B:TYR:HB2	1:53:A:LEU:HA	16	0.25
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	5	0.24
(3,300)	2:396:B:ASP:OD2	2:382:B:ARG:HH21	16	0.24
(3,300)	2:396:B:ASP:OD2	2:382:B:ARG:HH22	16	0.24
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	11	0.24
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	2	0.24
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	13	0.24
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	19	0.24
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	19	0.24
(3,222)	2:335:B:LEU:O	2:338:B:LEU:H	10	0.24
(3,222)	2:335:B:LEU:O	2:338:B:LEU:H	17	0.24
(3,211)	2:327:B:ALA:O	2:349:B:ARG:N	3	0.24
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	8	0.24
(3,147)	2:269:B:GLU:O	2:273:B:LYS:N	8	0.24
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ1	7	0.24
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ2	7	0.24
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ3	7	0.24
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH21	2	0.24
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH22	2	0.24
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	14	0.24
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	16	0.24
(3,27)	2:206:B:ALA:O	2:210:B:GLU:N	20	0.24
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	4	0.24
(2,594)	2:408:B:LEU:H	2:406:B:GLN:H	10	0.24
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	3	0.24
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	12	0.24
(2,592)	2:407:B:ARG:H	2:405:B:TYR:H	16	0.24
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	13	0.24
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	3	0.24
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	8	0.24
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	14	0.24
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	19	0.24
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	4	0.24
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	1	0.24
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	2	0.24
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	5	0.24
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	20	0.24
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	12	0.24
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	8	0.24
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	18	0.24
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	11	0.24
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	5	0.24
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	15	0.24
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	18	0.24
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	11	0.24
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	18	0.24
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	19	0.24
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	3	0.24
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	7	0.24
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	19	0.24
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	3	0.24
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	15	0.24
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	7	0.24
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	8	0.24
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	11	0.24
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	7	0.24
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	16	0.24
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	13	0.24
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	5	0.24
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	15	0.24
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	14	0.24
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	13	0.24
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	9	0.24
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	14	0.24
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	17	0.24
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	2	0.24
(2,156)	2:247:B:HIS:H	2:248:B:LEU:H	10	0.24
(2,139)	2:240:B:ALA:H	2:241:B:ILE:H	12	0.24
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	15	0.24
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	1	0.24
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	4	0.24
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	6	0.24
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	2	0.24
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	14	0.24
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	2	0.24
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	2	0.24
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	6	0.24
(2,49)	2:201:B:SER:H	2:202:B:THR:H	2	0.24
(2,49)	2:201:B:SER:H	2:202:B:THR:H	17	0.24
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	17	0.24
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	12	0.24
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	1	0.24
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:53:A:LEU:HD22	2:292:B:LYS:N	20	0.24
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	14	0.23
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	6	0.23
(3,282)	2:384:B:LEU:O	2:183:B:ALA:H	3	0.23
(3,236)	2:347:B:VAL:O	2:327:B:ALA:H	2	0.23
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	14	0.23
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	16	0.23
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	16	0.23
(3,168)	2:280:B:ALA:O	2:284:B:ALA:H	7	0.23
(3,127)	2:257:B:GLU:OE1	2:278:B:LYS:NZ	5	0.23
(3,105)	2:247:B:HIS:O	2:250:B:SER:OG	3	0.23
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	6	0.23
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	4	0.23
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	10	0.23
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	18	0.23
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	18	0.23
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	13	0.23
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	13	0.23
(3,31)	2:208:B:GLU:OE1	2:211:B:ARG:NH2	13	0.23
(2,607)	2:413:B:ILE:H	2:414:B:GLU:H	12	0.23
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	3	0.23
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	11	0.23
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	14	0.23
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	17	0.23
(2,565)	2:401:B:LEU:H	2:398:B:GLU:H	18	0.23
(2,561)	2:398:B:GLU:H	2:401:B:LEU:H	18	0.23
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	5	0.23
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	7	0.23
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	17	0.23
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	6	0.23
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	11	0.23
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	5	0.23
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	14	0.23
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	4	0.23
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	10	0.23
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	19	0.23
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	14	0.23
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	4	0.23
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	3	0.23
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	16	0.23
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	7	0.23
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	9	0.23
(2,351)	2:315:B:GLY:H	2:314:B:GLN:H	11	0.23
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	8	0.23
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	11	0.23
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	9	0.23
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	10	0.23
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	19	0.23
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	16	0.23
(2,225)	2:414:B:GLU:H	2:413:B:ILE:H	12	0.23
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	12	0.23
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	14	0.23
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	11	0.23
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	11	0.23
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	5	0.23
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	2	0.23
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	13	0.23
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	8	0.23
(2,168)	2:253:B:ARG:H	2:256:B:ARG:H	3	0.23
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	16	0.23
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	1	0.23
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	14	0.23
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	7	0.23
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	6	0.23
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	14	0.23
(2,49)	2:201:B:SER:H	2:202:B:THR:H	12	0.23
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	19	0.23
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	5	0.23
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	18	0.23
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	4	0.23
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	7	0.22
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	8	0.22
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	3	0.22
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	19	0.22
(3,273)	2:373:B:ASP:O	2:349:B:ARG:NH1	18	0.22
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	18	0.22
(3,258)	2:361:B:VAL:O	2:365:B:GLY:H	12	0.22
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	18	0.22
(3,241)	2:352:B:ALA:O	2:355:B:SER:OG	7	0.22
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	16	0.22
(3,222)	2:335:B:LEU:O	2:338:B:LEU:H	7	0.22
(3,214)	2:328:B:ASP:O	2:350:B:ASP:H	18	0.22
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	3	0.22
(3,172)	2:283:B:PHE:O	2:286:B:LEU:H	7	0.22
(3,167)	2:280:B:ALA:O	2:284:B:ALA:N	18	0.22
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	1	0.22
(3,136)	2:261:B:GLU:O	2:266:B:SER:H	6	0.22
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	18	0.22
(3,101)	2:246:B:SER:O	2:250:B:SER:OG	4	0.22
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	14	0.22
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	3	0.22
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	15	0.22
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	6	0.22
(2,608)	2:413:B:ILE:H	2:411:B:GLU:H	16	0.22
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	5	0.22
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	11	0.22
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	5	0.22
(2,526)	2:385:B:ILE:H	2:394:B:LEU:H	4	0.22
(2,526)	2:385:B:ILE:H	2:394:B:LEU:H	17	0.22
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	9	0.22
(2,506)	2:381:B:ARG:H	2:185:B:GLY:H	5	0.22
(2,501)	2:380:B:HIS:H	2:379:B:LEU:H	15	0.22
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	5	0.22
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	9	0.22
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	19	0.22
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	15	0.22
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	2	0.22
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	7	0.22
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	11	0.22
(2,444)	2:358:B:ALA:H	2:357:B:ALA:H	16	0.22
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	2	0.22
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	12	0.22
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	3	0.22
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	13	0.22
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	13	0.22
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	1	0.22
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	14	0.22
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	6	0.22
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	2	0.22
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	6	0.22
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	8	0.22
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	12	0.22
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	16	0.22
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	6	0.22
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	2	0.22
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	17	0.22
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	1	0.22
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	8	0.22
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	1	0.22
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	7	0.22
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	16	0.22
(2,168)	2:253:B:ARG:H	2:256:B:ARG:H	4	0.22
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	12	0.22
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	20	0.22
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	9	0.22
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	19	0.22
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	9	0.22
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	8	0.22
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	9	0.22
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	9	0.22
(2,49)	2:201:B:SER:H	2:202:B:THR:H	16	0.22
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	15	0.22
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	16	0.22
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	2	0.22
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	10	0.22
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	14	0.22
(2,30)	2:185:B:GLY:H	2:381:B:ARG:H	5	0.22
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	3	0.22
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	9	0.22
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	7	0.22
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	3	0.21
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	10	0.21
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	7	0.21
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	19	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	10	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	10	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	16	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	16	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	19	0.21
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	19	0.21
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	3	0.21
(3,110)	2:251:B:ASP:OD1	2:253:B:ARG:H	15	0.21
(3,109)	2:251:B:ASP:OD1	2:253:B:ARG:N	13	0.21
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	16	0.21
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	15	0.21
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	20	0.21
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	9	0.21
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE21	9	0.21
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE22	9	0.21
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	12	0.21
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	4	0.21
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	2	0.21
(3,53)	2:218:B:GLU:O	2:222:B:GLU:N	20	0.21
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	13	0.21
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	19	0.21
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	11	0.21
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	19	0.21
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	19	0.21
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	16	0.21
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	16	0.21
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	10	0.21
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	10	0.21
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	10	0.21
(3,8)	2:177:B:ALA:O	2:368:B:THR:H	5	0.21
(2,607)	2:413:B:ILE:H	2:414:B:GLU:H	20	0.21
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	7	0.21
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	17	0.21
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	13	0.21
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	6	0.21
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	9	0.21
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	2	0.21
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	5	0.21
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	18	0.21
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	9	0.21
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	13	0.21
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	20	0.21
(2,501)	2:380:B:HIS:H	2:379:B:LEU:H	8	0.21
(2,500)	2:379:B:LEU:H	2:380:B:HIS:H	4	0.21
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	1	0.21
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	2	0.21
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	14	0.21
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	2	0.21
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	8	0.21
(2,450)	2:360:B:MET:H	2:361:B:VAL:H	6	0.21
(2,448)	2:361:B:VAL:H	2:360:B:MET:H	6	0.21
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	13	0.21
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	13	0.21
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	2	0.21
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	16	0.21
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	13	0.21
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	17	0.21
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	11	0.21
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	16	0.21
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	20	0.21
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	5	0.21
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	10	0.21
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	6	0.21
(2,305)	2:298:B:LEU:H	2:297:B:ASP:H	10	0.21
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	10	0.21
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	9	0.21
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	13	0.21
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	6	0.21
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	3	0.21
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	14	0.21
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	15	0.21
(2,225)	2:414:B:GLU:H	2:413:B:ILE:H	20	0.21
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	6	0.21
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	2	0.21
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	16	0.21
(2,220)	2:270:B:TRP:H	2:272:B:VAL:H	20	0.21
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	5	0.21
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	11	0.21
(2,193)	2:261:B:GLU:H	2:259:B:PHE:H	14	0.21
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	5	0.21
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	5	0.21
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	11	0.21
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	17	0.21
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	9	0.21
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	7	0.21
(2,168)	2:253:B:ARG:H	2:256:B:ARG:H	17	0.21
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	4	0.21
(2,107)	2:222:B:GLU:H	2:223:B:PHE:H	9	0.21
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	2	0.21
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	19	0.21
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	2	0.21
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	13	0.21
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	18	0.21
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	5	0.21
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	19	0.21
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	1	0.21
(2,40)	2:193:B:LEU:H	2:194:B:MET:H	18	0.21
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	6	0.21
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	12	0.21
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	14	0.21
(1,27)	1:53:A:LEU:HD23	2:293:B:GLU:N	2	0.21
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	7	0.2
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	1	0.2
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	1	0.2
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	16	0.2
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	16	0.2
(3,243)	2:353:B:ALA:O	2:362:B:ARG:NH1	18	0.2
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	16	0.2
(3,229)	2:342:B:ARG:O	2:323:B:PHE:N	5	0.2
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	12	0.2
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	12	0.2
(3,190)	2:299:B:ARG:O	2:303:B:GLN:H	16	0.2
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	13	0.2
(3,173)	2:284:B:ALA:O	2:292:B:LYS:NZ	8	0.2
(3,166)	2:279:B:PHE:O	2:283:B:PHE:H	6	0.2
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	14	0.2
(3,145)	2:269:B:GLU:OE2	2:211:B:ARG:NH1	7	0.2
(3,127)	2:257:B:GLU:OE1	2:278:B:LYS:NZ	4	0.2
(3,102)	2:246:B:SER:O	2:250:B:SER:HG	10	0.2
(3,95)	2:244:B:LEU:O	2:247:B:HIS:N	19	0.2
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	15	0.2
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	20	0.2
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	16	0.2
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	4	0.2
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	10	0.2
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	12	0.2
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	19	0.2
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	19	0.2
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	13	0.2
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	13	0.2
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	13	0.2
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	18	0.2
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	16	0.2
(2,586)	2:405:B:TYR:H	2:402:B:LEU:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,579)	2:404:B:GLU:H	2:402:B:LEU:H	10	0.2
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	11	0.2
(2,560)	2:396:B:ASP:H	2:383:B:THR:H	20	0.2
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	3	0.2
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	19	0.2
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	20	0.2
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	13	0.2
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	14	0.2
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	17	0.2
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	17	0.2
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	17	0.2
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	3	0.2
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	9	0.2
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	9	0.2
(2,433)	2:349:B:ARG:H	2:350:B:ASP:H	5	0.2
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	4	0.2
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	3	0.2
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	20	0.2
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	13	0.2
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	19	0.2
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	14	0.2
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	5	0.2
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	5	0.2
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	4	0.2
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	20	0.2
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	18	0.2
(2,348)	2:314:B:GLN:H	2:313:B:ASN:H	3	0.2
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	14	0.2
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	18	0.2
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	8	0.2
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	10	0.2
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	13	0.2
(2,252)	2:277:B:GLU:H	2:278:B:LYS:H	18	0.2
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	3	0.2
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	19	0.2
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	1	0.2
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	4	0.2
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	8	0.2
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	4	0.2
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	4	0.2
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	8	0.2
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	1	0.2
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	2	0.2
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	11	0.2
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	2	0.2
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	11	0.2
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	18	0.2
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	6	0.2
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	17	0.2
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	13	0.2
(2,49)	2:201:B:SER:H	2:202:B:THR:H	3	0.2
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	10	0.2
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	1	0.2
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	3	0.2
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	9	0.2
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	11	0.2
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	17	0.2
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	16	0.2
(1,7)	1:53:A:LEU:HD22	2:248:B:LEU:HD13	15	0.2
(3,281)	2:384:B:LEU:O	2:183:B:ALA:N	18	0.19
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	5	0.19
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	5	0.19
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	14	0.19
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	14	0.19
(3,228)	2:339:B:PRO:O	2:343:B:LEU:H	12	0.19
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	8	0.19
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	8	0.19
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	14	0.19
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	14	0.19
(3,188)	2:298:B:LEU:O	2:302:B:GLY:H	16	0.19
(3,168)	2:280:B:ALA:O	2:284:B:ALA:H	9	0.19
(3,159)	2:274:B:THR:O	2:278:B:LYS:N	11	0.19
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	17	0.19
(3,93)	2:244:B:LEU:O	2:248:B:LEU:N	7	0.19
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE21	10	0.19
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE22	10	0.19
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	15	0.19
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	9	0.19
(3,52)	2:217:B:GLU:O	2:221:B:ASN:H	15	0.19
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	15	0.19
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	15	0.19
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	12	0.19
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	2:194:B:MET:O	2:273:B:LYS:NZ	20	0.19
(3,7)	2:177:B:ALA:O	2:368:B:THR:N	16	0.19
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	9	0.19
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	1	0.19
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	8	0.19
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	12	0.19
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	10	0.19
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	20	0.19
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	10	0.19
(2,519)	2:384:B:LEU:H	2:184:B:GLU:H	2	0.19
(2,519)	2:384:B:LEU:H	2:184:B:GLU:H	20	0.19
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	19	0.19
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	13	0.19
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	19	0.19
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	20	0.19
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	3	0.19
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	4	0.19
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	7	0.19
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	12	0.19
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	13	0.19
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	15	0.19
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	20	0.19
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	5	0.19
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	18	0.19
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	2	0.19
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	6	0.19
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	9	0.19
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	15	0.19
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	15	0.19
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	2	0.19
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	3	0.19
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	13	0.19
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	8	0.19
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	20	0.19
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	15	0.19
(2,283)	2:286:B:LEU:H	2:283:B:PHE:H	18	0.19
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	20	0.19
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	15	0.19
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	6	0.19
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	16	0.19
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	17	0.19
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	12	0.19
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	12	0.19
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	11	0.19
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	4	0.19
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	6	0.19
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	19	0.19
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	5	0.19
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	12	0.19
(2,128)	2:230:B:PHE:H	2:229:B:ARG:H	10	0.19
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	13	0.19
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	7	0.19
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	13	0.19
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	12	0.19
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	5	0.19
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	5	0.19
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	8	0.19
(2,50)	2:202:B:THR:H	2:203:B:LEU:H	14	0.19
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	2	0.19
(2,42)	2:194:B:MET:H	2:193:B:LEU:H	1	0.19
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	3	0.19
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	12	0.19
(2,36)	2:188:B:ASP:H	2:326:B:VAL:H	7	0.19
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	6	0.19
(2,28)	2:184:B:GLU:H	2:384:B:LEU:H	2	0.19
(2,28)	2:184:B:GLU:H	2:384:B:LEU:H	20	0.19
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	1	0.19
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	4	0.19
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	15	0.19
(1,37)	2:279:B:PHE:HE2	1:48:A:SER:OG	19	0.19
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	9	0.18
(3,294)	2:392:B:GLU:O	2:387:B:ASP:H	7	0.18
(3,277)	2:379:B:LEU:O	2:382:B:ARG:N	9	0.18
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	11	0.18
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	11	0.18
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	17	0.18
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	17	0.18
(3,261)	2:366:B:ILE:O	2:368:B:THR:OG1	12	0.18
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	12	0.18
(3,229)	2:342:B:ARG:O	2:323:B:PHE:N	4	0.18
(3,227)	2:339:B:PRO:O	2:343:B:LEU:N	7	0.18
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	18	0.18
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	9	0.18
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	11	0.18
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	12	0.18
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	4	0.18
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	4	0.18
(3,184)	2:296:B:GLY:O	2:300:B:ALA:H	14	0.18
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	14	0.18
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	2	0.18
(3,149)	2:270:B:TRP:O	2:274:B:THR:OG1	4	0.18
(3,139)	2:267:B:VAL:O	2:271:B:ALA:N	1	0.18
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ1	14	0.18
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ2	14	0.18
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ3	14	0.18
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	8	0.18
(3,105)	2:247:B:HIS:O	2:250:B:SER:OG	4	0.18
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	14	0.18
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	1	0.18
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH21	20	0.18
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH22	20	0.18
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	5	0.18
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	18	0.18
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	1	0.18
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	11	0.18
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	7	0.18
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	20	0.18
(3,8)	2:177:B:ALA:O	2:368:B:THR:H	4	0.18
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	19	0.18
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	16	0.18
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	6	0.18
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	15	0.18
(2,528)	2:386:B:VAL:H	2:181:B:ALA:H	12	0.18
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	12	0.18
(2,526)	2:385:B:ILE:H	2:394:B:LEU:H	12	0.18
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	16	0.18
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	13	0.18
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	9	0.18
(2,481)	2:372:B:ALA:H	2:373:B:ASP:H	16	0.18
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	5	0.18
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	6	0.18
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	9	0.18
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	20	0.18
(2,453)	2:362:B:ARG:H	2:360:B:MET:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,444)	2:358:B:ALA:H	2:357:B:ALA:H	8	0.18
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	11	0.18
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	8	0.18
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	7	0.18
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	12	0.18
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	18	0.18
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	18	0.18
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	19	0.18
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	4	0.18
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	5	0.18
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	10	0.18
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	13	0.18
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	1	0.18
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	11	0.18
(2,283)	2:286:B:LEU:H	2:283:B:PHE:H	7	0.18
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	1	0.18
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	18	0.18
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	1	0.18
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	7	0.18
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	4	0.18
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	7	0.18
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	9	0.18
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	19	0.18
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	2	0.18
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	5	0.18
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	17	0.18
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	17	0.18
(2,186)	2:259:B:PHE:H	2:262:B:VAL:H	16	0.18
(2,184)	2:259:B:PHE:H	2:256:B:ARG:H	8	0.18
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	20	0.18
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	14	0.18
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	12	0.18
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	11	0.18
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	3	0.18
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	4	0.18
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	14	0.18
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	11	0.18
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	17	0.18
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	16	0.18
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	14	0.18
(2,56)	2:207:B:LEU:H	2:209:B:ARG:H	12	0.18
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	2:201:B:SER:H	2:202:B:THR:H	20	0.18
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	4	0.18
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	19	0.18
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	13	0.18
(2,18)	2:181:B:ALA:H	2:386:B:VAL:H	12	0.18
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	8	0.17
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	12	0.17
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	9	0.17
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	9	0.17
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	9	0.17
(3,268)	2:368:B:THR:O	2:176:B:ALA:H	3	0.17
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	3	0.17
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	13	0.17
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	13	0.17
(3,185)	2:297:B:ASP:OD1	2:356:B:GLN:NE2	9	0.17
(3,171)	2:283:B:PHE:O	2:286:B:LEU:N	7	0.17
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	11	0.17
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	19	0.17
(3,102)	2:246:B:SER:O	2:250:B:SER:HG	14	0.17
(3,86)	2:239:B:ALA:O	2:243:B:ASP:H	12	0.17
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH21	19	0.17
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH22	19	0.17
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	1	0.17
(3,53)	2:218:B:GLU:O	2:222:B:GLU:N	16	0.17
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	2	0.17
(3,23)	2:204:B:ASP:O	2:208:B:GLU:N	20	0.17
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	18	0.17
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	18	0.17
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	18	0.17
(3,7)	2:177:B:ALA:O	2:368:B:THR:N	5	0.17
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	3	0.17
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	16	0.17
(2,560)	2:396:B:ASP:H	2:383:B:THR:H	9	0.17
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	6	0.17
(2,545)	2:392:B:GLU:H	2:388:B:GLY:H	8	0.17
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	12	0.17
(2,526)	2:385:B:ILE:H	2:394:B:LEU:H	11	0.17
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	7	0.17
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	11	0.17
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	19	0.17
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	7	0.17
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	16	0.17
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	10	0.17
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	7	0.17
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	16	0.17
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	20	0.17
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	1	0.17
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	11	0.17
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	11	0.17
(2,436)	2:350:B:ASP:H	2:349:B:ARG:H	3	0.17
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	14	0.17
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	4	0.17
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	12	0.17
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	20	0.17
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	9	0.17
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	12	0.17
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	16	0.17
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	18	0.17
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	1	0.17
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	20	0.17
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	2	0.17
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	5	0.17
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	9	0.17
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	3	0.17
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	14	0.17
(2,244)	2:275:B:VAL:H	2:273:B:LYS:H	5	0.17
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	9	0.17
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	7	0.17
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	6	0.17
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	4	0.17
(2,221)	2:271:B:ALA:H	2:270:B:TRP:H	7	0.17
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	3	0.17
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	13	0.17
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	13	0.17
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	2	0.17
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	13	0.17
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	18	0.17
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	10	0.17
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	10	0.17
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	1	0.17
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	5	0.17
(2,118)	2:227:B:SER:H	2:229:B:ARG:H	12	0.17
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	9	0.17
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	10	0.17
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	4	0.17
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	13	0.17
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	15	0.17
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	17	0.17
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	10	0.17
(2,59)	2:209:B:ARG:H	2:211:B:ARG:H	6	0.17
(2,56)	2:207:B:LEU:H	2:209:B:ARG:H	3	0.17
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	13	0.17
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	15	0.17
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	16	0.17
(2,4)	2:173:B:ALA:H	2:172:B:ARG:H	15	0.17
(1,10)	1:47:A:ASN:HD22	2:252:B:THR:HG1	12	0.17
(4,6)	2:328:B:ASP:OD1	2:328:B:ASP:H	15	0.16
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	10	0.16
(3,302)	2:399:B:PRO:O	2:403:B:GLN:H	16	0.16
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	17	0.16
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	20	0.16
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	15	0.16
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	6	0.16
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	6	0.16
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	9	0.16
(3,260)	2:361:B:VAL:O	2:366:B:ILE:H	14	0.16
(3,259)	2:361:B:VAL:O	2:366:B:ILE:N	10	0.16
(3,230)	2:342:B:ARG:O	2:323:B:PHE:H	10	0.16
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	13	0.16
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	13	0.16
(3,165)	2:279:B:PHE:O	2:283:B:PHE:N	6	0.16
(3,109)	2:251:B:ASP:OD1	2:253:B:ARG:N	4	0.16
(3,107)	2:251:B:ASP:O	2:253:B:ARG:N	10	0.16
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	7	0.16
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	16	0.16
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	4	0.16
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	15	0.16
(3,72)	2:223:B:PHE:O	2:227:B:SER:HG	5	0.16
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	17	0.16
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	6	0.16
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	19	0.16
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	6	0.16
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	13	0.16
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	15	0.16
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	15	0.16
(3,26)	2:205:B:PRO:O	2:209:B:ARG:H	11	0.16
(3,21)	2:194:B:MET:O	2:273:B:LYS:NZ	1	0.16
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	6	0.16
(3,19)	2:188:B:ASP:OD1	2:190:B:THR:N	9	0.16
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	14	0.16
(2,602)	2:411:B:GLU:H	2:409:B:ILE:H	11	0.16
(2,584)	2:405:B:TYR:H	2:408:B:LEU:H	10	0.16
(2,584)	2:405:B:TYR:H	2:408:B:LEU:H	18	0.16
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	5	0.16
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	1	0.16
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	1	0.16
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	10	0.16
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	15	0.16
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	17	0.16
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	10	0.16
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	15	0.16
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	17	0.16
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	6	0.16
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	13	0.16
(2,450)	2:360:B:MET:H	2:361:B:VAL:H	12	0.16
(2,448)	2:361:B:VAL:H	2:360:B:MET:H	12	0.16
(2,446)	2:359:B:ILE:H	2:361:B:VAL:H	2	0.16
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	20	0.16
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	20	0.16
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	10	0.16
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	4	0.16
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	20	0.16
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	4	0.16
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	2	0.16
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	4	0.16
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	12	0.16
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	2	0.16
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	4	0.16
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	12	0.16
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	7	0.16
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	8	0.16
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	4	0.16
(2,356)	2:323:B:PHE:H	2:344:B:VAL:H	4	0.16
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	9	0.16
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	2:285:B:ALA:H	2:284:B:ALA:H	11	0.16
(2,275)	2:284:B:ALA:H	2:285:B:ALA:H	11	0.16
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	3	0.16
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	4	0.16
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	2	0.16
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	8	0.16
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	16	0.16
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	20	0.16
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	1	0.16
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	5	0.16
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	15	0.16
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	6	0.16
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	11	0.16
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	18	0.16
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	9	0.16
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	9	0.16
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	14	0.16
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	16	0.16
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	6	0.16
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	12	0.16
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	16	0.16
(2,168)	2:253:B:ARG:H	2:256:B:ARG:H	16	0.16
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	9	0.16
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	17	0.16
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	9	0.16
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	17	0.16
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	1	0.16
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	7	0.16
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	19	0.16
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	8	0.16
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	16	0.16
(2,139)	2:240:B:ALA:H	2:241:B:ILE:H	10	0.16
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	3	0.16
(2,45)	2:195:B:GLU:H	2:197:B:VAL:H	1	0.16
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	5	0.16
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	9	0.16
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	17	0.16
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	20	0.16
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	9	0.16
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	1	0.16
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	4	0.16
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	19	0.15
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	15	0.15
(3,278)	2:379:B:LEU:O	2:382:B:ARG:H	9	0.15
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	1	0.15
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	1	0.15
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	13	0.15
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	13	0.15
(3,271)	2:370:B:MET:O	2:174:B:LEU:N	6	0.15
(3,258)	2:361:B:VAL:O	2:365:B:GLY:H	6	0.15
(3,240)	2:348:B:VAL:O	2:372:B:ALA:H	16	0.15
(3,236)	2:347:B:VAL:O	2:327:B:ALA:H	18	0.15
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	18	0.15
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	9	0.15
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	9	0.15
(3,190)	2:299:B:ARG:O	2:303:B:GLN:H	13	0.15
(3,172)	2:283:B:PHE:O	2:286:B:LEU:H	9	0.15
(3,147)	2:269:B:GLU:O	2:273:B:LYS:N	10	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ1	4	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ2	4	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ3	4	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ1	11	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ2	11	0.15
(3,128)	2:257:B:GLU:OE1	2:278:B:LYS:HZ3	11	0.15
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	5	0.15
(3,98)	2:245:B:TYR:O	2:249:B:LEU:H	10	0.15
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	13	0.15
(3,76)	2:235:B:GLN:O	2:238:B:THR:HG1	6	0.15
(3,75)	2:235:B:GLN:O	2:238:B:THR:OG1	19	0.15
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	4	0.15
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	9	0.15
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	4	0.15
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	4	0.15
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ1	11	0.15
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ2	11	0.15
(3,22)	2:194:B:MET:O	2:273:B:LYS:HZ3	11	0.15
(3,21)	2:194:B:MET:O	2:273:B:LYS:NZ	13	0.15
(3,9)	2:179:B:GLY:O	2:388:B:GLY:N	1	0.15
(2,602)	2:411:B:GLU:H	2:409:B:ILE:H	4	0.15
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	14	0.15
(2,564)	2:400:B:VAL:H	2:401:B:LEU:H	20	0.15
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	4	0.15
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,530)	2:386:B:VAL:H	2:385:B:ILE:H	20	0.15
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	3	0.15
(2,514)	2:383:B:THR:H	2:185:B:GLY:H	11	0.15
(2,502)	2:380:B:HIS:H	2:378:B:VAL:H	15	0.15
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	15	0.15
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	7	0.15
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	1	0.15
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	8	0.15
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	15	0.15
(2,471)	2:369:B:VAL:H	2:346:B:VAL:H	19	0.15
(2,468)	2:368:B:THR:H	2:346:B:VAL:H	1	0.15
(2,432)	2:349:B:ARG:H	2:327:B:ALA:H	5	0.15
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	1	0.15
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	20	0.15
(2,410)	2:341:B:ASP:H	2:342:B:ARG:H	6	0.15
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	15	0.15
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	8	0.15
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	8	0.15
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	5	0.15
(2,362)	2:324:B:ILE:H	2:184:B:GLU:H	18	0.15
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	5	0.15
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	7	0.15
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	11	0.15
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	1	0.15
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	8	0.15
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	1	0.15
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	10	0.15
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	4	0.15
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	20	0.15
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	9	0.15
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	14	0.15
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	17	0.15
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	19	0.15
(2,297)	2:294:B:ARG:H	2:292:B:LYS:H	7	0.15
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	6	0.15
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	3	0.15
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	6	0.15
(2,289)	2:292:B:LYS:H	2:291:B:LEU:H	1	0.15
(2,267)	2:282:B:GLN:H	2:281:B:GLU:H	9	0.15
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	15	0.15
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	5	0.15
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	12	0.15
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	7	0.15
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	10	0.15
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	6	0.15
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	1	0.15
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	18	0.15
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	12	0.15
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	18	0.15
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	2	0.15
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	3	0.15
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	9	0.15
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	6	0.15
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	9	0.15
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	20	0.15
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	1	0.15
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	1	0.15
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	3	0.15
(2,141)	2:241:B:ILE:H	2:243:B:ASP:H	18	0.15
(2,118)	2:227:B:SER:H	2:229:B:ARG:H	3	0.15
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	3	0.15
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	16	0.15
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	20	0.15
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	20	0.15
(2,90)	2:217:B:GLU:H	2:219:B:ALA:H	2	0.15
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	5	0.15
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	9	0.15
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	6	0.15
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	19	0.15
(2,60)	2:209:B:ARG:H	2:206:B:ALA:H	5	0.15
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	20	0.15
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	13	0.15
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	15	0.15
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	16	0.15
(2,38)	2:190:B:THR:H	2:189:B:ALA:H	15	0.15
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	18	0.15
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	10	0.15
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	2	0.15
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	6	0.15
(1,44)	2:290:B:TYR:H	1:59:A:LYS:HZ3	20	0.15
(1,36)	2:247:B:HIS:HE2	1:47:A:ASN:OD1	7	0.15
(1,6)	1:47:A:ASN:OD1	2:247:B:HIS:HE2	7	0.15
(4,5)	2:328:B:ASP:OD1	2:328:B:ASP:N	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,324)	2:407:B:ARG:O	2:411:B:GLU:H	13	0.14
(3,322)	2:407:B:ARG:O	2:410:B:SER:HG	17	0.14
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	18	0.14
(3,275)	2:375:B:GLN:O	2:378:B:VAL:N	1	0.14
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	1	0.14
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	10	0.14
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	20	0.14
(3,254)	2:359:B:ILE:O	2:363:B:ALA:H	6	0.14
(3,229)	2:342:B:ARG:O	2:323:B:PHE:N	8	0.14
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	2	0.14
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	2	0.14
(3,225)	2:337:B:GLU:OE2	2:303:B:GLN:NE2	2	0.14
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH21	12	0.14
(3,224)	2:336:B:ALA:O	2:304:B:ARG:HH22	12	0.14
(3,206)	2:323:B:PHE:O	2:344:B:VAL:H	12	0.14
(3,206)	2:323:B:PHE:O	2:344:B:VAL:H	16	0.14
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	10	0.14
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	10	0.14
(3,145)	2:269:B:GLU:OE2	2:211:B:ARG:NH1	4	0.14
(3,143)	2:269:B:GLU:OE1	2:211:B:ARG:NH2	6	0.14
(3,140)	2:267:B:VAL:O	2:271:B:ALA:H	1	0.14
(3,106)	2:247:B:HIS:O	2:250:B:SER:HG	7	0.14
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	15	0.14
(3,63)	2:222:B:GLU:OE1	2:308:B:HIS:NE2	7	0.14
(3,63)	2:222:B:GLU:OE1	2:308:B:HIS:NE2	20	0.14
(3,54)	2:218:B:GLU:O	2:222:B:GLU:H	8	0.14
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	8	0.14
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	14	0.14
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	10	0.14
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	11	0.14
(3,27)	2:206:B:ALA:O	2:210:B:GLU:N	9	0.14
(3,25)	2:205:B:PRO:O	2:209:B:ARG:N	14	0.14
(3,21)	2:194:B:MET:O	2:273:B:LYS:NZ	5	0.14
(3,18)	2:186:B:TRP:O	2:326:B:VAL:H	16	0.14
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	10	0.14
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	20	0.14
(2,579)	2:404:B:GLU:H	2:402:B:LEU:H	19	0.14
(2,576)	2:403:B:GLN:H	2:400:B:VAL:H	1	0.14
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	1	0.14
(2,554)	2:394:B:LEU:H	2:386:B:VAL:H	19	0.14
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	8	0.14
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	4	0.14
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	15	0.14
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	13	0.14
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	12	0.14
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	18	0.14
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	20	0.14
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	8	0.14
(2,490)	2:375:B:GLN:H	2:374:B:ILE:H	7	0.14
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	18	0.14
(2,475)	2:370:B:MET:H	2:174:B:LEU:H	9	0.14
(2,467)	2:368:B:THR:H	2:388:B:GLY:H	8	0.14
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	8	0.14
(2,433)	2:349:B:ARG:H	2:350:B:ASP:H	16	0.14
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	3	0.14
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	16	0.14
(2,422)	2:345:B:GLY:H	2:323:B:PHE:H	16	0.14
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	8	0.14
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	11	0.14
(2,399)	2:337:B:GLU:H	2:335:B:LEU:H	3	0.14
(2,382)	2:330:B:LEU:H	2:352:B:ALA:H	18	0.14
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	8	0.14
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	12	0.14
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	10	0.14
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	1	0.14
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	7	0.14
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	11	0.14
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	15	0.14
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	19	0.14
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	17	0.14
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	3	0.14
(2,342)	2:311:B:ASP:H	2:310:B:ASP:H	5	0.14
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	4	0.14
(2,297)	2:294:B:ARG:H	2:292:B:LYS:H	15	0.14
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	19	0.14
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	7	0.14
(2,281)	2:285:B:ALA:H	2:286:B:LEU:H	8	0.14
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	8	0.14
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	4	0.14
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	14	0.14
(2,263)	2:281:B:GLU:H	2:280:B:ALA:H	12	0.14
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	11	0.14
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	13	0.14
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	15	0.14
(2,220)	2:270:B:TRP:H	2:272:B:VAL:H	12	0.14
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	15	0.14
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	3	0.14
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	10	0.14
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	14	0.14
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	15	0.14
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	18	0.14
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	4	0.14
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	8	0.14
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	10	0.14
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	16	0.14
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	14	0.14
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	15	0.14
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	18	0.14
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	4	0.14
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	8	0.14
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	10	0.14
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	16	0.14
(2,185)	2:259:B:PHE:H	2:261:B:GLU:H	19	0.14
(2,184)	2:259:B:PHE:H	2:256:B:ARG:H	19	0.14
(2,174)	2:256:B:ARG:H	2:258:B:LEU:H	15	0.14
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	7	0.14
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	10	0.14
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	13	0.14
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	13	0.14
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	10	0.14
(2,151)	2:244:B:LEU:H	2:243:B:ASP:H	17	0.14
(2,145)	2:242:B:PHE:H	2:241:B:ILE:H	10	0.14
(2,142)	2:241:B:ILE:H	2:239:B:ALA:H	17	0.14
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	12	0.14
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	18	0.14
(2,82)	2:215:B:ALA:H	2:217:B:GLU:H	3	0.14
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	12	0.14
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	4	0.14
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	7	0.14
(2,49)	2:201:B:SER:H	2:202:B:THR:H	13	0.14
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	8	0.14
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	12	0.14
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	13	0.14
(2,42)	2:194:B:MET:H	2:193:B:LEU:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	13	0.14
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	14	0.14
(2,7)	2:174:B:LEU:H	2:370:B:MET:H	19	0.14
(1,29)	1:53:A:LEU:HD13	2:295:B:ALA:H	19	0.14
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	4	0.13
(4,2)	2:269:B:GLU:OE1	2:269:B:GLU:H	16	0.13
(3,310)	2:403:B:GLN:O	2:407:B:ARG:H	2	0.13
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	16	0.13
(3,273)	2:373:B:ASP:O	2:349:B:ARG:NH1	2	0.13
(3,271)	2:370:B:MET:O	2:174:B:LEU:N	18	0.13
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	18	0.13
(3,225)	2:337:B:GLU:OE2	2:303:B:GLN:NE2	8	0.13
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	4	0.13
(3,213)	2:328:B:ASP:O	2:350:B:ASP:N	18	0.13
(3,211)	2:327:B:ALA:O	2:349:B:ARG:N	8	0.13
(3,211)	2:327:B:ALA:O	2:349:B:ARG:N	13	0.13
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	6	0.13
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	6	0.13
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	3	0.13
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	17	0.13
(3,151)	2:270:B:TRP:O	2:274:B:THR:N	12	0.13
(3,136)	2:261:B:GLU:O	2:266:B:SER:H	9	0.13
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ1	1	0.13
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ2	1	0.13
(3,134)	2:261:B:GLU:OE2	2:264:B:LYS:HZ3	1	0.13
(3,91)	2:243:B:ASP:O	2:247:B:HIS:N	18	0.13
(3,67)	2:222:B:GLU:OE2	2:304:B:ARG:NH1	2	0.13
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	19	0.13
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH21	4	0.13
(3,60)	2:221:B:ASN:OD1	2:224:B:ARG:HH22	4	0.13
(3,59)	2:221:B:ASN:OD1	2:224:B:ARG:NH2	4	0.13
(3,53)	2:218:B:GLU:O	2:222:B:GLU:N	9	0.13
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	2	0.13
(3,34)	2:208:B:GLU:OE1	2:268:B:ALA:H	16	0.13
(3,24)	2:204:B:ASP:O	2:208:B:GLU:H	20	0.13
(3,12)	2:181:B:ALA:O	2:386:B:VAL:H	12	0.13
(2,608)	2:413:B:ILE:H	2:411:B:GLU:H	1	0.13
(2,604)	2:411:B:GLU:H	2:412:B:GLU:H	5	0.13
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	15	0.13
(2,579)	2:404:B:GLU:H	2:402:B:LEU:H	13	0.13
(2,579)	2:404:B:GLU:H	2:402:B:LEU:H	17	0.13
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,550)	2:393:B:LEU:H	2:173:B:ALA:H	4	0.13
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	3	0.13
(2,544)	2:392:B:GLU:H	2:389:B:TYR:H	14	0.13
(2,528)	2:386:B:VAL:H	2:181:B:ALA:H	2	0.13
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	18	0.13
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	5	0.13
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	5	0.13
(2,493)	2:377:B:SER:H	2:379:B:LEU:H	4	0.13
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	6	0.13
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	11	0.13
(2,466)	2:366:B:ILE:H	2:364:B:LEU:H	4	0.13
(2,450)	2:360:B:MET:H	2:361:B:VAL:H	10	0.13
(2,448)	2:361:B:VAL:H	2:360:B:MET:H	10	0.13
(2,441)	2:357:B:ALA:H	2:356:B:GLN:H	9	0.13
(2,437)	2:350:B:ASP:H	2:351:B:GLY:H	6	0.13
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	8	0.13
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	10	0.13
(2,407)	2:340:B:GLN:H	2:341:B:ASP:H	7	0.13
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	1	0.13
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	1	0.13
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	17	0.13
(2,365)	2:325:B:LEU:H	2:345:B:GLY:H	7	0.13
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	6	0.13
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	9	0.13
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	2	0.13
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	3	0.13
(2,349)	2:374:B:ILE:H	2:375:B:GLN:H	11	0.13
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	7	0.13
(2,290)	2:292:B:LYS:H	2:294:B:ARG:H	12	0.13
(2,285)	2:288:B:ASP:H	2:287:B:SER:H	17	0.13
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	10	0.13
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	10	0.13
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	11	0.13
(2,243)	2:275:B:VAL:H	2:277:B:GLU:H	9	0.13
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	6	0.13
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	20	0.13
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	11	0.13
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	12	0.13
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	14	0.13
(2,218)	2:270:B:TRP:H	2:273:B:LYS:H	4	0.13
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	10	0.13
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,195)	2:261:B:GLU:H	2:258:B:LEU:H	6	0.13
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	19	0.13
(2,184)	2:259:B:PHE:H	2:256:B:ARG:H	6	0.13
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	8	0.13
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	5	0.13
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	16	0.13
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	5	0.13
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	16	0.13
(2,107)	2:222:B:GLU:H	2:223:B:PHE:H	17	0.13
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	12	0.13
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	8	0.13
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	3	0.13
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	14	0.13
(2,56)	2:207:B:LEU:H	2:209:B:ARG:H	13	0.13
(2,51)	2:202:B:THR:H	2:267:B:VAL:H	15	0.13
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	18	0.13
(2,18)	2:181:B:ALA:H	2:386:B:VAL:H	2	0.13
(1,26)	1:53:A:LEU:HD21	2:292:B:LYS:N	5	0.13
(4,9)	2:375:B:GLN:OE1	2:375:B:GLN:N	4	0.12
(4,9)	2:375:B:GLN:OE1	2:375:B:GLN:N	14	0.12
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	16	0.12
(4,4)	2:281:B:GLU:OE1	2:281:B:GLU:H	8	0.12
(3,320)	2:406:B:GLN:O	2:410:B:SER:HG	18	0.12
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH11	10	0.12
(3,312)	2:404:B:GLU:OE2	2:407:B:ARG:HH12	10	0.12
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	2	0.12
(3,276)	2:375:B:GLN:O	2:378:B:VAL:H	3	0.12
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	2	0.12
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	2	0.12
(3,271)	2:370:B:MET:O	2:174:B:LEU:N	5	0.12
(3,271)	2:370:B:MET:O	2:174:B:LEU:N	17	0.12
(3,243)	2:353:B:ALA:O	2:362:B:ARG:NH1	14	0.12
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	12	0.12
(3,238)	2:348:B:VAL:O	2:371:B:GLY:H	15	0.12
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	4	0.12
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	4	0.12
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	13	0.12
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	19	0.12
(3,206)	2:323:B:PHE:O	2:344:B:VAL:H	1	0.12
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	15	0.12
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	15	0.12
(3,179)	2:291:B:LEU:O	2:294:B:ARG:N	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,178)	2:288:B:ASP:O	2:292:B:LYS:H	17	0.12
(3,177)	2:288:B:ASP:O	2:292:B:LYS:N	20	0.12
(3,170)	2:281:B:GLU:O	2:285:B:ALA:H	8	0.12
(3,149)	2:270:B:TRP:O	2:274:B:THR:OG1	9	0.12
(3,141)	2:268:B:ALA:O	2:272:B:VAL:N	5	0.12
(3,108)	2:251:B:ASP:O	2:253:B:ARG:H	11	0.12
(3,107)	2:251:B:ASP:O	2:253:B:ARG:N	12	0.12
(3,96)	2:244:B:LEU:O	2:247:B:HIS:H	14	0.12
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	1	0.12
(3,68)	2:222:B:GLU:OE2	2:304:B:ARG:HH11	16	0.12
(3,68)	2:222:B:GLU:OE2	2:304:B:ARG:HH12	16	0.12
(3,49)	2:217:B:GLU:O	2:221:B:ASN:ND2	12	0.12
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	10	0.12
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	16	0.12
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	19	0.12
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	3	0.12
(3,23)	2:204:B:ASP:O	2:208:B:GLU:N	3	0.12
(3,23)	2:204:B:ASP:O	2:208:B:GLU:N	16	0.12
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	1	0.12
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	8	0.12
(3,18)	2:186:B:TRP:O	2:326:B:VAL:H	17	0.12
(3,8)	2:177:B:ALA:O	2:368:B:THR:H	6	0.12
(3,5)	2:176:B:ALA:O	2:362:B:ARG:NH2	11	0.12
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	19	0.12
(2,586)	2:405:B:TYR:H	2:402:B:LEU:H	13	0.12
(2,563)	2:400:B:VAL:H	2:402:B:LEU:H	10	0.12
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	4	0.12
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	18	0.12
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	19	0.12
(2,542)	2:391:B:GLY:H	2:387:B:ASP:H	18	0.12
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	8	0.12
(2,532)	2:387:B:ASP:H	2:394:B:LEU:H	6	0.12
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	8	0.12
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	9	0.12
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	13	0.12
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	7	0.12
(2,523)	2:384:B:LEU:H	2:185:B:GLY:H	18	0.12
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	8	0.12
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	9	0.12
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	13	0.12
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	12	0.12
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	12	0.12
(2,494)	2:377:B:SER:H	2:380:B:HIS:H	11	0.12
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	5	0.12
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	9	0.12
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	19	0.12
(2,480)	2:371:B:GLY:H	2:372:B:ALA:H	9	0.12
(2,465)	2:366:B:ILE:H	2:365:B:GLY:H	5	0.12
(2,446)	2:359:B:ILE:H	2:361:B:VAL:H	15	0.12
(2,434)	2:350:B:ASP:H	2:371:B:GLY:H	5	0.12
(2,432)	2:349:B:ARG:H	2:327:B:ALA:H	4	0.12
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	5	0.12
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	5	0.12
(2,424)	2:347:B:VAL:H	2:327:B:ALA:H	12	0.12
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	9	0.12
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	4	0.12
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	13	0.12
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	15	0.12
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	10	0.12
(2,403)	2:338:B:LEU:H	2:337:B:GLU:H	11	0.12
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	10	0.12
(2,398)	2:337:B:GLU:H	2:338:B:LEU:H	11	0.12
(2,381)	2:330:B:LEU:H	2:331:B:SER:H	1	0.12
(2,362)	2:324:B:ILE:H	2:184:B:GLU:H	3	0.12
(2,359)	2:324:B:ILE:H	2:185:B:GLY:H	8	0.12
(2,356)	2:323:B:PHE:H	2:344:B:VAL:H	1	0.12
(2,356)	2:323:B:PHE:H	2:344:B:VAL:H	15	0.12
(2,350)	2:314:B:GLN:H	2:315:B:GLY:H	15	0.12
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	1	0.12
(2,341)	2:311:B:ASP:H	2:313:B:ASN:H	12	0.12
(2,323)	2:304:B:ARG:H	2:303:B:GLN:H	14	0.12
(2,323)	2:304:B:ARG:H	2:303:B:GLN:H	15	0.12
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	2	0.12
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	13	0.12
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	5	0.12
(2,278)	2:285:B:ALA:H	2:284:B:ALA:H	7	0.12
(2,277)	2:284:B:ALA:H	2:281:B:GLU:H	14	0.12
(2,275)	2:284:B:ALA:H	2:285:B:ALA:H	7	0.12
(2,273)	2:284:B:ALA:H	2:283:B:PHE:H	6	0.12
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	13	0.12
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	18	0.12
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	2	0.12
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,240)	2:274:B:THR:H	2:273:B:LYS:H	5	0.12
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	8	0.12
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	10	0.12
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	2	0.12
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	3	0.12
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	15	0.12
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	20	0.12
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	1	0.12
(2,229)	2:272:B:VAL:H	2:270:B:TRP:H	17	0.12
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	11	0.12
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	19	0.12
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	13	0.12
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	14	0.12
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	15	0.12
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	14	0.12
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	15	0.12
(2,184)	2:259:B:PHE:H	2:256:B:ARG:H	16	0.12
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	1	0.12
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	20	0.12
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	5	0.12
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	20	0.12
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	8	0.12
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	14	0.12
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	8	0.12
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	14	0.12
(2,149)	2:243:B:ASP:H	2:241:B:ILE:H	10	0.12
(2,128)	2:230:B:PHE:H	2:229:B:ARG:H	12	0.12
(2,118)	2:227:B:SER:H	2:229:B:ARG:H	9	0.12
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	3	0.12
(2,116)	2:226:B:TYR:H	2:227:B:SER:H	7	0.12
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	5	0.12
(2,95)	2:218:B:GLU:H	2:221:B:ASN:H	16	0.12
(2,56)	2:207:B:LEU:H	2:209:B:ARG:H	4	0.12
(2,48)	2:198:B:TYR:H	2:270:B:TRP:HE1	8	0.12
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	8	0.12
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	11	0.12
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	15	0.12
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	9	0.12
(1,37)	2:247:B:HIS:HE2	1:48:A:SER:HA	1	0.12
(1,19)	1:53:A:LEU:HD23	2:284:B:ALA:N	4	0.12
(1,19)	1:53:A:LEU:HD21	2:284:B:ALA:HA	18	0.12
(1,3)	1:16:A:HIS:HE1	2:241:B:ILE:HD11	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,2)	2:269:B:GLU:OE1	2:269:B:GLU:H	18	0.11
(3,298)	2:394:B:LEU:O	2:385:B:ILE:H	4	0.11
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	15	0.11
(3,297)	2:394:B:LEU:O	2:385:B:ILE:N	20	0.11
(3,290)	2:387:B:ASP:O	2:392:B:GLU:H	14	0.11
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH11	20	0.11
(3,274)	2:373:B:ASP:O	2:349:B:ARG:HH12	20	0.11
(3,264)	2:367:B:PRO:O	2:346:B:VAL:H	15	0.11
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	5	0.11
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	5	0.11
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	8	0.11
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	8	0.11
(3,242)	2:352:B:ALA:O	2:355:B:SER:HG	1	0.11
(3,240)	2:348:B:VAL:O	2:372:B:ALA:H	12	0.11
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE21	13	0.11
(3,226)	2:337:B:GLU:OE2	2:303:B:GLN:HE22	13	0.11
(3,225)	2:337:B:GLU:OE2	2:303:B:GLN:NE2	12	0.11
(3,212)	2:327:B:ALA:O	2:349:B:ARG:H	15	0.11
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE21	3	0.11
(3,186)	2:297:B:ASP:OD1	2:356:B:GLN:HE22	3	0.11
(3,181)	2:294:B:ARG:O	2:297:B:ASP:N	3	0.11
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	7	0.11
(3,148)	2:269:B:GLU:O	2:273:B:LYS:H	18	0.11
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	5	0.11
(3,94)	2:244:B:LEU:O	2:248:B:LEU:H	18	0.11
(3,92)	2:243:B:ASP:O	2:247:B:HIS:H	12	0.11
(3,88)	2:240:B:ALA:O	2:244:B:LEU:H	12	0.11
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE21	18	0.11
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE22	18	0.11
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE21	19	0.11
(3,80)	2:237:B:GLU:OE1	2:235:B:GLN:HE22	19	0.11
(3,77)	2:236:B:LYS:O	2:240:B:ALA:N	17	0.11
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	1	0.11
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	8	0.11
(3,74)	2:229:B:ARG:O	2:232:B:ALA:H	20	0.11
(3,64)	2:222:B:GLU:OE1	2:308:B:HIS:HE2	9	0.11
(3,53)	2:218:B:GLU:O	2:222:B:GLU:N	11	0.11
(3,52)	2:217:B:GLU:O	2:221:B:ASN:H	2	0.11
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	11	0.11
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	12	0.11
(3,48)	2:216:B:LEU:O	2:220:B:ALA:H	18	0.11
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,44)	2:214:B:GLY:O	2:218:B:GLU:H	12	0.11
(3,33)	2:208:B:GLU:OE1	2:268:B:ALA:N	19	0.11
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH21	12	0.11
(3,32)	2:208:B:GLU:OE1	2:211:B:ARG:HH22	12	0.11
(3,28)	2:206:B:ALA:O	2:210:B:GLU:H	17	0.11
(3,20)	2:188:B:ASP:OD1	2:190:B:THR:H	12	0.11
(3,6)	2:176:B:ALA:O	2:362:B:ARG:HH21	7	0.11
(3,6)	2:176:B:ALA:O	2:362:B:ARG:HH22	7	0.11
(2,609)	2:415:B:LEU:H	2:414:B:GLU:H	6	0.11
(2,607)	2:413:B:ILE:H	2:414:B:GLU:H	4	0.11
(2,601)	2:409:B:ILE:H	2:406:B:GLN:H	4	0.11
(2,586)	2:405:B:TYR:H	2:402:B:LEU:H	18	0.11
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	12	0.11
(2,577)	2:403:B:GLN:H	2:406:B:GLN:H	20	0.11
(2,570)	2:402:B:LEU:H	2:401:B:LEU:H	18	0.11
(2,568)	2:402:B:LEU:H	2:400:B:VAL:H	12	0.11
(2,563)	2:400:B:VAL:H	2:402:B:LEU:H	19	0.11
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	16	0.11
(2,552)	2:394:B:LEU:H	2:385:B:ILE:H	19	0.11
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	13	0.11
(2,549)	2:393:B:LEU:H	2:394:B:LEU:H	20	0.11
(2,527)	2:385:B:ILE:H	2:396:B:ASP:H	11	0.11
(2,525)	2:385:B:ILE:H	2:384:B:LEU:H	12	0.11
(2,522)	2:384:B:LEU:H	2:396:B:ASP:H	12	0.11
(2,521)	2:384:B:LEU:H	2:385:B:ILE:H	12	0.11
(2,518)	2:384:B:LEU:H	2:183:B:ALA:H	2	0.11
(2,515)	2:383:B:THR:H	2:396:B:ASP:H	8	0.11
(2,510)	2:382:B:ARG:H	2:379:B:LEU:H	19	0.11
(2,490)	2:375:B:GLN:H	2:374:B:ILE:H	6	0.11
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	2	0.11
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	14	0.11
(2,465)	2:366:B:ILE:H	2:365:B:GLY:H	3	0.11
(2,465)	2:366:B:ILE:H	2:365:B:GLY:H	8	0.11
(2,446)	2:359:B:ILE:H	2:361:B:VAL:H	11	0.11
(2,444)	2:358:B:ALA:H	2:357:B:ALA:H	7	0.11
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	8	0.11
(2,439)	2:352:B:ALA:H	2:351:B:GLY:H	10	0.11
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	8	0.11
(2,438)	2:351:B:GLY:H	2:352:B:ALA:H	10	0.11
(2,429)	2:348:B:VAL:H	2:370:B:MET:H	7	0.11
(2,426)	2:347:B:VAL:H	2:348:B:VAL:H	9	0.11
(2,423)	2:345:B:GLY:H	2:325:B:LEU:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	2:345:B:GLY:H	2:325:B:LEU:H	10	0.11
(2,422)	2:345:B:GLY:H	2:323:B:PHE:H	17	0.11
(2,420)	2:344:B:VAL:H	2:325:B:LEU:H	16	0.11
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	12	0.11
(2,416)	2:343:B:LEU:H	2:340:B:GLN:H	18	0.11
(2,410)	2:341:B:ASP:H	2:342:B:ARG:H	16	0.11
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	3	0.11
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	16	0.11
(2,399)	2:337:B:GLU:H	2:335:B:LEU:H	8	0.11
(2,357)	2:323:B:PHE:H	2:345:B:GLY:H	2	0.11
(2,346)	2:313:B:ASN:H	2:312:B:ALA:H	6	0.11
(2,322)	2:304:B:ARG:H	2:305:B:LEU:H	19	0.11
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	15	0.11
(2,301)	2:296:B:GLY:H	2:297:B:ASP:H	16	0.11
(2,292)	2:293:B:GLU:H	2:290:B:TYR:H	12	0.11
(2,272)	2:283:B:PHE:H	2:284:B:ALA:H	11	0.11
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	2	0.11
(2,267)	2:282:B:GLN:H	2:281:B:GLU:H	7	0.11
(2,259)	2:280:B:ALA:H	2:281:B:GLU:H	13	0.11
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	17	0.11
(2,243)	2:275:B:VAL:H	2:277:B:GLU:H	2	0.11
(2,225)	2:414:B:GLU:H	2:413:B:ILE:H	4	0.11
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	2	0.11
(2,219)	2:270:B:TRP:H	2:271:B:ALA:H	16	0.11
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	4	0.11
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	12	0.11
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	15	0.11
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	17	0.11
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	18	0.11
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	3	0.11
(2,198)	2:262:B:VAL:H	2:260:B:ALA:H	7	0.11
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	3	0.11
(2,187)	2:260:B:ALA:H	2:262:B:VAL:H	7	0.11
(2,185)	2:259:B:PHE:H	2:261:B:GLU:H	1	0.11
(2,180)	2:258:B:LEU:H	2:256:B:ARG:H	7	0.11
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	14	0.11
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	3	0.11
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	3	0.11
(2,99)	2:220:B:ALA:H	2:219:B:ALA:H	17	0.11
(2,98)	2:219:B:ALA:H	2:218:B:GLU:H	3	0.11
(2,94)	2:218:B:GLU:H	2:219:B:ALA:H	3	0.11
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	11	0.11
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	15	0.11
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	16	0.11
(2,44)	2:195:B:GLU:H	2:196:B:GLN:H	14	0.11
(2,41)	2:193:B:LEU:H	2:196:B:GLN:H	10	0.11
(2,38)	2:190:B:THR:H	2:189:B:ALA:H	3	0.11
(2,29)	2:185:B:GLY:H	2:383:B:THR:H	4	0.11
(2,27)	2:184:B:GLU:H	2:324:B:ILE:H	8	0.11
(2,22)	2:183:B:ALA:H	2:384:B:LEU:H	2	0.11
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	12	0.11
(1,29)	1:53:A:LEU:HD23	2:295:B:ALA:H	14	0.11
(4,8)	2:341:B:ASP:OD1	2:341:B:ASP:H	4	0.1
(4,5)	2:328:B:ASP:OD1	2:328:B:ASP:N	11	0.1
(3,309)	2:403:B:GLN:O	2:407:B:ARG:N	6	0.1
(3,288)	2:387:B:ASP:OD1	2:389:B:TYR:H	18	0.1
(3,286)	2:386:B:VAL:O	2:181:B:ALA:H	10	0.1
(3,281)	2:384:B:LEU:O	2:183:B:ALA:N	3	0.1
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH11	19	0.1
(3,244)	2:353:B:ALA:O	2:362:B:ARG:HH12	19	0.1
(3,223)	2:336:B:ALA:O	2:304:B:ARG:NH2	8	0.1
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE21	7	0.1
(3,204)	2:313:B:ASN:O	2:314:B:GLN:HE22	7	0.1
(3,139)	2:267:B:VAL:O	2:271:B:ALA:N	5	0.1
(3,102)	2:246:B:SER:O	2:250:B:SER:HG	1	0.1
(3,66)	2:222:B:GLU:OE1	2:304:B:ARG:HE	18	0.1
(3,49)	2:217:B:GLU:O	2:221:B:ASN:ND2	14	0.1
(3,49)	2:217:B:GLU:O	2:221:B:ASN:ND2	18	0.1
(3,47)	2:216:B:LEU:O	2:220:B:ALA:N	5	0.1
(2,586)	2:405:B:TYR:H	2:402:B:LEU:H	20	0.1
(2,576)	2:403:B:GLN:H	2:400:B:VAL:H	13	0.1
(2,556)	2:395:B:VAL:H	2:171:B:ILE:H	20	0.1
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	8	0.1
(2,540)	2:390:B:ARG:H	2:388:B:GLY:H	13	0.1
(2,533)	2:387:B:ASP:H	2:389:B:TYR:H	7	0.1
(2,513)	2:382:B:ARG:H	2:185:B:GLY:H	1	0.1
(2,511)	2:382:B:ARG:H	2:381:B:ARG:H	20	0.1
(2,507)	2:381:B:ARG:H	2:382:B:ARG:H	20	0.1
(2,486)	2:373:B:ASP:H	2:372:B:ALA:H	17	0.1
(2,470)	2:369:B:VAL:H	2:368:B:THR:H	4	0.1
(2,470)	2:369:B:VAL:H	2:368:B:THR:H	16	0.1
(2,465)	2:366:B:ILE:H	2:365:B:GLY:H	13	0.1
(2,451)	2:361:B:VAL:H	2:363:B:ALA:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,436)	2:350:B:ASP:H	2:349:B:ARG:H	5	0.1
(2,419)	2:344:B:VAL:H	2:345:B:GLY:H	8	0.1
(2,409)	2:341:B:ASP:H	2:340:B:GLN:H	1	0.1
(2,408)	2:172:B:ARG:H	2:171:B:ILE:H	16	0.1
(2,407)	2:340:B:GLN:H	2:341:B:ASP:H	19	0.1
(2,360)	2:324:B:ILE:H	2:344:B:VAL:H	2	0.1
(2,304)	2:297:B:ASP:H	2:296:B:GLY:H	11	0.1
(2,284)	2:286:B:LEU:H	2:284:B:ALA:H	15	0.1
(2,271)	2:283:B:PHE:H	2:282:B:GLN:H	12	0.1
(2,254)	2:278:B:LYS:H	2:276:B:ILE:H	4	0.1
(2,235)	2:273:B:LYS:H	2:270:B:TRP:H	16	0.1
(2,234)	2:273:B:LYS:H	2:275:B:VAL:H	8	0.1
(2,224)	2:414:B:GLU:H	2:415:B:LEU:H	18	0.1
(2,214)	2:269:B:GLU:H	2:268:B:ALA:H	7	0.1
(2,209)	2:265:B:GLY:H	2:264:B:LYS:H	20	0.1
(2,201)	2:263:B:ASP:H	2:261:B:GLU:H	19	0.1
(2,196)	2:261:B:GLU:H	2:263:B:ASP:H	19	0.1
(2,185)	2:259:B:PHE:H	2:261:B:GLU:H	17	0.1
(2,177)	2:257:B:GLU:H	2:255:B:ARG:H	10	0.1
(2,175)	2:256:B:ARG:H	2:253:B:ARG:H	8	0.1
(2,171)	2:255:B:ARG:H	2:256:B:ARG:H	1	0.1
(2,157)	2:247:B:HIS:H	2:246:B:SER:H	6	0.1
(2,155)	2:246:B:SER:H	2:247:B:HIS:H	6	0.1
(2,77)	2:214:B:GLY:H	2:212:B:LEU:H	20	0.1
(2,76)	2:214:B:GLY:H	2:216:B:LEU:H	10	0.1
(2,65)	2:210:B:GLU:H	2:208:B:GLU:H	10	0.1
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	5	0.1
(2,43)	2:195:B:GLU:H	2:194:B:MET:H	15	0.1
(2,33)	2:185:B:GLY:H	2:382:B:ARG:H	19	0.1
(2,31)	2:185:B:GLY:H	2:384:B:LEU:H	3	0.1
(2,16)	2:177:B:ALA:H	2:176:B:ALA:H	20	0.1
(2,6)	2:173:B:ALA:H	2:392:B:GLU:H	18	0.1
(2,1)	2:345:B:GLY:H	2:344:B:VAL:H	8	0.1

10 Dihedral-angle violation analysis [i](#)

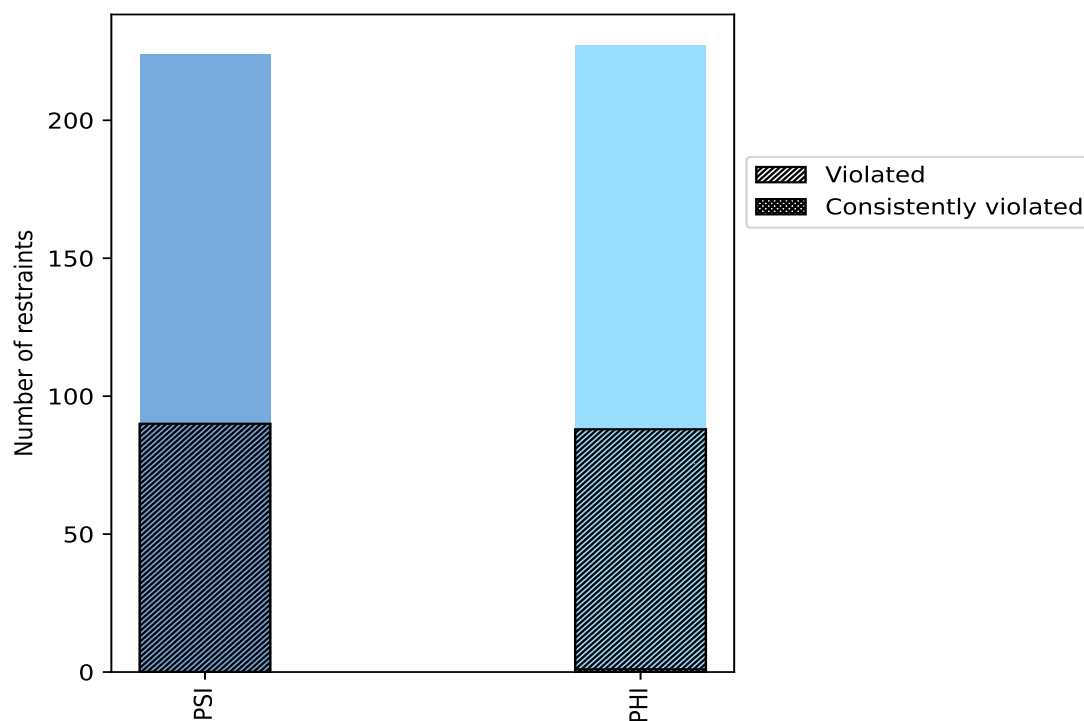
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	224	49.7	90	40.2	20.0	0	0.0	0.0
PHI	227	50.3	88	38.8	19.5	1	0.4	0.2
Total	451	100.0	178	39.5	39.5	1	0.2	0.2

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



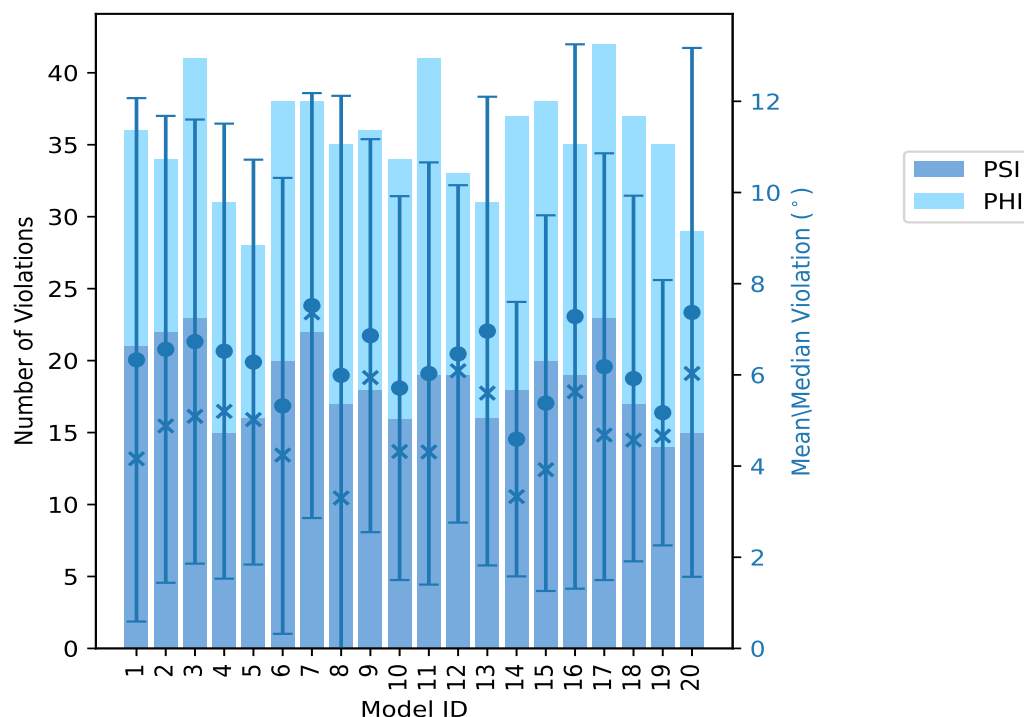
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	21	15	36	6.33	26.18	5.74	4.16
2	22	12	34	6.56	19.65	5.12	4.88
3	23	18	41	6.73	21.08	4.87	5.09
4	15	16	31	6.52	21.34	4.99	5.2
5	16	12	28	6.28	16.4	4.44	5.02
6	20	18	38	5.32	29.11	5.0	4.24
7	22	16	38	7.52	18.72	4.66	7.36
8	17	18	35	5.99	24.93	6.13	3.3
9	18	18	36	6.86	16.67	4.31	5.94
10	16	18	34	5.71	17.25	4.21	4.32
11	19	22	41	6.03	23.01	4.63	4.31
12	19	14	33	6.46	17.77	3.7	6.09
13	16	15	31	6.96	20.58	5.14	5.6
14	18	19	37	4.59	11.55	3.01	3.33
15	20	18	38	5.38	19.44	4.12	3.92
16	19	16	35	7.28	22.49	5.97	5.63
17	23	19	42	6.18	20.9	4.68	4.68
18	17	20	37	5.92	17.45	4.01	4.57
19	14	21	35	5.17	10.93	2.91	4.66
20	15	14	29	7.37	25.37	5.8	6.03

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
28	31	59	1	5.0
19	19	38	2	10.0
8	8	16	3	15.0
7	9	16	4	20.0
5	5	10	5	25.0
5	0	5	6	30.0
3	2	5	7	35.0
3	0	3	8	40.0
3	5	8	9	45.0
2	2	4	10	50.0
0	1	1	11	55.0

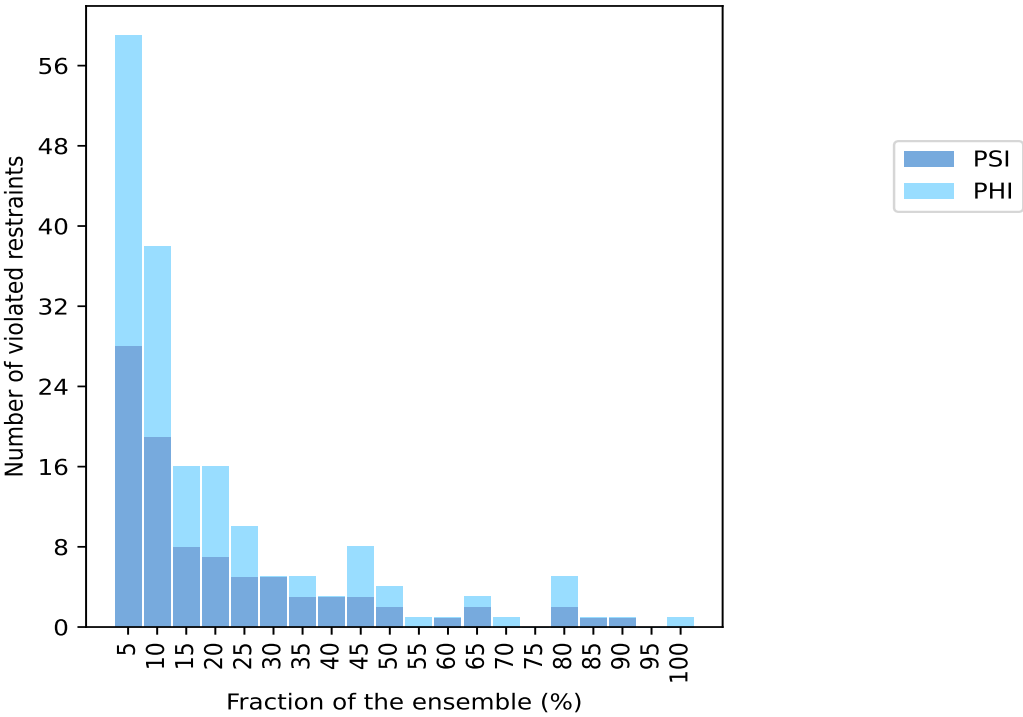
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	0	1	12	60.0
2	1	3	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
2	3	5	16	80.0
1	0	1	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

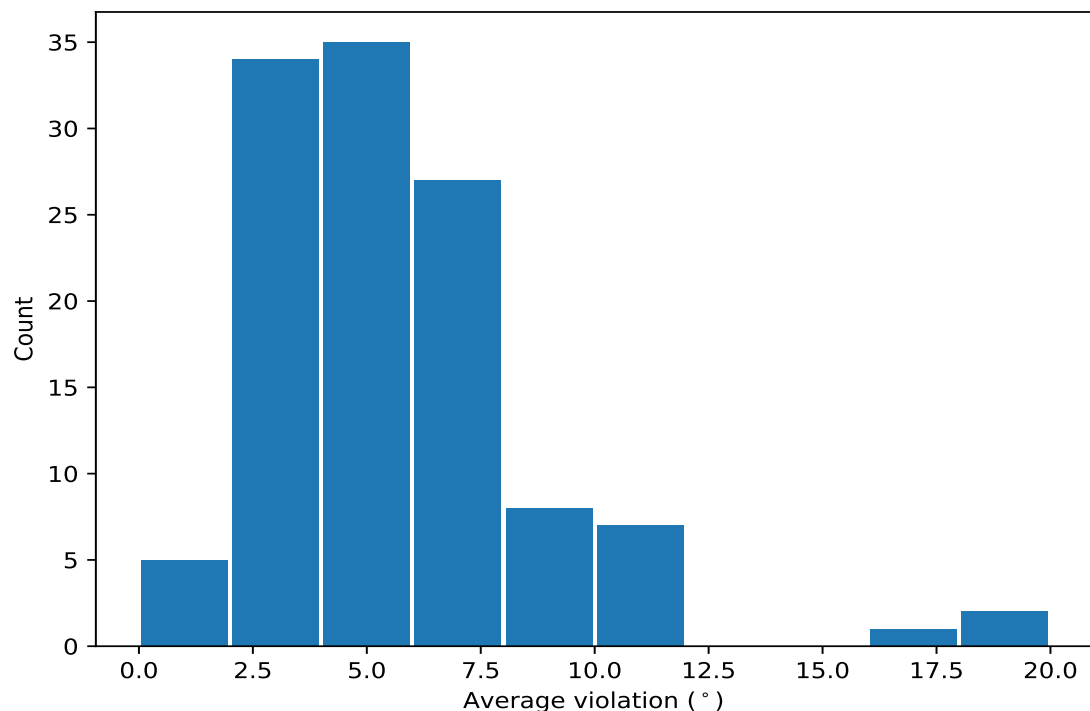


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	20	8.49	3.2	8.6
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	18	17.43	4.81	17.55
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	17	11.58	4.31	11.55
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	16	18.06	3.7	18.24
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	16	7.76	3.31	7.52
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	16	5.96	3.44	5.2
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	16	5.09	2.72	5.23
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	16	4.78	1.89	5.01
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	14	7.68	4.33	6.82
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	13	7.18	3.87	8.34
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	13	4.34	1.66	3.91
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	13	4.26	1.61	4.25
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	12	2.96	1.68	2.24
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	11	5.93	3.33	5.63
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	10	7.31	4.35	5.78
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	10	5.07	3.12	4.36
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	10	4.04	1.96	3.7
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	10	3.02	1.83	2.52
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	9	7.09	3.43	6.32
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	9	6.16	3.58	4.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	9	5.86	3.95	5.59
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	9	5.73	2.66	5.29
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	9	5.43	3.16	6.33
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	9	5.14	4.13	3.56
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	9	3.62	2.23	3.3
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	9	2.94	1.79	2.42
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	8	8.45	3.08	8.68
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	8	8.26	5.19	8.91
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	8	6.12	4.07	4.98
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	7	10.36	2.21	10.88
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	7	6.84	3.38	8.22
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	7	6.32	5.17	3.86
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	7	6.01	2.61	6.04
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	7	2.02	1.34	1.27
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	6	10.08	4.36	10.24
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	6	7.08	3.14	7.74
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	6	5.93	3.62	5.15
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	6	4.95	2.75	4.04
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	6	3.11	2.59	2.0
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	5	8.21	2.37	8.94
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	5	6.49	5.03	5.91
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	5	6.16	4.46	4.41
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	5	5.92	2.79	7.3
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	5	5.63	4.5	4.0
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	5	4.69	3.2	3.14
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	5	4.57	2.43	3.71
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	5	4.05	1.44	4.36
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	5	3.97	1.62	4.14
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	5	3.3	0.94	2.97
(1,269)	2:344:B:VAL:C	2:345:B:GLY:N	2:345:B:GLY:CA	2:345:B:GLY:C	4	10.46	9.32	6.21
(1,402)	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2:205:B:PRO:N	4	8.07	2.1	7.7
(1,38)	2:205:B:PRO:N	2:205:B:PRO:CA	2:205:B:PRO:C	2:206:B:ALA:N	4	6.74	4.57	6.38
(1,312)	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	2:376:B:PRO:N	4	6.68	2.88	6.44
(1,219)	2:318:B:ALA:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	4	6.1	6.55	2.75
(1,321)	2:384:B:LEU:C	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	4	5.3	2.51	4.88
(1,34)	2:201:B:SER:N	2:201:B:SER:CA	2:201:B:SER:C	2:202:B:THR:N	4	4.74	1.28	4.63
(1,231)	2:325:B:LEU:C	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	4	4.62	1.37	5.23
(1,372)	2:413:B:ILE:C	2:414:B:GLU:N	2:414:B:GLU:CA	2:414:B:GLU:C	4	4.5	3.64	3.07
(1,229)	2:324:B:ILE:C	2:325:B:LEU:N	2:325:B:LEU:CA	2:325:B:LEU:C	4	3.84	1.59	3.82
(1,350)	2:402:B:LEU:N	2:402:B:LEU:CA	2:402:B:LEU:C	2:403:B:GLN:N	4	3.66	1.79	3.0
(1,327)	2:387:B:ASP:C	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	4	3.56	1.59	3.19
(1,256)	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	2:339:B:PRO:N	4	3.34	1.85	2.5
(1,223)	2:321:B:GLU:C	2:322:B:ARG:N	2:322:B:ARG:CA	2:322:B:ARG:C	4	3.25	1.51	3.08
(1,186)	2:291:B:LEU:N	2:291:B:LEU:CA	2:291:B:LEU:C	2:292:B:LYS:N	4	3.21	0.36	3.32
(1,365)	2:409:B:ILE:C	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	4	3.04	1.63	2.46
(1,222)	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	2:322:B:ARG:N	3	9.54	2.56	11.18
(1,39)	2:205:B:PRO:C	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	3	8.75	6.55	5.2
(1,409)	2:232:B:ALA:C	2:233:B:GLY:N	2:233:B:GLY:CA	2:233:B:GLY:C	3	7.88	2.25	7.3
(1,355)	2:404:B:GLU:C	2:405:B:TYR:N	2:405:B:TYR:CA	2:405:B:TYR:C	3	6.95	2.18	6.86
(1,14)	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	2:184:B:GLU:N	3	4.98	3.98	2.94
(1,260)	2:340:B:GLN:N	2:340:B:GLN:CA	2:340:B:GLN:C	2:341:B:ASP:N	3	4.14	2.67	2.5

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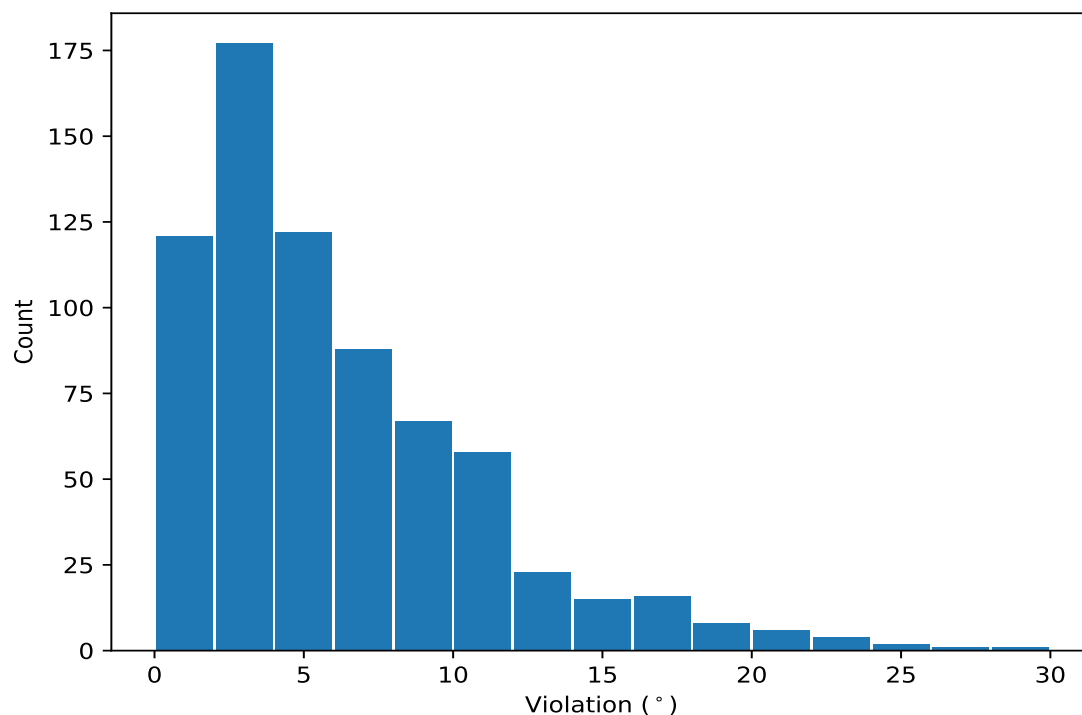
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,395)	2:195:B:GLU:C	2:196:B:GLN:N	2:196:B:GLN:CA	2:196:B:GLN:C	3	3.5	2.22	2.27
(1,393)	2:194:B:MET:C	2:195:B:GLU:N	2:195:B:GLU:CA	2:195:B:GLU:C	3	3.21	2.46	1.89
(1,316)	2:377:B:SER:N	2:377:B:SER:CA	2:377:B:SER:C	2:378:B:VAL:N	3	3.2	2.68	1.43
(1,165)	2:278:B:LYS:C	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	3	3.08	0.86	2.51
(1,107)	2:245:B:TYR:C	2:246:B:SER:N	2:246:B:SER:CA	2:246:B:SER:C	3	2.84	1.31	2.19
(1,437)	2:378:B:VAL:N	2:378:B:VAL:CA	2:378:B:VAL:C	2:379:B:LEU:N	3	2.53	1.97	1.14
(1,92)	2:238:B:THR:N	2:238:B:THR:CA	2:238:B:THR:C	2:239:B:ALA:N	3	2.01	0.92	1.39
(1,228)	2:324:B:ILE:N	2:324:B:ILE:CA	2:324:B:ILE:C	2:325:B:LEU:N	3	1.87	0.81	1.57
(1,438)	2:378:B:VAL:C	2:379:B:LEU:N	2:379:B:LEU:CA	2:379:B:LEU:C	3	1.62	0.42	1.76
(1,278)	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2:353:B:ALA:N	3	1.47	0.39	1.42
(1,411)	2:233:B:GLY:C	2:234:B:ALA:N	2:234:B:ALA:CA	2:234:B:ALA:C	2	18.35	10.76	18.35
(1,340)	2:394:B:LEU:N	2:394:B:LEU:CA	2:394:B:LEU:C	2:395:B:VAL:N	2	11.62	1.4	11.62
(1,220)	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	2:320:B:PRO:N	2	11.28	9.8	11.28
(1,169)	2:280:B:ALA:C	2:281:B:GLU:N	2:281:B:GLU:CA	2:281:B:GLU:C	2	10.96	0.93	10.96
(1,347)	2:400:B:VAL:C	2:401:B:LEU:N	2:401:B:LEU:CA	2:401:B:LEU:C	2	9.3	8.15	9.3
(1,440)	2:380:B:HIS:C	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2	7.5	5.8	7.5
(1,447)	2:397:B:PRO:N	2:397:B:PRO:CA	2:397:B:PRO:C	2:398:B:GLU:N	2	7.07	1.37	7.07
(1,332)	2:390:B:ARG:N	2:390:B:ARG:CA	2:390:B:ARG:C	2:391:B:GLY:N	2	7.06	2.8	7.06
(1,29)	2:197:B:VAL:C	2:198:B:TYR:N	2:198:B:TYR:CA	2:198:B:TYR:C	2	7.02	4.05	7.02
(1,63)	2:217:B:GLU:C	2:218:B:GLU:N	2:218:B:GLU:CA	2:218:B:GLU:C	2	6.8	1.12	6.8
(1,369)	2:412:B:GLU:N	2:412:B:GLU:CA	2:412:B:GLU:C	2:413:B:ILE:N	2	6.52	0.49	6.52
(1,451)	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	2:418:B:LEU:N	2	6.46	4.96	6.46
(1,218)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:ALA:N	2	6.26	2.41	6.26
(1,314)	2:376:B:PRO:N	2:376:B:PRO:CA	2:376:B:PRO:C	2:377:B:SER:N	2	6.0	2.5	6.0
(1,25)	2:193:B:LEU:C	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	2	5.91	2.95	5.91
(1,427)	2:310:B:ASP:N	2:310:B:ASP:CA	2:310:B:ASP:C	2:311:B:ASP:N	2	5.83	3.47	5.83
(1,27)	2:196:B:GLN:C	2:197:B:VAL:N	2:197:B:VAL:CA	2:197:B:VAL:C	2	5.58	1.42	5.58
(1,388)	2:188:B:ASP:N	2:188:B:ASP:CA	2:188:B:ASP:C	2:189:B:ALA:N	2	5.42	4.04	5.42
(1,226)	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	2:324:B:ILE:N	2	5.08	3.26	5.08
(1,41)	2:206:B:ALA:C	2:207:B:LEU:N	2:207:B:LEU:CA	2:207:B:LEU:C	2	4.52	1.52	4.52
(1,26)	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	2:195:B:GLU:N	2	4.48	0.27	4.48
(1,277)	2:351:B:GLY:C	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2	4.39	0.86	4.39
(1,239)	2:329:B:GLU:C	2:330:B:LEU:N	2:330:B:LEU:CA	2:330:B:LEU:C	2	4.38	1.09	4.38
(1,450)	2:416:B:SER:C	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	2	4.08	0.33	4.08
(1,273)	2:346:B:VAL:C	2:347:B:VAL:N	2:347:B:VAL:CA	2:347:B:VAL:C	2	3.96	2.33	3.96
(1,319)	2:383:B:THR:C	2:384:B:LEU:N	2:384:B:LEU:CA	2:384:B:LEU:C	2	3.82	2.8	3.82
(1,40)	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	2:207:B:LEU:N	2	3.49	0.17	3.49
(1,31)	2:199:B:GLN:C	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2	3.3	0.52	3.3
(1,17)	2:186:B:TRP:C	2:187:B:GLN:N	2:187:B:GLN:CA	2:187:B:GLN:C	2	2.87	0.18	2.87
(1,419)	2:288:B:ASP:N	2:288:B:ASP:CA	2:288:B:ASP:C	2:289:B:ASN:N	2	2.66	0.44	2.66
(1,303)	2:367:B:PRO:C	2:368:B:THR:N	2:368:B:THR:CA	2:368:B:THR:C	2	2.6	1.58	2.6
(1,308)	2:370:B:MET:N	2:370:B:MET:CA	2:370:B:MET:C	2:371:B:GLY:N	2	2.18	1.02	2.18
(1,366)	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	2:411:B:GLU:N	2	2.14	0.88	2.14
(1,241)	2:330:B:LEU:C	2:331:B:SER:N	2:331:B:SER:CA	2:331:B:SER:C	2	2.12	0.45	2.12
(1,1)	2:170:B:ARG:C	2:171:B:ILE:N	2:171:B:ILE:CA	2:171:B:ILE:C	2	2.12	0.99	2.12
(1,433)	2:373:B:ASP:N	2:373:B:ASP:CA	2:373:B:ASP:C	2:374:B:ILE:N	2	2.1	0.76	2.1
(1,88)	2:236:B:LYS:N	2:236:B:LYS:CA	2:236:B:LYS:C	2:237:B:GLU:N	2	1.42	0.15	1.42
(1,16)	2:184:B:GLU:N	2:184:B:GLU:CA	2:184:B:GLU:C	2:185:B:GLY:N	2	1.38	0.27	1.38

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,411)	2:233:B:GLY:C	2:234:B:ALA:N	2:234:B:ALA:CA	2:234:B:ALA:C	6	29.11
(1,269)	2:344:B:VAL:C	2:345:B:GLY:N	2:345:B:GLY:CA	2:345:B:GLY:C	1	26.18
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	20	25.37
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	8	24.93
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	8	23.2
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	20	23.04
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	11	23.01
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	16	22.49
(1,299)	2:365:B:GLY:C	2:366:B:ILE:N	2:366:B:ILE:CA	2:366:B:ILE:C	16	21.65
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	4	21.34
(1,220)	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	2:320:B:PRO:N	3	21.08
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	17	20.9
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	4	20.82
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	13	20.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2	19.65
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	15	19.44
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	1	19.27
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	3	19.12
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	13	18.99
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	1	18.83
(1,298)	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	2:366:B:ILE:N	16	18.77
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	7	18.72
(1,39)	2:205:B:PRO:C	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	8	17.94
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	2	17.85
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	12	17.77
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	13	17.47
(1,347)	2:400:B:VAL:C	2:401:B:LEU:N	2:401:B:LEU:CA	2:401:B:LEU:C	18	17.45
(1,219)	2:318:B:ALA:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	3	17.4
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	10	17.25
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	7	17.09
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	16	16.89
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	9	16.67
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	5	16.4
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	3	16.29
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	5	16.24
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	16	16.22
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	9	16.21
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	2	16.07
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	7	15.93
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	17	15.68
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	17	15.64
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	5	15.39
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2	15.25
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	11	15.18
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	16	15.1
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	7	14.7
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	7	14.54
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	8	14.44
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	4	14.4
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	10	14.31
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	13	14.27
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	9	14.22
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2	14.01
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	15	13.91
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	17	13.84
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	4	13.69
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	17	13.67
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	16	13.61
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	15	13.48
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	12	13.31
(1,440)	2:380:B:HIS:C	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	7	13.3
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	1	13.16
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	6	13.13
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	20	13.12
(1,340)	2:394:B:LEU:N	2:394:B:LEU:CA	2:394:B:LEU:C	2:395:B:VAL:N	10	13.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	2:205:B:PRO:N	2:205:B:PRO:CA	2:205:B:PRO:C	2:206:B:ALA:N	8	12.98
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	12	12.94
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	9	12.91
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	20	12.7
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	20	12.68
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	18	12.56
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	17	12.46
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	3	12.27
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	11	12.15
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	10	12.09
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	11	12.08
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	9	11.97
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	11	11.94
(1,169)	2:280:B:ALA:C	2:281:B:GLU:N	2:281:B:GLU:CA	2:281:B:GLU:C	7	11.89
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	18	11.83
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	18	11.82
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	10	11.73
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	13	11.7
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	3	11.68
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	11	11.63
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	5	11.57
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	14	11.55
(1,222)	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	2:322:B:ARG:N	2	11.52
(1,451)	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	2:418:B:LEU:N	9	11.41
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	1	11.32
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	6	11.21
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	8	11.2
(1,222)	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	2:322:B:ARG:N	15	11.18
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	10	11.17
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	20	11.09
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	12	11.07
(1,29)	2:197:B:VAL:C	2:198:B:TYR:N	2:198:B:TYR:CA	2:198:B:TYR:C	13	11.07
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	18	11.03
(1,402)	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2:205:B:PRO:N	2	11.01
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	18	11.0
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	8	10.99
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	3	10.99
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	13	10.97
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	7	10.96
(1,444)	2:395:B:VAL:C	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	19	10.93
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	19	10.93
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	13	10.93
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	9	10.93
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	7	10.93
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	19	10.9
(1,409)	2:232:B:ALA:C	2:233:B:GLY:N	2:233:B:GLY:CA	2:233:B:GLY:C	18	10.89
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	15	10.88
(1,312)	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	2:376:B:PRO:N	5	10.82
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	2	10.73
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	6	10.72
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	1	10.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	20	10.66
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	7	10.65
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	14	10.6
(1,372)	2:413:B:ILE:C	2:414:B:GLU:N	2:414:B:GLU:CA	2:414:B:GLU:C	18	10.58
(1,14)	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	2:184:B:GLU:N	20	10.55
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	15	10.51
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	19	10.38
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	15	10.32
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	17	10.31
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	12	10.22
(1,340)	2:394:B:LEU:N	2:394:B:LEU:CA	2:394:B:LEU:C	2:395:B:VAL:N	11	10.22
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	3	10.22
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	5	10.14
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	2	10.12
(1,375)	2:415:B:LEU:C	2:416:B:SER:N	2:416:B:SER:CA	2:416:B:SER:C	20	10.1
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	18	10.06
(1,169)	2:280:B:ALA:C	2:281:B:GLU:N	2:281:B:GLU:CA	2:281:B:GLU:C	9	10.03
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	11	10.01
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	4	9.94
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	9	9.93
(1,332)	2:390:B:ARG:N	2:390:B:ARG:CA	2:390:B:ARG:C	2:391:B:GLY:N	18	9.86
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	9	9.82
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	5	9.81
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	17	9.78
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	9	9.77
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	8	9.7
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	14	9.7
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	12	9.7
(1,355)	2:404:B:GLU:C	2:405:B:TYR:N	2:405:B:TYR:CA	2:405:B:TYR:C	17	9.66
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	11	9.63
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	3	9.63
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	7	9.49
(1,388)	2:188:B:ASP:N	2:188:B:ASP:CA	2:188:B:ASP:C	2:189:B:ALA:N	9	9.46
(1,428)	2:311:B:ASP:C	2:312:B:ALA:N	2:312:B:ALA:CA	2:312:B:ALA:C	14	9.41
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	1	9.39
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	16	9.38
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	11	9.36
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	3	9.31
(1,427)	2:310:B:ASP:N	2:310:B:ASP:CA	2:310:B:ASP:C	2:311:B:ASP:N	12	9.3
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	17	9.23
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	9	9.22
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	1	9.21
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	12	9.16
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	11	9.13
(1,110)	2:247:B:HIS:N	2:247:B:HIS:CA	2:247:B:HIS:C	2:248:B:LEU:N	7	9.11
(1,402)	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2:205:B:PRO:N	1	9.09
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	10	9.04
(1,38)	2:205:B:PRO:N	2:205:B:PRO:CA	2:205:B:PRO:C	2:206:B:ALA:N	19	9.02
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	4	8.95
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	6	8.94
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	7	8.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	14	8.93
(1,321)	2:384:B:LEU:C	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	10	8.88
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	8	8.87
(1,25)	2:193:B:LEU:C	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	19	8.86
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	10	8.85
(1,161)	2:276:B:ILE:C	2:277:B:GLU:N	2:277:B:GLU:CA	2:277:B:GLU:C	18	8.83
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	17	8.76
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	11	8.74
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	16	8.73
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	17	8.71
(1,269)	2:344:B:VAL:C	2:345:B:GLY:N	2:345:B:GLY:CA	2:345:B:GLY:C	16	8.68
(1,218)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:ALA:N	14	8.67
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	16	8.66
(1,442)	2:381:B:ARG:C	2:382:B:ARG:N	2:382:B:ARG:CA	2:382:B:ARG:C	7	8.65
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	13	8.62
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	6	8.61
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	11	8.59
(1,374)	2:415:B:LEU:N	2:415:B:LEU:CA	2:415:B:LEU:C	2:416:B:SER:N	1	8.59
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	7	8.59
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	3	8.53
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	2	8.51
(1,314)	2:376:B:PRO:N	2:376:B:PRO:CA	2:376:B:PRO:C	2:377:B:SER:N	3	8.51
(1,390)	2:189:B:ALA:N	2:189:B:ALA:CA	2:189:B:ALA:C	2:190:B:THR:N	2	8.5
(1,447)	2:397:B:PRO:N	2:397:B:PRO:CA	2:397:B:PRO:C	2:398:B:GLU:N	6	8.45
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	4	8.34
(1,226)	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	2:324:B:ILE:N	1	8.34
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	1	8.32
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	4	8.31
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	5	8.27
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	7	8.26
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	9	8.23
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	4	8.22
(1,429)	2:312:B:ALA:N	2:312:B:ALA:CA	2:312:B:ALA:C	2:313:B:ASN:N	15	8.13
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	14	8.09
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	20	7.93
(1,63)	2:217:B:GLU:C	2:218:B:GLU:N	2:218:B:GLU:CA	2:218:B:GLU:C	3	7.92
(1,260)	2:340:B:GLN:N	2:340:B:GLN:CA	2:340:B:GLN:C	2:341:B:ASP:N	14	7.9
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	3	7.81
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	12	7.81
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	15	7.79
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	17	7.79
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	9	7.79
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	1	7.78
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	6	7.77
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	7	7.76
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	5	7.75
(1,168)	2:280:B:ALA:N	2:280:B:ALA:CA	2:280:B:ALA:C	2:281:B:GLU:N	11	7.73
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	12	7.72
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	14	7.71
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	16	7.71
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	7	7.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	8	7.66
(1,411)	2:233:B:GLY:C	2:234:B:ALA:N	2:234:B:ALA:CA	2:234:B:ALA:C	16	7.59
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	6	7.59
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	12	7.59
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	7	7.56
(1,312)	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	2:376:B:PRO:N	17	7.51
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	19	7.48
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	16	7.44
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	13	7.43
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	14	7.39
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	18	7.38
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	9	7.33
(1,409)	2:232:B:ALA:C	2:233:B:GLY:N	2:233:B:GLY:CA	2:233:B:GLY:C	4	7.3
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	5	7.3
(1,439)	2:379:B:LEU:N	2:379:B:LEU:CA	2:379:B:LEU:C	2:380:B:HIS:N	3	7.29
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	13	7.26
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	12	7.25
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	17	7.17
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	7	7.15
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	16	7.14
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	3	7.08
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	9	7.07
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	20	7.04
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	4	7.04
(1,369)	2:412:B:GLU:N	2:412:B:GLU:CA	2:412:B:GLU:C	2:413:B:ILE:N	4	7.01
(1,27)	2:196:B:GLN:C	2:197:B:VAL:N	2:197:B:VAL:CA	2:197:B:VAL:C	19	7.0
(1,316)	2:377:B:SER:N	2:377:B:SER:CA	2:377:B:SER:C	2:378:B:VAL:N	7	6.99
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	19	6.97
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	10	6.95
(1,271)	2:345:B:GLY:C	2:346:B:VAL:N	2:346:B:VAL:CA	2:346:B:VAL:C	1	6.92
(1,376)	2:416:B:SER:N	2:416:B:SER:CA	2:416:B:SER:C	2:417:B:ARG:N	1	6.91
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	2	6.87
(1,355)	2:404:B:GLU:C	2:405:B:TYR:N	2:405:B:TYR:CA	2:405:B:TYR:C	10	6.86
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	6	6.85
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	7	6.81
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	8	6.77
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	17	6.76
(1,350)	2:402:B:LEU:N	2:402:B:LEU:CA	2:402:B:LEU:C	2:403:B:GLN:N	10	6.68
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	19	6.66
(1,393)	2:194:B:MET:C	2:195:B:GLU:N	2:195:B:GLU:CA	2:195:B:GLU:C	6	6.65
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	12	6.65
(1,319)	2:383:B:THR:C	2:384:B:LEU:N	2:384:B:LEU:CA	2:384:B:LEU:C	20	6.63
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	19	6.63
(1,395)	2:195:B:GLU:C	2:196:B:GLN:N	2:196:B:GLN:CA	2:196:B:GLN:C	18	6.62
(1,256)	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	2:339:B:PRO:N	12	6.5
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	3	6.48
(1,279)	2:355:B:SER:C	2:356:B:GLN:N	2:356:B:GLN:CA	2:356:B:GLN:C	15	6.48
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	19	6.44
(1,321)	2:384:B:LEU:C	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	11	6.38
(1,34)	2:201:B:SER:N	2:201:B:SER:CA	2:201:B:SER:C	2:202:B:THR:N	17	6.38
(1,368)	2:411:B:GLU:N	2:411:B:GLU:CA	2:411:B:GLU:C	2:412:B:GLU:N	15	6.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	13	6.33
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	2	6.33
(1,402)	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2:205:B:PRO:N	3	6.32
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	14	6.32
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	11	6.32
(1,94)	2:239:B:ALA:N	2:239:B:ALA:CA	2:239:B:ALA:C	2:240:B:ALA:N	12	6.32
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	13	6.31
(1,273)	2:346:B:VAL:C	2:347:B:VAL:N	2:347:B:VAL:CA	2:347:B:VAL:C	13	6.28
(1,32)	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	2:201:B:SER:N	9	6.24
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	12	6.21
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	20	6.18
(1,385)	2:185:B:GLY:C	2:186:B:TRP:N	2:186:B:TRP:CA	2:186:B:TRP:C	3	6.17
(1,327)	2:387:B:ASP:C	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	11	6.1
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	12	6.09
(1,90)	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	2:238:B:THR:N	6	6.08
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	20	6.04
(1,369)	2:412:B:GLU:N	2:412:B:GLU:CA	2:412:B:GLU:C	2:413:B:ILE:N	20	6.03
(1,41)	2:206:B:ALA:C	2:207:B:LEU:N	2:207:B:LEU:CA	2:207:B:LEU:C	20	6.03
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	12	6.02
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	16	6.0
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	19	5.96
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	2	5.95
(1,222)	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	2:322:B:ARG:N	5	5.92
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	16	5.91
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	6	5.91
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	10	5.9
(1,402)	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2:205:B:PRO:N	12	5.86
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	19	5.82
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	14	5.79
(1,365)	2:409:B:ILE:C	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	10	5.75
(1,35)	2:201:B:SER:C	2:202:B:THR:N	2:202:B:THR:CA	2:202:B:THR:C	4	5.75
(1,447)	2:397:B:PRO:N	2:397:B:PRO:CA	2:397:B:PRO:C	2:398:B:GLU:N	18	5.7
(1,231)	2:325:B:LEU:C	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	15	5.7
(1,63)	2:217:B:GLU:C	2:218:B:GLU:N	2:218:B:GLU:CA	2:218:B:GLU:C	15	5.68
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	9	5.65
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	13	5.63
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	16	5.63
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	16	5.62
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	4	5.61
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	5	5.6
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	13	5.6
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	5	5.59
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	17	5.59
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	16	5.58
(1,34)	2:201:B:SER:N	2:201:B:SER:CA	2:201:B:SER:C	2:202:B:THR:N	18	5.58
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	5	5.56
(1,231)	2:325:B:LEU:C	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	4	5.54
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	17	5.51
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	2	5.5
(1,229)	2:324:B:ILE:C	2:325:B:LEU:N	2:325:B:LEU:CA	2:325:B:LEU:C	19	5.49
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	9	5.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,239)	2:329:B:GLU:C	2:330:B:LEU:N	2:330:B:LEU:CA	2:330:B:LEU:C	6	5.47
(1,409)	2:232:B:ALA:C	2:233:B:GLY:N	2:233:B:GLY:CA	2:233:B:GLY:C	19	5.46
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	1	5.38
(1,223)	2:321:B:GLU:C	2:322:B:ARG:N	2:322:B:ARG:CA	2:322:B:ARG:C	9	5.38
(1,312)	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	2:376:B:PRO:N	18	5.37
(1,229)	2:324:B:ILE:C	2:325:B:LEU:N	2:325:B:LEU:CA	2:325:B:LEU:C	14	5.37
(1,398)	2:199:B:GLN:N	2:199:B:GLN:CA	2:199:B:GLN:C	2:200:B:ALA:N	9	5.35
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	3	5.34
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	2	5.33
(1,437)	2:378:B:VAL:N	2:378:B:VAL:CA	2:378:B:VAL:C	2:379:B:LEU:N	8	5.31
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	13	5.31
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	10	5.29
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	12	5.29
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	16	5.28
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	11	5.28
(1,112)	2:248:B:LEU:N	2:248:B:LEU:CA	2:248:B:LEU:C	2:249:B:LEU:N	1	5.27
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	17	5.26
(1,277)	2:351:B:GLY:C	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	18	5.25
(1,175)	2:283:B:PHE:C	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	6	5.25
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	6	5.24
(1,39)	2:205:B:PRO:C	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	4	5.2
(1,182)	2:289:B:ASN:N	2:289:B:ASN:CA	2:289:B:ASN:C	2:290:B:TYR:N	12	5.18
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	15	5.17
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	2	5.16
(1,116)	2:250:B:SER:N	2:250:B:SER:CA	2:250:B:SER:C	2:251:B:ASP:N	7	5.13
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	3	5.09
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	19	5.08
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	11	5.07
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	15	5.01
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	7	4.98
(1,91)	2:237:B:GLU:C	2:238:B:THR:N	2:238:B:THR:CA	2:238:B:THR:C	7	4.98
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	17	4.95
(1,231)	2:325:B:LEU:C	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	18	4.92
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	15	4.84
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	3	4.82
(1,26)	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	2:195:B:GLU:N	6	4.76
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	13	4.74
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	14	4.72
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	14	4.69
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	6	4.67
(1,107)	2:245:B:TYR:C	2:246:B:SER:N	2:246:B:SER:CA	2:246:B:SER:C	12	4.67
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	19	4.66
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	9	4.63
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	10	4.63
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	2	4.6
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	15	4.59
(1,445)	2:396:B:ASP:N	2:396:B:ASP:CA	2:396:B:ASP:C	2:397:B:PRO:N	18	4.57
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	15	4.57
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	20	4.55
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	11	4.53
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	4	4.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	14	4.52
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	3	4.49
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	8	4.49
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	5	4.48
(1,261)	2:340:B:GLN:C	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	1	4.47
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2	4.44
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	3	4.42
(1,450)	2:416:B:SER:C	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	15	4.41
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	8	4.41
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	13	4.41
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	17	4.4
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	10	4.36
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	4	4.35
(1,355)	2:404:B:GLU:C	2:405:B:TYR:N	2:405:B:TYR:CA	2:405:B:TYR:C	6	4.32
(1,341)	2:394:B:LEU:C	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	11	4.31
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	19	4.31
(1,165)	2:278:B:LYS:C	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	19	4.3
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	10	4.29
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	17	4.28
(1,332)	2:390:B:ARG:N	2:390:B:ARG:CA	2:390:B:ARG:C	2:391:B:GLY:N	2	4.27
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	9	4.27
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	12	4.25
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	13	4.21
(1,26)	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	2:195:B:GLU:N	19	4.21
(1,152)	2:272:B:VAL:N	2:272:B:VAL:CA	2:272:B:VAL:C	2:273:B:LYS:N	16	4.19
(1,303)	2:367:B:PRO:C	2:368:B:THR:N	2:368:B:THR:CA	2:368:B:THR:C	19	4.18
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	7	4.17
(1,27)	2:196:B:GLN:C	2:197:B:VAL:N	2:197:B:VAL:CA	2:197:B:VAL:C	6	4.16
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	3	4.14
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	3	4.13
(1,189)	2:292:B:LYS:C	2:293:B:GLU:N	2:293:B:GLU:CA	2:293:B:GLU:C	8	4.13
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	11	4.11
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	12	4.08
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	3	4.06
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	5	4.06
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	19	4.06
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	4	4.05
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	11	4.01
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	11	4.0
(1,166)	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	2:280:B:ALA:N	18	4.0
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	3	3.99
(1,85)	2:230:B:PHE:C	2:231:B:ALA:N	2:231:B:ALA:CA	2:231:B:ALA:C	16	3.96
(1,372)	2:413:B:ILE:C	2:414:B:GLU:N	2:414:B:GLU:CA	2:414:B:GLU:C	20	3.94
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	20	3.91
(1,223)	2:321:B:GLU:C	2:322:B:ARG:N	2:322:B:ARG:CA	2:322:B:ARG:C	13	3.9
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	5	3.89
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	11	3.86
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	11	3.85
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	1	3.85
(1,218)	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	2:312:B:ALA:N	1	3.85
(1,31)	2:199:B:GLN:C	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	6	3.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	2:267:B:VAL:C	2:268:B:ALA:N	2:268:B:ALA:CA	2:268:B:ALA:C	20	3.8
(1,450)	2:416:B:SER:C	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	18	3.76
(1,269)	2:344:B:VAL:C	2:345:B:GLY:N	2:345:B:GLY:CA	2:345:B:GLY:C	10	3.74
(1,38)	2:205:B:PRO:N	2:205:B:PRO:CA	2:205:B:PRO:C	2:206:B:ALA:N	17	3.74
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	4	3.71
(1,258)	2:339:B:PRO:N	2:339:B:PRO:CA	2:339:B:PRO:C	2:340:B:GLN:N	8	3.68
(1,34)	2:201:B:SER:N	2:201:B:SER:CA	2:201:B:SER:C	2:202:B:THR:N	7	3.68
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	13	3.66
(1,40)	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	2:207:B:LEU:N	13	3.66
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	7	3.62
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	5	3.61
(1,392)	2:190:B:THR:N	2:190:B:THR:CA	2:190:B:THR:C	2:191:B:LEU:N	18	3.6
(1,186)	2:291:B:LEU:N	2:291:B:LEU:CA	2:291:B:LEU:C	2:292:B:LYS:N	7	3.57
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	20	3.56
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	10	3.54
(1,277)	2:351:B:GLY:C	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2	3.54
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	17	3.53
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	19	3.53
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	4	3.53
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	10	3.51
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	12	3.51
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	14	3.51
(1,327)	2:387:B:ASP:C	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	12	3.5
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	3	3.5
(1,314)	2:376:B:PRO:N	2:376:B:PRO:CA	2:376:B:PRO:C	2:377:B:SER:N	1	3.5
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	17	3.48
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	4	3.46
(1,183)	2:289:B:ASN:C	2:290:B:TYR:N	2:290:B:TYR:CA	2:290:B:TYR:C	14	3.46
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	15	3.44
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	2	3.44
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	1	3.43
(1,36)	2:202:B:THR:N	2:202:B:THR:CA	2:202:B:THR:C	2:203:B:LEU:N	5	3.42
(1,186)	2:291:B:LEU:N	2:291:B:LEU:CA	2:291:B:LEU:C	2:292:B:LYS:N	12	3.4
(1,321)	2:384:B:LEU:C	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	8	3.38
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	6	3.36
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	17	3.34
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	5	3.34
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	14	3.33
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	14	3.33
(1,34)	2:201:B:SER:N	2:201:B:SER:CA	2:201:B:SER:C	2:202:B:THR:N	15	3.33
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	10	3.32
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	7	3.32
(1,40)	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	2:207:B:LEU:N	3	3.32
(1,92)	2:238:B:THR:N	2:238:B:THR:CA	2:238:B:THR:C	2:239:B:ALA:N	7	3.31
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	7	3.3
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	8	3.3
(1,239)	2:329:B:GLU:C	2:330:B:LEU:N	2:330:B:LEU:CA	2:330:B:LEU:C	4	3.29
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	18	3.26
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	2	3.26
(1,186)	2:291:B:LEU:N	2:291:B:LEU:CA	2:291:B:LEU:C	2:292:B:LYS:N	18	3.25
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	15	3.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	16	3.24
(1,269)	2:344:B:VAL:C	2:345:B:GLY:N	2:345:B:GLY:CA	2:345:B:GLY:C	3	3.23
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	17	3.22
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	1	3.21
(1,308)	2:370:B:MET:N	2:370:B:MET:CA	2:370:B:MET:C	2:371:B:GLY:N	15	3.2
(1,2)	2:171:B:ILE:N	2:171:B:ILE:CA	2:171:B:ILE:C	2:172:B:ARG:N	11	3.2
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	4	3.14
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	20	3.14
(1,232)	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	2:327:B:ALA:N	12	3.13
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	14	3.13
(1,350)	2:402:B:LEU:N	2:402:B:LEU:CA	2:402:B:LEU:C	2:403:B:GLN:N	3	3.11
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	6	3.11
(1,39)	2:205:B:PRO:C	2:206:B:ALA:N	2:206:B:ALA:CA	2:206:B:ALA:C	17	3.11
(1,419)	2:288:B:ASP:N	2:288:B:ASP:CA	2:288:B:ASP:C	2:289:B:ASN:N	3	3.1
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	3	3.1
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	2	3.1
(1,1)	2:170:B:ARG:C	2:171:B:ILE:N	2:171:B:ILE:CA	2:171:B:ILE:C	13	3.1
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	20	3.09
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	9	3.08
(1,219)	2:318:B:ALA:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	18	3.07
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	4	3.07
(1,17)	2:186:B:TRP:C	2:187:B:GLN:N	2:187:B:GLN:CA	2:187:B:GLN:C	17	3.05
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	20	3.04
(1,366)	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	2:411:B:GLU:N	14	3.02
(1,312)	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	2:376:B:PRO:N	6	3.0
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	11	3.0
(1,41)	2:206:B:ALA:C	2:207:B:LEU:N	2:207:B:LEU:CA	2:207:B:LEU:C	9	3.0
(1,228)	2:324:B:ILE:N	2:324:B:ILE:CA	2:324:B:ILE:C	2:325:B:LEU:N	15	2.98
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	2	2.97
(1,29)	2:197:B:VAL:C	2:198:B:TYR:N	2:198:B:TYR:CA	2:198:B:TYR:C	11	2.97
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	4	2.96
(1,253)	2:336:B:ALA:C	2:337:B:GLU:N	2:337:B:GLU:CA	2:337:B:GLU:C	12	2.96
(1,25)	2:193:B:LEU:C	2:194:B:MET:N	2:194:B:MET:CA	2:194:B:MET:C	8	2.96
(1,14)	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	2:184:B:GLU:N	8	2.94
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	1	2.93
(1,350)	2:402:B:LEU:N	2:402:B:LEU:CA	2:402:B:LEU:C	2:403:B:GLN:N	8	2.9
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	18	2.89
(1,327)	2:387:B:ASP:C	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	10	2.88
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	9	2.88
(1,433)	2:373:B:ASP:N	2:373:B:ASP:CA	2:373:B:ASP:C	2:374:B:ILE:N	3	2.85
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	16	2.85
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	5	2.83
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	17	2.81
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	20	2.78
(1,365)	2:409:B:ILE:C	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	19	2.77
(1,31)	2:199:B:GLN:C	2:200:B:ALA:N	2:200:B:ALA:CA	2:200:B:ALA:C	19	2.77
(1,331)	2:389:B:TYR:C	2:390:B:ARG:N	2:390:B:ARG:CA	2:390:B:ARG:C	18	2.73
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	6	2.73
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	9	2.72
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	15	2.7
(1,17)	2:186:B:TRP:C	2:187:B:GLN:N	2:187:B:GLN:CA	2:187:B:GLN:C	18	2.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	9	2.67
(1,9)	2:180:B:VAL:C	2:181:B:ALA:N	2:181:B:ALA:CA	2:181:B:ALA:C	15	2.62
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	6	2.61
(1,186)	2:291:B:LEU:N	2:291:B:LEU:CA	2:291:B:LEU:C	2:292:B:LYS:N	15	2.61
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	15	2.6
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	15	2.6
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	18	2.58
(1,241)	2:330:B:LEU:C	2:331:B:SER:N	2:331:B:SER:CA	2:331:B:SER:C	18	2.57
(1,326)	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	2:388:B:GLY:N	13	2.56
(1,321)	2:384:B:LEU:C	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	15	2.55
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	11	2.55
(1,256)	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	2:339:B:PRO:N	11	2.51
(1,165)	2:278:B:LYS:C	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	8	2.51
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	20	2.5
(1,260)	2:340:B:GLN:N	2:340:B:GLN:CA	2:340:B:GLN:C	2:341:B:ASP:N	6	2.5
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	5	2.49
(1,256)	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	2:339:B:PRO:N	17	2.48
(1,79)	2:227:B:SER:C	2:228:B:LYS:N	2:228:B:LYS:CA	2:228:B:LYS:C	10	2.48
(1,324)	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	2:387:B:ASP:N	18	2.46
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	19	2.43
(1,219)	2:318:B:ALA:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	17	2.43
(1,165)	2:278:B:LYS:C	2:279:B:PHE:N	2:279:B:PHE:CA	2:279:B:PHE:C	7	2.43
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	15	2.42
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	14	2.38
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	8	2.37
(1,427)	2:310:B:ASP:N	2:310:B:ASP:CA	2:310:B:ASP:C	2:311:B:ASP:N	14	2.36
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	1	2.36
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	11	2.35
(1,424)	2:308:B:HIS:C	2:309:B:LEU:N	2:309:B:LEU:CA	2:309:B:LEU:C	10	2.33
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	11	2.32
(1,266)	2:343:B:LEU:N	2:343:B:LEU:CA	2:343:B:LEU:C	2:344:B:VAL:N	14	2.31
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	18	2.31
(1,231)	2:325:B:LEU:C	2:326:B:VAL:N	2:326:B:VAL:CA	2:326:B:VAL:C	5	2.3
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	16	2.28
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	9	2.28
(1,395)	2:195:B:GLU:C	2:196:B:GLN:N	2:196:B:GLN:CA	2:196:B:GLN:C	13	2.27
(1,229)	2:324:B:ILE:C	2:325:B:LEU:N	2:325:B:LEU:CA	2:325:B:LEU:C	9	2.27
(1,52)	2:212:B:LEU:N	2:212:B:LEU:CA	2:212:B:LEU:C	2:213:B:THR:N	8	2.26
(1,223)	2:321:B:GLU:C	2:322:B:ARG:N	2:322:B:ARG:CA	2:322:B:ARG:C	14	2.25
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	5	2.24
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	15	2.24
(1,229)	2:324:B:ILE:C	2:325:B:LEU:N	2:325:B:LEU:CA	2:325:B:LEU:C	6	2.23
(1,419)	2:288:B:ASP:N	2:288:B:ASP:CA	2:288:B:ASP:C	2:289:B:ASN:N	2	2.22
(1,255)	2:337:B:GLU:C	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	19	2.21
(1,372)	2:413:B:ILE:C	2:414:B:GLU:N	2:414:B:GLU:CA	2:414:B:GLU:C	19	2.2
(1,238)	2:329:B:GLU:N	2:329:B:GLU:CA	2:329:B:GLU:C	2:330:B:LEU:N	3	2.2
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	16	2.2
(1,107)	2:245:B:TYR:C	2:246:B:SER:N	2:246:B:SER:CA	2:246:B:SER:C	7	2.19
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	10	2.18
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	12	2.17
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	9	2.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	18	2.17
(1,365)	2:409:B:ILE:C	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	17	2.14
(1,24)	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	2:194:B:MET:N	10	2.13
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	14	2.11
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	10	2.09
(1,438)	2:378:B:VAL:C	2:379:B:LEU:N	2:379:B:LEU:CA	2:379:B:LEU:C	15	2.05
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	17	2.03
(1,401)	2:203:B:LEU:C	2:204:B:ASP:N	2:204:B:ASP:CA	2:204:B:ASP:C	8	2.02
(1,367)	2:410:B:SER:C	2:411:B:GLU:N	2:411:B:GLU:CA	2:411:B:GLU:C	15	2.02
(1,260)	2:340:B:GLN:N	2:340:B:GLN:CA	2:340:B:GLN:C	2:341:B:ASP:N	16	2.01
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	11	2.01
(1,225)	2:322:B:ARG:C	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	4	2.0
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	1	2.0
(1,371)	2:413:B:ILE:N	2:413:B:ILE:CA	2:413:B:ILE:C	2:414:B:GLU:N	13	1.99
(1,350)	2:402:B:LEU:N	2:402:B:LEU:CA	2:402:B:LEU:C	2:403:B:GLN:N	5	1.97
(1,278)	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2:353:B:ALA:N	9	1.97
(1,74)	2:223:B:PHE:N	2:223:B:PHE:CA	2:223:B:PHE:C	2:224:B:ARG:N	14	1.97
(1,44)	2:208:B:GLU:N	2:208:B:GLU:CA	2:208:B:GLU:C	2:209:B:ARG:N	3	1.97
(1,311)	2:374:B:ILE:C	2:375:B:GLN:N	2:375:B:GLN:CA	2:375:B:GLN:C	17	1.96
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	14	1.95
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	14	1.94
(1,98)	2:241:B:ILE:N	2:241:B:ILE:CA	2:241:B:ILE:C	2:242:B:PHE:N	8	1.94
(1,431)	2:320:B:PRO:N	2:320:B:PRO:CA	2:320:B:PRO:C	2:321:B:GLU:N	6	1.91
(1,393)	2:194:B:MET:C	2:195:B:GLU:N	2:195:B:GLU:CA	2:195:B:GLU:C	10	1.89
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2	1.88
(1,176)	2:284:B:ALA:N	2:284:B:ALA:CA	2:284:B:ALA:C	2:285:B:ALA:N	5	1.88
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	16	1.87
(1,256)	2:338:B:LEU:N	2:338:B:LEU:CA	2:338:B:LEU:C	2:339:B:PRO:N	2	1.85
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	19	1.84
(1,226)	2:323:B:PHE:N	2:323:B:PHE:CA	2:323:B:PHE:C	2:324:B:ILE:N	14	1.81
(1,323)	2:385:B:ILE:C	2:386:B:VAL:N	2:386:B:VAL:CA	2:386:B:VAL:C	13	1.8
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	4	1.8
(1,180)	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	2:288:B:ASP:N	1	1.8
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	18	1.79
(1,327)	2:387:B:ASP:C	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	19	1.77
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	14	1.77
(1,438)	2:378:B:VAL:C	2:379:B:LEU:N	2:379:B:LEU:CA	2:379:B:LEU:C	14	1.76
(1,195)	2:295:B:ALA:C	2:296:B:GLY:N	2:296:B:GLY:CA	2:296:B:GLY:C	13	1.75
(1,3)	2:171:B:ILE:C	2:172:B:ARG:N	2:172:B:ARG:CA	2:172:B:ARG:C	8	1.75
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	5	1.74
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	2	1.73
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	4	1.72
(1,440)	2:380:B:HIS:C	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	16	1.7
(1,297)	2:364:B:LEU:C	2:365:B:GLY:N	2:365:B:GLY:CA	2:365:B:GLY:C	6	1.7
(1,20)	2:191:B:LEU:N	2:191:B:LEU:CA	2:191:B:LEU:C	2:192:B:PRO:N	11	1.69
(1,325)	2:386:B:VAL:C	2:387:B:ASP:N	2:387:B:ASP:CA	2:387:B:ASP:C	14	1.68
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	8	1.68
(1,173)	2:282:B:GLN:C	2:283:B:PHE:N	2:283:B:PHE:CA	2:283:B:PHE:C	19	1.68
(1,241)	2:330:B:LEU:C	2:331:B:SER:N	2:331:B:SER:CA	2:331:B:SER:C	10	1.67
(1,333)	2:390:B:ARG:C	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	6	1.66
(1,145)	2:268:B:ALA:C	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	2:245:B:TYR:C	2:246:B:SER:N	2:246:B:SER:CA	2:246:B:SER:C	18	1.66
(1,16)	2:184:B:GLU:N	2:184:B:GLU:CA	2:184:B:GLU:C	2:185:B:GLY:N	6	1.65
(1,273)	2:346:B:VAL:C	2:347:B:VAL:N	2:347:B:VAL:CA	2:347:B:VAL:C	14	1.63
(1,22)	2:192:B:PRO:N	2:192:B:PRO:CA	2:192:B:PRO:C	2:193:B:LEU:N	4	1.63
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	15	1.62
(1,395)	2:195:B:GLU:C	2:196:B:GLN:N	2:196:B:GLN:CA	2:196:B:GLN:C	20	1.61
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	10	1.6
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	14	1.59
(1,228)	2:324:B:ILE:N	2:324:B:ILE:CA	2:324:B:ILE:C	2:325:B:LEU:N	17	1.57
(1,88)	2:236:B:LYS:N	2:236:B:LYS:CA	2:236:B:LYS:C	2:237:B:GLU:N	19	1.57
(1,157)	2:274:B:THR:C	2:275:B:VAL:N	2:275:B:VAL:CA	2:275:B:VAL:C	16	1.56
(1,274)	2:347:B:VAL:N	2:347:B:VAL:CA	2:347:B:VAL:C	2:348:B:VAL:N	2	1.55
(1,153)	2:272:B:VAL:C	2:273:B:LYS:N	2:273:B:LYS:CA	2:273:B:LYS:C	18	1.54
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	8	1.52
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	13	1.52
(1,286)	2:359:B:ILE:N	2:359:B:ILE:CA	2:359:B:ILE:C	2:360:B:MET:N	13	1.51
(1,451)	2:417:B:ARG:N	2:417:B:ARG:CA	2:417:B:ARG:C	2:418:B:LEU:N	7	1.5
(1,65)	2:218:B:GLU:C	2:219:B:ALA:N	2:219:B:ALA:CA	2:219:B:ALA:C	19	1.5
(1,365)	2:409:B:ILE:C	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	18	1.49
(1,219)	2:318:B:ALA:C	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	1	1.49
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	9	1.49
(1,280)	2:356:B:GLN:N	2:356:B:GLN:CA	2:356:B:GLN:C	2:357:B:ALA:N	2	1.48
(1,220)	2:319:B:TRP:N	2:319:B:TRP:CA	2:319:B:TRP:C	2:320:B:PRO:N	1	1.48
(1,223)	2:321:B:GLU:C	2:322:B:ARG:N	2:322:B:ARG:CA	2:322:B:ARG:C	10	1.46
(1,14)	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	2:184:B:GLU:N	17	1.46
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	1	1.45
(1,262)	2:341:B:ASP:N	2:341:B:ASP:CA	2:341:B:ASP:C	2:342:B:ARG:N	11	1.44
(1,404)	2:226:B:TYR:N	2:226:B:TYR:CA	2:226:B:TYR:C	2:227:B:SER:N	7	1.43
(1,316)	2:377:B:SER:N	2:377:B:SER:CA	2:377:B:SER:C	2:378:B:VAL:N	20	1.43
(1,278)	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2:353:B:ALA:N	2	1.42
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	15	1.42
(1,322)	2:385:B:ILE:N	2:385:B:ILE:CA	2:385:B:ILE:C	2:386:B:VAL:N	4	1.39
(1,92)	2:238:B:THR:N	2:238:B:THR:CA	2:238:B:THR:C	2:239:B:ALA:N	3	1.39
(1,388)	2:188:B:ASP:N	2:188:B:ASP:CA	2:188:B:ASP:C	2:189:B:ALA:N	6	1.38
(1,342)	2:395:B:VAL:N	2:395:B:VAL:CA	2:395:B:VAL:C	2:396:B:ASP:N	16	1.37
(1,433)	2:373:B:ASP:N	2:373:B:ASP:CA	2:373:B:ASP:C	2:374:B:ILE:N	8	1.34
(1,310)	2:372:B:ALA:N	2:372:B:ALA:CA	2:372:B:ALA:C	2:373:B:ASP:N	8	1.34
(1,146)	2:269:B:GLU:N	2:269:B:GLU:CA	2:269:B:GLU:C	2:270:B:TRP:N	17	1.34
(1,92)	2:238:B:THR:N	2:238:B:THR:CA	2:238:B:THR:C	2:239:B:ALA:N	8	1.33
(1,191)	2:293:B:GLU:C	2:294:B:ARG:N	2:294:B:ARG:CA	2:294:B:ARG:C	9	1.32
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	3	1.31
(1,193)	2:294:B:ARG:C	2:295:B:ALA:N	2:295:B:ALA:CA	2:295:B:ALA:C	1	1.31
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	1	1.3
(1,221)	2:320:B:PRO:C	2:321:B:GLU:N	2:321:B:GLU:CA	2:321:B:GLU:C	1	1.3
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	8	1.29
(1,117)	2:250:B:SER:C	2:251:B:ASP:N	2:251:B:ASP:CA	2:251:B:ASP:C	2	1.28
(1,88)	2:236:B:LYS:N	2:236:B:LYS:CA	2:236:B:LYS:C	2:237:B:GLU:N	16	1.28
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	15	1.27
(1,372)	2:413:B:ILE:C	2:414:B:GLU:N	2:414:B:GLU:CA	2:414:B:GLU:C	7	1.27
(1,366)	2:410:B:SER:N	2:410:B:SER:CA	2:410:B:SER:C	2:411:B:GLU:N	1	1.27
(1,84)	2:230:B:PHE:N	2:230:B:PHE:CA	2:230:B:PHE:C	2:231:B:ALA:N	12	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	2:192:B:PRO:C	2:193:B:LEU:N	2:193:B:LEU:CA	2:193:B:LEU:C	8	1.25
(1,38)	2:205:B:PRO:N	2:205:B:PRO:CA	2:205:B:PRO:C	2:206:B:ALA:N	11	1.24
(1,328)	2:388:B:GLY:N	2:388:B:GLY:CA	2:388:B:GLY:C	2:389:B:TYR:N	12	1.23
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	3	1.22
(1,378)	2:173:B:ALA:N	2:173:B:ALA:CA	2:173:B:ALA:C	2:174:B:LEU:N	6	1.22
(1,334)	2:391:B:GLY:N	2:391:B:GLY:CA	2:391:B:GLY:C	2:392:B:GLU:N	9	1.21
(1,380)	2:175:B:PRO:N	2:175:B:PRO:CA	2:175:B:PRO:C	2:176:B:ALA:N	17	1.19
(1,316)	2:377:B:SER:N	2:377:B:SER:CA	2:377:B:SER:C	2:378:B:VAL:N	17	1.19
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	12	1.18
(1,308)	2:370:B:MET:N	2:370:B:MET:CA	2:370:B:MET:C	2:371:B:GLY:N	1	1.17
(1,89)	2:236:B:LYS:C	2:237:B:GLU:N	2:237:B:GLU:CA	2:237:B:GLU:C	11	1.17
(1,415)	2:264:B:LYS:C	2:265:B:GLY:N	2:265:B:GLY:CA	2:265:B:GLY:C	6	1.16
(1,441)	2:381:B:ARG:N	2:381:B:ARG:CA	2:381:B:ARG:C	2:382:B:ARG:N	10	1.15
(1,347)	2:400:B:VAL:C	2:401:B:LEU:N	2:401:B:LEU:CA	2:401:B:LEU:C	11	1.15
(1,437)	2:378:B:VAL:N	2:378:B:VAL:CA	2:378:B:VAL:C	2:379:B:LEU:N	1	1.14
(1,437)	2:378:B:VAL:N	2:378:B:VAL:CA	2:378:B:VAL:C	2:379:B:LEU:N	15	1.14
(1,217)	2:310:B:ASP:C	2:311:B:ASP:N	2:311:B:ASP:CA	2:311:B:ASP:C	3	1.13
(1,1)	2:170:B:ARG:C	2:171:B:ILE:N	2:171:B:ILE:CA	2:171:B:ILE:C	11	1.13
(1,181)	2:288:B:ASP:C	2:289:B:ASN:N	2:289:B:ASN:CA	2:289:B:ASN:C	5	1.11
(1,16)	2:184:B:GLU:N	2:184:B:GLU:CA	2:184:B:GLU:C	2:185:B:GLY:N	17	1.11
(1,329)	2:388:B:GLY:C	2:389:B:TYR:N	2:389:B:TYR:CA	2:389:B:TYR:C	16	1.09
(1,296)	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	2:365:B:GLY:N	16	1.09
(1,393)	2:194:B:MET:C	2:195:B:GLU:N	2:195:B:GLU:CA	2:195:B:GLU:C	11	1.08
(1,295)	2:363:B:ALA:C	2:364:B:LEU:N	2:364:B:LEU:CA	2:364:B:LEU:C	14	1.08
(1,268)	2:344:B:VAL:N	2:344:B:VAL:CA	2:344:B:VAL:C	2:345:B:GLY:N	10	1.07
(1,228)	2:324:B:ILE:N	2:324:B:ILE:CA	2:324:B:ILE:C	2:325:B:LEU:N	20	1.07
(1,438)	2:378:B:VAL:C	2:379:B:LEU:N	2:379:B:LEU:CA	2:379:B:LEU:C	8	1.04
(1,13)	2:182:B:ILE:C	2:183:B:ALA:N	2:183:B:ALA:CA	2:183:B:ALA:C	19	1.04
(1,319)	2:383:B:THR:C	2:384:B:LEU:N	2:384:B:LEU:CA	2:384:B:LEU:C	6	1.02
(1,278)	2:352:B:ALA:N	2:352:B:ALA:CA	2:352:B:ALA:C	2:353:B:ALA:N	7	1.02
(1,303)	2:367:B:PRO:C	2:368:B:THR:N	2:368:B:THR:CA	2:368:B:THR:C	6	1.01
(1,179)	2:286:B:LEU:C	2:287:B:SER:N	2:287:B:SER:CA	2:287:B:SER:C	6	1.01