



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:30 pm GMT

PDB ID : 2KXP
Title : Solution NMR structure of V-1 bound to capping protein (CP)
Authors : Zwolak, A.; Fujiwara, I.; Hammer III, J.A.; Tjandra, N.
Deposited on : 2010-05-11

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

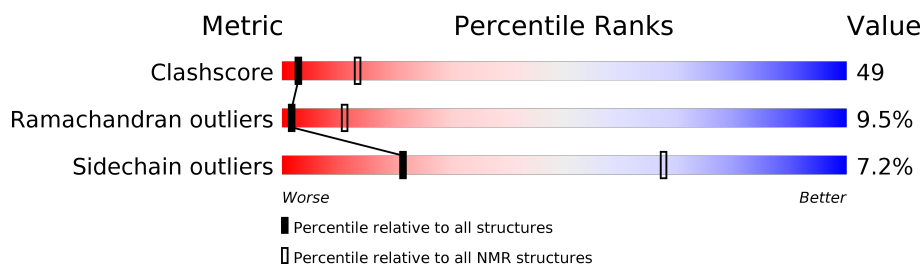
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	270	
3	C	118	

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:281, B:302-B:571 (545)	0.00	7
2	C:601-C:718 (118)	0.00	8

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 9
2	7, 10
3	4, 8
Single-model clusters	5

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10511 atoms, of which 5229 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						Trace
1	A	275	Total	C	H	N	O	S	0
			4416	1413	2177	392	429	5	

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms						Trace
2	B	270	Total	C	H	N	O	S	0
			4276	1334	2135	374	423	10	

- Molecule 3 is a protein called Myotrophin.

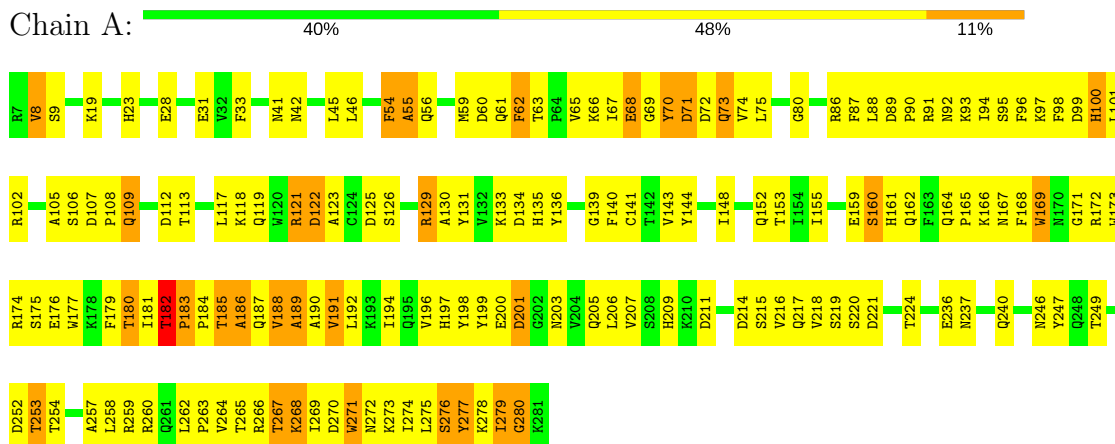
Mol	Chain	Residues	Atoms						Trace
3	C	118	Total	C	H	N	O	S	0
			1819	570	917	152	175	5	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

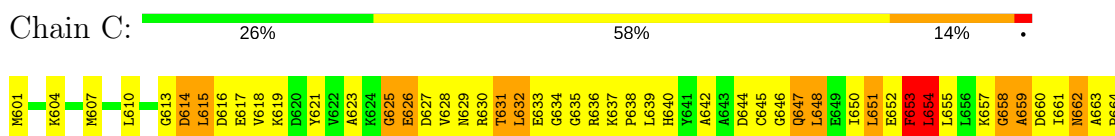
- Molecule 1: F-actin-capping protein subunit alpha-1

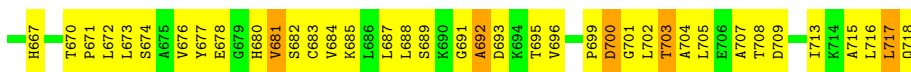


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Myotrophin



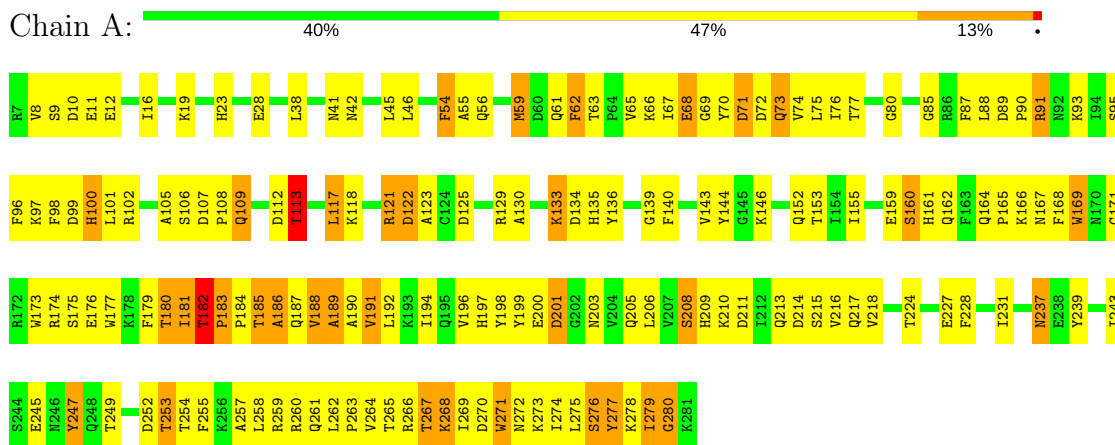


4.2 Scores per residue for each member of the ensemble

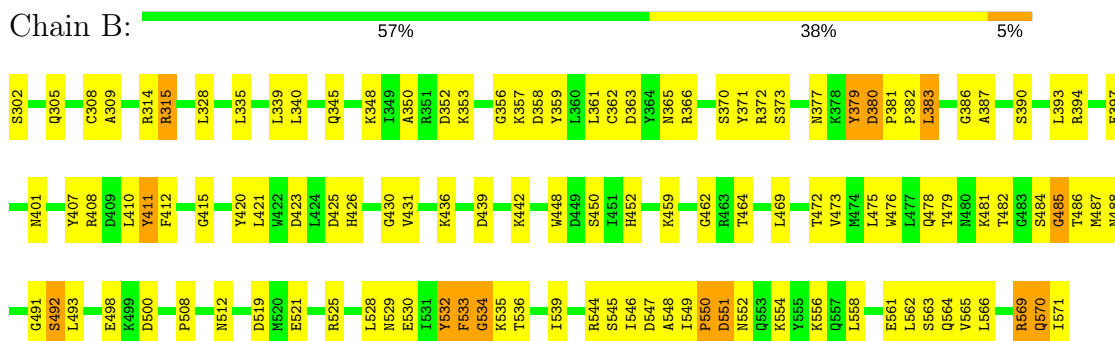
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

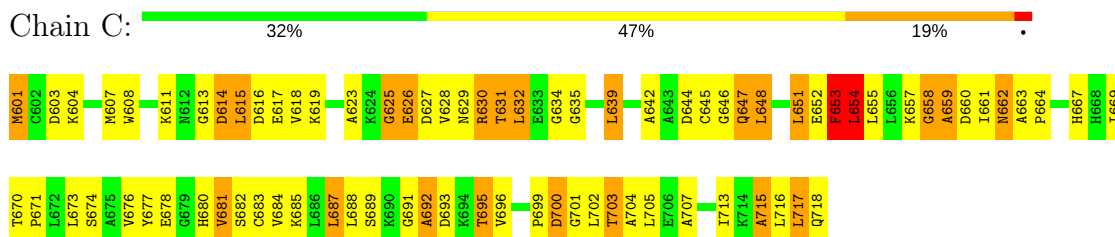
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

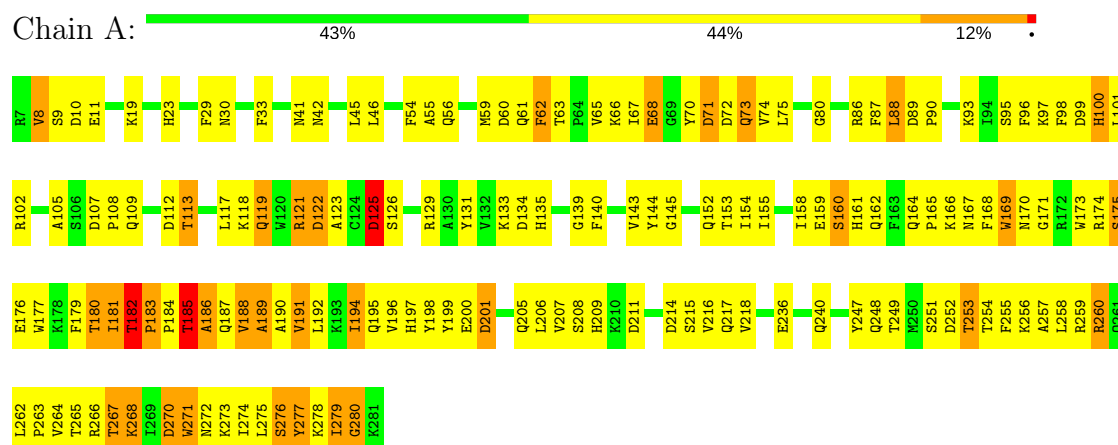


- Molecule 3: Myotrophin

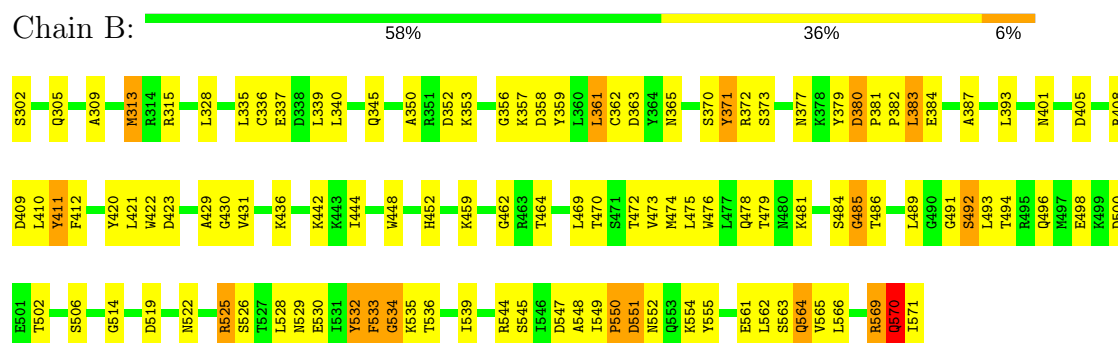


4.2.2 Score per residue for model 2

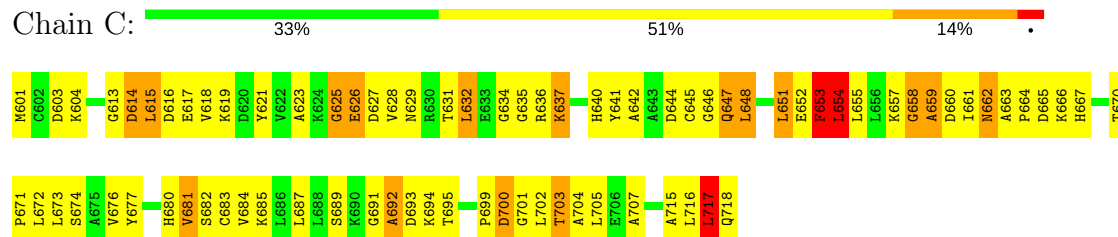
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

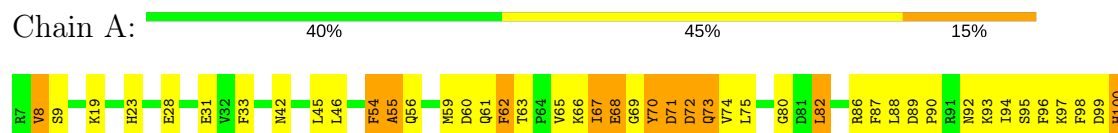


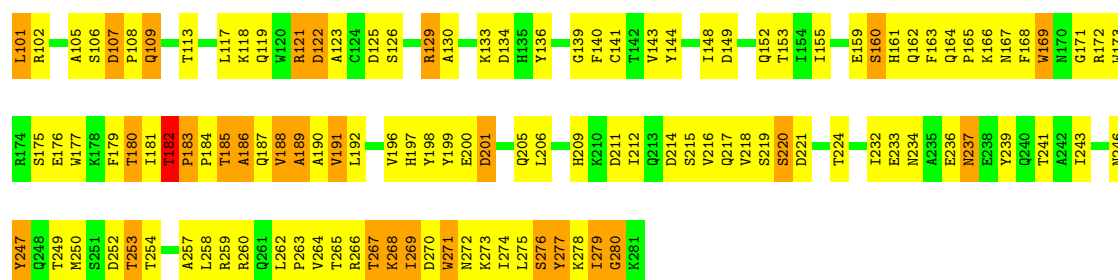
- Molecule 3: Myotrophin



4.2.3 Score per residue for model 3

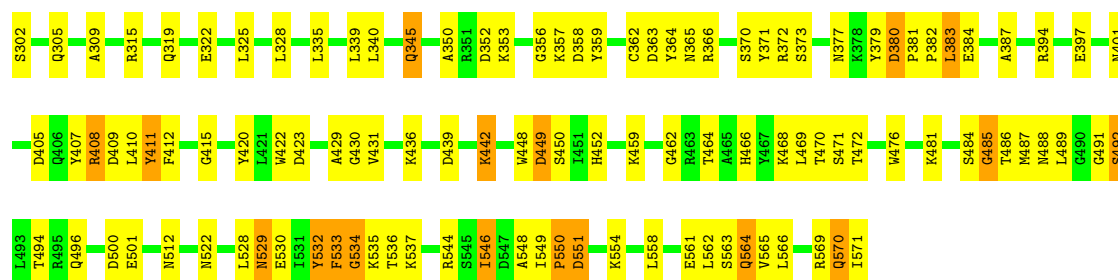
- Molecule 1: F-actin-capping protein subunit alpha-1





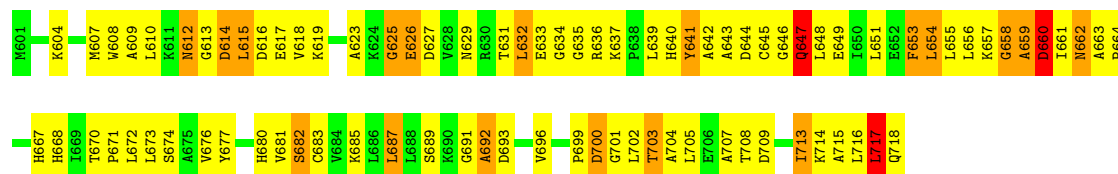
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 59% 34% 7%



- Molecule 3: Myotrophin

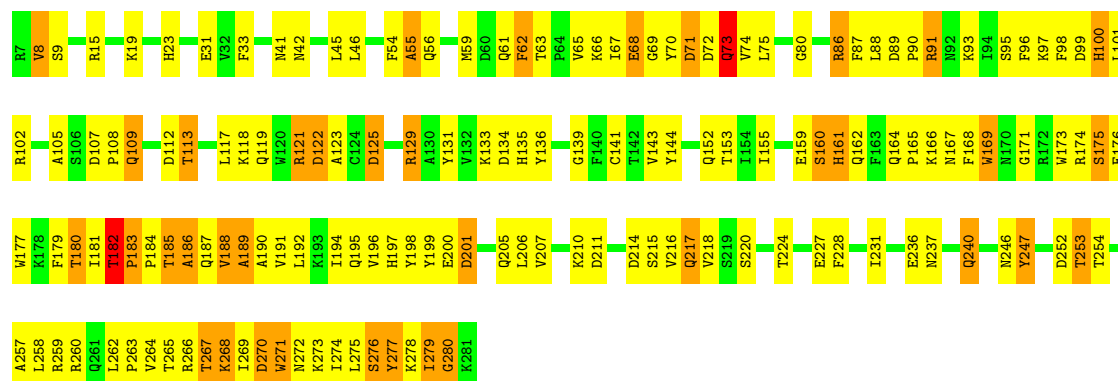
Chain C: 28% 54% 15%



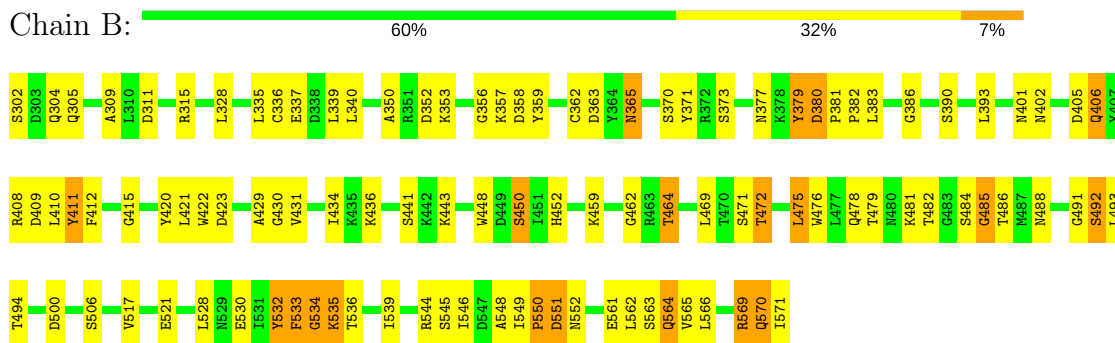
4.2.4 Score per residue for model 4

- Molecule 1: F-actin-capping protein subunit alpha-1

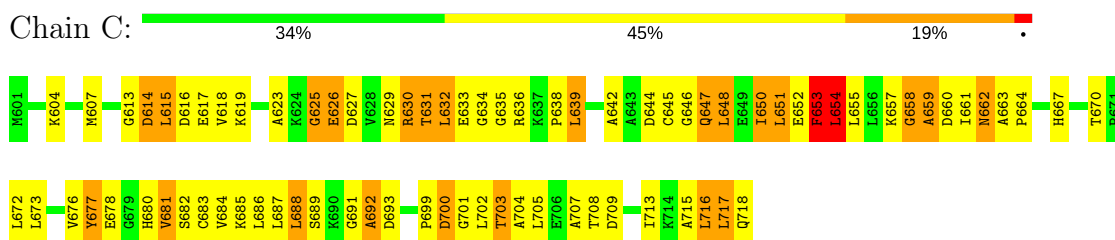
Chain A: 44% 42% 13%



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

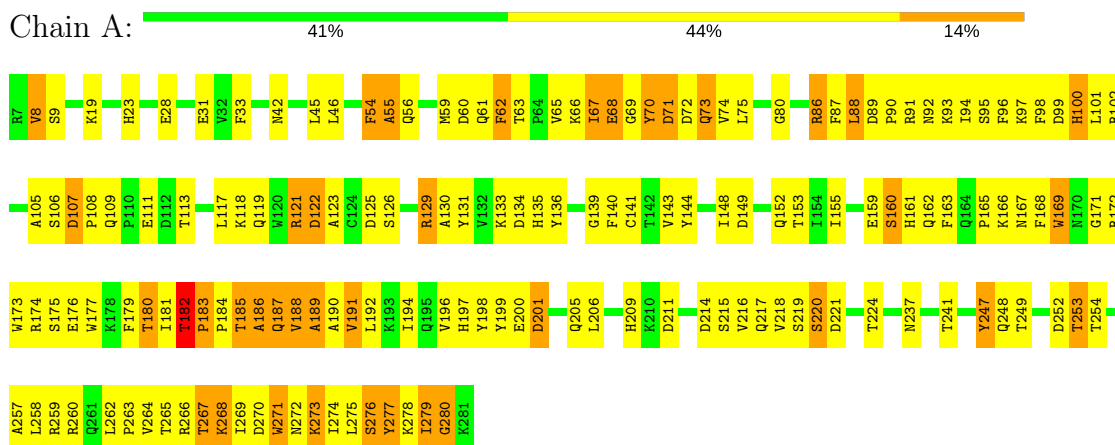


- Molecule 3: Myotrophin

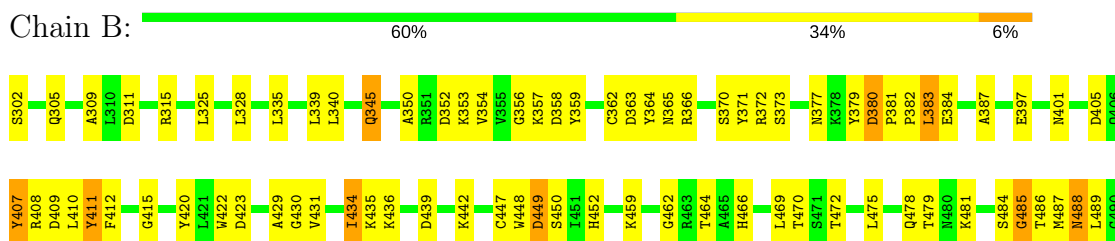


4.2.5 Score per residue for model 5

- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



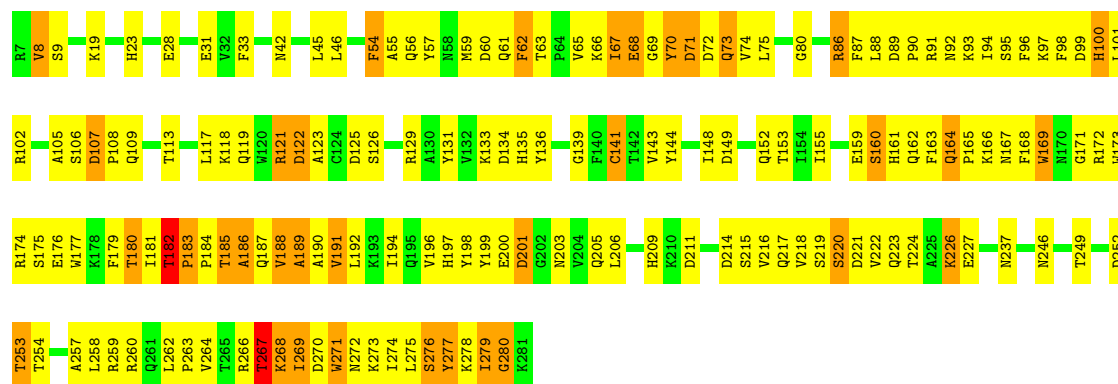


• Molecule 3: Myotrophin

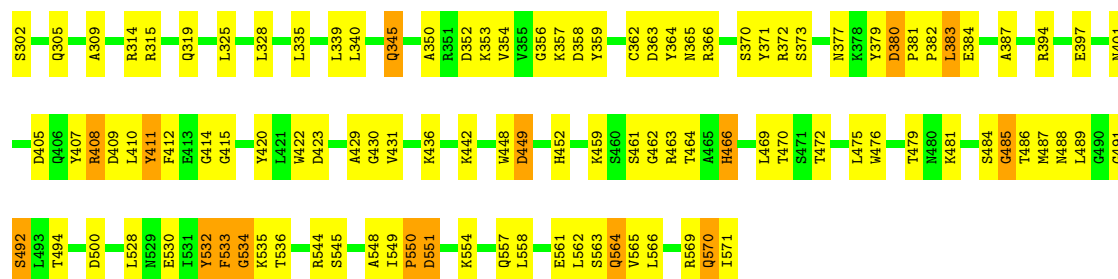


4.2.6 Score per residue for model 6

• Molecule 1: F-actin-capping protein subunit alpha-1



• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



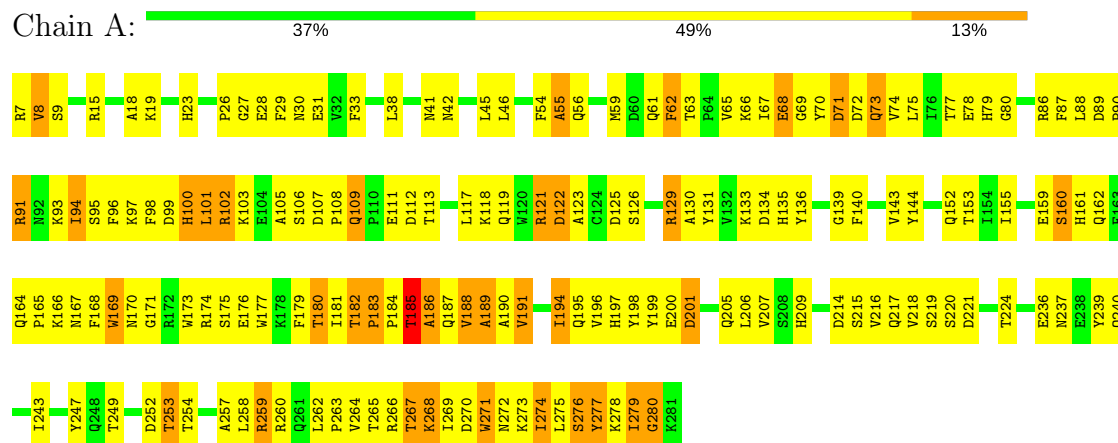
• Molecule 3: Myotrophin





4.2.7 Score per residue for model 7 (medoid)

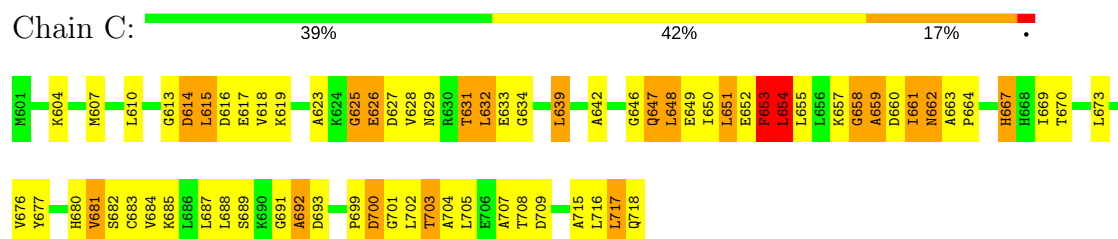
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

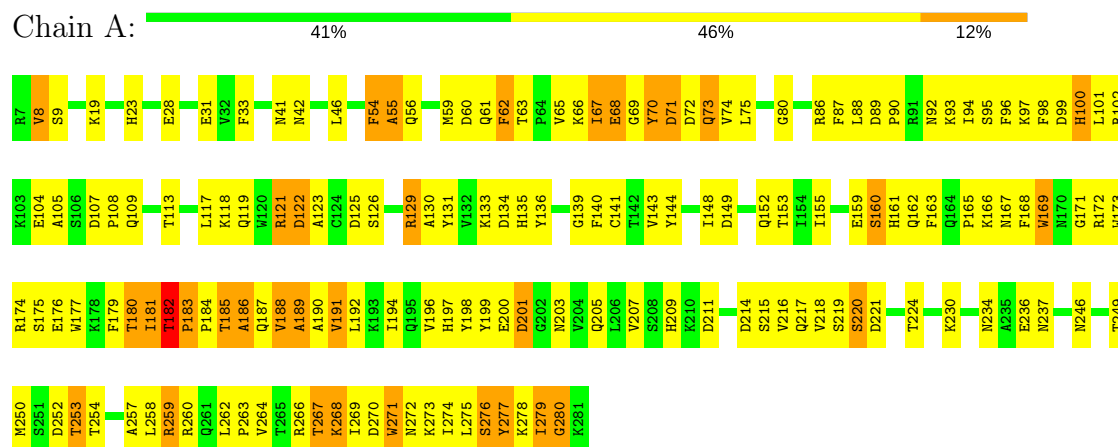


- Molecule 3: Myotrophin



4.2.8 Score per residue for model 8

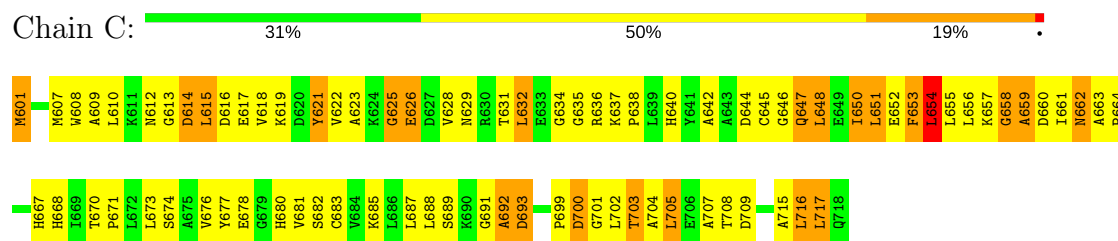
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

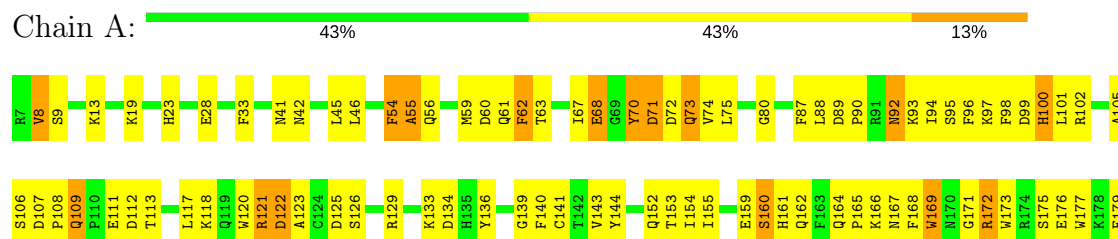


- Molecule 3: Myotrophin



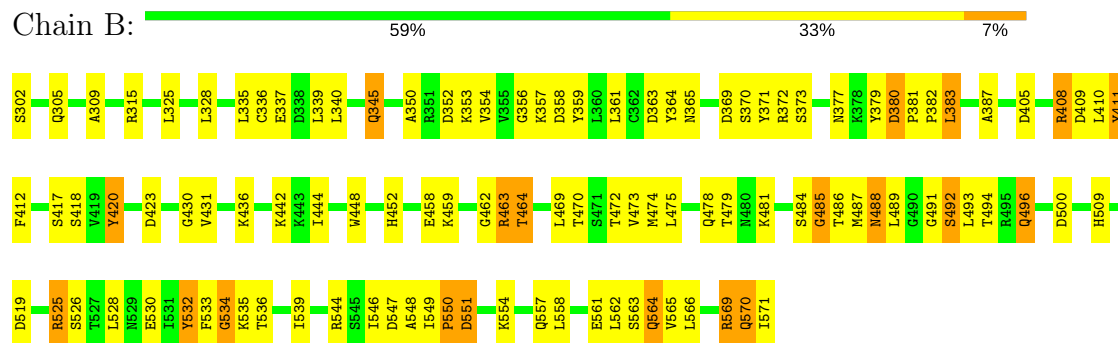
4.2.9 Score per residue for model 9

- Molecule 1: F-actin-capping protein subunit alpha-1

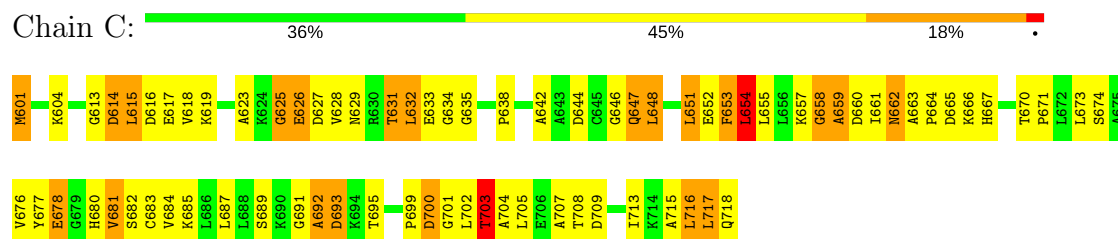




- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

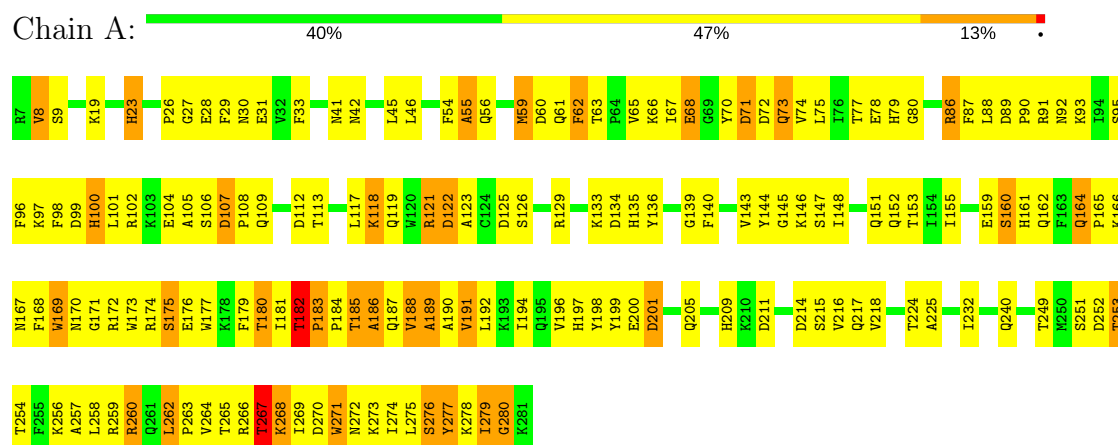


- Molecule 3: Myotrophin



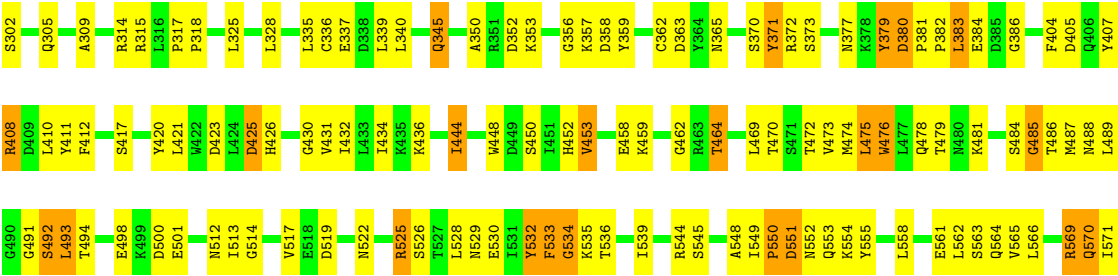
4.2.10 Score per residue for model 10

- Molecule 1: F-actin-capping protein subunit alpha-1

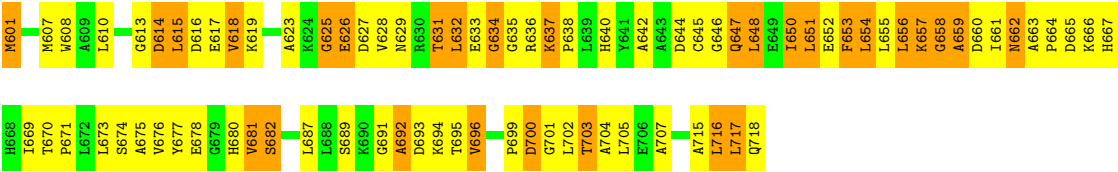
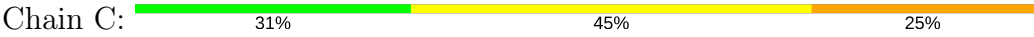


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2





• Molecule 3: Myotrophin



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.23

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	2239	2177	2166	269±10
2	B	2141	2135	2128	148±7
3	C	902	917	909	118±8
All	All	52820	52290	52030	5123

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:SER:O	1:A:278:LYS:N	1.32	1.62	4	10
1:A:182:THR:OG1	1:A:184:PRO:HG3	1.25	1.30	7	1
3:C:688:LEU:HD13	3:C:689:SER:N	1.23	1.49	4	2
1:A:273:LYS:O	1:A:277:TYR:HB3	1.22	1.35	8	10
3:C:673:LEU:O	3:C:676:VAL:HG22	1.18	0.99	3	1
3:C:673:LEU:O	3:C:676:VAL:CG2	1.14	1.95	3	1
1:A:186:ALA:O	1:A:216:VAL:O	1.11	1.68	7	10
1:A:186:ALA:HB3	1:A:216:VAL:O	1.10	1.47	5	10
3:C:691:GLY:O	3:C:693:ASP:N	1.09	1.85	9	10
1:A:187:GLN:O	1:A:188:VAL:HG23	1.09	1.44	4	10
1:A:186:ALA:HB3	1:A:216:VAL:C	1.08	1.69	3	10
1:A:279:ILE:O	1:A:280:GLY:O	1.08	1.72	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:273:LYS:O	1:A:277:TYR:CB	1.08	2.02	8	10
1:A:72:ASP:O	1:A:74:VAL:N	1.07	1.87	2	10
1:A:182:THR:OG1	1:A:184:PRO:CG	1.07	2.01	7	1
1:A:200:GLU:O	1:A:201:ASP:CG	1.07	1.92	10	7
1:A:183:PRO:HA	1:A:218:VAL:HB	1.06	1.28	1	10
1:A:187:GLN:HA	1:A:215:SER:HA	1.05	1.28	5	10
3:C:651:LEU:N	3:C:651:LEU:HD13	1.05	1.66	9	5
3:C:716:LEU:O	3:C:717:LEU:HB2	1.04	1.52	10	9
2:B:371:TYR:O	2:B:379:TYR:HA	1.04	1.52	9	10
3:C:651:LEU:HD13	3:C:651:LEU:H	1.04	0.99	8	4
3:C:651:LEU:H	3:C:651:LEU:HD13	1.03	1.08	4	4
1:A:186:ALA:CB	1:A:216:VAL:O	1.03	2.07	3	10
3:C:662:ASN:C	3:C:664:PRO:HD2	1.03	1.74	3	10
1:A:185:THR:O	1:A:217:GLN:HA	1.03	1.54	6	10
1:A:152:GLN:O	1:A:181:ILE:HG13	1.01	1.55	10	1
1:A:186:ALA:HB1	1:A:216:VAL:HG13	1.01	1.32	3	4
3:C:651:LEU:HD13	3:C:651:LEU:N	1.00	1.67	10	3
1:A:260:ARG:O	2:B:411:TYR:CZ	1.00	2.14	7	1
3:C:651:LEU:CD1	3:C:651:LEU:H	1.00	1.67	9	5
1:A:186:ALA:CA	1:A:216:VAL:O	0.99	2.11	3	10
3:C:653:PHE:O	3:C:655:LEU:N	0.99	1.96	8	10
1:A:186:ALA:HB2	1:A:218:VAL:HG23	0.98	1.35	1	10
3:C:716:LEU:O	3:C:717:LEU:HB3	0.98	1.54	3	1
3:C:688:LEU:C	3:C:688:LEU:HD22	0.98	1.79	4	1
2:B:352:ASP:O	2:B:356:GLY:N	0.97	1.97	8	10
3:C:688:LEU:HD22	3:C:688:LEU:O	0.97	1.59	4	1
3:C:688:LEU:HD22	3:C:688:LEU:C	0.97	1.79	6	1
2:B:444:ILE:H	2:B:444:ILE:HD13	0.97	1.20	10	1
2:B:370:SER:HB3	2:B:381:PRO:HD2	0.96	1.37	3	4
3:C:651:LEU:H	3:C:651:LEU:CD1	0.96	1.68	10	3
3:C:688:LEU:O	3:C:688:LEU:HD22	0.95	1.60	6	1
1:A:187:GLN:O	1:A:188:VAL:CG2	0.95	2.15	4	10
2:B:370:SER:HB2	2:B:381:PRO:HD2	0.94	1.38	5	6
1:A:186:ALA:C	1:A:216:VAL:O	0.92	2.08	8	10
3:C:688:LEU:HD13	3:C:689:SER:H	0.92	1.25	6	2
3:C:615:LEU:HD13	3:C:615:LEU:O	0.91	1.65	8	5
3:C:680:HIS:O	3:C:682:SER:N	0.91	2.04	3	10
3:C:654:LEU:HD22	3:C:654:LEU:O	0.90	1.65	6	1
2:B:530:GLU:O	2:B:534:GLY:HA3	0.90	1.67	7	10
3:C:648:LEU:HD13	3:C:682:SER:OG	0.90	1.67	3	1
1:A:252:ASP:O	1:A:253:THR:OG1	0.89	1.91	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:621:TYR:CD1	3:C:622:VAL:N	0.89	2.40	5	2
2:B:481:LYS:O	2:B:485:GLY:N	0.89	2.06	5	10
3:C:717:LEU:HD12	3:C:718:GLN:N	0.88	1.83	3	1
3:C:615:LEU:O	3:C:615:LEU:HD13	0.88	1.68	10	2
1:A:153:THR:HG23	1:A:179:PHE:C	0.88	1.89	4	3
1:A:152:GLN:O	1:A:181:ILE:CG1	0.87	2.23	10	1
3:C:621:TYR:OH	3:C:628:VAL:HG22	0.87	1.68	8	2
2:B:422:TRP:NE1	2:B:429:ALA:HB3	0.87	1.85	8	5
1:A:185:THR:O	1:A:217:GLN:CA	0.87	2.21	5	10
3:C:621:TYR:CG	3:C:622:VAL:N	0.86	2.43	8	2
1:A:106:SER:O	1:A:107:ASP:OD1	0.86	1.92	3	3
1:A:274:ILE:O	1:A:274:ILE:HD12	0.86	1.69	7	1
3:C:648:LEU:C	3:C:651:LEU:HD21	0.86	1.91	6	8
1:A:107:ASP:CG	1:A:107:ASP:O	0.86	2.14	5	3
1:A:152:GLN:N	1:A:181:ILE:HG12	0.85	1.86	10	1
2:B:569:ARG:O	2:B:570:GLN:HB3	0.85	1.67	2	2
2:B:493:LEU:HD13	2:B:494:THR:H	0.85	1.29	10	1
1:A:192:LEU:HD22	1:A:192:LEU:N	0.85	1.87	1	1
2:B:570:GLN:O	2:B:571:ILE:HB	0.85	1.72	9	10
3:C:648:LEU:HD13	3:C:648:LEU:N	0.84	1.88	5	6
2:B:561:GLU:O	2:B:565:VAL:HG23	0.84	1.72	7	10
1:A:186:ALA:O	1:A:216:VAL:N	0.84	2.11	8	10
1:A:182:THR:HB	1:A:184:PRO:CG	0.84	2.03	1	9
2:B:422:TRP:CE2	2:B:429:ALA:HB3	0.84	2.08	4	7
1:A:153:THR:OG1	1:A:180:THR:HA	0.84	1.71	3	3
3:C:654:LEU:HD22	3:C:654:LEU:H	0.83	1.32	1	2
3:C:653:PHE:C	3:C:655:LEU:H	0.83	1.77	5	10
1:A:152:GLN:H	1:A:181:ILE:HG12	0.83	1.32	10	1
1:A:95:SER:O	1:A:109:GLN:N	0.83	2.12	6	10
2:B:361:LEU:HD23	2:B:362:CYS:H	0.82	1.34	2	1
1:A:95:SER:O	1:A:108:PRO:CA	0.82	2.28	4	10
1:A:186:ALA:CB	1:A:216:VAL:HG13	0.82	2.05	6	4
3:C:716:LEU:O	3:C:717:LEU:CB	0.82	2.28	3	10
3:C:676:VAL:HG23	3:C:677:TYR:H	0.81	1.32	3	1
1:A:219:SER:H	1:A:224:THR:CG2	0.81	1.88	5	5
1:A:185:THR:C	1:A:217:GLN:HA	0.81	1.96	10	10
3:C:654:LEU:H	3:C:654:LEU:HD22	0.81	1.31	7	1
2:B:570:GLN:O	2:B:571:ILE:CB	0.81	2.29	5	10
1:A:200:GLU:O	1:A:201:ASP:CB	0.81	2.29	5	10
1:A:95:SER:O	1:A:108:PRO:HA	0.80	1.77	4	10
1:A:252:ASP:O	1:A:252:ASP:OD1	0.80	2.00	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:662:ASN:C	3:C:664:PRO:CD	0.80	2.50	5	10
1:A:70:TYR:O	1:A:72:ASP:N	0.80	2.15	1	10
2:B:563:SER:O	2:B:565:VAL:N	0.80	2.15	2	10
3:C:703:THR:O	3:C:707:ALA:HB2	0.79	1.78	9	10
3:C:676:VAL:HG23	3:C:677:TYR:N	0.79	1.88	3	1
1:A:74:VAL:C	1:A:75:LEU:HD22	0.79	1.97	9	1
3:C:651:LEU:N	3:C:651:LEU:HD22	0.79	1.93	6	6
2:B:570:GLN:O	2:B:571:ILE:HG22	0.79	1.77	7	5
3:C:680:HIS:C	3:C:682:SER:H	0.79	1.81	10	10
2:B:570:GLN:O	2:B:571:ILE:CG2	0.79	2.31	7	5
2:B:493:LEU:HD13	2:B:494:THR:N	0.79	1.91	10	1
3:C:685:LYS:O	3:C:688:LEU:HD12	0.79	1.78	6	2
1:A:270:ASP:O	1:A:273:LYS:N	0.79	2.14	6	10
2:B:562:LEU:O	2:B:565:VAL:HB	0.78	1.78	4	10
1:A:181:ILE:O	1:A:182:THR:HG23	0.78	1.78	1	9
3:C:648:LEU:N	3:C:648:LEU:HD13	0.78	1.94	7	2
1:A:181:ILE:O	1:A:181:ILE:HD12	0.78	1.77	10	1
3:C:650:ILE:O	3:C:654:LEU:HD12	0.78	1.78	6	2
3:C:663:ALA:N	3:C:664:PRO:CD	0.78	2.47	5	10
3:C:648:LEU:HD12	3:C:648:LEU:O	0.78	1.79	8	1
1:A:188:VAL:CG1	1:A:189:ALA:N	0.78	2.47	10	10
3:C:688:LEU:CD1	3:C:689:SER:N	0.77	2.42	4	2
1:A:168:PHE:O	1:A:169:TRP:HB3	0.77	1.80	8	10
1:A:208:SER:OG	2:B:487:MET:HA	0.77	1.79	1	1
1:A:177:TRP:CZ2	1:A:232:ILE:HG23	0.77	2.15	10	1
1:A:173:TRP:CE3	1:A:194:ILE:HD11	0.77	2.15	7	1
1:A:98:PHE:HA	1:A:105:ALA:HB1	0.77	1.57	5	10
1:A:77:THR:O	1:A:87:PHE:CE2	0.76	2.38	1	1
2:B:372:ARG:NH1	2:B:387:ALA:O	0.76	2.18	1	1
1:A:67:ILE:HD12	1:A:68:GLU:N	0.76	1.95	5	4
3:C:651:LEU:HD22	3:C:651:LEU:N	0.76	1.94	2	2
2:B:408:ARG:HE	2:B:415:GLY:C	0.76	1.83	6	2
1:A:98:PHE:HA	1:A:105:ALA:CB	0.76	2.11	10	10
2:B:444:ILE:N	2:B:444:ILE:HD13	0.75	1.95	10	1
1:A:117:LEU:O	1:A:117:LEU:HG	0.75	1.80	9	4
2:B:370:SER:HB2	2:B:381:PRO:CD	0.75	2.12	9	6
1:A:249:THR:HA	1:A:252:ASP:OD1	0.75	1.81	6	1
1:A:173:TRP:CZ3	1:A:194:ILE:HD11	0.75	2.17	10	5
2:B:569:ARG:O	2:B:570:GLN:CB	0.75	2.35	1	10
1:A:160:SER:O	1:A:173:TRP:N	0.74	2.20	3	10
3:C:621:TYR:CD1	3:C:621:TYR:C	0.74	2.61	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:648:LEU:CD1	3:C:648:LEU:N	0.74	2.50	5	4
2:B:379:TYR:CE2	2:B:386:GLY:HA3	0.74	2.17	7	3
2:B:370:SER:HB3	2:B:381:PRO:CD	0.74	2.12	2	4
1:A:201:ASP:OD1	2:B:493:LEU:HD21	0.74	1.82	10	1
1:A:274:ILE:HD11	2:B:403:ALA:HB1	0.74	1.59	7	1
1:A:169:TRP:CD2	1:A:169:TRP:O	0.74	2.41	9	7
3:C:651:LEU:N	3:C:651:LEU:CD1	0.73	2.40	1	6
3:C:601:MET:O	3:C:602:CYS:SG	0.73	2.47	5	1
3:C:691:GLY:C	3:C:693:ASP:N	0.73	2.41	9	10
1:A:148:ILE:O	1:A:151:GLN:CG	0.73	2.36	10	1
3:C:651:LEU:CD2	3:C:652:GLU:H	0.73	1.97	9	8
2:B:379:TYR:CZ	2:B:386:GLY:HA3	0.73	2.19	1	3
1:A:275:LEU:O	1:A:276:SER:CB	0.73	2.37	1	10
2:B:371:TYR:O	2:B:379:TYR:CA	0.73	2.36	5	10
1:A:259:ARG:CZ	2:B:448:TRP:CZ2	0.73	2.71	7	1
1:A:201:ASP:CG	2:B:493:LEU:HD11	0.73	2.03	10	1
1:A:181:ILE:O	1:A:182:THR:HB	0.73	1.83	7	1
1:A:67:ILE:HD12	1:A:68:GLU:H	0.72	1.44	3	4
1:A:187:GLN:CA	1:A:215:SER:HA	0.72	2.13	9	10
2:B:380:ASP:HB3	2:B:381:PRO:HD3	0.72	1.58	7	6
2:B:569:ARG:O	2:B:570:GLN:HB2	0.72	1.83	3	8
1:A:256:LYS:NZ	3:C:636:ARG:NE	0.72	2.37	2	1
1:A:181:ILE:O	1:A:182:THR:OG1	0.72	2.07	2	9
3:C:688:LEU:C	3:C:688:LEU:HD13	0.71	2.05	4	1
1:A:72:ASP:O	1:A:73:GLN:C	0.71	2.29	5	10
3:C:628:VAL:O	3:C:628:VAL:HG23	0.71	1.85	2	1
3:C:699:PRO:O	3:C:700:ASP:CG	0.71	2.29	4	3
3:C:688:LEU:HD13	3:C:688:LEU:C	0.71	2.05	6	1
3:C:654:LEU:HD13	3:C:655:LEU:N	0.71	2.00	6	1
3:C:691:GLY:C	3:C:693:ASP:H	0.71	1.89	8	10
1:A:183:PRO:HA	1:A:218:VAL:CB	0.71	2.14	2	10
1:A:8:VAL:HG13	1:A:8:VAL:O	0.71	1.86	7	6
1:A:192:LEU:N	1:A:192:LEU:CD1	0.71	2.54	3	5
2:B:470:THR:O	2:B:470:THR:HG23	0.71	1.85	7	2
1:A:95:SER:HB3	1:A:109:GLN:O	0.71	1.86	8	2
3:C:628:VAL:HG23	3:C:628:VAL:O	0.70	1.85	1	1
3:C:615:LEU:HD11	3:C:653:PHE:CE2	0.70	2.20	10	1
2:B:571:ILE:O	2:B:571:ILE:HG23	0.70	1.86	6	2
2:B:379:TYR:CE1	2:B:383:LEU:HB3	0.70	2.20	4	1
2:B:571:ILE:HG23	2:B:571:ILE:O	0.70	1.86	8	3
1:A:169:TRP:HA	1:A:197:HIS:O	0.70	1.87	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:350:ALA:CB	2:B:359:TYR:CZ	0.70	2.74	9	10
3:C:654:LEU:C	3:C:654:LEU:HD22	0.70	2.06	6	1
3:C:683:CYS:SG	3:C:684:VAL:N	0.70	2.65	5	3
1:A:219:SER:H	1:A:224:THR:HG22	0.70	1.46	7	5
1:A:200:GLU:O	1:A:201:ASP:HB2	0.70	1.87	1	9
1:A:263:PRO:O	1:A:266:ARG:N	0.70	2.24	8	10
1:A:111:GLU:O	1:A:111:GLU:CG	0.70	2.40	7	1
1:A:121:ARG:HE	1:A:122:ASP:N	0.70	1.85	4	1
1:A:187:GLN:O	1:A:216:VAL:HG12	0.70	1.86	8	4
1:A:187:GLN:O	1:A:188:VAL:CB	0.70	2.40	6	10
3:C:655:LEU:C	3:C:655:LEU:HD23	0.70	2.07	8	2
1:A:182:THR:HG1	1:A:184:PRO:HG3	0.69	1.42	7	1
3:C:618:VAL:O	3:C:621:TYR:CD2	0.69	2.45	8	2
3:C:615:LEU:HD13	3:C:615:LEU:C	0.69	2.07	9	4
3:C:676:VAL:CG2	3:C:677:TYR:H	0.69	2.01	3	1
3:C:648:LEU:N	3:C:648:LEU:CD1	0.69	2.56	10	4
2:B:532:TYR:O	2:B:536:THR:OG1	0.69	2.10	5	8
1:A:165:PRO:O	1:A:167:ASN:N	0.69	2.26	3	10
3:C:680:HIS:C	3:C:682:SER:N	0.69	2.46	7	10
1:A:259:ARG:HG3	2:B:412:PHE:CE1	0.69	2.22	5	1
1:A:275:LEU:O	1:A:276:SER:OG	0.69	2.11	10	9
3:C:642:ALA:O	3:C:646:GLY:N	0.69	2.26	7	10
1:A:180:THR:O	1:A:181:ILE:HG23	0.69	1.88	10	1
1:A:107:ASP:OD1	1:A:107:ASP:O	0.69	2.11	6	1
1:A:276:SER:C	1:A:278:LYS:N	0.68	2.47	1	10
1:A:179:PHE:O	1:A:180:THR:O	0.68	2.12	9	10
1:A:8:VAL:O	1:A:8:VAL:HG13	0.68	1.88	2	3
1:A:107:ASP:O	1:A:107:ASP:OD1	0.68	2.12	5	2
1:A:181:ILE:O	1:A:182:THR:CG2	0.68	2.41	1	9
3:C:653:PHE:C	3:C:655:LEU:N	0.68	2.43	1	10
1:A:259:ARG:HG2	1:A:260:ARG:H	0.68	1.47	5	5
1:A:194:ILE:HD13	1:A:195:GLN:N	0.68	2.03	2	1
1:A:90:PRO:O	1:A:121:ARG:NH1	0.68	2.27	4	1
1:A:161:HIS:CG	1:A:163:PHE:CZ	0.68	2.82	5	4
2:B:380:ASP:CB	2:B:381:PRO:HD3	0.68	2.19	8	10
1:A:184:PRO:O	1:A:185:THR:HG23	0.68	1.88	7	1
2:B:361:LEU:HD11	2:B:371:TYR:CD1	0.68	2.24	2	1
1:A:168:PHE:HB3	1:A:199:TYR:O	0.68	1.89	5	10
2:B:412:PHE:CD1	2:B:436:LYS:HG3	0.68	2.23	5	1
3:C:651:LEU:HD22	3:C:652:GLU:H	0.68	1.47	9	8
1:A:188:VAL:HG12	1:A:189:ALA:N	0.68	2.03	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ARG:NH2	1:A:133:LYS:HZ2	0.68	1.86	6	1
1:A:70:TYR:CZ	1:A:92:ASN:OD1	0.68	2.47	3	4
1:A:278:LYS:O	1:A:279:ILE:CG1	0.67	2.42	8	3
1:A:182:THR:HB	1:A:184:PRO:HG3	0.67	1.66	1	9
1:A:279:ILE:HD12	1:A:279:ILE:N	0.67	2.03	1	1
3:C:663:ALA:N	3:C:664:PRO:HD2	0.67	2.04	9	10
3:C:681:VAL:O	3:C:684:VAL:HG22	0.67	1.89	1	6
1:A:67:ILE:O	1:A:68:GLU:C	0.67	2.33	5	10
3:C:676:VAL:CG2	3:C:677:TYR:N	0.67	2.58	3	1
1:A:129:ARG:NH2	1:A:133:LYS:NZ	0.67	2.42	6	1
2:B:422:TRP:CZ3	2:B:424:LEU:HD21	0.67	2.24	7	1
3:C:672:LEU:C	3:C:672:LEU:HD23	0.67	2.09	2	2
2:B:488:ASN:N	2:B:488:ASN:ND2	0.67	2.43	9	1
3:C:648:LEU:HA	3:C:651:LEU:HD21	0.67	1.66	5	1
1:A:186:ALA:HB2	1:A:218:VAL:CG2	0.67	2.18	9	10
1:A:172:ARG:NH1	1:A:174:ARG:NE	0.67	2.43	10	1
2:B:571:ILE:CG2	2:B:571:ILE:O	0.66	2.43	6	1
1:A:74:VAL:HG22	1:A:75:LEU:N	0.66	2.05	7	10
3:C:615:LEU:O	3:C:615:LEU:HD22	0.66	1.90	9	4
3:C:602:CYS:SG	3:C:606:PHE:CD2	0.66	2.89	5	1
2:B:350:ALA:O	2:B:358:ASP:HA	0.66	1.91	7	10
1:A:169:TRP:O	1:A:169:TRP:CD2	0.66	2.49	6	3
2:B:571:ILE:O	2:B:571:ILE:CG2	0.66	2.43	10	4
2:B:371:TYR:N	2:B:371:TYR:CD1	0.66	2.64	2	1
1:A:192:LEU:N	1:A:192:LEU:HD12	0.66	2.05	10	2
3:C:654:LEU:H	3:C:654:LEU:HD12	0.66	1.51	10	1
3:C:615:LEU:C	3:C:615:LEU:HD13	0.66	2.10	2	3
3:C:651:LEU:CD1	3:C:651:LEU:N	0.66	2.46	2	2
2:B:452:HIS:CG	2:B:471:SER:HG	0.66	2.08	8	1
2:B:569:ARG:C	2:B:570:GLN:CD	0.66	2.54	2	1
2:B:415:GLY:HA3	2:B:436:LYS:HD3	0.66	1.67	5	1
3:C:693:ASP:CG	3:C:696:VAL:HG13	0.66	2.10	10	1
1:A:121:ARG:HH21	1:A:145:GLY:H	0.66	1.31	2	2
3:C:602:CYS:SG	3:C:606:PHE:CE2	0.66	2.89	5	1
1:A:89:ASP:O	1:A:93:LYS:HA	0.65	1.92	5	10
1:A:135:HIS:O	2:B:544:ARG:HG2	0.65	1.90	7	7
3:C:702:LEU:O	3:C:703:THR:C	0.65	2.35	5	10
1:A:88:LEU:HD23	1:A:89:ASP:H	0.65	1.49	5	1
2:B:340:LEU:O	2:B:363:ASP:CB	0.65	2.45	3	10
1:A:75:LEU:CD2	1:A:75:LEU:N	0.65	2.59	9	1
1:A:75:LEU:HD22	1:A:75:LEU:N	0.65	2.06	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:MET:SD	1:A:59:MET:C	0.65	2.75	10	1
2:B:350:ALA:HB1	2:B:359:TYR:CZ	0.65	2.27	5	10
3:C:654:LEU:N	3:C:654:LEU:CD1	0.65	2.59	6	1
2:B:528:LEU:O	2:B:532:TYR:HB2	0.65	1.92	2	10
2:B:379:TYR:CD1	2:B:383:LEU:HB2	0.65	2.27	4	2
2:B:361:LEU:HD11	2:B:371:TYR:CG	0.65	2.27	2	1
1:A:192:LEU:HD12	1:A:192:LEU:N	0.64	2.08	9	5
2:B:361:LEU:HD12	2:B:361:LEU:N	0.64	2.08	9	1
1:A:187:GLN:HA	1:A:215:SER:CA	0.64	2.17	8	10
1:A:100:HIS:N	1:A:100:HIS:CD2	0.64	2.63	7	1
1:A:267:THR:O	1:A:268:LYS:C	0.64	2.36	3	10
1:A:161:HIS:CD2	1:A:163:PHE:CZ	0.64	2.86	3	4
2:B:544:ARG:HG2	2:B:545:SER:H	0.64	1.50	1	8
1:A:59:MET:HG3	1:A:60:ASP:N	0.64	2.07	10	1
2:B:475:LEU:HD23	2:B:476:TRP:N	0.64	2.07	4	3
1:A:129:ARG:O	1:A:129:ARG:NE	0.64	2.30	7	1
3:C:654:LEU:HD23	3:C:654:LEU:H	0.64	1.51	4	1
1:A:153:THR:HA	1:A:179:PHE:O	0.64	1.93	2	10
1:A:198:TYR:CD1	1:A:198:TYR:O	0.64	2.51	3	5
2:B:377:ASN:ND2	2:B:394:ARG:NE	0.64	2.46	3	3
3:C:685:LYS:O	3:C:688:LEU:CD1	0.64	2.46	6	2
2:B:361:LEU:HD23	2:B:362:CYS:N	0.64	2.07	2	1
1:A:181:ILE:O	1:A:182:THR:CB	0.64	2.46	3	10
2:B:362:CYS:HG	2:B:365:ASN:CG	0.64	1.95	1	6
3:C:615:LEU:HD22	3:C:615:LEU:O	0.63	1.93	2	2
1:A:117:LEU:HD12	1:A:120:TRP:CD1	0.63	2.29	9	1
1:A:260:ARG:O	2:B:411:TYR:CE2	0.63	2.50	7	1
3:C:650:ILE:CD1	3:C:650:ILE:N	0.63	2.60	5	1
1:A:165:PRO:O	1:A:168:PHE:N	0.63	2.31	5	10
1:A:152:GLN:CB	1:A:181:ILE:HG21	0.63	2.24	10	1
1:A:198:TYR:O	1:A:198:TYR:CD1	0.63	2.51	5	2
1:A:59:MET:SD	1:A:59:MET:N	0.63	2.71	1	1
1:A:172:ARG:HH11	1:A:174:ARG:NE	0.63	1.91	10	1
1:A:100:HIS:CD2	1:A:100:HIS:H	0.63	2.11	1	2
1:A:148:ILE:O	1:A:151:GLN:HG2	0.63	1.93	10	1
1:A:152:GLN:HB2	1:A:181:ILE:HG21	0.63	1.69	10	1
3:C:654:LEU:HD13	3:C:654:LEU:C	0.63	2.13	6	1
1:A:195:GLN:NE2	1:A:205:GLN:NE2	0.63	2.46	9	1
2:B:530:GLU:O	2:B:534:GLY:CA	0.63	2.46	1	10
1:A:74:VAL:C	1:A:75:LEU:HD12	0.63	2.14	1	2
3:C:688:LEU:HD12	3:C:691:GLY:O	0.63	1.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:364:TYR:CD1	2:B:422:TRP:CH2	0.62	2.87	8	4
1:A:263:PRO:HG3	2:B:411:TYR:CZ	0.62	2.29	10	1
2:B:570:GLN:OE1	2:B:570:GLN:O	0.62	2.16	2	1
3:C:688:LEU:C	3:C:688:LEU:CD2	0.62	2.52	4	1
1:A:117:LEU:HG	1:A:117:LEU:O	0.62	1.94	5	5
1:A:70:TYR:CE1	1:A:92:ASN:CG	0.62	2.73	5	4
1:A:196:VAL:O	1:A:205:GLN:HA	0.62	1.95	9	10
1:A:273:LYS:O	1:A:277:TYR:HB2	0.62	1.94	10	10
1:A:277:TYR:CD2	1:A:277:TYR:O	0.62	2.53	7	5
3:C:636:ARG:NH1	3:C:641:TYR:CE2	0.62	2.68	2	1
1:A:259:ARG:NE	2:B:411:TYR:CD1	0.62	2.67	5	4
1:A:279:ILE:HG22	1:A:279:ILE:O	0.62	1.93	1	2
2:B:362:CYS:H	2:B:365:ASN:HD21	0.62	1.35	4	1
1:A:70:TYR:O	1:A:71:ASP:C	0.62	2.38	4	10
2:B:381:PRO:O	2:B:383:LEU:N	0.62	2.33	5	10
3:C:651:LEU:HD12	3:C:652:GLU:N	0.62	2.10	5	1
1:A:29:PHE:CD2	1:A:30:ASN:N	0.62	2.68	10	3
1:A:61:GLN:NE2	1:A:172:ARG:NH2	0.62	2.47	8	2
2:B:371:TYR:CD1	2:B:371:TYR:N	0.62	2.66	10	2
3:C:716:LEU:O	3:C:717:LEU:CG	0.62	2.48	7	3
2:B:412:PHE:CD1	2:B:412:PHE:N	0.62	2.68	6	4
1:A:192:LEU:CD2	1:A:192:LEU:N	0.62	2.59	1	1
2:B:372:ARG:NH2	2:B:397:GLU:OE2	0.62	2.32	5	2
3:C:636:ARG:NH1	3:C:641:TYR:CZ	0.62	2.67	2	1
1:A:92:ASN:HD22	1:A:92:ASN:N	0.62	1.92	9	1
3:C:695:THR:HG23	3:C:695:THR:O	0.61	1.95	9	1
1:A:92:ASN:OD1	1:A:94:ILE:HD13	0.61	1.95	6	4
3:C:659:ALA:C	3:C:661:ILE:H	0.61	1.99	3	10
3:C:673:LEU:HA	3:C:676:VAL:CG1	0.61	2.26	3	1
3:C:610:LEU:CD2	3:C:618:VAL:HG11	0.61	2.25	8	2
2:B:361:LEU:N	2:B:361:LEU:HD12	0.61	2.10	1	1
2:B:420:TYR:C	2:B:421:LEU:HD12	0.61	2.15	1	2
1:A:59:MET:SD	1:A:78:GLU:N	0.61	2.72	10	1
1:A:118:LYS:HZ3	1:A:121:ARG:NE	0.61	1.93	5	2
2:B:563:SER:C	2:B:565:VAL:N	0.61	2.53	5	10
1:A:186:ALA:CB	1:A:218:VAL:HG23	0.61	2.21	2	10
1:A:263:PRO:HD3	2:B:411:TYR:CZ	0.61	2.31	4	8
1:A:277:TYR:O	1:A:277:TYR:CG	0.61	2.54	6	6
1:A:100:HIS:CD2	1:A:100:HIS:N	0.61	2.69	1	2
2:B:492:SER:C	2:B:493:LEU:HD22	0.61	2.15	2	5
1:A:59:MET:SD	1:A:60:ASP:N	0.61	2.74	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:GLN:O	1:A:181:ILE:HB	0.61	1.95	1	9
1:A:187:GLN:O	1:A:188:VAL:HB	0.61	1.95	1	8
2:B:496:GLN:N	2:B:496:GLN:NE2	0.61	2.48	2	1
1:A:46:LEU:O	1:A:46:LEU:HD23	0.61	1.95	1	1
2:B:350:ALA:HB2	2:B:361:LEU:HD11	0.61	1.72	9	2
2:B:453:VAL:O	2:B:470:THR:HG22	0.61	1.96	10	2
1:A:270:ASP:O	1:A:271:TRP:C	0.61	2.39	5	10
3:C:699:PRO:O	3:C:700:ASP:HB2	0.61	1.96	8	7
3:C:680:HIS:O	3:C:681:VAL:HG22	0.61	1.96	6	5
1:A:206:LEU:HD12	1:A:247:TYR:OH	0.61	1.94	9	3
1:A:199:TYR:CG	1:A:199:TYR:O	0.61	2.54	10	4
1:A:278:LYS:O	1:A:279:ILE:HG12	0.61	1.96	8	3
2:B:564:GLN:NE2	2:B:568:GLN:NE2	0.61	2.49	7	1
3:C:651:LEU:CD2	3:C:651:LEU:H	0.61	2.07	6	4
1:A:149:ASP:O	1:A:149:ASP:OD1	0.61	2.19	6	1
1:A:91:ARG:NH2	1:A:141:CYS:SG	0.61	2.73	6	1
3:C:673:LEU:HA	3:C:676:VAL:HG13	0.61	1.72	3	1
1:A:152:GLN:O	1:A:181:ILE:HG23	0.60	1.96	10	1
1:A:271:TRP:O	1:A:274:ILE:N	0.60	2.33	1	10
1:A:274:ILE:N	1:A:274:ILE:HD12	0.60	2.11	1	1
1:A:198:TYR:CD2	1:A:198:TYR:O	0.60	2.54	2	1
1:A:256:LYS:NZ	3:C:636:ARG:HE	0.60	1.92	2	1
1:A:184:PRO:O	1:A:185:THR:OG1	0.60	2.19	5	9
1:A:216:VAL:HG22	1:A:217:GLN:N	0.60	2.12	8	4
1:A:177:TRP:CE3	1:A:190:ALA:CB	0.60	2.85	10	1
1:A:149:ASP:OD1	1:A:149:ASP:O	0.60	2.19	5	2
3:C:651:LEU:N	3:C:651:LEU:CD2	0.60	2.61	7	5
1:A:118:LYS:HZ3	1:A:121:ARG:HE	0.60	1.40	5	2
1:A:97:LYS:O	1:A:105:ALA:HB1	0.60	1.97	9	10
2:B:469:LEU:HD12	2:B:470:THR:H	0.60	1.57	2	6
2:B:450:SER:OG	2:B:452:HIS:CE1	0.60	2.54	3	1
1:A:121:ARG:HH21	1:A:145:GLY:N	0.60	1.93	2	2
3:C:651:LEU:HD22	3:C:651:LEU:H	0.60	1.57	6	2
1:A:188:VAL:HG13	1:A:189:ALA:N	0.60	2.10	1	4
1:A:86:ARG:NH2	1:A:107:ASP:O	0.60	2.35	2	1
1:A:168:PHE:CD1	1:A:199:TYR:O	0.60	2.54	9	6
1:A:262:LEU:O	1:A:262:LEU:HD12	0.60	1.96	10	1
2:B:379:TYR:CE1	2:B:383:LEU:CB	0.60	2.85	4	1
3:C:613:GLY:O	3:C:615:LEU:N	0.60	2.33	7	10
1:A:279:ILE:O	1:A:279:ILE:HG22	0.60	1.97	2	3
3:C:695:THR:O	3:C:695:THR:HG23	0.60	1.97	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLN:O	1:A:63:THR:N	0.60	2.35	1	10
1:A:177:TRP:HB3	1:A:179:PHE:CZ	0.60	2.32	8	7
1:A:216:VAL:HG12	1:A:217:GLN:N	0.60	2.12	1	6
2:B:336:CYS:SG	2:B:337:GLU:N	0.60	2.75	9	4
2:B:459:LYS:CG	2:B:464:THR:O	0.59	2.50	9	6
1:A:274:ILE:O	1:A:274:ILE:HG22	0.59	1.97	3	3
2:B:452:HIS:ND1	2:B:471:SER:OG	0.59	2.34	8	1
3:C:644:ASP:O	3:C:644:ASP:OD1	0.59	2.21	6	2
2:B:313:MET:N	2:B:313:MET:SD	0.59	2.75	2	1
2:B:491:GLY:O	2:B:492:SER:HB3	0.59	1.98	8	7
1:A:61:GLN:O	1:A:62:PHE:C	0.59	2.41	9	10
1:A:277:TYR:CG	1:A:277:TYR:O	0.59	2.54	2	4
1:A:186:ALA:CB	1:A:216:VAL:C	0.59	2.58	5	10
3:C:650:ILE:HD12	3:C:650:ILE:N	0.59	2.10	5	1
1:A:239:TYR:CE2	1:A:243:ILE:HD11	0.59	2.33	7	3
1:A:182:THR:OG1	1:A:184:PRO:CD	0.59	2.50	7	1
2:B:422:TRP:CD1	2:B:422:TRP:N	0.59	2.69	7	2
1:A:65:VAL:HG22	1:A:66:LYS:N	0.59	2.12	1	9
2:B:487:MET:SD	2:B:487:MET:O	0.59	2.61	3	1
2:B:370:SER:OG	2:B:381:PRO:HB2	0.59	1.96	10	4
1:A:159:GLU:OE2	1:A:173:TRP:O	0.59	2.19	1	1
1:A:148:ILE:O	1:A:151:GLN:HG3	0.59	1.97	10	1
1:A:169:TRP:O	1:A:169:TRP:CE3	0.59	2.56	9	6
2:B:310:LEU:HD23	2:B:310:LEU:O	0.59	1.98	8	1
1:A:95:SER:N	1:A:109:GLN:O	0.59	2.35	1	10
2:B:383:LEU:HD23	2:B:384:GLU:H	0.59	1.58	10	6
3:C:651:LEU:H	3:C:651:LEU:CD2	0.59	2.09	2	3
1:A:199:TYR:OH	2:B:314:ARG:NH2	0.59	2.35	10	1
2:B:463:ARG:CG	2:B:463:ARG:HH11	0.59	2.11	9	1
2:B:488:ASN:HD22	2:B:488:ASN:N	0.59	1.95	9	1
2:B:370:SER:OG	2:B:383:LEU:HD12	0.59	1.98	5	3
1:A:165:PRO:C	1:A:167:ASN:N	0.59	2.56	3	10
2:B:563:SER:C	2:B:565:VAL:H	0.59	2.01	6	10
2:B:544:ARG:HG2	2:B:545:SER:N	0.59	2.13	1	7
3:C:699:PRO:HG2	3:C:702:LEU:HD22	0.59	1.74	8	1
1:A:61:GLN:OE1	1:A:172:ARG:NH2	0.59	2.35	5	2
3:C:672:LEU:HD12	3:C:684:VAL:HG13	0.59	1.73	5	1
3:C:691:GLY:O	3:C:692:ALA:C	0.59	2.41	5	10
3:C:636:ARG:HH21	3:C:640:HIS:CD2	0.59	2.15	10	2
2:B:408:ARG:NH1	2:B:415:GLY:O	0.59	2.36	1	2
3:C:651:LEU:CD2	3:C:651:LEU:N	0.59	2.60	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:274:ILE:O	1:A:274:ILE:CG2	0.59	2.51	4	2
3:C:717:LEU:HD12	3:C:718:GLN:H	0.58	1.53	3	1
3:C:717:LEU:CD1	3:C:718:GLN:N	0.58	2.63	3	1
3:C:648:LEU:O	3:C:651:LEU:HD21	0.58	1.98	10	8
2:B:564:GLN:NE2	2:B:568:GLN:HE22	0.58	1.95	7	1
1:A:165:PRO:C	1:A:167:ASN:H	0.58	2.02	9	10
2:B:370:SER:HA	2:B:381:PRO:HG2	0.58	1.75	4	10
2:B:442:LYS:NZ	3:C:644:ASP:OD2	0.58	2.35	9	2
3:C:642:ALA:O	3:C:646:GLY:HA3	0.58	1.99	10	10
3:C:642:ALA:O	3:C:646:GLY:CA	0.58	2.52	3	10
1:A:72:ASP:OD1	1:A:91:ARG:NE	0.58	2.36	5	2
1:A:205:GLN:NE2	1:A:207:VAL:CG2	0.58	2.66	7	2
3:C:677:TYR:CD1	3:C:677:TYR:O	0.58	2.56	2	1
3:C:630:ARG:CG	3:C:630:ARG:HH11	0.58	2.11	4	1
1:A:177:TRP:CD2	1:A:190:ALA:CB	0.58	2.87	7	8
1:A:274:ILE:HG22	1:A:274:ILE:O	0.58	1.97	1	2
1:A:176:GLU:O	1:A:190:ALA:HB1	0.58	1.99	5	10
3:C:688:LEU:CD2	3:C:688:LEU:C	0.58	2.53	6	1
1:A:248:GLN:O	1:A:252:ASP:OD2	0.58	2.21	5	2
1:A:131:TYR:OH	2:B:544:ARG:NH2	0.58	2.37	4	6
2:B:570:GLN:O	2:B:571:ILE:CG1	0.58	2.51	1	5
2:B:566:LEU:HD22	2:B:566:LEU:N	0.58	2.13	7	1
1:A:161:HIS:CD2	1:A:163:PHE:CE2	0.58	2.92	3	4
2:B:377:ASN:ND2	2:B:394:ARG:CZ	0.58	2.66	3	3
3:C:630:ARG:CD	3:C:630:ARG:H	0.58	2.12	1	1
1:A:91:ARG:HH22	1:A:129:ARG:NH2	0.58	1.95	10	1
3:C:648:LEU:O	3:C:648:LEU:CD1	0.58	2.51	8	1
2:B:422:TRP:CZ2	2:B:429:ALA:HB3	0.58	2.33	4	3
1:A:236:GLU:OE2	1:A:237:ASN:ND2	0.58	2.37	9	1
2:B:478:GLN:NE2	2:B:479:THR:H	0.58	1.97	9	1
2:B:525:ARG:CG	2:B:525:ARG:HH11	0.58	2.12	8	2
1:A:121:ARG:O	1:A:122:ASP:C	0.58	2.42	5	10
1:A:169:TRP:CE3	1:A:169:TRP:O	0.58	2.57	10	4
1:A:180:THR:OG1	1:A:181:ILE:N	0.58	2.37	2	7
1:A:164:GLN:HB3	1:A:169:TRP:CE2	0.58	2.33	1	7
1:A:253:THR:OG1	3:C:636:ARG:NH2	0.58	2.36	8	1
2:B:422:TRP:N	2:B:422:TRP:CD1	0.58	2.71	2	1
1:A:251:SER:OG	2:B:533:PHE:HB3	0.58	1.98	2	1
1:A:146:LYS:CG	1:A:147:SER:N	0.57	2.67	10	1
1:A:173:TRP:CH2	1:A:194:ILE:HD11	0.57	2.34	4	2
2:B:442:LYS:NZ	3:C:640:HIS:NE2	0.57	2.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:ILE:HG12	2:B:487:MET:SD	0.57	2.39	7	1
3:C:678:GLU:CD	3:C:678:GLU:O	0.57	2.43	9	1
2:B:550:PRO:O	2:B:551:ASP:O	0.57	2.23	5	10
1:A:19:LYS:O	1:A:23:HIS:CG	0.57	2.57	4	10
1:A:216:VAL:CG2	1:A:217:GLN:N	0.57	2.67	3	4
1:A:74:VAL:HG22	1:A:75:LEU:H	0.57	1.60	9	10
1:A:237:ASN:ND2	1:A:237:ASN:O	0.57	2.37	1	1
3:C:717:LEU:HG	3:C:718:GLN:H	0.57	1.58	1	2
2:B:432:ILE:O	2:B:452:HIS:ND1	0.57	2.36	10	1
1:A:277:TYR:O	1:A:277:TYR:CD2	0.57	2.57	5	5
2:B:550:PRO:O	2:B:551:ASP:C	0.57	2.43	8	10
3:C:701:GLY:O	3:C:705:LEU:CB	0.57	2.53	10	10
1:A:89:ASP:O	1:A:93:LYS:CA	0.57	2.53	1	10
1:A:224:THR:OG1	1:A:228:PHE:CZ	0.57	2.56	1	1
1:A:246:ASN:HD21	2:B:481:LYS:NZ	0.57	1.97	4	1
1:A:121:ARG:HG2	1:A:122:ASP:N	0.57	2.14	2	1
1:A:206:LEU:HD23	1:A:206:LEU:O	0.57	1.99	5	3
2:B:439:ASP:OD1	2:B:441:SER:N	0.57	2.37	8	1
3:C:651:LEU:HD12	3:C:652:GLU:H	0.57	1.60	5	1
2:B:439:ASP:OD1	2:B:442:LYS:N	0.57	2.37	8	1
1:A:259:ARG:HG2	1:A:260:ARG:N	0.57	2.15	5	3
1:A:261:GLN:O	1:A:262:LEU:HG	0.57	1.99	1	1
1:A:192:LEU:CD1	1:A:192:LEU:N	0.57	2.67	8	2
1:A:263:PRO:HA	2:B:410:LEU:O	0.57	2.00	8	10
2:B:412:PHE:O	2:B:436:LYS:NZ	0.57	2.38	10	8
1:A:55:ALA:O	1:A:59:MET:SD	0.57	2.62	1	1
2:B:569:ARG:HH11	2:B:569:ARG:CG	0.57	2.11	1	2
1:A:155:ILE:N	1:A:155:ILE:HD12	0.57	2.14	9	1
3:C:700:ASP:CG	3:C:701:GLY:N	0.57	2.58	5	7
1:A:129:ARG:HH11	1:A:129:ARG:CG	0.57	2.13	3	3
1:A:61:GLN:OE1	1:A:174:ARG:NH2	0.57	2.37	1	2
3:C:674:SER:O	3:C:678:GLU:HG2	0.57	2.00	6	2
1:A:188:VAL:HG13	1:A:189:ALA:H	0.57	1.59	2	10
2:B:544:ARG:CG	2:B:545:SER:N	0.57	2.68	1	4
2:B:493:LEU:CD1	2:B:494:THR:N	0.57	2.66	10	1
1:A:260:ARG:NH1	3:C:633:GLU:OE1	0.57	2.38	9	1
1:A:188:VAL:O	1:A:189:ALA:HB2	0.56	2.01	6	10
2:B:448:TRP:CD1	2:B:448:TRP:C	0.56	2.79	8	6
1:A:236:GLU:CG	2:B:544:ARG:NH1	0.56	2.68	2	1
3:C:662:ASN:CA	3:C:664:PRO:HD2	0.56	2.30	9	10
3:C:651:LEU:O	3:C:655:LEU:HB2	0.56	2.00	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:394:ARG:NH1	2:B:397:GLU:OE1	0.56	2.38	8	1
1:A:249:THR:OG1	3:C:677:TYR:CZ	0.56	2.59	6	1
2:B:493:LEU:N	2:B:493:LEU:HD22	0.56	2.14	2	1
1:A:181:ILE:C	1:A:182:THR:OG1	0.56	2.43	2	9
2:B:340:LEU:O	2:B:363:ASP:CG	0.56	2.44	8	4
1:A:86:ARG:CG	1:A:86:ARG:HH11	0.56	2.14	10	5
1:A:216:VAL:CG1	1:A:217:GLN:N	0.56	2.67	4	6
2:B:379:TYR:CD1	2:B:383:LEU:CB	0.56	2.88	4	2
3:C:651:LEU:O	3:C:655:LEU:HB3	0.56	2.00	7	2
1:A:158:ILE:HD13	1:A:175:SER:OG	0.56	2.00	2	1
1:A:184:PRO:C	1:A:185:THR:HG22	0.56	2.19	2	1
2:B:362:CYS:O	2:B:365:ASN:ND2	0.56	2.39	4	1
2:B:379:TYR:OH	2:B:387:ALA:O	0.56	2.21	6	6
1:A:89:ASP:O	1:A:93:LYS:N	0.56	2.39	9	10
1:A:199:TYR:N	1:A:199:TYR:CD1	0.56	2.73	8	3
1:A:255:PHE:CE2	2:B:525:ARG:CZ	0.56	2.89	1	1
2:B:562:LEU:HD23	2:B:562:LEU:O	0.56	2.00	10	1
1:A:89:ASP:HB3	1:A:94:ILE:HD13	0.56	1.77	7	1
2:B:549:ILE:O	2:B:551:ASP:N	0.56	2.39	6	10
1:A:89:ASP:OD1	1:A:92:ASN:N	0.56	2.38	9	3
1:A:199:TYR:O	1:A:199:TYR:CG	0.56	2.59	9	2
1:A:266:ARG:O	1:A:267:THR:OG1	0.56	2.22	8	4
2:B:372:ARG:NH1	2:B:377:ASN:OD1	0.56	2.39	5	2
1:A:28:GLU:OE2	1:A:170:ASN:ND2	0.56	2.38	7	1
2:B:525:ARG:O	2:B:529:ASN:ND2	0.56	2.39	2	1
1:A:199:TYR:CD1	1:A:199:TYR:N	0.56	2.73	5	1
1:A:148:ILE:O	1:A:149:ASP:OD1	0.56	2.24	6	4
2:B:570:GLN:OE1	2:B:570:GLN:N	0.56	2.38	2	1
1:A:279:ILE:O	1:A:280:GLY:C	0.56	2.44	5	10
3:C:649:GLU:O	3:C:653:PHE:CD1	0.56	2.59	3	1
2:B:552:ASN:ND2	2:B:555:TYR:CD1	0.56	2.74	10	2
1:A:91:ARG:CG	1:A:91:ARG:HH11	0.56	2.12	4	1
1:A:153:THR:HG23	1:A:180:THR:N	0.56	2.15	4	3
1:A:29:PHE:CG	1:A:30:ASN:N	0.56	2.73	10	3
2:B:411:TYR:N	2:B:411:TYR:CD1	0.56	2.73	10	1
3:C:651:LEU:O	3:C:655:LEU:CB	0.56	2.54	9	10
2:B:325:LEU:CD2	2:B:345:GLN:NE2	0.56	2.69	6	5
2:B:452:HIS:CE1	2:B:471:SER:OG	0.56	2.59	8	1
3:C:667:HIS:ND1	3:C:667:HIS:N	0.56	2.53	7	1
1:A:113:THR:OG1	1:A:118:LYS:NZ	0.56	2.38	4	1
2:B:448:TRP:C	2:B:448:TRP:CD1	0.55	2.79	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:661:ILE:HD11	3:C:672:LEU:CD2	0.55	2.32	5	1
1:A:267:THR:O	1:A:268:LYS:O	0.55	2.24	7	10
1:A:118:LYS:HZ2	1:A:121:ARG:HH21	0.55	1.44	3	2
1:A:159:GLU:OE2	1:A:160:SER:N	0.55	2.35	1	1
2:B:444:ILE:HG22	2:B:479:THR:OG1	0.55	2.01	2	1
1:A:206:LEU:C	1:A:206:LEU:HD23	0.55	2.21	9	2
3:C:699:PRO:O	3:C:700:ASP:CB	0.55	2.54	10	10
1:A:210:LYS:NZ	2:B:482:THR:O	0.55	2.39	4	2
1:A:184:PRO:O	1:A:185:THR:CG2	0.55	2.54	7	1
2:B:380:ASP:OD1	2:B:381:PRO:N	0.55	2.40	7	1
1:A:188:VAL:HB	1:A:214:ASP:O	0.55	2.01	3	10
1:A:129:ARG:HG3	1:A:130:ALA:N	0.55	2.16	8	4
1:A:169:TRP:CZ3	2:B:539:ILE:HD12	0.55	2.37	1	5
1:A:26:PRO:O	1:A:170:ASN:ND2	0.55	2.40	10	1
2:B:412:PHE:N	2:B:412:PHE:CD1	0.55	2.74	10	1
1:A:148:ILE:O	1:A:149:ASP:CG	0.55	2.45	8	4
1:A:179:PHE:CD1	1:A:179:PHE:C	0.55	2.78	1	1
3:C:642:ALA:O	3:C:651:LEU:HD12	0.55	2.02	2	8
1:A:179:PHE:CD2	1:A:179:PHE:O	0.55	2.60	9	1
2:B:418:SER:OG	2:B:420:TYR:OH	0.55	2.19	9	1
1:A:129:ARG:NH1	1:A:129:ARG:CG	0.55	2.69	3	3
3:C:717:LEU:CG	3:C:718:GLN:H	0.55	2.14	1	2
3:C:654:LEU:H	3:C:654:LEU:HD23	0.55	1.61	8	1
3:C:630:ARG:NH1	3:C:630:ARG:CG	0.55	2.68	4	1
3:C:639:LEU:HD22	3:C:660:ASP:OD1	0.55	2.02	3	1
3:C:640:HIS:CE1	3:C:644:ASP:OD2	0.55	2.59	2	2
1:A:261:GLN:CG	2:B:525:ARG:NH1	0.55	2.69	1	1
2:B:439:ASP:CG	3:C:611:LYS:HZ1	0.55	2.04	1	1
2:B:553:GLN:CD	2:B:553:GLN:H	0.55	2.05	10	1
1:A:111:GLU:O	1:A:111:GLU:HG3	0.55	2.01	7	1
1:A:229:ILE:O	1:A:232:ILE:HG12	0.55	2.02	9	1
1:A:42:ASN:ND2	1:A:45:LEU:CD1	0.55	2.70	5	3
3:C:673:LEU:O	3:C:676:VAL:HB	0.55	2.02	9	9
1:A:274:ILE:CG2	1:A:274:ILE:O	0.55	2.54	1	3
3:C:656:LEU:O	3:C:656:LEU:HD23	0.55	2.00	10	1
2:B:420:TYR:CD1	2:B:420:TYR:N	0.55	2.74	9	1
3:C:659:ALA:O	3:C:661:ILE:N	0.55	2.40	2	10
2:B:340:LEU:O	2:B:363:ASP:HB2	0.55	2.02	6	4
2:B:383:LEU:CD2	2:B:384:GLU:H	0.55	2.15	10	6
2:B:449:ASP:N	2:B:449:ASP:OD1	0.55	2.37	3	2
3:C:716:LEU:O	3:C:717:LEU:HD13	0.55	2.02	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:478:GLN:CD	2:B:479:THR:H	0.55	2.05	9	1
1:A:126:SER:O	1:A:129:ARG:CG	0.55	2.55	7	4
2:B:350:ALA:CB	2:B:359:TYR:CE1	0.55	2.90	9	9
1:A:247:TYR:CE2	2:B:537:LYS:NZ	0.55	2.71	3	1
1:A:31:GLU:OE1	2:B:315:ARG:NE	0.55	2.39	10	2
2:B:449:ASP:OD1	2:B:449:ASP:N	0.55	2.40	5	1
3:C:675:ALA:O	3:C:678:GLU:HB2	0.55	2.02	10	3
1:A:152:GLN:N	1:A:181:ILE:CG1	0.55	2.69	10	1
3:C:628:VAL:HG11	3:C:654:LEU:O	0.55	2.02	7	4
2:B:443:LYS:NZ	3:C:677:TYR:CD2	0.55	2.75	7	1
1:A:173:TRP:CZ3	2:B:544:ARG:NH1	0.55	2.75	9	1
2:B:533:PHE:CD1	2:B:533:PHE:N	0.54	2.74	5	8
1:A:19:LYS:O	1:A:23:HIS:ND1	0.54	2.40	2	9
1:A:159:GLU:CD	1:A:160:SER:N	0.54	2.61	10	9
3:C:701:GLY:O	3:C:705:LEU:HB3	0.54	2.01	1	10
1:A:136:TYR:N	1:A:136:TYR:CD1	0.54	2.75	1	1
1:A:61:GLN:NE2	1:A:174:ARG:NH2	0.54	2.55	1	2
2:B:476:TRP:C	2:B:476:TRP:CD1	0.54	2.80	4	2
1:A:67:ILE:CD1	1:A:68:GLU:N	0.54	2.69	5	4
2:B:415:GLY:HA3	2:B:436:LYS:CD	0.54	2.33	5	1
2:B:422:TRP:CD1	2:B:422:TRP:O	0.54	2.61	8	4
1:A:72:ASP:C	1:A:74:VAL:N	0.54	2.61	8	9
3:C:635:GLY:O	3:C:667:HIS:NE2	0.54	2.40	3	8
1:A:201:ASP:OD1	2:B:493:LEU:CD2	0.54	2.55	10	1
2:B:459:LYS:HB2	2:B:464:THR:O	0.54	2.03	4	6
1:A:159:GLU:OE2	1:A:161:HIS:ND1	0.54	2.41	9	6
3:C:654:LEU:H	3:C:654:LEU:CD2	0.54	2.13	4	2
2:B:409:ASP:OD2	3:C:604:LYS:NZ	0.54	2.39	4	2
3:C:699:PRO:HB2	3:C:702:LEU:HD13	0.54	1.79	8	1
1:A:70:TYR:CE1	1:A:92:ASN:ND2	0.54	2.76	5	4
1:A:260:ARG:O	2:B:411:TYR:CE1	0.54	2.61	8	9
1:A:237:ASN:C	1:A:237:ASN:ND2	0.54	2.61	3	1
3:C:647:GLN:C	3:C:648:LEU:HG	0.54	2.22	3	1
3:C:678:GLU:OE1	3:C:680:HIS:ND1	0.54	2.40	9	1
3:C:688:LEU:C	3:C:688:LEU:CD1	0.54	2.72	4	1
2:B:439:ASP:OD1	3:C:611:LYS:NZ	0.54	2.41	1	1
1:A:255:PHE:CE1	2:B:529:ASN:OD1	0.54	2.61	2	1
1:A:271:TRP:CE2	2:B:514:GLY:HA3	0.54	2.37	2	1
1:A:232:ILE:O	1:A:236:GLU:HG2	0.54	2.03	3	1
1:A:246:ASN:O	1:A:250:MET:SD	0.54	2.65	8	2
2:B:566:LEU:CD2	2:B:566:LEU:N	0.54	2.71	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:OE1	2:B:315:ARG:NH1	0.54	2.41	3	3
1:A:121:ARG:O	1:A:123:ALA:N	0.54	2.41	6	10
1:A:68:GLU:OE1	1:A:69:GLY:N	0.54	2.41	8	7
1:A:169:TRP:CB	1:A:198:TYR:CD2	0.54	2.91	1	2
1:A:179:PHE:CE2	1:A:228:PHE:CZ	0.54	2.95	1	1
1:A:259:ARG:NH2	2:B:407:TYR:OH	0.54	2.41	1	1
3:C:627:ASP:O	3:C:630:ARG:NE	0.54	2.41	1	1
3:C:662:ASN:OD1	3:C:663:ALA:N	0.54	2.41	2	6
1:A:240:GLN:HA	1:A:243:ILE:HD12	0.54	1.79	7	1
2:B:525:ARG:HH11	2:B:525:ARG:CG	0.54	2.15	9	3
3:C:644:ASP:C	3:C:644:ASP:OD1	0.54	2.45	6	2
3:C:639:LEU:HD23	3:C:671:PRO:HG3	0.54	1.80	6	1
1:A:75:LEU:HD12	1:A:75:LEU:N	0.54	2.18	2	1
2:B:444:ILE:HG23	2:B:479:THR:OG1	0.54	2.03	9	1
1:A:136:TYR:CD1	1:A:136:TYR:N	0.54	2.75	4	1
3:C:658:GLY:O	3:C:659:ALA:HB2	0.54	2.03	5	10
3:C:664:PRO:O	3:C:697:LYS:NZ	0.54	2.40	5	1
3:C:612:ASN:HD22	3:C:612:ASN:N	0.54	2.00	3	1
1:A:76:ILE:HG23	1:A:87:PHE:CE2	0.54	2.37	1	1
1:A:73:GLN:OE1	1:A:140:PHE:CZ	0.54	2.61	9	1
2:B:443:LYS:CD	2:B:443:LYS:H	0.54	2.16	4	1
1:A:86:ARG:CG	1:A:86:ARG:NH1	0.54	2.70	7	4
2:B:547:ASP:OD1	2:B:548:ALA:N	0.54	2.41	1	2
1:A:73:GLN:OE1	1:A:73:GLN:N	0.54	2.41	4	2
1:A:28:GLU:OE2	2:B:315:ARG:NE	0.54	2.40	9	1
2:B:435:LYS:O	2:B:436:LYS:HD3	0.53	2.03	5	1
2:B:478:GLN:HG3	2:B:479:THR:N	0.53	2.18	5	1
1:A:148:ILE:HG22	1:A:149:ASP:OD2	0.53	2.04	8	3
1:A:99:ASP:O	1:A:102:ARG:O	0.53	2.26	3	10
2:B:466:HIS:ND1	2:B:500:ASP:OD1	0.53	2.41	6	3
1:A:177:TRP:CD2	1:A:190:ALA:HB2	0.53	2.38	7	8
3:C:615:LEU:O	3:C:615:LEU:CD1	0.53	2.51	8	6
1:A:152:GLN:O	1:A:181:ILE:CG2	0.53	2.57	10	1
1:A:167:ASN:OD1	1:A:169:TRP:NE1	0.53	2.41	7	1
2:B:372:ARG:NH2	2:B:420:TYR:OH	0.53	2.40	7	1
2:B:472:THR:HG23	2:B:494:THR:HG22	0.53	1.79	7	1
1:A:99:ASP:OD2	1:A:102:ARG:NE	0.53	2.41	6	1
1:A:251:SER:OG	2:B:533:PHE:CG	0.53	2.60	2	1
2:B:418:SER:OG	2:B:420:TYR:CZ	0.53	2.59	9	1
1:A:129:ARG:CG	1:A:129:ARG:HH11	0.53	2.16	4	1
2:B:452:HIS:NE2	2:B:521:GLU:OE2	0.53	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:ALA:HB3	1:A:217:GLN:N	0.53	2.18	5	10
1:A:59:MET:CG	1:A:60:ASP:N	0.53	2.70	10	1
3:C:633:GLU:OE1	3:C:634:GLY:N	0.53	2.42	10	1
1:A:246:ASN:OD1	2:B:481:LYS:NZ	0.53	2.40	6	1
2:B:466:HIS:CG	2:B:500:ASP:OD1	0.53	2.61	6	4
1:A:144:TYR:N	1:A:155:ILE:O	0.53	2.41	6	10
1:A:33:PHE:CZ	1:A:46:LEU:HD21	0.53	2.39	2	9
1:A:237:ASN:HD21	2:B:546:ILE:CD1	0.53	2.17	1	1
2:B:425:ASP:OD1	2:B:426:HIS:N	0.53	2.42	10	2
2:B:373:SER:O	2:B:377:ASN:HA	0.53	2.04	5	10
3:C:604:LYS:NZ	3:C:607:MET:CE	0.53	2.72	5	1
1:A:184:PRO:O	1:A:185:THR:CB	0.53	2.57	6	10
1:A:70:TYR:CE2	1:A:92:ASN:OD1	0.53	2.62	8	4
1:A:152:GLN:HB2	1:A:181:ILE:HG13	0.53	1.80	1	1
1:A:200:GLU:C	1:A:201:ASP:CG	0.53	2.66	10	1
1:A:274:ILE:CD1	2:B:403:ALA:HB1	0.53	2.31	7	1
1:A:73:GLN:OE1	1:A:140:PHE:CE1	0.53	2.61	9	1
1:A:91:ARG:CG	1:A:91:ARG:NH1	0.53	2.69	4	1
3:C:610:LEU:H	3:C:610:LEU:HD12	0.53	1.63	5	3
1:A:273:LYS:O	1:A:273:LYS:HG3	0.53	2.04	7	3
2:B:350:ALA:HB3	2:B:359:TYR:CZ	0.53	2.38	9	10
1:A:237:ASN:HD21	2:B:546:ILE:HD12	0.53	1.64	1	1
3:C:695:THR:CG2	3:C:703:THR:OG1	0.53	2.57	1	1
2:B:340:LEU:O	2:B:363:ASP:HB3	0.53	2.03	10	6
3:C:646:GLY:O	3:C:650:ILE:HD13	0.53	2.03	5	1
1:A:70:TYR:CE2	1:A:94:ILE:HD13	0.53	2.39	8	4
1:A:188:VAL:CG1	1:A:189:ALA:H	0.53	2.16	7	6
1:A:152:GLN:H	1:A:181:ILE:HG21	0.53	1.63	2	7
2:B:322:GLU:CD	2:B:322:GLU:H	0.53	2.06	3	1
1:A:209:HIS:CE1	2:B:486:THR:OG1	0.53	2.62	2	6
3:C:716:LEU:O	3:C:717:LEU:HD23	0.53	2.03	9	3
1:A:75:LEU:N	1:A:75:LEU:HD12	0.53	2.19	1	1
2:B:372:ARG:HG3	2:B:372:ARG:HH11	0.53	1.63	1	1
1:A:126:SER:O	1:A:129:ARG:HB3	0.53	2.04	10	4
2:B:473:VAL:O	2:B:492:SER:OG	0.53	2.23	10	2
1:A:259:ARG:NH2	2:B:521:GLU:OE2	0.53	2.42	7	1
3:C:667:HIS:O	3:C:668:HIS:CG	0.53	2.62	6	1
1:A:139:GLY:CA	1:A:159:GLU:O	0.53	2.57	5	10
1:A:220:SER:O	1:A:224:THR:HG23	0.53	2.04	7	5
1:A:86:ARG:NH2	1:A:107:ASP:OD2	0.53	2.40	3	1
2:B:569:ARG:NH1	2:B:569:ARG:CG	0.53	2.68	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:693:ASP:CG	3:C:694:LYS:N	0.53	2.62	10	1
1:A:194:ILE:HD13	1:A:195:GLN:H	0.53	1.60	2	1
1:A:253:THR:CG2	3:C:636:ARG:HH21	0.53	2.17	4	1
1:A:260:ARG:NH1	3:C:633:GLU:OE2	0.53	2.42	4	1
1:A:121:ARG:NH1	1:A:122:ASP:OD1	0.53	2.42	6	4
1:A:136:TYR:OH	1:A:173:TRP:CE2	0.53	2.55	9	3
1:A:10:ASP:OD1	1:A:11:GLU:N	0.53	2.41	1	2
1:A:67:ILE:HD12	1:A:67:ILE:N	0.53	2.19	9	1
1:A:54:PHE:CD1	1:A:54:PHE:N	0.53	2.74	4	1
2:B:569:ARG:CG	2:B:569:ARG:HH11	0.53	2.16	4	1
1:A:92:ASN:OD1	1:A:94:ILE:CD1	0.53	2.57	6	4
3:C:703:THR:OG1	3:C:704:ALA:N	0.53	2.42	9	4
1:A:203:ASN:ND2	2:B:314:ARG:O	0.53	2.41	1	1
3:C:693:ASP:OD2	3:C:695:THR:N	0.53	2.42	10	1
3:C:603:ASP:OD1	3:C:604:LYS:N	0.53	2.42	2	1
1:A:72:ASP:O	1:A:91:ARG:NH2	0.52	2.41	5	1
1:A:164:GLN:OE1	1:A:167:ASN:ND2	0.52	2.42	3	1
3:C:668:HIS:ND1	3:C:668:HIS:O	0.52	2.43	3	1
2:B:408:ARG:CD	2:B:408:ARG:C	0.52	2.78	8	1
2:B:439:ASP:OD1	2:B:441:SER:OG	0.52	2.26	8	1
2:B:475:LEU:HD23	2:B:532:TYR:CD2	0.52	2.40	2	5
2:B:450:SER:OG	2:B:452:HIS:NE2	0.52	2.43	1	2
1:A:182:THR:O	1:A:182:THR:HG23	0.52	2.03	7	1
2:B:458:GLU:OE2	2:B:509:HIS:NE2	0.52	2.42	9	1
1:A:173:TRP:CZ3	2:B:544:ARG:CZ	0.52	2.92	9	1
1:A:206:LEU:HD23	1:A:206:LEU:C	0.52	2.23	5	2
2:B:350:ALA:CB	2:B:359:TYR:CE2	0.52	2.92	1	2
1:A:237:ASN:ND2	2:B:546:ILE:CD1	0.52	2.73	1	1
3:C:651:LEU:H	3:C:651:LEU:HD22	0.52	1.60	7	2
1:A:252:ASP:OD1	1:A:252:ASP:C	0.52	2.47	6	1
3:C:686:LEU:N	3:C:686:LEU:CD2	0.52	2.72	5	1
1:A:168:PHE:O	1:A:169:TRP:CB	0.52	2.55	8	8
3:C:680:HIS:O	3:C:681:VAL:CG2	0.52	2.57	7	5
2:B:525:ARG:NH1	2:B:525:ARG:CG	0.52	2.72	9	3
3:C:659:ALA:C	3:C:661:ILE:N	0.52	2.63	3	10
1:A:92:ASN:ND2	1:A:92:ASN:O	0.52	2.43	3	3
1:A:71:ASP:O	1:A:73:GLN:NE2	0.52	2.43	1	1
1:A:91:ARG:CZ	1:A:141:CYS:O	0.52	2.58	6	1
1:A:125:ASP:CG	1:A:143:VAL:HB	0.52	2.24	2	1
2:B:569:ARG:CG	2:B:569:ARG:NH1	0.52	2.71	2	2
1:A:129:ARG:CG	1:A:129:ARG:NH1	0.52	2.72	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:GLN:N	1:A:187:GLN:OE1	0.52	2.42	5	1
1:A:172:ARG:NH1	1:A:174:ARG:CZ	0.52	2.72	10	1
2:B:491:GLY:O	2:B:492:SER:HB2	0.52	2.04	10	3
1:A:271:TRP:CZ2	2:B:514:GLY:CA	0.52	2.93	7	2
1:A:184:PRO:C	1:A:185:THR:OG1	0.52	2.47	7	1
3:C:674:SER:O	3:C:678:GLU:CG	0.52	2.58	6	2
2:B:442:LYS:NZ	3:C:677:TYR:O	0.52	2.42	1	1
1:A:86:ARG:HH11	1:A:86:ARG:HG2	0.52	1.63	7	2
1:A:99:ASP:OD2	1:A:102:ARG:NH2	0.52	2.42	6	1
1:A:195:GLN:HE21	1:A:205:GLN:NE2	0.52	2.03	9	1
1:A:232:ILE:CG1	1:A:233:GLU:N	0.52	2.72	9	1
1:A:260:ARG:NH1	3:C:633:GLU:CD	0.52	2.64	9	1
1:A:93:LYS:CE	1:A:121:ARG:HH12	0.52	2.17	4	1
1:A:93:LYS:CE	1:A:121:ARG:HH22	0.52	2.17	4	1
3:C:647:GLN:O	3:C:648:LEU:HB2	0.52	2.05	6	8
1:A:221:ASP:N	1:A:221:ASP:OD1	0.52	2.43	7	2
2:B:449:ASP:OD2	2:B:476:TRP:NE1	0.52	2.42	3	2
1:A:167:ASN:O	1:A:168:PHE:HB2	0.52	2.05	1	6
3:C:718:GLN:NE2	3:C:718:GLN:OXT	0.52	2.43	10	1
3:C:640:HIS:CE1	3:C:674:SER:OG	0.52	2.63	6	1
3:C:693:ASP:OD1	3:C:693:ASP:N	0.52	2.40	9	1
2:B:362:CYS:H	2:B:365:ASN:ND2	0.52	2.02	4	1
2:B:478:GLN:NE2	2:B:488:ASN:OD1	0.52	2.43	4	1
3:C:693:ASP:N	3:C:693:ASP:OD1	0.52	2.42	5	1
1:A:161:HIS:O	1:A:162:GLN:NE2	0.52	2.43	8	10
2:B:309:ALA:HB1	2:B:328:LEU:HD21	0.52	1.82	3	10
1:A:70:TYR:C	1:A:72:ASP:N	0.52	2.64	3	10
1:A:259:ARG:HH22	2:B:521:GLU:CA	0.52	2.18	8	1
2:B:439:ASP:OD2	2:B:441:SER:OG	0.52	2.27	8	1
2:B:366:ARG:NH1	2:B:371:TYR:OH	0.52	2.43	7	1
1:A:70:TYR:CD2	1:A:94:ILE:CD1	0.52	2.93	9	1
1:A:74:VAL:CG2	1:A:75:LEU:N	0.51	2.73	7	10
1:A:129:ARG:C	1:A:129:ARG:NE	0.51	2.64	7	1
1:A:121:ARG:NH2	1:A:145:GLY:H	0.51	2.03	2	1
1:A:254:THR:OG1	2:B:444:ILE:CD1	0.51	2.59	2	1
3:C:607:MET:CE	3:C:633:GLU:OE2	0.51	2.58	5	2
1:A:28:GLU:OE2	2:B:315:ARG:NH2	0.51	2.43	1	1
3:C:601:MET:N	3:C:601:MET:SD	0.51	2.84	1	3
3:C:715:ALA:O	3:C:716:LEU:HG	0.51	2.05	1	1
2:B:458:GLU:CD	2:B:459:LYS:N	0.51	2.63	10	1
1:A:169:TRP:CD1	2:B:535:LYS:NZ	0.51	2.76	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:O	1:A:82:LEU:HD13	0.51	2.05	3	1
3:C:677:TYR:O	3:C:677:TYR:HD1	0.51	1.89	2	1
2:B:463:ARG:NH1	2:B:463:ARG:CG	0.51	2.68	9	1
3:C:686:LEU:N	3:C:686:LEU:HD22	0.51	2.20	5	1
1:A:279:ILE:CG2	1:A:279:ILE:O	0.51	2.58	1	2
1:A:174:ARG:C	1:A:175:SER:HG	0.51	2.09	10	1
2:B:407:TYR:O	2:B:411:TYR:CD1	0.51	2.64	10	1
1:A:271:TRP:CZ2	2:B:514:GLY:C	0.51	2.84	7	2
1:A:260:ARG:CG	2:B:411:TYR:O	0.51	2.59	9	2
1:A:247:TYR:O	1:A:251:SER:OG	0.51	2.19	2	1
1:A:173:TRP:CD1	1:A:174:ARG:N	0.51	2.79	5	8
1:A:149:ASP:OD2	1:A:149:ASP:O	0.51	2.28	3	1
3:C:651:LEU:CD2	3:C:652:GLU:N	0.51	2.71	9	8
2:B:408:ARG:NE	2:B:414:GLY:O	0.51	2.43	6	2
3:C:688:LEU:CD1	3:C:691:GLY:O	0.51	2.58	7	1
1:A:173:TRP:CH2	2:B:544:ARG:NH1	0.51	2.79	9	1
1:A:237:ASN:O	1:A:241:THR:HG23	0.51	2.04	5	2
1:A:253:THR:HG22	1:A:254:THR:N	0.51	2.21	5	8
3:C:646:GLY:C	3:C:648:LEU:H	0.51	2.09	4	10
1:A:62:PHE:N	1:A:62:PHE:CD1	0.51	2.78	8	2
2:B:372:ARG:HH11	2:B:372:ARG:CG	0.51	2.18	1	1
3:C:625:GLY:O	3:C:626:GLU:O	0.51	2.29	2	10
3:C:631:THR:O	3:C:632:LEU:C	0.51	2.49	10	10
1:A:61:GLN:NE2	1:A:174:ARG:HH21	0.51	2.03	1	2
3:C:717:LEU:CG	3:C:718:GLN:N	0.51	2.73	1	2
3:C:618:VAL:CG1	3:C:654:LEU:HD21	0.51	2.36	10	1
1:A:275:LEU:O	1:A:276:SER:HB2	0.51	2.05	2	2
2:B:496:GLN:NE2	2:B:496:GLN:H	0.51	2.03	2	1
3:C:621:TYR:CE2	3:C:627:ASP:OD2	0.51	2.63	2	1
2:B:496:GLN:CD	2:B:496:GLN:H	0.51	2.07	9	1
3:C:646:GLY:C	3:C:648:LEU:N	0.51	2.64	8	10
1:A:96:PHE:HA	1:A:108:PRO:HA	0.51	1.83	10	10
1:A:226:LYS:HG3	1:A:227:GLU:N	0.51	2.20	6	1
3:C:674:SER:HA	3:C:677:TYR:CE2	0.51	2.40	2	1
3:C:633:GLU:OE1	3:C:636:ARG:NH2	0.51	2.44	3	1
1:A:279:ILE:CD1	1:A:279:ILE:N	0.51	2.73	1	1
2:B:498:GLU:OE1	2:B:498:GLU:N	0.51	2.44	10	1
2:B:493:LEU:CD2	2:B:493:LEU:N	0.51	2.73	2	1
3:C:601:MET:SD	3:C:601:MET:N	0.51	2.84	9	2
1:A:90:PRO:CG	1:A:143:VAL:O	0.51	2.59	5	8
1:A:220:SER:O	1:A:224:THR:CG2	0.51	2.59	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:372:ARG:HB2	2:B:379:TYR:CZ	0.51	2.41	9	6
2:B:439:ASP:O	2:B:442:LYS:CG	0.51	2.59	3	1
1:A:167:ASN:OD1	1:A:169:TRP:CD1	0.51	2.64	7	1
1:A:136:TYR:OH	1:A:173:TRP:NE1	0.50	2.44	10	4
3:C:655:LEU:HD23	3:C:656:LEU:N	0.50	2.20	3	2
2:B:372:ARG:NH1	2:B:372:ARG:CG	0.50	2.73	1	1
2:B:470:THR:CG2	2:B:470:THR:O	0.50	2.59	10	1
2:B:364:TYR:O	2:B:420:TYR:CE2	0.50	2.64	7	1
1:A:196:VAL:O	1:A:205:GLN:CG	0.50	2.60	4	4
1:A:240:GLN:NE2	2:B:546:ILE:HD11	0.50	2.21	4	1
1:A:86:ARG:HG2	1:A:86:ARG:HH11	0.50	1.66	5	1
1:A:237:ASN:ND2	1:A:237:ASN:C	0.50	2.63	1	1
3:C:630:ARG:HH11	3:C:630:ARG:CB	0.50	2.19	1	1
1:A:266:ARG:C	1:A:267:THR:OG1	0.50	2.50	6	2
1:A:121:ARG:HD2	1:A:122:ASP:N	0.50	2.21	9	4
3:C:644:ASP:O	3:C:645:CYS:SG	0.50	2.69	10	2
1:A:237:ASN:ND2	2:B:546:ILE:HD12	0.50	2.22	1	1
2:B:550:PRO:O	2:B:552:ASN:ND2	0.50	2.44	1	1
3:C:645:CYS:O	3:C:645:CYS:SG	0.50	2.70	1	2
1:A:134:ASP:O	1:A:135:HIS:CD2	0.50	2.64	7	2
2:B:380:ASP:CB	2:B:381:PRO:CD	0.50	2.90	6	10
1:A:246:ASN:HD21	2:B:484:SER:CB	0.50	2.19	8	2
1:A:274:ILE:CD1	1:A:274:ILE:N	0.50	2.74	1	1
2:B:546:ILE:HG23	2:B:547:ASP:N	0.50	2.21	7	3
1:A:169:TRP:C	1:A:169:TRP:CE3	0.50	2.85	9	3
1:A:61:GLN:NE2	1:A:61:GLN:O	0.50	2.44	10	1
1:A:195:GLN:NE2	1:A:205:GLN:OE1	0.50	2.45	7	1
2:B:352:ASP:N	2:B:357:LYS:O	0.50	2.45	2	10
1:A:70:TYR:O	1:A:72:ASP:OD1	0.50	2.29	3	1
2:B:372:ARG:NH2	2:B:397:GLU:OE1	0.50	2.41	8	2
3:C:705:LEU:C	3:C:705:LEU:HD23	0.50	2.26	2	2
2:B:363:ASP:OD1	2:B:364:TYR:CE1	0.50	2.65	7	1
2:B:472:THR:HG22	2:B:472:THR:O	0.50	2.06	7	1
1:A:269:ILE:CG2	1:A:270:ASP:N	0.50	2.75	3	3
3:C:668:HIS:CG	3:C:668:HIS:O	0.50	2.61	8	2
1:A:200:GLU:O	1:A:201:ASP:OD1	0.50	2.29	10	1
1:A:169:TRP:O	1:A:169:TRP:CG	0.50	2.65	2	4
1:A:251:SER:OG	2:B:533:PHE:CB	0.50	2.60	2	1
3:C:644:ASP:OD2	3:C:678:GLU:OE2	0.50	2.29	5	2
3:C:614:ASP:O	3:C:617:GLU:N	0.50	2.41	3	10
3:C:630:ARG:HH11	3:C:630:ARG:CG	0.50	2.20	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:637:LYS:H	3:C:637:LYS:CD	0.50	2.19	6	2
1:A:200:GLU:O	1:A:201:ASP:HB3	0.50	2.04	2	3
1:A:272:ASN:HD22	1:A:272:ASN:H	0.50	1.50	2	1
3:C:646:GLY:O	3:C:648:LEU:N	0.50	2.45	6	10
2:B:407:TYR:C	2:B:407:TYR:CD1	0.50	2.85	6	3
1:A:173:TRP:CH2	1:A:236:GLU:OE1	0.50	2.65	3	1
1:A:59:MET:SD	1:A:77:THR:HA	0.50	2.47	10	1
2:B:525:ARG:HH11	2:B:525:ARG:HG2	0.50	1.67	7	1
3:C:702:LEU:HG	3:C:703:THR:N	0.50	2.21	7	2
1:A:67:ILE:CD1	1:A:67:ILE:N	0.50	2.75	9	1
3:C:636:ARG:NH1	3:C:641:TYR:OH	0.49	2.45	5	1
1:A:54:PHE:CG	1:A:100:HIS:CB	0.49	2.95	8	6
2:B:464:THR:HG23	2:B:464:THR:O	0.49	2.06	3	2
1:A:65:VAL:CG2	1:A:66:LYS:N	0.49	2.75	1	9
2:B:379:TYR:CE1	2:B:386:GLY:HA3	0.49	2.41	1	1
1:A:201:ASP:OD2	2:B:493:LEU:HD11	0.49	2.07	10	1
1:A:134:ASP:C	1:A:135:HIS:CD2	0.49	2.85	7	1
2:B:525:ARG:CG	2:B:525:ARG:NH1	0.49	2.73	7	2
1:A:90:PRO:HG2	1:A:143:VAL:O	0.49	2.08	9	2
1:A:169:TRP:CG	1:A:169:TRP:O	0.49	2.65	5	6
1:A:62:PHE:CD1	1:A:62:PHE:N	0.49	2.79	5	4
1:A:186:ALA:O	1:A:215:SER:C	0.49	2.50	10	10
2:B:315:ARG:HH11	2:B:315:ARG:HG2	0.49	1.67	1	3
2:B:407:TYR:CE2	2:B:411:TYR:CZ	0.49	3.00	10	1
1:A:104:GLU:N	1:A:104:GLU:OE1	0.49	2.45	8	1
3:C:716:LEU:O	3:C:717:LEU:CD1	0.49	2.61	8	3
2:B:393:LEU:CD2	2:B:393:LEU:N	0.49	2.76	7	2
1:A:259:ARG:CZ	2:B:448:TRP:CH2	0.49	2.95	7	1
1:A:278:LYS:C	1:A:280:GLY:H	0.49	2.11	5	10
2:B:498:GLU:CD	2:B:498:GLU:N	0.49	2.65	2	2
2:B:525:ARG:HG2	2:B:525:ARG:HH11	0.49	1.67	2	3
3:C:610:LEU:HD21	3:C:618:VAL:HG11	0.49	1.84	8	1
3:C:654:LEU:O	3:C:654:LEU:CD2	0.49	2.50	6	1
3:C:708:THR:HG22	3:C:709:ASP:H	0.49	1.67	8	4
3:C:630:ARG:CG	3:C:630:ARG:NH1	0.49	2.75	1	1
1:A:259:ARG:NH1	2:B:448:TRP:CH2	0.49	2.81	7	1
3:C:642:ALA:C	3:C:651:LEU:HD12	0.49	2.28	2	4
1:A:217:GLN:CD	1:A:217:GLN:N	0.49	2.66	4	1
2:B:406:GLN:O	2:B:410:LEU:HD13	0.49	2.08	4	1
2:B:469:LEU:HG	2:B:470:THR:N	0.49	2.22	5	6
1:A:31:GLU:OE1	2:B:315:ARG:NH2	0.49	2.44	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:464:THR:O	2:B:464:THR:HG23	0.49	2.06	8	2
3:C:615:LEU:CD1	3:C:615:LEU:O	0.49	2.52	2	1
1:A:252:ASP:C	1:A:252:ASP:OD1	0.49	2.51	2	2
3:C:704:ALA:HB3	3:C:717:LEU:HD23	0.49	1.82	3	1
2:B:372:ARG:CB	2:B:372:ARG:CZ	0.49	2.88	1	1
2:B:478:GLN:CG	2:B:488:ASN:ND2	0.49	2.76	1	1
1:A:8:VAL:CG1	1:A:8:VAL:O	0.49	2.59	4	5
3:C:673:LEU:HD21	3:C:703:THR:HA	0.49	1.83	9	1
1:A:187:GLN:C	1:A:214:ASP:O	0.49	2.51	5	10
3:C:692:ALA:O	3:C:693:ASP:C	0.49	2.51	5	10
3:C:636:ARG:NH2	3:C:640:HIS:CD2	0.49	2.80	10	2
2:B:442:LYS:CB	2:B:442:LYS:NZ	0.49	2.76	3	1
1:A:195:GLN:HE21	1:A:205:GLN:HE21	0.49	1.51	9	1
2:B:442:LYS:NZ	3:C:644:ASP:OD1	0.49	2.46	9	1
2:B:569:ARG:O	2:B:570:GLN:CG	0.49	2.61	9	1
3:C:653:PHE:CD2	3:C:654:LEU:N	0.49	2.80	9	1
2:B:311:ASP:OD1	2:B:315:ARG:NH1	0.49	2.46	4	1
2:B:406:GLN:OE1	2:B:406:GLN:N	0.49	2.45	4	1
1:A:177:TRP:HA	1:A:190:ALA:HB2	0.49	1.85	3	10
2:B:498:GLU:N	2:B:498:GLU:CD	0.49	2.65	7	2
1:A:230:LYS:O	1:A:234:ASN:ND2	0.49	2.45	8	1
2:B:309:ALA:O	2:B:313:MET:SD	0.49	2.71	2	1
2:B:313:MET:SD	2:B:328:LEU:HD22	0.49	2.47	2	1
1:A:205:GLN:OE1	1:A:207:VAL:CG2	0.49	2.61	9	2
1:A:201:ASP:O	1:A:201:ASP:OD1	0.49	2.31	4	2
1:A:186:ALA:O	1:A:216:VAL:C	0.48	2.48	5	10
1:A:278:LYS:C	1:A:280:GLY:N	0.48	2.67	8	10
3:C:615:LEU:HD22	3:C:618:VAL:CG1	0.48	2.38	4	5
1:A:67:ILE:CD1	1:A:94:ILE:HD11	0.48	2.38	7	1
3:C:688:LEU:HD13	3:C:693:ASP:O	0.48	2.08	7	1
1:A:92:ASN:N	1:A:92:ASN:ND2	0.48	2.57	9	1
2:B:561:GLU:O	2:B:564:GLN:HG2	0.48	2.08	3	5
1:A:80:GLY:O	1:A:87:PHE:HA	0.48	2.08	4	10
1:A:118:LYS:HZ2	1:A:121:ARG:NH2	0.48	2.05	3	1
1:A:88:LEU:CD1	1:A:144:TYR:OH	0.48	2.62	10	1
1:A:27:GLY:C	1:A:28:GLU:OE1	0.48	2.52	10	2
3:C:615:LEU:C	3:C:615:LEU:CD1	0.48	2.80	9	3
2:B:442:LYS:NZ	3:C:644:ASP:CG	0.48	2.67	9	1
2:B:405:ASP:O	2:B:408:ARG:NH1	0.48	2.46	5	1
2:B:469:LEU:CG	2:B:470:THR:N	0.48	2.77	5	6
2:B:478:GLN:OE1	2:B:487:MET:O	0.48	2.31	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:664:PRO:O	3:C:697:LYS:CE	0.48	2.62	5	1
1:A:80:GLY:O	1:A:88:LEU:N	0.48	2.47	1	10
1:A:55:ALA:O	1:A:56:GLN:C	0.48	2.52	9	10
3:C:700:ASP:CG	3:C:701:GLY:H	0.48	2.10	3	7
1:A:70:TYR:O	1:A:71:ASP:OD1	0.48	2.31	1	1
3:C:618:VAL:HG11	3:C:654:LEU:HD11	0.48	1.85	10	1
1:A:255:PHE:CZ	2:B:529:ASN:ND2	0.48	2.81	2	1
2:B:365:ASN:HB3	2:B:420:TYR:CD2	0.48	2.43	9	1
2:B:434:ILE:HG23	2:B:436:LYS:NZ	0.48	2.23	5	1
3:C:717:LEU:O	3:C:718:GLN:HB2	0.48	2.09	2	7
1:A:191:VAL:HG23	1:A:211:ASP:OD1	0.48	2.08	10	6
1:A:245:GLU:OE2	3:C:677:TYR:CE1	0.48	2.66	1	1
1:A:91:ARG:NE	1:A:129:ARG:NH2	0.48	2.60	1	1
3:C:628:VAL:CG2	3:C:628:VAL:O	0.48	2.58	1	1
3:C:715:ALA:C	3:C:716:LEU:HD12	0.48	2.29	1	1
3:C:671:PRO:O	3:C:674:SER:OG	0.48	2.26	10	4
3:C:651:LEU:HD22	3:C:652:GLU:N	0.48	2.21	9	4
2:B:335:LEU:O	2:B:339:LEU:CG	0.48	2.62	1	10
1:A:246:ASN:ND2	2:B:484:SER:OG	0.48	2.46	8	2
1:A:41:ASN:O	1:A:42:ASN:CG	0.48	2.51	7	7
1:A:72:ASP:OD2	1:A:89:ASP:OD2	0.48	2.32	7	4
2:B:452:HIS:CE1	2:B:471:SER:HG	0.48	2.21	8	1
1:A:169:TRP:CE3	1:A:169:TRP:C	0.48	2.87	2	2
3:C:672:LEU:C	3:C:672:LEU:CD2	0.48	2.82	2	1
3:C:661:ILE:CD1	3:C:687:LEU:HD11	0.48	2.39	2	1
3:C:673:LEU:N	3:C:673:LEU:HD12	0.48	2.23	7	2
2:B:431:VAL:HG13	2:B:431:VAL:O	0.48	2.09	10	2
3:C:655:LEU:CD2	3:C:655:LEU:C	0.48	2.78	3	2
1:A:262:LEU:CD1	1:A:262:LEU:O	0.48	2.62	10	1
2:B:407:TYR:CD2	2:B:411:TYR:CE1	0.48	3.01	10	1
1:A:61:GLN:CD	1:A:172:ARG:NH2	0.48	2.66	6	2
1:A:201:ASP:OD1	1:A:201:ASP:O	0.48	2.32	7	1
1:A:252:ASP:OD1	1:A:252:ASP:O	0.48	2.32	6	2
3:C:661:ILE:O	3:C:661:ILE:HG23	0.48	2.07	9	3
2:B:442:LYS:NZ	3:C:645:CYS:SG	0.48	2.86	2	1
1:A:233:GLU:O	1:A:236:GLU:HG3	0.48	2.08	9	1
2:B:442:LYS:HZ3	3:C:678:GLU:HG2	0.48	1.69	9	1
1:A:129:ARG:NH2	1:A:130:ALA:HB2	0.48	2.23	3	3
2:B:481:LYS:O	2:B:485:GLY:CA	0.48	2.62	3	10
1:A:54:PHE:CG	1:A:100:HIS:HB2	0.48	2.44	8	6
1:A:237:ASN:OD1	2:B:546:ILE:CD1	0.48	2.62	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:408:ARG:O	2:B:412:PHE:HB2	0.48	2.09	8	5
2:B:554:LYS:HG3	2:B:555:TYR:H	0.48	1.69	2	1
2:B:418:SER:CB	2:B:420:TYR:OH	0.48	2.62	9	1
2:B:443:LYS:CD	2:B:443:LYS:N	0.48	2.77	4	1
3:C:644:ASP:OD1	3:C:644:ASP:C	0.48	2.51	5	1
3:C:614:ASP:O	3:C:616:ASP:N	0.48	2.47	1	10
3:C:610:LEU:CD2	3:C:638:PRO:O	0.48	2.61	10	3
1:A:169:TRP:CD2	1:A:169:TRP:C	0.48	2.87	9	6
1:A:213:GLN:CD	1:A:213:GLN:N	0.48	2.67	1	1
3:C:654:LEU:CD2	3:C:654:LEU:H	0.48	2.09	7	3
2:B:434:ILE:HB	2:B:450:SER:OG	0.48	2.09	8	2
3:C:716:LEU:O	3:C:717:LEU:HD12	0.48	2.09	7	1
2:B:409:ASP:O	2:B:409:ASP:OD1	0.48	2.32	6	1
1:A:125:ASP:OD1	1:A:143:VAL:HG11	0.48	2.09	2	1
1:A:70:TYR:CZ	1:A:92:ASN:CG	0.48	2.87	8	4
2:B:370:SER:CA	2:B:381:PRO:HG2	0.48	2.39	4	10
2:B:319:GLN:NE2	2:B:488:ASN:CG	0.48	2.67	3	2
2:B:366:ARG:CZ	2:B:371:TYR:OH	0.48	2.62	7	2
2:B:448:TRP:CZ2	2:B:473:VAL:HG11	0.48	2.44	9	2
1:A:177:TRP:CE2	1:A:232:ILE:HG23	0.48	2.44	10	1
1:A:101:LEU:N	1:A:101:LEU:CD2	0.48	2.76	7	1
3:C:628:VAL:O	3:C:628:VAL:CG2	0.48	2.58	2	1
2:B:364:TYR:CG	2:B:431:VAL:HG21	0.48	2.43	9	1
2:B:491:GLY:O	2:B:492:SER:CB	0.48	2.62	3	10
2:B:420:TYR:O	2:B:430:GLY:HA2	0.48	2.09	6	10
1:A:192:LEU:CD2	1:A:236:GLU:OE1	0.48	2.62	3	1
1:A:136:TYR:CE1	1:A:173:TRP:CD1	0.48	3.02	9	2
2:B:315:ARG:HH11	2:B:315:ARG:CG	0.48	2.22	1	2
3:C:673:LEU:HD12	3:C:673:LEU:N	0.48	2.24	10	1
2:B:448:TRP:CZ2	2:B:473:VAL:HG21	0.48	2.44	2	1
1:A:203:ASN:C	1:A:203:ASN:ND2	0.48	2.67	9	1
1:A:236:GLU:CG	1:A:237:ASN:N	0.48	2.77	9	1
2:B:478:GLN:NE2	2:B:488:ASN:CG	0.47	2.67	5	1
1:A:101:LEU:N	1:A:101:LEU:HD12	0.47	2.24	3	1
3:C:672:LEU:CD1	3:C:692:ALA:HB1	0.47	2.39	3	1
2:B:569:ARG:HH11	2:B:569:ARG:HG2	0.47	1.69	2	2
1:A:100:HIS:H	1:A:100:HIS:CD2	0.47	2.27	7	1
3:C:672:LEU:CD1	3:C:684:VAL:HG13	0.47	2.40	5	1
3:C:625:GLY:O	3:C:626:GLU:C	0.47	2.53	6	10
1:A:198:TYR:OH	1:A:200:GLU:OE1	0.47	2.32	10	6
1:A:164:GLN:CB	1:A:169:TRP:CZ2	0.47	2.97	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:388:MET:O	2:B:388:MET:SD	0.47	2.73	7	1
2:B:442:LYS:CE	3:C:644:ASP:OD2	0.47	2.62	6	1
3:C:644:ASP:OD1	3:C:678:GLU:OE1	0.47	2.31	6	1
3:C:621:TYR:CE2	3:C:627:ASP:CG	0.47	2.88	2	1
3:C:614:ASP:C	3:C:616:ASP:N	0.47	2.68	5	10
1:A:73:GLN:CD	1:A:73:GLN:N	0.47	2.67	1	1
1:A:199:TYR:CD1	1:A:199:TYR:C	0.47	2.88	10	2
2:B:478:GLN:OE1	2:B:488:ASN:CG	0.47	2.52	9	1
3:C:639:LEU:HD23	3:C:639:LEU:O	0.47	2.09	5	2
2:B:439:ASP:CG	3:C:611:LYS:NZ	0.47	2.67	1	1
1:A:273:LYS:O	1:A:273:LYS:CG	0.47	2.61	5	1
1:A:275:LEU:O	1:A:276:SER:HB3	0.47	2.10	5	6
3:C:713:ILE:O	3:C:716:LEU:CD2	0.47	2.63	5	1
1:A:197:HIS:CE1	1:A:199:TYR:CD1	0.47	3.03	8	4
1:A:61:GLN:CD	1:A:174:ARG:NH2	0.47	2.67	1	2
3:C:627:ASP:OD1	3:C:627:ASP:O	0.47	2.32	2	2
1:A:77:THR:OG1	1:A:78:GLU:N	0.47	2.48	7	1
1:A:121:ARG:O	1:A:125:ASP:OD1	0.47	2.31	2	1
1:A:192:LEU:HD22	1:A:236:GLU:OE1	0.47	2.09	4	1
1:A:70:TYR:CZ	1:A:92:ASN:ND2	0.47	2.83	8	4
2:B:393:LEU:N	2:B:393:LEU:CD2	0.47	2.78	1	2
2:B:478:GLN:CD	2:B:479:THR:N	0.47	2.68	1	2
3:C:615:LEU:HD22	3:C:618:VAL:HG23	0.47	1.85	8	1
3:C:713:ILE:O	3:C:716:LEU:HD21	0.47	2.10	5	1
1:A:247:TYR:HH	2:B:536:THR:CB	0.47	2.21	5	2
1:A:95:SER:O	1:A:108:PRO:C	0.47	2.53	5	10
1:A:248:GLN:O	1:A:252:ASP:CG	0.47	2.53	2	2
1:A:199:TYR:C	1:A:199:TYR:CD1	0.47	2.88	1	4
1:A:79:HIS:O	1:A:144:TYR:CZ	0.47	2.67	10	1
3:C:648:LEU:CD2	3:C:682:SER:OG	0.47	2.63	10	1
3:C:665:ASP:OD1	3:C:665:ASP:N	0.47	2.47	9	3
1:A:101:LEU:N	1:A:101:LEU:HD22	0.47	2.22	7	1
1:A:89:ASP:CB	1:A:94:ILE:HD13	0.47	2.40	7	1
3:C:674:SER:HA	3:C:677:TYR:CZ	0.47	2.44	2	1
1:A:121:ARG:CG	1:A:125:ASP:OD2	0.47	2.62	2	1
1:A:161:HIS:HB2	1:A:171:GLY:O	0.47	2.09	4	10
2:B:315:ARG:NH1	2:B:315:ARG:CG	0.47	2.76	1	2
3:C:717:LEU:HD23	3:C:718:GLN:N	0.47	2.24	1	2
1:A:265:THR:HG22	1:A:265:THR:O	0.47	2.10	10	2
2:B:487:MET:C	2:B:488:ASN:HD22	0.47	2.13	7	2
2:B:449:ASP:OD1	2:B:474:MET:O	0.47	2.33	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:272:ASN:ND2	2:B:506:SER:O	0.47	2.48	4	1
2:B:535:LYS:O	2:B:536:THR:C	0.47	2.53	8	10
2:B:362:CYS:O	2:B:365:ASN:OD1	0.47	2.32	2	8
1:A:221:ASP:OD1	1:A:221:ASP:N	0.47	2.45	3	3
3:C:713:ILE:CG2	3:C:714:LYS:N	0.47	2.78	3	1
1:A:75:LEU:CD1	1:A:75:LEU:N	0.47	2.78	2	2
2:B:422:TRP:CZ2	2:B:429:ALA:CB	0.47	2.97	4	3
1:A:260:ARG:O	2:B:411:TYR:CD1	0.47	2.68	8	8
1:A:259:ARG:HH22	2:B:521:GLU:C	0.47	2.13	8	1
3:C:638:PRO:O	3:C:654:LEU:CD1	0.47	2.62	4	2
2:B:563:SER:O	2:B:566:LEU:N	0.46	2.48	5	10
3:C:645:CYS:SG	3:C:645:CYS:O	0.46	2.72	5	3
2:B:358:ASP:O	2:B:358:ASP:OD1	0.46	2.33	4	2
3:C:654:LEU:HD13	3:C:654:LEU:N	0.46	2.23	6	3
3:C:627:ASP:O	3:C:627:ASP:OD1	0.46	2.32	7	1
3:C:607:MET:SD	3:C:633:GLU:OE2	0.46	2.74	7	2
2:B:362:CYS:SG	2:B:365:ASN:CG	0.46	2.93	10	8
2:B:408:ARG:CD	2:B:414:GLY:O	0.46	2.63	8	1
1:A:256:LYS:HZ1	3:C:636:ARG:HE	0.46	1.53	2	1
1:A:120:TRP:HB2	1:A:154:ILE:HD11	0.46	1.86	9	1
2:B:365:ASN:ND2	2:B:365:ASN:C	0.46	2.68	4	1
3:C:607:MET:HE2	3:C:633:GLU:OE2	0.46	2.10	5	1
1:A:133:LYS:CG	1:A:133:LYS:O	0.46	2.63	1	1
2:B:478:GLN:NE2	2:B:479:THR:C	0.46	2.69	1	1
2:B:508:PRO:O	2:B:512:ASN:ND2	0.46	2.48	1	1
3:C:667:HIS:N	3:C:667:HIS:ND1	0.46	2.64	1	1
1:A:70:TYR:CE2	1:A:94:ILE:CD1	0.46	2.98	9	1
1:A:86:ARG:NH1	1:A:86:ARG:CG	0.46	2.72	4	1
3:C:615:LEU:CD1	3:C:615:LEU:C	0.46	2.84	8	2
1:A:177:TRP:CD2	1:A:232:ILE:HG12	0.46	2.46	10	1
2:B:434:ILE:HB	2:B:450:SER:CB	0.46	2.41	8	3
2:B:570:GLN:CD	2:B:570:GLN:N	0.46	2.66	2	1
1:A:87:PHE:HB2	1:A:96:PHE:CZ	0.46	2.46	5	9
1:A:129:ARG:CD	1:A:129:ARG:C	0.46	2.83	3	1
1:A:95:SER:CB	1:A:109:GLN:O	0.46	2.63	5	10
1:A:169:TRP:CA	1:A:197:HIS:O	0.46	2.62	5	10
1:A:194:ILE:CG2	1:A:208:SER:HB3	0.46	2.41	1	1
1:A:273:LYS:C	1:A:274:ILE:HD12	0.46	2.29	1	1
2:B:478:GLN:CG	2:B:479:THR:N	0.46	2.79	9	4
2:B:315:ARG:HG2	2:B:315:ARG:HH11	0.46	1.70	9	5
2:B:463:ARG:HG2	2:B:463:ARG:HH11	0.46	1.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:609:ALA:HB3	3:C:618:VAL:HG13	0.46	1.87	5	3
1:A:8:VAL:O	1:A:8:VAL:CG1	0.46	2.61	9	3
1:A:209:HIS:CE1	2:B:486:THR:HG1	0.46	2.29	9	4
1:A:85:GLY:O	1:A:98:PHE:CE1	0.46	2.68	1	1
1:A:28:GLU:OE2	1:A:170:ASN:OD1	0.46	2.34	10	1
3:C:693:ASP:OD1	3:C:696:VAL:HG22	0.46	2.10	10	1
1:A:273:LYS:CG	1:A:273:LYS:O	0.46	2.60	7	1
1:A:117:LEU:O	1:A:117:LEU:CG	0.46	2.60	9	1
2:B:479:THR:HG23	2:B:479:THR:O	0.46	2.11	4	1
1:A:266:ARG:CG	1:A:266:ARG:O	0.46	2.62	5	1
3:C:661:ILE:HG13	3:C:661:ILE:O	0.46	2.11	1	2
2:B:487:MET:CG	2:B:487:MET:O	0.46	2.63	3	1
2:B:425:ASP:OD1	2:B:425:ASP:N	0.46	2.47	1	1
2:B:458:GLU:OE1	2:B:459:LYS:N	0.46	2.48	10	1
2:B:525:ARG:HG3	2:B:526:SER:N	0.46	2.25	10	5
1:A:259:ARG:NH2	2:B:521:GLU:HB3	0.46	2.25	7	1
1:A:94:ILE:C	1:A:111:GLU:OE1	0.46	2.53	7	1
1:A:121:ARG:C	1:A:125:ASP:OD1	0.46	2.54	2	1
1:A:121:ARG:CG	1:A:125:ASP:OD1	0.46	2.63	2	1
1:A:236:GLU:OE1	1:A:236:GLU:C	0.46	2.53	9	1
1:A:247:TYR:OH	2:B:489:LEU:HD11	0.46	2.10	5	1
1:A:133:LYS:O	1:A:134:ASP:OD1	0.46	2.34	4	9
1:A:153:THR:HG23	1:A:179:PHE:O	0.46	2.10	4	3
1:A:173:TRP:CD1	1:A:173:TRP:C	0.46	2.90	6	3
1:A:181:ILE:C	1:A:181:ILE:HD12	0.46	2.32	10	1
1:A:259:ARG:HH22	2:B:521:GLU:CB	0.46	2.23	8	1
1:A:26:PRO:O	1:A:28:GLU:OE1	0.46	2.34	7	1
3:C:640:HIS:CE1	3:C:674:SER:HG	0.46	2.26	6	1
1:A:59:MET:C	1:A:59:MET:SD	0.46	2.93	9	1
2:B:365:ASN:CB	2:B:420:TYR:CD2	0.46	2.99	9	1
2:B:402:ASN:O	2:B:406:GLN:NE2	0.46	2.49	4	1
2:B:434:ILE:HG23	2:B:436:LYS:CE	0.46	2.41	5	1
3:C:609:ALA:CB	3:C:618:VAL:HG13	0.46	2.40	5	3
3:C:700:ASP:OD2	3:C:701:GLY:N	0.46	2.49	5	1
2:B:484:SER:O	2:B:486:THR:N	0.46	2.49	6	10
3:C:621:TYR:CZ	3:C:622:VAL:HB	0.46	2.46	8	2
2:B:431:VAL:CG1	2:B:431:VAL:O	0.46	2.64	10	1
1:A:57:TYR:O	1:A:60:ASP:OD1	0.46	2.32	6	1
1:A:184:PRO:O	1:A:185:THR:HB	0.46	2.11	2	1
2:B:496:GLN:CD	2:B:496:GLN:N	0.46	2.70	9	1
1:A:179:PHE:CD1	1:A:228:PHE:CE1	0.46	3.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:GLN:O	1:A:60:ASP:OD2	0.45	2.34	3	3
1:A:206:LEU:HD12	2:B:488:ASN:O	0.45	2.11	3	2
1:A:91:ARG:HE	1:A:129:ARG:NH2	0.45	2.08	1	1
2:B:379:TYR:CZ	2:B:386:GLY:CA	0.45	2.96	1	1
3:C:693:ASP:CG	3:C:694:LYS:H	0.45	2.14	10	2
3:C:661:ILE:CD1	3:C:692:ALA:HB2	0.45	2.41	6	3
1:A:59:MET:SD	1:A:60:ASP:OD1	0.45	2.74	9	1
2:B:462:GLY:C	2:B:464:THR:H	0.45	2.15	8	10
2:B:350:ALA:HB3	2:B:359:TYR:CE2	0.45	2.46	2	6
1:A:45:LEU:N	1:A:45:LEU:CD1	0.45	2.79	9	4
2:B:513:ILE:O	2:B:517:VAL:HG23	0.45	2.12	10	1
1:A:207:VAL:HG21	2:B:319:GLN:NE2	0.45	2.26	7	2
2:B:388:MET:C	2:B:388:MET:SD	0.45	2.95	7	1
2:B:546:ILE:CG2	2:B:547:ASP:N	0.45	2.79	7	1
3:C:640:HIS:ND1	3:C:674:SER:OG	0.45	2.46	6	1
1:A:198:TYR:CZ	1:A:200:GLU:HB3	0.45	2.45	2	2
1:A:13:LYS:CB	1:A:13:LYS:NZ	0.45	2.80	9	1
3:C:672:LEU:CD2	3:C:672:LEU:C	0.45	2.82	4	1
3:C:686:LEU:HD22	3:C:686:LEU:N	0.45	2.26	4	1
1:A:269:ILE:HG22	1:A:270:ASP:N	0.45	2.26	5	3
1:A:267:THR:HG23	1:A:267:THR:O	0.45	2.11	3	3
3:C:699:PRO:O	3:C:700:ASP:OD2	0.45	2.34	2	2
1:A:144:TYR:CE2	1:A:146:LYS:HB2	0.45	2.46	10	1
2:B:405:ASP:OD2	2:B:408:ARG:NH2	0.45	2.47	10	1
1:A:31:GLU:H	1:A:31:GLU:CD	0.45	2.15	8	1
1:A:256:LYS:HZ1	3:C:636:ARG:NE	0.45	2.07	2	1
2:B:564:GLN:O	2:B:564:GLN:OE1	0.45	2.35	9	1
3:C:607:MET:C	3:C:607:MET:SD	0.45	2.95	4	1
1:A:173:TRP:C	1:A:173:TRP:CD1	0.45	2.90	5	2
2:B:350:ALA:O	2:B:358:ASP:CA	0.45	2.64	5	10
3:C:654:LEU:HD23	3:C:654:LEU:N	0.45	2.27	5	1
1:A:136:TYR:CE1	2:B:544:ARG:HB2	0.45	2.46	7	4
1:A:80:GLY:O	1:A:87:PHE:CA	0.45	2.65	8	10
2:B:404:PHE:CZ	2:B:432:ILE:HD13	0.45	2.47	10	1
2:B:408:ARG:NE	2:B:415:GLY:O	0.45	2.48	6	1
2:B:484:SER:O	2:B:485:GLY:C	0.45	2.55	8	10
3:C:643:ALA:HB2	3:C:651:LEU:CD1	0.45	2.41	3	1
1:A:113:THR:OG1	1:A:118:LYS:CE	0.45	2.64	1	1
3:C:715:ALA:O	3:C:716:LEU:CG	0.45	2.65	1	1
1:A:112:ASP:O	1:A:112:ASP:OD1	0.45	2.35	10	4
1:A:167:ASN:OD1	1:A:167:ASN:O	0.45	2.35	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:552:ASN:OD1	2:B:552:ASN:O	0.45	2.35	10	3
3:C:692:ALA:C	3:C:693:ASP:OD1	0.45	2.55	10	1
1:A:45:LEU:N	1:A:45:LEU:HD12	0.45	2.27	9	3
1:A:279:ILE:O	1:A:279:ILE:CG2	0.45	2.64	7	3
2:B:393:LEU:N	2:B:393:LEU:HD22	0.45	2.26	7	1
1:A:71:ASP:N	1:A:71:ASP:OD1	0.45	2.50	2	1
2:B:409:ASP:OD1	3:C:604:LYS:NZ	0.45	2.49	9	1
3:C:686:LEU:CD2	3:C:686:LEU:N	0.45	2.79	4	1
1:A:88:LEU:HD23	1:A:89:ASP:N	0.45	2.23	5	1
1:A:107:ASP:N	1:A:108:PRO:CD	0.45	2.79	4	10
1:A:99:ASP:O	1:A:100:HIS:C	0.45	2.55	3	10
2:B:319:GLN:NE2	2:B:488:ASN:OD1	0.45	2.49	3	2
3:C:661:ILE:O	3:C:661:ILE:HG13	0.45	2.12	10	1
1:A:194:ILE:CD1	1:A:195:GLN:N	0.45	2.79	2	1
3:C:628:VAL:O	3:C:660:ASP:OD2	0.45	2.35	5	1
3:C:616:ASP:OD1	3:C:616:ASP:N	0.45	2.45	3	1
1:A:45:LEU:HD12	1:A:45:LEU:N	0.45	2.27	1	3
2:B:489:LEU:O	2:B:489:LEU:HG	0.45	2.11	9	3
1:A:260:ARG:HB2	2:B:411:TYR:O	0.45	2.12	2	1
2:B:315:ARG:CG	2:B:315:ARG:NH1	0.45	2.79	9	1
1:A:129:ARG:C	1:A:129:ARG:CD	0.45	2.84	5	3
2:B:412:PHE:CG	2:B:436:LYS:CE	0.45	3.00	5	1
2:B:472:THR:HG23	2:B:494:THR:OG1	0.45	2.12	5	6
3:C:662:ASN:O	3:C:697:LYS:NZ	0.45	2.47	5	1
1:A:249:THR:O	1:A:253:THR:HB	0.45	2.12	8	9
1:A:75:LEU:HD21	1:A:140:PHE:HB2	0.45	1.88	10	5
1:A:129:ARG:HH11	1:A:129:ARG:HG2	0.45	1.72	8	3
1:A:237:ASN:C	1:A:237:ASN:HD22	0.45	2.13	3	1
2:B:348:LYS:O	2:B:361:LEU:HD12	0.45	2.11	1	1
1:A:269:ILE:CG1	1:A:270:ASP:N	0.45	2.79	10	4
1:A:240:GLN:CB	2:B:544:ARG:NH2	0.45	2.80	10	1
1:A:45:LEU:CD1	1:A:45:LEU:N	0.45	2.80	2	2
1:A:274:ILE:O	1:A:274:ILE:CD1	0.45	2.56	7	1
3:C:638:PRO:O	3:C:654:LEU:HD22	0.45	2.12	9	1
3:C:630:ARG:HG2	3:C:630:ARG:HH11	0.45	1.71	4	1
1:A:237:ASN:OD1	2:B:544:ARG:NH2	0.45	2.50	8	4
1:A:153:THR:HG1	1:A:180:THR:HA	0.45	1.70	3	1
3:C:644:ASP:OD2	3:C:678:GLU:OE1	0.45	2.35	1	2
1:A:180:THR:O	1:A:181:ILE:CG2	0.45	2.65	10	1
3:C:644:ASP:OD1	3:C:678:GLU:OE2	0.45	2.35	4	2
1:A:41:ASN:O	1:A:42:ASN:ND2	0.45	2.50	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:370:SER:CB	2:B:381:PRO:HD2	0.45	2.31	7	1
1:A:92:ASN:O	1:A:92:ASN:ND2	0.45	2.50	6	1
2:B:479:THR:O	2:B:479:THR:HG23	0.45	2.11	6	1
1:A:60:ASP:O	1:A:174:ARG:NH1	0.45	2.49	2	1
2:B:547:ASP:O	2:B:547:ASP:OD1	0.45	2.35	2	1
1:A:232:ILE:HG13	1:A:233:GLU:N	0.45	2.26	9	1
1:A:259:ARG:CD	2:B:448:TRP:CH2	0.45	3.00	9	1
1:A:270:ASP:O	1:A:272:ASN:N	0.45	2.50	5	10
1:A:278:LYS:O	1:A:280:GLY:N	0.45	2.50	6	10
1:A:267:THR:O	1:A:267:THR:HG23	0.45	2.12	9	3
3:C:654:LEU:N	3:C:654:LEU:HD12	0.45	2.27	3	1
1:A:130:ALA:HA	1:A:133:LYS:HG2	0.45	1.88	1	1
1:A:75:LEU:HD11	1:A:140:PHE:CB	0.45	2.42	1	2
1:A:54:PHE:HB3	1:A:100:HIS:CB	0.45	2.42	10	3
1:A:92:ASN:HD22	1:A:92:ASN:H	0.45	1.52	9	1
2:B:535:LYS:CD	2:B:535:LYS:N	0.45	2.80	4	1
3:C:610:LEU:HG	3:C:618:VAL:HG11	0.44	1.88	5	1
2:B:556:LYS:N	2:B:556:LYS:CD	0.44	2.80	1	1
2:B:564:GLN:HE21	2:B:568:GLN:NE2	0.44	2.09	7	1
1:A:119:GLN:OE1	1:A:119:GLN:N	0.44	2.47	2	1
2:B:372:ARG:CZ	2:B:377:ASN:OD1	0.44	2.65	5	2
1:A:74:VAL:CG2	1:A:75:LEU:H	0.44	2.25	7	9
3:C:626:GLU:O	3:C:627:ASP:OD1	0.44	2.34	3	3
1:A:169:TRP:HB3	1:A:198:TYR:CD2	0.44	2.47	1	2
2:B:370:SER:CB	2:B:381:PRO:HG2	0.44	2.42	4	6
1:A:251:SER:O	1:A:256:LYS:NZ	0.44	2.51	10	1
2:B:500:ASP:O	2:B:500:ASP:OD1	0.44	2.35	4	5
1:A:41:ASN:O	1:A:42:ASN:OD1	0.44	2.35	9	3
3:C:716:LEU:O	3:C:717:LEU:CD2	0.44	2.65	9	2
1:A:117:LEU:HD13	1:A:152:GLN:HB3	0.44	1.90	8	2
3:C:626:GLU:OE1	3:C:626:GLU:O	0.44	2.34	6	1
1:A:95:SER:OG	1:A:109:GLN:O	0.44	2.31	9	1
2:B:469:LEU:CD1	2:B:470:THR:H	0.44	2.25	6	4
1:A:254:THR:O	1:A:257:ALA:HB3	0.44	2.13	1	10
3:C:614:ASP:OD1	3:C:616:ASP:CG	0.44	2.56	3	1
1:A:107:ASP:OD1	1:A:107:ASP:N	0.44	2.48	10	1
1:A:86:ARG:N	1:A:86:ARG:CD	0.44	2.77	4	2
1:A:71:ASP:OD1	1:A:71:ASP:O	0.44	2.36	8	2
1:A:259:ARG:HH22	2:B:521:GLU:CG	0.44	2.25	7	1
1:A:192:LEU:HD21	1:A:236:GLU:OE1	0.44	2.11	2	1
1:A:161:HIS:N	1:A:161:HIS:ND1	0.44	2.66	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:HIS:O	1:A:209:HIS:ND1	0.44	2.50	5	1
1:A:273:LYS:CA	1:A:277:TYR:HB2	0.44	2.43	5	10
3:C:621:TYR:OH	3:C:628:VAL:CG2	0.44	2.56	8	2
1:A:117:LEU:HD22	1:A:152:GLN:HB3	0.44	1.89	7	5
1:A:76:ILE:CG2	1:A:87:PHE:CE2	0.44	3.01	1	1
3:C:630:ARG:CD	3:C:630:ARG:N	0.44	2.81	1	1
1:A:28:GLU:OE2	2:B:315:ARG:NH1	0.44	2.50	8	1
3:C:708:THR:O	3:C:709:ASP:OD1	0.44	2.35	8	2
2:B:452:HIS:N	2:B:452:HIS:CD2	0.44	2.84	4	2
3:C:718:GLN:OXT	3:C:718:GLN:OE1	0.44	2.35	2	2
1:A:74:VAL:C	1:A:75:LEU:CD2	0.44	2.81	9	1
1:A:273:LYS:NZ	1:A:277:TYR:CE2	0.44	2.83	5	1
2:B:412:PHE:CG	2:B:436:LYS:HE2	0.44	2.48	5	1
3:C:621:TYR:CD1	3:C:622:VAL:CA	0.44	3.01	5	2
1:A:191:VAL:CG2	1:A:211:ASP:OD1	0.44	2.66	3	5
2:B:522:ASN:O	2:B:525:ARG:HG3	0.44	2.12	7	3
3:C:694:LYS:O	3:C:695:THR:HG23	0.44	2.13	6	1
2:B:434:ILE:HB	2:B:450:SER:HB3	0.44	1.90	4	1
1:A:95:SER:O	1:A:108:PRO:CB	0.44	2.66	5	10
1:A:129:ARG:CZ	1:A:130:ALA:HB2	0.44	2.42	3	3
1:A:177:TRP:HA	1:A:190:ALA:CB	0.44	2.43	9	10
2:B:409:ASP:OD1	2:B:409:ASP:O	0.44	2.35	3	1
2:B:489:LEU:HG	2:B:489:LEU:O	0.44	2.12	8	2
2:B:525:ARG:CD	2:B:525:ARG:C	0.44	2.85	8	1
1:A:201:ASP:OD2	2:B:494:THR:O	0.44	2.35	7	3
1:A:119:GLN:CD	1:A:119:GLN:H	0.44	2.15	2	1
1:A:131:TYR:O	1:A:135:HIS:ND1	0.44	2.47	2	1
1:A:217:GLN:CD	1:A:217:GLN:H	0.44	2.16	4	1
3:C:661:ILE:HD11	3:C:672:LEU:HD23	0.44	1.90	5	1
3:C:644:ASP:CG	3:C:678:GLU:OE1	0.44	2.56	5	1
2:B:370:SER:CB	2:B:381:PRO:CG	0.44	2.95	4	10
2:B:554:LYS:O	2:B:558:LEU:N	0.44	2.49	6	8
1:A:167:ASN:N	1:A:167:ASN:HD22	0.44	2.11	3	1
1:A:212:ILE:N	1:A:212:ILE:HD12	0.44	2.28	3	1
2:B:380:ASP:OD1	2:B:381:PRO:CD	0.44	2.65	7	1
3:C:654:LEU:C	3:C:654:LEU:CD2	0.44	2.77	6	1
1:A:252:ASP:C	1:A:253:THR:OG1	0.44	2.56	4	1
1:A:240:GLN:HE21	2:B:546:ILE:CD1	0.44	2.26	4	1
1:A:31:GLU:CD	1:A:31:GLU:H	0.44	2.16	5	4
1:A:211:ASP:OD1	1:A:211:ASP:O	0.44	2.35	1	2
2:B:519:ASP:OD1	2:B:519:ASP:O	0.44	2.35	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:688:LEU:HD12	3:C:693:ASP:O	0.44	2.13	8	2
1:A:117:LEU:CD1	1:A:120:TRP:CD1	0.44	3.00	9	1
1:A:237:ASN:O	1:A:241:THR:OG1	0.44	2.34	9	1
1:A:211:ASP:O	1:A:211:ASP:OD1	0.44	2.36	4	1
3:C:650:ILE:CG2	3:C:654:LEU:HD21	0.44	2.43	4	1
2:B:302:SER:O	2:B:305:GLN:N	0.44	2.51	5	10
2:B:554:LYS:O	2:B:558:LEU:HD13	0.44	2.12	3	2
1:A:188:VAL:O	1:A:189:ALA:CB	0.44	2.66	10	9
3:C:717:LEU:O	3:C:718:GLN:HB3	0.44	2.12	3	1
1:A:133:LYS:HD2	1:A:133:LYS:O	0.44	2.13	1	1
2:B:478:GLN:NE2	2:B:479:THR:N	0.44	2.66	1	1
1:A:272:ASN:OD1	2:B:506:SER:O	0.44	2.36	2	2
1:A:56:GLN:O	1:A:60:ASP:OD1	0.44	2.36	6	1
2:B:408:ARG:NH2	2:B:415:GLY:O	0.44	2.49	6	1
1:A:179:PHE:C	1:A:179:PHE:CD1	0.44	2.86	2	1
2:B:528:LEU:CD1	2:B:532:TYR:CE1	0.44	3.00	2	1
1:A:176:GLU:O	1:A:190:ALA:CB	0.43	2.66	8	10
1:A:91:ARG:NH2	1:A:129:ARG:NH2	0.43	2.66	10	1
1:A:60:ASP:OD1	1:A:60:ASP:O	0.43	2.36	10	1
2:B:478:GLN:CD	2:B:488:ASN:HD21	0.43	2.17	8	1
3:C:668:HIS:CD2	3:C:668:HIS:O	0.43	2.71	8	1
1:A:136:TYR:OH	1:A:236:GLU:OE2	0.43	2.36	7	1
2:B:478:GLN:OE1	2:B:487:MET:C	0.43	2.57	5	1
2:B:462:GLY:C	2:B:464:THR:N	0.43	2.72	1	10
1:A:233:GLU:OE1	1:A:234:ASN:OD1	0.43	2.36	3	1
3:C:648:LEU:CD1	3:C:682:SER:OG	0.43	2.56	3	1
2:B:501:GLU:OE2	2:B:512:ASN:OD1	0.43	2.36	8	3
1:A:169:TRP:CZ3	2:B:539:ILE:HG23	0.43	2.48	10	3
1:A:131:TYR:OH	1:A:236:GLU:OE1	0.43	2.34	8	2
2:B:401:ASN:O	2:B:405:ASP:OD2	0.43	2.36	5	1
1:A:90:PRO:HG3	1:A:143:VAL:O	0.43	2.13	3	7
2:B:364:TYR:CE1	2:B:422:TRP:CZ2	0.43	3.06	8	2
2:B:397:GLU:O	2:B:401:ASN:ND2	0.43	2.52	8	2
1:A:136:TYR:OH	1:A:173:TRP:CD1	0.43	2.68	10	1
2:B:458:GLU:OE1	2:B:459:LYS:O	0.43	2.37	10	1
3:C:654:LEU:CD1	3:C:654:LEU:H	0.43	2.19	10	1
2:B:519:ASP:O	2:B:519:ASP:OD1	0.43	2.36	7	2
3:C:654:LEU:N	3:C:654:LEU:HD13	0.43	2.28	7	1
1:A:112:ASP:OD1	1:A:112:ASP:O	0.43	2.36	2	2
1:A:121:ARG:HH21	1:A:145:GLY:CA	0.43	2.26	2	1
1:A:86:ARG:HH12	1:A:109:GLN:NE2	0.43	2.10	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:441:SER:O	3:C:677:TYR:CD1	0.43	2.71	4	1
2:B:366:ARG:CD	2:B:371:TYR:CZ	0.43	3.02	3	3
2:B:408:ARG:HG2	2:B:409:ASP:N	0.43	2.28	2	2
1:A:259:ARG:NH2	2:B:411:TYR:CD2	0.43	2.86	3	1
2:B:372:ARG:CZ	2:B:387:ALA:O	0.43	2.65	1	1
3:C:693:ASP:OD2	3:C:696:VAL:HG13	0.43	2.13	10	1
2:B:408:ARG:HH12	2:B:417:SER:N	0.43	2.11	9	2
1:A:274:ILE:CD1	2:B:403:ALA:CB	0.43	2.96	7	1
2:B:551:ASP:OD1	2:B:551:ASP:O	0.43	2.37	7	1
1:A:236:GLU:CD	1:A:237:ASN:N	0.43	2.71	9	1
2:B:434:ILE:O	2:B:434:ILE:HG22	0.43	2.12	5	1
3:C:664:PRO:O	3:C:697:LYS:CD	0.43	2.67	5	1
2:B:352:ASP:O	2:B:353:LYS:C	0.43	2.57	3	10
3:C:671:PRO:O	3:C:674:SER:HB2	0.43	2.13	3	2
3:C:713:ILE:HD13	3:C:713:ILE:O	0.43	2.12	3	1
1:A:172:ARG:HH11	1:A:174:ARG:CD	0.43	2.26	10	1
1:A:161:HIS:ND1	1:A:161:HIS:C	0.43	2.71	7	1
1:A:237:ASN:ND2	2:B:544:ARG:NH2	0.43	2.65	4	1
2:B:304:GLN:CD	2:B:304:GLN:H	0.43	2.17	4	1
2:B:563:SER:O	2:B:564:GLN:C	0.43	2.56	3	7
2:B:401:ASN:O	2:B:405:ASP:CG	0.43	2.56	6	5
3:C:607:MET:SD	3:C:641:TYR:CE2	0.43	3.11	3	1
2:B:500:ASP:OD1	2:B:500:ASP:O	0.43	2.36	1	1
3:C:647:GLN:O	3:C:649:GLU:OE1	0.43	2.36	7	1
2:B:350:ALA:HB1	2:B:359:TYR:CE1	0.43	2.48	9	1
2:B:517:VAL:O	2:B:521:GLU:OE1	0.43	2.36	4	1
3:C:705:LEU:HD13	3:C:705:LEU:C	0.43	2.34	8	2
2:B:335:LEU:O	2:B:339:LEU:HG	0.43	2.14	10	6
2:B:380:ASP:OD1	2:B:380:ASP:C	0.43	2.57	3	1
1:A:12:GLU:O	1:A:16:ILE:HG12	0.43	2.13	1	1
3:C:639:LEU:O	3:C:639:LEU:HD23	0.43	2.13	4	2
2:B:350:ALA:HB3	2:B:359:TYR:CE1	0.43	2.47	9	2
2:B:401:ASN:O	2:B:401:ASN:OD1	0.43	2.37	2	2
1:A:111:GLU:OE1	1:A:111:GLU:O	0.43	2.37	9	1
2:B:362:CYS:SG	2:B:365:ASN:ND2	0.43	2.92	4	1
3:C:687:LEU:C	3:C:689:SER:N	0.43	2.72	5	10
2:B:302:SER:O	2:B:305:GLN:HB2	0.43	2.14	1	10
3:C:648:LEU:HD22	3:C:682:SER:CB	0.43	2.44	3	1
3:C:704:ALA:HB3	3:C:717:LEU:CD2	0.43	2.43	3	1
3:C:692:ALA:O	3:C:693:ASP:OD1	0.43	2.37	10	1
1:A:243:ILE:HG12	2:B:487:MET:CE	0.43	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:407:TYR:CG	2:B:407:TYR:O	0.43	2.72	6	1
2:B:408:ARG:NH1	2:B:408:ARG:CG	0.43	2.81	6	1
2:B:489:LEU:C	2:B:489:LEU:CD2	0.43	2.87	5	1
1:A:263:PRO:O	1:A:264:VAL:C	0.43	2.57	3	10
1:A:134:ASP:O	2:B:548:ALA:HA	0.43	2.14	10	10
3:C:667:HIS:O	3:C:669:ILE:HG22	0.43	2.13	7	3
3:C:705:LEU:HD23	3:C:705:LEU:C	0.43	2.34	9	2
2:B:478:GLN:NE2	2:B:479:THR:CA	0.43	2.82	1	1
3:C:625:GLY:C	3:C:626:GLU:CG	0.43	2.87	4	6
1:A:136:TYR:CD1	1:A:160:SER:CB	0.43	3.02	10	2
2:B:475:LEU:HD23	2:B:476:TRP:H	0.43	1.72	4	3
2:B:439:ASP:CG	2:B:441:SER:OG	0.43	2.57	8	1
3:C:648:LEU:O	3:C:648:LEU:CG	0.43	2.65	8	1
3:C:628:VAL:O	3:C:660:ASP:OD1	0.43	2.36	5	1
3:C:661:ILE:O	3:C:662:ASN:CG	0.43	2.57	5	2
1:A:191:VAL:O	1:A:191:VAL:HG13	0.43	2.14	2	4
2:B:407:TYR:O	2:B:407:TYR:CG	0.43	2.72	3	2
1:A:168:PHE:CG	1:A:199:TYR:O	0.43	2.72	9	5
2:B:352:ASP:OD1	2:B:359:TYR:CE1	0.43	2.72	8	1
1:A:79:HIS:CE1	1:A:155:ILE:HD13	0.43	2.48	7	1
1:A:274:ILE:HD11	2:B:403:ALA:CB	0.43	2.39	7	1
1:A:223:GLN:O	1:A:226:LYS:HG3	0.43	2.14	6	1
3:C:705:LEU:CD2	3:C:705:LEU:C	0.43	2.87	2	1
1:A:175:SER:OG	1:A:175:SER:O	0.43	2.37	4	1
3:C:672:LEU:O	3:C:672:LEU:HD23	0.43	2.14	4	1
2:B:372:ARG:HB2	2:B:379:TYR:CE2	0.42	2.49	5	3
1:A:161:HIS:NE2	1:A:163:PHE:CE2	0.42	2.87	3	4
1:A:117:LEU:CD1	1:A:146:LYS:C	0.42	2.87	1	1
1:A:61:GLN:OE1	1:A:63:THR:OG1	0.42	2.37	10	1
2:B:422:TRP:HE1	2:B:429:ALA:HB3	0.42	1.69	8	1
3:C:647:GLN:O	3:C:648:LEU:CG	0.42	2.66	8	1
1:A:129:ARG:C	1:A:129:ARG:HE	0.42	2.16	7	1
1:A:89:ASP:OD1	1:A:89:ASP:C	0.42	2.56	7	2
3:C:688:LEU:O	3:C:688:LEU:CD2	0.42	2.51	6	1
3:C:673:LEU:N	3:C:673:LEU:CD1	0.42	2.82	5	2
3:C:619:LYS:O	3:C:623:ALA:HB2	0.42	2.14	6	10
2:B:372:ARG:HH22	2:B:397:GLU:CD	0.42	2.17	3	1
3:C:680:HIS:C	3:C:681:VAL:HG22	0.42	2.34	7	4
1:A:146:LYS:HG2	1:A:147:SER:N	0.42	2.28	10	1
2:B:436:LYS:HD2	2:B:437:ALA:N	0.42	2.29	8	1
1:A:28:GLU:OE1	1:A:28:GLU:N	0.42	2.52	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:672:LEU:HD23	3:C:672:LEU:O	0.42	2.14	2	1
2:B:475:LEU:HB3	2:B:532:TYR:CZ	0.42	2.49	9	1
3:C:654:LEU:C	3:C:654:LEU:HD12	0.42	2.35	9	1
1:A:259:ARG:HD2	2:B:448:TRP:CH2	0.42	2.49	4	2
1:A:179:PHE:CD1	1:A:188:VAL:HG22	0.42	2.49	5	4
2:B:489:LEU:HD23	2:B:489:LEU:C	0.42	2.34	5	1
2:B:411:TYR:OH	2:B:522:ASN:ND2	0.42	2.51	3	2
3:C:705:LEU:CD1	3:C:705:LEU:C	0.42	2.88	8	2
1:A:59:MET:C	1:A:61:GLN:H	0.42	2.18	3	10
3:C:701:GLY:O	3:C:705:LEU:HB2	0.42	2.14	3	4
3:C:630:ARG:HH11	3:C:630:ARG:HB2	0.42	1.74	1	1
3:C:705:LEU:HD23	3:C:717:LEU:HD23	0.42	1.92	8	1
1:A:169:TRP:O	1:A:170:ASN:OD1	0.42	2.37	7	1
1:A:91:ARG:HG2	1:A:91:ARG:HH11	0.42	1.73	4	2
3:C:644:ASP:CG	3:C:678:GLU:OE2	0.42	2.58	6	1
1:A:206:LEU:HD22	1:A:247:TYR:OH	0.42	2.13	2	1
1:A:227:GLU:O	1:A:231:ILE:CD1	0.42	2.67	4	1
2:B:475:LEU:HD23	2:B:532:TYR:CE2	0.42	2.49	5	1
2:B:404:PHE:CZ	2:B:432:ILE:CD1	0.42	3.03	10	1
3:C:665:ASP:OD1	3:C:666:LYS:N	0.42	2.51	9	3
1:A:259:ARG:NH2	2:B:521:GLU:O	0.42	2.51	8	1
1:A:15:ARG:NH2	1:A:18:ALA:CB	0.42	2.82	7	1
1:A:206:LEU:HG	1:A:206:LEU:O	0.42	2.13	6	1
2:B:552:ASN:O	2:B:552:ASN:OD1	0.42	2.37	2	1
1:A:260:ARG:HG2	2:B:411:TYR:O	0.42	2.14	9	1
3:C:702:LEU:O	3:C:704:ALA:N	0.42	2.53	2	10
3:C:615:LEU:HA	3:C:618:VAL:CG2	0.42	2.45	3	3
1:A:177:TRP:CE3	1:A:190:ALA:HB2	0.42	2.49	7	5
3:C:705:LEU:C	3:C:705:LEU:CD2	0.42	2.87	1	1
1:A:227:GLU:O	1:A:231:ILE:HD13	0.42	2.14	4	2
1:A:117:LEU:HD21	1:A:154:ILE:HD13	0.42	1.92	2	1
1:A:117:LEU:HD21	1:A:154:ILE:CD1	0.42	2.44	2	1
3:C:700:ASP:OD1	3:C:701:GLY:N	0.42	2.53	9	1
1:A:264:VAL:HG23	1:A:265:THR:N	0.42	2.30	5	6
3:C:616:ASP:O	3:C:616:ASP:OD1	0.42	2.37	5	1
2:B:431:VAL:HA	2:B:452:HIS:O	0.42	2.15	7	10
1:A:191:VAL:HG13	1:A:191:VAL:O	0.42	2.15	3	4
3:C:672:LEU:HD11	3:C:692:ALA:HB1	0.42	1.90	3	1
1:A:269:ILE:HG23	1:A:270:ASP:N	0.42	2.29	6	2
1:A:38:LEU:CD1	2:B:308:CYS:SG	0.42	3.08	1	2
1:A:75:LEU:HD11	1:A:140:PHE:HB2	0.42	1.91	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:GLN:N	1:A:187:GLN:CD	0.42	2.73	10	2
2:B:474:MET:HA	2:B:492:SER:HB2	0.42	1.92	2	3
2:B:431:VAL:O	2:B:431:VAL:HG13	0.42	2.15	8	2
1:A:201:ASP:CG	2:B:494:THR:O	0.42	2.58	7	3
1:A:253:THR:HG23	3:C:636:ARG:HH21	0.42	1.72	4	1
1:A:273:LYS:NZ	1:A:277:TYR:CD2	0.42	2.83	5	1
2:B:434:ILE:HG23	2:B:436:LYS:HE2	0.42	1.92	5	1
1:A:173:TRP:CZ2	1:A:236:GLU:OE1	0.42	2.73	3	1
1:A:169:TRP:HB2	1:A:198:TYR:CD2	0.42	2.50	1	2
3:C:677:TYR:O	3:C:677:TYR:CD2	0.42	2.73	1	1
3:C:673:LEU:CD1	3:C:673:LEU:N	0.42	2.83	10	1
1:A:198:TYR:OH	2:B:535:LYS:NZ	0.42	2.50	7	1
1:A:252:ASP:O	1:A:252:ASP:CG	0.42	2.57	6	1
3:C:630:ARG:HG2	3:C:631:THR:N	0.42	2.29	6	1
3:C:637:LYS:CD	3:C:637:LYS:H	0.42	2.27	2	1
1:A:172:ARG:HE	1:A:172:ARG:C	0.42	2.18	9	1
2:B:569:ARG:O	2:B:570:GLN:OE1	0.42	2.37	9	1
2:B:459:LYS:CB	2:B:464:THR:O	0.42	2.68	5	10
1:A:136:TYR:CE1	2:B:544:ARG:HB3	0.42	2.50	3	1
1:A:99:ASP:OD2	1:A:104:GLU:O	0.42	2.37	10	1
2:B:325:LEU:CD2	2:B:345:GLN:OE1	0.42	2.68	10	1
2:B:466:HIS:CE1	2:B:500:ASP:OD2	0.42	2.73	6	1
1:A:177:TRP:CD1	1:A:177:TRP:N	0.42	2.88	9	1
3:C:685:LYS:C	3:C:687:LEU:H	0.42	2.19	1	9
1:A:95:SER:HB3	1:A:109:GLN:CB	0.42	2.45	7	4
1:A:264:VAL:HG13	1:A:265:THR:N	0.42	2.30	3	1
2:B:452:HIS:HD1	2:B:471:SER:CB	0.42	2.28	3	1
3:C:607:MET:CG	3:C:608:TRP:N	0.42	2.82	10	2
1:A:95:SER:HB2	1:A:109:GLN:CB	0.42	2.45	9	1
1:A:195:GLN:OE1	1:A:205:GLN:OE1	0.42	2.37	4	1
3:C:647:GLN:O	3:C:647:GLN:OE1	0.42	2.37	3	1
1:A:192:LEU:HD22	1:A:192:LEU:H	0.42	1.65	1	1
3:C:687:LEU:C	3:C:687:LEU:HD23	0.42	2.35	8	1
2:B:405:ASP:O	2:B:405:ASP:OD1	0.42	2.37	9	1
1:A:121:ARG:HE	1:A:122:ASP:CA	0.42	2.28	4	1
1:A:107:ASP:C	1:A:107:ASP:OD1	0.41	2.59	5	1
2:B:439:ASP:O	2:B:442:LYS:HG2	0.41	2.15	3	1
1:A:275:LEU:C	1:A:276:SER:OG	0.41	2.58	8	5
1:A:31:GLU:CD	2:B:315:ARG:HH21	0.41	2.19	10	1
3:C:627:ASP:CG	3:C:627:ASP:O	0.41	2.58	10	1
1:A:203:ASN:OD1	2:B:314:ARG:O	0.41	2.37	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:610:LEU:HD21	3:C:618:VAL:HG21	0.41	1.92	7	1
1:A:144:TYR:HB2	1:A:155:ILE:HB	0.41	1.91	4	1
1:A:111:GLU:O	1:A:111:GLU:OE1	0.41	2.38	5	1
1:A:206:LEU:O	1:A:206:LEU:CD2	0.41	2.67	5	1
1:A:70:TYR:CD2	1:A:94:ILE:HD13	0.41	2.50	6	4
1:A:273:LYS:HA	1:A:277:TYR:HB2	0.41	1.92	1	7
1:A:91:ARG:C	1:A:91:ARG:CD	0.41	2.88	7	1
3:C:642:ALA:O	3:C:651:LEU:CD1	0.41	2.69	6	2
2:B:569:ARG:O	2:B:570:GLN:CD	0.41	2.58	2	1
1:A:90:PRO:O	1:A:121:ARG:CZ	0.41	2.69	9	1
1:A:253:THR:CG2	3:C:636:ARG:NH2	0.41	2.83	4	1
1:A:169:TRP:C	1:A:169:TRP:CD2	0.41	2.94	5	1
1:A:70:TYR:CE1	1:A:92:ASN:OD1	0.41	2.73	3	2
2:B:364:TYR:CD1	2:B:422:TRP:CZ2	0.41	3.08	3	2
3:C:604:LYS:O	3:C:608:TRP:N	0.41	2.41	3	2
1:A:224:THR:CG2	1:A:225:ALA:N	0.41	2.83	10	1
3:C:648:LEU:CA	3:C:651:LEU:HD21	0.41	2.44	6	2
1:A:125:ASP:OD1	1:A:125:ASP:N	0.41	2.53	2	1
1:A:233:GLU:O	1:A:237:ASN:OD1	0.41	2.37	9	1
3:C:661:ILE:O	3:C:662:ASN:OD1	0.41	2.38	4	1
2:B:434:ILE:HG23	2:B:436:LYS:HZ3	0.41	1.74	5	1
2:B:350:ALA:HB1	2:B:359:TYR:CE2	0.41	2.49	1	1
2:B:478:GLN:C	2:B:479:THR:HG22	0.41	2.36	8	1
1:A:274:ILE:C	1:A:274:ILE:HD12	0.41	2.35	7	1
1:A:107:ASP:OD1	1:A:107:ASP:C	0.41	2.59	6	1
2:B:459:LYS:NZ	2:B:461:SER:O	0.41	2.41	6	1
2:B:557:GLN:CD	2:B:557:GLN:O	0.41	2.59	6	1
2:B:470:THR:HG22	2:B:470:THR:O	0.41	2.15	2	1
3:C:615:LEU:CD2	3:C:615:LEU:O	0.41	2.65	9	2
2:B:304:GLN:CD	2:B:304:GLN:N	0.41	2.74	4	1
1:A:118:LYS:O	1:A:119:GLN:C	0.41	2.59	4	8
1:A:192:LEU:CD2	1:A:192:LEU:H	0.41	2.24	1	1
1:A:264:VAL:CG2	1:A:265:THR:N	0.41	2.82	1	3
1:A:161:HIS:N	1:A:161:HIS:CD2	0.41	2.89	10	1
2:B:444:ILE:HG22	2:B:479:THR:HB	0.41	1.91	10	1
1:A:256:LYS:NZ	3:C:636:ARG:CZ	0.41	2.84	2	1
2:B:408:ARG:CG	2:B:409:ASP:N	0.41	2.83	2	1
3:C:603:ASP:OD1	3:C:603:ASP:N	0.41	2.53	2	1
3:C:650:ILE:HG22	3:C:654:LEU:HD21	0.41	1.93	4	1
1:A:262:LEU:HD23	1:A:263:PRO:HD2	0.41	1.91	1	1
1:A:164:GLN:OE1	1:A:164:GLN:O	0.41	2.39	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:ASP:HB2	2:B:381:PRO:HD3	0.41	1.92	6	1
2:B:377:ASN:ND2	2:B:394:ARG:NH2	0.41	2.69	6	1
1:A:125:ASP:OD1	1:A:143:VAL:CG1	0.41	2.69	2	1
1:A:270:ASP:N	1:A:270:ASP:OD1	0.41	2.53	2	1
3:C:693:ASP:OD1	3:C:696:VAL:CG2	0.41	2.68	10	1
1:A:54:PHE:CD1	1:A:100:HIS:CB	0.41	3.04	8	1
3:C:610:LEU:HD23	3:C:650:ILE:HG21	0.41	1.91	8	1
1:A:129:ARG:CA	1:A:129:ARG:HE	0.41	2.27	7	1
1:A:203:ASN:C	1:A:203:ASN:HD22	0.41	2.19	9	1
1:A:206:LEU:CD2	1:A:206:LEU:C	0.41	2.87	9	1
2:B:458:GLU:OE2	2:B:509:HIS:CD2	0.41	2.73	9	1
1:A:262:LEU:HD12	1:A:262:LEU:O	0.41	2.15	4	1
2:B:529:ASN:ND2	2:B:529:ASN:C	0.41	2.74	3	1
3:C:648:LEU:HD13	3:C:682:SER:CB	0.41	2.44	3	1
2:B:557:GLN:O	2:B:557:GLN:CD	0.41	2.60	8	2
3:C:603:ASP:O	3:C:603:ASP:OD1	0.41	2.39	6	1
3:C:626:GLU:OE2	3:C:628:VAL:HG22	0.41	2.16	6	1
2:B:442:LYS:NZ	3:C:644:ASP:HB3	0.41	2.31	2	1
2:B:471:SER:C	2:B:472:THR:HG22	0.41	2.35	4	1
1:A:197:HIS:CD2	1:A:198:TYR:N	0.41	2.89	5	1
1:A:88:LEU:CD2	1:A:89:ASP:H	0.41	2.26	5	1
2:B:353:LYS:O	2:B:354:VAL:C	0.41	2.59	6	2
3:C:658:GLY:O	3:C:659:ALA:CB	0.41	2.69	3	2
3:C:662:ASN:HD22	3:C:696:VAL:HG11	0.41	1.76	3	1
2:B:421:LEU:N	2:B:421:LEU:HD12	0.41	2.30	1	1
2:B:444:ILE:CD1	2:B:444:ILE:N	0.41	2.68	10	1
3:C:681:VAL:HG23	3:C:681:VAL:O	0.41	2.15	10	1
2:B:372:ARG:NH1	2:B:420:TYR:OH	0.41	2.49	10	1
3:C:628:VAL:HG11	3:C:654:LEU:HB2	0.41	1.93	8	1
3:C:621:TYR:OH	3:C:627:ASP:OD2	0.41	2.36	6	1
2:B:408:ARG:CG	2:B:408:ARG:HH11	0.41	2.27	6	1
1:A:121:ARG:CG	1:A:122:ASP:N	0.41	2.82	2	1
2:B:361:LEU:CD2	2:B:362:CYS:N	0.41	2.82	2	1
2:B:311:ASP:OD1	2:B:315:ARG:NE	0.41	2.54	5	1
2:B:439:ASP:OD2	2:B:442:LYS:NZ	0.41	2.44	5	1
1:A:61:GLN:CG	1:A:61:GLN:O	0.41	2.69	10	1
3:C:608:TRP:NE1	3:C:612:ASN:OD1	0.41	2.53	8	1
1:A:126:SER:O	1:A:129:ARG:HG3	0.41	2.16	7	1
1:A:198:TYR:HD1	1:A:198:TYR:O	0.41	1.98	6	1
2:B:479:THR:HG22	2:B:487:MET:HB3	0.41	1.92	6	1
3:C:688:LEU:CD1	3:C:688:LEU:C	0.41	2.72	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ILE:CG2	1:A:194:ILE:O	0.41	2.67	2	1
2:B:359:TYR:OH	2:B:380:ASP:OD1	0.41	2.36	2	1
2:B:570:GLN:CG	2:B:570:GLN:O	0.41	2.69	2	1
1:A:91:ARG:NE	1:A:125:ASP:OD2	0.41	2.54	4	1
3:C:662:ASN:O	3:C:663:ALA:C	0.40	2.59	5	4
2:B:452:HIS:ND1	2:B:471:SER:CB	0.40	2.84	3	1
3:C:717:LEU:O	3:C:718:GLN:CB	0.40	2.70	4	3
1:A:172:ARG:HH12	1:A:174:ARG:CZ	0.40	2.28	10	1
1:A:188:VAL:HG23	1:A:216:VAL:HG12	0.40	1.94	6	1
1:A:221:ASP:CG	1:A:222:VAL:H	0.40	2.19	6	1
3:C:673:LEU:HD23	3:C:676:VAL:HG21	0.40	1.91	9	1
1:A:173:TRP:NE1	1:A:236:GLU:OE2	0.40	2.54	4	1
1:A:42:ASN:ND2	1:A:45:LEU:HD12	0.40	2.31	5	1
1:A:272:ASN:OD1	1:A:272:ASN:O	0.40	2.38	3	1
1:A:106:SER:O	1:A:107:ASP:CB	0.40	2.70	1	5
2:B:468:LYS:CE	2:B:496:GLN:NE2	0.40	2.85	8	2
3:C:603:ASP:O	3:C:607:MET:HG3	0.40	2.15	1	1
2:B:408:ARG:HH11	2:B:408:ARG:HG3	0.40	1.76	10	1
2:B:553:GLN:H	2:B:553:GLN:NE2	0.40	2.14	10	1
2:B:510:ILE:HD12	2:B:510:ILE:H	0.40	1.76	7	1
2:B:408:ARG:CZ	2:B:414:GLY:O	0.40	2.69	6	1
2:B:405:ASP:OD1	2:B:405:ASP:O	0.40	2.39	2	1
3:C:676:VAL:HG12	3:C:677:TYR:N	0.40	2.30	9	1
1:A:240:GLN:OE1	1:A:240:GLN:O	0.40	2.40	4	1
3:C:666:LYS:N	3:C:666:LYS:CD	0.40	2.84	5	1
1:A:266:ARG:O	1:A:267:THR:HB	0.40	2.17	3	1
2:B:401:ASN:O	2:B:405:ASP:OD1	0.40	2.39	3	1
1:A:250:MET:SD	2:B:489:LEU:CD2	0.40	3.09	3	1
2:B:473:VAL:CG2	2:B:521:GLU:OE1	0.40	2.69	1	1
2:B:479:THR:CG2	2:B:487:MET:HB3	0.40	2.46	1	1
3:C:637:LYS:H	3:C:637:LYS:HD2	0.40	1.76	6	1
3:C:695:THR:O	3:C:695:THR:CG2	0.40	2.67	2	1
2:B:464:THR:O	2:B:464:THR:CG2	0.40	2.69	3	2
1:A:72:ASP:OD2	1:A:89:ASP:OD1	0.40	2.40	1	1
1:A:274:ILE:HG23	1:A:274:ILE:O	0.40	2.15	10	1
1:A:30:ASN:CG	1:A:31:GLU:N	0.40	2.75	7	1
1:A:152:GLN:O	1:A:180:THR:C	0.40	2.60	6	2
1:A:221:ASP:CG	1:A:222:VAL:N	0.40	2.75	6	1
2:B:369:ASP:O	2:B:369:ASP:OD1	0.40	2.39	9	1
2:B:551:ASP:O	2:B:551:ASP:OD1	0.40	2.39	4	1
2:B:317:PRO:HA	2:B:318:PRO:HD3	0.40	1.79	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:687:LEU:O	3:C:689:SER:N	0.40	2.55	10	2
2:B:434:ILE:CB	2:B:450:SER:OG	0.40	2.69	8	1
2:B:464:THR:CG2	2:B:464:THR:O	0.40	2.70	8	1
1:A:89:ASP:OD2	1:A:94:ILE:CD1	0.40	2.69	7	1
2:B:379:TYR:N	2:B:379:TYR:CD1	0.40	2.90	9	1
1:A:220:SER:O	1:A:224:THR:OG1	0.40	2.30	4	1
1:A:135:HIS:HB3	2:B:544:ARG:HE	0.40	1.77	4	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	273/275 (99%)	194±0 (71±0%)	48±0 (17±0%)	32±0 (12±0%)	1	8
2	B	268/270 (99%)	227±0 (85±0%)	31±0 (12±0%)	10±0 (4±0%)	7	35
3	C	116/118 (98%)	62±0 (53±0%)	33±0 (28±0%)	21±0 (18±0%)	0	3
All	All	6570/6630 (99%)	4827 (73%)	1116 (17%)	627 (10%)	2	11

All 63 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	662	ASN	10
1	A	166	LYS	10
1	A	121	ARG	10
1	A	258	LEU	10
1	A	71	ASP	10
2	B	485	GLY	10
3	C	703	THR	10
1	A	183	PRO	10
2	B	532	TYR	10
1	A	73	GLN	10
1	A	185	THR	10
3	C	615	LEU	10

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Mol	Chain	Res	Type	Models (Total)
3	C	700	ASP	10
1	A	188	VAL	10
1	A	277	TYR	10
1	A	191	VAL	10
3	C	625	GLY	10
2	B	423	ASP	10
1	A	189	ALA	10
1	A	279	ILE	10
1	A	122	ASP	10
1	A	125	ASP	10
3	C	654	LEU	10
1	A	101	LEU	10
3	C	653	PHE	10
3	C	681	VAL	10
3	C	717	LEU	10
3	C	692	ALA	10
3	C	614	ASP	10
3	C	660	ASP	10
1	A	9	SER	10
2	B	570	GLN	10
2	B	382	PRO	10
1	A	271	TRP	10
3	C	629	ASN	10
2	B	564	GLN	10
1	A	268	LYS	10
1	A	113	THR	10
1	A	8	VAL	10
2	B	492	SER	10
3	C	632	LEU	10
2	B	551	ASP	10
3	C	658	GLY	10
1	A	62	PHE	10
3	C	626	GLU	10
3	C	715	ALA	10
1	A	182	THR	10
3	C	634	GLY	10
1	A	253	THR	10
1	A	267	THR	10
1	A	280	GLY	10
1	A	201	ASP	10
3	C	647	GLN	10
2	B	550	PRO	10

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Mol	Chain	Res	Type	Models (Total)
1	A	180	THR	10
3	C	657	LYS	10
2	B	534	GLY	10
3	C	659	ALA	10
1	A	186	ALA	10
1	A	169	TRP	10
1	A	68	GLU	10
1	A	276	SER	10
1	A	55	ALA	7

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/243 (100%)	227±1 (93±1%)	16±1 (7±1%)	24	70
2	B	241/241 (100%)	228±3 (95±1%)	13±3 (5±1%)	30	76
3	C	96/96 (100%)	83±2 (87±3%)	13±2 (13±3%)	9	50
All	All	5800/5800 (100%)	5384 (93%)	416 (7%)	21	67

All 145 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	175	SER	10
2	B	533	PHE	10
1	A	100	HIS	10
2	B	380	ASP	10
1	A	160	SER	10
3	C	670	THR	10
1	A	182	THR	9
3	C	651	LEU	9
3	C	648	LEU	9
2	B	345	GLN	9
1	A	262	LEU	8
2	B	411	TYR	8
2	B	383	LEU	8
3	C	654	LEU	8

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Mol	Chain	Res	Type	Models (Total)
3	C	631	THR	7
3	C	683	CYS	6
1	A	54	PHE	6
1	A	247	TYR	6
1	A	141	CYS	6
2	B	408	ARG	5
1	A	70	TYR	5
1	A	109	GLN	5
2	B	569	ARG	5
2	B	525	ARG	5
3	C	637	LYS	5
3	C	716	LEU	5
1	A	129	ARG	5
3	C	653	PHE	5
1	A	86	ARG	5
2	B	469	LEU	4
3	C	601	MET	4
1	A	107	ASP	4
1	A	67	ILE	4
2	B	449	ASP	4
3	C	677	TYR	4
1	A	220	SER	4
3	C	639	LEU	4
2	B	379	TYR	4
3	C	713	ILE	4
3	C	650	ILE	4
2	B	450	SER	3
2	B	464	THR	3
1	A	91	ARG	3
1	A	259	ARG	3
1	A	270	ASP	3
1	A	181	ILE	3
2	B	475	LEU	3
3	C	693	ASP	3
2	B	472	THR	3
3	C	687	LEU	3
2	B	421	LEU	3
2	B	390	SER	3
3	C	696	VAL	3
2	B	529	ASN	3
3	C	621	TYR	2
3	C	688	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	88	LEU	2
1	A	208	SER	2
3	C	682	SER	2
1	A	185	THR	2
2	B	447	CYS	2
1	A	269	ILE	2
1	A	113	THR	2
1	A	59	MET	2
1	A	237	ASN	2
2	B	488	ASN	2
1	A	217	GLN	2
3	C	703	THR	2
3	C	630	ARG	2
2	B	453	VAL	2
1	A	260	ARG	2
1	A	118	LYS	2
3	C	705	LEU	2
1	A	194	ILE	2
1	A	267	THR	2
1	A	164	GLN	2
1	A	92	ASN	2
2	B	476	TRP	2
2	B	371	TYR	2
3	C	717	LEU	2
1	A	240	GLN	2
2	B	463	ARG	2
2	B	354	VAL	2
3	C	695	THR	2
1	A	102	ARG	1
1	A	23	HIS	1
3	C	602	CYS	1
1	A	119	GLN	1
3	C	612	ASN	1
1	A	15	ARG	1
3	C	697	LYS	1
2	B	444	ILE	1
3	C	647	GLN	1
3	C	657	LYS	1
1	A	187	GLN	1
2	B	493	LEU	1
1	A	7	ARG	1
1	A	274	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	103	LYS	1
3	C	708	THR	1
1	A	125	ASP	1
3	C	641	TYR	1
1	A	133	LYS	1
1	A	273	LYS	1
3	C	678	GLU	1
3	C	656	LEU	1
2	B	570	GLN	1
2	B	313	MET	1
2	B	436	LYS	1
2	B	442	LYS	1
3	C	604	LYS	1
2	B	535	LYS	1
3	C	618	VAL	1
1	A	94	ILE	1
1	A	226	LYS	1
2	B	365	ASN	1
3	C	669	ILE	1
2	B	407	TYR	1
1	A	117	LEU	1
2	B	478	GLN	1
1	A	73	GLN	1
2	B	315	ARG	1
2	B	388	MET	1
2	B	420	TYR	1
2	B	479	THR	1
1	A	72	ASP	1
2	B	496	GLN	1
3	C	667	HIS	1
3	C	660	ASP	1
2	B	406	GLN	1
2	B	434	ILE	1
1	A	82	LEU	1
2	B	502	THR	1
2	B	546	ILE	1
1	A	161	HIS	1
1	A	170	ASN	1
1	A	172	ARG	1
2	B	466	HIS	1
3	C	606	PHE	1
1	A	203	ASN	1

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Mol	Chain	Res	Type	Models (Total)
2	B	361	LEU	1
2	B	425	ASP	1
2	B	474	MET	1
3	C	672	LEU	1
3	C	661	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided