WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 11:24 AM EST

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

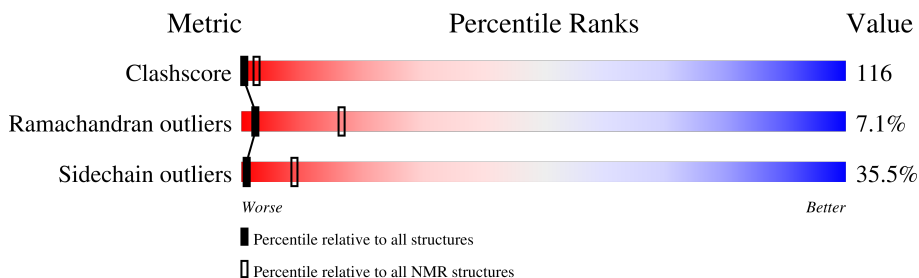|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	Percentile Ranks	Value
Clashscore		116
Ramachandran outliers		7.1%
Sidechain outliers		35.5%

Worse ... *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	87	10% 53% 23% 14%
1	B	87	10% 53% 23% 14%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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 (i)

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, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

● Molecule 1: GENE V PROTEIN
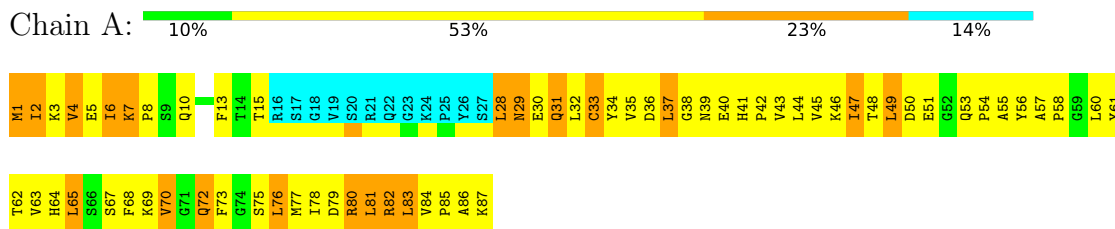
Chain A:

● Molecule 1: GENE V PROTEIN
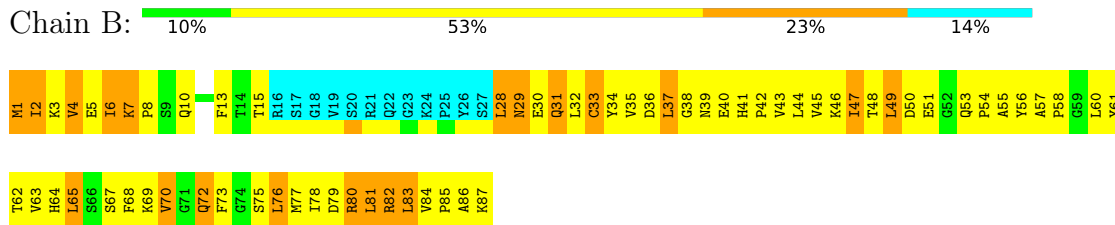
Chain B:

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.
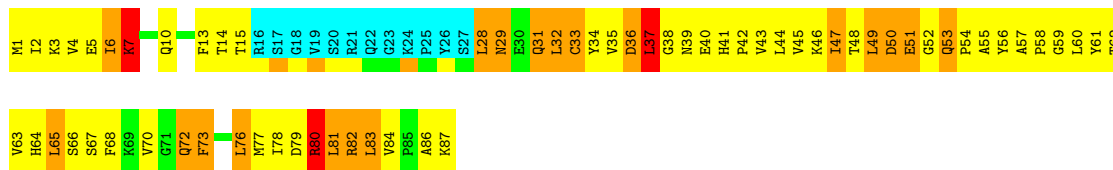
4.2.1 Score per residue for model 1

● Molecule 1: GENE V PROTEIN
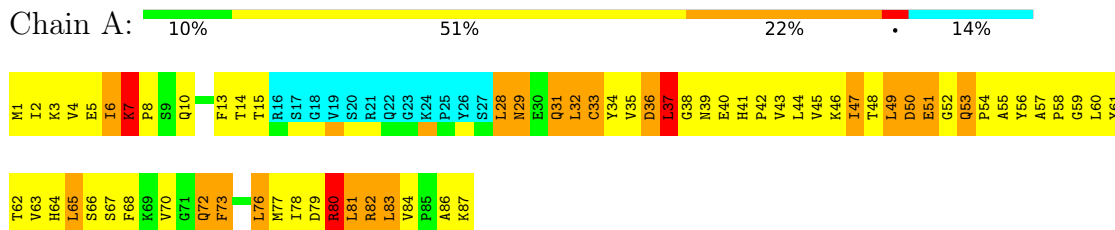
Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

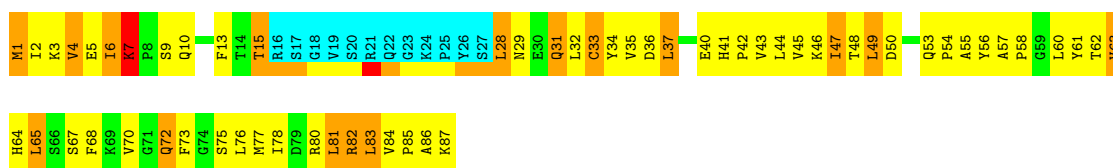
4.2.2 Score per residue for model 2

• 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:

T62 V63 H64 L65 S66 S67 F68 K69 V70 G71 Q72 F73 L76 M77 I78 D79 R80 L81 R82 L83 V84 P85 A86 K87
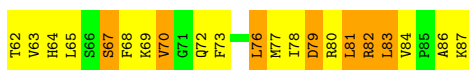
4.2.4 Score per residue for model 4

• Molecule 1: GENE V PROTEIN

Chain A: 14% 48% 23% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 T62

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

• Molecule 1: GENE V PROTEIN

Chain B: 13% 49% 23% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 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

4.2.5 Score per residue for model 5

• Molecule 1: GENE V PROTEIN

Chain A: 16% 46% 23% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 G52 Q53 P54 A55 Y56 A57 P58 G59 L60

Y61 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

• Molecule 1: GENE V PROTEIN

Chain B: 16% 46% 23% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 G52 Q53 P54 A55 Y56 A57 P58 G59 L60

Y61 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

4.2.6 Score per residue for model 6

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

4.2.8 Score per residue for model 8

• Molecule 1: GENE V PROTEIN

Chain A:

● Molecule 1: GENE V PROTEIN
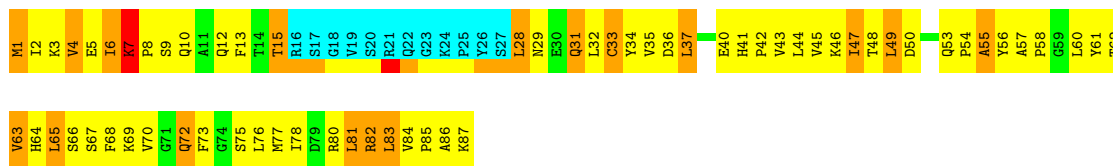
Chain B:

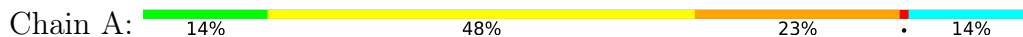### 4.2.9 Score per residue for model 9

● Molecule 1: GENE V PROTEIN

Chain A:

● Molecule 1: GENE V PROTEIN
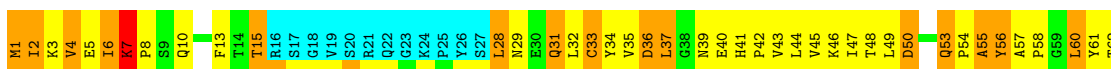
Chain B:

4.2.10 Score per residue for model 10

● Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

4.2.12 Score per residue for model 12

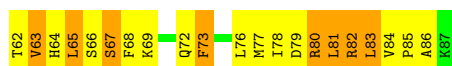• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

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

4.2.13　Score per residue for model 13

• Molecule 1: GENE V PROTEIN

Chain A:　15%　47%　21%　•　14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 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

• Molecule 1: GENE V PROTEIN

Chain B:　15%　47%　21%　•　14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 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

4.2.14　Score per residue for model 14 (medoid)

• Molecule 1: GENE V PROTEIN

Chain A:　13%　48%　23%　•　14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 P54 A55 Y56 A57 P58 G59 L60 Y61

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

• Molecule 1: GENE V PROTEIN

Chain B:　13%　49%　22%　•　14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 P54 A55 Y56 A57 P58 G59 L60 Y61

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

4.2.15 Score per residue for model 15

• Molecule 1: GENE V PROTEIN
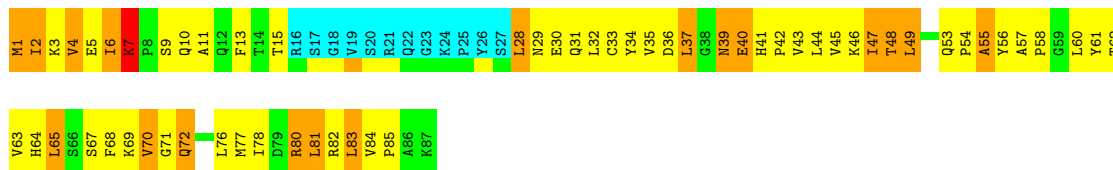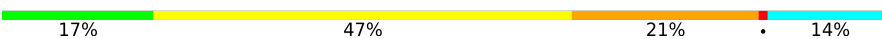
Chain A:

• Molecule 1: GENE V PROTEIN
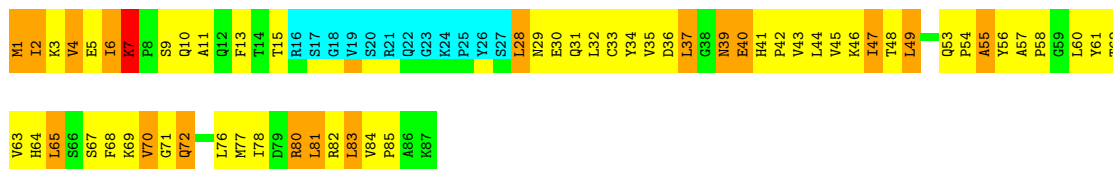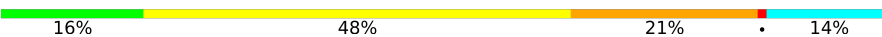
Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: GENE V PROTEIN
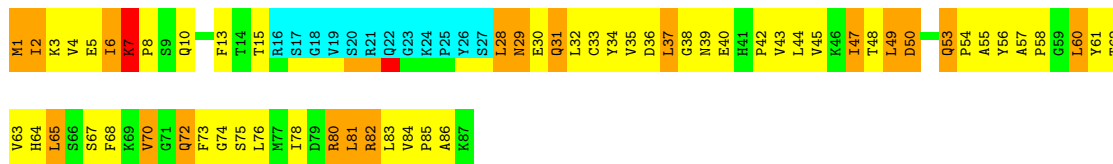
Chain A:

• Molecule 1: GENE V PROTEIN
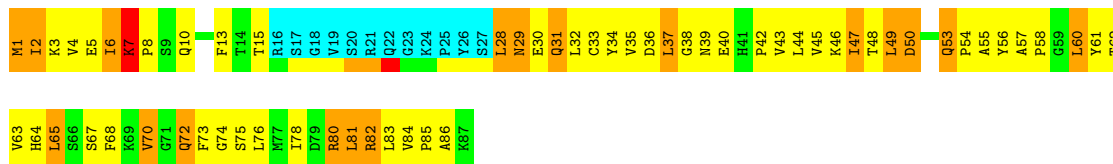
Chain B:

4.2.17 Score per residue for model 17

• Molecule 1: GENE V PROTEIN
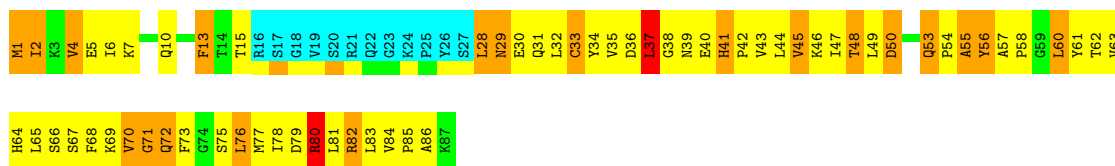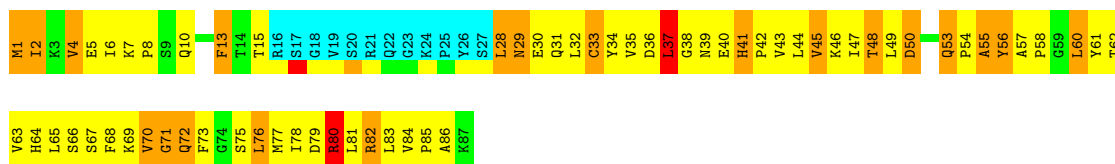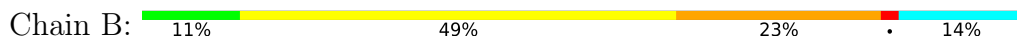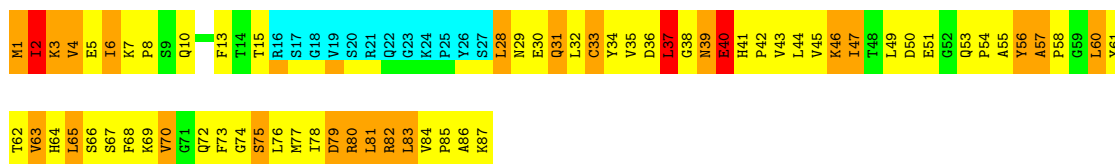
Chain A:

- Molecule 1: GENE V PROTEIN

Chain B:
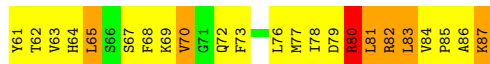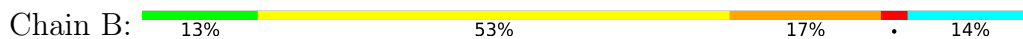
4.2.18 Score per residue for model 18

- Molecule 1: GENE V PROTEIN

Chain A:

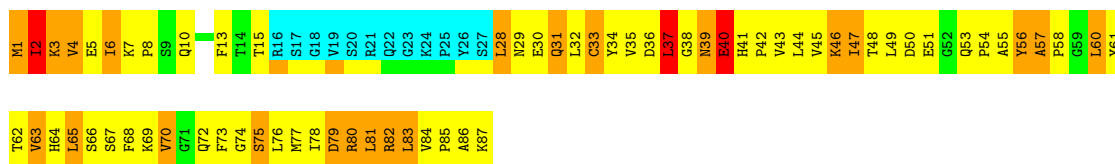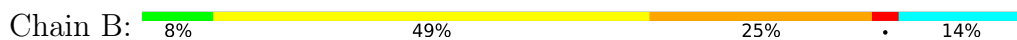- Molecule 1: GENE V PROTEIN

Chain B:
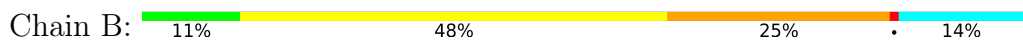
4.2.19 Score per residue for model 19
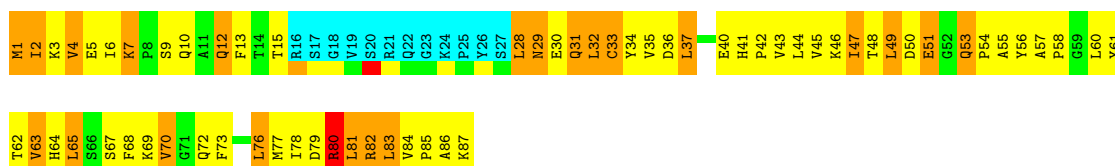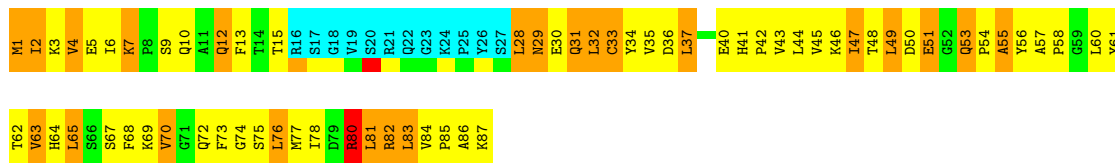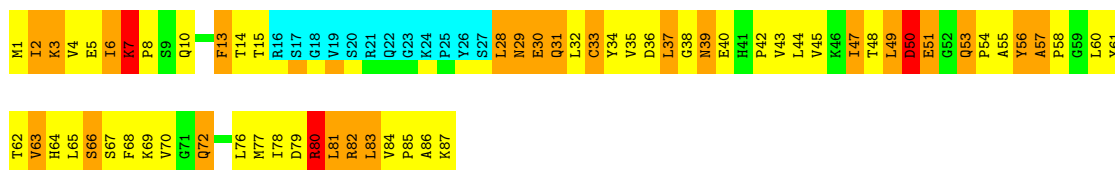
- Molecule 1: GENE V PROTEIN

Chain A:

- Molecule 1: GENE V PROTEIN

Chain B:
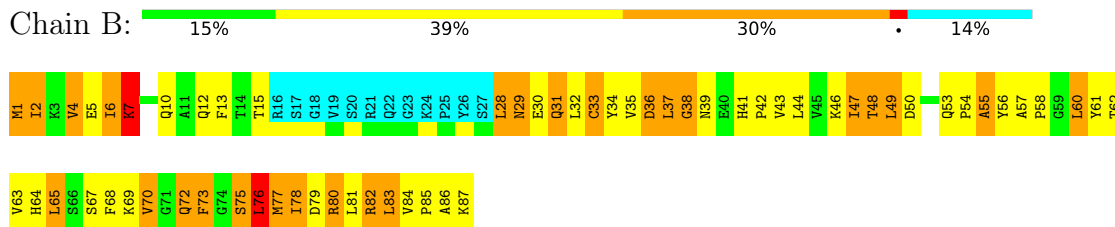
4.2.20 Score per residue for model 20

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:
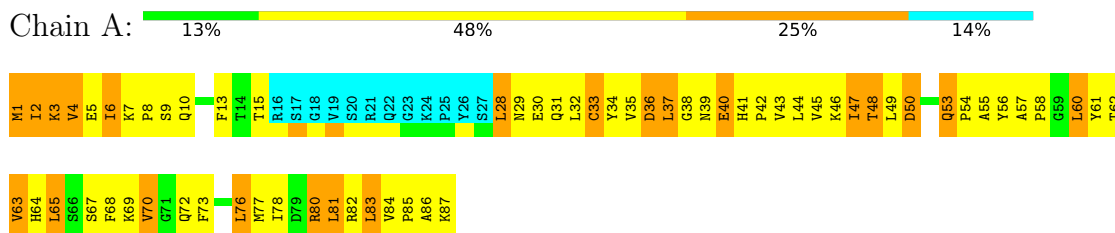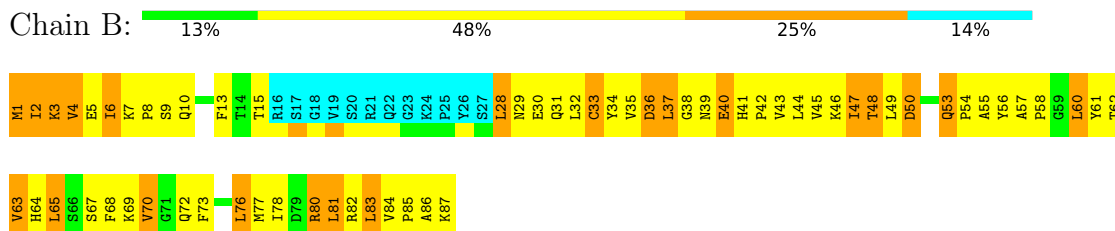
4.2.21 Score per residue for model 21

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:

T62 V63 H64 L65 S66 S67 F68 K69 V70 G71 Q72 F73 G74 S75 L76 M77 I78 D79 R80 L81 R82 L83 V84 K87
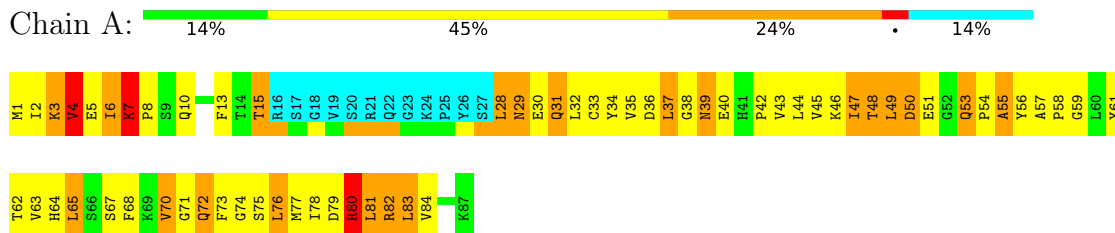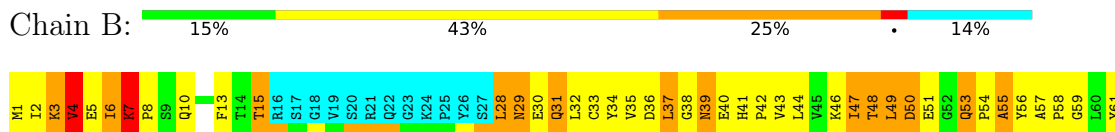
4.2.22 Score per residue for model 22

• Molecule 1: GENE V PROTEIN

Chain A: 11% 53% 20% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 A11 Q12 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 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

• Molecule 1: GENE V PROTEIN

Chain B: 14% 51% 20% • 14%

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61 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

4.2.23 Score per residue for model 23

• Molecule 1: GENE V PROTEIN

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

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 G52 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61

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

• Molecule 1: GENE V PROTEIN

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

M1 I2 K3 V4 E5 I6 K7 P8 S9 Q10 F13 T14 T15 R16 S17 G18 V19 S20 R21 Q22 G23 K24 P25 Y26 S27 L28 N29 E30 Q31 L32 C33 Y34 V35 D36 L37 G38 N39 E40 H41 P42 V43 L44 V45 K46 I47 T48 L49 D50 E51 G52 Q53 P54 A55 Y56 A57 P58 G59 L60 Y61

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

4.2.24 Score per residue for model 24

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:
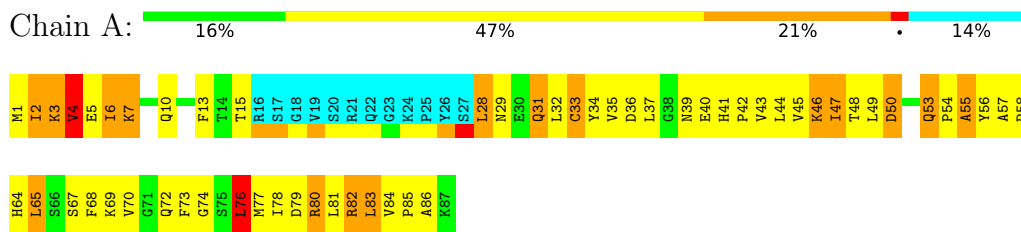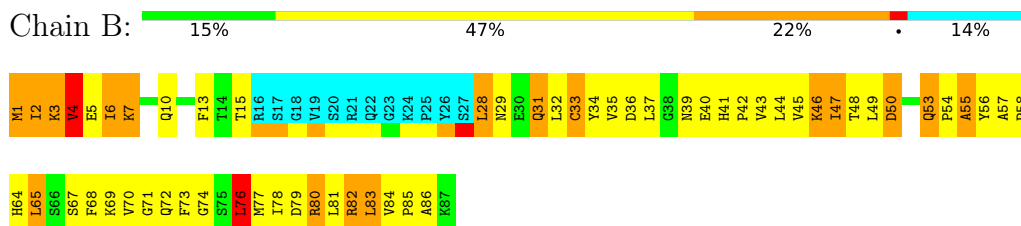
4.2.25 Score per residue for model 25

• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B:
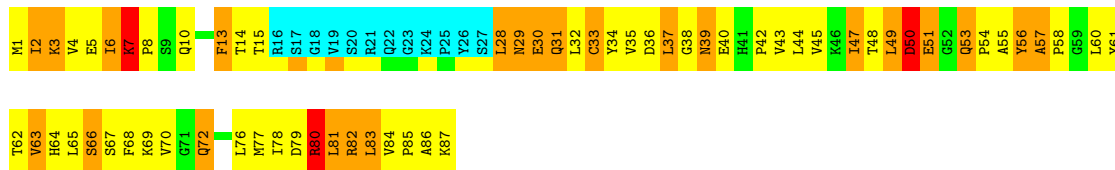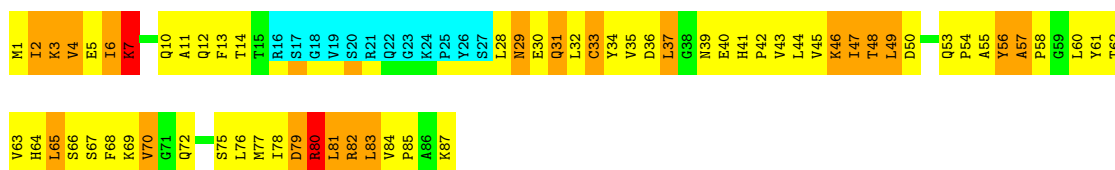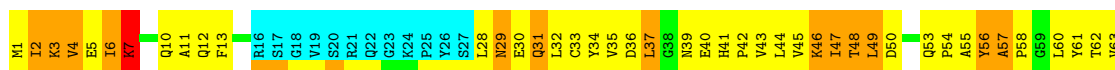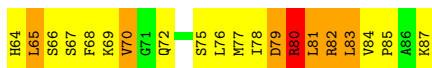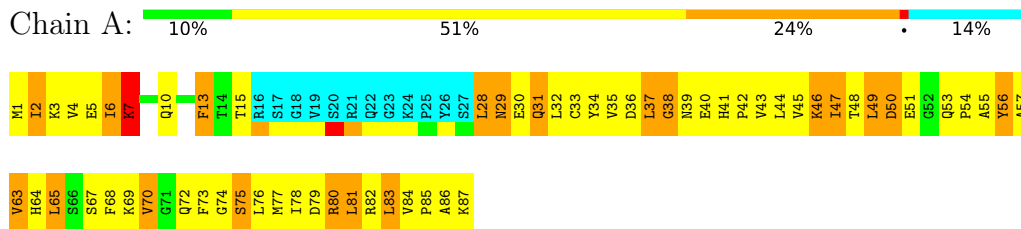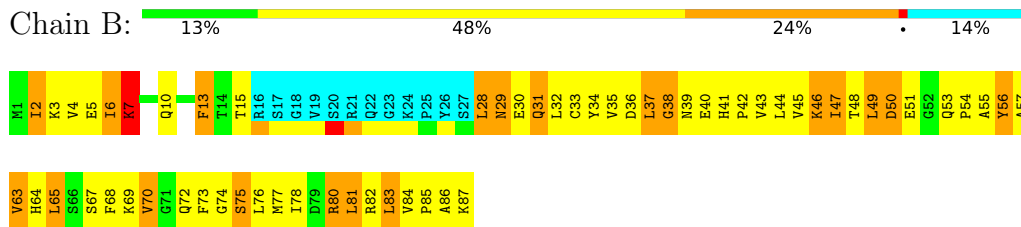

4.2.26 Score per residue for model 26

• Molecule 1: GENE V PROTEIN
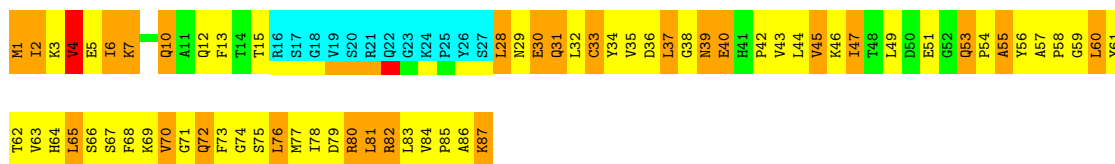
Chain A:

• Molecule 1: GENE V PROTEIN
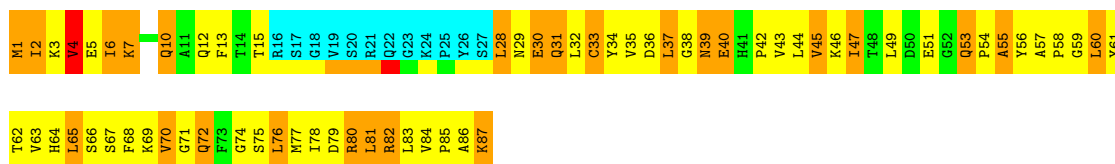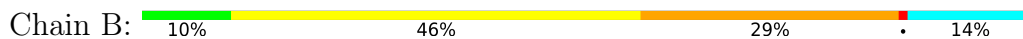
Chain B:

4.2.27   Score per residue for model 27

• Molecule 1: GENE V PROTEIN
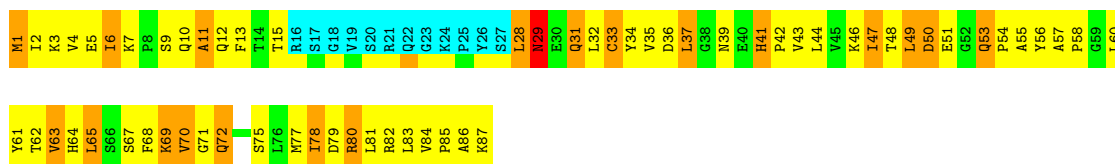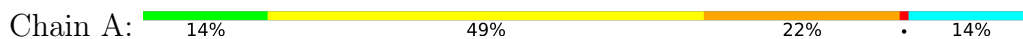
Chain A:

• Molecule 1: GENE V PROTEIN
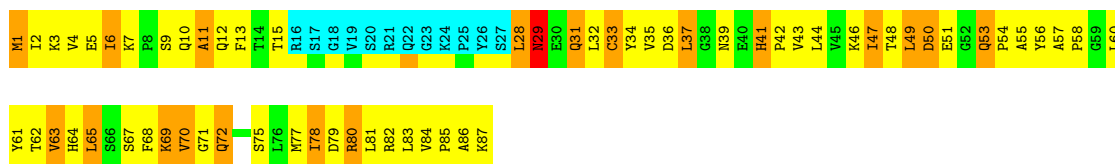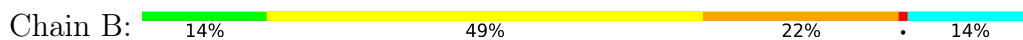
Chain B:

4.2.28   Score per residue for model 28

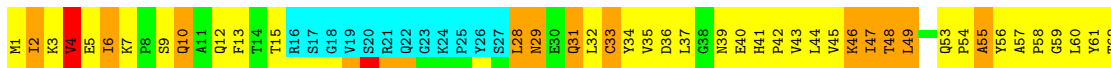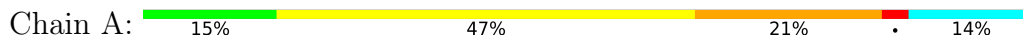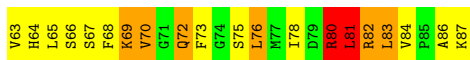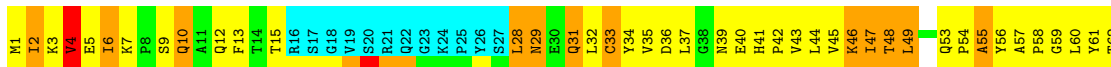• Molecule 1: GENE V PROTEIN

Chain A:

• Molecule 1: GENE V PROTEIN

Chain B: 14%   49%   18%   5%   14%
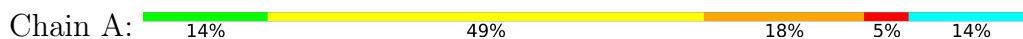
4.2.29   Score per residue for model 29

● Molecule 1: GENE V PROTEIN

Chain A: 15%   45%   25%   •   14%

● Molecule 1: GENE V PROTEIN

Chain B: 14%   46%   25%   •   14%
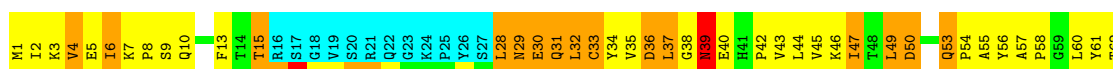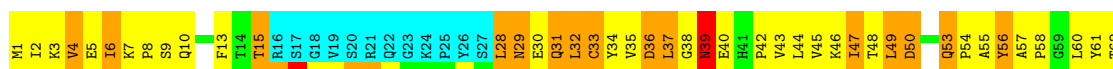
4.2.30   Score per residue for model 30

● Molecule 1: GENE V PROTEIN

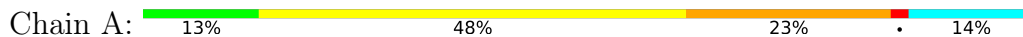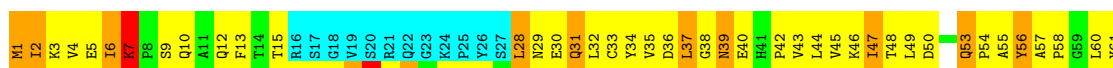Chain A: 15%   51%   20%   •   14%

● Molecule 1: GENE V PROTEIN

Chain B: 14%   51%   21%   •   14%

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.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	Models 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:10:GLN:OE1	1:A:32:LEU:HD13	0.94	1.61	27	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:HG13	1:A:61:TYR:CB	0.94	1.92	13	12
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:A:63:VAL:CG1	1:A:81:LEU:HD12	0.88	1.99	18	7
1:B:47:ILE:CD1	1:B:83:LEU:HD12	0.88	1.99	17	15
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:36:ASP:O	1:B:37:LEU:HD12	0.85	1.70	3	4
1:B:33:CYS:SG	1:B:47:ILE:HD13	0.85	2.10	5	5
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:A:65:LEU:HD22	1:B:2:ILE:HA	0.84	1.47	28	14
1:B:76:LEU:HD23	1:B:77:MET:N	0.84	1.87	9	5
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:43:VAL:CG2	1:B:70:VAL:HG11	0.81	2.05	4	4
1:A:70:VAL:HG11	1:B:43:VAL:CG2	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:31:GLN:HG3	1:A:55:ALA:HB1	0.80	1.53	5	17
1:A:70:VAL:HG11	1:B:43:VAL:HG21	0.80	1.53	4	4
1:A:70:VAL:HG21	1:B:43:VAL:CG2	0.80	2.04	29	4
1:A:2:ILE:CA	1:B:65:LEU:HD22	0.80	2.07	29	21
1:A:2:ILE:HG23	1:B:65:LEU:CD1	0.80	2.06	2	5
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:A:3:LYS:O	1:A:4:VAL:HG23	0.76	1.80	1	7
1:B:6:ILE:HD13	1:B:61:TYR:CE1	0.76	2.16	26	17

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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:A:76:LEU:HD11	1:B:37:LEU:HD21	0.75	1.55	3	2
1:A:47:ILE:HD11	1:A:83:LEU:CB	0.75	2.11	8	6
1:B:34:TYR:CE2	1:B:44:LEU:HD13	0.75	2.16	17	6
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:2:ILE:H	1:B:65:LEU:HD22	0.73	1.43	5	5
1:A:65:LEU:HD22	1:B:2:ILE:H	0.73	1.43	15	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:A:63:VAL:HG11	1:A:81:LEU:HB2	0.72	1.60	13	16
1:B:57:ALA:HB1	1:B:58:PRO:CD	0.72	2.13	1	28
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:A:2:ILE:HD12	1:A:63:VAL:HB	0.72	1.58	8	3
1:B:48:THR:HG21	1:B:80:ARG:NH1	0.72	1.99	12	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:HD12	1:B:37:LEU:O	0.71	1.85	20	1
1:B:28:LEU:C	1:B:28:LEU:HD22	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:49:LEU:HD12	1:A:53:GLN:O	0.71	1.85	22	7
1:A:76:LEU:CD1	1:B:35:VAL:HG11	0.71	2.16	10	4
1:B:37:LEU:HD23	1:B:37:LEU:N	0.71	2.00	25	1
1:A:33:CYS:SG	1:A:47:ILE:HD12	0.71	2.24	22	2
1:A:35:VAL:HG11	1:B:76:LEU:CD1	0.71	2.15	10	4
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	2
1:B:1:MET:SD	1:B:62:THR:HG21	0.70	2.25	6	9
1:B:49:LEU:HD13	1:B:49:LEU:O	0.70	1.86	23	2
1:A:68:PHE:C	1:B:37:LEU:HD11	0.70	2.05	6	9
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:C	1:A:28:LEU:HD12	0.70	2.07	17	1
1:B:28:LEU:C	1:B:28:LEU:HD12	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	2
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:A:6:ILE:HD11	1:A:33:CYS:SG	0.69	2.28	16	5
1:B:33:CYS:SG	1:B:47:ILE:HD11	0.69	2.27	15	1
1:B:36:ASP:C	1:B:37:LEU:HD12	0.69	2.07	3	2
1:A:47:ILE:HD11	1:A:83:LEU:HB3	0.69	1.65	22	1
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:A:37:LEU:CG	1:B:65:LEU:HD13	0.69	2.18	11	1
1:B:6:ILE:HD11	1:B:33:CYS:SG	0.69	2.27	21	5
1:B:35:VAL:HG12	1:B:37:LEU:H	0.69	1.48	25	3
1:B:35:VAL:HG13	1:B:37:LEU:HD11	0.69	1.65	1	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:A:65:LEU:HD13	1:B:37:LEU:CG	0.69	2.18	11	1
1:A:33:CYS:SG	1:A:47:ILE:HD11	0.69	2.28	15	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:81:LEU:HD12	1:A:81:LEU:C	0.68	2.08	8	1
1:A:37:LEU:HG	1:B:65:LEU:HD21	0.68	1.65	16	3
1:B:81:LEU:C	1:B:81:LEU:HD12	0.68	2.09	8	1
1:A:36:ASP:C	1:A:37:LEU:HD12	0.68	2.07	3	2
1:A:76:LEU:HD13	1:B:35:VAL:HG21	0.68	1.64	26	1
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:O	1:A:81:LEU:HD23	0.68	1.88	7	23
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:A:32:LEU:N	1:A:32:LEU:HD12	0.68	2.03	28	4
1:A:35:VAL:HG13	1:A:37:LEU:HD11	0.68	1.65	1	1
1:B:81:LEU:HD23	1:B:81:LEU:O	0.68	1.89	7	23
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:B:32:LEU:HD12	1:B:32:LEU:N	0.67	2.03	28	5
1:A:28:LEU:HD11	1:A:30:GLU:HG3	0.67	1.65	10	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:N	1:B:29:ASN:OD1	0.67	2.28	13	14
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:B:35:VAL:HG12	1:B:37:LEU:HG	0.67	1.67	23	4
1:A:61:TYR:CD2	1:A:83:LEU:HD23	0.67	2.25	26	3
1:B:7:LYS:CD	1:B:34:TYR:CD2	0.66	2.79	11	15
1:B:37:LEU:HD23	1:B:37:LEU:O	0.66	1.90	13	4
1:A:37:LEU:O	1:A:37:LEU:HD23	0.66	1.90	13	5
1:A:65:LEU:HD23	1:A:68:PHE:HD2	0.66	1.47	9	1
1:A:28:LEU:HD12	1:A:28:LEU:C	0.66	2.10	10	1
1:B:65:LEU:CB	1:B:68:PHE:CD2	0.66	2.79	30	20
1:B:37:LEU:HD12	1:B:37:LEU:N	0.66	2.06	17	1
1:A:29:ASN:OD1	1:A:29:ASN:N	0.66	2.28	13	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LEU:CD2	1:B:48:THR:HG22	0.66	2.21	1	3
1:A:35:VAL:HG12	1:A:37:LEU:HG	0.66	1.67	23	4
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:B:28:LEU:HD12	1:B:28:LEU:C	0.66	2.10	10	1
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:HG23	1:A:43:VAL:O	0.65	1.92	18	27
1:A:28:LEU:CD2	1:A:48:THR:HG22	0.65	2.21	1	3
1:B:36:ASP:C	1:B:37:LEU:HD23	0.65	2.11	7	1
1:A:37:LEU:HD21	1:B:69:LYS:HA	0.65	1.67	13	7
1:A:37:LEU:N	1:A:37:LEU:HD12	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:A:65:LEU:HB2	1:A:68:PHE:CD2	0.64	2.26	19	27
1:B:47:ILE:CG2	1:B:56:TYR:CE1	0.64	2.79	15	19
1:A:36:ASP:C	1:A:37:LEU:HD23	0.64	2.11	7	1
1:B:43:VAL:HG23	1:B:43:VAL:O	0.64	1.92	18	26
1:B:65:LEU:HB2	1:B:68:PHE:CD2	0.64	2.27	27	27
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: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:A:68:PHE:N	1:A:68:PHE:CD1	0.64	2.65	19	30
1:B:68:PHE:CD1	1:B:68:PHE:N	0.64	2.64	28	30
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:A:7:LYS:HD3	1:A:34:TYR:CD2	0.64	2.28	19	18
1:B:43:VAL:HG23	1:B:45:VAL:HG23	0.64	1.70	15	2
1:B:4:VAL:HG11	1:B:83:LEU:CD1	0.64	2.23	29	1
1:A:13:PHE:CD2	1:A:55:ALA:HB2	0.64	2.28	10	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:59:GLY:O	1:B:61:TYR:CD1	0.64	2.51	1	5
1:A:13:PHE:CE1	1:A:29:ASN:ND2	0.64	2.67	9	12
1:B:35:VAL:O	1:B:43:VAL:HG13	0.64	1.93	3	4
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:A:13:PHE:CD1	1:A: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:B:13:PHE:CD1	1:B:29:ASN:CB	0.63	2.81	19	20
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:40:GLU:O	1:B:41:HIS:CG	0.63	2.52	22	12
1:B:56:TYR:CE2	1:B:83:LEU:CB	0.63	2.81	26	19
1:A:37:LEU:HD13	1:A:37:LEU:H	0.63	1.54	1	1
1:A:56:TYR:CE2	1:A:83:LEU:CB	0.63	2.82	26	19
1:B:13:PHE:CE1	1:B:29:ASN:ND2	0.63	2.67	5	12
1:A:43:VAL:HG23	1:A:45:VAL:HG23	0.63	1.70	15	2
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: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:B:13:PHE:CD2	1:B:55:ALA:HB2	0.62	2.29	10	27
1:A:69:LYS:HA	1:B:37:LEU:HD21	0.62	1.70	13	7
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:A:81:LEU:N	1:A:81:LEU:HD23	0.62	2.10	3	4
1:A:45:VAL:HG12	1:B:70:VAL:CG1	0.62	2.25	20	3
1:A:76:LEU:HD11	1:B:37:LEU:HD22	0.62	1.70	20	1
1:A:35:VAL:O	1:A:43:VAL:HG13	0.62	1.94	3	4
1:A:76:LEU:C	1:A:76:LEU:HD23	0.62	2.15	15	2
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:C	1:B:76:LEU:HD23	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:NE2	1:A:72:GLN:N	0.61	2.48	13	3
1:A:32:LEU:HD12	1:A:44:LEU:HG	0.61	1.72	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:70:VAL:CG1	1:B:45:VAL:HG12	0.61	2.25	20	4
1:B:6:ILE:HD11	1:B:83:LEU:CD2	0.61	2.25	22	3
1:A:13:PHE:CG	1:A:49:LEU:HD12	0.61	2.31	6	4
1:B:7:LYS:HD2	1:B:34:TYR:CE2	0.61	2.31	20	5
1:A:32:LEU:HD22	1:A:44:LEU:HD21	0.61	1.71	10	3
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:A:13:PHE:CD1	1:A:29:ASN:HB3	0.60	2.31	10	25
1:A:47:ILE:HD12	1:A:56:TYR:CE1	0.60	2.31	29	3
1:A:13:PHE:CD2	1:A:49:LEU:HD12	0.60	2.31	18	5
1:B:72:GLN:N	1:B:72:GLN:NE2	0.60	2.48	13	3
1:B:31:GLN:CB	1:B:47:ILE:HG22	0.60	2.24	5	18
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:A:37:LEU:CB	1:B:65:LEU:HD21	0.60	2.26	21	1
1:B:10:GLN:NE2	1:B:32:LEU:HD22	0.60	2.12	27	1
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:B:47:ILE:HG21	1:B:56:TYR:CD1	0.60	2.31	27	19
1:A:45:VAL:CG2	1:B:70:VAL:CG1	0.60	2.80	18	11
1:A:45:VAL:CG1	1:B:70:VAL:CG1	0.60	2.79	14	5
1:B:47:ILE:HG12	1:B:56:TYR:CE2	0.60	2.32	9	4
1:B:40:GLU:O	1:B:41:HIS:CB	0.60	2.49	22	4
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	18
1:B:6:ILE:O	1:B:6:ILE:HG22	0.60	1.96	14	22
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:78:ILE:CG2	1:A:81:LEU:N	0.60	2.65	18	3
1:A:7:LYS:HD2	1:A:34:TYR:CE2	0.60	2.31	20	5
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:10:GLN:NE2	1:A:32:LEU:HD22	0.60	2.12	27	1
1:A:47:ILE:HG21	1:A:56:TYR:CD1	0.59	2.33	27	19
1:A:2:ILE:CG1	1:B:65:LEU:HD21	0.59	2.27	9	2
1:A:65:LEU:HD21	1:B:2:ILE:CG1	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:A:37:LEU:HA	1:B:65:LEU:HD13	0.59	1.74	3	1
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: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:B:39:ASN:O	1:B:41:HIS:CE1	0.59	2.56	27	3
1:A:70:VAL:HG11	1:B:45:VAL:HG23	0.59	1.74	26	1
1:A:31:GLN:HE21	1:A:55:ALA:HB1	0.59	1.58	21	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:72:GLN:O	1:A:73:PHE:CG	0.59	2.55	28	2
1:A:39:ASN:HD22	1:A:43:VAL:HG11	0.59	1.57	27	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:A:47:ILE:HG12	1:A:56:TYR:CE2	0.59	2.33	9	4
1:B:7:LYS:HD3	1:B:34:TYR:CD1	0.59	2.33	18	2
1:B:29:ASN:OD1	1:B:29:ASN:N	0.59	2.36	14	2
1:A:37:LEU:CD2	1:A:38:GLY:N	0.59	2.65	1	2
1:A:78:ILE:CD1	1:B:78:ILE:HD12	0.59	2.28	2	18
1:A:63:VAL:HG11	1:A:81:LEU:HD12	0.59	1.73	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:70:VAL:CG1	1:B:43:VAL:HG21	0.59	2.27	4	2
1:A:68:PHE:HB3	1:A:76:LEU:HD21	0.59	1.74	13	3
1:B:76:LEU:O	1:B:76:LEU:HD23	0.59	1.98	23	1
1:A:34:TYR:CD1	1:A:42:PRO:HB2	0.58	2.33	14	16
1:A:45:VAL:CG1	1:A:46:LYS:N	0.58	2.66	22	11
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:65:LEU:HD22	1:B:2:ILE:HG13	0.58	1.75	4	3
1:A:2:ILE:CG1	1:B:65:LEU:CD2	0.58	2.81	13	1
1:B:39:ASN:HD22	1:B:43:VAL:HG11	0.58	1.57	27	2
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:6:ILE:CD1	1:B:61:TYR:CD1	0.58	2.87	7	12
1:A:37:LEU:HD11	1:B:69:LYS:HA	0.58	1.75	8	4
1:B:65:LEU:HD23	1:B:68:PHE:CE2	0.58	2.33	13	2
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:2:ILE:CG2	1:A:63:VAL:CG2	0.58	2.82	5	10
1:A:34:TYR:CD2	1:A:42:PRO:HB2	0.58	2.33	22	14
1:A:76:LEU:HD12	1:B:35:VAL:HG11	0.58	1.74	11	1
1:A:65:LEU:HD13	1:B:2:ILE:HG12	0.58	1.75	25	1
1:A:79:ASP:O	1:A:80:ARG:CB	0.58	2.52	9	7
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:4:VAL:CB	1:B:35:VAL:HG22	0.58	2.29	14	6
1:B:34:TYR:CD2	1:B:42:PRO:HB2	0.58	2.33	22	14
1:A:65:LEU:CD2	1:B:2:ILE:N	0.58	2.66	30	2
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	8	19
1:A:28:LEU:HD22	1:A:50:ASP:HB3	0.58	1.76	6	1
1:A:39:ASN:OD1	1:A:41:HIS:CD2	0.58	2.57	8	1
1:B:10:GLN:OE1	1:B:44:LEU:HD13	0.58	1.99	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1:MET:O	1:B:37:LEU:HD22	0.58	1.98	21	1
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:A:65:LEU:HD13	1:B:37:LEU:HA	0.57	1.75	3	1
1:B:2:ILE:CG2	1:B:63:VAL:CG2	0.57	2.82	5	10
1:B:28:LEU:HD22	1:B:29:ASN:N	0.57	2.14	18	1
1:B:28:LEU:CD1	1:B:28:LEU:N	0.57	2.67	18	1
1:B:4:VAL:CG1	1:B:5:GLU:N	0.57	2.67	1	10
1:B:36:ASP:O	1:B:38:GLY:N	0.57	2.37	3	19
1:B:70:VAL:HG22	1:B:76:LEU:CD1	0.57	2.29	4	1
1:A:3:LYS:C	1:A:4:VAL:HG12	0.57	2.19	21	4
1:A:81:LEU:N	1:A:81:LEU:CD2	0.57	2.67	3	4
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:B:4:VAL:N	1:B:61:TYR:O	0.57	2.38	30	17
1:A:37:LEU:HD11	1:B:69:LYS:N	0.57	2.14	5	6
1:A:4:VAL:N	1:A:61:TYR:O	0.57	2.38	30	18
1:A:34:TYR:CE1	1:A:44:LEU:HB2	0.57	2.35	27	27
1:A:68:PHE:O	1:B:37:LEU:HD11	0.57	1.99	6	2
1:B:3:LYS:C	1:B:4:VAL:HG12	0.57	2.20	21	4
1:A:1:MET:O	1:A:37:LEU:HD22	0.57	1.99	21	1
1:B:31:GLN:HB2	1:B:49:LEU:HD23	0.57	1.76	29	2
1:A:45:VAL:HG23	1:B:70:VAL:HG11	0.57	1.77	26	1
1:B:40:GLU:O	1:B:41:HIS:ND1	0.57	2.38	23	10
1:A:70:VAL:HG22	1:A:76:LEU:CD1	0.57	2.30	4	1
1:A:28:LEU:N	1:A:28:LEU:CD1	0.57	2.67	18	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:4:VAL:CB	1:A:35:VAL:HG22	0.57	2.29	14	7
1:B:6:ILE:HG23	1:B:10:GLN:O	0.57	2.00	24	4
1:B:81:LEU:N	1:B:81:LEU:CD2	0.57	2.67	3	4
1:A:6:ILE:HG23	1:A:10:GLN:O	0.57	2.00	24	3
1:B:35:VAL:CG1	1:B:37:LEU:HD23	0.57	2.29	20	1
1:A:76:LEU:HD23	1:A:76:LEU:O	0.57	1.98	23	1
1:A:36:ASP:O	1:A:38:GLY:N	0.57	2.37	3	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:3:LYS:O	1:B:4:VAL:CG2	0.57	2.53	1	11
1:A:13:PHE:CD1	1:A:13:PHE:N	0.57	2.73	8	3
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:3:LYS:O	1:A:4:VAL:CG2	0.56	2.53	1	11
1:A:2:ILE:HG21	1:B:76:LEU:HD22	0.56	1.76	16	1
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: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: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:47:ILE:HG21	1:B:56:TYR:OH	0.56	2.00	15	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:B:13:PHE:N	1:B:13:PHE:CD1	0.56	2.73	8	3
1:A:35:VAL:CG1	1:A:37:LEU:HD23	0.56	2.30	20	1
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
1:B:37:LEU:N	1:B:37:LEU:CD2	0.56	2.68	25	1
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:A:45:VAL:HG12	1:A:46:LYS:N	0.56	2.16	5	10
1:A:65:LEU:HD12	1:B:37:LEU:HG	0.56	1.76	6	1
1:B:37:LEU:HD22	1:B:39:ASN:HD21	0.56	1.60	13	2
1:B:3:LYS:H	1:B:37:LEU:HD12	0.56	1.56	1	1
1:B:32:LEU:HD23	1:B:46:LYS:HA	0.56	1.76	5	3
1:B:6:ILE:HG12	1:B:61:TYR:CD1	0.56	2.36	10	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	23
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:76:LEU:HD22	1:B:2:ILE:HG21	0.55	1.79	16	1
1:A:39:ASN:O	1:A:41:HIS:CD2	0.55	2.59	27	1
1:A:7:LYS:CG	1:A:34:TYR:CE2	0.55	2.90	11	15
1:A:28:LEU:HD23	1:A:49:LEU:O	0.55	2.01	13	2
1:B:6:ILE:HG13	1:B:61:TYR:CE1	0.55	2.37	10	3
1:A:81:LEU:O	1:A:81:LEU:CD2	0.55	2.55	2	23
1:B:6:ILE:O	1:B:6:ILE:CG2	0.55	2.55	21	5
1:B:65:LEU:HA	1:B:68:PHE:CD2	0.55	2.37	14	24
1:B:45:VAL:HG12	1:B:46:LYS:N	0.55	2.16	5	10
1:B:72:GLN:O	1:B:73:PHE:CD2	0.55	2.59	28	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	20
1:A:63:VAL:HG13	1:A:81:LEU:CD1	0.55	2.31	18	5
1:B:78:ILE:O	1:B:79:ASP:CB	0.55	2.54	7	5
1:A:6:ILE:HG12	1:A:61:TYR:CD1	0.55	2.36	10	2
1:A:29:ASN:N	1:A:29:ASN:OD1	0.55	2.40	10	2
1:A:37:LEU:HD22	1:A:38:GLY:N	0.55	2.17	1	1
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
1:B:43:VAL:O	1:B:43:VAL:CG2	0.55	2.55	25	18
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:6:ILE:O	1:A:6:ILE:CG2	0.55	2.55	21	5
1:B:37:LEU:HD22	1:B:37:LEU:N	0.55	2.17	1	1
1:A:37:LEU:O	1:B:65:LEU:CD1	0.55	2.55	19	2
1:A:2:ILE:CG2	1:A:63:VAL:HG21	0.55	2.31	5	3
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:2:ILE:CA	1:B:65:LEU:HD21	0.55	2.31	11	1
1:A:13:PHE:N	1:A:55:ALA:HB2	0.55	2.17	17	12
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:2:ILE:HG23	1:B:65:LEU:HD21	0.55	1.78	11	1
1:A:65:LEU:HD11	1:B:37:LEU:CA	0.55	2.32	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:A:37:LEU:HG	1:B:65:LEU:HD12	0.54	1.78	6	1
1:A:37:LEU:CD1	1:A:39:ASN:ND2	0.54	2.70	9	1
1:A:47:ILE:HG21	1:A:56:TYR:OH	0.54	2.00	15	1
1:B:39:ASN:O	1:B:41:HIS:CD2	0.54	2.59	27	1
1:A:35:VAL:CG1	1:A:37:LEU:HD21	0.54	2.32	1	1
1:A:76:LEU:O	1:A:77:MET:CG	0.54	2.55	26	18
1:B:57:ALA:CB	1:B:58:PRO:CD	0.54	2.84	13	20
1:B:43:VAL:HG23	1:B:45:VAL:HG13	0.54	1.79	14	3
1:A:70:VAL:HG21	1:B:43:VAL:HG11	0.54	1.78	3	3
1:A:13:PHE:CD1	1:A:29:ASN:CG	0.54	2.81	30	10
1:B:7:LYS:HG2	1:B:34:TYR:CE1	0.54	2.38	5	2
1:A:37:LEU:CA	1:B:65:LEU:HD11	0.54	2.32	25	1
1:A:3:LYS:O	1:A:37:LEU:CD1	0.54	2.56	1	1
1:A:62:THR:O	1:A:84:VAL:CG2	0.54	2.56	13	17
1:A:29:ASN:CB	1:A:49:LEU:HB3	0.54	2.32	5	5
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:7:LYS:HG3	1:A:34:TYR:CD2	0.54	2.37	20	1
1:B:10:GLN:O	1:B:31:GLN:NE2	0.54	2.41	22	28
1:A:29:ASN:HB2	1:A:49:LEU:CB	0.54	2.32	15	4
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:29:ASN:HB2	1:B:49:LEU:CB	0.54	2.32	15	3
1:B:61:TYR:CD2	1:B:84:VAL:C	0.54	2.81	13	18
1:B:2:ILE:CG2	1:B:63:VAL:HG21	0.54	2.31	5	2
1:A:3:LYS:H	1:A:37:LEU:HD12	0.54	1.55	1	1
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:7:LYS:HG2	1:A:34:TYR:CE2	0.54	2.37	11	15
1:A:37:LEU:HD22	1:A:37:LEU:N	0.54	2.16	1	1
1:B:31:GLN:HB3	1:B:47:ILE:CG2	0.54	2.33	29	27
1:A:69:LYS:HA	1:B:37:LEU:HD11	0.54	1.78	8	4
1:B:4:VAL:HG21	1:B:83:LEU:HD11	0.54	1.79	22	2
1:B:81:LEU:N	1:B:81:LEU:HD23	0.54	2.18	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:CG1	1:B:45:VAL:HG21	0.54	2.32	9	4
1:A:32:LEU:N	1:A:32:LEU:CD2	0.54	2.70	9	2
1:A:1:MET:C	1:B:65:LEU:HD22	0.54	2.22	18	5
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: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:A:72:GLN:O	1:A:72:GLN:CG	0.54	2.56	29	6
1:B:68:PHE:CD1	1:B:78:ILE:HG13	0.54	2.38	4	1
1:B:6:ILE:CD1	1:B:61:TYR:CG	0.54	2.91	7	4
1:B:28:LEU:HD12	1:B:29:ASN:C	0.54	2.23	10	2
1:B:33:CYS:SG	1:B:47:ILE:CG1	0.54	2.96	15	3
1:B:10:GLN:HE22	1:B:32:LEU:HD22	0.54	1.63	27	1
1:B:49:LEU:CD1	1:B:53:GLN:O	0.54	2.56	1	8
1:A:62:THR:HG23	1:A:86:ALA:HA	0.54	1.80	8	12
1:B:29:ASN:CB	1:B:49:LEU:HB3	0.54	2.32	5	5
1:B:32:LEU:N	1:B:32:LEU:CD2	0.54	2.70	9	2
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:7:LYS:HG3	1:B:34:TYR:CD1	0.54	2.38	28	1
1:A:65:LEU:HD13	1:B:2:ILE:HG22	0.54	1.77	30	1
1:B:3:LYS:O	1:B:37:LEU:CD1	0.54	2.56	1	1
1:A:29:ASN:O	1:A:49:LEU:CB	0.53	2.56	14	8
1:A:61:TYR:CD2	1:A:84:VAL:C	0.53	2.81	13	18
1:B:72:GLN:CG	1:B:72:GLN:O	0.53	2.56	29	6
1:A:1:MET:O	1:A:3:LYS:N	0.53	2.41	24	12
1:B:36:ASP:O	1:B:39:ASN:N	0.53	2.41	26	6
1:A:28:LEU:HD12	1:A:29:ASN:C	0.53	2.23	10	2
1:A:38:GLY:O	1:A:39:ASN:CB	0.53	2.55	26	1
1:A:49:LEU:CD1	1:A:53:GLN:O	0.53	2.56	1	8
1:A:65:LEU:CD1	1:B:37:LEU:HG	0.53	2.33	1	4
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:B:38:GLY:O	1:B:39:ASN:CB	0.53	2.55	26	1
1:B:1:MET:O	1:B:3:LYS:N	0.53	2.42	24	12
1:A:4:VAL:HG21	1:A:83:LEU:HD11	0.53	1.79	22	2
1:A:33:CYS:SG	1:A:47:ILE:CG1	0.53	2.96	15	3
1:B:68:PHE:CD1	1:B:78:ILE:HG12	0.53	2.37	13	1
1:B:29:ASN:O	1:B:49:LEU:CB	0.53	2.57	3	8
1:B:62:THR:HG23	1:B:86:ALA:CA	0.53	2.34	8	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:A:65:LEU:HD21	1:B:2:ILE:HG13	0.53	1.81	13	1
1:A:31:GLN:HB3	1:A:47:ILE:CG2	0.53	2.33	29	27
1:A:33:CYS:O	1:A:44:LEU:HD12	0.53	2.03	18	8
1:B:62:THR:HG23	1:B:86:ALA:CB	0.53	2.34	28	11
1:B:1:MET:CG	1:B:1:MET:O	0.53	2.56	9	1
1:B:65:LEU:HG	1:B:68:PHE:CD2	0.53	2.39	11	1
1:B:49:LEU:O	1:B:49:LEU:CD1	0.53	2.56	23	1
1:B:81:LEU:O	1:B:81:LEU:CG	0.53	2.57	16	24
1:B:31:GLN:CB	1:B:47:ILE:CG2	0.53	2.86	8	11
1:B:40:GLU:C	1:B:41:HIS:CG	0.53	2.80	7	4
1:B:67:SER:O	1:B:79:ASP:CB	0.53	2.57	9	2
1:B:65:LEU:O	1:B:65:LEU:HD12	0.53	2.04	8	4
1:A:48:THR:HG21	1:A:80:ARG:CZ	0.53	2.33	22	2
1:B:10:GLN:O	1:B:11:ALA:C	0.53	2.47	27	1
1:A:1:MET:SD	1:A:62:THR:CG2	0.53	2.97	2	4
1:B:65:LEU:HA	1:B:68:PHE:CG	0.53	2.39	3	18
1:B:33:CYS:O	1:B:44:LEU:HD12	0.53	2.04	15	8
1:A:43:VAL:O	1:A:43:VAL:HG23	0.53	2.04	9	2
1:B:69:LYS:CG	1:B:77:MET:O	0.53	2.57	7	1
1:A:45:VAL:HG21	1:B:70:VAL:CG1	0.53	2.33	9	3
1:A:65:LEU:HG	1:A:68:PHE:CD2	0.53	2.38	11	1
1:B:35:VAL:CG1	1:B:37:LEU:HG	0.53	2.34	28	2
1:A:62:THR:HG23	1:A:86:ALA:CA	0.53	2.34	8	16
1:A:81:LEU:O	1:A:81:LEU:CG	0.53	2.57	29	23
1:B:35:VAL:CG1	1:B:37:LEU:HD21	0.53	2.33	1	1
1:A:40:GLU:C	1:A:41:HIS:CG	0.53	2.80	7	4
1:A:56:TYR:CE1	1:A:83:LEU:HB3	0.53	2.39	8	1
1:B:47:ILE:HD12	1:B:56:TYR:CZ	0.53	2.39	29	4
1:A:10:GLN:O	1:A:12:GLN:N	0.53	2.42	27	1
1:B:29:ASN:ND2	1:B:49:LEU:O	0.53	2.42	18	6
1:B:47:ILE:HG13	1:B:56:TYR:CE2	0.53	2.39	11	5
1:A:39:ASN:O	1:A:41:HIS:N	0.53	2.42	18	6
1:B:43:VAL:CG2	1:B:43:VAL:O	0.53	2.57	7	7
1:A:47:ILE:HD12	1:A:56:TYR:CZ	0.53	2.39	29	4
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:HD12	1:A:37:LEU:C	0.53	2.23	28	1
1:A:29:ASN:ND2	1:A:49:LEU:O	0.53	2.42	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:GLN:HB3	1:A:47:ILE:HG22	0.53	1.80	14	15
1:A:47:ILE:O	1:A:47:ILE:CG2	0.53	2.56	1	3
1:A:65:LEU:HA	1:A:68:PHE:CG	0.53	2.39	8	19
1:B:1:MET:SD	1:B:62:THR:CG2	0.53	2.97	2	4
1:B:64:HIS:N	1:B:82:ARG:O	0.53	2.42	13	8
1:B:31:GLN:OE1	1:B:56:TYR:N	0.53	2.41	8	2
1:B:56:TYR:CE1	1:B:83:LEU:HB3	0.53	2.39	8	1
1:A:65:LEU:HD22	1:B:1:MET:C	0.53	2.23	18	5
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:49:LEU:O	1:A:49:LEU:CD1	0.53	2.56	23	1
1:A:80:ARG:O	1:A:81:LEU:C	0.52	2.48	4	23
1:B:4:VAL:O	1:B:61:TYR:N	0.52	2.40	15	8
1:A:4:VAL:HG21	1:A:35:VAL:HG22	0.52	1.79	7	3
1:A:31:GLN:OE1	1:A:55:ALA:CB	0.52	2.55	7	2
1:B:7:LYS:HE2	1:B:34:TYR:CD2	0.52	2.39	10	2
1:A:37:LEU:CD1	1:A:37:LEU:C	0.52	2.78	29	4
1:B:39:ASN:O	1:B:41:HIS:ND1	0.52	2.42	19	1
1:A:10:GLN:HE22	1:A:32:LEU:HD22	0.52	1.63	27	1
1:B:37:LEU:HD12	1:B:37:LEU:C	0.52	2.23	28	1
1:B:31:GLN:HB3	1:B:47:ILE:HG22	0.52	1.80	14	16
1:A:47:ILE:CG2	1:A:48:THR:N	0.52	2.72	2	4
1:B:39:ASN:O	1:B:41:HIS:N	0.52	2.43	9	6
1:B:72:GLN:C	1:B:73:PHE:CG	0.52	2.81	8	3
1:B:33:CYS:SG	1:B:47:ILE:CD1	0.52	2.97	9	5
1:A:31:GLN:OE1	1:A:56:TYR:N	0.52	2.41	8	2
1:A:7:LYS:HE2	1:A:34:TYR:CD2	0.52	2.39	10	2
1:A:64:HIS:N	1:A:82:ARG:O	0.52	2.42	13	8
1:B:80:ARG:O	1:B:81:LEU:C	0.52	2.47	4	23
1:A:72:GLN:C	1:A:73:PHE:CG	0.52	2.81	8	3
1:A:12:GLN:HA	1:A:55:ALA:HB3	0.52	1.82	17	4
1:B:7:LYS:CD	1:B:34:TYR:CE2	0.52	2.92	11	4
1:A:6:ILE:CD1	1:A:83:LEU:CD2	0.52	2.88	22	3
1:A:62:THR:HG23	1:A:86:ALA:CB	0.52	2.34	28	13
1:B:47:ILE:CG2	1:B:47:ILE:O	0.52	2.56	1	3
1:B:31:GLN:O	1:B:47:ILE:N	0.52	2.43	13	6
1:A:43:VAL:CG2	1:A:43:VAL:O	0.52	2.57	19	4
1:B:7:LYS:CG	1:B:34:TYR:CE1	0.52	2.92	18	2
1:A:65:LEU:HD12	1:A:65:LEU:O	0.52	2.04	8	4
1:B:31:GLN:OE1	1:B:55:ALA:CB	0.52	2.55	7	2
1:A:68:PHE:CD1	1:A:78:ILE:HG12	0.52	2.38	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:TYR:CE1	1:B:83:LEU:O	0.52	2.63	13	1
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: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:36:ASP:OD1	1:A:36:ASP:N	0.52	2.43	14	3
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:37:LEU:O	1:A:37:LEU:CD1	0.52	2.57	26	2
1:A:37:LEU:HG	1:B:65:LEU:CD1	0.52	2.34	1	3
1:A:39:ASN:O	1:A:40:GLU:C	0.52	2.48	15	15
1:B:3:LYS:N	1:B:37:LEU:CD1	0.52	2.64	1	1
1:A:31:GLN:O	1:A:47:ILE:N	0.52	2.43	9	6
1:B:47:ILE:CG2	1:B:48:THR:N	0.52	2.73	2	4
1:A:68:PHE:CD1	1:A:78:ILE:HG13	0.52	2.40	4	1
1:A:6:ILE:CD1	1:A:61:TYR:CG	0.52	2.92	7	3
1:A:1:MET:CG	1:A:1:MET:O	0.52	2.56	9	1
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
1:B:36:ASP:OD1	1:B:36:ASP:N	0.52	2.42	28	6
1:A:35:VAL:O	1:A:37:LEU:CD2	0.52	2.57	7	1
1:A:39:ASN:O	1:A:41:HIS:ND1	0.52	2.43	19	1
1:B:39:ASN:O	1:B:41:HIS:NE2	0.52	2.42	27	1
1:A:35:VAL:CG1	1:A:37:LEU:HG	0.52	2.34	28	1
1:B:28:LEU:HD22	1:B:48:THR:CG2	0.52	2.35	4	4
1:B:47:ILE:HG12	1:B:56:TYR:CZ	0.52	2.40	26	18
1:B:63:VAL:CG1	1:B:81:LEU:CD1	0.52	2.87	4	2
1:B:72:GLN:O	1:B:72:GLN:NE2	0.52	2.43	18	5
1:A:76:LEU:HB2	1:B:81:LEU:HD13	0.52	1.79	14	5
1:B:6:ILE:CD1	1:B:83:LEU:CD2	0.52	2.88	22	3
1:A:70:VAL:HG11	1:B:45:VAL:CG1	0.52	2.35	28	3
1:B:43:VAL:O	1:B:43:VAL:HG23	0.52	2.03	7	3
1:A:7:LYS:CG	1:A:34:TYR:CE1	0.52	2.93	18	2
1:A:33:CYS:SG	1:A:47:ILE:CD1	0.52	2.97	9	5
1:A:62:THR:O	1:A:84:VAL:HG23	0.52	2.05	13	1
1:B:31:GLN:NE2	1:B:56:TYR:O	0.52	2.41	17	12
1:B:32:LEU:CD2	1:B:44:LEU:CD1	0.52	2.87	10	1
1:B:47:ILE:HG21	1:B:56:TYR:CE2	0.52	2.40	13	1
1:B:70:VAL:HG13	1:B:76:LEU:HD12	0.52	1.82	18	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ASP:O	1:A:39:ASN:N	0.51	2.41	26	6
1:B:6:ILE:CD1	1:B:33:CYS:SG	0.51	2.98	16	2
1:B:39:ASN:N	1:B:39:ASN:OD1	0.51	2.43	28	3
1:B:35:VAL:CG1	1:B:36:ASP:N	0.51	2.73	26	2
1:A:28:LEU:HD22	1:A:48:THR:CG2	0.51	2.35	4	4
1:B:67:SER:OG	1:B:82:ARG:N	0.51	2.43	28	7
1:A:65:LEU:CD1	1:B:37:LEU:CA	0.51	2.88	19	4
1:A:67:SER:O	1:A:79:ASP:N	0.51	2.43	9	2
1:B:34:TYR:CE2	1:B:44:LEU:HB2	0.51	2.40	28	3
1:A:35:VAL:CG1	1:A:36:ASP:N	0.51	2.73	26	2
1:B:71:GLY:O	1:B:72:GLN:CG	0.51	2.59	28	1
1:A:2:ILE:HG22	1:B:65:LEU:HD13	0.51	1.81	30	1
1:B:62:THR:N	1:B:84:VAL:O	0.51	2.39	26	25
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
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:37:LEU:HD22	1:B:65:LEU:CD2	0.51	2.35	21	1
1:A:72:GLN:O	1:A:72:GLN:NE2	0.51	2.44	27	5
1:A:70:VAL:HG11	1:B:45:VAL:CG2	0.51	2.36	9	2
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:CD1	1:B:37:LEU:C	0.51	2.78	29	4
1:A:2:ILE:HG22	1:A:37:LEU:CD2	0.51	2.36	28	1
1:A:36:ASP:N	1:A:36:ASP:OD1	0.51	2.43	28	4
1:A:67:SER:OG	1:A:82:ARG:N	0.51	2.43	28	7
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:2:ILE:HA	1:B:65:LEU:CD2	0.51	2.36	11	2
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:A:65:LEU:O	1:A:68:PHE:N	0.51	2.43	13	3
1:A:56:TYR:CE1	1:A:83:LEU:O	0.51	2.63	13	1
1:B:2:ILE:HG22	1:B:37:LEU:CD2	0.51	2.36	28	1
1:A:4:VAL:HB	1:A:61:TYR:CB	0.51	2.36	25	11
1:A:63:VAL:HG13	1:A:81:LEU:CG	0.51	2.36	4	1
1:B:76:LEU:C	1:B:77:MET:CG	0.51	2.79	4	6
1:B:7:LYS:HE2	1:B:34:TYR:CE2	0.51	2.41	6	3
1:A:57:ALA:CB	1:A:58:PRO:CD	0.51	2.88	15	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:O	1:A:61:TYR:N	0.51	2.43	2	8
1:A:37:LEU:HD23	1:A:39:ASN:OD1	0.51	2.06	4	1
1:A:65:LEU:HB2	1:A:68:PHE:CE2	0.51	2.41	25	2
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:B:65:LEU:O	1:B:68:PHE:N	0.51	2.43	13	3
1:A:56:TYR:CZ	1:A:83:LEU:HB3	0.51	2.41	13	1
1:B:76:LEU:HD23	1:B:76:LEU:C	0.51	2.26	25	2
1:B:4:VAL:HB	1:B:61:TYR:CB	0.51	2.36	25	11
1:B:54:PRO:O	1:B:55:ALA:C	0.51	2.48	8	30
1:A:37:LEU:CA	1:B:65:LEU:CD1	0.51	2.89	19	4
1:B:63:VAL:HG13	1:B:81:LEU:CG	0.51	2.36	4	1
1:A:29:ASN:ND2	1:A:50:ASP:O	0.51	2.43	11	6
1:B:62:THR:O	1:B:84:VAL:HG23	0.51	2.06	13	1
1:A:6:ILE:CD1	1:A:33:CYS:SG	0.51	2.98	16	2
1:A:7:LYS:HD2	1:A:34:TYR:CZ	0.51	2.41	28	2
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:65:LEU:HA	1:B:68:PHE:CE2	0.51	2.41	5	19
1:B:67:SER:O	1:B:79:ASP:N	0.51	2.43	9	3
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:A:40:GLU:O	1:A:41:HIS:HB3	0.51	2.06	8	1
1:A:76:LEU:HD23	1:A:76:LEU:C	0.51	2.27	25	2
1:A:2:ILE:HA	1:A:37:LEU:HD22	0.51	1.83	28	1
1:A:35:VAL:HG12	1:A:37:LEU:CD2	0.50	2.36	1	1
1:A:65:LEU:CD2	1:B:1:MET:C	0.50	2.80	22	9
1:A:39:ASN:OD1	1:A:39:ASN:N	0.50	2.42	28	6
1:B:39:ASN:O	1:B:40:GLU:CB	0.50	2.59	4	2
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:54:PRO:O	1:A:55:ALA:C	0.50	2.48	8	29
1:B:37:LEU:HD23	1:B:39:ASN:OD1	0.50	2.06	4	1
1:A:13:PHE:CB	1:A:30:GLU:O	0.50	2.60	12	4
1:A:37:LEU:HA	1:B:65:LEU:HD11	0.50	1.83	25	2
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:HD21	1:B:37:LEU:HD22	0.50	1.82	21	1
1:A:65:LEU:CD2	1:B:37:LEU:HD22	0.50	2.36	21	1
1:A:29:ASN:HD22	1:A:49:LEU:HD12	0.50	1.67	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:7:LYS:HD2	1:B:34:TYR:CZ	0.50	2.42	28	2
1:B:49:LEU:CD1	1:B:50:ASP:O	0.50	2.59	24	2
1:A:64:HIS:HB2	1:A:82:ARG:O	0.50	2.07	2	22
1:A:13:PHE:CD1	1:A:29:ASN:HB2	0.50	2.41	17	6
1:B:35:VAL:O	1:B:43:VAL:CG2	0.50	2.58	23	8
1:A:76:LEU:C	1:A:77:MET:CG	0.50	2.79	4	6
1:B:7:LYS:HE2	1:B:34:TYR:CE1	0.50	2.42	5	1
1:A:1:MET:C	1:B:65:LEU:CD2	0.50	2.80	18	8
1:B:40:GLU:O	1:B:41:HIS:HB3	0.50	2.06	8	1
1:A:37:LEU:HD22	1:B:65:LEU:HD21	0.50	1.82	21	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
1:A:83:LEU:O	1:A:84:VAL:CG1	0.50	2.60	1	2
1:B:83:LEU:O	1:B:84:VAL:CG1	0.50	2.59	1	2
1:A:4:VAL:HG22	1:A:35:VAL:HG13	0.50	1.83	17	2
1:A:6:ILE:CG1	1:A:61:TYR:CE1	0.50	2.94	10	3
1:B:37:LEU:N	1:B:37:LEU:CD1	0.50	2.72	17	1
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:B:31:GLN:OE1	1:B:32:LEU:N	0.50	2.45	19	2
1:A:1:MET:O	1:A:2:ILE:CB	0.50	2.60	26	5
1:B:13:PHE:CB	1:B:30:GLU:O	0.50	2.59	12	4
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:28:LEU:CD2	1:B:48:THR:CG2	0.50	2.90	1	1
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:49:LEU:CD2	1:B:56:TYR:CE1	0.49	2.95	1	1
1:B:63:VAL:HG12	1:B:64:HIS:N	0.49	2.22	5	10
1:A:55:ALA:O	1:A:57:ALA:N	0.49	2.45	12	6
1:B:4:VAL:HG22	1:B:35:VAL:HG13	0.49	1.83	17	2
1:A:32:LEU:HD13	1:A:45:VAL:O	0.49	2.07	9	1
1:B:6:ILE:CD1	1:B:56:TYR:CB	0.49	2.90	13	3
1:B:47:ILE:HD12	1:B:56:TYR:HE2	0.49	1.67	13	1
1:A:45:VAL:CG1	1:B:70:VAL:HG11	0.49	2.37	28	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:HA	1:A:34:TYR:O	0.49	2.08	20	24
1:B:7:LYS:HB2	1:B:10:GLN:CG	0.49	2.38	26	3
1:A:37:LEU:CG	1:A:37:LEU:O	0.49	2.60	8	3
1:B:4:VAL:HG21	1:B:35:VAL:HG22	0.49	1.79	7	3
1:B:29:ASN:OD1	1:B:49:LEU:O	0.49	2.30	7	6
1:A:32:LEU:HD23	1:A:44:LEU:HD11	0.49	1.81	10	2
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: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:39:ASN:O	1:A:41:HIS:O	0.49	2.30	15	6
1:B:67:SER:O	1:B:78:ILE:O	0.49	2.31	7	4
1:A:70:VAL:HG13	1:B:45:VAL:CG2	0.49	2.37	22	2
1:A:31:GLN:OE1	1:A:32:LEU:O	0.49	2.31	17	18
1:A:49:LEU:CD2	1:A:56:TYR:CE1	0.49	2.95	1	1
1:A:62:THR:N	1:A:84:VAL:O	0.49	2.40	1	30
1:A:65:LEU:CB	1:B:2:ILE:HG12	0.49	2.38	1	8
1:B:39:ASN:O	1:B:41:HIS:O	0.49	2.31	18	7
1:A:7:LYS:HE2	1:A:34:TYR:CE1	0.49	2.42	5	1
1:A:67:SER:O	1:A:78:ILE:O	0.49	2.30	7	4
1:A:49:LEU:CD2	1:A:55:ALA:HA	0.49	2.38	8	7
1:B:10:GLN:O	1:B:31:GLN:OE1	0.49	2.30	16	8
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:68:PHE:CE1	1:A:78:ILE:HG13	0.49	2.43	4	1
1:A:79:ASP:O	1:A:80:ARG:HB3	0.49	2.08	18	3
1:B:37:LEU:C	1:B:37:LEU:HD13	0.49	2.28	16	2
1:A:67:SER:HB3	1:A:80:ARG:C	0.49	2.28	13	19
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:B:6:ILE:HD12	1:B:56:TYR:CB	0.49	2.38	23	3
1:B:31:GLN:OE1	1:B:49:LEU:HD23	0.49	2.08	8	1
1:A:1:MET:C	1:A:2:ILE:CG1	0.49	2.81	9	1
1:A:7:LYS:HD3	1:A:34:TYR:CG	0.49	2.43	10	2
1:A:6:ILE:HD13	1:A:56:TYR:CB	0.49	2.36	13	1
1:A:47:ILE:HD12	1:A:56:TYR:HE2	0.49	1.68	13	1
1:B:6:ILE:HD13	1:B:56:TYR:CB	0.49	2.37	13	1
1:A:12:GLN:HA	1:A:55:ALA:CB	0.49	2.38	17	2
1:A:38:GLY:O	1:A:39:ASN:ND2	0.49	2.45	26	1
1:A:60:LEU:O	1:A:85:PRO:HA	0.49	2.08	6	26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:PHE:CE1	1:B:78:ILE:HG13	0.49	2.42	4	1
1:B:78:ILE:HG22	1:B:79:ASP:N	0.49	2.23	19	4
1:A:7:LYS:HG3	1:A:34:TYR:CE1	0.49	2.43	27	3
1:A:47:ILE:HD11	1:A:83:LEU:HD12	0.49	1.83	24	3
1:B:34:TYR:CE2	1:B:44:LEU:CD1	0.49	2.93	17	1
1:B:29:ASN:CB	1:B:49:LEU:O	0.49	2.61	18	1
1:A:65:LEU:HD11	1:B:37:LEU:HA	0.49	1.83	25	2
1:A:37:LEU:HA	1:B:65:LEU:CD1	0.49	2.37	3	4
1:B:2:ILE:HG21	1:B:63:VAL:CG2	0.49	2.36	5	1
1:B:1:MET:O	1:B:2:ILE:CB	0.49	2.60	26	4
1:B:61:TYR:CD2	1:B:83:LEU:CD2	0.49	2.96	8	4
1:B:7:LYS:HD3	1:B:34:TYR:CG	0.49	2.43	24	2
1:B:47:ILE:HG23	1:B:56:TYR:CE1	0.49	2.43	1	4
1:B:6:ILE:HD13	1:B:61:TYR:CZ	0.49	2.43	11	6
1:B:37:LEU:O	1:B:37:LEU:CG	0.49	2.60	8	6
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:A:6:ILE:HD12	1:A:56:TYR:CB	0.49	2.38	23	3
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:32:LEU:HD13	1:B:45:VAL:O	0.49	2.07	9	1
1:A:32:LEU:HD23	1:A:44:LEU:CD1	0.49	2.37	10	1
1:B:83:LEU:HG	1:B:84:VAL:N	0.49	2.23	29	4
1:A:33:CYS:O	1:A:44:LEU:HA	0.48	2.08	15	22
1:A:67:SER:OG	1:A:80:ARG:O	0.48	2.31	20	20
1:B:29:ASN:HD22	1:B:49:LEU:HD12	0.48	1.67	1	1
1:B:35:VAL:HG12	1:B:37:LEU:CD2	0.48	2.38	1	1
1:A:65:LEU:CD1	1:B:37:LEU:HA	0.48	2.38	3	4
1:A:37:LEU:CD1	1:B:69:LYS:CA	0.48	2.90	5	3
1:A:6:ILE:CG1	1:A:61:TYR:CD1	0.48	2.96	23	2
1:B:5:GLU:N	1:B:34:TYR:O	0.48	2.46	28	3
1:B:55:ALA:O	1:B:57:ALA:N	0.48	2.46	9	7
1:B:36:ASP:O	1:B:39:ASN:OD1	0.48	2.32	8	2
1:B:47:ILE:CG2	1:B:56:TYR:CE2	0.48	2.96	13	2
1:B:6:ILE:CG1	1:B:61:TYR:CD1	0.48	2.96	23	2
1:A:83:LEU:HG	1:A:84:VAL:N	0.48	2.22	29	4
1:A:2:ILE:HG12	1:B:65:LEU:CB	0.48	2.38	1	9
1:B:47:ILE:CD1	1:B:56:TYR:OH	0.48	2.61	1	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:A:10:GLN:O	1:A:31:GLN:OE1	0.48	2.31	16	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:SER:HB3	1:B:80:ARG:O	0.48	2.08	8	12
1:A:49:LEU:HD13	1:A:49:LEU:C	0.48	2.29	6	4
1:B:1:MET:C	1:B:2:ILE:CG1	0.48	2.81	9	1
1:A:28:LEU:C	1:A:28:LEU:CD1	0.48	2.78	17	2
1:B:71:GLY:C	1:B:72:GLN:NE2	0.48	2.67	21	2
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:13:PHE:CD1	1:A:13:PHE:C	0.48	2.87	18	12
1:A:32:LEU:N	1:A:32:LEU:CD1	0.48	2.74	28	2
1:B:31:GLN:OE1	1:B:32:LEU:O	0.48	2.31	9	18
1:B:34:TYR:CZ	1:B:44:LEU:HB2	0.48	2.44	11	13
1:B:82:ARG:NH1	1:B:82:ARG:HG3	0.48	2.24	1	2
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:3:LYS:O	1:A:35:VAL:HG13	0.48	2.09	21	2
1:B:3:LYS:O	1:B:35:VAL:HG13	0.48	2.08	21	2
1:A:7:LYS:CE	1:A:34:TYR:CD2	0.48	2.97	24	2
1:A:37:LEU:HD13	1:B:70:VAL:HG22	0.48	1.84	13	2
1:B:47:ILE:HD12	1:B:83:LEU:HD12	0.48	1.85	15	1
1:A:37:LEU:C	1:A:37:LEU:HD13	0.48	2.28	16	2
1:A:48:THR:OG1	1:A:80:ARG:CZ	0.48	2.62	18	1
1:A:2:ILE:HG21	1:B:76:LEU:CD2	0.48	2.37	16	2
1:A:7:LYS:HG3	1:A:34:TYR:CZ	0.48	2.44	27	3
1:A:37:LEU:HD22	1:A:39:ASN:ND2	0.48	2.23	13	2
1:B:33:CYS:O	1:B:44:LEU:HA	0.48	2.08	15	20
1:B:72:GLN:HA	1:B:72:GLN:NE2	0.48	2.23	3	3
1:A:2:ILE:CG1	1:B:65:LEU:HB3	0.48	2.39	4	2
1:A:11:ALA:O	1:A:55:ALA:HB3	0.48	2.09	15	3
1:B:32:LEU:HD23	1:B:44:LEU:CD1	0.48	2.38	10	1
1:A:31:GLN:OE1	1:A:32:LEU:N	0.48	2.45	19	2
1:A:76:LEU:HD22	1:B:81:LEU:CD1	0.48	2.38	23	1
1:A:3:LYS:O	1:A:37:LEU:HD11	0.48	2.09	1	1
1:A:6:ILE:O	1:A:7:LYS:O	0.48	2.32	2	16
1:A:47:ILE:CD1	1:A:56:TYR:OH	0.48	2.62	1	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:A:31:GLN:OE1	1:A:49:LEU:HD23	0.48	2.08	8	1
1:B:28:LEU:C	1:B:28:LEU:CD1	0.48	2.77	17	2
1:A:71:GLY:C	1:A:72:GLN:NE2	0.48	2.67	15	2
1:A:37:LEU:HD22	1:B:69:LYS:CA	0.48	2.38	17	1
1:B:12:GLN:HA	1:B:55:ALA:CB	0.48	2.38	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:ND2	1:A:43:VAL:CG1	0.48	2.76	29	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:79:ASP:O	1:B:80:ARG:HB3	0.48	2.08	18	3
1:B:70:VAL:O	1:B:71:GLY:O	0.48	2.32	8	1
1:B:80:ARG:CG	1:B:80:ARG:O	0.48	2.62	12	1
1:A:38:GLY:O	1:A:39:ASN:OD1	0.48	2.32	16	2
1:A:49:LEU:CD1	1:A:50:ASP:O	0.48	2.61	30	2
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:65:LEU:CB	1:B:2:ILE:HG23	0.48	2.38	30	1
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:B:4:VAL:HA	1:B:34:TYR:O	0.48	2.08	19	25
1:A:37:LEU:CD1	1:B:69:LYS:HA	0.48	2.39	8	3
1:B:29:ASN:O	1:B:49:LEU:HB2	0.48	2.09	25	6
1:B:32:LEU:HD22	1:B:44:LEU:HD11	0.48	1.82	10	2
1:A:65:LEU:CD2	1:B:2:ILE:HA	0.48	2.36	11	4
1:A:5:GLU:N	1:A:34:TYR:O	0.48	2.47	28	4
1:A:72:GLN:N	1:A:72:GLN:CD	0.48	2.67	15	1
1:A:45:VAL:CG2	1:B:75:SER:CA	0.48	2.92	16	1
1:A:2:ILE:HG23	1:B:65:LEU:CB	0.48	2.39	30	1
1:A:6:ILE:CD1	1:A:56:TYR:HB3	0.48	2.39	14	10
1:A:67:SER:HB3	1:A:80:ARG:O	0.48	2.09	24	14
1:A:65:LEU:HB3	1:B:2:ILE:CG1	0.48	2.39	4	2
1:B:49:LEU:HD13	1:B:49:LEU:C	0.48	2.29	6	5
1:B:72:GLN:N	1:B:72:GLN:CD	0.48	2.67	15	1
1:A:12:GLN:CA	1:A:55:ALA:CB	0.48	2.92	27	2
1:A:13:PHE:CG	1:A:29:ASN:HB2	0.47	2.44	1	1
1:A:78:ILE:HG22	1:A:79:ASP:N	0.47	2.23	19	4
1:A:36:ASP:O	1:A:39:ASN:OD1	0.47	2.32	8	2
1:A:74:GLY:O	1:A:75:SER:OG	0.47	2.32	9	2
1:A:79:ASP:O	1:A:80:ARG:HB2	0.47	2.08	12	7
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	3
1:A:81:LEU:C	1:A:81:LEU:CD1	0.47	2.78	8	1
1:B:32:LEU:HD23	1:B:44:LEU:HD11	0.47	1.82	10	2
1:A:31:GLN:C	1:A:32:LEU:HD22	0.47	2.30	9	2
1:A:73:PHE:CG	1:A:73:PHE:O	0.47	2.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:7:LYS:HD3	1:B:34:TYR:CE2	0.47	2.45	22	3
1:B:12:GLN:CA	1:B:55:ALA:CB	0.47	2.92	27	2
1:B:13:PHE:CD1	1:B:13:PHE:C	0.47	2.87	18	11
1:B:62:THR:CG2	1:B:86:ALA:HA	0.47	2.40	8	11
1:B:67:SER:CB	1:B:80:ARG:C	0.47	2.83	1	5
1:B:7:LYS:CE	1:B:34:TYR:CD2	0.47	2.97	24	2
1:A:68:PHE:CE1	1:A:78:ILE:HG23	0.47	2.45	13	1
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:B:79:ASP:O	1:B:80:ARG:HB2	0.47	2.09	12	4
1:B:83:LEU:O	1:B:84:VAL:HG13	0.47	2.10	1	1
1:A:3:LYS:C	1:A:4:VAL:HG23	0.47	2.30	25	10
1:A:6:ILE:HD12	1:A:56:TYR:HB2	0.47	1.85	8	2
1:A:45:VAL:CG2	1:B:70:VAL:HG11	0.47	2.39	9	3
1:B:38:GLY:O	1:B:39:ASN:OD1	0.47	2.32	16	2
1:A:28:LEU:N	1:A:28:LEU:HD13	0.47	2.24	18	1
1:A:80:ARG:NH1	1:A:80:ARG:HG3	0.47	2.24	18	2
1:B:65:LEU:O	1:B:67:SER:N	0.47	2.48	2	3
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:B:6:ILE:HG21	1:B:57:ALA:O	0.47	2.10	16	5
1:B:6:ILE:HD12	1:B:61:TYR:CD1	0.47	2.45	7	2
1:A:61:TYR:CD2	1:A:83:LEU:CD2	0.47	2.97	8	4
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: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:B:15:THR:HG23	1:B:28:LEU:C	0.47	2.30	29	1
1:A:82:ARG:NH1	1:A:82:ARG:HG3	0.47	2.24	1	2
1:B:50:ASP:CB	1:B:53:GLN:HB2	0.47	2.40	16	9
1:B:3:LYS:C	1:B:4:VAL:HG23	0.47	2.30	25	10
1:B:11:ALA:O	1:B:55:ALA:HB3	0.47	2.09	15	3
1:B:73:PHE:O	1:B:73:PHE:CG	0.47	2.67	10	1
1:B:56:TYR:CD1	1:B:61:TYR:CE2	0.47	3.03	13	1
1:B:36:ASP:CB	1:B:41:HIS:O	0.47	2.63	14	1
1:A:39:ASN:ND2	1:A:43:VAL:HG21	0.47	2.24	26	1
1:B:33:CYS:SG	1:B:83:LEU:HD12	0.47	2.50	1	1
1:B:67:SER:OG	1:B:80:ARG:O	0.47	2.33	3	20
1:A:76:LEU:CD2	1:B:2:ILE:HG21	0.47	2.39	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LYS:O	1:B:74:GLY:O	0.47	2.33	5	2
1:A:82:ARG:NH1	1:A:82:ARG:HG2	0.47	2.25	7	3
1:B:36:ASP:O	1:B:37:LEU:C	0.47	2.53	19	11
1:B:81:LEU:HD12	1:B:83:LEU:N	0.47	2.25	8	1
1:A:7:LYS:HD3	1:A:34:TYR:CE2	0.47	2.44	22	3
1:B:37:LEU:HD22	1:B:39:ASN:ND2	0.47	2.24	13	2
1:A:37:LEU:HD12	1:A:38:GLY:H	0.47	1.69	17	1
1:A:65:LEU:CD1	1:B:37:LEU:HB2	0.47	2.40	20	2
1:B:60:LEU:O	1:B:86:ALA:N	0.47	2.43	23	1
1:A:75:SER:N	1:B:45:VAL:HG23	0.47	2.25	29	1
1:A:34:TYR:CZ	1:A:44:LEU:HB2	0.47	2.45	28	13
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:39:ASN:O	1:B:40:GLU:HB2	0.47	2.10	4	1
1:B:31:GLN:C	1:B:32:LEU:HD22	0.47	2.30	9	2
1:A:29:ASN:O	1:A:49:LEU:HB2	0.47	2.09	25	6
1:A:56:TYR:CD1	1:A:61:TYR:CE2	0.47	3.03	13	1
1:A:47:ILE:HD12	1:A:83:LEU:HD12	0.47	1.85	15	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: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:39:ASN:OD1	1:A:41:HIS:O	0.47	2.32	8	1
1:A:10:GLN:OE1	1:A:34:TYR:CD2	0.47	2.68	26	1
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: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	3
1:A:39:ASN:O	1:A:40:GLU:HB2	0.47	2.10	4	1
1:A:70:VAL:O	1:A:71:GLY:O	0.47	2.32	8	1
1:B:10:GLN:NE2	1:B:33:CYS:HA	0.47	2.25	10	1
1:A:80:ARG:O	1:A:80:ARG:CG	0.47	2.62	12	1
1:A:50:ASP:CB	1:A:53:GLN:HB2	0.46	2.40	16	9
1:A:63:VAL:HG12	1:A:64:HIS:H	0.46	1.70	24	8
1:B:60:LEU:O	1:B:61:TYR:CD1	0.46	2.68	2	3
1:A:80:ARG:O	1:A:81:LEU:O	0.46	2.33	4	1
1:A:33:CYS:SG	1:A:83:LEU:HD12	0.46	2.50	1	1
1:A:67:SER:CB	1:A:80:ARG:C	0.46	2.83	1	6
1:A:36:ASP:O	1:A:37:LEU:C	0.46	2.52	9	11
1:A:4:VAL:HG22	1:A:5:GLU:N	0.46	2.25	8	3
1:A:68:PHE:O	1:A:69:LYS:CG	0.46	2.63	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:PHE:O	1:B:69:LYS:CG	0.46	2.63	9	2
1:A:70:VAL:HG22	1:B:37:LEU:HD13	0.46	1.86	13	2
1:B:80:ARG:HG3	1:B:80:ARG:NH1	0.46	2.24	18	1
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
1:A:7:LYS:CE	1:A:7:LYS:HA	0.46	2.40	13	3
1:A:65:LEU:HA	1:A:68:PHE:CD1	0.46	2.44	30	9
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: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:A:60:LEU:O	1:A:61:TYR:CD1	0.46	2.68	2	3
1:B:47:ILE:CD1	1:B:83:LEU:HB2	0.46	2.39	23	7
1:B:80:ARG:O	1:B:81:LEU:O	0.46	2.33	4	1
1:B:54:PRO:O	1:B:55:ALA:O	0.46	2.33	13	1
1:A:36:ASP:CB	1:A:41:HIS:O	0.46	2.63	14	1
1:B:28:LEU:N	1:B:28:LEU:HD13	0.46	2.24	18	1
1:B:10:GLN:OE1	1:B:34:TYR:CD2	0.46	2.68	26	1
1:B:82:ARG:NH1	1:B:82:ARG:CG	0.46	2.78	9	6
1:B:36:ASP:HA	1:B:41:HIS:O	0.46	2.11	6	11
1:B:39:ASN:OD1	1:B:39:ASN:N	0.46	2.49	3	3
1:B:78:ILE:HG21	1:B:81:LEU:HB3	0.46	1.87	18	4
1:B:6:ILE:HD12	1:B:56:TYR:HB2	0.46	1.85	8	2
1:A:37:LEU:HB3	1:B:65:LEU:CD1	0.46	2.40	30	1
1:A:37:LEU:CD2	1:A:37:LEU:C	0.46	2.84	1	1
1:A:82:ARG:NH1	1:A:82:ARG:CG	0.46	2.79	24	5
1:B:37:LEU:HD22	1:B:38:GLY:H	0.46	1.70	1	1
1:A:37:LEU:CD2	1:B:69:LYS:HA	0.46	2.40	15	7
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:B:56:TYR:O	1:B:57:ALA:O	0.46	2.33	7	5
1:A:35:VAL:HG12	1:A:37:LEU:N	0.46	2.26	8	1
1:A:73:PHE:CD1	1:A:73:PHE:N	0.46	2.84	8	3
1:B:35:VAL:HG12	1:B:37:LEU:N	0.46	2.26	8	1
1:A:65:LEU:HG	1:A:68:PHE:CE2	0.46	2.46	11	1
1:A:37:LEU:HB2	1:B:65:LEU:CD1	0.46	2.41	20	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:A:69:LYS:HA	1:B:37:LEU:CD1	0.46	2.41	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:68:PHE:CE1	1:B:78:ILE:HG23	0.46	2.45	13	1
1:B:80:ARG:NH1	1:B:80:ARG:CG	0.46	2.78	18	3
1:A:71:GLY:N	1:A:77:MET:SD	0.46	2.89	27	1
1:B:1:MET:O	1:B:2:ILE:C	0.46	2.54	30	1
1:B:35:VAL:HG13	1:B:37:LEU:CD1	0.46	2.38	1	1
1:A:37:LEU:O	1:A:37:LEU:CG	0.46	2.62	15	4
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
1:B:32:LEU:N	1:B:32:LEU:HD22	0.46	2.25	9	1
1:B:76:LEU:O	1:B:77:MET:HG2	0.46	2.11	19	11
1:B:48:THR:O	1:B:48:THR:CG2	0.46	2.61	25	1
1:B:71:GLY:N	1:B:77:MET:SD	0.46	2.89	27	1
1:A:33:CYS:SG	1:A:45:VAL:HG13	0.46	2.51	1	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:A:67:SER:HG	1:A:80:ARG:C	0.46	2.13	4	1
1:B:82:ARG:NH1	1:B:82:ARG:HG2	0.46	2.25	7	3
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:31:GLN:OE1	1:A:33:CYS:SG	0.46	2.74	15	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:83:LEU:C	1:A:84:VAL:HG13	0.46	2.32	1	2
1:B:37:LEU:CD2	1:B:37:LEU:C	0.46	2.84	1	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:6:ILE:O	1:A:6:ILE:HG22	0.46	2.11	30	4
1:A:36:ASP:O	1:A:39:ASN:CG	0.46	2.54	15	5
1:A:82:ARG:CG	1:A:82:ARG:NH1	0.46	2.78	9	3
1:A:45:VAL:CG1	1:B:75:SER:HA	0.46	2.41	13	1
1:B:31:GLN:OE1	1:B:33:CYS:SG	0.46	2.74	15	1
1:A:81:LEU:CG	1:A:81:LEU:O	0.46	2.64	27	1
1:A:7:LYS:CB	1:A:8:PRO:HD2	0.45	2.42	11	10
1:A:10:GLN:O	1:A:31:GLN:CD	0.45	2.54	29	7
1:A:81:LEU:O	1:A:81:LEU:HG	0.45	2.11	29	22
1:B:81:LEU:O	1:B:81:LEU:HG	0.45	2.11	17	22
1:B:32:LEU:C	1:B:33:CYS:SG	0.45	2.94	21	21
1:B:37:LEU:HD23	1:B:37:LEU:C	0.45	2.31	6	1
1:A:78:ILE:HG21	1:A:81:LEU:HB3	0.45	1.87	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ILE:CD1	1:B:78:ILE:HG13	0.45	2.40	13	2
1:B:37:LEU:CD1	1:B:38:GLY:N	0.45	2.64	28	1
1:A:33:CYS:SG	1:A:83:LEU:CD1	0.45	3.04	1	1
1:A:35:VAL:HG13	1:A:37:LEU:CD1	0.45	2.38	1	1
1:A:65:LEU:O	1:A:67:SER:N	0.45	2.49	2	3
1:A:2:ILE:CD1	1:A:63:VAL:HB	0.45	2.41	11	8
1:A:13:PHE:HD2	1:A:49:LEU:HD12	0.45	1.71	8	1
1:B:36:ASP:O	1:B:39:ASN:CG	0.45	2.55	15	5
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:HG2	0.45	2.11	9	11
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:54:PRO:O	1:A:55:ALA:O	0.45	2.33	13	1
1:B:37:LEU:HD12	1:B:38:GLY:H	0.45	1.69	17	1
1:B:29:ASN:CG	1:B:49:LEU:O	0.45	2.55	22	1
1:A:74:GLY:O	1:B:46:LYS:N	0.45	2.49	24	1
1:B:10:GLN:O	1:B:31:GLN:CD	0.45	2.54	29	7
1:B:51:GLU:O	1:B:52:GLY:C	0.45	2.53	6	3
1:B:59:GLY:O	1:B:60:LEU:C	0.45	2.55	13	2
1:B:40:GLU:C	1:B:41:HIS:ND1	0.45	2.69	2	1
1:A:13:PHE:CD2	1:A:49:LEU:CG	0.45	2.99	26	5
1:A:29:ASN:HB2	1:A:49:LEU:HB3	0.45	1.88	15	6
1:B:4:VAL:HG13	1:B:61:TYR:O	0.45	2.10	23	3
1:A:10:GLN:NE2	1:A:33:CYS:HA	0.45	2.26	10	1
1:A:13:PHE:HB2	1:A:30:GLU:O	0.45	2.12	12	1
1:A:37:LEU:N	1:A:37:LEU:CD1	0.45	2.72	17	1
1:A:28:LEU:C	1:A:28:LEU:CD2	0.45	2.78	18	1
1:B:7:LYS:HD2	1:B:34:TYR:CD1	0.45	2.45	18	1
1:A:31:GLN:CA	1:A:47:ILE:HG22	0.45	2.42	22	3
1:A:35:VAL:CG1	1:A:37:LEU:CD2	0.45	2.94	1	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: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	2
1:A:39:ASN:HB3	1:A:41:HIS:NE2	0.45	2.27	19	1
1:B:81:LEU:CG	1:B:81:LEU:O	0.45	2.64	27	1
1:A:65:LEU:C	1:A:67:SER:N	0.45	2.69	2	11
1:B:35:VAL:CG1	1:B:37:LEU:HD11	0.45	2.38	1	1
1:A:40:GLU:C	1:A:41:HIS:ND1	0.45	2.69	2	1
1:A:4:VAL:HG23	1:A:34:TYR:O	0.45	2.12	15	8
1:A:6:ILE:HG13	1:A:33:CYS:CB	0.45	2.42	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:A:36:ASP:OD2	1:A:42:PRO:CA	0.45	2.65	19	2
1:A:29:ASN:CG	1:A:49:LEU:O	0.45	2.55	22	1
1:A:70:VAL:CG1	1:B:45:VAL:HG11	0.45	2.42	23	1
1:A:65:LEU:CD1	1:B:37:LEU:CG	0.45	2.95	1	1
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
1:B:4:VAL:HG23	1:B:34:TYR:O	0.45	2.12	15	8
1:B:13:PHE:HD2	1:B:49:LEU:HD12	0.45	1.72	8	1
1:A:2:ILE:O	1:A:62:THR:HA	0.45	2.11	30	4
1:B:65:LEU:HG	1:B:68:PHE:CE2	0.45	2.46	11	1
1:A:32:LEU:O	1:A:33:CYS:SG	0.45	2.74	30	2
1:A:45:VAL:CG2	1:B:74:GLY:C	0.45	2.85	16	1
1:B:4:VAL:HG21	1:B:83:LEU:CD1	0.45	2.41	22	2
1:A:45:VAL:HG11	1:B:70:VAL:CG1	0.45	2.42	23	1
1:B:65:LEU:C	1:B:67:SER:N	0.45	2.70	11	10
1:A:72:GLN:O	1:A:72:GLN:CD	0.45	2.55	11	2
1:A:56:TYR:N	1:A:56:TYR:CD1	0.45	2.85	9	3
1:B:38:GLY:C	1:B:39:ASN:OD1	0.45	2.55	9	2
1:B:74:GLY:O	1:B:75:SER:OG	0.45	2.32	9	3
1:B:76:LEU:O	1:B:77:MET:SD	0.45	2.75	12	1
1:B:6:ILE:HG13	1:B:33:CYS:SG	0.45	2.52	15	1
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:A:37:LEU:HD21	1:B:68:PHE:O	0.45	2.11	27	3
1:A:68:PHE:O	1:B:37:LEU:HD21	0.45	2.11	27	3
1:B:63:VAL:HG12	1:B:64:HIS:H	0.45	1.71	24	8
1:B:72:GLN:O	1:B:72:GLN:CD	0.45	2.55	2	2
1:B:78:ILE:CG2	1:B:81:LEU:HB3	0.45	2.42	18	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:36:ASP:O	1:A:37:LEU:HG	0.45	2.12	7	1
1:B:73:PHE:CD1	1:B:73:PHE:N	0.45	2.84	21	3
1:A:49:LEU:O	1:A:50:ASP:O	0.45	2.34	11	1
1:B:48:THR:O	1:B:49:LEU:C	0.45	2.55	25	3
1:B:80:ARG:NH1	1:B:80:ARG:HG2	0.45	2.27	17	1
1:B:81:LEU:O	1:B:81:LEU:HD23	0.45	2.10	19	1
1:A:3:LYS:N	1:A:37:LEU:HD11	0.45	2.27	21	1
1:A:29:ASN:HB3	1:A:49:LEU:CB	0.45	2.42	2	2
1:B:7:LYS:CB	1:B:8:PRO:HD2	0.45	2.42	11	10

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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:2:ILE:HB	1:B:63:VAL:CG2	0.45	2.41	8	3
1:B:13:PHE:HA	1:B:31:GLN:CG	0.45	2.42	8	1
1:B:36:ASP:O	1:B:37:LEU:CB	0.45	2.65	29	4
1:B:49:LEU:O	1:B:50:ASP:O	0.45	2.34	11	1
1:A:78:ILE:HG13	1:B:78:ILE:CD1	0.45	2.42	24	2
1:A:6:ILE:HG13	1:A:33:CYS:SG	0.45	2.52	15	2
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: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:56:TYR:CE2	1:A:83:LEU:HB2	0.45	2.46	10	3
1:B:34:TYR:HB3	1:B:42:PRO:CB	0.45	2.41	14	7
1:A:40:GLU:O	1:A:41:HIS:HB2	0.45	2.11	23	3
1:A:55:ALA:O	1:A:56:TYR:C	0.45	2.56	8	9
1:B:31:GLN:OE1	1:B:55:ALA:HA	0.45	2.12	8	1
1:A:38:GLY:C	1:A:39:ASN:OD1	0.45	2.55	9	2
1:A:80:ARG:NH1	1:A:80:ARG:CG	0.45	2.79	28	2
1:B:7:LYS:HD3	1:B:34:TYR:CE1	0.45	2.47	18	1
1:A:74:GLY:O	1:B:46:LYS:CB	0.45	2.65	24	1
1:B:80:ARG:NH1	1:B:80:ARG:HG3	0.45	2.26	28	1
1:A:69:LYS:HB2	1:A:69:LYS:NZ	0.45	2.27	30	1
1:B:35:VAL:CG1	1:B:37:LEU:CD2	0.44	2.95	1	1
1:A:69:LYS:CA	1:B:37:LEU:CD1	0.44	2.95	5	3
1:B:6:ILE:HG13	1:B:33:CYS:CB	0.44	2.42	15	2
1:B:1:MET:O	1:B:2:ILE:HB	0.44	2.12	26	3
1:B:67:SER:O	1:B:79:ASP:HB2	0.44	2.12	9	1
1:A:86:ALA:O	1:A:87:LYS:CB	0.44	2.65	17	1
1:B:31:GLN:CA	1:B:47:ILE:HG22	0.44	2.42	22	3
1:A:65:LEU:HD13	1:B:37:LEU:HD22	0.44	1.87	28	1
1:B:4:VAL:HB	1:B:61:TYR:HB2	0.44	1.89	16	11
1:A:77:MET:O	1:A:78:ILE:C	0.44	2.54	27	7
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:B:55:ALA:O	1:B:56:TYR:C	0.44	2.56	8	8
1:A:69:LYS:HA	1:B:37:LEU:CD2	0.44	2.41	15	5
1:A:67:SER:O	1:A:79:ASP:HB2	0.44	2.12	9	1
1:A:2:ILE:CG2	1:B:76:LEU:HD13	0.44	2.42	11	1
1:A:51:GLU:O	1:A:52:GLY:C	0.44	2.55	23	3
1:B:83:LEU:C	1:B:84:VAL:HG13	0.44	2.32	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HA	1:B:65:LEU:CD1	0.44	2.39	10	3
1:B:76:LEU:HD23	1:B:77:MET:H	0.44	1.66	9	1
1:A:80:ARG:CG	1:A:80:ARG:NH1	0.44	2.78	17	1
1:B:39:ASN:HB3	1:B:41:HIS:NE2	0.44	2.26	19	1
1:B:65:LEU:O	1:B:66:SER:C	0.44	2.56	11	3
1:A:78:ILE:O	1:A:79:ASP:C	0.44	2.55	8	3
1:B:2:ILE:CD1	1:B:63:VAL:HB	0.44	2.41	11	8
1:B:56:TYR:N	1:B:56:TYR:CD1	0.44	2.85	9	3
1:A:1:MET:O	1:A:2:ILE:HB	0.44	2.12	26	3
1:B:36:ASP:O	1:B:37:LEU:HG	0.44	2.12	7	1
1:A:37:LEU:HB3	1:A:39:ASN:ND2	0.44	2.27	8	2
1:B:13:PHE:HA	1:B:31:GLN:HG3	0.44	1.89	8	1
1:A:2:ILE:H	1:B:65:LEU:HD11	0.44	1.73	9	1
1:A:47:ILE:HD12	1:A:56:TYR:CE2	0.44	2.47	10	1
1:B:10:GLN:CB	1:B:32:LEU:HB2	0.44	2.42	13	1
1:A:79:ASP:OD1	1:A:79:ASP:O	0.44	2.35	26	1
1:A:3:LYS:HD3	1:A:60:LEU:HD21	0.44	1.89	28	1
1:A:47:ILE:O	1:A:47:ILE:HG23	0.44	2.13	1	3
1:A:4:VAL:CA	1:A:34:TYR:O	0.44	2.65	20	5
1:A:28:LEU:CD2	1:A:50:ASP:HB3	0.44	2.43	6	1
1:B:81:LEU:HD12	1:B:82:ARG:N	0.44	2.28	8	1
1:B:47:ILE:HD12	1:B:56:TYR:CE2	0.44	2.48	10	1
1:A:36:ASP:O	1:A:39:ASN:ND2	0.44	2.51	15	1
1:A:80:ARG:NH1	1:A:80:ARG:HG2	0.44	2.28	17	1
1:B:3:LYS:N	1:B:37:LEU:HD11	0.44	2.28	21	1
1:B:71:GLY:O	1:B:72:GLN:CB	0.44	2.66	28	2
1:A:1:MET:O	1:A:2:ILE:C	0.44	2.54	30	1
1:A:65:LEU:HB3	1:B:2:ILE:HG12	0.44	1.90	1	7
1:B:72:GLN:O	1:B:73:PHE:HB2	0.44	2.13	1	7
1:B:29:ASN:HB2	1:B:49:LEU:HB3	0.44	1.89	25	7
1:B:29:ASN:HB3	1:B:49:LEU:CB	0.44	2.42	15	2
1:B:65:LEU:CA	1:B:68:PHE:CD2	0.44	3.01	14	10
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:6:ILE:CG1	1:A:33:CYS:SG	0.44	3.06	30	2
1:B:32:LEU:O	1:B:33:CYS:SG	0.44	2.74	30	2
1:A:74:GLY:O	1:B:45:VAL:HG22	0.44	2.13	24	1
1:A:65:LEU:CD1	1:B:37:LEU:HB3	0.44	2.41	30	2
1:A:2:ILE:HG12	1:B:65:LEU:HB3	0.44	1.88	1	5
1:A:7:LYS:CB	1:A:8:PRO:CD	0.44	2.96	5	8
1:A:37:LEU:HD23	1:B:65:LEU:CD1	0.44	2.42	1	1

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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: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:48:THR:O	1:A:49:LEU:C	0.44	2.55	11	4
1:B:82:ARG:CG	1:B:82:ARG:NH1	0.44	2.78	26	2
1:B:37:LEU:O	1:B:37:LEU:CD2	0.44	2.66	15	2
1:B:4:VAL:CA	1:B:34:TYR:O	0.44	2.66	20	4
1:B:6:ILE:CG1	1:B:33:CYS:SG	0.44	3.06	30	2
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:B:37:LEU:O	1:B:39:ASN:OD1	0.44	2.35	18	1
1:A:37:LEU:HD22	1:B:65:LEU:HD13	0.44	1.88	28	1
1:B:51:GLU:HG2	1:B:52:GLY:N	0.44	2.28	1	1
1:B:36:ASP:C	1:B:37:LEU:CD1	0.44	2.83	3	1
1:B:77:MET:O	1:B:78:ILE:C	0.44	2.56	14	8
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:36:ASP:O	1:A:37:LEU:CB	0.44	2.66	11	3
1:B:34:TYR:HA	1:B:43:VAL:O	0.44	2.13	20	5
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:B:41:HIS:ND1	1:B:41:HIS:N	0.44	2.64	28	1
1:A:2:ILE:HG13	1:A:63:VAL:CB	0.44	2.43	30	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:4:VAL:HG21	1:A:83:LEU:CD1	0.43	2.42	22	2
1:A:74:GLY:O	1:B:46:LYS:HB3	0.43	2.13	16	1
1:A:65:LEU:CD1	1:B:37:LEU:HD23	0.43	2.42	1	1
1:B:15:THR:HG23	1:B:29:ASN:OD1	0.43	2.13	2	1
1:B:56:TYR:CE2	1:B:83:LEU:HB2	0.43	2.49	2	3
1:A:65:LEU:CA	1:A:68:PHE:CD2	0.43	3.01	14	11
1:A:62:THR:O	1:A:63:VAL:O	0.43	2.36	11	3
1:A:65:LEU:HA	1:A:68:PHE:CZ	0.43	2.48	17	4
1:A:13:PHE:CG	1:A:49:LEU:CD1	0.43	2.99	6	1
1:A:4:VAL:HB	1:A:61:TYR:HB2	0.43	1.90	11	9
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:A:75:SER:HA	1:B:45:VAL:CG1	0.43	2.43	13	1
1:A:36:ASP:OD2	1:A:41:HIS:C	0.43	2.57	14	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:B:36:ASP:OD2	1:B:42:PRO:CA	0.43	2.66	19	2
1:B:79:ASP:O	1:B:79:ASP:OD1	0.43	2.35	26	1
1:B:12:GLN:O	1:B:12:GLN:CG	0.43	2.66	27	1
1:B:3:LYS:C	1:B:4:VAL:CG2	0.43	2.86	30	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: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:A:33:CYS:SG	1:A:47:ILE:HG12	0.43	2.54	10	3
1:B:36:ASP:O	1:B:39:ASN:ND2	0.43	2.51	15	1
1:B:65:LEU:HA	1:B:68:PHE:CZ	0.43	2.48	25	3
1:A:81:LEU:HD23	1:A:81:LEU:N	0.43	2.28	19	1
1:A:46:LYS:CB	1:B:74:GLY:O	0.43	2.66	24	1
1:B:2:ILE:HG13	1:B:63:VAL:CB	0.43	2.43	30	1
1:A:29:ASN:HB3	1:A:49:LEU:HB2	0.43	1.90	15	2
1:A:68:PHE:O	1:A:69:LYS:HG2	0.43	2.13	8	1
1:B:37:LEU:HB3	1:B:39:ASN:ND2	0.43	2.27	8	2
1:A:13:PHE:CA	1:A:30:GLU:O	0.43	2.66	12	2
1:A:34:TYR:HA	1:A:43:VAL:O	0.43	2.13	20	6
1:A:6:ILE:CG2	1:A:57:ALA:O	0.43	2.66	16	2
1:A:45:VAL:HG22	1:B:74:GLY:C	0.43	2.33	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:B:31:GLN:NE2	1:B:56:TYR:HB2	0.43	2.28	26	2
1:A:41:HIS:ND1	1:A:41:HIS:N	0.43	2.65	28	1
1:A:36:ASP:O	1:A:37:LEU:CD1	0.43	2.56	3	1
1:A:31:GLN:OE1	1:A:55:ALA:HA	0.43	2.13	8	1
1:B:47:ILE:HD11	1:B:83:LEU:HD12	0.43	1.89	15	4
1:B:38:GLY:O	1:B:39:ASN:CG	0.43	2.57	16	1
1:B:75:SER:O	1:B:76:LEU:O	0.43	2.37	18	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: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:45:VAL:HG23	1:B:75:SER:N	0.43	2.28	29	1
1:A:4:VAL:CG1	1:A:33:CYS:HB2	0.43	2.43	1	1
1:A:47:ILE:CG1	1:A:83:LEU:HB2	0.43	2.43	1	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:B:73:PHE:O	1:B:75:SER:OG	0.43	2.34	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD12	1:A:32:LEU:N	0.43	2.27	23	1
1:A:47:ILE:HD11	1:A:56:TYR:OH	0.43	2.13	1	1
1:B:7:LYS:NZ	1:B:7:LYS:HA	0.43	2.29	2	7
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:81:LEU:HD21	1:B:83:LEU:HG	0.43	1.90	4	1
1:A:7:LYS:HB3	1:A:8:PRO:HD2	0.43	1.91	9	7
1:A:13:PHE:HA	1:A:31:GLN:HG3	0.43	1.89	8	1
1:A:2:ILE:CB	1:B:65:LEU:HD21	0.43	2.44	11	1
1:B:1:MET:SD	1:B:62:THR:HB	0.43	2.54	29	8
1:A:76:LEU:C	1:A:77:MET:HG3	0.43	2.34	20	3
1:A:75:SER:CA	1:B:45:VAL:CG2	0.43	2.96	16	1
1:B:86:ALA:O	1:B:87:LYS:C	0.43	2.57	18	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:4:VAL:HG21	1:B:33:CYS:HB2	0.43	1.90	29	2
1:A:49:LEU:HD11	1:A:54:PRO:C	0.43	2.34	1	1
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:B:6:ILE:O	1:B:7:LYS:C	0.43	2.56	8	4
1:B:29:ASN:HB2	1:B:49:LEU:O	0.43	2.13	23	2
1:A:4:VAL:HG22	1:A:35:VAL:CB	0.43	2.43	7	2
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:74:GLY:C	1:A:75:SER:OG	0.43	2.57	25	2
1:A:62:THR:CG2	1:A:86:ALA:CB	0.43	2.96	11	3
1:B:36:ASP:OD1	1:B:37:LEU:N	0.43	2.52	12	1
1:A:81:LEU:HD13	1:B:76:LEU:CB	0.43	2.44	13	1
1:A:4:VAL:CG1	1:A:83:LEU:HD21	0.43	2.44	20	1
1:A:78:ILE:HD11	1:B:78:ILE:HG13	0.43	1.90	28	1
1:A:49:LEU:HD13	1:A:50:ASP:N	0.43	2.29	30	1
1:A:37:LEU:CG	1:B:65:LEU:CD1	0.43	2.96	1	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: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:49:LEU:O	1:B:50:ASP:C	0.43	2.56	9	2
1:B:3:LYS:HB3	1:B:36:ASP:OD2	0.43	2.14	12	1
1:B:2:ILE:CG2	1:B:63:VAL:HG23	0.43	2.44	13	1
1:A:37:LEU:CD1	1:A:38:GLY:N	0.43	2.64	28	1
1:B:47:ILE:O	1:B:47:ILE:HG23	0.43	2.13	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LYS:HA	1:A:7:LYS:NZ	0.43	2.29	19	6
1:B:5:GLU:O	1:B:34:TYR:HB2	0.43	2.14	6	14
1:A:50:ASP:O	1:A:51:GLU:CB	0.43	2.65	6	1
1:B:1:MET:HG3	1:B:62:THR:CG2	0.43	2.43	17	3
1:A:76:LEU:HD13	1:B:2:ILE:CG2	0.43	2.43	11	1
1:A:10:GLN:OE1	1:A:32:LEU:HB2	0.43	2.14	15	1
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:A:7:LYS:CB	1:A:10:GLN:HG2	0.42	2.44	2	1
1:B:7:LYS:CB	1:B:10:GLN:HG2	0.42	2.44	2	1
1:B:63:VAL:HG13	1:B:81:LEU:HG	0.42	1.88	4	1
1:B:56:TYR:O	1:B:57:ALA:C	0.42	2.57	7	2
1:A:81:LEU:HD11	1:A:83:LEU:HB2	0.42	1.91	8	1
1:A:65:LEU:HD11	1:B:2:ILE:H	0.42	1.73	9	1
1:A:43:VAL:CG1	1:B:70:VAL:HG21	0.42	2.44	14	1
1:B:76:LEU:C	1:B:76:LEU:CD2	0.42	2.86	17	2
1:B:4:VAL:CG1	1:B:83:LEU:HD21	0.42	2.44	20	1
1:A:65:LEU:HD13	1:B:37:LEU:HD13	0.42	1.82	28	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:1:MET:SD	1:A:62:THR:HB	0.42	2.54	14	8
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: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: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:76:LEU:HG	1:B:77:MET:N	0.42	2.27	28	1
1:B:49:LEU:HD13	1:B:50:ASP:N	0.42	2.29	30	1
1:A:31:GLN:HB2	1:A:47:ILE:HG22	0.42	1.90	2	1
1:B:47:ILE:CG1	1:B:56:TYR:CE2	0.42	3.02	2	4
1:A:2:ILE:CG2	1:B:65:LEU:CD2	0.42	2.86	9	1
1:A:65:LEU:HD22	1:B:37:LEU:HB3	0.42	1.91	11	1
1:B:75:SER:O	1:B:76:LEU:C	0.42	2.57	19	3
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
1:B:41:HIS:HB2	1:B:42:PRO:HD2	0.42	1.91	27	1
1:A:78:ILE:HG13	1:B:78:ILE:HD11	0.42	1.90	28	1
1:A:36:ASP:HB2	1:A:39:ASN:O	0.42	2.14	3	1
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

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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: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:B:4:VAL:O	1:B:5:GLU:HG3	0.42	2.14	27	3
1:A:6:ILE:HD11	1:A:56:TYR:HD2	0.42	1.74	26	1
1:A:81:LEU:HD21	1:A:83:LEU:HG	0.42	1.89	4	1
1:A:69:LYS:HG2	1:A:77:MET:O	0.42	2.14	7	1
1:B:7:LYS:HB3	1:B:8:PRO:HD2	0.42	1.91	9	7
1:A:2:ILE:HB	1:A:63:VAL:CG2	0.42	2.41	8	3
1:B:37:LEU:O	1:B:37:LEU:HD23	0.42	2.14	8	1
1:B:68:PHE:N	1:B:68:PHE:HD1	0.42	2.12	18	3
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:A:75:SER:O	1:A:76:LEU:O	0.42	2.37	18	1
1:B:28:LEU:C	1:B:28:LEU:CD2	0.42	2.78	18	1
1:A:28:LEU:O	1:A:29:ASN:C	0.42	2.58	27	2
1:B:6:ILE:HG12	1:B:56:TYR:CB	0.42	2.44	26	1
1:A:12:GLN:O	1:A:12:GLN:CG	0.42	2.67	27	1
1:A:4:VAL:HG21	1:A:33:CYS:HB2	0.42	1.90	29	1
1:B:36:ASP:HB2	1:B:39:ASN:O	0.42	2.14	3	1
1:B:76:LEU:C	1:B:77:MET:HG3	0.42	2.34	20	3
1:B:62:THR:O	1:B:63:VAL:O	0.42	2.37	5	3
1:B:6:ILE:O	1:B:58:PRO:HA	0.42	2.14	7	1
1:A:13:PHE:CA	1:A:31:GLN:HG3	0.42	2.44	8	1
1:A:65:LEU:HD21	1:B:2:ILE:CB	0.42	2.45	11	1
1:A:47:ILE:HD13	1:A:48:THR:H	0.42	1.75	19	1
1:B:7:LYS:N	1:B:7:LYS:HD2	0.42	2.29	19	2
1:B:4:VAL:CG1	1:B:61:TYR:O	0.42	2.68	23	1
1:A:71:GLY:O	1:A:72:GLN:C	0.42	2.55	26	1
1:A:41:HIS:HB2	1:A:42:PRO:HD2	0.42	1.91	27	1
1:A:13:PHE:H	1:A:55:ALA:HB2	0.42	1.75	17	4
1:A:13:PHE:CE1	1:A:29:ASN:CG	0.42	2.93	26	2
1:A:49:LEU:O	1:A:50:ASP:C	0.42	2.57	9	2
1:B:33:CYS:SG	1:B:47:ILE:HG12	0.42	2.54	10	3
1:A:36:ASP:OD1	1:A:37:LEU:N	0.42	2.52	12	1
1:A:29:ASN:O	1:A:49:LEU:O	0.42	2.38	18	1
1:A:56:TYR:CD2	1:A:83:LEU:HD22	0.42	2.50	26	1
1:A:51:GLU:HG2	1:A:52:GLY:N	0.42	2.28	1	1
1:A:41:HIS:CD2	1:A:41:HIS:O	0.42	2.73	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:37:LEU:HD11	1:B:69:LYS:C	0.42	2.35	13	1
1:B:29:ASN:ND2	1:B:49:LEU:HB3	0.42	2.30	13	1
1:B:36:ASP:OD2	1:B:41:HIS:C	0.42	2.57	14	1
1:B:72:GLN:O	1:B:72:GLN:HG2	0.42	2.14	29	2
1:A:3:LYS:HA	1:A:61:TYR:O	0.42	2.14	21	1
1:A:31:GLN:N	1:A:47:ILE:O	0.42	2.46	23	1
1:B:37:LEU:O	1:B:37:LEU:HD12	0.42	2.14	26	1
1:A:63:VAL:HA	1:A:83:LEU:HD12	0.42	1.92	27	1
1:A:4:VAL:HG23	1:A:34:TYR:C	0.42	2.35	2	1
1:B:65:LEU:O	1:B:65:LEU:HG	0.42	2.13	2	3
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: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:B:41:HIS:CD2	1:B:41:HIS:O	0.42	2.73	8	1
1:A:76:LEU:HD11	1:B:37:LEU:HD12	0.42	1.92	10	1
1:A:37:LEU:HD12	1:B:76:LEU:HD11	0.42	1.90	12	1
1:A:36:ASP:HB3	1:A:41:HIS:O	0.42	2.15	14	1
1:A:37:LEU:HG	1:B:65:LEU:CD2	0.42	2.45	26	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:49:LEU:HD22	1:A:49:LEU:HA	0.42	1.69	17	5
1:A:6:ILE:HB	1:A:57:ALA:O	0.42	2.15	10	1
1:A:28:LEU:HD13	1:A:28:LEU:O	0.42	2.14	18	1
1:A:37:LEU:HG	1:A:37:LEU:O	0.42	2.15	22	1
1:A:50:ASP:O	1:A:51:GLU:C	0.41	2.57	1	1
1:B:4:VAL:HG23	1:B:34:TYR:C	0.41	2.36	2	1
1:A:2:ILE:CG1	1:B:65:LEU:HD22	0.41	2.45	3	1
1:B:1:MET:O	1:B:1:MET:HG3	0.41	2.15	5	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:A:10:GLN:O	1:A:10:GLN:HG3	0.41	2.14	10	1
1:A:68:PHE:O	1:A:69:LYS:HG3	0.41	2.15	17	1
1:A:49:LEU:HD21	1:A:54:PRO:C	0.41	2.36	23	1
1:B:13:PHE:CE1	1:B:29:ASN:CG	0.41	2.93	26	1
1:B:4:VAL:CG1	1:B:61:TYR:HB2	0.41	2.45	1	1
1:A:33:CYS:SG	1:A:47:ILE:HG13	0.41	2.55	20	3
1:A:65:LEU:O	1:A:65:LEU:HG	0.41	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:74:GLY:C	1:B:75:SER:OG	0.41	2.57	25	2
1:A:6:ILE:HG13	1:A:61:TYR:CZ	0.41	2.50	10	1
1:A:3:LYS:HB3	1:A:36:ASP:OD2	0.41	2.14	12	1
1:B:49:LEU:HD22	1:B:49:LEU:HA	0.41	1.71	12	2
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:38:GLY:C	1:A:39:ASN:CG	0.41	2.79	16	2
1:B:28:LEU:HD13	1:B:28:LEU:O	0.41	2.14	18	1
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:A:2:ILE:CG2	1:A:37:LEU:HD22	0.41	2.46	28	1
1:B:15:THR:CG2	1:B:28:LEU:O	0.41	2.59	29	1
1:A:65:LEU:HD21	1:B:2:ILE:CG2	0.41	2.44	11	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:71:GLY:O	1:A:72:GLN:CB	0.41	2.66	28	1
1:A:13:PHE:CG	1:A:29:ASN:HB3	0.41	2.50	30	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: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:A:53:GLN:OE1	1:A:82:ARG:NH2	0.41	2.54	8	1
1:A:32:LEU:HA	1:A:45:VAL:O	0.41	2.16	9	2
1:B:38:GLY:C	1:B:39:ASN:CG	0.41	2.79	16	2
1:A:81:LEU:HD23	1:A:81:LEU:O	0.41	2.14	27	2
1:A:1:MET:O	1:A:37:LEU:CD2	0.41	2.67	21	1
1:B:10:GLN:OE1	1:B:34:TYR:CE2	0.41	2.74	26	1
1:B:69:LYS:O	1:B:77:MET:HG3	0.41	2.15	27	1
1:A:6:ILE:HD11	1:A:83:LEU:HD23	0.41	1.92	29	1
1:A:67:SER:OG	1:A:80:ARG:C	0.41	2.59	4	1
1:A:4:VAL:HB	1:A:35:VAL:CG2	0.41	2.42	12	2
1:A:76:LEU:O	1:A:77:MET:HG3	0.41	2.16	11	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:76:LEU:C	1:A:76:LEU:CD2	0.41	2.85	15	1
1:A:49:LEU:HG	1:A:55:ALA:HA	0.41	1.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:ASN:O	1:B:49:LEU:O	0.41	2.38	18	1
1:A:7:LYS:N	1:A:7:LYS:HD2	0.41	2.29	19	1
1:A:3:LYS:C	1:A:4:VAL:CG1	0.41	2.89	21	1
1:B:37:LEU:O	1:B:37:LEU:HG	0.41	2.15	22	1
1:A:86:ALA:O	1:A:87:LYS:O	0.41	2.38	26	1
1:A:73:PHE:O	1:A:73:PHE:CD1	0.41	2.74	29	1
1:A:36:ASP:O	1:A:37:LEU:HB3	0.41	2.15	6	2
1:A:6:ILE:O	1:A:58:PRO:HA	0.41	2.15	7	1
1:A:36:ASP:C	1:A:38:GLY:N	0.41	2.74	8	2
1:B:32:LEU:HA	1:B:45:VAL:O	0.41	2.16	26	2
1:B:6:ILE:HG13	1:B:61:TYR:CZ	0.41	2.49	10	1
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:B:2:ILE:HG22	1:B:35:VAL:CG1	0.41	2.46	23	1
1:A:4:VAL:O	1:A:5:GLU:HG3	0.41	2.14	27	2
1:B:6:ILE:HD11	1:B:56:TYR:HD2	0.41	1.76	26	1
1:B:2:ILE:CG2	1:B:37:LEU:HD22	0.41	2.46	28	1
1:B:13:PHE:CG	1:B:29:ASN:HB3	0.41	2.50	30	1
1:A:13:PHE:HB3	1:A:49:LEU:HG	0.41	1.93	1	2
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:B:4:VAL:HB	1:B:35:VAL:HA	0.41	1.92	5	1
1:A:2:ILE:HG21	1:B:76:LEU:HD13	0.41	1.92	11	2
1:A:37:LEU:HB3	1:B:65:LEU:HD22	0.41	1.91	11	1
1:A:63:VAL:HG22	1:A:83:LEU:HD12	0.41	1.92	13	1
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: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:63:VAL:CG1	1:B:81:LEU:CG	0.41	2.99	4	1
1:A:70:VAL:HG13	1:B:45:VAL:HG21	0.41	1.93	6	1
1:B:13:PHE:H	1:B:55:ALA:HB2	0.41	1.76	11	4
1:B:69:LYS:HG3	1:B:77:MET:O	0.41	2.14	7	1
1:B:6:ILE:HB	1:B:57:ALA:O	0.41	2.16	10	1
1:A:48:THR:O	1:A:48:THR:CG2	0.41	2.61	25	1
1:B:13:PHE:N	1:B:55:ALA:CB	0.41	2.84	26	1
1:B:36:ASP:HA	1:B:39:ASN:OD1	0.41	2.16	28	1
1:B:73:PHE:O	1:B:73:PHE:CD1	0.41	2.74	29	1
1:B:78:ILE:HG23	1:B:81:LEU:N	0.41	2.31	3	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLY:O	1:B:46:LYS:O	0.41	2.39	5	1
1:B:36:ASP:C	1:B:38:GLY:N	0.41	2.74	25	4
1:B:13:PHE:CA	1:B:31:GLN:HG3	0.41	2.45	8	1
1:B:53:GLN:OE1	1:B:82:ARG:NH2	0.41	2.54	8	1
1:A:65:LEU:O	1:A:66:SER:C	0.41	2.56	11	2
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:A:72:GLN:O	1:A:72:GLN:HG2	0.41	2.14	29	2
1:B:36:ASP:OD2	1:B:42:PRO:N	0.41	2.54	19	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:HD21	1:B:43:VAL:HG11	0.41	1.91	7	1
1:B:81:LEU:CD1	1:B:83:LEU:N	0.41	2.84	8	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:A:28:LEU:CD1	1:A:28:LEU:H	0.41	2.29	18	1
1:B:80:ARG:O	1:B:80:ARG:CG	0.40	2.69	1	1
1:B:1:MET:SD	1:B:62:THR:CB	0.40	3.09	23	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:75:SER:O	1:B:77:MET:HG3	0.40	2.16	4	1
1:A:76:LEU:HD23	1:A:77:MET:H	0.40	1.67	9	1
1:A:12:GLN:O	1:A:31:GLN:HG2	0.40	2.16	22	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: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:37:LEU:CD2	1:B:65:LEU:CD1	0.40	2.99	1	1
1:B:13:PHE:HB3	1:B:49:LEU:HG	0.40	1.93	14	2
1:B:71:GLY:O	1:B:75:SER:O	0.40	2.39	6	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:A:49:LEU:C	1:A:49:LEU:HD13	0.40	2.35	28	1
1:A:35:VAL:CG1	1:A:37:LEU:CD1	0.40	2.99	1	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: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:7:LYS:NZ	1:A:7:LYS:HA	0.40	2.31	15	2
1:A:74:GLY:C	1:B:45:VAL:HG22	0.40	2.37	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:2:ILE:HG22	1:A:35:VAL:CG1	0.40	2.46	23	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:B:71:GLY:O	1:B:75:SER:N	0.40	2.41	7	1
1:A:32:LEU:HD23	1:A:44:LEU:CG	0.40	2.47	8	1
1:A:14:THR:O	1:A:29:ASN:HA	0.40	2.17	12	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

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/87 (84%)	55±3 (76±3%)	13±2 (17±3%)	5±2 (7±2%)	2	17
1	B	73/87 (84%)	55±3 (76±4%)	13±2 (17±3%)	5±2 (7±2%)	2	16
All	All	4380/5220 (84%)	3319 (76%)	752 (17%)	309 (7%)	2	16

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	B	63	VAL	13
1	A	56	TYR	13
1	B	55	ALA	11
1	A	37	LEU	9
1	B	37	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	55	ALA	9
1	A	57	ALA	6
1	B	57	ALA	6
1	A	51	GLU	5
1	B	51	GLU	5
1	A	40	GLU	5
1	B	40	GLU	5
1	A	38	GLY	5
1	B	38	GLY	5
1	A	76	LEU	5
1	B	76	LEU	5
1	A	41	HIS	4
1	B	41	HIS	4
1	A	4	VAL	4
1	B	4	VAL	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	71	GLY	1
1	B	71	GLY	1
1	A	50	ASP	1
1	B	50	ASP	1
1	A	11	ALA	1
1	A	29	ASN	1
1	A	78	ILE	1
1	B	11	ALA	1
1	B	29	ASN	1
1	B	78	ILE	1
1	A	72	GLN	1
1	A	73	PHE	1
1	B	72	GLN	1
1	B	73	PHE	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	A	28	LEU	28
1	B	28	LEU	28
1	A	6	ILE	27
1	A	31	GLN	27
1	A	47	ILE	27
1	B	6	ILE	27
1	B	31	GLN	27
1	B	47	ILE	27
1	A	65	LEU	26
1	B	65	LEU	26
1	A	72	GLN	24
1	A	81	LEU	24
1	A	82	ARG	24
1	A	83	LEU	24
1	B	72	GLN	24
1	B	81	LEU	24
1	B	82	ARG	24
1	B	83	LEU	24
1	A	37	LEU	23
1	B	37	LEU	23
1	A	70	VAL	21
1	B	70	VAL	21
1	A	33	CYS	20
1	A	87	LYS	20
1	B	33	CYS	20
1	B	87	LYS	20
1	A	49	LEU	19
1	B	49	LEU	19
1	A	4	VAL	19
1	B	4	VAL	19
1	A	29	ASN	18
1	A	46	LYS	18

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Mol	Chain	Res	Type	Models (Total)
1	A	50	ASP	18
1	B	29	ASN	18
1	B	46	LYS	18
1	B	50	ASP	18
1	B	1	MET	18
1	A	7	LYS	17
1	A	53	GLN	17
1	B	7	LYS	17
1	B	53	GLN	17
1	A	1	MET	17
1	A	80	ARG	16
1	B	80	ARG	16
1	A	60	LEU	16
1	B	60	LEU	16
1	A	73	PHE	14
1	A	76	LEU	14
1	B	73	PHE	14
1	B	76	LEU	14
1	A	69	LYS	14
1	B	69	LYS	14
1	A	9	SER	13
1	B	9	SER	13
1	A	48	THR	13
1	B	48	THR	13
1	A	3	LYS	12
1	A	75	SER	12
1	B	3	LYS	12
1	B	75	SER	12
1	A	51	GLU	11
1	B	51	GLU	11
1	A	66	SER	9
1	B	66	SER	9
1	A	39	ASN	9
1	B	39	ASN	9
1	A	36	ASP	8
1	B	36	ASP	8
1	A	12	GLN	8
1	B	12	GLN	8
1	A	79	ASP	7
1	B	79	ASP	7
1	A	30	GLU	6
1	B	30	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	41	HIS	5
1	B	41	HIS	5
1	A	67	SER	5
1	B	67	SER	5
1	A	32	LEU	4
1	B	32	LEU	4
1	A	2	ILE	4
1	B	2	ILE	4
1	A	13	PHE	3
1	B	13	PHE	3
1	A	40	GLU	3
1	B	40	GLU	3
1	A	14	THR	2
1	B	14	THR	2
1	A	45	VAL	2
1	B	45	VAL	2
1	A	10	GLN	2
1	B	10	GLN	2
1	A	77	MET	2
1	B	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 ⓘ

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided