



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:01 pm GMT

PDB ID : 2GVA
Title : REFINED SOLUTION STRUCTURE OF THE TYR 41-> HIS MUTANT OF THE M13 GENE V PROTEIN. A COMPARISON WITH THE CRYSTAL STRUCTURE
Authors : Folkers, P.J.M.; Nilges, M.; Folmer, R.H.A.; Prompers, J.J.; Konings, R.N.H.; Hilbers, C.W.
Deposited on : 1995-07-27

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

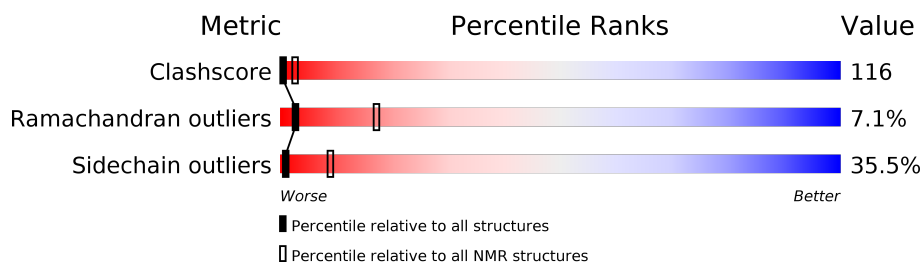
1 Overall quality at a glance

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	87	
1	B	87	

2 Ensemble composition and analysis

This entry contains 30 models. Model 14 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:1-A:15, A:28-A:87, B:1-B:15, B:28-B:87 (150)	0.49	14

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

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

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

Cluster number	Models
1	2, 3, 4, 5, 7, 10, 14, 15, 17, 19, 20, 24, 25, 26, 27, 28
2	1, 12, 16, 21, 29, 30
3	6, 22, 23
4	9, 13
Single-model clusters	8; 11; 18

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2760 atoms, of which 1400 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GENE V PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1380	435	700	117	125	3	
1	B	87	Total	C	H	N	O	S	0
			1380	435	700	117	125	3	

There are 2 discrepancies between the modelled and reference sequences:

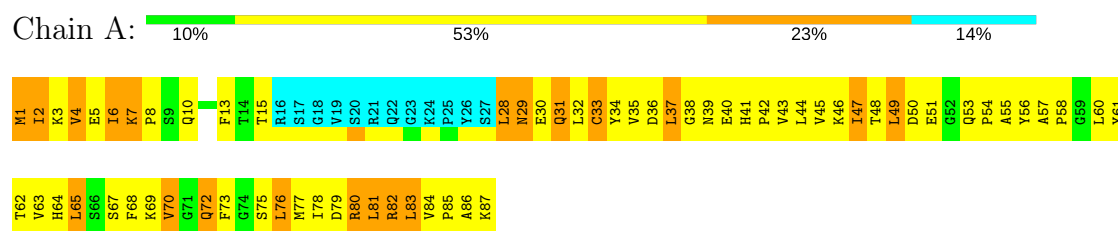
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	HIS	TYR	CONFLICT	UNP P69544
B	41	HIS	TYR	CONFLICT	UNP P69544

4 Residue-property plots

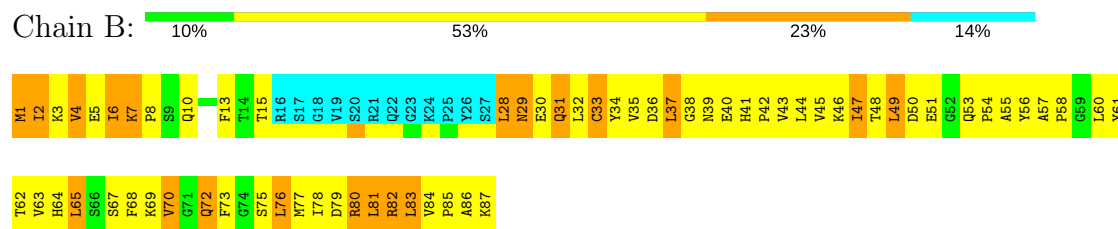
4.1 Average score per residue in the NMR ensemble

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: GENE V PROTEIN



• Molecule 1: GENE V PROTEIN

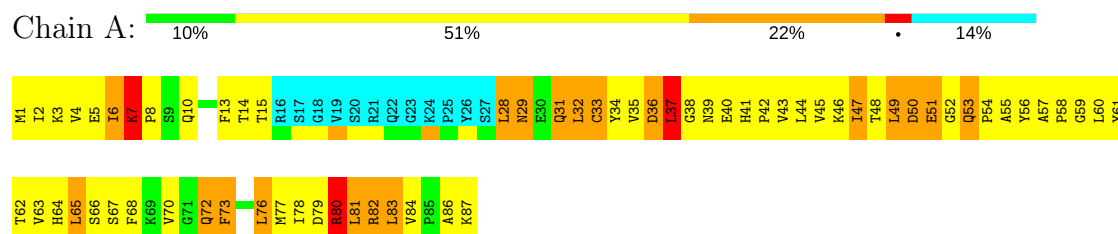


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

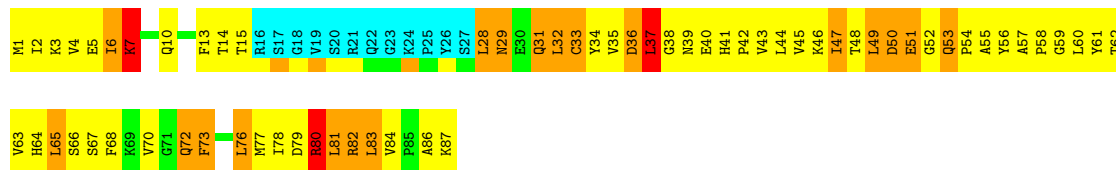
4.2.1 Score per residue for model 1

• Molecule 1: GENE V PROTEIN



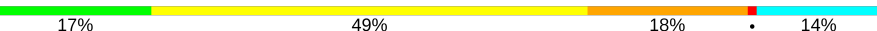
- Molecule 1: GENE V PROTEIN

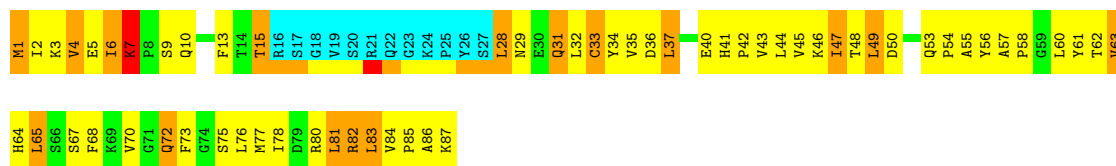
Chain B: 




4.2.2 Score per residue for model 2

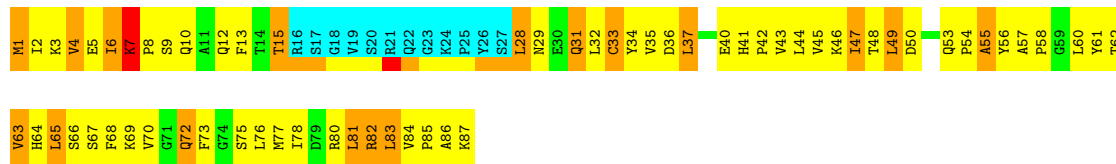
- Molecule 1: GENE V PROTEIN

Chain A: 



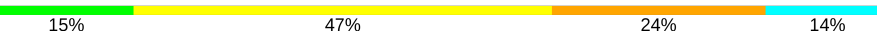
- Molecule 1: GENE V PROTEIN

Chain B: 



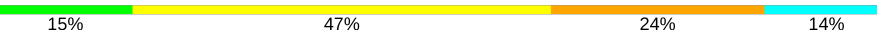
4.2.3 Score per residue for model 3

- Molecule 1: GENE V PROTEIN

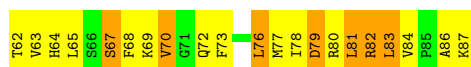
Chain A: 



- Molecule 1: GENE V PROTEIN

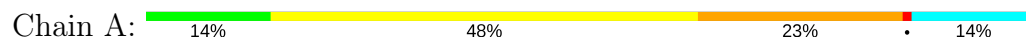
Chain B: 



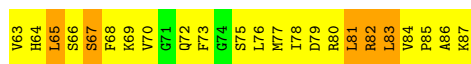
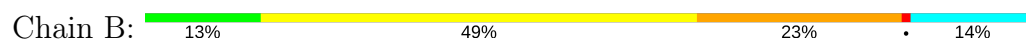


4.2.4 Score per residue for model 4

- Molecule 1: GENE V PROTEIN

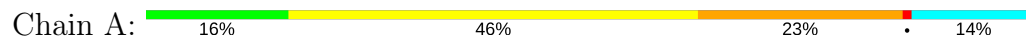


- Molecule 1: GENE V PROTEIN

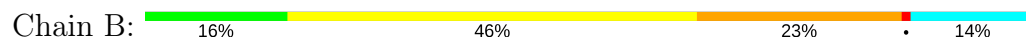


4.2.5 Score per residue for model 5

- Molecule 1: GENE V PROTEIN

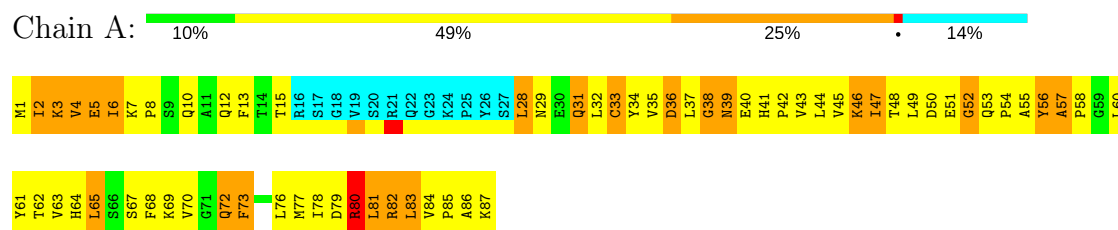


- Molecule 1: GENE V PROTEIN

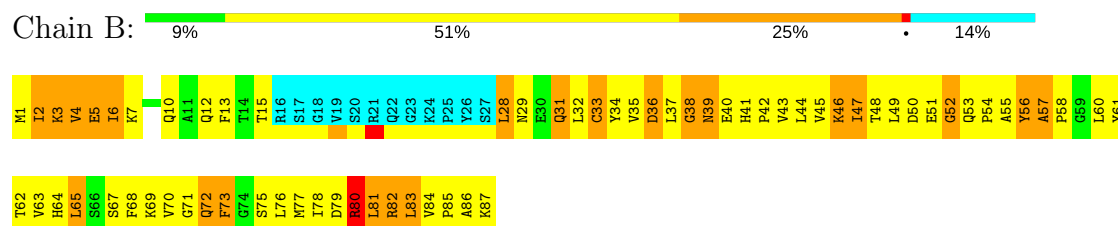


4.2.6 Score per residue for model 6

- Molecule 1: GENE V PROTEIN

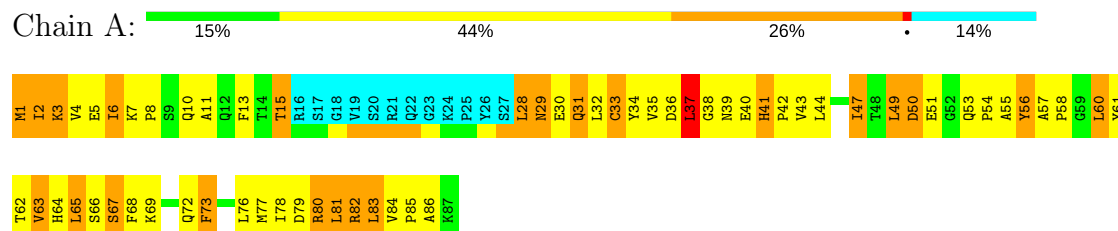


- Molecule 1: GENE V PROTEIN

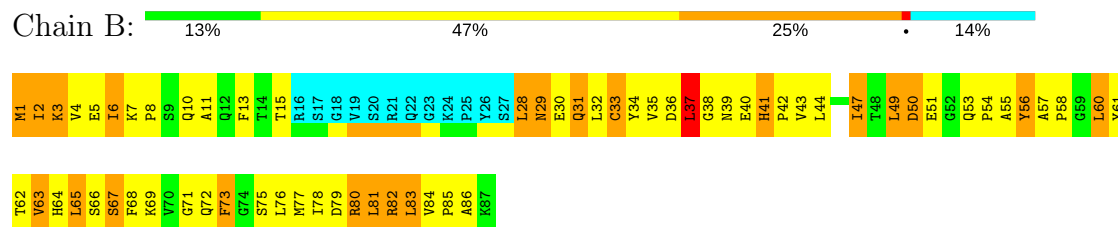


4.2.7 Score per residue for model 7

- Molecule 1: GENE V PROTEIN



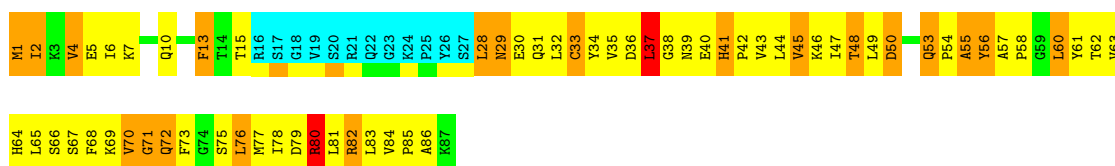
- Molecule 1: GENE V PROTEIN



4.2.8 Score per residue for model 8

- Molecule 1: GENE V PROTEIN





• Molecule 1: GENE V PROTEIN

Chain B: 11% 49% 23% • 14%



4.2.9 Score per residue for model 9

• Molecule 1: GENE V PROTEIN

Chain A: 9% 48% 25% • 14%



• Molecule 1: GENE V PROTEIN

Chain B: 8% 49% 25% • 14%



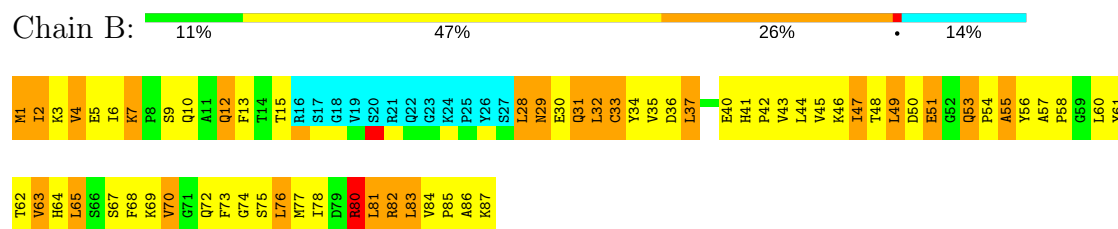
4.2.10 Score per residue for model 10

• Molecule 1: GENE V PROTEIN

Chain A: 13% 47% 25% • 14%

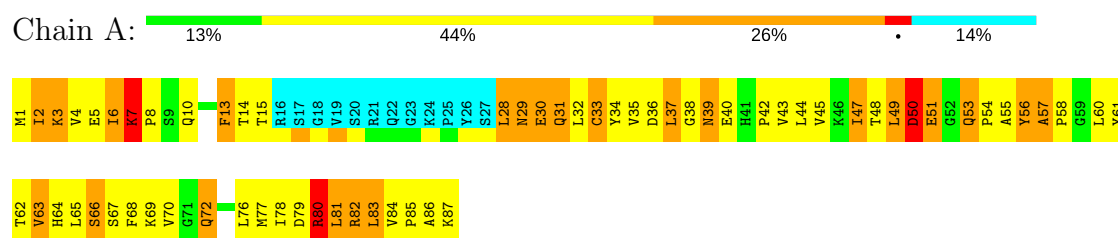


- Molecule 1: GENE V PROTEIN

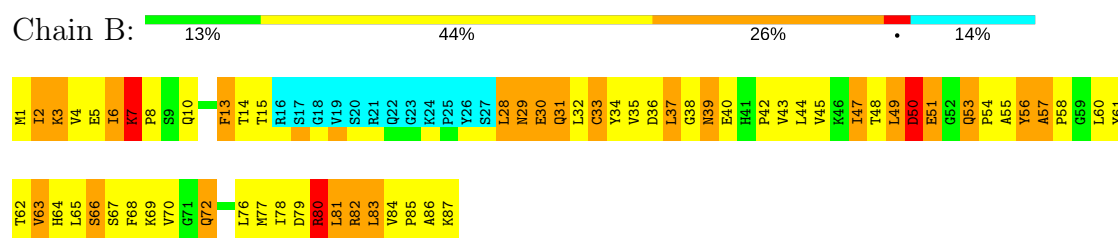


4.2.11 Score per residue for model 11

- Molecule 1: GENE V PROTEIN

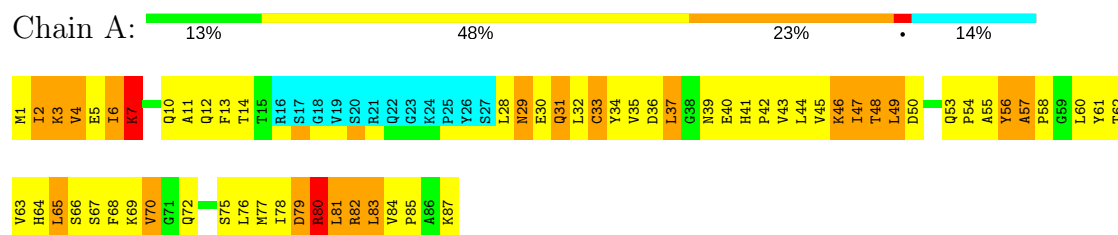


- Molecule 1: GENE V PROTEIN

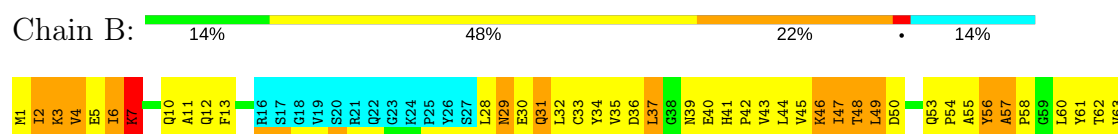


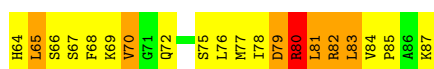
4.2.12 Score per residue for model 12

- Molecule 1: GENE V PROTEIN



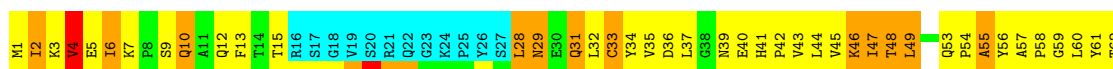
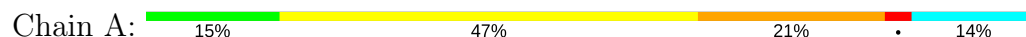
- Molecule 1: GENE V PROTEIN



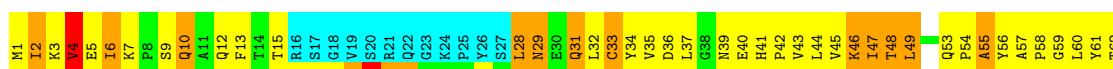
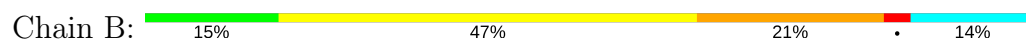


4.2.13 Score per residue for model 13

- Molecule 1: GENE V PROTEIN

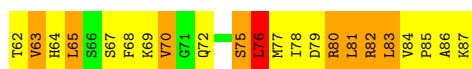
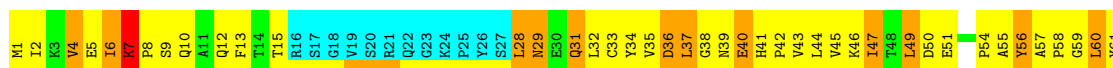


- Molecule 1: GENE V PROTEIN

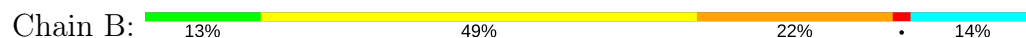


4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: GENE V PROTEIN

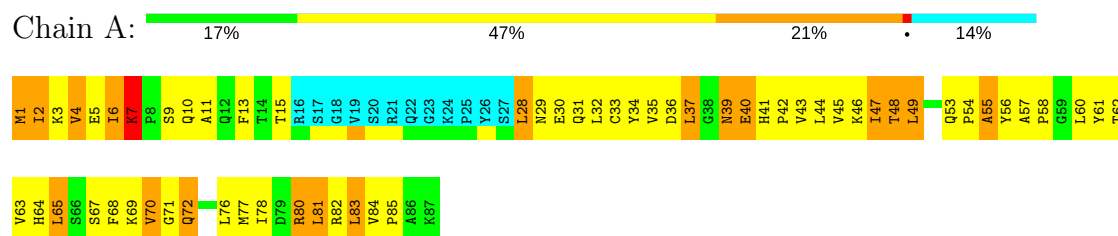


- Molecule 1: GENE V PROTEIN

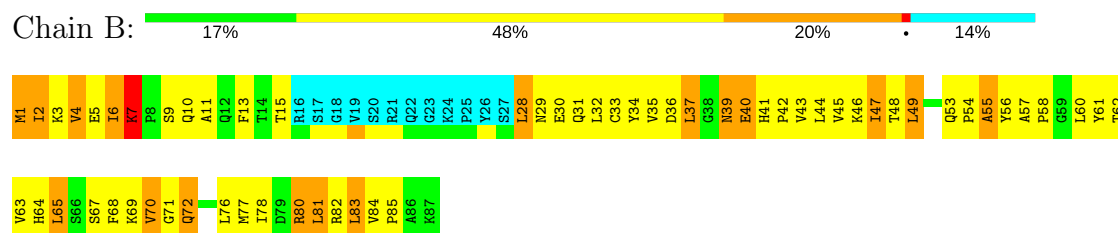


4.2.15 Score per residue for model 15

• Molecule 1: GENE V PROTEIN

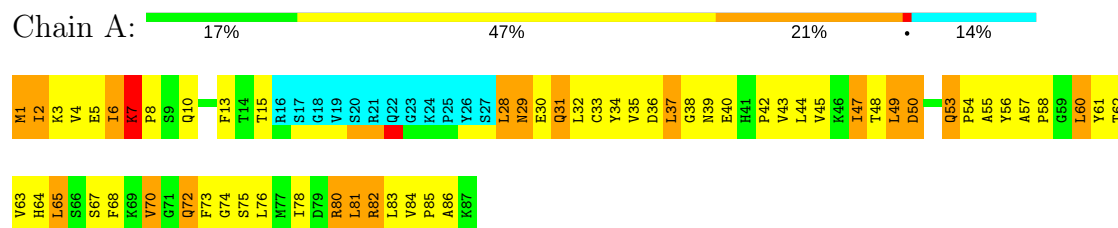


• Molecule 1: GENE V PROTEIN

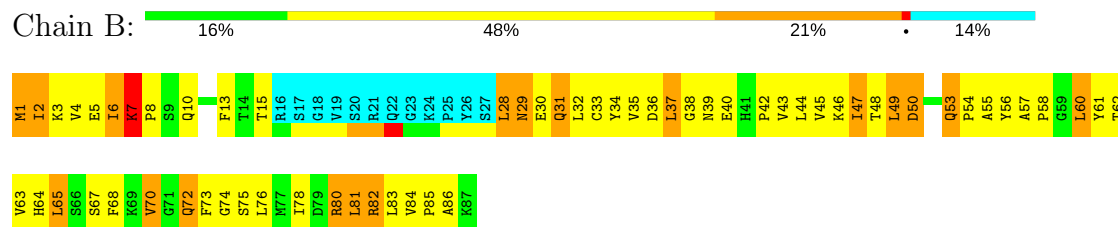


4.2.16 Score per residue for model 16

• Molecule 1: GENE V PROTEIN

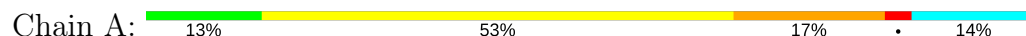


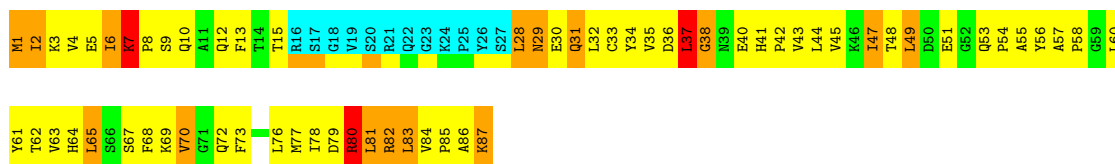
• Molecule 1: GENE V PROTEIN



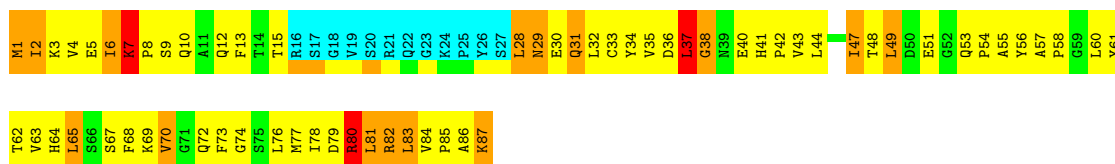
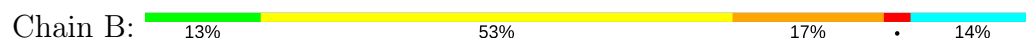
4.2.17 Score per residue for model 17

• Molecule 1: GENE V PROTEIN



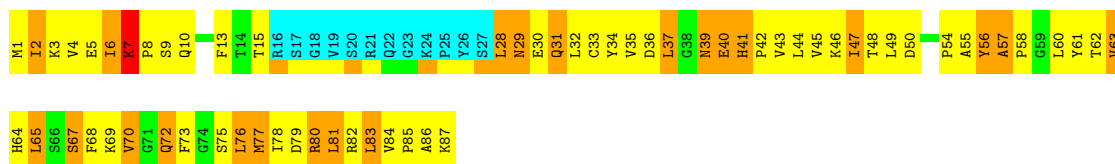


• Molecule 1: GENE V PROTEIN

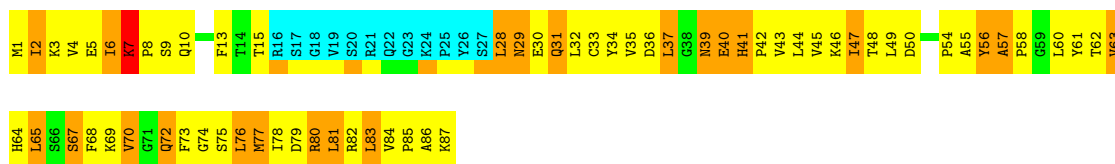


4.2.18 Score per residue for model 18

• Molecule 1: GENE V PROTEIN

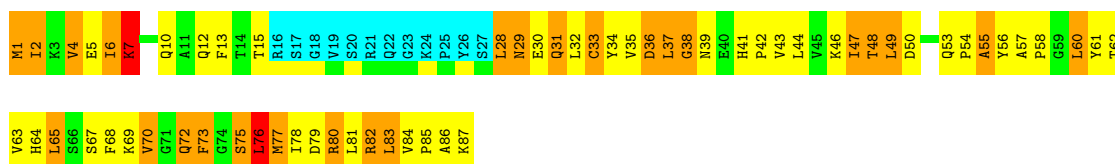


• Molecule 1: GENE V PROTEIN

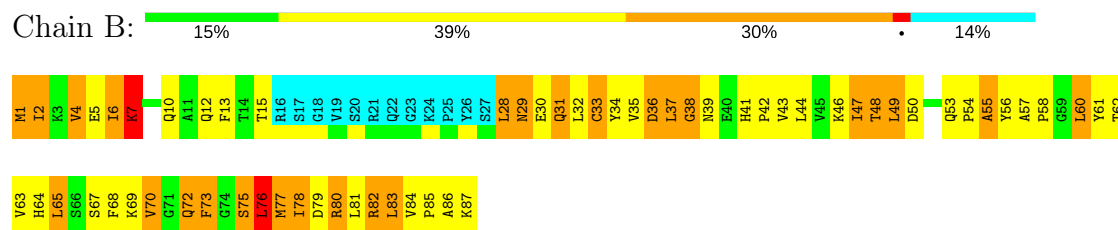


4.2.19 Score per residue for model 19

• Molecule 1: GENE V PROTEIN

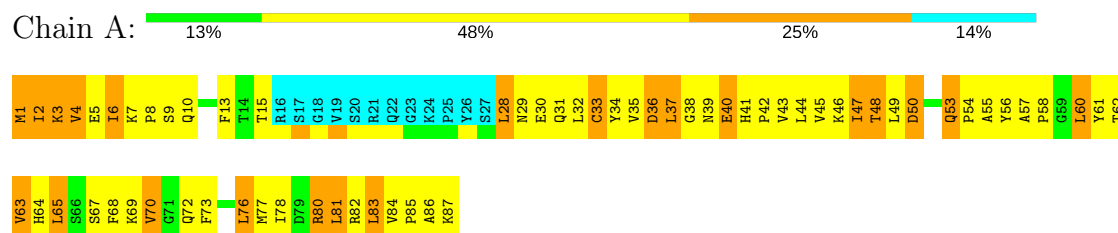


• Molecule 1: GENE V PROTEIN

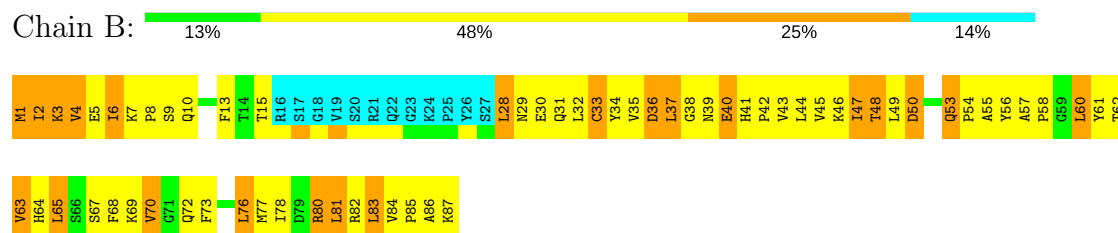


4.2.20 Score per residue for model 20

- Molecule 1: GENE V PROTEIN

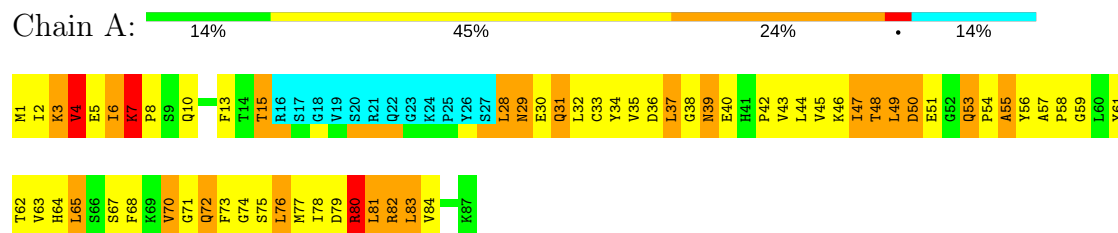


- Molecule 1: GENE V PROTEIN

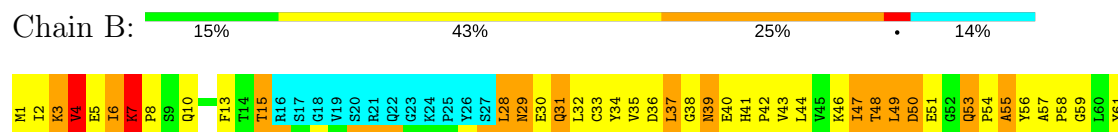


4.2.21 Score per residue for model 21

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN





4.2.22 Score per residue for model 22

- Molecule 1: GENE V PROTEIN

Chain A: 11% 53% 20% • 14%



- Molecule 1: GENE V PROTEIN

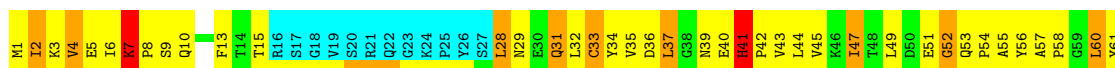
Chain B: 14% 51% 20% • 14%



4.2.23 Score per residue for model 23

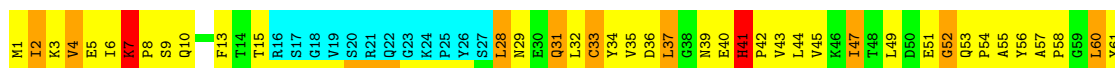
- Molecule 1: GENE V PROTEIN

Chain A: 14% 51% 17% 5% 14%



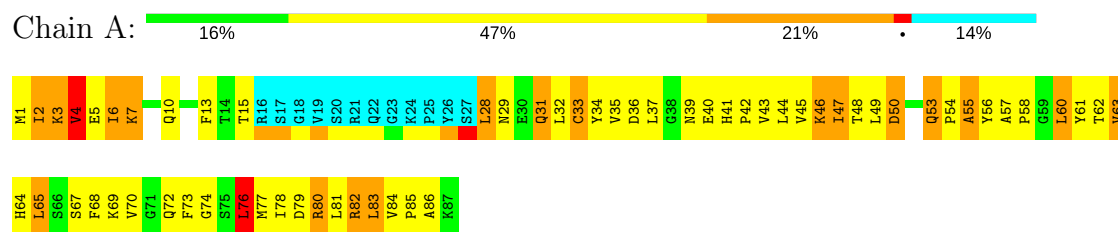
- Molecule 1: GENE V PROTEIN

Chain B: 16% 48% 17% 5% 14%

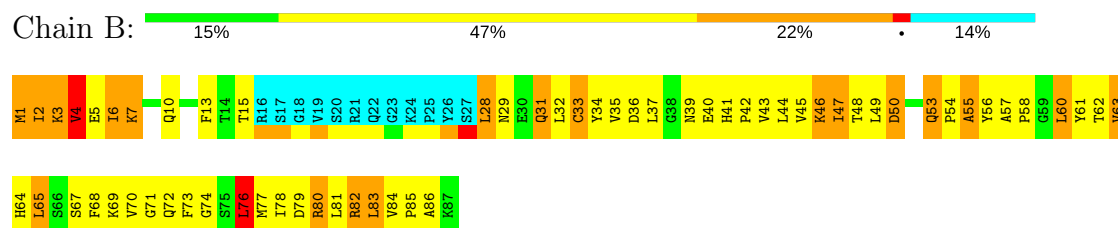


4.2.24 Score per residue for model 24

• Molecule 1: GENE V PROTEIN

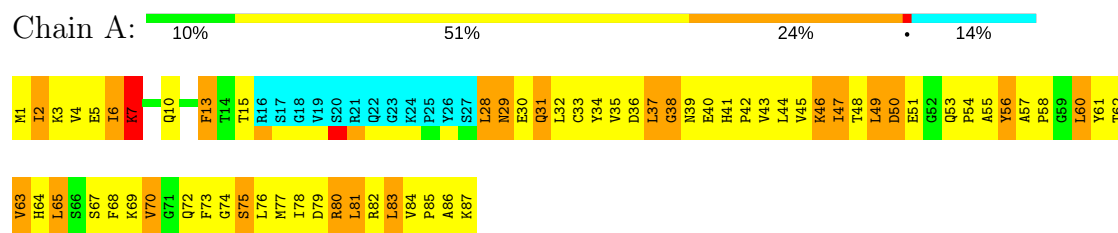


• Molecule 1: GENE V PROTEIN

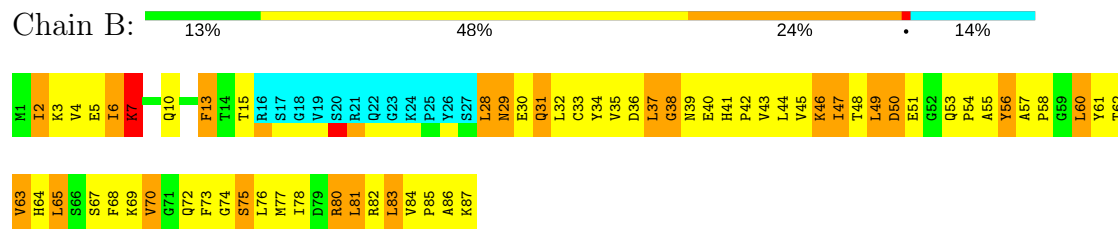


4.2.25 Score per residue for model 25

• Molecule 1: GENE V PROTEIN



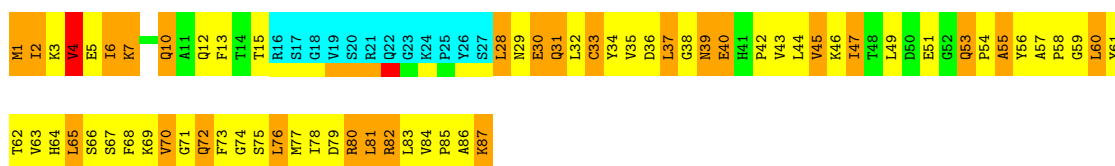
• Molecule 1: GENE V PROTEIN



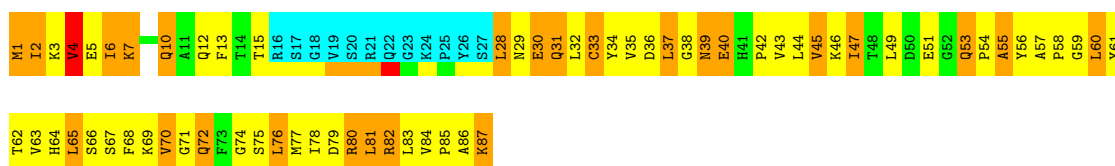
4.2.26 Score per residue for model 26

• Molecule 1: GENE V PROTEIN



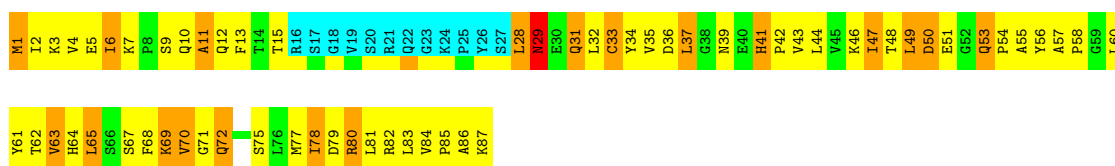
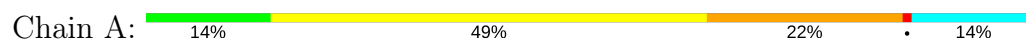


• Molecule 1: GENE V PROTEIN

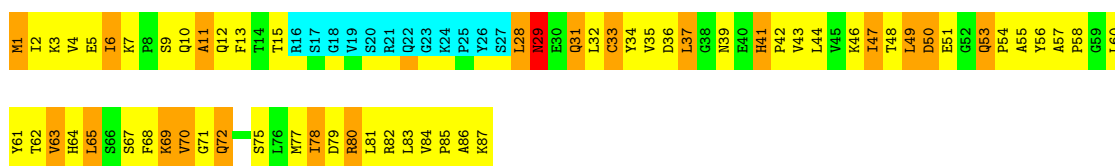
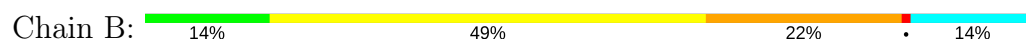


4.2.27 Score per residue for model 27

• Molecule 1: GENE V PROTEIN

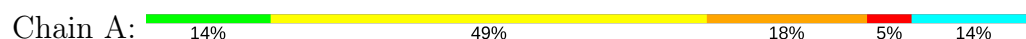


• Molecule 1: GENE V PROTEIN

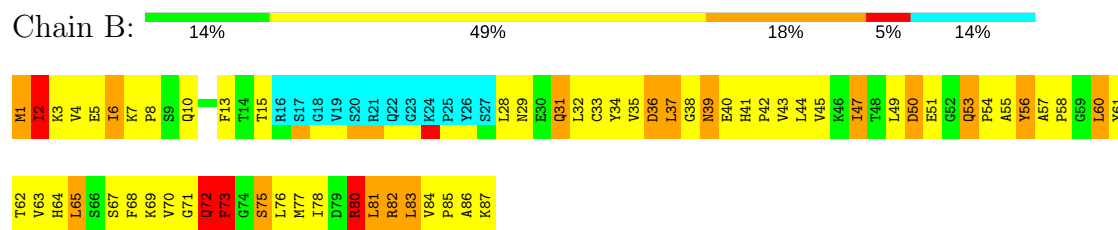


4.2.28 Score per residue for model 28

• Molecule 1: GENE V PROTEIN

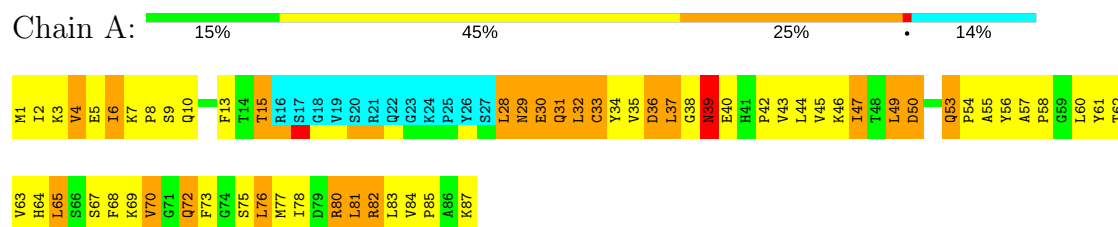


• Molecule 1: GENE V PROTEIN

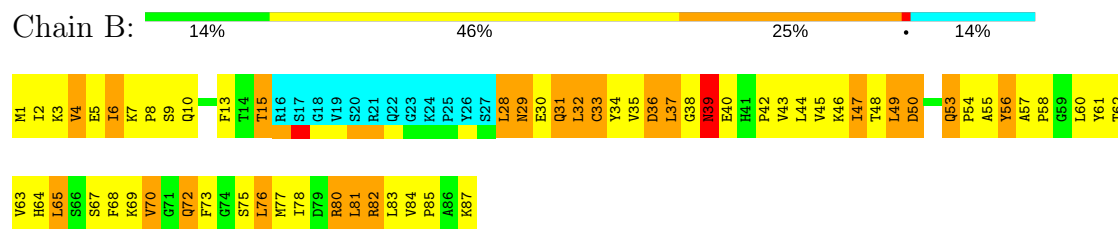


4.2.29 Score per residue for model 29

- Molecule 1: GENE V PROTEIN

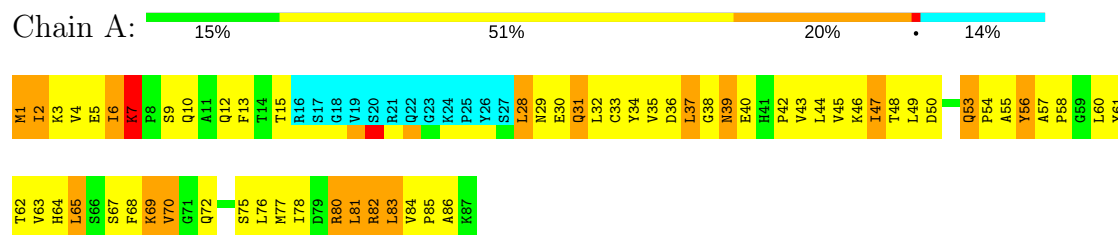


- Molecule 1: GENE V PROTEIN

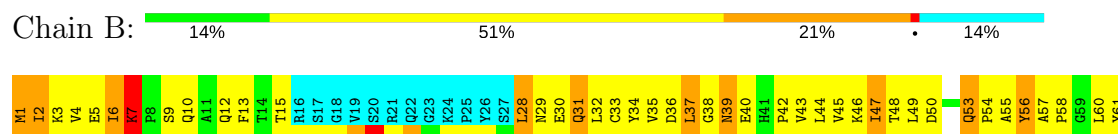


4.2.30 Score per residue for model 30

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN



T62	V63	H64	L65	S66	S67	F68	K69	V70	G71	Q72	F73	G74	S75	L76	M77	I78	D79	R80	L81	R82	L83	V84	P85	A86	K87
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

5 Refinement protocol and experimental data overview

Of the ? calculated structures, 30 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	
X-PLOR	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	588	607	607	153±10
1	B	588	607	607	152±10
All	All	35280	36420	36420	8286

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 116.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:VAL:HG22	1:B:35:VAL:HG22	1.14	1.20	1	11
1:A:43:VAL:HG21	1:B:70:VAL:HG21	1.12	1.18	29	19
1:A:4:VAL:HG22	1:A:35:VAL:HG22	1.06	1.20	1	11
1:A:70:VAL:HG21	1:B:43:VAL:HG21	1.05	1.15	29	17
1:A:63:VAL:HG13	1:A:81:LEU:HD13	1.03	1.29	8	1
1:B:63:VAL:HG13	1:B:81:LEU:HD13	1.01	1.29	8	1
1:A:37:LEU:HD12	1:A:38:GLY:N	0.98	1.72	28	2
1:B:37:LEU:HD12	1:B:38:GLY:N	0.98	1.73	28	2
1:A:4:VAL:CG2	1:A:35:VAL:HG22	0.98	1.89	7	11
1:A:65:LEU:CD1	1:B:37:LEU:HD13	0.97	1.89	28	1
1:B:4:VAL:CG2	1:B:35:VAL:HG22	0.97	1.89	7	11
1:A:37:LEU:HD13	1:B:65:LEU:CD1	0.97	1.89	28	1
1:A:4:VAL:HG13	1:A:61:TYR:CB	0.94	1.92	13	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:OE1	1:A:32:LEU:HD13	0.94	1.61	27	3
1:B:4:VAL:HG13	1:B:61:TYR:CB	0.94	1.92	13	12
1:A:47:ILE:HD11	1:A:83:LEU:HB2	0.93	1.40	8	16
1:B:10:GLN:OE1	1:B:32:LEU:HD13	0.93	1.61	27	3
1:A:47:ILE:HG21	1:A:56:TYR:CE1	0.92	1.99	15	11
1:A:3:LYS:N	1:A:37:LEU:HD12	0.91	1.79	1	1
1:B:47:ILE:HD11	1:B:83:LEU:HB2	0.91	1.40	8	16
1:B:3:LYS:N	1:B:37:LEU:HD12	0.91	1.79	1	1
1:B:47:ILE:HG21	1:B:56:TYR:CE1	0.91	1.99	15	11
1:B:47:ILE:HG21	1:B:56:TYR:CZ	0.90	2.01	15	1
1:A:65:LEU:CD2	1:B:2:ILE:HG23	0.90	1.96	9	2
1:B:35:VAL:O	1:B:43:VAL:HG22	0.90	1.66	10	28
1:A:47:ILE:HD13	1:A:83:LEU:HD12	0.90	1.43	28	13
1:B:65:LEU:HD23	1:B:68:PHE:CD2	0.90	2.02	9	2
1:A:65:LEU:HD23	1:A:68:PHE:CD2	0.89	2.02	9	2
1:A:2:ILE:HG23	1:B:65:LEU:CD2	0.89	1.97	9	2
1:A:47:ILE:HG21	1:A:56:TYR:CZ	0.89	2.02	15	1
1:A:35:VAL:O	1:A:43:VAL:HG22	0.89	1.67	18	28
1:B:4:VAL:HG13	1:B:61:TYR:HB2	0.89	1.44	24	7
1:B:47:ILE:HD13	1:B:83:LEU:HD12	0.89	1.43	28	13
1:A:2:ILE:N	1:B:65:LEU:HD22	0.89	1.83	18	23
1:B:57:ALA:HB1	1:B:58:PRO:HD2	0.88	1.44	1	30
1:A:49:LEU:HD11	1:A:53:GLN:O	0.88	1.67	20	8
1:A:57:ALA:HB1	1:A:58:PRO:HD2	0.88	1.44	1	30
1:A:65:LEU:HD22	1:B:2:ILE:N	0.88	1.84	18	24
1:A:4:VAL:HG13	1:A:61:TYR:HB2	0.88	1.44	24	7
1:B:47:ILE:CD1	1:B:83:LEU:HD12	0.88	1.99	17	15
1:A:63:VAL:CG1	1:A:81:LEU:HD12	0.88	1.99	18	7
1:B:49:LEU:HD11	1:B:53:GLN:O	0.88	1.67	20	8
1:A:6:ILE:HG21	1:A:56:TYR:O	0.88	1.68	7	24
1:A:47:ILE:CD1	1:A:83:LEU:HD12	0.88	1.99	24	15
1:B:63:VAL:CG1	1:B:81:LEU:HD12	0.88	1.99	18	7
1:B:6:ILE:HG21	1:B:56:TYR:O	0.87	1.68	7	24
1:A:31:GLN:OE1	1:A:55:ALA:HB1	0.87	1.69	22	2
1:A:33:CYS:SG	1:A:47:ILE:HD13	0.86	2.11	5	5
1:A:37:LEU:CG	1:B:65:LEU:HD11	0.86	2.00	30	4
1:A:2:ILE:HA	1:B:65:LEU:HD22	0.86	1.47	28	14
1:B:31:GLN:OE1	1:B:55:ALA:HB1	0.85	1.69	22	2
1:B:33:CYS:SG	1:B:47:ILE:HD13	0.85	2.10	5	5
1:B:36:ASP:O	1:B:37:LEU:HD12	0.85	1.70	3	4
1:A:15:THR:HG23	1:A:28:LEU:O	0.85	1.71	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:THR:HG23	1:B:28:LEU:O	0.84	1.72	29	1
1:A:36:ASP:O	1:A:37:LEU:HD12	0.84	1.70	3	4
1:A:65:LEU:HD11	1:B:37:LEU:CG	0.84	2.03	30	5
1:B:76:LEU:HD23	1:B:77:MET:N	0.84	1.87	9	5
1:A:65:LEU:HD22	1:B:2:ILE:HA	0.84	1.47	28	14
1:A:78:ILE:HD12	1:B:78:ILE:HD12	0.84	1.49	23	20
1:A:76:LEU:HD23	1:A:77:MET:N	0.83	1.88	9	5
1:A:2:ILE:HG23	1:B:65:LEU:HD13	0.83	1.49	21	8
1:A:65:LEU:CD1	1:B:2:ILE:HG23	0.82	2.04	2	5
1:B:62:THR:O	1:B:84:VAL:HG22	0.82	1.75	26	29
1:A:62:THR:O	1:A:84:VAL:HG22	0.81	1.75	26	29
1:A:65:LEU:HD13	1:B:37:LEU:HG	0.81	1.51	11	2
1:A:65:LEU:HD22	1:B:2:ILE:HG23	0.81	1.52	9	1
1:A:65:LEU:HD13	1:B:2:ILE:HG23	0.81	1.49	21	9
1:A:70:VAL:HG11	1:B:43:VAL:CG2	0.81	2.05	4	4
1:A:43:VAL:CG2	1:B:70:VAL:HG11	0.81	2.05	4	4
1:A:37:LEU:HG	1:B:65:LEU:HD13	0.81	1.51	11	1
1:A:32:LEU:HB3	1:A:44:LEU:HD11	0.80	1.54	3	29
1:A:43:VAL:HG21	1:B:70:VAL:HG11	0.80	1.54	4	4
1:A:70:VAL:HG11	1:B:43:VAL:HG21	0.80	1.53	4	4
1:A:31:GLN:HG3	1:A:55:ALA:HB1	0.80	1.53	5	17
1:A:70:VAL:HG21	1:B:43:VAL:CG2	0.80	2.04	29	4
1:A:2:ILE:HG23	1:B:65:LEU:CD1	0.80	2.06	2	5
1:A:2:ILE:CA	1:B:65:LEU:HD22	0.80	2.07	29	21
1:B:32:LEU:HB3	1:B:44:LEU:HD11	0.80	1.54	3	29
1:B:4:VAL:HG11	1:B:83:LEU:HD21	0.79	1.55	6	12
1:A:37:LEU:HG	1:B:65:LEU:HD11	0.79	1.54	30	4
1:A:37:LEU:HB3	1:B:65:LEU:HD11	0.79	1.54	29	4
1:A:4:VAL:HG11	1:A:83:LEU:HD21	0.78	1.55	6	12
1:B:31:GLN:HG3	1:B:55:ALA:HB1	0.78	1.54	5	17
1:A:2:ILE:HG23	1:B:65:LEU:HD22	0.78	1.54	9	1
1:A:37:LEU:HD13	1:B:65:LEU:HD11	0.78	1.55	28	1
1:A:65:LEU:HD22	1:B:2:ILE:CA	0.78	2.07	29	21
1:A:37:LEU:HD23	1:A:38:GLY:N	0.78	1.94	6	2
1:B:37:LEU:HD23	1:B:38:GLY:N	0.78	1.94	6	2
1:A:65:LEU:HD11	1:B:37:LEU:HD13	0.77	1.55	28	1
1:A:2:ILE:HG12	1:B:65:LEU:HD21	0.77	1.57	9	1
1:A:65:LEU:HD11	1:B:37:LEU:HB3	0.77	1.56	29	4
1:A:34:TYR:CE2	1:A:44:LEU:HD13	0.77	2.15	17	6
1:B:6:ILE:HD13	1:B:61:TYR:CE1	0.76	2.16	26	17
1:A:3:LYS:O	1:A:4:VAL:HG23	0.76	1.80	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:HG11	1:A:83:LEU:HD11	0.76	1.57	13	9
1:A:65:LEU:HD21	1:B:2:ILE:HG12	0.76	1.57	9	1
1:B:3:LYS:O	1:B:4:VAL:HG23	0.76	1.80	1	8
1:B:47:ILE:HD11	1:B:83:LEU:CB	0.76	2.11	22	6
1:A:65:LEU:HD11	1:B:37:LEU:HG	0.76	1.57	30	4
1:A:4:VAL:HB	1:A:35:VAL:HG22	0.76	1.58	3	18
1:B:4:VAL:HG11	1:B:83:LEU:HD11	0.76	1.58	29	9
1:A:43:VAL:CG2	1:B:70:VAL:HG21	0.76	2.06	29	5
1:B:34:TYR:CE2	1:B:44:LEU:HD13	0.75	2.16	17	6
1:A:47:ILE:HD11	1:A:83:LEU:CB	0.75	2.11	8	6
1:A:76:LEU:HD11	1:B:37:LEU:HD21	0.75	1.55	3	2
1:A:6:ILE:HD13	1:A:61:TYR:CE1	0.75	2.16	26	17
1:B:32:LEU:CD2	1:B:44:LEU:HD11	0.75	2.12	10	3
1:B:4:VAL:HB	1:B:35:VAL:HG22	0.75	1.58	9	18
1:A:32:LEU:CD2	1:A:44:LEU:HD11	0.75	2.11	10	3
1:A:63:VAL:HG13	1:A:81:LEU:HD12	0.75	1.59	18	4
1:B:2:ILE:HD12	1:B:63:VAL:HB	0.74	1.58	8	3
1:B:61:TYR:HB3	1:B:83:LEU:HD22	0.74	1.58	23	23
1:B:63:VAL:HG11	1:B:81:LEU:HB2	0.74	1.59	13	17
1:A:4:VAL:O	1:A:60:LEU:HD23	0.74	1.82	22	12
1:B:4:VAL:O	1:B:60:LEU:HD23	0.74	1.82	22	12
1:A:57:ALA:HB1	1:A:58:PRO:CD	0.74	2.13	1	28
1:A:61:TYR:HB3	1:A:83:LEU:HD22	0.74	1.58	23	23
1:A:70:VAL:CG2	1:B:43:VAL:HG21	0.73	2.08	29	11
1:A:65:LEU:HD22	1:B:2:ILE:H	0.73	1.43	15	5
1:A:2:ILE:H	1:B:65:LEU:HD22	0.73	1.43	5	5
1:A:2:ILE:HG21	1:A:63:VAL:HG21	0.73	1.61	5	11
1:B:63:VAL:HG13	1:B:81:LEU:HD12	0.73	1.59	18	4
1:A:37:LEU:CB	1:B:65:LEU:HD11	0.73	2.13	29	4
1:B:57:ALA:HB1	1:B:58:PRO:CD	0.72	2.13	1	28
1:A:63:VAL:HG11	1:A:81:LEU:HB2	0.72	1.60	13	16
1:A:48:THR:HG21	1:A:80:ARG:NH1	0.72	1.99	12	3
1:B:2:ILE:HG21	1:B:63:VAL:HG21	0.72	1.61	5	11
1:B:48:THR:HG21	1:B:80:ARG:NH1	0.72	1.99	12	3
1:A:2:ILE:HD12	1:A:63:VAL:HB	0.72	1.58	8	3
1:A:65:LEU:HD11	1:B:37:LEU:CB	0.72	2.12	29	4
1:B:31:GLN:O	1:B:32:LEU:HD23	0.72	1.83	21	2
1:A:37:LEU:N	1:A:37:LEU:HD23	0.72	2.00	25	1
1:B:49:LEU:HD12	1:B:53:GLN:O	0.72	1.85	22	7
1:A:43:VAL:HG21	1:B:70:VAL:CG2	0.72	2.10	29	12
1:A:37:LEU:HD11	1:B:69:LYS:CA	0.72	2.15	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:C	1:A:28:LEU:HD22	0.71	2.05	18	1
1:B:37:LEU:O	1:B:37:LEU:HD12	0.71	1.85	20	2
1:B:28:LEU:HD22	1:B:28:LEU:C	0.71	2.05	18	1
1:A:31:GLN:O	1:A:32:LEU:HD23	0.71	1.83	21	2
1:A:1:MET:SD	1:A:62:THR:HG21	0.71	2.25	6	9
1:B:33:CYS:SG	1:B:47:ILE:HD12	0.71	2.25	22	2
1:A:76:LEU:CD1	1:B:35:VAL:HG11	0.71	2.16	10	4
1:A:49:LEU:HD12	1:A:53:GLN:O	0.71	1.85	22	7
1:B:37:LEU:HD23	1:B:37:LEU:N	0.71	2.00	25	1
1:A:35:VAL:HG11	1:B:76:LEU:CD1	0.71	2.15	10	4
1:A:33:CYS:SG	1:A:47:ILE:HD12	0.71	2.24	22	2
1:B:39:ASN:ND2	1:B:43:VAL:HG11	0.71	2.01	29	2
1:A:4:VAL:HG22	1:A:35:VAL:CG2	0.71	2.15	7	9
1:A:37:LEU:HD11	1:B:68:PHE:C	0.70	2.06	6	9
1:A:39:ASN:ND2	1:A:43:VAL:HG11	0.70	2.01	29	2
1:A:65:LEU:HD11	1:B:37:LEU:O	0.70	1.86	19	6
1:A:37:LEU:O	1:A:37:LEU:HD12	0.70	1.86	20	1
1:B:1:MET:SD	1:B:62:THR:HG21	0.70	2.25	6	9
1:B:49:LEU:O	1:B:49:LEU:HD13	0.70	1.86	23	1
1:A:68:PHE:C	1:B:37:LEU:HD11	0.70	2.05	6	9
1:B:28:LEU:C	1:B:28:LEU:HD12	0.70	2.07	17	2
1:A:37:LEU:HD21	1:B:76:LEU:HD11	0.70	1.60	3	2
1:A:2:ILE:HA	1:B:65:LEU:HD21	0.70	1.62	11	1
1:A:28:LEU:HD12	1:A:28:LEU:C	0.70	2.07	17	1
1:A:37:LEU:O	1:B:65:LEU:HD11	0.70	1.86	19	6
1:A:49:LEU:HD13	1:A:49:LEU:O	0.70	1.86	23	1
1:A:35:VAL:HG12	1:A:37:LEU:H	0.69	1.47	25	3
1:A:49:LEU:HD13	1:A:50:ASP:O	0.69	1.87	24	3
1:B:49:LEU:HD13	1:B:50:ASP:O	0.69	1.87	24	3
1:A:35:VAL:HG21	1:B:76:LEU:HD13	0.69	1.64	26	1
1:B:33:CYS:SG	1:B:47:ILE:HD11	0.69	2.27	15	1
1:A:6:ILE:HD11	1:A:33:CYS:SG	0.69	2.28	16	5
1:A:47:ILE:HD11	1:A:83:LEU:HB3	0.69	1.65	22	1
1:B:36:ASP:C	1:B:37:LEU:HD12	0.69	2.07	3	2
1:B:4:VAL:HG22	1:B:35:VAL:CG2	0.69	2.15	7	9
1:A:69:LYS:CA	1:B:37:LEU:HD11	0.69	2.17	8	5
1:B:6:ILE:HD11	1:B:33:CYS:SG	0.69	2.27	21	5
1:A:37:LEU:CG	1:B:65:LEU:HD13	0.69	2.18	11	1
1:B:35:VAL:HG12	1:B:37:LEU:H	0.69	1.48	25	3
1:A:33:CYS:SG	1:A:47:ILE:HD11	0.69	2.28	15	1
1:A:2:ILE:HA	1:B:65:LEU:HD13	0.69	1.64	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LEU:HD11	1:B:30:GLU:HG3	0.69	1.64	10	2
1:B:35:VAL:HG13	1:B:37:LEU:HD11	0.69	1.65	1	1
1:A:65:LEU:HD13	1:B:37:LEU:CG	0.69	2.18	11	1
1:A:65:LEU:HD21	1:B:2:ILE:HA	0.69	1.62	11	1
1:B:28:LEU:HD12	1:B:29:ASN:N	0.69	2.02	10	1
1:A:37:LEU:HG	1:B:65:LEU:HD21	0.68	1.65	16	3
1:A:81:LEU:HD12	1:A:81:LEU:C	0.68	2.08	8	1
1:B:81:LEU:C	1:B:81:LEU:HD12	0.68	2.09	8	1
1:A:76:LEU:HD13	1:B:35:VAL:HG21	0.68	1.64	26	1
1:A:36:ASP:C	1:A:37:LEU:HD12	0.68	2.07	3	2
1:A:65:LEU:HD13	1:B:2:ILE:HA	0.68	1.65	10	5
1:B:6:ILE:HD13	1:B:61:TYR:CD1	0.68	2.23	26	7
1:A:48:THR:O	1:A:48:THR:HG22	0.68	1.89	25	1
1:A:6:ILE:HD13	1:A:56:TYR:HB3	0.68	1.64	13	16
1:A:6:ILE:HD13	1:A:61:TYR:CD1	0.68	2.24	26	8
1:A:81:LEU:HD23	1:A:81:LEU:O	0.68	1.88	7	18
1:A:28:LEU:HD12	1:A:29:ASN:N	0.68	2.02	10	1
1:B:47:ILE:HD11	1:B:83:LEU:HB3	0.68	1.65	22	1
1:B:81:LEU:O	1:B:81:LEU:HD23	0.68	1.89	7	10
1:A:7:LYS:CD	1:A:34:TYR:CD1	0.68	2.77	18	2
1:A:65:LEU:HD21	1:B:37:LEU:HG	0.68	1.64	16	3
1:A:35:VAL:HG13	1:A:37:LEU:HD11	0.68	1.65	1	1
1:A:32:LEU:HD12	1:A:32:LEU:N	0.68	2.03	28	1
1:A:28:LEU:HD11	1:A:30:GLU:HG3	0.67	1.65	10	2
1:B:32:LEU:HD12	1:B:32:LEU:N	0.67	2.03	28	2
1:B:6:ILE:HD13	1:B:56:TYR:HB3	0.67	1.65	13	17
1:B:7:LYS:CD	1:B:34:TYR:CD1	0.67	2.77	18	2
1:B:48:THR:HG22	1:B:48:THR:O	0.67	1.89	25	1
1:B:29:ASN:OD1	1:B:29:ASN:N	0.67	2.28	13	7
1:A:28:LEU:HD12	1:A:29:ASN:O	0.67	1.90	2	2
1:B:28:LEU:HD12	1:B:29:ASN:O	0.67	1.90	2	1
1:A:61:TYR:CD2	1:A:83:LEU:HD23	0.67	2.25	26	3
1:B:35:VAL:HG12	1:B:37:LEU:HG	0.67	1.67	23	4
1:B:7:LYS:CD	1:B:34:TYR:CD2	0.66	2.79	11	15
1:B:29:ASN:N	1:B:29:ASN:OD1	0.66	2.28	22	9
1:B:37:LEU:HD23	1:B:37:LEU:O	0.66	1.90	13	3
1:A:28:LEU:C	1:A:28:LEU:HD12	0.66	2.10	10	1
1:A:37:LEU:O	1:A:37:LEU:HD23	0.66	1.90	13	4
1:A:65:LEU:HD23	1:A:68:PHE:HD2	0.66	1.47	9	1
1:B:65:LEU:CB	1:B:68:PHE:CD2	0.66	2.79	30	20
1:B:37:LEU:N	1:B:37:LEU:HD12	0.66	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:N	1:A:29:ASN:OD1	0.66	2.28	13	7
1:A:35:VAL:HG12	1:A:37:LEU:HG	0.66	1.67	23	4
1:B:28:LEU:CD2	1:B:48:THR:HG22	0.66	2.21	1	3
1:A:32:LEU:CB	1:A:44:LEU:HD11	0.66	2.20	28	7
1:B:61:TYR:CD2	1:B:83:LEU:HD23	0.66	2.26	26	3
1:A:7:LYS:CD	1:A:34:TYR:CD2	0.66	2.79	4	15
1:B:32:LEU:CB	1:B:44:LEU:HD11	0.66	2.20	28	7
1:A:34:TYR:CE1	1:A:44:LEU:HD13	0.66	2.26	8	12
1:A:35:VAL:O	1:A:37:LEU:HD23	0.65	1.91	7	1
1:B:34:TYR:CE1	1:B:44:LEU:HD13	0.65	2.27	8	12
1:A:37:LEU:HD22	1:B:69:LYS:HA	0.65	1.69	17	1
1:A:65:LEU:CB	1:A:68:PHE:CD2	0.65	2.79	30	20
1:A:43:VAL:O	1:A:43:VAL:HG23	0.65	1.92	18	19
1:B:36:ASP:C	1:B:37:LEU:HD23	0.65	2.11	7	1
1:A:28:LEU:CD2	1:A:48:THR:HG22	0.65	2.21	1	3
1:A:37:LEU:HD21	1:B:69:LYS:HA	0.65	1.67	13	7
1:A:37:LEU:HD12	1:A:37:LEU:N	0.65	2.05	17	1
1:B:35:VAL:O	1:B:37:LEU:HD23	0.65	1.91	7	1
1:B:4:VAL:CG1	1:B:83:LEU:HD11	0.65	2.21	29	1
1:B:47:ILE:CG2	1:B:56:TYR:CE1	0.64	2.79	15	19
1:A:65:LEU:HB2	1:A:68:PHE:CD2	0.64	2.26	19	27
1:A:36:ASP:C	1:A:37:LEU:HD23	0.64	2.11	7	1
1:B:65:LEU:HB2	1:B:68:PHE:CD2	0.64	2.27	27	27
1:B:43:VAL:HG23	1:B:43:VAL:O	0.64	1.92	18	15
1:A:4:VAL:CG1	1:A:83:LEU:HD11	0.64	2.21	29	1
1:B:2:ILE:HB	1:B:63:VAL:HG23	0.64	1.68	8	3
1:B:7:LYS:HD3	1:B:34:TYR:CD2	0.64	2.28	26	18
1:A:13:PHE:CD2	1:A:49:LEU:CD1	0.64	2.81	4	8
1:A:2:ILE:HB	1:A:63:VAL:HG23	0.64	1.68	8	4
1:A:37:LEU:HD21	1:B:70:VAL:HG22	0.64	1.69	17	3
1:A:49:LEU:O	1:A:49:LEU:HD13	0.64	1.93	6	1
1:A:49:LEU:HD21	1:A:55:ALA:HA	0.64	1.70	29	13
1:B:13:PHE:CD2	1:B:49:LEU:CD1	0.64	2.80	26	8
1:A:4:VAL:HG11	1:A:83:LEU:CD1	0.64	2.23	29	1
1:B:68:PHE:N	1:B:68:PHE:CD1	0.64	2.64	28	17
1:A:68:PHE:N	1:A:68:PHE:CD1	0.64	2.65	19	18
1:A:70:VAL:HG11	1:B:45:VAL:HG12	0.64	1.69	30	4
1:A:81:LEU:HD13	1:B:76:LEU:HD22	0.64	1.68	23	1
1:B:43:VAL:HG23	1:B:45:VAL:HG23	0.64	1.70	15	2
1:A:7:LYS:HD3	1:A:34:TYR:CD2	0.64	2.28	19	18
1:B:4:VAL:HG11	1:B:83:LEU:CD1	0.64	2.23	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:PHE:CE1	1:A:29:ASN:ND2	0.64	2.67	9	12
1:A:13:PHE:CD2	1:A:55:ALA:HB2	0.64	2.28	10	27
1:B:59:GLY:O	1:B:61:TYR:CD1	0.64	2.51	1	5
1:B:35:VAL:O	1:B:43:VAL:HG13	0.64	1.93	3	4
1:A:68:PHE:CD1	1:A:68:PHE:N	0.63	2.65	20	12
1:A:10:GLN:NE2	1:A:32:LEU:HD12	0.63	2.08	20	1
1:A:76:LEU:HD22	1:B:81:LEU:HD13	0.63	1.68	23	1
1:B:49:LEU:HD13	1:B:49:LEU:O	0.63	1.93	6	1
1:A:13:PHE:CD1	1:A:29:ASN:CB	0.63	2.81	19	20
1:B:13:PHE:CD1	1:B:29:ASN:CB	0.63	2.81	19	20
1:A:59:GLY:O	1:A:61:TYR:CD1	0.63	2.52	1	5
1:A:43:VAL:HG11	1:B:70:VAL:HG21	0.63	1.70	14	3
1:B:10:GLN:NE2	1:B:32:LEU:HD12	0.63	2.08	20	1
1:B:56:TYR:CE2	1:B:83:LEU:CB	0.63	2.81	26	19
1:B:40:GLU:O	1:B:41:HIS:CG	0.63	2.52	22	12
1:A:43:VAL:HG23	1:A:45:VAL:HG23	0.63	1.70	15	2
1:B:13:PHE:CE1	1:B:29:ASN:ND2	0.63	2.67	5	12
1:A:56:TYR:CE2	1:A:83:LEU:CB	0.63	2.82	26	19
1:B:68:PHE:CD1	1:B:68:PHE:N	0.63	2.65	19	13
1:A:37:LEU:H	1:A:37:LEU:HD13	0.63	1.54	1	1
1:A:40:GLU:O	1:A:41:HIS:CG	0.63	2.52	22	12
1:B:56:TYR:CE2	1:B:83:LEU:HB3	0.63	2.29	26	28
1:B:68:PHE:CE1	1:B:78:ILE:CG1	0.63	2.82	4	10
1:A:13:PHE:CD2	1:A:29:ASN:CB	0.63	2.82	8	3
1:B:13:PHE:CD2	1:B:29:ASN:CB	0.63	2.82	8	3
1:A:68:PHE:CE1	1:A:78:ILE:CG1	0.62	2.82	4	10
1:A:31:GLN:CB	1:A:47:ILE:HG22	0.62	2.24	5	18
1:B:49:LEU:HD21	1:B:55:ALA:HA	0.62	1.71	14	12
1:A:43:VAL:HG23	1:A:43:VAL:O	0.62	1.93	17	10
1:B:32:LEU:HD12	1:B:44:LEU:HG	0.62	1.72	19	1
1:B:32:LEU:HD22	1:B:44:LEU:HD21	0.62	1.71	10	3
1:A:69:LYS:HA	1:B:37:LEU:HD21	0.62	1.70	13	7
1:B:13:PHE:CD2	1:B:55:ALA:HB2	0.62	2.29	10	27
1:A:56:TYR:CE2	1:A:83:LEU:HB3	0.62	2.29	26	28
1:B:37:LEU:HD13	1:B:37:LEU:H	0.62	1.54	1	1
1:B:81:LEU:HD23	1:B:81:LEU:O	0.62	1.94	9	14
1:A:81:LEU:N	1:A:81:LEU:HD23	0.62	2.10	3	3
1:A:76:LEU:HD11	1:B:37:LEU:HD22	0.62	1.70	20	1
1:A:45:VAL:HG12	1:B:70:VAL:CG1	0.62	2.25	20	3
1:B:43:VAL:O	1:B:43:VAL:HG23	0.62	1.95	12	14
1:A:32:LEU:N	1:A:32:LEU:HD12	0.62	2.10	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:N	1:B:32:LEU:HD12	0.62	2.10	1	3
1:A:76:LEU:HD23	1:A:76:LEU:C	0.62	2.15	15	2
1:A:35:VAL:O	1:A:43:VAL:HG13	0.62	1.94	3	4
1:A:28:LEU:HD13	1:A:48:THR:HG23	0.62	1.72	17	1
1:A:37:LEU:HD22	1:B:76:LEU:HD11	0.61	1.71	20	1
1:B:76:LEU:HD23	1:B:76:LEU:C	0.61	2.15	15	2
1:A:6:ILE:HD11	1:A:83:LEU:CD2	0.61	2.26	22	3
1:A:72:GLN:N	1:A:72:GLN:NE2	0.61	2.48	13	2
1:A:32:LEU:HD12	1:A:44:LEU:HG	0.61	1.72	19	1
1:A:70:VAL:CG1	1:B:45:VAL:CG2	0.61	2.79	9	10
1:B:63:VAL:HG11	1:B:81:LEU:HD12	0.61	1.73	18	5
1:B:4:VAL:HG13	1:B:61:TYR:C	0.61	2.16	6	12
1:B:6:ILE:HD11	1:B:83:LEU:CD2	0.61	2.25	22	3
1:A:70:VAL:CG1	1:B:45:VAL:HG12	0.61	2.25	20	4
1:A:32:LEU:HD22	1:A:44:LEU:HD21	0.61	1.71	10	3
1:B:7:LYS:HD2	1:B:34:TYR:CE2	0.61	2.31	20	5
1:A:13:PHE:CG	1:A:49:LEU:HD12	0.61	2.31	6	4
1:A:60:LEU:HB3	1:A:86:ALA:HB3	0.61	1.72	22	18
1:A:45:VAL:HG12	1:B:70:VAL:HG11	0.61	1.70	30	5
1:A:69:LYS:HA	1:B:37:LEU:HD22	0.61	1.72	17	1
1:B:68:PHE:CE1	1:B:78:ILE:HG12	0.61	2.31	11	30
1:A:47:ILE:CD1	1:A:56:TYR:CE2	0.61	2.84	10	6
1:A:76:LEU:CD1	1:B:37:LEU:HD21	0.61	2.25	3	2
1:B:81:LEU:HD23	1:B:81:LEU:N	0.61	2.10	3	3
1:B:28:LEU:HD13	1:B:48:THR:HG23	0.61	1.72	17	1
1:B:65:LEU:HD23	1:B:68:PHE:HD2	0.61	1.48	9	1
1:B:72:GLN:NE2	1:B:72:GLN:N	0.60	2.48	13	2
1:A:13:PHE:CD1	1:A:29:ASN:HB3	0.60	2.31	10	25
1:A:13:PHE:CD2	1:A:49:LEU:HD12	0.60	2.31	18	5
1:A:47:ILE:HD12	1:A:56:TYR:CE1	0.60	2.31	29	3
1:B:31:GLN:CB	1:B:47:ILE:HG22	0.60	2.24	5	18
1:A:81:LEU:O	1:A:81:LEU:HD23	0.60	1.95	23	7
1:B:28:LEU:HD11	1:B:30:GLU:CG	0.60	2.27	17	1
1:B:13:PHE:CG	1:B:49:LEU:HD12	0.60	2.31	6	4
1:B:10:GLN:NE2	1:B:32:LEU:HD22	0.60	2.12	27	1
1:A:37:LEU:CB	1:B:65:LEU:HD21	0.60	2.26	21	1
1:A:76:LEU:C	1:A:76:LEU:HD23	0.60	2.16	17	2
1:B:13:PHE:CD2	1:B:49:LEU:HD12	0.60	2.31	18	6
1:A:68:PHE:CE1	1:A:78:ILE:HG12	0.60	2.31	11	30
1:A:45:VAL:CG2	1:B:70:VAL:CG1	0.60	2.80	18	11
1:B:40:GLU:O	1:B:41:HIS:CB	0.60	2.49	22	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:HG21	1:B:56:TYR:CD1	0.60	2.31	27	19
1:B:47:ILE:HG12	1:B:56:TYR:CE2	0.60	2.32	9	4
1:A:45:VAL:CG1	1:B:70:VAL:CG1	0.60	2.79	14	5
1:A:47:ILE:CG2	1:A:56:TYR:CE1	0.60	2.80	15	18
1:A:4:VAL:HG13	1:A:61:TYR:C	0.60	2.17	29	12
1:B:78:ILE:CG2	1:B:81:LEU:N	0.60	2.65	18	3
1:B:68:PHE:HB3	1:B:76:LEU:HD21	0.60	1.73	13	4
1:A:6:ILE:HG22	1:A:6:ILE:O	0.60	1.96	14	10
1:B:6:ILE:O	1:B:6:ILE:HG22	0.60	1.96	14	12
1:B:47:ILE:HD12	1:B:56:TYR:CE1	0.60	2.31	29	3
1:A:35:VAL:HG11	1:B:76:LEU:HD12	0.60	1.73	11	1
1:A:78:ILE:CD1	1:B:78:ILE:CD1	0.60	2.79	20	18
1:B:13:PHE:CD1	1:B:29:ASN:HB3	0.60	2.31	10	25
1:A:10:GLN:OE1	1:A:32:LEU:HD12	0.60	1.97	17	2
1:A:7:LYS:HD2	1:A:34:TYR:CE2	0.60	2.31	20	5
1:A:78:ILE:CG2	1:A:81:LEU:N	0.60	2.65	18	3
1:A:10:GLN:NE2	1:A:32:LEU:HD22	0.60	2.12	27	1
1:A:39:ASN:O	1:A:41:HIS:CE1	0.60	2.55	27	3
1:A:70:VAL:HG22	1:B:37:LEU:HD21	0.60	1.73	17	3
1:A:47:ILE:HG21	1:A:56:TYR:CD1	0.59	2.33	27	19
1:A:65:LEU:HD21	1:B:2:ILE:CG1	0.59	2.27	9	2
1:A:2:ILE:CG1	1:B:65:LEU:HD21	0.59	2.27	9	2
1:A:13:PHE:HD2	1:A:55:ALA:HB2	0.59	1.57	26	20
1:A:65:LEU:HD23	1:A:68:PHE:CE2	0.59	2.32	13	2
1:B:10:GLN:OE1	1:B:32:LEU:HD12	0.59	1.97	17	2
1:B:47:ILE:CD1	1:B:56:TYR:CE2	0.59	2.85	10	6
1:A:40:GLU:O	1:A:41:HIS:CB	0.59	2.49	23	4
1:B:34:TYR:HE1	1:B:44:LEU:HD13	0.59	1.57	8	11
1:B:60:LEU:HB3	1:B:86:ALA:HB3	0.59	1.72	22	18
1:A:37:LEU:HA	1:B:65:LEU:HD13	0.59	1.74	3	1
1:A:2:ILE:HD13	1:A:63:VAL:HB	0.59	1.74	18	7
1:B:28:LEU:HD22	1:B:48:THR:HG22	0.59	1.74	11	2
1:A:65:LEU:HD21	1:B:37:LEU:CB	0.59	2.27	21	1
1:A:29:ASN:CB	1:A:49:LEU:CB	0.59	2.81	2	3
1:A:70:VAL:HG11	1:B:45:VAL:HG23	0.59	1.74	26	1
1:B:39:ASN:O	1:B:41:HIS:CE1	0.59	2.56	27	3
1:B:29:ASN:CB	1:B:49:LEU:CB	0.59	2.81	15	3
1:B:45:VAL:CG1	1:B:46:LYS:N	0.59	2.66	13	11
1:A:70:VAL:CG1	1:B:45:VAL:CG1	0.59	2.80	14	5
1:A:31:GLN:HE21	1:A:55:ALA:HB1	0.59	1.58	21	3
1:A:39:ASN:HD22	1:A:43:VAL:HG11	0.59	1.57	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLN:O	1:A:73:PHE:CG	0.59	2.55	28	2
1:B:31:GLN:HE21	1:B:55:ALA:HB1	0.59	1.58	21	3
1:B:37:LEU:CD2	1:B:38:GLY:N	0.59	2.65	1	2
1:A:28:LEU:HD22	1:A:48:THR:HG22	0.59	1.74	11	2
1:A:28:LEU:HD11	1:A:30:GLU:CG	0.59	2.27	17	1
1:B:7:LYS:HD3	1:B:34:TYR:CD1	0.59	2.33	18	2
1:A:47:ILE:HG12	1:A:56:TYR:CE2	0.59	2.33	9	4
1:A:37:LEU:HD23	1:A:37:LEU:O	0.59	1.98	15	1
1:A:78:ILE:CD1	1:B:78:ILE:HD12	0.59	2.28	2	18
1:A:70:VAL:CG1	1:B:43:VAL:HG21	0.59	2.27	4	2
1:A:63:VAL:HG11	1:A:81:LEU:HD12	0.59	1.73	18	5
1:A:68:PHE:HB3	1:A:76:LEU:HD21	0.59	1.74	13	3
1:A:37:LEU:CD2	1:A:38:GLY:N	0.59	2.65	1	2
1:B:76:LEU:O	1:B:76:LEU:HD23	0.59	1.98	23	1
1:A:45:VAL:CG1	1:A:46:LYS:N	0.58	2.66	22	11
1:A:34:TYR:CD1	1:A:42:PRO:HB2	0.58	2.33	14	16
1:B:34:TYR:CD1	1:B:42:PRO:HB2	0.58	2.33	23	16
1:A:10:GLN:OE1	1:A:44:LEU:HD13	0.58	1.99	13	1
1:A:65:LEU:CD2	1:B:2:ILE:CG1	0.58	2.81	13	1
1:B:2:ILE:HD13	1:B:63:VAL:HB	0.58	1.73	18	8
1:B:4:VAL:CG2	1:B:5:GLU:N	0.58	2.67	26	19
1:A:29:ASN:OD1	1:A:29:ASN:N	0.58	2.37	27	9
1:A:2:ILE:CG1	1:B:65:LEU:CD2	0.58	2.81	13	1
1:A:65:LEU:HD22	1:B:2:ILE:HG13	0.58	1.75	4	3
1:B:39:ASN:HD22	1:B:43:VAL:HG11	0.58	1.57	27	2
1:B:6:ILE:CD1	1:B:61:TYR:CD1	0.58	2.87	7	12
1:A:67:SER:CB	1:A:80:ARG:O	0.58	2.52	19	28
1:A:72:GLN:O	1:A:73:PHE:CB	0.58	2.51	28	8
1:B:65:LEU:HD23	1:B:68:PHE:CE2	0.58	2.33	13	2
1:A:37:LEU:HD11	1:B:69:LYS:HA	0.58	1.75	8	4
1:A:45:VAL:CG2	1:B:75:SER:N	0.58	2.66	16	1
1:A:7:LYS:HD3	1:A:34:TYR:CD1	0.58	2.33	18	2
1:A:2:ILE:N	1:B:65:LEU:CD2	0.58	2.66	30	1
1:B:72:GLN:O	1:B:73:PHE:CB	0.58	2.51	28	8
1:A:2:ILE:HG13	1:B:65:LEU:HD22	0.58	1.76	4	3
1:B:72:GLN:O	1:B:73:PHE:CG	0.58	2.56	28	2
1:A:2:ILE:CG2	1:B:65:LEU:HD13	0.58	2.24	21	5
1:A:6:ILE:CD1	1:A:61:TYR:CD1	0.58	2.86	7	12
1:A:34:TYR:CD2	1:A:42:PRO:HB2	0.58	2.33	22	14
1:A:2:ILE:CG2	1:A:63:VAL:CG2	0.58	2.82	5	10
1:A:65:LEU:HD13	1:B:2:ILE:HG12	0.58	1.75	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:HD12	1:B:35:VAL:HG11	0.58	1.74	11	1
1:B:13:PHE:HD2	1:B:55:ALA:HB2	0.58	1.57	26	22
1:A:34:TYR:HE1	1:A:44:LEU:HD13	0.58	1.58	9	11
1:B:34:TYR:CD2	1:B:42:PRO:HB2	0.58	2.33	22	14
1:A:79:ASP:O	1:A:80:ARG:CB	0.58	2.52	9	7
1:A:65:LEU:CD2	1:B:2:ILE:N	0.58	2.66	30	2
1:B:4:VAL:CB	1:B:35:VAL:HG22	0.58	2.29	14	6
1:A:2:ILE:HG12	1:B:65:LEU:HD13	0.58	1.75	25	1
1:A:4:VAL:CG2	1:A:5:GLU:N	0.58	2.67	13	19
1:B:10:GLN:OE1	1:B:44:LEU:HD13	0.58	1.99	13	1
1:A:28:LEU:HD22	1:A:50:ASP:HB3	0.58	1.76	6	1
1:B:1:MET:O	1:B:37:LEU:HD22	0.58	1.98	21	1
1:A:39:ASN:OD1	1:A:41:HIS:CD2	0.58	2.57	8	1
1:B:37:LEU:O	1:B:37:LEU:HD23	0.57	1.99	15	2
1:B:29:ASN:O	1:B:49:LEU:N	0.57	2.37	10	21
1:A:65:LEU:HD13	1:B:2:ILE:CG2	0.57	2.24	21	4
1:B:7:LYS:HD2	1:B:34:TYR:CE1	0.57	2.34	28	1
1:A:29:ASN:O	1:A:49:LEU:N	0.57	2.37	10	20
1:B:67:SER:CB	1:B:80:ARG:O	0.57	2.52	7	28
1:B:2:ILE:CG2	1:B:63:VAL:CG2	0.57	2.82	5	10
1:B:28:LEU:CD1	1:B:28:LEU:N	0.57	2.67	18	1
1:B:28:LEU:HD22	1:B:29:ASN:N	0.57	2.14	18	1
1:A:65:LEU:HD13	1:B:37:LEU:HA	0.57	1.75	3	1
1:B:36:ASP:O	1:B:38:GLY:N	0.57	2.37	3	19
1:B:4:VAL:CG1	1:B:5:GLU:N	0.57	2.67	1	10
1:A:3:LYS:C	1:A:4:VAL:HG12	0.57	2.19	21	4
1:B:70:VAL:HG22	1:B:76:LEU:CD1	0.57	2.29	4	1
1:A:81:LEU:CD2	1:A:81:LEU:N	0.57	2.67	3	2
1:A:49:LEU:HD21	1:A:53:GLN:O	0.57	1.99	6	1
1:B:28:LEU:HD22	1:B:50:ASP:HB3	0.57	1.76	6	1
1:B:49:LEU:HD21	1:B:53:GLN:O	0.57	1.99	6	1
1:A:37:LEU:HD11	1:B:69:LYS:N	0.57	2.14	5	6
1:B:4:VAL:N	1:B:61:TYR:O	0.57	2.38	30	17
1:A:34:TYR:CE1	1:A:44:LEU:HB2	0.57	2.35	27	27
1:A:4:VAL:N	1:A:61:TYR:O	0.57	2.38	30	18
1:A:68:PHE:O	1:B:37:LEU:HD11	0.57	1.99	6	2
1:B:31:GLN:HB2	1:B:49:LEU:HD23	0.57	1.76	29	2
1:B:3:LYS:C	1:B:4:VAL:HG12	0.57	2.20	21	4
1:A:6:ILE:O	1:A:6:ILE:HG22	0.57	1.99	1	12
1:A:45:VAL:HG23	1:B:70:VAL:HG11	0.57	1.77	26	1
1:A:1:MET:O	1:A:37:LEU:HD22	0.57	1.99	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:GLU:O	1:B:41:HIS:ND1	0.57	2.38	23	10
1:A:28:LEU:CD1	1:A:28:LEU:N	0.57	2.67	18	1
1:A:70:VAL:HG22	1:A:76:LEU:CD1	0.57	2.30	4	1
1:A:4:VAL:CG1	1:A:5:GLU:N	0.57	2.67	1	10
1:A:32:LEU:HD23	1:A:46:LYS:HA	0.57	1.76	5	3
1:B:35:VAL:HG12	1:B:36:ASP:N	0.57	2.15	26	2
1:B:79:ASP:O	1:B:80:ARG:CB	0.57	2.53	8	7
1:A:6:ILE:HG23	1:A:10:GLN:O	0.57	2.00	24	3
1:B:6:ILE:HG23	1:B:10:GLN:O	0.57	2.00	24	4
1:B:81:LEU:CD2	1:B:81:LEU:N	0.57	2.67	3	1
1:A:4:VAL:CB	1:A:35:VAL:HG22	0.57	2.29	14	7
1:B:35:VAL:CG1	1:B:37:LEU:HD23	0.57	2.29	20	1
1:A:76:LEU:O	1:A:76:LEU:HD23	0.57	1.98	23	1
1:B:3:LYS:O	1:B:4:VAL:CG2	0.57	2.53	1	11
1:A:36:ASP:O	1:A:38:GLY:N	0.57	2.37	3	19
1:A:28:LEU:HD22	1:A:29:ASN:N	0.57	2.14	18	1
1:A:7:LYS:HD2	1:A:34:TYR:CE1	0.57	2.35	28	1
1:A:13:PHE:N	1:A:13:PHE:CD1	0.57	2.73	8	2
1:B:6:ILE:HG22	1:B:6:ILE:O	0.56	1.99	1	10
1:A:3:LYS:O	1:A:4:VAL:CG2	0.56	2.53	1	11
1:A:31:GLN:HB2	1:A:49:LEU:HD23	0.56	1.76	29	3
1:A:37:LEU:N	1:A:37:LEU:CD2	0.56	2.68	25	1
1:A:2:ILE:HG21	1:B:76:LEU:HD22	0.56	1.76	16	1
1:A:4:VAL:HG12	1:A:5:GLU:N	0.56	2.16	16	11
1:A:81:LEU:HD13	1:B:76:LEU:HB2	0.56	1.76	14	5
1:B:39:ASN:OD1	1:B:41:HIS:CD2	0.56	2.58	8	1
1:B:47:ILE:HG21	1:B:56:TYR:OH	0.56	2.00	15	1
1:A:40:GLU:O	1:A:41:HIS:ND1	0.56	2.38	23	10
1:A:62:THR:HG23	1:A:86:ALA:HB2	0.56	1.78	28	10
1:A:78:ILE:O	1:A:79:ASP:CB	0.56	2.53	19	5
1:A:65:LEU:HD21	1:B:2:ILE:HG23	0.56	1.77	11	1
1:B:64:HIS:CB	1:B:82:ARG:O	0.56	2.54	5	29
1:B:34:TYR:CE1	1:B:44:LEU:HB2	0.56	2.36	22	27
1:A:6:ILE:HG13	1:A:61:TYR:CE1	0.56	2.36	23	3
1:B:4:VAL:CG1	1:B:61:TYR:CB	0.56	2.81	8	3
1:A:76:LEU:CD1	1:B:37:LEU:HD22	0.56	2.31	20	1
1:A:43:VAL:HG21	1:B:70:VAL:CG1	0.56	2.28	4	2
1:A:35:VAL:CG1	1:A:37:LEU:HD23	0.56	2.30	20	1
1:B:13:PHE:CD1	1:B:13:PHE:N	0.56	2.73	8	2
1:B:47:ILE:HG12	1:B:56:TYR:CE1	0.56	2.36	4	16
1:A:37:LEU:HD11	1:B:68:PHE:O	0.56	2.00	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:LEU:N	1:B:37:LEU:CD2	0.56	2.68	25	1
1:A:45:VAL:HG12	1:A:46:LYS:N	0.56	2.16	5	10
1:A:64:HIS:CB	1:A:82:ARG:O	0.56	2.54	5	29
1:A:65:LEU:HA	1:A:68:PHE:CD2	0.56	2.36	14	24
1:B:37:LEU:HD22	1:B:39:ASN:HD21	0.56	1.60	13	2
1:A:65:LEU:HD12	1:B:37:LEU:HG	0.56	1.76	6	1
1:B:6:ILE:HG12	1:B:61:TYR:CD1	0.56	2.36	10	2
1:B:32:LEU:HD23	1:B:46:LYS:HA	0.56	1.76	5	3
1:B:3:LYS:H	1:B:37:LEU:HD12	0.56	1.56	1	1
1:B:34:TYR:CZ	1:B:44:LEU:HD13	0.56	2.36	17	1
1:A:4:VAL:HG13	1:A:61:TYR:HB3	0.56	1.76	13	2
1:A:37:LEU:HD22	1:B:76:LEU:CD1	0.56	2.30	20	1
1:A:78:ILE:HD12	1:B:78:ILE:CD1	0.55	2.30	2	14
1:B:4:VAL:HG12	1:B:5:GLU:N	0.55	2.16	1	11
1:A:47:ILE:HG12	1:A:56:TYR:CE1	0.55	2.35	4	16
1:A:34:TYR:CZ	1:A:44:LEU:HD13	0.55	2.35	17	1
1:B:81:LEU:O	1:B:81:LEU:CD2	0.55	2.55	15	11
1:A:72:GLN:O	1:A:73:PHE:CD2	0.55	2.59	28	1
1:B:4:VAL:HG13	1:B:61:TYR:HB3	0.55	1.76	13	1
1:A:39:ASN:O	1:A:41:HIS:CD2	0.55	2.59	27	1
1:A:76:LEU:HD22	1:B:2:ILE:HG21	0.55	1.79	16	1
1:A:7:LYS:CG	1:A:34:TYR:CE2	0.55	2.90	11	15
1:B:6:ILE:HG13	1:B:61:TYR:CE1	0.55	2.37	10	3
1:A:28:LEU:HD23	1:A:49:LEU:O	0.55	2.01	13	2
1:A:81:LEU:CD2	1:A:81:LEU:O	0.55	2.55	2	14
1:B:45:VAL:HG12	1:B:46:LYS:N	0.55	2.16	5	10
1:B:65:LEU:HA	1:B:68:PHE:CD2	0.55	2.37	14	24
1:B:6:ILE:O	1:B:6:ILE:CG2	0.55	2.55	21	3
1:B:72:GLN:O	1:B:73:PHE:CD2	0.55	2.59	28	1
1:B:72:GLN:N	1:B:72:GLN:NE2	0.55	2.55	21	1
1:B:37:LEU:HD22	1:B:38:GLY:N	0.55	2.16	1	1
1:B:37:LEU:CD1	1:B:39:ASN:ND2	0.55	2.70	9	1
1:A:1:MET:O	1:B:65:LEU:HD22	0.55	2.02	21	1
1:A:13:PHE:CD2	1:A:49:LEU:HG	0.55	2.37	7	24
1:A:43:VAL:O	1:A:43:VAL:CG2	0.55	2.55	25	14
1:A:6:ILE:HG12	1:A:61:TYR:CD1	0.55	2.36	10	2
1:B:81:LEU:CD2	1:B:81:LEU:O	0.55	2.55	23	12
1:B:78:ILE:O	1:B:79:ASP:CB	0.55	2.54	7	5
1:A:63:VAL:HG13	1:A:81:LEU:CD1	0.55	2.31	18	5
1:B:63:VAL:CG1	1:B:81:LEU:HB2	0.55	2.32	27	29
1:B:76:LEU:O	1:B:77:MET:CG	0.55	2.55	3	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:VAL:O	1:B:43:VAL:CG2	0.55	2.55	25	12
1:A:37:LEU:HD22	1:A:38:GLY:N	0.55	2.17	1	1
1:A:75:SER:N	1:B:45:VAL:CG2	0.55	2.70	16	1
1:A:65:LEU:CD1	1:B:37:LEU:O	0.55	2.55	19	1
1:A:69:LYS:N	1:B:37:LEU:HD11	0.55	2.17	5	6
1:B:28:LEU:HD23	1:B:49:LEU:O	0.55	2.02	13	2
1:A:6:ILE:O	1:A:6:ILE:CG2	0.55	2.55	21	4
1:A:2:ILE:CG2	1:A:63:VAL:HG21	0.55	2.31	5	3
1:A:37:LEU:O	1:B:65:LEU:CD1	0.55	2.55	19	2
1:B:37:LEU:N	1:B:37:LEU:HD22	0.55	2.17	1	1
1:A:2:ILE:CA	1:B:65:LEU:HD21	0.55	2.31	11	1
1:B:13:PHE:CD2	1:B:49:LEU:HG	0.55	2.37	7	24
1:A:2:ILE:CA	1:B:65:LEU:HD13	0.55	2.32	10	4
1:A:13:PHE:N	1:A:55:ALA:HB2	0.55	2.17	17	12
1:A:81:LEU:O	1:A:81:LEU:CD2	0.55	2.55	23	9
1:B:13:PHE:N	1:B:13:PHE:CD1	0.55	2.73	25	1
1:A:65:LEU:HD11	1:B:37:LEU:CA	0.55	2.32	25	1
1:A:2:ILE:HG23	1:B:65:LEU:HD21	0.55	1.78	11	1
1:A:47:ILE:HG21	1:A:56:TYR:OH	0.54	2.00	15	1
1:A:63:VAL:CG1	1:A:81:LEU:HB2	0.54	2.32	27	29
1:B:62:THR:HG23	1:B:86:ALA:HB2	0.54	1.77	28	10
1:A:37:LEU:HD21	1:B:76:LEU:CD1	0.54	2.32	3	2
1:B:39:ASN:O	1:B:41:HIS:CD2	0.54	2.59	27	1
1:A:37:LEU:CD1	1:A:39:ASN:ND2	0.54	2.70	9	1
1:A:37:LEU:HG	1:B:65:LEU:HD12	0.54	1.78	6	1
1:B:57:ALA:CB	1:B:58:PRO:CD	0.54	2.84	13	20
1:A:76:LEU:O	1:A:77:MET:CG	0.54	2.55	26	18
1:B:43:VAL:HG23	1:B:45:VAL:HG13	0.54	1.79	14	3
1:B:7:LYS:HG2	1:B:34:TYR:CE1	0.54	2.38	5	2
1:A:13:PHE:CD1	1:A:29:ASN:CG	0.54	2.81	30	10
1:A:70:VAL:HG21	1:B:43:VAL:HG11	0.54	1.78	3	3
1:A:35:VAL:CG1	1:A:37:LEU:HD21	0.54	2.32	1	1
1:A:13:PHE:CD1	1:A:13:PHE:N	0.54	2.73	25	1
1:A:37:LEU:CA	1:B:65:LEU:HD11	0.54	2.32	25	1
1:A:72:GLN:NE2	1:A:72:GLN:N	0.54	2.55	21	1
1:A:29:ASN:CB	1:A:49:LEU:HB3	0.54	2.32	5	5
1:A:62:THR:O	1:A:84:VAL:CG2	0.54	2.56	13	17
1:B:63:VAL:HG13	1:B:81:LEU:CD1	0.54	2.31	18	4
1:A:7:LYS:HG2	1:A:34:TYR:CE1	0.54	2.37	5	2
1:A:4:VAL:CG1	1:A:61:TYR:CB	0.54	2.82	8	3
1:A:3:LYS:O	1:A:37:LEU:CD1	0.54	2.56	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LYS:HG3	1:A:34:TYR:CD2	0.54	2.37	20	1
1:A:29:ASN:HB2	1:A:49:LEU:CB	0.54	2.32	15	4
1:B:29:ASN:HB2	1:B:49:LEU:CB	0.54	2.32	15	3
1:B:10:GLN:O	1:B:31:GLN:NE2	0.54	2.41	22	28
1:B:61:TYR:CD2	1:B:84:VAL:C	0.54	2.81	13	18
1:A:31:GLN:CB	1:A:47:ILE:CG2	0.54	2.86	8	12
1:A:43:VAL:HG23	1:A:45:VAL:HG13	0.54	1.78	14	3
1:B:13:PHE:CD1	1:B:29:ASN:CG	0.54	2.81	6	11
1:B:2:ILE:CG2	1:B:63:VAL:HG21	0.54	2.31	5	2
1:B:7:LYS:HG2	1:B:34:TYR:CE2	0.54	2.37	11	15
1:B:13:PHE:N	1:B:55:ALA:HB2	0.54	2.17	17	12
1:A:37:LEU:HD22	1:A:39:ASN:HD21	0.54	1.60	13	2
1:A:35:VAL:HG12	1:A:36:ASP:N	0.54	2.15	26	2
1:A:3:LYS:H	1:A:37:LEU:HD12	0.54	1.55	1	1
1:A:7:LYS:HG2	1:A:34:TYR:CE2	0.54	2.38	23	15
1:B:31:GLN:HB3	1:B:47:ILE:CG2	0.54	2.33	29	27
1:B:4:VAL:HG21	1:B:83:LEU:HD11	0.54	1.79	22	2
1:A:1:MET:C	1:B:65:LEU:HD22	0.54	2.22	18	5
1:B:81:LEU:N	1:B:81:LEU:HD23	0.54	2.18	18	2
1:A:70:VAL:CG1	1:B:45:VAL:HG21	0.54	2.32	9	4
1:A:69:LYS:HA	1:B:37:LEU:HD11	0.54	1.78	8	4
1:B:6:ILE:CG2	1:B:6:ILE:O	0.54	2.56	14	2
1:A:37:LEU:HD22	1:A:37:LEU:N	0.54	2.16	1	1
1:A:32:LEU:N	1:A:32:LEU:CD2	0.54	2.70	9	2
1:A:7:LYS:HG3	1:A:34:TYR:CD1	0.54	2.38	28	1
1:B:48:THR:HG21	1:B:80:ARG:CZ	0.54	2.33	22	2
1:B:7:LYS:HG3	1:B:34:TYR:CD2	0.54	2.37	20	1
1:B:33:CYS:SG	1:B:47:ILE:CG1	0.54	2.96	15	3
1:B:43:VAL:CG2	1:B:43:VAL:O	0.54	2.56	18	13
1:A:10:GLN:O	1:A:31:GLN:NE2	0.54	2.41	7	28
1:B:7:LYS:CG	1:B:34:TYR:CE2	0.54	2.90	11	15
1:B:28:LEU:HD12	1:B:29:ASN:C	0.54	2.23	10	2
1:A:72:GLN:CG	1:A:72:GLN:O	0.54	2.56	29	3
1:B:6:ILE:CD1	1:B:61:TYR:CG	0.54	2.91	7	4
1:B:10:GLN:HE22	1:B:32:LEU:HD22	0.54	1.63	27	1
1:B:68:PHE:CD1	1:B:78:ILE:HG13	0.54	2.38	4	1
1:B:29:ASN:CB	1:B:49:LEU:HB3	0.54	2.32	5	5
1:A:62:THR:HG23	1:A:86:ALA:HA	0.54	1.80	8	12
1:B:49:LEU:CD1	1:B:53:GLN:O	0.54	2.56	1	8
1:A:65:LEU:HD13	1:B:2:ILE:HG22	0.54	1.77	30	1
1:B:32:LEU:N	1:B:32:LEU:CD2	0.54	2.70	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:LYS:HG3	1:B:34:TYR:CD1	0.54	2.38	28	1
1:A:65:LEU:HD21	1:B:2:ILE:CA	0.54	2.32	11	1
1:A:65:LEU:HD22	1:B:1:MET:O	0.54	2.02	21	1
1:B:3:LYS:O	1:B:37:LEU:CD1	0.54	2.56	1	1
1:B:36:ASP:O	1:B:39:ASN:N	0.53	2.41	26	6
1:A:61:TYR:CD2	1:A:84:VAL:C	0.53	2.81	13	18
1:A:28:LEU:HD12	1:A:29:ASN:C	0.53	2.23	10	2
1:A:1:MET:O	1:A:3:LYS:N	0.53	2.41	24	12
1:B:72:GLN:O	1:B:72:GLN:CG	0.53	2.56	29	3
1:A:38:GLY:O	1:A:39:ASN:CB	0.53	2.55	26	1
1:A:29:ASN:O	1:A:49:LEU:CB	0.53	2.56	14	8
1:B:62:THR:O	1:B:84:VAL:CG2	0.53	2.56	13	16
1:B:62:THR:HG23	1:B:86:ALA:HA	0.53	1.80	2	12
1:A:49:LEU:CD1	1:A:53:GLN:O	0.53	2.56	1	8
1:B:38:GLY:O	1:B:39:ASN:CB	0.53	2.55	26	1
1:A:65:LEU:CD1	1:B:37:LEU:HG	0.53	2.33	1	4
1:A:33:CYS:SG	1:A:47:ILE:CG1	0.53	2.96	15	3
1:A:4:VAL:HG21	1:A:83:LEU:HD11	0.53	1.79	22	2
1:B:1:MET:O	1:B:3:LYS:N	0.53	2.42	24	12
1:A:43:VAL:CG2	1:A:43:VAL:O	0.53	2.56	18	10
1:A:81:LEU:HD23	1:A:81:LEU:N	0.53	2.18	18	2
1:B:68:PHE:CD1	1:B:78:ILE:HG12	0.53	2.37	13	1
1:A:47:ILE:HG13	1:A:56:TYR:CE2	0.53	2.38	2	5
1:A:31:GLN:NE2	1:A:56:TYR:O	0.53	2.40	17	11
1:A:7:LYS:CD	1:A:34:TYR:CE2	0.53	2.92	11	4
1:B:62:THR:HG23	1:B:86:ALA:CA	0.53	2.34	8	16
1:B:72:GLN:CG	1:B:72:GLN:O	0.53	2.56	16	3
1:A:65:LEU:HD21	1:B:2:ILE:HG13	0.53	1.81	13	1
1:B:29:ASN:O	1:B:49:LEU:CB	0.53	2.57	3	8
1:A:33:CYS:O	1:A:44:LEU:HD12	0.53	2.03	18	8
1:A:31:GLN:HB3	1:A:47:ILE:CG2	0.53	2.33	29	27
1:B:62:THR:HG23	1:B:86:ALA:CB	0.53	2.34	28	11
1:B:1:MET:O	1:B:1:MET:CG	0.53	2.56	9	1
1:B:49:LEU:O	1:B:49:LEU:CD1	0.53	2.56	23	1
1:B:65:LEU:HG	1:B:68:PHE:CD2	0.53	2.39	11	1
1:B:81:LEU:O	1:B:81:LEU:CG	0.53	2.57	16	13
1:B:31:GLN:CB	1:B:47:ILE:CG2	0.53	2.86	8	11
1:A:48:THR:HG21	1:A:80:ARG:CZ	0.53	2.33	22	2
1:B:40:GLU:C	1:B:41:HIS:CG	0.53	2.80	7	4
1:B:65:LEU:HD12	1:B:65:LEU:O	0.53	2.04	8	2
1:B:10:GLN:O	1:B:11:ALA:C	0.53	2.47	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:SER:O	1:B:79:ASP:CB	0.53	2.57	9	2
1:B:33:CYS:O	1:B:44:LEU:HD12	0.53	2.04	15	8
1:B:81:LEU:CG	1:B:81:LEU:O	0.53	2.57	17	12
1:A:1:MET:SD	1:A:62:THR:CG2	0.53	2.97	2	4
1:B:69:LYS:CG	1:B:77:MET:O	0.53	2.57	7	1
1:B:65:LEU:HA	1:B:68:PHE:CG	0.53	2.39	3	18
1:A:72:GLN:O	1:A:72:GLN:CG	0.53	2.56	18	3
1:A:45:VAL:HG21	1:B:70:VAL:CG1	0.53	2.33	9	3
1:B:35:VAL:CG1	1:B:37:LEU:HG	0.53	2.34	28	2
1:A:65:LEU:HG	1:A:68:PHE:CD2	0.53	2.38	11	1
1:A:81:LEU:O	1:A:81:LEU:CG	0.53	2.57	29	15
1:B:47:ILE:HD12	1:B:56:TYR:CZ	0.53	2.39	29	4
1:A:62:THR:HG23	1:A:86:ALA:CA	0.53	2.34	8	16
1:A:40:GLU:C	1:A:41:HIS:CG	0.53	2.80	7	4
1:A:10:GLN:O	1:A:12:GLN:N	0.53	2.42	27	1
1:B:35:VAL:CG1	1:B:37:LEU:HD21	0.53	2.33	1	1
1:A:56:TYR:CE1	1:A:83:LEU:HB3	0.53	2.39	8	1
1:A:39:ASN:O	1:A:41:HIS:N	0.53	2.42	18	6
1:B:47:ILE:HG13	1:B:56:TYR:CE2	0.53	2.39	11	5
1:A:47:ILE:HD12	1:A:56:TYR:CZ	0.53	2.39	29	4
1:B:29:ASN:ND2	1:B:49:LEU:O	0.53	2.42	18	6
1:B:7:LYS:CD	1:B:34:TYR:CE1	0.53	2.92	18	2
1:A:39:ASN:O	1:A:41:HIS:NE2	0.53	2.42	27	1
1:A:37:LEU:C	1:A:37:LEU:HD12	0.53	2.23	28	1
1:B:64:HIS:N	1:B:82:ARG:O	0.53	2.42	13	8
1:A:65:LEU:HD22	1:B:1:MET:C	0.53	2.23	18	5
1:B:1:MET:SD	1:B:62:THR:CG2	0.53	2.97	2	4
1:B:31:GLN:OE1	1:B:56:TYR:N	0.53	2.41	8	2
1:A:65:LEU:HA	1:A:68:PHE:CG	0.53	2.39	8	19
1:A:31:GLN:HB3	1:A:47:ILE:HG22	0.53	1.80	14	15
1:A:29:ASN:ND2	1:A:49:LEU:O	0.53	2.42	3	6
1:A:65:LEU:CD2	1:B:2:ILE:HG12	0.53	2.34	13	1
1:B:37:LEU:O	1:B:37:LEU:CD1	0.53	2.57	26	2
1:A:47:ILE:CG2	1:A:47:ILE:O	0.53	2.56	1	2
1:A:49:LEU:CD1	1:A:49:LEU:O	0.53	2.56	23	1
1:B:56:TYR:CE1	1:B:83:LEU:HB3	0.53	2.39	8	1
1:B:4:VAL:O	1:B:61:TYR:N	0.52	2.40	15	8
1:A:80:ARG:O	1:A:81:LEU:C	0.52	2.48	4	23
1:B:7:LYS:HE2	1:B:34:TYR:CD2	0.52	2.39	10	2
1:A:31:GLN:OE1	1:A:55:ALA:CB	0.52	2.55	7	2
1:A:4:VAL:HG21	1:A:35:VAL:HG22	0.52	1.79	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:HE22	1:A:32:LEU:HD22	0.52	1.63	27	1
1:B:37:LEU:C	1:B:37:LEU:HD12	0.52	2.23	28	1
1:A:37:LEU:C	1:A:37:LEU:CD1	0.52	2.78	29	1
1:B:39:ASN:O	1:B:41:HIS:ND1	0.52	2.42	19	1
1:B:33:CYS:SG	1:B:47:ILE:CD1	0.52	2.97	9	5
1:B:39:ASN:O	1:B:41:HIS:N	0.52	2.43	9	6
1:A:7:LYS:HE2	1:A:34:TYR:CD2	0.52	2.39	10	2
1:A:47:ILE:CG2	1:A:48:THR:N	0.52	2.72	2	4
1:A:31:GLN:OE1	1:A:56:TYR:N	0.52	2.41	8	2
1:B:31:GLN:HB3	1:B:47:ILE:HG22	0.52	1.80	14	16
1:B:72:GLN:C	1:B:73:PHE:CG	0.52	2.81	8	3
1:B:80:ARG:O	1:B:81:LEU:C	0.52	2.47	4	23
1:A:12:GLN:HA	1:A:55:ALA:HB3	0.52	1.82	17	4
1:A:64:HIS:N	1:A:82:ARG:O	0.52	2.42	13	8
1:A:6:ILE:CD1	1:A:83:LEU:CD2	0.52	2.88	22	3
1:B:7:LYS:CD	1:B:34:TYR:CE2	0.52	2.92	11	4
1:A:72:GLN:C	1:A:73:PHE:CG	0.52	2.81	8	3
1:A:81:LEU:CG	1:A:81:LEU:O	0.52	2.57	16	9
1:B:31:GLN:OE1	1:B:55:ALA:CB	0.52	2.55	7	2
1:A:62:THR:HG23	1:A:86:ALA:CB	0.52	2.34	28	13
1:B:31:GLN:O	1:B:47:ILE:N	0.52	2.43	13	6
1:A:65:LEU:HD12	1:A:65:LEU:O	0.52	2.04	8	4
1:B:7:LYS:CG	1:B:34:TYR:CE1	0.52	2.92	18	2
1:A:68:PHE:CD1	1:A:78:ILE:HG12	0.52	2.38	13	1
1:B:56:TYR:CE1	1:B:83:LEU:O	0.52	2.63	13	1
1:B:47:ILE:CG2	1:B:47:ILE:O	0.52	2.56	1	2
1:A:69:LYS:CG	1:A:77:MET:O	0.52	2.57	7	1
1:B:35:VAL:O	1:B:37:LEU:CD2	0.52	2.57	7	1
1:A:7:LYS:CD	1:A:34:TYR:CE1	0.52	2.92	18	2
1:A:70:VAL:HG13	1:A:76:LEU:HD12	0.52	1.82	18	1
1:A:2:ILE:HG12	1:B:65:LEU:CD2	0.52	2.35	13	1
1:A:2:ILE:HG13	1:B:65:LEU:HD21	0.52	1.81	13	1
1:A:37:LEU:CD1	1:A:37:LEU:O	0.52	2.57	26	2
1:A:36:ASP:OD1	1:A:36:ASP:N	0.52	2.43	14	4
1:A:39:ASN:O	1:A:40:GLU:C	0.52	2.48	15	15
1:B:47:ILE:CG2	1:B:48:THR:N	0.52	2.73	2	4
1:A:31:GLN:O	1:A:47:ILE:N	0.52	2.43	9	6
1:A:6:ILE:CD1	1:A:61:TYR:CG	0.52	2.92	7	3
1:A:37:LEU:HG	1:B:65:LEU:CD1	0.52	2.34	1	3
1:A:10:GLN:O	1:A:11:ALA:C	0.52	2.47	27	1
1:B:10:GLN:O	1:B:12:GLN:N	0.52	2.42	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:LYS:N	1:B:37:LEU:CD1	0.52	2.64	1	1
1:A:1:MET:O	1:A:1:MET:CG	0.52	2.56	9	1
1:A:68:PHE:CD1	1:A:78:ILE:HG13	0.52	2.40	4	1
1:A:35:VAL:O	1:A:37:LEU:CD2	0.52	2.57	7	1
1:B:39:ASN:O	1:B:41:HIS:NE2	0.52	2.42	27	1
1:B:36:ASP:N	1:B:36:ASP:OD1	0.52	2.42	28	3
1:A:35:VAL:CG1	1:A:37:LEU:HG	0.52	2.34	28	1
1:A:39:ASN:O	1:A:41:HIS:ND1	0.52	2.43	19	1
1:B:6:ILE:CD1	1:B:83:LEU:CD2	0.52	2.88	22	3
1:B:47:ILE:HG12	1:B:56:TYR:CZ	0.52	2.40	26	18
1:A:76:LEU:HB2	1:B:81:LEU:HD13	0.52	1.79	14	5
1:B:72:GLN:NE2	1:B:72:GLN:O	0.52	2.43	18	3
1:B:63:VAL:CG1	1:B:81:LEU:CD1	0.52	2.87	4	2
1:A:70:VAL:HG11	1:B:45:VAL:CG1	0.52	2.35	28	3
1:B:28:LEU:HD22	1:B:48:THR:CG2	0.52	2.35	4	4
1:A:33:CYS:SG	1:A:47:ILE:CD1	0.52	2.98	15	5
1:A:7:LYS:CG	1:A:34:TYR:CE1	0.52	2.93	18	2
1:A:62:THR:O	1:A:84:VAL:HG23	0.52	2.05	13	1
1:B:32:LEU:CD2	1:B:44:LEU:CD1	0.52	2.87	10	1
1:B:31:GLN:NE2	1:B:56:TYR:O	0.52	2.41	17	12
1:B:70:VAL:HG13	1:B:76:LEU:HD12	0.52	1.82	18	1
1:B:47:ILE:HG21	1:B:56:TYR:CE2	0.52	2.40	13	1
1:A:36:ASP:O	1:A:39:ASN:N	0.51	2.41	26	6
1:A:65:LEU:HA	1:A:68:PHE:CE2	0.51	2.41	5	21
1:A:63:VAL:CG1	1:A:81:LEU:CD1	0.51	2.87	4	2
1:B:35:VAL:CG1	1:B:36:ASP:N	0.51	2.73	26	2
1:B:39:ASN:N	1:B:39:ASN:OD1	0.51	2.43	28	3
1:B:6:ILE:CD1	1:B:33:CYS:SG	0.51	2.98	16	2
1:B:34:TYR:CE2	1:B:44:LEU:HB2	0.51	2.40	28	3
1:B:67:SER:OG	1:B:82:ARG:N	0.51	2.43	28	7
1:A:35:VAL:CG1	1:A:36:ASP:N	0.51	2.73	26	2
1:A:37:LEU:CD1	1:A:37:LEU:C	0.51	2.79	26	3
1:A:2:ILE:HG22	1:B:65:LEU:HD13	0.51	1.81	30	1
1:A:65:LEU:CD1	1:B:37:LEU:CA	0.51	2.88	19	4
1:A:28:LEU:HD22	1:A:48:THR:CG2	0.51	2.35	4	4
1:A:67:SER:O	1:A:79:ASP:N	0.51	2.43	9	2
1:B:71:GLY:O	1:B:72:GLN:CG	0.51	2.59	28	1
1:B:62:THR:N	1:B:84:VAL:O	0.51	2.39	26	25
1:B:81:LEU:N	1:B:81:LEU:CD2	0.51	2.73	18	3
1:A:34:TYR:CE2	1:A:44:LEU:HB2	0.51	2.40	28	3
1:B:47:ILE:HG21	1:B:56:TYR:CD2	0.51	2.41	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:B:65:LEU:CD2	0.51	2.35	21	1
1:B:81:LEU:C	1:B:81:LEU:CD1	0.51	2.78	8	1
1:A:34:TYR:CE2	1:A:44:LEU:CD1	0.51	2.92	17	1
1:A:65:LEU:HD13	1:B:2:ILE:CA	0.51	2.33	10	3
1:B:6:ILE:CG1	1:B:61:TYR:CE1	0.51	2.94	10	2
1:A:47:ILE:HG21	1:A:56:TYR:CE2	0.51	2.40	13	1
1:B:37:LEU:C	1:B:37:LEU:CD1	0.51	2.78	29	2
1:A:70:VAL:HG11	1:B:45:VAL:CG2	0.51	2.36	9	2
1:A:72:GLN:O	1:A:72:GLN:NE2	0.51	2.44	27	2
1:A:2:ILE:HG22	1:A:37:LEU:CD2	0.51	2.36	28	1
1:B:12:GLN:HA	1:B:55:ALA:HB3	0.51	1.82	17	5
1:A:35:VAL:O	1:A:43:VAL:CG2	0.51	2.57	14	8
1:A:67:SER:OG	1:A:82:ARG:N	0.51	2.43	28	7
1:A:2:ILE:HA	1:B:65:LEU:CD2	0.51	2.36	11	2
1:A:36:ASP:N	1:A:36:ASP:OD1	0.51	2.43	28	3
1:A:56:TYR:CE1	1:A:83:LEU:O	0.51	2.63	13	1
1:A:65:LEU:O	1:A:68:PHE:N	0.51	2.43	13	3
1:A:67:SER:O	1:A:79:ASP:CB	0.51	2.57	9	2
1:A:51:GLU:O	1:A:53:GLN:N	0.51	2.43	6	2
1:B:51:GLU:O	1:B:53:GLN:N	0.51	2.43	6	2
1:B:2:ILE:HG22	1:B:37:LEU:CD2	0.51	2.36	28	1
1:B:76:LEU:C	1:B:77:MET:CG	0.51	2.79	4	6
1:A:4:VAL:HB	1:A:61:TYR:CB	0.51	2.36	25	11
1:B:7:LYS:HE2	1:B:34:TYR:CE2	0.51	2.41	6	3
1:B:37:LEU:CD1	1:B:37:LEU:C	0.51	2.79	16	2
1:A:63:VAL:HG13	1:A:81:LEU:CG	0.51	2.36	4	1
1:A:57:ALA:CB	1:A:58:PRO:CD	0.51	2.88	15	21
1:A:4:VAL:O	1:A:61:TYR:N	0.51	2.43	2	8
1:A:7:LYS:HE2	1:A:34:TYR:CE2	0.51	2.41	6	3
1:A:47:ILE:HG21	1:A:56:TYR:CD2	0.51	2.41	13	2
1:A:56:TYR:CZ	1:A:83:LEU:HB3	0.51	2.41	13	1
1:B:65:LEU:O	1:B:68:PHE:N	0.51	2.43	13	3
1:A:65:LEU:HB2	1:A:68:PHE:CE2	0.51	2.41	25	2
1:A:37:LEU:HD23	1:A:39:ASN:OD1	0.51	2.06	4	1
1:B:76:LEU:C	1:B:76:LEU:HD23	0.51	2.26	25	2
1:B:54:PRO:O	1:B:55:ALA:C	0.51	2.48	8	30
1:B:4:VAL:HB	1:B:61:TYR:CB	0.51	2.36	25	11
1:B:62:THR:O	1:B:84:VAL:HG23	0.51	2.06	13	1
1:A:29:ASN:ND2	1:A:50:ASP:O	0.51	2.43	11	6
1:A:37:LEU:CA	1:B:65:LEU:CD1	0.51	2.89	19	4
1:A:7:LYS:HD2	1:A:34:TYR:CZ	0.51	2.41	28	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:VAL:HG13	1:B:81:LEU:CG	0.51	2.36	4	1
1:A:6:ILE:CD1	1:A:33:CYS:SG	0.51	2.98	16	2
1:B:65:LEU:HA	1:B:68:PHE:CE2	0.51	2.41	5	19
1:A:47:ILE:HG12	1:A:56:TYR:CZ	0.51	2.40	26	18
1:B:29:ASN:ND2	1:B:50:ASP:O	0.51	2.43	11	6
1:B:36:ASP:OD1	1:B:36:ASP:N	0.51	2.43	19	3
1:A:3:LYS:N	1:A:37:LEU:CD1	0.51	2.64	1	1
1:B:33:CYS:SG	1:B:45:VAL:CG1	0.51	2.99	1	1
1:B:67:SER:O	1:B:79:ASP:N	0.51	2.43	9	3
1:A:2:ILE:HA	1:A:37:LEU:HD22	0.51	1.83	28	1
1:A:40:GLU:O	1:A:41:HIS:HB3	0.51	2.06	8	1
1:A:32:LEU:CD2	1:A:44:LEU:CD1	0.50	2.87	10	1
1:A:32:LEU:HD22	1:A:44:LEU:HD11	0.50	1.81	10	2
1:A:65:LEU:CD2	1:B:1:MET:C	0.50	2.80	22	9
1:B:39:ASN:O	1:B:40:GLU:CB	0.50	2.59	4	2
1:A:39:ASN:N	1:A:39:ASN:OD1	0.50	2.42	28	5
1:A:35:VAL:HG12	1:A:37:LEU:CD2	0.50	2.36	1	1
1:A:54:PRO:O	1:A:55:ALA:C	0.50	2.48	8	29
1:B:72:GLN:O	1:B:72:GLN:NE2	0.50	2.43	27	2
1:A:37:LEU:HA	1:B:65:LEU:HD11	0.50	1.83	25	2
1:A:13:PHE:CB	1:A:30:GLU:O	0.50	2.60	12	4
1:B:37:LEU:HD23	1:B:39:ASN:OD1	0.50	2.06	4	1
1:A:37:LEU:HB3	1:B:65:LEU:HD21	0.50	1.81	21	1
1:A:33:CYS:SG	1:A:45:VAL:CG1	0.50	3.00	1	1
1:B:13:PHE:CD2	1:B:29:ASN:HB2	0.50	2.41	11	3
1:A:65:LEU:CD2	1:B:37:LEU:HD22	0.50	2.36	21	1
1:A:65:LEU:HD21	1:B:37:LEU:HD22	0.50	1.82	21	1
1:A:72:GLN:NE2	1:A:72:GLN:O	0.50	2.45	16	3
1:B:49:LEU:CD1	1:B:50:ASP:O	0.50	2.59	24	2
1:A:29:ASN:HD22	1:A:49:LEU:HD12	0.50	1.67	1	1
1:B:7:LYS:HD2	1:B:34:TYR:CZ	0.50	2.42	28	2
1:B:63:VAL:CG1	1:B:81:LEU:HG	0.50	2.37	4	1
1:A:13:PHE:CD2	1:A:29:ASN:HB2	0.50	2.42	8	3
1:A:76:LEU:C	1:A:77:MET:CG	0.50	2.79	4	6
1:A:64:HIS:HB2	1:A:82:ARG:O	0.50	2.07	2	22
1:A:1:MET:C	1:B:65:LEU:CD2	0.50	2.80	18	8
1:B:35:VAL:O	1:B:43:VAL:CG2	0.50	2.58	23	8
1:A:13:PHE:CD1	1:A:29:ASN:HB2	0.50	2.41	17	6
1:B:7:LYS:HE2	1:B:34:TYR:CE1	0.50	2.42	5	1
1:A:81:LEU:CD1	1:B:76:LEU:HD22	0.50	2.36	23	1
1:B:65:LEU:HB2	1:B:68:PHE:CE2	0.50	2.41	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:B:65:LEU:HD21	0.50	1.82	21	1
1:B:40:GLU:O	1:B:41:HIS:HB3	0.50	2.06	8	1
1:A:6:ILE:CG1	1:A:61:TYR:CE1	0.50	2.94	10	3
1:A:4:VAL:HG22	1:A:35:VAL:HG13	0.50	1.83	17	2
1:B:83:LEU:O	1:B:84:VAL:CG1	0.50	2.59	1	2
1:A:83:LEU:O	1:A:84:VAL:CG1	0.50	2.60	1	2
1:B:37:LEU:N	1:B:37:LEU:CD1	0.50	2.72	17	1
1:B:31:GLN:OE1	1:B:32:LEU:N	0.50	2.45	19	2
1:A:28:LEU:CD2	1:A:48:THR:CG2	0.50	2.90	1	1
1:A:63:VAL:CG1	1:A:81:LEU:HG	0.50	2.37	4	1
1:A:1:MET:O	1:A:2:ILE:CB	0.50	2.60	26	5
1:A:6:ILE:CD1	1:A:56:TYR:CB	0.50	2.90	13	3
1:B:56:TYR:CZ	1:B:83:LEU:HB3	0.50	2.41	13	1
1:B:13:PHE:CB	1:B:30:GLU:O	0.50	2.59	12	4
1:B:64:HIS:HB2	1:B:82:ARG:O	0.50	2.07	2	22
1:B:13:PHE:CD1	1:B:29:ASN:HB2	0.50	2.42	19	6
1:B:28:LEU:CD2	1:B:48:THR:CG2	0.50	2.90	1	1
1:B:63:VAL:HG12	1:B:64:HIS:N	0.49	2.22	5	10
1:B:4:VAL:HG22	1:B:35:VAL:HG13	0.49	1.83	17	2
1:A:55:ALA:O	1:A:57:ALA:N	0.49	2.45	12	6
1:B:47:ILE:HD12	1:B:56:TYR:HE2	0.49	1.67	13	1
1:B:6:ILE:CD1	1:B:56:TYR:CB	0.49	2.90	13	3
1:A:45:VAL:CG1	1:B:70:VAL:HG11	0.49	2.37	28	3
1:B:49:LEU:CD2	1:B:56:TYR:CE1	0.49	2.95	1	1
1:A:32:LEU:HD13	1:A:45:VAL:O	0.49	2.07	9	1
1:B:39:ASN:O	1:B:40:GLU:C	0.49	2.48	15	16
1:A:29:ASN:CB	1:A:49:LEU:O	0.49	2.61	18	1
1:B:38:GLY:O	1:B:39:ASN:ND2	0.49	2.45	26	1
1:A:71:GLY:O	1:A:72:GLN:CG	0.49	2.59	28	1
1:A:4:VAL:HA	1:A:34:TYR:O	0.49	2.08	20	24
1:A:37:LEU:CG	1:A:37:LEU:O	0.49	2.60	8	3
1:A:32:LEU:HD23	1:A:44:LEU:HD11	0.49	1.81	10	2
1:B:29:ASN:OD1	1:B:49:LEU:O	0.49	2.30	7	6
1:B:7:LYS:HB2	1:B:10:GLN:CG	0.49	2.38	26	3
1:B:4:VAL:HG21	1:B:35:VAL:HG22	0.49	1.79	7	3
1:B:49:LEU:CD2	1:B:55:ALA:HA	0.49	2.37	8	5
1:B:2:ILE:HA	1:B:37:LEU:HD22	0.49	1.83	28	1
1:A:39:ASN:O	1:A:41:HIS:O	0.49	2.30	15	6
1:A:61:TYR:HB3	1:A:83:LEU:CD2	0.49	2.38	5	21
1:B:60:LEU:O	1:B:85:PRO:HA	0.49	2.07	6	26
1:A:70:VAL:HG13	1:B:45:VAL:CG2	0.49	2.37	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:SER:O	1:B:78:ILE:O	0.49	2.31	7	4
1:B:39:ASN:O	1:B:41:HIS:O	0.49	2.31	18	7
1:A:62:THR:N	1:A:84:VAL:O	0.49	2.40	1	30
1:A:31:GLN:OE1	1:A:32:LEU:O	0.49	2.31	17	18
1:A:67:SER:O	1:A:78:ILE:O	0.49	2.30	7	4
1:A:7:LYS:HE2	1:A:34:TYR:CE1	0.49	2.42	5	1
1:A:65:LEU:CB	1:B:2:ILE:HG12	0.49	2.38	1	8
1:B:10:GLN:O	1:B:31:GLN:OE1	0.49	2.30	16	8
1:A:49:LEU:CD2	1:A:55:ALA:HA	0.49	2.38	8	7
1:A:49:LEU:CD2	1:A:56:TYR:CE1	0.49	2.95	1	1
1:A:65:LEU:HD21	1:B:37:LEU:HB3	0.49	1.83	21	1
1:A:63:VAL:HG12	1:A:64:HIS:N	0.49	2.23	9	10
1:A:39:ASN:O	1:A:40:GLU:CB	0.49	2.59	4	2
1:A:79:ASP:O	1:A:80:ARG:HB3	0.49	2.08	18	3
1:A:68:PHE:CE1	1:A:78:ILE:HG13	0.49	2.43	4	1
1:B:37:LEU:C	1:B:37:LEU:HD13	0.49	2.28	16	1
1:A:67:SER:HB3	1:A:80:ARG:C	0.49	2.28	13	19
1:A:7:LYS:HD3	1:A:34:TYR:CG	0.49	2.43	10	2
1:B:6:ILE:HD12	1:B:56:TYR:CB	0.49	2.38	23	3
1:A:6:ILE:HD13	1:A:61:TYR:CZ	0.49	2.43	2	7
1:A:7:LYS:HB2	1:A:10:GLN:CG	0.49	2.38	26	4
1:A:47:ILE:HD12	1:A:56:TYR:HE2	0.49	1.68	13	1
1:A:6:ILE:HD13	1:A:56:TYR:CB	0.49	2.36	13	1
1:B:6:ILE:HD13	1:B:56:TYR:CB	0.49	2.37	13	1
1:A:38:GLY:O	1:A:39:ASN:ND2	0.49	2.45	26	1
1:A:12:GLN:HA	1:A:55:ALA:CB	0.49	2.38	17	2
1:A:1:MET:C	1:A:2:ILE:CG1	0.49	2.81	9	1
1:B:31:GLN:OE1	1:B:49:LEU:HD23	0.49	2.08	8	1
1:A:60:LEU:O	1:A:85:PRO:HA	0.49	2.08	6	26
1:A:47:ILE:HD11	1:A:83:LEU:HD12	0.49	1.83	24	3
1:B:78:ILE:HG22	1:B:79:ASP:N	0.49	2.23	19	4
1:B:29:ASN:CB	1:B:49:LEU:O	0.49	2.61	18	1
1:A:7:LYS:HG3	1:A:34:TYR:CE1	0.49	2.43	27	3
1:A:65:LEU:HD11	1:B:37:LEU:HA	0.49	1.83	25	2
1:B:68:PHE:CE1	1:B:78:ILE:HG13	0.49	2.42	4	1
1:A:47:ILE:O	1:A:47:ILE:CG2	0.49	2.60	16	1
1:B:34:TYR:CE2	1:B:44:LEU:CD1	0.49	2.93	17	1
1:B:7:LYS:HD3	1:B:34:TYR:CG	0.49	2.43	24	2
1:B:61:TYR:CD2	1:B:83:LEU:CD2	0.49	2.96	8	4
1:B:1:MET:O	1:B:2:ILE:CB	0.49	2.60	26	4
1:B:2:ILE:HG21	1:B:63:VAL:CG2	0.49	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HA	1:B:65:LEU:CD1	0.49	2.37	3	4
1:B:37:LEU:O	1:B:37:LEU:CG	0.49	2.60	8	3
1:A:32:LEU:HD23	1:A:44:LEU:CD1	0.49	2.37	10	1
1:A:6:ILE:HD12	1:A:56:TYR:CB	0.49	2.38	23	3
1:A:45:VAL:CG2	1:B:70:VAL:HG13	0.49	2.38	22	2
1:A:29:ASN:OD1	1:A:49:LEU:O	0.49	2.31	7	6
1:B:83:LEU:HG	1:B:84:VAL:N	0.49	2.23	29	4
1:B:6:ILE:HD13	1:B:61:TYR:CZ	0.49	2.43	11	6
1:A:47:ILE:CG2	1:A:56:TYR:CE2	0.49	2.96	13	2
1:B:7:LYS:HG3	1:B:34:TYR:CE1	0.49	2.43	8	3
1:B:47:ILE:HG23	1:B:56:TYR:CE1	0.49	2.43	1	4
1:B:32:LEU:HD13	1:B:45:VAL:O	0.49	2.07	9	1
1:A:33:CYS:O	1:A:44:LEU:HA	0.48	2.08	15	22
1:A:6:ILE:CG1	1:A:61:TYR:CD1	0.48	2.96	23	2
1:A:67:SER:OG	1:A:80:ARG:O	0.48	2.31	20	20
1:A:37:LEU:CD1	1:B:69:LYS:CA	0.48	2.90	5	3
1:A:65:LEU:CD1	1:B:37:LEU:HA	0.48	2.38	3	4
1:B:35:VAL:HG12	1:B:37:LEU:CD2	0.48	2.38	1	1
1:B:29:ASN:HD22	1:B:49:LEU:HD12	0.48	1.67	1	1
1:B:5:GLU:N	1:B:34:TYR:O	0.48	2.46	28	3
1:B:47:ILE:O	1:B:47:ILE:CG2	0.48	2.60	16	1
1:B:6:ILE:CG1	1:B:61:TYR:CD1	0.48	2.96	23	2
1:B:36:ASP:O	1:B:39:ASN:OD1	0.48	2.32	8	2
1:A:83:LEU:HG	1:A:84:VAL:N	0.48	2.22	29	4
1:B:55:ALA:O	1:B:57:ALA:N	0.48	2.46	9	7
1:B:47:ILE:CG2	1:B:56:TYR:CE2	0.48	2.96	13	2
1:B:71:GLY:C	1:B:72:GLN:NE2	0.48	2.67	21	2
1:B:61:TYR:HB3	1:B:83:LEU:CD2	0.48	2.38	5	21
1:B:34:TYR:HB3	1:B:42:PRO:HB2	0.48	1.85	18	21
1:B:67:SER:HB3	1:B:80:ARG:O	0.48	2.08	8	12
1:B:48:THR:OG1	1:B:80:ARG:CZ	0.48	2.62	18	1
1:B:10:GLN:OE1	1:B:44:LEU:CD1	0.48	2.62	26	1
1:A:2:ILE:HG12	1:B:65:LEU:CB	0.48	2.38	1	9
1:A:10:GLN:O	1:A:31:GLN:OE1	0.48	2.32	30	9
1:A:49:LEU:C	1:A:49:LEU:HD13	0.48	2.29	6	4
1:B:47:ILE:CD1	1:B:56:TYR:OH	0.48	2.61	1	2
1:B:1:MET:C	1:B:2:ILE:CG1	0.48	2.81	9	1
1:A:28:LEU:CD1	1:A:28:LEU:C	0.48	2.78	17	1
1:B:47:ILE:HD12	1:B:83:LEU:HD12	0.48	1.85	15	1
1:B:31:GLN:OE1	1:B:32:LEU:O	0.48	2.31	9	18
1:A:7:LYS:CE	1:A:34:TYR:CD2	0.48	2.97	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:TYR:CZ	1:B:44:LEU:HB2	0.48	2.44	11	13
1:A:41:HIS:HB3	1:A:42:PRO:HD2	0.48	1.86	7	1
1:B:41:HIS:HB3	1:B:42:PRO:HD2	0.48	1.86	7	1
1:A:13:PHE:CD1	1:A:13:PHE:C	0.48	2.87	18	5
1:A:48:THR:OG1	1:A:80:ARG:CZ	0.48	2.62	18	1
1:A:37:LEU:HD13	1:B:70:VAL:HG22	0.48	1.84	13	2
1:B:82:ARG:NH1	1:B:82:ARG:HG3	0.48	2.24	1	1
1:A:32:LEU:CD1	1:A:32:LEU:N	0.48	2.74	28	2
1:B:3:LYS:O	1:B:35:VAL:HG13	0.48	2.08	21	2
1:A:3:LYS:O	1:A:35:VAL:HG13	0.48	2.09	21	2
1:A:37:LEU:C	1:A:37:LEU:HD13	0.48	2.28	16	1
1:A:37:LEU:HD22	1:A:39:ASN:ND2	0.48	2.23	13	2
1:A:7:LYS:HG3	1:A:34:TYR:CZ	0.48	2.44	27	3
1:A:2:ILE:HG21	1:B:76:LEU:CD2	0.48	2.37	16	2
1:A:11:ALA:O	1:A:55:ALA:HB3	0.48	2.09	15	3
1:B:33:CYS:O	1:B:44:LEU:HA	0.48	2.08	15	20
1:B:32:LEU:HD23	1:B:44:LEU:CD1	0.48	2.38	10	1
1:B:72:GLN:NE2	1:B:72:GLN:HA	0.48	2.23	3	3
1:A:31:GLN:OE1	1:A:32:LEU:N	0.48	2.45	19	2
1:A:2:ILE:CG1	1:B:65:LEU:HB3	0.48	2.39	4	2
1:A:76:LEU:HD22	1:B:81:LEU:CD1	0.48	2.38	23	1
1:A:71:GLY:C	1:A:72:GLN:NE2	0.48	2.67	15	2
1:B:67:SER:HB3	1:B:80:ARG:C	0.48	2.29	13	19
1:A:34:TYR:HB3	1:A:42:PRO:HB2	0.48	1.85	17	22
1:B:28:LEU:C	1:B:28:LEU:CD1	0.48	2.77	17	2
1:A:6:ILE:O	1:A:7:LYS:O	0.48	2.32	2	16
1:B:12:GLN:HA	1:B:55:ALA:CB	0.48	2.38	17	2
1:A:3:LYS:O	1:A:37:LEU:HD11	0.48	2.09	1	1
1:A:47:ILE:CD1	1:A:56:TYR:OH	0.48	2.62	1	2
1:A:31:GLN:OE1	1:A:49:LEU:HD23	0.48	2.08	8	1
1:A:39:ASN:ND2	1:A:43:VAL:CG1	0.48	2.76	29	1
1:A:37:LEU:HD22	1:B:69:LYS:CA	0.48	2.38	17	1
1:B:79:ASP:O	1:B:80:ARG:HB3	0.48	2.08	18	3
1:A:10:GLN:OE1	1:A:44:LEU:CD1	0.48	2.61	26	1
1:B:39:ASN:ND2	1:B:43:VAL:HG21	0.48	2.24	26	1
1:A:49:LEU:CD1	1:A:50:ASP:O	0.48	2.61	30	2
1:A:65:LEU:CB	1:B:2:ILE:HG23	0.48	2.38	30	1
1:A:47:ILE:HG23	1:A:56:TYR:CE1	0.48	2.44	1	3
1:B:3:LYS:O	1:B:37:LEU:HD11	0.48	2.09	1	1
1:B:80:ARG:CG	1:B:80:ARG:O	0.48	2.62	12	2
1:A:38:GLY:O	1:A:39:ASN:OD1	0.48	2.32	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:VAL:O	1:B:71:GLY:O	0.48	2.32	8	1
1:A:72:GLN:N	1:A:72:GLN:CD	0.48	2.67	15	1
1:B:4:VAL:HA	1:B:34:TYR:O	0.48	2.08	19	25
1:A:5:GLU:N	1:A:34:TYR:O	0.48	2.47	28	4
1:B:32:LEU:HD22	1:B:44:LEU:HD11	0.48	1.82	10	2
1:B:29:ASN:O	1:B:49:LEU:HB2	0.48	2.09	25	6
1:A:37:LEU:CD1	1:B:69:LYS:HA	0.48	2.39	8	3
1:A:2:ILE:HG23	1:B:65:LEU:CB	0.48	2.39	30	1
1:A:65:LEU:CD2	1:B:2:ILE:HA	0.48	2.36	11	4
1:B:13:PHE:CG	1:B:29:ASN:HB2	0.48	2.44	1	1
1:B:32:LEU:N	1:B:32:LEU:CD1	0.48	2.74	28	2
1:A:45:VAL:CG2	1:B:75:SER:CA	0.48	2.92	16	1
1:B:72:GLN:CD	1:B:72:GLN:N	0.48	2.67	15	1
1:A:67:SER:HB3	1:A:80:ARG:O	0.48	2.09	24	14
1:A:6:ILE:CD1	1:A:56:TYR:HB3	0.48	2.39	14	10
1:B:49:LEU:HD13	1:B:49:LEU:C	0.48	2.29	6	2
1:A:12:GLN:CA	1:A:55:ALA:CB	0.48	2.92	27	2
1:A:65:LEU:HB3	1:B:2:ILE:CG1	0.48	2.39	4	2
1:A:36:ASP:O	1:A:39:ASN:OD1	0.47	2.32	8	2
1:A:78:ILE:HG22	1:A:79:ASP:N	0.47	2.24	24	4
1:A:74:GLY:O	1:A:75:SER:OG	0.47	2.32	9	2
1:A:13:PHE:CG	1:A:29:ASN:HB2	0.47	2.44	1	1
1:A:73:PHE:CG	1:A:73:PHE:O	0.47	2.67	10	1
1:B:32:LEU:HD23	1:B:44:LEU:HD11	0.47	1.82	10	2
1:A:79:ASP:O	1:A:80:ARG:HB2	0.47	2.08	12	7
1:B:7:LYS:HD3	1:B:34:TYR:CE2	0.47	2.45	22	3
1:B:6:ILE:O	1:B:7:LYS:O	0.47	2.31	2	16
1:B:6:ILE:CD1	1:B:56:TYR:HB3	0.47	2.39	14	12
1:B:32:LEU:HB3	1:B:44:LEU:CD1	0.47	2.39	20	6
1:A:72:GLN:HA	1:A:72:GLN:NE2	0.47	2.23	3	1
1:B:12:GLN:CA	1:B:55:ALA:CB	0.47	2.92	27	2
1:A:31:GLN:C	1:A:32:LEU:HD22	0.47	2.30	9	2
1:A:81:LEU:C	1:A:81:LEU:CD1	0.47	2.78	8	1
1:B:7:LYS:CE	1:B:34:TYR:CD2	0.47	2.97	24	2
1:B:62:THR:CG2	1:B:86:ALA:HA	0.47	2.40	8	11
1:B:13:PHE:C	1:B:13:PHE:CD1	0.47	2.87	18	3
1:A:68:PHE:CE1	1:A:78:ILE:HG23	0.47	2.45	13	1
1:B:67:SER:CB	1:B:80:ARG:C	0.47	2.83	1	5
1:B:7:LYS:HG3	1:B:34:TYR:CZ	0.47	2.44	27	2
1:A:31:GLN:C	1:A:32:LEU:HD12	0.47	2.30	23	1
1:A:3:LYS:C	1:A:4:VAL:HG23	0.47	2.30	25	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD13	1:A:28:LEU:N	0.47	2.24	18	1
1:A:80:ARG:NH1	1:A:80:ARG:HG3	0.47	2.24	18	2
1:A:45:VAL:CG2	1:B:70:VAL:HG11	0.47	2.39	9	3
1:B:49:LEU:C	1:B:49:LEU:HD13	0.47	2.30	30	3
1:B:83:LEU:O	1:B:84:VAL:HG13	0.47	2.10	1	1
1:B:79:ASP:O	1:B:80:ARG:HB2	0.47	2.09	12	4
1:A:6:ILE:HD12	1:A:56:TYR:HB2	0.47	1.85	8	2
1:B:38:GLY:O	1:B:39:ASN:OD1	0.47	2.32	16	2
1:B:6:ILE:HG21	1:B:57:ALA:O	0.47	2.10	16	5
1:A:61:TYR:CB	1:A:83:LEU:HD21	0.47	2.39	22	3
1:B:61:TYR:CB	1:B:83:LEU:HD21	0.47	2.39	22	4
1:A:61:TYR:CD2	1:A:83:LEU:CD2	0.47	2.97	8	4
1:B:65:LEU:O	1:B:67:SER:N	0.47	2.48	2	3
1:B:6:ILE:HD12	1:B:61:TYR:CD1	0.47	2.45	7	2
1:A:56:TYR:O	1:A:57:ALA:O	0.47	2.33	12	7
1:B:65:LEU:HA	1:B:68:PHE:CD1	0.47	2.44	30	8
1:A:47:ILE:CD1	1:A:83:LEU:HB2	0.47	2.39	12	6
1:A:63:VAL:CG1	1:A:81:LEU:HD11	0.47	2.40	4	1
1:A:81:LEU:HD12	1:A:83:LEU:N	0.47	2.25	8	1
1:B:39:ASN:OD1	1:B:41:HIS:O	0.47	2.32	8	1
1:B:15:THR:HG23	1:B:28:LEU:C	0.47	2.30	29	1
1:B:11:ALA:O	1:B:55:ALA:HB3	0.47	2.09	15	3
1:B:73:PHE:CG	1:B:73:PHE:O	0.47	2.67	10	1
1:B:3:LYS:C	1:B:4:VAL:HG23	0.47	2.30	25	10
1:B:56:TYR:CD1	1:B:61:TYR:CE2	0.47	3.03	13	1
1:A:39:ASN:ND2	1:A:43:VAL:HG21	0.47	2.24	26	1
1:B:50:ASP:CB	1:B:53:GLN:HB2	0.47	2.40	16	9
1:B:36:ASP:CB	1:B:41:HIS:O	0.47	2.63	14	1
1:A:82:ARG:HG3	1:A:82:ARG:NH1	0.47	2.24	1	2
1:B:67:SER:OG	1:B:80:ARG:O	0.47	2.33	3	20
1:A:7:LYS:HD3	1:A:34:TYR:CE2	0.47	2.44	22	3
1:B:36:ASP:O	1:B:37:LEU:C	0.47	2.53	19	11
1:A:82:ARG:NH1	1:A:82:ARG:HG2	0.47	2.25	7	2
1:A:46:LYS:O	1:B:74:GLY:O	0.47	2.33	5	2
1:B:37:LEU:HD22	1:B:39:ASN:ND2	0.47	2.24	13	2
1:B:33:CYS:SG	1:B:83:LEU:HD12	0.47	2.50	1	1
1:A:65:LEU:CD1	1:B:37:LEU:HB2	0.47	2.40	20	2
1:A:76:LEU:CD2	1:B:2:ILE:HG21	0.47	2.39	16	2
1:B:60:LEU:O	1:B:86:ALA:N	0.47	2.43	23	1
1:B:81:LEU:HD12	1:B:83:LEU:N	0.47	2.25	8	1
1:A:75:SER:N	1:B:45:VAL:HG23	0.47	2.25	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD12	1:A:38:GLY:H	0.47	1.69	17	1
1:A:47:ILE:HD12	1:A:83:LEU:HD12	0.47	1.85	15	1
1:A:28:LEU:C	1:A:28:LEU:CD1	0.47	2.79	10	1
1:A:29:ASN:O	1:A:49:LEU:HB2	0.47	2.09	25	6
1:A:34:TYR:CZ	1:A:44:LEU:HB2	0.47	2.45	28	13
1:A:56:TYR:CD1	1:A:61:TYR:CE2	0.47	3.03	13	1
1:A:83:LEU:O	1:A:84:VAL:HG13	0.47	2.10	1	1
1:B:33:CYS:SG	1:B:45:VAL:HG13	0.47	2.50	1	1
1:B:31:GLN:C	1:B:32:LEU:HD22	0.47	2.30	9	2
1:B:39:ASN:O	1:B:40:GLU:HB2	0.47	2.10	4	1
1:A:62:THR:CG2	1:A:86:ALA:HA	0.47	2.40	2	10
1:B:78:ILE:HG23	1:B:81:LEU:CA	0.47	2.40	18	3
1:A:81:LEU:N	1:A:81:LEU:CD2	0.47	2.77	27	2
1:A:10:GLN:OE1	1:A:34:TYR:CD2	0.47	2.68	26	1
1:A:35:VAL:CG1	1:A:37:LEU:HD11	0.47	2.37	1	1
1:A:37:LEU:HD22	1:A:38:GLY:H	0.47	1.70	1	1
1:A:39:ASN:OD1	1:A:41:HIS:O	0.47	2.32	8	1
1:B:10:GLN:NE2	1:B:33:CYS:HA	0.47	2.25	10	1
1:B:47:ILE:HG23	1:B:48:THR:N	0.47	2.25	2	2
1:B:7:LYS:HA	1:B:7:LYS:CE	0.47	2.40	13	2
1:A:32:LEU:HB3	1:A:44:LEU:CD1	0.47	2.40	23	6
1:A:47:ILE:CD1	1:A:56:TYR:CZ	0.47	2.98	29	2
1:A:39:ASN:O	1:A:40:GLU:HB2	0.47	2.10	4	1
1:A:80:ARG:O	1:A:80:ARG:CG	0.47	2.62	12	1
1:A:70:VAL:O	1:A:71:GLY:O	0.47	2.32	8	1
1:B:60:LEU:O	1:B:61:TYR:CD1	0.46	2.68	2	3
1:A:63:VAL:HG12	1:A:64:HIS:H	0.46	1.70	24	8
1:A:50:ASP:CB	1:A:53:GLN:HB2	0.46	2.40	16	9
1:A:80:ARG:O	1:A:81:LEU:O	0.46	2.33	4	1
1:A:36:ASP:O	1:A:37:LEU:C	0.46	2.52	9	11
1:B:80:ARG:NH1	1:B:80:ARG:HG3	0.46	2.24	18	2
1:A:70:VAL:HG22	1:B:37:LEU:HD13	0.46	1.86	13	2
1:A:67:SER:CB	1:A:80:ARG:C	0.46	2.83	1	6
1:A:4:VAL:HG22	1:A:5:GLU:N	0.46	2.25	8	3
1:A:33:CYS:SG	1:A:83:LEU:HD12	0.46	2.50	1	1
1:A:68:PHE:O	1:A:69:LYS:CG	0.46	2.63	9	2
1:B:68:PHE:O	1:B:69:LYS:CG	0.46	2.63	9	2
1:A:2:ILE:CG2	1:A:37:LEU:CD2	0.46	2.94	28	1
1:A:37:LEU:HD13	1:B:65:LEU:HD13	0.46	1.81	28	1
1:A:15:THR:HG23	1:A:28:LEU:C	0.46	2.29	29	1
1:B:39:ASN:ND2	1:B:43:VAL:CG1	0.46	2.76	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HA	1:A:68:PHE:CD1	0.46	2.44	30	9
1:A:7:LYS:HA	1:A:7:LYS:CE	0.46	2.40	13	2
1:B:63:VAL:CG1	1:B:81:LEU:HD11	0.46	2.40	4	1
1:B:31:GLN:C	1:B:32:LEU:HD12	0.46	2.30	23	1
1:A:60:LEU:O	1:A:61:TYR:CD1	0.46	2.68	2	3
1:B:28:LEU:HD13	1:B:28:LEU:N	0.46	2.24	18	1
1:B:47:ILE:CD1	1:B:83:LEU:HB2	0.46	2.39	23	7
1:B:54:PRO:O	1:B:55:ALA:O	0.46	2.33	13	1
1:B:10:GLN:OE1	1:B:34:TYR:CD2	0.46	2.68	26	1
1:A:36:ASP:CB	1:A:41:HIS:O	0.46	2.63	14	1
1:A:47:ILE:HD13	1:A:48:THR:N	0.46	2.26	1	1
1:B:47:ILE:CD1	1:B:56:TYR:CZ	0.46	2.98	29	2
1:B:80:ARG:O	1:B:81:LEU:O	0.46	2.33	4	1
1:B:36:ASP:HA	1:B:41:HIS:O	0.46	2.11	6	11
1:B:78:ILE:HG21	1:B:81:LEU:HB3	0.46	1.87	18	4
1:B:82:ARG:NH1	1:B:82:ARG:CG	0.46	2.78	9	4
1:A:37:LEU:HB3	1:B:65:LEU:CD1	0.46	2.40	30	1
1:B:6:ILE:HD12	1:B:56:TYR:HB2	0.46	1.85	8	2
1:A:37:LEU:CD2	1:B:69:LYS:HA	0.46	2.40	15	7
1:B:56:TYR:O	1:B:57:ALA:O	0.46	2.33	7	5
1:A:78:ILE:HG23	1:A:81:LEU:CA	0.46	2.40	18	3
1:B:78:ILE:O	1:B:79:ASP:C	0.46	2.54	8	3
1:A:82:ARG:CG	1:A:82:ARG:NH1	0.46	2.79	24	6
1:A:73:PHE:CD1	1:A:73:PHE:N	0.46	2.84	8	3
1:A:37:LEU:CD2	1:A:37:LEU:C	0.46	2.84	1	1
1:B:37:LEU:HD22	1:B:38:GLY:H	0.46	1.70	1	1
1:A:37:LEU:HB2	1:B:65:LEU:CD1	0.46	2.41	20	2
1:A:65:LEU:HG	1:A:68:PHE:CE2	0.46	2.46	11	1
1:A:35:VAL:HG12	1:A:37:LEU:N	0.46	2.26	8	1
1:B:35:VAL:HG12	1:B:37:LEU:N	0.46	2.26	8	1
1:A:72:GLN:NE2	1:A:72:GLN:HA	0.46	2.25	22	2
1:A:6:ILE:HD12	1:A:61:TYR:CD1	0.46	2.45	7	2
1:A:78:ILE:O	1:A:79:ASP:HB3	0.46	2.11	7	5
1:B:80:ARG:NH1	1:B:80:ARG:CG	0.46	2.78	18	2
1:B:68:PHE:CE1	1:B:78:ILE:HG23	0.46	2.45	13	1
1:B:1:MET:O	1:B:2:ILE:C	0.46	2.54	30	1
1:A:71:GLY:N	1:A:77:MET:SD	0.46	2.89	27	1
1:A:69:LYS:HA	1:B:37:LEU:CD1	0.46	2.41	8	2
1:B:76:LEU:O	1:B:77:MET:HG2	0.46	2.11	19	11
1:A:6:ILE:HG21	1:A:57:ALA:O	0.46	2.11	13	4
1:B:4:VAL:HG22	1:B:5:GLU:N	0.46	2.25	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:71:GLY:N	1:B:77:MET:SD	0.46	2.89	27	1
1:B:35:VAL:HG13	1:B:37:LEU:CD1	0.46	2.38	1	1
1:B:32:LEU:N	1:B:32:LEU:HD22	0.46	2.25	9	1
1:B:48:THR:O	1:B:48:THR:CG2	0.46	2.61	25	1
1:A:31:GLN:OE1	1:A:33:CYS:SG	0.46	2.74	15	1
1:A:32:LEU:C	1:A:33:CYS:SG	0.46	2.94	18	23
1:A:36:ASP:HA	1:A:41:HIS:O	0.46	2.11	6	11
1:B:82:ARG:NH1	1:B:82:ARG:HG2	0.46	2.25	7	1
1:A:33:CYS:SG	1:A:45:VAL:HG13	0.46	2.51	1	1
1:A:32:LEU:N	1:A:32:LEU:HD22	0.46	2.24	9	1
1:A:65:LEU:CD2	1:B:2:ILE:CG2	0.46	2.85	9	1
1:B:1:MET:C	1:B:2:ILE:HG13	0.46	2.32	9	1
1:A:67:SER:HG	1:A:80:ARG:C	0.46	2.13	4	1
1:A:1:MET:CG	1:A:62:THR:HB	0.46	2.41	16	3
1:B:1:MET:CG	1:B:62:THR:HB	0.46	2.41	16	3
1:B:2:ILE:CG2	1:B:37:LEU:CD2	0.46	2.94	28	1
1:A:36:ASP:O	1:A:39:ASN:CG	0.46	2.54	15	5
1:B:31:GLN:OE1	1:B:33:CYS:SG	0.46	2.74	15	1
1:A:47:ILE:HG23	1:A:48:THR:N	0.46	2.25	2	2
1:A:78:ILE:CG2	1:A:81:LEU:HB3	0.46	2.41	3	3
1:A:45:VAL:CG1	1:B:75:SER:HA	0.46	2.41	13	1
1:A:83:LEU:C	1:A:84:VAL:HG13	0.46	2.32	1	2
1:B:37:LEU:C	1:B:37:LEU:CD2	0.46	2.84	1	1
1:B:81:LEU:O	1:B:81:LEU:HG	0.45	2.11	20	11
1:B:32:LEU:C	1:B:33:CYS:SG	0.45	2.94	21	21
1:A:81:LEU:HG	1:A:81:LEU:O	0.45	2.11	29	12
1:B:81:LEU:HG	1:B:81:LEU:O	0.45	2.11	17	11
1:A:78:ILE:HG21	1:A:81:LEU:HB3	0.45	1.87	18	2
1:A:7:LYS:CB	1:A:8:PRO:HD2	0.45	2.42	11	10
1:A:78:ILE:CD1	1:B:78:ILE:HG13	0.45	2.40	13	2
1:A:10:GLN:O	1:A:31:GLN:CD	0.45	2.54	29	7
1:B:37:LEU:CD1	1:B:38:GLY:N	0.45	2.64	28	1
1:B:37:LEU:HD23	1:B:37:LEU:C	0.45	2.31	6	1
1:B:82:ARG:HG3	1:B:82:ARG:NH1	0.45	2.26	12	1
1:B:36:ASP:O	1:B:39:ASN:CG	0.45	2.55	15	5
1:A:76:LEU:O	1:A:77:MET:HG2	0.45	2.11	9	11
1:A:2:ILE:CD1	1:A:63:VAL:HB	0.45	2.41	11	8
1:B:29:ASN:CG	1:B:49:LEU:O	0.45	2.55	22	1
1:A:65:LEU:O	1:A:67:SER:N	0.45	2.49	2	3
1:A:54:PRO:O	1:A:55:ALA:O	0.45	2.33	13	1
1:A:74:GLY:O	1:B:46:LYS:N	0.45	2.49	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG13	1:A:37:LEU:CD1	0.45	2.38	1	1
1:A:33:CYS:SG	1:A:83:LEU:CD1	0.45	3.04	1	1
1:A:1:MET:C	1:A:2:ILE:HG13	0.45	2.31	9	1
1:A:76:LEU:O	1:A:77:MET:SD	0.45	2.74	12	1
1:B:13:PHE:HB2	1:B:30:GLU:O	0.45	2.12	12	1
1:A:13:PHE:HD2	1:A:49:LEU:HD12	0.45	1.71	8	1
1:B:37:LEU:HD12	1:B:38:GLY:H	0.45	1.69	17	1
1:A:29:ASN:HB2	1:A:49:LEU:HB3	0.45	1.88	15	6
1:A:10:GLN:NE2	1:A:33:CYS:HA	0.45	2.26	10	1
1:A:31:GLN:CA	1:A:47:ILE:HG22	0.45	2.42	22	3
1:B:40:GLU:C	1:B:41:HIS:ND1	0.45	2.69	2	1
1:A:28:LEU:CD2	1:A:28:LEU:C	0.45	2.78	18	1
1:B:7:LYS:HD2	1:B:34:TYR:CD1	0.45	2.45	18	1
1:B:59:GLY:O	1:B:60:LEU:C	0.45	2.55	13	2
1:A:13:PHE:CD2	1:A:49:LEU:CG	0.45	2.99	26	5
1:B:10:GLN:O	1:B:31:GLN:CD	0.45	2.54	29	7
1:A:49:LEU:HD13	1:A:49:LEU:C	0.45	2.32	24	1
1:B:51:GLU:O	1:B:52:GLY:C	0.45	2.53	6	3
1:B:4:VAL:HG13	1:B:61:TYR:O	0.45	2.10	23	3
1:A:13:PHE:HB2	1:A:30:GLU:O	0.45	2.12	12	1
1:A:37:LEU:CD1	1:A:37:LEU:N	0.45	2.72	17	1
1:B:40:GLU:O	1:B:41:HIS:HB2	0.45	2.11	23	3
1:A:37:LEU:O	1:A:37:LEU:CD2	0.45	2.63	13	1
1:A:59:GLY:O	1:A:60:LEU:C	0.45	2.55	13	2
1:B:13:PHE:CD2	1:B:49:LEU:CG	0.45	2.99	26	5
1:A:35:VAL:CG1	1:A:37:LEU:CD2	0.45	2.94	1	1
1:A:39:ASN:HB3	1:A:41:HIS:NE2	0.45	2.27	19	1
1:A:6:ILE:HG13	1:A:33:CYS:CB	0.45	2.42	15	2
1:A:4:VAL:HG23	1:A:34:TYR:O	0.45	2.12	15	8
1:A:65:LEU:C	1:A:67:SER:N	0.45	2.69	2	11
1:A:29:ASN:CG	1:A:49:LEU:O	0.45	2.55	22	1
1:A:40:GLU:C	1:A:41:HIS:ND1	0.45	2.69	2	1
1:B:78:ILE:O	1:B:79:ASP:HB3	0.45	2.10	7	5
1:B:2:ILE:O	1:B:62:THR:HA	0.45	2.12	28	5
1:B:35:VAL:CG1	1:B:37:LEU:HD11	0.45	2.38	1	1
1:A:70:VAL:CG1	1:B:45:VAL:HG11	0.45	2.42	23	1
1:A:36:ASP:OD2	1:A:42:PRO:CA	0.45	2.65	19	2
1:B:4:VAL:HG23	1:B:34:TYR:O	0.45	2.12	15	8
1:B:4:VAL:HG21	1:B:83:LEU:CD1	0.45	2.41	22	2
1:A:72:GLN:O	1:A:73:PHE:HB2	0.45	2.11	7	7
1:A:34:TYR:HB3	1:A:42:PRO:CB	0.45	2.42	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:O	1:A:62:THR:HA	0.45	2.11	30	4
1:A:32:LEU:O	1:A:33:CYS:SG	0.45	2.74	30	2
1:A:65:LEU:CD1	1:B:37:LEU:CG	0.45	2.95	1	1
1:A:45:VAL:HG11	1:B:70:VAL:CG1	0.45	2.42	23	1
1:B:65:LEU:HG	1:B:68:PHE:CE2	0.45	2.46	11	1
1:B:13:PHE:HD2	1:B:49:LEU:HD12	0.45	1.72	8	1
1:A:45:VAL:CG2	1:B:74:GLY:C	0.45	2.85	16	1
1:B:6:ILE:HG13	1:B:33:CYS:SG	0.45	2.52	15	1
1:B:65:LEU:C	1:B:67:SER:N	0.45	2.70	11	10
1:B:74:GLY:O	1:B:75:SER:OG	0.45	2.32	9	3
1:A:72:GLN:CD	1:A:72:GLN:O	0.45	2.55	11	2
1:A:37:LEU:O	1:A:39:ASN:OD1	0.45	2.35	18	1
1:B:69:LYS:HB2	1:B:69:LYS:NZ	0.45	2.27	30	1
1:B:38:GLY:C	1:B:39:ASN:OD1	0.45	2.55	9	2
1:A:56:TYR:CD1	1:A:56:TYR:N	0.45	2.85	9	1
1:B:76:LEU:O	1:B:77:MET:SD	0.45	2.75	12	1
1:A:68:PHE:O	1:B:37:LEU:HD21	0.45	2.11	27	3
1:A:37:LEU:HD21	1:B:68:PHE:O	0.45	2.11	27	3
1:B:63:VAL:HG12	1:B:64:HIS:H	0.45	1.71	24	8
1:A:37:LEU:O	1:A:37:LEU:CG	0.45	2.64	27	4
1:B:72:GLN:CD	1:B:72:GLN:O	0.45	2.55	2	1
1:A:36:ASP:O	1:A:37:LEU:HG	0.45	2.12	7	1
1:B:82:ARG:CG	1:B:82:ARG:NH1	0.45	2.78	24	4
1:B:78:ILE:CG2	1:B:81:LEU:HB3	0.45	2.42	18	3
1:B:73:PHE:CD1	1:B:73:PHE:N	0.45	2.84	21	2
1:B:48:THR:O	1:B:49:LEU:C	0.45	2.55	25	3
1:B:70:VAL:HG22	1:B:76:LEU:HD12	0.45	1.88	4	1
1:A:4:VAL:HG13	1:A:61:TYR:O	0.45	2.11	23	3
1:A:49:LEU:O	1:A:50:ASP:O	0.45	2.34	11	1
1:A:3:LYS:N	1:A:37:LEU:HD11	0.45	2.27	21	1
1:B:80:ARG:HG2	1:B:80:ARG:NH1	0.45	2.27	17	1
1:A:6:ILE:HG13	1:A:33:CYS:SG	0.45	2.52	15	2
1:A:29:ASN:HB3	1:A:49:LEU:CB	0.45	2.42	2	2
1:B:37:LEU:CG	1:B:37:LEU:O	0.45	2.65	27	3
1:B:7:LYS:CB	1:B:8:PRO:HD2	0.45	2.42	11	10
1:A:78:ILE:HG13	1:B:78:ILE:CD1	0.45	2.42	24	2
1:B:2:ILE:HB	1:B:63:VAL:CG2	0.45	2.41	8	3
1:A:76:LEU:HG	1:A:77:MET:N	0.45	2.27	28	1
1:B:3:LYS:HD3	1:B:60:LEU:HD21	0.45	1.89	28	1
1:B:49:LEU:O	1:B:50:ASP:O	0.45	2.34	11	1
1:B:36:ASP:O	1:B:37:LEU:CB	0.45	2.65	29	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:PHE:HA	1:A:31:GLN:CG	0.45	2.42	8	1
1:B:13:PHE:HA	1:B:31:GLN:CG	0.45	2.42	8	1
1:A:56:TYR:CE2	1:A:83:LEU:HB2	0.45	2.46	10	3
1:A:40:GLU:O	1:A:41:HIS:HB2	0.45	2.11	23	3
1:B:34:TYR:HB3	1:B:42:PRO:CB	0.45	2.41	14	7
1:A:55:ALA:O	1:A:56:TYR:C	0.45	2.56	8	9
1:B:7:LYS:HD3	1:B:34:TYR:CE1	0.45	2.47	18	1
1:A:69:LYS:NZ	1:A:69:LYS:HB2	0.45	2.27	30	1
1:A:74:GLY:O	1:B:46:LYS:CB	0.45	2.65	24	1
1:B:33:CYS:SG	1:B:83:LEU:CD1	0.45	3.04	1	1
1:B:47:ILE:HD13	1:B:48:THR:N	0.45	2.26	1	1
1:A:38:GLY:C	1:A:39:ASN:OD1	0.45	2.55	9	2
1:A:80:ARG:CG	1:A:80:ARG:NH1	0.45	2.79	28	2
1:B:65:LEU:O	1:B:65:LEU:HD12	0.45	2.12	17	2
1:B:31:GLN:OE1	1:B:55:ALA:HA	0.45	2.12	8	1
1:B:6:ILE:HG13	1:B:33:CYS:CB	0.44	2.42	15	2
1:B:31:GLN:CA	1:B:47:ILE:HG22	0.44	2.42	22	3
1:B:1:MET:O	1:B:2:ILE:HB	0.44	2.12	26	3
1:A:69:LYS:CA	1:B:37:LEU:CD1	0.44	2.95	5	3
1:B:35:VAL:CG1	1:B:37:LEU:CD2	0.44	2.95	1	1
1:B:67:SER:O	1:B:79:ASP:HB2	0.44	2.12	9	1
1:A:65:LEU:HD13	1:B:37:LEU:HD22	0.44	1.87	28	1
1:A:86:ALA:O	1:A:87:LYS:CB	0.44	2.65	17	1
1:A:69:LYS:HA	1:B:37:LEU:CD2	0.44	2.41	15	5
1:B:4:VAL:HB	1:B:61:TYR:HB2	0.44	1.89	16	11
1:B:55:ALA:O	1:B:56:TYR:C	0.44	2.56	8	8
1:A:77:MET:O	1:A:78:ILE:C	0.44	2.54	27	7
1:A:67:SER:O	1:A:79:ASP:HB2	0.44	2.12	9	1
1:A:63:VAL:HG13	1:A:81:LEU:HG	0.44	1.88	4	1
1:A:37:LEU:HD23	1:A:37:LEU:C	0.44	2.30	6	1
1:B:13:PHE:CG	1:B:49:LEU:CD1	0.44	2.99	6	1
1:A:2:ILE:CG2	1:B:76:LEU:HD13	0.44	2.42	11	1
1:A:2:ILE:HA	1:B:65:LEU:CD1	0.44	2.39	10	3
1:A:82:ARG:NH1	1:A:82:ARG:CG	0.44	2.79	11	2
1:B:83:LEU:C	1:B:84:VAL:HG13	0.44	2.32	1	2
1:A:51:GLU:O	1:A:52:GLY:C	0.44	2.55	23	3
1:B:76:LEU:HD23	1:B:77:MET:H	0.44	1.66	9	1
1:B:39:ASN:HB3	1:B:41:HIS:NE2	0.44	2.26	19	1
1:A:81:LEU:O	1:A:81:LEU:HG	0.44	2.11	17	10
1:A:47:ILE:HD12	1:A:56:TYR:CE2	0.44	2.47	10	1
1:B:2:ILE:CD1	1:B:63:VAL:HB	0.44	2.41	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HB3	1:A:39:ASN:ND2	0.44	2.27	8	2
1:B:65:LEU:O	1:B:66:SER:C	0.44	2.56	11	3
1:B:36:ASP:O	1:B:37:LEU:HG	0.44	2.12	7	1
1:A:1:MET:O	1:A:2:ILE:HB	0.44	2.12	26	3
1:A:78:ILE:O	1:A:79:ASP:C	0.44	2.55	8	3
1:B:10:GLN:CB	1:B:32:LEU:HB2	0.44	2.42	13	1
1:A:79:ASP:O	1:A:79:ASP:OD1	0.44	2.35	26	1
1:B:56:TYR:CD1	1:B:56:TYR:N	0.44	2.85	9	2
1:A:2:ILE:H	1:B:65:LEU:HD11	0.44	1.73	9	1
1:A:3:LYS:HD3	1:A:60:LEU:HD21	0.44	1.89	28	1
1:B:72:GLN:O	1:B:72:GLN:CD	0.44	2.55	11	1
1:B:13:PHE:HA	1:B:31:GLN:HG3	0.44	1.89	8	1
1:A:36:ASP:O	1:A:39:ASN:ND2	0.44	2.51	15	1
1:A:4:VAL:CA	1:A:34:TYR:O	0.44	2.65	20	5
1:B:47:ILE:HD12	1:B:56:TYR:CE2	0.44	2.48	10	1
1:A:1:MET:O	1:A:2:ILE:C	0.44	2.54	30	1
1:B:71:GLY:O	1:B:72:GLN:CB	0.44	2.66	28	2
1:A:47:ILE:O	1:A:47:ILE:HG23	0.44	2.13	1	1
1:A:28:LEU:CD2	1:A:50:ASP:HB3	0.44	2.43	6	1
1:B:3:LYS:N	1:B:37:LEU:HD11	0.44	2.28	21	1
1:B:81:LEU:HD12	1:B:82:ARG:N	0.44	2.28	8	1
1:A:80:ARG:HG2	1:A:80:ARG:NH1	0.44	2.28	17	1
1:B:29:ASN:HB3	1:B:49:LEU:CB	0.44	2.42	15	2
1:A:6:ILE:CG1	1:A:33:CYS:SG	0.44	3.06	30	2
1:B:29:ASN:HB2	1:B:49:LEU:HB3	0.44	1.89	25	7
1:B:72:GLN:O	1:B:73:PHE:HB2	0.44	2.13	1	7
1:B:7:LYS:CB	1:B:8:PRO:CD	0.44	2.95	11	5
1:B:62:THR:CG2	1:B:86:ALA:CB	0.44	2.96	11	3
1:A:65:LEU:HB3	1:B:2:ILE:HG12	0.44	1.90	1	7
1:B:32:LEU:O	1:B:33:CYS:SG	0.44	2.74	30	2
1:A:65:LEU:CD1	1:B:37:LEU:HB3	0.44	2.41	30	2
1:B:65:LEU:CA	1:B:68:PHE:CD2	0.44	3.01	14	10
1:A:74:GLY:O	1:B:45:VAL:HG22	0.44	2.13	24	1
1:B:37:LEU:O	1:B:37:LEU:CD2	0.44	2.66	15	1
1:A:48:THR:O	1:A:49:LEU:C	0.44	2.55	11	4
1:B:6:ILE:CG1	1:B:33:CYS:SG	0.44	3.06	30	2
1:B:4:VAL:CA	1:B:34:TYR:O	0.44	2.66	20	4
1:A:65:LEU:CD1	1:B:2:ILE:HA	0.44	2.40	10	1
1:B:13:PHE:CA	1:B:30:GLU:O	0.44	2.66	12	2
1:A:7:LYS:CB	1:A:8:PRO:CD	0.44	2.96	5	8
1:A:2:ILE:HG12	1:B:65:LEU:HB3	0.44	1.88	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:VAL:CG1	1:B:33:CYS:HB2	0.44	2.43	1	1
1:A:37:LEU:HD23	1:B:65:LEU:CD1	0.44	2.42	1	1
1:A:69:LYS:CA	1:B:37:LEU:HD22	0.44	2.42	17	1
1:B:28:LEU:CD2	1:B:49:LEU:O	0.44	2.66	7	1
1:A:7:LYS:HD3	1:A:34:TYR:CE1	0.44	2.47	18	1
1:A:80:ARG:NH1	1:A:80:ARG:CG	0.44	2.78	18	1
1:B:37:LEU:O	1:B:39:ASN:OD1	0.44	2.35	18	1
1:B:39:ASN:OD1	1:B:39:ASN:N	0.44	2.51	20	3
1:A:37:LEU:HD22	1:B:65:LEU:HD13	0.44	1.88	28	1
1:B:77:MET:O	1:B:78:ILE:C	0.44	2.56	14	8
1:A:10:GLN:CB	1:A:32:LEU:HB2	0.44	2.43	13	1
1:A:76:LEU:CB	1:B:81:LEU:HD13	0.44	2.43	13	2
1:A:2:ILE:HG13	1:A:63:VAL:CB	0.44	2.43	30	1
1:B:36:ASP:C	1:B:37:LEU:CD1	0.44	2.83	3	1
1:B:51:GLU:HG2	1:B:52:GLY:N	0.44	2.28	1	1
1:B:34:TYR:HA	1:B:43:VAL:O	0.44	2.13	20	5
1:B:41:HIS:N	1:B:41:HIS:ND1	0.44	2.64	28	1
1:A:36:ASP:O	1:A:37:LEU:CB	0.44	2.66	11	3
1:A:68:PHE:CD1	1:A:78:ILE:HA	0.44	2.47	8	2
1:B:68:PHE:CD1	1:B:78:ILE:HA	0.44	2.48	8	2
1:A:4:VAL:HG21	1:A:83:LEU:CD1	0.43	2.42	22	2
1:A:56:TYR:N	1:A:56:TYR:CD1	0.43	2.86	5	2
1:B:56:TYR:N	1:B:56:TYR:CD1	0.43	2.86	5	1
1:B:49:LEU:HD11	1:B:54:PRO:C	0.43	2.34	1	1
1:A:70:VAL:HG22	1:A:76:LEU:HD12	0.43	1.88	4	1
1:A:74:GLY:O	1:B:46:LYS:HB3	0.43	2.13	16	1
1:B:80:ARG:CG	1:B:80:ARG:NH1	0.43	2.78	17	1
1:A:13:PHE:HA	1:A:30:GLU:O	0.43	2.13	15	13
1:B:13:PHE:HA	1:B:30:GLU:O	0.43	2.13	15	12
1:B:56:TYR:CE2	1:B:83:LEU:HB2	0.43	2.49	2	3
1:A:4:VAL:HB	1:A:61:TYR:HB2	0.43	1.90	11	9
1:B:15:THR:HG23	1:B:29:ASN:OD1	0.43	2.13	2	1
1:A:65:LEU:HA	1:A:68:PHE:CZ	0.43	2.48	17	4
1:A:75:SER:HA	1:B:45:VAL:CG1	0.43	2.43	13	1
1:A:62:THR:O	1:A:63:VAL:O	0.43	2.36	11	3
1:B:79:ASP:O	1:B:79:ASP:OD1	0.43	2.35	26	1
1:B:3:LYS:C	1:B:4:VAL:CG2	0.43	2.86	30	1
1:A:65:LEU:CA	1:A:68:PHE:CD2	0.43	3.01	14	11
1:A:36:ASP:OD2	1:A:41:HIS:C	0.43	2.57	14	1
1:B:12:GLN:CG	1:B:12:GLN:O	0.43	2.66	27	1
1:B:6:ILE:CG2	1:B:57:ALA:O	0.43	2.66	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:CD1	1:B:37:LEU:HD23	0.43	2.42	1	1
1:B:36:ASP:OD2	1:B:42:PRO:CA	0.43	2.66	19	2
1:A:13:PHE:CG	1:A:49:LEU:CD1	0.43	2.99	6	1
1:A:37:LEU:CD2	1:A:37:LEU:O	0.43	2.65	15	1
1:B:36:ASP:O	1:B:39:ASN:ND2	0.43	2.51	15	1
1:A:33:CYS:SG	1:A:47:ILE:HG12	0.43	2.54	10	3
1:A:15:THR:HG23	1:A:29:ASN:OD1	0.43	2.13	2	1
1:A:28:LEU:CD2	1:A:49:LEU:O	0.43	2.66	7	1
1:B:65:LEU:HA	1:B:68:PHE:CZ	0.43	2.48	25	3
1:B:2:ILE:HG13	1:B:63:VAL:CB	0.43	2.43	30	1
1:A:46:LYS:CB	1:B:74:GLY:O	0.43	2.66	24	1
1:B:47:ILE:HD11	1:B:56:TYR:OH	0.43	2.13	1	1
1:B:47:ILE:CG1	1:B:83:LEU:HB2	0.43	2.43	1	1
1:A:29:ASN:HB3	1:A:49:LEU:HB2	0.43	1.90	15	2
1:A:13:PHE:CA	1:A:30:GLU:O	0.43	2.66	12	2
1:B:37:LEU:HB3	1:B:39:ASN:ND2	0.43	2.27	8	2
1:A:34:TYR:HA	1:A:43:VAL:O	0.43	2.13	20	6
1:B:31:GLN:NE2	1:B:56:TYR:HB2	0.43	2.28	26	2
1:A:6:ILE:CG2	1:A:57:ALA:O	0.43	2.66	16	2
1:A:65:LEU:CD1	1:B:37:LEU:CB	0.43	2.96	20	2
1:A:65:LEU:HD13	1:B:37:LEU:CB	0.43	2.44	20	1
1:A:41:HIS:N	1:A:41:HIS:ND1	0.43	2.65	28	1
1:A:68:PHE:O	1:A:69:LYS:HG2	0.43	2.13	8	1
1:A:45:VAL:HG22	1:B:74:GLY:C	0.43	2.33	16	2
1:B:47:ILE:HD11	1:B:83:LEU:HD12	0.43	1.89	15	4
1:B:75:SER:O	1:B:76:LEU:O	0.43	2.37	18	1
1:A:31:GLN:NE2	1:A:56:TYR:HB2	0.43	2.29	26	2
1:A:45:VAL:HG22	1:B:75:SER:N	0.43	2.29	26	1
1:B:71:GLY:O	1:B:72:GLN:C	0.43	2.55	26	1
1:A:36:ASP:O	1:A:37:LEU:CD1	0.43	2.56	3	1
1:A:45:VAL:HG22	1:B:74:GLY:O	0.43	2.14	24	1
1:A:46:LYS:N	1:B:74:GLY:O	0.43	2.51	24	1
1:A:31:GLN:OE1	1:A:55:ALA:HA	0.43	2.13	8	1
1:B:38:GLY:O	1:B:39:ASN:CG	0.43	2.57	16	1
1:A:45:VAL:HG23	1:B:75:SER:N	0.43	2.28	29	1
1:A:2:ILE:CG2	1:A:63:VAL:HG23	0.43	2.44	13	1
1:A:75:SER:O	1:A:76:LEU:C	0.43	2.57	19	4
1:A:47:ILE:CG1	1:A:83:LEU:HB2	0.43	2.43	1	1
1:A:4:VAL:CG1	1:A:33:CYS:HB2	0.43	2.43	1	1
1:B:73:PHE:O	1:B:75:SER:OG	0.43	2.34	21	1
1:B:7:LYS:NZ	1:B:7:LYS:HA	0.43	2.29	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:C	1:A:77:MET:HG3	0.43	2.34	20	3
1:A:7:LYS:HB3	1:A:8:PRO:HD2	0.43	1.91	9	7
1:B:7:LYS:HA	1:B:7:LYS:NZ	0.43	2.29	2	4
1:B:86:ALA:O	1:B:87:LYS:C	0.43	2.57	18	1
1:B:1:MET:SD	1:B:62:THR:HB	0.43	2.54	29	8
1:A:36:ASP:C	1:A:37:LEU:CD1	0.43	2.83	3	1
1:B:36:ASP:O	1:B:37:LEU:CD1	0.43	2.56	3	1
1:B:4:VAL:HG21	1:B:33:CYS:HB2	0.43	1.90	29	2
1:A:47:ILE:HD11	1:A:56:TYR:OH	0.43	2.13	1	1
1:A:37:LEU:CB	1:B:65:LEU:CD1	0.43	2.97	20	2
1:A:37:LEU:CB	1:B:65:LEU:HD13	0.43	2.44	20	1
1:B:81:LEU:HD21	1:B:83:LEU:HG	0.43	1.90	4	1
1:A:2:ILE:CB	1:B:65:LEU:HD21	0.43	2.44	11	1
1:A:13:PHE:HA	1:A:31:GLN:HG3	0.43	1.89	8	1
1:A:75:SER:CA	1:B:45:VAL:CG2	0.43	2.96	16	1
1:B:13:PHE:CD1	1:B:13:PHE:C	0.43	2.90	10	8
1:A:47:ILE:CG1	1:A:56:TYR:CE2	0.43	3.02	2	4
1:B:31:GLN:HB2	1:B:47:ILE:HG22	0.43	1.90	2	1
1:A:4:VAL:HG22	1:A:35:VAL:CB	0.43	2.43	7	2
1:A:81:LEU:HD13	1:B:76:LEU:CB	0.43	2.44	13	1
1:A:62:THR:CG2	1:A:86:ALA:CB	0.43	2.96	11	3
1:A:49:LEU:HD13	1:A:50:ASP:N	0.43	2.29	30	1
1:B:6:ILE:O	1:B:7:LYS:C	0.43	2.56	8	4
1:A:49:LEU:HD11	1:A:54:PRO:C	0.43	2.34	1	1
1:A:4:VAL:CG1	1:A:83:LEU:HD21	0.43	2.44	20	1
1:A:74:GLY:C	1:A:75:SER:OG	0.43	2.57	25	2
1:B:29:ASN:HB2	1:B:49:LEU:O	0.43	2.13	23	2
1:A:78:ILE:HD11	1:B:78:ILE:HG13	0.43	1.90	28	1
1:B:36:ASP:OD1	1:B:37:LEU:N	0.43	2.52	12	1
1:A:6:ILE:O	1:A:7:LYS:C	0.43	2.56	8	1
1:A:81:LEU:HD12	1:A:82:ARG:N	0.43	2.28	8	1
1:A:5:GLU:O	1:A:34:TYR:HB2	0.43	2.14	7	14
1:A:29:ASN:HB2	1:A:49:LEU:O	0.43	2.14	23	3
1:B:2:ILE:CG2	1:B:63:VAL:HG23	0.43	2.44	13	1
1:B:82:ARG:HG2	1:B:82:ARG:NH1	0.43	2.29	24	2
1:A:37:LEU:CG	1:B:65:LEU:CD1	0.43	2.96	1	1
1:B:49:LEU:O	1:B:50:ASP:C	0.43	2.56	9	2
1:A:37:LEU:CD1	1:A:38:GLY:N	0.43	2.64	28	1
1:B:28:LEU:CD2	1:B:50:ASP:HB3	0.43	2.43	6	1
1:B:50:ASP:O	1:B:51:GLU:CB	0.43	2.65	6	1
1:B:3:LYS:HB3	1:B:36:ASP:OD2	0.43	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:OE1	1:A:32:LEU:HB2	0.43	2.14	15	1
1:B:1:MET:HG3	1:B:62:THR:CG2	0.43	2.43	17	3
1:A:7:LYS:NZ	1:A:7:LYS:HA	0.43	2.29	19	4
1:B:5:GLU:O	1:B:34:TYR:HB2	0.43	2.14	6	14
1:A:6:ILE:HG12	1:A:56:TYR:CB	0.43	2.44	26	1
1:A:3:LYS:C	1:A:4:VAL:CG2	0.43	2.86	30	1
1:B:47:ILE:HG23	1:B:47:ILE:O	0.43	2.13	1	2
1:A:50:ASP:O	1:A:51:GLU:CB	0.43	2.65	6	1
1:A:76:LEU:HD13	1:B:2:ILE:CG2	0.43	2.43	11	1
1:B:76:LEU:CD2	1:B:76:LEU:C	0.42	2.86	17	2
1:A:13:PHE:C	1:A:13:PHE:CD1	0.42	2.91	10	7
1:A:7:LYS:CB	1:A:10:GLN:HG2	0.42	2.44	2	1
1:A:7:LYS:HA	1:A:7:LYS:NZ	0.42	2.29	2	4
1:B:7:LYS:CB	1:B:10:GLN:HG2	0.42	2.44	2	1
1:B:56:TYR:O	1:B:57:ALA:C	0.42	2.57	7	2
1:A:43:VAL:CG1	1:B:70:VAL:HG21	0.42	2.44	14	1
1:B:4:VAL:CG1	1:B:83:LEU:HD21	0.42	2.44	20	1
1:A:65:LEU:HD11	1:B:2:ILE:H	0.42	1.73	9	1
1:B:63:VAL:HG13	1:B:81:LEU:HG	0.42	1.88	4	1
1:A:65:LEU:HD13	1:B:37:LEU:HD13	0.42	1.82	28	1
1:A:81:LEU:HD11	1:A:83:LEU:HB2	0.42	1.91	8	1
1:A:37:LEU:HD21	1:A:43:VAL:HG11	0.42	1.91	7	1
1:B:4:VAL:HG22	1:B:35:VAL:CB	0.42	2.43	7	2
1:A:7:LYS:HD2	1:A:34:TYR:CD1	0.42	2.46	18	1
1:A:86:ALA:O	1:A:87:LYS:C	0.42	2.57	18	1
1:A:1:MET:SD	1:A:62:THR:HB	0.42	2.54	14	8
1:A:39:ASN:ND2	1:A:43:VAL:CG2	0.42	2.82	26	1
1:B:56:TYR:CD2	1:B:83:LEU:HD22	0.42	2.49	26	1
1:B:49:LEU:HD13	1:B:50:ASP:N	0.42	2.29	30	1
1:B:76:LEU:HG	1:B:77:MET:N	0.42	2.27	28	1
1:B:68:PHE:O	1:B:69:LYS:HG3	0.42	2.14	17	1
1:B:86:ALA:O	1:B:87:LYS:CB	0.42	2.65	17	1
1:B:47:ILE:CG1	1:B:56:TYR:CE2	0.42	3.02	2	4
1:A:31:GLN:HB2	1:A:47:ILE:HG22	0.42	1.90	2	1
1:B:41:HIS:HB2	1:B:42:PRO:HD2	0.42	1.91	27	1
1:A:2:ILE:CG2	1:B:65:LEU:CD2	0.42	2.86	9	1
1:B:75:SER:O	1:B:76:LEU:C	0.42	2.57	19	3
1:A:78:ILE:HG13	1:B:78:ILE:HD11	0.42	1.90	28	1
1:A:65:LEU:HD22	1:B:37:LEU:HB3	0.42	1.91	11	1
1:B:1:MET:O	1:B:37:LEU:CD2	0.42	2.67	21	1
1:B:3:LYS:HA	1:B:61:TYR:O	0.42	2.14	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HG3	1:A:62:THR:CG2	0.42	2.44	15	4
1:B:10:GLN:OE1	1:B:32:LEU:HB2	0.42	2.15	15	2
1:A:2:ILE:CB	1:B:65:LEU:HD13	0.42	2.44	10	2
1:A:6:ILE:HD11	1:A:56:TYR:HD2	0.42	1.74	26	1
1:A:37:LEU:HD13	1:A:37:LEU:C	0.42	2.35	30	1
1:A:36:ASP:HB2	1:A:39:ASN:O	0.42	2.14	3	1
1:B:4:VAL:O	1:B:5:GLU:HG3	0.42	2.14	27	3
1:A:63:VAL:HG13	1:A:81:LEU:HD11	0.42	1.90	4	1
1:B:63:VAL:HG13	1:B:81:LEU:HD11	0.42	1.90	4	1
1:A:38:GLY:O	1:A:39:ASN:CG	0.42	2.57	16	1
1:B:47:ILE:HD13	1:B:48:THR:H	0.42	1.74	19	1
1:A:65:LEU:HD13	1:B:2:ILE:CB	0.42	2.44	10	2
1:A:29:ASN:ND2	1:A:49:LEU:HB3	0.42	2.30	13	2
1:B:7:LYS:HB3	1:B:8:PRO:HD2	0.42	1.91	9	7
1:A:69:LYS:HG2	1:A:77:MET:O	0.42	2.14	7	1
1:A:75:SER:O	1:A:76:LEU:O	0.42	2.37	18	1
1:B:28:LEU:CD2	1:B:28:LEU:C	0.42	2.78	18	1
1:B:68:PHE:N	1:B:68:PHE:HD1	0.42	2.12	18	2
1:A:2:ILE:HB	1:A:63:VAL:CG2	0.42	2.41	8	3
1:B:6:ILE:HG12	1:B:56:TYR:CB	0.42	2.44	26	1
1:A:28:LEU:O	1:A:29:ASN:C	0.42	2.58	27	2
1:A:12:GLN:CG	1:A:12:GLN:O	0.42	2.67	27	1
1:A:81:LEU:HD21	1:A:83:LEU:HG	0.42	1.89	4	1
1:A:47:ILE:HG23	1:A:47:ILE:O	0.42	2.13	23	2
1:A:4:VAL:HG21	1:A:33:CYS:HB2	0.42	1.90	29	1
1:B:76:LEU:C	1:B:77:MET:HG3	0.42	2.34	20	3
1:B:6:ILE:O	1:B:58:PRO:HA	0.42	2.14	7	1
1:B:62:THR:O	1:B:63:VAL:O	0.42	2.37	5	3
1:A:71:GLY:O	1:A:72:GLN:C	0.42	2.55	26	1
1:B:36:ASP:HB2	1:B:39:ASN:O	0.42	2.14	3	1
1:A:82:ARG:HG2	1:A:82:ARG:NH1	0.42	2.29	24	1
1:A:41:HIS:HB2	1:A:42:PRO:HD2	0.42	1.91	27	1
1:B:4:VAL:CG1	1:B:61:TYR:O	0.42	2.68	23	1
1:A:65:LEU:HD21	1:B:2:ILE:CB	0.42	2.45	11	1
1:A:13:PHE:CA	1:A:31:GLN:HG3	0.42	2.44	8	1
1:A:47:ILE:HD13	1:A:48:THR:H	0.42	1.75	19	1
1:B:7:LYS:HD2	1:B:7:LYS:N	0.42	2.29	19	1
1:B:33:CYS:SG	1:B:47:ILE:HG12	0.42	2.54	10	3
1:A:13:PHE:H	1:A:55:ALA:HB2	0.42	1.75	17	4
1:A:29:ASN:O	1:A:49:LEU:O	0.42	2.38	18	1
1:A:13:PHE:CE1	1:A:29:ASN:CG	0.42	2.93	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TYR:CD2	1:A:83:LEU:HD22	0.42	2.50	26	1
1:A:49:LEU:O	1:A:50:ASP:C	0.42	2.57	9	2
1:A:36:ASP:OD1	1:A:37:LEU:N	0.42	2.52	12	1
1:B:29:ASN:ND2	1:B:49:LEU:HB3	0.42	2.30	13	1
1:A:37:LEU:HD11	1:B:69:LYS:C	0.42	2.35	13	1
1:B:36:ASP:OD2	1:B:41:HIS:C	0.42	2.57	14	1
1:A:63:VAL:HA	1:A:83:LEU:HD12	0.42	1.92	27	1
1:A:51:GLU:HG2	1:A:52:GLY:N	0.42	2.28	1	1
1:A:31:GLN:N	1:A:47:ILE:O	0.42	2.46	23	1
1:A:3:LYS:HA	1:A:61:TYR:O	0.42	2.14	21	1
1:A:41:HIS:O	1:A:41:HIS:CD2	0.42	2.73	8	1
1:B:68:PHE:O	1:B:69:LYS:HG2	0.42	2.15	8	1
1:B:81:LEU:HD11	1:B:83:LEU:HB2	0.42	1.91	8	1
1:B:72:GLN:O	1:B:72:GLN:HG2	0.42	2.14	29	1
1:A:76:LEU:HD11	1:B:37:LEU:HD12	0.42	1.92	10	1
1:A:4:VAL:HG23	1:A:34:TYR:C	0.42	2.35	2	1
1:B:65:LEU:HG	1:B:65:LEU:O	0.42	2.13	2	2
1:A:50:ASP:HB2	1:A:53:GLN:NE2	0.42	2.30	7	1
1:A:69:LYS:HG3	1:A:77:MET:O	0.42	2.15	7	1
1:B:69:LYS:HG2	1:B:77:MET:O	0.42	2.14	7	1
1:A:62:THR:O	1:A:63:VAL:C	0.42	2.58	9	4
1:B:62:THR:O	1:B:63:VAL:C	0.42	2.57	9	5
1:A:37:LEU:HG	1:B:65:LEU:CD2	0.42	2.45	26	1
1:A:37:LEU:HD12	1:A:37:LEU:O	0.42	2.14	26	1
1:A:36:ASP:HB3	1:A:41:HIS:O	0.42	2.15	14	1
1:A:37:LEU:HD12	1:B:76:LEU:HD11	0.42	1.90	12	1
1:B:41:HIS:O	1:B:41:HIS:CD2	0.42	2.73	8	1
1:B:6:ILE:HD11	1:B:83:LEU:HD23	0.42	1.92	29	1
1:B:29:ASN:HB3	1:B:49:LEU:HB2	0.42	1.90	15	2
1:A:6:ILE:HB	1:A:57:ALA:O	0.42	2.15	10	1
1:A:37:LEU:HG	1:A:37:LEU:O	0.42	2.15	22	1
1:A:6:ILE:CG2	1:A:6:ILE:O	0.42	2.68	2	1
1:A:49:LEU:HA	1:A:49:LEU:HD22	0.42	1.69	17	3
1:A:28:LEU:HD13	1:A:28:LEU:O	0.42	2.14	18	1
1:A:10:GLN:HG3	1:A:10:GLN:O	0.41	2.14	10	1
1:B:4:VAL:HG23	1:B:34:TYR:C	0.41	2.36	2	1
1:A:56:TYR:O	1:A:57:ALA:C	0.41	2.57	7	2
1:B:50:ASP:HB2	1:B:53:GLN:NE2	0.41	2.30	7	1
1:B:1:MET:HG3	1:B:1:MET:O	0.41	2.15	5	1
1:B:13:PHE:CE1	1:B:29:ASN:CG	0.41	2.93	26	1
1:A:2:ILE:CG1	1:B:65:LEU:HD22	0.41	2.45	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ASP:O	1:A:51:GLU:C	0.41	2.57	1	1
1:A:49:LEU:HD21	1:A:54:PRO:C	0.41	2.36	23	1
1:B:73:PHE:N	1:B:73:PHE:CD1	0.41	2.84	8	1
1:A:68:PHE:O	1:A:69:LYS:HG3	0.41	2.15	17	1
1:B:49:LEU:HA	1:B:49:LEU:HD22	0.41	1.71	12	2
1:A:6:ILE:HG13	1:A:61:TYR:CZ	0.41	2.50	10	1
1:A:65:LEU:HG	1:A:65:LEU:O	0.41	2.13	2	1
1:A:33:CYS:SG	1:A:47:ILE:HG13	0.41	2.55	20	3
1:B:28:LEU:O	1:B:28:LEU:HD13	0.41	2.14	18	1
1:A:47:ILE:HG13	1:A:56:TYR:CD2	0.41	2.50	13	1
1:A:60:LEU:O	1:A:86:ALA:N	0.41	2.45	13	1
1:A:1:MET:O	1:A:1:MET:HG3	0.41	2.15	5	1
1:A:2:ILE:CG1	1:B:65:LEU:HB2	0.41	2.46	5	1
1:B:36:ASP:O	1:B:37:LEU:HB3	0.41	2.15	6	2
1:A:73:PHE:O	1:A:74:GLY:C	0.41	2.59	26	3
1:B:39:ASN:ND2	1:B:43:VAL:CG2	0.41	2.82	26	1
1:A:69:LYS:O	1:A:77:MET:HG3	0.41	2.15	27	1
1:B:4:VAL:CG1	1:B:61:TYR:HB2	0.41	2.45	1	1
1:B:68:PHE:HD1	1:B:68:PHE:N	0.41	2.13	9	1
1:B:74:GLY:C	1:B:75:SER:OG	0.41	2.57	25	2
1:A:2:ILE:CG2	1:A:37:LEU:HD22	0.41	2.46	28	1
1:A:38:GLY:C	1:A:39:ASN:CG	0.41	2.79	16	2
1:A:3:LYS:HB3	1:A:36:ASP:OD2	0.41	2.14	12	1
1:B:47:ILE:O	1:B:47:ILE:HG23	0.41	2.14	16	1
1:B:15:THR:CG2	1:B:28:LEU:O	0.41	2.59	29	1
1:A:6:ILE:HB	1:A:61:TYR:CE1	0.41	2.51	13	2
1:B:63:VAL:HG22	1:B:83:LEU:HD12	0.41	1.91	13	1
1:A:10:GLN:OE1	1:A:34:TYR:CE2	0.41	2.74	26	1
1:A:13:PHE:CG	1:A:29:ASN:HB3	0.41	2.50	30	1
1:A:71:GLY:O	1:A:72:GLN:CB	0.41	2.66	28	1
1:A:65:LEU:HD21	1:B:2:ILE:CG2	0.41	2.44	11	1
1:B:33:CYS:SG	1:B:47:ILE:HG13	0.41	2.55	20	3
1:A:4:VAL:HB	1:A:35:VAL:HA	0.41	1.92	5	1
1:B:10:GLN:OE1	1:B:34:TYR:CE2	0.41	2.74	26	1
1:A:32:LEU:HA	1:A:45:VAL:O	0.41	2.16	9	2
1:B:69:LYS:O	1:B:77:MET:HG3	0.41	2.15	27	1
1:B:7:LYS:CE	1:B:7:LYS:HA	0.41	2.46	27	1
1:A:4:VAL:CG1	1:A:61:TYR:HB2	0.41	2.45	1	1
1:B:76:LEU:O	1:B:77:MET:HG3	0.41	2.16	1	1
1:A:1:MET:O	1:A:37:LEU:CD2	0.41	2.67	21	1
1:B:38:GLY:C	1:B:39:ASN:CG	0.41	2.79	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:OE1	1:A:82:ARG:NH2	0.41	2.54	8	1
1:A:6:ILE:HD11	1:A:83:LEU:HD23	0.41	1.92	29	1
1:A:76:LEU:C	1:A:76:LEU:CD2	0.41	2.85	15	1
1:A:4:VAL:HB	1:A:35:VAL:CG2	0.41	2.42	12	2
1:B:37:LEU:HG	1:B:37:LEU:O	0.41	2.15	22	1
1:A:49:LEU:HG	1:A:55:ALA:HA	0.41	1.92	18	1
1:B:29:ASN:O	1:B:49:LEU:O	0.41	2.38	18	1
1:A:4:VAL:CG1	1:A:61:TYR:HB3	0.41	2.44	13	1
1:A:68:PHE:N	1:A:68:PHE:HD1	0.41	2.13	13	1
1:A:86:ALA:O	1:A:87:LYS:O	0.41	2.38	26	1
1:A:67:SER:OG	1:A:80:ARG:C	0.41	2.59	4	1
1:A:76:LEU:O	1:A:77:MET:HG3	0.41	2.16	11	1
1:A:3:LYS:C	1:A:4:VAL:CG1	0.41	2.89	21	1
1:A:73:PHE:CD1	1:A:73:PHE:O	0.41	2.74	29	1
1:A:7:LYS:N	1:A:7:LYS:HD2	0.41	2.29	19	1
1:B:6:ILE:HG13	1:B:61:TYR:CZ	0.41	2.49	10	1
1:A:6:ILE:O	1:A:58:PRO:HA	0.41	2.15	7	1
1:A:36:ASP:O	1:A:37:LEU:HB3	0.41	2.15	6	2
1:B:32:LEU:HA	1:B:45:VAL:O	0.41	2.16	26	2
1:B:6:ILE:HD11	1:B:56:TYR:HD2	0.41	1.76	26	1
1:B:13:PHE:CG	1:B:29:ASN:HB3	0.41	2.50	30	1
1:A:4:VAL:O	1:A:5:GLU:HG3	0.41	2.14	27	2
1:A:7:LYS:CE	1:A:7:LYS:HA	0.41	2.46	27	1
1:B:2:ILE:HG22	1:B:35:VAL:CG1	0.41	2.46	23	1
1:B:2:ILE:CG2	1:B:37:LEU:HD22	0.41	2.46	28	1
1:A:36:ASP:C	1:A:38:GLY:N	0.41	2.74	8	2
1:A:2:ILE:CG2	1:B:65:LEU:HD21	0.41	2.44	11	1
1:A:36:ASP:OD2	1:A:42:PRO:N	0.41	2.53	19	1
1:A:2:ILE:HG21	1:B:76:LEU:HD13	0.41	1.92	11	2
1:B:49:LEU:HG	1:B:55:ALA:HA	0.41	1.92	18	1
1:B:65:LEU:HA	1:B:68:PHE:CE1	0.41	2.50	18	1
1:A:63:VAL:HG22	1:A:83:LEU:HD12	0.41	1.92	13	1
1:B:4:VAL:HB	1:B:35:VAL:HA	0.41	1.92	5	1
1:A:13:PHE:HB3	1:A:49:LEU:HG	0.41	1.93	1	2
1:B:28:LEU:O	1:B:29:ASN:C	0.41	2.58	27	1
1:B:71:GLY:CA	1:B:77:MET:SD	0.41	3.09	27	1
1:B:4:VAL:HG11	1:B:33:CYS:HB2	0.41	1.93	1	1
1:B:50:ASP:O	1:B:51:GLU:C	0.41	2.57	1	1
1:A:37:LEU:HB3	1:B:65:LEU:HD22	0.41	1.91	11	1
1:B:6:ILE:HB	1:B:57:ALA:O	0.41	2.16	10	1
1:B:69:LYS:HG3	1:B:77:MET:O	0.41	2.14	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:PHE:H	1:B:55:ALA:HB2	0.41	1.76	11	4
1:A:49:LEU:HD22	1:A:49:LEU:HA	0.41	1.75	18	2
1:B:13:PHE:N	1:B:55:ALA:CB	0.41	2.84	26	1
1:B:63:VAL:CG1	1:B:81:LEU:CG	0.41	2.99	4	1
1:B:36:ASP:HA	1:B:39:ASN:OD1	0.41	2.16	28	1
1:A:70:VAL:HG13	1:B:45:VAL:HG21	0.41	1.93	6	1
1:A:48:THR:O	1:A:48:THR:CG2	0.41	2.61	25	1
1:A:39:ASN:OD1	1:A:39:ASN:N	0.41	2.54	29	1
1:B:73:PHE:CD1	1:B:73:PHE:O	0.41	2.74	29	1
1:B:36:ASP:C	1:B:38:GLY:N	0.41	2.74	25	4
1:B:72:GLN:HG2	1:B:72:GLN:O	0.41	2.16	18	1
1:A:35:VAL:HG11	1:B:76:LEU:HD11	0.41	1.91	13	1
1:B:68:PHE:HB3	1:B:76:LEU:CD2	0.41	2.44	13	1
1:B:37:LEU:CD2	1:B:37:LEU:O	0.41	2.64	13	1
1:A:74:GLY:O	1:B:46:LYS:O	0.41	2.39	5	1
1:A:36:ASP:O	1:A:39:ASN:O	0.41	2.38	26	1
1:A:35:VAL:HG11	1:B:76:LEU:HD13	0.41	1.93	30	1
1:B:37:LEU:HD13	1:B:37:LEU:C	0.41	2.35	30	1
1:B:78:ILE:HG23	1:B:81:LEU:N	0.41	2.31	3	1
1:A:65:LEU:O	1:A:66:SER:C	0.41	2.56	11	2
1:A:32:LEU:HD23	1:A:45:VAL:O	0.41	2.16	4	1
1:B:67:SER:OG	1:B:80:ARG:C	0.41	2.59	4	1
1:B:53:GLN:OE1	1:B:82:ARG:NH2	0.41	2.54	8	1
1:B:13:PHE:CA	1:B:31:GLN:HG3	0.41	2.45	8	1
1:A:72:GLN:O	1:A:72:GLN:HG2	0.41	2.14	29	1
1:B:36:ASP:OD2	1:B:42:PRO:N	0.41	2.54	19	1
1:A:60:LEU:C	1:A:61:TYR:CD1	0.41	2.95	10	1
1:B:10:GLN:O	1:B:10:GLN:HG3	0.41	2.14	10	1
1:B:37:LEU:HD21	1:B:43:VAL:HG11	0.41	1.91	7	1
1:A:28:LEU:CD1	1:A:28:LEU:H	0.41	2.29	18	1
1:B:7:LYS:N	1:B:7:LYS:HD2	0.41	2.30	25	1
1:B:65:LEU:O	1:B:65:LEU:HG	0.41	2.16	21	1
1:B:81:LEU:CD1	1:B:83:LEU:N	0.41	2.84	8	1
1:A:38:GLY:O	1:A:39:ASN:HB3	0.40	2.16	26	1
1:B:86:ALA:O	1:B:87:LYS:O	0.40	2.39	26	1
1:A:71:GLY:CA	1:A:77:MET:SD	0.40	3.09	27	1
1:B:1:MET:SD	1:B:62:THR:CB	0.40	3.09	23	1
1:A:12:GLN:O	1:A:31:GLN:HG2	0.40	2.16	22	1
1:B:36:ASP:O	1:B:39:ASN:O	0.40	2.38	26	1
1:B:74:GLY:O	1:B:75:SER:CB	0.40	2.68	30	1
1:A:76:LEU:HD23	1:A:77:MET:H	0.40	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:SER:O	1:B:77:MET:HG3	0.40	2.16	4	1
1:A:1:MET:SD	1:A:62:THR:CB	0.40	3.09	23	1
1:A:4:VAL:CG1	1:A:61:TYR:O	0.40	2.69	23	1
1:A:1:MET:HG3	1:A:62:THR:HB	0.40	1.92	22	1
1:B:62:THR:OG1	1:B:84:VAL:HG23	0.40	2.16	26	1
1:B:13:PHE:HB3	1:B:49:LEU:HG	0.40	1.93	14	2
1:A:37:LEU:CD2	1:B:65:LEU:CD1	0.40	2.99	1	1
1:B:71:GLY:O	1:B:75:SER:O	0.40	2.39	6	1
1:A:72:GLN:HG2	1:A:72:GLN:O	0.40	2.16	16	1
1:A:4:VAL:HG22	1:A:35:VAL:CG1	0.40	2.46	7	2
1:B:47:ILE:HG13	1:B:56:TYR:CD2	0.40	2.50	13	1
1:A:67:SER:HB2	1:A:82:ARG:N	0.40	2.31	5	1
1:B:7:LYS:HE2	1:B:34:TYR:CD1	0.40	2.52	5	1
1:A:35:VAL:CG1	1:A:37:LEU:CD1	0.40	2.99	1	1
1:A:2:ILE:HG22	1:A:35:VAL:CG1	0.40	2.46	23	1
1:A:74:GLY:C	1:B:45:VAL:HG22	0.40	2.37	16	1
1:B:71:GLY:O	1:B:75:SER:N	0.40	2.41	7	1
1:B:6:ILE:HB	1:B:61:TYR:CE1	0.40	2.51	13	2
1:A:35:VAL:O	1:A:42:PRO:HA	0.40	2.17	26	1
1:A:63:VAL:CG1	1:A:81:LEU:CG	0.40	2.99	4	1
1:A:65:LEU:HD22	1:B:2:ILE:CG1	0.40	2.47	4	1
1:A:14:THR:O	1:A:29:ASN:HA	0.40	2.17	12	1
1:A:32:LEU:HD23	1:A:44:LEU:CG	0.40	2.47	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/87 (84%)	55±3 (76±3%)	13±2 (17±3%)	5±2 (7±2%)	3	17
1	B	73/87 (84%)	55±3 (76±4%)	13±2 (17±3%)	5±2 (7±2%)	3	17
All	All	4380/5220 (84%)	3319 (76%)	752 (17%)	309 (7%)	3	17

All 48 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	80	ARG	24
1	B	80	ARG	24
1	A	2	ILE	21
1	B	2	ILE	21
1	A	7	LYS	16
1	B	7	LYS	16
1	B	56	TYR	14
1	A	63	VAL	13
1	A	56	TYR	13
1	B	63	VAL	13
1	B	55	ALA	11
1	A	37	LEU	9
1	B	37	LEU	9
1	A	55	ALA	9
1	B	57	ALA	6
1	A	57	ALA	6
1	B	76	LEU	5
1	A	51	GLU	5
1	B	51	GLU	5
1	A	76	LEU	5
1	B	38	GLY	5
1	B	40	GLU	5
1	A	40	GLU	5
1	A	38	GLY	5
1	B	4	VAL	4
1	A	4	VAL	4
1	A	41	HIS	4
1	B	41	HIS	4
1	A	39	ASN	3
1	B	39	ASN	3
1	A	81	LEU	2
1	B	81	LEU	2
1	A	52	GLY	2
1	B	52	GLY	2
1	A	11	ALA	1
1	B	11	ALA	1
1	B	73	PHE	1
1	B	71	GLY	1
1	A	72	GLN	1
1	A	71	GLY	1
1	A	78	ILE	1
1	B	72	GLN	1
1	A	73	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	50	ASP	1
1	B	50	ASP	1
1	B	78	ILE	1
1	B	29	ASN	1
1	A	29	ASN	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	66/76 (87%)	43±3 (65±4%)	23±3 (35±4%)	1	9
1	B	66/76 (87%)	43±3 (64±4%)	23±3 (36±4%)	1	9
All	All	3960/4560 (87%)	2554 (64%)	1406 (36%)	1	9

All 99 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	THR	29
1	B	15	THR	29
1	B	28	LEU	28
1	A	28	LEU	28
1	B	47	ILE	27
1	B	6	ILE	27
1	A	31	GLN	27
1	B	31	GLN	27
1	A	47	ILE	27
1	A	6	ILE	27
1	B	65	LEU	26
1	A	65	LEU	26
1	A	81	LEU	24
1	B	82	ARG	24
1	B	83	LEU	24
1	A	83	LEU	24
1	A	72	GLN	24
1	B	81	LEU	24
1	B	72	GLN	24

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ARG	24
1	A	37	LEU	23
1	B	37	LEU	23
1	B	70	VAL	21
1	A	70	VAL	21
1	A	33	CYS	20
1	B	33	CYS	20
1	A	87	LYS	20
1	B	87	LYS	20
1	B	49	LEU	19
1	B	4	VAL	19
1	A	4	VAL	19
1	A	49	LEU	19
1	A	46	LYS	18
1	A	50	ASP	18
1	B	50	ASP	18
1	A	29	ASN	18
1	B	46	LYS	18
1	B	29	ASN	18
1	B	1	MET	18
1	B	53	GLN	17
1	A	53	GLN	17
1	B	7	LYS	17
1	A	1	MET	17
1	A	7	LYS	17
1	A	80	ARG	16
1	B	60	LEU	16
1	B	80	ARG	16
1	A	60	LEU	16
1	B	76	LEU	14
1	A	76	LEU	14
1	B	73	PHE	14
1	A	69	LYS	14
1	B	69	LYS	14
1	A	73	PHE	14
1	B	9	SER	13
1	A	48	THR	13
1	A	9	SER	13
1	B	48	THR	13
1	B	3	LYS	12
1	A	75	SER	12
1	B	75	SER	12

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Mol	Chain	Res	Type	Models (Total)
1	A	3	LYS	12
1	A	51	GLU	11
1	B	51	GLU	11
1	B	66	SER	9
1	A	66	SER	9
1	A	39	ASN	9
1	B	39	ASN	9
1	A	12	GLN	8
1	B	12	GLN	8
1	A	36	ASP	8
1	B	36	ASP	8
1	A	79	ASP	7
1	B	79	ASP	7
1	A	30	GLU	6
1	B	30	GLU	6
1	B	67	SER	5
1	B	41	HIS	5
1	A	41	HIS	5
1	A	67	SER	5
1	A	32	LEU	4
1	A	2	ILE	4
1	B	32	LEU	4
1	B	2	ILE	4
1	B	13	PHE	3
1	A	40	GLU	3
1	B	40	GLU	3
1	A	13	PHE	3
1	B	77	MET	2
1	A	45	VAL	2
1	A	14	THR	2
1	B	14	THR	2
1	A	10	GLN	2
1	B	10	GLN	2
1	B	45	VAL	2
1	A	77	MET	2
1	A	5	GLU	1
1	B	5	GLU	1
1	B	78	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided