



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 10:46 PM UTC

PDB ID : 1X9X / pdb_00001x9x
Title : Solution Structure of Dimeric SAM Domain from MAPKKK Ste11
Authors : Bhattacharjya, S.; Xu, P.; Gingras, R.; Shaykhutdinov, R.; Wu, C.; Whiteway, M.; Ni, F.
Deposited on : 2004-08-24

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

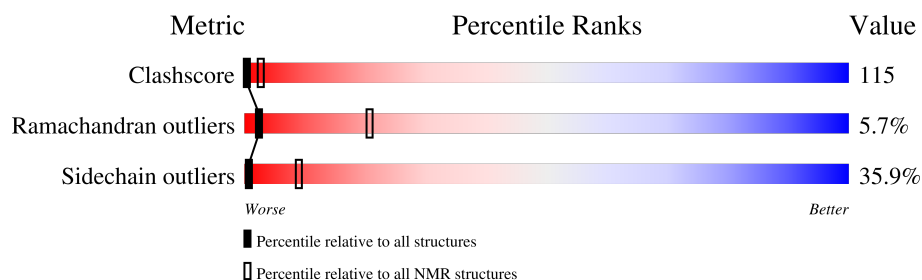
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	68	19% 43% 24% 6% 9%
1	B	68	9% 44% 31% 7% 9%

2 Ensemble composition and analysis

This entry contains 8 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:66, B:93-B:149 (115)	0.56	4

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 8
2	1, 3, 5
3	6, 7

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2088 atoms, of which 1070 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase STE11.

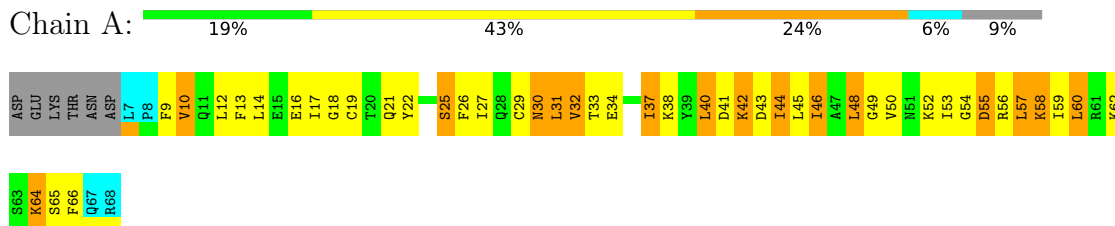
Mol	Chain	Residues	Atoms						Trace
1	A	62	Total	C	H	N	O	S	0
			1044	331	535	83	93	2	
1	B	62	Total	C	H	N	O	S	0
			1044	331	535	83	93	2	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Serine/threonine-protein kinase STE11



- Molecule 1: Serine/threonine-protein kinase STE11

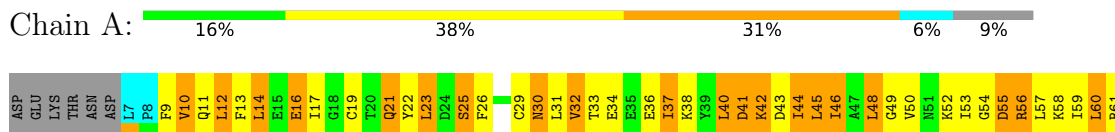


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

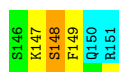
- Molecule 1: Serine/threonine-protein kinase STE11





- Molecule 1: Serine/threonine-protein kinase STE11

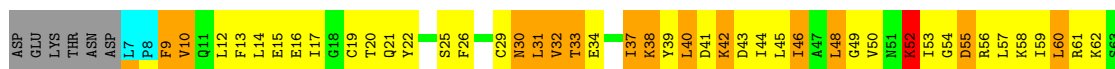
Chain B: 13% 40% 31% 7% 9%



4.2.2 Score per residue for model 2

- Molecule 1: Serine/threonine-protein kinase STE11

Chain A: 16% 46% 22% 6% 9%



- Molecule 1: Serine/threonine-protein kinase STE11

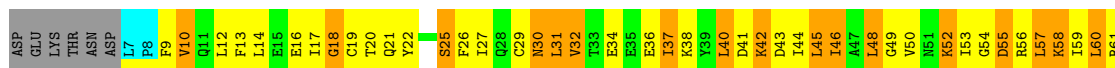
Chain B: 10% 43% 31% 7% 9%



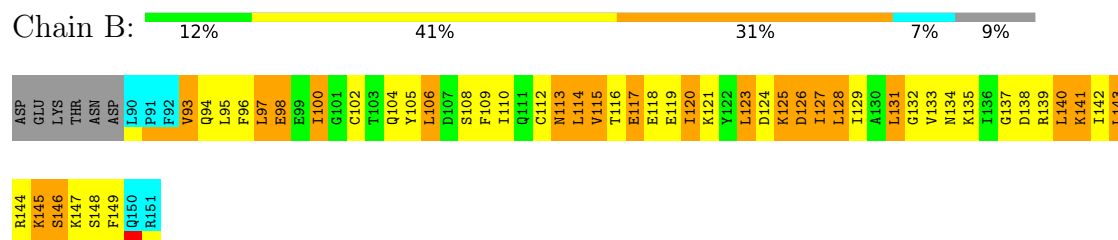
4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase STE11

Chain A: 16% 43% 26% 6% 9%

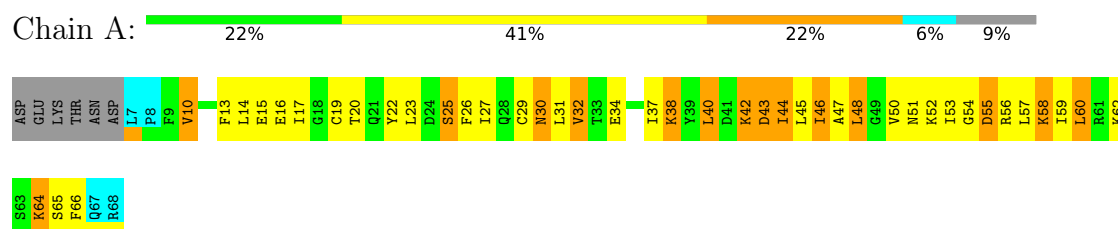


- Molecule 1: Serine/threonine-protein kinase STE11

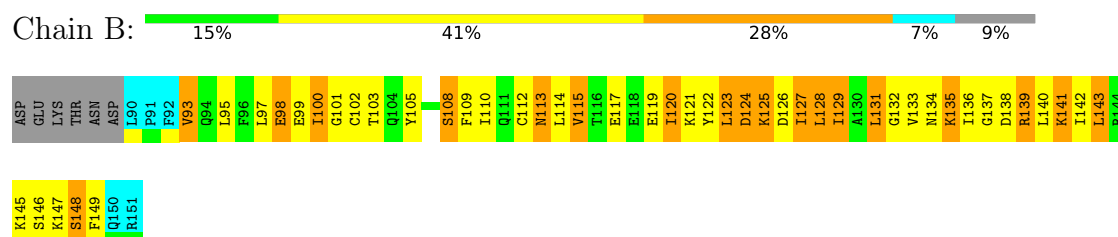


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Serine/threonine-protein kinase STE11

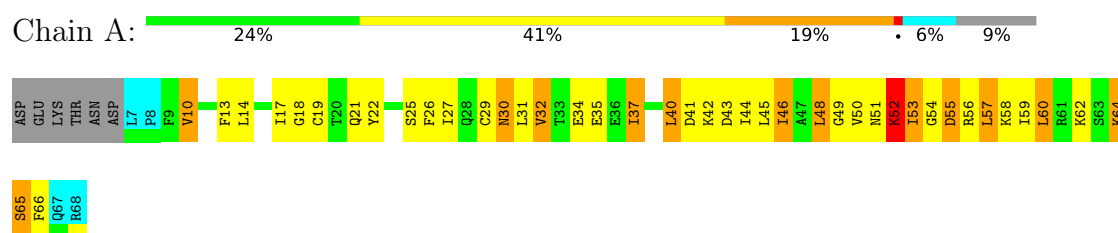


- Molecule 1: Serine/threonine-protein kinase STE11

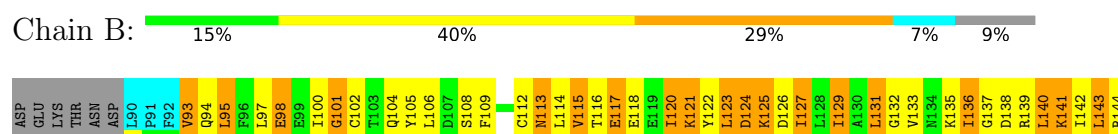


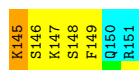
4.2.5 Score per residue for model 5

- Molecule 1: Serine/threonine-protein kinase STE11



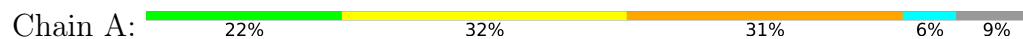
- Molecule 1: Serine/threonine-protein kinase STE11



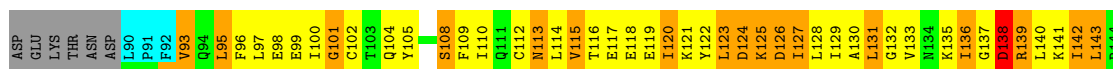


4.2.6 Score per residue for model 6

- Molecule 1: Serine/threonine-protein kinase STE11

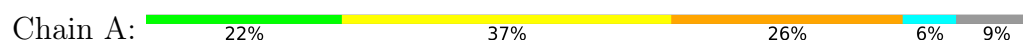


- Molecule 1: Serine/threonine-protein kinase STE11

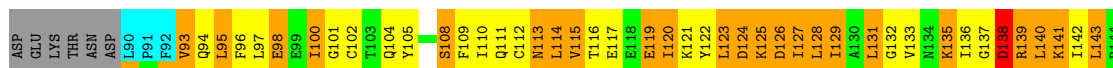


4.2.7 Score per residue for model 7

- Molecule 1: Serine/threonine-protein kinase STE11

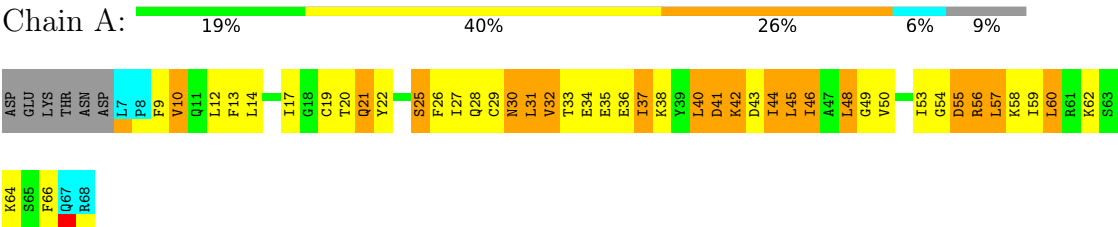


- Molecule 1: Serine/threonine-protein kinase STE11

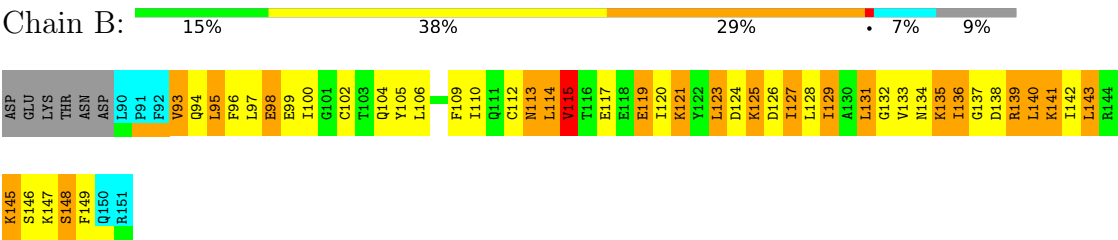


4.2.8 Score per residue for model 8

- Molecule 1: Serine/threonine-protein kinase STE11



- Molecule 1: Serine/threonine-protein kinase STE11



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distant geometry*.

Of the 20 calculated structures, 8 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
CYANA	refinement	1.0.6

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	474	497	496	117±13
1	B	463	488	487	129±14
All	All	7496	7880	7864	1760

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 115.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:120:ILE:HD11	1:B:149:PHE:CZ	1.17	1.73	7	8
1:A:37:ILE:HD11	1:A:66:PHE:CZ	1.06	1.84	4	8
1:A:14:LEU:HD21	1:A:26:PHE:CD2	1.06	1.86	1	1
1:A:14:LEU:HD11	1:A:26:PHE:CD2	1.04	1.85	7	6
1:B:131:LEU:HD22	1:B:133:VAL:HG13	1.03	1.29	2	3
1:A:48:LEU:HD22	1:A:50:VAL:HG13	0.98	1.35	1	1
1:B:123:LEU:HD13	1:B:123:LEU:C	0.96	1.85	1	1
1:B:105:TYR:CD2	1:B:133:VAL:HG11	0.96	1.96	4	4
1:B:131:LEU:CD2	1:B:133:VAL:HG13	0.96	1.90	1	4
1:A:10:VAL:HG13	1:A:14:LEU:HD22	0.95	1.36	1	1
1:A:48:LEU:CD2	1:A:50:VAL:HG13	0.95	1.90	1	2
1:A:57:LEU:HD12	1:A:57:LEU:O	0.95	1.62	6	2
1:A:48:LEU:HD22	1:A:50:VAL:HG23	0.94	1.38	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:HG21	1:A:31:LEU:O	0.94	1.61	3	7
1:B:125:LYS:O	1:B:129:ILE:HG23	0.94	1.62	2	1
1:B:131:LEU:HD22	1:B:133:VAL:HG23	0.93	1.40	3	3
1:A:22:TYR:CD2	1:A:50:VAL:HG11	0.93	1.99	5	2
1:A:46:ILE:HG21	1:B:125:LYS:NZ	0.92	1.78	4	1
1:A:19:CYS:SG	1:A:59:ILE:HD11	0.92	2.05	8	8
1:A:56:ARG:NH2	1:B:129:ILE:HD13	0.91	1.79	4	2
1:B:131:LEU:HD23	1:B:131:LEU:C	0.91	1.90	2	8
1:B:93:VAL:HG21	1:B:114:LEU:O	0.90	1.64	7	8
1:B:97:LEU:HD21	1:B:109:PHE:CD2	0.89	2.03	3	2
1:B:109:PHE:CE1	1:B:128:LEU:HD11	0.89	2.02	6	1
1:B:128:LEU:O	1:B:133:VAL:HG22	0.88	1.66	7	4
1:B:128:LEU:HD22	1:B:142:ILE:CG2	0.87	1.99	2	1
1:A:42:LYS:O	1:A:46:ILE:HG22	0.87	1.70	1	1
1:A:45:LEU:HD22	1:A:59:ILE:HG21	0.87	1.44	2	1
1:A:40:LEU:C	1:A:40:LEU:HD12	0.86	1.96	1	4
1:A:48:LEU:C	1:A:48:LEU:HD23	0.86	1.95	3	7
1:A:60:LEU:HD11	1:B:124:ASP:OD1	0.84	1.72	3	1
1:B:123:LEU:HD12	1:B:127:ILE:CG2	0.84	2.02	8	4
1:A:41:ASP:HB2	1:A:44:ILE:HD13	0.84	1.50	2	1
1:A:22:TYR:CE2	1:A:50:VAL:HG11	0.84	2.08	5	2
1:A:14:LEU:HD21	1:A:26:PHE:CE2	0.83	2.09	1	8
1:B:123:LEU:C	1:B:123:LEU:CD1	0.82	2.52	1	2
1:B:105:TYR:CE2	1:B:133:VAL:HG21	0.82	2.10	6	1
1:B:143:LEU:C	1:B:143:LEU:HD13	0.82	2.00	4	1
1:B:135:LYS:O	1:B:139:ARG:NH1	0.81	2.12	6	1
1:A:46:ILE:HD11	1:B:136:ILE:HD13	0.81	1.51	1	1
1:A:27:ILE:HG12	1:A:32:VAL:HG21	0.81	1.50	4	3
1:B:125:LYS:HZ1	1:B:139:ARG:HE	0.81	1.18	2	1
1:B:123:LEU:HD11	1:B:128:LEU:HD22	0.81	1.51	4	1
1:B:120:ILE:HA	1:B:123:LEU:HD22	0.81	1.53	8	3
1:A:48:LEU:HD23	1:A:49:GLY:N	0.81	1.90	2	7
1:B:123:LEU:HD11	1:B:128:LEU:CD2	0.80	2.06	4	1
1:A:57:LEU:HD12	1:A:57:LEU:C	0.80	2.02	8	2
1:B:105:TYR:CE2	1:B:133:VAL:HG11	0.80	2.11	7	4
1:A:57:LEU:C	1:A:57:LEU:HD13	0.80	2.02	5	1
1:A:60:LEU:HD21	1:B:124:ASP:CG	0.80	2.02	3	5
1:A:44:ILE:HD12	1:B:140:LEU:HD11	0.79	1.52	4	1
1:B:114:LEU:HD11	1:B:123:LEU:HD23	0.79	1.54	3	1
1:B:102:CYS:SG	1:B:142:ILE:HD11	0.78	2.18	8	7
1:A:50:VAL:HG23	1:A:50:VAL:O	0.78	1.78	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:PHE:CE1	1:A:45:LEU:HD11	0.77	2.14	8	1
1:B:110:ILE:HG12	1:B:115:VAL:HG21	0.77	1.53	6	1
1:B:131:LEU:HD23	1:B:132:GLY:N	0.77	1.95	8	8
1:B:133:VAL:HG23	1:B:133:VAL:O	0.77	1.77	2	3
1:A:45:LEU:HD22	1:A:59:ILE:CG2	0.77	2.08	2	1
1:B:129:ILE:C	1:B:129:ILE:HD13	0.77	2.05	1	1
1:A:48:LEU:HD22	1:A:50:VAL:CG2	0.77	2.10	7	2
1:B:128:LEU:C	1:B:133:VAL:HG22	0.76	2.05	7	3
1:B:140:LEU:O	1:B:140:LEU:HD23	0.76	1.80	7	2
1:A:45:LEU:HD13	1:A:48:LEU:HD13	0.76	1.57	8	1
1:A:46:ILE:HG22	1:A:56:ARG:HG2	0.75	1.59	2	2
1:B:125:LYS:NZ	1:B:139:ARG:HE	0.75	1.80	2	1
1:A:53:ILE:HG23	1:B:129:ILE:CD1	0.75	2.10	4	3
1:B:125:LYS:HB3	1:B:143:LEU:HD13	0.74	1.59	5	2
1:B:115:VAL:HG22	1:B:115:VAL:O	0.74	1.81	3	3
1:A:42:LYS:HD2	1:A:60:LEU:HD13	0.74	1.59	3	1
1:A:46:ILE:HD13	1:B:139:ARG:NH2	0.74	1.97	2	1
1:A:37:ILE:O	1:A:40:LEU:HD22	0.74	1.83	8	4
1:B:131:LEU:CD2	1:B:133:VAL:HG23	0.74	2.13	3	3
1:B:97:LEU:HD21	1:B:109:PHE:CE2	0.74	2.16	7	4
1:B:128:LEU:HD21	1:B:142:ILE:HD12	0.74	1.58	6	1
1:A:15:GLU:CG	1:A:20:THR:HG22	0.73	2.13	2	1
1:A:46:ILE:CD1	1:B:139:ARG:HH21	0.73	1.95	2	1
1:A:46:ILE:HD12	1:A:46:ILE:C	0.73	2.09	2	1
1:A:41:ASP:HB3	1:B:143:LEU:HD21	0.73	1.57	8	1
1:B:114:LEU:HD22	1:B:120:ILE:HG22	0.73	1.60	4	2
1:A:48:LEU:CD2	1:A:50:VAL:HG23	0.73	2.12	8	3
1:B:120:ILE:O	1:B:123:LEU:HD22	0.73	1.84	5	3
1:A:42:LYS:O	1:A:46:ILE:HG23	0.73	1.84	4	2
1:B:125:LYS:NZ	1:B:139:ARG:NE	0.73	2.37	2	1
1:B:120:ILE:CD1	1:B:149:PHE:CZ	0.72	2.66	7	5
1:B:140:LEU:HD23	1:B:140:LEU:C	0.72	2.09	7	1
1:B:95:LEU:HD13	1:B:95:LEU:O	0.72	1.83	3	3
1:B:120:ILE:HD11	1:B:149:PHE:CE1	0.72	2.18	7	3
1:A:42:LYS:CB	1:A:42:LYS:HZ3	0.72	1.96	3	1
1:A:26:PHE:CE1	1:A:45:LEU:CD2	0.72	2.72	3	3
1:A:31:LEU:HD11	1:A:40:LEU:HD13	0.72	1.61	8	3
1:B:112:CYS:O	1:B:113:ASN:CB	0.72	2.38	8	8
1:A:37:ILE:CD1	1:A:66:PHE:CZ	0.71	2.73	8	6
1:B:122:TYR:CG	1:B:122:TYR:O	0.71	2.43	4	1
1:A:26:PHE:CZ	1:A:45:LEU:CD2	0.71	2.73	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:O	1:A:12:LEU:HD23	0.71	1.85	3	2
1:B:129:ILE:C	1:B:129:ILE:HD12	0.71	2.11	2	2
1:B:112:CYS:HB3	1:B:114:LEU:HD22	0.70	1.62	7	1
1:A:46:ILE:HD13	1:B:139:ARG:HH21	0.70	1.45	2	1
1:B:131:LEU:HD22	1:B:133:VAL:CG2	0.70	2.16	3	2
1:A:29:CYS:O	1:A:30:ASN:CB	0.70	2.40	1	8
1:B:124:ASP:O	1:B:128:LEU:HD22	0.70	1.87	7	2
1:B:140:LEU:C	1:B:140:LEU:HD23	0.70	2.11	2	1
1:B:140:LEU:O	1:B:143:LEU:HD23	0.70	1.86	3	1
1:B:125:LYS:HZ1	1:B:139:ARG:NE	0.70	1.84	2	1
1:A:22:TYR:CE2	1:A:50:VAL:CG1	0.70	2.74	5	2
1:A:13:PHE:O	1:A:17:ILE:HG23	0.70	1.87	8	1
1:A:31:LEU:HD11	1:A:40:LEU:HD23	0.70	1.64	2	2
1:A:46:ILE:HD13	1:B:136:ILE:HB	0.69	1.62	6	1
1:B:97:LEU:HD11	1:B:109:PHE:CE2	0.69	2.22	8	1
1:A:43:ASP:HA	1:A:46:ILE:CG2	0.69	2.17	1	2
1:A:14:LEU:CD2	1:A:17:ILE:HD11	0.69	2.18	5	4
1:B:93:VAL:HG13	1:B:97:LEU:HD22	0.69	1.61	3	2
1:A:46:ILE:HG21	1:B:125:LYS:HE2	0.69	1.63	6	1
1:A:12:LEU:C	1:A:12:LEU:HD13	0.69	2.13	7	1
1:A:10:VAL:CG1	1:A:14:LEU:HD22	0.69	2.14	1	1
1:A:32:VAL:O	1:A:32:VAL:HG23	0.69	1.87	1	5
1:A:43:ASP:O	1:A:46:ILE:HG22	0.69	1.88	7	2
1:A:42:LYS:CB	1:A:42:LYS:NZ	0.69	2.55	3	1
1:A:40:LEU:C	1:A:40:LEU:CD1	0.68	2.66	1	3
1:B:109:PHE:CD2	1:B:114:LEU:HB2	0.68	2.22	2	5
1:A:12:LEU:HD23	1:A:12:LEU:C	0.68	2.14	3	1
1:A:10:VAL:HG12	1:A:32:VAL:HG13	0.68	1.65	6	2
1:B:97:LEU:HD23	1:B:100:ILE:HD11	0.68	1.66	1	3
1:B:109:PHE:CD2	1:B:114:LEU:CB	0.68	2.76	1	8
1:B:95:LEU:HD13	1:B:95:LEU:C	0.67	2.13	1	3
1:A:46:ILE:HG22	1:A:56:ARG:NE	0.67	2.04	6	1
1:A:26:PHE:CD1	1:A:48:LEU:HD11	0.67	2.24	2	6
1:B:131:LEU:HD22	1:B:133:VAL:HG12	0.67	1.63	8	1
1:A:41:ASP:OD1	1:B:143:LEU:HD21	0.67	1.89	5	1
1:A:48:LEU:HD22	1:A:50:VAL:HG12	0.67	1.67	2	2
1:B:131:LEU:HD22	1:B:133:VAL:CG1	0.67	2.19	1	2
1:A:26:PHE:CD2	1:A:31:LEU:HB2	0.67	2.25	4	4
1:A:40:LEU:CD1	1:A:40:LEU:C	0.67	2.67	7	1
1:B:115:VAL:O	1:B:115:VAL:HG23	0.67	1.88	1	4
1:A:46:ILE:HD11	1:B:136:ILE:CD1	0.66	2.19	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:128:LEU:HD22	1:B:142:ILE:HG22	0.66	1.67	2	1
1:A:27:ILE:CG1	1:A:32:VAL:HG21	0.66	2.20	4	3
1:A:42:LYS:O	1:A:45:LEU:HG	0.66	1.90	4	1
1:A:40:LEU:HD23	1:A:40:LEU:C	0.66	2.16	8	2
1:A:25:SER:C	1:A:48:LEU:HD13	0.66	2.15	4	1
1:A:42:LYS:HE2	1:B:129:ILE:HG21	0.66	1.67	1	1
1:B:105:TYR:CE2	1:B:133:VAL:CG1	0.66	2.78	4	4
1:B:131:LEU:C	1:B:131:LEU:CD2	0.66	2.67	8	5
1:B:96:PHE:CE1	1:B:100:ILE:HG21	0.66	2.25	3	1
1:A:57:LEU:HD13	1:A:60:LEU:HD22	0.66	1.65	6	1
1:B:108:SER:HB3	1:B:131:LEU:HD21	0.65	1.66	2	5
1:A:45:LEU:O	1:A:50:VAL:HG12	0.65	1.91	2	2
1:A:57:LEU:HD23	1:A:57:LEU:O	0.65	1.92	7	2
1:B:131:LEU:HD22	1:B:133:VAL:HG22	0.65	1.67	4	1
1:B:109:PHE:CD1	1:B:131:LEU:HD11	0.65	2.26	2	7
1:A:53:ILE:HG23	1:B:129:ILE:HD11	0.65	1.66	1	2
1:B:129:ILE:HD13	1:B:130:ALA:N	0.65	2.07	1	1
1:B:114:LEU:HB3	1:B:120:ILE:HG22	0.65	1.68	6	2
1:B:114:LEU:CB	1:B:120:ILE:HG22	0.64	2.23	7	2
1:B:115:VAL:O	1:B:115:VAL:CG2	0.64	2.46	2	6
1:A:26:PHE:CD1	1:A:48:LEU:CD1	0.64	2.81	2	6
1:B:109:PHE:CD1	1:B:131:LEU:CD1	0.64	2.81	2	7
1:B:97:LEU:CD2	1:B:100:ILE:HD11	0.63	2.22	1	3
1:B:133:VAL:O	1:B:133:VAL:CG2	0.63	2.45	2	3
1:A:14:LEU:HD22	1:A:17:ILE:HD11	0.63	1.70	5	1
1:B:110:ILE:CG1	1:B:115:VAL:HG21	0.63	2.22	6	1
1:A:10:VAL:CG2	1:A:37:ILE:CD1	0.63	2.76	6	3
1:B:105:TYR:O	1:B:109:PHE:N	0.63	2.29	8	6
1:B:93:VAL:CG2	1:B:120:ILE:CD1	0.63	2.77	3	3
1:A:42:LYS:NZ	1:B:126:ASP:CG	0.63	2.57	5	1
1:B:123:LEU:HD12	1:B:127:ILE:HG22	0.63	1.71	8	1
1:B:120:ILE:CD1	1:B:149:PHE:CE1	0.63	2.80	7	4
1:B:123:LEU:HD13	1:B:124:ASP:N	0.62	2.09	1	1
1:A:46:ILE:HG21	1:B:125:LYS:HZ1	0.62	1.54	4	1
1:B:128:LEU:CB	1:B:139:ARG:CZ	0.62	2.76	4	1
1:A:26:PHE:CD2	1:A:31:LEU:CB	0.62	2.82	4	8
1:B:112:CYS:O	1:B:113:ASN:CG	0.62	2.42	8	8
1:B:114:LEU:HD11	1:B:123:LEU:HD13	0.62	1.72	4	2
1:A:32:VAL:O	1:A:32:VAL:CG2	0.62	2.46	1	3
1:A:22:TYR:O	1:A:26:PHE:N	0.62	2.30	3	6
1:A:45:LEU:HD23	1:A:48:LEU:HD13	0.62	1.71	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:96:PHE:O	1:B:100:ILE:HG23	0.62	1.94	7	3
1:B:114:LEU:HD22	1:B:120:ILE:CG2	0.61	2.25	1	2
1:B:95:LEU:HD12	1:B:95:LEU:C	0.61	2.20	2	2
1:A:25:SER:HB3	1:A:48:LEU:HD11	0.61	1.71	4	1
1:A:31:LEU:HB3	1:A:37:ILE:CG2	0.61	2.25	7	7
1:A:14:LEU:HD11	1:A:26:PHE:CG	0.61	2.29	8	5
1:A:50:VAL:O	1:A:50:VAL:CG2	0.61	2.48	1	1
1:A:45:LEU:HD13	1:A:56:ARG:NH2	0.61	2.11	1	1
1:A:57:LEU:HB2	1:B:126:ASP:CG	0.61	2.20	5	6
1:A:46:ILE:HD12	1:A:56:ARG:NH1	0.61	2.10	5	1
1:A:45:LEU:HD13	1:A:59:ILE:HG22	0.61	1.73	2	1
1:B:100:ILE:HG22	1:B:145:LYS:HD2	0.61	1.71	3	3
1:A:25:SER:HB3	1:A:48:LEU:HD21	0.61	1.71	7	7
1:A:37:ILE:HD11	1:A:66:PHE:CE2	0.61	2.31	1	1
1:A:15:GLU:HG2	1:A:20:THR:HG22	0.61	1.72	2	1
1:B:109:PHE:CD2	1:B:114:LEU:HB3	0.60	2.31	7	6
1:A:48:LEU:C	1:A:48:LEU:CD2	0.60	2.71	5	6
1:A:42:LYS:CB	1:A:42:LYS:HZ2	0.60	2.08	7	1
1:B:123:LEU:HD22	1:B:124:ASP:O	0.60	1.96	1	1
1:A:42:LYS:CG	1:B:125:LYS:CG	0.60	2.79	6	6
1:A:42:LYS:NZ	1:A:60:LEU:HD22	0.60	2.11	2	1
1:A:43:ASP:CG	1:B:140:LEU:HB2	0.60	2.21	2	4
1:A:40:LEU:HD23	1:A:40:LEU:O	0.60	1.95	3	1
1:A:34:GLU:HA	1:A:66:PHE:CE2	0.60	2.32	4	6
1:A:17:ILE:HG21	1:A:62:LYS:CG	0.60	2.27	8	2
1:B:105:TYR:CE2	1:B:133:VAL:CG2	0.60	2.85	6	1
1:A:48:LEU:HD22	1:A:50:VAL:CG1	0.60	2.21	1	1
1:A:57:LEU:CB	1:B:126:ASP:CB	0.60	2.80	8	2
1:A:45:LEU:O	1:A:50:VAL:HG22	0.60	1.96	5	2
1:B:104:GLN:OE1	1:B:105:TYR:CE1	0.60	2.54	1	1
1:B:123:LEU:HD23	1:B:127:ILE:HG21	0.60	1.72	1	1
1:B:122:TYR:O	1:B:122:TYR:CD2	0.60	2.55	4	1
1:A:43:ASP:OD1	1:B:139:ARG:C	0.60	2.45	8	1
1:A:29:CYS:O	1:A:30:ASN:CG	0.60	2.45	1	6
1:A:45:LEU:C	1:A:50:VAL:HG22	0.60	2.22	1	1
1:B:139:ARG:HH21	1:B:142:ILE:HB	0.60	1.57	4	1
1:A:37:ILE:HA	1:A:40:LEU:HD22	0.60	1.74	6	1
1:A:45:LEU:HD22	1:A:59:ILE:HG22	0.60	1.72	4	1
1:A:12:LEU:HD13	1:A:12:LEU:C	0.59	2.22	2	1
1:B:138:ASP:CB	1:B:139:ARG:NH2	0.59	2.65	6	1
1:B:112:CYS:O	1:B:113:ASN:HB2	0.59	1.97	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:CG2	1:B:129:ILE:HD11	0.59	2.27	1	1
1:A:56:ARG:HH21	1:B:129:ILE:HD13	0.59	1.53	4	1
1:A:14:LEU:HD11	1:A:26:PHE:CE2	0.59	2.32	8	4
1:A:37:ILE:CD1	1:A:66:PHE:CE2	0.59	2.86	2	2
1:A:41:ASP:CG	1:B:143:LEU:HD11	0.59	2.22	2	1
1:B:140:LEU:HD23	1:B:141:LYS:N	0.59	2.12	3	1
1:B:141:LYS:HG3	1:B:142:ILE:N	0.59	2.11	4	5
1:A:42:LYS:HZ2	1:B:125:LYS:HG3	0.59	1.56	3	2
1:A:37:ILE:CD1	1:A:66:PHE:CE1	0.59	2.85	8	5
1:A:43:ASP:CB	1:B:140:LEU:HB3	0.59	2.28	5	2
1:B:96:PHE:CE1	1:B:100:ILE:CG2	0.59	2.86	3	1
1:A:31:LEU:CD1	1:A:40:LEU:CD1	0.59	2.80	4	1
1:B:139:ARG:CZ	1:B:139:ARG:H	0.59	2.10	6	1
1:B:120:ILE:O	1:B:123:LEU:HD12	0.58	1.98	1	1
1:A:57:LEU:HB2	1:B:126:ASP:CB	0.58	2.28	6	7
1:B:95:LEU:HD12	1:B:95:LEU:O	0.58	1.96	2	2
1:A:41:ASP:OD2	1:B:140:LEU:HD13	0.58	1.97	5	1
1:A:42:LYS:HG2	1:B:125:LYS:CG	0.58	2.27	5	3
1:A:60:LEU:HD21	1:B:124:ASP:CB	0.58	2.29	1	1
1:B:93:VAL:HG21	1:B:120:ILE:HD13	0.58	1.73	3	2
1:A:57:LEU:CA	1:B:126:ASP:CG	0.58	2.76	1	1
1:A:51:ASN:O	1:A:52:LYS:C	0.58	2.47	5	1
1:A:43:ASP:CG	1:B:140:LEU:HA	0.58	2.24	8	1
1:B:102:CYS:HB3	1:B:105:TYR:CG	0.58	2.34	2	8
1:B:114:LEU:HB3	1:B:120:ILE:CG2	0.58	2.29	3	6
1:A:19:CYS:HA	1:A:22:TYR:CD1	0.58	2.34	2	4
1:A:25:SER:O	1:A:48:LEU:HD13	0.57	1.99	4	1
1:A:44:ILE:CD1	1:B:140:LEU:CD1	0.57	2.81	8	2
1:A:43:ASP:CB	1:B:140:LEU:HB2	0.57	2.30	2	3
1:A:60:LEU:HD21	1:B:124:ASP:HB3	0.57	1.76	1	1
1:B:129:ILE:HG13	1:B:139:ARG:HH21	0.57	1.58	1	1
1:A:45:LEU:O	1:A:50:VAL:CG1	0.57	2.53	2	2
1:A:56:ARG:NH2	1:B:129:ILE:CD1	0.57	2.67	3	3
1:A:37:ILE:HD11	1:A:66:PHE:CE1	0.57	2.33	4	2
1:A:41:ASP:OD2	1:B:140:LEU:HD21	0.57	1.98	1	1
1:B:108:SER:HB2	1:B:131:LEU:HD21	0.57	1.76	4	2
1:A:53:ILE:HG23	1:B:129:ILE:HD12	0.57	1.75	4	1
1:A:17:ILE:HG21	1:A:62:LYS:HG2	0.57	1.77	8	1
1:A:31:LEU:CD1	1:A:40:LEU:HD13	0.57	2.27	8	3
1:A:40:LEU:HD12	1:A:44:ILE:CG2	0.57	2.30	4	2
1:A:57:LEU:C	1:A:57:LEU:CD1	0.57	2.76	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:139:ARG:CZ	1:B:139:ARG:N	0.57	2.68	6	1
1:A:37:ILE:HA	1:A:40:LEU:HD23	0.57	1.76	1	2
1:B:94:GLN:HB2	1:B:106:LEU:HD11	0.57	1.77	2	1
1:A:37:ILE:HG13	1:A:66:PHE:CE1	0.57	2.35	8	6
1:A:10:VAL:HG21	1:A:37:ILE:HD13	0.57	1.77	6	2
1:B:140:LEU:C	1:B:140:LEU:CD2	0.57	2.78	7	2
1:B:140:LEU:HA	1:B:143:LEU:HD23	0.57	1.75	2	1
1:A:56:ARG:HH21	1:B:129:ILE:CD1	0.57	2.12	4	2
1:B:125:LYS:HZ3	1:B:139:ARG:HD3	0.57	1.60	3	1
1:A:45:LEU:CD1	1:A:48:LEU:HD13	0.57	2.28	8	1
1:A:34:GLU:HA	1:A:66:PHE:CE1	0.56	2.35	2	2
1:A:41:ASP:OD2	1:A:44:ILE:HD12	0.56	1.99	1	1
1:A:57:LEU:N	1:B:126:ASP:CG	0.56	2.63	1	1
1:B:120:ILE:HG13	1:B:149:PHE:CE1	0.56	2.36	4	7
1:B:93:VAL:CG2	1:B:114:LEU:O	0.56	2.49	7	2
1:A:43:ASP:CB	1:B:140:LEU:CB	0.56	2.83	5	3
1:B:102:CYS:HA	1:B:105:TYR:CD1	0.56	2.35	3	3
1:A:48:LEU:HD22	1:A:50:VAL:HG22	0.56	1.77	5	1
1:B:97:LEU:HD21	1:B:109:PHE:CG	0.56	2.34	8	1
1:B:129:ILE:HD12	1:B:130:ALA:N	0.56	2.16	6	2
1:B:125:LYS:CD	1:B:139:ARG:NH1	0.56	2.67	4	1
1:B:125:LYS:HE2	1:B:129:ILE:HG21	0.56	1.77	4	1
1:B:100:ILE:HG22	1:B:145:LYS:HD3	0.56	1.75	5	1
1:B:120:ILE:CA	1:B:123:LEU:HD22	0.56	2.28	8	1
1:B:114:LEU:CD1	1:B:123:LEU:CD1	0.56	2.83	5	2
1:A:29:CYS:O	1:A:30:ASN:HB2	0.56	2.00	1	6
1:B:109:PHE:O	1:B:113:ASN:N	0.56	2.36	3	7
1:B:137:GLY:O	1:B:140:LEU:N	0.56	2.28	2	3
1:B:109:PHE:HE1	1:B:128:LEU:HD11	0.56	1.54	6	1
1:A:48:LEU:HD12	1:A:48:LEU:C	0.56	2.26	4	1
1:B:94:GLN:CB	1:B:106:LEU:HD11	0.56	2.30	2	1
1:B:104:GLN:HG2	1:B:105:TYR:CE1	0.56	2.36	8	5
1:A:15:GLU:HG3	1:A:20:THR:HG22	0.56	1.77	2	1
1:A:42:LYS:HZ3	1:A:42:LYS:HB3	0.56	1.60	3	1
1:B:140:LEU:O	1:B:140:LEU:HD12	0.56	2.01	5	1
1:B:123:LEU:HD23	1:B:123:LEU:O	0.56	2.00	7	1
1:A:48:LEU:CD2	1:A:50:VAL:CG1	0.55	2.78	1	1
1:A:13:PHE:CZ	1:A:62:LYS:HB3	0.55	2.37	8	8
1:A:26:PHE:HE1	1:A:45:LEU:HD11	0.55	1.55	8	1
1:A:57:LEU:HD23	1:A:57:LEU:C	0.55	2.27	7	2
1:A:37:ILE:HG13	1:A:66:PHE:CD1	0.55	2.37	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:SER:CB	1:A:48:LEU:HD21	0.55	2.31	1	5
1:B:135:LYS:O	1:B:139:ARG:CD	0.55	2.54	1	1
1:A:38:LYS:CB	1:A:66:PHE:HB2	0.55	2.32	6	4
1:A:43:ASP:HB3	1:B:140:LEU:HD12	0.55	1.77	1	3
1:B:137:GLY:O	1:B:139:ARG:N	0.55	2.39	7	6
1:A:10:VAL:HG11	1:A:31:LEU:O	0.55	2.02	5	3
1:A:43:ASP:OD2	1:A:46:ILE:HG21	0.55	2.02	3	1
1:A:46:ILE:HG21	1:B:125:LYS:CE	0.55	2.32	6	1
1:A:25:SER:O	1:A:28:GLN:CG	0.55	2.55	8	1
1:B:129:ILE:CG1	1:B:139:ARG:HH21	0.55	2.15	1	1
1:A:40:LEU:HD22	1:A:44:ILE:CG2	0.55	2.32	2	1
1:A:46:ILE:HG21	1:B:125:LYS:HZ3	0.55	1.59	4	1
1:A:35:GLU:O	1:A:38:LYS:CG	0.55	2.55	6	1
1:A:43:ASP:OD1	1:B:139:ARG:CB	0.55	2.55	7	1
1:A:40:LEU:HD12	1:A:40:LEU:O	0.55	2.00	1	2
1:A:57:LEU:HD11	1:B:127:ILE:HD12	0.55	1.77	1	1
1:B:125:LYS:NZ	1:B:139:ARG:HH11	0.55	2.00	5	1
1:A:44:ILE:HD11	1:B:140:LEU:HD11	0.55	1.77	7	1
1:A:26:PHE:CD2	1:A:31:LEU:HB3	0.55	2.37	7	7
1:A:54:GLY:O	1:A:56:ARG:N	0.55	2.40	5	8
1:A:58:LYS:C	1:A:58:LYS:CD	0.55	2.79	6	2
1:A:31:LEU:CD2	1:A:40:LEU:HD13	0.55	2.32	4	1
1:A:60:LEU:CD2	1:B:124:ASP:CG	0.55	2.79	4	2
1:B:138:ASP:O	1:B:141:LYS:CG	0.55	2.54	4	1
1:B:125:LYS:HA	1:B:128:LEU:HD12	0.54	1.78	1	1
1:B:131:LEU:CD2	1:B:133:VAL:CG1	0.54	2.78	1	2
1:A:42:LYS:CB	1:A:60:LEU:CD1	0.54	2.86	6	1
1:A:26:PHE:O	1:A:30:ASN:N	0.54	2.39	6	6
1:B:104:GLN:HG3	1:B:105:TYR:CE1	0.54	2.37	1	1
1:B:128:LEU:HD12	1:B:131:LEU:HD13	0.54	1.79	6	3
1:A:31:LEU:HB3	1:A:37:ILE:HG22	0.54	1.79	4	1
1:B:133:VAL:O	1:B:139:ARG:NE	0.54	2.41	5	1
1:B:108:SER:O	1:B:111:GLN:CG	0.54	2.56	7	1
1:B:93:VAL:CG2	1:B:120:ILE:HD13	0.54	2.33	6	6
1:A:42:LYS:HG3	1:B:125:LYS:CG	0.54	2.32	6	3
1:B:133:VAL:O	1:B:139:ARG:CD	0.54	2.55	4	1
1:B:128:LEU:O	1:B:133:VAL:HG12	0.54	2.02	8	1
1:B:141:LYS:CD	1:B:141:LYS:C	0.54	2.81	8	3
1:A:23:LEU:CD1	1:A:23:LEU:N	0.54	2.71	1	1
1:B:100:ILE:O	1:B:101:GLY:C	0.54	2.51	6	3
1:A:27:ILE:HA	1:A:32:VAL:HG12	0.54	1.78	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:118:GLU:O	1:B:121:LYS:CG	0.54	2.56	5	1
1:A:46:ILE:HD12	1:B:136:ILE:HD12	0.54	1.79	7	1
1:B:108:SER:CB	1:B:131:LEU:HD21	0.54	2.32	2	5
1:B:117:GLU:HA	1:B:149:PHE:CE2	0.54	2.38	3	6
1:B:102:CYS:CA	1:B:105:TYR:CD1	0.54	2.91	8	4
1:B:110:ILE:HA	1:B:115:VAL:CG1	0.54	2.33	7	2
1:B:145:LYS:O	1:B:148:SER:CB	0.53	2.56	1	8
1:B:100:ILE:HD12	1:B:142:ILE:HG12	0.53	1.81	8	2
1:B:125:LYS:NZ	1:B:139:ARG:NH1	0.53	2.56	5	1
1:B:109:PHE:HD1	1:B:131:LEU:HD11	0.53	1.64	7	7
1:A:43:ASP:CG	1:B:140:LEU:HD12	0.53	2.27	2	1
1:A:19:CYS:CA	1:A:22:TYR:CD1	0.53	2.91	2	5
1:A:43:ASP:OD1	1:B:137:GLY:O	0.53	2.25	3	2
1:A:21:GLN:HG2	1:A:22:TYR:CE1	0.53	2.38	5	6
1:B:126:ASP:HA	1:B:129:ILE:CG1	0.53	2.34	4	3
1:B:124:ASP:O	1:B:128:LEU:CD2	0.53	2.56	3	2
1:A:14:LEU:HD23	1:A:17:ILE:HD11	0.53	1.78	7	3
1:A:37:ILE:HG13	1:A:66:PHE:CE2	0.53	2.38	1	2
1:A:14:LEU:HD13	1:A:22:TYR:HB2	0.53	1.81	5	2
1:A:42:LYS:HZ2	1:B:126:ASP:CG	0.53	2.11	5	1
1:B:121:LYS:CB	1:B:149:PHE:HB2	0.53	2.34	5	3
1:A:10:VAL:CG2	1:A:31:LEU:O	0.53	2.49	3	1
1:A:31:LEU:HD11	1:A:40:LEU:CD1	0.53	2.33	4	1
1:A:41:ASP:CB	1:B:143:LEU:HD21	0.53	2.33	8	1
1:B:134:ASN:O	1:B:136:ILE:N	0.53	2.41	1	4
1:B:95:LEU:C	1:B:95:LEU:HD23	0.53	2.29	5	1
1:B:128:LEU:C	1:B:133:VAL:CG2	0.53	2.80	7	1
1:A:19:CYS:HB3	1:A:22:TYR:CG	0.53	2.39	8	7
1:A:54:GLY:C	1:A:56:ARG:N	0.53	2.65	5	8
1:A:62:LYS:O	1:A:65:SER:CB	0.53	2.56	5	7
1:B:95:LEU:O	1:B:98:GLU:CG	0.53	2.57	2	8
1:B:137:GLY:O	1:B:138:ASP:C	0.53	2.52	7	8
1:A:42:LYS:CG	1:B:125:LYS:HB3	0.53	2.32	7	5
1:A:42:LYS:HZ3	1:A:42:LYS:HB2	0.53	1.62	3	1
1:B:123:LEU:HD22	1:B:127:ILE:CG2	0.53	2.34	3	1
1:B:133:VAL:HG11	1:B:139:ARG:NE	0.53	2.18	6	1
1:B:135:LYS:O	1:B:139:ARG:NH2	0.53	2.40	7	1
1:A:26:PHE:HD1	1:A:48:LEU:HD11	0.53	1.64	7	7
1:B:120:ILE:CG1	1:B:149:PHE:CE1	0.53	2.92	7	4
1:A:33:THR:HG23	1:A:36:GLU:H	0.53	1.63	8	1
1:B:102:CYS:HB3	1:B:105:TYR:CD1	0.52	2.39	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:HG21	1:A:37:ILE:CD1	0.52	2.35	7	2
1:A:10:VAL:CG2	1:A:37:ILE:HD13	0.52	2.34	1	3
1:A:26:PHE:CE1	1:A:45:LEU:HD21	0.52	2.39	1	1
1:A:37:ILE:O	1:A:40:LEU:CD1	0.52	2.57	2	2
1:B:124:ASP:OD2	1:B:127:ILE:CD1	0.52	2.57	4	1
1:B:109:PHE:CG	1:B:114:LEU:HB2	0.52	2.40	6	5
1:B:123:LEU:CD2	1:B:127:ILE:CG2	0.52	2.88	1	1
1:A:42:LYS:CG	1:B:125:LYS:HG2	0.52	2.34	2	1
1:A:27:ILE:HA	1:A:32:VAL:CG1	0.52	2.34	3	2
1:A:25:SER:C	1:A:48:LEU:CD1	0.52	2.83	4	1
1:B:123:LEU:HD12	1:B:127:ILE:HG21	0.52	1.82	5	3
1:A:48:LEU:CD2	1:A:48:LEU:C	0.52	2.72	1	1
1:B:106:LEU:C	1:B:110:ILE:HD12	0.52	2.29	8	1
1:B:147:LYS:C	1:B:149:PHE:N	0.52	2.65	4	8
1:A:54:GLY:O	1:A:55:ASP:C	0.52	2.53	3	8
1:B:105:TYR:O	1:B:109:PHE:HB2	0.52	2.04	6	4
1:B:125:LYS:NZ	1:B:139:ARG:HB3	0.52	2.20	1	1
1:A:42:LYS:CB	1:A:60:LEU:HD12	0.52	2.35	6	1
1:A:46:ILE:C	1:A:46:ILE:HD13	0.52	2.29	1	1
1:B:114:LEU:CG	1:B:120:ILE:HG22	0.52	2.34	7	2
1:A:48:LEU:HD21	1:A:50:VAL:HG13	0.52	1.82	5	1
1:A:46:ILE:CD1	1:A:46:ILE:C	0.52	2.80	2	1
1:B:143:LEU:C	1:B:143:LEU:CD1	0.52	2.75	4	1
1:B:114:LEU:CD2	1:B:120:ILE:HG22	0.52	2.35	6	1
1:A:42:LYS:HB3	1:B:125:LYS:CG	0.52	2.35	5	2
1:B:97:LEU:O	1:B:101:GLY:N	0.52	2.43	2	3
1:A:37:ILE:HA	1:A:40:LEU:HG	0.52	1.81	7	1
1:B:114:LEU:HD12	1:B:120:ILE:HG22	0.52	1.81	8	1
1:A:41:ASP:CG	1:B:143:LEU:CD2	0.51	2.84	1	1
1:B:123:LEU:HD21	1:B:146:SER:OG	0.51	2.05	2	1
1:A:42:LYS:HG3	1:B:125:LYS:HG2	0.51	1.82	4	2
1:B:128:LEU:HB2	1:B:139:ARG:NH1	0.51	2.20	4	1
1:A:43:ASP:HA	1:A:46:ILE:HG22	0.51	1.82	5	1
1:B:109:PHE:O	1:B:114:LEU:N	0.51	2.38	8	1
1:A:57:LEU:HD12	1:B:126:ASP:HB3	0.51	1.81	1	1
1:A:46:ILE:HG22	1:A:56:ARG:CG	0.51	2.32	4	2
1:B:97:LEU:HD13	1:B:105:TYR:HB2	0.51	1.82	2	1
1:B:112:CYS:HB3	1:B:114:LEU:CD2	0.51	2.35	8	2
1:B:125:LYS:HD3	1:B:139:ARG:NH1	0.51	2.19	4	1
1:A:13:PHE:O	1:A:16:GLU:CG	0.51	2.59	1	1
1:A:64:LYS:C	1:A:66:PHE:N	0.51	2.68	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ASP:HB2	1:B:140:LEU:CB	0.51	2.36	5	1
1:A:57:LEU:N	1:B:126:ASP:OD1	0.51	2.42	8	2
1:B:131:LEU:CD2	1:B:131:LEU:C	0.51	2.75	1	3
1:A:42:LYS:HB2	1:A:60:LEU:CD1	0.51	2.36	6	2
1:A:58:LYS:HG3	1:A:59:ILE:N	0.51	2.19	3	2
1:A:19:CYS:SG	1:A:22:TYR:CG	0.51	2.97	6	1
1:B:145:LYS:O	1:B:148:SER:N	0.51	2.43	3	8
1:A:31:LEU:CD1	1:A:40:LEU:HD23	0.51	2.36	2	1
1:A:37:ILE:C	1:A:40:LEU:HD22	0.51	2.30	6	1
1:A:46:ILE:HG22	1:A:56:ARG:CD	0.51	2.36	6	1
1:B:137:GLY:C	1:B:139:ARG:N	0.51	2.66	6	7
1:A:43:ASP:HB3	1:B:140:LEU:CG	0.51	2.36	4	2
1:A:33:THR:O	1:A:34:GLU:C	0.51	2.53	7	2
1:B:104:GLN:HG3	1:B:105:TYR:CD1	0.51	2.41	1	1
1:A:37:ILE:O	1:A:40:LEU:CD2	0.51	2.59	4	4
1:B:123:LEU:HD23	1:B:123:LEU:C	0.51	2.30	5	2
1:B:140:LEU:HD12	1:B:140:LEU:C	0.51	2.30	5	1
1:A:56:ARG:CB	1:B:126:ASP:OD1	0.51	2.59	8	1
1:A:21:GLN:HG2	1:A:22:TYR:CD1	0.51	2.41	5	5
1:A:29:CYS:C	1:A:30:ASN:CG	0.51	2.79	5	6
1:B:133:VAL:HG23	1:B:139:ARG:CD	0.51	2.36	4	1
1:B:123:LEU:CD1	1:B:128:LEU:HD13	0.51	2.35	6	1
1:A:40:LEU:HD12	1:A:44:ILE:HG21	0.50	1.82	6	1
1:A:26:PHE:CZ	1:A:45:LEU:HD21	0.50	2.41	3	3
1:A:51:ASN:O	1:A:53:ILE:N	0.50	2.44	5	1
1:A:57:LEU:O	1:A:60:LEU:HB3	0.50	2.06	8	1
1:A:44:ILE:CD1	1:B:140:LEU:HD13	0.50	2.37	8	1
1:A:26:PHE:CZ	1:A:45:LEU:HD23	0.50	2.42	2	1
1:A:33:THR:O	1:A:37:ILE:HD13	0.50	2.06	2	2
1:A:42:LYS:HE3	1:A:56:ARG:C	0.50	2.32	2	1
1:A:42:LYS:HZ1	1:A:60:LEU:HD22	0.50	1.67	2	1
1:B:139:ARG:NH2	1:B:142:ILE:HB	0.50	2.22	4	1
1:B:120:ILE:HD11	1:B:149:PHE:HZ	0.50	1.49	6	1
1:A:56:ARG:NH2	1:A:56:ARG:O	0.50	2.45	1	1
1:A:37:ILE:HG13	1:A:66:PHE:CD2	0.50	2.42	2	1
1:B:110:ILE:HA	1:B:115:VAL:HG12	0.50	1.82	2	1
1:B:116:THR:O	1:B:117:GLU:C	0.50	2.54	3	2
1:B:128:LEU:O	1:B:131:LEU:HB3	0.50	2.06	8	1
1:B:100:ILE:O	1:B:141:LYS:CE	0.50	2.60	4	1
1:B:135:LYS:O	1:B:139:ARG:CG	0.50	2.59	4	1
1:B:139:ARG:HA	1:B:139:ARG:NE	0.50	2.21	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:142:ILE:O	1:B:146:SER:CB	0.50	2.59	6	2
1:A:43:ASP:OD1	1:B:140:LEU:N	0.50	2.45	6	1
1:B:139:ARG:NH1	1:B:139:ARG:HB2	0.50	2.21	6	1
1:A:43:ASP:OD1	1:B:140:LEU:HD12	0.50	2.06	2	1
1:A:34:GLU:O	1:A:66:PHE:CD2	0.50	2.65	3	1
1:A:14:LEU:HD21	1:A:26:PHE:CZ	0.50	2.41	4	2
1:A:42:LYS:HB3	1:A:60:LEU:HD11	0.50	1.83	5	1
1:B:125:LYS:CD	1:B:129:ILE:CG2	0.50	2.90	6	1
1:A:17:ILE:O	1:A:18:GLY:C	0.49	2.55	3	2
1:B:95:LEU:O	1:B:98:GLU:HG3	0.49	2.07	3	8
1:B:114:LEU:CD1	1:B:123:LEU:HD13	0.49	2.36	4	2
1:A:33:THR:O	1:A:35:GLU:N	0.49	2.45	6	2
1:A:42:LYS:HG2	1:B:125:LYS:HG3	0.49	1.83	1	1
1:B:104:GLN:HG2	1:B:105:TYR:CD1	0.49	2.42	6	5
1:B:138:ASP:HB3	1:B:139:ARG:HH21	0.49	1.66	6	1
1:B:96:PHE:CE2	1:B:120:ILE:HD12	0.49	2.42	8	1
1:A:42:LYS:HD3	1:B:125:LYS:CB	0.49	2.36	3	2
1:A:10:VAL:O	1:A:14:LEU:N	0.49	2.39	7	3
1:B:128:LEU:HB2	1:B:139:ARG:CZ	0.49	2.38	4	1
1:B:96:PHE:HE2	1:B:120:ILE:HD12	0.49	1.67	8	1
1:A:29:CYS:HB3	1:A:31:LEU:CD2	0.49	2.37	7	6
1:B:112:CYS:C	1:B:113:ASN:CG	0.49	2.80	5	8
1:A:43:ASP:OD2	1:B:125:LYS:NZ	0.49	2.45	2	1
1:A:12:LEU:HD12	1:A:12:LEU:C	0.49	2.33	1	1
1:B:96:PHE:CZ	1:B:145:LYS:HB3	0.49	2.42	6	4
1:A:50:VAL:HG23	1:A:52:LYS:CG	0.49	2.36	2	1
1:B:129:ILE:HG12	1:B:139:ARG:CZ	0.49	2.38	5	1
1:A:17:ILE:C	1:A:58:LYS:NZ	0.49	2.71	6	1
1:A:42:LYS:HB2	1:A:42:LYS:NZ	0.49	2.22	8	1
1:A:50:VAL:O	1:A:56:ARG:HD2	0.49	2.08	4	2
1:B:125:LYS:O	1:B:128:LEU:HG	0.49	2.08	2	2
1:B:129:ILE:C	1:B:129:ILE:CD1	0.49	2.77	1	2
1:B:93:VAL:HG11	1:B:114:LEU:O	0.49	2.07	7	2
1:A:26:PHE:CG	1:A:31:LEU:HB2	0.49	2.43	5	3
1:B:140:LEU:O	1:B:143:LEU:HG	0.49	2.08	2	1
1:B:114:LEU:CD1	1:B:123:LEU:HD23	0.49	2.32	3	1
1:A:46:ILE:CD1	1:A:56:ARG:NH1	0.49	2.76	5	1
1:A:37:ILE:CA	1:A:40:LEU:HD22	0.49	2.37	6	1
1:B:100:ILE:CG2	1:B:145:LYS:HD2	0.48	2.38	6	2
1:B:94:GLN:C	1:B:94:GLN:CD	0.48	2.80	8	1
1:A:42:LYS:CG	1:B:125:LYS:HG3	0.48	2.38	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:123:LEU:CD2	1:B:127:ILE:HG21	0.48	2.38	1	1
1:B:126:ASP:HA	1:B:129:ILE:CG2	0.48	2.38	1	2
1:A:45:LEU:O	1:A:48:LEU:HB3	0.48	2.08	2	3
1:B:141:LYS:C	1:B:141:LYS:HD3	0.48	2.33	7	3
1:A:25:SER:CB	1:A:48:LEU:HD11	0.48	2.37	4	1
1:B:128:LEU:HB3	1:B:139:ARG:CZ	0.48	2.37	4	1
1:A:31:LEU:HD12	1:A:37:ILE:CG2	0.48	2.38	3	5
1:A:12:LEU:C	1:A:12:LEU:CD2	0.48	2.86	3	1
1:A:43:ASP:OD1	1:B:140:LEU:HB3	0.48	2.09	3	1
1:A:14:LEU:CD2	1:A:26:PHE:CD2	0.48	2.79	1	1
1:A:60:LEU:CD2	1:B:124:ASP:HB3	0.48	2.38	7	2
1:B:114:LEU:HD22	1:B:123:LEU:HD13	0.48	1.85	2	2
1:B:128:LEU:CD2	1:B:142:ILE:HG22	0.48	2.36	2	1
1:A:40:LEU:HD11	1:A:45:LEU:HD11	0.48	1.86	3	1
1:B:123:LEU:HD22	1:B:127:ILE:HG22	0.48	1.85	3	1
1:B:106:LEU:O	1:B:110:ILE:HD12	0.48	2.08	8	1
1:A:19:CYS:SG	1:A:59:ILE:CD1	0.48	3.01	1	4
1:A:37:ILE:CG1	1:A:66:PHE:CE2	0.48	2.96	1	2
1:B:117:GLU:HB3	1:B:149:PHE:CE2	0.48	2.44	7	4
1:B:128:LEU:HD22	1:B:142:ILE:HG21	0.48	1.80	2	1
1:A:53:ILE:HD12	1:B:129:ILE:HD11	0.48	1.84	1	1
1:B:116:THR:O	1:B:118:GLU:N	0.48	2.47	5	2
1:A:57:LEU:HD13	1:A:60:LEU:CD2	0.48	2.37	6	1
1:A:43:ASP:OD2	1:B:143:LEU:HD22	0.48	2.07	8	1
1:A:62:LYS:O	1:A:65:SER:N	0.48	2.44	3	6
1:B:135:LYS:O	1:B:139:ARG:HD3	0.48	2.07	1	2
1:A:34:GLU:HB3	1:A:66:PHE:CE2	0.48	2.44	5	2
1:B:94:GLN:CD	1:B:106:LEU:HD11	0.48	2.34	3	1
1:B:123:LEU:C	1:B:123:LEU:HD12	0.48	2.33	3	1
1:A:53:ILE:HA	1:A:56:ARG:HH21	0.48	1.67	5	1
1:A:38:LYS:HB2	1:A:66:PHE:CB	0.48	2.39	4	2
1:B:112:CYS:C	1:B:113:ASN:OD1	0.48	2.57	3	1
1:B:134:ASN:C	1:B:139:ARG:HH21	0.48	2.16	3	1
1:B:138:ASP:O	1:B:141:LYS:N	0.48	2.46	3	5
1:B:100:ILE:HG21	1:B:145:LYS:CG	0.48	2.39	1	1
1:A:22:TYR:O	1:A:26:PHE:HB2	0.48	2.09	4	2
1:B:143:LEU:O	1:B:146:SER:OG	0.48	2.32	5	5
1:B:139:ARG:NH1	1:B:139:ARG:HB3	0.48	2.23	4	1
1:A:16:GLU:HG2	1:A:17:ILE:HG23	0.48	1.86	6	1
1:B:120:ILE:O	1:B:123:LEU:CD1	0.47	2.61	3	2
1:B:147:LYS:O	1:B:149:PHE:N	0.47	2.47	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:114:LEU:CD2	1:B:123:LEU:HD13	0.47	2.38	5	2
1:B:137:GLY:O	1:B:140:LEU:HB3	0.47	2.09	2	1
1:B:94:GLN:CG	1:B:106:LEU:HD11	0.47	2.39	3	1
1:A:42:LYS:HE3	1:A:56:ARG:CZ	0.47	2.39	5	1
1:A:60:LEU:CD1	1:B:124:ASP:HB3	0.47	2.39	4	2
1:A:35:GLU:O	1:A:38:LYS:HG2	0.47	2.09	8	1
1:A:31:LEU:HD13	1:A:36:GLU:HB3	0.47	1.85	1	1
1:A:41:ASP:HB3	1:B:143:LEU:CD2	0.47	2.39	1	1
1:B:140:LEU:O	1:B:143:LEU:HB3	0.47	2.09	1	1
1:B:125:LYS:HZ1	1:B:139:ARG:HG3	0.47	1.68	2	1
1:B:125:LYS:CD	1:B:125:LYS:C	0.47	2.87	6	2
1:A:45:LEU:HD22	1:A:56:ARG:NH1	0.47	2.24	1	1
1:A:54:GLY:O	1:A:57:LEU:N	0.47	2.45	1	1
1:B:123:LEU:HD23	1:B:127:ILE:CG2	0.47	2.38	1	1
1:A:56:ARG:NH2	1:B:129:ILE:HG12	0.47	2.23	2	1
1:B:102:CYS:SG	1:B:142:ILE:CD1	0.47	2.98	8	1
1:B:113:ASN:O	1:B:114:LEU:HD13	0.47	2.09	8	1
1:A:14:LEU:O	1:A:19:CYS:N	0.47	2.48	1	2
1:A:45:LEU:HD13	1:A:56:ARG:CZ	0.47	2.39	1	1
1:A:19:CYS:HA	1:A:22:TYR:CE1	0.47	2.44	2	1
1:A:37:ILE:HA	1:A:40:LEU:CD2	0.47	2.40	5	2
1:A:41:ASP:CB	1:B:143:LEU:HD22	0.47	2.40	1	1
1:A:42:LYS:HZ1	1:B:126:ASP:HB2	0.47	1.69	3	1
1:A:58:LYS:C	1:A:58:LYS:HD3	0.47	2.35	6	2
1:B:116:THR:C	1:B:118:GLU:N	0.47	2.72	5	2
1:A:33:THR:C	1:A:35:GLU:N	0.47	2.70	6	1
1:B:104:GLN:OE1	1:B:105:TYR:CD1	0.47	2.68	1	1
1:A:17:ILE:HG22	1:A:62:LYS:CD	0.47	2.39	5	3
1:A:34:GLU:CB	1:A:66:PHE:CE1	0.47	2.99	1	2
1:B:106:LEU:O	1:B:110:ILE:HG13	0.47	2.10	3	2
1:A:34:GLU:CB	1:A:66:PHE:CE2	0.47	2.98	5	2
1:B:114:LEU:HD11	1:B:123:LEU:CD1	0.47	2.39	5	2
1:B:120:ILE:HA	1:B:123:LEU:CD2	0.47	2.40	4	1
1:A:17:ILE:CG2	1:A:62:LYS:CD	0.46	2.93	1	6
1:A:42:LYS:HG3	1:B:125:LYS:CE	0.46	2.41	1	1
1:B:125:LYS:CE	1:B:129:ILE:HG21	0.46	2.40	4	2
1:B:128:LEU:HB3	1:B:133:VAL:HG21	0.46	1.86	7	1
1:A:44:ILE:HD13	1:B:140:LEU:CD1	0.46	2.39	8	1
1:A:42:LYS:HG2	1:B:125:LYS:HG2	0.46	1.86	2	1
1:B:131:LEU:CD2	1:B:133:VAL:CG2	0.46	2.85	3	1
1:B:143:LEU:C	1:B:146:SER:OG	0.46	2.58	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LYS:CB	1:A:60:LEU:HB2	0.46	2.40	7	2
1:A:45:LEU:HD13	1:A:59:ILE:CG2	0.46	2.40	7	1
1:A:12:LEU:HD12	1:A:12:LEU:O	0.46	2.10	1	1
1:B:97:LEU:O	1:B:102:CYS:N	0.46	2.49	8	2
1:A:46:ILE:HG13	1:A:47:ALA:N	0.46	2.25	6	2
1:B:114:LEU:HD22	1:B:123:LEU:HD22	0.46	1.86	6	1
1:B:120:ILE:O	1:B:123:LEU:CD2	0.46	2.63	2	2
1:A:41:ASP:CG	1:B:143:LEU:HD21	0.46	2.34	5	2
1:A:42:LYS:NZ	1:A:42:LYS:HB2	0.46	2.21	3	1
1:B:105:TYR:CD1	1:B:105:TYR:N	0.46	2.84	8	2
1:B:100:ILE:HG22	1:B:145:LYS:HG3	0.46	1.87	8	2
1:A:50:VAL:HG23	1:A:52:LYS:HG2	0.46	1.86	2	1
1:B:114:LEU:HD13	1:B:123:LEU:CD1	0.46	2.40	2	1
1:A:43:ASP:OD1	1:B:137:GLY:CA	0.46	2.63	3	1
1:A:55:ASP:O	1:A:58:LYS:N	0.46	2.48	8	4
1:B:135:LYS:C	1:B:139:ARG:NH2	0.46	2.74	5	1
1:B:140:LEU:HD23	1:B:140:LEU:O	0.46	2.10	4	1
1:A:42:LYS:HD3	1:B:126:ASP:CA	0.46	2.39	5	1
1:B:102:CYS:HA	1:B:105:TYR:CE1	0.46	2.45	8	1
1:B:145:LYS:O	1:B:148:SER:HB2	0.46	2.11	5	4
1:B:141:LYS:CB	1:B:141:LYS:NZ	0.46	2.78	4	1
1:A:38:LYS:HB3	1:A:66:PHE:CB	0.46	2.41	6	1
1:A:42:LYS:HD3	1:B:125:LYS:CG	0.46	2.40	3	1
1:A:46:ILE:HD12	1:B:136:ILE:HG23	0.46	1.88	1	1
1:B:117:GLU:CB	1:B:149:PHE:CE2	0.46	2.99	2	6
1:A:46:ILE:HA	1:A:50:VAL:HG13	0.46	1.86	2	1
1:B:139:ARG:CZ	1:B:139:ARG:HB3	0.46	2.41	4	1
1:B:138:ASP:CB	1:B:139:ARG:HH21	0.46	2.23	6	1
1:A:42:LYS:HG2	1:B:125:LYS:HB3	0.45	1.88	2	1
1:A:29:CYS:O	1:A:30:ASN:HB3	0.45	2.10	5	3
1:B:120:ILE:HG13	1:B:149:PHE:CD1	0.45	2.47	5	1
1:B:125:LYS:HB2	1:B:143:LEU:CB	0.45	2.41	5	1
1:A:42:LYS:HG3	1:B:125:LYS:CD	0.45	2.40	2	1
1:B:121:LYS:HB2	1:B:149:PHE:CB	0.45	2.41	8	4
1:B:120:ILE:HA	1:B:123:LEU:HG	0.45	1.88	3	1
1:A:43:ASP:OD1	1:B:137:GLY:N	0.45	2.49	5	1
1:A:46:ILE:HD13	1:B:136:ILE:CB	0.45	2.39	6	1
1:A:17:ILE:CG2	1:A:62:LYS:HG3	0.45	2.42	3	3
1:A:41:ASP:HB3	1:B:143:LEU:HD22	0.45	1.88	1	1
1:A:40:LEU:HD22	1:A:44:ILE:HG22	0.45	1.86	2	1
1:B:113:ASN:O	1:B:119:GLU:CD	0.45	2.59	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:CD1	1:B:136:ILE:HD11	0.45	2.40	8	1
1:B:128:LEU:CD1	1:B:139:ARG:HB2	0.45	2.42	2	1
1:A:48:LEU:HD12	1:A:48:LEU:O	0.45	2.12	4	1
1:B:131:LEU:HD21	1:B:133:VAL:HG13	0.45	1.87	4	1
1:A:13:PHE:CE1	1:A:62:LYS:HB3	0.45	2.46	7	2
1:B:112:CYS:SG	1:B:127:ILE:HG23	0.45	2.52	1	1
1:B:134:ASN:HA	1:B:139:ARG:NH2	0.45	2.25	3	1
1:B:135:LYS:C	1:B:139:ARG:HH21	0.45	2.19	5	1
1:A:57:LEU:CB	1:B:126:ASP:HB3	0.45	2.41	8	1
1:B:112:CYS:SG	1:B:114:LEU:HD21	0.45	2.51	8	1
1:B:108:SER:HB3	1:B:131:LEU:CD2	0.45	2.41	2	1
1:B:116:THR:HG23	1:B:119:GLU:H	0.45	1.72	7	1
1:B:108:SER:OG	1:B:131:LEU:HD21	0.45	2.12	1	1
1:B:116:THR:O	1:B:120:ILE:HD13	0.45	2.12	1	1
1:A:45:LEU:O	1:A:48:LEU:N	0.45	2.49	5	3
1:B:125:LYS:HD2	1:B:125:LYS:O	0.45	2.12	4	1
1:B:120:ILE:O	1:B:123:LEU:HD23	0.45	2.12	6	1
1:A:56:ARG:NH1	1:A:56:ARG:HA	0.45	2.26	1	1
1:B:142:ILE:O	1:B:146:SER:N	0.45	2.43	5	3
1:A:43:ASP:HB3	1:B:140:LEU:CB	0.45	2.41	4	1
1:B:143:LEU:HD13	1:B:143:LEU:O	0.45	2.11	4	1
1:A:46:ILE:CD1	1:B:136:ILE:CG1	0.45	2.95	6	1
1:A:43:ASP:HB2	1:B:125:LYS:CE	0.45	2.42	2	1
1:B:128:LEU:O	1:B:131:LEU:N	0.45	2.49	8	2
1:B:125:LYS:HZ3	1:B:139:ARG:HB3	0.45	1.72	5	1
1:B:126:ASP:O	1:B:129:ILE:HG22	0.45	2.11	5	1
1:A:17:ILE:CG2	1:A:62:LYS:HG2	0.45	2.41	8	1
1:B:106:LEU:O	1:B:110:ILE:CD1	0.45	2.65	8	1
1:A:17:ILE:CG2	1:A:62:LYS:CG	0.44	2.94	1	3
1:A:46:ILE:CD1	1:B:136:ILE:CG2	0.44	2.95	1	1
1:A:46:ILE:HG13	1:A:56:ARG:NH1	0.44	2.27	3	1
1:B:134:ASN:CA	1:B:139:ARG:HH21	0.44	2.25	3	1
1:A:17:ILE:O	1:A:58:LYS:NZ	0.44	2.47	6	1
1:A:42:LYS:HB2	1:A:60:LEU:HD12	0.44	1.89	6	1
1:B:133:VAL:CG1	1:B:139:ARG:NE	0.44	2.80	6	1
1:B:106:LEU:CD1	1:B:106:LEU:N	0.44	2.81	8	1
1:A:25:SER:HB3	1:A:48:LEU:CD2	0.44	2.41	6	4
1:B:100:ILE:CG2	1:B:145:LYS:HG3	0.44	2.42	1	3
1:B:129:ILE:HG13	1:B:139:ARG:NH2	0.44	2.27	1	1
1:A:31:LEU:HD22	1:A:40:LEU:HD13	0.44	1.90	4	1
1:B:134:ASN:O	1:B:135:LYS:C	0.44	2.60	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:VAL:HG21	1:B:120:ILE:CD1	0.44	2.40	5	1
1:A:17:ILE:CG2	1:A:62:LYS:HD2	0.44	2.42	7	6
1:A:56:ARG:HH21	1:B:129:ILE:HG12	0.44	1.71	2	1
1:A:64:LYS:O	1:A:66:PHE:N	0.44	2.49	3	2
1:B:135:LYS:O	1:B:139:ARG:HG2	0.44	2.12	4	1
1:A:46:ILE:HD13	1:B:136:ILE:HD12	0.44	1.87	5	1
1:A:46:ILE:CD1	1:B:136:ILE:CD1	0.44	2.95	8	1
1:B:126:ASP:HA	1:B:129:ILE:HG22	0.44	1.90	8	1
1:B:97:LEU:HA	1:B:100:ILE:CG1	0.44	2.41	1	3
1:A:43:ASP:OD2	1:B:139:ARG:HD2	0.44	2.11	3	1
1:B:123:LEU:HG	1:B:124:ASP:N	0.44	2.27	4	2
1:A:17:ILE:HA	1:A:58:LYS:HZ1	0.44	1.70	6	1
1:B:100:ILE:CG2	1:B:145:LYS:CG	0.44	2.96	6	2
1:A:38:LYS:HB2	1:A:66:PHE:HB2	0.44	1.89	3	1
1:B:105:TYR:CE2	1:B:142:ILE:HD11	0.44	2.47	5	1
1:B:93:VAL:CG1	1:B:115:VAL:HA	0.44	2.42	3	2
1:A:25:SER:CB	1:A:48:LEU:CD1	0.44	2.95	4	1
1:A:26:PHE:CE1	1:A:48:LEU:HD21	0.44	2.48	4	1
1:B:122:TYR:CD2	1:B:122:TYR:O	0.44	2.70	6	1
1:A:37:ILE:CG1	1:A:66:PHE:CE1	0.44	3.01	5	4
1:B:108:SER:HB2	1:B:131:LEU:CD2	0.44	2.42	4	1
1:A:42:LYS:HZ2	1:A:42:LYS:C	0.44	2.20	7	1
1:A:42:LYS:HE3	1:B:125:LYS:CG	0.44	2.43	8	1
1:B:123:LEU:CD2	1:B:124:ASP:O	0.44	2.65	1	1
1:B:127:ILE:O	1:B:131:LEU:N	0.44	2.51	1	1
1:A:42:LYS:HB2	1:A:60:LEU:HD13	0.44	1.90	2	1
1:A:15:GLU:CG	1:A:20:THR:OG1	0.44	2.66	4	1
1:A:57:LEU:CD1	1:A:60:LEU:CD2	0.44	2.95	6	1
1:B:139:ARG:N	1:B:139:ARG:CZ	0.44	2.80	7	1
1:A:30:ASN:O	1:A:31:LEU:HD13	0.44	2.13	3	2
1:B:102:CYS:CB	1:B:105:TYR:CD1	0.44	3.01	6	3
1:B:104:GLN:CD	1:B:105:TYR:CE1	0.44	2.96	1	1
1:B:129:ILE:HG22	1:B:139:ARG:CB	0.44	2.42	3	1
1:A:10:VAL:CG1	1:A:32:VAL:HA	0.44	2.43	7	2
1:A:43:ASP:O	1:A:46:ILE:HG13	0.44	2.12	6	1
1:A:29:CYS:SG	1:A:31:LEU:CD2	0.44	3.06	8	1
1:A:41:ASP:CG	1:B:143:LEU:HD22	0.43	2.38	1	1
1:A:17:ILE:HG22	1:A:62:LYS:CE	0.43	2.43	4	3
1:A:46:ILE:CG2	1:A:56:ARG:NE	0.43	2.80	6	1
1:A:45:LEU:HD11	1:A:59:ILE:CG2	0.43	2.44	1	1
1:A:43:ASP:CB	1:B:140:LEU:HD12	0.43	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LYS:HB2	1:B:125:LYS:HG2	0.43	1.88	3	1
1:B:129:ILE:CG2	1:B:139:ARG:HB2	0.43	2.43	3	1
1:B:114:LEU:HD12	1:B:120:ILE:CG2	0.43	2.43	8	1
1:B:125:LYS:O	1:B:125:LYS:HD2	0.43	2.12	8	1
1:A:22:TYR:CD1	1:A:22:TYR:N	0.43	2.86	2	2
1:A:43:ASP:HB3	1:B:140:LEU:HB2	0.43	1.90	4	1
1:A:42:LYS:HG3	1:A:43:ASP:N	0.43	2.27	7	2
1:A:34:GLU:HB3	1:A:66:PHE:CE1	0.43	2.49	1	1
1:A:34:GLU:CA	1:A:66:PHE:CE1	0.43	3.01	2	2
1:B:104:GLN:CG	1:B:105:TYR:CE1	0.43	3.01	1	1
1:B:105:TYR:HB3	1:B:109:PHE:CD1	0.43	2.49	2	1
1:A:25:SER:HB3	1:A:48:LEU:CG	0.43	2.44	3	1
1:B:125:LYS:CE	1:B:139:ARG:HB3	0.43	2.43	1	1
1:A:60:LEU:HD21	1:B:124:ASP:OD1	0.43	2.13	3	1
1:B:133:VAL:C	1:B:135:LYS:N	0.43	2.75	7	1
1:A:43:ASP:OD1	1:B:125:LYS:HD3	0.43	2.12	8	1
1:A:21:GLN:C	1:A:22:TYR:CD1	0.43	2.97	2	1
1:B:96:PHE:CE2	1:B:149:PHE:CE1	0.43	3.06	3	1
1:A:42:LYS:NZ	1:A:42:LYS:HB3	0.43	2.23	3	1
1:A:43:ASP:CA	1:A:46:ILE:HG22	0.43	2.44	5	1
1:B:125:LYS:CB	1:B:143:LEU:HB2	0.43	2.43	5	1
1:B:139:ARG:NH1	1:B:140:LEU:HB2	0.43	2.29	8	1
1:A:53:ILE:HG12	1:B:129:ILE:HD13	0.43	1.90	2	1
1:A:42:LYS:NZ	1:B:126:ASP:HB2	0.43	2.28	3	1
1:A:42:LYS:CE	1:A:56:ARG:CZ	0.43	2.96	5	1
1:A:25:SER:O	1:A:28:GLN:HG3	0.43	2.13	8	1
1:A:56:ARG:C	1:B:126:ASP:OD2	0.43	2.61	1	1
1:A:46:ILE:HA	1:A:50:VAL:O	0.43	2.13	4	2
1:A:42:LYS:CG	1:B:125:LYS:CB	0.43	2.97	6	1
1:A:42:LYS:HG3	1:B:125:LYS:HB3	0.43	1.89	6	1
1:B:106:LEU:HD23	1:B:106:LEU:N	0.43	2.28	5	1
1:B:128:LEU:HB3	1:B:139:ARG:CG	0.43	2.44	6	1
1:B:116:THR:CG2	1:B:119:GLU:HB2	0.43	2.43	7	1
1:B:126:ASP:O	1:B:129:ILE:HG23	0.42	2.13	1	1
1:A:57:LEU:O	1:A:60:LEU:HD23	0.42	2.14	3	2
1:B:95:LEU:O	1:B:95:LEU:HD12	0.42	2.14	7	1
1:B:118:GLU:O	1:B:122:TYR:N	0.42	2.52	1	1
1:A:12:LEU:C	1:A:12:LEU:CD1	0.42	2.86	7	2
1:A:22:TYR:HB3	1:A:26:PHE:CD1	0.42	2.49	3	2
1:A:62:LYS:O	1:A:65:SER:HB2	0.42	2.14	2	1
1:B:126:ASP:O	1:B:126:ASP:OD2	0.42	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:CYS:SG	1:A:31:LEU:HD21	0.42	2.55	1	2
1:A:42:LYS:NZ	1:B:126:ASP:OD1	0.42	2.53	5	1
1:B:136:ILE:N	1:B:139:ARG:NH2	0.42	2.67	5	1
1:A:58:LYS:CD	1:A:62:LYS:HG3	0.42	2.44	6	1
1:B:114:LEU:CB	1:B:120:ILE:CG2	0.42	2.97	8	1
1:A:13:PHE:O	1:A:16:GLU:HG3	0.42	2.14	1	1
1:A:42:LYS:HB3	1:B:125:LYS:HG3	0.42	1.90	1	1
1:A:53:ILE:HD12	1:B:129:ILE:CD1	0.42	2.44	1	1
1:B:96:PHE:CE1	1:B:145:LYS:HB3	0.42	2.49	6	3
1:B:129:ILE:HA	1:B:133:VAL:O	0.42	2.13	6	1
1:B:139:ARG:CZ	1:B:139:ARG:HB2	0.42	2.45	6	1
1:B:95:LEU:C	1:B:95:LEU:CD1	0.42	2.91	3	3
1:B:123:LEU:CD1	1:B:127:ILE:CG2	0.42	2.93	4	1
1:A:10:VAL:HG23	1:A:34:GLU:HG2	0.42	1.91	7	1
1:A:46:ILE:HG12	1:A:56:ARG:CZ	0.42	2.44	7	1
1:B:139:ARG:NH1	1:B:140:LEU:CB	0.42	2.83	8	1
1:B:137:GLY:H	1:B:139:ARG:CG	0.42	2.28	8	2
1:A:34:GLU:CA	1:A:66:PHE:CE2	0.42	3.02	4	1
1:A:51:ASN:OD1	1:B:136:ILE:HD11	0.42	2.14	4	1
1:B:142:ILE:O	1:B:146:SER:OG	0.42	2.38	6	2
1:B:98:GLU:HG3	1:B:99:GLU:N	0.42	2.30	4	3
1:B:114:LEU:HD11	1:B:123:LEU:HD12	0.42	1.90	2	2
1:A:38:LYS:CB	1:A:66:PHE:CB	0.42	2.98	6	1
1:B:129:ILE:HD12	1:B:129:ILE:C	0.42	2.40	6	1
1:A:53:ILE:HB	1:B:129:ILE:HD13	0.42	1.91	6	1
1:B:139:ARG:HA	1:B:139:ARG:NH1	0.42	2.30	7	1
1:A:42:LYS:HZ1	1:A:56:ARG:HB3	0.42	1.75	8	1
1:A:57:LEU:HB2	1:B:126:ASP:HB3	0.42	1.91	8	1
1:A:16:GLU:HG3	1:A:17:ILE:N	0.42	2.28	1	1
1:A:43:ASP:CA	1:A:46:ILE:CG2	0.42	2.96	1	1
1:B:94:GLN:HG2	1:B:106:LEU:HD11	0.42	1.92	3	1
1:A:31:LEU:CB	1:A:37:ILE:CG2	0.42	2.98	6	2
1:A:42:LYS:CE	1:B:125:LYS:HG3	0.42	2.45	8	1
1:B:128:LEU:HD12	1:B:129:ILE:N	0.42	2.30	8	1
1:A:40:LEU:HB2	1:A:44:ILE:HG21	0.41	1.91	2	1
1:A:50:VAL:O	1:A:50:VAL:HG22	0.41	2.15	4	1
1:B:97:LEU:HD23	1:B:100:ILE:CD1	0.41	2.42	4	1
1:B:108:SER:O	1:B:111:GLN:HG2	0.41	2.15	7	1
1:B:123:LEU:HB2	1:B:127:ILE:HG21	0.41	1.91	7	1
1:A:44:ILE:O	1:A:48:LEU:N	0.41	2.54	8	1
1:A:42:LYS:HG2	1:B:125:LYS:CB	0.41	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LYS:CE	1:B:126:ASP:HB2	0.41	2.45	4	1
1:A:14:LEU:O	1:A:18:GLY:N	0.41	2.53	5	1
1:A:17:ILE:CA	1:A:58:LYS:NZ	0.41	2.83	6	1
1:A:56:ARG:HB2	1:B:126:ASP:OD1	0.41	2.14	8	1
1:A:42:LYS:CE	1:B:139:ARG:NH2	0.41	2.83	1	1
1:A:12:LEU:HD13	1:A:12:LEU:O	0.41	2.14	2	2
1:B:121:LYS:HB2	1:B:149:PHE:HB2	0.41	1.91	2	3
1:A:27:ILE:CG1	1:A:32:VAL:CG2	0.41	2.97	4	1
1:B:147:LYS:C	1:B:149:PHE:H	0.41	2.23	8	2
1:A:62:LYS:O	1:A:65:SER:HB3	0.41	2.15	7	1
1:B:117:GLU:CA	1:B:149:PHE:CE2	0.41	3.03	3	2
1:B:93:VAL:HB	1:B:115:VAL:HA	0.41	1.93	4	1
1:A:13:PHE:CD2	1:A:14:LEU:CD1	0.41	3.04	1	1
1:B:100:ILE:CG2	1:B:145:LYS:CD	0.41	2.99	1	1
1:A:27:ILE:HG12	1:A:32:VAL:CG1	0.41	2.46	3	1
1:B:135:LYS:O	1:B:139:ARG:CZ	0.41	2.68	6	1
1:A:57:LEU:HB3	1:B:126:ASP:CB	0.41	2.43	8	1
1:A:45:LEU:HD13	1:A:56:ARG:HH22	0.41	1.73	1	1
1:A:45:LEU:CB	1:A:56:ARG:CZ	0.41	2.99	1	1
1:B:141:LYS:NZ	1:B:145:LYS:NZ	0.41	2.68	3	1
1:B:133:VAL:O	1:B:133:VAL:HG23	0.41	2.16	4	1
1:A:64:LYS:C	1:A:66:PHE:H	0.41	2.24	5	1
1:A:43:ASP:HA	1:A:46:ILE:CG1	0.41	2.46	2	1
1:A:23:LEU:O	1:A:27:ILE:HG13	0.41	2.16	4	1
1:B:114:LEU:HD21	1:B:123:LEU:HD13	0.41	1.93	4	1
1:B:136:ILE:CA	1:B:139:ARG:NH2	0.41	2.84	5	1
1:A:10:VAL:CG1	1:A:32:VAL:HG13	0.41	2.43	6	1
1:B:110:ILE:CG1	1:B:115:VAL:CG2	0.41	2.98	6	1
1:A:56:ARG:NH2	1:B:125:LYS:HZ1	0.41	2.14	8	1
1:A:60:LEU:HD21	1:B:124:ASP:OD2	0.41	2.16	2	1
1:A:60:LEU:CD1	1:B:124:ASP:OD1	0.41	2.59	3	1
1:A:43:ASP:HB3	1:B:140:LEU:CD1	0.41	2.45	4	1
1:B:93:VAL:HG13	1:B:97:LEU:CD1	0.41	2.46	4	1
1:B:125:LYS:HD2	1:B:139:ARG:NH1	0.41	2.30	4	1
1:B:126:ASP:HA	1:B:129:ILE:HD11	0.41	1.92	4	1
1:A:13:PHE:CZ	1:A:66:PHE:CE1	0.41	3.09	7	1
1:A:44:ILE:CD1	1:B:140:LEU:HD11	0.41	2.46	7	1
1:A:43:ASP:OD1	1:B:137:GLY:HA2	0.41	2.15	3	1
1:B:94:GLN:CD	1:B:106:LEU:CD1	0.41	2.94	3	1
1:B:94:GLN:HG2	1:B:106:LEU:CD1	0.41	2.46	3	1
1:A:23:LEU:O	1:A:27:ILE:CG1	0.41	2.69	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:141:LYS:NZ	1:B:141:LYS:HB2	0.41	2.31	4	1
1:B:125:LYS:CD	1:B:129:ILE:HG23	0.41	2.46	6	1
1:A:25:SER:O	1:A:48:LEU:HG	0.41	2.16	8	1
1:B:128:LEU:O	1:B:133:VAL:CG1	0.41	2.67	8	1
1:B:104:GLN:OE1	1:B:104:GLN:O	0.41	2.39	1	1
1:B:117:GLU:O	1:B:149:PHE:CD2	0.41	2.74	1	1
1:A:57:LEU:CD2	1:B:127:ILE:HD12	0.41	2.46	6	1
1:B:141:LYS:CG	1:B:142:ILE:N	0.41	2.83	7	1
1:A:30:ASN:O	1:A:36:GLU:CB	0.41	2.69	8	1
1:B:96:PHE:CD1	1:B:96:PHE:C	0.41	2.98	8	1
1:B:138:ASP:C	1:B:140:LEU:N	0.40	2.76	2	1
1:A:42:LYS:HB3	1:B:125:LYS:HG2	0.40	1.93	5	1
1:B:124:ASP:N	1:B:124:ASP:OD2	0.40	2.55	5	1
1:A:41:ASP:OD2	1:A:41:ASP:N	0.40	2.54	7	1
1:A:43:ASP:O	1:A:43:ASP:OD2	0.40	2.39	7	1
1:A:40:LEU:C	1:A:40:LEU:CD2	0.40	2.87	8	1
1:A:42:LYS:NZ	1:A:42:LYS:CB	0.40	2.83	8	1
1:B:104:GLN:C	1:B:105:TYR:CD1	0.40	2.99	8	1
1:B:104:GLN:N	1:B:104:GLN:OE1	0.40	2.54	2	1
1:A:42:LYS:HD3	1:B:125:LYS:HG3	0.40	1.92	3	1
1:A:53:ILE:HG23	1:B:129:ILE:HD13	0.40	1.89	4	1
1:B:125:LYS:HE2	1:B:129:ILE:CG2	0.40	2.46	4	1
1:B:113:ASN:O	1:B:119:GLU:CB	0.40	2.70	8	1
1:A:37:ILE:O	1:A:40:LEU:HD11	0.40	2.15	2	1
1:B:138:ASP:O	1:B:141:LYS:HG3	0.40	2.17	2	2
1:B:119:GLU:O	1:B:122:TYR:CD1	0.40	2.74	4	1
1:B:136:ILE:HA	1:B:139:ARG:NH2	0.40	2.30	5	1
1:A:58:LYS:CG	1:A:59:ILE:N	0.40	2.84	6	1
1:A:13:PHE:CE2	1:A:62:LYS:HB3	0.40	2.51	8	1
1:A:40:LEU:HD13	1:A:41:ASP:O	0.40	2.17	2	1
1:B:123:LEU:CD2	1:B:146:SER:HB2	0.40	2.47	5	1
1:B:129:ILE:CG2	1:B:139:ARG:HD2	0.40	2.47	6	1
1:A:43:ASP:OD1	1:B:139:ARG:HB3	0.40	2.15	7	1
1:A:46:ILE:CD1	1:B:136:ILE:HD12	0.40	2.45	7	1
1:A:57:LEU:C	1:A:57:LEU:CD2	0.40	2.95	7	1
1:B:114:LEU:CD1	1:B:120:ILE:HG22	0.40	2.46	8	1
1:B:147:LYS:O	1:B:148:SER:C	0.40	2.65	1	1
1:B:123:LEU:CD1	1:B:127:ILE:HG22	0.40	2.46	4	1
1:A:42:LYS:HD3	1:B:126:ASP:H	0.40	1.76	7	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/68 (85%)	44±1 (77±1%)	10±0 (18±1%)	3±1 (6±1%)	2	20
1	B	57/68 (84%)	44±1 (77±2%)	10±1 (17±2%)	3±1 (5±1%)	2	21
All	All	920/1088 (85%)	707 (77%)	161 (18%)	52 (6%)	2	21

All 14 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	30	ASN	8
1	A	55	ASP	8
1	B	113	ASN	8
1	A	52	LYS	5
1	B	135	LYS	5
1	B	101	GLY	3
1	B	148	SER	3
1	A	18	GLY	2
1	B	117	GLU	2
1	A	34	GLU	2
1	B	115	VAL	2
1	B	138	ASP	2
1	A	32	VAL	1
1	A	65	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/64 (84%)	36±3 (67±6%)	18±3 (33±6%)	1	12
1	B	53/64 (83%)	32±3 (61±5%)	20±3 (39±5%)	0	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	856/1024 (84%)	549 (64%)	307 (36%)	1 9

All 77 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	10	VAL	8
1	A	40	LEU	8
1	A	46	ILE	8
1	A	48	LEU	8
1	A	60	LEU	8
1	B	93	VAL	8
1	B	123	LEU	8
1	B	125	LYS	8
1	B	127	ILE	8
1	B	131	LEU	8
1	B	141	LYS	8
1	B	143	LEU	8
1	A	32	VAL	7
1	A	37	ILE	7
1	A	42	LYS	7
1	A	44	ILE	7
1	A	58	LYS	7
1	B	115	VAL	7
1	B	120	ILE	7
1	A	25	SER	6
1	B	95	LEU	6
1	B	129	ILE	6
1	B	139	ARG	6
1	B	98	GLU	6
1	A	16	GLU	5
1	A	64	LYS	5
1	B	128	LEU	5
1	A	31	LEU	5
1	B	140	LEU	5
1	B	124	ASP	5
1	A	9	PHE	4
1	A	61	ARG	4
1	B	126	ASP	4
1	A	38	LYS	4
1	B	100	ILE	4
1	B	108	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	57	LEU	4
1	B	119	GLU	4
1	A	41	ASP	3
1	A	45	LEU	3
1	B	118	GLU	3
1	B	121	LYS	3
1	B	122	TYR	3
1	A	52	LYS	3
1	B	144	ARG	3
1	B	147	LYS	3
1	B	114	LEU	3
1	B	145	LYS	3
1	B	136	ILE	3
1	A	12	LEU	2
1	A	21	GLN	2
1	A	33	THR	2
1	A	56	ARG	2
1	B	104	GLN	2
1	A	20	THR	2
1	A	53	ILE	2
1	B	94	GLN	2
1	B	138	ASP	2
1	A	11	GLN	1
1	A	14	LEU	1
1	A	23	LEU	1
1	A	39	TYR	1
1	B	133	VAL	1
1	A	36	GLU	1
1	B	97	LEU	1
1	B	106	LEU	1
1	B	146	SER	1
1	A	43	ASP	1
1	B	103	THR	1
1	A	35	GLU	1
1	A	17	ILE	1
1	A	19	CYS	1
1	B	116	THR	1
1	B	142	ILE	1
1	A	15	GLU	1
1	B	135	LYS	1
1	B	99	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided