



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:26 pm GMT

PDB ID : 1ISK
Title : 3-OXO-DELTA5-STEROID ISOMERASE, NMR, 20 STRUCTURES
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Deposited on : 1997-03-12

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

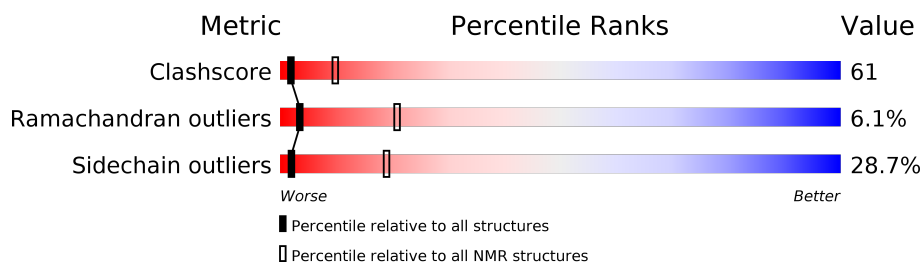
1 Overall quality at a glance

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	125	
1	B	125	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:87, A:92-A:104, A:108-A:125, B:1-B:87, B:91-B:103, B:108-B:125 (235)	0.69	12

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3750 atoms, of which 1862 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 3-OXO-DELTA5-STEROID ISOMERASE.

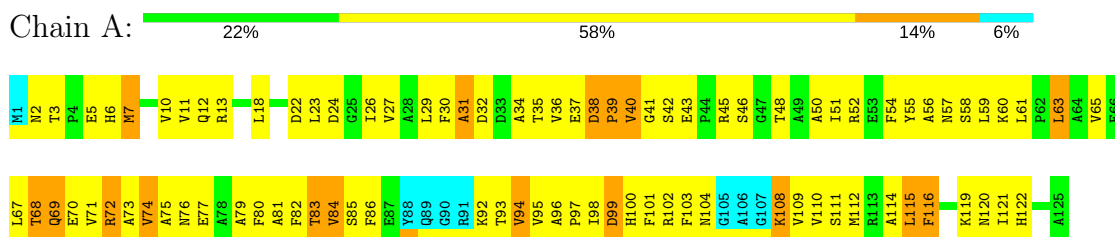
Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			1875	597	931	165	179	3	
1	B	125	Total	C	H	N	O	S	0
			1875	597	931	165	179	3	

4 Residue-property plots

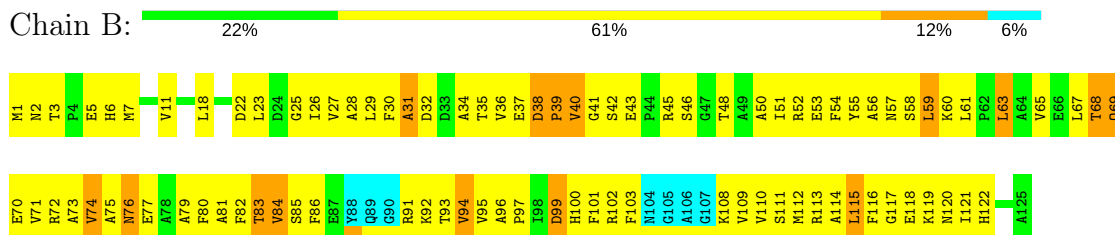
4.1 Average score per residue in the NMR ensemble

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: 3-OXO-DELTA5-STERIOD ISOMERASE



• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

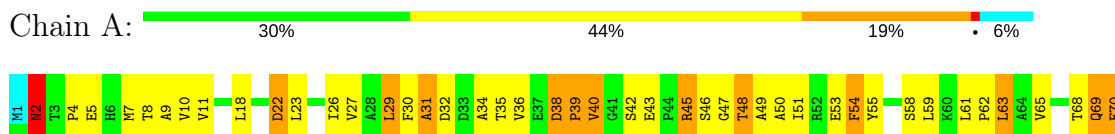


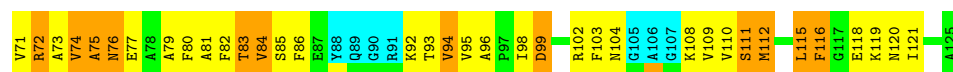
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

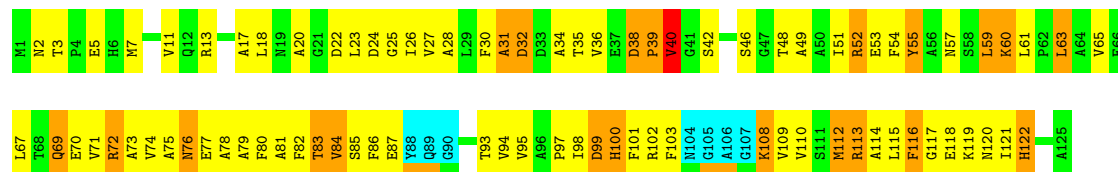
• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE





• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

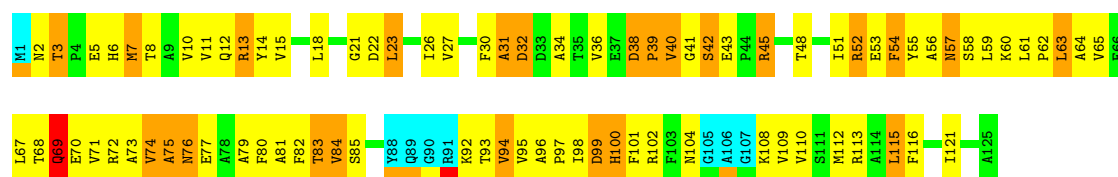
Chain B: 27% 50% 17% 6%



4.2.2 Score per residue for model 2

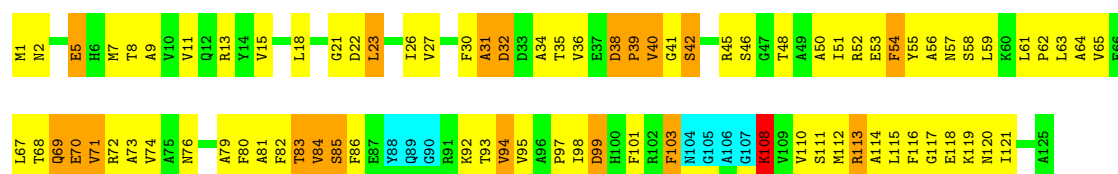
• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 26% 47% 19% 6%



• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

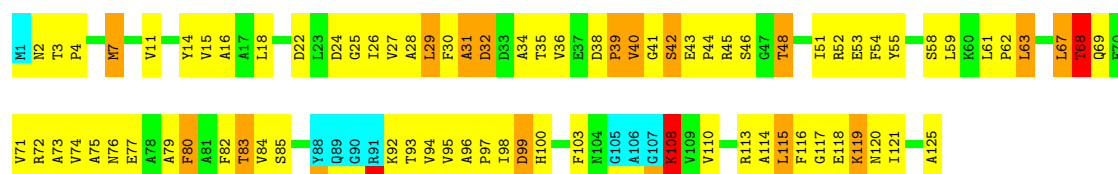
Chain B: 28% 50% 15% 6%



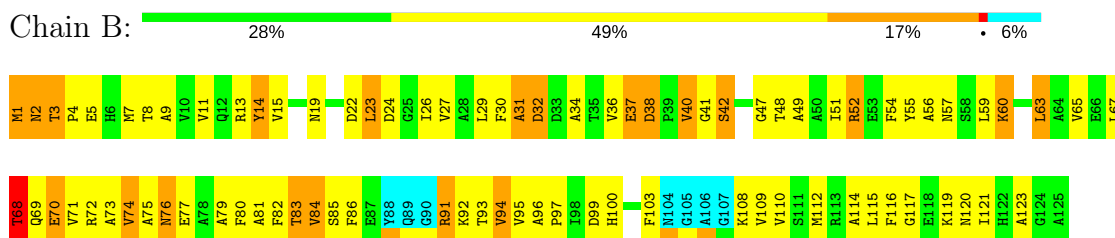
4.2.3 Score per residue for model 3

• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 30% 50% 12% 6%

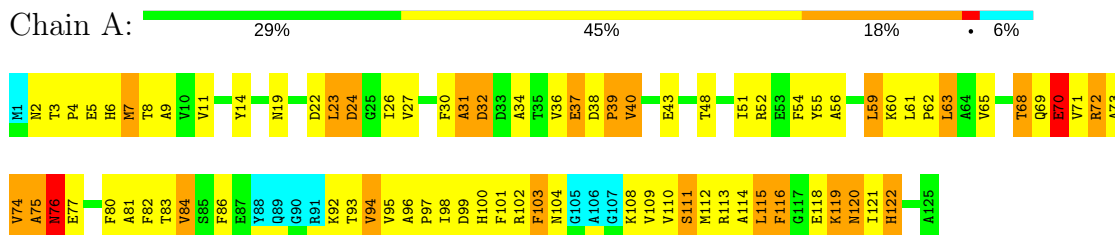


• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

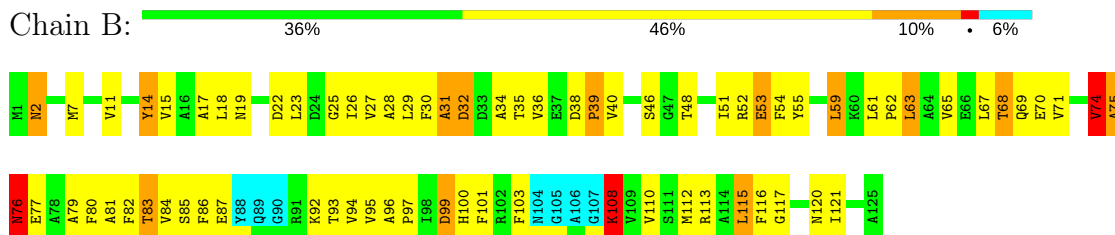


4.2.4 Score per residue for model 4

- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

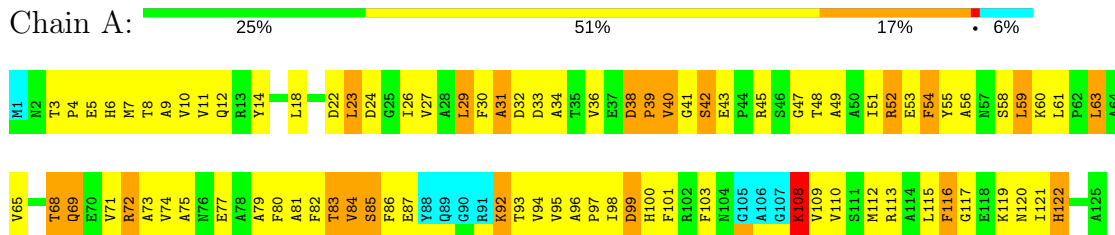


- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

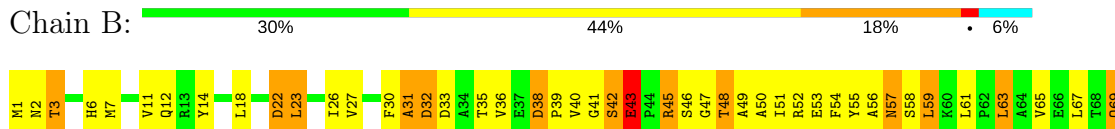


4.2.5 Score per residue for model 5

- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE



- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

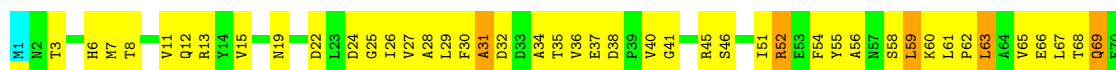




4.2.6 Score per residue for model 6

- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 32% 49% 12% 6%



- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

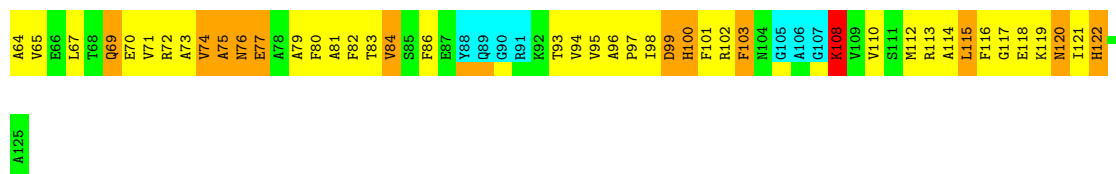
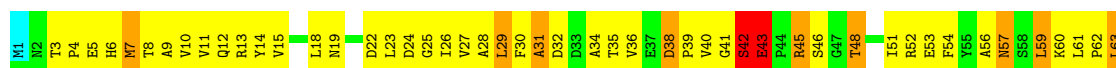
Chain B: 29% 47% 17% 6%



4.2.7 Score per residue for model 7

- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 20% 54% 17% 6%



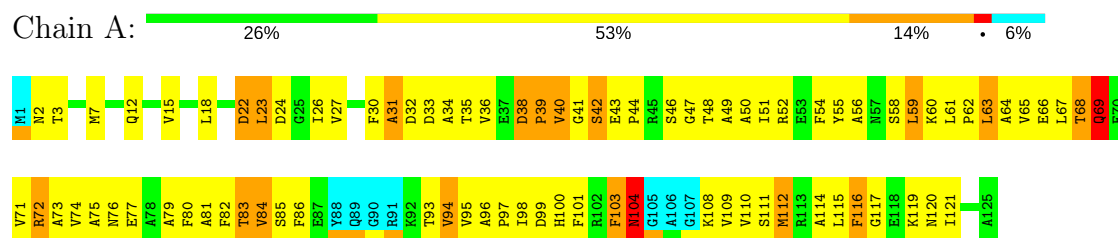
- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain B: 25% 53% 15% 6%

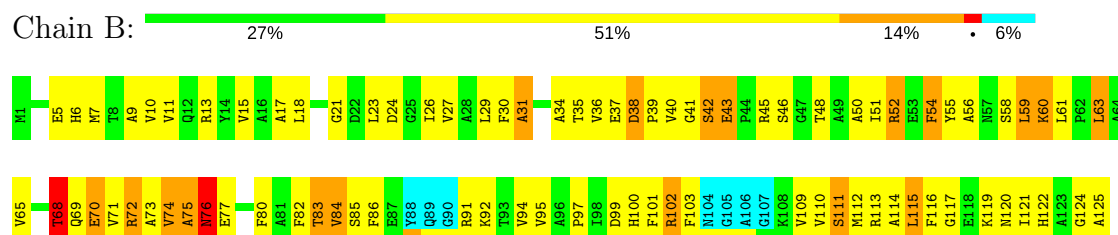


4.2.8 Score per residue for model 8

- Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

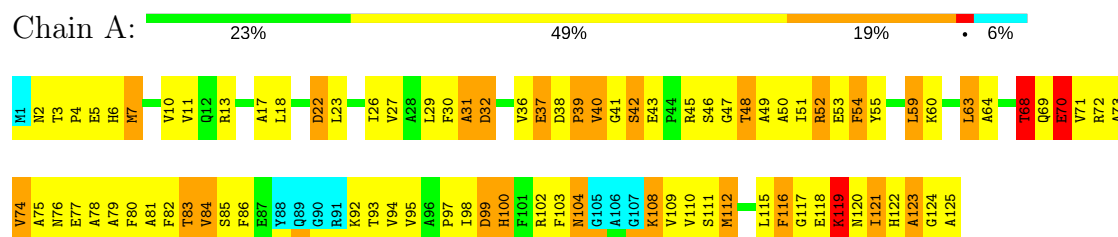


- Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

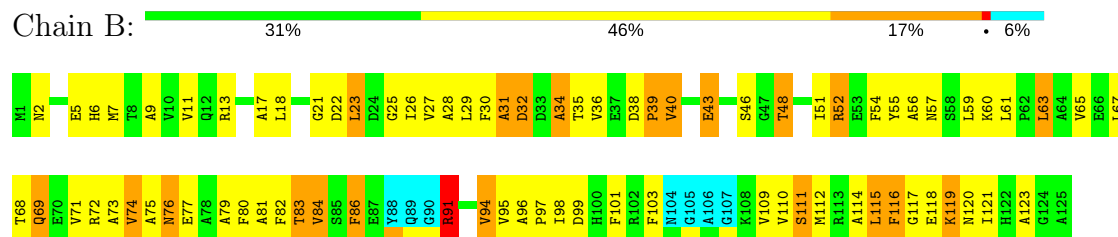


4.2.9 Score per residue for model 9

- Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



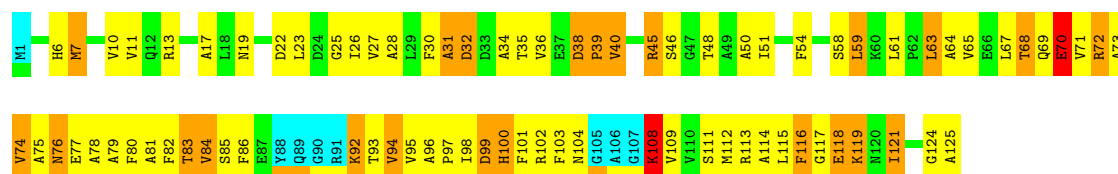
- Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



4.2.10 Score per residue for model 10

- Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE





• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

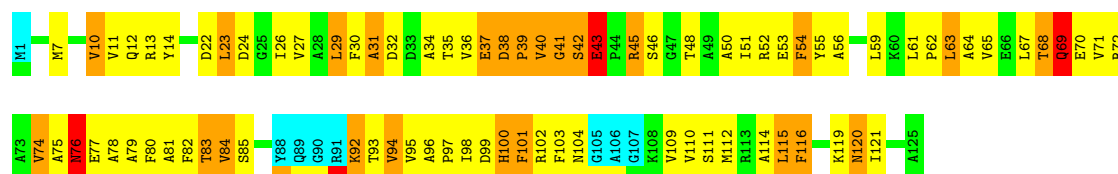
Chain B: 29% 50% 16% 6%



4.2.11 Score per residue for model 11

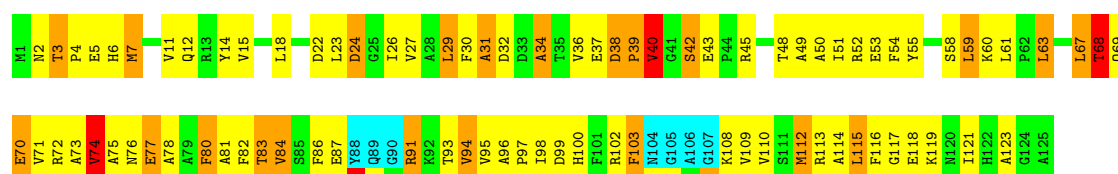
• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 28% 44% 19% 6%



• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

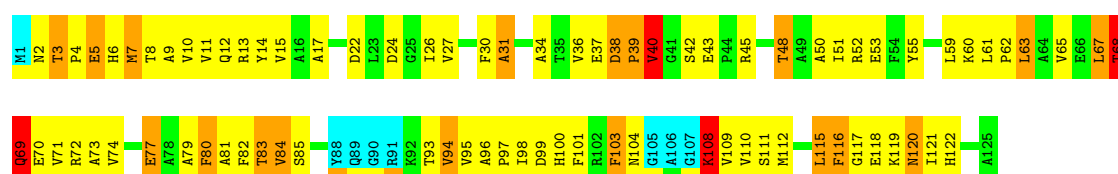
Chain B: 26% 48% 18% 6%



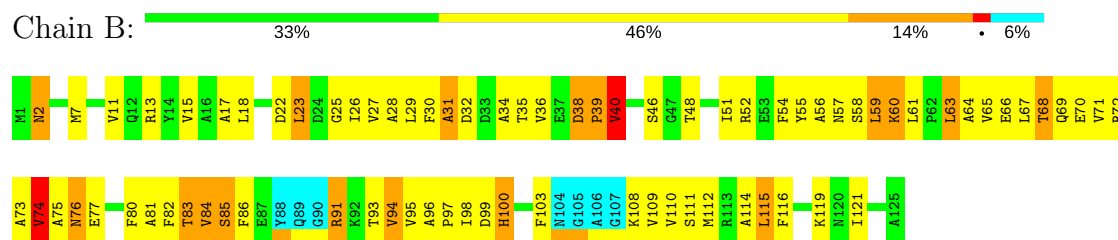
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 28% 48% 14% 6%

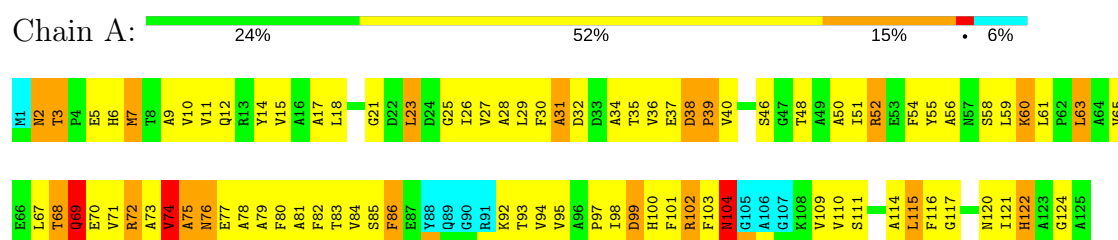


• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

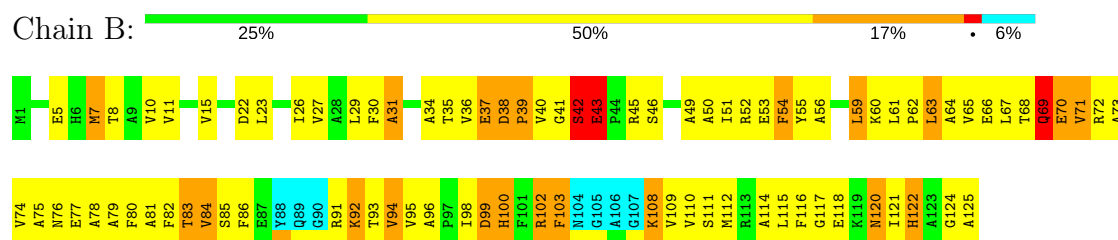


4.2.13 Score per residue for model 13

• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

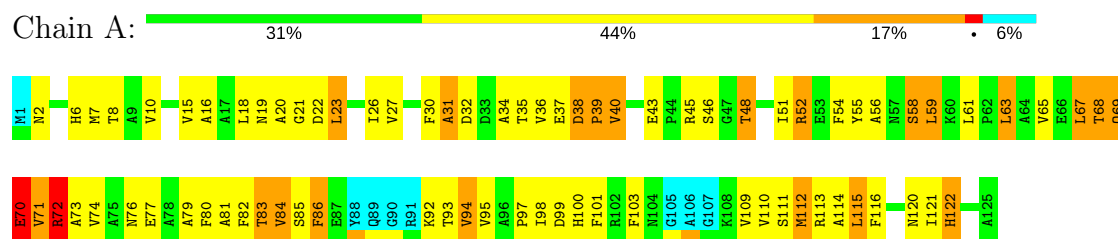


• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



4.2.14 Score per residue for model 14

• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

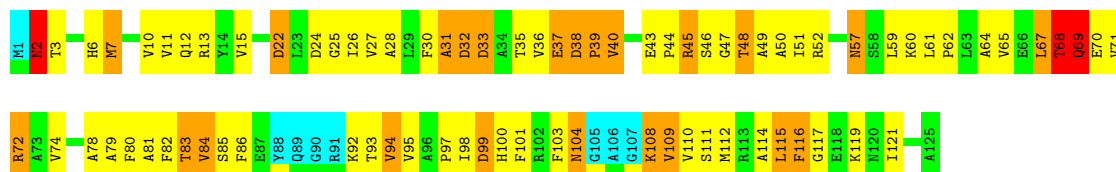




4.2.15 Score per residue for model 15

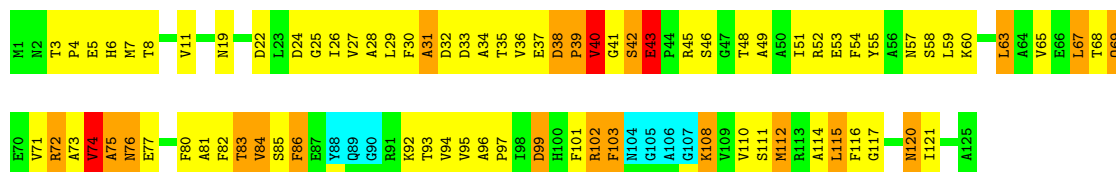
- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 30% 43% 18% 6%



- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

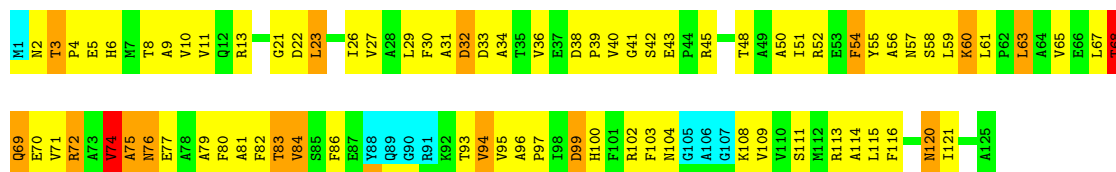
Chain B: 30% 46% 16% 6%



4.2.16 Score per residue for model 16

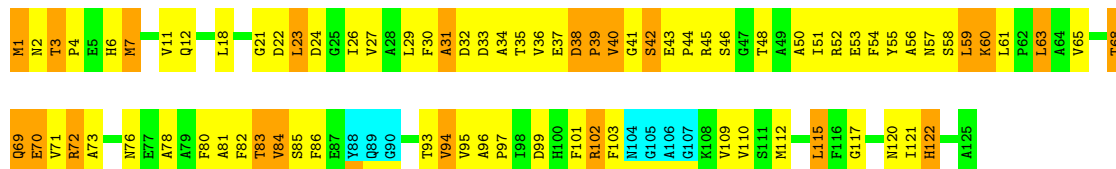
- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 30% 50% 12% 6%



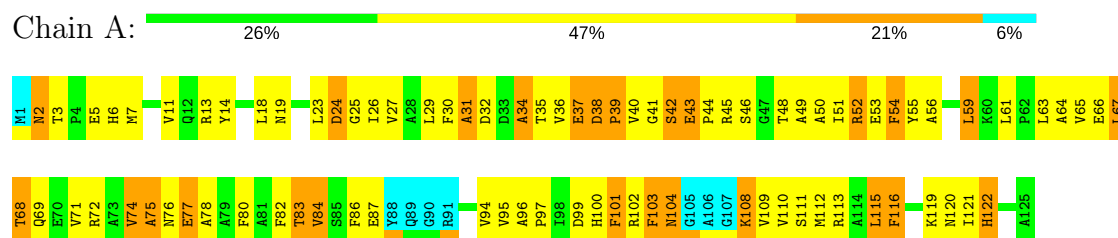
- Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain B: 30% 46% 18% 6%

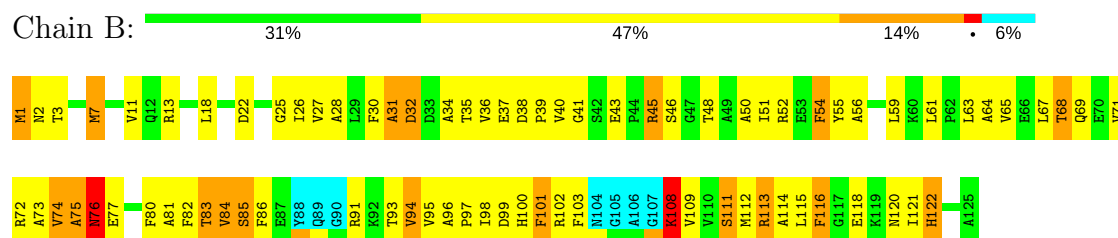


4.2.17 Score per residue for model 17

• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

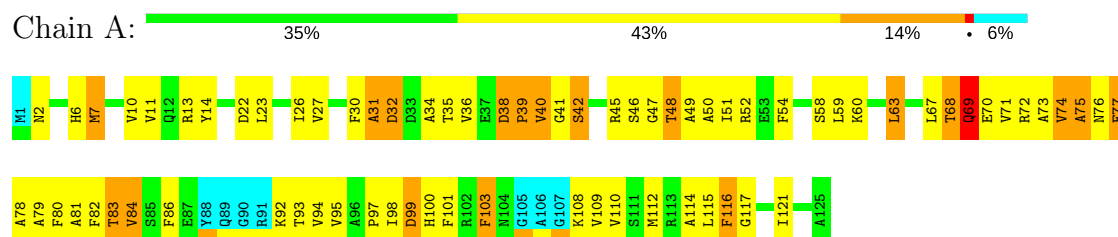


• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE

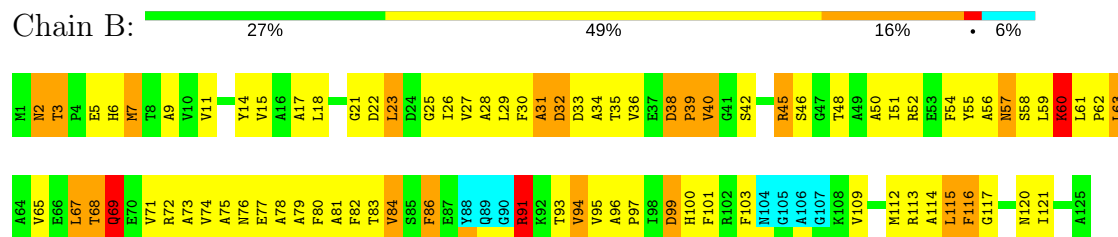


4.2.18 Score per residue for model 18

• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



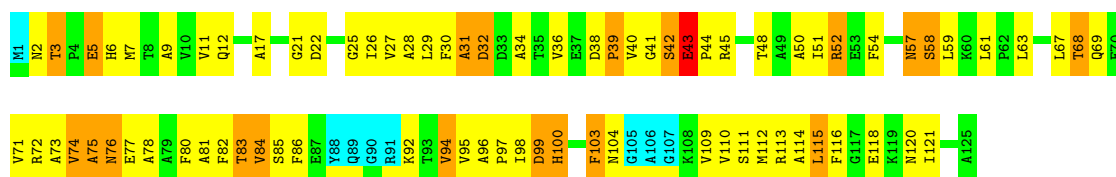
• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE



4.2.19 Score per residue for model 19

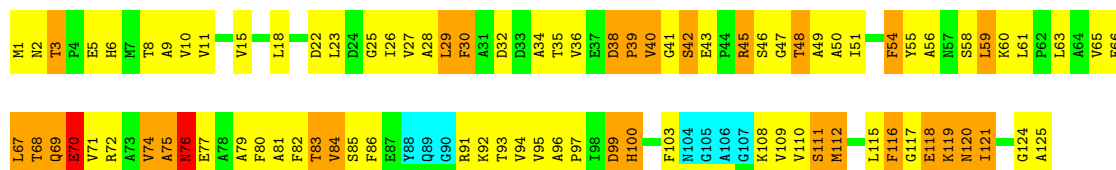
• Molecule 1: 3-OXO-DELTA5-STEROID ISOMERASE





• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

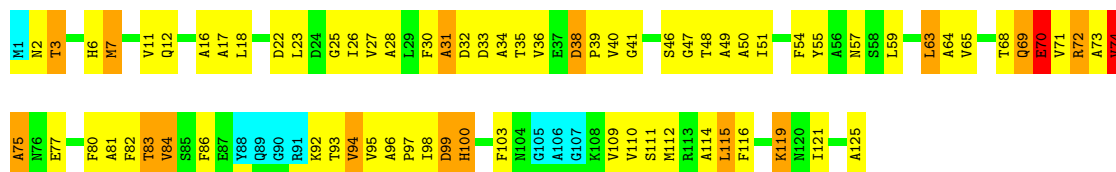
Chain B: 24% 47% 22% 6%



4.2.20 Score per residue for model 20

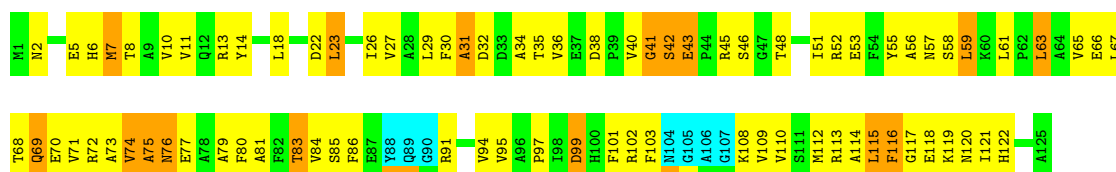
• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain A: 34% 46% 12% 6%



• Molecule 1: 3-OXO-DELTA5-STERIOD ISOMERASE

Chain B: 30% 52% 13% 6%



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	refinement	

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	887	879	874	114±15
1	B	898	894	892	113±11
All	All	35700	35460	35320	4298

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:LEU:HD23	1:B:86:PHE:CE1	1.09	1.83	8	2
1:A:40:VAL:HG21	1:B:74:VAL:HG11	1.05	1.21	7	10
1:B:65:VAL:HG22	1:B:84:VAL:HG12	1.04	1.08	20	2
1:B:15:VAL:HG21	1:B:82:PHE:CE2	1.03	1.89	11	1
1:A:74:VAL:HG11	1:B:40:VAL:HG21	1.01	1.10	13	8
1:A:8:THR:HG23	1:A:71:VAL:HG11	0.99	1.33	2	5
1:A:79:ALA:HB1	1:A:100:HIS:CE1	0.98	1.93	7	1
1:B:8:THR:HG23	1:B:71:VAL:HG11	0.98	1.31	2	3
1:A:40:VAL:CG2	1:B:74:VAL:HG11	0.98	1.89	20	8
1:A:40:VAL:HG21	1:B:74:VAL:CG1	0.97	1.89	20	5
1:B:30:PHE:CE1	1:B:51:ILE:HG21	0.96	1.96	19	10
1:A:74:VAL:CG1	1:B:40:VAL:HG21	0.95	1.89	13	4
1:B:67:LEU:HD12	1:B:68:THR:N	0.93	1.77	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:HD12	1:A:82:PHE:CZ	0.93	1.99	12	2
1:A:30:PHE:CZ	1:A:51:ILE:HG21	0.93	1.99	13	14
1:A:15:VAL:HG21	1:A:82:PHE:CZ	0.93	1.99	12	2
1:A:18:LEU:HD23	1:A:65:VAL:HG11	0.92	1.41	14	1
1:B:103:PHE:CB	1:B:109:VAL:HG22	0.92	1.95	17	4
1:A:17:ALA:HB1	1:A:22:ASP:OD1	0.92	1.64	9	2
1:A:95:VAL:HG22	1:A:121:ILE:HG23	0.92	1.38	9	6
1:B:86:PHE:CE1	1:B:95:VAL:HG23	0.91	2.00	16	11
1:A:32:ASP:O	1:A:48:THR:HG23	0.91	1.65	20	11
1:B:32:ASP:O	1:B:48:THR:HG23	0.90	1.64	4	12
1:B:72:ARG:NH2	1:B:98:ILE:HG21	0.90	1.82	9	1
1:A:79:ALA:HB2	1:A:100:HIS:CD2	0.89	2.02	5	6
1:A:74:VAL:HG11	1:B:40:VAL:CG2	0.89	1.97	13	4
1:B:65:VAL:CG2	1:B:84:VAL:HG12	0.89	1.98	20	1
1:B:71:VAL:H	1:B:72:ARG:HH21	0.89	1.07	17	1
1:B:45:ARG:CG	1:B:50:ALA:HB1	0.88	1.98	6	5
1:A:95:VAL:HG22	1:A:121:ILE:CG1	0.88	1.99	12	7
1:B:103:PHE:CE2	1:B:109:VAL:HG22	0.87	2.05	11	6
1:B:36:VAL:HG11	1:B:54:PHE:CE2	0.87	2.05	9	4
1:A:100:HIS:CE1	1:A:115:LEU:HD12	0.86	2.04	17	2
1:B:79:ALA:HB2	1:B:100:HIS:CD2	0.86	2.04	18	4
1:B:26:ILE:HG21	1:B:55:TYR:CE2	0.86	2.06	18	3
1:A:103:PHE:CD1	1:A:109:VAL:HG22	0.86	2.06	14	4
1:B:61:LEU:HD11	1:B:87:GLU:O	0.86	1.70	11	2
1:A:71:VAL:HG22	1:A:80:PHE:CB	0.86	2.01	2	17
1:A:63:LEU:HD11	1:A:65:VAL:HG23	0.85	1.44	8	4
1:A:77:GLU:OE1	1:B:115:LEU:HD21	0.85	1.72	16	4
1:A:30:PHE:CE1	1:A:51:ILE:HG21	0.85	2.06	1	10
1:A:15:VAL:HG21	1:A:82:PHE:CE2	0.85	2.06	12	2
1:B:55:TYR:O	1:B:59:LEU:HD12	0.85	1.71	8	12
1:A:96:ALA:HB3	1:A:120:ASN:ND2	0.85	1.86	7	1
1:B:7:MET:SD	1:B:73:ALA:HB1	0.85	2.12	6	2
1:A:63:LEU:O	1:A:63:LEU:HD13	0.85	1.72	11	2
1:A:84:VAL:HG22	1:A:86:PHE:CZ	0.84	2.07	14	2
1:A:23:LEU:HD11	1:A:56:ALA:HB2	0.84	1.49	8	3
1:B:71:VAL:HG22	1:B:80:PHE:CB	0.84	2.02	9	16
1:A:15:VAL:HG21	1:A:67:LEU:HD23	0.84	1.47	15	2
1:A:6:HIS:O	1:A:10:VAL:HG23	0.84	1.71	10	6
1:B:30:PHE:CE2	1:B:51:ILE:HG21	0.83	2.07	14	1
1:B:27:VAL:HG13	1:B:48:THR:HG23	0.83	1.51	14	2
1:A:34:ALA:O	1:A:51:ILE:HD11	0.82	1.74	16	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ARG:O	1:A:109:VAL:HG13	0.82	1.75	2	2
1:B:63:LEU:O	1:B:63:LEU:HD13	0.82	1.73	13	1
1:A:79:ALA:HB2	1:A:100:HIS:ND1	0.82	1.88	9	1
1:A:7:MET:CE	1:A:73:ALA:HB1	0.82	2.05	6	13
1:A:86:PHE:CE1	1:A:95:VAL:HG23	0.82	2.10	10	8
1:B:95:VAL:HG22	1:B:121:ILE:HG23	0.82	1.50	19	2
1:B:34:ALA:O	1:B:51:ILE:HD11	0.82	1.74	15	5
1:A:72:ARG:HH21	1:B:120:ASN:HD21	0.82	1.11	16	1
1:A:15:VAL:HG21	1:A:67:LEU:CD2	0.81	2.05	7	3
1:A:7:MET:HG2	1:A:78:ALA:HB2	0.81	1.50	13	3
1:A:73:ALA:O	1:A:74:VAL:HG23	0.81	1.75	3	2
1:A:98:ILE:HG21	1:B:72:ARG:NH2	0.81	1.89	10	2
1:B:98:ILE:HG22	1:B:100:HIS:CE1	0.81	2.10	12	1
1:A:15:VAL:HG11	1:A:82:PHE:CE2	0.81	2.10	12	1
1:B:63:LEU:HD23	1:B:86:PHE:CE2	0.81	2.10	20	1
1:A:11:VAL:O	1:A:15:VAL:HG23	0.81	1.75	3	1
1:B:78:ALA:HB3	1:B:101:PHE:CE1	0.81	2.11	16	2
1:A:95:VAL:HG12	1:A:97:PRO:HD3	0.81	1.51	13	5
1:A:23:LEU:O	1:A:27:VAL:HG23	0.81	1.76	8	10
1:B:23:LEU:O	1:B:27:VAL:HG23	0.81	1.75	18	9
1:B:71:VAL:HG22	1:B:80:PHE:HB2	0.81	1.52	12	17
1:A:115:LEU:HD23	1:B:74:VAL:CG2	0.81	2.06	4	3
1:A:71:VAL:HG22	1:A:80:PHE:HB2	0.80	1.52	20	17
1:A:40:VAL:HB	1:B:75:ALA:HB2	0.80	1.53	11	2
1:A:108:LYS:O	1:A:110:VAL:HG23	0.80	1.75	15	5
1:A:74:VAL:HG21	1:B:116:PHE:O	0.80	1.74	5	2
1:B:117:GLY:O	1:B:121:ILE:HD11	0.80	1.74	2	5
1:A:92:LYS:HB3	1:A:125:ALA:HB3	0.80	1.53	9	2
1:B:95:VAL:HG22	1:B:121:ILE:CG1	0.80	2.06	4	5
1:A:95:VAL:HG22	1:A:121:ILE:HG12	0.80	1.54	6	10
1:A:79:ALA:HB2	1:A:100:HIS:CE1	0.80	2.12	9	2
1:B:7:MET:O	1:B:11:VAL:HG23	0.80	1.76	16	1
1:B:27:VAL:HG21	1:B:52:ARG:CB	0.80	2.07	5	3
1:B:73:ALA:O	1:B:74:VAL:HG23	0.80	1.75	10	2
1:B:65:VAL:HG22	1:B:84:VAL:HB	0.79	1.52	15	4
1:B:64:ALA:HB3	1:B:85:SER:HB3	0.79	1.53	7	2
1:A:71:VAL:HG13	1:A:79:ALA:O	0.79	1.78	11	1
1:A:84:VAL:HG22	1:A:86:PHE:CE2	0.79	2.13	14	2
1:A:67:LEU:HD23	1:A:68:THR:N	0.79	1.92	2	1
1:A:27:VAL:HG21	1:A:52:ARG:HB2	0.79	1.54	14	1
1:A:84:VAL:HG21	1:A:86:PHE:CZ	0.79	2.12	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:HD2	1:B:98:ILE:HD12	0.79	1.54	1	2
1:B:15:VAL:HG21	1:B:82:PHE:CZ	0.79	2.12	11	1
1:B:34:ALA:HB1	1:B:112:MET:HE1	0.79	1.55	19	1
1:B:79:ALA:HB2	1:B:100:HIS:CE1	0.79	2.13	10	2
1:A:98:ILE:HD12	1:B:72:ARG:HD2	0.79	1.55	5	2
1:B:6:HIS:O	1:B:10:VAL:HG23	0.79	1.76	8	3
1:B:23:LEU:HD11	1:B:52:ARG:O	0.79	1.77	18	2
1:B:96:ALA:HB3	1:B:120:ASN:HB2	0.78	1.55	15	2
1:A:63:LEU:HD22	1:A:64:ALA:N	0.78	1.93	8	6
1:B:96:ALA:HB3	1:B:120:ASN:OD1	0.78	1.79	9	1
1:A:71:VAL:H	1:A:72:ARG:HH21	0.77	1.22	14	1
1:A:115:LEU:HD21	1:B:77:GLU:OE1	0.77	1.79	6	1
1:B:67:LEU:CD1	1:B:82:PHE:CZ	0.77	2.67	11	1
1:A:71:VAL:H	1:A:72:ARG:NH2	0.77	1.76	14	1
1:B:45:ARG:HD3	1:B:50:ALA:HB1	0.77	1.56	2	1
1:A:71:VAL:HG22	1:A:80:PHE:HB3	0.77	1.54	11	13
1:B:45:ARG:HG2	1:B:50:ALA:HB1	0.77	1.56	6	2
1:A:115:LEU:HD21	1:B:77:GLU:OE2	0.77	1.79	20	4
1:B:10:VAL:HG13	1:B:29:LEU:HD22	0.77	1.55	7	1
1:B:71:VAL:N	1:B:72:ARG:HH21	0.77	1.77	17	1
1:A:79:ALA:HB1	1:A:100:HIS:CD2	0.77	2.15	15	2
1:B:36:VAL:HG22	1:B:112:MET:SD	0.76	2.21	19	3
1:A:74:VAL:HG13	1:B:40:VAL:HG21	0.76	1.57	8	2
1:A:63:LEU:HD21	1:A:65:VAL:HG23	0.76	1.56	20	3
1:A:45:ARG:HB3	1:A:50:ALA:HB1	0.76	1.57	17	4
1:A:27:VAL:HG21	1:A:52:ARG:HG3	0.76	1.56	9	2
1:B:64:ALA:HB3	1:B:85:SER:HB2	0.76	1.58	14	2
1:A:30:PHE:CE2	1:A:51:ILE:HG21	0.76	2.16	13	2
1:B:22:ASP:O	1:B:26:ILE:HD12	0.76	1.81	18	16
1:B:63:LEU:HD22	1:B:84:VAL:CG2	0.76	2.11	15	2
1:B:38:ASP:OD1	1:B:114:ALA:HB2	0.76	1.81	3	1
1:A:67:LEU:CD1	1:A:82:PHE:CZ	0.76	2.68	12	2
1:A:103:PHE:CE1	1:A:109:VAL:HG22	0.75	2.16	19	3
1:B:95:VAL:HG12	1:B:97:PRO:HD3	0.75	1.58	8	4
1:B:35:THR:HG22	1:B:46:SER:HB3	0.75	1.57	8	3
1:B:95:VAL:HG22	1:B:121:ILE:HG12	0.75	1.57	8	10
1:B:102:ARG:O	1:B:109:VAL:HG13	0.75	1.81	16	3
1:B:35:THR:HG22	1:B:46:SER:CB	0.75	2.12	9	17
1:B:84:VAL:CG2	1:B:86:PHE:CE2	0.75	2.70	8	1
1:B:27:VAL:CG1	1:B:48:THR:HG23	0.74	2.12	6	2
1:A:84:VAL:CG2	1:A:86:PHE:CE2	0.74	2.70	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:11:VAL:HG22	1:B:101:PHE:CZ	0.74	2.17	17	3
1:A:65:VAL:HG22	1:A:84:VAL:HB	0.74	1.58	5	6
1:B:10:VAL:HG13	1:B:29:LEU:CD2	0.74	2.13	7	2
1:B:92:LYS:HB2	1:B:125:ALA:HB3	0.74	1.58	19	1
1:B:72:ARG:CG	1:B:79:ALA:HB3	0.74	2.11	5	2
1:A:23:LEU:HD11	1:A:52:ARG:O	0.74	1.83	2	2
1:B:11:VAL:O	1:B:15:VAL:HG23	0.74	1.81	11	4
1:A:23:LEU:CD1	1:A:56:ALA:HB2	0.74	2.13	8	1
1:A:115:LEU:HD22	1:B:79:ALA:HB2	0.73	1.60	19	1
1:A:103:PHE:CZ	1:A:109:VAL:CG2	0.73	2.71	9	6
1:A:67:LEU:HD12	1:A:68:THR:N	0.73	1.98	14	1
1:B:39:PRO:O	1:B:114:ALA:HB3	0.73	1.84	10	4
1:A:74:VAL:HG13	1:A:75:ALA:N	0.73	1.99	4	3
1:A:26:ILE:HG21	1:A:55:TYR:CE2	0.73	2.18	13	4
1:A:23:LEU:HD11	1:A:56:ALA:HA	0.73	1.60	4	2
1:B:74:VAL:HG13	1:B:75:ALA:N	0.73	1.99	19	2
1:A:79:ALA:HB2	1:A:100:HIS:NE2	0.73	1.98	3	2
1:B:27:VAL:HG21	1:B:52:ARG:HB2	0.73	1.60	14	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.73	2.04	8	3
1:A:120:ASN:CG	1:B:72:ARG:HH21	0.73	1.87	16	1
1:A:38:ASP:HB3	1:A:114:ALA:HB3	0.73	1.58	10	1
1:B:63:LEU:HD22	1:B:84:VAL:HG23	0.72	1.61	15	4
1:A:103:PHE:CD2	1:A:109:VAL:HG22	0.72	2.19	4	10
1:A:103:PHE:CZ	1:A:109:VAL:HG23	0.72	2.19	8	3
1:B:27:VAL:HG21	1:B:52:ARG:HB3	0.72	1.59	5	1
1:B:23:LEU:HD21	1:B:56:ALA:HA	0.72	1.61	18	2
1:B:63:LEU:C	1:B:63:LEU:HD13	0.72	2.05	13	1
1:A:55:TYR:O	1:A:59:LEU:HD12	0.72	1.85	20	5
1:A:22:ASP:O	1:A:26:ILE:HD12	0.72	1.85	9	17
1:A:23:LEU:HD23	1:A:59:LEU:HD13	0.72	1.61	14	2
1:B:67:LEU:C	1:B:67:LEU:HD12	0.72	2.05	18	2
1:B:45:ARG:HG3	1:B:50:ALA:HB1	0.72	1.61	10	3
1:A:121:ILE:HD12	1:A:121:ILE:N	0.72	2.00	13	2
1:B:23:LEU:HD11	1:B:56:ALA:HB2	0.71	1.59	16	6
1:A:63:LEU:HD13	1:A:63:LEU:C	0.71	2.06	20	3
1:A:74:VAL:HG12	1:B:40:VAL:HG21	0.71	1.62	5	1
1:B:65:VAL:HG13	1:B:82:PHE:CD2	0.71	2.20	10	12
1:A:103:PHE:CE2	1:A:109:VAL:CG2	0.71	2.73	9	8
1:A:95:VAL:CG2	1:A:121:ILE:HG23	0.71	2.14	9	3
1:B:103:PHE:CE1	1:B:109:VAL:HG22	0.71	2.20	14	3
1:A:70:GLU:OE1	1:B:98:ILE:HD11	0.71	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG22	1:A:46:SER:HB3	0.71	1.61	20	4
1:A:92:LYS:CB	1:A:125:ALA:HB3	0.71	2.15	9	1
1:B:103:PHE:CE1	1:B:109:VAL:HG23	0.71	2.21	5	2
1:A:35:THR:HG22	1:A:46:SER:CB	0.71	2.16	3	12
1:A:115:LEU:HD21	1:B:77:GLU:CD	0.71	2.06	11	3
1:A:11:VAL:HG21	1:A:80:PHE:CE1	0.70	2.20	12	2
1:B:31:ALA:HB2	1:B:110:VAL:HG22	0.70	1.63	13	8
1:A:11:VAL:HG22	1:A:101:PHE:CZ	0.70	2.20	11	4
1:A:103:PHE:CE2	1:A:109:VAL:HG22	0.70	2.20	4	7
1:B:103:PHE:CE2	1:B:109:VAL:CG2	0.70	2.74	7	7
1:B:69:GLN:NE2	1:B:81:ALA:HB3	0.70	2.02	3	1
1:B:79:ALA:CB	1:B:100:HIS:CE1	0.70	2.74	13	1
1:A:61:LEU:HD23	1:A:63:LEU:HD23	0.70	1.61	7	3
1:B:18:LEU:HD12	1:B:59:LEU:HD11	0.70	1.62	20	2
1:B:3:THR:HG23	1:B:6:HIS:HB2	0.70	1.61	7	6
1:A:34:ALA:HA	1:A:110:VAL:HG13	0.70	1.64	4	4
1:A:30:PHE:CZ	1:A:51:ILE:CG2	0.70	2.75	13	3
1:A:79:ALA:CB	1:A:100:HIS:CD2	0.69	2.74	15	4
1:A:18:LEU:HD23	1:A:65:VAL:CG1	0.69	2.17	14	1
1:B:7:MET:CE	1:B:73:ALA:HB1	0.69	2.17	3	9
1:B:84:VAL:CG2	1:B:86:PHE:CE1	0.69	2.74	11	2
1:B:30:PHE:CG	1:B:112:MET:HE1	0.69	2.22	5	2
1:A:11:VAL:HG22	1:A:101:PHE:CD2	0.69	2.23	5	5
1:A:39:PRO:O	1:A:114:ALA:HB3	0.69	1.86	7	4
1:B:70:GLU:CD	1:B:72:ARG:HH21	0.69	1.90	14	2
1:A:27:VAL:HG21	1:A:52:ARG:CG	0.69	2.17	4	3
1:A:7:MET:HE3	1:A:73:ALA:HB1	0.69	1.64	4	9
1:B:84:VAL:HG21	1:B:86:PHE:CE2	0.69	2.23	8	1
1:B:23:LEU:HD11	1:B:56:ALA:HA	0.69	1.63	14	1
1:B:80:PHE:CZ	1:B:99:ASP:CB	0.69	2.75	13	11
1:A:115:LEU:HD13	1:B:72:ARG:NH1	0.69	2.03	2	1
1:B:7:MET:CG	1:B:103:PHE:CZ	0.69	2.75	17	2
1:B:103:PHE:CG	1:B:109:VAL:HG22	0.69	2.23	17	2
1:B:72:ARG:NE	1:B:79:ALA:HB3	0.69	2.03	20	3
1:A:80:PHE:CE1	1:A:99:ASP:CB	0.68	2.77	6	6
1:A:27:VAL:HG21	1:A:52:ARG:HG2	0.68	1.65	18	1
1:B:96:ALA:HB3	1:B:120:ASN:CG	0.68	2.08	9	1
1:A:115:LEU:HD23	1:B:74:VAL:HG21	0.68	1.64	4	2
1:A:113:ARG:HD3	1:A:115:LEU:HD12	0.68	1.65	4	1
1:A:95:VAL:HG22	1:A:121:ILE:HG13	0.68	1.62	12	3
1:A:98:ILE:HD13	1:B:72:ARG:NE	0.68	2.03	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:VAL:HG13	1:A:82:PHE:CD2	0.68	2.23	8	7
1:A:45:ARG:CG	1:A:50:ALA:HB1	0.68	2.19	15	2
1:B:94:VAL:HG12	1:B:94:VAL:O	0.68	1.86	20	2
1:B:118:GLU:HA	1:B:121:ILE:HD12	0.68	1.63	1	2
1:B:94:VAL:O	1:B:94:VAL:HG12	0.67	1.88	4	2
1:A:80:PHE:CZ	1:A:99:ASP:CB	0.67	2.77	1	13
1:B:27:VAL:CG1	1:B:48:THR:HG22	0.67	2.19	8	2
1:A:63:LEU:HD22	1:A:84:VAL:HG23	0.67	1.64	13	2
1:A:81:ALA:HB2	1:A:98:ILE:HG12	0.67	1.66	10	7
1:B:71:VAL:HG13	1:B:80:PHE:CD1	0.67	2.23	11	1
1:A:18:LEU:HD23	1:A:65:VAL:CG2	0.67	2.19	7	1
1:A:18:LEU:CD2	1:A:65:VAL:HG11	0.67	2.19	14	1
1:A:75:ALA:CB	1:B:40:VAL:HG12	0.67	2.19	19	1
1:B:36:VAL:HG13	1:B:112:MET:HB2	0.67	1.66	8	1
1:A:27:VAL:HG13	1:A:48:THR:CG2	0.67	2.19	12	1
1:B:35:THR:HG22	1:B:46:SER:HB2	0.67	1.65	9	9
1:A:94:VAL:O	1:A:94:VAL:HG13	0.67	1.89	13	4
1:A:19:ASN:ND2	1:A:64:ALA:HB1	0.67	2.05	7	1
1:A:72:ARG:HH21	1:B:120:ASN:HB3	0.67	1.50	4	1
1:A:27:VAL:HG13	1:A:48:THR:HG22	0.67	1.65	1	1
1:A:45:ARG:CD	1:A:50:ALA:HB1	0.67	2.20	19	1
1:B:11:VAL:HG22	1:B:80:PHE:CD1	0.67	2.24	18	1
1:A:11:VAL:HG13	1:A:80:PHE:CE1	0.67	2.25	10	5
1:A:63:LEU:HD13	1:A:63:LEU:O	0.67	1.90	20	3
1:A:103:PHE:CG	1:A:109:VAL:HG22	0.67	2.24	17	1
1:A:118:GLU:HB2	1:B:74:VAL:HG23	0.67	1.65	9	2
1:A:67:LEU:HD23	1:A:81:ALA:O	0.66	1.89	11	2
1:A:117:GLY:O	1:A:121:ILE:HD11	0.66	1.89	12	4
1:A:117:GLY:O	1:A:121:ILE:HD13	0.66	1.90	13	1
1:B:120:ASN:C	1:B:121:ILE:HD12	0.66	2.10	10	2
1:A:80:PHE:CE2	1:A:82:PHE:CD1	0.66	2.83	19	3
1:A:70:GLU:HB2	1:A:81:ALA:HB3	0.66	1.67	2	2
1:A:94:VAL:HG12	1:A:94:VAL:O	0.66	1.89	6	2
1:A:7:MET:CG	1:A:78:ALA:HB2	0.66	2.20	13	1
1:B:108:LYS:O	1:B:110:VAL:HG23	0.66	1.90	4	2
1:B:30:PHE:CE1	1:B:51:ILE:HD13	0.66	2.26	8	3
1:B:63:LEU:C	1:B:63:LEU:HD12	0.66	2.11	8	4
1:A:38:ASP:HB2	1:A:114:ALA:HB3	0.66	1.65	18	3
1:B:15:VAL:HG13	1:B:65:VAL:CG1	0.65	2.21	8	1
1:B:64:ALA:HB3	1:B:85:SER:CB	0.65	2.21	7	3
1:B:36:VAL:HG23	1:B:51:ILE:HG12	0.65	1.68	14	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD23	1:A:63:LEU:CD2	0.65	2.21	7	2
1:A:65:VAL:HG22	1:A:84:VAL:HG12	0.65	1.67	6	2
1:B:80:PHE:CE2	1:B:99:ASP:CB	0.65	2.80	11	2
1:B:45:ARG:NH2	1:B:54:PHE:CE1	0.65	2.65	15	2
1:A:94:VAL:O	1:A:94:VAL:HG12	0.65	1.92	14	3
1:B:7:MET:HE3	1:B:73:ALA:HB1	0.65	1.68	20	3
1:B:45:ARG:CZ	1:B:54:PHE:CG	0.65	2.80	15	2
1:B:32:ASP:O	1:B:48:THR:HG22	0.65	1.92	5	3
1:A:11:VAL:CG2	1:A:80:PHE:CE1	0.65	2.79	12	4
1:B:103:PHE:CD2	1:B:109:VAL:HG22	0.65	2.26	12	5
1:A:45:ARG:NH1	1:A:54:PHE:CE1	0.65	2.65	7	1
1:A:72:ARG:NH2	1:B:120:ASN:HD21	0.65	1.89	16	2
1:B:103:PHE:CZ	1:B:109:VAL:CG2	0.65	2.79	8	4
1:B:14:TYR:CE1	1:B:18:LEU:HD21	0.65	2.26	6	1
1:B:14:TYR:O	1:B:18:LEU:HD23	0.65	1.91	6	2
1:B:27:VAL:HG13	1:B:48:THR:CG2	0.65	2.22	14	2
1:A:70:GLU:HB3	1:A:72:ARG:HH21	0.65	1.51	20	1
1:A:72:ARG:HH21	1:B:120:ASN:CB	0.65	2.05	4	1
1:A:63:LEU:H	1:A:63:LEU:HD12	0.65	1.52	5	1
1:B:72:ARG:CD	1:B:79:ALA:HB3	0.65	2.22	5	2
1:B:36:VAL:HG13	1:B:112:MET:HG3	0.65	1.66	16	1
1:A:40:VAL:CB	1:B:75:ALA:HB2	0.65	2.22	11	2
1:A:36:VAL:HG13	1:A:112:MET:HG3	0.65	1.66	9	3
1:A:98:ILE:HG22	1:A:100:HIS:CE1	0.65	2.27	11	2
1:A:78:ALA:HB3	1:A:101:PHE:HB2	0.65	1.69	18	2
1:A:86:PHE:CZ	1:A:95:VAL:HG23	0.65	2.27	10	2
1:B:71:VAL:HG13	1:B:80:PHE:HB3	0.65	1.68	18	18
1:A:63:LEU:HD22	1:A:64:ALA:H	0.65	1.51	8	1
1:A:103:PHE:CE1	1:A:109:VAL:HG23	0.65	2.27	20	3
1:A:36:VAL:HG13	1:A:112:MET:HE2	0.65	1.69	4	1
1:A:36:VAL:HG21	1:A:51:ILE:HG23	0.64	1.69	11	11
1:B:97:PRO:CB	1:B:116:PHE:CZ	0.64	2.80	8	3
1:A:109:VAL:HG12	1:A:112:MET:SD	0.64	2.32	14	1
1:A:36:VAL:HG23	1:A:51:ILE:HG12	0.64	1.68	17	14
1:A:3:THR:HG23	1:A:6:HIS:HB2	0.64	1.69	12	6
1:B:38:ASP:HB2	1:B:114:ALA:HB3	0.64	1.68	6	2
1:B:103:PHE:CD1	1:B:109:VAL:HG22	0.64	2.27	18	3
1:B:95:VAL:CG2	1:B:121:ILE:HG23	0.64	2.21	20	2
1:B:36:VAL:HG23	1:B:51:ILE:CD1	0.64	2.22	20	3
1:B:11:VAL:CG2	1:B:80:PHE:CD1	0.64	2.81	18	2
1:B:11:VAL:HG22	1:B:101:PHE:CD2	0.64	2.28	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:HH21	1:B:120:ASN:ND2	0.64	1.87	16	2
1:B:95:VAL:HG22	1:B:121:ILE:HG13	0.64	1.70	10	3
1:A:11:VAL:HG22	1:A:80:PHE:CE2	0.64	2.28	13	2
1:A:84:VAL:CG2	1:A:86:PHE:CZ	0.64	2.80	13	5
1:A:77:GLU:CD	1:B:115:LEU:HD21	0.64	2.13	19	2
1:B:63:LEU:HD22	1:B:64:ALA:N	0.64	2.08	13	1
1:B:7:MET:HG2	1:B:78:ALA:HB2	0.64	1.70	13	2
1:A:80:PHE:CE2	1:A:99:ASP:CB	0.64	2.81	12	5
1:A:71:VAL:HG13	1:A:80:PHE:CD1	0.64	2.27	3	2
1:B:72:ARG:HB2	1:B:79:ALA:HB3	0.64	1.67	9	1
1:A:70:GLU:CB	1:A:72:ARG:HH21	0.64	2.06	20	1
1:B:30:PHE:CG	1:B:112:MET:HE2	0.64	2.27	13	1
1:B:30:PHE:HE1	1:B:51:ILE:HD13	0.64	1.52	8	2
1:B:2:ASN:HD22	1:B:2:ASN:N	0.64	1.91	4	1
1:B:103:PHE:HB3	1:B:109:VAL:HG22	0.64	1.70	9	3
1:A:84:VAL:O	1:A:86:PHE:CE1	0.64	2.51	14	2
1:B:15:VAL:HG13	1:B:65:VAL:HG12	0.63	1.69	6	3
1:A:79:ALA:CB	1:A:100:HIS:CE1	0.63	2.78	7	1
1:B:14:TYR:CZ	1:B:18:LEU:HD21	0.63	2.29	6	2
1:B:45:ARG:CZ	1:B:54:PHE:CD1	0.63	2.82	15	2
1:A:23:LEU:CD2	1:A:59:LEU:HD13	0.63	2.23	5	1
1:A:86:PHE:HE1	1:A:95:VAL:HG23	0.63	1.52	7	4
1:A:92:LYS:NZ	1:A:125:ALA:HB2	0.63	2.07	20	1
1:B:82:PHE:CE2	1:B:84:VAL:CG1	0.63	2.81	4	1
1:A:120:ASN:C	1:A:121:ILE:HD12	0.63	2.14	14	2
1:A:63:LEU:HD22	1:A:64:ALA:O	0.63	1.94	9	2
1:B:23:LEU:HD12	1:B:52:ARG:HG3	0.63	1.71	9	3
1:A:40:VAL:HG12	1:A:41:GLY:H	0.63	1.54	19	5
1:B:103:PHE:CE1	1:B:109:VAL:CG2	0.63	2.81	8	5
1:B:67:LEU:HD12	1:B:82:PHE:CZ	0.63	2.29	11	1
1:A:45:ARG:HG2	1:A:50:ALA:HB1	0.63	1.68	15	1
1:B:73:ALA:C	1:B:74:VAL:HG22	0.63	2.13	15	1
1:A:30:PHE:CG	1:A:112:MET:HE2	0.63	2.29	10	1
1:A:103:PHE:CE1	1:A:109:VAL:CG2	0.63	2.82	19	5
1:A:63:LEU:HD22	1:A:86:PHE:CE1	0.63	2.28	17	1
1:A:75:ALA:O	1:A:76:ASN:C	0.62	2.37	2	11
1:A:113:ARG:CD	1:A:115:LEU:HD12	0.62	2.23	4	1
1:B:124:GLY:O	1:B:125:ALA:HB3	0.62	1.94	13	1
1:A:15:VAL:HG11	1:A:67:LEU:H	0.62	1.53	14	2
1:B:30:PHE:CZ	1:B:51:ILE:HG21	0.62	2.29	7	12
1:A:26:ILE:CG2	1:A:55:TYR:CE1	0.62	2.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:PRO:HA	1:B:72:ARG:HH21	0.62	1.52	11	1
1:B:71:VAL:HG22	1:B:80:PHE:HB3	0.62	1.68	20	13
1:B:34:ALA:HB2	1:B:109:VAL:O	0.62	1.94	17	2
1:B:93:THR:HG22	1:B:121:ILE:CG2	0.62	2.24	15	6
1:B:61:LEU:HD21	1:B:87:GLU:H	0.62	1.53	11	2
1:A:95:VAL:HG13	1:A:121:ILE:HG13	0.62	1.71	13	5
1:A:36:VAL:HG11	1:A:54:PHE:CE2	0.62	2.29	18	2
1:B:63:LEU:HD21	1:B:65:VAL:HG23	0.62	1.71	13	1
1:B:97:PRO:CB	1:B:116:PHE:CE1	0.62	2.82	8	4
1:A:64:ALA:HB3	1:A:85:SER:HB3	0.62	1.70	15	1
1:A:94:VAL:CG1	1:A:94:VAL:O	0.62	2.47	13	8
1:A:15:VAL:CG2	1:A:82:PHE:CZ	0.62	2.81	12	1
1:B:15:VAL:CG2	1:B:82:PHE:CE2	0.62	2.77	11	1
1:B:114:ALA:O	1:B:115:LEU:HD12	0.62	1.94	15	1
1:B:3:THR:O	1:B:7:MET:HE2	0.62	1.95	6	1
1:A:18:LEU:CD2	1:A:65:VAL:HG21	0.62	2.25	7	1
1:B:23:LEU:CD1	1:B:56:ALA:HB2	0.62	2.24	20	3
1:A:30:PHE:CD1	1:A:31:ALA:O	0.62	2.52	13	1
1:A:116:PHE:CD1	1:A:116:PHE:O	0.62	2.53	5	3
1:A:30:PHE:CD2	1:A:112:MET:CE	0.62	2.83	9	3
1:B:11:VAL:CG1	1:B:80:PHE:CD1	0.62	2.83	5	3
1:B:11:VAL:HG13	1:B:80:PHE:CZ	0.62	2.30	12	6
1:A:116:PHE:O	1:A:116:PHE:CD1	0.62	2.53	1	4
1:B:80:PHE:CE2	1:B:82:PHE:CD1	0.62	2.88	18	2
1:A:84:VAL:O	1:A:84:VAL:HG22	0.62	1.94	15	3
1:A:7:MET:O	1:A:11:VAL:HG23	0.62	1.95	11	1
1:A:110:VAL:O	1:A:110:VAL:HG12	0.62	1.94	9	5
1:B:18:LEU:HD23	1:B:65:VAL:HG21	0.61	1.70	2	2
1:A:3:THR:HG23	1:A:6:HIS:CB	0.61	2.25	12	7
1:A:7:MET:CG	1:A:103:PHE:CE1	0.61	2.83	3	1
1:B:41:GLY:O	1:B:42:SER:CB	0.61	2.48	19	8
1:B:11:VAL:HG13	1:B:80:PHE:CE1	0.61	2.30	6	7
1:A:4:PRO:HB3	1:A:73:ALA:HB3	0.61	1.71	9	2
1:B:82:PHE:CE2	1:B:84:VAL:HG12	0.61	2.29	14	2
1:B:18:LEU:HA	1:B:26:ILE:HD11	0.61	1.71	10	13
1:B:80:PHE:CZ	1:B:99:ASP:CG	0.61	2.74	14	1
1:A:23:LEU:HG	1:A:56:ALA:HB2	0.61	1.71	13	1
1:A:23:LEU:HD21	1:A:56:ALA:HA	0.61	1.72	5	2
1:B:26:ILE:O	1:B:30:PHE:CE1	0.61	2.54	14	2
1:A:41:GLY:O	1:A:42:SER:CB	0.61	2.49	3	7
1:A:71:VAL:HG13	1:A:80:PHE:HB3	0.61	1.72	6	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:11:VAL:HG22	1:B:101:PHE:HZ	0.61	1.55	17	3
1:B:31:ALA:CB	1:B:110:VAL:HG22	0.61	2.24	13	8
1:A:15:VAL:HG11	1:A:66:GLU:HA	0.61	1.73	8	1
1:B:11:VAL:HG21	1:B:78:ALA:HB1	0.61	1.73	1	1
1:B:67:LEU:HD23	1:B:81:ALA:O	0.61	1.95	19	2
1:A:14:TYR:CE1	1:A:26:ILE:HG23	0.61	2.30	17	1
1:B:21:GLY:HA2	1:B:59:LEU:HD22	0.61	1.72	18	4
1:A:26:ILE:O	1:A:30:PHE:CE1	0.61	2.54	12	1
1:B:15:VAL:HG11	1:B:67:LEU:N	0.61	2.11	2	1
1:A:81:ALA:HB2	1:A:98:ILE:CG1	0.61	2.26	9	2
1:A:31:ALA:CB	1:A:110:VAL:HG22	0.61	2.25	4	8
1:B:30:PHE:HE1	1:B:51:ILE:HG21	0.61	1.51	16	3
1:A:23:LEU:HD11	1:A:56:ALA:CB	0.61	2.25	8	1
1:A:98:ILE:HD11	1:B:70:GLU:OE1	0.61	1.96	13	1
1:A:26:ILE:O	1:A:30:PHE:CE2	0.60	2.54	18	17
1:B:26:ILE:O	1:B:30:PHE:CE2	0.60	2.54	9	15
1:B:26:ILE:O	1:B:30:PHE:CD1	0.60	2.54	1	1
1:B:116:PHE:CD1	1:B:116:PHE:O	0.60	2.54	19	1
1:A:75:ALA:HB3	1:B:40:VAL:HG12	0.60	1.73	19	1
1:B:77:GLU:OE1	1:B:100:HIS:CD2	0.60	2.54	11	1
1:B:45:ARG:NH2	1:B:54:PHE:CD1	0.60	2.69	15	2
1:B:116:PHE:O	1:B:116:PHE:CD1	0.60	2.54	14	2
1:B:69:GLN:HG3	1:B:81:ALA:HB3	0.60	1.73	19	2
1:B:11:VAL:HG22	1:B:80:PHE:CE1	0.60	2.31	4	7
1:A:38:ASP:O	1:A:54:PHE:CZ	0.60	2.54	1	1
1:B:82:PHE:CD1	1:B:99:ASP:OD1	0.60	2.54	14	1
1:A:118:GLU:O	1:A:119:LYS:CB	0.60	2.48	9	2
1:B:79:ALA:HB2	1:B:100:HIS:ND1	0.60	2.11	10	1
1:A:93:THR:CG2	1:A:121:ILE:CG2	0.60	2.79	1	8
1:A:7:MET:SD	1:A:78:ALA:HB2	0.60	2.37	11	1
1:B:75:ALA:O	1:B:76:ASN:C	0.60	2.40	20	11
1:B:86:PHE:CD1	1:B:86:PHE:C	0.60	2.74	10	2
1:A:72:ARG:HG3	1:B:98:ILE:HD12	0.60	1.74	7	1
1:B:8:THR:OG1	1:B:73:ALA:HB2	0.60	1.96	3	1
1:B:38:ASP:O	1:B:54:PHE:CZ	0.60	2.54	1	3
1:B:84:VAL:CG1	1:B:97:PRO:CD	0.60	2.80	2	6
1:B:39:PRO:C	1:B:40:VAL:HG22	0.60	2.16	15	9
1:B:61:LEU:HD23	1:B:63:LEU:HD23	0.60	1.72	9	2
1:A:79:ALA:HB1	1:A:100:HIS:NE2	0.60	2.11	15	1
1:B:11:VAL:HG11	1:B:80:PHE:CD1	0.60	2.32	20	4
1:A:31:ALA:HB2	1:A:110:VAL:HG22	0.60	1.72	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:71:VAL:H	1:B:72:ARG:NH2	0.60	1.88	17	1
1:A:30:PHE:CD2	1:A:112:MET:HE1	0.60	2.32	9	2
1:A:93:THR:HG23	1:A:123:ALA:HA	0.60	1.74	9	1
1:B:38:ASP:CG	1:B:54:PHE:CZ	0.60	2.75	13	1
1:B:82:PHE:CE1	1:B:99:ASP:OD2	0.60	2.55	15	3
1:B:93:THR:CG2	1:B:121:ILE:CG2	0.60	2.80	13	11
1:B:84:VAL:O	1:B:84:VAL:HG22	0.60	1.95	7	3
1:B:48:THR:HA	1:B:51:ILE:HD12	0.60	1.71	6	1
1:A:45:ARG:CZ	1:A:54:PHE:CZ	0.60	2.84	7	2
1:B:18:LEU:HD23	1:B:65:VAL:HG11	0.60	1.73	4	1
1:B:82:PHE:CE1	1:B:99:ASP:OD1	0.60	2.54	4	1
1:A:100:HIS:NE2	1:B:115:LEU:HD11	0.60	2.12	9	1
1:A:8:THR:HG23	1:A:71:VAL:CG1	0.60	2.20	2	4
1:B:7:MET:HE2	1:B:73:ALA:HB1	0.60	1.73	7	3
1:B:38:ASP:OD2	1:B:54:PHE:CZ	0.60	2.55	13	1
1:B:38:ASP:HB3	1:B:114:ALA:HB3	0.60	1.74	2	3
1:B:84:VAL:HG22	1:B:84:VAL:O	0.60	1.97	2	2
1:A:61:LEU:HD12	1:A:62:PRO:HD2	0.60	1.74	7	10
1:A:7:MET:HE1	1:A:73:ALA:HB1	0.60	1.74	3	4
1:B:38:ASP:O	1:B:54:PHE:CE2	0.60	2.55	10	2
1:A:93:THR:HG22	1:A:121:ILE:HG23	0.59	1.74	12	3
1:B:68:THR:CG2	1:B:83:THR:OG1	0.59	2.49	11	15
1:A:84:VAL:CG1	1:A:97:PRO:CD	0.59	2.80	15	4
1:A:11:VAL:HG22	1:A:101:PHE:HZ	0.59	1.56	17	4
1:B:40:VAL:HG12	1:B:41:GLY:H	0.59	1.55	13	5
1:B:95:VAL:HG13	1:B:121:ILE:HG13	0.59	1.74	11	7
1:A:36:VAL:HG22	1:A:112:MET:SD	0.59	2.37	11	3
1:A:82:PHE:CE1	1:A:99:ASP:OD2	0.59	2.55	15	1
1:A:11:VAL:HG22	1:A:80:PHE:CE1	0.59	2.32	9	4
1:B:103:PHE:CZ	1:B:109:VAL:HG23	0.59	2.33	8	2
1:A:103:PHE:CB	1:A:109:VAL:HG22	0.59	2.27	10	1
1:B:36:VAL:HG21	1:B:51:ILE:HG23	0.59	1.74	6	4
1:B:27:VAL:HG13	1:B:48:THR:HG22	0.59	1.74	8	1
1:B:69:GLN:HE21	1:B:81:ALA:HB3	0.59	1.57	3	1
1:A:81:ALA:CB	1:A:98:ILE:CG1	0.59	2.80	9	1
1:A:26:ILE:O	1:A:30:PHE:CD1	0.59	2.55	12	1
1:B:46:SER:O	1:B:50:ALA:HB3	0.59	1.98	16	1
1:A:32:ASP:O	1:A:48:THR:HG22	0.59	1.97	14	6
1:B:99:ASP:OD2	1:B:101:PHE:CZ	0.59	2.55	8	2
1:B:116:PHE:C	1:B:116:PHE:CD1	0.59	2.74	17	3
1:B:38:ASP:OD1	1:B:54:PHE:CD2	0.59	2.55	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:LEU:CD1	1:B:59:LEU:HD11	0.59	2.27	10	1
1:B:67:LEU:HG	1:B:82:PHE:CZ	0.59	2.33	11	1
1:A:77:GLU:OE1	1:A:100:HIS:CE1	0.59	2.55	13	1
1:B:72:ARG:CZ	1:B:79:ALA:HB3	0.59	2.28	10	1
1:A:30:PHE:HE1	1:A:51:ILE:HG21	0.59	1.58	16	4
1:B:26:ILE:O	1:B:30:PHE:CD2	0.59	2.56	9	2
1:A:86:PHE:CD1	1:A:93:THR:O	0.59	2.55	5	4
1:B:102:ARG:HD3	1:B:113:ARG:HH21	0.59	1.58	10	1
1:B:93:THR:HG22	1:B:121:ILE:HG23	0.59	1.75	5	5
1:A:63:LEU:N	1:A:63:LEU:HD12	0.59	2.12	5	1
1:B:84:VAL:HG21	1:B:86:PHE:CZ	0.59	2.33	11	2
1:A:52:ARG:O	1:A:56:ALA:HB2	0.59	1.97	17	4
1:B:95:VAL:HG22	1:B:121:ILE:CD1	0.59	2.28	6	2
1:B:96:ALA:HB3	1:B:120:ASN:ND2	0.59	2.13	5	1
1:B:30:PHE:CD1	1:B:112:MET:CE	0.59	2.86	9	2
1:A:38:ASP:O	1:A:54:PHE:CE1	0.59	2.56	10	1
1:A:103:PHE:CD2	1:A:109:VAL:CG2	0.59	2.84	17	3
1:A:18:LEU:HD23	1:A:65:VAL:HG21	0.59	1.75	7	1
1:B:84:VAL:CG2	1:B:86:PHE:CZ	0.59	2.86	4	1
1:B:23:LEU:HD21	1:B:56:ALA:CA	0.58	2.28	18	2
1:B:63:LEU:C	1:B:63:LEU:CD1	0.58	2.71	8	5
1:A:30:PHE:CE2	1:A:112:MET:CE	0.58	2.85	19	1
1:A:14:TYR:CZ	1:A:18:LEU:HD21	0.58	2.33	13	1
1:B:121:ILE:HD12	1:B:121:ILE:N	0.58	2.13	10	2
1:B:3:THR:HG23	1:B:6:HIS:CB	0.58	2.28	6	6
1:B:86:PHE:CD1	1:B:93:THR:O	0.58	2.56	6	3
1:A:10:VAL:HG13	1:A:29:LEU:HD22	0.58	1.76	7	2
1:A:69:GLN:NE2	1:A:81:ALA:HB3	0.58	2.14	4	2
1:A:101:PHE:CD1	1:A:109:VAL:HG11	0.58	2.32	13	1
1:A:45:ARG:CD	1:A:54:PHE:CD2	0.58	2.87	1	1
1:B:63:LEU:CD2	1:B:84:VAL:HG23	0.58	2.29	19	1
1:A:103:PHE:HB3	1:A:109:VAL:HG22	0.58	1.73	10	1
1:A:39:PRO:C	1:A:40:VAL:HG22	0.58	2.17	12	8
1:A:98:ILE:HG22	1:A:100:HIS:NE2	0.58	2.14	12	2
1:A:97:PRO:CA	1:B:72:ARG:HH21	0.58	2.11	11	1
1:A:3:THR:OG1	1:A:6:HIS:CD2	0.58	2.56	6	1
1:A:11:VAL:HG11	1:A:80:PHE:CD2	0.58	2.33	7	1
1:A:34:ALA:C	1:A:51:ILE:HD11	0.58	2.19	17	1
1:A:117:GLY:HA3	1:B:72:ARG:HH21	0.58	1.56	18	1
1:A:95:VAL:HG12	1:A:97:PRO:CD	0.58	2.28	13	2
1:A:45:ARG:HD3	1:A:50:ALA:HB1	0.58	1.75	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:VAL:HG21	1:B:86:PHE:CE1	0.58	2.32	11	1
1:B:11:VAL:CG2	1:B:80:PHE:CE1	0.58	2.87	14	3
1:B:36:VAL:HG21	1:B:51:ILE:HG12	0.58	1.75	8	2
1:A:98:ILE:HD12	1:B:72:ARG:HG3	0.58	1.76	14	4
1:B:63:LEU:HD12	1:B:63:LEU:H	0.58	1.59	15	1
1:A:15:VAL:HG11	1:A:67:LEU:N	0.58	2.13	2	1
1:A:8:THR:OG1	1:A:73:ALA:HB2	0.58	1.99	5	4
1:A:21:GLY:C	1:A:59:LEU:HD11	0.58	2.18	16	1
1:B:103:PHE:C	1:B:103:PHE:CD1	0.58	2.77	6	1
1:A:40:VAL:HG12	1:A:113:ARG:HH21	0.58	1.59	5	1
1:A:38:ASP:HA	1:A:39:PRO:O	0.57	1.99	9	13
1:A:67:LEU:HG	1:A:82:PHE:CZ	0.57	2.34	3	2
1:B:34:ALA:HA	1:B:110:VAL:HG13	0.57	1.74	11	2
1:A:75:ALA:HB2	1:B:40:VAL:CG1	0.57	2.29	3	1
1:B:11:VAL:HG22	1:B:80:PHE:CZ	0.57	2.34	11	1
1:A:63:LEU:HD11	1:A:65:VAL:CG2	0.57	2.25	8	1
1:A:26:ILE:HG21	1:A:55:TYR:CD2	0.57	2.34	13	1
1:B:80:PHE:CE1	1:B:99:ASP:CB	0.57	2.88	18	5
1:B:36:VAL:HG13	1:B:112:MET:CB	0.57	2.28	8	1
1:A:98:ILE:HG21	1:B:72:ARG:HH21	0.57	1.56	10	1
1:A:100:HIS:CG	1:A:100:HIS:O	0.57	2.58	2	1
1:A:86:PHE:CD1	1:A:86:PHE:C	0.57	2.78	16	2
1:A:103:PHE:CE2	1:A:109:VAL:HG23	0.57	2.35	15	1
1:B:19:ASN:OD1	1:B:64:ALA:HB1	0.57	1.99	6	1
1:A:116:PHE:O	1:B:74:VAL:HG21	0.57	1.99	10	1
1:A:23:LEU:HD12	1:A:52:ARG:HG3	0.57	1.76	2	2
1:A:63:LEU:CD1	1:A:63:LEU:C	0.57	2.73	13	8
1:B:86:PHE:HE1	1:B:95:VAL:HG23	0.57	1.58	16	3
1:A:30:PHE:CG	1:A:112:MET:CE	0.57	2.87	10	3
1:A:67:LEU:HG	1:A:82:PHE:CE1	0.57	2.35	12	2
1:A:84:VAL:HG21	1:A:86:PHE:CE2	0.57	2.32	17	2
1:A:14:TYR:HA	1:A:29:LEU:HD13	0.57	1.77	3	2
1:A:36:VAL:HG23	1:A:51:ILE:CD1	0.57	2.30	10	2
1:B:72:ARG:NH2	1:B:98:ILE:HD13	0.57	2.14	9	1
1:A:69:GLN:N	1:A:69:GLN:NE2	0.57	2.53	2	1
1:A:74:VAL:O	1:A:76:ASN:N	0.57	2.37	19	8
1:A:11:VAL:HG13	1:A:80:PHE:CZ	0.57	2.34	13	4
1:B:38:ASP:CG	1:B:54:PHE:CE1	0.57	2.78	8	1
1:B:61:LEU:HD23	1:B:63:LEU:CD2	0.57	2.29	9	2
1:A:116:PHE:CD1	1:A:117:GLY:N	0.57	2.73	9	1
1:B:95:VAL:HG13	1:B:121:ILE:CG1	0.56	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:PHE:CE1	1:B:74:VAL:HG21	0.56	2.34	19	1
1:A:14:TYR:OH	1:A:55:TYR:CZ	0.56	2.58	17	2
1:A:68:THR:CG2	1:A:83:THR:OG1	0.56	2.53	12	14
1:B:91:ARG:HD2	1:B:123:ALA:HB1	0.56	1.76	3	1
1:A:100:HIS:CD2	1:A:100:HIS:O	0.56	2.58	2	1
1:B:80:PHE:CE2	1:B:99:ASP:HB3	0.56	2.36	11	3
1:A:100:HIS:N	1:A:100:HIS:ND1	0.56	2.54	11	1
1:B:38:ASP:CG	1:B:54:PHE:CD1	0.56	2.79	8	1
1:B:63:LEU:HD23	1:B:86:PHE:CD1	0.56	2.34	8	1
1:B:110:VAL:HG12	1:B:110:VAL:O	0.56	2.00	13	3
1:B:77:GLU:OE2	1:B:100:HIS:CE1	0.56	2.58	4	1
1:A:45:ARG:CB	1:A:50:ALA:HB1	0.56	2.30	17	2
1:B:86:PHE:CD1	1:B:86:PHE:O	0.56	2.58	19	1
1:B:80:PHE:CZ	1:B:99:ASP:HB2	0.56	2.35	19	13
1:B:80:PHE:CE2	1:B:99:ASP:HB2	0.56	2.36	11	6
1:B:14:TYR:HA	1:B:29:LEU:HD13	0.56	1.77	11	1
1:A:18:LEU:HD12	1:A:59:LEU:HD11	0.56	1.78	7	1
1:B:80:PHE:CE2	1:B:99:ASP:OD2	0.56	2.58	14	2
1:A:5:GLU:O	1:A:9:ALA:HB2	0.56	2.01	7	8
1:B:80:PHE:CZ	1:B:99:ASP:HB3	0.56	2.36	19	9
1:A:98:ILE:CG2	1:A:100:HIS:NE2	0.56	2.69	4	4
1:A:72:ARG:CZ	1:B:120:ASN:ND2	0.56	2.69	7	3
1:A:27:VAL:HG21	1:A:52:ARG:CB	0.56	2.30	14	1
1:B:11:VAL:CG1	1:B:80:PHE:CG	0.56	2.88	5	2
1:B:61:LEU:HD23	1:B:63:LEU:HG	0.56	1.78	17	3
1:B:23:LEU:HG	1:B:56:ALA:HB2	0.56	1.78	12	1
1:B:18:LEU:HD23	1:B:65:VAL:HB	0.56	1.78	16	1
1:B:86:PHE:CZ	1:B:93:THR:CG2	0.56	2.89	1	2
1:A:17:ALA:O	1:A:26:ILE:HD11	0.56	2.00	10	2
1:B:80:PHE:CE2	1:B:99:ASP:CG	0.56	2.80	14	2
1:A:74:VAL:HG12	1:A:75:ALA:H	0.56	1.60	19	1
1:A:40:VAL:HG12	1:A:113:ARG:NH2	0.56	2.15	5	1
1:A:74:VAL:CG1	1:A:75:ALA:N	0.56	2.69	7	4
1:B:84:VAL:HG23	1:B:86:PHE:CE1	0.56	2.35	11	2
1:B:95:VAL:HG22	1:B:121:ILE:CG2	0.56	2.31	20	1
1:A:95:VAL:HG13	1:A:121:ILE:CG1	0.56	2.31	1	3
1:B:38:ASP:CG	1:B:54:PHE:CD2	0.56	2.80	5	1
1:A:103:PHE:O	1:A:104:ASN:CB	0.56	2.54	9	3
1:B:117:GLY:O	1:B:121:ILE:HD12	0.56	2.00	8	2
1:A:3:THR:OG1	1:A:6:HIS:CG	0.56	2.59	5	1
1:B:69:GLN:HB2	1:B:81:ALA:HB3	0.56	1.78	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:PHE:CE2	1:A:51:ILE:CG2	0.56	2.89	13	1
1:B:38:ASP:HA	1:B:39:PRO:O	0.55	2.02	2	9
1:B:98:ILE:CG2	1:B:100:HIS:CE1	0.55	2.88	12	1
1:A:40:VAL:CG1	1:B:75:ALA:CB	0.55	2.84	13	2
1:A:27:VAL:CG1	1:A:48:THR:HG22	0.55	2.30	8	2
1:B:116:PHE:CG	1:B:116:PHE:O	0.55	2.59	13	1
1:A:26:ILE:O	1:A:30:PHE:CD2	0.55	2.59	3	5
1:B:5:GLU:O	1:B:9:ALA:HB2	0.55	2.01	3	6
1:A:80:PHE:CE2	1:A:99:ASP:HB3	0.55	2.36	12	6
1:B:1:MET:O	1:B:3:THR:HG22	0.55	2.00	16	1
1:A:74:VAL:HG13	1:A:75:ALA:H	0.55	1.62	2	3
1:A:116:PHE:O	1:A:116:PHE:CG	0.55	2.59	8	6
1:A:74:VAL:HG12	1:B:115:LEU:HD23	0.55	1.78	9	1
1:B:91:ARG:CD	1:B:123:ALA:HB1	0.55	2.32	9	1
1:B:69:GLN:HE22	1:B:81:ALA:HB3	0.55	1.62	13	1
1:A:80:PHE:CZ	1:A:99:ASP:HB3	0.55	2.37	2	7
1:B:69:GLN:NE2	1:B:81:ALA:CB	0.55	2.70	4	3
1:B:74:VAL:O	1:B:76:ASN:N	0.55	2.39	7	8
1:B:69:GLN:CB	1:B:81:ALA:HB3	0.55	2.31	9	3
1:A:96:ALA:HB3	1:A:120:ASN:OD1	0.55	2.01	1	1
1:B:30:PHE:CD1	1:B:112:MET:HE2	0.55	2.37	9	2
1:B:17:ALA:HB1	1:B:22:ASP:OD1	0.55	2.02	9	1
1:A:95:VAL:HG22	1:A:121:ILE:CG2	0.55	2.31	13	2
1:B:80:PHE:N	1:B:80:PHE:CD1	0.55	2.75	11	2
1:B:103:PHE:HB3	1:B:109:VAL:HG13	0.55	1.78	17	3
1:B:7:MET:HA	1:B:103:PHE:CZ	0.55	2.36	3	2
1:B:84:VAL:HG23	1:B:95:VAL:HB	0.55	1.79	20	1
1:A:69:GLN:HG3	1:A:81:ALA:HB3	0.55	1.78	1	1
1:A:117:GLY:O	1:A:121:ILE:HD12	0.55	2.01	5	1
1:A:80:PHE:CZ	1:A:99:ASP:HB2	0.55	2.37	9	17
1:A:80:PHE:CE1	1:A:99:ASP:HB3	0.55	2.37	10	13
1:A:18:LEU:HA	1:A:26:ILE:HD11	0.55	1.78	7	8
1:A:80:PHE:CE2	1:A:99:ASP:HB2	0.55	2.37	3	6
1:B:86:PHE:CZ	1:B:95:VAL:HG23	0.55	2.37	16	1
1:A:79:ALA:HB3	1:B:115:LEU:HD22	0.55	1.77	10	3
1:A:27:VAL:CG1	1:A:48:THR:CG2	0.55	2.85	12	1
1:B:23:LEU:CD2	1:B:59:LEU:CD1	0.55	2.85	12	1
1:A:38:ASP:O	1:A:54:PHE:CE2	0.55	2.60	16	1
1:B:102:ARG:NE	1:B:111:SER:CB	0.55	2.70	15	1
1:B:27:VAL:HG21	1:B:52:ARG:CA	0.55	2.32	5	2
1:A:45:ARG:CZ	1:A:54:PHE:CE2	0.55	2.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD22	1:A:84:VAL:CG2	0.55	2.32	13	2
1:A:14:TYR:CE1	1:A:18:LEU:HD21	0.55	2.37	13	1
1:B:67:LEU:HD11	1:B:80:PHE:CD2	0.55	2.37	9	2
1:A:67:LEU:HD12	1:A:68:THR:H	0.55	1.60	14	1
1:A:40:VAL:HG11	1:B:74:VAL:CG1	0.55	2.31	19	1
1:A:121:ILE:N	1:A:121:ILE:CD1	0.55	2.70	13	1
1:A:100:HIS:CD2	1:A:100:HIS:C	0.54	2.80	10	3
1:A:63:LEU:HD12	1:A:63:LEU:C	0.54	2.22	19	3
1:B:7:MET:HG3	1:B:103:PHE:CZ	0.54	2.37	17	1
1:B:110:VAL:O	1:B:110:VAL:HG12	0.54	2.02	12	6
1:A:86:PHE:CZ	1:A:93:THR:HB	0.54	2.37	8	9
1:B:63:LEU:CD2	1:B:86:PHE:CE1	0.54	2.75	8	3
1:B:54:PHE:CD1	1:B:54:PHE:C	0.54	2.79	13	2
1:A:80:PHE:CE1	1:A:99:ASP:HB2	0.54	2.37	6	3
1:A:41:GLY:O	1:A:42:SER:C	0.54	2.45	17	1
1:A:72:ARG:HH21	1:B:97:PRO:HA	0.54	1.63	18	1
1:B:70:GLU:HB2	1:B:81:ALA:HB3	0.54	1.80	2	1
1:B:74:VAL:CG1	1:B:75:ALA:N	0.54	2.70	6	3
1:B:37:GLU:O	1:B:37:GLU:CG	0.54	2.55	14	1
1:B:68:THR:HG23	1:B:69:GLN:NE2	0.54	2.17	19	1
1:B:10:VAL:HG21	1:B:103:PHE:CZ	0.54	2.37	13	1
1:B:122:HIS:CD2	1:B:122:HIS:N	0.54	2.75	13	3
1:A:69:GLN:NE2	1:A:70:GLU:O	0.54	2.40	9	3
1:B:70:GLU:O	1:B:80:PHE:HA	0.54	2.03	2	2
1:A:67:LEU:CG	1:A:82:PHE:CZ	0.54	2.91	12	2
1:A:40:VAL:CG1	1:B:75:ALA:HB2	0.54	2.32	11	3
1:B:79:ALA:HB2	1:B:100:HIS:NE2	0.54	2.16	18	1
1:B:11:VAL:HG13	1:B:80:PHE:CD1	0.54	2.38	5	2
1:B:86:PHE:CZ	1:B:93:THR:HB	0.54	2.37	16	7
1:B:95:VAL:HG11	1:B:116:PHE:CZ	0.54	2.38	6	1
1:A:72:ARG:CZ	1:B:96:ALA:O	0.54	2.56	4	1
1:A:23:LEU:CD2	1:A:59:LEU:HD12	0.54	2.33	2	2
1:B:39:PRO:O	1:B:114:ALA:CB	0.54	2.56	8	4
1:B:94:VAL:O	1:B:94:VAL:CG1	0.54	2.56	20	12
1:A:63:LEU:HD12	1:A:63:LEU:H	0.54	1.63	16	1
1:B:67:LEU:HG	1:B:82:PHE:CE1	0.54	2.38	11	1
1:A:73:ALA:O	1:B:118:GLU:CB	0.54	2.55	19	1
1:A:116:PHE:CD1	1:A:116:PHE:C	0.54	2.78	11	1
1:B:30:PHE:CG	1:B:112:MET:CE	0.54	2.90	5	3
1:A:86:PHE:CD1	1:A:86:PHE:N	0.54	2.76	14	1
1:A:84:VAL:CG2	1:A:84:VAL:O	0.53	2.56	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:97:PRO:HB3	1:B:116:PHE:CZ	0.53	2.38	8	3
1:B:27:VAL:HG22	1:B:51:ILE:CG2	0.53	2.33	13	2
1:A:115:LEU:HD22	1:B:79:ALA:HB3	0.53	1.80	1	1
1:A:115:LEU:HD22	1:B:79:ALA:CB	0.53	2.33	19	2
1:A:10:VAL:HG21	1:A:103:PHE:HZ	0.53	1.63	15	2
1:A:92:LYS:CE	1:A:125:ALA:HB2	0.53	2.32	20	1
1:A:98:ILE:HD12	1:B:72:ARG:CD	0.53	2.31	5	1
1:B:31:ALA:HB3	1:B:109:VAL:O	0.53	2.03	17	1
1:B:38:ASP:CB	1:B:54:PHE:CZ	0.53	2.92	8	2
1:A:110:VAL:O	1:A:110:VAL:CG1	0.53	2.55	9	3
1:A:45:ARG:HD3	1:A:54:PHE:CD2	0.53	2.39	1	2
1:B:14:TYR:C	1:B:14:TYR:CD1	0.53	2.81	4	1
1:B:65:VAL:HG22	1:B:84:VAL:CB	0.53	2.32	15	1
1:B:23:LEU:HD21	1:B:59:LEU:HD12	0.53	1.80	7	2
1:B:65:VAL:HG13	1:B:82:PHE:HD2	0.53	1.63	14	5
1:B:7:MET:HG2	1:B:103:PHE:CZ	0.53	2.37	17	2
1:B:118:GLU:O	1:B:119:LYS:CB	0.53	2.56	19	1
1:B:72:ARG:HH21	1:B:98:ILE:HG21	0.53	1.62	9	1
1:B:79:ALA:HB2	1:B:100:HIS:CG	0.53	2.38	10	1
1:A:15:VAL:CG2	1:A:82:PHE:CE2	0.53	2.87	12	2
1:A:7:MET:HG2	1:A:103:PHE:CE1	0.53	2.38	3	1
1:A:40:VAL:HG12	1:B:75:ALA:HB2	0.53	1.80	1	1
1:A:70:GLU:O	1:A:71:VAL:CG2	0.53	2.57	14	1
1:A:98:ILE:HG21	1:B:72:ARG:NH1	0.53	2.18	9	1
1:B:18:LEU:CA	1:B:26:ILE:HD11	0.53	2.34	10	1
1:B:36:VAL:HG13	1:B:112:MET:HG2	0.53	1.78	2	1
1:A:95:VAL:HG22	1:A:121:ILE:CD1	0.53	2.33	16	3
1:A:68:THR:HG22	1:A:83:THR:OG1	0.53	2.04	14	7
1:B:11:VAL:HG21	1:B:80:PHE:CE1	0.53	2.38	14	2
1:B:4:PRO:O	1:B:8:THR:CB	0.53	2.57	7	3
1:A:15:VAL:HG21	1:A:67:LEU:HD21	0.53	1.79	6	1
1:B:8:THR:HG23	1:B:71:VAL:HB	0.53	1.80	19	2
1:B:39:PRO:C	1:B:40:VAL:CG2	0.53	2.77	14	12
1:A:98:ILE:HG22	1:A:100:HIS:CD2	0.53	2.38	12	1
1:B:74:VAL:O	1:B:77:GLU:CG	0.53	2.57	11	2
1:A:35:THR:HG22	1:A:46:SER:HB2	0.53	1.80	17	7
1:A:121:ILE:N	1:A:121:ILE:HD12	0.53	2.19	14	1
1:A:36:VAL:HG11	1:A:55:TYR:CE2	0.53	2.39	17	1
1:B:84:VAL:HG13	1:B:95:VAL:HB	0.53	1.81	12	3
1:B:97:PRO:HB3	1:B:116:PHE:CE1	0.53	2.39	15	3
1:B:80:PHE:CE1	1:B:99:ASP:HB3	0.53	2.38	18	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:CB	1:A:79:ALA:O	0.53	2.57	1	1
1:A:26:ILE:HG22	1:A:30:PHE:HE2	0.53	1.64	17	4
1:A:75:ALA:O	1:A:77:GLU:N	0.53	2.41	19	12
1:B:17:ALA:HB1	1:B:26:ILE:HG13	0.53	1.80	18	3
1:A:103:PHE:C	1:A:103:PHE:CD1	0.53	2.82	10	1
1:A:72:ARG:NH2	1:B:117:GLY:N	0.53	2.58	15	1
1:A:69:GLN:CG	1:A:81:ALA:O	0.53	2.57	8	2
1:B:84:VAL:CG2	1:B:84:VAL:O	0.53	2.57	13	7
1:B:32:ASP:C	1:B:48:THR:OG1	0.53	2.47	14	2
1:A:7:MET:HG3	1:A:103:PHE:CE1	0.53	2.38	3	1
1:A:7:MET:HA	1:A:103:PHE:CZ	0.53	2.39	5	1
1:B:64:ALA:HB3	1:B:85:SER:O	0.53	2.04	17	1
1:B:34:ALA:HB2	1:B:110:VAL:HA	0.52	1.80	14	4
1:B:11:VAL:CG1	1:B:80:PHE:CE1	0.52	2.93	7	4
1:B:122:HIS:N	1:B:122:HIS:CD2	0.52	2.76	17	5
1:A:39:PRO:O	1:A:114:ALA:CB	0.52	2.57	7	3
1:A:97:PRO:CB	1:A:116:PHE:CZ	0.52	2.92	3	1
1:A:11:VAL:HG11	1:A:80:PHE:CD1	0.52	2.39	4	2
1:A:118:GLU:CB	1:B:74:VAL:HG23	0.52	2.34	9	1
1:B:52:ARG:O	1:B:56:ALA:HB2	0.52	2.04	5	4
1:A:42:SER:O	1:A:43:GLU:CB	0.52	2.57	17	4
1:B:27:VAL:CG1	1:B:48:THR:CG2	0.52	2.87	14	4
1:A:18:LEU:CA	1:A:26:ILE:HD11	0.52	2.35	7	2
1:B:68:THR:CG2	1:B:69:GLN:NE2	0.52	2.72	19	1
1:B:72:ARG:HG2	1:B:79:ALA:HB3	0.52	1.80	5	1
1:A:23:LEU:HD12	1:A:52:ARG:HG2	0.52	1.81	13	1
1:A:72:ARG:NH2	1:B:120:ASN:ND2	0.52	2.57	7	5
1:A:71:VAL:CG1	1:A:79:ALA:O	0.52	2.55	11	1
1:B:38:ASP:HB2	1:B:54:PHE:CZ	0.52	2.39	5	2
1:A:30:PHE:CD2	1:A:112:MET:HE3	0.52	2.40	19	2
1:A:72:ARG:HH21	1:B:96:ALA:C	0.52	2.08	5	1
1:A:63:LEU:CD2	1:A:64:ALA:O	0.52	2.57	10	2
1:A:86:PHE:CZ	1:A:93:THR:CG2	0.52	2.93	5	5
1:A:78:ALA:HB3	1:A:101:PHE:CE1	0.52	2.40	10	2
1:A:98:ILE:CG2	1:B:72:ARG:NH2	0.52	2.69	10	2
1:A:94:VAL:O	1:A:94:VAL:CG1	0.52	2.58	14	10
1:A:63:LEU:CB	1:A:85:SER:O	0.52	2.57	5	2
1:A:32:ASP:HA	1:A:48:THR:HG23	0.52	1.82	1	1
1:A:63:LEU:O	1:A:63:LEU:HD12	0.52	2.05	12	2
1:B:86:PHE:C	1:B:86:PHE:CD1	0.52	2.83	19	1
1:B:79:ALA:HB1	1:B:100:HIS:CE1	0.52	2.39	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:C	1:A:63:LEU:CD1	0.52	2.79	11	5
1:A:45:ARG:HD2	1:A:54:PHE:CE1	0.52	2.40	11	1
1:A:92:LYS:HE3	1:A:125:ALA:HB2	0.52	1.82	20	1
1:B:63:LEU:CD1	1:B:63:LEU:C	0.52	2.77	3	4
1:B:22:ASP:O	1:B:26:ILE:CG1	0.52	2.58	6	11
1:A:3:THR:O	1:A:7:MET:SD	0.52	2.68	7	6
1:B:73:ALA:C	1:B:74:VAL:CG2	0.52	2.79	15	4
1:A:69:GLN:NE2	1:A:81:ALA:CB	0.52	2.73	19	3
1:A:97:PRO:HB3	1:A:116:PHE:CE1	0.52	2.40	3	3
1:A:15:VAL:CG1	1:A:82:PHE:CE2	0.52	2.90	12	1
1:B:61:LEU:HD23	1:B:86:PHE:HD1	0.52	1.65	8	1
1:B:72:ARG:CB	1:B:79:ALA:O	0.52	2.58	3	2
1:A:72:ARG:NH2	1:B:120:ASN:CB	0.52	2.73	5	2
1:A:68:THR:HG21	1:A:83:THR:HG23	0.52	1.81	1	1
1:B:117:GLY:HA2	1:B:121:ILE:HD11	0.52	1.81	19	1
1:B:45:ARG:NH2	1:B:54:PHE:CD2	0.52	2.78	19	1
1:A:27:VAL:HG13	1:A:48:THR:OG1	0.52	2.04	13	1
1:B:40:VAL:HG13	1:B:115:LEU:HG	0.52	1.81	10	1
1:A:93:THR:HG22	1:A:121:ILE:CG2	0.52	2.35	2	4
1:A:63:LEU:HD21	1:A:84:VAL:HB	0.52	1.81	8	3
1:B:39:PRO:HB3	1:B:116:PHE:CD1	0.52	2.40	7	3
1:B:69:GLN:NE2	1:B:81:ALA:C	0.52	2.63	4	9
1:B:100:HIS:CD2	1:B:100:HIS:O	0.52	2.63	6	1
1:B:8:THR:OG1	1:B:73:ALA:CB	0.52	2.58	3	1
1:A:39:PRO:HB3	1:A:116:PHE:CD1	0.52	2.40	10	3
1:A:22:ASP:C	1:A:26:ILE:HD12	0.52	2.24	4	1
1:B:77:GLU:HG2	1:B:100:HIS:CE1	0.52	2.40	19	3
1:B:111:SER:N	1:B:112:MET:CE	0.52	2.73	19	1
1:B:70:GLU:O	1:B:71:VAL:CG2	0.51	2.58	2	2
1:B:93:THR:CG2	1:B:121:ILE:HG22	0.51	2.36	2	2
1:B:94:VAL:CG1	1:B:94:VAL:O	0.51	2.58	8	5
1:A:116:PHE:CG	1:A:116:PHE:O	0.51	2.62	15	3
1:B:67:LEU:HD22	1:B:82:PHE:HB3	0.51	1.83	9	1
1:A:23:LEU:CD2	1:A:59:LEU:CD1	0.51	2.88	2	1
1:A:80:PHE:CZ	1:A:101:PHE:CZ	0.51	2.98	2	1
1:A:122:HIS:N	1:A:122:HIS:CD2	0.51	2.78	14	3
1:A:10:VAL:HG11	1:A:103:PHE:CZ	0.51	2.40	14	1
1:A:5:GLU:O	1:A:9:ALA:CB	0.51	2.58	12	8
1:A:39:PRO:CB	1:A:116:PHE:CD1	0.51	2.94	10	3
1:B:40:VAL:HG22	1:B:114:ALA:O	0.51	2.05	3	2
1:B:70:GLU:CB	1:B:72:ARG:HH21	0.51	2.18	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:PHE:CE1	1:A:101:PHE:CZ	0.51	2.98	2	2
1:A:74:VAL:O	1:A:75:ALA:C	0.51	2.48	2	2
1:B:113:ARG:CD	1:B:113:ARG:N	0.51	2.73	2	1
1:A:80:PHE:CE1	1:A:82:PHE:CD1	0.51	2.98	18	3
1:A:74:VAL:HG12	1:A:75:ALA:N	0.51	2.21	19	1
1:B:116:PHE:CE1	1:B:117:GLY:O	0.51	2.64	9	1
1:A:52:ARG:O	1:A:56:ALA:CB	0.51	2.58	17	7
1:A:98:ILE:HD11	1:B:72:ARG:CZ	0.51	2.36	8	1
1:B:11:VAL:HG13	1:B:80:PHE:CE2	0.51	2.40	1	2
1:B:38:ASP:OD2	1:B:114:ALA:CB	0.51	2.59	18	2
1:B:31:ALA:CB	1:B:109:VAL:O	0.51	2.59	17	1
1:A:27:VAL:HA	1:A:30:PHE:CE2	0.51	2.40	13	1
1:A:11:VAL:HG13	1:A:80:PHE:CE2	0.51	2.39	16	4
1:A:63:LEU:CD2	1:A:86:PHE:CE1	0.51	2.94	19	3
1:B:110:VAL:C	1:B:112:MET:CE	0.51	2.79	19	1
1:A:11:VAL:CG1	1:A:80:PHE:CD1	0.51	2.93	2	3
1:A:48:THR:O	1:A:52:ARG:CB	0.51	2.59	17	7
1:A:67:LEU:HB2	1:A:82:PHE:CE2	0.51	2.40	12	1
1:B:63:LEU:CB	1:B:85:SER:O	0.51	2.59	12	5
1:A:32:ASP:C	1:A:48:THR:HG23	0.51	2.26	4	3
1:B:38:ASP:CB	1:B:114:ALA:HB3	0.51	2.36	17	3
1:A:27:VAL:HG11	1:A:48:THR:OG1	0.51	2.04	9	1
1:B:100:HIS:ND1	1:B:100:HIS:N	0.51	2.58	12	1
1:B:3:THR:OG1	1:B:6:HIS:CG	0.51	2.64	15	1
1:B:42:SER:O	1:B:43:GLU:CB	0.51	2.59	5	5
1:B:116:PHE:O	1:B:116:PHE:CG	0.51	2.62	20	2
1:B:69:GLN:CD	1:B:70:GLU:N	0.51	2.64	3	1
1:B:23:LEU:HD21	1:B:55:TYR:CB	0.51	2.36	13	1
1:A:22:ASP:O	1:A:26:ILE:CD1	0.51	2.59	16	13
1:A:79:ALA:HB2	1:B:115:LEU:HD22	0.51	1.82	12	1
1:A:84:VAL:HG22	1:A:95:VAL:HB	0.51	1.83	17	3
1:A:39:PRO:HB2	1:A:116:PHE:CD1	0.51	2.41	5	4
1:B:97:PRO:HB3	1:B:116:PHE:CD1	0.51	2.41	7	5
1:B:23:LEU:CD2	1:B:55:TYR:CB	0.51	2.88	13	2
1:A:22:ASP:O	1:A:26:ILE:CG1	0.51	2.59	8	15
1:A:72:ARG:CZ	1:B:120:ASN:OD1	0.51	2.59	16	3
1:A:100:HIS:CE1	1:A:115:LEU:CD1	0.51	2.94	11	1
1:A:120:ASN:OD1	1:B:72:ARG:CZ	0.51	2.59	7	1
1:B:10:VAL:HG21	1:B:103:PHE:HZ	0.51	1.64	13	2
1:A:39:PRO:C	1:A:40:VAL:CG2	0.50	2.78	3	11
1:B:52:ARG:O	1:B:56:ALA:CB	0.50	2.59	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:GLY:O	1:A:121:ILE:CD1	0.50	2.59	8	6
1:A:45:ARG:HG2	1:A:54:PHE:CE1	0.50	2.41	6	1
1:A:67:LEU:HD22	1:A:82:PHE:CB	0.50	2.36	6	1
1:A:98:ILE:HD12	1:B:72:ARG:HE	0.50	1.64	3	1
1:B:69:GLN:NE2	1:B:81:ALA:HB1	0.50	2.21	4	1
1:B:124:GLY:O	1:B:125:ALA:HB2	0.50	2.06	14	1
1:B:33:ASP:O	1:B:34:ALA:O	0.50	2.29	14	1
1:A:45:ARG:NE	1:A:54:PHE:CZ	0.50	2.79	17	1
1:B:103:PHE:HB2	1:B:109:VAL:HG22	0.50	1.82	17	2
1:A:72:ARG:CZ	1:B:120:ASN:CG	0.50	2.79	18	1
1:B:22:ASP:O	1:B:26:ILE:CD1	0.50	2.59	16	11
1:A:84:VAL:HG13	1:A:95:VAL:HB	0.50	1.82	14	3
1:A:23:LEU:HD21	1:A:56:ALA:CA	0.50	2.36	5	1
1:A:72:ARG:CD	1:B:115:LEU:O	0.50	2.59	5	1
1:B:38:ASP:OD1	1:B:54:PHE:CE2	0.50	2.64	13	1
1:A:115:LEU:HD22	1:B:72:ARG:HH11	0.50	1.66	10	1
1:A:70:GLU:O	1:A:80:PHE:HA	0.50	2.06	14	2
1:A:8:THR:OG1	1:A:73:ALA:CB	0.50	2.59	12	2
1:B:95:VAL:HG12	1:B:96:ALA:N	0.50	2.22	6	12
1:A:7:MET:HE2	1:A:73:ALA:HB1	0.50	1.83	9	4
1:B:34:ALA:CB	1:B:110:VAL:HA	0.50	2.36	14	5
1:B:75:ALA:O	1:B:77:GLU:CG	0.50	2.60	8	1
1:A:57:ASN:ND2	1:A:58:SER:N	0.50	2.60	2	2
1:B:84:VAL:O	1:B:84:VAL:CG2	0.50	2.60	7	4
1:A:115:LEU:CD2	1:B:77:GLU:OE1	0.50	2.59	12	2
1:A:32:ASP:O	1:A:48:THR:CG2	0.50	2.59	13	3
1:B:23:LEU:HG	1:B:59:LEU:HD13	0.50	1.83	14	1
1:B:38:ASP:OD2	1:B:54:PHE:CE1	0.50	2.64	13	1
1:B:48:THR:O	1:B:52:ARG:CB	0.50	2.59	12	7
1:B:5:GLU:O	1:B:9:ALA:CB	0.50	2.60	3	8
1:A:50:ALA:O	1:A:54:PHE:CB	0.50	2.60	8	3
1:B:102:ARG:CZ	1:B:111:SER:OG	0.50	2.60	8	1
1:B:40:VAL:CG2	1:B:114:ALA:O	0.50	2.60	17	3
1:B:39:PRO:HB2	1:B:116:PHE:CD1	0.50	2.42	14	3
1:B:38:ASP:CG	1:B:114:ALA:HB3	0.50	2.26	9	1
1:A:72:ARG:NE	1:B:120:ASN:ND2	0.50	2.60	10	2
1:A:23:LEU:O	1:A:27:VAL:CG2	0.50	2.59	2	8
1:A:45:ARG:HG3	1:A:54:PHE:CD1	0.50	2.41	6	2
1:B:78:ALA:O	1:B:80:PHE:CE1	0.50	2.64	11	1
1:B:67:LEU:HG	1:B:82:PHE:CE2	0.50	2.41	11	1
1:A:84:VAL:O	1:A:84:VAL:CG2	0.50	2.59	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:VAL:HG21	1:B:116:PHE:CZ	0.50	2.42	6	1
1:A:14:TYR:CE1	1:A:26:ILE:CG2	0.50	2.93	17	1
1:A:11:VAL:CG2	1:A:80:PHE:CD2	0.50	2.94	13	1
1:B:55:TYR:OH	1:B:112:MET:CE	0.50	2.60	12	2
1:B:57:ASN:O	1:B:60:LYS:CG	0.50	2.60	3	2
1:A:45:ARG:CD	1:A:54:PHE:CE1	0.50	2.95	11	1
1:A:36:VAL:HG11	1:A:55:TYR:HE1	0.50	1.66	11	2
1:B:45:ARG:CB	1:B:50:ALA:HB1	0.50	2.37	11	1
1:B:49:ALA:O	1:B:53:GLU:CG	0.50	2.60	11	3
1:A:36:VAL:O	1:A:44:PRO:CB	0.50	2.60	15	2
1:A:64:ALA:HB3	1:A:85:SER:CB	0.50	2.36	15	1
1:B:49:ALA:O	1:B:53:GLU:CB	0.50	2.60	15	2
1:A:67:LEU:C	1:A:67:LEU:HD12	0.50	2.26	8	1
1:A:69:GLN:HE21	1:A:81:ALA:HB3	0.50	1.65	4	1
1:A:96:ALA:HB3	1:A:120:ASN:HB2	0.50	1.84	4	1
1:B:72:ARG:CG	1:B:79:ALA:O	0.50	2.60	19	2
1:A:69:GLN:NE2	1:A:81:ALA:C	0.50	2.65	8	7
1:B:75:ALA:O	1:B:77:GLU:N	0.50	2.45	6	11
1:A:116:PHE:O	1:B:74:VAL:CG2	0.50	2.60	14	1
1:A:48:THR:O	1:A:52:ARG:CG	0.50	2.60	5	1
1:B:63:LEU:HD23	1:B:86:PHE:HB3	0.50	1.83	17	1
1:B:26:ILE:CG2	1:B:55:TYR:CE2	0.50	2.94	16	1
1:B:7:MET:HB3	1:B:73:ALA:HB1	0.50	1.83	16	1
1:B:67:LEU:CG	1:B:82:PHE:CZ	0.50	2.94	11	1
1:B:84:VAL:O	1:B:94:VAL:CG2	0.50	2.59	11	1
1:B:7:MET:HA	1:B:103:PHE:CE2	0.50	2.42	7	2
1:A:2:ASN:ND2	1:A:103:PHE:CB	0.50	2.75	9	1
1:A:94:VAL:HG13	1:A:94:VAL:O	0.49	2.07	5	2
1:B:37:GLU:OE1	1:B:44:PRO:CA	0.49	2.60	16	1
1:B:68:THR:HG22	1:B:83:THR:OG1	0.49	2.07	8	3
1:A:38:ASP:OD1	1:A:114:ALA:CB	0.49	2.60	15	2
1:A:72:ARG:NH1	1:B:120:ASN:ND2	0.49	2.60	6	1
1:B:36:VAL:HG23	1:B:51:ILE:CG1	0.49	2.37	9	3
1:A:68:THR:HG21	1:A:83:THR:CG2	0.49	2.37	1	1
1:B:30:PHE:HE2	1:B:51:ILE:HG21	0.49	1.63	14	1
1:A:49:ALA:O	1:A:53:GLU:CG	0.49	2.59	17	1
1:A:95:VAL:HG12	1:A:96:ALA:N	0.49	2.22	16	11
1:A:45:ARG:HD2	1:A:54:PHE:CZ	0.49	2.42	11	1
1:B:34:ALA:CB	1:B:112:MET:CE	0.49	2.90	8	1
1:B:55:TYR:O	1:B:59:LEU:CG	0.49	2.60	17	2
1:A:92:LYS:O	1:A:92:LYS:CG	0.49	2.60	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:THR:CG2	1:B:6:HIS:CD2	0.49	2.95	18	1
1:A:38:ASP:HB3	1:A:54:PHE:CZ	0.49	2.42	9	1
1:A:69:GLN:NE2	1:A:70:GLU:N	0.49	2.59	9	2
1:B:72:ARG:NH1	1:B:79:ALA:HB3	0.49	2.22	10	1
1:B:23:LEU:O	1:B:27:VAL:CG2	0.49	2.60	7	4
1:A:65:VAL:HG13	1:A:82:PHE:HD2	0.49	1.66	7	2
1:B:45:ARG:HB3	1:B:50:ALA:HB1	0.49	1.84	19	2
1:B:96:ALA:O	1:B:120:ASN:ND2	0.49	2.45	19	5
1:A:67:LEU:HG	1:A:82:PHE:CE2	0.49	2.42	3	1
1:A:80:PHE:N	1:A:80:PHE:CD1	0.49	2.80	3	1
1:A:65:VAL:HG13	1:A:84:VAL:HG12	0.49	1.84	5	1
1:A:8:THR:HG23	1:A:71:VAL:HB	0.49	1.84	6	1
1:A:103:PHE:CD1	1:A:109:VAL:CG2	0.49	2.91	14	1
1:B:124:GLY:O	1:B:125:ALA:CB	0.49	2.60	13	1
1:B:27:VAL:HA	1:B:30:PHE:CZ	0.49	2.42	9	18
1:B:53:GLU:O	1:B:57:ASN:CB	0.49	2.61	16	2
1:B:27:VAL:HG11	1:B:48:THR:HB	0.49	1.85	11	1
1:A:50:ALA:O	1:A:54:PHE:CD2	0.49	2.66	20	1
1:A:97:PRO:HG3	1:A:116:PHE:CE2	0.49	2.43	3	4
1:A:30:PHE:CD2	1:A:31:ALA:O	0.49	2.65	12	1
1:B:97:PRO:HB3	1:B:116:PHE:CE2	0.49	2.42	15	2
1:A:69:GLN:CD	1:A:81:ALA:CB	0.49	2.81	8	1
1:A:18:LEU:CD1	1:A:59:LEU:HD11	0.49	2.38	7	1
1:B:7:MET:HB2	1:B:103:PHE:CE1	0.49	2.42	3	2
1:A:69:GLN:O	1:A:70:GLU:CB	0.49	2.60	20	4
1:A:51:ILE:CG2	1:A:55:TYR:CE2	0.49	2.96	3	1
1:A:7:MET:HG3	1:A:103:PHE:CZ	0.49	2.42	3	2
1:A:80:PHE:CD2	1:A:82:PHE:CE1	0.49	3.00	3	1
1:B:108:LYS:O	1:B:108:LYS:CG	0.49	2.61	1	1
1:A:70:GLU:OE2	1:B:119:LYS:CD	0.49	2.60	1	1
1:A:120:ASN:ND2	1:B:72:ARG:NE	0.49	2.60	14	2
1:A:77:GLU:CG	1:A:78:ALA:N	0.49	2.75	19	1
1:A:110:VAL:CG1	1:A:110:VAL:O	0.49	2.60	5	2
1:A:54:PHE:CD2	1:A:55:TYR:CD1	0.49	3.00	5	1
1:A:39:PRO:HB3	1:A:116:PHE:CD2	0.49	2.43	18	2
1:A:117:GLY:HA2	1:A:121:ILE:HD11	0.49	1.83	9	2
1:B:67:LEU:HD11	1:B:80:PHE:HD2	0.49	1.66	9	1
1:A:67:LEU:HD23	1:A:68:THR:H	0.49	1.66	2	2
1:B:42:SER:O	1:B:43:GLU:CG	0.49	2.60	10	3
1:A:86:PHE:CE1	1:A:93:THR:HB	0.49	2.43	9	4
1:A:75:ALA:HB2	1:B:40:VAL:HB	0.49	1.83	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PHE:CD1	1:A:112:MET:HB2	0.49	2.42	7	1
1:A:71:VAL:O	1:A:72:ARG:CZ	0.49	2.60	9	2
1:B:100:HIS:ND1	1:B:100:HIS:C	0.49	2.66	19	1
1:A:74:VAL:HG22	1:A:75:ALA:H	0.49	1.67	2	2
1:A:15:VAL:HG11	1:A:82:PHE:CD2	0.49	2.41	12	1
1:B:27:VAL:HA	1:B:30:PHE:CE1	0.49	2.43	5	10
1:A:97:PRO:HB3	1:A:116:PHE:CZ	0.49	2.42	3	1
1:B:99:ASP:HB2	1:B:101:PHE:CZ	0.49	2.42	14	1
1:A:30:PHE:CE2	1:A:112:MET:HE3	0.49	2.42	19	1
1:A:77:GLU:OE2	1:A:102:ARG:CG	0.49	2.61	13	1
1:B:23:LEU:HD12	1:B:52:ARG:CG	0.49	2.38	12	2
1:B:97:PRO:HB2	1:B:116:PHE:CE1	0.49	2.42	8	3
1:B:117:GLY:O	1:B:121:ILE:CD1	0.49	2.61	8	3
1:A:38:ASP:OD1	1:A:54:PHE:CE2	0.49	2.66	4	1
1:B:54:PHE:CD2	1:B:55:TYR:N	0.49	2.81	4	1
1:B:45:ARG:CZ	1:B:54:PHE:CD2	0.49	2.96	19	1
1:B:26:ILE:HG21	1:B:55:TYR:CD2	0.49	2.42	18	1
1:B:70:GLU:O	1:B:80:PHE:CA	0.49	2.61	2	2
1:A:69:GLN:O	1:A:70:GLU:CG	0.49	2.60	20	2
1:A:72:ARG:HD3	1:B:98:ILE:HD12	0.49	1.85	11	1
1:B:77:GLU:OE1	1:B:102:ARG:CD	0.49	2.60	8	1
1:A:55:TYR:O	1:A:59:LEU:CD1	0.49	2.60	20	1
1:B:84:VAL:HG22	1:B:95:VAL:O	0.49	2.07	20	1
1:A:102:ARG:CB	1:A:111:SER:O	0.49	2.60	4	1
1:B:11:VAL:HG22	1:B:101:PHE:CE1	0.49	2.42	17	1
1:B:30:PHE:CE1	1:B:112:MET:HE1	0.49	2.43	9	1
1:B:118:GLU:O	1:B:118:GLU:CG	0.49	2.60	9	1
1:A:121:ILE:C	1:A:122:HIS:CD2	0.48	2.86	7	4
1:A:98:ILE:HD11	1:B:70:GLU:CD	0.48	2.28	13	1
1:A:15:VAL:HG21	1:A:82:PHE:CE1	0.48	2.40	12	1
1:B:110:VAL:O	1:B:110:VAL:CG1	0.48	2.61	12	4
1:B:14:TYR:C	1:B:18:LEU:HD23	0.48	2.28	18	2
1:A:39:PRO:HB3	1:A:116:PHE:CE1	0.48	2.42	7	2
1:B:36:VAL:HG11	1:B:55:TYR:CE1	0.48	2.43	7	1
1:B:45:ARG:HB2	1:B:50:ALA:HB1	0.48	1.84	18	1
1:B:100:HIS:NE2	1:B:113:ARG:NE	0.48	2.60	6	1
1:B:18:LEU:O	1:B:59:LEU:CD2	0.48	2.62	9	1
1:A:63:LEU:HD22	1:A:64:ALA:C	0.48	2.29	10	2
1:A:7:MET:CB	1:A:73:ALA:HB1	0.48	2.38	10	1
1:B:69:GLN:CB	1:B:81:ALA:O	0.48	2.61	6	2
1:A:67:LEU:HD21	1:A:80:PHE:HB2	0.48	1.86	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:SER:O	1:A:43:GLU:CG	0.48	2.61	17	3
1:B:4:PRO:HA	1:B:7:MET:CG	0.48	2.38	7	1
1:A:39:PRO:HG2	1:A:116:PHE:CE1	0.48	2.44	20	1
1:B:11:VAL:HG11	1:B:80:PHE:CG	0.48	2.43	5	2
1:B:32:ASP:OD1	1:B:48:THR:HG21	0.48	2.08	3	1
1:B:86:PHE:CE1	1:B:93:THR:HB	0.48	2.43	5	4
1:B:63:LEU:HD13	1:B:65:VAL:HG23	0.48	1.84	12	2
1:A:4:PRO:O	1:A:8:THR:CB	0.48	2.62	1	6
1:B:103:PHE:CZ	1:B:109:VAL:HG22	0.48	2.44	7	1
1:A:104:ASN:CB	1:A:110:VAL:CG2	0.48	2.92	19	1
1:A:115:LEU:HD23	1:B:74:VAL:HG23	0.48	1.82	4	2
1:A:86:PHE:N	1:A:86:PHE:CD1	0.48	2.81	8	4
1:B:95:VAL:HG12	1:B:97:PRO:CD	0.48	2.35	20	2
1:B:101:PHE:CD1	1:B:112:MET:HB2	0.48	2.43	20	1
1:B:84:VAL:HB	1:B:86:PHE:CZ	0.48	2.44	20	1
1:A:61:LEU:HD21	1:A:87:GLU:H	0.48	1.68	17	1
1:B:3:THR:HG21	1:B:6:HIS:CD2	0.48	2.43	18	1
1:B:97:PRO:HG3	1:B:116:PHE:CE2	0.48	2.44	2	4
1:A:27:VAL:HA	1:A:30:PHE:CZ	0.48	2.44	7	18
1:A:84:VAL:CG1	1:A:97:PRO:HD3	0.48	2.39	16	1
1:A:97:PRO:CB	1:A:116:PHE:CE1	0.48	2.96	3	4
1:A:97:PRO:HB3	1:A:116:PHE:CD1	0.48	2.43	7	5
1:A:102:ARG:CG	1:A:103:PHE:N	0.48	2.76	11	1
1:B:93:THR:OG1	1:B:123:ALA:CB	0.48	2.61	11	1
1:B:37:GLU:CA	1:B:37:GLU:OE1	0.48	2.61	15	1
1:A:119:LYS:CE	1:B:71:VAL:O	0.48	2.62	4	1
1:A:69:GLN:CD	1:A:70:GLU:N	0.48	2.67	4	3
1:B:116:PHE:CD1	1:B:116:PHE:C	0.48	2.83	19	3
1:A:77:GLU:HB3	1:A:100:HIS:CE1	0.48	2.44	9	1
1:B:69:GLN:NE2	1:B:69:GLN:C	0.48	2.67	13	1
1:B:18:LEU:CD2	1:B:65:VAL:HG21	0.48	2.38	2	1
1:B:32:ASP:O	1:B:48:THR:CG2	0.48	2.62	1	7
1:A:41:GLY:O	1:A:43:GLU:N	0.48	2.47	17	4
1:A:67:LEU:HD11	1:A:80:PHE:CD2	0.48	2.43	11	1
1:B:45:ARG:NH1	1:B:54:PHE:CD1	0.48	2.81	11	1
1:B:77:GLU:CD	1:B:100:HIS:CD2	0.48	2.87	11	1
1:A:14:TYR:C	1:A:14:TYR:CD1	0.48	2.87	3	2
1:B:38:ASP:HB2	1:B:54:PHE:CE1	0.48	2.43	5	2
1:B:103:PHE:N	1:B:103:PHE:CD1	0.48	2.80	9	2
1:A:82:PHE:CZ	1:A:97:PRO:HG2	0.48	2.44	13	8
1:A:98:ILE:CG2	1:A:100:HIS:CE1	0.48	2.97	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:PRO:O	1:A:114:ALA:CA	0.48	2.61	7	3
1:B:39:PRO:HB3	1:B:116:PHE:CE1	0.48	2.44	7	1
1:A:39:PRO:CG	1:A:116:PHE:CE1	0.48	2.97	10	1
1:B:54:PHE:O	1:B:58:SER:CB	0.48	2.62	5	2
1:A:7:MET:O	1:A:10:VAL:HG12	0.48	2.08	11	1
1:B:83:THR:C	1:B:84:VAL:CG1	0.48	2.83	8	1
1:B:41:GLY:O	1:B:43:GLU:N	0.48	2.46	13	3
1:A:86:PHE:CE2	1:A:93:THR:HB	0.48	2.44	7	2
1:A:86:PHE:CD1	1:A:86:PHE:O	0.48	2.67	20	1
1:A:74:VAL:O	1:A:77:GLU:CG	0.48	2.62	3	2
1:A:103:PHE:CD1	1:A:103:PHE:N	0.48	2.80	14	1
1:A:104:ASN:HB2	1:A:110:VAL:HG23	0.48	1.86	19	1
1:A:7:MET:HA	1:A:103:PHE:CE2	0.48	2.43	5	1
1:B:103:PHE:CZ	1:B:108:LYS:HD3	0.47	2.44	2	1
1:B:37:GLU:N	1:B:112:MET:O	0.47	2.47	3	5
1:A:63:LEU:HD12	1:A:63:LEU:O	0.47	2.09	3	1
1:B:36:VAL:HG11	1:B:54:PHE:CD2	0.47	2.44	3	1
1:A:42:SER:OG	1:A:43:GLU:N	0.47	2.47	5	1
1:B:67:LEU:HD22	1:B:82:PHE:CB	0.47	2.38	9	1
1:A:67:LEU:N	1:A:82:PHE:CD2	0.47	2.82	12	1
1:A:63:LEU:C	1:A:63:LEU:HD12	0.47	2.30	1	5
1:B:74:VAL:HG13	1:B:75:ALA:H	0.47	1.67	19	2
1:A:118:GLU:HA	1:A:121:ILE:HD12	0.47	1.86	4	1
1:A:70:GLU:C	1:A:71:VAL:HG23	0.47	2.30	14	1
1:A:63:LEU:HD12	1:A:64:ALA:N	0.47	2.24	17	1
1:B:73:ALA:O	1:B:74:VAL:CG2	0.47	2.58	18	2
1:A:45:ARG:CZ	1:A:54:PHE:CD1	0.47	2.96	10	1
1:A:84:VAL:HG13	1:A:97:PRO:CD	0.47	2.40	2	9
1:B:117:GLY:CA	1:B:120:ASN:OD1	0.47	2.62	2	1
1:A:7:MET:CE	1:A:77:GLU:O	0.47	2.62	7	3
1:A:45:ARG:HD2	1:A:54:PHE:CD1	0.47	2.45	16	1
1:B:36:VAL:HG22	1:B:112:MET:CE	0.47	2.39	3	2
1:B:26:ILE:HG22	1:B:30:PHE:HE2	0.47	1.70	7	2
1:A:70:GLU:OE1	1:B:98:ILE:CD1	0.47	2.60	2	1
1:A:11:VAL:CG1	1:A:80:PHE:CE2	0.47	2.97	16	1
1:B:54:PHE:CD2	1:B:55:TYR:CD1	0.47	3.02	16	1
1:A:27:VAL:HA	1:A:30:PHE:CE1	0.47	2.44	4	6
1:A:67:LEU:HD13	1:A:81:ALA:O	0.47	2.09	7	1
1:B:3:THR:CG2	1:B:6:HIS:CG	0.47	2.97	7	1
1:A:65:VAL:HG13	1:A:82:PHE:CD1	0.47	2.44	1	1
1:A:120:ASN:CG	1:B:72:ARG:CZ	0.47	2.83	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:SER:HA	1:A:94:VAL:HG23	0.47	1.85	3	1
1:A:73:ALA:C	1:A:74:VAL:CG2	0.47	2.83	13	3
1:B:103:PHE:CB	1:B:109:VAL:CG2	0.47	2.84	17	1
1:B:61:LEU:HD23	1:B:63:LEU:CG	0.47	2.39	9	1
1:B:46:SER:O	1:B:50:ALA:CB	0.47	2.63	16	1
1:B:86:PHE:CE2	1:B:93:THR:HB	0.47	2.45	16	1
1:A:36:VAL:CG2	1:A:51:ILE:CD1	0.47	2.93	8	2
1:B:14:TYR:HE1	1:B:55:TYR:HH	0.47	1.52	20	1
1:B:67:LEU:CD2	1:B:81:ALA:O	0.47	2.63	4	1
1:B:71:VAL:CG2	1:B:80:PHE:CB	0.47	2.88	5	1
1:B:36:VAL:CG1	1:B:54:PHE:CE2	0.47	2.97	18	2
1:A:57:ASN:O	1:A:60:LYS:CB	0.47	2.63	2	1
1:B:15:VAL:HG11	1:B:67:LEU:HB2	0.47	1.87	2	1
1:B:55:TYR:O	1:B:59:LEU:CD1	0.47	2.61	17	3
1:A:26:ILE:HG22	1:A:30:PHE:HE1	0.47	1.70	12	1
1:A:37:GLU:N	1:A:112:MET:O	0.47	2.48	12	4
1:B:86:PHE:CD1	1:B:86:PHE:N	0.47	2.83	16	1
1:A:120:ASN:CB	1:B:72:ARG:HH21	0.47	2.23	16	1
1:B:3:THR:O	1:B:7:MET:SD	0.47	2.73	3	4
1:A:99:ASP:C	1:A:100:HIS:ND1	0.47	2.68	11	1
1:A:120:ASN:CG	1:B:72:ARG:NH1	0.47	2.68	1	2
1:A:86:PHE:CE1	1:A:95:VAL:CG2	0.47	2.98	15	2
1:A:69:GLN:CD	1:A:81:ALA:HB3	0.47	2.30	8	1
1:B:75:ALA:C	1:B:77:GLU:N	0.47	2.68	6	11
1:B:36:VAL:CG1	1:B:38:ASP:OD2	0.47	2.63	3	1
1:B:54:PHE:CG	1:B:55:TYR:N	0.47	2.82	13	2
1:B:80:PHE:CE1	1:B:99:ASP:HB2	0.47	2.45	19	3
1:B:100:HIS:C	1:B:100:HIS:ND1	0.47	2.67	14	1
1:B:96:ALA:HB3	1:B:120:ASN:HD22	0.47	1.70	5	1
1:B:14:TYR:CD2	1:B:101:PHE:CZ	0.47	3.02	5	1
1:A:66:GLU:CG	1:A:67:LEU:N	0.47	2.78	17	1
1:A:82:PHE:CD1	1:A:82:PHE:N	0.47	2.82	9	1
1:B:72:ARG:HH21	1:B:98:ILE:HD13	0.47	1.67	9	1
1:A:14:TYR:O	1:A:18:LEU:HD23	0.47	2.10	13	1
1:A:93:THR:CG2	1:A:94:VAL:N	0.47	2.78	13	1
1:A:26:ILE:CG2	1:A:55:TYR:CD1	0.47	2.97	16	1
1:A:83:THR:C	1:A:84:VAL:CG1	0.47	2.83	5	3
1:A:45:ARG:HG2	1:A:54:PHE:CZ	0.47	2.45	6	1
1:A:11:VAL:CG2	1:A:101:PHE:CD2	0.47	2.98	4	2
1:B:11:VAL:CG1	1:B:80:PHE:CD2	0.47	2.98	1	1
1:B:77:GLU:CG	1:B:100:HIS:CE1	0.47	2.97	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:PHE:O	1:A:96:ALA:HA	0.47	2.10	3	5
1:B:23:LEU:CD2	1:B:59:LEU:HD12	0.47	2.40	12	1
1:A:103:PHE:CZ	1:A:108:LYS:CG	0.47	2.98	7	1
1:B:7:MET:CE	1:B:77:GLU:O	0.47	2.63	3	1
1:A:27:VAL:CG1	1:A:48:THR:HB	0.47	2.40	4	1
1:B:103:PHE:CD2	1:B:108:LYS:HA	0.47	2.45	4	1
1:B:82:PHE:CE1	1:B:97:PRO:HG2	0.47	2.45	14	1
1:B:36:VAL:CG2	1:B:112:MET:SD	0.47	3.00	19	1
1:A:54:PHE:CG	1:A:55:TYR:N	0.47	2.80	9	2
1:A:100:HIS:NE2	1:B:115:LEU:CD1	0.47	2.78	9	1
1:A:23:LEU:HD12	1:A:52:ARG:CG	0.47	2.39	2	1
1:B:70:GLU:C	1:B:71:VAL:HG23	0.47	2.30	2	2
1:B:59:LEU:C	1:B:61:LEU:N	0.47	2.69	18	16
1:A:14:TYR:OH	1:A:55:TYR:CE1	0.47	2.68	12	2
1:B:69:GLN:NE2	1:B:81:ALA:O	0.47	2.48	20	5
1:A:34:ALA:HB2	1:A:110:VAL:HA	0.47	1.87	19	2
1:B:63:LEU:N	1:B:63:LEU:HD12	0.47	2.24	5	2
1:A:11:VAL:HG22	1:A:80:PHE:CZ	0.47	2.45	3	1
1:B:100:HIS:C	1:B:100:HIS:CD2	0.47	2.88	1	1
1:A:77:GLU:CG	1:A:101:PHE:O	0.47	2.63	14	1
1:A:70:GLU:O	1:A:80:PHE:CA	0.47	2.62	14	1
1:B:30:PHE:CE2	1:B:112:MET:SD	0.47	3.08	18	1
1:A:118:GLU:O	1:A:119:LYS:CD	0.47	2.63	10	1
1:A:31:ALA:HB3	1:A:34:ALA:HB2	0.46	1.85	2	15
1:B:8:THR:HG23	1:B:71:VAL:CG1	0.46	2.22	2	2
1:B:84:VAL:CG1	1:B:97:PRO:HD3	0.46	2.40	19	4
1:A:72:ARG:NE	1:B:115:LEU:O	0.46	2.49	5	1
1:B:32:ASP:OD2	1:B:48:THR:HG21	0.46	2.10	9	1
1:B:110:VAL:CG1	1:B:110:VAL:O	0.46	2.62	13	1
1:A:45:ARG:HD2	1:A:50:ALA:HB1	0.46	1.87	12	2
1:B:55:TYR:OH	1:B:112:MET:HE1	0.46	2.10	12	1
1:B:74:VAL:O	1:B:75:ALA:C	0.46	2.54	20	3
1:B:120:ASN:N	1:B:120:ASN:HD22	0.46	2.08	8	1
1:B:95:VAL:HG11	1:B:116:PHE:CE1	0.46	2.46	9	2
1:B:101:PHE:CD1	1:B:101:PHE:N	0.46	2.82	20	2
1:A:36:VAL:HG11	1:A:54:PHE:HE2	0.46	1.69	5	1
1:B:10:VAL:HG13	1:B:29:LEU:HD21	0.46	1.86	10	1
1:B:82:PHE:CE2	1:B:97:PRO:HG2	0.46	2.46	6	4
1:A:69:GLN:NE2	1:A:81:ALA:O	0.46	2.48	6	5
1:A:122:HIS:CD2	1:A:122:HIS:N	0.46	2.84	13	4
1:B:14:TYR:O	1:B:18:LEU:CD2	0.46	2.62	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:THR:O	1:B:7:MET:CE	0.46	2.63	6	1
1:A:63:LEU:HD23	1:A:84:VAL:HG23	0.46	1.87	20	1
1:A:71:VAL:N	1:A:72:ARG:HH21	0.46	2.02	14	1
1:A:110:VAL:HG12	1:A:110:VAL:O	0.46	2.09	18	1
1:B:31:ALA:HB3	1:B:34:ALA:HB2	0.46	1.87	2	13
1:A:79:ALA:CB	1:B:115:LEU:HD22	0.46	2.40	12	2
1:B:63:LEU:H	1:B:63:LEU:HD12	0.46	1.69	12	2
1:B:25:GLY:O	1:B:28:ALA:N	0.46	2.48	14	12
1:A:75:ALA:C	1:A:77:GLU:N	0.46	2.68	4	10
1:B:82:PHE:CZ	1:B:97:PRO:HG2	0.46	2.46	14	7
1:A:103:PHE:CE1	1:A:108:LYS:HG2	0.46	2.46	6	1
1:A:96:ALA:O	1:A:120:ASN:ND2	0.46	2.49	1	2
1:B:20:ALA:HB3	1:B:22:ASP:OD2	0.46	2.10	1	1
1:A:82:PHE:CE2	1:A:97:PRO:HG2	0.46	2.46	14	7
1:A:67:LEU:CD1	1:A:82:PHE:CE1	0.46	2.98	12	2
1:A:71:VAL:HG13	1:A:80:PHE:HD1	0.46	1.70	3	2
1:B:84:VAL:HG13	1:B:97:PRO:CD	0.46	2.41	11	7
1:B:7:MET:HG3	1:B:8:THR:N	0.46	2.26	6	2
1:B:38:ASP:HB3	1:B:54:PHE:CE2	0.46	2.46	8	1
1:A:26:ILE:CG2	1:A:55:TYR:CE2	0.46	2.98	5	3
1:A:39:PRO:HB3	1:A:116:PHE:CE2	0.46	2.45	9	1
1:A:10:VAL:O	1:A:14:TYR:CB	0.46	2.64	12	1
1:B:37:GLU:OE2	1:B:43:GLU:N	0.46	2.48	15	1
1:B:121:ILE:C	1:B:122:HIS:CD2	0.46	2.89	14	3
1:A:36:VAL:HG23	1:A:51:ILE:CG1	0.46	2.41	10	1
1:B:80:PHE:CD2	1:B:82:PHE:CE1	0.46	3.03	11	1
1:A:75:ALA:HB3	1:B:40:VAL:HG11	0.46	1.87	8	1
1:B:17:ALA:O	1:B:21:GLY:N	0.46	2.48	18	2
1:A:71:VAL:HA	1:A:80:PHE:CB	0.46	2.40	19	7
1:A:101:PHE:CD1	1:A:101:PHE:N	0.46	2.82	11	1
1:A:45:ARG:NH1	1:A:54:PHE:CD1	0.46	2.83	7	1
1:B:57:ASN:O	1:B:60:LYS:CD	0.46	2.64	1	1
1:B:47:GLY:O	1:B:50:ALA:N	0.46	2.48	19	1
1:B:51:ILE:O	1:B:55:TYR:CD1	0.46	2.69	17	2
1:A:93:THR:HG22	1:A:94:VAL:N	0.46	2.26	13	1
1:A:59:LEU:C	1:A:61:LEU:N	0.46	2.69	5	11
1:A:51:ILE:HG23	1:A:55:TYR:CE2	0.46	2.46	12	1
1:A:67:LEU:CB	1:A:82:PHE:CE2	0.46	2.99	12	1
1:A:23:LEU:HD21	1:A:55:TYR:CB	0.46	2.41	4	2
1:A:72:ARG:NH2	1:B:120:ASN:OD1	0.46	2.49	15	2
1:B:48:THR:O	1:B:52:ARG:CG	0.46	2.64	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:GLU:CD	1:B:72:ARG:NH2	0.46	2.69	8	1
1:A:63:LEU:CD1	1:A:65:VAL:HG23	0.46	2.40	17	2
1:A:103:PHE:CZ	1:A:109:VAL:HG22	0.46	2.46	1	1
1:A:36:VAL:HG11	1:A:55:TYR:CE1	0.46	2.46	1	1
1:B:15:VAL:HG11	1:B:66:GLU:HA	0.46	1.88	12	2
1:A:77:GLU:CD	1:A:100:HIS:NE2	0.46	2.70	3	2
1:B:11:VAL:CG2	1:B:80:PHE:CZ	0.46	2.98	11	1
1:B:67:LEU:CD1	1:B:82:PHE:CE1	0.46	3.00	11	1
1:A:65:VAL:CG1	1:A:82:PHE:CD2	0.46	2.98	7	1
1:B:51:ILE:HG23	1:B:55:TYR:CE2	0.46	2.46	9	2
1:A:10:VAL:HG13	1:A:29:LEU:CD2	0.46	2.41	5	1
1:A:72:ARG:NH1	1:B:116:PHE:C	0.46	2.70	5	1
1:B:120:ASN:ND2	1:B:120:ASN:N	0.46	2.60	13	1
1:A:23:LEU:CD1	1:A:52:ARG:O	0.45	2.65	13	2
1:A:2:ASN:ND2	1:A:103:PHE:CD2	0.45	2.85	12	1
1:A:103:PHE:CE2	1:A:108:LYS:HA	0.45	2.46	12	2
1:A:101:PHE:N	1:A:101:PHE:CD1	0.45	2.83	8	1
1:B:56:ALA:O	1:B:59:LEU:N	0.45	2.50	19	3
1:B:76:ASN:N	1:B:76:ASN:ND2	0.45	2.63	4	1
1:B:71:VAL:HA	1:B:80:PHE:CB	0.45	2.41	1	2
1:A:120:ASN:CG	1:B:72:ARG:NH2	0.45	2.70	14	1
1:A:21:GLY:O	1:A:23:LEU:N	0.45	2.49	14	1
1:B:99:ASP:OD2	1:B:99:ASP:N	0.45	2.49	14	1
1:A:120:ASN:OD1	1:B:72:ARG:NH2	0.45	2.49	13	2
1:B:57:ASN:ND2	1:B:58:SER:N	0.45	2.64	18	2
1:A:84:VAL:HG23	1:A:86:PHE:CE2	0.45	2.45	19	2
1:A:103:PHE:O	1:A:104:ASN:CG	0.45	2.53	9	2
1:A:120:ASN:ND2	1:B:72:ARG:CD	0.45	2.79	13	1
1:A:120:ASN:ND2	1:B:70:GLU:OE1	0.45	2.50	16	2
1:A:120:ASN:ND2	1:B:70:GLU:CD	0.45	2.69	11	1
1:A:98:ILE:CG2	1:A:100:HIS:CD2	0.45	2.99	15	1
1:A:15:VAL:CG2	1:A:67:LEU:HD23	0.45	2.32	15	1
1:A:25:GLY:O	1:A:28:ALA:N	0.45	2.49	13	8
1:B:52:ARG:CD	1:B:52:ARG:C	0.45	2.84	6	1
1:B:4:PRO:HA	1:B:7:MET:SD	0.45	2.51	7	1
1:B:68:THR:O	1:B:69:GLN:CG	0.45	2.65	7	1
1:A:80:PHE:CD2	1:A:99:ASP:HB2	0.45	2.46	3	1
1:B:80:PHE:CD2	1:B:99:ASP:OD2	0.45	2.69	14	2
1:B:7:MET:CG	1:B:78:ALA:HB2	0.45	2.40	13	2
1:B:69:GLN:N	1:B:69:GLN:NE2	0.45	2.64	2	1
1:A:103:PHE:CE1	1:A:108:LYS:HB3	0.45	2.46	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:PRO:O	1:B:114:ALA:CA	0.45	2.64	8	2
1:A:74:VAL:HG11	1:B:116:PHE:O	0.45	2.11	8	1
1:A:61:LEU:CD2	1:A:63:LEU:HD23	0.45	2.39	7	1
1:B:57:ASN:ND2	1:B:57:ASN:C	0.45	2.70	18	2
1:A:17:ALA:O	1:A:21:GLY:N	0.45	2.49	13	2
1:A:81:ALA:CB	1:A:98:ILE:HG12	0.45	2.41	10	2
1:A:76:ASN:OD1	1:A:76:ASN:N	0.45	2.50	10	1
1:B:39:PRO:O	1:B:40:VAL:HG22	0.45	2.11	14	5
1:A:14:TYR:CD2	1:A:15:VAL:N	0.45	2.85	12	1
1:B:70:GLU:OE2	1:B:72:ARG:NH2	0.45	2.50	16	1
1:A:120:ASN:ND2	1:B:70:GLU:OE2	0.45	2.50	11	3
1:B:59:LEU:O	1:B:61:LEU:N	0.45	2.49	18	7
1:B:34:ALA:HB1	1:B:112:MET:CE	0.45	2.41	8	2
1:A:15:VAL:O	1:A:18:LEU:N	0.45	2.49	3	3
1:B:96:ALA:C	1:B:120:ASN:OD1	0.45	2.55	7	2
1:B:35:THR:HG22	1:B:46:SER:HA	0.45	1.87	4	2
1:A:2:ASN:ND2	1:A:76:ASN:OD1	0.45	2.50	1	2
1:B:11:VAL:CG2	1:B:78:ALA:CB	0.45	2.95	1	1
1:A:115:LEU:CB	1:B:72:ARG:CD	0.45	2.94	10	1
1:A:11:VAL:HG13	1:A:80:PHE:CD1	0.45	2.47	2	2
1:B:86:PHE:N	1:B:86:PHE:CD1	0.45	2.81	11	2
1:A:10:VAL:HG21	1:A:103:PHE:CZ	0.45	2.46	15	1
1:A:96:ALA:O	1:B:72:ARG:NH1	0.45	2.50	8	1
1:A:77:GLU:OE1	1:A:100:HIS:NE2	0.45	2.50	13	3
1:B:112:MET:SD	1:B:112:MET:N	0.45	2.89	14	2
1:A:119:LYS:O	1:A:120:ASN:ND2	0.45	2.50	6	1
1:B:111:SER:OG	1:B:113:ARG:NH2	0.45	2.50	7	2
1:A:120:ASN:OD1	1:B:72:ARG:NH1	0.45	2.49	7	1
1:A:54:PHE:O	1:A:57:ASN:ND2	0.45	2.50	19	2
1:B:19:ASN:ND2	1:B:65:VAL:O	0.45	2.50	3	1
1:B:40:VAL:HG12	1:B:41:GLY:N	0.45	2.26	17	2
1:B:2:ASN:CG	1:B:76:ASN:ND2	0.45	2.70	18	1
1:A:2:ASN:ND2	1:A:7:MET:SD	0.45	2.90	9	1
1:B:45:ARG:HD3	1:B:54:PHE:CD1	0.45	2.47	10	1
1:A:115:LEU:HD13	1:B:72:ARG:HH12	0.45	1.70	2	1
1:B:70:GLU:O	1:B:80:PHE:CB	0.45	2.64	13	2
1:A:118:GLU:HA	1:A:121:ILE:HD13	0.45	1.86	12	1
1:A:72:ARG:NH1	1:B:96:ALA:O	0.45	2.49	12	2
1:B:36:VAL:C	1:B:37:GLU:CG	0.45	2.85	11	1
1:A:115:LEU:CD2	1:B:77:GLU:CD	0.45	2.83	11	1
1:B:2:ASN:OD1	1:B:76:ASN:ND2	0.45	2.50	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:HD2	1:A:54:PHE:CD2	0.45	2.47	10	2
1:A:98:ILE:HG21	1:B:72:ARG:CZ	0.45	2.41	9	1
1:B:32:ASP:O	1:B:48:THR:N	0.45	2.48	9	1
1:A:80:PHE:O	1:A:98:ILE:HG23	0.45	2.11	12	1
1:B:98:ILE:HG22	1:B:100:HIS:NE2	0.45	2.26	12	1
1:B:30:PHE:CZ	1:B:51:ILE:CG2	0.45	2.99	19	6
1:A:11:VAL:CG1	1:A:80:PHE:CD2	0.45	2.99	7	2
1:B:84:VAL:HG12	1:B:97:PRO:CD	0.45	2.42	7	2
1:A:38:ASP:O	1:A:45:ARG:NH1	0.45	2.49	10	2
1:A:44:PRO:O	1:A:45:ARG:NE	0.45	2.50	3	2
1:A:75:ALA:O	1:A:76:ASN:ND2	0.45	2.50	3	1
1:B:14:TYR:CD1	1:B:15:VAL:N	0.45	2.84	3	1
1:B:1:MET:O	1:B:2:ASN:ND2	0.45	2.50	3	1
1:B:2:ASN:ND2	1:B:76:ASN:OD1	0.45	2.50	14	1
1:A:39:PRO:O	1:A:114:ALA:O	0.45	2.35	10	3
1:A:38:ASP:HB3	1:A:54:PHE:CE1	0.45	2.47	9	1
1:B:22:ASP:N	1:B:22:ASP:OD2	0.45	2.50	10	1
1:A:115:LEU:CB	1:B:72:ARG:HD3	0.45	2.42	10	1
1:B:21:GLY:O	1:B:23:LEU:N	0.45	2.50	16	1
1:B:77:GLU:OE2	1:B:100:HIS:NE2	0.45	2.50	11	2
1:A:2:ASN:OD1	1:A:103:PHE:CB	0.45	2.65	15	1
1:B:7:MET:SD	1:B:77:GLU:O	0.45	2.75	15	3
1:A:72:ARG:NH1	1:B:115:LEU:O	0.45	2.50	8	1
1:A:84:VAL:CG2	1:A:86:PHE:CE1	0.45	3.00	6	1
1:B:7:MET:SD	1:B:73:ALA:CB	0.45	2.96	6	1
1:B:7:MET:HE3	1:B:77:GLU:O	0.45	2.11	3	1
1:A:119:LYS:NZ	1:A:119:LYS:O	0.45	2.49	4	1
1:A:23:LEU:CD2	1:A:55:TYR:CB	0.45	2.95	4	1
1:A:69:GLN:NE2	1:A:81:ALA:HB1	0.45	2.26	19	1
1:A:65:VAL:HG22	1:A:84:VAL:CB	0.45	2.35	5	1
1:A:100:HIS:HE1	1:B:115:LEU:HD11	0.45	1.72	5	1
1:B:76:ASN:ND2	1:B:103:PHE:O	0.45	2.50	13	1
1:A:57:ASN:ND2	1:A:57:ASN:C	0.45	2.70	15	2
1:B:94:VAL:HG13	1:B:94:VAL:O	0.45	2.12	12	4
1:B:52:ARG:O	1:B:56:ALA:HB3	0.45	2.11	16	2
1:A:70:GLU:CD	1:A:72:ARG:NH1	0.45	2.70	11	1
1:B:38:ASP:OD2	1:B:45:ARG:NH2	0.45	2.50	15	1
1:B:119:LYS:O	1:B:120:ASN:ND2	0.45	2.50	20	1
1:A:93:THR:CG2	1:A:122:HIS:O	0.45	2.64	4	1
1:A:115:LEU:HD13	1:B:100:HIS:NE2	0.45	2.27	13	1
1:A:7:MET:HG3	1:A:103:PHE:CE2	0.45	2.47	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1:MET:C	1:B:2:ASN:ND2	0.45	2.71	2	1
1:B:93:THR:CG2	1:B:121:ILE:HG23	0.45	2.40	16	1
1:A:99:ASP:OD1	1:A:114:ALA:CB	0.45	2.65	11	1
1:A:56:ALA:O	1:A:59:LEU:N	0.45	2.50	8	1
1:A:3:THR:OG1	1:A:6:HIS:CB	0.45	2.65	4	2
1:A:70:GLU:OE1	1:B:120:ASN:ND2	0.45	2.50	20	1
1:B:84:VAL:HG23	1:B:86:PHE:HE1	0.45	1.72	20	1
1:A:72:ARG:NH1	1:B:117:GLY:N	0.45	2.63	4	2
1:A:72:ARG:CZ	1:B:120:ASN:CB	0.45	2.95	18	1
1:A:17:ALA:CB	1:A:22:ASP:OD1	0.44	2.59	12	1
1:B:76:ASN:OD1	1:B:76:ASN:N	0.44	2.50	9	2
1:B:63:LEU:O	1:B:63:LEU:HD12	0.44	2.12	8	1
1:A:82:PHE:N	1:A:82:PHE:CD1	0.44	2.84	10	2
1:A:104:ASN:CB	1:A:110:VAL:HG23	0.44	2.42	19	1
1:A:39:PRO:CB	1:A:116:PHE:CE1	0.44	3.00	10	1
1:B:44:PRO:O	1:B:45:ARG:NE	0.44	2.50	10	1
1:B:15:VAL:O	1:B:18:LEU:N	0.44	2.50	12	1
1:B:84:VAL:O	1:B:94:VAL:HG22	0.44	2.10	11	1
1:A:51:ILE:HG23	1:A:55:TYR:CE1	0.44	2.47	5	2
1:B:18:LEU:HD13	1:B:26:ILE:HD13	0.44	1.89	6	1
1:A:43:GLU:O	1:A:45:ARG:NH2	0.44	2.50	7	1
1:B:71:VAL:CG2	1:B:80:PHE:HB3	0.44	2.42	20	3
1:B:37:GLU:HG3	1:B:37:GLU:O	0.44	2.11	14	1
1:B:11:VAL:CG1	1:B:80:PHE:CZ	0.44	3.00	14	1
1:B:72:ARG:O	1:B:72:ARG:CG	0.44	2.66	5	1
1:A:116:PHE:O	1:B:72:ARG:NE	0.44	2.50	18	1
1:A:14:TYR:C	1:A:18:LEU:HD23	0.44	2.33	13	1
1:A:45:ARG:CZ	1:A:54:PHE:CG	0.44	3.00	10	1
1:B:57:ASN:OD1	1:B:58:SER:N	0.44	2.49	2	1
1:B:70:GLU:C	1:B:71:VAL:CG2	0.44	2.86	2	2
1:A:33:ASP:N	1:A:33:ASP:OD1	0.44	2.50	15	1
1:A:69:GLN:CB	1:A:81:ALA:O	0.44	2.65	15	2
1:A:51:ILE:O	1:A:55:TYR:CD1	0.44	2.70	8	1
1:A:72:ARG:CG	1:A:79:ALA:O	0.44	2.65	7	2
1:A:72:ARG:NH2	1:B:120:ASN:CG	0.44	2.70	7	1
1:B:32:ASP:C	1:B:48:THR:HG23	0.44	2.27	4	1
1:A:10:VAL:HG13	1:A:29:LEU:HD21	0.44	1.90	1	1
1:B:103:PHE:CD1	1:B:103:PHE:N	0.44	2.86	1	1
1:B:93:THR:HG23	1:B:123:ALA:HA	0.44	1.87	14	1
1:B:80:PHE:O	1:B:98:ILE:HG23	0.44	2.13	13	1
1:A:57:ASN:CG	1:A:58:SER:N	0.44	2.70	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:GLU:O	1:B:57:ASN:ND2	0.44	2.50	2	1
1:B:7:MET:CB	1:B:73:ALA:HB1	0.44	2.42	16	1
1:B:69:GLN:C	1:B:70:GLU:CG	0.44	2.84	11	1
1:B:68:THR:HG21	1:B:83:THR:CG2	0.44	2.43	15	1
1:B:39:PRO:O	1:B:114:ALA:C	0.44	2.55	8	4
1:B:95:VAL:CG1	1:B:96:ALA:N	0.44	2.80	6	1
1:A:97:PRO:HB3	1:A:116:PHE:CE2	0.44	2.47	3	1
1:A:19:ASN:OD1	1:A:65:VAL:N	0.44	2.50	17	1
1:B:95:VAL:CG1	1:B:116:PHE:CE1	0.44	3.00	9	1
1:A:80:PHE:CD2	1:A:80:PHE:O	0.44	2.71	2	1
1:B:33:ASP:OD2	1:B:33:ASP:N	0.44	2.50	16	1
1:B:61:LEU:HD21	1:B:86:PHE:HB2	0.44	1.87	6	1
1:A:59:LEU:O	1:A:61:LEU:N	0.44	2.50	13	7
1:B:38:ASP:OD2	1:B:38:ASP:N	0.44	2.49	3	1
1:B:27:VAL:CG1	1:B:48:THR:OG1	0.44	2.66	5	1
1:A:2:ASN:OD1	1:A:76:ASN:ND2	0.44	2.50	18	1
1:A:61:LEU:O	1:A:63:LEU:HD12	0.44	2.13	10	1
1:B:101:PHE:CE1	1:B:112:MET:SD	0.44	3.11	2	2
1:B:102:ARG:CD	1:B:113:ARG:HH21	0.44	2.24	10	1
1:B:76:ASN:ND2	1:B:76:ASN:O	0.44	2.51	10	1
1:A:104:ASN:ND2	1:A:108:LYS:O	0.44	2.50	2	1
1:A:39:PRO:O	1:A:114:ALA:C	0.44	2.56	16	4
1:A:11:VAL:HG22	1:A:101:PHE:CE1	0.44	2.48	11	1
1:A:45:ARG:CG	1:A:54:PHE:CE1	0.44	3.01	6	1
1:B:101:PHE:CB	1:B:112:MET:HA	0.44	2.42	6	1
1:B:117:GLY:O	1:B:120:ASN:ND2	0.44	2.50	3	1
1:B:77:GLU:OE2	1:B:100:HIS:CD2	0.44	2.71	1	1
1:A:70:GLU:O	1:A:80:PHE:CB	0.44	2.65	14	1
1:B:1:MET:SD	1:B:2:ASN:N	0.44	2.91	14	1
1:B:77:GLU:OE1	1:B:100:HIS:NE2	0.44	2.50	17	1
1:B:30:PHE:CE1	1:B:112:MET:HE3	0.44	2.48	18	1
1:A:45:ARG:HB2	1:A:50:ALA:HB1	0.44	1.90	10	1
1:A:32:ASP:N	1:A:32:ASP:OD1	0.44	2.50	15	2
1:A:7:MET:HE1	1:A:73:ALA:C	0.44	2.33	8	1
1:A:119:LYS:CD	1:B:70:GLU:OE2	0.44	2.66	3	1
1:A:104:ASN:HD21	1:A:110:VAL:HG21	0.44	1.73	1	1
1:B:63:LEU:HD12	1:B:63:LEU:O	0.44	2.12	1	1
1:B:30:PHE:CD1	1:B:31:ALA:O	0.44	2.71	9	1
1:A:93:THR:HG23	1:A:122:HIS:O	0.44	2.13	4	1
1:B:35:THR:HG22	1:B:46:SER:CA	0.44	2.42	9	2
1:A:71:VAL:CG2	1:A:80:PHE:HB3	0.44	2.43	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:86:PHE:CZ	1:B:93:THR:HG22	0.44	2.48	1	1
1:B:70:GLU:HB3	1:B:72:ARG:HH21	0.44	1.71	19	1
1:B:64:ALA:CB	1:B:85:SER:O	0.44	2.66	17	1
1:A:7:MET:HB3	1:A:73:ALA:HB1	0.44	1.88	10	1
1:A:39:PRO:O	1:A:40:VAL:HG22	0.43	2.12	3	4
1:A:32:ASP:HA	1:A:48:THR:CG2	0.43	2.42	16	4
1:B:97:PRO:CG	1:B:116:PHE:CZ	0.43	3.01	15	2
1:A:36:VAL:CG2	1:A:51:ILE:HD13	0.43	2.43	8	1
1:A:24:ASP:OD2	1:A:52:ARG:NH2	0.43	2.51	7	1
1:B:67:LEU:O	1:B:68:THR:CB	0.43	2.66	3	1
1:B:34:ALA:HA	1:B:110:VAL:O	0.43	2.13	14	1
1:A:54:PHE:C	1:A:54:PHE:CD1	0.43	2.89	5	1
1:B:103:PHE:HB3	1:B:109:VAL:CG2	0.43	2.42	9	2
1:A:23:LEU:HD11	1:A:56:ALA:N	0.43	2.28	13	1
1:B:61:LEU:HD12	1:B:62:PRO:HD2	0.43	1.89	4	6
1:B:97:PRO:HB3	1:B:116:PHE:CG	0.43	2.48	10	2
1:A:67:LEU:HG	1:A:82:PHE:CD1	0.43	2.49	12	2
1:A:67:LEU:HD11	1:A:71:VAL:CG2	0.43	2.43	12	1
1:B:18:LEU:HD12	1:B:26:ILE:HD13	0.43	1.90	16	1
1:B:57:ASN:O	1:B:60:LYS:CB	0.43	2.67	16	2
1:B:97:PRO:HB3	1:B:116:PHE:CD2	0.43	2.49	15	2
1:B:120:ASN:N	1:B:120:ASN:ND2	0.43	2.65	8	1
1:B:32:ASP:O	1:B:48:THR:CB	0.43	2.65	14	2
1:A:38:ASP:O	1:A:45:ARG:NH2	0.43	2.50	10	2
1:B:101:PHE:N	1:B:101:PHE:CD1	0.43	2.86	4	2
1:B:117:GLY:N	1:B:120:ASN:OD1	0.43	2.48	14	2
1:B:37:GLU:OE2	1:B:37:GLU:C	0.43	2.57	14	1
1:A:80:PHE:CE1	1:A:101:PHE:CE2	0.43	3.06	2	1
1:A:101:PHE:CE1	1:A:112:MET:HB3	0.43	2.48	12	1
1:B:74:VAL:O	1:B:77:GLU:O	0.43	2.36	12	2
1:A:45:ARG:HD3	1:A:54:PHE:CG	0.43	2.48	7	1
1:B:63:LEU:CD2	1:B:86:PHE:CE2	0.43	2.96	20	1
1:B:38:ASP:OD1	1:B:114:ALA:CB	0.43	2.62	3	1
1:A:47:GLY:O	1:A:50:ALA:N	0.43	2.52	9	2
1:B:1:MET:SD	1:B:3:THR:CG2	0.43	3.06	17	1
1:B:71:VAL:HG13	1:B:80:PHE:HD1	0.43	1.71	11	1
1:B:7:MET:CG	1:B:8:THR:N	0.43	2.81	15	2
1:A:19:ASN:ND2	1:A:65:VAL:O	0.43	2.50	4	1
1:B:111:SER:N	1:B:112:MET:HE2	0.43	2.29	19	1
1:A:98:ILE:HD13	1:B:72:ARG:HH21	0.43	1.74	10	1
1:A:104:ASN:O	1:A:108:LYS:CG	0.43	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ASN:N	1:A:120:ASN:OD1	0.43	2.51	12	2
1:B:77:GLU:CD	1:B:77:GLU:C	0.43	2.77	12	1
1:A:30:PHE:CE1	1:A:51:ILE:CG2	0.43	2.97	16	1
1:A:57:ASN:O	1:A:60:LYS:CG	0.43	2.66	16	1
1:A:21:GLY:CA	1:A:59:LEU:HD11	0.43	2.43	16	1
1:A:84:VAL:HG12	1:A:97:PRO:CD	0.43	2.44	16	1
1:A:72:ARG:NH1	1:B:120:ASN:OD1	0.43	2.52	15	2
1:A:47:GLY:O	1:A:49:ALA:N	0.43	2.51	1	5
1:B:66:GLU:OE2	1:B:67:LEU:N	0.43	2.52	20	1
1:A:98:ILE:CG2	1:B:72:ARG:NH1	0.43	2.82	20	1
1:B:116:PHE:CG	1:B:117:GLY:N	0.43	2.86	1	1
1:A:23:LEU:HD11	1:A:52:ARG:HG2	0.43	1.89	14	1
1:A:68:THR:OG1	1:A:69:GLN:CD	0.43	2.56	14	1
1:A:104:ASN:HB2	1:A:110:VAL:CG2	0.43	2.43	19	1
1:A:100:HIS:CE1	1:A:113:ARG:HG2	0.43	2.48	17	1
1:A:11:VAL:HG22	1:A:101:PHE:CE2	0.43	2.48	18	1
1:B:69:GLN:O	1:B:70:GLU:O	0.43	2.37	2	1
1:A:68:THR:OG1	1:A:68:THR:O	0.43	2.35	16	1
1:A:95:VAL:HG11	1:A:116:PHE:CE1	0.43	2.49	11	1
1:A:120:ASN:HB2	1:B:72:ARG:CZ	0.43	2.44	11	2
1:B:103:PHE:CE2	1:B:108:LYS:HA	0.43	2.49	15	1
1:B:74:VAL:HG22	1:B:75:ALA:H	0.43	1.73	6	2
1:A:36:VAL:CG2	1:A:51:ILE:HG12	0.43	2.44	13	3
1:B:2:ASN:N	1:B:2:ASN:OD1	0.43	2.51	18	1
1:A:68:THR:OG1	1:A:81:ALA:O	0.43	2.34	2	1
1:B:36:VAL:CG2	1:B:51:ILE:HG12	0.43	2.42	14	4
1:A:38:ASP:CB	1:A:114:ALA:HB3	0.43	2.43	6	1
1:B:26:ILE:HG21	1:B:55:TYR:CE1	0.43	2.49	4	1
1:B:30:PHE:CD2	1:B:31:ALA:O	0.43	2.72	1	1
1:B:7:MET:HG2	1:B:103:PHE:CE1	0.43	2.49	17	1
1:B:18:LEU:HD23	1:B:65:VAL:CG2	0.43	2.40	2	1
1:A:37:GLU:OE2	1:A:41:GLY:N	0.43	2.50	11	1
1:A:47:GLY:C	1:A:49:ALA:N	0.43	2.71	1	7
1:B:76:ASN:N	1:B:76:ASN:OD1	0.43	2.51	8	1
1:A:70:GLU:CB	1:A:72:ARG:NH2	0.43	2.80	20	1
1:A:27:VAL:CG1	1:A:48:THR:OG1	0.43	2.67	3	2
1:A:24:ASP:O	1:A:27:VAL:N	0.43	2.52	4	1
1:A:72:ARG:O	1:A:78:ALA:HA	0.43	2.14	19	1
1:A:14:TYR:HB2	1:A:29:LEU:HD13	0.43	1.90	5	1
1:A:18:LEU:O	1:A:59:LEU:HD21	0.43	2.14	9	1
1:A:100:HIS:O	1:A:113:ARG:CG	0.43	2.66	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:100:HIS:O	1:B:100:HIS:ND1	0.43	2.49	11	1
1:B:68:THR:OG1	1:B:68:THR:O	0.43	2.34	7	1
1:B:63:LEU:CD2	1:B:86:PHE:HB3	0.43	2.44	7	1
1:B:7:MET:CA	1:B:103:PHE:CZ	0.43	3.02	3	1
1:B:70:GLU:C	1:B:70:GLU:CD	0.43	2.78	5	1
1:B:85:SER:CB	1:B:94:VAL:HG23	0.43	2.44	17	1
1:A:11:VAL:HG21	1:A:80:PHE:CD1	0.43	2.48	9	1
1:B:69:GLN:NE2	1:B:69:GLN:O	0.43	2.52	13	1
1:A:95:VAL:CG1	1:A:96:ALA:N	0.43	2.82	16	2
1:B:80:PHE:CD2	1:B:99:ASP:HB2	0.43	2.48	11	1
1:A:14:TYR:CD1	1:A:14:TYR:C	0.43	2.92	7	3
1:B:3:THR:HG23	1:B:6:HIS:CG	0.43	2.49	7	1
1:A:93:THR:CG2	1:A:121:ILE:HG22	0.43	2.44	3	1
1:B:22:ASP:C	1:B:26:ILE:HD12	0.43	2.34	3	1
1:B:63:LEU:HD12	1:B:63:LEU:C	0.43	2.34	3	3
1:B:83:THR:HA	1:B:95:VAL:O	0.43	2.14	1	1
1:A:97:PRO:HB3	1:A:116:PHE:CB	0.43	2.44	9	1
1:A:14:TYR:O	1:A:18:LEU:CD2	0.43	2.67	13	1
1:B:4:PRO:HB3	1:B:73:ALA:HB3	0.42	1.91	11	1
1:A:77:GLU:CD	1:A:100:HIS:HE2	0.42	2.17	20	1
1:B:69:GLN:OE1	1:B:70:GLU:CB	0.42	2.67	3	1
1:B:32:ASP:CA	1:B:48:THR:HG23	0.42	2.43	4	2
1:A:74:VAL:O	1:A:77:GLU:O	0.42	2.36	10	1
1:A:10:VAL:O	1:A:13:ARG:N	0.42	2.51	2	1
1:B:96:ALA:N	1:B:120:ASN:OD1	0.42	2.50	6	1
1:A:115:LEU:HD21	1:B:77:GLU:HB3	0.42	1.91	7	1
1:B:23:LEU:CD2	1:B:55:TYR:HB3	0.42	2.44	4	3
1:B:70:GLU:CD	1:B:71:VAL:N	0.42	2.73	5	1
1:B:78:ALA:HB3	1:B:101:PHE:HB2	0.42	1.91	18	1
1:A:11:VAL:HG12	1:A:67:LEU:CD1	0.42	2.45	2	1
1:A:120:ASN:ND2	1:B:72:ARG:CG	0.42	2.82	12	1
1:A:101:PHE:CE1	1:A:112:MET:SD	0.42	3.12	15	1
1:B:71:VAL:CG1	1:B:80:PHE:HB3	0.42	2.43	19	3
1:A:70:GLU:C	1:A:71:VAL:CG2	0.42	2.88	14	1
1:B:30:PHE:CD2	1:B:112:MET:CE	0.42	3.01	5	1
1:A:67:LEU:CD2	1:A:81:ALA:O	0.42	2.68	18	1
1:B:82:PHE:N	1:B:82:PHE:CD1	0.42	2.88	6	1
1:B:47:GLY:C	1:B:49:ALA:N	0.42	2.72	19	4
1:B:60:LYS:C	1:B:60:LYS:CD	0.42	2.87	3	1
1:B:61:LEU:CD1	1:B:87:GLU:O	0.42	2.61	4	1
1:B:97:PRO:HB3	1:B:116:PHE:CB	0.42	2.44	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:CZ	1:B:98:ILE:HD11	0.42	2.45	12	1
1:B:101:PHE:HB3	1:B:112:MET:CB	0.42	2.44	6	3
1:B:36:VAL:HG11	1:B:55:TYR:HE1	0.42	1.73	7	1
1:A:79:ALA:HB2	1:A:100:HIS:CG	0.42	2.48	3	1
1:B:100:HIS:CG	1:B:100:HIS:O	0.42	2.72	19	1
1:B:11:VAL:HG13	1:B:80:PHE:CG	0.42	2.50	2	2
1:A:26:ILE:HG22	1:A:55:TYR:CE1	0.42	2.48	16	1
1:B:45:ARG:NH1	1:B:55:TYR:CD1	0.42	2.87	11	1
1:A:108:LYS:O	1:A:109:VAL:C	0.42	2.57	15	1
1:B:73:ALA:O	1:B:74:VAL:HG22	0.42	2.14	15	1
1:A:30:PHE:CG	1:A:112:MET:HE1	0.42	2.49	8	2
1:B:30:PHE:HB2	1:B:112:MET:CE	0.42	2.45	8	1
1:A:40:VAL:HG22	1:A:114:ALA:O	0.42	2.15	6	1
1:B:53:GLU:O	1:B:57:ASN:OD1	0.42	2.38	5	1
1:A:103:PHE:CE1	1:A:108:LYS:HA	0.42	2.49	18	1
1:B:26:ILE:HG22	1:B:30:PHE:CE2	0.42	2.49	13	1
1:B:27:VAL:HG22	1:B:51:ILE:HG21	0.42	1.91	13	1
1:A:41:GLY:O	1:A:42:SER:OG	0.42	2.38	2	1
1:A:2:ASN:OD1	1:A:76:ASN:N	0.42	2.52	16	1
1:B:15:VAL:HG13	1:B:65:VAL:HG11	0.42	1.90	8	1
1:B:63:LEU:HD23	1:B:86:PHE:CD2	0.42	2.49	20	1
1:B:93:THR:CG2	1:B:94:VAL:N	0.42	2.83	4	1
1:A:40:VAL:HG11	1:B:74:VAL:HG13	0.42	1.91	19	1
1:A:2:ASN:N	1:A:2:ASN:OD1	0.42	2.52	17	1
1:A:63:LEU:HB2	1:A:86:PHE:CB	0.42	2.45	9	1
1:B:45:ARG:NE	1:B:54:PHE:CD2	0.42	2.88	2	1
1:A:38:ASP:HA	1:A:39:PRO:C	0.42	2.35	12	10
1:A:69:GLN:NE2	1:A:69:GLN:N	0.42	2.68	14	1
1:A:26:ILE:HG21	1:A:55:TYR:HE2	0.42	1.75	8	1
1:A:34:ALA:HB3	1:A:51:ILE:HD11	0.42	1.91	6	1
1:A:97:PRO:HG3	1:A:116:PHE:CZ	0.42	2.49	7	1
1:A:30:PHE:CG	1:A:112:MET:HE3	0.42	2.50	18	1
1:B:26:ILE:CD1	1:B:59:LEU:HD11	0.42	2.45	18	1
1:B:38:ASP:HA	1:B:39:PRO:C	0.42	2.35	15	12
1:B:61:LEU:HD23	1:B:86:PHE:CD1	0.42	2.49	8	1
1:B:68:THR:O	1:B:69:GLN:CD	0.42	2.59	7	1
1:A:119:LYS:O	1:A:119:LYS:NZ	0.42	2.50	20	1
1:A:27:VAL:CG1	1:A:48:THR:CB	0.42	2.98	4	1
1:B:102:ARG:CG	1:B:111:SER:OG	0.42	2.68	14	1
1:B:68:THR:HG21	1:B:83:THR:HG23	0.42	1.92	19	1
1:B:14:TYR:CG	1:B:101:PHE:CZ	0.42	3.08	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:LEU:CD1	1:B:52:ARG:HA	0.42	2.45	18	1
1:B:27:VAL:HA	1:B:30:PHE:CE2	0.42	2.50	9	1
1:A:97:PRO:HB3	1:A:116:PHE:CG	0.41	2.49	16	1
1:A:34:ALA:CB	1:A:110:VAL:HA	0.41	2.45	13	3
1:B:111:SER:C	1:B:112:MET:SD	0.41	2.98	14	2
1:A:120:ASN:CB	1:B:72:ARG:NH1	0.41	2.83	6	1
1:B:92:LYS:HD2	1:B:125:ALA:HB3	0.41	1.92	6	1
1:B:95:VAL:CG2	1:B:121:ILE:HG13	0.41	2.44	4	1
1:A:102:ARG:HG3	1:A:111:SER:CB	0.41	2.45	1	1
1:A:75:ALA:CB	1:B:40:VAL:CG1	0.41	2.96	19	1
1:A:81:ALA:HB2	1:A:98:ILE:CD1	0.41	2.45	9	1
1:B:67:LEU:HD13	1:B:81:ALA:O	0.41	2.15	9	1
1:B:92:LYS:HD3	1:B:125:ALA:HB2	0.41	1.91	13	1
1:A:97:PRO:HB2	1:A:116:PHE:CE1	0.41	2.50	16	1
1:A:30:PHE:O	1:A:31:ALA:O	0.41	2.39	17	9
1:A:45:ARG:NH2	1:A:54:PHE:CZ	0.41	2.88	7	1
1:B:3:THR:OG1	1:B:4:PRO:HD2	0.41	2.15	7	1
1:B:7:MET:HE2	1:B:73:ALA:CB	0.41	2.43	7	1
1:B:56:ALA:C	1:B:58:SER:N	0.41	2.73	19	2
1:A:71:VAL:CG1	1:A:80:PHE:HB3	0.41	2.45	1	1
1:A:96:ALA:O	1:A:120:ASN:OD1	0.41	2.38	1	1
1:A:85:SER:HA	1:A:93:THR:O	0.41	2.14	14	1
1:A:72:ARG:HH12	1:B:117:GLY:N	0.41	2.12	18	1
1:B:23:LEU:CD2	1:B:55:TYR:HB2	0.41	2.43	13	1
1:B:77:GLU:OE1	1:B:102:ARG:CG	0.41	2.68	13	1
1:A:72:ARG:NH1	1:B:98:ILE:CG1	0.41	2.84	12	1
1:B:82:PHE:O	1:B:96:ALA:HA	0.41	2.15	11	2
1:A:103:PHE:C	1:A:104:ASN:OD1	0.41	2.59	8	1
1:A:109:VAL:HG12	1:A:112:MET:CE	0.41	2.46	6	1
1:A:66:GLU:O	1:A:66:GLU:CG	0.41	2.67	6	1
1:B:27:VAL:HG21	1:B:52:ARG:HA	0.41	1.93	6	1
1:A:92:LYS:C	1:A:93:THR:HG1	0.41	2.16	3	1
1:B:11:VAL:CG1	1:B:80:PHE:CE2	0.41	3.03	14	1
1:A:49:ALA:O	1:A:53:GLU:CB	0.41	2.68	17	1
1:A:72:ARG:NE	1:B:120:ASN:HD22	0.41	2.13	9	2
1:A:61:LEU:HD21	1:A:86:PHE:HB3	0.41	1.91	13	1
1:A:34:ALA:HB2	1:A:109:VAL:O	0.41	2.15	10	1
1:A:21:GLY:HA2	1:A:59:LEU:HD21	0.41	1.91	2	1
1:A:23:LEU:CD2	1:A:55:TYR:HB3	0.41	2.45	11	1
1:A:36:VAL:CG2	1:A:51:ILE:HG23	0.41	2.43	11	1
1:A:56:ALA:C	1:A:58:SER:N	0.41	2.73	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:ALA:O	1:B:26:ILE:HD11	0.41	2.16	7	1
1:A:72:ARG:NH1	1:B:116:PHE:HA	0.41	2.30	4	1
1:B:52:ARG:NH1	1:B:53:GLU:OE1	0.41	2.53	4	1
1:B:66:GLU:O	1:B:83:THR:OG1	0.41	2.37	19	1
1:A:52:ARG:O	1:A:56:ALA:HB3	0.41	2.16	5	1
1:A:100:HIS:CE1	1:B:115:LEU:HD11	0.41	2.50	5	1
1:B:35:THR:O	1:B:112:MET:N	0.41	2.53	17	1
1:B:26:ILE:O	1:B:30:PHE:CZ	0.41	2.74	18	1
1:B:38:ASP:OD1	1:B:38:ASP:C	0.41	2.59	18	1
1:B:67:LEU:HD12	1:B:68:THR:CA	0.41	2.43	18	1
1:A:72:ARG:NH1	1:B:119:LYS:C	0.41	2.74	9	1
1:B:91:ARG:HD3	1:B:123:ALA:HB1	0.41	1.92	9	1
1:A:92:LYS:O	1:A:124:GLY:O	0.41	2.38	13	2
1:A:39:PRO:HG3	1:A:116:PHE:CE1	0.41	2.50	10	1
1:A:118:GLU:C	1:A:119:LYS:CG	0.41	2.87	10	1
1:B:39:PRO:O	1:B:114:ALA:O	0.41	2.38	6	5
1:A:67:LEU:HD21	1:A:80:PHE:CD1	0.41	2.50	16	1
1:A:37:GLU:O	1:A:39:PRO:O	0.41	2.39	13	2
1:B:100:HIS:CE1	1:B:113:ARG:HB2	0.41	2.50	6	1
1:B:32:ASP:O	1:B:48:THR:OG1	0.41	2.38	14	2
1:A:75:ALA:O	1:A:76:ASN:CG	0.41	2.59	3	1
1:B:54:PHE:CE2	1:B:55:TYR:CE1	0.41	3.09	3	1
1:B:67:LEU:O	1:B:68:THR:HB	0.41	2.16	3	1
1:B:69:GLN:CG	1:B:81:ALA:O	0.41	2.68	1	1
1:A:58:SER:OG	1:A:59:LEU:N	0.41	2.52	14	1
1:B:45:ARG:HD2	1:B:54:PHE:CG	0.41	2.50	18	1
1:A:104:ASN:HD21	1:A:110:VAL:HG23	0.41	1.76	2	1
1:A:95:VAL:CG2	1:A:121:ILE:HG12	0.41	2.39	2	1
1:A:40:VAL:HG11	1:A:115:LEU:HG	0.41	1.91	2	1
1:A:92:LYS:C	1:A:93:THR:OG1	0.41	2.59	2	2
1:B:72:ARG:HG3	1:B:79:ALA:HB3	0.41	1.91	2	1
1:A:2:ASN:CB	1:A:76:ASN:OD1	0.41	2.68	16	1
1:B:86:PHE:CZ	1:B:93:THR:CB	0.41	3.03	1	2
1:B:103:PHE:CE2	1:B:109:VAL:HG23	0.41	2.51	8	1
1:B:40:VAL:HG22	1:B:115:LEU:HA	0.41	1.91	8	1
1:B:59:LEU:O	1:B:60:LYS:C	0.41	2.58	18	2
1:B:100:HIS:CD2	1:B:100:HIS:C	0.41	2.93	6	1
1:A:32:ASP:CA	1:A:48:THR:HG23	0.41	2.46	1	1
1:A:23:LEU:CD1	1:A:52:ARG:HG2	0.41	2.45	14	1
1:A:63:LEU:CA	1:A:85:SER:O	0.41	2.69	5	1
1:B:95:VAL:CG2	1:B:121:ILE:HG12	0.41	2.40	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ASP:CG	1:B:54:PHE:CE2	0.41	2.93	13	1
1:A:118:GLU:O	1:A:119:LYS:HB2	0.41	2.15	10	1
1:B:112:MET:C	1:B:113:ARG:CG	0.41	2.89	10	1
1:A:70:GLU:O	1:A:79:ALA:O	0.41	2.39	2	1
1:B:24:ASP:OD1	1:B:24:ASP:N	0.41	2.53	11	1
1:B:101:PHE:CB	1:B:112:MET:CB	0.41	2.99	6	1
1:B:65:VAL:HG13	1:B:83:THR:O	0.41	2.15	7	2
1:A:119:LYS:O	1:A:119:LYS:CD	0.41	2.69	20	1
1:B:38:ASP:C	1:B:38:ASP:OD2	0.41	2.59	14	2
1:B:37:GLU:CD	1:B:37:GLU:O	0.41	2.59	14	1
1:A:75:ALA:HB2	1:B:40:VAL:HG12	0.41	1.93	19	1
1:A:72:ARG:NH2	1:B:120:ASN:HB3	0.41	2.31	5	1
1:A:24:ASP:OD1	1:A:25:GLY:N	0.41	2.51	17	1
1:A:45:ARG:CZ	1:A:54:PHE:CE1	0.41	3.04	17	1
1:A:61:LEU:HD23	1:A:86:PHE:HD1	0.41	1.76	17	1
1:A:36:VAL:CG1	1:A:38:ASP:OD2	0.41	2.69	10	1
1:B:30:PHE:O	1:B:31:ALA:O	0.41	2.39	20	8
1:A:27:VAL:HG12	1:A:48:THR:HG22	0.41	1.93	8	1
1:A:75:ALA:CB	1:B:40:VAL:HB	0.41	2.46	8	1
1:B:37:GLU:CG	1:B:113:ARG:CB	0.41	2.99	8	1
1:B:47:GLY:O	1:B:49:ALA:N	0.41	2.54	3	1
1:A:99:ASP:OD2	1:A:114:ALA:HB2	0.41	2.16	14	1
1:B:117:GLY:HA2	1:B:121:ILE:CD1	0.41	2.46	19	1
1:B:30:PHE:CD2	1:B:112:MET:SD	0.41	3.14	18	1
1:B:67:LEU:CD1	1:B:67:LEU:C	0.41	2.78	18	1
1:A:95:VAL:C	1:A:97:PRO:HD3	0.41	2.36	13	1
1:B:39:PRO:HA	1:B:114:ALA:HB3	0.41	1.92	13	1
1:B:27:VAL:HG22	1:B:51:ILE:HG22	0.41	1.93	8	2
1:A:36:VAL:HG13	1:A:112:MET:CG	0.41	2.45	11	1
1:B:70:GLU:CD	1:B:70:GLU:C	0.41	2.80	8	1
1:B:3:THR:OG1	1:B:5:GLU:CG	0.41	2.69	7	1
1:A:19:ASN:ND2	1:A:64:ALA:CB	0.41	2.81	7	1
1:A:86:PHE:CZ	1:A:93:THR:CB	0.41	3.04	7	1
1:A:72:ARG:NH2	1:B:97:PRO:HA	0.41	2.30	7	1
1:A:40:VAL:HG22	1:A:115:LEU:HA	0.41	1.93	20	2
1:A:15:VAL:O	1:A:16:ALA:C	0.41	2.59	3	1
1:A:73:ALA:O	1:A:74:VAL:CG2	0.41	2.59	3	1
1:A:24:ASP:C	1:A:26:ILE:N	0.41	2.74	4	1
1:A:72:ARG:NH2	1:B:120:ASN:HB2	0.41	2.31	4	1
1:B:2:ASN:ND2	1:B:2:ASN:N	0.41	2.64	4	1
1:A:104:ASN:C	1:A:104:ASN:OD1	0.41	2.60	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:HG22	1:A:112:MET:CE	0.41	2.45	1	1
1:B:17:ALA:O	1:B:22:ASP:OD2	0.41	2.39	1	1
1:A:7:MET:SD	1:A:77:GLU:O	0.41	2.79	19	3
1:A:71:VAL:O	1:A:73:ALA:N	0.41	2.54	14	1
1:B:92:LYS:O	1:B:124:GLY:O	0.41	2.39	19	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.41	2.81	5	1
1:B:79:ALA:HB2	1:B:100:HIS:HD2	0.41	1.76	5	1
1:A:96:ALA:O	1:A:120:ASN:CG	0.41	2.60	5	1
1:A:75:ALA:O	1:A:77:GLU:CG	0.41	2.68	5	1
1:A:3:THR:CG2	1:A:6:HIS:HB2	0.41	2.46	17	1
1:B:23:LEU:CD1	1:B:52:ARG:O	0.41	2.69	9	1
1:A:4:PRO:CB	1:A:73:ALA:HB3	0.41	2.43	9	1
1:B:111:SER:C	1:B:112:MET:CG	0.41	2.89	9	1
1:B:92:LYS:CD	1:B:125:ALA:HB2	0.41	2.46	13	1
1:A:59:LEU:O	1:A:60:LYS:C	0.41	2.59	13	1
1:B:44:PRO:O	1:B:45:ARG:CD	0.41	2.69	10	1
1:A:21:GLY:HA2	1:A:59:LEU:CD2	0.41	2.46	2	1
1:B:117:GLY:C	1:B:120:ASN:OD1	0.41	2.60	2	1
1:B:77:GLU:O	1:B:77:GLU:OE1	0.41	2.39	12	1
1:B:45:ARG:NH2	1:B:54:PHE:CZ	0.41	2.89	11	1
1:B:37:GLU:HG3	1:B:113:ARG:CG	0.41	2.46	8	1
1:B:92:LYS:HD2	1:B:125:ALA:CB	0.41	2.45	6	1
1:A:67:LEU:HD22	1:A:82:PHE:HB3	0.41	1.93	7	1
1:A:16:ALA:C	1:A:18:LEU:N	0.41	2.75	20	1
1:B:37:GLU:C	1:B:38:ASP:OD2	0.41	2.59	3	1
1:B:67:LEU:C	1:B:68:THR:HG22	0.41	2.36	3	1
1:A:38:ASP:HB2	1:A:114:ALA:CB	0.41	2.46	4	1
1:A:93:THR:HA	1:A:122:HIS:O	0.41	2.16	4	1
1:A:98:ILE:CG2	1:A:99:ASP:N	0.41	2.84	4	1
1:B:11:VAL:HG11	1:B:80:PHE:CD2	0.41	2.51	1	1
1:B:37:GLU:HG3	1:B:113:ARG:CB	0.41	2.46	14	1
1:B:79:ALA:CB	1:B:100:HIS:CD2	0.41	2.93	18	1
1:B:63:LEU:HD21	1:B:84:VAL:HB	0.41	1.92	13	1
1:A:53:GLU:O	1:A:57:ASN:OD1	0.40	2.40	2	2
1:A:119:LYS:C	1:A:120:ASN:OD1	0.40	2.58	11	1
1:A:63:LEU:HA	1:A:85:SER:O	0.40	2.15	19	2
1:A:103:PHE:CZ	1:A:108:LYS:HG2	0.40	2.51	7	1
1:A:119:LYS:HE2	1:B:70:GLU:CG	0.40	2.46	20	1
1:B:84:VAL:CG2	1:B:95:VAL:HB	0.40	2.47	20	1
1:A:115:LEU:HD23	1:B:74:VAL:HG12	0.40	1.93	3	1
1:A:26:ILE:O	1:A:30:PHE:CZ	0.40	2.74	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:GLU:OE1	1:A:37:GLU:O	0.40	2.39	4	1
1:B:84:VAL:HG23	1:B:86:PHE:CZ	0.40	2.50	4	1
1:A:102:ARG:CD	1:A:111:SER:HB3	0.40	2.46	1	1
1:A:93:THR:CG2	1:A:121:ILE:HG23	0.40	2.46	5	1
1:A:41:GLY:N	1:B:75:ALA:HB2	0.40	2.31	5	1
1:B:67:LEU:CD1	1:B:68:THR:N	0.40	2.68	18	1
1:B:37:GLU:C	1:B:37:GLU:OE1	0.40	2.59	15	1
1:B:52:ARG:CG	1:B:53:GLU:N	0.40	2.83	15	1
1:B:32:ASP:HA	1:B:48:THR:CG2	0.40	2.46	3	1
1:B:92:LYS:C	1:B:93:THR:OG1	0.40	2.59	3	3
1:A:23:LEU:CD2	1:A:55:TYR:HB2	0.40	2.46	4	1
1:B:38:ASP:C	1:B:38:ASP:OD1	0.40	2.59	1	1
1:A:19:ASN:CG	1:A:65:VAL:O	0.40	2.60	14	1
1:A:16:ALA:O	1:A:20:ALA:CB	0.40	2.69	14	1
1:A:70:GLU:O	1:A:80:PHE:HB2	0.40	2.16	14	1
1:A:84:VAL:N	1:A:95:VAL:O	0.40	2.54	14	1
1:B:27:VAL:HG11	1:B:48:THR:OG1	0.40	2.16	19	1
1:A:45:ARG:N	1:A:45:ARG:CD	0.40	2.84	17	1
1:A:97:PRO:HA	1:B:72:ARG:NH1	0.40	2.31	18	1
1:A:15:VAL:HG13	1:A:65:VAL:HG12	0.40	1.92	13	1
1:B:124:GLY:O	1:B:125:ALA:C	0.40	2.60	8	3
1:B:111:SER:OG	1:B:113:ARG:NH1	0.40	2.54	7	1
1:A:54:PHE:O	1:A:57:ASN:OD1	0.40	2.40	20	1
1:A:74:VAL:HG22	1:B:117:GLY:CA	0.40	2.47	20	1
1:A:117:GLY:O	1:A:120:ASN:OD1	0.40	2.40	3	1
1:A:35:THR:O	1:A:112:MET:SD	0.40	2.80	1	1
1:A:69:GLN:O	1:A:70:GLU:O	0.40	2.40	14	1
1:B:120:ASN:O	1:B:122:HIS:NE2	0.40	2.54	14	1
1:A:73:ALA:HA	1:A:77:GLU:O	0.40	2.16	19	1
1:A:37:GLU:CG	1:A:44:PRO:HB3	0.40	2.46	17	1
1:B:86:PHE:O	1:B:93:THR:O	0.40	2.40	18	1
1:A:2:ASN:CG	1:A:7:MET:SD	0.40	3.00	9	1
1:A:37:GLU:O	1:A:37:GLU:OE1	0.40	2.40	9	1
1:B:63:LEU:HD11	1:B:65:VAL:HG23	0.40	1.93	13	1
1:A:67:LEU:HD21	1:A:80:PHE:HD1	0.40	1.76	16	1
1:A:74:VAL:HG12	1:B:115:LEU:CD2	0.40	2.46	11	1
1:B:45:ARG:HD2	1:B:50:ALA:CB	0.40	2.46	8	1
1:B:92:LYS:CD	1:B:125:ALA:HB3	0.40	2.47	6	1
1:B:39:PRO:CB	1:B:116:PHE:CD1	0.40	3.05	7	1
1:A:92:LYS:HE3	1:A:125:ALA:CB	0.40	2.47	20	1
1:B:72:ARG:NE	1:B:79:ALA:CB	0.40	2.82	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1:MET:C	1:B:2:ASN:CG	0.40	2.80	3	1
1:B:37:GLU:HB3	1:B:113:ARG:CG	0.40	2.46	17	1
1:B:81:ALA:HB2	1:B:98:ILE:HG12	0.40	1.94	17	1
1:A:72:ARG:CZ	1:B:116:PHE:HA	0.40	2.47	18	1
1:A:122:HIS:O	1:A:123:ALA:O	0.40	2.40	9	1
1:A:124:GLY:O	1:A:125:ALA:C	0.40	2.60	9	1
1:A:118:GLU:OE1	1:B:73:ALA:O	0.40	2.40	9	1
1:B:45:ARG:CD	1:B:50:ALA:HB1	0.40	2.47	13	1
1:B:42:SER:C	1:B:43:GLU:CG	0.40	2.90	16	1
1:B:100:HIS:O	1:B:100:HIS:CG	0.40	2.74	6	1
1:B:85:SER:HA	1:B:93:THR:O	0.40	2.16	4	1
1:B:100:HIS:O	1:B:113:ARG:O	0.40	2.39	1	1
1:A:16:ALA:O	1:A:20:ALA:HB2	0.40	2.17	14	1
1:A:11:VAL:CG1	1:A:80:PHE:CE1	0.40	3.04	5	1
1:B:36:VAL:CG1	1:B:38:ASP:OD1	0.40	2.69	17	1
1:A:4:PRO:HA	1:A:73:ALA:CB	0.40	2.47	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	116/125 (93%)	92±4 (80±3%)	16±4 (14±4%)	7±1 (6±1%)	3	20
1	B	116/125 (93%)	94±3 (81±3%)	16±3 (13±3%)	7±2 (6±1%)	4	22
All	All	4640/5000 (93%)	3719 (80%)	639 (14%)	282 (6%)	3	21

All 43 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	31	ALA	20
1	B	31	ALA	19
1	A	39	PRO	16
1	B	39	PRO	14
1	A	68	THR	13

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Mol	Chain	Res	Type	Models (Total)
1	B	74	VAL	12
1	B	42	SER	12
1	A	74	VAL	11
1	A	42	SER	11
1	B	68	THR	11
1	A	75	ALA	11
1	A	69	GLN	11
1	B	76	ASN	10
1	A	108	LYS	9
1	A	76	ASN	9
1	B	75	ALA	9
1	A	2	ASN	8
1	B	43	GLU	8
1	B	91	ARG	7
1	B	2	ASN	7
1	B	69	GLN	6
1	A	104	ASN	6
1	A	43	GLU	5
1	A	70	GLU	5
1	B	108	LYS	5
1	B	70	GLU	4
1	B	40	VAL	4
1	B	34	ALA	3
1	B	71	VAL	2
1	B	41	GLY	1
1	A	40	VAL	1
1	A	41	GLY	1
1	A	72	ARG	1
1	A	71	VAL	1
1	A	119	LYS	1
1	A	84	VAL	1
1	A	34	ALA	1
1	A	48	THR	1
1	B	60	LYS	1
1	A	109	VAL	1
1	B	22	ASP	1
1	A	123	ALA	1
1	B	4	PRO	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/95 (96%)	64±4 (71±4%)	27±4 (29±4%)	2	18
1	B	92/95 (97%)	66±4 (72±4%)	26±4 (28±4%)	2	20
All	All	3660/3800 (96%)	2610 (71%)	1050 (29%)	2	19

All 129 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	B	83	THR	20
1	A	83	THR	20
1	A	115	LEU	19
1	B	115	LEU	18
1	B	84	VAL	18
1	A	63	LEU	17
1	A	84	VAL	16
1	B	63	LEU	16
1	B	38	ASP	16
1	A	99	ASP	15
1	A	38	ASP	15
1	B	59	LEU	14
1	A	111	SER	14
1	B	29	LEU	14
1	B	40	VAL	13
1	A	94	VAL	13
1	A	69	GLN	13
1	B	108	LYS	13
1	B	99	ASP	13
1	A	40	VAL	13
1	B	94	VAL	13
1	B	85	SER	12
1	B	69	GLN	12
1	B	60	LYS	12
1	B	76	ASN	12
1	A	59	LEU	12
1	A	7	MET	12
1	A	72	ARG	12

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Mol	Chain	Res	Type	Models (Total)
1	A	119	LYS	12
1	B	111	SER	11
1	A	60	LYS	11
1	A	68	THR	11
1	B	70	GLU	11
1	A	13	ARG	11
1	A	29	LEU	11
1	A	70	GLU	11
1	A	116	PHE	11
1	B	91	ARG	11
1	A	12	GLN	11
1	A	58	SER	10
1	B	67	LEU	10
1	A	23	LEU	10
1	A	108	LYS	10
1	A	32	ASP	10
1	A	52	ARG	10
1	A	43	GLU	10
1	B	13	ARG	10
1	A	85	SER	10
1	A	24	ASP	9
1	B	32	ASP	9
1	B	23	LEU	9
1	B	1	MET	9
1	A	74	VAL	9
1	A	92	LYS	9
1	A	120	ASN	9
1	A	54	PHE	9
1	B	45	ARG	9
1	B	102	ARG	9
1	B	7	MET	9
1	B	3	THR	9
1	B	119	LYS	9
1	B	54	PHE	8
1	A	103	PHE	8
1	A	3	THR	8
1	B	116	PHE	8
1	A	100	HIS	8
1	A	67	LEU	8
1	A	45	ARG	8
1	B	113	ARG	7
1	B	52	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	B	68	THR	7
1	B	2	ASN	7
1	B	5	GLU	7
1	B	100	HIS	7
1	B	58	SER	7
1	A	48	THR	7
1	B	92	LYS	7
1	B	74	VAL	7
1	B	118	GLU	7
1	B	43	GLU	7
1	B	24	ASP	7
1	A	112	MET	7
1	A	113	ARG	6
1	B	122	HIS	6
1	A	37	GLU	6
1	A	53	GLU	6
1	B	112	MET	6
1	A	122	HIS	6
1	A	102	ARG	6
1	B	72	ARG	6
1	A	5	GLU	5
1	A	76	ASN	5
1	A	33	ASP	5
1	A	118	GLU	5
1	B	57	ASN	5
1	B	103	PHE	5
1	A	2	ASN	5
1	B	120	ASN	5
1	B	86	PHE	4
1	B	48	THR	4
1	B	77	GLU	4
1	B	42	SER	4
1	A	77	GLU	4
1	A	57	ASN	4
1	A	22	ASP	4
1	A	101	PHE	3
1	B	37	GLU	3
1	A	42	SER	3
1	B	33	ASP	3
1	B	12	GLN	3
1	A	121	ILE	2
1	B	55	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	19	ASN	2
1	A	19	ASN	2
1	B	30	PHE	2
1	A	104	ASN	2
1	A	86	PHE	2
1	B	22	ASP	2
1	A	80	PHE	2
1	B	14	TYR	2
1	B	27	VAL	1
1	B	87	GLU	1
1	A	46	SER	1
1	B	101	PHE	1
1	A	10	VAL	1
1	A	55	TYR	1
1	B	121	ILE	1
1	B	80	PHE	1
1	B	53	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided