Full wwPDB NMR Structure Validation Report (i)

Dec 20, 2023 – 09:27 AM EST

PDB ID	:	1JOY
Title	:	SOLUTION STRUCTURE OF THE HOMODIMERIC DOMAIN OF ENVZ FROM ESCHERICHIA COLI BY MULTI-DIMENSIONAL NMR.
Authors	:	Tomomori, C.; Tanaka, T.; Dutta, R.; Park, H.; Saha, S.K.; Zhu, Y.; Ishima, R.; Liu, D.; Tong, K.I.; Kurokawa, H.; Qian, H.; Inouye, M.; Ikura, M.
Deposited on	:	1998-12-28

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

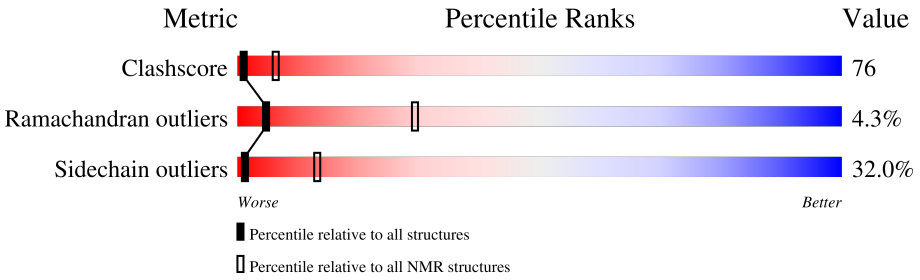
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	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	67	10% 57% 15% • 16%
1	B	67	10% 57% 15% • 16%

2 Ensemble composition and analysis

This entry contains 21 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 as representative.

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:232-A:287, B:232-B:287 (112)	1.07	13

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 7 single-model clusters were found.

Cluster number	Models
1	1, 11, 12, 13, 15, 21
2	2, 4, 14, 16
3	5, 6
4	10, 17, 20
Single-model clusters	3; 7; 8; 9; 18; 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2116 atoms, of which 1060 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (ENVZ_ECOLI).

Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1058	326	530	91	106	5	
1	B	67	Total	C	H	N	O	S	0
			1058	326	530	91	106	5	

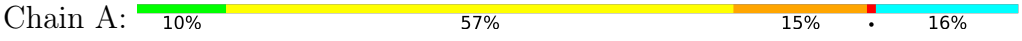
4 Residue-property plots

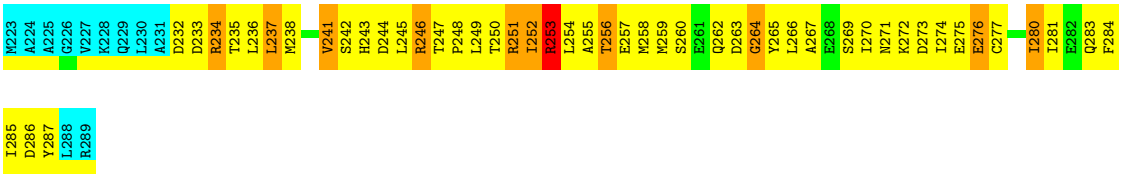
4.1 Average score per residue in the NMR ensemble

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: PROTEIN (ENVZ_ECOLI)

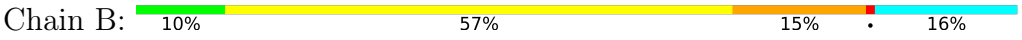
Chain A:





• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B:



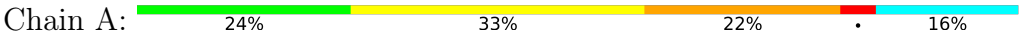
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

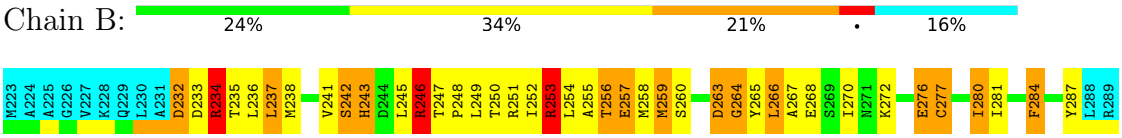
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

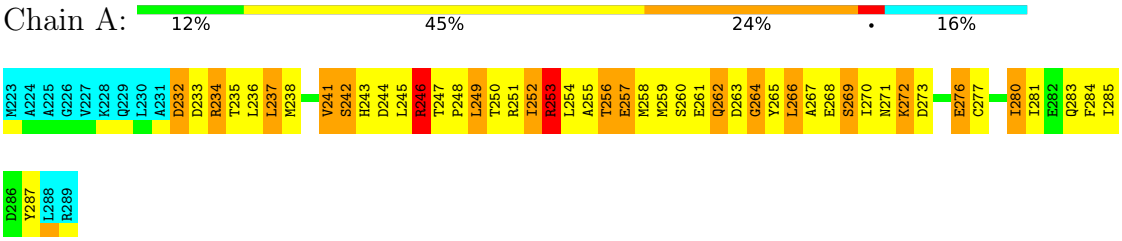
Chain B:



4.2.2 Score per residue for model 2

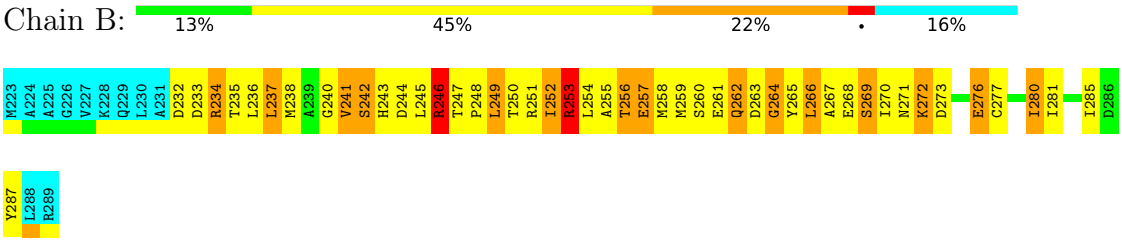
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

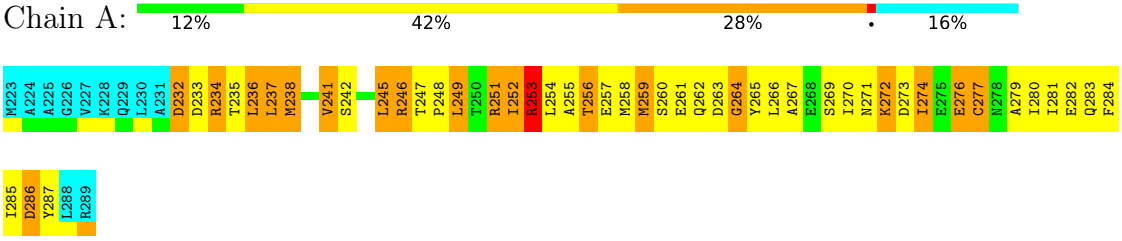
Chain B:



4.2.3 Score per residue for model 3

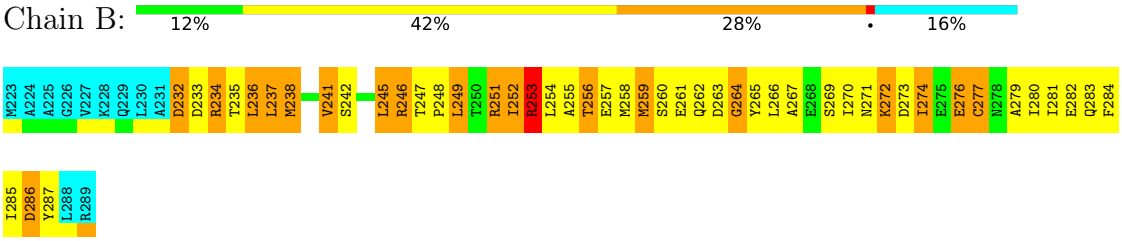
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

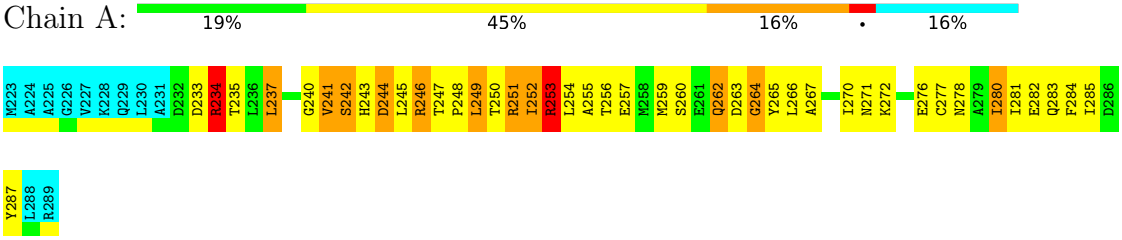
Chain B:



4.2.4 Score per residue for model 4

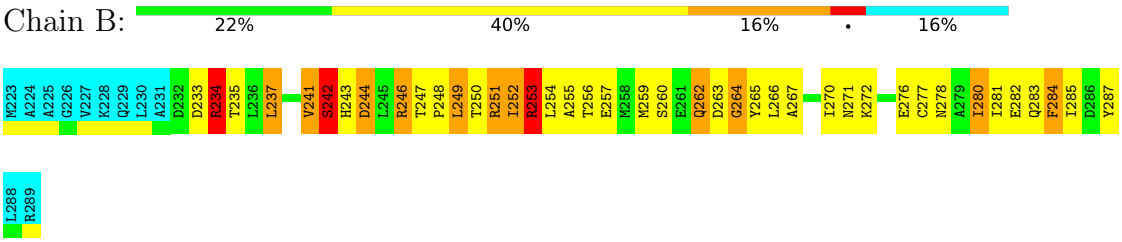
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

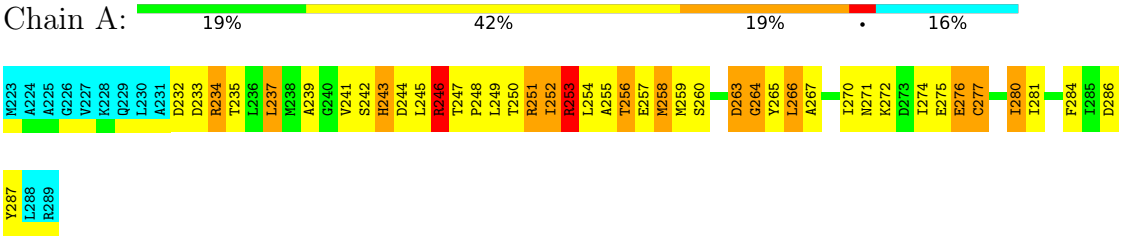
Chain B:



4.2.5 Score per residue for model 5

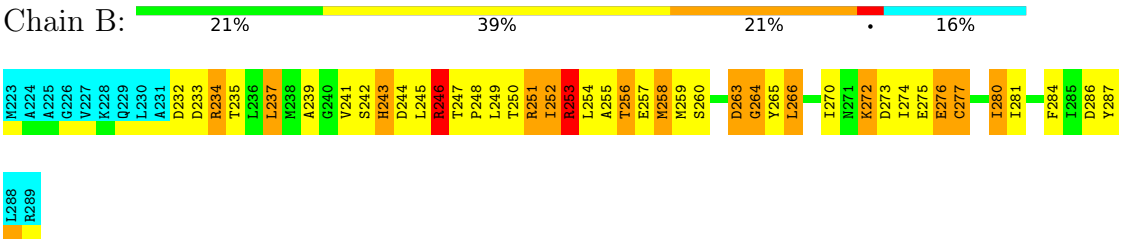
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

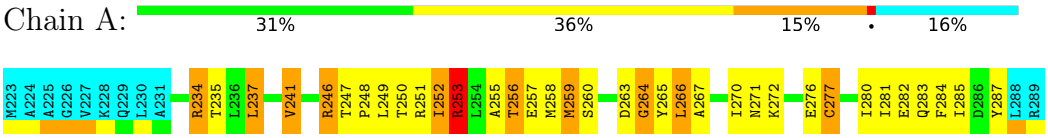
Chain B:



4.2.6 Score per residue for model 6

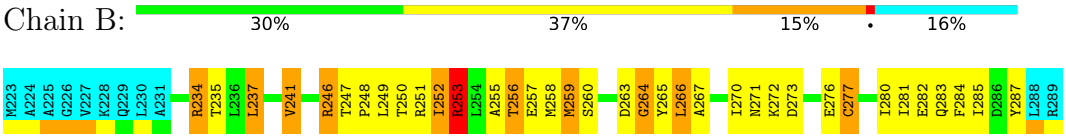
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

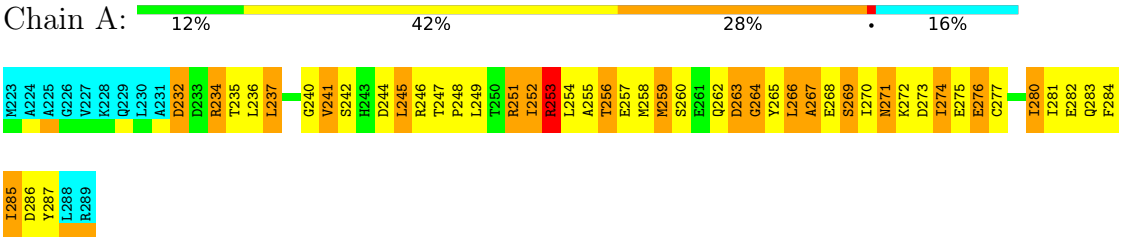
Chain B:



4.2.7 Score per residue for model 7

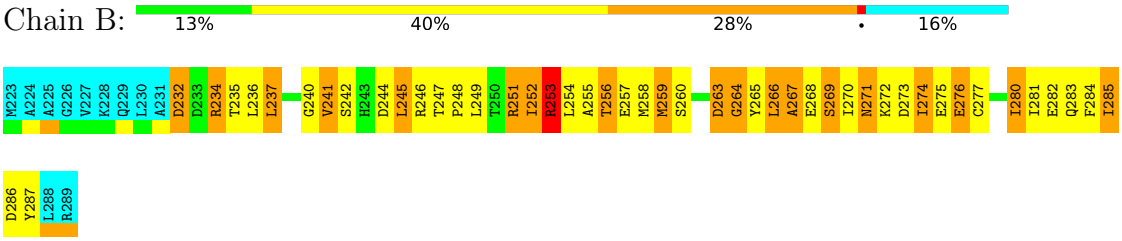
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

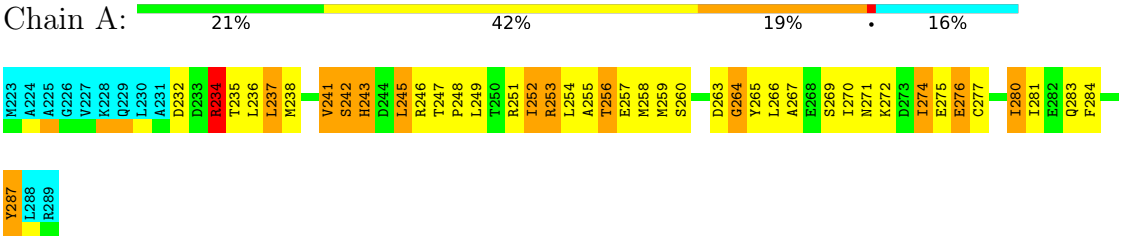
Chain B:



4.2.8 Score per residue for model 8

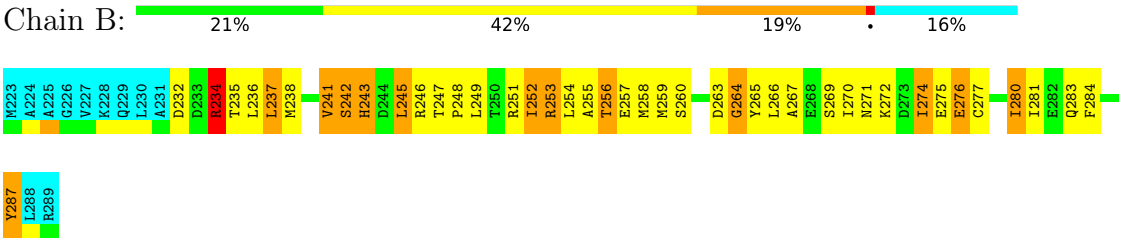
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

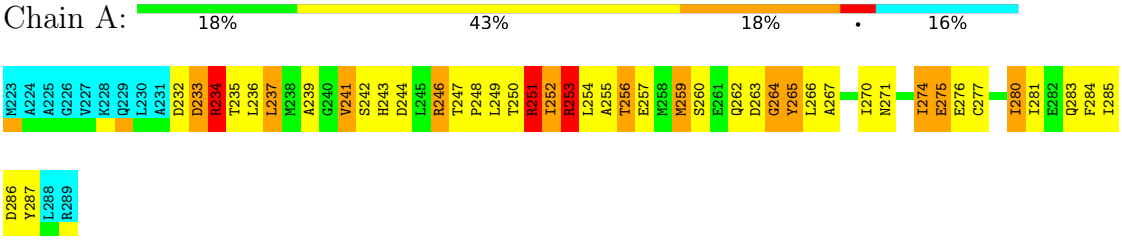
Chain B:



4.2.9 Score per residue for model 9

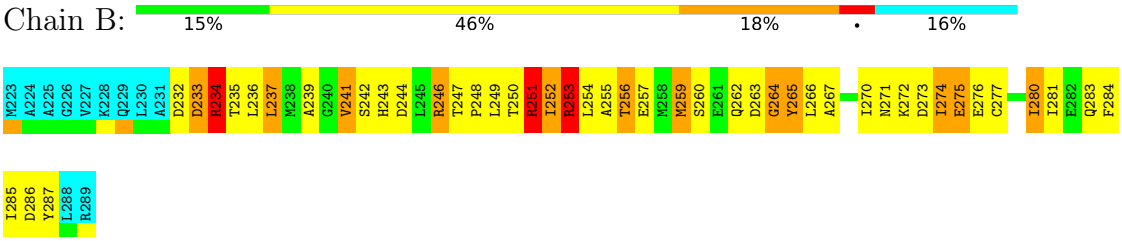
- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



- Molecule 1: PROTEIN (ENVZ_ECOLI)

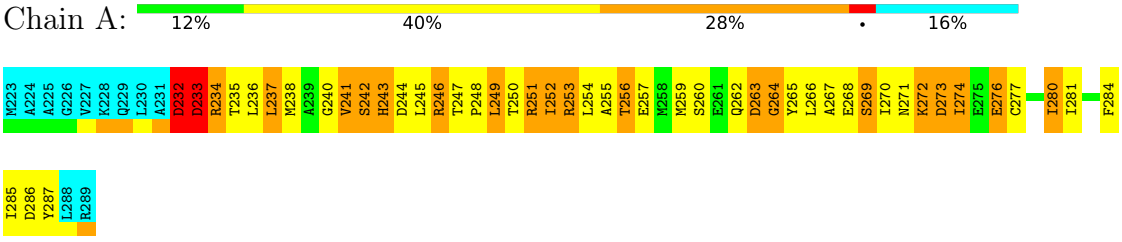
Chain B:



4.2.10 Score per residue for model 10

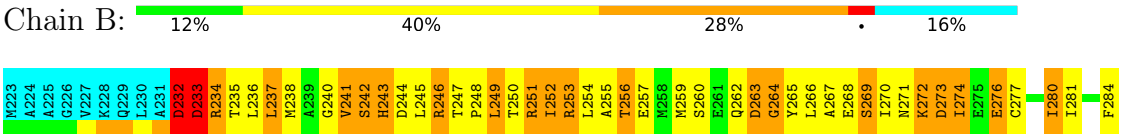
- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



- Molecule 1: PROTEIN (ENVZ_ECOLI)

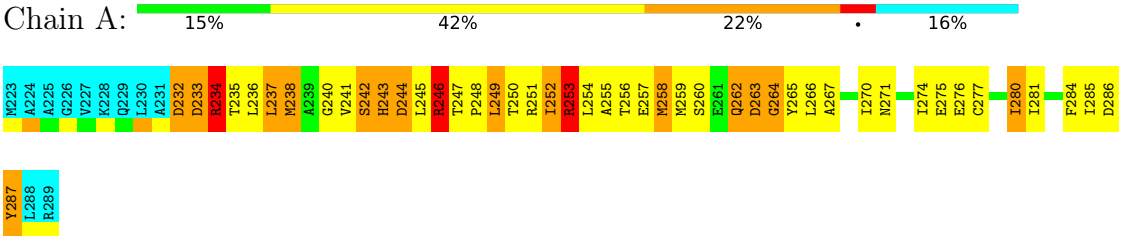
Chain B:



4.2.11 Score per residue for model 11

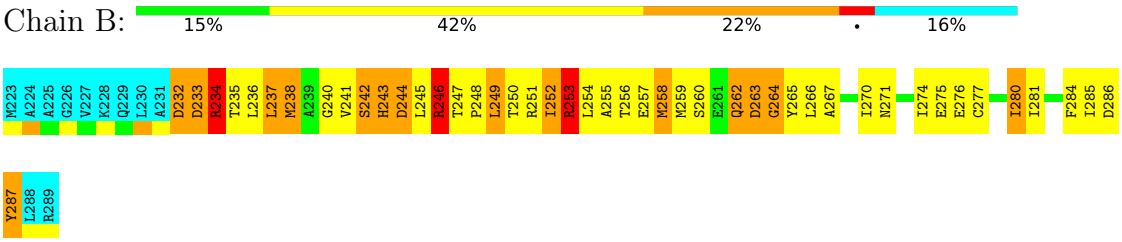
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

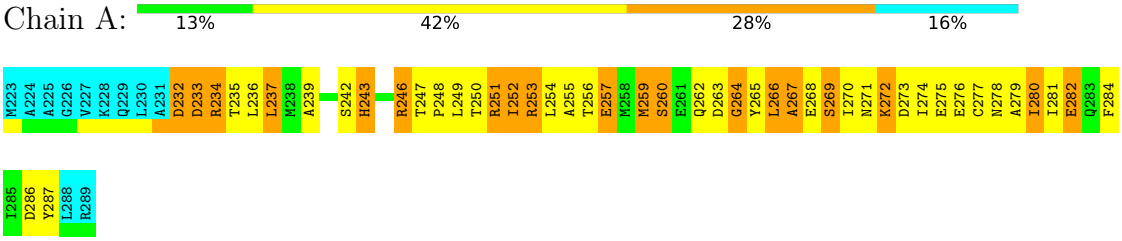
Chain B:



4.2.12 Score per residue for model 12

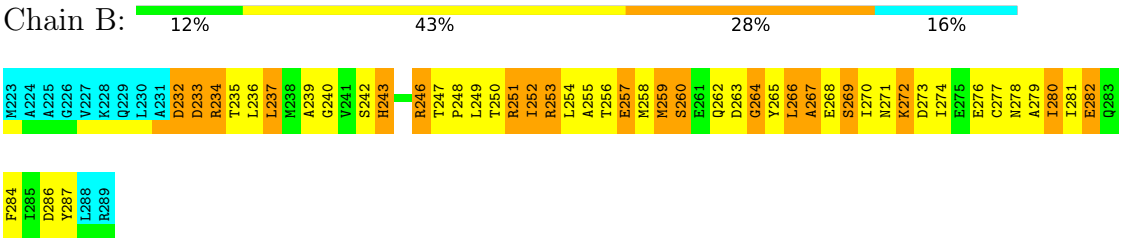
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

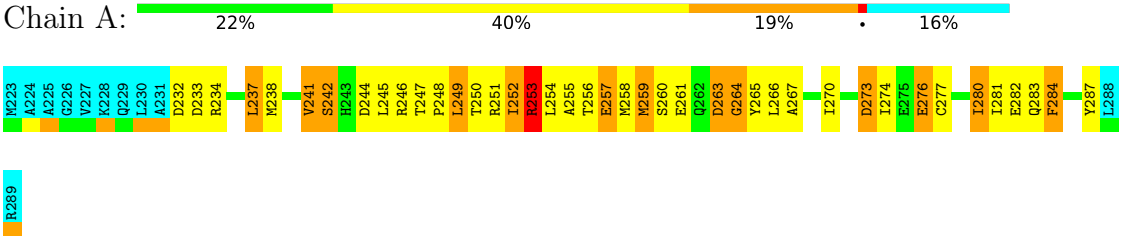
Chain B:



4.2.13 Score per residue for model 13 (medoid)

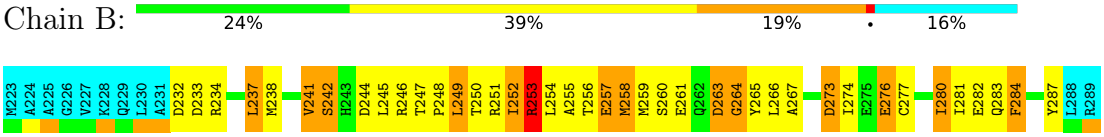
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

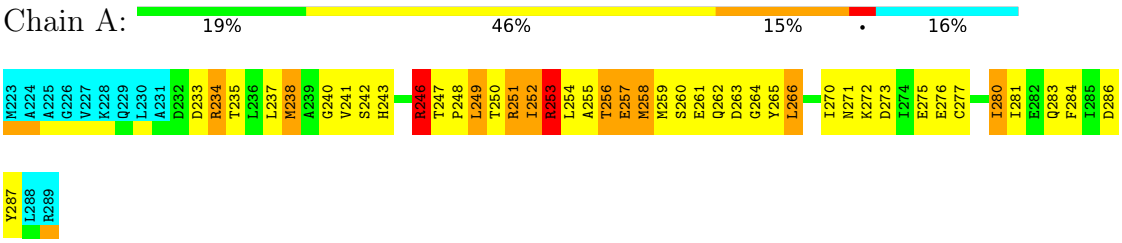
Chain B:



4.2.14 Score per residue for model 14

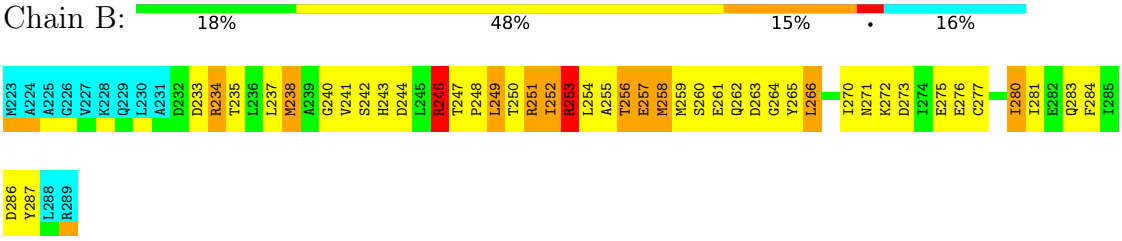
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

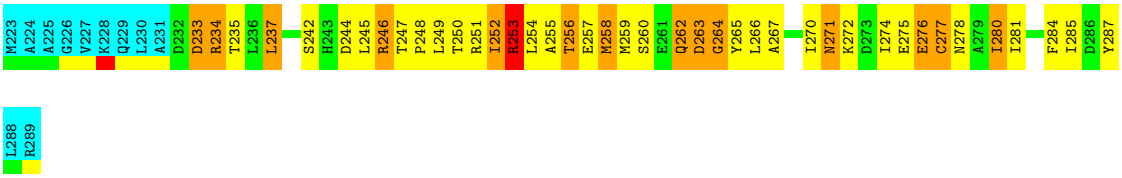
Chain B:



4.2.15 Score per residue for model 15

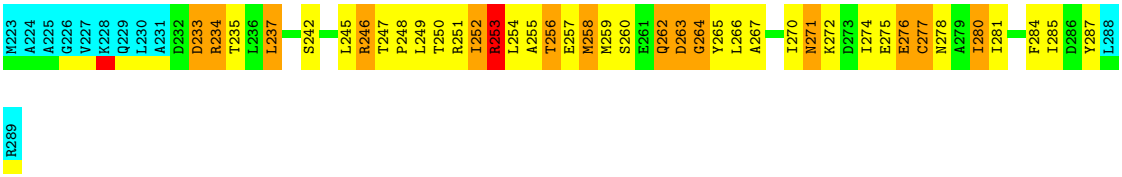
• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



• Molecule 1: PROTEIN (ENVZ_ECOLI)

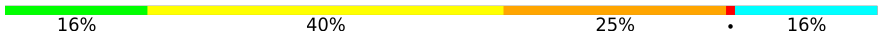
Chain B:

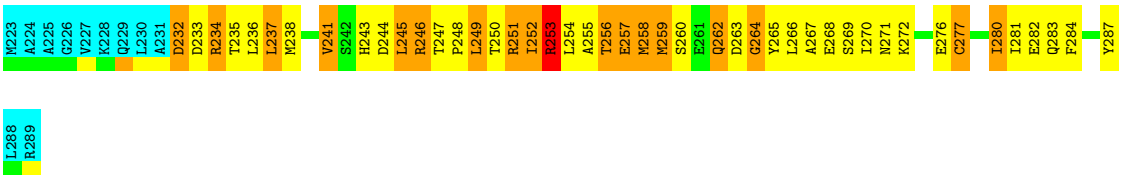


4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (ENVZ_ECOLI)

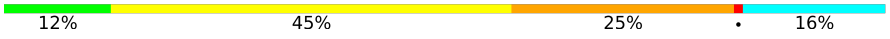
Chain A:

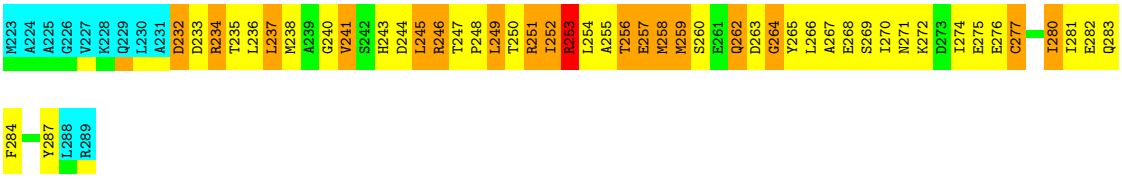




• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B:

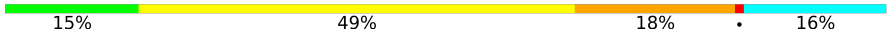




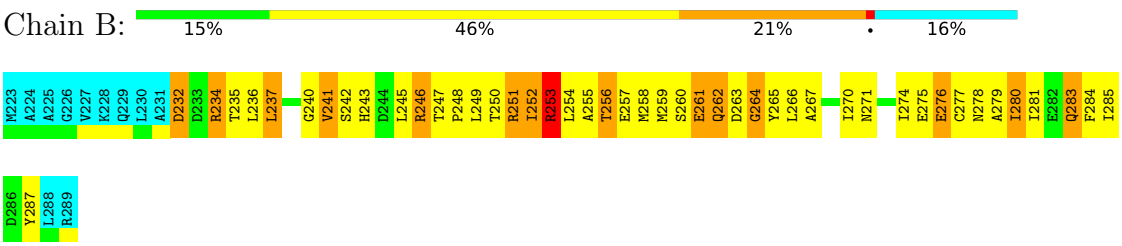
4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:

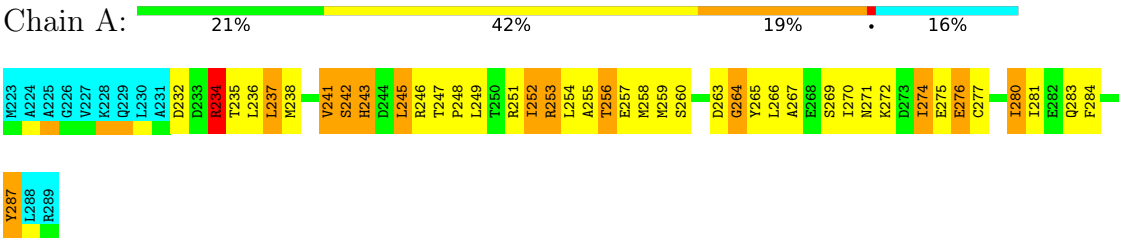


• Molecule 1: PROTEIN (ENVZ_ECOLI)

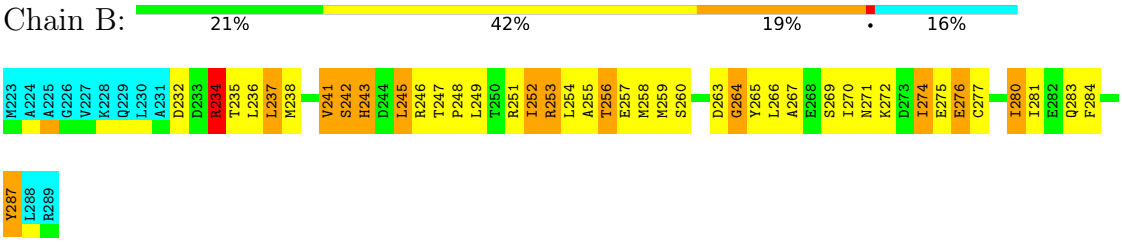


4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN (ENVZ_ECOLI)

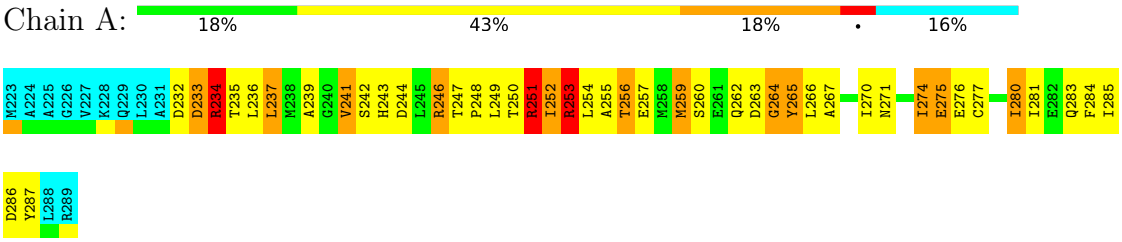


• Molecule 1: PROTEIN (ENVZ_ECOLI)



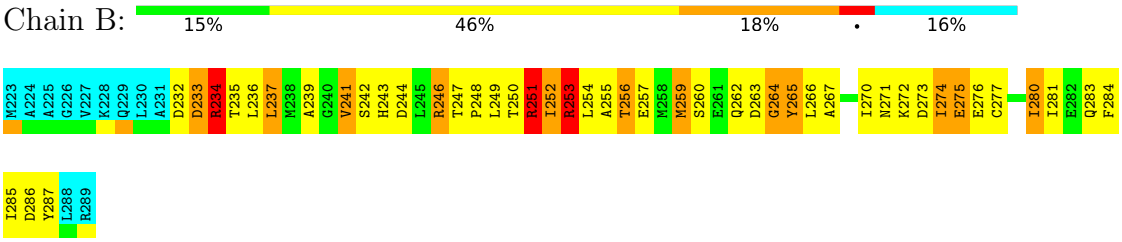
4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN (ENVZ_ECOLI)



• Molecule 1: PROTEIN (ENVZ_ECOLI)

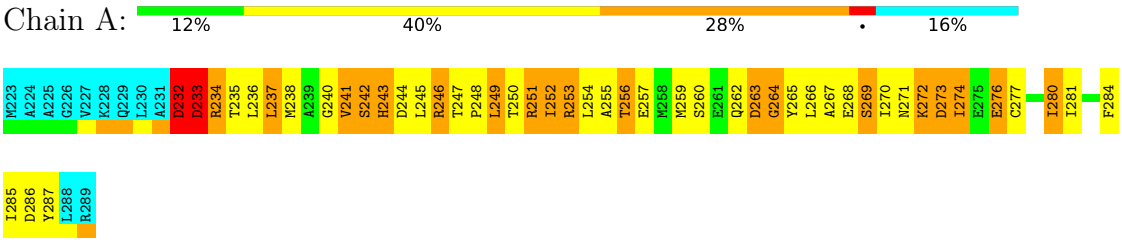
Chain B:



4.2.20 Score per residue for model 20

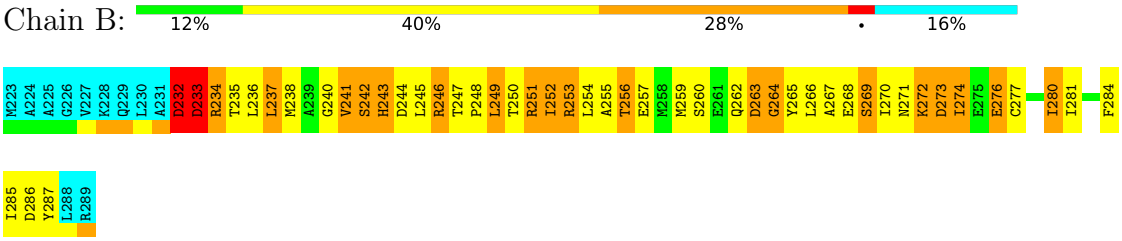
- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



- Molecule 1: PROTEIN (ENVZ_ECOLI)

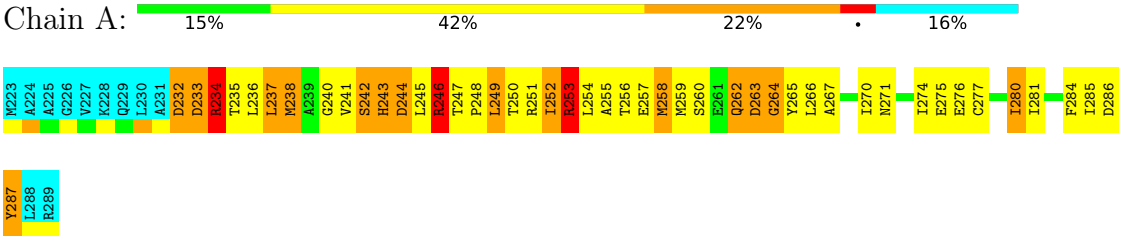
Chain B:



4.2.21 Score per residue for model 21

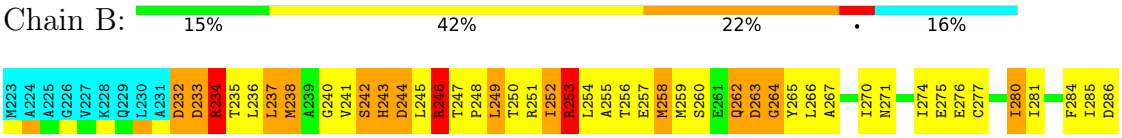
- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A:



- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B:




Y287
L288
R289

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 21 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
NMRPipe	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.0±0.2
1	B	0.0±0.0	4.0±0.2
All	All	0	166

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	234	ARG	Sidechain	21
1	A	251	ARG	Sidechain	21
1	A	253	ARG	Sidechain	21
1	B	234	ARG	Sidechain	21
1	B	251	ARG	Sidechain	21
1	B	253	ARG	Sidechain	21
1	A	246	ARG	Sidechain	20
1	B	246	ARG	Sidechain	20

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	448	436	436	71±8
1	B	448	436	436	71±9
All	All	18816	18312	18312	2824

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 76.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:LEU:HD13	1:A:250:THR:N	1.00	1.70	16	1
1:B:249:LEU:HD13	1:B:250:THR:N	0.99	1.70	16	1
1:A:266:LEU:HD12	1:A:267:ALA:N	0.98	1.74	17	4
1:B:266:LEU:HD12	1:B:267:ALA:N	0.96	1.74	17	4
1:B:245:LEU:O	1:B:249:LEU:HD21	0.96	1.60	3	3
1:A:245:LEU:O	1:A:249:LEU:HD21	0.95	1.60	3	3
1:A:254:LEU:HD12	1:A:255:ALA:N	0.93	1.78	9	2
1:B:280:ILE:N	1:B:280:ILE:HD13	0.93	1.79	12	1
1:A:280:ILE:HD13	1:A:280:ILE:N	0.92	1.79	12	1
1:B:254:LEU:HD12	1:B:255:ALA:N	0.92	1.78	9	2
1:A:266:LEU:HB2	1:B:255:ALA:HB1	0.91	1.42	9	12
1:A:256:THR:HG22	1:A:266:LEU:HD13	0.90	1.43	17	3
1:B:236:LEU:HD12	1:B:236:LEU:O	0.89	1.67	3	2
1:A:236:LEU:HD12	1:A:236:LEU:O	0.88	1.67	3	2
1:B:256:THR:HG22	1:B:266:LEU:HD13	0.88	1.43	17	3
1:A:256:THR:CG2	1:A:266:LEU:HD22	0.87	2.00	14	1
1:A:256:THR:HG22	1:A:266:LEU:CD1	0.87	2.00	8	9
1:B:256:THR:HG22	1:B:266:LEU:CD1	0.87	2.00	8	9
1:B:256:THR:CG2	1:B:266:LEU:HD22	0.87	1.99	14	1
1:B:256:THR:HG21	1:B:270:ILE:HD12	0.86	1.46	11	10
1:A:256:THR:HG21	1:A:270:ILE:CD1	0.85	2.02	4	13
1:A:256:THR:HG21	1:A:270:ILE:HD12	0.85	1.46	11	10
1:B:256:THR:HG21	1:B:270:ILE:CD1	0.84	2.02	4	13
1:A:266:LEU:CB	1:B:255:ALA:HB1	0.83	2.03	8	9
1:A:241:VAL:HG22	1:B:284:PHE:CE2	0.83	2.08	5	4
1:A:256:THR:HG22	1:A:266:LEU:HD22	0.81	1.52	14	2
1:A:256:THR:HG22	1:A:266:LEU:HD12	0.81	1.51	8	8
1:A:255:ALA:HB1	1:B:266:LEU:HB2	0.81	1.50	9	9
1:B:256:THR:HG22	1:B:266:LEU:HD22	0.80	1.52	14	2
1:B:259:MET:HB3	1:B:266:LEU:HD11	0.80	1.54	3	3
1:B:256:THR:HG22	1:B:266:LEU:HD12	0.79	1.51	8	8
1:B:249:LEU:HB3	1:B:274:ILE:HD11	0.79	1.54	8	3
1:B:246:ARG:O	1:B:249:LEU:HD22	0.79	1.77	14	4
1:A:259:MET:HB3	1:A:266:LEU:HD11	0.78	1.54	3	3
1:A:246:ARG:O	1:A:249:LEU:HD22	0.78	1.77	14	4
1:A:270:ILE:CG1	1:B:252:ILE:HD11	0.78	2.08	15	6
1:A:249:LEU:HB3	1:A:274:ILE:HD11	0.77	1.54	8	3
1:A:255:ALA:HB1	1:B:266:LEU:CB	0.77	2.09	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:249:LEU:HD22	1:B:249:LEU:O	0.76	1.81	16	1
1:A:256:THR:HG21	1:A:270:ILE:HG13	0.75	1.57	6	5
1:B:238:MET:CE	1:B:285:ILE:HG21	0.75	2.11	10	2
1:B:256:THR:HG21	1:B:270:ILE:HG13	0.75	1.57	6	5
1:A:238:MET:CE	1:A:285:ILE:HG21	0.75	2.11	10	2
1:B:249:LEU:HD22	1:B:249:LEU:C	0.75	2.01	16	1
1:A:249:LEU:HD22	1:A:249:LEU:O	0.75	1.81	16	1
1:B:233:ASP:HA	1:B:236:LEU:HD12	0.74	1.58	10	2
1:A:249:LEU:HD22	1:A:249:LEU:C	0.73	2.02	16	1
1:A:233:ASP:HA	1:A:236:LEU:HD12	0.73	1.58	10	2
1:A:245:LEU:HD11	1:B:245:LEU:HD11	0.73	1.60	8	2
1:A:284:PHE:CE2	1:B:241:VAL:HG22	0.73	2.19	5	4
1:B:281:ILE:O	1:B:285:ILE:HD13	0.72	1.84	4	3
1:A:281:ILE:O	1:A:285:ILE:HD13	0.71	1.84	4	3
1:B:266:LEU:HD12	1:B:267:ALA:H	0.71	1.46	6	2
1:A:277:CYS:HA	1:A:280:ILE:HD11	0.71	1.63	9	12
1:A:249:LEU:CB	1:A:274:ILE:HD11	0.71	2.16	8	3
1:A:237:LEU:HA	1:A:241:VAL:HG23	0.70	1.63	7	1
1:B:254:LEU:HD12	1:B:254:LEU:C	0.70	2.06	9	2
1:B:237:LEU:HA	1:B:241:VAL:HG23	0.70	1.63	7	2
1:A:232:ASP:O	1:A:236:LEU:HD23	0.70	1.86	12	4
1:B:252:ILE:HD13	1:B:255:ALA:HB3	0.70	1.63	15	19
1:A:266:LEU:HD12	1:A:267:ALA:H	0.70	1.46	6	2
1:B:277:CYS:HA	1:B:280:ILE:HD11	0.70	1.63	9	12
1:B:260:SER:HB2	1:B:267:ALA:HB2	0.70	1.64	11	2
1:A:247:THR:N	1:A:248:PRO:CD	0.70	2.54	9	21
1:B:247:THR:N	1:B:248:PRO:CD	0.70	2.54	9	21
1:B:249:LEU:CB	1:B:274:ILE:HD11	0.70	2.16	8	3
1:A:254:LEU:HD12	1:A:254:LEU:C	0.70	2.06	9	2
1:B:232:ASP:O	1:B:236:LEU:HD23	0.70	1.86	12	4
1:A:249:LEU:HD23	1:A:250:THR:N	0.70	2.02	14	4
1:B:249:LEU:HD23	1:B:250:THR:N	0.69	2.02	14	4
1:A:249:LEU:N	1:A:249:LEU:HD23	0.69	2.03	3	2
1:A:252:ILE:HD13	1:A:255:ALA:HB3	0.69	1.63	5	19
1:A:260:SER:HB2	1:A:267:ALA:HB2	0.68	1.64	11	2
1:B:249:LEU:HD23	1:B:249:LEU:N	0.68	2.03	3	2
1:B:256:THR:OG1	1:B:270:ILE:HD12	0.67	1.89	3	4
1:A:259:MET:HB2	1:A:266:LEU:HD11	0.67	1.66	4	3
1:A:256:THR:OG1	1:A:270:ILE:HD12	0.67	1.89	3	4
1:A:249:LEU:HD13	1:A:274:ILE:HG12	0.66	1.66	13	2
1:B:259:MET:HB2	1:B:266:LEU:HD11	0.66	1.66	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:265:TYR:CD1	1:A:266:LEU:N	0.66	2.64	17	4
1:B:265:TYR:CD1	1:B:266:LEU:N	0.66	2.64	17	5
1:B:249:LEU:HD13	1:B:274:ILE:HG12	0.66	1.66	13	2
1:A:284:PHE:CE1	1:B:240:GLY:CA	0.66	2.79	2	2
1:A:280:ILE:N	1:A:280:ILE:CD1	0.65	2.52	12	1
1:A:287:TYR:CD1	1:A:287:TYR:N	0.65	2.64	13	6
1:A:237:LEU:N	1:A:237:LEU:CD2	0.64	2.61	17	8
1:A:240:GLY:CA	1:B:284:PHE:CE1	0.64	2.80	14	1
1:B:256:THR:HG22	1:B:266:LEU:HB3	0.64	1.70	7	1
1:B:252:ILE:HD13	1:B:255:ALA:CB	0.64	2.22	2	19
1:B:284:PHE:HA	1:B:287:TYR:CE2	0.64	2.28	10	12
1:A:252:ILE:HD13	1:A:255:ALA:CB	0.63	2.22	2	19
1:A:284:PHE:HA	1:A:287:TYR:CE2	0.63	2.28	10	12
1:B:287:TYR:CD1	1:B:287:TYR:N	0.63	2.63	16	6
1:A:270:ILE:HG12	1:B:252:ILE:HD11	0.63	1.71	15	2
1:A:256:THR:HG22	1:A:266:LEU:CG	0.62	2.24	8	2
1:A:252:ILE:O	1:A:256:THR:HG22	0.62	1.94	13	1
1:B:249:LEU:HD23	1:B:250:THR:H	0.62	1.53	14	4
1:B:237:LEU:CD2	1:B:237:LEU:N	0.62	2.61	17	4
1:B:252:ILE:O	1:B:256:THR:HG22	0.62	1.94	13	1
1:A:246:ARG:O	1:A:249:LEU:HD12	0.62	1.94	16	1
1:A:249:LEU:HD23	1:A:250:THR:H	0.62	1.53	14	4
1:A:256:THR:HG22	1:A:266:LEU:HB3	0.62	1.70	7	1
1:B:256:THR:HG21	1:B:270:ILE:HD11	0.62	1.72	4	2
1:B:259:MET:SD	1:B:266:LEU:HD22	0.62	2.35	1	1
1:A:270:ILE:HG13	1:B:252:ILE:HD11	0.61	1.71	9	3
1:B:246:ARG:O	1:B:249:LEU:HD12	0.61	1.94	16	1
1:A:259:MET:SD	1:A:266:LEU:HD22	0.61	2.35	1	1
1:B:237:LEU:O	1:B:241:VAL:HG23	0.61	1.95	10	13
1:A:256:THR:HG21	1:A:270:ILE:HD11	0.61	1.71	4	2
1:A:249:LEU:HD13	1:A:250:THR:H	0.61	1.53	16	1
1:B:256:THR:HG22	1:B:266:LEU:CG	0.61	2.24	8	2
1:A:249:LEU:HD13	1:A:249:LEU:C	0.61	2.16	16	1
1:B:246:ARG:O	1:B:249:LEU:HD21	0.61	1.96	17	5
1:A:237:LEU:O	1:A:241:VAL:HG23	0.61	1.96	10	14
1:A:259:MET:CG	1:B:259:MET:CG	0.61	2.79	12	2
1:A:284:PHE:O	1:A:287:TYR:CE1	0.61	2.54	12	5
1:A:284:PHE:O	1:A:287:TYR:CZ	0.60	2.54	17	6
1:B:284:PHE:O	1:B:287:TYR:CE1	0.60	2.54	12	5
1:A:283:GLN:O	1:A:287:TYR:CE1	0.60	2.54	13	8
1:B:283:GLN:O	1:B:287:TYR:CE1	0.60	2.54	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:249:LEU:HD13	1:B:250:THR:H	0.60	1.53	16	1
1:B:284:PHE:O	1:B:287:TYR:CZ	0.60	2.54	17	6
1:A:246:ARG:O	1:A:249:LEU:HD21	0.60	1.96	17	5
1:B:260:SER:O	1:B:264:GLY:CA	0.60	2.50	13	21
1:B:263:ASP:OD1	1:B:265:TYR:CZ	0.60	2.55	15	1
1:A:270:ILE:CG1	1:B:252:ILE:CD1	0.59	2.81	9	3
1:B:249:LEU:HD13	1:B:274:ILE:HG13	0.59	1.74	3	1
1:A:280:ILE:O	1:A:284:PHE:CG	0.59	2.55	5	2
1:A:260:SER:O	1:A:264:GLY:CA	0.59	2.50	1	21
1:A:263:ASP:OD1	1:A:265:TYR:CZ	0.59	2.55	15	1
1:A:263:ASP:O	1:A:265:TYR:N	0.59	2.36	1	20
1:A:241:VAL:O	1:A:245:LEU:HD23	0.59	1.98	13	1
1:B:263:ASP:O	1:B:265:TYR:N	0.59	2.36	1	20
1:B:280:ILE:N	1:B:280:ILE:CD1	0.59	2.52	12	1
1:B:249:LEU:HD13	1:B:249:LEU:C	0.59	2.16	16	1
1:A:236:LEU:O	1:A:240:GLY:HA3	0.59	1.98	10	4
1:B:247:THR:N	1:B:248:PRO:HD2	0.59	2.13	11	20
1:A:252:ILE:CG2	1:A:270:ILE:HD13	0.59	2.28	7	12
1:B:280:ILE:O	1:B:284:PHE:CG	0.59	2.55	5	2
1:B:241:VAL:O	1:B:245:LEU:HD23	0.59	1.98	13	1
1:B:263:ASP:OD2	1:B:265:TYR:CZ	0.59	2.56	15	1
1:B:237:LEU:N	1:B:237:LEU:HD23	0.58	2.13	11	14
1:A:263:ASP:OD2	1:A:265:TYR:CZ	0.58	2.56	15	1
1:B:280:ILE:O	1:B:284:PHE:CD1	0.58	2.56	6	2
1:B:276:GLU:O	1:B:280:ILE:CD1	0.58	2.52	15	7
1:A:247:THR:N	1:A:248:PRO:HD2	0.58	2.14	6	20
1:B:252:ILE:CG2	1:B:270:ILE:HD12	0.58	2.29	6	4
1:A:276:GLU:O	1:A:280:ILE:CD1	0.58	2.51	16	7
1:B:287:TYR:CD1	1:B:287:TYR:O	0.58	2.57	8	3
1:B:252:ILE:CG2	1:B:270:ILE:HD13	0.58	2.29	15	12
1:A:287:TYR:CD1	1:A:287:TYR:O	0.58	2.57	8	3
1:A:237:LEU:N	1:A:237:LEU:HD23	0.58	2.13	11	6
1:B:256:THR:O	1:B:260:SER:N	0.58	2.37	5	17
1:B:236:LEU:O	1:B:240:GLY:HA3	0.58	1.98	10	5
1:A:256:THR:O	1:A:260:SER:N	0.57	2.37	5	17
1:A:284:PHE:CE1	1:B:240:GLY:HA2	0.57	2.34	2	1
1:A:249:LEU:HD13	1:A:274:ILE:HG13	0.57	1.74	3	1
1:A:270:ILE:HG12	1:B:252:ILE:CD1	0.57	2.29	15	3
1:B:277:CYS:HA	1:B:280:ILE:CD1	0.57	2.30	11	9
1:A:243:HIS:CD2	1:A:243:HIS:C	0.57	2.78	16	2
1:B:256:THR:O	1:B:260:SER:CB	0.57	2.53	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:ILE:O	1:A:284:PHE:CD1	0.57	2.56	6	1
1:A:252:ILE:CG2	1:A:270:ILE:HD12	0.57	2.29	6	4
1:A:260:SER:CB	1:A:267:ALA:HB2	0.57	2.30	8	4
1:A:284:PHE:CD2	1:A:287:TYR:OH	0.57	2.57	17	6
1:A:240:GLY:C	1:B:284:PHE:CZ	0.57	2.77	4	2
1:A:259:MET:O	1:A:266:LEU:HD11	0.57	2.00	6	1
1:B:284:PHE:CD2	1:B:287:TYR:OH	0.57	2.57	17	6
1:B:284:PHE:O	1:B:287:TYR:CE2	0.57	2.58	15	1
1:B:243:HIS:CD2	1:B:244:ASP:N	0.57	2.73	16	1
1:B:284:PHE:HA	1:B:287:TYR:CZ	0.57	2.35	12	6
1:B:250:THR:HG23	1:B:253:ARG:HD3	0.57	1.77	15	1
1:A:256:THR:O	1:A:260:SER:CB	0.56	2.53	11	3
1:A:243:HIS:CD2	1:A:244:ASP:N	0.56	2.73	16	1
1:A:277:CYS:HA	1:A:280:ILE:CD1	0.56	2.30	16	9
1:A:263:ASP:O	1:A:266:LEU:CD2	0.56	2.53	12	9
1:A:277:CYS:O	1:A:281:ILE:CG1	0.56	2.53	4	20
1:A:284:PHE:HA	1:A:287:TYR:CZ	0.56	2.35	12	6
1:B:277:CYS:O	1:B:281:ILE:CG1	0.56	2.54	2	20
1:B:247:THR:HG22	1:B:248:PRO:HD3	0.56	1.77	5	2
1:B:260:SER:CB	1:B:267:ALA:HB2	0.56	2.30	8	4
1:A:284:PHE:O	1:A:287:TYR:CE2	0.56	2.58	15	1
1:A:266:LEU:HB3	1:B:255:ALA:HB1	0.56	1.77	12	2
1:A:246:ARG:HA	1:A:249:LEU:CD2	0.56	2.31	17	5
1:B:284:PHE:C	1:B:284:PHE:CD1	0.56	2.79	12	1
1:B:263:ASP:O	1:B:266:LEU:CD2	0.56	2.53	12	9
1:A:281:ILE:HD13	1:B:241:VAL:HG11	0.56	1.77	2	1
1:B:236:LEU:HD12	1:B:236:LEU:C	0.56	2.21	3	1
1:B:283:GLN:O	1:B:287:TYR:CD1	0.56	2.59	7	2
1:A:236:LEU:HD12	1:A:236:LEU:C	0.56	2.21	3	1
1:B:243:HIS:CD2	1:B:243:HIS:C	0.56	2.78	16	2
1:B:259:MET:O	1:B:266:LEU:HD11	0.56	2.00	6	1
1:A:260:SER:HA	1:A:264:GLY:HA2	0.56	1.78	13	21
1:B:246:ARG:HA	1:B:249:LEU:CD2	0.56	2.31	17	5
1:A:283:GLN:O	1:A:287:TYR:CD1	0.56	2.59	7	1
1:A:250:THR:HG23	1:A:253:ARG:HD3	0.56	1.76	15	1
1:B:268:GLU:O	1:B:272:LYS:CG	0.55	2.54	2	1
1:A:265:TYR:C	1:A:265:TYR:CD1	0.55	2.78	6	2
1:B:234:ARG:CG	1:B:235:THR:N	0.55	2.69	17	20
1:A:287:TYR:CD1	1:A:287:TYR:C	0.55	2.80	8	4
1:A:246:ARG:CD	1:A:249:LEU:HD11	0.55	2.31	11	2
1:A:263:ASP:CB	1:A:266:LEU:HD23	0.55	2.32	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:ARG:CG	1:A:235:THR:N	0.55	2.69	17	20
1:B:237:LEU:N	1:B:237:LEU:CD2	0.55	2.69	1	4
1:B:249:LEU:HD13	1:B:274:ILE:CG1	0.55	2.32	3	1
1:B:263:ASP:CB	1:B:266:LEU:HD23	0.55	2.32	16	1
1:A:277:CYS:O	1:A:281:ILE:HG12	0.55	2.02	14	17
1:A:252:ILE:CG2	1:A:270:ILE:HG21	0.55	2.32	12	4
1:A:247:THR:HG22	1:A:248:PRO:HD3	0.55	1.77	5	2
1:A:256:THR:HG22	1:A:266:LEU:CD2	0.55	2.31	7	1
1:B:260:SER:OG	1:B:267:ALA:CB	0.55	2.55	12	3
1:B:287:TYR:CD1	1:B:287:TYR:C	0.55	2.80	8	2
1:A:238:MET:HE1	1:A:285:ILE:HG21	0.55	1.78	10	2
1:A:260:SER:OG	1:A:267:ALA:CB	0.55	2.55	12	3
1:A:268:GLU:O	1:A:272:LYS:CG	0.55	2.54	2	1
1:A:249:LEU:HD12	1:A:250:THR:N	0.55	2.16	10	2
1:B:249:LEU:HD12	1:B:250:THR:N	0.55	2.16	10	2
1:B:243:HIS:CD2	1:B:243:HIS:O	0.55	2.60	14	1
1:B:252:ILE:CG2	1:B:270:ILE:HG21	0.55	2.32	12	4
1:B:265:TYR:CD1	1:B:265:TYR:C	0.55	2.78	6	4
1:A:263:ASP:OD2	1:A:265:TYR:CE2	0.55	2.60	15	2
1:B:287:TYR:O	1:B:287:TYR:CG	0.55	2.59	8	2
1:A:252:ILE:HD11	1:B:270:ILE:HG12	0.55	1.78	15	2
1:B:277:CYS:O	1:B:281:ILE:HG12	0.55	2.02	5	17
1:A:284:PHE:C	1:A:284:PHE:CD1	0.55	2.79	12	1
1:B:284:PHE:CD1	1:B:287:TYR:CE2	0.55	2.95	13	3
1:A:263:ASP:OD1	1:A:265:TYR:CD2	0.55	2.60	8	2
1:B:263:ASP:O	1:B:266:LEU:HD23	0.55	2.02	11	5
1:A:280:ILE:HD12	1:A:281:ILE:HG12	0.54	1.78	7	11
1:A:249:LEU:O	1:A:253:ARG:HB3	0.54	2.02	2	2
1:B:249:LEU:O	1:B:253:ARG:HB3	0.54	2.02	2	2
1:B:246:ARG:O	1:B:249:LEU:CD2	0.54	2.56	4	8
1:B:263:ASP:OD2	1:B:265:TYR:CE2	0.54	2.60	15	2
1:B:256:THR:HG22	1:B:266:LEU:CD2	0.54	2.31	7	1
1:A:272:LYS:CD	1:A:273:ASP:N	0.54	2.71	2	1
1:A:284:PHE:CD1	1:A:287:TYR:CE2	0.54	2.95	13	2
1:A:287:TYR:O	1:A:287:TYR:CG	0.54	2.59	8	2
1:A:287:TYR:OH	1:B:236:LEU:CD1	0.54	2.56	8	2
1:A:243:HIS:O	1:A:243:HIS:CD2	0.54	2.60	14	2
1:B:246:ARG:CD	1:B:249:LEU:HD11	0.54	2.31	11	2
1:A:259:MET:CE	1:B:258:MET:CG	0.54	2.86	2	1
1:A:249:LEU:HD13	1:A:274:ILE:CG1	0.54	2.32	3	1
1:A:246:ARG:O	1:A:249:LEU:CD2	0.54	2.56	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:232:ASP:O	1:B:236:LEU:CD2	0.54	2.56	12	4
1:B:260:SER:HA	1:B:264:GLY:HA2	0.54	1.78	13	21
1:A:263:ASP:O	1:A:266:LEU:HD23	0.54	2.02	11	5
1:A:252:ILE:O	1:A:256:THR:OG1	0.54	2.25	14	18
1:B:252:ILE:O	1:B:256:THR:OG1	0.54	2.25	14	18
1:B:283:GLN:O	1:B:287:TYR:CZ	0.54	2.61	14	3
1:A:260:SER:O	1:A:264:GLY:HA2	0.54	2.03	14	16
1:B:272:LYS:CD	1:B:273:ASP:N	0.54	2.71	2	1
1:A:253:ARG:O	1:A:257:GLU:CB	0.54	2.56	12	16
1:A:265:TYR:CD1	1:A:265:TYR:C	0.54	2.82	17	2
1:B:262:GLN:N	1:B:262:GLN:OE1	0.54	2.41	4	1
1:A:259:MET:SD	1:A:266:LEU:CD1	0.54	2.96	7	1
1:A:272:LYS:CG	1:A:273:ASP:N	0.54	2.71	7	1
1:B:263:ASP:OD1	1:B:265:TYR:CD2	0.54	2.60	8	2
1:B:260:SER:O	1:B:264:GLY:HA2	0.53	2.03	14	16
1:A:262:GLN:OE1	1:A:262:GLN:N	0.53	2.41	4	1
1:A:273:ASP:O	1:A:276:GLU:CG	0.53	2.56	14	2
1:A:249:LEU:N	1:A:249:LEU:CD2	0.53	2.69	3	1
1:B:253:ARG:O	1:B:257:GLU:CB	0.53	2.56	13	16
1:B:272:LYS:CG	1:B:273:ASP:N	0.53	2.71	7	1
1:A:245:LEU:N	1:A:245:LEU:CD2	0.53	2.72	17	2
1:B:249:LEU:HD22	1:B:249:LEU:N	0.53	2.19	7	1
1:B:238:MET:HE1	1:B:285:ILE:HG21	0.53	1.78	10	2
1:B:245:LEU:N	1:B:245:LEU:CD2	0.53	2.71	17	2
1:B:259:MET:SD	1:B:266:LEU:CD1	0.53	2.97	7	1
1:A:259:MET:HA	1:A:259:MET:HE2	0.53	1.79	11	2
1:B:280:ILE:HD12	1:B:281:ILE:HG12	0.53	1.78	7	11
1:B:263:ASP:HB3	1:B:266:LEU:HD23	0.53	1.80	3	1
1:B:253:ARG:O	1:B:257:GLU:HB2	0.53	2.04	13	21
1:A:281:ILE:O	1:A:285:ILE:CD1	0.53	2.56	4	1
1:B:259:MET:O	1:B:266:LEU:CD2	0.53	2.57	4	1
1:A:283:GLN:O	1:A:287:TYR:CZ	0.53	2.61	14	3
1:B:263:ASP:HB2	1:B:266:LEU:CD2	0.53	2.34	16	1
1:A:249:LEU:O	1:A:253:ARG:CB	0.53	2.57	2	1
1:A:280:ILE:O	1:A:284:PHE:CB	0.53	2.57	8	3
1:B:280:ILE:O	1:B:284:PHE:CB	0.53	2.57	8	4
1:A:284:PHE:CZ	1:B:240:GLY:O	0.53	2.62	2	2
1:B:281:ILE:O	1:B:285:ILE:CD1	0.53	2.56	4	1
1:A:259:MET:SD	1:A:266:LEU:CD2	0.53	2.97	1	1
1:B:257:GLU:O	1:B:260:SER:CB	0.53	2.57	13	2
1:A:259:MET:O	1:A:266:LEU:CD2	0.53	2.57	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:LEU:O	1:A:258:MET:CG	0.53	2.57	14	6
1:B:250:THR:O	1:B:253:ARG:CB	0.53	2.56	6	4
1:A:232:ASP:O	1:A:236:LEU:CD1	0.53	2.57	7	2
1:A:249:LEU:HD22	1:A:249:LEU:N	0.53	2.19	7	1
1:B:259:MET:HB3	1:B:266:LEU:HD13	0.53	1.80	7	1
1:B:273:ASP:O	1:B:276:GLU:CG	0.53	2.56	14	2
1:A:250:THR:O	1:A:253:ARG:CB	0.52	2.57	6	4
1:A:277:CYS:O	1:A:280:ILE:HG13	0.52	2.05	1	12
1:A:257:GLU:O	1:A:260:SER:CB	0.52	2.57	13	2
1:A:259:MET:HB3	1:A:266:LEU:HD13	0.52	1.80	7	1
1:B:232:ASP:O	1:B:236:LEU:CD1	0.52	2.57	7	2
1:A:236:LEU:CD1	1:B:287:TYR:OH	0.52	2.56	8	2
1:A:232:ASP:O	1:A:236:LEU:CD2	0.52	2.57	16	4
1:B:245:LEU:O	1:B:249:LEU:CD2	0.52	2.57	11	2
1:A:253:ARG:O	1:A:257:GLU:HB2	0.52	2.04	13	21
1:A:241:VAL:O	1:A:243:HIS:N	0.52	2.42	4	4
1:B:241:VAL:O	1:B:243:HIS:N	0.52	2.42	4	4
1:A:249:LEU:HB3	1:A:274:ILE:CG1	0.52	2.35	3	1
1:B:249:LEU:HB3	1:B:274:ILE:CG1	0.52	2.35	3	1
1:A:256:THR:CG2	1:A:266:LEU:HD12	0.52	2.31	8	2
1:B:254:LEU:O	1:B:258:MET:CG	0.52	2.57	15	6
1:A:242:SER:OG	1:A:243:HIS:N	0.52	2.42	10	5
1:B:259:MET:SD	1:B:266:LEU:CD2	0.52	2.97	1	1
1:B:249:LEU:O	1:B:253:ARG:CB	0.52	2.57	2	1
1:A:249:LEU:HB2	1:A:274:ILE:HD11	0.52	1.81	7	1
1:A:263:ASP:HB2	1:A:266:LEU:CD2	0.52	2.34	16	1
1:B:242:SER:OG	1:B:243:HIS:N	0.52	2.42	10	5
1:B:277:CYS:O	1:B:280:ILE:HG13	0.52	2.05	1	12
1:B:263:ASP:HB3	1:B:265:TYR:CE2	0.52	2.40	17	3
1:A:241:VAL:HG22	1:B:284:PHE:HE2	0.52	1.58	5	2
1:A:284:PHE:HE2	1:B:241:VAL:HG22	0.52	1.64	5	2
1:A:259:MET:CG	1:B:259:MET:HG2	0.52	2.35	12	2
1:B:272:LYS:HG3	1:B:273:ASP:N	0.52	2.20	7	4
1:A:260:SER:CA	1:A:264:GLY:HA2	0.51	2.36	12	19
1:A:263:ASP:HB3	1:A:265:TYR:CE2	0.51	2.40	4	3
1:B:249:LEU:HB2	1:B:274:ILE:HD11	0.51	1.81	7	1
1:B:277:CYS:HA	1:B:280:ILE:CG1	0.51	2.36	10	8
1:A:246:ARG:HA	1:A:249:LEU:HD23	0.51	1.82	1	2
1:A:233:ASP:O	1:A:237:LEU:HG	0.51	2.06	9	10
1:A:259:MET:CE	1:A:262:GLN:HB2	0.51	2.35	9	2
1:B:274:ILE:O	1:B:277:CYS:CB	0.51	2.58	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:LEU:HA	1:A:257:GLU:HB3	0.51	1.82	9	18
1:B:254:LEU:HA	1:B:257:GLU:HB3	0.51	1.83	13	18
1:A:252:ILE:HD11	1:B:270:ILE:CG1	0.51	2.36	9	6
1:A:263:ASP:HB3	1:A:266:LEU:HD23	0.51	1.80	3	2
1:A:238:MET:O	1:A:242:SER:CB	0.51	2.59	8	6
1:A:246:ARG:O	1:A:249:LEU:CD1	0.51	2.59	16	1
1:A:237:LEU:HD23	1:A:237:LEU:N	0.51	2.21	10	8
1:A:234:ARG:HG3	1:A:235:THR:N	0.50	2.20	17	11
1:B:254:LEU:O	1:B:258:MET:HG3	0.50	2.05	5	5
1:A:255:ALA:HB1	1:B:266:LEU:HB3	0.50	1.80	6	1
1:B:260:SER:HB2	1:B:267:ALA:CB	0.50	2.36	8	2
1:A:274:ILE:O	1:A:277:CYS:CB	0.50	2.58	9	2
1:A:277:CYS:HA	1:A:280:ILE:CG1	0.50	2.36	10	8
1:A:244:ASP:O	1:A:248:PRO:HD3	0.50	2.07	2	6
1:B:249:LEU:C	1:B:249:LEU:CD2	0.50	2.74	16	1
1:A:259:MET:CE	1:B:258:MET:HG3	0.50	2.37	2	1
1:B:281:ILE:O	1:B:285:ILE:CG1	0.50	2.60	15	3
1:B:237:LEU:O	1:B:241:VAL:CG2	0.50	2.60	16	2
1:B:238:MET:O	1:B:242:SER:CB	0.50	2.59	8	6
1:A:266:LEU:HG	1:A:267:ALA:N	0.50	2.20	4	11
1:B:259:MET:CE	1:B:262:GLN:HB2	0.50	2.35	9	2
1:B:260:SER:CA	1:B:264:GLY:HA2	0.50	2.36	12	19
1:B:264:GLY:O	1:B:265:TYR:C	0.50	2.49	14	15
1:B:285:ILE:O	1:B:286:ASP:C	0.50	2.50	3	3
1:A:259:MET:O	1:A:266:LEU:HD21	0.50	2.07	4	2
1:A:254:LEU:O	1:A:258:MET:HG3	0.50	2.05	5	5
1:A:272:LYS:HG3	1:A:273:ASP:N	0.50	2.20	7	4
1:B:277:CYS:CA	1:B:280:ILE:HD11	0.50	2.34	9	7
1:B:233:ASP:O	1:B:237:LEU:CG	0.50	2.60	1	4
1:A:237:LEU:O	1:A:241:VAL:CG2	0.50	2.60	16	2
1:A:264:GLY:O	1:A:267:ALA:HB3	0.50	2.06	9	2
1:B:246:ARG:O	1:B:249:LEU:CD1	0.50	2.59	16	1
1:B:259:MET:O	1:B:266:LEU:HD21	0.50	2.07	4	2
1:A:260:SER:OG	1:A:267:ALA:HB2	0.50	2.07	12	1
1:B:246:ARG:HA	1:B:249:LEU:HD23	0.50	1.82	1	2
1:A:281:ILE:O	1:A:285:ILE:CG1	0.50	2.60	15	3
1:B:234:ARG:HG3	1:B:235:THR:N	0.50	2.22	15	11
1:A:263:ASP:CG	1:A:265:TYR:CZ	0.50	2.85	15	1
1:B:263:ASP:CG	1:B:265:TYR:CZ	0.50	2.85	15	1
1:A:266:LEU:O	1:A:267:ALA:C	0.50	2.50	12	4
1:B:244:ASP:O	1:B:248:PRO:HD3	0.50	2.07	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:258:MET:HB2	1:A:259:MET:CE	0.50	2.37	15	1
1:A:280:ILE:HG21	1:B:244:ASP:OD2	0.50	2.07	16	1
1:B:233:ASP:O	1:B:237:LEU:HG	0.50	2.06	9	10
1:A:259:MET:CG	1:B:259:MET:HB3	0.50	2.37	5	1
1:A:245:LEU:O	1:A:249:LEU:CD2	0.50	2.57	11	2
1:B:258:MET:HG2	1:B:259:MET:N	0.49	2.22	2	1
1:A:285:ILE:O	1:A:286:ASP:C	0.49	2.50	3	3
1:A:259:MET:HG3	1:B:259:MET:CG	0.49	2.37	12	1
1:B:270:ILE:O	1:B:272:LYS:N	0.49	2.45	15	8
1:A:239:ALA:O	1:A:243:HIS:CB	0.49	2.61	5	3
1:B:264:GLY:O	1:B:267:ALA:HB3	0.49	2.06	9	2
1:B:249:LEU:CD2	1:B:274:ILE:HG12	0.49	2.37	12	1
1:A:233:ASP:O	1:A:237:LEU:CG	0.49	2.60	1	4
1:B:266:LEU:HG	1:B:267:ALA:N	0.49	2.22	9	11
1:B:256:THR:CG2	1:B:266:LEU:HD12	0.49	2.31	8	2
1:B:266:LEU:O	1:B:267:ALA:C	0.49	2.50	12	5
1:B:252:ILE:CD1	1:B:255:ALA:HB3	0.49	2.37	2	1
1:B:263:ASP:HB3	1:B:266:LEU:HD12	0.49	1.85	7	1
1:A:277:CYS:CA	1:A:280:ILE:HD11	0.49	2.34	9	7
1:B:258:MET:HB2	1:B:259:MET:CE	0.49	2.37	15	1
1:A:258:MET:HG2	1:A:259:MET:N	0.49	2.22	2	1
1:A:276:GLU:HG3	1:A:277:CYS:N	0.49	2.22	13	2
1:A:259:MET:SD	1:B:259:MET:SD	0.49	3.11	17	5
1:A:240:GLY:O	1:B:284:PHE:CZ	0.49	2.66	14	2
1:A:260:SER:HB2	1:A:267:ALA:CB	0.49	2.36	8	2
1:A:246:ARG:HA	1:A:249:LEU:HD11	0.49	1.85	11	2
1:A:254:LEU:C	1:A:254:LEU:CD1	0.49	2.79	9	2
1:A:264:GLY:O	1:A:265:TYR:C	0.49	2.49	14	15
1:A:276:GLU:O	1:A:280:ILE:HG12	0.49	2.08	7	12
1:A:284:PHE:O	1:A:284:PHE:CD1	0.49	2.66	1	1
1:B:254:LEU:C	1:B:254:LEU:CD1	0.49	2.79	9	2
1:B:277:CYS:CA	1:B:280:ILE:CD1	0.49	2.91	15	4
1:A:250:THR:HA	1:A:253:ARG:CD	0.49	2.38	15	1
1:A:270:ILE:O	1:A:272:LYS:N	0.49	2.46	7	8
1:B:239:ALA:O	1:B:243:HIS:CB	0.49	2.61	5	3
1:A:277:CYS:CA	1:A:280:ILE:CD1	0.49	2.91	15	4
1:A:259:MET:CG	1:B:259:MET:HB2	0.48	2.38	1	1
1:A:258:MET:O	1:A:262:GLN:OE1	0.48	2.31	11	2
1:B:258:MET:O	1:B:262:GLN:OE1	0.48	2.31	11	2
1:A:250:THR:HA	1:A:253:ARG:HB2	0.48	1.85	5	12
1:B:260:SER:O	1:B:264:GLY:N	0.48	2.47	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:249:LEU:HB3	1:B:274:ILE:CD1	0.48	2.34	8	3
1:B:260:SER:OG	1:B:267:ALA:HB2	0.48	2.07	12	1
1:A:236:LEU:HD11	1:B:287:TYR:OH	0.48	2.07	8	2
1:A:249:LEU:CD2	1:A:274:ILE:HG12	0.48	2.37	12	1
1:B:276:GLU:O	1:B:280:ILE:HG12	0.48	2.09	2	12
1:B:274:ILE:HG22	1:B:275:GLU:N	0.48	2.23	8	2
1:A:260:SER:O	1:A:264:GLY:N	0.48	2.47	13	4
1:B:250:THR:HA	1:B:253:ARG:CD	0.48	2.38	15	1
1:B:250:THR:HA	1:B:253:ARG:HB2	0.48	1.85	5	13
1:B:249:LEU:O	1:B:253:ARG:HB2	0.48	2.09	6	13
1:B:284:PHE:O	1:B:284:PHE:CD1	0.48	2.66	1	1
1:A:263:ASP:HB3	1:A:266:LEU:HD12	0.48	1.85	7	1
1:A:274:ILE:HG22	1:A:275:GLU:N	0.48	2.23	8	2
1:B:276:GLU:HG3	1:B:277:CYS:N	0.48	2.22	13	2
1:B:252:ILE:HA	1:B:255:ALA:HB3	0.47	1.86	1	1
1:A:263:ASP:HB3	1:A:265:TYR:CE1	0.47	2.44	16	1
1:A:252:ILE:HD12	1:B:270:ILE:HD11	0.47	1.86	1	1
1:A:270:ILE:HG12	1:B:252:ILE:HG13	0.47	1.86	13	3
1:B:249:LEU:HD22	1:B:274:ILE:HG12	0.47	1.86	12	1
1:A:277:CYS:O	1:A:280:ILE:CD1	0.47	2.63	4	6
1:A:273:ASP:O	1:A:276:GLU:HG3	0.47	2.09	13	2
1:A:280:ILE:O	1:A:284:PHE:HB3	0.47	2.09	8	2
1:B:246:ARG:HA	1:B:249:LEU:HD11	0.47	1.85	11	2
1:B:280:ILE:O	1:B:284:PHE:HB3	0.47	2.09	8	2
1:A:252:ILE:HD11	1:B:270:ILE:HG13	0.47	1.86	9	2
1:B:276:GLU:C	1:B:280:ILE:HD11	0.47	2.30	16	4
1:A:270:ILE:HG12	1:B:252:ILE:CG1	0.47	2.40	13	2
1:A:249:LEU:O	1:A:253:ARG:HB2	0.47	2.09	6	13
1:B:270:ILE:HG22	1:B:271:ASN:N	0.47	2.24	11	3
1:A:249:LEU:HB3	1:A:274:ILE:CD1	0.47	2.34	8	3
1:A:259:MET:HB3	1:B:259:MET:CG	0.47	2.39	5	2
1:A:270:ILE:O	1:A:271:ASN:C	0.47	2.53	15	18
1:A:259:MET:HB3	1:B:259:MET:HG3	0.47	1.85	15	1
1:B:263:ASP:O	1:B:264:GLY:C	0.47	2.53	12	17
1:B:277:CYS:O	1:B:280:ILE:CD1	0.47	2.63	4	6
1:A:270:ILE:HG22	1:A:271:ASN:N	0.47	2.24	11	3
1:A:236:LEU:C	1:A:236:LEU:CD1	0.47	2.83	3	1
1:A:237:LEU:CA	1:A:241:VAL:HG23	0.47	2.36	7	1
1:B:273:ASP:O	1:B:276:GLU:HG3	0.47	2.09	13	2
1:B:259:MET:HA	1:B:259:MET:HE2	0.47	1.85	11	2
1:B:239:ALA:O	1:B:243:HIS:HB2	0.47	2.10	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:263:ASP:OD2	1:B:266:LEU:CD2	0.47	2.63	6	1
1:A:266:LEU:CD2	1:B:255:ALA:HB1	0.47	2.39	7	1
1:A:263:ASP:O	1:A:264:GLY:C	0.47	2.54	1	17
1:A:248:PRO:O	1:A:249:LEU:C	0.47	2.53	11	6
1:A:252:ILE:CD1	1:A:255:ALA:HB3	0.47	2.37	2	1
1:B:246:ARG:HA	1:B:249:LEU:HD21	0.47	1.86	11	3
1:A:263:ASP:HB2	1:A:265:TYR:CE2	0.47	2.45	6	1
1:A:237:LEU:HD12	1:A:284:PHE:CE2	0.47	2.45	8	2
1:B:263:ASP:HB3	1:B:266:LEU:CD2	0.47	2.40	3	1
1:A:249:LEU:HD22	1:A:274:ILE:HG12	0.47	1.87	12	1
1:A:240:GLY:HA3	1:B:284:PHE:CE1	0.47	2.43	14	1
1:B:263:ASP:HB3	1:B:265:TYR:CE1	0.47	2.44	16	1
1:A:273:ASP:OD1	1:B:248:PRO:HB3	0.47	2.10	17	1
1:A:252:ILE:HA	1:A:255:ALA:HB3	0.46	1.86	1	1
1:A:259:MET:HG2	1:B:259:MET:CG	0.46	2.40	6	1
1:A:263:ASP:OD2	1:A:266:LEU:CD2	0.46	2.63	6	1
1:B:249:LEU:CG	1:B:274:ILE:HD11	0.46	2.40	7	1
1:B:240:GLY:O	1:B:244:ASP:CG	0.46	2.54	11	2
1:A:258:MET:HB2	1:B:259:MET:CE	0.46	2.40	16	1
1:B:256:THR:CG2	1:B:270:ILE:HD12	0.46	2.39	7	4
1:B:263:ASP:HB2	1:B:265:TYR:CE2	0.46	2.45	6	1
1:B:237:LEU:CA	1:B:241:VAL:HG23	0.46	2.36	7	1
1:B:272:LYS:O	1:B:275:GLU:HG3	0.46	2.10	8	2
1:A:240:GLY:O	1:A:244:ASP:CG	0.46	2.54	11	2
1:B:270:ILE:O	1:B:271:ASN:C	0.46	2.52	3	18
1:B:240:GLY:O	1:B:244:ASP:OD2	0.46	2.34	7	1
1:B:284:PHE:CE1	1:B:287:TYR:CE2	0.46	3.03	7	1
1:A:272:LYS:O	1:A:275:GLU:HG3	0.46	2.10	8	2
1:B:257:GLU:O	1:B:260:SER:OG	0.46	2.32	13	1
1:A:239:ALA:O	1:A:243:HIS:HB2	0.46	2.10	5	3
1:A:252:ILE:CD1	1:B:270:ILE:HG13	0.46	2.40	11	2
1:A:263:ASP:CG	1:A:265:TYR:OH	0.46	2.54	16	1
1:A:246:ARG:HA	1:A:249:LEU:HD21	0.46	1.87	11	3
1:A:259:MET:SD	1:B:258:MET:SD	0.46	3.14	2	1
1:A:240:GLY:CA	1:B:284:PHE:CZ	0.46	2.99	14	2
1:B:250:THR:O	1:B:253:ARG:HB2	0.46	2.10	6	8
1:B:237:LEU:HD12	1:B:284:PHE:CE2	0.46	2.45	8	2
1:B:249:LEU:CD1	1:B:274:ILE:HG12	0.46	2.40	12	1
1:B:245:LEU:N	1:B:245:LEU:HD22	0.46	2.26	17	2
1:B:250:THR:HA	1:B:253:ARG:HB3	0.46	1.88	2	1
1:A:262:GLN:O	1:A:263:ASP:OD1	0.46	2.34	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:279:ALA:O	1:B:283:GLN:HG2	0.46	2.11	3	1
1:A:256:THR:CG2	1:A:270:ILE:HD12	0.46	2.39	4	5
1:B:287:TYR:C	1:B:287:TYR:CD1	0.46	2.89	5	2
1:A:249:LEU:CG	1:A:274:ILE:HD11	0.46	2.40	7	1
1:A:276:GLU:C	1:A:280:ILE:HD11	0.46	2.31	15	4
1:A:249:LEU:CD1	1:A:274:ILE:HG12	0.46	2.40	12	1
1:B:249:LEU:N	1:B:249:LEU:CD2	0.46	2.69	3	1
1:A:250:THR:O	1:A:253:ARG:HB2	0.46	2.11	6	8
1:A:270:ILE:CG1	1:B:252:ILE:HG13	0.46	2.40	7	1
1:B:280:ILE:CD1	1:B:281:ILE:HG12	0.46	2.41	5	6
1:A:232:ASP:O	1:A:232:ASP:OD1	0.46	2.34	13	2
1:A:279:ALA:O	1:A:283:GLN:HG2	0.46	2.11	3	1
1:B:232:ASP:O	1:B:232:ASP:OD1	0.46	2.34	13	2
1:B:263:ASP:CG	1:B:265:TYR:OH	0.46	2.54	16	1
1:A:249:LEU:HG	1:A:250:THR:N	0.46	2.26	1	2
1:A:256:THR:O	1:A:260:SER:HB2	0.46	2.11	6	8
1:B:251:ARG:O	1:B:254:LEU:HG	0.46	2.11	9	2
1:A:279:ALA:C	1:A:280:ILE:HD13	0.46	2.30	12	1
1:A:263:ASP:CB	1:B:259:MET:HE3	0.46	2.40	15	1
1:A:245:LEU:N	1:A:245:LEU:HD22	0.46	2.26	17	2
1:B:262:GLN:O	1:B:263:ASP:OD1	0.46	2.34	14	3
1:A:284:PHE:CE1	1:A:287:TYR:CE2	0.46	3.04	7	1
1:B:256:THR:HG22	1:B:266:LEU:HG	0.46	1.87	8	3
1:A:259:MET:HB2	1:B:259:MET:HG3	0.46	1.87	9	2
1:A:262:GLN:O	1:A:263:ASP:CG	0.46	2.55	12	1
1:A:258:MET:HB3	1:B:259:MET:CE	0.45	2.41	1	1
1:A:279:ALA:O	1:A:283:GLN:CG	0.45	2.64	3	1
1:B:259:MET:C	1:B:266:LEU:HD21	0.45	2.32	4	1
1:A:239:ALA:HA	1:A:243:HIS:CG	0.45	2.47	5	1
1:B:256:THR:O	1:B:260:SER:HB2	0.45	2.11	6	5
1:A:240:GLY:O	1:A:244:ASP:OD2	0.45	2.34	7	1
1:A:270:ILE:HG13	1:B:252:ILE:HG13	0.45	1.88	11	2
1:A:258:MET:HB2	1:B:259:MET:SD	0.45	2.51	1	1
1:A:280:ILE:CD1	1:A:281:ILE:HG12	0.45	2.42	7	7
1:A:252:ILE:HG21	1:A:270:ILE:HD12	0.45	1.86	5	1
1:B:266:LEU:CD1	1:B:267:ALA:N	0.45	2.78	6	2
1:A:282:GLU:O	1:A:286:ASP:OD2	0.45	2.35	7	1
1:B:259:MET:O	1:B:263:ASP:N	0.45	2.49	7	1
1:B:282:GLU:O	1:B:286:ASP:OD2	0.45	2.35	7	1
1:B:279:ALA:O	1:B:283:GLN:CG	0.45	2.64	3	1
1:A:236:LEU:HG	1:A:237:LEU:CD2	0.45	2.41	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:242:SER:O	1:B:243:HIS:C	0.45	2.55	1	3
1:B:236:LEU:HG	1:B:237:LEU:HD23	0.45	1.89	3	3
1:A:259:MET:O	1:A:263:ASP:N	0.45	2.49	7	1
1:B:276:GLU:O	1:B:280:ILE:CG1	0.45	2.65	3	4
1:B:248:PRO:O	1:B:249:LEU:C	0.45	2.53	11	5
1:B:237:LEU:HA	1:B:241:VAL:CG2	0.45	2.40	7	1
1:A:256:THR:HG22	1:A:266:LEU:HG	0.45	1.87	8	3
1:A:270:ILE:HG13	1:B:252:ILE:CD1	0.45	2.42	11	2
1:A:238:MET:O	1:A:242:SER:OG	0.45	2.34	11	3
1:A:271:ASN:ND2	1:A:271:ASN:N	0.45	2.63	8	2
1:B:273:ASP:O	1:B:276:GLU:HG2	0.45	2.11	14	1
1:A:276:GLU:O	1:A:280:ILE:CG1	0.45	2.65	6	5
1:B:249:LEU:HG	1:B:250:THR:N	0.45	2.26	1	2
1:A:259:MET:HB3	1:A:266:LEU:CD1	0.45	2.42	9	4
1:A:239:ALA:C	1:A:243:HIS:HB2	0.45	2.32	9	3
1:A:259:MET:SD	1:B:259:MET:HG3	0.45	2.52	7	1
1:A:246:ARG:C	1:A:248:PRO:HD2	0.45	2.33	14	4
1:B:256:THR:CG2	1:B:270:ILE:CD1	0.45	2.89	4	2
1:A:249:LEU:O	1:A:253:ARG:N	0.45	2.50	17	2
1:B:262:GLN:O	1:B:263:ASP:CG	0.45	2.55	12	1
1:B:259:MET:HB3	1:B:266:LEU:CD1	0.45	2.42	9	4
1:B:239:ALA:HA	1:B:243:HIS:CG	0.45	2.47	5	1
1:B:254:LEU:O	1:B:258:MET:HG2	0.45	2.12	14	1
1:A:257:GLU:O	1:A:260:SER:HB3	0.45	2.12	16	9
1:B:252:ILE:HG21	1:B:270:ILE:HD12	0.45	1.86	5	2
1:A:250:THR:HA	1:A:253:ARG:HB3	0.45	1.88	2	1
1:A:252:ILE:HG23	1:A:270:ILE:HD13	0.45	1.89	2	1
1:B:249:LEU:O	1:B:253:ARG:N	0.45	2.50	17	2
1:A:257:GLU:O	1:A:260:SER:OG	0.45	2.32	13	1
1:B:265:TYR:CG	1:B:266:LEU:N	0.45	2.84	14	1
1:A:263:ASP:OD1	1:A:265:TYR:CE1	0.45	2.70	15	1
1:A:284:PHE:CZ	1:B:240:GLY:C	0.45	2.90	16	1
1:B:257:GLU:O	1:B:260:SER:HB3	0.44	2.12	16	9
1:A:250:THR:CA	1:A:253:ARG:HB3	0.44	2.42	2	1
1:A:263:ASP:HB3	1:A:266:LEU:CD2	0.44	2.40	3	1
1:A:270:ILE:HD11	1:B:252:ILE:HD12	0.44	1.87	8	2
1:A:236:LEU:O	1:A:240:GLY:CA	0.44	2.65	10	2
1:A:259:MET:C	1:A:266:LEU:HD21	0.44	2.32	4	1
1:B:238:MET:O	1:B:242:SER:HB3	0.44	2.12	11	2
1:A:242:SER:O	1:A:243:HIS:C	0.44	2.55	1	3
1:A:259:MET:HG3	1:B:259:MET:HG3	0.44	1.88	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:239:ALA:C	1:B:243:HIS:HB2	0.44	2.32	9	3
1:A:251:ARG:O	1:A:254:LEU:HG	0.44	2.11	9	2
1:A:278:ASN:C	1:A:280:ILE:N	0.44	2.71	12	1
1:A:271:ASN:O	1:A:274:ILE:HB	0.44	2.13	8	8
1:A:262:GLN:OE1	1:A:262:GLN:HA	0.44	2.12	10	2
1:B:256:THR:HB	1:B:266:LEU:HD12	0.44	1.89	12	1
1:A:280:ILE:CD1	1:B:245:LEU:HD21	0.44	2.43	2	1
1:B:245:LEU:C	1:B:248:PRO:HD2	0.44	2.33	10	6
1:A:237:LEU:HB3	1:A:285:ILE:HD11	0.44	1.89	9	2
1:A:269:SER:O	1:A:273:ASP:HB2	0.44	2.13	10	3
1:A:282:GLU:OE1	1:A:282:GLU:CA	0.44	2.64	12	1
1:A:265:TYR:CG	1:A:266:LEU:N	0.44	2.84	14	1
1:A:258:MET:CG	1:A:259:MET:N	0.44	2.81	2	1
1:B:250:THR:CA	1:B:253:ARG:HB3	0.44	2.43	2	1
1:A:236:LEU:HG	1:A:237:LEU:HD23	0.44	1.89	3	3
1:A:285:ILE:HD13	1:A:285:ILE:N	0.44	2.27	3	1
1:B:256:THR:CG2	1:B:266:LEU:HB3	0.44	2.42	7	1
1:B:269:SER:O	1:B:273:ASP:HB2	0.44	2.13	10	3
1:A:273:ASP:OD2	1:B:248:PRO:HB2	0.44	2.12	17	1
1:B:236:LEU:HG	1:B:237:LEU:CD2	0.44	2.42	11	3
1:B:246:ARG:C	1:B:248:PRO:HD2	0.44	2.33	14	4
1:B:236:LEU:O	1:B:240:GLY:CA	0.44	2.65	10	2
1:A:273:ASP:O	1:A:276:GLU:HG2	0.44	2.11	14	1
1:B:263:ASP:OD1	1:B:265:TYR:CE1	0.44	2.71	15	1
1:A:259:MET:SD	1:B:259:MET:HB2	0.44	2.53	2	1
1:A:259:MET:SD	1:B:259:MET:CG	0.44	3.06	7	1
1:A:238:MET:O	1:A:242:SER:HB3	0.44	2.12	11	2
1:A:284:PHE:HZ	1:B:237:LEU:HD13	0.44	1.73	9	2
1:A:276:GLU:O	1:A:277:CYS:C	0.44	2.56	15	4
1:B:274:ILE:O	1:B:277:CYS:HB3	0.44	2.13	11	2
1:B:276:GLU:O	1:B:277:CYS:C	0.44	2.55	16	4
1:A:241:VAL:O	1:A:242:SER:C	0.43	2.56	4	4
1:B:258:MET:HG3	1:B:259:MET:CE	0.43	2.43	6	1
1:B:277:CYS:HA	1:B:280:ILE:HG12	0.43	1.90	6	2
1:A:237:LEU:HA	1:A:241:VAL:CG2	0.43	2.40	7	1
1:B:260:SER:CB	1:B:267:ALA:CB	0.43	2.96	8	2
1:B:252:ILE:HG22	1:B:270:ILE:HG21	0.43	1.89	9	2
1:B:275:GLU:OE1	1:B:275:GLU:O	0.43	2.36	9	2
1:B:248:PRO:O	1:B:250:THR:N	0.43	2.51	11	2
1:A:256:THR:HB	1:A:266:LEU:HD12	0.43	1.89	12	1
1:A:281:ILE:O	1:A:285:ILE:HG12	0.43	2.13	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:CYS:HA	1:A:280:ILE:HG12	0.43	1.90	6	1
1:A:252:ILE:HG22	1:A:270:ILE:HG21	0.43	1.89	9	2
1:B:260:SER:C	1:B:264:GLY:HA2	0.43	2.34	16	2
1:B:252:ILE:HG23	1:B:270:ILE:HD13	0.43	1.89	2	1
1:B:281:ILE:O	1:B:285:ILE:HG12	0.43	2.13	3	3
1:A:245:LEU:C	1:A:248:PRO:HD2	0.43	2.33	10	6
1:A:275:GLU:OE1	1:A:275:GLU:CA	0.43	2.66	9	2
1:B:262:GLN:HA	1:B:262:GLN:OE1	0.43	2.12	10	2
1:B:257:GLU:O	1:B:260:SER:HB2	0.43	2.13	12	1
1:A:254:LEU:O	1:A:258:MET:HG2	0.43	2.12	14	1
1:A:260:SER:C	1:A:264:GLY:HA2	0.43	2.34	16	2
1:A:236:LEU:O	1:A:236:LEU:CD1	0.43	2.56	3	1
1:B:280:ILE:O	1:B:284:PHE:HB2	0.43	2.13	9	4
1:A:266:LEU:CD1	1:A:267:ALA:N	0.43	2.78	6	1
1:A:259:MET:SD	1:A:266:LEU:HD11	0.43	2.52	7	1
1:B:249:LEU:O	1:B:253:ARG:HD3	0.43	2.14	7	1
1:B:259:MET:SD	1:B:266:LEU:HD11	0.43	2.52	7	1
1:B:268:GLU:O	1:B:269:SER:C	0.43	2.56	7	2
1:B:265:TYR:O	1:B:266:LEU:C	0.43	2.57	14	3
1:A:262:GLN:OE1	1:A:262:GLN:CA	0.43	2.66	10	2
1:B:262:GLN:OE1	1:B:262:GLN:CA	0.43	2.66	10	2
1:A:274:ILE:O	1:A:277:CYS:HB3	0.43	2.13	11	2
1:B:279:ALA:C	1:B:280:ILE:HD13	0.43	2.31	12	1
1:A:250:THR:O	1:A:253:ARG:HG2	0.43	2.13	15	1
1:A:232:ASP:O	1:A:236:LEU:HB3	0.43	2.14	9	6
1:B:271:ASN:O	1:B:274:ILE:HB	0.43	2.13	8	9
1:A:247:THR:N	1:A:248:PRO:HD3	0.43	2.28	4	1
1:B:247:THR:N	1:B:248:PRO:HD3	0.43	2.28	4	1
1:A:256:THR:HG21	1:A:270:ILE:CG1	0.43	2.38	6	1
1:A:260:SER:CB	1:A:267:ALA:CB	0.43	2.96	8	2
1:A:283:GLN:O	1:A:287:TYR:HB3	0.43	2.14	8	2
1:A:265:TYR:O	1:A:266:LEU:C	0.43	2.57	9	3
1:A:246:ARG:CG	1:A:249:LEU:HD11	0.43	2.43	11	2
1:B:282:GLU:OE1	1:B:282:GLU:CA	0.43	2.64	12	1
1:A:244:ASP:OD2	1:A:245:LEU:HD22	0.43	2.14	2	1
1:B:241:VAL:O	1:B:242:SER:C	0.43	2.56	4	2
1:B:258:MET:CG	1:B:259:MET:N	0.43	2.81	2	1
1:B:241:VAL:HA	1:B:244:ASP:OD2	0.43	2.14	7	1
1:B:250:THR:O	1:B:253:ARG:HG2	0.43	2.13	15	1
1:B:263:ASP:HB3	1:B:265:TYR:CZ	0.43	2.49	16	1
1:A:252:ILE:HD13	1:A:252:ILE:HA	0.43	1.66	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:250:THR:O	1:B:253:ARG:HB3	0.43	2.14	2	3
1:B:238:MET:O	1:B:242:SER:HB2	0.43	2.14	3	1
1:B:237:LEU:HB3	1:B:285:ILE:HD11	0.43	1.89	9	2
1:A:284:PHE:HA	1:A:287:TYR:OH	0.43	2.14	11	3
1:A:262:GLN:O	1:A:262:GLN:CD	0.43	2.57	15	1
1:B:262:GLN:CD	1:B:262:GLN:O	0.43	2.57	15	1
1:B:279:ALA:O	1:B:283:GLN:HB3	0.43	2.13	17	1
1:B:232:ASP:O	1:B:236:LEU:HB3	0.43	2.14	9	6
1:A:238:MET:O	1:A:242:SER:HB2	0.43	2.14	3	1
1:B:285:ILE:N	1:B:285:ILE:HD13	0.43	2.27	3	1
1:A:266:LEU:CG	1:A:267:ALA:N	0.43	2.82	9	4
1:B:271:ASN:ND2	1:B:271:ASN:N	0.43	2.63	8	2
1:A:253:ARG:HG3	1:A:271:ASN:OD1	0.43	2.14	12	1
1:A:263:ASP:HB3	1:A:265:TYR:CZ	0.43	2.49	16	1
1:A:279:ALA:O	1:A:283:GLN:HB3	0.43	2.13	17	1
1:B:270:ILE:C	1:B:272:LYS:N	0.43	2.72	3	1
1:B:287:TYR:N	1:B:287:TYR:CD1	0.43	2.87	4	1
1:A:256:THR:HB	1:A:267:ALA:N	0.43	2.29	7	1
1:A:268:GLU:O	1:A:269:SER:C	0.43	2.56	7	4
1:A:276:GLU:O	1:A:280:ILE:HG13	0.43	2.13	9	2
1:A:261:GLU:O	1:A:262:GLN:C	0.43	2.57	2	1
1:A:280:ILE:O	1:A:284:PHE:HB2	0.43	2.13	9	4
1:A:259:MET:HG2	1:B:259:MET:HG2	0.43	1.91	6	1
1:B:256:THR:HG21	1:B:270:ILE:CG1	0.43	2.38	6	1
1:B:285:ILE:N	1:B:285:ILE:CD1	0.43	2.82	6	2
1:B:241:VAL:O	1:B:244:ASP:CG	0.43	2.57	7	1
1:B:256:THR:HB	1:B:267:ALA:N	0.43	2.29	7	1
1:A:240:GLY:O	1:A:244:ASP:HB2	0.43	2.14	10	2
1:B:246:ARG:CG	1:B:249:LEU:HD11	0.43	2.43	11	2
1:A:259:MET:CB	1:B:259:MET:HG3	0.43	2.44	15	1
1:A:258:MET:HG3	1:A:259:MET:CE	0.42	2.43	6	1
1:B:275:GLU:OE1	1:B:275:GLU:CA	0.42	2.66	9	2
1:A:248:PRO:O	1:A:250:THR:N	0.42	2.51	11	2
1:A:257:GLU:O	1:A:260:SER:HB2	0.42	2.13	12	1
1:B:278:ASN:C	1:B:280:ILE:N	0.42	2.71	12	1
1:B:256:THR:O	1:B:257:GLU:C	0.42	2.57	13	1
1:B:263:ASP:HB2	1:B:266:LEU:HD23	0.42	1.90	16	1
1:B:261:GLU:O	1:B:262:GLN:C	0.42	2.57	2	2
1:A:270:ILE:O	1:A:273:ASP:N	0.42	2.52	7	2
1:A:256:THR:CG2	1:A:266:LEU:HB3	0.42	2.42	7	1
1:B:284:PHE:HA	1:B:287:TYR:OH	0.42	2.14	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:THR:O	1:A:253:ARG:HB3	0.42	2.14	10	3
1:A:249:LEU:O	1:A:253:ARG:HD3	0.42	2.14	7	1
1:A:287:TYR:OH	1:B:236:LEU:HD11	0.42	2.15	8	2
1:B:275:GLU:OE1	1:B:275:GLU:C	0.42	2.57	9	2
1:B:277:CYS:C	1:B:280:ILE:HG12	0.42	2.34	12	1
1:A:263:ASP:CG	1:A:265:TYR:CE2	0.42	2.93	15	1
1:B:277:CYS:O	1:B:280:ILE:CG1	0.42	2.67	1	1
1:A:259:MET:HE1	1:B:258:MET:HG3	0.42	1.91	2	1
1:A:283:GLN:O	1:A:286:ASP:HB2	0.42	2.15	3	1
1:A:275:GLU:OE1	1:A:275:GLU:C	0.42	2.57	9	2
1:A:275:GLU:OE1	1:A:275:GLU:O	0.42	2.36	9	2
1:B:263:ASP:O	1:B:266:LEU:HG	0.42	2.15	17	1
1:A:285:ILE:CD1	1:A:285:ILE:N	0.42	2.82	6	1
1:A:257:GLU:HA	1:A:260:SER:HB2	0.42	1.92	9	2
1:A:277:CYS:C	1:A:280:ILE:HG12	0.42	2.34	12	1
1:B:246:ARG:NH1	1:B:278:ASN:OD1	0.42	2.53	17	1
1:A:277:CYS:O	1:A:280:ILE:CG1	0.42	2.67	1	1
1:B:266:LEU:CG	1:B:267:ALA:N	0.42	2.82	13	4
1:B:272:LYS:O	1:B:273:ASP:C	0.42	2.58	5	4
1:A:241:VAL:HA	1:A:244:ASP:OD2	0.42	2.14	7	1
1:A:245:LEU:O	1:A:249:LEU:HD23	0.42	2.14	7	1
1:B:276:GLU:O	1:B:280:ILE:HG13	0.42	2.13	9	2
1:B:240:GLY:O	1:B:244:ASP:HB2	0.42	2.14	10	2
1:A:246:ARG:NH1	1:A:278:ASN:OD1	0.42	2.53	17	1
1:A:263:ASP:O	1:A:266:LEU:HG	0.42	2.15	17	1
1:B:245:LEU:O	1:B:249:LEU:HD23	0.42	2.14	7	1
1:A:249:LEU:CD2	1:A:250:THR:N	0.42	2.80	14	1
1:A:233:ASP:O	1:A:237:LEU:HB2	0.42	2.15	15	1
1:B:244:ASP:OD2	1:B:245:LEU:HD22	0.42	2.14	2	1
1:B:268:GLU:O	1:B:272:LYS:HG3	0.42	2.14	2	1
1:B:270:ILE:O	1:B:273:ASP:N	0.42	2.53	7	2
1:A:256:THR:HB	1:A:267:ALA:CA	0.42	2.45	12	1
1:B:253:ARG:HG3	1:B:271:ASN:OD1	0.42	2.14	12	1
1:A:256:THR:O	1:A:257:GLU:C	0.42	2.57	13	1
1:A:259:MET:SD	1:B:258:MET:HB2	0.42	2.55	13	1
1:A:287:TYR:N	1:A:287:TYR:CD1	0.42	2.87	4	1
1:A:241:VAL:O	1:A:244:ASP:CG	0.42	2.57	7	1
1:B:245:LEU:CD2	1:B:277:CYS:SG	0.42	3.08	16	1
1:B:238:MET:O	1:B:242:SER:OG	0.42	2.35	3	1
1:A:249:LEU:HD22	1:A:249:LEU:H	0.42	1.73	7	1
1:B:283:GLN:O	1:B:287:TYR:HB3	0.42	2.14	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:274:ILE:O	1:A:275:GLU:C	0.42	2.59	9	5
1:A:276:GLU:O	1:A:280:ILE:HD11	0.42	2.14	12	1
1:B:263:ASP:CG	1:B:265:TYR:CE2	0.42	2.93	15	1
1:B:260:SER:HA	1:B:266:LEU:HD11	0.41	1.92	6	1
1:B:272:LYS:C	1:B:274:ILE:N	0.41	2.72	8	2
1:B:276:GLU:O	1:B:280:ILE:HD11	0.41	2.15	8	3
1:A:256:THR:CB	1:A:266:LEU:HD12	0.41	2.45	12	1
1:A:266:LEU:O	1:A:269:SER:N	0.41	2.53	12	1
1:A:258:MET:SD	1:B:259:MET:SD	0.41	3.19	2	1
1:A:268:GLU:O	1:A:272:LYS:HG3	0.41	2.14	2	1
1:A:285:ILE:N	1:A:285:ILE:CD1	0.41	2.83	7	1
1:B:274:ILE:O	1:B:275:GLU:C	0.41	2.59	9	5
1:B:266:LEU:O	1:B:269:SER:N	0.41	2.53	12	1
1:B:284:PHE:CD1	1:B:284:PHE:C	0.41	2.94	1	1
1:A:252:ILE:CD1	1:B:270:ILE:CG1	0.41	2.98	9	2
1:B:265:TYR:N	1:B:265:TYR:CD1	0.41	2.87	9	2
1:B:277:CYS:CA	1:B:280:ILE:HG12	0.41	2.45	12	1
1:A:272:LYS:HD3	1:A:273:ASP:N	0.41	2.31	2	1
1:B:283:GLN:O	1:B:286:ASP:HB2	0.41	2.15	3	1
1:B:249:LEU:HD22	1:B:249:LEU:H	0.41	1.73	7	1
1:A:259:MET:SD	1:B:259:MET:HE3	0.41	2.56	17	1
1:A:245:LEU:CD1	1:B:277:CYS:SG	0.41	3.09	4	1
1:A:241:VAL:HG22	1:B:284:PHE:CD2	0.41	2.50	5	1
1:A:245:LEU:CD2	1:A:277:CYS:SG	0.41	3.08	16	1
1:B:257:GLU:HA	1:B:260:SER:HB2	0.41	1.92	9	2
1:A:268:GLU:O	1:A:272:LYS:HB3	0.41	2.15	10	2
1:A:262:GLN:O	1:A:263:ASP:CB	0.41	2.69	11	2
1:A:258:MET:HB2	1:A:259:MET:HE2	0.41	1.93	15	1
1:A:274:ILE:O	1:A:277:CYS:HB2	0.41	2.15	15	1
1:B:233:ASP:O	1:B:237:LEU:HB2	0.41	2.15	15	1
1:B:274:ILE:O	1:B:277:CYS:HB2	0.41	2.15	15	1
1:A:256:THR:O	1:A:260:SER:HB3	0.41	2.16	5	1
1:B:275:GLU:HG3	1:B:276:GLU:N	0.41	2.30	9	2
1:A:277:CYS:C	1:A:280:ILE:HG13	0.41	2.36	10	2
1:A:284:PHE:CG	1:A:287:TYR:OH	0.41	2.71	11	2
1:A:270:ILE:C	1:A:272:LYS:N	0.41	2.72	3	1
1:A:245:LEU:O	1:A:248:PRO:HD2	0.41	2.16	4	1
1:A:270:ILE:HD13	1:B:252:ILE:HG13	0.41	1.92	8	2
1:A:259:MET:HG2	1:B:259:MET:HB3	0.41	1.93	12	1
1:B:239:ALA:HA	1:B:243:HIS:HB2	0.41	1.93	12	1
1:B:238:MET:C	1:B:240:GLY:N	0.41	2.73	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:244:ASP:O	1:B:247:THR:HG22	0.41	2.16	14	1
1:A:245:LEU:HD21	1:B:280:ILE:CD1	0.41	2.45	2	1
1:B:281:ILE:O	1:B:284:PHE:HB3	0.41	2.16	3	1
1:A:260:SER:HA	1:A:266:LEU:HD11	0.41	1.92	6	1
1:A:262:GLN:O	1:A:263:ASP:HB2	0.41	2.16	7	1
1:A:272:LYS:C	1:A:274:ILE:N	0.41	2.72	8	2
1:A:254:LEU:HA	1:A:257:GLU:CB	0.41	2.45	9	2
1:A:239:ALA:HA	1:A:243:HIS:HB2	0.41	1.93	12	1
1:A:232:ASP:O	1:A:236:LEU:HD11	0.41	2.15	17	1
1:B:232:ASP:O	1:B:236:LEU:HD11	0.41	2.15	17	1
1:A:252:ILE:CD1	1:B:270:ILE:CD1	0.41	2.99	1	1
1:A:250:THR:CA	1:A:253:ARG:HB2	0.41	2.46	5	2
1:B:263:ASP:OD2	1:B:266:LEU:HG	0.41	2.16	6	1
1:A:259:MET:HG3	1:B:259:MET:SD	0.41	2.56	7	1
1:A:277:CYS:CA	1:A:280:ILE:HG12	0.41	2.45	12	1
1:A:269:SER:C	1:A:272:LYS:HG3	0.40	2.37	2	1
1:B:272:LYS:HD3	1:B:273:ASP:N	0.40	2.31	2	1
1:A:259:MET:HG3	1:B:259:MET:HB3	0.40	1.93	4	1
1:A:265:TYR:N	1:A:265:TYR:CD1	0.40	2.87	9	2
1:B:277:CYS:C	1:B:280:ILE:HG13	0.40	2.36	10	2
1:B:263:ASP:OD1	1:B:266:LEU:HD21	0.40	2.16	6	1
1:B:256:THR:CB	1:B:266:LEU:HD12	0.40	2.45	12	1
1:B:278:ASN:O	1:B:279:ALA:C	0.40	2.59	12	1
1:B:269:SER:C	1:B:272:LYS:HG3	0.40	2.37	2	1
1:B:250:THR:CA	1:B:253:ARG:HB2	0.40	2.47	6	1
1:B:258:MET:HG3	1:B:259:MET:SD	0.40	2.56	12	1
1:B:268:GLU:O	1:B:272:LYS:HB2	0.40	2.17	1	1
1:A:281:ILE:O	1:A:284:PHE:HB3	0.40	2.16	3	1
1:A:267:ALA:O	1:A:270:ILE:HB	0.40	2.16	5	1
1:B:268:GLU:O	1:B:272:LYS:HB3	0.40	2.15	10	2
1:B:256:THR:HB	1:B:267:ALA:CA	0.40	2.45	12	1
1:B:270:ILE:O	1:B:273:ASP:HB3	0.40	2.16	12	1
1:A:284:PHE:HD2	1:A:287:TYR:HH	0.40	1.58	15	1
1:A:249:LEU:C	1:A:249:LEU:CD2	0.40	2.74	16	1
1:A:268:GLU:O	1:A:272:LYS:HB2	0.40	2.17	1	1
1:A:284:PHE:CD1	1:A:284:PHE:C	0.40	2.94	1	1
1:B:243:HIS:O	1:B:243:HIS:CD2	0.40	2.74	1	1
1:A:259:MET:CG	1:B:259:MET:SD	0.40	3.10	7	1
1:A:238:MET:C	1:A:240:GLY:N	0.40	2.73	14	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	56/67 (84%)	46±2 (83±3%)	7±2 (13±3%)	2±1 (4±2%)	5	29
1	B	56/67 (84%)	46±2 (83±3%)	7±2 (13±3%)	2±1 (4±2%)	5	29
All	All	2352/2814 (84%)	1946 (83%)	306 (13%)	100 (4%)	5	29

All 20 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	264	GLY	20
1	B	264	GLY	20
1	A	232	ASP	9
1	B	232	ASP	9
1	A	263	ASP	6
1	B	263	ASP	6
1	A	242	SER	5
1	B	242	SER	5
1	A	267	ALA	2
1	A	271	ASN	2
1	B	267	ALA	2
1	B	271	ASN	2
1	A	265	TYR	2
1	B	265	TYR	2
1	A	233	ASP	2
1	B	233	ASP	2
1	A	243	HIS	1
1	B	243	HIS	1
1	A	266	LEU	1
1	B	266	LEU	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	50/57 (88%)	34±3 (68±6%)	16±3 (32±6%)	1 13
1	B	50/57 (88%)	34±3 (68±6%)	16±3 (32±6%)	1 13
All	All	2100/2394 (88%)	1429 (68%)	671 (32%)	1 13

All 82 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	237	LEU	21
1	B	237	LEU	21
1	A	252	ILE	20
1	B	252	ILE	20
1	A	280	ILE	19
1	B	280	ILE	19
1	A	241	VAL	16
1	A	253	ARG	16
1	A	256	THR	16
1	B	241	VAL	16
1	B	253	ARG	16
1	B	256	THR	16
1	A	276	GLU	13
1	B	276	GLU	13
1	B	242	SER	12
1	A	233	ASP	12
1	B	233	ASP	12
1	A	251	ARG	12
1	B	251	ARG	12
1	A	242	SER	11
1	A	258	MET	11
1	A	259	MET	11
1	B	258	MET	11
1	B	259	MET	11
1	A	249	LEU	10
1	B	249	LEU	10
1	A	246	ARG	9
1	B	246	ARG	9
1	A	269	SER	9
1	B	269	SER	9
1	A	274	ILE	9
1	B	274	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	243	HIS	9
1	B	243	HIS	9
1	A	234	ARG	8
1	B	234	ARG	8
1	A	286	ASP	8
1	B	286	ASP	8
1	A	232	ASP	7
1	A	238	MET	7
1	B	232	ASP	7
1	B	238	MET	7
1	A	262	GLN	7
1	A	272	LYS	7
1	B	262	GLN	7
1	B	272	LYS	7
1	A	275	GLU	7
1	B	275	GLU	7
1	A	257	GLU	6
1	A	266	LEU	6
1	A	277	CYS	6
1	B	257	GLU	6
1	B	266	LEU	6
1	B	277	CYS	6
1	A	245	LEU	6
1	A	282	GLU	6
1	B	245	LEU	6
1	B	282	GLU	6
1	A	261	GLU	4
1	B	261	GLU	4
1	A	244	ASP	4
1	B	244	ASP	4
1	A	287	TYR	4
1	B	287	TYR	4
1	A	284	PHE	3
1	B	284	PHE	3
1	A	263	ASP	3
1	B	263	ASP	3
1	A	273	ASP	3
1	B	273	ASP	3
1	A	236	LEU	2
1	B	236	LEU	2
1	A	278	ASN	2
1	B	278	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	283	GLN	2
1	B	283	GLN	2
1	A	285	ILE	1
1	B	285	ILE	1
1	A	260	SER	1
1	B	260	SER	1
1	A	268	GLU	1
1	B	268	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no 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