Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 10:26 PM EDT

PDB ID	:	2M6I
BMRB ID	:	19126
Title	:	Putative pentameric open-channel structure of full-length transmembrane domains of human glycine receptor alpha1 subunit
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Deposited on	:	2013-03-29

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 (i) 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 (1)) were used in the production of this report:

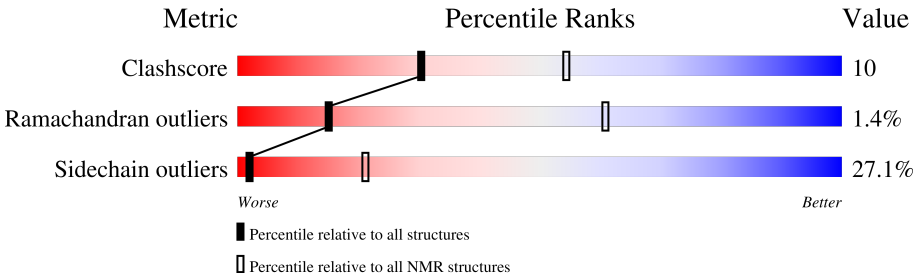
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 11%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	150	53% 38% · 8%
1	B	150	52% 39% · 8%
1	C	150	57% 35% · 7%
1	D	150	53% 39% · 7%
1	E	150	51% 41% · 7%

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:216-A:318, A:389-A:423, B:216-B:318, B:389-B:423, C:215-C:318, C:389-C:423, D:215-D:318, D:389-D:423, E:215-E:318, E:389-E:423 (693)	1.00	1

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12445 atoms, of which 6300 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	B	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	C	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	D	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	E	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	

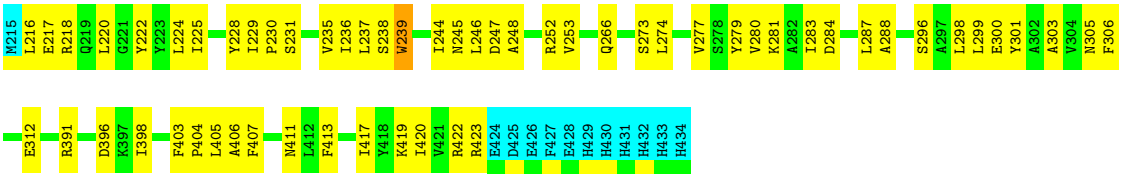
4 Residue-property plots

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.

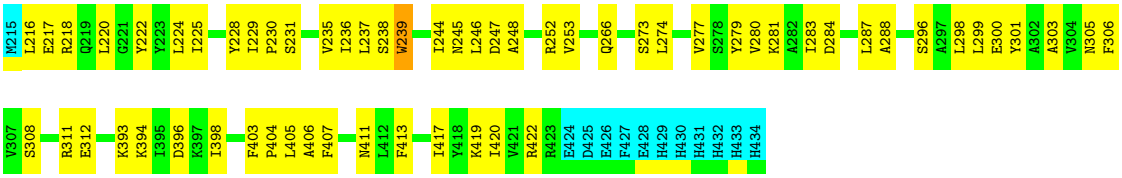
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



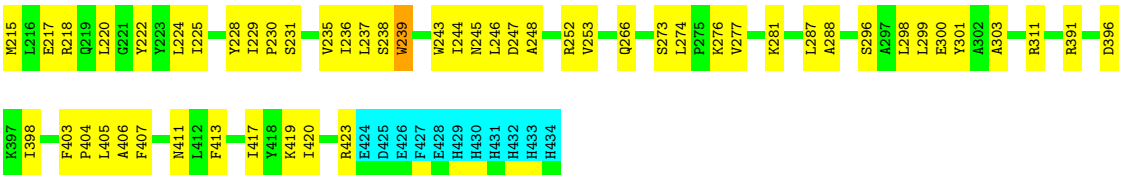
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



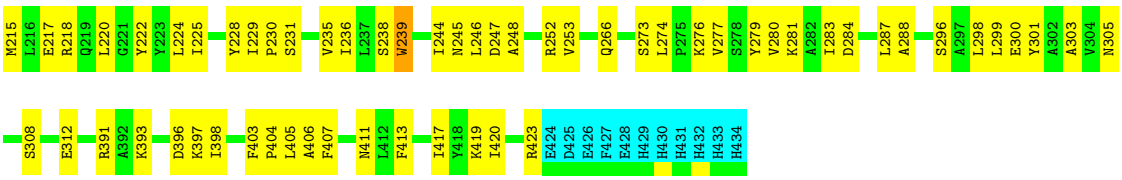
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

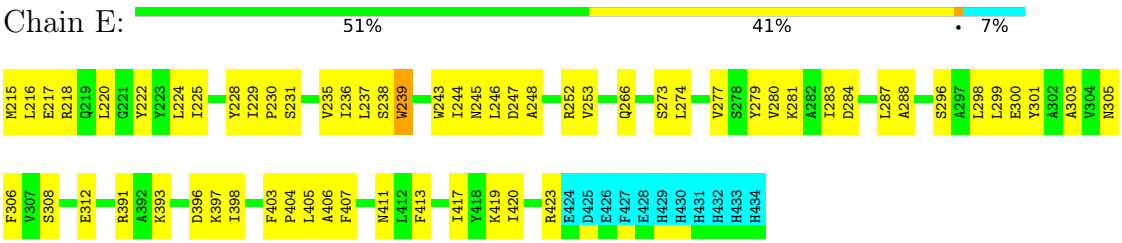


• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

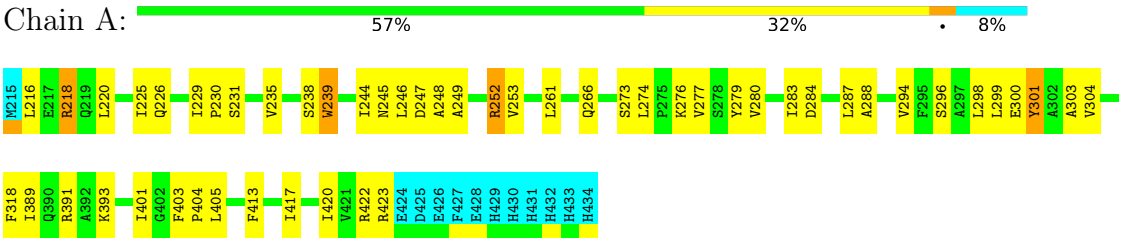


4.2 Scores per residue for each member of the ensemble

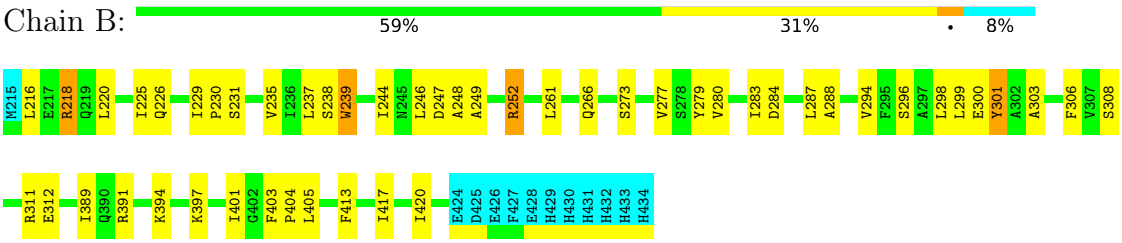
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

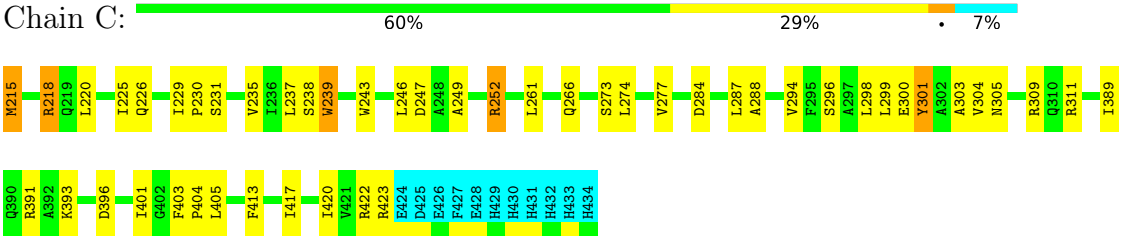


• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit



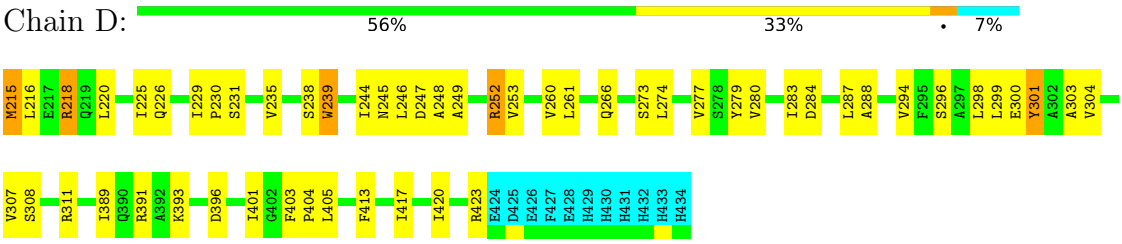
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



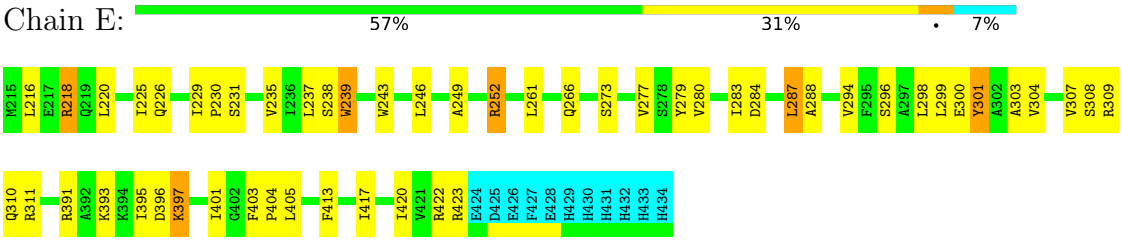
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

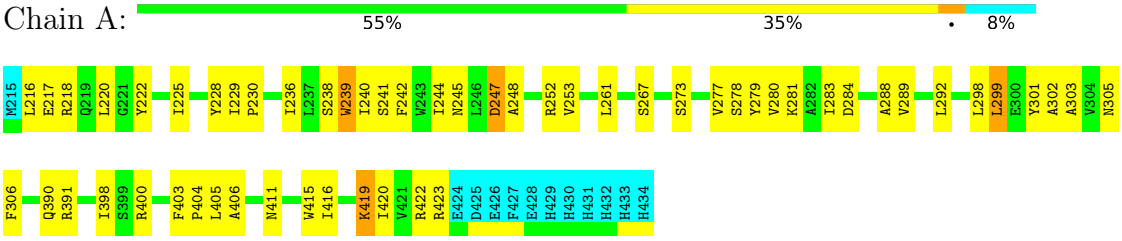
Chain E:



4.2.2 Score per residue for model 2

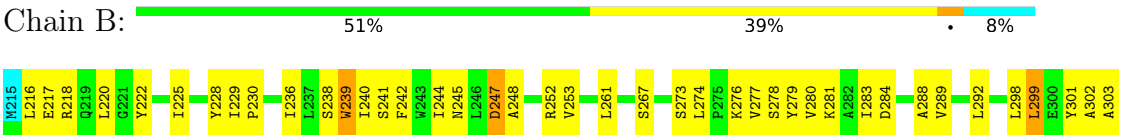
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

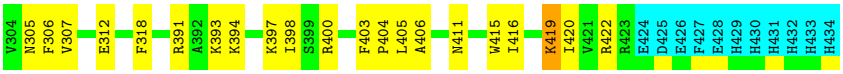
Chain A:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

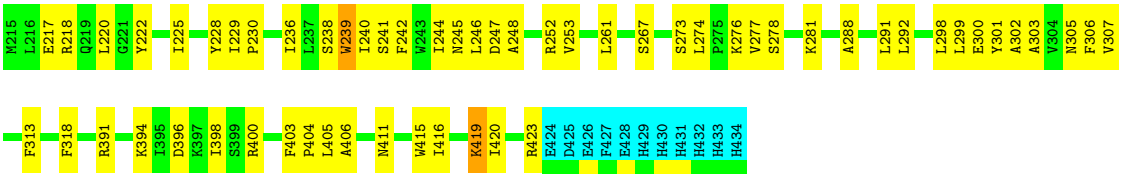
Chain B:





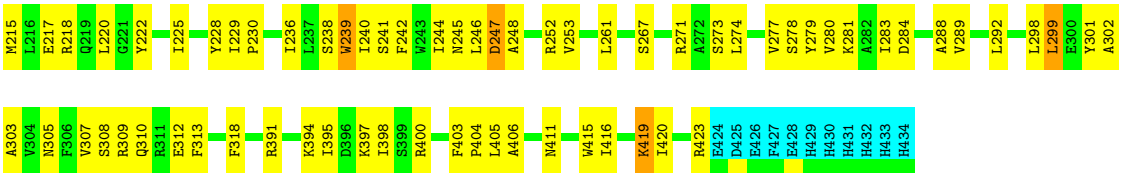
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



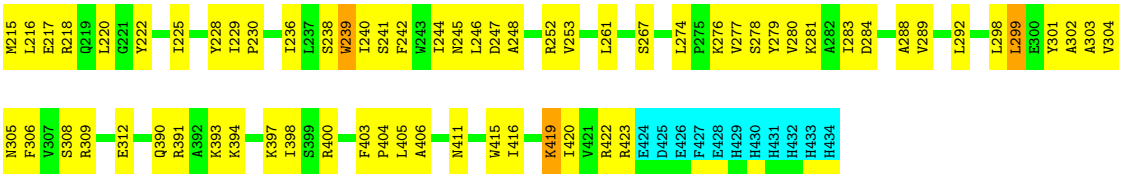
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

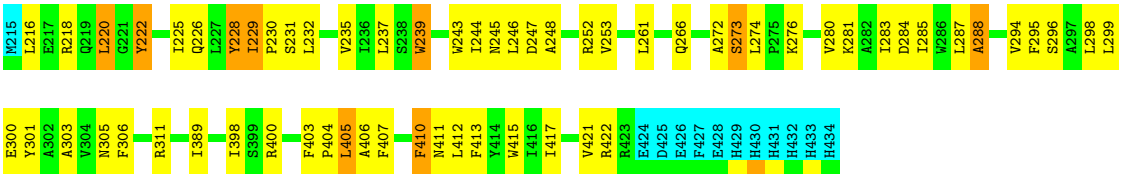
Chain E:



4.2.3 Score per residue for model 3

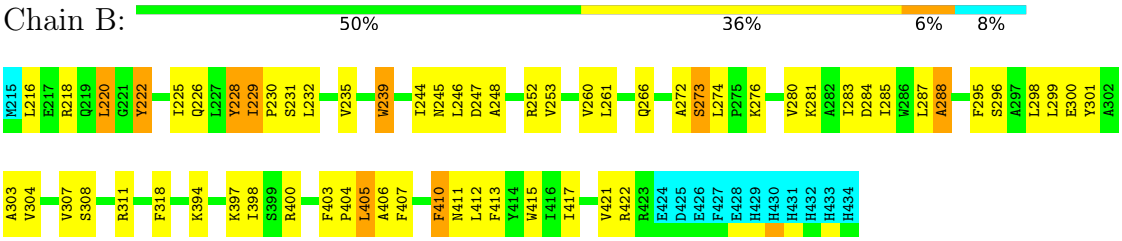
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



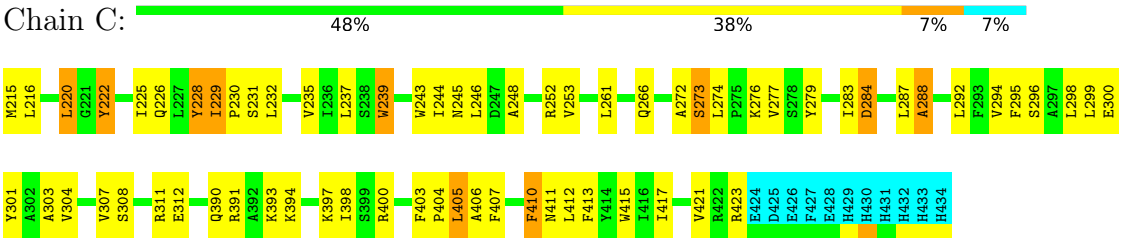
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



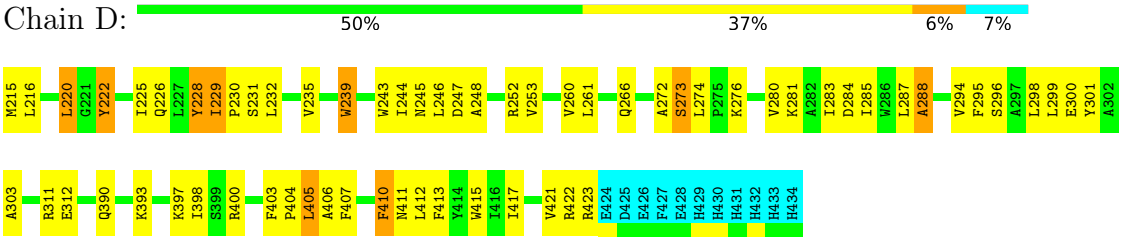
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



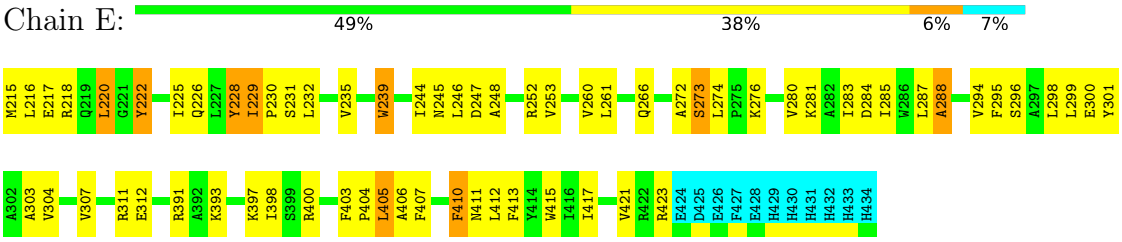
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

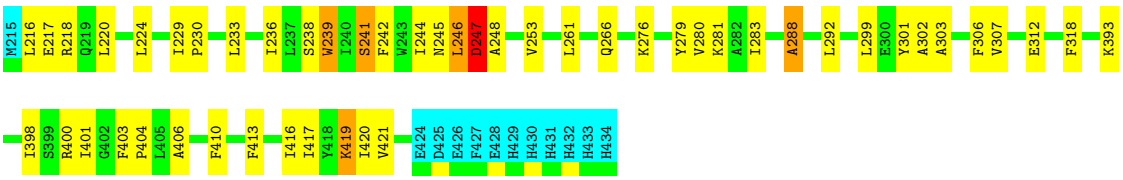
Chain E:



4.2.4 Score per residue for model 4

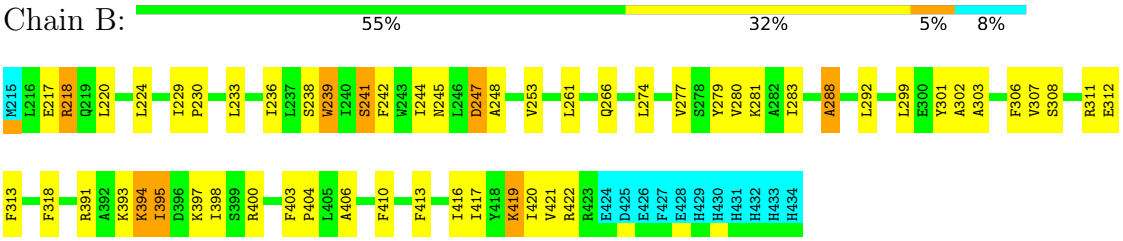
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



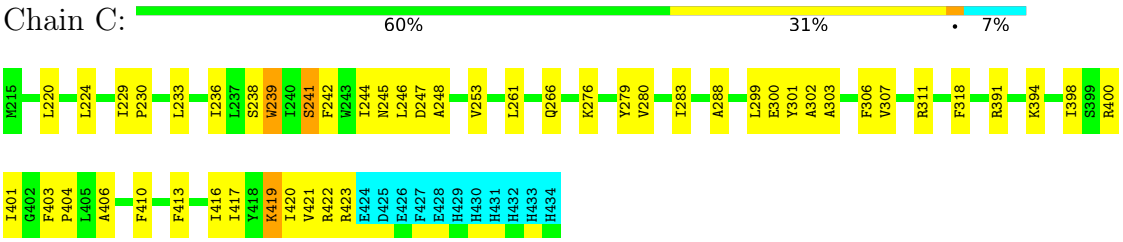
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



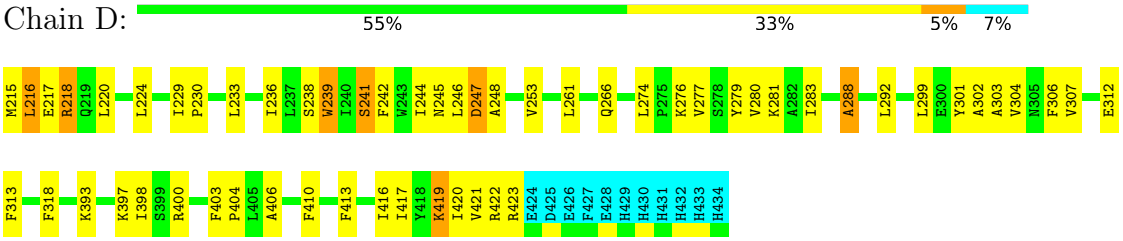
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



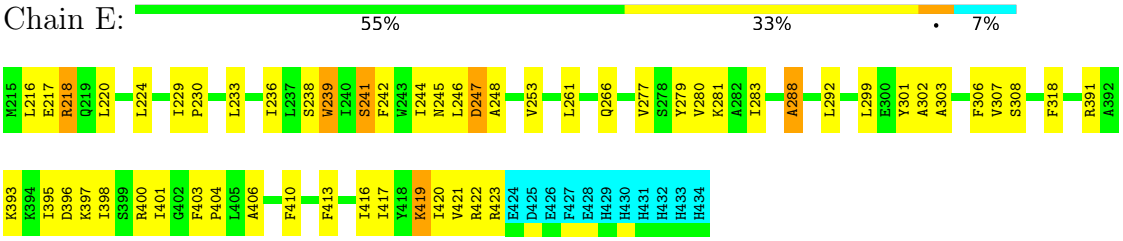
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

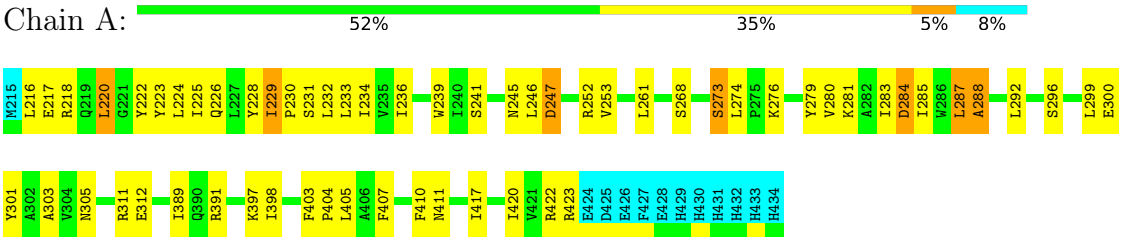
Chain E:



4.2.5 Score per residue for model 5

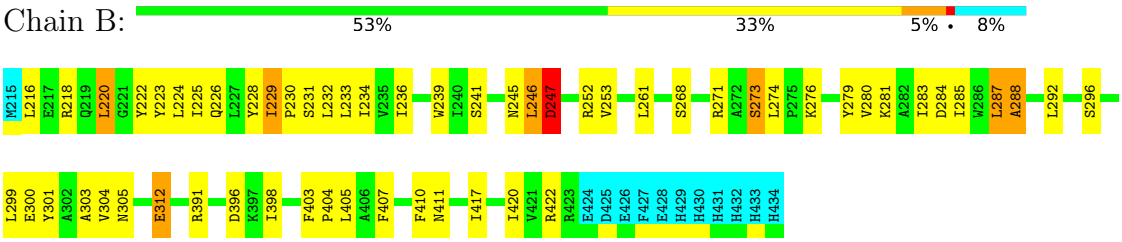
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



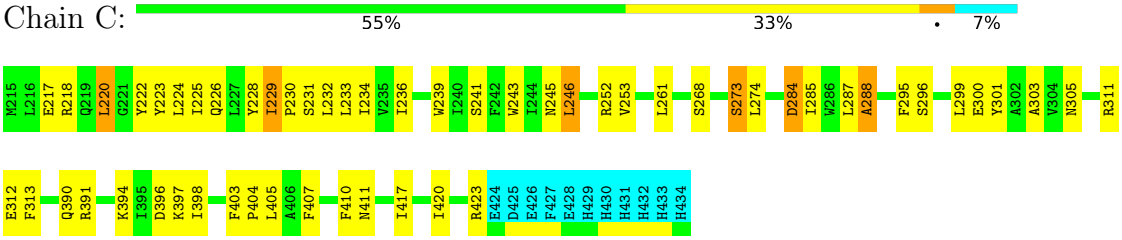
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



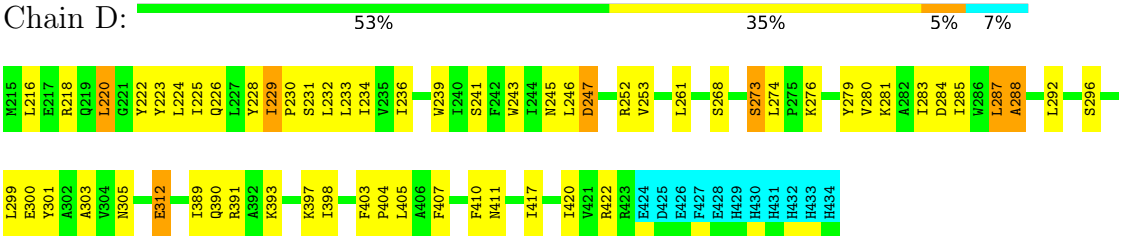
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



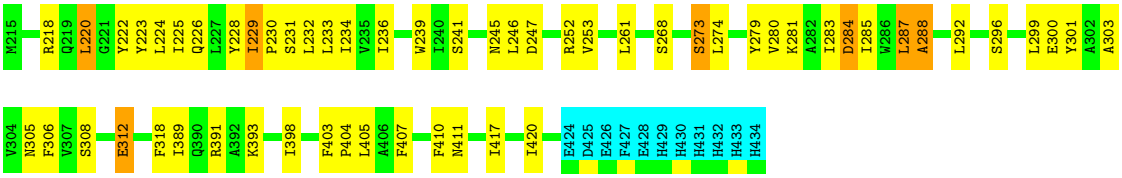
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

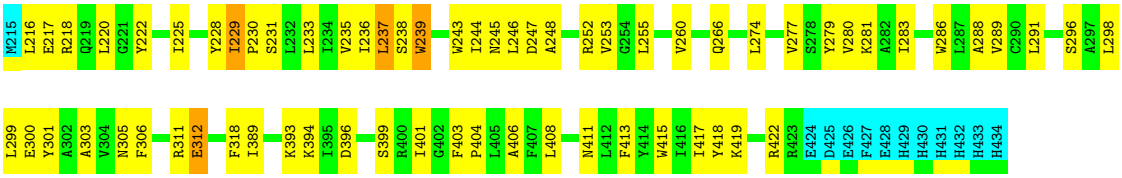
Chain E:



4.2.6 Score per residue for model 6

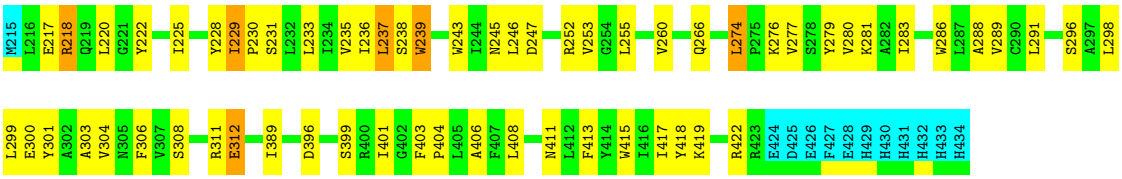
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



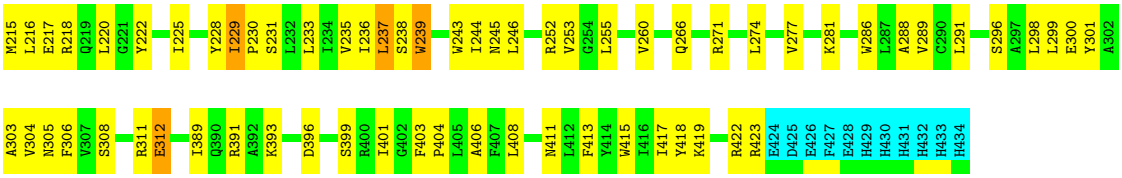
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



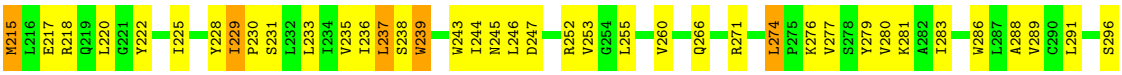
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



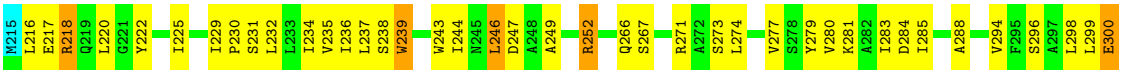
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2.7 Score per residue for model 7

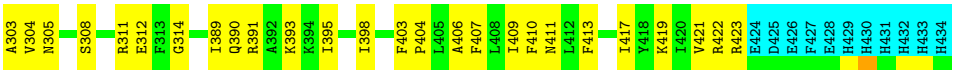
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



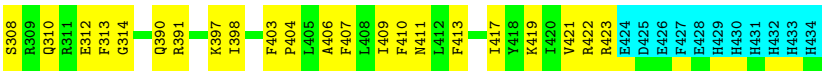
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



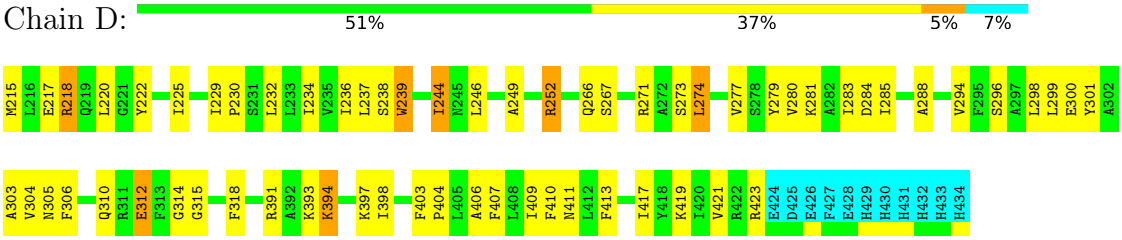
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



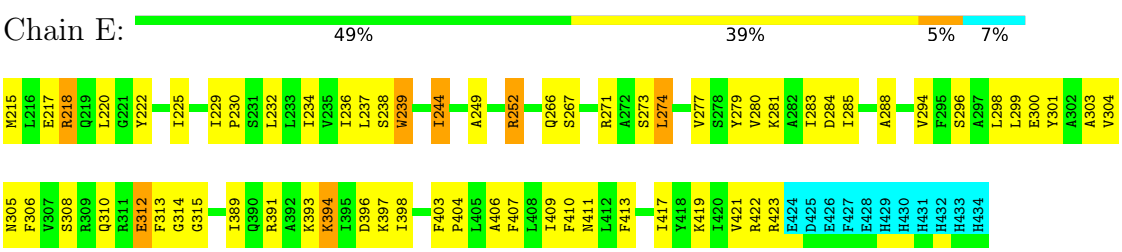
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

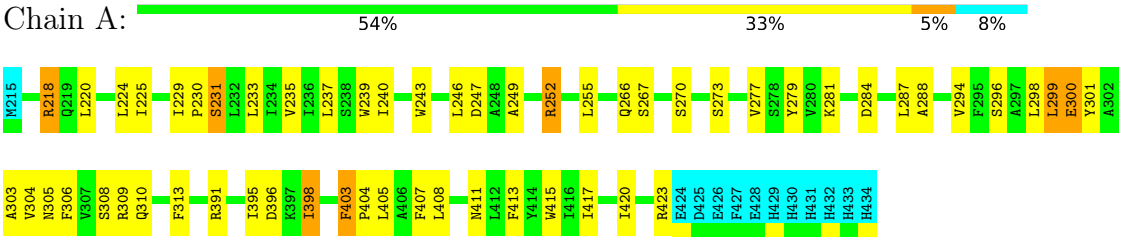
Chain E:



4.2.8 Score per residue for model 8

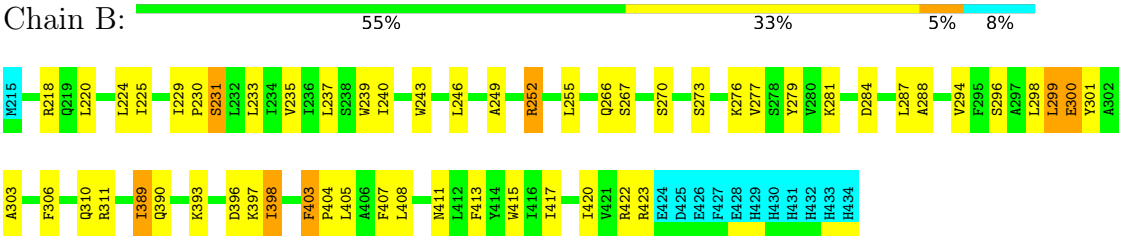
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



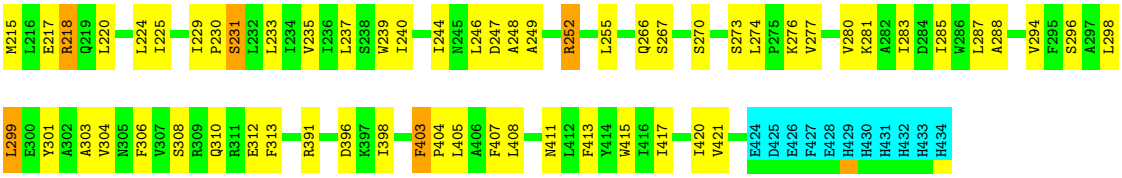
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



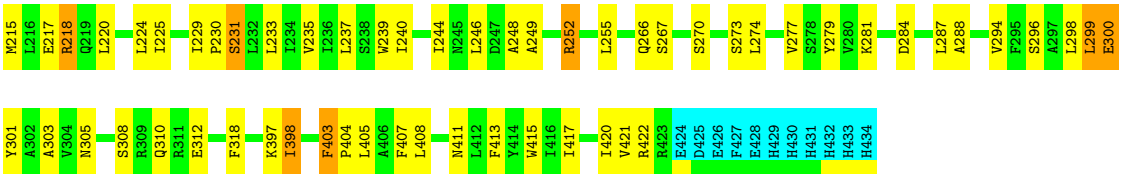
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



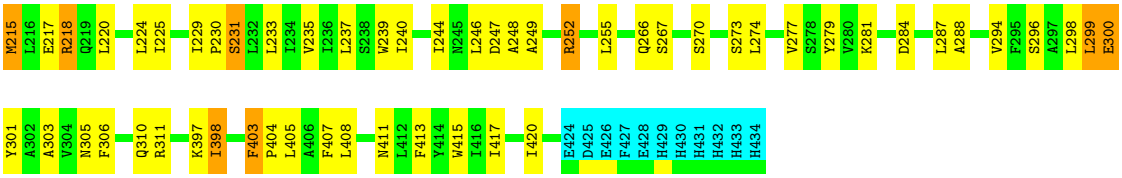
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

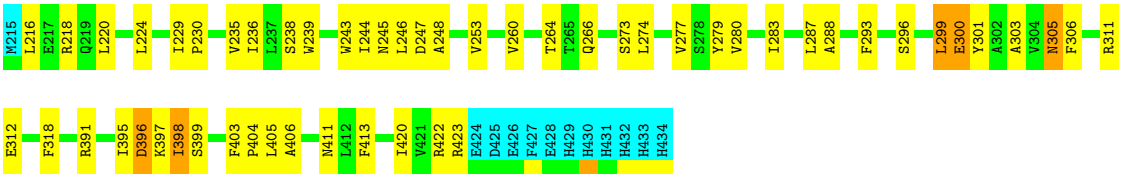
Chain E:



4.2.9 Score per residue for model 9

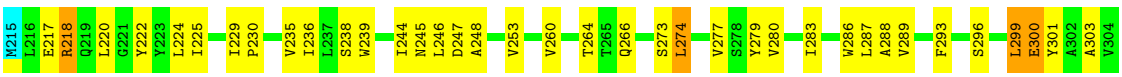
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

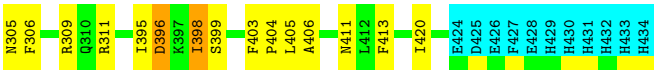
Chain A:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

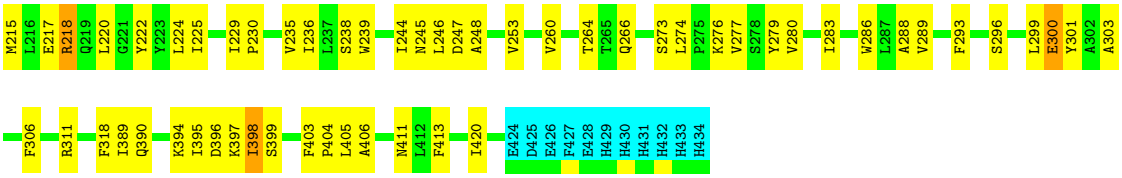
Chain B:





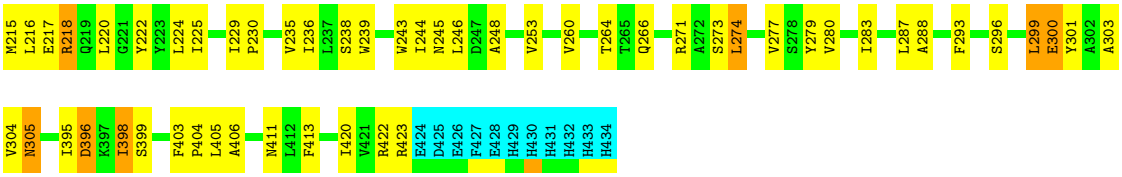
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



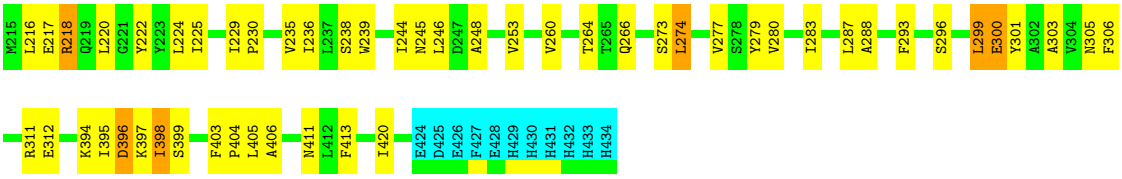
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

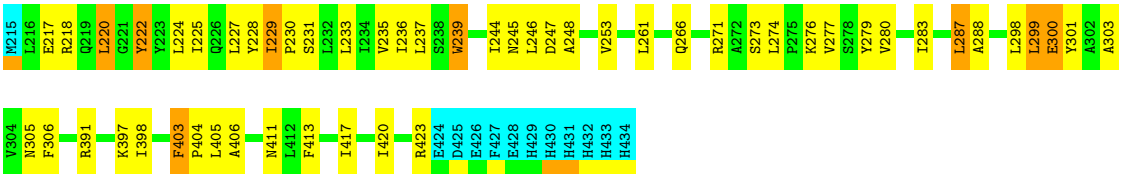
Chain E:



4.2.10 Score per residue for model 10

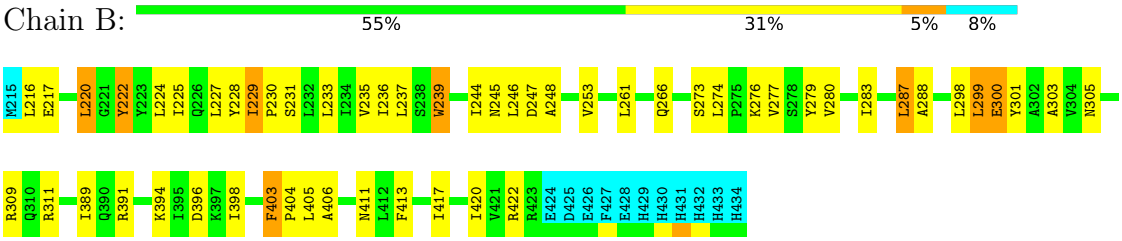
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



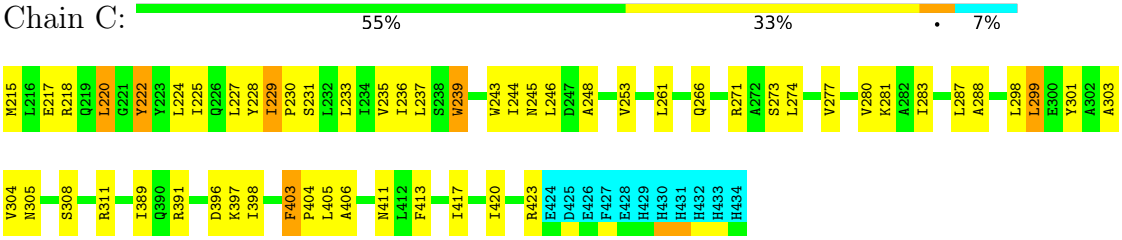
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



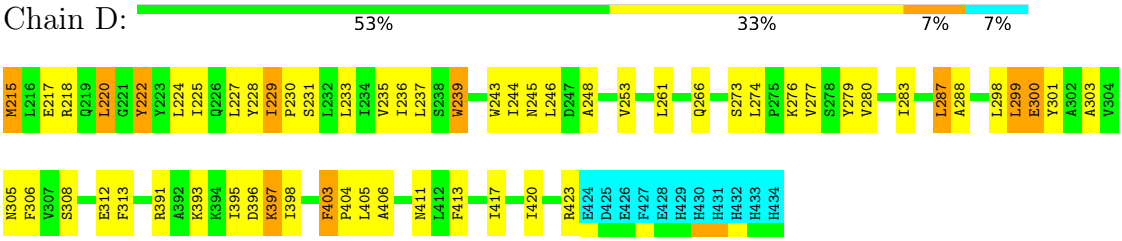
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



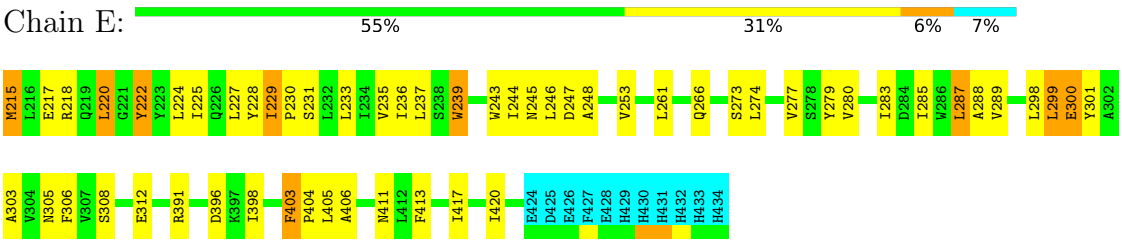
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

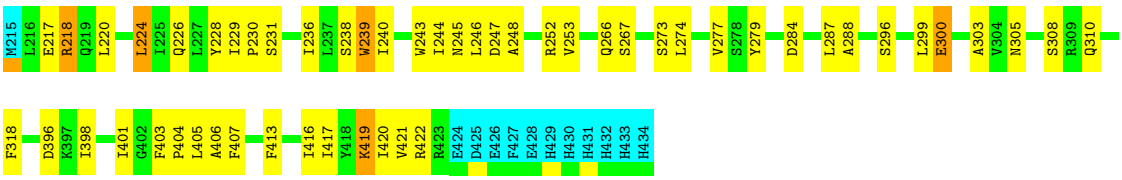
Chain E:



4.2.11 Score per residue for model 11

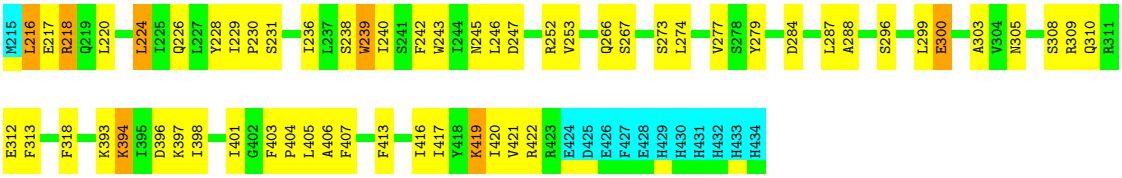
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



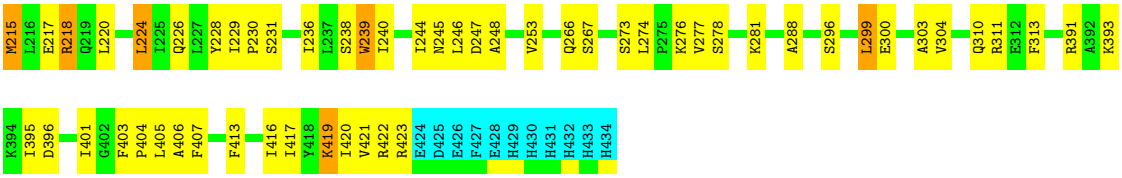
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



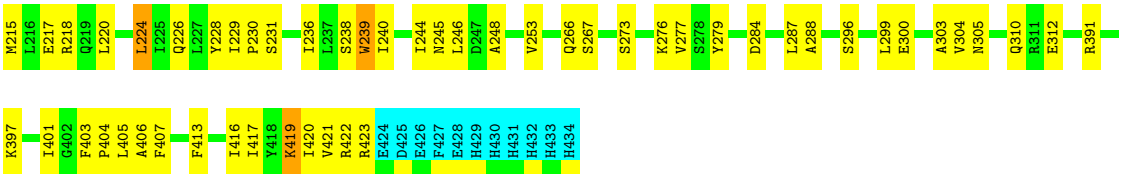
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



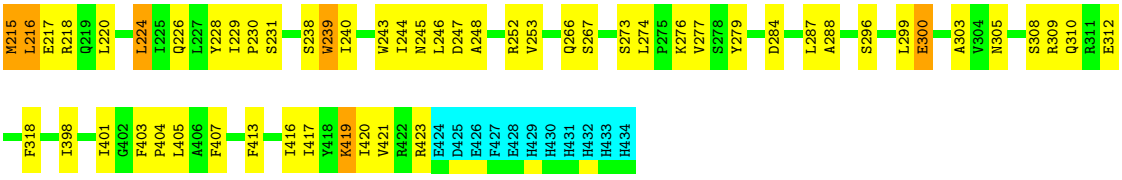
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

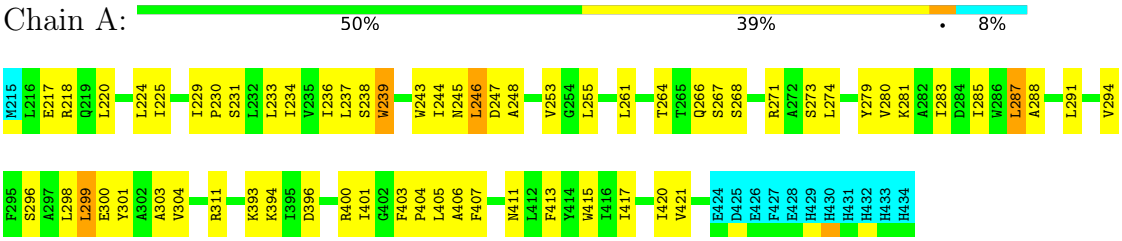
Chain E:



4.2.12 Score per residue for model 12

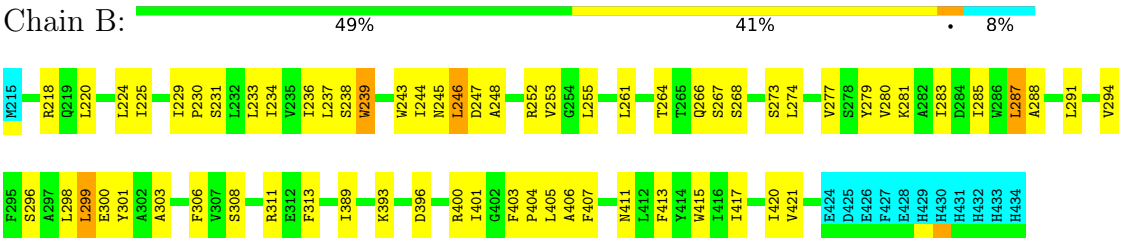
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



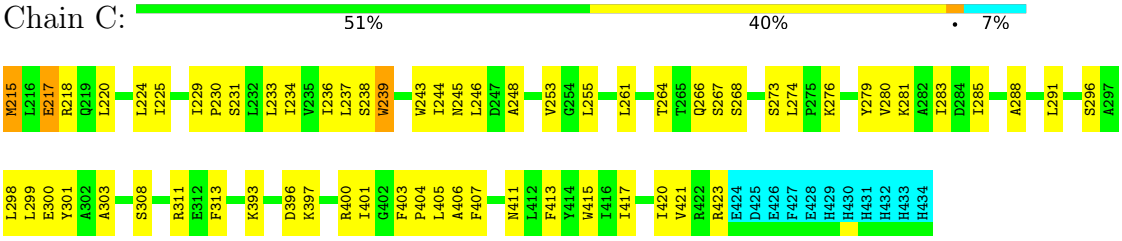
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



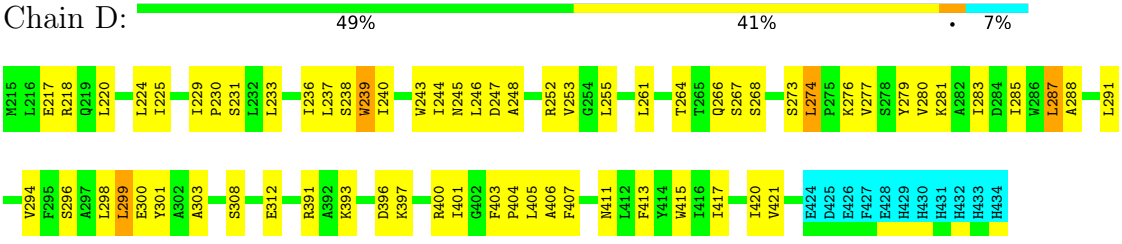
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



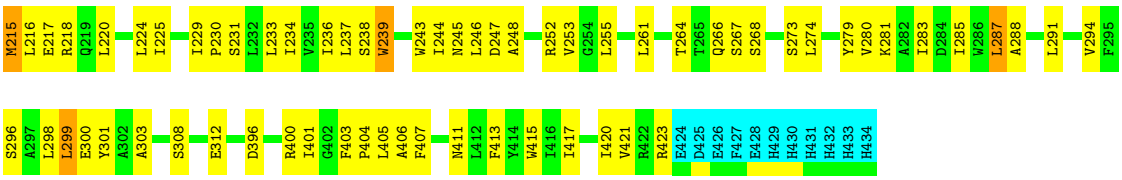
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

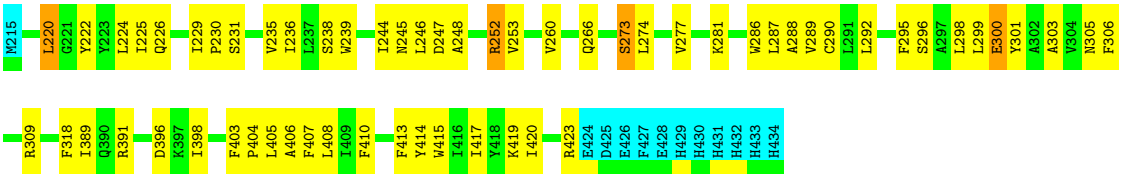
Chain E:



4.2.13 Score per residue for model 13

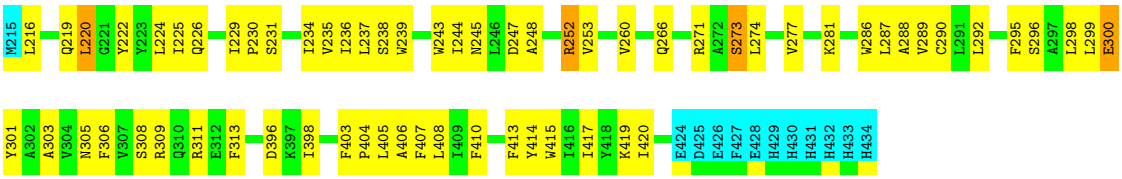
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



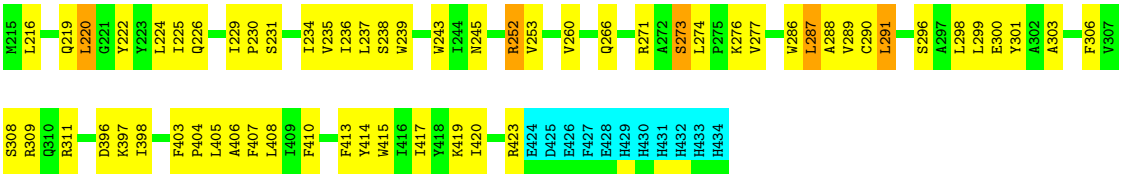
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

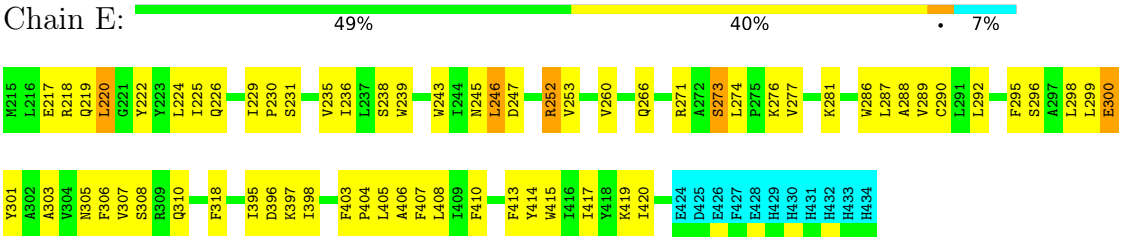
Chain C:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

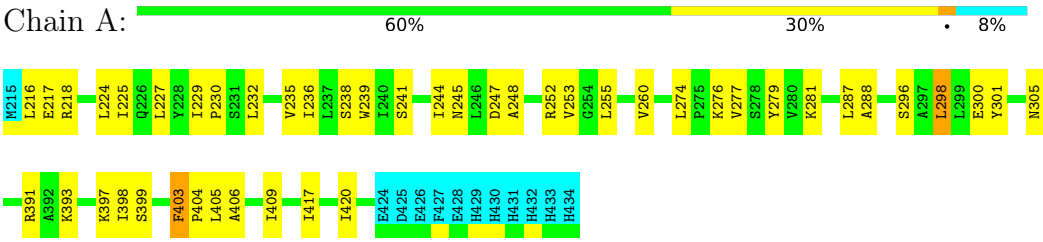
Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

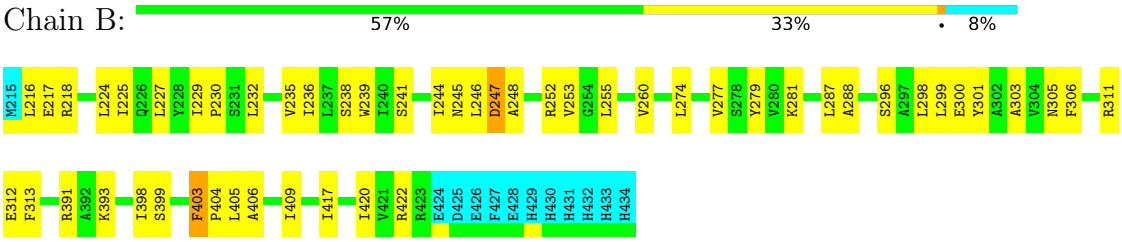


4.2.14 Score per residue for model 14

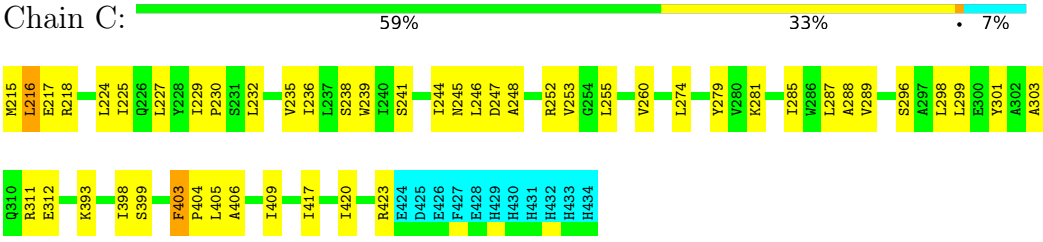
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

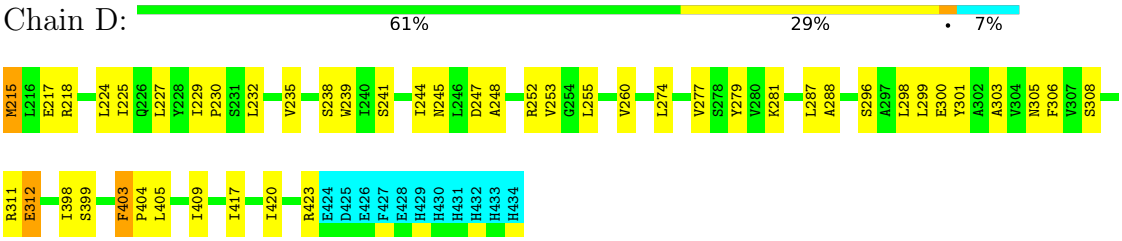


• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit



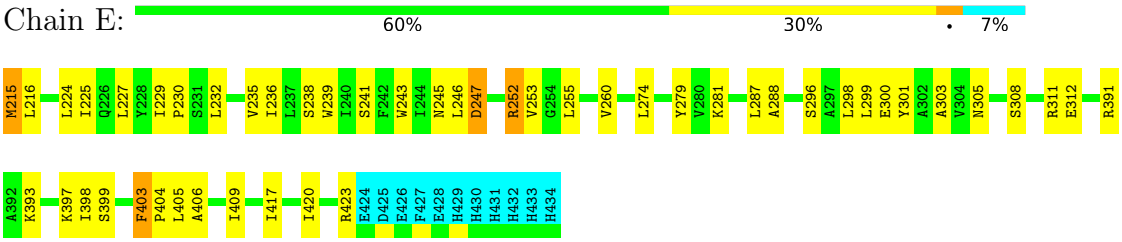
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

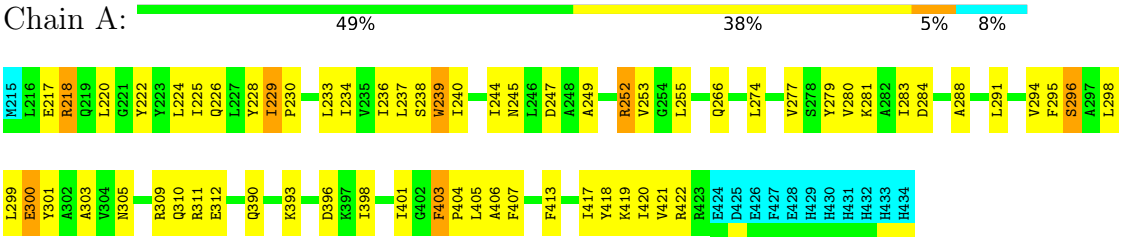
Chain E:



4.2.15 Score per residue for model 15

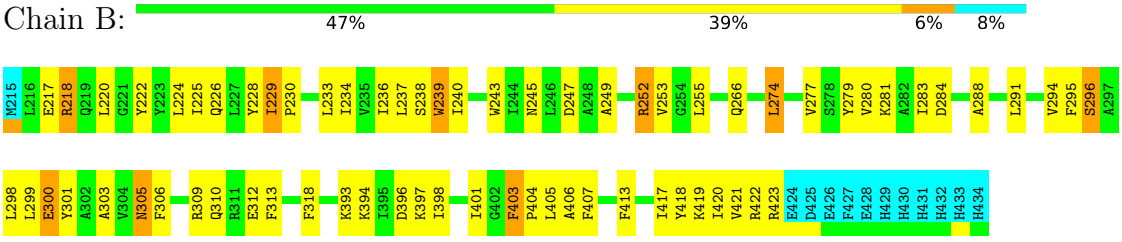
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:



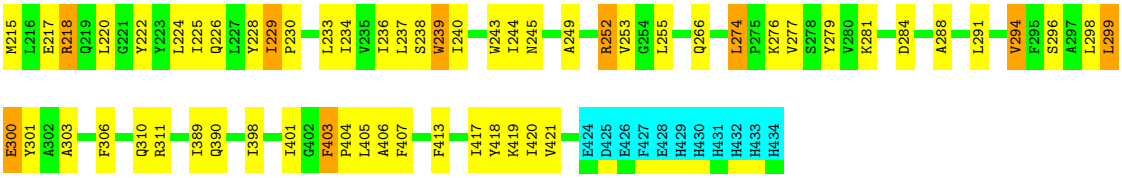
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:



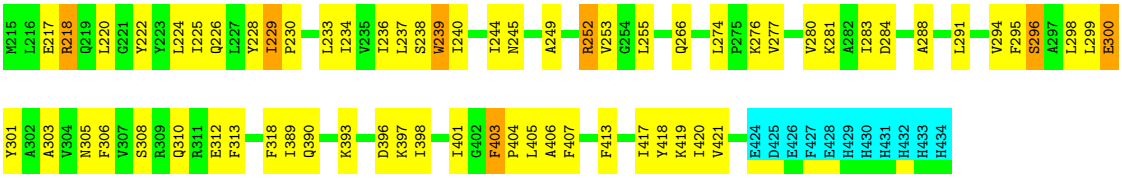
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:



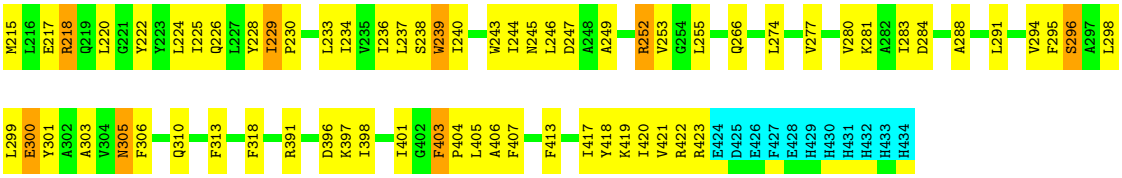
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:



• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	3.0

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	1
Total number of shifts	1145
Number of shifts mapped to atoms	1145
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	11%

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	1115	1178	1178	25±6
1	B	1115	1178	1178	25±6
1	C	1123	1187	1186	25±5
1	D	1123	1187	1186	25±6
1	E	1123	1187	1186	25±6
All	All	83985	88755	88710	1705

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:246:LEU:HD21	1:D:304:VAL:HG21	0.93	1.39	6	2
1:E:246:LEU:HD21	1:E:304:VAL:HG21	0.89	1.42	6	1
1:B:246:LEU:HD21	1:B:304:VAL:HG21	0.89	1.45	6	2
1:C:246:LEU:HD21	1:C:304:VAL:HG21	0.84	1.46	3	4
1:A:225:ILE:HG23	1:A:417:ILE:HD13	0.68	1.65	8	5
1:A:246:LEU:HD21	1:A:304:VAL:CG2	0.67	2.19	8	2
1:E:225:ILE:HG23	1:E:417:ILE:HD13	0.67	1.66	8	5
1:C:225:ILE:HG23	1:C:417:ILE:HD13	0.67	1.65	8	5
1:D:218:ARG:HD2	1:D:277:VAL:HG11	0.66	1.68	8	5
1:A:298:LEU:HD13	1:E:237:LEU:HB3	0.66	1.68	15	5

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Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:225:ILE:HG23	1:B:417:ILE:HD13	0.66	1.67	14	5
1:B:237:LEU:HB3	1:C:298:LEU:HD13	0.65	1.68	7	5
1:D:225:ILE:HG23	1:D:417:ILE:HD13	0.65	1.68	1	5
1:C:237:LEU:HB3	1:D:298:LEU:HD13	0.65	1.69	15	5
1:D:218:ARG:CD	1:D:277:VAL:HG11	0.65	2.22	8	6
1:E:218:ARG:CD	1:E:277:VAL:HG11	0.65	2.22	9	6
1:E:218:ARG:HD2	1:E:277:VAL:HG11	0.65	1.69	8	5
1:C:218:ARG:HD2	1:C:277:VAL:HG11	0.64	1.69	8	5
1:B:300:GLU:OE2	1:B:398:ILE:HD12	0.64	1.93	15	1
1:C:246:LEU:HD21	1:C:304:VAL:CG2	0.64	2.22	11	2
1:C:218:ARG:CD	1:C:277:VAL:HG11	0.63	2.24	15	8
1:E:218:ARG:HD3	1:E:277:VAL:HG11	0.63	1.69	9	1
1:B:218:ARG:CD	1:B:277:VAL:HG11	0.63	2.24	15	9
1:A:218:ARG:HD3	1:A:277:VAL:HG11	0.63	1.71	9	3
1:B:218:ARG:HD3	1:B:277:VAL:HG11	0.62	1.71	2	4
1:C:225:ILE:CG1	1:C:417:ILE:HG21	0.62	2.23	3	3
1:B:389:ILE:HG23	1:B:390:GLN:HG2	0.62	1.72	8	2
1:A:300:GLU:OE2	1:A:398:ILE:HD12	0.62	1.94	15	1
1:E:300:GLU:OE2	1:E:398:ILE:HD12	0.62	1.93	15	1
1:A:218:ARG:CD	1:A:277:VAL:HG11	0.62	2.25	15	7
1:B:242:PHE:CD1	1:B:253:VAL:HG22	0.62	2.29	11	1
1:C:300:GLU:OE2	1:C:398:ILE:HD12	0.62	1.94	15	1
1:B:218:ARG:HD2	1:B:277:VAL:HG11	0.62	1.72	1	4
1:D:246:LEU:HD21	1:D:304:VAL:CG2	0.62	2.25	11	4
1:C:218:ARG:HD3	1:C:277:VAL:HG11	0.61	1.70	2	3
1:D:300:GLU:OE2	1:D:398:ILE:HD12	0.61	1.94	15	1
1:A:298:LEU:HD12	1:E:252:ARG:NH1	0.61	2.11	13	2
1:D:237:LEU:HB3	1:E:298:LEU:HD13	0.61	1.72	7	5
1:A:218:ARG:HD2	1:A:277:VAL:HG11	0.61	1.70	8	4
1:C:246:LEU:HD13	1:C:300:GLU:OE1	0.61	1.95	2	2
1:C:225:ILE:HG12	1:C:417:ILE:HG21	0.61	1.73	15	5
1:D:225:ILE:CG1	1:D:417:ILE:HG21	0.61	2.26	3	3
1:D:215:MET:N	1:D:274:LEU:HD13	0.61	2.11	8	4
1:A:280:VAL:HA	1:A:283:ILE:HD12	0.61	1.73	2	11
1:E:215:MET:N	1:E:274:LEU:HD13	0.61	2.11	12	5
1:A:225:ILE:HG12	1:A:417:ILE:HG21	0.61	1.73	15	5
1:B:281:LYS:HE3	1:B:285:ILE:HD11	0.60	1.74	3	1
1:C:215:MET:N	1:C:274:LEU:HD13	0.60	2.12	12	5
1:D:280:VAL:HA	1:D:283:ILE:HD12	0.60	1.73	1	11
1:B:239:TRP:CH2	1:B:398:ILE:HD11	0.60	2.32	3	5
1:D:218:ARG:HD3	1:D:277:VAL:HG11	0.60	1.72	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:280:VAL:HA	1:B:283:ILE:HD12	0.60	1.73	2	11
1:A:281:LYS:HE3	1:A:285:ILE:HD11	0.60	1.74	3	1
1:A:239:TRP:CH2	1:A:401:ILE:HD11	0.60	2.32	6	5
1:E:239:TRP:CH2	1:E:401:ILE:HD11	0.60	2.31	6	5
1:E:280:VAL:HA	1:E:283:ILE:HD12	0.60	1.73	2	11
1:D:225:ILE:HG12	1:D:417:ILE:HG21	0.60	1.74	15	5
1:C:239:TRP:CH2	1:C:401:ILE:HD11	0.59	2.32	6	5
1:E:239:TRP:CH2	1:E:398:ILE:HD11	0.59	2.32	3	5
1:A:225:ILE:CG1	1:A:417:ILE:HG21	0.59	2.27	3	4
1:E:225:ILE:HG12	1:E:417:ILE:HG21	0.59	1.74	15	5
1:D:215:MET:O	1:D:274:LEU:HD13	0.59	1.97	2	3
1:A:237:LEU:HB3	1:B:298:LEU:HD13	0.59	1.75	15	5
1:A:300:GLU:OE2	1:A:398:ILE:HD13	0.59	1.98	10	3
1:B:225:ILE:HG12	1:B:417:ILE:HG21	0.59	1.75	15	5
1:E:279:TYR:CZ	1:E:283:ILE:HD11	0.59	2.33	5	1
1:B:239:TRP:CH2	1:B:401:ILE:HD11	0.59	2.33	6	5
1:E:215:MET:O	1:E:274:LEU:HD13	0.59	1.97	6	1
1:A:236:ILE:HG12	1:A:406:ALA:HB1	0.58	1.73	10	3
1:A:244:ILE:HD13	1:B:305:ASN:OD1	0.58	1.97	7	1
1:A:299:LEU:HD23	1:A:300:GLU:OE1	0.58	1.98	10	1
1:A:252:ARG:NH1	1:B:298:LEU:HD12	0.58	2.13	13	1
1:E:281:LYS:HE3	1:E:285:ILE:HD11	0.58	1.75	3	1
1:B:225:ILE:CG1	1:B:417:ILE:HG21	0.58	2.28	3	3
1:D:244:ILE:HD13	1:E:305:ASN:CG	0.58	2.19	13	1
1:D:239:TRP:CH2	1:D:401:ILE:HD11	0.58	2.32	6	4
1:E:225:ILE:CG1	1:E:417:ILE:HG21	0.58	2.29	5	3
1:D:279:TYR:CZ	1:D:283:ILE:HD11	0.58	2.33	5	1
1:B:279:TYR:CZ	1:B:283:ILE:HD11	0.58	2.33	5	1
1:D:281:LYS:HE3	1:D:285:ILE:HD11	0.58	1.74	3	1
1:D:300:GLU:OE2	1:D:398:ILE:HD13	0.58	1.99	10	2
1:E:307:VAL:HG12	1:E:318:PHE:CZ	0.58	2.33	13	1
1:B:296:SER:HA	1:B:299:LEU:HD12	0.57	1.75	15	1
1:E:215:MET:HA	1:E:274:LEU:HD13	0.57	1.77	10	1
1:C:234:ILE:HA	1:C:237:LEU:HD12	0.57	1.75	15	3
1:D:296:SER:HA	1:D:299:LEU:HD12	0.57	1.76	15	1
1:E:220:LEU:HD13	1:E:273:SER:CB	0.57	2.29	11	6
1:A:305:ASN:OD1	1:E:244:ILE:HD12	0.57	2.00	9	2
1:A:296:SER:HA	1:A:299:LEU:HD12	0.57	1.76	15	1
1:D:220:LEU:HD13	1:D:273:SER:CB	0.57	2.30	7	7
1:D:299:LEU:HD23	1:D:300:GLU:OE1	0.57	2.00	10	1
1:E:299:LEU:HD23	1:E:300:GLU:OE1	0.57	2.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:236:ILE:HG12	1:C:406:ALA:HB1	0.57	1.75	10	3
1:B:279:TYR:CD2	1:B:283:ILE:HD11	0.57	2.35	12	1
1:E:234:ILE:HA	1:E:237:LEU:HD12	0.57	1.75	15	2
1:D:252:ARG:NH1	1:E:298:LEU:HD12	0.57	2.15	13	1
1:E:300:GLU:OE2	1:E:398:ILE:HD13	0.57	2.00	10	3
1:E:279:TYR:CD2	1:E:283:ILE:HD11	0.57	2.35	12	1
1:D:244:ILE:HD13	1:E:305:ASN:OD1	0.57	1.99	13	1
1:A:220:LEU:HD11	1:A:272:ALA:HB3	0.56	1.76	3	1
1:A:279:TYR:CD2	1:A:283:ILE:HD11	0.56	2.35	12	1
1:D:279:TYR:CD2	1:D:283:ILE:HD11	0.56	2.35	12	1
1:B:220:LEU:HD11	1:B:272:ALA:HB3	0.56	1.76	3	1
1:B:234:ILE:HA	1:B:237:LEU:HD12	0.56	1.75	15	3
1:E:236:ILE:HG12	1:E:406:ALA:HB1	0.56	1.76	10	3
1:E:296:SER:HA	1:E:299:LEU:HD12	0.56	1.76	15	1
1:B:220:LEU:HD13	1:B:273:SER:CB	0.56	2.31	7	7
1:C:215:MET:O	1:C:274:LEU:HD13	0.56	2.00	14	1
1:A:239:TRP:CH2	1:A:398:ILE:HD11	0.56	2.35	3	5
1:D:220:LEU:HD11	1:D:272:ALA:HB3	0.56	1.76	3	1
1:B:236:ILE:HG12	1:B:406:ALA:HB1	0.56	1.76	10	3
1:E:232:LEU:HD11	1:E:409:ILE:CG2	0.56	2.31	14	2
1:D:239:TRP:CH2	1:D:398:ILE:HD11	0.55	2.36	3	5
1:D:243:TRP:O	1:D:246:LEU:HD22	0.55	2.00	5	1
1:C:232:LEU:HD11	1:C:409:ILE:CG2	0.55	2.31	14	2
1:A:246:LEU:HD11	1:A:304:VAL:CG2	0.55	2.32	12	1
1:D:220:LEU:HD22	1:D:273:SER:HB2	0.55	1.77	3	2
1:A:232:LEU:HD11	1:A:409:ILE:CG2	0.55	2.31	14	2
1:C:220:LEU:HD13	1:C:273:SER:CB	0.55	2.32	7	6
1:C:294:VAL:O	1:C:298:LEU:HD12	0.55	2.02	15	5
1:A:246:LEU:HD23	1:A:247:ASP:HB3	0.55	1.79	4	1
1:D:236:ILE:HG12	1:D:406:ALA:HB1	0.55	1.77	10	3
1:A:236:ILE:HD13	1:A:406:ALA:HB1	0.55	1.79	4	7
1:B:307:VAL:HG11	1:B:318:PHE:CE1	0.55	2.36	4	2
1:E:220:LEU:HD22	1:E:273:SER:HB2	0.55	1.79	3	2
1:D:246:LEU:HD23	1:D:246:LEU:O	0.55	2.02	8	1
1:C:239:TRP:CH2	1:C:398:ILE:HD11	0.55	2.36	3	5
1:E:288:ALA:O	1:E:292:LEU:HD12	0.55	2.02	4	2
1:C:215:MET:HA	1:C:274:LEU:HD13	0.55	1.78	11	1
1:C:249:ALA:HB1	1:D:301:TYR:OH	0.54	2.01	15	4
1:A:302:ALA:HB2	1:E:241:SER:HB3	0.54	1.79	2	1
1:D:288:ALA:O	1:D:292:LEU:HD12	0.54	2.02	4	2
1:A:220:LEU:HD13	1:A:273:SER:CB	0.54	2.32	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:288:ALA:O	1:A:292:LEU:HD12	0.54	2.03	4	2
1:E:307:VAL:HG11	1:E:318:PHE:CD1	0.54	2.38	4	1
1:E:220:LEU:HD11	1:E:272:ALA:HB3	0.54	1.80	3	1
1:A:307:VAL:HG11	1:A:318:PHE:CD1	0.54	2.38	4	1
1:D:217:GLU:OE1	1:D:274:LEU:HD22	0.54	2.02	12	2
1:C:244:ILE:HD13	1:D:305:ASN:ND2	0.54	2.17	15	1
1:B:231:SER:O	1:B:235:VAL:HG23	0.54	2.03	13	6
1:D:233:LEU:HA	1:D:236:ILE:HD12	0.54	1.80	5	2
1:E:233:LEU:HA	1:E:236:ILE:HD12	0.54	1.80	5	2
1:B:232:LEU:HD11	1:B:409:ILE:CG2	0.54	2.33	14	2
1:A:318:PHE:CD2	1:A:389:ILE:HG23	0.54	2.37	6	3
1:B:220:LEU:HD22	1:B:273:SER:HB2	0.54	1.80	3	2
1:E:417:ILE:O	1:E:421:VAL:HG23	0.54	2.02	3	6
1:B:252:ARG:NH1	1:C:298:LEU:HD12	0.54	2.17	13	1
1:C:231:SER:O	1:C:235:VAL:HG23	0.54	2.03	13	7
1:D:307:VAL:HG11	1:D:318:PHE:CE1	0.54	2.38	2	2
1:D:231:SER:O	1:D:235:VAL:HG23	0.54	2.03	13	6
1:D:307:VAL:HG11	1:D:318:PHE:CD1	0.54	2.38	4	2
1:B:299:LEU:HD23	1:B:300:GLU:OE1	0.54	2.03	10	1
1:C:252:ARG:NH1	1:D:298:LEU:HD12	0.54	2.17	13	1
1:E:231:SER:O	1:E:235:VAL:HG23	0.54	2.03	13	6
1:C:280:VAL:HA	1:C:283:ILE:HD12	0.54	1.79	10	5
1:E:307:VAL:HG11	1:E:318:PHE:CE1	0.54	2.38	4	1
1:A:233:LEU:HA	1:A:236:ILE:HD12	0.54	1.80	5	2
1:E:246:LEU:HD23	1:E:246:LEU:O	0.54	2.02	8	2
1:E:217:GLU:OE1	1:E:274:LEU:HD22	0.54	2.03	12	2
1:E:252:ARG:HA	1:E:255:LEU:HD12	0.54	1.80	15	1
1:C:307:VAL:HG11	1:C:318:PHE:CE1	0.54	2.37	2	2
1:C:228:TYR:O	1:C:232:LEU:HD12	0.54	2.03	3	2
1:E:228:TYR:O	1:E:232:LEU:HD12	0.54	2.03	3	2
1:B:300:GLU:OE2	1:B:398:ILE:HD13	0.54	2.02	10	3
1:D:294:VAL:O	1:D:298:LEU:HD12	0.53	2.03	15	6
1:D:232:LEU:HD11	1:D:409:ILE:CG2	0.53	2.33	14	2
1:D:235:VAL:HG22	1:D:260:VAL:HG21	0.53	1.80	13	6
1:C:220:LEU:HD11	1:C:272:ALA:HB3	0.53	1.81	3	1
1:A:301:TYR:OH	1:E:249:ALA:HB1	0.53	2.02	7	4
1:B:236:ILE:HD13	1:B:406:ALA:HB1	0.53	1.80	2	7
1:B:307:VAL:HG11	1:B:318:PHE:CD1	0.53	2.38	4	3
1:B:228:TYR:O	1:B:232:LEU:HD12	0.53	2.03	3	2
1:C:233:LEU:HA	1:C:236:ILE:HD12	0.53	1.80	5	2
1:B:235:VAL:HG22	1:B:260:VAL:HG21	0.53	1.80	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:ILE:HA	1:A:237:LEU:HD12	0.53	1.81	15	2
1:B:233:LEU:HD22	1:C:291:LEU:HD11	0.53	1.80	12	1
1:A:231:SER:O	1:A:235:VAL:HG23	0.53	2.03	13	7
1:B:245:ASN:CB	1:B:253:VAL:HG23	0.53	2.34	11	11
1:A:220:LEU:HD22	1:A:273:SER:HB2	0.53	1.80	3	2
1:E:235:VAL:HG22	1:E:260:VAL:HG21	0.53	1.79	13	5
1:C:235:VAL:HG22	1:C:260:VAL:HG21	0.53	1.80	13	4
1:A:232:LEU:HD11	1:A:409:ILE:HG21	0.53	1.80	7	1
1:A:294:VAL:O	1:A:298:LEU:HD12	0.53	2.03	15	6
1:A:228:TYR:O	1:A:232:LEU:HD12	0.53	2.03	3	2
1:A:417:ILE:O	1:A:421:VAL:HG23	0.53	2.04	3	6
1:D:228:TYR:O	1:D:232:LEU:HD12	0.53	2.03	3	2
1:E:294:VAL:O	1:E:298:LEU:HD12	0.52	2.04	8	6
1:E:236:ILE:HD13	1:E:406:ALA:HB1	0.52	1.80	4	7
1:A:279:TYR:CZ	1:A:283:ILE:HD11	0.52	2.39	5	1
1:C:233:LEU:HD22	1:D:291:LEU:HD11	0.52	1.80	12	1
1:C:220:LEU:HD22	1:C:273:SER:HB2	0.52	1.80	3	2
1:C:232:LEU:HD11	1:C:409:ILE:HG21	0.52	1.81	7	1
1:B:220:LEU:HD13	1:B:273:SER:HB3	0.52	1.80	9	5
1:D:416:ILE:HD13	1:D:419:LYS:HE2	0.52	1.82	4	2
1:A:233:LEU:HD22	1:B:291:LEU:HD11	0.52	1.79	12	1
1:A:246:LEU:HD23	1:A:246:LEU:O	0.52	2.04	11	5
1:D:233:LEU:HD22	1:E:291:LEU:HD11	0.52	1.80	12	1
1:C:307:VAL:HG11	1:C:318:PHE:CD1	0.52	2.38	4	2
1:B:237:LEU:CB	1:C:298:LEU:HD13	0.52	2.33	7	4
1:D:236:ILE:HD13	1:D:406:ALA:HB1	0.52	1.82	2	6
1:B:233:LEU:HD13	1:C:291:LEU:CD2	0.52	2.35	15	2
1:D:249:ALA:HB1	1:E:301:TYR:OH	0.52	2.05	7	4
1:A:235:VAL:HG22	1:A:260:VAL:HG21	0.52	1.80	13	4
1:D:241:SER:HB3	1:E:302:ALA:HB2	0.52	1.81	2	1
1:A:302:ALA:HB2	1:E:241:SER:CB	0.52	2.34	4	1
1:A:307:VAL:HG11	1:A:318:PHE:CE1	0.52	2.39	4	1
1:C:233:LEU:HD13	1:D:291:LEU:CD2	0.52	2.35	15	2
1:B:252:ARG:HA	1:B:255:LEU:HD12	0.52	1.80	15	1
1:C:236:ILE:HD13	1:C:406:ALA:HB1	0.52	1.80	4	6
1:E:235:VAL:HG22	1:E:260:VAL:CG2	0.52	2.35	13	2
1:B:294:VAL:O	1:B:298:LEU:HD12	0.52	2.03	15	5
1:D:417:ILE:O	1:D:421:VAL:HG23	0.52	2.04	3	7
1:B:288:ALA:O	1:B:292:LEU:HD12	0.52	2.04	4	2
1:B:233:LEU:HA	1:B:236:ILE:HD12	0.52	1.80	5	2
1:A:300:GLU:HG3	1:A:398:ILE:HD12	0.52	1.82	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:305:ASN:ND2	1:E:244:ILE:HD13	0.52	2.20	15	1
1:C:252:ARG:HA	1:C:255:LEU:HD12	0.52	1.80	15	1
1:C:220:LEU:HD23	1:C:278:SER:CB	0.51	2.35	2	1
1:D:217:GLU:HG3	1:D:277:VAL:HG21	0.51	1.81	6	8
1:E:284:ASP:O	1:E:288:ALA:HB3	0.51	2.05	3	2
1:A:416:ILE:HD13	1:A:419:LYS:HE2	0.51	1.82	4	2
1:C:417:ILE:O	1:C:421:VAL:HG23	0.51	2.04	3	7
1:A:298:LEU:HD21	1:E:252:ARG:NH1	0.51	2.20	8	3
1:A:241:SER:HB3	1:B:302:ALA:HB2	0.51	1.81	2	1
1:B:241:SER:HB3	1:C:302:ALA:HB2	0.51	1.82	2	1
1:B:417:ILE:O	1:B:421:VAL:HG23	0.51	2.04	3	6
1:A:241:SER:CB	1:B:302:ALA:HB2	0.51	2.35	4	1
1:D:235:VAL:HG22	1:D:260:VAL:CG2	0.51	2.35	13	2
1:A:298:LEU:HD13	1:E:237:LEU:CB	0.51	2.34	15	4
1:C:237:LEU:CB	1:D:298:LEU:HD13	0.51	2.35	12	5
1:C:241:SER:HB3	1:D:302:ALA:HB2	0.51	1.83	2	1
1:C:241:SER:CB	1:D:302:ALA:HB2	0.51	2.35	4	1
1:B:235:VAL:HG22	1:B:260:VAL:CG2	0.51	2.35	13	1
1:A:245:ASN:CB	1:A:253:VAL:HG23	0.51	2.36	10	12
1:B:246:LEU:O	1:B:246:LEU:HD23	0.51	2.06	1	3
1:D:245:ASN:CB	1:D:253:VAL:HG23	0.51	2.36	10	13
1:B:217:GLU:HG3	1:B:277:VAL:HG21	0.51	1.82	6	8
1:B:246:LEU:HD23	1:B:247:ASP:HB3	0.51	1.82	5	1
1:A:235:VAL:HG22	1:A:260:VAL:CG2	0.51	2.35	13	1
1:D:234:ILE:HA	1:D:237:LEU:HD12	0.51	1.81	15	1
1:B:416:ILE:HD13	1:B:419:LYS:HE2	0.51	1.82	4	2
1:C:222:TYR:HA	1:C:225:ILE:HD12	0.51	1.83	10	9
1:E:217:GLU:HG3	1:E:277:VAL:HG21	0.51	1.83	11	7
1:C:405:LEU:HD23	1:C:406:ALA:N	0.51	2.21	3	1
1:D:252:ARG:HA	1:D:255:LEU:HD12	0.51	1.83	15	1
1:D:220:LEU:HD13	1:D:273:SER:HB3	0.51	1.83	9	6
1:A:217:GLU:HG3	1:A:277:VAL:HG21	0.51	1.83	11	7
1:D:405:LEU:HD23	1:D:406:ALA:N	0.51	2.21	3	1
1:E:220:LEU:HD13	1:E:273:SER:HB3	0.51	1.83	9	4
1:B:232:LEU:HD21	1:B:409:ILE:HG22	0.51	1.83	7	1
1:A:403:PHE:N	1:A:404:PRO:HD2	0.50	2.21	2	15
1:A:405:LEU:HD23	1:A:406:ALA:N	0.50	2.21	3	1
1:B:224:LEU:HD23	1:B:228:TYR:CE1	0.50	2.42	11	1
1:C:403:PHE:N	1:C:404:PRO:HD2	0.50	2.21	2	15
1:E:239:TRP:CZ3	1:E:401:ILE:HD11	0.50	2.41	6	3
1:B:244:ILE:HG13	1:B:248:ALA:HB3	0.50	1.83	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:245:ASN:CB	1:E:253:VAL:HG23	0.50	2.36	10	11
1:E:416:ILE:HD13	1:E:419:LYS:HE2	0.50	1.82	2	2
1:C:232:LEU:HD21	1:C:409:ILE:HG22	0.50	1.83	7	1
1:C:224:LEU:HD23	1:C:228:TYR:CE1	0.50	2.42	11	1
1:A:246:LEU:HD21	1:A:304:VAL:HG21	0.50	1.82	8	3
1:B:249:ALA:HB1	1:C:301:TYR:OH	0.50	2.05	7	4
1:D:239:TRP:CZ3	1:D:401:ILE:HD11	0.50	2.42	6	3
1:A:222:TYR:HA	1:A:225:ILE:HD12	0.50	1.83	6	8
1:A:244:ILE:HG13	1:A:248:ALA:HB3	0.50	1.82	2	4
1:C:279:TYR:CZ	1:C:283:ILE:HD11	0.50	2.42	3	1
1:D:220:LEU:HD22	1:D:273:SER:CB	0.50	2.36	3	2
1:A:232:LEU:HD21	1:A:409:ILE:HG22	0.50	1.83	7	1
1:B:222:TYR:HA	1:B:225:ILE:HD12	0.50	1.84	15	9
1:E:244:ILE:HG13	1:E:248:ALA:HB3	0.50	1.82	2	2
1:D:233:LEU:HD13	1:E:291:LEU:CD2	0.50	2.36	15	2
1:A:224:LEU:HD23	1:A:228:TYR:CE1	0.50	2.42	11	1
1:C:300:GLU:HG2	1:C:398:ILE:HD12	0.50	1.82	13	1
1:C:244:ILE:HG13	1:C:248:ALA:HB3	0.50	1.82	2	3
1:C:245:ASN:CB	1:C:253:VAL:HG23	0.50	2.36	10	10
1:B:232:LEU:HD11	1:B:409:ILE:HG21	0.50	1.82	7	1
1:C:220:LEU:HD13	1:C:273:SER:HB3	0.50	1.81	9	6
1:B:220:LEU:HD23	1:B:278:SER:CB	0.50	2.37	2	1
1:A:284:ASP:O	1:A:288:ALA:HB3	0.50	2.07	3	2
1:E:405:LEU:HD23	1:E:406:ALA:N	0.50	2.21	3	1
1:C:416:ILE:HD13	1:C:419:LYS:HE2	0.50	1.82	2	2
1:E:222:TYR:HA	1:E:225:ILE:HD12	0.50	1.83	6	9
1:D:403:PHE:N	1:D:404:PRO:HD2	0.50	2.21	2	15
1:B:284:ASP:O	1:B:288:ALA:HB3	0.50	2.06	3	1
1:A:239:TRP:CZ3	1:A:401:ILE:HD11	0.50	2.41	1	3
1:A:249:ALA:HB1	1:B:301:TYR:OH	0.50	2.07	7	4
1:B:244:ILE:HG12	1:B:248:ALA:HB3	0.50	1.84	3	5
1:B:403:PHE:N	1:B:404:PRO:HD2	0.50	2.21	2	15
1:D:222:TYR:HA	1:D:225:ILE:HD12	0.50	1.83	6	9
1:C:284:ASP:O	1:C:288:ALA:HB3	0.50	2.06	3	2
1:D:284:ASP:O	1:D:288:ALA:HB3	0.50	2.06	3	1
1:C:246:LEU:HD11	1:C:300:GLU:HG3	0.50	1.82	5	1
1:C:235:VAL:HG22	1:C:260:VAL:CG2	0.50	2.35	13	2
1:D:224:LEU:HD23	1:D:228:TYR:CE1	0.49	2.42	11	1
1:C:217:GLU:HG3	1:C:277:VAL:HG21	0.49	1.83	9	8
1:E:244:ILE:HG12	1:E:248:ALA:HB3	0.49	1.84	3	6
1:B:300:GLU:HG3	1:B:398:ILE:HD12	0.49	1.85	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:220:LEU:HD13	1:A:273:SER:HB3	0.49	1.84	9	5
1:D:220:LEU:HD13	1:D:273:SER:CA	0.49	2.37	5	1
1:A:233:LEU:HD13	1:B:291:LEU:CD2	0.49	2.37	15	2
1:D:232:LEU:HD11	1:D:409:ILE:HG21	0.49	1.83	7	1
1:E:403:PHE:N	1:E:404:PRO:HD2	0.49	2.21	2	15
1:D:220:LEU:HD13	1:D:273:SER:N	0.49	2.22	3	1
1:E:395:ILE:HD13	1:E:397:LYS:NZ	0.49	2.22	1	1
1:D:244:ILE:HG13	1:D:248:ALA:HB3	0.49	1.83	4	4
1:C:220:LEU:HD22	1:C:273:SER:CB	0.49	2.38	3	2
1:A:252:ARG:NH1	1:B:298:LEU:HD21	0.49	2.23	8	4
1:B:239:TRP:CZ3	1:B:401:ILE:HD11	0.49	2.42	6	3
1:D:244:ILE:HG12	1:D:248:ALA:HB3	0.49	1.85	3	7
1:D:241:SER:CB	1:E:302:ALA:HB2	0.49	2.37	4	1
1:B:252:ARG:NH1	1:C:298:LEU:HD21	0.49	2.22	8	3
1:A:302:ALA:HB1	1:E:240:ILE:HG22	0.49	1.85	2	1
1:E:245:ASN:HB2	1:E:253:VAL:HG23	0.49	1.85	2	5
1:B:405:LEU:HD23	1:B:406:ALA:N	0.49	2.21	3	1
1:E:224:LEU:HD23	1:E:228:TYR:CE1	0.49	2.42	11	1
1:E:229:ILE:N	1:E:230:PRO:HD2	0.49	2.23	5	15
1:A:232:LEU:HD22	1:A:410:PHE:HB2	0.49	1.84	3	1
1:C:279:TYR:CD2	1:C:283:ILE:HD11	0.49	2.42	4	1
1:D:232:LEU:HD21	1:D:409:ILE:HG22	0.49	1.84	7	1
1:E:246:LEU:O	1:E:246:LEU:HD13	0.49	2.07	13	1
1:C:239:TRP:CZ3	1:C:401:ILE:HD11	0.49	2.42	1	2
1:A:220:LEU:HD23	1:A:278:SER:CB	0.49	2.38	2	1
1:B:416:ILE:HD13	1:B:419:LYS:HE3	0.49	1.85	11	1
1:A:237:LEU:CB	1:B:298:LEU:HD13	0.48	2.37	12	4
1:D:237:LEU:CB	1:E:298:LEU:HD13	0.48	2.38	7	3
1:A:416:ILE:HD13	1:A:419:LYS:HE3	0.48	1.85	11	1
1:A:229:ILE:N	1:A:230:PRO:HD2	0.48	2.23	5	15
1:C:299:LEU:O	1:C:303:ALA:HB2	0.48	2.08	10	15
1:B:220:LEU:HD22	1:B:273:SER:CB	0.48	2.38	3	2
1:A:237:LEU:HD23	1:B:298:LEU:HD13	0.48	1.86	6	1
1:B:229:ILE:N	1:B:230:PRO:HD2	0.48	2.24	13	15
1:C:229:ILE:N	1:C:230:PRO:HD2	0.48	2.24	9	15
1:B:232:LEU:HD22	1:B:410:PHE:HB2	0.48	1.85	3	1
1:D:300:GLU:HG3	1:D:398:ILE:HD12	0.48	1.85	13	1
1:A:252:ARG:HA	1:A:255:LEU:HD12	0.48	1.83	15	1
1:D:229:ILE:N	1:D:230:PRO:HD2	0.48	2.23	5	15
1:A:220:LEU:HD22	1:A:273:SER:CB	0.48	2.38	3	2
1:A:230:PRO:O	1:A:234:ILE:HD12	0.48	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:ARG:CZ	1:B:298:LEU:HD21	0.48	2.39	2	1
1:C:230:PRO:O	1:C:234:ILE:HD12	0.48	2.08	7	1
1:A:299:LEU:O	1:A:303:ALA:HB2	0.48	2.08	2	14
1:B:299:LEU:O	1:B:303:ALA:HB2	0.48	2.09	2	15
1:D:252:ARG:NH1	1:E:298:LEU:HD21	0.48	2.24	8	4
1:D:220:LEU:HD23	1:D:278:SER:CB	0.48	2.38	2	1
1:D:279:TYR:CE1	1:D:283:ILE:HD11	0.48	2.44	5	1
1:B:237:LEU:HD23	1:C:298:LEU:HD13	0.48	1.85	6	1
1:C:252:ARG:NH1	1:D:298:LEU:HD21	0.48	2.24	8	3
1:B:241:SER:CB	1:C:302:ALA:HB2	0.48	2.39	4	1
1:A:298:LEU:HD11	1:E:237:LEU:O	0.48	2.08	6	2
1:D:230:PRO:O	1:D:234:ILE:HD12	0.48	2.08	7	1
1:E:299:LEU:O	1:E:303:ALA:HB2	0.48	2.09	12	15
1:E:232:LEU:HD21	1:E:409:ILE:HG22	0.48	1.85	7	1
1:E:416:ILE:HD13	1:E:419:LYS:HE3	0.48	1.85	11	1
1:E:295:PHE:CZ	1:E:299:LEU:HD11	0.48	2.44	15	1
1:D:237:LEU:HD23	1:E:298:LEU:HD13	0.48	1.85	6	1
1:C:287:LEU:HD21	1:C:291:LEU:HD13	0.48	1.85	13	1
1:D:245:ASN:HB2	1:D:253:VAL:HG23	0.48	1.85	2	5
1:B:220:LEU:HD13	1:B:273:SER:CA	0.48	2.39	5	1
1:E:232:LEU:HD11	1:E:409:ILE:HG21	0.48	1.85	7	1
1:D:220:LEU:HD12	1:D:273:SER:CB	0.47	2.39	10	1
1:A:236:ILE:CD1	1:A:406:ALA:HB1	0.47	2.39	2	6
1:E:220:LEU:HD13	1:E:273:SER:N	0.47	2.24	3	1
1:B:230:PRO:O	1:B:234:ILE:HD12	0.47	2.10	7	1
1:B:300:GLU:CD	1:B:398:ILE:HD13	0.47	2.30	9	1
1:A:291:LEU:HD11	1:E:233:LEU:HD22	0.47	1.86	12	1
1:E:300:GLU:HG3	1:E:398:ILE:HD12	0.47	1.87	13	1
1:C:244:ILE:HG12	1:C:248:ALA:HB3	0.47	1.86	11	6
1:E:232:LEU:HD22	1:E:410:PHE:HB2	0.47	1.86	3	1
1:E:279:TYR:CE1	1:E:283:ILE:HD11	0.47	2.44	5	1
1:C:217:GLU:OE1	1:C:274:LEU:HD22	0.47	2.09	7	2
1:C:416:ILE:HD13	1:C:419:LYS:HE3	0.47	1.85	11	1
1:A:245:ASN:HB2	1:A:253:VAL:HG23	0.47	1.85	2	8
1:D:246:LEU:HD13	1:D:246:LEU:O	0.47	2.09	2	1
1:B:237:LEU:O	1:C:298:LEU:HD11	0.47	2.10	6	2
1:C:304:VAL:HG23	1:C:391:ARG:CZ	0.47	2.39	8	1
1:E:300:GLU:CD	1:E:398:ILE:HD13	0.47	2.30	9	1
1:D:295:PHE:CZ	1:D:299:LEU:HD11	0.47	2.44	15	1
1:C:240:ILE:HG22	1:D:302:ALA:HB1	0.47	1.87	2	1
1:A:237:LEU:O	1:B:298:LEU:HD11	0.47	2.09	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:246:LEU:HD21	1:B:304:VAL:CG2	0.47	2.39	7	1
1:C:287:LEU:CD2	1:C:291:LEU:HD13	0.47	2.40	13	1
1:D:299:LEU:O	1:D:303:ALA:HB2	0.47	2.10	10	15
1:B:220:LEU:HD13	1:B:273:SER:N	0.47	2.25	3	1
1:B:394:LYS:C	1:B:395:ILE:HD12	0.47	2.30	4	1
1:C:220:LEU:HD13	1:C:273:SER:CA	0.47	2.40	5	1
1:D:246:LEU:HD23	1:D:247:ASP:N	0.47	2.24	5	1
1:A:291:LEU:CD2	1:E:233:LEU:HD13	0.47	2.40	15	2
1:B:234:ILE:HD11	1:C:291:LEU:CD2	0.47	2.39	7	1
1:A:300:GLU:CD	1:A:398:ILE:HD13	0.47	2.30	9	1
1:A:244:ILE:HG12	1:A:248:ALA:HB3	0.47	1.85	3	7
1:A:298:LEU:HD21	1:E:252:ARG:CZ	0.47	2.40	2	1
1:B:245:ASN:HB2	1:B:253:VAL:HG23	0.47	1.86	4	6
1:D:252:ARG:CZ	1:E:298:LEU:HD21	0.47	2.38	2	1
1:E:220:LEU:HD23	1:E:278:SER:CB	0.47	2.40	2	1
1:E:220:LEU:HD22	1:E:273:SER:CB	0.47	2.40	3	2
1:E:220:LEU:HD12	1:E:273:SER:CB	0.47	2.39	10	1
1:A:295:PHE:CZ	1:A:299:LEU:HD11	0.47	2.45	15	1
1:B:295:PHE:CZ	1:B:299:LEU:HD11	0.47	2.44	15	1
1:B:217:GLU:OE1	1:B:274:LEU:HD22	0.47	2.09	7	1
1:C:245:ASN:HB2	1:C:253:VAL:HG23	0.47	1.85	2	6
1:E:220:LEU:HD13	1:E:273:SER:CA	0.47	2.39	5	1
1:A:220:LEU:HD13	1:A:273:SER:N	0.46	2.25	3	1
1:B:279:TYR:CE1	1:B:283:ILE:HD11	0.46	2.44	5	1
1:D:237:LEU:O	1:E:298:LEU:HD11	0.46	2.11	6	2
1:C:215:MET:C	1:C:216:LEU:HD22	0.46	2.30	14	1
1:B:237:LEU:HB3	1:C:298:LEU:HD22	0.46	1.86	10	1
1:B:242:PHE:CE1	1:B:253:VAL:HG22	0.46	2.45	11	1
1:C:232:LEU:HD22	1:C:410:PHE:HB2	0.46	1.86	3	1
1:D:215:MET:C	1:D:216:LEU:HD22	0.46	2.31	4	1
1:D:416:ILE:HD13	1:D:419:LYS:HE3	0.46	1.85	11	1
1:D:232:LEU:HD22	1:D:410:PHE:HB2	0.46	1.86	3	1
1:D:300:GLU:CD	1:D:398:ILE:HD13	0.46	2.31	9	1
1:C:220:LEU:HD13	1:C:273:SER:N	0.46	2.26	3	1
1:A:302:ALA:HB2	1:E:241:SER:OG	0.46	2.10	4	1
1:E:236:ILE:CD1	1:E:406:ALA:HB1	0.46	2.41	4	4
1:C:287:LEU:HD13	1:C:291:LEU:HD22	0.46	1.87	13	1
1:B:236:ILE:CD1	1:B:406:ALA:HB1	0.46	2.40	2	6
1:B:240:ILE:HG22	1:C:302:ALA:HB1	0.46	1.88	2	1
1:A:220:LEU:HD13	1:A:273:SER:CA	0.46	2.40	5	1
1:C:237:LEU:O	1:D:298:LEU:HD11	0.46	2.11	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:233:LEU:HD21	1:A:410:PHE:CZ	0.45	2.46	4	1
1:C:246:LEU:HD23	1:C:246:LEU:O	0.45	2.11	14	1
1:B:403:PHE:CB	1:B:404:PRO:CD	0.45	2.94	4	14
1:A:298:LEU:HD13	1:E:237:LEU:HD23	0.45	1.89	6	1
1:D:236:ILE:CD1	1:D:406:ALA:HB1	0.45	2.41	4	5
1:D:244:ILE:HD12	1:E:305:ASN:HB2	0.45	1.87	6	2
1:C:236:ILE:CD1	1:C:406:ALA:HB1	0.45	2.40	4	7
1:C:220:LEU:HD12	1:C:273:SER:CB	0.45	2.41	10	1
1:B:252:ARG:CZ	1:C:298:LEU:HD21	0.45	2.41	2	1
1:C:233:LEU:HD21	1:C:410:PHE:CZ	0.45	2.47	4	1
1:A:220:LEU:HD12	1:A:273:SER:CB	0.45	2.42	10	1
1:C:403:PHE:CB	1:C:404:PRO:CD	0.45	2.95	6	14
1:C:252:ARG:CZ	1:D:298:LEU:HD21	0.45	2.42	2	1
1:D:403:PHE:CB	1:D:404:PRO:CD	0.45	2.95	7	14
1:A:403:PHE:CB	1:A:404:PRO:CD	0.45	2.95	7	14
1:E:403:PHE:CB	1:E:404:PRO:CD	0.45	2.95	6	14
1:E:233:LEU:HD21	1:E:410:PHE:CZ	0.44	2.47	4	1
1:A:237:LEU:HB3	1:B:298:LEU:HD22	0.44	1.89	10	1
1:C:237:LEU:HB3	1:D:298:LEU:HD22	0.44	1.89	10	1
1:C:285:ILE:O	1:C:289:VAL:HG12	0.44	2.12	14	1
1:B:233:LEU:HD21	1:B:410:PHE:CZ	0.44	2.48	4	1
1:C:237:LEU:HD23	1:D:298:LEU:HD13	0.44	1.87	6	1
1:C:300:GLU:CD	1:C:398:ILE:HD13	0.44	2.32	9	1
1:E:220:LEU:HD13	1:E:273:SER:HB2	0.44	1.88	11	1
1:D:412:LEU:O	1:D:412:LEU:HD12	0.44	2.13	3	1
1:E:217:GLU:CG	1:E:274:LEU:HD22	0.44	2.43	9	1
1:E:412:LEU:HD12	1:E:412:LEU:O	0.44	2.13	3	1
1:B:286:TRP:HA	1:B:289:VAL:HG12	0.44	1.90	6	2
1:C:244:ILE:HD13	1:D:304:VAL:HB	0.44	1.89	7	1
1:C:244:ILE:HD12	1:D:305:ASN:OD1	0.44	2.12	9	1
1:B:220:LEU:HD12	1:B:273:SER:CB	0.44	2.42	10	1
1:D:395:ILE:HD12	1:D:397:LYS:CG	0.44	2.43	10	1
1:A:412:LEU:HD12	1:A:412:LEU:O	0.44	2.12	3	1
1:B:220:LEU:HD13	1:B:273:SER:HB2	0.44	1.90	11	1
1:B:412:LEU:HD12	1:B:412:LEU:O	0.44	2.13	3	1
1:E:286:TRP:HA	1:E:289:VAL:HG12	0.44	1.90	6	1
1:B:300:GLU:CD	1:B:398:ILE:HD12	0.44	2.33	15	1
1:E:216:LEU:HD11	1:E:273:SER:OG	0.44	2.13	11	1
1:C:412:LEU:HD12	1:C:412:LEU:O	0.44	2.13	3	1
1:A:246:LEU:HD12	1:A:246:LEU:O	0.44	2.13	8	1
1:C:299:LEU:O	1:C:299:LEU:HD23	0.43	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:286:TRP:HA	1:C:289:VAL:HG12	0.43	1.89	6	2
1:C:236:ILE:HG23	1:C:406:ALA:CB	0.43	2.43	6	1
1:C:225:ILE:HG12	1:C:417:ILE:HD12	0.43	1.90	7	1
1:E:300:GLU:CD	1:E:398:ILE:HD12	0.43	2.33	15	1
1:A:287:LEU:O	1:A:287:LEU:HD23	0.43	2.14	10	2
1:A:286:TRP:HA	1:A:289:VAL:HG12	0.43	1.90	6	1
1:B:236:ILE:HG23	1:B:406:ALA:CB	0.43	2.44	6	1
1:D:217:GLU:CG	1:D:274:LEU:HD22	0.43	2.44	9	1
1:D:229:ILE:HG22	1:D:230:PRO:N	0.43	2.29	15	11
1:E:244:ILE:O	1:E:246:LEU:HD23	0.43	2.13	15	1
1:D:244:ILE:HD13	1:E:304:VAL:HB	0.43	1.91	7	1
1:D:246:LEU:HD12	1:D:246:LEU:O	0.43	2.14	11	1
1:D:300:GLU:CD	1:D:398:ILE:HD12	0.43	2.34	15	1
1:C:229:ILE:HG22	1:C:230:PRO:N	0.43	2.29	15	8
1:C:241:SER:OG	1:D:302:ALA:HB2	0.43	2.13	4	1
1:D:233:LEU:HD21	1:D:410:PHE:CZ	0.43	2.49	4	1
1:D:237:LEU:HB3	1:E:298:LEU:HD22	0.43	1.91	10	1
1:D:236:ILE:HG23	1:D:406:ALA:CB	0.43	2.44	6	1
1:B:287:LEU:HD23	1:B:287:LEU:O	0.43	2.14	10	2
1:A:300:GLU:CD	1:A:398:ILE:HD12	0.43	2.34	15	1
1:B:287:LEU:O	1:B:287:LEU:HD12	0.43	2.14	5	1
1:E:236:ILE:HG23	1:E:406:ALA:CB	0.43	2.43	6	1
1:B:229:ILE:HG22	1:B:230:PRO:N	0.42	2.29	5	14
1:E:229:ILE:HG22	1:E:230:PRO:N	0.42	2.30	5	13
1:D:220:LEU:CD1	1:D:272:ALA:HB3	0.42	2.44	3	1
1:C:220:LEU:HD22	1:C:273:SER:OG	0.42	2.14	5	1
1:A:229:ILE:HG22	1:A:230:PRO:N	0.42	2.29	3	14
1:E:287:LEU:O	1:E:287:LEU:HD23	0.42	2.14	10	3
1:A:287:LEU:HD12	1:A:287:LEU:O	0.42	2.13	5	1
1:D:220:LEU:HD22	1:D:273:SER:OG	0.42	2.14	5	1
1:E:215:MET:N	1:E:274:LEU:HD22	0.42	2.29	14	1
1:D:287:LEU:HD12	1:D:287:LEU:O	0.42	2.14	5	1
1:A:236:ILE:HG23	1:A:406:ALA:CB	0.42	2.45	6	1
1:A:227:LEU:O	1:A:227:LEU:HD23	0.42	2.14	10	1
1:C:246:LEU:HD11	1:C:300:GLU:CG	0.42	2.43	5	1
1:E:220:LEU:HD22	1:E:273:SER:OG	0.42	2.15	5	1
1:E:287:LEU:HD12	1:E:287:LEU:O	0.42	2.14	5	1
1:C:244:ILE:HD12	1:D:305:ASN:HB2	0.42	1.90	6	1
1:D:287:LEU:O	1:D:287:LEU:HD23	0.42	2.14	10	2
1:A:246:LEU:HD11	1:A:304:VAL:HG21	0.42	1.91	12	1
1:D:286:TRP:HA	1:D:289:VAL:HG12	0.42	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:244:ILE:HD13	1:C:304:VAL:HB	0.42	1.91	7	1
1:C:227:LEU:HD23	1:C:227:LEU:O	0.42	2.14	10	1
1:E:227:LEU:O	1:E:227:LEU:HD23	0.42	2.14	10	1
1:D:227:LEU:HD23	1:D:227:LEU:O	0.42	2.14	10	1
1:A:236:ILE:CG1	1:A:406:ALA:HB1	0.42	2.44	11	2
1:A:241:SER:OG	1:B:302:ALA:HB2	0.42	2.15	4	1
1:E:398:ILE:HD12	1:E:401:ILE:HD11	0.42	1.92	4	1
1:E:285:ILE:O	1:E:289:VAL:HG13	0.42	2.15	10	1
1:C:246:LEU:O	1:C:246:LEU:HD12	0.41	2.14	11	3
1:A:398:ILE:HD12	1:A:401:ILE:HD11	0.41	1.92	4	1
1:B:394:LYS:O	1:B:395:ILE:HD12	0.41	2.15	4	1
1:A:279:TYR:CE1	1:A:283:ILE:HD11	0.41	2.49	5	1
1:B:216:LEU:HD11	1:B:273:SER:OG	0.41	2.15	11	1
1:B:246:LEU:O	1:B:246:LEU:HD13	0.41	2.15	12	1
1:C:239:TRP:HH2	1:C:401:ILE:HD11	0.41	1.74	15	1
1:E:304:VAL:O	1:E:307:VAL:HG23	0.41	2.16	3	2
1:E:246:LEU:HD21	1:E:304:VAL:CG2	0.41	2.46	2	1
1:C:398:ILE:HD12	1:C:401:ILE:HD11	0.41	1.92	4	1
1:B:227:LEU:O	1:B:227:LEU:HD23	0.41	2.14	10	1
1:B:220:LEU:HD22	1:B:273:SER:OG	0.41	2.15	5	1
1:E:310:GLN:NE2	1:E:315:GLY:H	0.41	2.14	7	1
1:E:225:ILE:HG12	1:E:417:ILE:HD12	0.41	1.92	7	1
1:D:229:ILE:CB	1:D:230:PRO:CD	0.41	2.99	2	8
1:E:229:ILE:CB	1:E:230:PRO:CD	0.41	2.99	15	10
1:C:304:VAL:O	1:C:307:VAL:HG23	0.41	2.16	3	1
1:A:237:LEU:CD2	1:B:298:LEU:HD22	0.41	2.46	6	1
1:B:218:ARG:NE	1:B:277:VAL:HG11	0.41	2.30	8	1
1:C:403:PHE:N	1:C:404:PRO:CD	0.41	2.84	2	1
1:D:240:ILE:HG22	1:E:302:ALA:HB1	0.41	1.92	2	1
1:E:403:PHE:N	1:E:404:PRO:CD	0.41	2.84	2	1
1:C:288:ALA:O	1:C:292:LEU:HD12	0.41	2.15	3	1
1:D:241:SER:OG	1:E:302:ALA:HB2	0.41	2.16	4	1
1:A:225:ILE:HG12	1:A:417:ILE:HD12	0.41	1.92	7	1
1:D:220:LEU:HD12	1:D:273:SER:HB3	0.41	1.91	10	1
1:E:220:LEU:HD12	1:E:273:SER:HB3	0.41	1.91	10	1
1:C:300:GLU:CD	1:C:398:ILE:HD12	0.41	2.37	15	1
1:C:229:ILE:CB	1:C:230:PRO:CD	0.41	2.99	2	7
1:A:220:LEU:CD1	1:A:272:ALA:HB3	0.41	2.44	3	1
1:B:220:LEU:CD1	1:B:272:ALA:HB3	0.41	2.44	3	1
1:A:220:LEU:HD22	1:A:273:SER:OG	0.41	2.16	5	1
1:E:395:ILE:HD13	1:E:397:LYS:CE	0.40	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:304:VAL:HB	1:E:244:ILE:HD13	0.40	1.92	7	1
1:D:217:GLU:CG	1:D:277:VAL:HG21	0.40	2.46	8	1
1:B:236:ILE:CG1	1:B:406:ALA:HB1	0.40	2.46	11	2
1:C:236:ILE:CG1	1:C:406:ALA:HB1	0.40	2.46	11	1
1:E:239:TRP:HH2	1:E:401:ILE:HD11	0.40	1.75	15	2
1:D:240:ILE:HD13	1:D:243:TRP:CZ2	0.40	2.51	12	1
1:A:229:ILE:CB	1:A:230:PRO:CD	0.40	2.99	1	3
1:B:229:ILE:CB	1:B:230:PRO:CD	0.40	2.99	1	3
1:A:240:ILE:HG22	1:B:302:ALA:HB1	0.40	1.94	2	1
1:B:304:VAL:O	1:B:307:VAL:HG23	0.40	2.16	3	1
1:B:237:LEU:CD2	1:C:298:LEU:HD22	0.40	2.46	6	1
1:C:217:GLU:CG	1:C:277:VAL:HG21	0.40	2.46	6	1
1:A:246:LEU:HD11	1:A:300:GLU:CD	0.40	2.37	7	1
1:C:220:LEU:HD12	1:C:273:SER:HB3	0.40	1.94	10	1
1:D:304:VAL:O	1:D:307:VAL:HG23	0.40	2.16	1	1
1:A:403:PHE:N	1:A:404:PRO:CD	0.40	2.84	2	1
1:B:403:PHE:N	1:B:404:PRO:CD	0.40	2.84	2	1
1:B:241:SER:OG	1:C:302:ALA:HB2	0.40	2.16	4	1
1:A:305:ASN:HB2	1:E:244:ILE:HD12	0.40	1.93	6	1
1:C:304:VAL:HG23	1:C:391:ARG:NH1	0.40	2.30	8	1
1:A:298:LEU:HD22	1:E:237:LEU:HB3	0.40	1.92	10	1
1:A:244:ILE:HD12	1:B:305:ASN:HB2	0.40	1.94	15	1
1:D:236:ILE:CG1	1:D:406:ALA:HB1	0.40	2.47	11	1
1:B:216:LEU:HD13	1:B:219:GLN:HE21	0.40	1.76	13	1
1:D:310:GLN:NE2	1:D:315:GLY:H	0.40	2.13	7	1
1:A:318:PHE:HD2	1:A:389:ILE:HG23	0.40	1.77	13	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/150 (92%)	129±1 (93±1%)	7±1 (5±1%)	2±1 (1±1%)	15	61
1	B	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	14	59
1	C	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	16	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	138/150 (92%)	129±1 (93±1%)	7±1 (5±1%)	2±1 (1±1%)	15	61
1	E	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	15	61
All	All	10350/11250 (92%)	9653 (93%)	553 (5%)	144 (1%)	15	61

All 44 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	288	ALA	15
1	B	288	ALA	15
1	C	288	ALA	15
1	D	288	ALA	15
1	E	288	ALA	15
1	A	247	ASP	4
1	B	247	ASP	4
1	D	247	ASP	4
1	E	247	ASP	4
1	A	312	GLU	4
1	B	312	GLU	4
1	C	312	GLU	4
1	D	312	GLU	4
1	E	312	GLU	4
1	C	247	ASP	3
1	B	394	LYS	2
1	B	395	ILE	1
1	A	314	GLY	1
1	B	314	GLY	1
1	C	314	GLY	1
1	D	314	GLY	1
1	D	394	LYS	1
1	E	314	GLY	1
1	E	394	LYS	1
1	A	396	ASP	1
1	B	396	ASP	1
1	C	396	ASP	1
1	D	396	ASP	1
1	E	396	ASP	1
1	A	289	VAL	1
1	A	290	CYS	1
1	B	289	VAL	1
1	B	290	CYS	1
1	C	289	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	C	290	CYS	1
1	D	289	VAL	1
1	D	290	CYS	1
1	E	289	VAL	1
1	E	290	CYS	1
1	A	398	ILE	1
1	B	398	ILE	1
1	C	398	ILE	1
1	D	398	ILE	1
1	E	398	ILE	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/130 (91%)	87±5 (74±4%)	31±5 (26±4%)	2	22
1	B	118/130 (91%)	86±4 (72±4%)	32±4 (28±4%)	2	20
1	C	119/130 (92%)	88±5 (74±4%)	31±5 (26±4%)	2	23
1	D	119/130 (92%)	87±4 (73±4%)	32±4 (27±4%)	2	21
1	E	119/130 (92%)	85±3 (72±3%)	34±3 (28±3%)	2	19
All	All	8895/9750 (91%)	6487 (73%)	2408 (27%)	2	21

All 435 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	239	TRP	15
1	B	239	TRP	15
1	C	239	TRP	15
1	D	239	TRP	15
1	E	239	TRP	15
1	A	247	ASP	14
1	B	247	ASP	14
1	E	218	ARG	14
1	A	300	GLU	13
1	B	300	GLU	13

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Mol	Chain	Res	Type	Models (Total)
1	D	300	GLU	13
1	E	300	GLU	13
1	E	420	ILE	13
1	D	312	GLU	13
1	A	218	ARG	12
1	A	266	GLN	12
1	A	296	SER	12
1	A	405	LEU	12
1	A	413	PHE	12
1	A	420	ILE	12
1	B	266	GLN	12
1	B	296	SER	12
1	B	405	LEU	12
1	B	413	PHE	12
1	B	420	ILE	12
1	C	266	GLN	12
1	C	296	SER	12
1	C	311	ARG	12
1	C	405	LEU	12
1	C	413	PHE	12
1	C	420	ILE	12
1	C	423	ARG	12
1	D	218	ARG	12
1	D	266	GLN	12
1	D	296	SER	12
1	D	405	LEU	12
1	D	413	PHE	12
1	D	420	ILE	12
1	E	266	GLN	12
1	E	296	SER	12
1	E	405	LEU	12
1	E	413	PHE	12
1	A	238	SER	11
1	A	279	TYR	11
1	A	301	TYR	11
1	B	238	SER	11
1	B	252	ARG	11
1	B	279	TYR	11
1	B	301	TYR	11
1	B	311	ARG	11
1	C	238	SER	11
1	C	301	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	D	238	SER	11
1	D	301	TYR	11
1	D	423	ARG	11
1	E	238	SER	11
1	E	252	ARG	11
1	E	301	TYR	11
1	B	422	ARG	11
1	D	397	LYS	11
1	A	252	ARG	10
1	A	287	LEU	10
1	B	218	ARG	10
1	B	287	LEU	10
1	B	306	PHE	10
1	C	218	ARG	10
1	D	252	ARG	10
1	D	279	TYR	10
1	D	287	LEU	10
1	E	279	TYR	10
1	E	287	LEU	10
1	E	308	SER	10
1	E	397	LYS	10
1	E	423	ARG	10
1	A	281	LYS	10
1	B	281	LYS	10
1	C	276	LYS	10
1	D	281	LYS	10
1	E	281	LYS	10
1	E	306	PHE	10
1	E	247	ASP	10
1	A	224	LEU	10
1	B	224	LEU	10
1	C	224	LEU	10
1	D	224	LEU	10
1	E	224	LEU	10
1	A	391	ARG	9
1	A	422	ARG	9
1	C	252	ARG	9
1	C	391	ARG	9
1	C	396	ASP	9
1	D	391	ARG	9
1	D	393	LYS	9
1	E	246	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	E	391	ARG	9
1	E	396	ASP	9
1	A	305	ASN	9
1	A	306	PHE	9
1	A	411	ASN	9
1	B	274	LEU	9
1	B	411	ASN	9
1	C	411	ASN	9
1	D	305	ASN	9
1	D	411	ASN	9
1	E	305	ASN	9
1	E	411	ASN	9
1	D	276	LYS	9
1	E	215	MET	9
1	B	396	ASP	9
1	A	423	ARG	8
1	B	308	SER	8
1	C	243	TRP	8
1	D	215	MET	8
1	D	308	SER	8
1	E	216	LEU	8
1	E	243	TRP	8
1	E	393	LYS	8
1	A	216	LEU	8
1	B	305	ASN	8
1	B	393	LYS	8
1	C	274	LEU	8
1	C	281	LYS	8
1	E	312	GLU	8
1	A	274	LEU	8
1	A	407	PHE	8
1	B	407	PHE	8
1	C	407	PHE	8
1	D	274	LEU	8
1	D	407	PHE	8
1	E	407	PHE	8
1	A	396	ASP	8
1	A	261	LEU	7
1	A	284	ASP	7
1	A	393	LYS	7
1	B	216	LEU	7
1	B	261	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	B	284	ASP	7
1	B	312	GLU	7
1	B	391	ARG	7
1	B	397	LYS	7
1	C	215	MET	7
1	C	261	LEU	7
1	C	287	LEU	7
1	C	300	GLU	7
1	C	305	ASN	7
1	D	247	ASP	7
1	D	261	LEU	7
1	D	284	ASP	7
1	D	396	ASP	7
1	E	261	LEU	7
1	E	284	ASP	7
1	A	419	LYS	7
1	B	276	LYS	7
1	B	419	LYS	7
1	C	306	PHE	7
1	C	419	LYS	7
1	D	419	LYS	7
1	E	419	LYS	7
1	A	220	LEU	7
1	A	243	TRP	7
1	B	220	LEU	7
1	C	220	LEU	7
1	C	308	SER	7
1	C	397	LYS	7
1	D	220	LEU	7
1	E	220	LEU	7
1	E	274	LEU	7
1	D	306	PHE	7
1	A	226	GLN	6
1	A	276	LYS	6
1	B	226	GLN	6
1	B	394	LYS	6
1	C	226	GLN	6
1	C	393	LYS	6
1	D	226	GLN	6
1	E	226	GLN	6
1	E	311	ARG	6
1	E	422	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	415	TRP	6
1	B	415	TRP	6
1	C	313	PHE	6
1	C	415	TRP	6
1	D	415	TRP	6
1	E	415	TRP	6
1	A	311	ARG	6
1	B	246	LEU	6
1	D	422	ARG	6
1	B	313	PHE	6
1	B	243	TRP	6
1	B	389	ILE	5
1	C	247	ASP	5
1	C	389	ILE	5
1	C	422	ARG	5
1	D	216	LEU	5
1	E	310	GLN	5
1	A	228	TYR	5
1	A	267	SER	5
1	A	299	LEU	5
1	B	228	TYR	5
1	B	267	SER	5
1	B	299	LEU	5
1	C	228	TYR	5
1	C	267	SER	5
1	C	394	LYS	5
1	D	228	TYR	5
1	D	267	SER	5
1	D	299	LEU	5
1	E	228	TYR	5
1	E	267	SER	5
1	E	276	LYS	5
1	E	299	LEU	5
1	A	229	ILE	5
1	B	229	ILE	5
1	C	229	ILE	5
1	C	390	GLN	5
1	D	229	ILE	5
1	D	243	TRP	5
1	E	229	ILE	5
1	A	246	LEU	5
1	A	312	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	C	299	LEU	5
1	B	309	ARG	5
1	C	284	ASP	4
1	D	311	ARG	4
1	A	400	ARG	4
1	B	400	ARG	4
1	C	400	ARG	4
1	D	271	ARG	4
1	D	310	GLN	4
1	D	313	PHE	4
1	D	400	ARG	4
1	E	394	LYS	4
1	E	400	ARG	4
1	A	410	PHE	4
1	B	410	PHE	4
1	C	216	LEU	4
1	C	410	PHE	4
1	D	246	LEU	4
1	D	410	PHE	4
1	E	410	PHE	4
1	A	231	SER	4
1	A	397	LYS	4
1	B	231	SER	4
1	C	231	SER	4
1	C	246	LEU	4
1	C	285	ILE	4
1	D	231	SER	4
1	E	231	SER	4
1	A	255	LEU	4
1	B	255	LEU	4
1	C	255	LEU	4
1	D	255	LEU	4
1	E	255	LEU	4
1	A	310	GLN	4
1	C	310	GLN	4
1	A	403	PHE	4
1	B	403	PHE	4
1	C	403	PHE	4
1	D	403	PHE	4
1	E	403	PHE	4
1	C	279	TYR	4
1	C	309	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	D	389	ILE	3
1	E	309	ARG	3
1	A	390	GLN	3
1	A	273	SER	3
1	B	273	SER	3
1	C	273	SER	3
1	C	312	GLU	3
1	D	273	SER	3
1	D	390	GLN	3
1	E	217	GLU	3
1	E	273	SER	3
1	A	217	GLU	3
1	A	241	SER	3
1	B	241	SER	3
1	C	241	SER	3
1	D	241	SER	3
1	E	241	SER	3
1	E	395	ILE	3
1	A	285	ILE	3
1	A	398	ILE	3
1	B	285	ILE	3
1	B	398	ILE	3
1	C	217	GLU	3
1	C	398	ILE	3
1	D	285	ILE	3
1	D	398	ILE	3
1	E	285	ILE	3
1	E	318	PHE	3
1	E	398	ILE	3
1	A	399	SER	3
1	A	408	LEU	3
1	B	399	SER	3
1	B	408	LEU	3
1	C	271	ARG	3
1	C	399	SER	3
1	C	408	LEU	3
1	D	399	SER	3
1	D	408	LEU	3
1	E	271	ARG	3
1	E	399	SER	3
1	E	408	LEU	3
1	A	271	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	318	PHE	3
1	B	423	ARG	3
1	D	318	PHE	3
1	A	240	ILE	3
1	A	308	SER	3
1	A	309	ARG	3
1	B	240	ILE	3
1	B	310	GLN	3
1	C	240	ILE	3
1	D	240	ILE	3
1	E	240	ILE	3
1	A	242	PHE	2
1	A	292	LEU	2
1	B	242	PHE	2
1	B	292	LEU	2
1	C	242	PHE	2
1	C	291	LEU	2
1	D	242	PHE	2
1	D	292	LEU	2
1	D	394	LYS	2
1	D	395	ILE	2
1	E	242	PHE	2
1	E	292	LEU	2
1	A	222	TYR	2
1	A	295	PHE	2
1	A	389	ILE	2
1	B	222	TYR	2
1	B	295	PHE	2
1	C	222	TYR	2
1	C	277	VAL	2
1	C	295	PHE	2
1	D	222	TYR	2
1	D	295	PHE	2
1	E	222	TYR	2
1	E	295	PHE	2
1	A	268	SER	2
1	B	268	SER	2
1	B	271	ARG	2
1	C	268	SER	2
1	D	268	SER	2
1	E	234	ILE	2
1	E	268	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	E	389	ILE	2
1	A	394	LYS	2
1	A	418	TYR	2
1	B	418	TYR	2
1	C	418	TYR	2
1	D	418	TYR	2
1	E	418	TYR	2
1	B	395	ILE	2
1	E	313	PHE	2
1	A	395	ILE	2
1	A	264	THR	2
1	B	264	THR	2
1	C	264	THR	2
1	C	395	ILE	2
1	D	264	THR	2
1	E	264	THR	2
1	B	318	PHE	2
1	A	289	VAL	1
1	B	289	VAL	1
1	C	292	LEU	1
1	D	289	VAL	1
1	D	309	ARG	1
1	E	289	VAL	1
1	E	390	GLN	1
1	B	217	GLU	1
1	D	217	GLU	1
1	A	223	TYR	1
1	A	234	ILE	1
1	B	223	TYR	1
1	B	234	ILE	1
1	C	223	TYR	1
1	C	234	ILE	1
1	D	223	TYR	1
1	D	234	ILE	1
1	E	223	TYR	1
1	A	237	LEU	1
1	B	237	LEU	1
1	C	237	LEU	1
1	D	237	LEU	1
1	E	237	LEU	1
1	B	244	ILE	1
1	C	244	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	D	244	ILE	1
1	E	244	ILE	1
1	A	233	LEU	1
1	A	270	SER	1
1	A	313	PHE	1
1	B	233	LEU	1
1	B	270	SER	1
1	C	233	LEU	1
1	C	270	SER	1
1	D	233	LEU	1
1	D	270	SER	1
1	E	233	LEU	1
1	E	270	SER	1
1	A	293	PHE	1
1	B	293	PHE	1
1	C	293	PHE	1
1	C	318	PHE	1
1	D	293	PHE	1
1	E	293	PHE	1
1	C	278	SER	1
1	A	277	VAL	1
1	A	286	TRP	1
1	A	414	TYR	1
1	B	277	VAL	1
1	B	286	TRP	1
1	B	414	TYR	1
1	C	219	GLN	1
1	C	286	TRP	1
1	C	414	TYR	1
1	D	277	VAL	1
1	D	286	TRP	1
1	D	414	TYR	1
1	E	219	GLN	1
1	E	277	VAL	1
1	E	286	TRP	1
1	E	414	TYR	1
1	A	227	LEU	1
1	A	298	LEU	1
1	B	227	LEU	1
1	B	298	LEU	1
1	C	227	LEU	1
1	C	298	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	D	227	LEU	1
1	D	298	LEU	1
1	E	227	LEU	1
1	E	298	LEU	1
1	C	294	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 11% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1145
Number of shifts mapped to atoms	1145
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	133	-0.30 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	112	0.27 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	18	—	None (insufficient data)
^{15}N	146	0.96 ± 0.20	Should be applied

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 11%, i.e. 1085 atoms were assigned a chemical shift out of a possible 10225. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	524/3470 (15%)	252/1411 (18%)	138/1386 (10%)	134/673 (20%)
Sidechain	544/5700 (10%)	414/3786 (11%)	121/1709 (7%)	9/205 (4%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	17/1055 (2%)	17/510 (3%)	0/525 (0%)	0/20 (0%)
Overall	1085/10225 (11%)	683/5707 (12%)	259/3620 (7%)	143/898 (16%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 1144 atoms were assigned a chemical shift out of a possible 11020. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	566/3755 (15%)	269/1525 (18%)	151/1500 (10%)	146/730 (20%)
Sidechain	561/5950 (9%)	420/3940 (11%)	132/1805 (7%)	9/205 (4%)
Aromatic	17/1315 (1%)	17/655 (3%)	0/610 (0%)	0/50 (0%)
Overall	1144/11020 (10%)	706/6120 (12%)	283/3915 (7%)	155/985 (16%)

7.1.4 Statistically unusual chemical shifts (i)

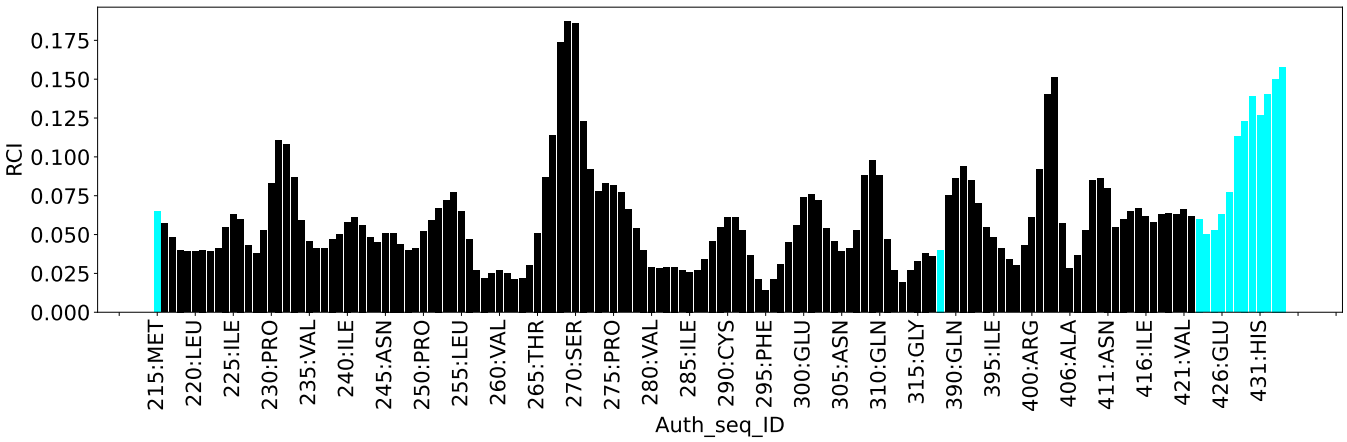
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	257	ILE	HB	3.24	0.35 – 3.22	5.1

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:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
215:MET
220:LEU
225:ILE
230:PRO
235:VAL
240:ILE
245:ASN
250:PRO
255:LEU
260:VAL
265:THR
270:SER
275:PRO
280:VAL
285:ILE
290:CYS
295:PHE
300:GLU
305:ASN
310:GLN
315:GLY
390:GLN
395:ILE
400:ARG
406:ALA
411:ASN
416:ILE
421:VAL
426:GLU
431:HIS
Auth_seq_ID

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	2070
Intra-residue (|i-j|=0)	320
Sequential (|i-j|=1)	341
Medium range (|i-j|>1 and |i-j|<5)	320
Long range (|i-j|≥5)	244
Inter-chain	335
Hydrogen bond restraints	510
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	5
Number of restraints per residue	2.8
Number of long range restraints per residue[1]	0.3

[1]Long 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)	18.4	0.2
0.2-0.5 (Medium)	43.7	0.5
>0.5 (Large)	279.0	7.82

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

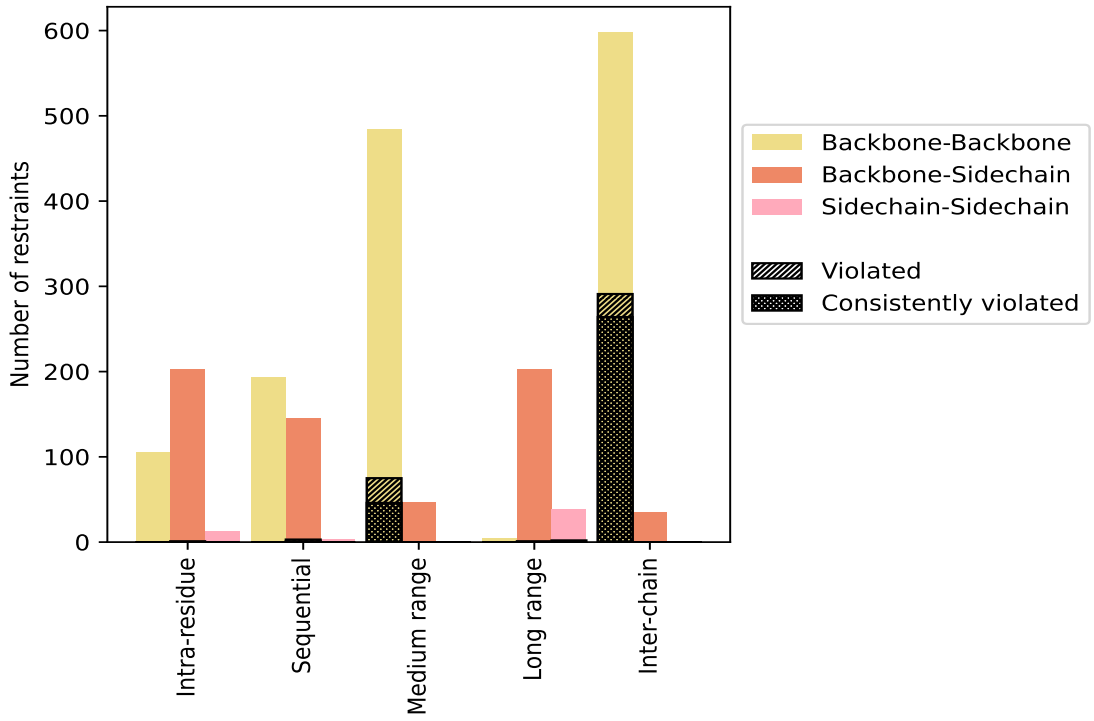
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	320	15.5	1	0.3	0.0	0	0.0	0.0
Backbone-Backbone	105	5.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	202	9.8	1	0.5	0.0	0	0.0	0.0
Sidechain-Sidechain	13	0.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	341	16.5	3	0.9	0.1	1	0.3	0.0
Backbone-Backbone	193	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	145	7.0	3	2.1	0.1	1	0.7	0.0
Sidechain-Sidechain	3	0.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	320	15.5	18	5.6	0.9	2	0.6	0.1
Backbone-Backbone	272	13.1	18	6.6	0.9	2	0.7	0.1
Backbone-Sidechain	47	2.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	244	11.8	3	1.2	0.1	0	0.0	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	202	9.8	1	0.5	0.0	0	0.0	0.0
Sidechain-Sidechain	38	1.8	2	5.3	0.1	0	0.0	0.0
Inter-chain	335	16.2	147	43.9	7.1	130	38.8	6.3
Backbone-Backbone	300	14.5	147	49.0	7.1	130	43.3	6.3
Backbone-Sidechain	35	1.7	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	510	24.6	201	39.4	9.7	178	34.9	8.6
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2070	100.0	373	18.0	18.0	311	15.0	15.0
Backbone-Backbone	1384	66.9	366	26.4	17.7	310	22.4	15.0
Backbone-Sidechain	631	30.5	5	0.8	0.2	1	0.2	0.0
Sidechain-Sidechain	55	2.7	2	3.6	0.1	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



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

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	2	63	3	277	345	2.36	7.74	1.96	2.07
2	1	1	53	1	284	340	2.49	7.82	1.83	2.35
3	0	1	61	3	286	351	2.26	7.78	1.92	1.95
4	1	2	55	2	279	339	2.45	7.8	1.88	2.21
5	0	1	59	3	284	347	2.49	7.82	1.87	2.22
6	0	1	59	2	279	341	2.36	7.55	1.94	2.16
7	0	2	58	2	269	331	2.41	7.3	1.91	2.15
8	0	3	59	2	274	338	2.4	7.49	1.93	2.05
9	0	1	59	2	284	346	2.36	7.79	1.94	2.1
10	0	1	60	3	279	343	2.34	7.65	1.95	2.1
11	0	1	57	3	269	330	2.38	7.57	1.95	2.14

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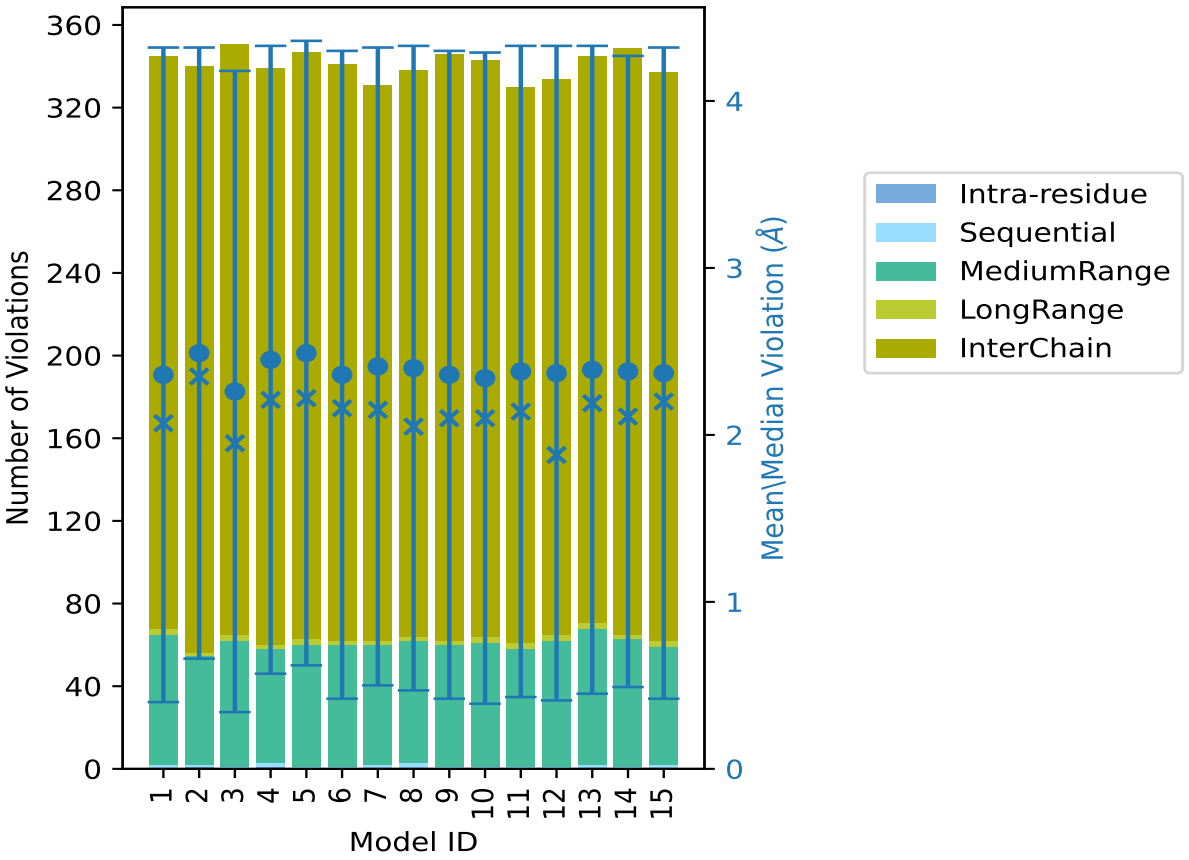
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	1	61	3	269	334	2.37	7.79	1.96	1.88
13	0	2	66	3	274	345	2.39	7.68	1.94	2.19
14	0	1	62	2	284	349	2.38	7.49	1.89	2.11
15	0	2	57	3	275	337	2.37	7.48	1.95	2.2

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

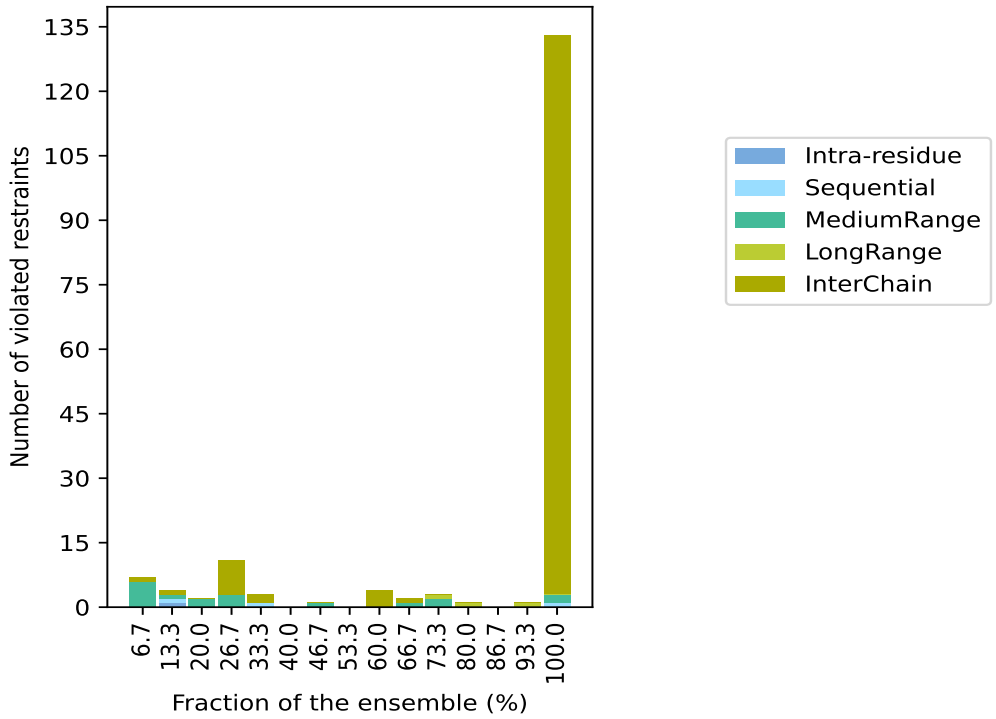
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints

for a given fraction of the ensemble. In total, 1388(IR:319, SQ:338, MR:302, LR:241, IC:188) 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]	%
0	0	6	0	1	7	1	6.7
1	1	1	0	1	4	2	13.3
0	0	2	0	0	2	3	20.0
0	0	3	0	8	11	4	26.7
0	1	0	0	2	3	5	33.3
0	0	0	0	0	0	6	40.0
0	0	1	0	0	1	7	46.7
0	0	0	0	0	0	8	53.3
0	0	0	0	4	4	9	60.0
0	0	1	0	1	2	10	66.7
0	0	2	1	0	3	11	73.3
0	0	0	1	0	1	12	80.0
0	0	0	0	0	0	13	86.7
0	0	0	1	0	1	14	93.3
0	1	2	0	130	133	15	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

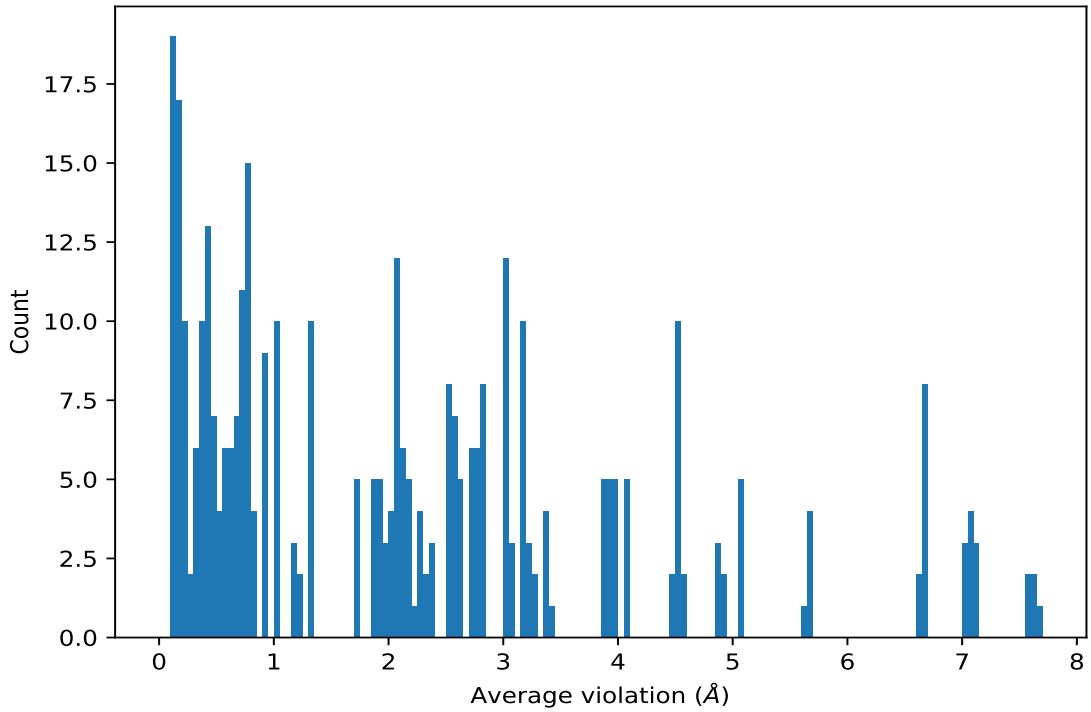
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance 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



9.4.2 Table: Most violated distance restraints (i)

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)
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	15	7.65	0.15	7.68
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	15	7.63	0.16	7.66
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	15	7.61	0.16	7.62
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	15	7.6	0.17	7.61
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	15	7.59	0.16	7.57
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	15	7.14	0.12	7.2
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	15	7.13	0.1	7.17
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	15	7.11	0.12	7.14
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	15	7.1	0.12	7.16
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	15	7.07	0.12	7.13
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	15	7.06	0.16	7.1
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	15	7.06	0.15	7.07
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	15	7.03	0.16	7.08
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	15	7.03	0.16	7.1
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	15	7.03	0.15	7.1
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	15	6.69	0.03	6.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	15	6.68	0.02	6.68
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	15	6.67	0.01	6.67
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	15	6.67	0.2	6.72
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	15	6.66	0.02	6.66
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	15	6.66	0.02	6.66
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	15	6.65	0.22	6.74
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	15	6.65	0.22	6.74
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	15	6.61	0.21	6.69
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	15	6.61	0.23	6.66
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	15	5.67	0.03	5.67
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	15	5.66	0.02	5.67
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	15	5.65	0.02	5.66
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	15	5.65	0.06	5.67
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	15	5.64	0.04	5.66
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	15	5.1	0.1	5.15
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	15	5.1	0.09	5.11
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	15	5.09	0.1	5.08
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	15	5.09	0.1	5.11
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	15	5.09	0.1	5.08
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	15	4.91	0.23	4.96
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	15	4.9	0.22	4.98
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	15	4.89	0.23	4.97
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	15	4.88	0.23	4.96
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	15	4.88	0.23	4.93
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	15	4.57	0.11	4.57
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	15	4.57	0.11	4.59
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	15	4.54	0.1	4.5
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	15	4.53	0.09	4.52
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	15	4.53	0.11	4.51
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	15	4.53	0.01	4.53
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	15	4.52	0.15	4.55
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	15	4.52	0.19	4.6
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	15	4.51	0.02	4.51
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	15	4.5	0.01	4.5
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	15	4.5	0.03	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	15	4.5	0.01	4.5
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	15	4.48	0.19	4.58
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	15	4.45	0.15	4.5
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	15	4.08	0.07	4.1
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	15	4.08	0.07	4.1
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	15	4.07	0.07	4.09
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	15	4.07	0.09	4.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	15	4.07	0.05	4.07
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	15	3.98	0.03	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	15	3.97	0.02	3.98
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	15	3.96	0.02	3.96
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	15	3.96	0.02	3.95
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	15	3.96	0.02	3.95
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	15	3.94	0.09	3.96
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	15	3.93	0.09	3.96
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	15	3.93	0.09	3.96
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	15	3.93	0.09	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	15	3.92	0.09	3.95
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	15	3.89	0.03	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	15	3.89	0.01	3.89
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	15	3.87	0.01	3.88
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	15	3.87	0.03	3.87
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	15	3.86	0.05	3.88
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	15	3.43	0.15	3.48
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	15	3.4	0.14	3.45
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	15	3.4	0.14	3.46
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	15	3.39	0.15	3.42
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	15	3.39	0.14	3.42
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	15	3.26	0.24	3.36
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	15	3.25	0.23	3.31
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	15	3.24	0.23	3.34
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	15	3.23	0.23	3.3
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	15	3.21	0.23	3.3
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	15	3.19	0.36	3.16
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	15	3.19	0.68	3.4
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	15	3.19	0.36	3.19
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	15	3.19	0.68	3.38
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	15	3.19	0.68	3.38
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	15	3.18	0.67	3.38
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	15	3.18	0.67	3.38
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	15	3.18	0.36	3.17
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	15	3.17	0.36	3.16
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	15	3.16	0.35	3.17
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	15	3.08	0.21	3.04
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	15	3.07	0.2	3.0
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	15	3.06	0.2	2.99
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	15	3.05	0.21	3.0
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	15	3.05	0.23	3.05
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	15	3.05	0.23	3.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	15	3.05	0.21	3.02
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	15	3.04	0.24	3.04
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	15	3.04	0.18	3.06
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	15	3.03	0.21	3.07
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	15	3.03	0.23	3.06
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	15	3.03	0.19	3.06
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	15	3.03	0.18	3.06
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	15	3.02	0.18	3.06
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	15	3.01	0.17	3.07
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	15	2.84	0.03	2.84
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	15	2.84	0.01	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	15	2.84	0.01	2.84
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	15	2.84	0.01	2.84
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	15	2.83	0.02	2.83
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	15	2.82	0.07	2.83
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	15	2.81	0.05	2.82
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	15	2.81	0.06	2.83
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	15	2.8	0.06	2.82
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	15	2.8	0.06	2.82
(5,428)	1:B:265:THR:O	1:E:265:THR:O	15	2.79	0.37	2.83
(5,468)	1:C:265:THR:O	1:E:265:THR:O	15	2.77	0.38	2.82
(5,348)	1:A:265:THR:O	1:D:265:THR:O	15	2.76	0.38	2.85
(5,408)	1:B:265:THR:O	1:D:265:THR:O	15	2.76	0.38	2.81
(5,328)	1:A:265:THR:O	1:C:265:THR:O	15	2.74	0.39	2.82
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	15	2.72	0.25	2.77
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	15	2.72	0.24	2.79
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	15	2.72	0.25	2.76
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	15	2.72	0.25	2.76
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	15	2.71	0.24	2.76
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	15	2.63	0.17	2.55
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	15	2.62	0.22	2.66
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	15	2.62	0.21	2.65
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	15	2.61	0.22	2.62
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	15	2.61	0.23	2.61
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	15	2.59	0.22	2.61
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	15	2.59	0.18	2.51
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	15	2.59	0.18	2.51
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	15	2.59	0.18	2.51
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	15	2.58	0.16	2.51
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	15	2.57	0.25	2.6
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	15	2.57	0.25	2.59
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	15	2.55	0.26	2.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	15	2.54	0.25	2.55
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	15	2.54	0.25	2.57
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	15	2.53	0.37	2.61
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	15	2.53	0.38	2.58
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	15	2.52	0.37	2.6
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	15	2.52	0.38	2.59
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	15	2.51	0.37	2.58
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	15	2.37	0.42	2.49
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	15	2.36	0.43	2.5
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	15	2.35	0.42	2.48
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	15	2.34	0.41	2.46
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	15	2.34	0.42	2.47
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	15	2.28	0.15	2.27
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	15	2.26	0.16	2.24
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	15	2.26	0.16	2.23
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	15	2.25	0.16	2.21
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	15	2.24	0.16	2.2
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	15	2.19	0.17	2.25
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	15	2.18	0.17	2.24
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	15	2.18	0.18	2.25
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	15	2.18	0.17	2.24
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	15	2.16	0.18	2.22
(5,368)	1:A:265:THR:O	1:E:265:THR:O	15	2.14	0.23	2.18
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	15	2.12	0.23	2.1
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	15	2.1	0.24	2.07
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	15	2.1	0.24	2.07
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	15	2.1	0.24	2.07
(5,448)	1:C:265:THR:O	1:D:265:THR:O	15	2.1	0.24	2.14
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	15	2.08	0.24	2.04
(5,308)	1:A:265:THR:O	1:B:265:THR:O	15	2.07	0.24	2.12
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	15	2.07	0.3	1.9
(5,488)	1:D:265:THR:O	1:E:265:THR:O	15	2.07	0.24	2.11
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	15	2.07	0.3	1.92
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	15	2.07	0.32	1.99
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	15	2.06	0.3	1.9
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	15	2.06	0.3	1.93
(5,388)	1:B:265:THR:O	1:C:265:THR:O	15	2.06	0.24	2.1
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	15	2.06	0.31	1.98
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	15	2.06	0.32	2.01
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	15	2.06	0.32	1.98
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	15	2.05	0.18	2.03
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	15	2.05	0.3	1.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	15	2.04	0.32	1.98
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	15	2.0	0.18	1.95
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	15	1.99	0.19	2.0
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	15	1.99	0.19	1.97
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	15	1.99	0.19	1.99
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	15	1.95	0.23	1.99
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	15	1.95	0.22	2.0
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	15	1.94	0.23	1.96
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	15	1.93	0.23	1.97
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	15	1.93	0.23	1.96
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	15	1.88	0.22	1.83
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	15	1.86	0.22	1.82
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	15	1.86	0.22	1.81
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	15	1.86	0.23	1.79
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	15	1.85	0.22	1.82
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	15	1.74	0.09	1.77
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	15	1.73	0.11	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	15	1.72	0.11	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	15	1.71	0.11	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	15	1.71	0.11	1.76
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	15	1.34	0.1	1.37
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	15	1.34	0.29	1.3
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	15	1.34	0.1	1.37
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	15	1.34	0.3	1.31
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	15	1.34	0.3	1.28
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	15	1.33	0.1	1.37
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	15	1.32	0.3	1.25
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	15	1.32	0.1	1.36
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	15	1.32	0.1	1.35
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	15	1.32	0.3	1.26
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	15	1.23	0.06	1.24
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	15	1.21	0.06	1.22
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	15	1.2	0.06	1.22
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	15	1.19	0.07	1.22
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	15	1.18	0.06	1.2
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	15	1.04	0.4	1.08
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	15	1.04	0.25	1.09
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	15	1.03	0.39	1.09
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	15	1.03	0.39	1.07
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	15	1.02	0.39	1.09
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	15	1.02	0.24	1.05
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	15	1.01	0.24	1.04

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	15	1.0	0.24	1.05
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	15	1.0	0.38	1.06
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	15	1.0	0.24	1.02
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	15	0.83	0.25	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	15	0.81	0.01	0.81
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	15	0.8	0.25	0.79
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	15	0.79	0.01	0.8
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	15	0.79	0.25	0.78
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	15	0.78	0.25	0.78
(5,361)	1:A:231:SER:O	1:E:231:SER:O	15	0.78	0.39	0.57
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	15	0.78	0.25	0.76
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	15	0.77	0.32	0.81
(5,301)	1:A:231:SER:O	1:B:231:SER:O	15	0.76	0.41	0.52
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	15	0.76	0.01	0.75
(5,441)	1:C:231:SER:O	1:D:231:SER:O	15	0.75	0.4	0.55
(5,481)	1:D:231:SER:O	1:E:231:SER:O	15	0.75	0.4	0.53
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	15	0.75	0.14	0.8
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	15	0.74	0.03	0.73
(5,381)	1:B:231:SER:O	1:C:231:SER:O	15	0.74	0.4	0.55
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	15	0.73	0.33	0.76
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	15	0.73	0.33	0.79
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	15	0.73	0.02	0.73
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	15	0.72	0.09	0.72
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	15	0.72	0.03	0.72
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	15	0.71	0.33	0.75
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	15	0.71	0.33	0.77
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	15	0.71	0.03	0.7
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	15	0.7	0.03	0.69
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	15	0.7	0.03	0.7
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	15	0.68	0.02	0.69
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	15	0.68	0.08	0.7
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	15	0.68	0.01	0.68
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	15	0.66	0.04	0.65
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	15	0.65	0.02	0.63
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	15	0.63	0.08	0.66
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	15	0.62	0.06	0.59
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	15	0.62	0.14	0.67
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	15	0.61	0.04	0.62
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	15	0.61	0.04	0.6
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	15	0.57	0.11	0.58
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	15	0.57	0.02	0.57
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	15	0.57	0.05	0.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	15	0.55	0.16	0.61
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	15	0.55	0.06	0.56
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	15	0.54	0.02	0.54
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	15	0.52	0.14	0.46
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	15	0.5	0.04	0.5
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	15	0.5	0.11	0.5
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	15	0.49	0.13	0.43
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	15	0.47	0.14	0.41
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	15	0.47	0.14	0.41
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	15	0.45	0.08	0.5
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	15	0.45	0.07	0.44
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	15	0.45	0.05	0.43
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	15	0.44	0.14	0.39
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	15	0.44	0.14	0.37
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	15	0.44	0.06	0.41
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	15	0.43	0.06	0.4
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	15	0.43	0.11	0.42
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	15	0.43	0.06	0.39
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	15	0.41	0.02	0.41
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	15	0.41	0.1	0.41
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	15	0.4	0.04	0.4
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	15	0.38	0.03	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	15	0.38	0.01	0.38
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	15	0.38	0.09	0.39
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	15	0.37	0.01	0.37
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	15	0.37	0.01	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	15	0.37	0.01	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	15	0.36	0.01	0.37
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	15	0.36	0.01	0.36
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	15	0.36	0.01	0.36
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	15	0.35	0.02	0.35
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	15	0.34	0.1	0.34
(2,22)	1:A:258:THR:O	1:A:262:THR:N	15	0.34	0.07	0.38
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	15	0.32	0.19	0.31
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	15	0.29	0.04	0.3
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	15	0.28	0.08	0.27
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	15	0.24	0.1	0.24
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	15	0.22	0.03	0.22
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	15	0.22	0.03	0.22
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	15	0.19	0.02	0.19
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	15	0.17	0.06	0.15
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	15	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	15	0.13	0.01	0.13
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	14	0.63	0.19	0.71
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	14	0.6	0.13	0.64
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	14	0.32	0.08	0.32
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	14	0.2	0.04	0.2
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	14	0.17	0.04	0.17
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	14	0.17	0.04	0.17
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	14	0.17	0.04	0.17
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	14	0.17	0.04	0.17
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	14	0.14	0.02	0.13
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	13	0.79	0.34	0.69
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	13	0.77	0.35	0.68
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	13	0.76	0.34	0.68
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	13	0.76	0.34	0.67
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	13	0.73	0.34	0.62
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	12	0.16	0.04	0.15
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	12	0.15	0.02	0.14
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	12	0.12	0.01	0.12
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	11	0.18	0.0	0.18
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	11	0.16	0.03	0.16
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	11	0.16	0.04	0.17
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	11	0.12	0.01	0.11
(5,341)	1:A:231:SER:O	1:D:231:SER:O	10	0.92	0.6	0.84
(5,421)	1:B:231:SER:O	1:E:231:SER:O	10	0.92	0.6	0.85
(5,321)	1:A:231:SER:O	1:C:231:SER:O	10	0.91	0.61	0.83
(5,461)	1:C:231:SER:O	1:E:231:SER:O	10	0.91	0.6	0.86
(5,401)	1:B:231:SER:O	1:D:231:SER:O	10	0.9	0.6	0.84
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	10	0.84	0.46	0.73
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	10	0.22	0.08	0.22
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	10	0.14	0.02	0.14
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	9	0.93	0.4	0.78
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	9	0.92	0.41	0.75
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	9	0.92	0.4	0.78
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	9	0.9	0.4	0.76
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	9	0.36	0.16	0.46
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	7	0.12	0.01	0.12
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	6	0.11	0.01	0.11

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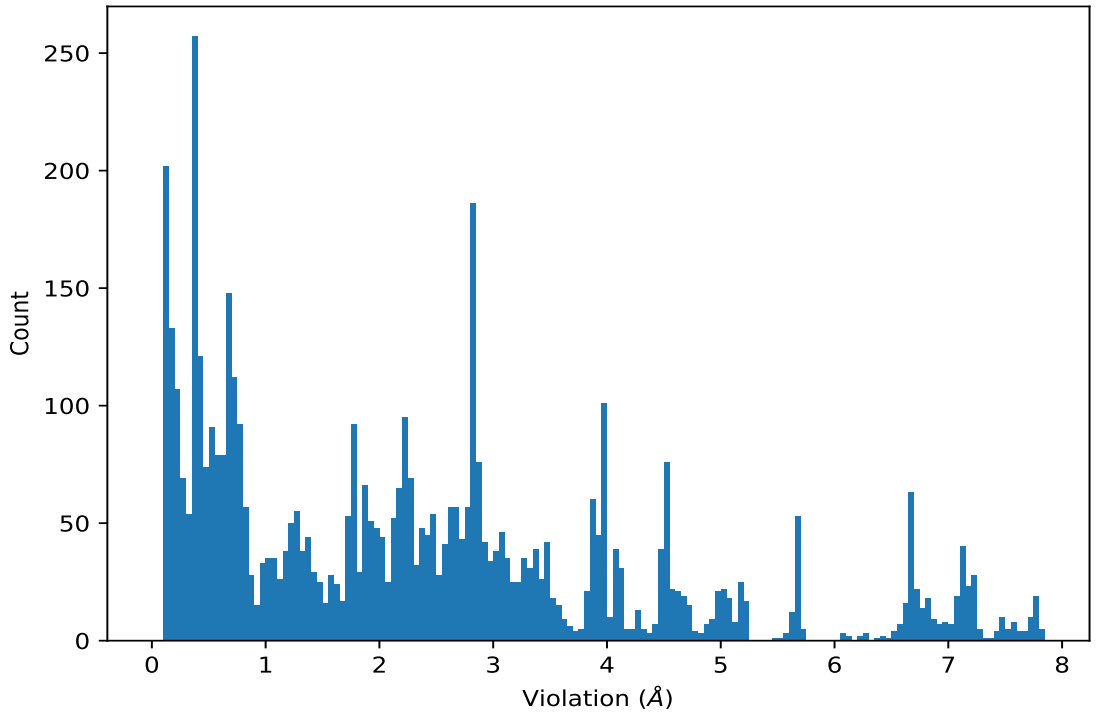
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	5	0.2	0.04	0.21
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	5	0.18	0.05	0.21
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	5	0.13	0.01	0.13
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	5	0.13	0.01	0.13
(5,423)	1:B:226:GLN:H	1:E:226:GLN:H	4	0.46	0.24	0.36
(5,343)	1:A:226:GLN:H	1:D:226:GLN:H	4	0.44	0.25	0.34
(5,463)	1:C:226:GLN:H	1:E:226:GLN:H	4	0.43	0.25	0.32
(5,323)	1:A:226:GLN:H	1:C:226:GLN:H	4	0.43	0.26	0.32
(5,403)	1:B:226:GLN:H	1:D:226:GLN:H	4	0.43	0.25	0.32
(5,404)	1:B:253:VAL:H	1:D:253:VAL:H	4	0.22	0.06	0.22
(5,344)	1:A:253:VAL:H	1:D:253:VAL:H	4	0.22	0.06	0.22
(5,324)	1:A:253:VAL:H	1:C:253:VAL:H	4	0.22	0.07	0.24
(2,708)	1:A:259:THR:H	1:A:261:LEU:H	4	0.12	0.0	0.12
(2,746)	1:A:304:VAL:HA	1:A:306:PHE:H	4	0.11	0.0	0.11
(2,696)	1:A:253:VAL:H	1:A:251:ALA:H	4	0.11	0.0	0.11
(2,30)	1:A:279:TYR:O	1:A:283:ILE:N	3	0.33	0.07	0.31
(2,795)	1:A:276:LYS:H	1:A:274:LEU:H	3	0.21	0.02	0.22
(2,749)	1:A:309:ARG:H	1:A:307:VAL:H	3	0.11	0.0	0.11
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD2	2	0.13	0.01	0.13
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD3	2	0.13	0.01	0.13
(2,553)	1:A:395:ILE:HB	1:A:396:ASP:H	2	0.12	0.02	0.12
(5,51)	1:A:297:ALA:H	1:D:297:ALA:H	2	0.12	0.0	0.12
(2,678)	1:A:220:LEU:H	1:A:222:TYR:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	2	7.82
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	5	7.82
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	2	7.81
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	5	7.8
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	4	7.8
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	12	7.79
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	9	7.79
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	12	7.79
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	4	7.78
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	9	7.78
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	9	7.78
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	12	7.78
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	5	7.78
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	3	7.78
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	4	7.78
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	3	7.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	3	7.77
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	9	7.77
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	4	7.76
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	5	7.75
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	4	7.75
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	2	7.75
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	3	7.75
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	9	7.75
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	2	7.74
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	12	7.74
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	1	7.74
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	3	7.73
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	2	7.72
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	5	7.72
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	1	7.72
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	1	7.72
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	1	7.71
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	12	7.71
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	1	7.69
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	13	7.68
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	13	7.66
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	10	7.65
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	10	7.63
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	13	7.62
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	13	7.61
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	10	7.61
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	10	7.58
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	13	7.57
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	11	7.57
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	10	7.56
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	11	7.56
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	11	7.56
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	6	7.55
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	6	7.55
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	6	7.53
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	11	7.53
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	6	7.53
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	6	7.53
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	11	7.51
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	14	7.49
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	8	7.49
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	8	7.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	15	7.48
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	8	7.47
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	8	7.46
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	8	7.46
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	14	7.46
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	15	7.46
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	14	7.45
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	14	7.43
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	14	7.43
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	15	7.42
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	15	7.4
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	15	7.39
(5,349)	1:A:300:GLU:O	1:D:300:GLU:O	7	7.3
(5,329)	1:A:300:GLU:O	1:C:300:GLU:O	7	7.28
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	12	7.27
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	1	7.27
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	1	7.26
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	1	7.25
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	14	7.24
(5,409)	1:B:300:GLU:O	1:D:300:GLU:O	7	7.24
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	12	7.23
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	15	7.23
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	9	7.23
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	11	7.23
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	5	7.23
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	10	7.23
(5,429)	1:B:300:GLU:O	1:E:300:GLU:O	7	7.23
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	1	7.22
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	13	7.22
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	12	7.22
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	9	7.22
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	12	7.22
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	12	7.22
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	13	7.22
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	6	7.21
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	15	7.21
(5,469)	1:C:300:GLU:O	1:E:300:GLU:O	7	7.21
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	10	7.2
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	12	7.2
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	10	7.2
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	1	7.2
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	3	7.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	3	7.2
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	6	7.2
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	10	7.2
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	13	7.2
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	6	7.19
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	1	7.19
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	15	7.19
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	11	7.18
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	6	7.18
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	3	7.18
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	8	7.18
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	11	7.18
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	11	7.17
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	1	7.17
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	11	7.17
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	10	7.17
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	6	7.17
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	10	7.17
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	8	7.16
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	13	7.16
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	13	7.16
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	9	7.16
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	6	7.15
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	13	7.15
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	11	7.15
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	15	7.15
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	11	7.15
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	9	7.14
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	15	7.14
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	6	7.14
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	12	7.14
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	15	7.14
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	15	7.14
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	11	7.14
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	15	7.14
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	10	7.14
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	13	7.14
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	6	7.14
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	3	7.13
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	1	7.13
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	13	7.13
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	8	7.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	14	7.13
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	1	7.13
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	9	7.13
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	10	7.13
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	12	7.13
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	6	7.13
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	9	7.12
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	15	7.12
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	9	7.12
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	6	7.12
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	8	7.11
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	8	7.11
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	11	7.11
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	13	7.11
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	15	7.11
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	13	7.11
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	8	7.11
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	10	7.1
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	12	7.1
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	1	7.1
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	11	7.1
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	3	7.1
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	14	7.1
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	14	7.1
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	8	7.1
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	8	7.09
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	5	7.09
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	14	7.09
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	14	7.09
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	10	7.08
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	9	7.08
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	8	7.08
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	3	7.07
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	8	7.07
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	9	7.07
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	7	7.07
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	12	7.07
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	5	7.06
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	14	7.06
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	5	7.06
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	3	7.06
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	3	7.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	14	7.05
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	14	7.05
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	3	7.04
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	5	7.04
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	9	7.04
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	14	7.03
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	3	7.03
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	7	7.01
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	5	7.0
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	5	6.99
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	5	6.98
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	7	6.97
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	7	6.97
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	5	6.96
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	5	6.96
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	4	6.95
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	7	6.95
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	7	6.94
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	4	6.94
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	4	6.94
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	7	6.94
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	4	6.92
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	4	6.91
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	7	6.91
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	7	6.89
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	14	6.89
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	15	6.88
(5,519)	1:A:240:ILE:O	1:D:300:GLU:O	2	6.87
(5,514)	1:A:300:GLU:O	1:C:240:ILE:O	2	6.87
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	11	6.87
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	7	6.86
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	8	6.86
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	14	6.85
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	11	6.84
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	15	6.84
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	8	6.84
(5,584)	1:C:300:GLU:O	1:E:240:ILE:O	2	6.83
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	15	6.83
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	7	6.83
(5,554)	1:B:300:GLU:O	1:D:240:ILE:O	2	6.82
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	6	6.82
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	11	6.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	11	6.82
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	6	6.81
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	11	6.81
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	1	6.81
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	6	6.81
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	10	6.81
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	6	6.8
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	6	6.8
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	15	6.8
(5,559)	1:B:240:ILE:O	1:E:300:GLU:O	2	6.79
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	1	6.79
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	10	6.79
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	10	6.79
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	15	6.79
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	4	6.78
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	13	6.78
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	8	6.78
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	12	6.76
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	4	6.75
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	4	6.75
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	13	6.75
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	8	6.75
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	9	6.75
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	8	6.74
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	12	6.74
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	14	6.74
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	13	6.74
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	4	6.73
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	14	6.73
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	1	6.73
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	1	6.73
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	4	6.72
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	14	6.72
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	8	6.71
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	12	6.71
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	13	6.71
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	11	6.71
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	15	6.71
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	1	6.7
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	8	6.7
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	12	6.7
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	7	6.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	15	6.7
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	11	6.7
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	12	6.7
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	4	6.69
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	13	6.69
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	12	6.69
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	1	6.69
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	9	6.69
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	9	6.69
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	2	6.69
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	4	6.69
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	7	6.69
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	10	6.69
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	11	6.68
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	12	6.68
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	1	6.68
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	9	6.68
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	8	6.68
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	11	6.68
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	14	6.68
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	2	6.68
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	4	6.68
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	8	6.68
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	10	6.68
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	14	6.68
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	5	6.68
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	8	6.68
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	13	6.68
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	5	6.68
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	7	6.68
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	2	6.67
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	7	6.67
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	14	6.67
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	4	6.67
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	14	6.67
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	4	6.67
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	7	6.67
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	13	6.67
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	10	6.67
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	12	6.67
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	14	6.67
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	3	6.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,509)	1:A:240:ILE:O	1:C:300:GLU:O	2	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	3	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	5	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	6	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	9	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	10	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	12	6.66
(5,474)	1:C:403:PHE:H	1:E:403:PHE:H	15	6.66
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	7	6.66
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	11	6.66
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	13	6.66
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	10	6.66
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	6	6.66
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	9	6.66
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	10	6.66
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	5	6.66
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	3	6.66
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	9	6.66
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	2	6.65
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	6	6.65
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	10	6.65
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	3	6.65
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	3	6.65
(5,334)	1:A:403:PHE:H	1:C:403:PHE:H	6	6.65
(5,524)	1:A:300:GLU:O	1:D:240:ILE:O	2	6.64
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	3	6.64
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	15	6.64
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	2	6.64
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	5	6.64
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	13	6.64
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	15	6.64
(5,354)	1:A:403:PHE:H	1:D:403:PHE:H	6	6.64
(5,414)	1:B:403:PHE:H	1:D:403:PHE:H	3	6.63
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	3	6.63
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	1	6.63
(5,434)	1:B:403:PHE:H	1:E:403:PHE:H	5	6.62
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	13	6.62
(5,579)	1:C:240:ILE:O	1:E:300:GLU:O	2	6.6
(5,549)	1:B:240:ILE:O	1:D:300:GLU:O	2	6.6
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	12	6.6
(5,564)	1:B:300:GLU:O	1:E:240:ILE:O	2	6.59
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	7	6.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	1	6.58
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	7	6.58
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	9	6.58
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	1	6.57
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	7	6.56
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	9	6.54
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	9	6.54
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	3	6.53
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	5	6.51
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	3	6.49
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	5	6.43
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	5	6.4
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	5	6.39
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	4	6.27
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	4	6.26
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	4	6.25
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	4	6.24
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	4	6.23
(5,319)	1:A:240:ILE:O	1:C:240:ILE:O	2	6.12
(5,339)	1:A:240:ILE:O	1:D:240:ILE:O	2	6.1
(5,459)	1:C:240:ILE:O	1:E:240:ILE:O	2	6.09
(5,419)	1:B:240:ILE:O	1:E:240:ILE:O	2	6.07
(5,399)	1:B:240:ILE:O	1:D:240:ILE:O	2	6.07
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	4	5.7
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	9	5.7
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	12	5.7
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	1	5.7
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	15	5.7
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	9	5.69
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	12	5.69
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	2	5.69
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	10	5.69
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	1	5.68
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	8	5.68
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	12	5.68
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	4	5.68
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	8	5.68
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	7	5.68
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	12	5.68
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	1	5.68
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	4	5.68
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	5	5.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	10	5.68
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	3	5.67
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	11	5.67
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	14	5.67
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	1	5.67
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	11	5.67
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	13	5.67
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	14	5.67
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	11	5.67
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	4	5.67
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	5	5.67
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	11	5.67
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	13	5.67
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	11	5.67
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	5	5.66
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	2	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	1	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	2	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	4	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	5	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	10	5.66
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	14	5.66
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	3	5.66
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	7	5.66
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	8	5.66
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	14	5.66
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	7	5.65
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	10	5.65
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	7	5.65
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	10	5.65
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	15	5.65
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	3	5.65
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	7	5.65
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	9	5.65
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	8	5.65
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	9	5.65
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	14	5.65
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	3	5.65
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	15	5.65
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	13	5.64
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	3	5.64
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	5	5.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	8	5.64
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	13	5.64
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	15	5.64
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	9	5.64
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	12	5.64
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	6	5.62
(5,432)	1:B:291:LEU:O	1:E:291:LEU:O	6	5.62
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	13	5.62
(5,412)	1:B:291:LEU:O	1:D:291:LEU:O	6	5.6
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	6	5.59
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	15	5.58
(5,352)	1:A:291:LEU:O	1:D:291:LEU:O	6	5.57
(5,332)	1:A:291:LEU:O	1:C:291:LEU:O	2	5.51
(5,472)	1:C:291:LEU:O	1:E:291:LEU:O	2	5.46
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	9	5.24
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	12	5.23
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	12	5.22
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	7	5.22
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	7	5.22
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	5	5.22
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	3	5.21
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	5	5.21
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	7	5.21
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	7	5.21
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	4	5.21
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	2	5.21
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	2	5.2
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	4	5.2
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	7	5.2
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	5	5.2
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	3	5.2
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	9	5.19
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	3	5.19
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	4	5.19
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	9	5.19
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	1	5.19
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	12	5.18
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	1	5.18
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	2	5.18
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	2	5.18
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	4	5.18
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	4	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	9	5.18
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	5	5.17
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	2	5.17
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	3	5.17
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	9	5.17
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	3	5.16
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	5	5.16
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	15	5.16
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	1	5.15
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	13	5.15
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	15	5.15
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	12	5.15
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	15	5.15
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	12	5.15
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	15	5.14
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	1	5.13
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	1	5.13
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	15	5.12
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	10	5.11
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	13	5.11
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	13	5.11
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	10	5.1
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	13	5.08
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	10	5.08
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	10	5.08
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	10	5.07
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	9	5.07
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	11	5.07
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	13	5.07
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	6	5.06
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	6	5.05
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	5	5.05
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	9	5.05
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	6	5.05
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	11	5.05
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	6	5.05
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	11	5.05
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	5	5.05
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	8	5.05
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	11	5.05
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	11	5.04
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	2	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	5	5.04
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	9	5.04
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	8	5.03
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	2	5.03
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	5	5.03
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	5	5.02
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	2	5.02
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	6	5.02
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	14	5.02
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	2	5.02
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	14	5.01
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	4	5.01
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	8	5.01
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	8	5.01
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	9	5.01
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	14	5.01
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	2	5.0
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	4	5.0
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	8	5.0
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	9	5.0
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	15	4.99
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	4	4.99
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	15	4.99
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	15	4.98
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	10	4.98
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	8	4.98
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	15	4.98
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	4	4.98
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	8	4.98
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	14	4.97
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	8	4.97
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	15	4.97
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	8	4.97
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	8	4.97
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	10	4.97
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	10	4.96
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	12	4.96
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	4	4.96
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	10	4.96
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	14	4.96
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	1	4.95
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	12	4.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	10	4.93
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	12	4.93
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	1	4.92
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	12	4.92
(5,309)	1:A:300:GLU:O	1:B:300:GLU:O	7	4.91
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	6	4.9
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	6	4.9
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	1	4.9
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	1	4.89
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	12	4.89
(5,369)	1:A:300:GLU:O	1:E:300:GLU:O	7	4.88
(5,489)	1:D:300:GLU:O	1:E:300:GLU:O	7	4.87
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	6	4.87
(5,449)	1:C:300:GLU:O	1:D:300:GLU:O	7	4.86
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	1	4.85
(5,389)	1:B:300:GLU:O	1:C:300:GLU:O	7	4.84
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	6	4.84
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	6	4.83
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	1	4.78
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	11	4.76
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	9	4.75
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	14	4.75
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	5	4.74
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	11	4.74
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	1	4.74
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	11	4.73
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	7	4.73
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	9	4.73
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	11	4.73
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	11	4.73
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	9	4.72
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	12	4.72
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	14	4.71
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	14	4.71
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	15	4.71
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	10	4.71
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	8	4.71
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	10	4.69
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	3	4.69
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	1	4.69
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	9	4.69
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	1	4.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	12	4.68
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	12	4.68
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	11	4.68
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	14	4.68
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	14	4.68
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	13	4.67
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	3	4.67
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	10	4.66
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	3	4.66
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	15	4.66
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	14	4.66
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	14	4.66
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	12	4.65
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	12	4.65
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	10	4.64
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	11	4.63
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	13	4.63
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	6	4.62
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	11	4.62
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	8	4.62
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	13	4.62
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	13	4.62
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	5	4.62
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	6	4.61
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	6	4.61
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	6	4.61
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	6	4.61
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	10	4.61
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	8	4.6
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	11	4.6
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	13	4.6
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	6	4.6
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	3	4.6
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	11	4.6
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	13	4.6
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	13	4.59
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	15	4.59
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	15	4.59
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	6	4.59
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	3	4.59
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	12	4.59
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	6	4.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	11	4.58
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	13	4.58
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	6	4.58
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	14	4.58
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	13	4.58
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	15	4.57
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	13	4.57
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	10	4.57
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	11	4.56
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	9	4.56
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	12	4.56
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	11	4.55
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	13	4.55
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	13	4.55
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	14	4.55
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	11	4.54
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	12	4.54
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	7	4.54
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	1	4.54
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	8	4.54
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	8	4.54
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	8	4.54
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	1	4.54
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	7	4.54
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	3	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	2	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	3	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	4	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	7	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	10	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	11	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	12	4.53
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	14	4.53
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	13	4.53
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	14	4.53
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	1	4.53
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	1	4.53
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	2	4.53
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	4	4.52
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	3	4.52
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	10	4.52
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	5	4.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	15	4.52
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	1	4.52
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	10	4.52
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	14	4.52
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	5	4.52
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	8	4.52
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	10	4.52
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	11	4.52
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	2	4.51
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	4	4.51
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	4	4.51
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	9	4.51
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	14	4.51
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	4	4.51
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	11	4.51
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	4	4.51
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	8	4.51
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	12	4.51
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	15	4.51
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	12	4.51
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	8	4.51
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	11	4.51
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	13	4.51
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	15	4.51
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	5	4.5
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	14	4.5
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	4	4.5
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	14	4.5
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	2	4.5
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	4	4.5
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	5	4.5
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	6	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	6	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	7	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	8	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	12	4.5
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	14	4.5
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	3	4.5
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	2	4.5
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	6	4.5
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	11	4.5
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	4	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	7	4.5
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	14	4.5
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	15	4.5
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	3	4.5
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	4	4.5
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	6	4.5
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	14	4.5
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	5	4.49
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	9	4.49
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	9	4.49
(5,494)	1:D:403:PHE:H	1:E:403:PHE:H	9	4.49
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	5	4.49
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	9	4.49
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	13	4.49
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	15	4.49
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	5	4.49
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	7	4.49
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	13	4.49
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	8	4.49
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	12	4.49
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	8	4.48
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	15	4.48
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	14	4.48
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	2	4.48
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	3	4.48
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	10	4.48
(5,454)	1:C:403:PHE:H	1:D:403:PHE:H	15	4.48
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	3	4.48
(5,394)	1:B:403:PHE:H	1:C:403:PHE:H	9	4.48
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	2	4.48
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	13	4.48
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	15	4.48
(5,314)	1:A:403:PHE:H	1:B:403:PHE:H	9	4.48
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	2	4.47
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	2	4.47
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	7	4.47
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	3	4.47
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	10	4.47
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	8	4.46
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	10	4.46
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	7	4.46
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	6	4.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	1	4.45
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	2	4.45
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	15	4.45
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	7	4.45
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	8	4.44
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	5	4.44
(5,374)	1:A:403:PHE:H	1:E:403:PHE:H	5	4.44
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	1	4.42
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	1	4.42
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	9	4.42
(5,529)	1:A:240:ILE:O	1:E:300:GLU:O	13	4.41
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	5	4.38
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	13	4.36
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	10	4.35
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	12	4.34
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	3	4.32
(5,594)	1:D:300:GLU:O	1:E:240:ILE:O	7	4.31
(5,504)	1:A:300:GLU:O	1:B:240:ILE:O	7	4.31
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	5	4.31
(5,574)	1:C:300:GLU:O	1:D:240:ILE:O	7	4.29
(5,473)	1:C:290:CYS:H	1:E:290:CYS:H	3	4.29
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	1	4.29
(5,544)	1:B:300:GLU:O	1:C:240:ILE:O	7	4.28
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	9	4.28
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	1	4.27
(5,353)	1:A:290:CYS:H	1:D:290:CYS:H	3	4.27
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	4	4.26
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	5	4.26
(5,433)	1:B:290:CYS:H	1:E:290:CYS:H	3	4.26
(5,413)	1:B:290:CYS:H	1:D:290:CYS:H	3	4.26
(5,333)	1:A:290:CYS:H	1:C:290:CYS:H	3	4.26
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	4	4.25
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	4	4.24
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	4	4.24
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	13	4.22
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	13	4.21
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	13	4.2
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	13	4.19
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	13	4.19
(5,479)	1:D:240:ILE:O	1:E:240:ILE:O	2	4.17
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	12	4.16
(5,379)	1:B:240:ILE:O	1:C:240:ILE:O	2	4.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	14	4.13
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	1	4.13
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	8	4.13
(5,439)	1:C:240:ILE:O	1:D:240:ILE:O	2	4.13
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	8	4.12
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	13	4.12
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	14	4.12
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	7	4.12
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	8	4.12
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	10	4.12
(5,359)	1:A:240:ILE:O	1:E:240:ILE:O	2	4.12
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	3	4.11
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	10	4.11
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	1	4.11
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	3	4.11
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	6	4.11
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	8	4.11
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	13	4.11
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	13	4.11
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	15	4.11
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	6	4.11
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	1	4.1
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	7	4.1
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	12	4.1
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	7	4.1
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	12	4.1
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	14	4.1
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	9	4.1
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	4	4.1
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	7	4.1
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	13	4.1
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	4	4.09
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	5	4.09
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	6	4.09
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	11	4.09
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	5	4.09
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	9	4.09
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	10	4.09
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	11	4.09
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	6	4.09
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	8	4.09
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	1	4.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	5	4.09
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	11	4.09
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	14	4.09
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	9	4.08
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	15	4.08
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	4	4.08
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	7	4.08
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	12	4.08
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	15	4.08
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	3	4.08
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	6	4.08
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	9	4.08
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	10	4.08
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	1	4.07
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	4	4.07
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	11	4.07
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	11	4.07
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	13	4.07
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	14	4.07
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	15	4.07
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	15	4.06
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	3	4.06
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	9	4.06
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	10	4.06
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	4	4.06
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	5	4.06
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	12	4.06
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	5	4.05
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	3	4.03
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	1	4.03
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	15	4.02
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	1	4.02
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	12	4.01
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	9	4.0
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	12	4.0
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	12	4.0
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	15	4.0
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	15	4.0
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	1	3.99
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	8	3.99
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	13	3.99
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	8	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	12	3.99
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	1	3.99
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	12	3.99
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	1	3.99
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	15	3.99
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	7	3.99
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	10	3.99
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	11	3.99
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	12	3.99
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	13	3.99
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	5	3.99
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	10	3.99
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	11	3.99
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	4	3.98
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	8	3.98
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	9	3.98
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	12	3.98
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	4	3.98
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	8	3.98
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	1	3.98
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	9	3.98
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	11	3.98
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	2	3.98
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	5	3.98
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	8	3.98
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	1	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	2	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	4	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	7	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	8	3.98
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	13	3.98
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	9	3.97
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	8	3.97
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	2	3.97
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	7	3.97
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	10	3.97
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	11	3.97
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	4	3.97
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	4	3.97
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	10	3.97
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	1	3.96
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	6	3.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	13	3.96
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	14	3.96
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	3	3.96
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	11	3.96
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	12	3.96
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	14	3.96
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	15	3.96
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	1	3.96
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	4	3.96
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	6	3.96
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	4	3.96
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	11	3.96
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	13	3.96
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	11	3.96
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	5	3.96
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	7	3.96
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	10	3.96
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	4	3.96
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	8	3.96
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	9	3.96
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	2	3.96
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	7	3.96
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	8	3.96
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	11	3.96
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	2	3.95
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	7	3.95
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	11	3.95
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	15	3.95
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	5	3.95
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	6	3.95
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	7	3.95
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	10	3.95
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	11	3.95
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	14	3.95
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	7	3.95
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	14	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	1	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	6	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	7	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	8	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	9	3.95
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	14	3.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	4	3.95
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	13	3.95
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	14	3.95
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	15	3.95
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	3	3.95
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	9	3.95
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	14	3.95
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	5	3.95
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	12	3.95
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	14	3.95
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	3	3.95
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	12	3.95
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	14	3.95
(5,470)	1:C:297:ALA:H	1:E:297:ALA:H	2	3.94
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	2	3.94
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	7	3.94
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	15	3.94
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	6	3.94
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	10	3.94
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	15	3.94
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	2	3.94
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	4	3.94
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	10	3.94
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	15	3.94
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	2	3.94
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	3	3.94
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	6	3.94
(5,410)	1:B:297:ALA:H	1:D:297:ALA:H	9	3.94
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	12	3.94
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	5	3.94
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	13	3.94
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	14	3.94
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	9	3.94
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	10	3.93
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	10	3.93
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	13	3.93
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	2	3.93
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	3	3.93
(5,430)	1:B:297:ALA:H	1:E:297:ALA:H	5	3.93
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	1	3.93
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	9	3.93
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	6	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	13	3.93
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	6	3.93
(5,330)	1:A:297:ALA:H	1:C:297:ALA:H	9	3.93
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	13	3.92
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	5	3.92
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	6	3.92
(5,350)	1:A:297:ALA:H	1:D:297:ALA:H	6	3.92
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	5	3.91
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	13	3.91
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	15	3.91
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	4	3.9
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	12	3.9
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	7	3.9
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	10	3.9
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	11	3.9
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	2	3.9
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	1	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	2	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	3	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	8	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	9	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	10	3.89
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	15	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	1	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	3	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	4	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	5	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	11	3.89
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	14	3.89
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	5	3.89
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	4	3.89
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	11	3.89
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	14	3.89
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	15	3.89
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	2	3.89
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	4	3.89
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	8	3.89
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	13	3.89
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	14	3.89
(5,542)	1:B:229:ILE:N	1:C:291:LEU:O	2	3.88
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	5	3.88
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	12	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	14	3.88
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	7	3.88
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	9	3.88
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	1	3.88
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	10	3.88
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	12	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	4	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	5	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	7	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	8	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	10	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	11	3.88
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	15	3.88
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	7	3.87
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	11	3.87
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	8	3.87
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	10	3.87
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	9	3.87
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	5	3.87
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	8	3.87
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	5	3.87
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	9	3.87
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	1	3.87
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	3	3.87
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	13	3.87
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	14	3.87
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	3	3.86
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	7	3.86
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	9	3.86
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	3	3.86
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	9	3.86
(5,492)	1:D:291:LEU:O	1:E:291:LEU:O	6	3.85
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	6	3.85
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	12	3.85
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	2	3.84
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	9	3.84
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	13	3.84
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	2	3.84
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	9	3.84
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	6	3.84
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	13	3.84
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	2	3.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	2	3.84
(5,312)	1:A:291:LEU:O	1:B:291:LEU:O	6	3.84
(5,502)	1:A:229:ILE:N	1:B:291:LEU:O	2	3.83
(5,372)	1:A:291:LEU:O	1:E:291:LEU:O	6	3.83
(5,592)	1:D:229:ILE:N	1:E:291:LEU:O	2	3.82
(5,572)	1:C:229:ILE:N	1:D:291:LEU:O	2	3.82
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	4	3.82
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	2	3.82
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	9	3.82
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	4	3.81
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	4	3.81
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	4	3.81
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	4	3.81
(5,392)	1:B:291:LEU:O	1:C:291:LEU:O	2	3.79
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	15	3.78
(5,537)	1:A:291:LEU:O	1:E:229:ILE:N	2	3.76
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	13	3.75
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	13	3.75
(5,452)	1:C:291:LEU:O	1:D:291:LEU:O	2	3.73
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	13	3.73
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	13	3.73
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	13	3.71
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	14	3.67
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	14	3.66
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	14	3.66
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	14	3.66
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	8	3.65
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	14	3.65
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	8	3.64
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	7	3.63
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	8	3.62
(5,471)	1:C:293:PHE:CA	1:E:293:PHE:CA	3	3.61
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	7	3.61
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	8	3.61
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	7	3.6
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	15	3.6
(5,351)	1:A:293:PHE:CA	1:D:293:PHE:CA	3	3.6
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	7	3.59
(5,431)	1:B:293:PHE:CA	1:E:293:PHE:CA	3	3.59
(5,411)	1:B:293:PHE:CA	1:D:293:PHE:CA	3	3.59
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	8	3.59
(5,331)	1:A:293:PHE:CA	1:C:293:PHE:CA	3	3.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	7	3.58
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	1	3.58
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	15	3.57
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	1	3.57
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	15	3.56
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	15	3.56
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	1	3.56
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	15	3.56
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	1	3.55
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	15	3.55
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	15	3.54
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	1	3.54
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	9	3.54
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	2	3.53
(5,428)	1:B:265:THR:O	1:E:265:THR:O	7	3.53
(5,468)	1:C:265:THR:O	1:E:265:THR:O	7	3.52
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	5	3.52
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	5	3.51
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	2	3.51
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	2	3.51
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	9	3.51
(5,408)	1:B:265:THR:O	1:D:265:THR:O	7	3.51
(5,348)	1:A:265:THR:O	1:D:265:THR:O	7	3.51
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	5	3.5
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	2	3.5
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	5	3.5
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	5	3.5
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	2	3.5
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	5	3.49
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	5	3.49
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	5	3.49
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	2	3.49
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	1	3.49
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	5	3.49
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	12	3.49
(5,328)	1:A:265:THR:O	1:C:265:THR:O	7	3.49
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	2	3.49
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	5	3.49
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	5	3.48
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	5	3.48
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	2	3.48
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	5	3.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	4	3.48
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	10	3.48
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	9	3.48
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	5	3.47
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	15	3.47
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	10	3.47
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	4	3.47
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	8	3.47
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	9	3.47
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	8	3.47
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	8	3.47
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	10	3.46
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	10	3.46
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	4	3.46
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	9	3.46
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	4	3.46
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	1	3.45
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	15	3.45
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	5	3.45
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	15	3.45
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	1	3.45
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	13	3.45
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	1	3.45
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	2	3.45
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	8	3.45
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	10	3.45
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	4	3.45
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	8	3.45
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	1	3.44
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	5	3.44
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	5	3.44
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	12	3.44
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	3	3.43
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	3	3.42
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	6	3.42
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	5	3.42
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	4	3.42
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	5	3.42
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	12	3.42
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	4	3.42
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	10	3.42
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	10	3.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	6	3.41
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	6	3.41
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	12	3.41
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	6	3.41
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	12	3.4
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	2	3.4
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	2	3.4
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	4	3.4
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	5	3.4
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	3	3.4
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	12	3.4
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	7	3.4
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	13	3.39
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	6	3.39
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	6	3.39
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	14	3.39
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	6	3.39
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	6	3.39
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	12	3.39
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	12	3.39
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	8	3.38
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	2	3.38
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	2	3.38
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	7	3.38
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	7	3.38
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	7	3.38
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	6	3.38
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	7	3.38
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	6	3.38
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	11	3.37
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	11	3.37
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	4	3.37
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	3	3.37
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	3	3.37
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	4	3.37
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	5	3.37
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	5	3.37
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	1	3.37
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	1	3.37
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	10	3.36
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	12	3.36
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	12	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	12	3.36
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	1	3.36
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	7	3.35
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	14	3.35
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	8	3.35
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	5	3.35
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	11	3.35
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	13	3.35
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	8	3.35
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	12	3.34
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	2	3.34
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	5	3.34
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	7	3.34
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	14	3.34
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	7	3.34
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	12	3.34
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	8	3.34
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	11	3.34
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	11	3.34
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	14	3.34
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	10	3.33
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	12	3.33
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	7	3.32
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	10	3.32
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	13	3.32
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	12	3.32
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	2	3.32
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	11	3.32
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	12	3.32
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	5	3.31
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	8	3.31
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	12	3.31
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	14	3.31
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	11	3.31
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	14	3.3
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	8	3.3
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	13	3.3
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	8	3.3
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	11	3.3
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	14	3.3
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	8	3.29
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	1	3.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	9	3.29
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	11	3.29
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	4	3.29
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	7	3.29
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	8	3.28
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	2	3.28
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	2	3.28
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	11	3.28
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	4	3.27
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	1	3.27
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	12	3.27
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	8	3.27
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	1	3.27
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	10	3.27
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	4	3.26
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	4	3.26
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	2	3.26
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	1	3.26
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	4	3.26
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	10	3.26
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	13	3.26
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	14	3.26
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	10	3.25
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	9	3.25
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	4	3.25
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	10	3.25
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	2	3.25
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	4	3.25
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	4	3.25
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	1	3.25
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	12	3.25
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	13	3.25
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	14	3.25
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	2	3.24
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	9	3.24
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	10	3.23
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	3	3.23
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	4	3.23
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	14	3.23
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	4	3.22
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	5	3.22
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	4	3.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	12	3.22
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	3	3.22
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	5	3.22
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	13	3.22
(5,428)	1:B:265:THR:O	1:E:265:THR:O	15	3.22
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	5	3.22
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	5	3.22
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	5	3.21
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	1	3.21
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	5	3.21
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	4	3.21
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	4	3.21
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	4	3.2
(5,468)	1:C:265:THR:O	1:E:265:THR:O	15	3.2
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	13	3.2
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	13	3.2
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	3	3.19
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	11	3.19
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	4	3.19
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	5	3.19
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	5	3.19
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	5	3.19
(5,348)	1:A:265:THR:O	1:D:265:THR:O	15	3.19
(5,328)	1:A:265:THR:O	1:C:265:THR:O	15	3.19
(5,408)	1:B:265:THR:O	1:D:265:THR:O	15	3.18
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	3	3.17
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	1	3.17
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	11	3.17
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	11	3.17
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	5	3.17
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	11	3.16
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	7	3.16
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	9	3.16
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	11	3.16
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	3	3.15
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	7	3.15
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	1	3.15
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	1	3.15
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	7	3.15
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	3	3.15
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	5	3.15
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	7	3.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	3	3.14
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	3	3.14
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	3	3.14
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	9	3.14
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	3	3.14
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	10	3.14
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	3	3.14
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	15	3.14
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	3	3.14
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	5	3.13
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	3	3.13
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	10	3.13
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	10	3.13
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	9	3.12
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	1	3.12
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	9	3.12
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	10	3.12
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	7	3.12
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	15	3.12
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	3	3.12
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	10	3.12
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	9	3.12
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	9	3.11
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	10	3.11
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	10	3.11
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	3	3.11
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	1	3.11
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	10	3.11
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	6	3.11
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	3	3.1
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	9	3.1
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	9	3.1
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	9	3.1
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	6	3.1
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	15	3.09
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	1	3.09
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	10	3.09
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	15	3.09
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	5	3.09
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	9	3.09
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	6	3.09
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	6	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	6	3.09
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	8	3.08
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	5	3.08
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	5	3.08
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	6	3.08
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	3	3.08
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	9	3.08
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	10	3.08
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	3	3.08
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	6	3.07
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	15	3.07
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	8	3.07
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	9	3.07
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	5	3.07
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	8	3.07
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	3	3.07
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	5	3.07
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	9	3.06
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	14	3.06
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	6	3.06
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	3	3.06
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	8	3.06
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	14	3.06
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	5	3.06
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	5	3.06
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	14	3.06
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	9	3.06
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	8	3.06
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	14	3.06
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	2	3.06
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	3	3.05
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	14	3.05
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	6	3.05
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	6	3.05
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	15	3.05
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	6	3.05
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	9	3.05
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	2	3.05
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	14	3.04
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	14	3.04
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	9	3.04
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	6	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,493)	1:D:290:CYS:H	1:E:290:CYS:H	3	3.04
(5,453)	1:C:290:CYS:H	1:D:290:CYS:H	3	3.04
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	15	3.03
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	6	3.03
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	14	3.03
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	9	3.03
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	3	3.03
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	2	3.03
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	2	3.03
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	3	3.02
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	14	3.02
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	14	3.02
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	14	3.02
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	14	3.02
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	15	3.02
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	2	3.02
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	11	3.02
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	15	3.01
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	5	3.01
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	3	3.01
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	3	3.01
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	6	3.01
(5,373)	1:A:290:CYS:H	1:E:290:CYS:H	3	3.01
(5,313)	1:A:290:CYS:H	1:B:290:CYS:H	3	3.01
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	14	3.0
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	15	3.0
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	15	3.0
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	14	3.0
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	11	3.0
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	11	3.0
(5,428)	1:B:265:THR:O	1:E:265:THR:O	13	3.0
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	11	3.0
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	11	3.0
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	15	3.0
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	13	2.99
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	13	2.99
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	13	2.99
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	6	2.99
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	15	2.99
(5,393)	1:B:290:CYS:H	1:C:290:CYS:H	3	2.99
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	15	2.99
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	2	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	15	2.98
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	15	2.98
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	14	2.98
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	14	2.98
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	13	2.98
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	13	2.98
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	2	2.98
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	15	2.98
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	13	2.97
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	1	2.97
(5,468)	1:C:265:THR:O	1:E:265:THR:O	13	2.97
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	1	2.96
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	2	2.96
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	2	2.96
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	1	2.96
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	15	2.96
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	15	2.96
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	14	2.95
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	6	2.95
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	1	2.95
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	2	2.95
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	2	2.95
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	14	2.95
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	14	2.95
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	13	2.95
(5,428)	1:B:265:THR:O	1:E:265:THR:O	6	2.95
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	6	2.94
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	14	2.94
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	6	2.94
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	13	2.94
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	13	2.94
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	2	2.94
(5,348)	1:A:265:THR:O	1:D:265:THR:O	13	2.94
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	2	2.93
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	15	2.93
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	13	2.93
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	6	2.93
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	6	2.93
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	4	2.93
(5,428)	1:B:265:THR:O	1:E:265:THR:O	11	2.93
(5,408)	1:B:265:THR:O	1:D:265:THR:O	6	2.93
(5,408)	1:B:265:THR:O	1:D:265:THR:O	13	2.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	4	2.93
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	10	2.92
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	14	2.92
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	10	2.92
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	14	2.92
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	10	2.92
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	10	2.92
(5,348)	1:A:265:THR:O	1:D:265:THR:O	11	2.92
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	10	2.91
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	8	2.91
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	1	2.91
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	2	2.91
(5,468)	1:C:265:THR:O	1:E:265:THR:O	6	2.91
(5,468)	1:C:265:THR:O	1:E:265:THR:O	11	2.91
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	4	2.91
(5,408)	1:B:265:THR:O	1:D:265:THR:O	11	2.91
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	4	2.91
(5,328)	1:A:265:THR:O	1:C:265:THR:O	13	2.91
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	8	2.9
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	13	2.9
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	6	2.9
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	12	2.9
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	6	2.9
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	12	2.9
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	12	2.9
(5,348)	1:A:265:THR:O	1:D:265:THR:O	6	2.9
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	6	2.89
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	4	2.89
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	1	2.89
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	12	2.89
(5,328)	1:A:265:THR:O	1:C:265:THR:O	11	2.89
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	7	2.88
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	13	2.88
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	14	2.88
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	7	2.88
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	8	2.88
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	6	2.88
(5,468)	1:C:265:THR:O	1:E:265:THR:O	3	2.88
(5,428)	1:B:265:THR:O	1:E:265:THR:O	3	2.88
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	9	2.88
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	9	2.88
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	7	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	6	2.87
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	7	2.87
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	10	2.87
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	14	2.87
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	13	2.87
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	1	2.87
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	1	2.87
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	10	2.86
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	7	2.86
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	7	2.86
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	2	2.86
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	8	2.86
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	12	2.86
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	9	2.86
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	15	2.86
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	11	2.86
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	2	2.86
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	1	2.86
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	8	2.86
(5,428)	1:B:265:THR:O	1:E:265:THR:O	5	2.86
(5,408)	1:B:265:THR:O	1:D:265:THR:O	3	2.86
(5,408)	1:B:265:THR:O	1:D:265:THR:O	5	2.86
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	11	2.86
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	11	2.86
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	15	2.86
(5,348)	1:A:265:THR:O	1:D:265:THR:O	3	2.86
(5,348)	1:A:265:THR:O	1:D:265:THR:O	5	2.86
(5,328)	1:A:265:THR:O	1:C:265:THR:O	6	2.86
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	8	2.86
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	4	2.85
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	14	2.85
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	11	2.85
(5,582)	1:C:229:ILE:N	1:E:291:LEU:O	12	2.85
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	11	2.85
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	7	2.85
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	11	2.85
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	13	2.85
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	10	2.85
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	4	2.85
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	8	2.85
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	11	2.85
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	1	2.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	11	2.85
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	1	2.85
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	11	2.85
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	7	2.85
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	15	2.85
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	4	2.85
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	15	2.85
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	12	2.85
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	10	2.85
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	15	2.85
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	7	2.85
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	8	2.85
(5,348)	1:A:265:THR:O	1:D:265:THR:O	1	2.85
(5,328)	1:A:265:THR:O	1:C:265:THR:O	5	2.85
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	2	2.85
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	5	2.85
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	13	2.85
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	15	2.85
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	15	2.84
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	2	2.84
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	4	2.84
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	10	2.84
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	9	2.84
(5,567)	1:B:291:LEU:O	1:E:229:ILE:N	11	2.84
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	11	2.84
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	15	2.84
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	4	2.84
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	9	2.84
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	9	2.84
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	8	2.84
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	12	2.84
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	13	2.84
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	2	2.84
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	3	2.84
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	7	2.84
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	10	2.84
(5,468)	1:C:265:THR:O	1:E:265:THR:O	5	2.84
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	2	2.84
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	14	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	1	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	3	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	4	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	5	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	7	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	8	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	11	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	12	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	13	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	14	2.84
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	15	2.84
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	15	2.84
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	4	2.84
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	5	2.84
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	8	2.84
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	12	2.84
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	9	2.84
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	4	2.84
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	8	2.84
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	11	2.84
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	4	2.84
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	10	2.84
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	2	2.84
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	8	2.84
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	1	2.84
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	7	2.84
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	10	2.84
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	9	2.83
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	1	2.83
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	13	2.83
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	8	2.83
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	7	2.83
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	12	2.83
(5,552)	1:B:229:ILE:N	1:D:291:LEU:O	7	2.83
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	2	2.83
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	10	2.83
(5,527)	1:A:291:LEU:O	1:D:229:ILE:N	13	2.83
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	11	2.83
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	12	2.83
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	15	2.83
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	13	2.83
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	4	2.83
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	2	2.83
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	4	2.83
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	9	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	15	2.83
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	5	2.83
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	9	2.83
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	11	2.83
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	12	2.83
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	14	2.83
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	1	2.83
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	4	2.83
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	6	2.83
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	7	2.83
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	11	2.83
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	6	2.83
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	9	2.83
(5,428)	1:B:265:THR:O	1:E:265:THR:O	1	2.83
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	4	2.83
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	10	2.83
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	12	2.83
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	6	2.83
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	7	2.83
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	14	2.83
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	7	2.83
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	10	2.83
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	13	2.83
(5,328)	1:A:265:THR:O	1:C:265:THR:O	3	2.83
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	7	2.83
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	15	2.83
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	3	2.83
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	4	2.83
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	11	2.83
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	8	2.82
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	8	2.82
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	11	2.82
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	13	2.82
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	11	2.82
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	12	2.82
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	13	2.82
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	9	2.82
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	2	2.82
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	10	2.82
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	8	2.82
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	15	2.82
(5,512)	1:A:229:ILE:N	1:C:291:LEU:O	12	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	13	2.82
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	1	2.82
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	7	2.82
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	10	2.82
(5,490)	1:D:297:ALA:H	1:E:297:ALA:H	6	2.82
(5,468)	1:C:265:THR:O	1:E:265:THR:O	1	2.82
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	8	2.82
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	9	2.82
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	2	2.82
(5,450)	1:C:297:ALA:H	1:D:297:ALA:H	10	2.82
(5,428)	1:B:265:THR:O	1:E:265:THR:O	8	2.82
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	1	2.82
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	8	2.82
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	11	2.82
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	14	2.82
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	2	2.82
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	13	2.82
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	15	2.82
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	2	2.82
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	13	2.82
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	14	2.82
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	2	2.82
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	5	2.82
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	14	2.82
(5,348)	1:A:265:THR:O	1:D:265:THR:O	10	2.82
(5,328)	1:A:265:THR:O	1:C:265:THR:O	1	2.82
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	1	2.82
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	5	2.82
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	10	2.82
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	11	2.82
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	6	2.82
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	12	2.82
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	14	2.82
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	12	2.81
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	1	2.81
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	1	2.81
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	11	2.81
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	13	2.81
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	8	2.81
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	13	2.81
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	7	2.81
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	11	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	8	2.81
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	5	2.81
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	6	2.81
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	11	2.81
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	14	2.81
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	5	2.81
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	13	2.81
(5,428)	1:B:265:THR:O	1:E:265:THR:O	10	2.81
(5,408)	1:B:265:THR:O	1:D:265:THR:O	1	2.81
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	6	2.81
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	7	2.81
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	9	2.81
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	3	2.81
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	6	2.81
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	3	2.81
(5,328)	1:A:265:THR:O	1:C:265:THR:O	10	2.81
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	4	2.81
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	6	2.81
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	9	2.81
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	12	2.81
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	14	2.81
(5,310)	1:A:297:ALA:H	1:B:297:ALA:H	9	2.81
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	7	2.8
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	11	2.8
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	4	2.8
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	8	2.8
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	8	2.8
(5,522)	1:A:229:ILE:N	1:D:291:LEU:O	7	2.8
(5,468)	1:C:265:THR:O	1:E:265:THR:O	10	2.8
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	10	2.8
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	15	2.8
(5,408)	1:B:265:THR:O	1:D:265:THR:O	10	2.8
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	5	2.8
(5,390)	1:B:297:ALA:H	1:C:297:ALA:H	9	2.8
(5,370)	1:A:297:ALA:H	1:E:297:ALA:H	6	2.8
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	13	2.8
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	4	2.79
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	15	2.79
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	9	2.79
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	7	2.79
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	8	2.79
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	13	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,538)	1:A:290:CYS:H	1:E:226:GLN:H	6	2.79
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	1	2.79
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	8	2.79
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	12	2.79
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	4	2.79
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	4	2.79
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	2	2.79
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	13	2.79
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	1	2.78
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	10	2.78
(5,587)	1:C:291:LEU:O	1:E:229:ILE:N	13	2.78
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	4	2.78
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	6	2.78
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	4	2.78
(5,562)	1:B:229:ILE:N	1:E:291:LEU:O	7	2.78
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	15	2.78
(5,517)	1:A:291:LEU:O	1:C:229:ILE:N	13	2.78
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	4	2.78
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	10	2.78
(5,468)	1:C:265:THR:O	1:E:265:THR:O	8	2.78
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	5	2.78
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	9	2.77
(5,573)	1:C:226:GLN:H	1:D:290:CYS:H	10	2.77
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	4	2.77
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	15	2.77
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	1	2.77
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	4	2.77
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	4	2.77
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	2	2.77
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	2	2.77
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	2	2.77
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	2	2.76
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	15	2.76
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	1	2.76
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	4	2.76
(5,557)	1:B:291:LEU:O	1:D:229:ILE:N	13	2.76
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	9	2.76
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	4	2.76
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	2	2.76
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	2	2.76
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	1	2.76
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	9	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	4	2.76
(5,348)	1:A:265:THR:O	1:D:265:THR:O	8	2.76
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	2	2.75
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	4	2.75
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	6	2.75
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	9	2.75
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	9	2.75
(5,408)	1:B:265:THR:O	1:D:265:THR:O	8	2.75
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	2	2.75
(5,593)	1:D:226:GLN:H	1:E:290:CYS:H	6	2.74
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	2	2.74
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	2	2.74
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	4	2.74
(5,543)	1:B:226:GLN:H	1:C:290:CYS:H	10	2.74
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	4	2.74
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	1	2.74
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	2	2.74
(5,503)	1:A:226:GLN:H	1:B:290:CYS:H	6	2.74
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	2	2.74
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	4	2.74
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	2	2.74
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	4	2.74
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	9	2.74
(5,328)	1:A:265:THR:O	1:C:265:THR:O	8	2.74
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	2	2.73
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	1	2.73
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	11	2.73
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	4	2.73
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	4	2.73
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	1	2.72
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	2	2.72
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	5	2.72
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	5	2.72
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	5	2.72
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	5	2.72
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	13	2.72
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	9	2.72
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	8	2.71
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	12	2.71
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	2	2.71
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	6	2.71
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	9	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	12	2.71
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	5	2.71
(5,499)	1:A:240:ILE:O	1:B:300:GLU:O	2	2.71
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	5	2.7
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	11	2.7
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	5	2.7
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	13	2.7
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	1	2.7
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	1	2.7
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	10	2.7
(5,589)	1:D:240:ILE:O	1:E:300:GLU:O	2	2.69
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	5	2.69
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	6	2.69
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	5	2.69
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	1	2.69
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	5	2.69
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	6	2.69
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	11	2.69
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	11	2.69
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	5	2.69
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	5	2.69
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	10	2.69
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	13	2.69
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	6	2.68
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	11	2.68
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	8	2.68
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	5	2.68
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	7	2.68
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	12	2.68
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	1	2.68
(5,520)	1:A:236:ILE:CA	1:D:297:ALA:H	12	2.68
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	15	2.68
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	1	2.68
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	13	2.68
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	15	2.67
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	12	2.67
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	15	2.67
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	5	2.67
(5,555)	1:B:297:ALA:H	1:D:236:ILE:CA	12	2.67
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	15	2.67
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	15	2.67
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	6	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	3	2.67
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	10	2.67
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	3	2.67
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	10	2.67
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	10	2.67
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	13	2.67
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	7	2.66
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	5	2.66
(5,539)	1:B:240:ILE:O	1:C:300:GLU:O	2	2.66
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	8	2.66
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	5	2.66
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	10	2.66
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	3	2.65
(5,585)	1:C:297:ALA:H	1:E:236:ILE:CA	12	2.65
(5,560)	1:B:236:ILE:CA	1:E:297:ALA:H	12	2.65
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	8	2.65
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	3	2.65
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	7	2.65
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	5	2.65
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	10	2.65
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	14	2.65
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	14	2.65
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	1	2.65
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	14	2.65
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	14	2.65
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	3	2.64
(5,569)	1:C:240:ILE:O	1:D:300:GLU:O	2	2.64
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	7	2.64
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	1	2.64
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	8	2.64
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	5	2.64
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	8	2.64
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	1	2.64
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	3	2.64
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	3	2.64
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	3	2.64
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	5	2.63
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	1	2.63
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	9	2.63
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	1	2.63
(5,534)	1:A:300:GLU:O	1:E:240:ILE:O	2	2.63
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	1	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	7	2.63
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	12	2.63
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	3	2.63
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	8	2.63
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	14	2.63
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	5	2.62
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	5	2.62
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	9	2.62
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	10	2.62
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	5	2.62
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	3	2.62
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	5	2.62
(5,515)	1:A:297:ALA:H	1:C:236:ILE:CA	12	2.62
(5,491)	1:D:293:PHE:CA	1:E:293:PHE:CA	3	2.62
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	9	2.62
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	8	2.62
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	9	2.61
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	10	2.61
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	5	2.61
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	8	2.61
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	10	2.61
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	8	2.61
(5,451)	1:C:293:PHE:CA	1:D:293:PHE:CA	3	2.61
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	14	2.61
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	8	2.61
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	9	2.61
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	14	2.61
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	14	2.61
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	8	2.6
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	2	2.6
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	9	2.6
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	5	2.6
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	8	2.6
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	9	2.6
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	1	2.6
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	8	2.6
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	14	2.6
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	1	2.6
(5,371)	1:A:293:PHE:CA	1:E:293:PHE:CA	3	2.6
(5,311)	1:A:293:PHE:CA	1:B:293:PHE:CA	3	2.6
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	2	2.59
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	9	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	8	2.59
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	14	2.59
(5,428)	1:B:265:THR:O	1:E:265:THR:O	4	2.59
(5,391)	1:B:293:PHE:CA	1:C:293:PHE:CA	3	2.59
(5,368)	1:A:265:THR:O	1:E:265:THR:O	7	2.59
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	9	2.58
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	1	2.58
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	2	2.58
(5,468)	1:C:265:THR:O	1:E:265:THR:O	4	2.58
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	9	2.58
(5,448)	1:C:265:THR:O	1:D:265:THR:O	7	2.58
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	9	2.58
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	1	2.58
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	8	2.58
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	9	2.58
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	1	2.58
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	7	2.57
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	2	2.57
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	8	2.57
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	7	2.57
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	1	2.57
(5,428)	1:B:265:THR:O	1:E:265:THR:O	12	2.57
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	8	2.57
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	7	2.56
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	8	2.56
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	9	2.56
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	7	2.56
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	9	2.56
(5,428)	1:B:265:THR:O	1:E:265:THR:O	14	2.56
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	8	2.56
(5,348)	1:A:265:THR:O	1:D:265:THR:O	4	2.56
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	7	2.55
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	14	2.55
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	2	2.55
(5,468)	1:C:265:THR:O	1:E:265:THR:O	14	2.55
(5,408)	1:B:265:THR:O	1:D:265:THR:O	4	2.55
(5,408)	1:B:265:THR:O	1:D:265:THR:O	12	2.55
(5,348)	1:A:265:THR:O	1:D:265:THR:O	12	2.55
(5,328)	1:A:265:THR:O	1:C:265:THR:O	4	2.55
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	4	2.54
(5,408)	1:B:265:THR:O	1:D:265:THR:O	14	2.54
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	12	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,488)	1:D:265:THR:O	1:E:265:THR:O	7	2.53
(5,468)	1:C:265:THR:O	1:E:265:THR:O	12	2.53
(5,308)	1:A:265:THR:O	1:B:265:THR:O	7	2.53
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	12	2.52
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	7	2.52
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	7	2.52
(5,388)	1:B:265:THR:O	1:C:265:THR:O	7	2.52
(5,348)	1:A:265:THR:O	1:D:265:THR:O	14	2.52
(5,328)	1:A:265:THR:O	1:C:265:THR:O	14	2.52
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	14	2.51
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	4	2.51
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	14	2.51
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	14	2.51
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	11	2.51
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	14	2.51
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	4	2.5
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	2	2.5
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	4	2.5
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	7	2.5
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	4	2.5
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	2	2.5
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	5	2.5
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	5	2.5
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	2	2.5
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	12	2.5
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	7	2.49
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	2	2.49
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	4	2.49
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	4	2.49
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	4	2.49
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	7	2.49
(5,428)	1:B:265:THR:O	1:E:265:THR:O	2	2.49
(5,328)	1:A:265:THR:O	1:C:265:THR:O	12	2.49
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	12	2.48
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	11	2.48
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	15	2.48
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	2	2.48
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	13	2.48
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	5	2.48
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	7	2.48
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	13	2.48
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	4	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	7	2.48
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	7	2.48
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	13	2.47
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	5	2.47
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	3	2.47
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	15	2.47
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	2	2.47
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	12	2.47
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	2	2.47
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	12	2.47
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	8	2.47
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	15	2.47
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	2	2.47
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	15	2.47
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	2	2.47
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	11	2.47
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	7	2.47
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	13	2.46
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	12	2.46
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	4	2.46
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	2	2.46
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	11	2.46
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	13	2.46
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	12	2.46
(5,408)	1:B:265:THR:O	1:D:265:THR:O	2	2.46
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	7	2.46
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	11	2.45
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	12	2.45
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	11	2.45
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	11	2.45
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	11	2.45
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	12	2.45
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	7	2.45
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	11	2.45
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	11	2.45
(5,468)	1:C:265:THR:O	1:E:265:THR:O	2	2.45
(5,348)	1:A:265:THR:O	1:D:265:THR:O	2	2.45
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	13	2.44
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	7	2.44
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	8	2.44
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	12	2.44
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	13	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	12	2.44
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	12	2.44
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	8	2.43
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	7	2.43
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	6	2.43
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	14	2.43
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	5	2.43
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	3	2.43
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	15	2.43
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	13	2.43
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	12	2.43
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	13	2.43
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	13	2.43
(5,328)	1:A:265:THR:O	1:C:265:THR:O	2	2.43
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	13	2.43
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	12	2.43
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	7	2.42
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	8	2.42
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	13	2.42
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	3	2.42
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	13	2.42
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	7	2.42
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	8	2.42
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	6	2.42
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	13	2.42
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	6	2.41
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	14	2.41
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	13	2.41
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	6	2.41
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	14	2.41
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	3	2.41
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	3	2.41
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	13	2.41
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	13	2.41
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	14	2.4
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	9	2.4
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	14	2.4
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	13	2.4
(5,532)	1:A:229:ILE:N	1:E:291:LEU:O	1	2.4
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	14	2.4
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	4	2.39
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	3	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	14	2.39
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	14	2.39
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	4	2.39
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	14	2.39
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	6	2.39
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	6	2.39
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	13	2.39
(5,368)	1:A:265:THR:O	1:E:265:THR:O	15	2.39
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	14	2.38
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	3	2.38
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	3	2.38
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	14	2.38
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	14	2.38
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	3	2.38
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	3	2.38
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	6	2.38
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	6	2.38
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	5	2.38
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	1	2.37
(5,577)	1:C:291:LEU:O	1:D:229:ILE:N	13	2.37
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	4	2.37
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	7	2.37
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	14	2.37
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	5	2.37
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	6	2.37
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	6	2.37
(5,597)	1:D:291:LEU:O	1:E:229:ILE:N	1	2.36
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	9	2.36
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	14	2.36
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	4	2.36
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	7	2.36
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	5	2.36
(5,308)	1:A:265:THR:O	1:B:265:THR:O	15	2.36
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	14	2.35
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	15	2.35
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	2	2.35
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	7	2.35
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	7	2.35
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	4	2.35
(5,547)	1:B:291:LEU:O	1:C:229:ILE:N	1	2.35
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	11	2.35
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	2	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	15	2.35
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	11	2.35
(5,507)	1:A:291:LEU:O	1:B:229:ILE:N	1	2.35
(5,448)	1:C:265:THR:O	1:D:265:THR:O	15	2.35
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	7	2.34
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	15	2.34
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	9	2.34
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	11	2.34
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	15	2.34
(5,488)	1:D:265:THR:O	1:E:265:THR:O	15	2.34
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	5	2.34
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	11	2.33
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	15	2.33
(5,388)	1:B:265:THR:O	1:C:265:THR:O	15	2.33
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	5	2.33
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	2	2.32
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	2	2.32
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	15	2.32
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	9	2.32
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	2	2.32
(5,595)	1:D:297:ALA:H	1:E:236:ILE:CA	6	2.31
(5,575)	1:C:297:ALA:H	1:D:236:ILE:CA	6	2.31
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	9	2.31
(5,545)	1:B:297:ALA:H	1:C:236:ILE:CA	6	2.31
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	9	2.31
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	15	2.31
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	14	2.3
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	11	2.3
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	8	2.3
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	10	2.3
(5,530)	1:A:236:ILE:CA	1:E:297:ALA:H	6	2.3
(5,505)	1:A:297:ALA:H	1:B:236:ILE:CA	6	2.3
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	6	2.3
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	6	2.3
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	6	2.3
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	6	2.3
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	15	2.29
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	8	2.29
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	12	2.29
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	8	2.28
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	15	2.28
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	10	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	9	2.28
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	9	2.28
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	15	2.28
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	15	2.28
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	12	2.28
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	13	2.28
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	12	2.28
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	6	2.28
(5,368)	1:A:265:THR:O	1:E:265:THR:O	13	2.28
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	2	2.28
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	10	2.27
(5,565)	1:B:297:ALA:H	1:E:236:ILE:CA	12	2.27
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	12	2.27
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	14	2.27
(5,525)	1:A:297:ALA:H	1:D:236:ILE:CA	12	2.27
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	8	2.27
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	4	2.27
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	8	2.27
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	13	2.27
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	2	2.27
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	1	2.27
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	11	2.27
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	13	2.26
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	9	2.26
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	14	2.26
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	12	2.26
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	10	2.26
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	14	2.26
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	11	2.26
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	2	2.26
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	1	2.26
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	1	2.26
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	4	2.26
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	11	2.26
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	6	2.26
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	8	2.26
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	11	2.26
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	15	2.26
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	9	2.25
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	8	2.25
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	13	2.25
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	6	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	9	2.25
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	12	2.25
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	9	2.25
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	8	2.25
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	10	2.25
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	2	2.25
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	11	2.25
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	15	2.25
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	6	2.25
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	14	2.25
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	15	2.25
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	1	2.25
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	2	2.25
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	4	2.25
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	14	2.25
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	11	2.25
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	2	2.25
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	2	2.25
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	13	2.25
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	1	2.25
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	15	2.25
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	12	2.24
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	13	2.24
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	9	2.24
(5,550)	1:B:236:ILE:CA	1:D:297:ALA:H	12	2.24
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	9	2.24
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	9	2.24
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	15	2.24
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	12	2.24
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	5	2.24
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	11	2.24
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	2	2.24
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	3	2.24
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	13	2.24
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	5	2.24
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	2	2.24
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	15	2.24
(5,368)	1:A:265:THR:O	1:E:265:THR:O	6	2.24
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	4	2.24
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	8	2.24
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	14	2.24
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	5	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	4	2.24
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	11	2.24
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	5	2.24
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	15	2.23
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	9	2.23
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	14	2.23
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	14	2.23
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	9	2.23
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	15	2.23
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	9	2.23
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	13	2.23
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	14	2.23
(5,510)	1:A:236:ILE:CA	1:C:297:ALA:H	12	2.23
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	13	2.23
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	15	2.23
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	3	2.23
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	6	2.23
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	14	2.23
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	3	2.23
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	15	2.23
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	11	2.23
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	15	2.23
(5,368)	1:A:265:THR:O	1:E:265:THR:O	11	2.23
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	6	2.23
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	2	2.23
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	12	2.23
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	13	2.23
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	11	2.23
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	1	2.22
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	6	2.22
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	15	2.22
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	10	2.22
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	14	2.22
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	13	2.22
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	10	2.22
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	9	2.22
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	10	2.22
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	10	2.22
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	12	2.22
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	5	2.22
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	3	2.22
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	8	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	15	2.22
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	10	2.21
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	10	2.21
(5,580)	1:C:236:ILE:CA	1:E:297:ALA:H	12	2.21
(5,568)	1:B:290:CYS:H	1:E:226:GLN:H	6	2.21
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	4	2.21
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	14	2.21
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	10	2.21
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	9	2.21
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	14	2.21
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	5	2.21
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	5	2.21
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	6	2.21
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	14	2.21
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	4	2.2
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	1	2.2
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	10	2.2
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	9	2.2
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	6	2.2
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	1	2.2
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	4	2.2
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	10	2.2
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	10	2.2
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	5	2.2
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	15	2.2
(5,448)	1:C:265:THR:O	1:D:265:THR:O	11	2.2
(5,448)	1:C:265:THR:O	1:D:265:THR:O	13	2.2
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	5	2.2
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	7	2.2
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	3	2.2
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	5	2.2
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	7	2.2
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	6	2.19
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	10	2.19
(5,583)	1:C:226:GLN:H	1:E:290:CYS:H	6	2.19
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	10	2.19
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	6	2.19
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	4	2.19
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	1	2.19
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	9	2.19
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	6	2.19
(5,488)	1:D:265:THR:O	1:E:265:THR:O	13	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,448)	1:C:265:THR:O	1:D:265:THR:O	6	2.19
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	4	2.19
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	10	2.18
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	6	2.18
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	10	2.18
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	4	2.18
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	4	2.18
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	7	2.18
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	4	2.18
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	7	2.18
(5,368)	1:A:265:THR:O	1:E:265:THR:O	1	2.18
(5,368)	1:A:265:THR:O	1:E:265:THR:O	3	2.18
(5,368)	1:A:265:THR:O	1:E:265:THR:O	5	2.18
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	4	2.18
(5,308)	1:A:265:THR:O	1:B:265:THR:O	13	2.18
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	13	2.17
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	5	2.17
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	9	2.17
(5,553)	1:B:226:GLN:H	1:D:290:CYS:H	10	2.17
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	5	2.17
(5,448)	1:C:265:THR:O	1:D:265:THR:O	3	2.17
(5,448)	1:C:265:THR:O	1:D:265:THR:O	5	2.17
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	7	2.17
(5,388)	1:B:265:THR:O	1:C:265:THR:O	13	2.17
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	4	2.17
(5,308)	1:A:265:THR:O	1:B:265:THR:O	11	2.17
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	4	2.16
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	9	2.16
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	6	2.16
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	4	2.16
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	1	2.16
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	4	2.16
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	4	2.16
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	9	2.16
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	4	2.16
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	9	2.16
(5,488)	1:D:265:THR:O	1:E:265:THR:O	11	2.16
(5,388)	1:B:265:THR:O	1:C:265:THR:O	6	2.16
(5,368)	1:A:265:THR:O	1:E:265:THR:O	8	2.16
(5,368)	1:A:265:THR:O	1:E:265:THR:O	10	2.16
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	3	2.15
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	13	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	11	2.15
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	6	2.15
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	5	2.15
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	10	2.15
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	6	2.15
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	10	2.15
(5,513)	1:A:226:GLN:H	1:C:290:CYS:H	6	2.15
(5,488)	1:D:265:THR:O	1:E:265:THR:O	6	2.15
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	7	2.15
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	11	2.15
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	7	2.15
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	11	2.15
(5,308)	1:A:265:THR:O	1:B:265:THR:O	6	2.15
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	6	2.14
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	6	2.14
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	11	2.14
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	13	2.14
(5,528)	1:A:290:CYS:H	1:D:226:GLN:H	6	2.14
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	11	2.14
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	10	2.14
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	10	2.14
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	5	2.14
(5,488)	1:D:265:THR:O	1:E:265:THR:O	3	2.14
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	7	2.14
(5,448)	1:C:265:THR:O	1:D:265:THR:O	1	2.14
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	11	2.14
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	7	2.14
(5,388)	1:B:265:THR:O	1:C:265:THR:O	11	2.14
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	11	2.14
(5,308)	1:A:265:THR:O	1:B:265:THR:O	5	2.14
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	10	2.13
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	3	2.13
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	10	2.13
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	10	2.13
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	6	2.13
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	11	2.13
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	13	2.13
(5,388)	1:B:265:THR:O	1:C:265:THR:O	5	2.13
(5,308)	1:A:265:THR:O	1:B:265:THR:O	3	2.13
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	5	2.12
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	9	2.12
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	6	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	9	2.12
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	3	2.12
(5,388)	1:B:265:THR:O	1:C:265:THR:O	3	2.12
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	7	2.12
(5,308)	1:A:265:THR:O	1:B:265:THR:O	1	2.12
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	10	2.11
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	9	2.11
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	14	2.11
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	1	2.11
(5,488)	1:D:265:THR:O	1:E:265:THR:O	1	2.11
(5,488)	1:D:265:THR:O	1:E:265:THR:O	5	2.11
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	11	2.11
(5,448)	1:C:265:THR:O	1:D:265:THR:O	10	2.11
(5,308)	1:A:265:THR:O	1:B:265:THR:O	10	2.11
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	11	2.1
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	10	2.1
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	10	2.1
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	3	2.1
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	6	2.1
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	6	2.1
(5,488)	1:D:265:THR:O	1:E:265:THR:O	10	2.1
(5,448)	1:C:265:THR:O	1:D:265:THR:O	8	2.1
(5,388)	1:B:265:THR:O	1:C:265:THR:O	10	2.1
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	9	2.09
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	3	2.09
(5,388)	1:B:265:THR:O	1:C:265:THR:O	1	2.09
(5,308)	1:A:265:THR:O	1:B:265:THR:O	8	2.09
(5,421)	1:B:231:SER:O	1:E:231:SER:O	2	2.08
(5,341)	1:A:231:SER:O	1:D:231:SER:O	2	2.08
(5,321)	1:A:231:SER:O	1:C:231:SER:O	2	2.08
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	1	2.07
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	1	2.07
(5,563)	1:B:226:GLN:H	1:E:290:CYS:H	3	2.07
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	1	2.07
(5,488)	1:D:265:THR:O	1:E:265:THR:O	8	2.07
(5,461)	1:C:231:SER:O	1:E:231:SER:O	2	2.07
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	4	2.06
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	3	2.06
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	3	2.06
(5,401)	1:B:231:SER:O	1:D:231:SER:O	2	2.06
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	9	2.06
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	10	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	4	2.05
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	4	2.05
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	8	2.05
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	4	2.05
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	3	2.05
(5,388)	1:B:265:THR:O	1:C:265:THR:O	8	2.05
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	8	2.04
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	1	2.04
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	4	2.04
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	7	2.04
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	3	2.04
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	7	2.04
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	8	2.04
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	10	2.04
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	1	2.04
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	1	2.04
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	15	2.04
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	1	2.04
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	8	2.03
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	3	2.03
(5,558)	1:B:290:CYS:H	1:D:226:GLN:H	14	2.03
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	2	2.03
(5,523)	1:A:226:GLN:H	1:D:290:CYS:H	14	2.03
(5,518)	1:A:290:CYS:H	1:C:226:GLN:H	14	2.03
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	1	2.03
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	10	2.03
(5,368)	1:A:265:THR:O	1:E:265:THR:O	12	2.03
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	15	2.03
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	3	2.03
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	14	2.02
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	10	2.02
(5,368)	1:A:265:THR:O	1:E:265:THR:O	4	2.02
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	10	2.02
(5,588)	1:C:290:CYS:H	1:E:226:GLN:H	14	2.01
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	3	2.01
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	7	2.01
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	7	2.01
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	3	2.01
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	7	2.0
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	8	2.0
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	9	2.0
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	2	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	15	2.0
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	14	2.0
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	15	2.0
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	15	2.0
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	1	2.0
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	3	2.0
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	3	2.0
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	14	2.0
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	2	1.99
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	14	1.99
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	3	1.99
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	15	1.99
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	14	1.99
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	8	1.99
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	8	1.99
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	14	1.99
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	15	1.98
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	14	1.98
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	3	1.98
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	14	1.98
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	3	1.98
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	3	1.98
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	15	1.98
(5,368)	1:A:265:THR:O	1:E:265:THR:O	14	1.98
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	15	1.97
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	2	1.97
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	15	1.97
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	14	1.97
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	11	1.97
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	14	1.97
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	14	1.97
(5,448)	1:C:265:THR:O	1:D:265:THR:O	4	1.97
(5,448)	1:C:265:THR:O	1:D:265:THR:O	14	1.97
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	9	1.97
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	10	1.97
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	13	1.96
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	12	1.96
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	8	1.96
(5,448)	1:C:265:THR:O	1:D:265:THR:O	12	1.96
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	8	1.96
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	8	1.96
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	9	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	10	1.96
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	9	1.96
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	3	1.95
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	2	1.95
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	13	1.95
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	3	1.95
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	1	1.95
(5,488)	1:D:265:THR:O	1:E:265:THR:O	4	1.95
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	9	1.95
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	10	1.95
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	10	1.95
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	10	1.95
(5,388)	1:B:265:THR:O	1:C:265:THR:O	4	1.95
(5,308)	1:A:265:THR:O	1:B:265:THR:O	4	1.95
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	8	1.94
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	12	1.94
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	3	1.94
(5,388)	1:B:265:THR:O	1:C:265:THR:O	14	1.94
(5,368)	1:A:265:THR:O	1:E:265:THR:O	2	1.94
(5,308)	1:A:265:THR:O	1:B:265:THR:O	14	1.94
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	10	1.93
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	6	1.93
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	10	1.93
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	13	1.93
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	3	1.93
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	1	1.93
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	10	1.93
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	2	1.93
(5,488)	1:D:265:THR:O	1:E:265:THR:O	12	1.93
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	6	1.92
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	9	1.92
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	3	1.92
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	6	1.92
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	13	1.92
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	14	1.92
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	10	1.92
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	13	1.92
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	11	1.92
(5,488)	1:D:265:THR:O	1:E:265:THR:O	14	1.92
(5,388)	1:B:265:THR:O	1:C:265:THR:O	12	1.92
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	2	1.91
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	1	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	10	1.91
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	1	1.91
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	11	1.91
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	3	1.91
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	11	1.91
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	14	1.91
(5,308)	1:A:265:THR:O	1:B:265:THR:O	12	1.91
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	9	1.9
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	3	1.9
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	11	1.9
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	2	1.9
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	8	1.9
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	9	1.9
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	2	1.9
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	7	1.9
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	1	1.9
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	6	1.9
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	1	1.9
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	6	1.9
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	8	1.9
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	9	1.9
(5,448)	1:C:265:THR:O	1:D:265:THR:O	2	1.9
(5,308)	1:A:265:THR:O	1:B:265:THR:O	2	1.9
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	3	1.89
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	14	1.89
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	11	1.89
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	1	1.89
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	8	1.89
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	1	1.89
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	12	1.89
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	11	1.89
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	13	1.89
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	8	1.88
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	12	1.88
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	6	1.88
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	1	1.88
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	8	1.88
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	8	1.88
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	7	1.88
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	12	1.88
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	6	1.88
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	8	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	3	1.88
(5,488)	1:D:265:THR:O	1:E:265:THR:O	2	1.88
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	13	1.88
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	10	1.88
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	13	1.88
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	11	1.87
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	11	1.87
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	7	1.87
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	8	1.87
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	12	1.87
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	14	1.87
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	5	1.87
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	11	1.87
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	6	1.87
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	6	1.87
(5,388)	1:B:265:THR:O	1:C:265:THR:O	2	1.87
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	10	1.87
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	15	1.86
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	1	1.86
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	1	1.86
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	3	1.86
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	5	1.86
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	2	1.86
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	12	1.86
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	8	1.86
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	15	1.86
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	8	1.86
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	5	1.86
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	7	1.86
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	6	1.86
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	10	1.86
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	6	1.86
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	13	1.86
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	10	1.86
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	13	1.86
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	5	1.85
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	8	1.85
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	12	1.85
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	15	1.85
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	8	1.85
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	15	1.85
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	8	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	12	1.85
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	6	1.85
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	10	1.85
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	6	1.85
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	6	1.85
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	12	1.84
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	1	1.84
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	8	1.84
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	7	1.84
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	15	1.84
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	12	1.84
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	12	1.84
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	6	1.84
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	12	1.83
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	12	1.83
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	5	1.83
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	12	1.83
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	15	1.82
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	12	1.82
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	15	1.82
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	15	1.82
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	12	1.82
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	15	1.82
(5,340)	1:A:236:ILE:CA	1:D:236:ILE:CA	12	1.82
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	12	1.81
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	12	1.81
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	13	1.81
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	11	1.81
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	15	1.8
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	13	1.8
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	13	1.8
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	12	1.8
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	1	1.8
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	13	1.8
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	11	1.79
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	11	1.79
(5,521)	1:A:231:SER:O	1:D:293:PHE:CA	7	1.79
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	7	1.79
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	11	1.79
(5,516)	1:A:293:PHE:CA	1:C:231:SER:O	13	1.79
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	12	1.79
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	8	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	13	1.79
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	5	1.79
(5,475)	1:C:406:ALA:C	1:E:406:ALA:C	3	1.79
(5,428)	1:B:265:THR:O	1:E:265:THR:O	9	1.79
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	8	1.79
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	11	1.79
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	15	1.79
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	11	1.78
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	7	1.78
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	8	1.78
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	1	1.78
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	2	1.78
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	4	1.78
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	11	1.78
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	12	1.78
(5,435)	1:B:406:ALA:C	1:E:406:ALA:C	3	1.78
(5,415)	1:B:406:ALA:C	1:D:406:ALA:C	3	1.78
(5,355)	1:A:406:ALA:C	1:D:406:ALA:C	3	1.78
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	5	1.78
(5,586)	1:C:293:PHE:CA	1:E:231:SER:O	7	1.77
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	7	1.77
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	7	1.77
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	1	1.77
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	7	1.77
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	3	1.77
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	15	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	4	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	6	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	11	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	13	1.77
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	14	1.77
(5,420)	1:B:236:ILE:CA	1:E:236:ILE:CA	12	1.77
(5,400)	1:B:236:ILE:CA	1:D:236:ILE:CA	12	1.77
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	2	1.77
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	4	1.77
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	14	1.77
(5,335)	1:A:406:ALA:C	1:C:406:ALA:C	3	1.77
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	2	1.77
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	1	1.76
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	14	1.76
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	14	1.76
(5,561)	1:B:231:SER:O	1:E:293:PHE:CA	7	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,556)	1:B:293:PHE:CA	1:D:231:SER:O	13	1.76
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	1	1.76
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	14	1.76
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	12	1.76
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	8	1.76
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	14	1.76
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	1	1.76
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	2	1.76
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	8	1.76
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	12	1.76
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	5	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	1	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	4	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	6	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	8	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	11	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	12	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	14	1.76
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	15	1.76
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	5	1.76
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	6	1.76
(5,320)	1:A:236:ILE:CA	1:C:236:ILE:CA	12	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	1	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	4	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	6	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	8	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	11	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	13	1.76
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	15	1.76
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	7	1.75
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	12	1.75
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	7	1.75
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	14	1.75
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	5	1.75
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	6	1.75
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	3	1.75
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	15	1.75
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	2	1.75
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	3	1.75
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	12	1.75
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	7	1.75
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	11	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	3	1.74
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	8	1.74
(5,571)	1:C:231:SER:O	1:D:293:PHE:CA	11	1.74
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	1	1.74
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	3	1.74
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	14	1.74
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	7	1.74
(5,468)	1:C:265:THR:O	1:E:265:THR:O	9	1.74
(5,460)	1:C:236:ILE:CA	1:E:236:ILE:CA	12	1.74
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	5	1.74
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	2	1.74
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	3	1.74
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	13	1.74
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	5	1.74
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	3	1.74
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	5	1.74
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	14	1.74
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	3	1.73
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	8	1.73
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	12	1.73
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	8	1.73
(5,536)	1:A:293:PHE:CA	1:E:231:SER:O	11	1.73
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	3	1.73
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	5	1.73
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	5	1.73
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	7	1.73
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	2	1.73
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	13	1.72
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	7	1.72
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	3	1.72
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	7	1.72
(5,501)	1:A:231:SER:O	1:B:293:PHE:CA	11	1.72
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	13	1.72
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	7	1.72
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	2	1.72
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	7	1.72
(5,408)	1:B:265:THR:O	1:D:265:THR:O	9	1.72
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	7	1.72
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	2	1.72
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	1	1.71
(5,591)	1:D:231:SER:O	1:E:293:PHE:CA	11	1.71
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	7	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	12	1.71
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	1	1.71
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	11	1.71
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	2	1.71
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	7	1.71
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	7	1.7
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	1	1.7
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	7	1.7
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	1	1.7
(5,348)	1:A:265:THR:O	1:D:265:THR:O	9	1.7
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	7	1.7
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	13	1.69
(5,541)	1:B:231:SER:O	1:C:293:PHE:CA	11	1.69
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	13	1.69
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	12	1.69
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	11	1.69
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	7	1.69
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	13	1.68
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	15	1.68
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	7	1.68
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	11	1.68
(5,301)	1:A:231:SER:O	1:B:231:SER:O	2	1.68
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	11	1.67
(5,361)	1:A:231:SER:O	1:E:231:SER:O	2	1.67
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	15	1.66
(5,481)	1:D:231:SER:O	1:E:231:SER:O	2	1.66
(5,441)	1:C:231:SER:O	1:D:231:SER:O	2	1.65
(5,328)	1:A:265:THR:O	1:C:265:THR:O	9	1.65
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	15	1.64
(5,381)	1:B:231:SER:O	1:C:231:SER:O	2	1.64
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	15	1.64
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	15	1.63
(5,533)	1:A:226:GLN:H	1:E:290:CYS:H	4	1.63
(5,511)	1:A:231:SER:O	1:C:293:PHE:CA	11	1.63
(5,436)	1:B:409:ILE:O	1:E:409:ILE:O	9	1.63
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	15	1.63
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	15	1.63
(5,526)	1:A:293:PHE:CA	1:D:231:SER:O	11	1.62
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	15	1.62
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	14	1.62
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	14	1.62
(5,581)	1:C:231:SER:O	1:E:293:PHE:CA	11	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,566)	1:B:293:PHE:CA	1:E:231:SER:O	11	1.61
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	15	1.61
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	6	1.61
(5,356)	1:A:409:ILE:O	1:D:409:ILE:O	9	1.61
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	6	1.6
(5,551)	1:B:231:SER:O	1:D:293:PHE:CA	11	1.6
(5,531)	1:A:231:SER:O	1:E:293:PHE:CA	13	1.6
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	14	1.6
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	15	1.6
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	14	1.6
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	13	1.59
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	6	1.59
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	10	1.59
(5,476)	1:C:409:ILE:O	1:E:409:ILE:O	9	1.59
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	5	1.59
(5,416)	1:B:409:ILE:O	1:D:409:ILE:O	9	1.59
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	10	1.59
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	10	1.59
(5,596)	1:D:293:PHE:CA	1:E:231:SER:O	6	1.58
(5,578)	1:C:290:CYS:H	1:D:226:GLN:H	4	1.58
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	5	1.58
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	5	1.58
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	14	1.58
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	10	1.58
(5,598)	1:D:290:CYS:H	1:E:226:GLN:H	4	1.57
(5,548)	1:B:290:CYS:H	1:C:226:GLN:H	4	1.57
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	6	1.57
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	10	1.57
(5,576)	1:C:293:PHE:CA	1:D:231:SER:O	13	1.56
(5,508)	1:A:290:CYS:H	1:B:226:GLN:H	4	1.56
(5,506)	1:A:293:PHE:CA	1:B:231:SER:O	13	1.56
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	5	1.56
(5,546)	1:B:293:PHE:CA	1:C:231:SER:O	13	1.55
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	10	1.55
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	10	1.55
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	5	1.55
(5,336)	1:A:409:ILE:O	1:C:409:ILE:O	9	1.55
(5,321)	1:A:231:SER:O	1:C:231:SER:O	5	1.55
(5,360)	1:A:236:ILE:CA	1:E:236:ILE:CA	12	1.54
(5,341)	1:A:231:SER:O	1:D:231:SER:O	5	1.54
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	10	1.53
(5,368)	1:A:265:THR:O	1:E:265:THR:O	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	10	1.53
(5,461)	1:C:231:SER:O	1:E:231:SER:O	4	1.52
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	10	1.52
(5,321)	1:A:231:SER:O	1:C:231:SER:O	4	1.52
(5,495)	1:D:406:ALA:C	1:E:406:ALA:C	3	1.51
(5,461)	1:C:231:SER:O	1:E:231:SER:O	5	1.51
(5,421)	1:B:231:SER:O	1:E:231:SER:O	4	1.51
(5,401)	1:B:231:SER:O	1:D:231:SER:O	5	1.51
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	1	1.51
(5,341)	1:A:231:SER:O	1:D:231:SER:O	4	1.51
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	8	1.5
(5,421)	1:B:231:SER:O	1:E:231:SER:O	5	1.5
(5,401)	1:B:231:SER:O	1:D:231:SER:O	4	1.49
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	1	1.49
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	1	1.48
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	8	1.48
(5,455)	1:C:406:ALA:C	1:D:406:ALA:C	3	1.48
(5,315)	1:A:406:ALA:C	1:B:406:ALA:C	3	1.48
(5,480)	1:D:236:ILE:CA	1:E:236:ILE:CA	12	1.47
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	1	1.47
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	1	1.47
(5,395)	1:B:406:ALA:C	1:C:406:ALA:C	3	1.47
(5,375)	1:A:406:ALA:C	1:E:406:ALA:C	3	1.47
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	2	1.47
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	8	1.47
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	2	1.47
(5,448)	1:C:265:THR:O	1:D:265:THR:O	9	1.46
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	9	1.46
(5,380)	1:B:236:ILE:CA	1:C:236:ILE:CA	12	1.46
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	8	1.46
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	2	1.45
(5,440)	1:C:236:ILE:CA	1:D:236:ILE:CA	12	1.45
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	8	1.45
(5,376)	1:A:409:ILE:O	1:E:409:ILE:O	9	1.45
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	5	1.45
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	5	1.45
(5,300)	1:A:236:ILE:CA	1:B:236:ILE:CA	12	1.45
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	2	1.44
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	13	1.44
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	13	1.44
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	13	1.44
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	13	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	5	1.43
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	9	1.43
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	1	1.42
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	5	1.42
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	9	1.42
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	5	1.42
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	2	1.42
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	13	1.42
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	15	1.42
(5,488)	1:D:265:THR:O	1:E:265:THR:O	9	1.41
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	9	1.41
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	6	1.41
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	15	1.41
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	13	1.41
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	13	1.41
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	15	1.41
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	13	1.41
(5,308)	1:A:265:THR:O	1:B:265:THR:O	9	1.41
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	1	1.4
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	1	1.4
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	1	1.4
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	15	1.4
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	6	1.4
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	13	1.4
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	1	1.39
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	6	1.39
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	15	1.39
(5,388)	1:B:265:THR:O	1:C:265:THR:O	9	1.39
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	7	1.39
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	10	1.39
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	13	1.39
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	10	1.39
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	4	1.38
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	3	1.38
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	7	1.38
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	14	1.38
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	3	1.38
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	7	1.38
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	7	1.38
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	14	1.38
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	6	1.38
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	4	1.37
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	4	1.37
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	5	1.37
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	14	1.37
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	10	1.37
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	10	1.37
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	10	1.37
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	14	1.37
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	3	1.37
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	4	1.36
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	4	1.36
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	3	1.36
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	5	1.36
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	5	1.36
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	9	1.36
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	6	1.36
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	14	1.36
(5,496)	1:D:409:ILE:O	1:E:409:ILE:O	9	1.35
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	5	1.35
(5,456)	1:C:409:ILE:O	1:D:409:ILE:O	9	1.35
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	5	1.35
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	5	1.35
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	5	1.35
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	9	1.35
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	3	1.35
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	5	1.35
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	7	1.34
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	5	1.34
(5,396)	1:B:409:ILE:O	1:C:409:ILE:O	9	1.34
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	5	1.34
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	7	1.33
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	8	1.33
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	8	1.33
(5,361)	1:A:231:SER:O	1:E:231:SER:O	4	1.33
(5,301)	1:A:231:SER:O	1:B:231:SER:O	5	1.33
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	7	1.32
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	9	1.32
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	10	1.32
(5,441)	1:C:231:SER:O	1:D:231:SER:O	5	1.32
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	14	1.32
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	14	1.32
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	1	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,361)	1:A:231:SER:O	1:E:231:SER:O	5	1.32
(5,316)	1:A:409:ILE:O	1:B:409:ILE:O	9	1.32
(5,301)	1:A:231:SER:O	1:B:231:SER:O	4	1.32
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	10	1.31
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	7	1.31
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	10	1.31
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	1	1.31
(5,441)	1:C:231:SER:O	1:D:231:SER:O	4	1.31
(5,381)	1:B:231:SER:O	1:C:231:SER:O	5	1.31
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	7	1.3
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	10	1.3
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	2	1.3
(5,481)	1:D:231:SER:O	1:E:231:SER:O	4	1.3
(5,481)	1:D:231:SER:O	1:E:231:SER:O	5	1.3
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	8	1.3
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	14	1.3
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	9	1.3
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	14	1.3
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	14	1.3
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	14	1.3
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	1	1.3
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	8	1.3
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	8	1.29
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	1	1.29
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	14	1.29
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	8	1.29
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	8	1.29
(5,381)	1:B:231:SER:O	1:C:231:SER:O	4	1.29
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	13	1.29
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	5	1.29
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	12	1.29
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	14	1.29
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	14	1.29
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	2	1.28
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	10	1.28
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	5	1.28
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	12	1.28
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	13	1.28
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	5	1.28
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	8	1.27
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	13	1.27
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	8	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	5	1.27
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	12	1.27
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	1	1.27
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	8	1.27
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	5	1.27
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	11	1.27
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	14	1.27
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	5	1.27
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	8	1.26
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	2	1.26
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	2	1.26
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	13	1.26
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	11	1.26
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	8	1.26
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	6	1.26
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	15	1.26
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	15	1.26
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	2	1.25
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	8	1.25
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	8	1.25
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	5	1.25
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	9	1.25
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	9	1.25
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	13	1.25
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	6	1.25
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	7	1.25
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	13	1.25
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	11	1.25
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	5	1.25
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	5	1.25
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	7	1.25
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	9	1.25
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	11	1.25
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	13	1.25
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	13	1.25
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	9	1.24
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	9	1.24
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	9	1.24
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	9	1.24
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	15	1.24
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	11	1.24
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	12	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	15	1.24
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	9	1.24
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	15	1.24
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	5	1.24
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	10	1.24
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	8	1.24
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	7	1.24
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	10	1.24
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	5	1.23
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	3	1.23
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	6	1.23
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	10	1.23
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	3	1.23
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	9	1.23
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	13	1.23
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	6	1.23
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	10	1.23
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	13	1.23
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	3	1.23
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	9	1.23
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	12	1.23
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	12	1.23
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	9	1.22
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	7	1.22
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	10	1.22
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	3	1.22
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	6	1.22
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	5	1.21
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	5	1.21
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	7	1.21
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	14	1.21
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	5	1.21
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	5	1.21
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	9	1.21
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	5	1.2
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	14	1.2
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	14	1.2
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	2	1.2
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	3	1.2
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	8	1.2
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	14	1.2
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	9	1.2
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	8	1.19
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	14	1.18
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	1	1.18
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	2	1.18
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	4	1.18
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	1	1.18
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	4	1.18
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	1	1.18
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	2	1.18
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	14	1.18
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	14	1.18
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	11	1.18
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	2	1.18
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	14	1.17
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	8	1.17
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	11	1.17
(5,426)	1:B:260:VAL:CA	1:E:260:VAL:CA	2	1.17
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	2	1.17
(5,346)	1:A:260:VAL:CA	1:D:260:VAL:CA	4	1.17
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	1	1.17
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	2	1.17
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	4	1.17
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	14	1.17
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	14	1.17
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	12	1.16
(5,466)	1:C:260:VAL:CA	1:E:260:VAL:CA	2	1.16
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	5	1.16
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	9	1.16
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	2	1.16
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	8	1.16
(5,326)	1:A:260:VAL:CA	1:C:260:VAL:CA	2	1.16
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	8	1.16
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	5	1.16
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	12	1.15
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	12	1.15
(5,406)	1:B:260:VAL:CA	1:D:260:VAL:CA	4	1.15
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	5	1.15
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	11	1.15
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	11	1.14
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	11	1.14
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	1	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	4	1.14
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	12	1.13
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	2	1.13
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	9	1.13
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	12	1.13
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	15	1.12
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	1	1.12
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	2	1.12
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	9	1.12
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	15	1.11
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	15	1.11
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	4	1.11
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	9	1.11
(5,366)	1:A:260:VAL:CA	1:E:260:VAL:CA	2	1.11
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	2	1.11
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	2	1.11
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	2	1.1
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	1	1.1
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	2	1.1
(5,446)	1:C:260:VAL:CA	1:D:260:VAL:CA	2	1.1
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	1	1.1
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	2	1.1
(5,306)	1:A:260:VAL:CA	1:B:260:VAL:CA	4	1.1
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	12	1.09
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	11	1.09
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	12	1.09
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	12	1.09
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	4	1.09
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	4	1.09
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	4	1.09
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	12	1.09
(5,361)	1:A:231:SER:O	1:E:231:SER:O	9	1.09
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	12	1.09
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	1	1.09
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	15	1.08
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	11	1.08
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	12	1.08
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	4	1.08
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	12	1.08
(5,386)	1:B:260:VAL:CA	1:C:260:VAL:CA	2	1.08
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	11	1.07
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	15	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	11	1.07
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	11	1.07
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	4	1.07
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	12	1.07
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	5	1.06
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	7	1.06
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	4	1.06
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	7	1.06
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	4	1.06
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	5	1.05
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	4	1.05
(5,486)	1:D:260:VAL:CA	1:E:260:VAL:CA	5	1.05
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	4	1.05
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	13	1.05
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	4	1.05
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	7	1.05
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	5	1.04
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	7	1.04
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	12	1.04
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	12	1.04
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	4	1.04
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	4	1.04
(5,421)	1:B:231:SER:O	1:E:231:SER:O	9	1.04
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	7	1.04
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	4	1.04
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	4	1.04
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	5	1.03
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	7	1.03
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	13	1.03
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	4	1.03
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	4	1.03
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	4	1.03
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	7	1.02
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	12	1.02
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	4	1.02
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	12	1.02
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	7	1.02
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	12	1.02
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	4	1.02
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	7	1.02
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	13	1.01
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	13	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,341)	1:A:231:SER:O	1:D:231:SER:O	9	1.01
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	12	1.01
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	5	1.0
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	4	1.0
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	13	1.0
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	4	1.0
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	7	1.0
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	4	1.0
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	10	1.0
(5,481)	1:D:231:SER:O	1:E:231:SER:O	14	0.99
(5,461)	1:C:231:SER:O	1:E:231:SER:O	9	0.99
(5,461)	1:C:231:SER:O	1:E:231:SER:O	14	0.99
(5,441)	1:C:231:SER:O	1:D:231:SER:O	9	0.99
(5,441)	1:C:231:SER:O	1:D:231:SER:O	14	0.99
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	13	0.99
(5,401)	1:B:231:SER:O	1:D:231:SER:O	9	0.99
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	13	0.99
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	10	0.99
(5,421)	1:B:231:SER:O	1:E:231:SER:O	14	0.98
(5,401)	1:B:231:SER:O	1:D:231:SER:O	14	0.98
(5,381)	1:B:231:SER:O	1:C:231:SER:O	14	0.98
(5,361)	1:A:231:SER:O	1:E:231:SER:O	14	0.98
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	10	0.98
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	10	0.98
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	10	0.97
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	10	0.97
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	13	0.97
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	10	0.97
(5,341)	1:A:231:SER:O	1:D:231:SER:O	14	0.97
(5,321)	1:A:231:SER:O	1:C:231:SER:O	9	0.97
(5,321)	1:A:231:SER:O	1:C:231:SER:O	14	0.97
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	13	0.97
(5,301)	1:A:231:SER:O	1:B:231:SER:O	9	0.97
(5,301)	1:A:231:SER:O	1:B:231:SER:O	14	0.97
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	10	0.96
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	10	0.96
(5,381)	1:B:231:SER:O	1:C:231:SER:O	9	0.96
(5,481)	1:D:231:SER:O	1:E:231:SER:O	9	0.95
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	10	0.95
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	8	0.95
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	5	0.95
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	13	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,590)	1:D:236:ILE:CA	1:E:297:ALA:H	3	0.94
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	11	0.94
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	8	0.93
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	11	0.93
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	5	0.93
(5,570)	1:C:236:ILE:CA	1:D:297:ALA:H	3	0.92
(5,500)	1:A:236:ILE:CA	1:B:297:ALA:H	3	0.92
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	8	0.92
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	11	0.91
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	8	0.91
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	5	0.91
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	8	0.9
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	11	0.9
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	9	0.9
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	11	0.9
(5,540)	1:B:236:ILE:CA	1:C:297:ALA:H	3	0.89
(5,535)	1:A:297:ALA:H	1:E:236:ILE:CA	3	0.89
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	5	0.89
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	7	0.89
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	8	0.89
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	7	0.88
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	5	0.88
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	8	0.88
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	11	0.88
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	11	0.87
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	8	0.87
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	2	0.87
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	3	0.87
(5,343)	1:A:226:GLN:H	1:D:226:GLN:H	5	0.87
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	2	0.86
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	3	0.86
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	11	0.86
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	7	0.86
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	3	0.86
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	11	0.86
(5,323)	1:A:226:GLN:H	1:C:226:GLN:H	5	0.86
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	7	0.86
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	3	0.86
(5,423)	1:B:226:GLN:H	1:E:226:GLN:H	5	0.85
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	12	0.85
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	11	0.85
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	5	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	13	0.85
(5,463)	1:C:226:GLN:H	1:E:226:GLN:H	5	0.84
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	2	0.84
(5,403)	1:B:226:GLN:H	1:D:226:GLN:H	5	0.84
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	2	0.84
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	7	0.84
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	8	0.84
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	2	0.84
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	3	0.83
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	15	0.83
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	15	0.83
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	6	0.83
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	14	0.83
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	10	0.83
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	11	0.83
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	3	0.83
(5,481)	1:D:231:SER:O	1:E:231:SER:O	3	0.82
(5,361)	1:A:231:SER:O	1:E:231:SER:O	3	0.82
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	5	0.82
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	8	0.82
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	10	0.82
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	13	0.82
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	1	0.82
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	9	0.82
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	14	0.82
(5,441)	1:C:231:SER:O	1:D:231:SER:O	3	0.81
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	3	0.81
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	6	0.81
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	8	0.81
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	15	0.81
(5,301)	1:A:231:SER:O	1:B:231:SER:O	3	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	1	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	3	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	7	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	9	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	12	0.81
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	15	0.81
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	8	0.81
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	12	0.81
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	3	0.8
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	15	0.8
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	3	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	7	0.8
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	1	0.8
(5,301)	1:A:231:SER:O	1:B:231:SER:O	10	0.8
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	11	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	1	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	6	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	8	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	9	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	10	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	11	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	12	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	14	0.8
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	15	0.8
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	6	0.8
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	7	0.8
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	15	0.8
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	12	0.79
(5,481)	1:D:231:SER:O	1:E:231:SER:O	10	0.79
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	6	0.79
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	9	0.79
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	15	0.79
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	7	0.79
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	15	0.79
(5,381)	1:B:231:SER:O	1:C:231:SER:O	3	0.79
(5,361)	1:A:231:SER:O	1:E:231:SER:O	10	0.79
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	7	0.79
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	13	0.79
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	3	0.79
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	5	0.79
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	7	0.79
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	2	0.79
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	1	0.78
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	15	0.78
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	7	0.78
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	3	0.78
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	12	0.78
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	15	0.78
(5,441)	1:C:231:SER:O	1:D:231:SER:O	10	0.78
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	2	0.78
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	3	0.78
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	3	0.78
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,381)	1:B:231:SER:O	1:C:231:SER:O	10	0.78
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	3	0.78
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	15	0.78
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	9	0.78
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	2	0.78
(2,39)	1:A:300:GLU:O	1:A:304:VAL:N	4	0.78
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	10	0.78
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	2	0.78
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	4	0.78
(2,3)	1:A:222:TYR:O	1:A:226:GLN:N	13	0.78
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	4	0.78
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	4	0.78
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	13	0.78
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	6	0.77
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	9	0.77
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	15	0.77
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	3	0.77
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	6	0.77
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	12	0.77
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	15	0.77
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	3	0.77
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	2	0.77
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	2	0.76
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	1	0.76
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	6	0.76
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	2	0.76
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	3	0.76
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	1	0.76
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	6	0.76
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	6	0.76
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	12	0.76
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	6	0.76
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	8	0.76
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	12	0.76
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	13	0.76
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	3	0.76
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	9	0.76
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	4	0.76
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	11	0.76
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	11	0.76
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	1	0.76
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	7	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	14	0.76
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	6	0.75
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	6	0.75
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	9	0.75
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	2	0.75
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	7	0.75
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	3	0.75
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	1	0.75
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	6	0.75
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	2	0.75
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	4	0.75
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	1	0.75
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	13	0.75
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	6	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	1	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	2	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	5	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	7	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	8	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	13	0.75
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	14	0.75
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	15	0.75
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	12	0.75
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	10	0.75
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	3	0.74
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	12	0.74
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	14	0.74
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	5	0.74
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	13	0.74
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	3	0.74
(2,32)	1:A:290:CYS:O	1:A:294:VAL:N	9	0.74
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	4	0.74
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	14	0.74
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	7	0.74
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	11	0.74
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	1	0.73
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	3	0.73
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	11	0.73
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	11	0.73
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	2	0.73
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	4	0.73
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	15	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	6	0.73
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	9	0.73
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	14	0.73
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	6	0.73
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	15	0.73
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	11	0.73
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	7	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	5	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	6	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	9	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	11	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	12	0.73
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	15	0.73
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	15	0.73
(5,461)	1:C:231:SER:O	1:E:231:SER:O	3	0.72
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	9	0.72
(5,421)	1:B:231:SER:O	1:E:231:SER:O	3	0.72
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	11	0.72
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	2	0.72
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	13	0.72
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	9	0.72
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	14	0.72
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	14	0.72
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	15	0.72
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	10	0.72
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	11	0.72
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	12	0.72
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	1	0.72
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	2	0.72
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	7	0.72
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	9	0.72
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	12	0.72
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	2	0.72
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	7	0.72
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	14	0.72
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	2	0.72
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	7	0.71
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	6	0.71
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	15	0.71
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	5	0.71
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	7	0.71
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	15	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	1	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	3	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	5	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	7	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	9	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	10	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	12	0.71
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	13	0.71
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	1	0.71
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	8	0.71
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	4	0.71
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	12	0.71
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	15	0.71
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	5	0.71
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	8	0.71
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	6	0.71
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	8	0.71
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	12	0.71
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	1	0.71
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	8	0.71
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	9	0.71
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	8	0.71
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	4	0.7
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	4	0.7
(5,401)	1:B:231:SER:O	1:D:231:SER:O	3	0.7
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	4	0.7
(5,341)	1:A:231:SER:O	1:D:231:SER:O	3	0.7
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	8	0.7
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	14	0.7
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	10	0.7
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	15	0.7
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	7	0.7
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	10	0.7
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	1	0.7
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	10	0.7
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	12	0.7
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	1	0.7
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	8	0.7
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	15	0.7
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	7	0.7
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	15	0.7
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	4	0.7
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	7	0.7
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	1	0.7
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	6	0.7
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	3	0.7
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	15	0.7
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	1	0.7
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	6	0.7
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	3	0.7
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	6	0.7
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	11	0.69
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	3	0.69
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	12	0.69
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	4	0.69
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	9	0.69
(5,341)	1:A:231:SER:O	1:D:231:SER:O	10	0.69
(5,321)	1:A:231:SER:O	1:C:231:SER:O	3	0.69
(5,321)	1:A:231:SER:O	1:C:231:SER:O	10	0.69
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	12	0.69
(2,53)	1:A:414:TYR:O	1:A:418:TYR:N	5	0.69
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	2	0.69
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	8	0.69
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	12	0.69
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	3	0.69
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	1	0.69
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	8	0.69
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	15	0.69
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	10	0.69
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	1	0.69
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	7	0.69
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	9	0.69
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	12	0.69
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	13	0.69
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	6	0.69
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	8	0.69
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	12	0.69
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	13	0.69
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	3	0.69
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	5	0.69
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	9	0.69
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	10	0.69
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	12	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	13	0.69
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	5	0.69
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	14	0.69
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	15	0.69
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	11	0.69
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	14	0.69
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	11	0.68
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	15	0.68
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	15	0.68
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	12	0.68
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	11	0.68
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	2	0.68
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	12	0.68
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	15	0.68
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	9	0.68
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	15	0.68
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	15	0.68
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	4	0.68
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	11	0.68
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	2	0.68
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	5	0.68
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	6	0.68
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	6	0.68
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	13	0.68
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	8	0.68
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	15	0.68
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	8	0.68
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	8	0.68
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	13	0.68
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	6	0.68
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	10	0.68
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	1	0.68
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	3	0.68
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	9	0.68
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	11	0.68
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	2	0.68
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	4	0.68
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	10	0.68
(2,16)	1:A:239:TRP:O	1:A:243:TRP:N	13	0.68
(2,14)	1:A:236:ILE:O	1:A:240:ILE:N	3	0.68
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	12	0.68
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	3	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	3	0.67
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	15	0.67
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	15	0.67
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	3	0.67
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	3	0.67
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	3	0.67
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	11	0.67
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	3	0.67
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	9	0.67
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	11	0.67
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	14	0.67
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	12	0.67
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	7	0.67
(2,33)	1:A:292:LEU:O	1:A:296:SER:N	1	0.67
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	13	0.67
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	11	0.67
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	4	0.67
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	11	0.67
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	2	0.67
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	4	0.67
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	10	0.67
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	14	0.67
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	15	0.67
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	9	0.67
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	3	0.67
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	13	0.67
(5,461)	1:C:231:SER:O	1:E:231:SER:O	10	0.66
(5,421)	1:B:231:SER:O	1:E:231:SER:O	10	0.66
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	9	0.66
(5,401)	1:B:231:SER:O	1:D:231:SER:O	10	0.66
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	3	0.66
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	15	0.66
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	1	0.66
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	5	0.66
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	4	0.66
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	4	0.66
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	13	0.66
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	6	0.66
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	11	0.66
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	2	0.66
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	4	0.66
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	11	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	12	0.66
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	10	0.66
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	13	0.66
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	3	0.66
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	2	0.66
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	5	0.66
(2,21)	1:A:256:GLY:O	1:A:260:VAL:N	7	0.66
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	4	0.66
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	10	0.66
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	13	0.66
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	14	0.66
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	1	0.66
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	9	0.65
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	6	0.65
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	15	0.65
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	15	0.65
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	3	0.65
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	3	0.65
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	2	0.65
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	4	0.65
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	6	0.65
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	14	0.65
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	5	0.65
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	11	0.65
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	8	0.65
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	3	0.65
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	6	0.65
(2,18)	1:A:251:ALA:O	1:A:255:LEU:N	2	0.65
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	4	0.65
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	10	0.65
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	11	0.65
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	5	0.65
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	12	0.64
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	2	0.64
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	1	0.64
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	6	0.64
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	15	0.64
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	1	0.64
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	6	0.64
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	9	0.64
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	10	0.64
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	8	0.64
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	9	0.64
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	13	0.64
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	5	0.64
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	5	0.64
(2,24)	1:A:260:VAL:O	1:A:264:THR:N	14	0.64
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	7	0.64
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	8	0.64
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	12	0.64
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	6	0.63
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	6	0.63
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	6	0.63
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	15	0.63
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	7	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	2	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	3	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	4	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	9	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	10	0.63
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	13	0.63
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	8	0.63
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	15	0.63
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	1	0.62
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	14	0.62
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	6	0.62
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	1	0.62
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	13	0.62
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	3	0.62
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	12	0.62
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	6	0.62
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	7	0.62
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	7	0.62
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	6	0.62
(2,34)	1:A:294:VAL:O	1:A:298:LEU:N	14	0.62
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	5	0.62
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	6	0.62
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	3	0.62
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	5	0.62
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	9	0.62
(2,12)	1:A:233:LEU:O	1:A:237:LEU:N	13	0.62
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	15	0.61
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	14	0.61
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	6	0.61
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	1	0.61
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	4	0.61
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	3	0.61
(2,48)	1:A:405:LEU:O	1:A:409:ILE:N	9	0.61
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	10	0.61
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	12	0.61
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	1	0.61
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	2	0.61
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	7	0.61
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	10	0.61
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	15	0.61
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	6	0.6
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	9	0.6
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	15	0.6
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	15	0.6
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	2	0.6
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	14	0.6
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	10	0.6
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	7	0.6
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	14	0.6
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	4	0.6
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	15	0.6
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	3	0.6
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	4	0.6
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	6	0.6
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	14	0.59
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	15	0.59
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	14	0.59
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	8	0.59
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	9	0.59
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	14	0.59
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	15	0.59
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	3	0.59
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	9	0.59
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	11	0.59
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	12	0.59
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	10	0.59
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	3	0.59
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	11	0.59
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	5	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	9	0.58
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	6	0.58
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	9	0.58
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	8	0.58
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	2	0.58
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	3	0.58
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	6	0.58
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	13	0.58
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	15	0.58
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	14	0.58
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	1	0.58
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	1	0.58
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	6	0.58
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	13	0.58
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	3	0.57
(5,361)	1:A:231:SER:O	1:E:231:SER:O	6	0.57
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	13	0.57
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	5	0.57
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	5	0.57
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	10	0.57
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	13	0.57
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	10	0.57
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	3	0.57
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	5	0.57
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	9	0.57
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	12	0.57
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	2	0.57
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	8	0.57
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	9	0.56
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	14	0.56
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	14	0.56
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	1	0.56
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	11	0.56
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	12	0.56
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	13	0.56
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	12	0.56
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	9	0.56
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	11	0.56
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	6	0.56
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	8	0.56
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	2	0.56
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	6	0.56
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	8	0.56
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	15	0.56
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	14	0.56
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	7	0.56
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	5	0.56
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	14	0.55
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	3	0.55
(5,441)	1:C:231:SER:O	1:D:231:SER:O	6	0.55
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	10	0.55
(5,381)	1:B:231:SER:O	1:C:231:SER:O	6	0.55
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	9	0.55
(2,6)	1:A:225:ILE:O	1:A:229:ILE:N	7	0.55
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	2	0.55
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	13	0.55
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	2	0.55
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	11	0.55
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	15	0.55
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	8	0.55
(2,13)	1:A:234:ILE:O	1:A:238:SER:N	14	0.55
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	3	0.55
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	4	0.55
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	10	0.54
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	14	0.54
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	14	0.54
(5,361)	1:A:231:SER:O	1:E:231:SER:O	1	0.54
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	9	0.54
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	3	0.54
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	4	0.54
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	11	0.54
(2,47)	1:A:404:PRO:O	1:A:408:LEU:N	9	0.54
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	1	0.54
(2,40)	1:A:302:ALA:O	1:A:306:PHE:N	14	0.54
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	1	0.54
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	8	0.54
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	9	0.54
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	12	0.54
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	12	0.54
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	2	0.54
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	5	0.54
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	8	0.54
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	15	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	6	0.54
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	3	0.53
(5,481)	1:D:231:SER:O	1:E:231:SER:O	6	0.53
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	13	0.53
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	7	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	2	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	3	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	4	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	7	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	11	0.53
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	14	0.53
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	4	0.53
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	7	0.53
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	10	0.53
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	6	0.52
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	6	0.52
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	4	0.52
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	6	0.52
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	9	0.52
(5,361)	1:A:231:SER:O	1:E:231:SER:O	8	0.52
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	13	0.52
(5,301)	1:A:231:SER:O	1:B:231:SER:O	1	0.52
(5,301)	1:A:231:SER:O	1:B:231:SER:O	6	0.52
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	9	0.52
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	5	0.52
(2,4)	1:A:223:TYR:O	1:A:227:LEU:N	5	0.52
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	3	0.52
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	9	0.52
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	10	0.52
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	13	0.52
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	4	0.52
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	12	0.52
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	4	0.52
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	1	0.52
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	13	0.52
(5,481)	1:D:231:SER:O	1:E:231:SER:O	1	0.51
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	4	0.51
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	10	0.51
(5,441)	1:C:231:SER:O	1:D:231:SER:O	1	0.51
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	11	0.51
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	6	0.51
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	10	0.51
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	6	0.51
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	1	0.51
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	5	0.51
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	5	0.51
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	6	0.51
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	15	0.51
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	9	0.51
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	10	0.51
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	1	0.51
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	2	0.51
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	9	0.5
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	4	0.5
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	11	0.5
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	13	0.5
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	12	0.5
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	11	0.5
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	2	0.5
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	4	0.5
(2,52)	1:A:410:PHE:O	1:A:414:TYR:N	14	0.5
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	5	0.5
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	2	0.5
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	4	0.5
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	12	0.5
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	9	0.5
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	11	0.5
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	10	0.5
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	6	0.5
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	15	0.5
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	13	0.49
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	11	0.49
(5,381)	1:B:231:SER:O	1:C:231:SER:O	1	0.49
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	12	0.49
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	4	0.49
(5,301)	1:A:231:SER:O	1:B:231:SER:O	8	0.49
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	5	0.49
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	10	0.49
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	7	0.49
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	3	0.48
(5,397)	1:B:411:ASN:O	1:C:411:ASN:O	10	0.48
(5,377)	1:A:411:ASN:O	1:E:411:ASN:O	10	0.48
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	5	0.48
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	3	0.48
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	10	0.48
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	7	0.48
(5,497)	1:D:411:ASN:O	1:E:411:ASN:O	10	0.47
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	11	0.47
(5,441)	1:C:231:SER:O	1:D:231:SER:O	8	0.47
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	3	0.47
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	9	0.47
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	8	0.47
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	1	0.47
(5,361)	1:A:231:SER:O	1:E:231:SER:O	12	0.47
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	11	0.47
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	2	0.47
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	3	0.47
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	3	0.47
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	14	0.47
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	6	0.47
(2,22)	1:A:258:THR:O	1:A:262:THR:N	9	0.47
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	9	0.47
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	13	0.47
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	5	0.47
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	12	0.47
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	3	0.46
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	11	0.46
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	3	0.46
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	12	0.46
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	1	0.46
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	6	0.46
(5,317)	1:A:411:ASN:O	1:B:411:ASN:O	10	0.46
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	9	0.46
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	14	0.46
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	10	0.46
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	11	0.46
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	14	0.46
(2,35)	1:A:295:PHE:O	1:A:299:LEU:N	9	0.46
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	1	0.46
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	10	0.46
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	12	0.46
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	5	0.45
(5,481)	1:D:231:SER:O	1:E:231:SER:O	8	0.45
(5,457)	1:C:411:ASN:O	1:D:411:ASN:O	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	3	0.45
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	9	0.45
(5,381)	1:B:231:SER:O	1:C:231:SER:O	8	0.45
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	12	0.45
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	3	0.45
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	12	0.45
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	15	0.45
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	8	0.45
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	13	0.45
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	3	0.45
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	3	0.45
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	13	0.45
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	6	0.45
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	6	0.45
(2,27)	1:A:276:LYS:O	1:A:280:VAL:N	10	0.45
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	6	0.45
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	2	0.45
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	13	0.45
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	11	0.45
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	1	0.44
(5,423)	1:B:226:GLN:H	1:E:226:GLN:H	2	0.44
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	10	0.44
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	8	0.44
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	9	0.44
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	8	0.44
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	4	0.44
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	7	0.44
(5,361)	1:A:231:SER:O	1:E:231:SER:O	13	0.44
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	9	0.44
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	15	0.44
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	1	0.44
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	2	0.44
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	11	0.44
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	15	0.44
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	8	0.44
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	13	0.44
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	11	0.44
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	9	0.43
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	12	0.43
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	15	0.43
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	3	0.43
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	10	0.43
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	5	0.43
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	10	0.43
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	11	0.43
(5,363)	1:A:226:GLN:H	1:E:226:GLN:H	14	0.43
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	7	0.43
(5,362)	1:A:229:ILE:N	1:E:229:ILE:N	11	0.43
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	3	0.43
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	8	0.43
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	11	0.43
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	12	0.43
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	3	0.43
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	1	0.43
(2,30)	1:A:279:TYR:O	1:A:283:ILE:N	13	0.43
(2,19)	1:A:253:VAL:O	1:A:257:ILE:N	3	0.43
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	7	0.43
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	9	0.43
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	10	0.42
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	8	0.42
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	13	0.42
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	8	0.42
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	6	0.42
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	11	0.42
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	4	0.42
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	13	0.42
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	4	0.42
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	8	0.42
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	8	0.42
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	10	0.42
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	6	0.42
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	11	0.42
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	11	0.42
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	4	0.42
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	8	0.42
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	1	0.41
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	1	0.41
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	6	0.41
(5,458)	1:C:413:PHE:O	1:D:413:PHE:O	10	0.41
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	1	0.41
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	4	0.41
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	7	0.41
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	11	0.41
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	15	0.41
(5,378)	1:A:413:PHE:O	1:E:413:PHE:O	6	0.41
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	1	0.41
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	6	0.41
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	11	0.41
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	14	0.41
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	11	0.41
(5,361)	1:A:231:SER:O	1:E:231:SER:O	7	0.41
(5,343)	1:A:226:GLN:H	1:D:226:GLN:H	2	0.41
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	1	0.41
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	7	0.41
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	1	0.41
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	11	0.41
(5,301)	1:A:231:SER:O	1:B:231:SER:O	11	0.41
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	15	0.41
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	4	0.41
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	10	0.41
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	3	0.41
(2,25)	1:A:261:LEU:O	1:A:265:THR:N	9	0.41
(2,15)	1:A:237:LEU:O	1:A:241:SER:N	14	0.41
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	9	0.41
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	7	0.4
(5,481)	1:D:231:SER:O	1:E:231:SER:O	13	0.4
(5,463)	1:C:226:GLN:H	1:E:226:GLN:H	2	0.4
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	14	0.4
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	5	0.4
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	7	0.4
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	8	0.4
(5,441)	1:C:231:SER:O	1:D:231:SER:O	11	0.4
(5,403)	1:B:226:GLN:H	1:D:226:GLN:H	2	0.4
(5,398)	1:B:413:PHE:O	1:C:413:PHE:O	6	0.4
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	6	0.4
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	1	0.4
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	2	0.4
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	7	0.4
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	4	0.4
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	8	0.4
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	5	0.4
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	13	0.4
(5,361)	1:A:231:SER:O	1:E:231:SER:O	11	0.4
(5,361)	1:A:231:SER:O	1:E:231:SER:O	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,323)	1:A:226:GLN:H	1:C:226:GLN:H	2	0.4
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	10	0.4
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	2	0.4
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	7	0.4
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	10	0.4
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	15	0.4
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	7	0.4
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	5	0.4
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	4	0.4
(2,42)	1:A:398:ILE:O	1:A:402:GLY:N	2	0.4
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	7	0.4
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	12	0.4
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	15	0.4
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	8	0.4
(5,498)	1:D:413:PHE:O	1:E:413:PHE:O	6	0.39
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	2	0.39
(5,484)	1:D:253:VAL:H	1:E:253:VAL:H	4	0.39
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	12	0.39
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	11	0.39
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	12	0.39
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	1	0.39
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	6	0.39
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	7	0.39
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	9	0.39
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	11	0.39
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	1	0.39
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	4	0.39
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	12	0.39
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	15	0.39
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	9	0.39
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	10	0.39
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	12	0.39
(5,443)	1:C:226:GLN:H	1:D:226:GLN:H	15	0.39
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	12	0.39
(5,441)	1:C:231:SER:O	1:D:231:SER:O	7	0.39
(5,441)	1:C:231:SER:O	1:D:231:SER:O	13	0.39
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	15	0.39
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	1	0.39
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	8	0.39
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	12	0.39
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	4	0.39
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	12	0.39
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	14	0.39
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	12	0.39
(5,381)	1:B:231:SER:O	1:C:231:SER:O	12	0.39
(5,381)	1:B:231:SER:O	1:C:231:SER:O	13	0.39
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	3	0.39
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	5	0.39
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	10	0.39
(5,367)	1:A:263:LEU:H	1:E:263:LEU:H	15	0.39
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	11	0.39
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	14	0.39
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	4	0.39
(5,318)	1:A:413:PHE:O	1:B:413:PHE:O	6	0.39
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	2	0.39
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	8	0.39
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	2	0.39
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	4	0.39
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	12	0.39
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	6	0.39
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	14	0.39
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	13	0.39
(5,301)	1:A:231:SER:O	1:B:231:SER:O	15	0.39
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	8	0.39
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	11	0.39
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	3	0.39
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	3	0.39
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	5	0.39
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	9	0.39
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	15	0.39
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	13	0.39
(2,28)	1:A:277:VAL:O	1:A:281:LYS:N	5	0.39
(2,22)	1:A:258:THR:O	1:A:262:THR:N	6	0.39
(2,22)	1:A:258:THR:O	1:A:262:THR:N	10	0.39
(2,22)	1:A:258:THR:O	1:A:262:THR:N	13	0.39
(2,22)	1:A:258:THR:O	1:A:262:THR:N	14	0.39
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	1	0.39
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	11	0.39
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	14	0.39
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	7	0.39
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	12	0.39
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	1	0.39
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	2	0.38
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	4	0.38
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	7	0.38
(5,481)	1:D:231:SER:O	1:E:231:SER:O	12	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	2	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	3	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	4	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	8	0.38
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	12	0.38
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	4	0.38
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	11	0.38
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	12	0.38
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	14	0.38
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	7	0.38
(5,442)	1:C:229:ILE:N	1:D:229:ILE:N	13	0.38
(5,441)	1:C:231:SER:O	1:D:231:SER:O	12	0.38
(5,438)	1:B:413:PHE:O	1:E:413:PHE:O	9	0.38
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	14	0.38
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	2	0.38
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	4	0.38
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	7	0.38
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	13	0.38
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	8	0.38
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	11	0.38
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	1	0.38
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	2	0.38
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	6	0.38
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	15	0.38
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	1	0.38
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	4	0.38
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	10	0.38
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	11	0.38
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	15	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	4	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	5	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	7	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	8	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	10	0.38
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	15	0.38
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	9	0.38
(5,303)	1:A:226:GLN:H	1:B:226:GLN:H	12	0.38
(5,301)	1:A:231:SER:O	1:B:231:SER:O	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,301)	1:A:231:SER:O	1:B:231:SER:O	13	0.38
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	7	0.38
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	7	0.38
(2,22)	1:A:258:THR:O	1:A:262:THR:N	1	0.38
(2,22)	1:A:258:THR:O	1:A:262:THR:N	3	0.38
(2,22)	1:A:258:THR:O	1:A:262:THR:N	8	0.38
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	4	0.38
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	2	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	3	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	4	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	12	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	13	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	14	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	15	0.37
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	3	0.37
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	4	0.37
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	12	0.37
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	13	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	1	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	7	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	8	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	10	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	11	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	14	0.37
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	15	0.37
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	8	0.37
(5,482)	1:D:229:ILE:N	1:E:229:ILE:N	13	0.37
(5,481)	1:D:231:SER:O	1:E:231:SER:O	7	0.37
(5,481)	1:D:231:SER:O	1:E:231:SER:O	11	0.37
(5,481)	1:D:231:SER:O	1:E:231:SER:O	15	0.37
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	15	0.37
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	5	0.37
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	10	0.37
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	13	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	1	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	2	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	5	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	7	0.37
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	9	0.37
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	2	0.37
(5,444)	1:C:253:VAL:H	1:D:253:VAL:H	13	0.37
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	6	0.37
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	10	0.37
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	15	0.37
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	4	0.37
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	11	0.37
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	14	0.37
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	9	0.37
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	10	0.37
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	11	0.37
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	15	0.37
(5,381)	1:B:231:SER:O	1:C:231:SER:O	15	0.37
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	7	0.37
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	13	0.37
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	1	0.37
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	15	0.37
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	5	0.37
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	7	0.37
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	13	0.37
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	14	0.37
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	1	0.37
(5,302)	1:A:229:ILE:N	1:B:229:ILE:N	12	0.37
(5,301)	1:A:231:SER:O	1:B:231:SER:O	12	0.37
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	2	0.37
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	11	0.37
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	14	0.37
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	6	0.36
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	7	0.36
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	8	0.36
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	10	0.36
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	11	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	1	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	5	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	7	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	10	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	11	0.36
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	15	0.36
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	6	0.36
(5,462)	1:C:229:ILE:N	1:E:229:ILE:N	14	0.36
(5,447)	1:C:263:LEU:H	1:D:263:LEU:H	15	0.36
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	3	0.36
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	6	0.36
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	10	0.36
(5,441)	1:C:231:SER:O	1:D:231:SER:O	15	0.36
(5,422)	1:B:229:ILE:N	1:E:229:ILE:N	14	0.36
(5,402)	1:B:229:ILE:N	1:D:229:ILE:N	14	0.36
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	2	0.36
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	5	0.36
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	12	0.36
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	2	0.36
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	5	0.36
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	12	0.36
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	15	0.36
(5,384)	1:B:253:VAL:H	1:C:253:VAL:H	11	0.36
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	1	0.36
(5,383)	1:B:226:GLN:H	1:C:226:GLN:H	7	0.36
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	7	0.36
(5,382)	1:B:229:ILE:N	1:C:229:ILE:N	13	0.36
(5,381)	1:B:231:SER:O	1:C:231:SER:O	7	0.36
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	10	0.36
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	15	0.36
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	2	0.36
(5,364)	1:A:253:VAL:H	1:E:253:VAL:H	7	0.36
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	3	0.36
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	9	0.36
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	3	0.36
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	12	0.36
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	14	0.36
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	13	0.36
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	7	0.36
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	2	0.36
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	9	0.36
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	5	0.35
(5,487)	1:D:263:LEU:H	1:E:263:LEU:H	9	0.35
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	6	0.35
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	8	0.35
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	14	0.35
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	15	0.35
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	15	0.35
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	1	0.35
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	3	0.35
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	7	0.35
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	8	0.35
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	13	0.35
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	6	0.35
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	7	0.35
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	10	0.35
(5,381)	1:B:231:SER:O	1:C:231:SER:O	11	0.35
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	3	0.35
(5,322)	1:A:229:ILE:N	1:C:229:ILE:N	14	0.35
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	6	0.35
(5,307)	1:A:263:LEU:H	1:B:263:LEU:H	12	0.35
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	9	0.35
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	11	0.35
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	13	0.35
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	1	0.35
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	3	0.35
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	12	0.35
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	7	0.35
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	15	0.35
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	8	0.35
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	4	0.35
(5,485)	1:D:256:GLY:O	1:E:256:GLY:O	9	0.34
(5,483)	1:D:226:GLN:H	1:E:226:GLN:H	9	0.34
(5,478)	1:C:413:PHE:O	1:E:413:PHE:O	9	0.34
(5,445)	1:C:256:GLY:O	1:D:256:GLY:O	13	0.34
(5,418)	1:B:413:PHE:O	1:D:413:PHE:O	9	0.34
(5,387)	1:B:263:LEU:H	1:C:263:LEU:H	9	0.34
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	1	0.34
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	8	0.34
(5,358)	1:A:413:PHE:O	1:D:413:PHE:O	9	0.34
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	14	0.34
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	15	0.34
(5,305)	1:A:256:GLY:O	1:B:256:GLY:O	6	0.34
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	1	0.34
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	2	0.34
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	6	0.34
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	4	0.34
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	14	0.34
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	3	0.33
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	13	0.33
(5,365)	1:A:256:GLY:O	1:E:256:GLY:O	5	0.33
(5,304)	1:A:253:VAL:H	1:B:253:VAL:H	11	0.33
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	12	0.33
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	1	0.33
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	8	0.33
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	15	0.33
(2,17)	1:A:250:PRO:O	1:A:254:GLY:N	5	0.33
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	9	0.33
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	12	0.33
(5,385)	1:B:256:GLY:O	1:C:256:GLY:O	9	0.32
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	14	0.32
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	8	0.32
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	1	0.32
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	7	0.32
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	13	0.32
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	4	0.32
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	5	0.32
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	7	0.32
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	5	0.31
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	12	0.31
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	11	0.31
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	14	0.31
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	9	0.31
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	10	0.31
(2,30)	1:A:279:TYR:O	1:A:283:ILE:N	5	0.31
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	2	0.31
(2,22)	1:A:258:THR:O	1:A:262:THR:N	5	0.31
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	1	0.31
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	2	0.31
(2,41)	1:A:303:ALA:O	1:A:307:VAL:N	2	0.3
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	6	0.3
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	8	0.3
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	14	0.3
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	8	0.3
(5,421)	1:B:231:SER:O	1:E:231:SER:O	6	0.29
(5,404)	1:B:253:VAL:H	1:D:253:VAL:H	14	0.29
(5,344)	1:A:253:VAL:H	1:D:253:VAL:H	14	0.29
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	10	0.29
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	6	0.29
(2,46)	1:A:403:PHE:O	1:A:407:PHE:N	5	0.29
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	15	0.29
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	6	0.29
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	11	0.29
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	13	0.29
(2,1)	1:A:220:LEU:O	1:A:224:LEU:N	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,401)	1:B:231:SER:O	1:D:231:SER:O	6	0.28
(5,341)	1:A:231:SER:O	1:D:231:SER:O	6	0.28
(5,338)	1:A:413:PHE:O	1:C:413:PHE:O	9	0.28
(5,324)	1:A:253:VAL:H	1:C:253:VAL:H	14	0.28
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	10	0.28
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	2	0.28
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	13	0.28
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	14	0.28
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	14	0.28
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	4	0.28
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	10	0.28
(2,36)	1:A:297:ALA:O	1:A:301:TYR:N	1	0.28
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	8	0.28
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	2	0.28
(5,461)	1:C:231:SER:O	1:E:231:SER:O	6	0.27
(5,423)	1:B:226:GLN:H	1:E:226:GLN:H	3	0.27
(5,423)	1:B:226:GLN:H	1:E:226:GLN:H	13	0.27
(5,324)	1:A:253:VAL:H	1:C:253:VAL:H	10	0.27
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	1	0.27
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	13	0.27
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	2	0.27
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	5	0.27
(2,22)	1:A:258:THR:O	1:A:262:THR:N	7	0.27
(2,22)	1:A:258:THR:O	1:A:262:THR:N	11	0.27
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	10	0.27
(5,343)	1:A:226:GLN:H	1:D:226:GLN:H	3	0.26
(5,321)	1:A:231:SER:O	1:C:231:SER:O	6	0.26
(2,7)	1:A:227:LEU:O	1:A:231:SER:N	15	0.26
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	13	0.26
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	4	0.26
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	5	0.26
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	5	0.26
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	10	0.26
(2,22)	1:A:258:THR:O	1:A:262:THR:N	12	0.26
(2,22)	1:A:258:THR:O	1:A:262:THR:N	15	0.26
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	7	0.26
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	7	0.26
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	7	0.26
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	7	0.26
(2,10)	1:A:230:PRO:O	1:A:234:ILE:N	14	0.26
(5,463)	1:C:226:GLN:H	1:E:226:GLN:H	3	0.25
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,404)	1:B:253:VAL:H	1:D:253:VAL:H	10	0.25
(5,403)	1:B:226:GLN:H	1:D:226:GLN:H	3	0.25
(5,344)	1:A:253:VAL:H	1:D:253:VAL:H	10	0.25
(5,341)	1:A:231:SER:O	1:D:231:SER:O	1	0.25
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	4	0.25
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	4	0.25
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	15	0.25
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	7	0.25
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	8	0.25
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	9	0.25
(2,30)	1:A:279:TYR:O	1:A:283:ILE:N	3	0.25
(2,22)	1:A:258:THR:O	1:A:262:THR:N	2	0.25
(2,22)	1:A:258:THR:O	1:A:262:THR:N	4	0.25
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	3	0.25
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	6	0.25
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	14	0.25
(5,343)	1:A:226:GLN:H	1:D:226:GLN:H	13	0.24
(5,321)	1:A:231:SER:O	1:C:231:SER:O	1	0.24
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	7	0.24
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	8	0.24
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	11	0.24
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	13	0.24
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	13	0.24
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	13	0.24
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	13	0.24
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	13	0.24
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	13	0.24
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	14	0.23
(5,463)	1:C:226:GLN:H	1:E:226:GLN:H	13	0.23
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	14	0.23
(5,323)	1:A:226:GLN:H	1:C:226:GLN:H	3	0.23
(2,795)	1:A:276:LYS:H	1:A:274:LEU:H	13	0.23
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	15	0.23
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	2	0.23
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	9	0.23
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	12	0.23
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	10	0.23
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	13	0.23
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	10	0.23
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	8	0.23
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	8	0.23
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	8	0.23
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	10	0.22
(5,461)	1:C:231:SER:O	1:E:231:SER:O	1	0.22
(5,403)	1:B:226:GLN:H	1:D:226:GLN:H	13	0.22
(5,323)	1:A:226:GLN:H	1:C:226:GLN:H	13	0.22
(2,795)	1:A:276:LYS:H	1:A:274:LEU:H	3	0.22
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	7	0.22
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	12	0.22
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	1	0.22
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	12	0.22
(2,50)	1:A:407:PHE:O	1:A:411:ASN:N	14	0.22
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	8	0.22
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	8	0.22
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	1	0.22
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	4	0.22
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	5	0.22
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	3	0.22
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	12	0.22
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	1	0.22
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	5	0.22
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	8	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	2	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	3	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	6	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	11	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	12	0.22
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	15	0.22
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	10	0.22
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	10	0.22
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	10	0.22
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	10	0.22
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	10	0.22
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	10	0.22
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	6	0.21
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	6	0.21
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	15	0.21
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	3	0.21
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	7	0.21
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	12	0.21
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	11	0.21
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	4	0.21
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	13	0.21
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	3	0.21
(2,38)	1:A:299:LEU:O	1:A:303:ALA:N	9	0.21
(2,26)	1:A:262:THR:O	1:A:266:GLN:N	9	0.21
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	15	0.21
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	1	0.21
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	5	0.21
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	7	0.21
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	15	0.21
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	15	0.21
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	15	0.21
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	15	0.21
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	15	0.21
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	15	0.21
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	9	0.21
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	9	0.21
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	9	0.21
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	9	0.21
(5,421)	1:B:231:SER:O	1:E:231:SER:O	1	0.2
(5,421)	1:B:231:SER:O	1:E:231:SER:O	8	0.2
(5,404)	1:B:253:VAL:H	1:D:253:VAL:H	6	0.2
(5,344)	1:A:253:VAL:H	1:D:253:VAL:H	6	0.2
(5,324)	1:A:253:VAL:H	1:C:253:VAL:H	6	0.2
(2,9)	1:A:229:ILE:O	1:A:233:LEU:N	6	0.2
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	7	0.2
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	8	0.2
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	9	0.2
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	10	0.2
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	11	0.2
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	1	0.2
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	13	0.2
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	4	0.2
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	9	0.2
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	12	0.2
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	12	0.2
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	12	0.2
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	12	0.2
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	3	0.2
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	10	0.2
(5,401)	1:B:231:SER:O	1:D:231:SER:O	1	0.19
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	11	0.19
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	1	0.19
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	9	0.19
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	14	0.19
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	15	0.19
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	1	0.19
(2,731)	1:A:289:VAL:H	1:A:291:LEU:H	13	0.19
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	6	0.19
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	11	0.19
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	3	0.19
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	11	0.19
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	2	0.19
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	4	0.19
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	7	0.19
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	2	0.19
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	4	0.19
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	7	0.19
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	11	0.19
(2,2)	1:A:221:GLY:O	1:A:225:ILE:N	13	0.19
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	6	0.19
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	6	0.19
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	6	0.19
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	6	0.19
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	11	0.19
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	11	0.19
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	11	0.19
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	11	0.19
(2,11)	1:A:232:LEU:O	1:A:236:ILE:N	6	0.19
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	9	0.18
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	1	0.18
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	11	0.18
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	12	0.18
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	15	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	2	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	4	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	6	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	8	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	10	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	11	0.18
(2,821)	1:A:422:ARG:H	1:A:424:GLU:H	12	0.18
(2,795)	1:A:276:LYS:H	1:A:274:LEU:H	5	0.18
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	2	0.18
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	13	0.18
(2,49)	1:A:406:ALA:O	1:A:410:PHE:N	9	0.18
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	4	0.18
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	9	0.18
(2,20)	1:A:255:LEU:O	1:A:259:THR:N	12	0.18
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	13	0.18
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	1	0.18
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	14	0.18
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	14	0.18
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	14	0.18
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	14	0.18
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	14	0.18
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	14	0.18
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	3	0.18
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	3	0.18
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	3	0.18
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	3	0.18
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	7	0.17
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	8	0.17
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	9	0.17
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	6	0.17
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	13	0.17
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	7	0.17
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	8	0.17
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	3	0.17
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	5	0.17
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	5	0.17
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	5	0.17
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	5	0.17
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	5	0.17
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	5	0.17
(5,461)	1:C:231:SER:O	1:E:231:SER:O	8	0.16
(5,341)	1:A:231:SER:O	1:D:231:SER:O	8	0.16
(5,321)	1:A:231:SER:O	1:C:231:SER:O	8	0.16
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	6	0.16
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	13	0.16
(2,808)	1:A:301:TYR:HA	1:A:303:ALA:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	10	0.16
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	1	0.16
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	8	0.16
(2,43)	1:A:399:SER:O	1:A:403:PHE:N	11	0.16
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	7	0.16
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	8	0.16
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	15	0.16
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	6	0.16
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	14	0.16
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	10	0.16
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	10	0.16
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	10	0.16
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	10	0.16
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	15	0.16
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	15	0.16
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	15	0.16
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	15	0.16
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	9	0.15
(5,401)	1:B:231:SER:O	1:D:231:SER:O	8	0.15
(5,357)	1:A:411:ASN:O	1:D:411:ASN:O	10	0.15
(5,337)	1:A:411:ASN:O	1:C:411:ASN:O	10	0.15
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	6	0.15
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	8	0.15
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	2	0.15
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	4	0.15
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	5	0.15
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	10	0.15
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	6	0.15
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	10	0.15
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	13	0.15
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	1	0.15
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	5	0.15
(2,623)	1:A:244:ILE:HB	1:A:245:ASN:H	14	0.15
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	15	0.15
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	1	0.15
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	5	0.15
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	11	0.15
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	5	0.15
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	10	0.15
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	14	0.15
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	6	0.15
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	14	0.15
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	10	0.15
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	15	0.15
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	15	0.15
(5,477)	1:C:411:ASN:O	1:E:411:ASN:O	10	0.14
(5,437)	1:B:411:ASN:O	1:E:411:ASN:O	10	0.14
(5,424)	1:B:253:VAL:H	1:E:253:VAL:H	3	0.14
(5,417)	1:B:411:ASN:O	1:D:411:ASN:O	10	0.14
(5,404)	1:B:253:VAL:H	1:D:253:VAL:H	9	0.14
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	13	0.14
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	1	0.14
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	9	0.14
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	12	0.14
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	5	0.14
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	6	0.14
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	3	0.14
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	5	0.14
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	11	0.14
(2,553)	1:A:395:ILE:HB	1:A:396:ASP:H	8	0.14
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	3	0.14
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	2	0.14
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	12	0.14
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	3	0.14
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	6	0.14
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	11	0.14
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	12	0.14
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	14	0.14
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	1	0.14
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	1	0.14
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	1	0.14
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	1	0.14
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD2	2	0.14
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD3	2	0.14
(5,344)	1:A:253:VAL:H	1:D:253:VAL:H	9	0.13
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	1	0.13
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	8	0.13
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	1	0.13
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	9	0.13
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	3	0.13
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	5	0.13
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	3	0.13
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	1	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	2	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	4	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	8	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	9	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	10	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	11	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	12	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	13	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	14	0.13
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	15	0.13
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	15	0.13
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	3	0.13
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	14	0.13
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	6	0.13
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	3	0.13
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	7	0.13
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	9	0.13
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	12	0.13
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	12	0.13
(2,31)	1:A:288:ALA:O	1:A:292:LEU:N	15	0.13
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	5	0.13
(2,29)	1:A:278:SER:O	1:A:282:ALA:N	6	0.13
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	10	0.13
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	13	0.13
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	1	0.13
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	3	0.13
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	8	0.13
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	9	0.13
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	13	0.13
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	13	0.13
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	13	0.13
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	13	0.13
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	7	0.13
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	7	0.13
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	13	0.13
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	13	0.13
(5,51)	1:A:297:ALA:H	1:D:297:ALA:H	1	0.12
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	5	0.12
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	6	0.12
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	7	0.12
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	8	0.12
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	10	0.12
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	13	0.12
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	10	0.12
(2,88)	1:A:251:ALA:O	1:A:255:LEU:H	13	0.12
(2,857)	1:A:257:ILE:HA	1:A:260:VAL:H	14	0.12
(2,810)	1:A:303:ALA:H	1:A:305:ASN:H	14	0.12
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	3	0.12
(2,782)	1:A:420:ILE:HA	1:A:422:ARG:H	7	0.12
(2,759)	1:A:397:LYS:HA	1:A:399:SER:H	14	0.12
(2,758)	1:A:396:ASP:HA	1:A:398:ILE:H	14	0.12
(2,755)	1:A:396:ASP:H	1:A:394:LYS:H	4	0.12
(2,746)	1:A:304:VAL:HA	1:A:306:PHE:H	14	0.12
(2,708)	1:A:259:THR:H	1:A:261:LEU:H	1	0.12
(2,708)	1:A:259:THR:H	1:A:261:LEU:H	8	0.12
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	9	0.12
(2,696)	1:A:253:VAL:H	1:A:251:ALA:H	1	0.12
(2,45)	1:A:402:GLY:O	1:A:406:ALA:N	13	0.12
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	8	0.12
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	11	0.12
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	5	0.12
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	15	0.12
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	5	0.12
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	7	0.12
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	2	0.12
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	3	0.12
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	4	0.12
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	4	0.12
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	4	0.12
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	4	0.12
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	4	0.12
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	11	0.12
(2,1150)	1:A:253:VAL:HG11	1:A:243:TRP:HD1	12	0.12
(2,1150)	1:A:253:VAL:HG12	1:A:243:TRP:HD1	12	0.12
(2,1150)	1:A:253:VAL:HG13	1:A:243:TRP:HD1	12	0.12
(2,1150)	1:A:253:VAL:HG21	1:A:243:TRP:HD1	12	0.12
(2,1150)	1:A:253:VAL:HG22	1:A:243:TRP:HD1	12	0.12
(2,1150)	1:A:253:VAL:HG23	1:A:243:TRP:HD1	12	0.12
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	5	0.12
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	5	0.12
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	5	0.12
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	5	0.12
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	8	0.12
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	8	0.12
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD2	4	0.12
(2,1072)	1:A:252:ARG:H	1:A:252:ARG:HD3	4	0.12
(5,51)	1:A:297:ALA:H	1:D:297:ALA:H	15	0.11
(5,464)	1:C:253:VAL:H	1:E:253:VAL:H	3	0.11
(5,342)	1:A:229:ILE:N	1:D:229:ILE:N	1	0.11
(5,324)	1:A:253:VAL:H	1:C:253:VAL:H	9	0.11
(5,31)	1:A:297:ALA:H	1:C:297:ALA:H	1	0.11
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	3	0.11
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	9	0.11
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	11	0.11
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	12	0.11
(3,104)	1:A:296:SER:HG	1:A:264:THR:H	15	0.11
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	6	0.11
(2,952)	1:A:258:THR:HA	1:A:262:THR:H	14	0.11
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	1	0.11
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	3	0.11
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	11	0.11
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	12	0.11
(2,84)	1:A:239:TRP:O	1:A:243:TRP:H	14	0.11
(2,777)	1:A:417:ILE:H	1:A:419:LYS:H	1	0.11
(2,749)	1:A:309:ARG:H	1:A:307:VAL:H	6	0.11
(2,749)	1:A:309:ARG:H	1:A:307:VAL:H	13	0.11
(2,749)	1:A:309:ARG:H	1:A:307:VAL:H	15	0.11
(2,746)	1:A:304:VAL:HA	1:A:306:PHE:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:A:304:VAL:HA	1:A:306:PHE:H	3	0.11
(2,746)	1:A:304:VAL:HA	1:A:306:PHE:H	7	0.11
(2,708)	1:A:259:THR:H	1:A:261:LEU:H	10	0.11
(2,708)	1:A:259:THR:H	1:A:261:LEU:H	13	0.11
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	12	0.11
(2,706)	1:A:258:THR:H	1:A:260:VAL:H	15	0.11
(2,696)	1:A:253:VAL:H	1:A:251:ALA:H	2	0.11
(2,696)	1:A:253:VAL:H	1:A:251:ALA:H	7	0.11
(2,696)	1:A:253:VAL:H	1:A:251:ALA:H	13	0.11
(2,678)	1:A:220:LEU:H	1:A:222:TYR:H	10	0.11
(2,678)	1:A:220:LEU:H	1:A:222:TYR:H	12	0.11
(2,553)	1:A:395:ILE:HB	1:A:396:ASP:H	4	0.11
(2,51)	1:A:409:ILE:O	1:A:413:PHE:N	10	0.11
(2,5)	1:A:224:LEU:O	1:A:228:TYR:N	13	0.11
(2,44)	1:A:401:ILE:O	1:A:405:LEU:N	14	0.11
(2,37)	1:A:298:LEU:O	1:A:302:ALA:N	8	0.11
(2,23)	1:A:259:THR:O	1:A:263:LEU:N	1	0.11
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	4	0.11
(2,134)	1:A:303:ALA:O	1:A:307:VAL:H	7	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	3	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	6	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	8	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	9	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	10	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	12	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	13	0.11
(2,130)	1:A:300:GLU:O	1:A:304:VAL:H	15	0.11
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	4	0.11
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	4	0.11
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	4	0.11
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	4	0.11
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG12	14	0.11
(2,1146)	1:A:250:PRO:HD2	1:A:244:ILE:HG13	14	0.11
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG12	14	0.11
(2,1146)	1:A:250:PRO:HD3	1:A:244:ILE:HG13	14	0.11
(2,114)	1:A:288:ALA:O	1:A:292:LEU:H	13	0.11
(2,1129)	1:A:252:ARG:HG2	1:A:253:VAL:H	1	0.11
(2,1129)	1:A:252:ARG:HG3	1:A:253:VAL:H	1	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value