



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 03:35 PM UTC

PDB ID : 1JOY / pdb_00001joy
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 ⓘ 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

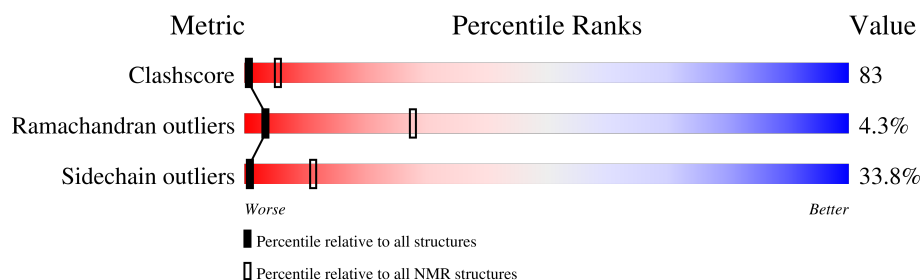
1 Overall quality at a glance

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	67	
1	B	67	

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).

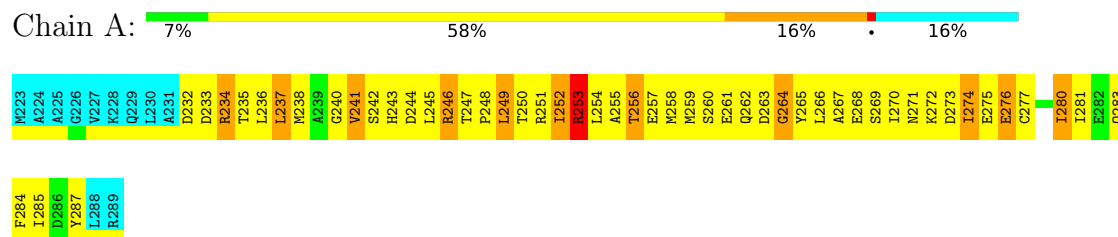
Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1058	326	530	91	106	5	
1	B	67	Total	C	H	N	O	S	0
			1058	326	530	91	106	5	

4 Residue-property plots [i](#)

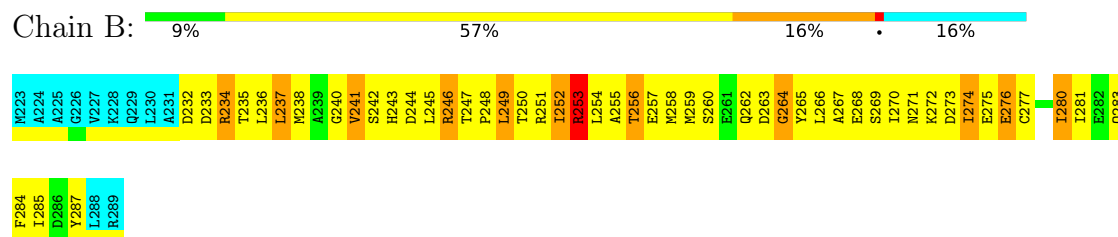
4.1 Average score per residue in the NMR ensemble

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)



- Molecule 1: PROTEIN (ENVZ_ECOLI)

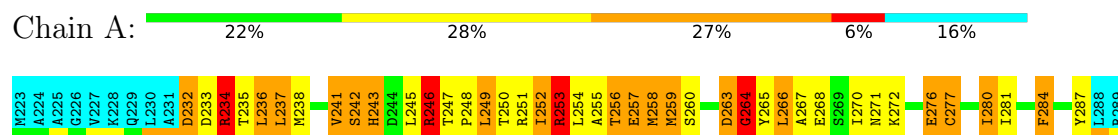


4.2 Scores per residue for each member of the ensemble

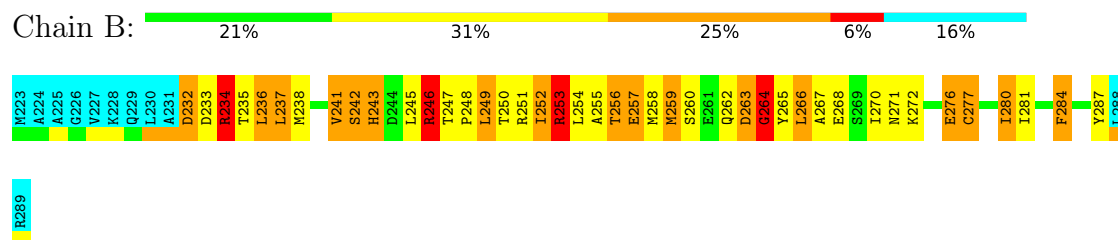
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (ENVZ_ECOLI)

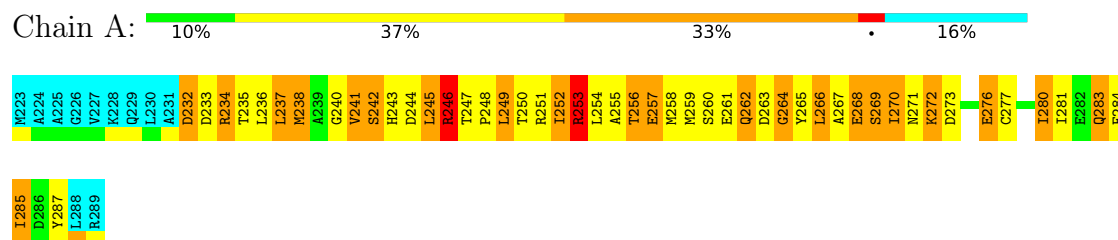


- Molecule 1: PROTEIN (ENVZ_ECOLI)

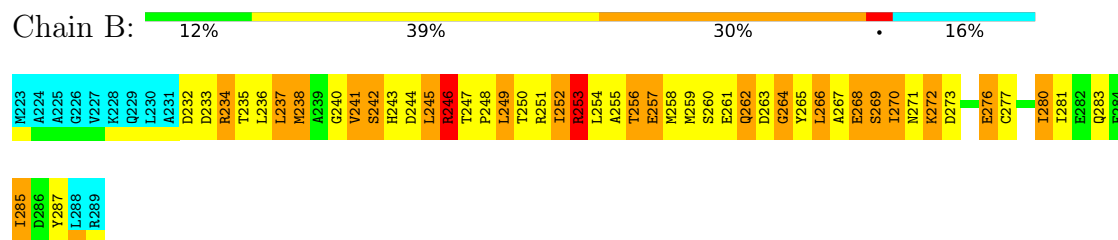


4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (ENVZ_ECOLI)

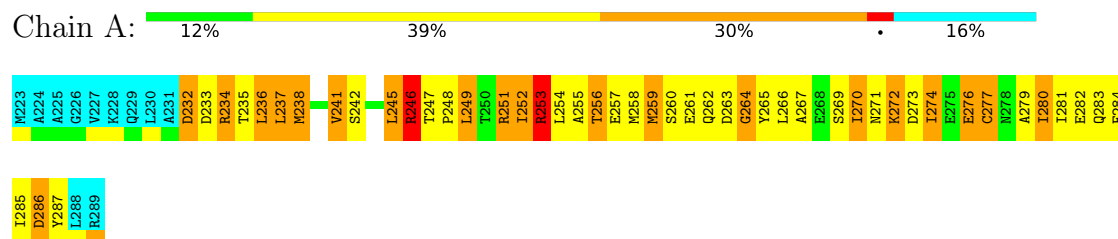


- Molecule 1: PROTEIN (ENVZ_ECOLI)

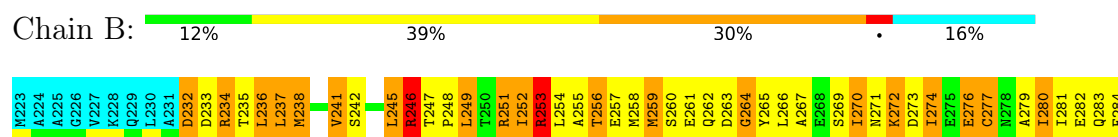


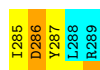
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (ENVZ_ECOLI)



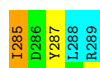
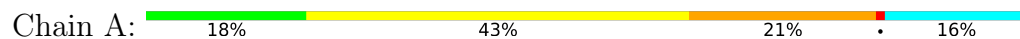
- Molecule 1: PROTEIN (ENVZ_ECOLI)



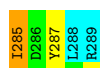
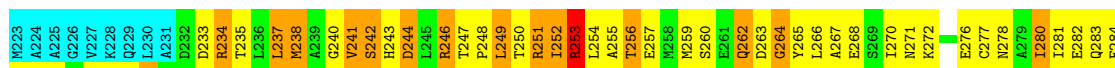
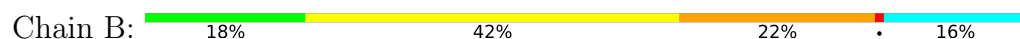


4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (ENVZ_ECOLI)

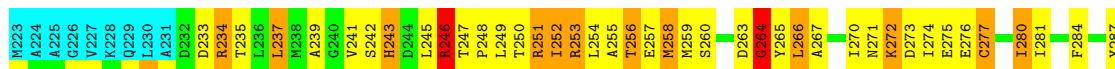
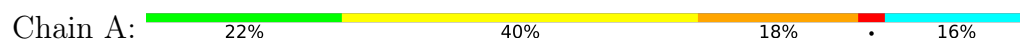


- Molecule 1: PROTEIN (ENVZ_ECOLI)

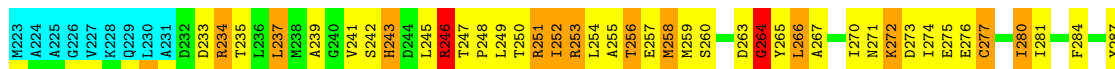
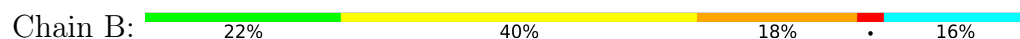


4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (ENVZ_ECOLI)

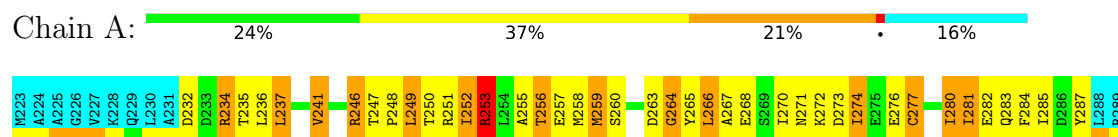


- Molecule 1: PROTEIN (ENVZ_ECOLI)

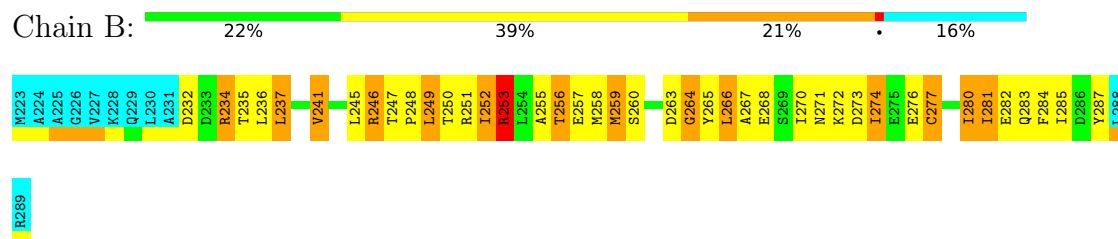


4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (ENVZ_ECOLI)

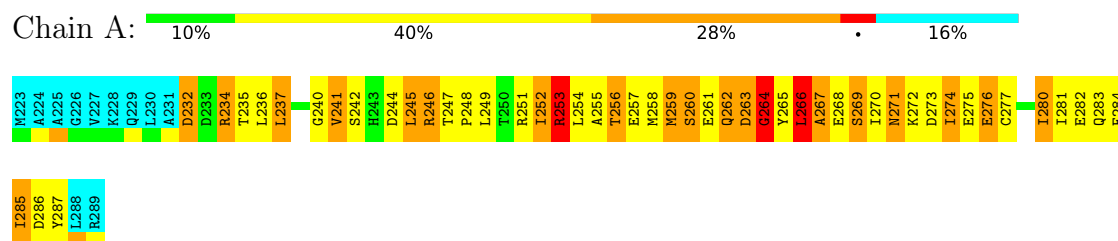


- Molecule 1: PROTEIN (ENVZ_ECOLI)

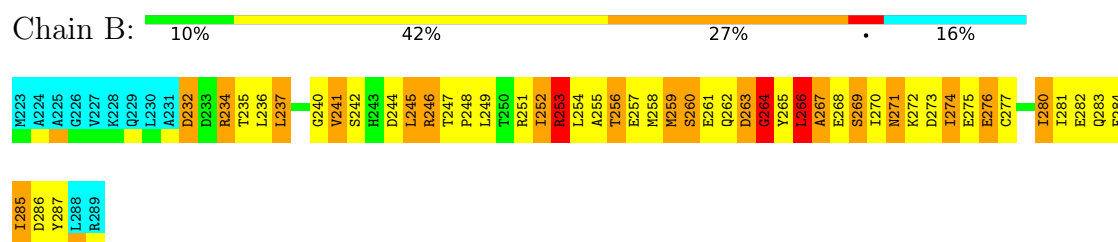


4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (ENVZ_ECOLI)

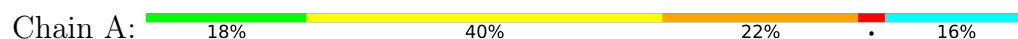


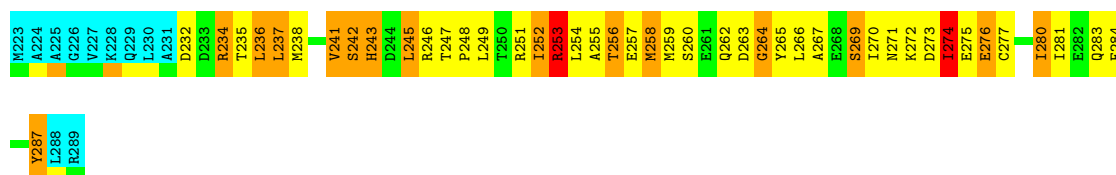
- Molecule 1: PROTEIN (ENVZ_ECOLI)



4.2.8 Score per residue for model 8

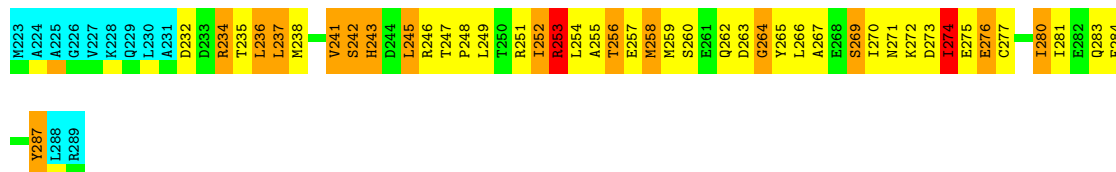
- Molecule 1: PROTEIN (ENVZ_ECOLI)





• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B: 18% 40% 22% 16%



4.2.9 Score per residue for model 9

• Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A: 10% 51% 22% 16%



• Molecule 1: PROTEIN (ENVZ_ECOLI)

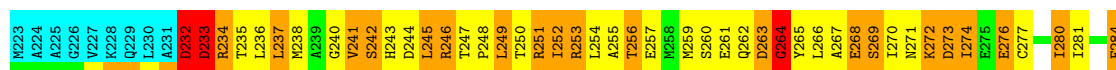
Chain B: 6% 55% 22% 16%



4.2.10 Score per residue for model 10

• Molecule 1: PROTEIN (ENVZ_ECOLI)

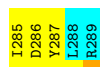
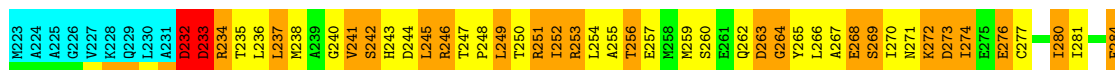
Chain A: 10% 39% 30% 16%





- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B: 12% 37% 31% • 16%



4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A: 10% 43% 25% • 16%



- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain B: 10% 43% 25% • 16%



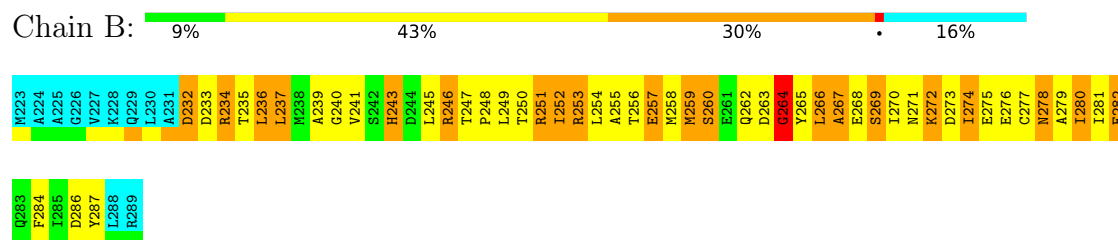
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (ENVZ_ECOLI)

Chain A: 10% 42% 30% • 16%

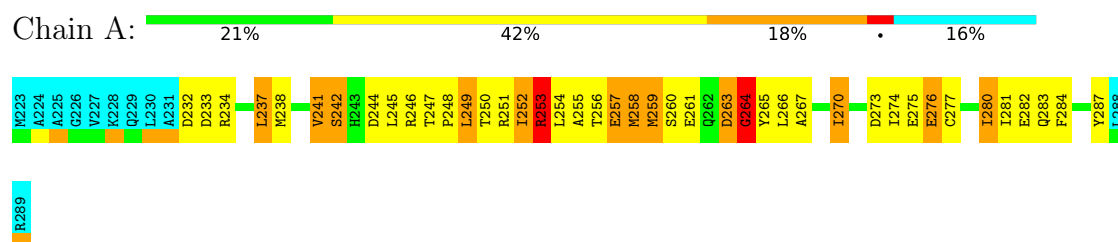


- Molecule 1: PROTEIN (ENVZ_ECOLI)

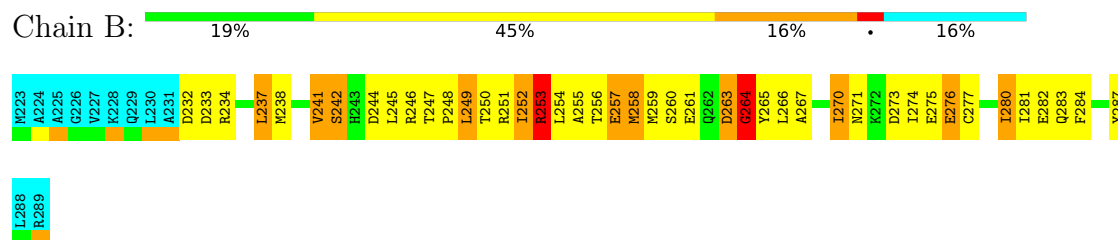


4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: PROTEIN (ENVZ_ECOLI)

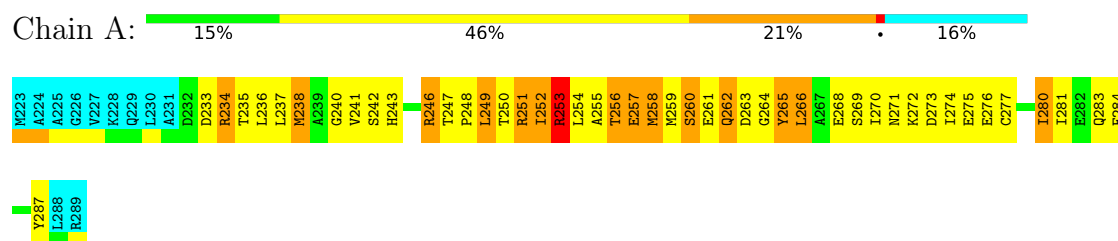


- Molecule 1: PROTEIN (ENVZ_ECOLI)

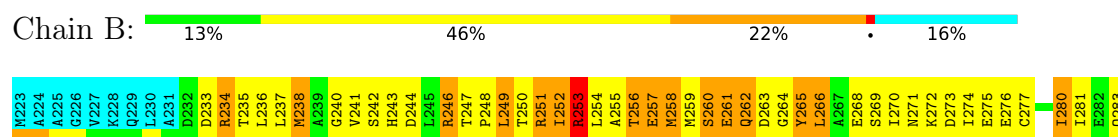


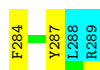
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (ENVZ_ECOLI)



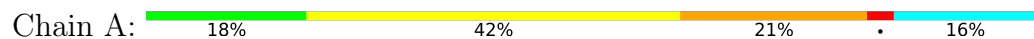
- Molecule 1: PROTEIN (ENVZ_ECOLI)



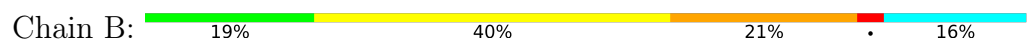


4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (ENVZ_ECOLI)



- Molecule 1: PROTEIN (ENVZ_ECOLI)

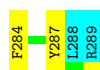


4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (ENVZ_ECOLI)

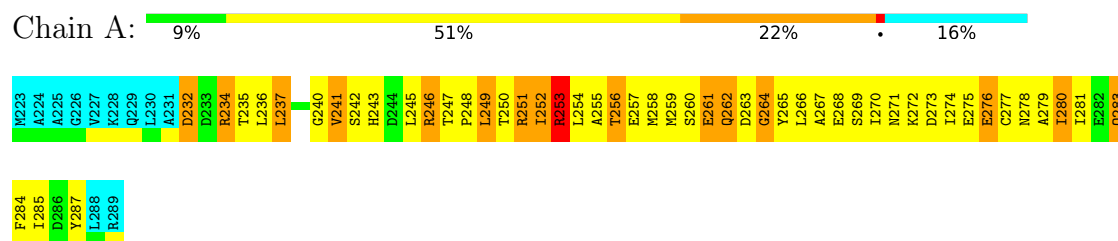


- Molecule 1: PROTEIN (ENVZ_ECOLI)

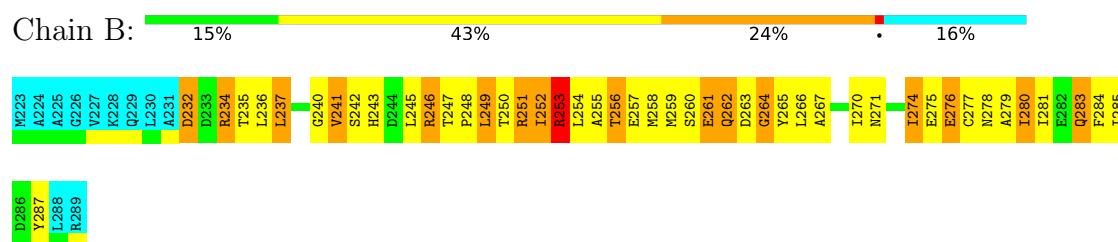


4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (ENVZ_ECOLI)

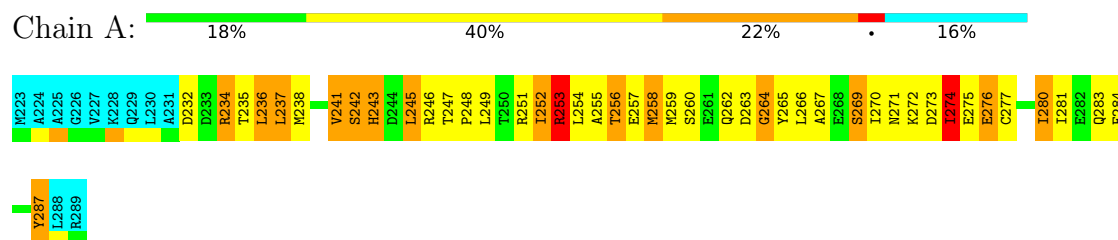


- Molecule 1: PROTEIN (ENVZ_ECOLI)

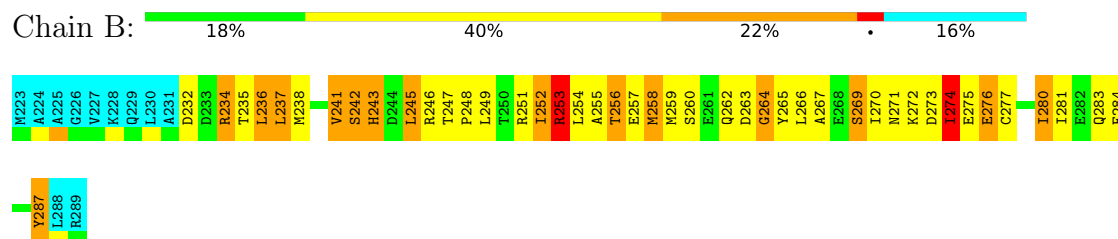


4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (ENVZ_ECOLI)

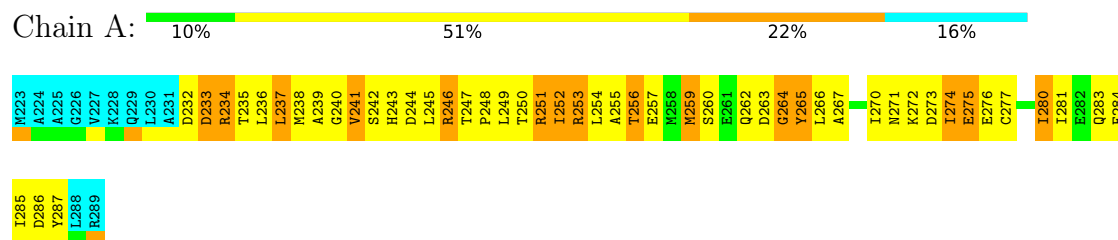


- Molecule 1: PROTEIN (ENVZ_ECOLI)

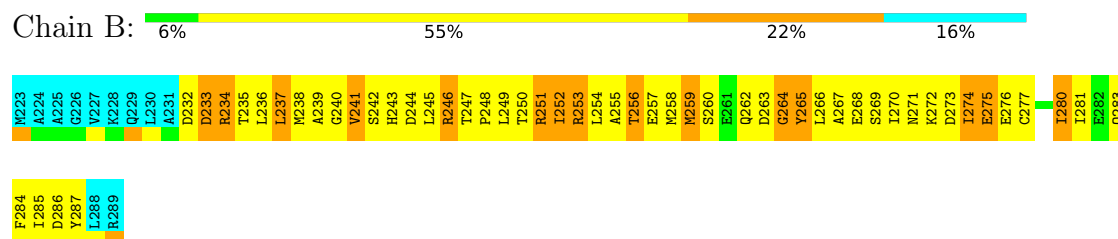


4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (ENVZ_ECOLI)

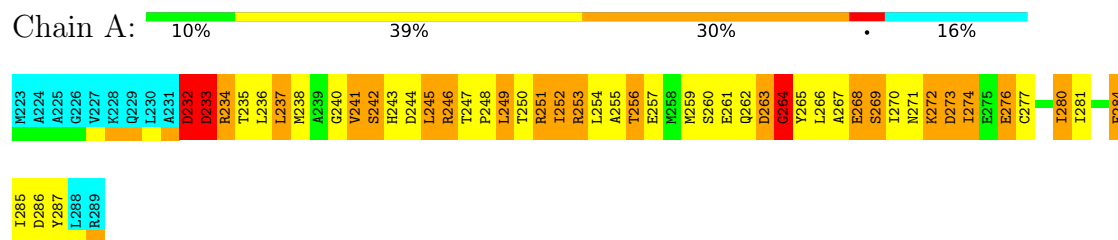


• Molecule 1: PROTEIN (ENVZ_ECOLI)

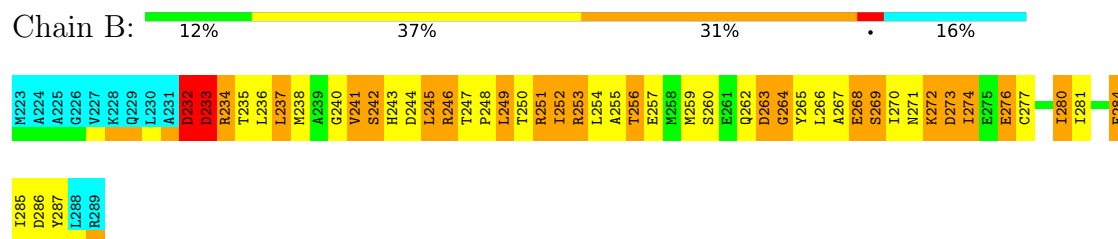


4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN (ENVZ_ECOLI)

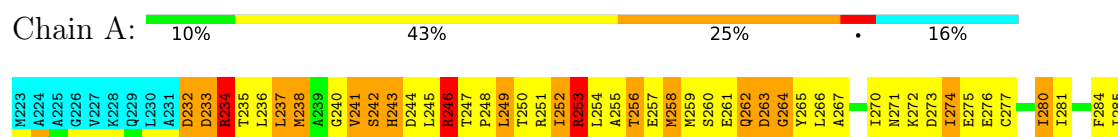


• Molecule 1: PROTEIN (ENVZ_ECOLI)



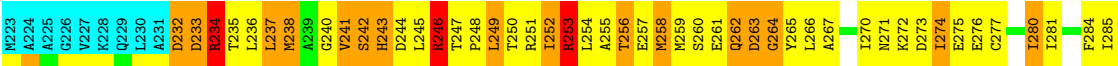
4.2.21 Score per residue for model 21

• Molecule 1: PROTEIN (ENVZ_ECOLI)





● Molecule 1: PROTEIN (ENVZ_ECOLI)



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 i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.51±0.02	0±0/453 (0.1± 0.1%)	1.60±0.01	1±1/612 (0.1± 0.1%)
1	B	1.51±0.02	0±0/453 (0.1± 0.1%)	1.60±0.02	1±1/612 (0.1± 0.2%)
All	All	1.51	14/19026 (0.1%)	1.60	34/25704 (0.1%)

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

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	264	GLY	N-CA	5.46	1.53	1.45	12	5
1	A	264	GLY	N-CA	5.40	1.53	1.45	12	7
1	B	265	TYR	N-CA	5.05	1.52	1.46	14	1
1	A	265	TYR	N-CA	5.04	1.52	1.46	14	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	274	ILE	N-CA-CB	-5.65	104.27	110.65	8	3
1	B	274	ILE	N-CA-CB	-5.62	104.30	110.65	8	3
1	A	262	GLN	N-CA-C	-5.45	105.89	112.54	14	3
1	B	281	ILE	N-CA-CB	-5.44	104.19	110.55	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	262	GLN	N-CA-C	-5.43	105.91	112.54	14	3
1	A	281	ILE	N-CA-CB	-5.41	104.22	110.55	6	1
1	B	261	GLU	N-CA-C	-5.41	106.62	113.43	14	2
1	A	284	PHE	CA-CB-CG	-5.39	108.41	113.80	10	2
1	B	284	PHE	CA-CB-CG	-5.38	108.42	113.80	10	2
1	B	253	ARG	N-CA-C	-5.27	105.95	112.38	15	4
1	A	253	ARG	N-CA-C	-5.26	105.96	112.38	15	4
1	B	260	SER	N-CA-C	-5.21	106.76	113.01	7	2
1	A	260	SER	N-CA-C	-5.17	106.81	113.01	7	2
1	A	261	GLU	N-CA-C	-5.05	106.80	113.12	7	1
1	B	236	LEU	N-CA-CB	-5.00	102.82	110.33	15	1

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	78±10
1	B	448	436	436	78±10
All	All	18816	18312	18312	3083

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 83.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:238:MET:HE3	1:B:285:ILE:HG21	1.03	1.30	10	2
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:238:MET:HE3	1:A:285:ILE:HG21	0.99	1.30	10	2
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:258:MET:HB2	1:B:259:MET:HE2	0.89	1.42	15	1
1:B:236:LEU:HD12	1:B:236:LEU:O	0.89	1.67	3	2
1:A:258:MET:HB2	1:B:259:MET:HE1	0.88	1.44	16	1
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:258:MET:HB2	1:A:259:MET:HE2	0.88	1.42	15	1
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:238:MET:HE3	1:A:285:ILE:CG2	0.81	2.06	10	2
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:238:MET:HE3	1:B:285:ILE:CG2	0.79	2.06	10	2
1:B:256:THR:HG22	1:B:266:LEU:HD12	0.79	1.51	8	8
1:B:249:LEU:C	1:B:249:LEU:HD22	0.79	2.01	16	1
1:B:249:LEU:HB3	1:B:274:ILE:HD11	0.79	1.54	8	3
1:A:249:LEU:C	1:A:249:LEU:HD22	0.79	2.02	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:246:ARG:O	1:B:249:LEU:HD22	0.79	1.77	14	4
1:A:259:MET:HE1	1:B:258:MET:HG3	0.78	1.54	2	1
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
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:254:LEU:HD12	1:B:254:LEU:C	0.75	2.06	9	2
1:B:256:THR:HG21	1:B:270:ILE:HG13	0.75	1.57	6	5
1:A:249:LEU:HD22	1:A:249:LEU:O	0.75	1.81	16	1
1:A:254:LEU:HD12	1:A:254:LEU:C	0.75	2.06	9	2
1:B:233:ASP:HA	1:B:236:LEU:HD12	0.74	1.58	10	2
1:A:238:MET:CE	1:A:285:ILE:HG21	0.74	2.11	10	2
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:259:MET:HE1	1:B:258:MET:HB2	0.72	1.58	16	1
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: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:A:259:MET:HE1	1:B:258:MET:CG	0.70	2.15	2	1
1:B:249:LEU:CB	1:B:274:ILE:HD11	0.70	2.16	8	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:259:MET:HE3	1:B:259:MET:HB3	0.67	1.66	17	1
1:A:249:LEU:HD13	1:A:274:ILE:HG12	0.66	1.66	13	2
1:A:258:MET:CB	1:A:259:MET:HE2	0.66	2.20	15	1
1:B:259:MET:HB2	1:B:266:LEU:HD11	0.66	1.66	4	3
1:B:258:MET:CB	1:B:259:MET:HE2	0.66	2.20	15	1
1:A:265:TYR:CD1	1:A:266:LEU:N	0.66	2.64	17	4
1:A:258:MET:HG3	1:B:259:MET:HE1	0.66	1.66	2	1
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:249:LEU:HD13	1:A:249:LEU:C	0.66	2.16	16	1
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:249:LEU:HD13	1:B:249:LEU:C	0.64	2.16	16	1
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:A:243:HIS:CD2	1:A:243:HIS:C	0.62	2.78	16	3
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:240:GLY:C	1:B:284:PHE:CZ	0.61	2.77	4	2
1:A:270:ILE:HG13	1:B:252:ILE:HD11	0.61	1.71	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:263:ASP:OD2	1:B:258:MET:HE1	0.61	1.95	9	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: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:B:284:PHE:C	1:B:284:PHE:CD1	0.61	2.79	12	1
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:B:236:LEU:HD12	1:B:236:LEU:C	0.60	2.21	3	1
1:A:283:GLN:O	1:A:287:TYR:CE1	0.60	2.54	13	8
1:A:236:LEU:HD12	1:A:236:LEU:C	0.60	2.21	3	1
1:B:243:HIS:CD2	1:B:243:HIS:C	0.60	2.78	16	3
1:B:283:GLN:O	1:B:287:TYR:CE1	0.60	2.54	13	7
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:A:265:TYR:C	1:A:265:TYR:CD1	0.60	2.78	6	3
1:A:287:TYR:CD1	1:A:287:TYR:C	0.60	2.80	8	6
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:B:287:TYR:C	1:B:287:TYR:CD1	0.60	2.80	8	6
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:B:265:TYR:CD1	1:B:265:TYR:C	0.59	2.78	6	4
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:284:PHE:C	1:A:284:PHE:CD1	0.59	2.79	12	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:265:TYR:CD1	1:A:265:TYR:C	0.58	2.82	17	1
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:B:258:MET:HE3	1:B:259:MET:HE1	0.57	1.76	12	1
1:B:256:THR:O	1:B:260:SER:CB	0.57	2.53	11	3
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:283:GLN:O	1:B:287:TYR:CD1	0.56	2.59	7	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:B:234:ARG:CG	1:B:235:THR:N	0.55	2.69	17	20
1:A:246:ARG:CD	1:A:249:LEU:HD11	0.55	2.31	11	2
1:A:258:MET:HE3	1:A:259:MET:HE1	0.55	1.76	12	1
1:A:259:MET:HE1	1:B:258:MET:CB	0.55	2.29	16	1
1:A:263:ASP:CB	1:A:266:LEU:HD23	0.55	2.32	16	1
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:A:260:SER:OG	1:A:267:ALA:CB	0.55	2.55	12	3
1:B:264:GLY:O	1:B:265:TYR:C	0.55	2.49	14	15
1:A:268:GLU:O	1:A:272:LYS:CG	0.55	2.54	2	1
1:B:285:ILE:O	1:B:286:ASP:C	0.55	2.50	3	3
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:A:259:MET:HA	1:A:259:MET:HE2	0.55	1.76	11	2
1:B:259:MET:HA	1:B:259:MET:HE2	0.55	1.77	11	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:277:CYS:O	1:B:281:ILE:HG12	0.55	2.02	5	17
1:A:266:LEU:O	1:A:267:ALA:C	0.55	2.50	12	8
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:B:263:ASP:CG	1:B:265:TYR:CZ	0.55	2.85	15	1
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:A:263:ASP:CG	1:A:265:TYR:CZ	0.54	2.85	15	1
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:A:285:ILE:O	1:A:286:ASP:C	0.54	2.50	3	3
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:B:246:ARG:CD	1:B:249:LEU:HD11	0.54	2.31	11	2
1:A:243:HIS:O	1:A:243:HIS:CD2	0.54	2.60	14	1
1:A:252:ILE:O	1:A:256:THR:OG1	0.54	2.25	14	18
1:B:266:LEU:O	1:B:267:ALA:C	0.54	2.50	12	8
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
1:B:232:ASP:O	1:B:236:LEU:CD2	0.54	2.56	12	4
1:B:249:LEU:C	1:B:249:LEU:CD2	0.54	2.74	16	1
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: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:A:264:GLY:O	1:A:265:TYR:C	0.54	2.49	14	15
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:259:MET:CE	1:B:258:MET:CG	0.53	2.86	2	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:254:LEU:C	1:A:254:LEU:CD1	0.52	2.79	9	2
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:B:276:GLU:C	1:B:280:ILE:HD11	0.52	2.30	16	6
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:A:270:ILE:O	1:A:271:ASN:C	0.52	2.53	15	20
1:B:263:ASP:O	1:B:264:GLY:C	0.52	2.53	12	17
1:A:236:LEU:C	1:A:236:LEU:CD1	0.52	2.83	3	1
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:A:263:ASP:O	1:A:264:GLY:C	0.51	2.54	1	17
1:A:248:PRO:O	1:A:249:LEU:C	0.51	2.53	11	8
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:B:240:GLY:O	1:B:244:ASP:CG	0.51	2.54	11	2
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
1:A:254:LEU:HA	1:A:257:GLU:HB3	0.51	1.82	9	18
1:B:270:ILE:O	1:B:271:ASN:C	0.51	2.52	3	21
1:A:258:MET:CB	1:B:259:MET:HE1	0.51	2.27	16	1
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:240:GLY:O	1:A:244:ASP:CG	0.51	2.54	11	2
1:A:263:ASP:CG	1:A:265:TYR:OH	0.51	2.54	16	1
1:A:238:MET:O	1:A:242:SER:CB	0.51	2.59	8	6
1:A:276:GLU:C	1:A:280:ILE:HD11	0.51	2.31	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:279:ALA:C	1:A:280:ILE:HD13	0.50	2.30	12	1
1:B:263:ASP:CG	1:B:265:TYR:OH	0.50	2.54	16	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:A:262:GLN:O	1:A:263:ASP:CG	0.50	2.55	12	3
1:B:260:SER:CA	1:B:264:GLY:HA2	0.50	2.36	12	19
1:A:259:MET:O	1:A:266:LEU:HD21	0.50	2.07	4	2
1:B:259:MET:C	1:B:266:LEU:HD21	0.50	2.32	4	1
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:242:SER:O	1:B:243:HIS:C	0.50	2.55	1	3
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:244:ASP:O	1:B:248:PRO:HD3	0.50	2.07	2	5
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:A:284:PHE:CZ	1:B:240:GLY:C	0.50	2.90	16	2
1:B:234:ARG:HG3	1:B:235:THR:N	0.49	2.20	17	11
1:B:258:MET:HG2	1:B:259:MET:N	0.49	2.22	2	1
1:A:239:ALA:C	1:A:243:HIS:HB2	0.49	2.32	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:254:LEU:C	1:B:254:LEU:CD1	0.49	2.79	9	2
1:B:262:GLN:O	1:B:263:ASP:CG	0.49	2.55	12	3
1:A:259:MET:HG3	1:B:259:MET:CG	0.49	2.37	12	1
1:A:246:ARG:C	1:A:248:PRO:HD2	0.49	2.33	14	16
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: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: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:259:MET:C	1:A:266:LEU:HD21	0.49	2.32	4	1
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:242:SER:O	1:A:243:HIS:C	0.49	2.55	1	3
1:A:276:GLU:O	1:A:280:ILE:HG12	0.49	2.08	7	12
1:B:239:ALA:C	1:B:243:HIS:HB2	0.49	2.32	9	3
1:A:284:PHE:O	1:A:284:PHE:CD1	0.49	2.66	1	1
1:B:245:LEU:C	1:B:248:PRO:HD2	0.49	2.33	10	14
1:B:248:PRO:O	1:B:249:LEU:C	0.49	2.53	11	8
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:B:246:ARG:C	1:B:248:PRO:HD2	0.48	2.33	14	16
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
1:B:249:LEU:HB3	1:B:274:ILE:CD1	0.48	2.34	8	3
1:A:276:GLU:O	1:A:277:CYS:C	0.48	2.56	15	6
1:B:260:SER:OG	1:B:267:ALA:HB2	0.48	2.07	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:LEU:HD11	1:B:287:TYR:OH	0.48	2.07	8	2
1:B:276:GLU:O	1:B:277:CYS:C	0.48	2.55	16	6
1:A:241:VAL:O	1:A:242:SER:C	0.48	2.56	4	9
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:260:SER:C	1:B:264:GLY:HA2	0.48	2.34	16	9
1:A:260:SER:C	1:A:264:GLY:HA2	0.48	2.34	16	7
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:A:245:LEU:C	1:A:248:PRO:HD2	0.48	2.33	10	13
1:B:250:THR:HA	1:B:253:ARG:HB2	0.48	1.85	5	13
1:B:268:GLU:O	1:B:269:SER:C	0.48	2.56	7	7
1:B:265:TYR:O	1:B:266:LEU:C	0.48	2.57	14	3
1:B:279:ALA:C	1:B:280:ILE:HD13	0.48	2.31	12	1
1:A:249:LEU:C	1:A:249:LEU:CD2	0.48	2.74	16	1
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:265:TYR:O	1:A:266:LEU:C	0.48	2.57	9	3
1:B:241:VAL:O	1:B:242:SER:C	0.48	2.56	4	9
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:A:262:GLN:O	1:A:262:GLN:CD	0.48	2.57	15	1
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:B:270:ILE:C	1:B:272:LYS:N	0.47	2.72	3	9
1:A:268:GLU:O	1:A:269:SER:C	0.47	2.56	7	7
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:261:GLU:O	1:A:262:GLN:C	0.47	2.57	2	4
1:A:273:ASP:O	1:A:276:GLU:HG3	0.47	2.09	13	2
1:B:241:VAL:O	1:B:244:ASP:CG	0.47	2.57	7	1
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:A:270:ILE:HG12	1:B:252:ILE:CG1	0.47	2.40	13	2
1:B:256:THR:O	1:B:257:GLU:C	0.47	2.57	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:LEU:O	1:A:253:ARG:HB2	0.47	2.09	6	13
1:B:261:GLU:O	1:B:262:GLN:C	0.47	2.57	2	2
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:275:GLU:C	1:A:275:GLU:OE1	0.47	2.57	9	2
1:B:277:CYS:C	1:B:280:ILE:HG12	0.47	2.34	12	1
1:B:275:GLU:OE1	1:B:275:GLU:C	0.47	2.57	9	2
1:A:259:MET:HB3	1:B:259:MET:HG3	0.47	1.85	15	1
1:A:263:ASP:CG	1:A:265:TYR:CE2	0.47	2.93	15	1
1:B:277:CYS:O	1:B:280:ILE:CD1	0.47	2.63	4	6
1:A:258:MET:CG	1:B:259:MET:HE1	0.47	2.39	2	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:262:GLN:CD	1:B:262:GLN:O	0.47	2.57	15	1
1:B:239:ALA:O	1:B:243:HIS:HB2	0.47	2.10	5	3
1:B:272:LYS:O	1:B:273:ASP:C	0.47	2.58	5	10
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:277:CYS:C	1:A:280:ILE:HG12	0.47	2.34	12	1
1:A:252:ILE:CD1	1:A:255:ALA:HB3	0.47	2.37	2	1
1:A:270:ILE:HG22	1:A:271:ASN:N	0.47	2.24	11	3
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:A:241:VAL:O	1:A:244:ASP:CG	0.46	2.57	7	1
1:B:249:LEU:CG	1:B:274:ILE:HD11	0.46	2.40	7	1
1:B:270:ILE:HG22	1:B:271:ASN:N	0.46	2.24	11	3
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:A:274:ILE:O	1:A:275:GLU:C	0.46	2.59	9	9
1:B:272:LYS:O	1:B:275:GLU:HG3	0.46	2.10	8	2
1:B:240:GLY:O	1:B:244:ASP:OD2	0.46	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	3
1:B:263:ASP:CG	1:B:265:TYR:CE2	0.46	2.93	15	1
1:A:239:ALA:O	1:A:243:HIS:HB2	0.46	2.10	5	3
1:B:272:LYS:C	1:B:274:ILE:N	0.46	2.72	8	4
1:B:274:ILE:O	1:B:275:GLU:C	0.46	2.59	9	9
1:A:252:ILE:CD1	1:B:270:ILE:HG13	0.46	2.40	11	2
1:B:284:PHE:CD1	1:B:284:PHE:C	0.46	2.94	1	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:A:262:GLN:OE1	1:B:259:MET:HE1	0.46	2.09	8	2
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
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:A:249:LEU:CG	1:A:274:ILE:HD11	0.46	2.40	7	1
1:B:259:MET:HE2	1:B:262:GLN:CB	0.46	2.41	9	2
1:A:249:LEU:CD1	1:A:274:ILE:HG12	0.46	2.40	12	1
1:A:238:MET:C	1:A:240:GLY:N	0.46	2.73	14	4
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:A:259:MET:HE1	1:B:262:GLN:OE1	0.46	2.10	8	2
1:A:256:THR:O	1:A:257:GLU:C	0.46	2.57	13	2
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: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:A:277:CYS:C	1:A:280:ILE:HG13	0.46	2.36	10	6
1:B:251:ARG:O	1:B:254:LEU:HG	0.46	2.11	9	2
1:A:245:LEU:N	1:A:245:LEU:HD22	0.46	2.26	17	2
1:A:270:ILE:C	1:A:272:LYS:N	0.46	2.72	3	9
1:B:262:GLN:O	1:B: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: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: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: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:272:LYS:C	1:A:274:ILE:N	0.45	2.72	8	4
1:A:270:ILE:HG13	1:B:252:ILE:HG13	0.45	1.88	11	2
1:B:278:ASN:C	1:B:280:ILE:N	0.45	2.71	12	1
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:A:259:MET:HE2	1:A:262:GLN:CB	0.45	2.41	9	2
1:A:278:ASN:C	1:A:280:ILE:N	0.45	2.71	12	1
1:B:277:CYS:C	1:B:280:ILE:HG13	0.45	2.36	10	6
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
1:A:269:SER:C	1:A:272:LYS:HG3	0.45	2.37	2	1
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: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:B:278:ASN:O	1:B:279:ALA:C	0.45	2.59	12	1
1:B:269:SER:C	1:B:272:LYS:HG3	0.45	2.37	2	1
1:A:271:ASN:ND2	1:A:271:ASN:N	0.45	2.63	8	2
1:A:238:MET:O	1:A:242:SER:OG	0.45	2.34	11	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:A:284:PHE:CD1	1:A:284:PHE:C	0.45	2.94	1	1
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:259:MET:SD	1:B:259:MET:HG3	0.45	2.52	7	1
1:B:256:THR:CG2	1:B:270:ILE:CD1	0.45	2.89	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:LEU:O	1:A:253:ARG:N	0.45	2.50	17	2
1:A:278:ASN:O	1:A:279:ALA:C	0.45	2.59	12	1
1:B:259:MET:HB3	1:B:266:LEU:CD1	0.45	2.42	9	4
1:A:272:LYS:O	1:A:273:ASP:C	0.45	2.60	9	10
1:B:239:ALA:HA	1:B:243:HIS:CG	0.45	2.47	5	1
1:B:275:GLU:CD	1:B:275:GLU:C	0.45	2.85	8	2
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: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:B:238:MET:O	1:B:242:SER:HB3	0.44	2.12	11	2
1:A:259:MET:HG3	1:B:259:MET:HG3	0.44	1.88	12	2
1:A:251:ARG:O	1:A:254:LEU:HG	0.44	2.11	9	2
1:A:272:LYS:C	1:A:272:LYS:HD3	0.44	2.37	2	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: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:CG	1:B:248:PRO:CB	0.44	2.90	17	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:MET:CE	1:B:258:MET:HG3	0.44	2.37	2	1
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:B:274:ILE:O	1:B:277:CYS:HB3	0.44	2.13	11	2
1:A:259:MET:HE3	1:B:263:ASP:HB2	0.43	1.90	4	1
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
1:A:277:CYS:HA	1:A:280:ILE:HG12	0.43	1.90	6	1
1:A:275:GLU:C	1:A:275:GLU:CD	0.43	2.85	8	2
1:A:252:ILE:HG22	1:A:270:ILE:HG21	0.43	1.89	9	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: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:259:MET:HE3	1:B:259:MET:HG3	0.43	1.90	2	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: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:A:250:THR:O	1:A:253:ARG:HG2	0.43	2.13	15	1
1:A:249:LEU:C	1:A:249:LEU:CD1	0.43	2.85	16	1
1:A:232:ASP:O	1:A:236:LEU:HB3	0.43	2.14	9	6
1:B:272:LYS:HD3	1:B:272:LYS:C	0.43	2.37	2	1
1:B:271:ASN:O	1:B:274:ILE:HB	0.43	2.13	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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
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:B:238:MET:C	1:B:238:MET:SD	0.43	3.02	16	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:A:263:ASP:C	1:A:265:TYR:N	0.43	2.76	1	8
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:275:GLU:OE1	1:A:275:GLU:CA	0.43	2.66	9	2
1:A:276:GLU:O	1:A:280:ILE:HG13	0.43	2.13	9	2
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: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:B:249:LEU:HD12	1:B:249:LEU:C	0.43	2.39	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:238:MET:SD	1:A:238:MET:C	0.42	3.02	16	1
1:B:263:ASP:HB2	1:B:266:LEU:HD23	0.42	1.90	16	1
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:259:MET:HE2	1:B:262:GLN:HB2	0.42	1.90	9	2
1:B:284:PHE:HA	1:B:287:TYR:OH	0.42	2.14	11	3
1:A:249:LEU:C	1:A:249:LEU:HD12	0.42	2.39	15	1
1:A:252:ILE:C	1:A:254:LEU:N	0.42	2.75	15	1
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:277:CYS:O	1:B:280:ILE:CG1	0.42	2.67	1	1
1:B:238:MET:C	1:B:240:GLY:N	0.42	2.75	4	5
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: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: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:263:ASP:C	1:B:265:TYR:N	0.42	2.76	1	6
1:B:266:LEU:CG	1:B:267:ALA:N	0.42	2.82	13	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:262:GLN:HB3	1:B:259:MET:HE1	0.42	1.91	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:B:272:LYS:HD2	1:B:272:LYS:C	0.42	2.40	10	2
1:A:284:PHE:C	1:A:286:ASP:N	0.42	2.77	11	2
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:252:ILE:C	1:B:254:LEU:N	0.42	2.75	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:B:245:LEU:CD2	1:B:277:CYS:SG	0.42	3.08	16	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
1:A:276:GLU:O	1:A:280:ILE:HD11	0.42	2.14	12	1
1:B:266:LEU:HD12	1:B:266:LEU:C	0.42	2.38	17	1
1:B:260:SER:HA	1:B:266:LEU:HD11	0.41	1.92	6	1
1:B:276:GLU:O	1:B:280:ILE:HD11	0.41	2.15	8	3
1:B:272:LYS:C	1:B:272:LYS:CD	0.41	2.92	10	2
1:B:284:PHE:C	1:B:286:ASP:N	0.41	2.77	11	2
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:A:259:MET:HE2	1:A:262:GLN:HB2	0.41	1.90	9	2
1:B:266:LEU:O	1:B:269:SER:N	0.41	2.53	12	1
1:A:243:HIS:C	1:A:243:HIS:CD2	0.41	2.98	1	1
1:B:241:VAL:C	1:B:243:HIS:N	0.41	2.78	4	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:268:GLU:C	1:B:270:ILE:N	0.41	2.78	12	1
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:243:HIS:CD2	1:A:243:HIS:O	0.41	2.74	1	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:248:PRO:C	1:B:250:THR:N	0.41	2.77	6	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:B:284:PHE:O	1:B:285:ILE:C	0.41	2.64	11	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:280:ILE:HA	1:B:283:GLN:CD	0.41	2.41	7	1
1:B:275:GLU:HG3	1:B:276:GLU:N	0.41	2.30	9	2
1:A:272:LYS:CD	1:A:272:LYS:C	0.41	2.92	10	2
1:A:284:PHE:CG	1:A:287:TYR:OH	0.41	2.71	11	2
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:244:ASP:O	1:B:247:THR:HG22	0.41	2.16	14	1
1:B:284:PHE:HD2	1:B:287:TYR:HH	0.41	1.55	15	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:B:269:SER:O	1:B:273:ASP:CG	0.41	2.64	8	2
1:A:254:LEU:HA	1:A:257:GLU:CB	0.41	2.45	9	2
1:A:272:LYS:C	1:A:272:LYS:HD2	0.41	2.40	10	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:241:VAL:C	1:A:243:HIS:N	0.41	2.78	4	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:B:262:GLN:N	1:B:262:GLN:CD	0.40	2.79	1	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:248:PRO:C	1:A:250:THR:N	0.40	2.77	6	3
1:A:265:TYR:N	1:A:265:TYR:CD1	0.40	2.87	9	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:250:THR:CA	1:B:253:ARG:HB2	0.40	2.47	6	1
1:A:280:ILE:HA	1:A:283:GLN:CD	0.40	2.40	7	1
1:A:269:SER:O	1:A:273:ASP:CG	0.40	2.64	8	2
1:B:258:MET:HG3	1:B:259:MET:SD	0.40	2.56	12	1
1:A:256:THR:C	1:A:258:MET:N	0.40	2.77	13	1
1:B:268:GLU:O	1:B:272:LYS:HB2	0.40	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:263:ASP:O	1:A:263:ASP:CG	0.40	2.65	6	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:268:GLU:O	1:A:272:LYS:HB2	0.40	2.17	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

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%)	3	28
1	B	56/67 (84%)	46±2 (83±3%)	7±2 (13±3%)	2±1 (4±2%)	3	28
All	All	2352/2814 (84%)	1946 (83%)	306 (13%)	100 (4%)	3	28

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

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Mol	Chain	Res	Type	Models (Total)
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 ⓘ

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%)	33±4 (66±7%)	17±4 (34±7%)	1	11
1	B	50/57 (88%)	33±4 (66±7%)	17±4 (34±7%)	1	11
All	All	2100/2394 (88%)	1390 (66%)	710 (34%)	1	11

All 84 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	A	252	ILE	21
1	A	280	ILE	21
1	B	237	LEU	21
1	B	252	ILE	21
1	B	280	ILE	21
1	A	241	VAL	20
1	B	241	VAL	20
1	A	256	THR	19
1	B	256	THR	19
1	A	274	ILE	16
1	B	274	ILE	16
1	A	253	ARG	15
1	B	253	ARG	15
1	A	249	LEU	13
1	A	258	MET	13

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Mol	Chain	Res	Type	Models (Total)
1	B	249	LEU	13
1	B	258	MET	13
1	A	276	GLU	12
1	B	276	GLU	12
1	A	259	MET	11
1	B	259	MET	11
1	A	242	SER	10
1	B	242	SER	10
1	A	233	ASP	10
1	B	233	ASP	10
1	A	245	LEU	9
1	A	269	SER	9
1	B	245	LEU	9
1	B	269	SER	9
1	A	236	LEU	8
1	A	246	ARG	8
1	B	236	LEU	8
1	B	246	ARG	8
1	A	251	ARG	8
1	B	251	ARG	8
1	A	275	GLU	8
1	B	275	GLU	8
1	A	238	MET	7
1	A	266	LEU	7
1	B	238	MET	7
1	B	266	LEU	7
1	A	262	GLN	7
1	A	272	LYS	7
1	B	262	GLN	7
1	B	272	LYS	7
1	A	243	HIS	7
1	B	243	HIS	7
1	A	232	ASP	6
1	A	257	GLU	6
1	A	277	CYS	6
1	B	232	ASP	6
1	B	257	GLU	6
1	B	277	CYS	6
1	A	268	GLU	6
1	B	268	GLU	6
1	A	261	GLU	6
1	A	282	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	286	ASP	6
1	B	261	GLU	6
1	B	282	GLU	6
1	B	286	ASP	6
1	A	287	TYR	4
1	B	287	TYR	4
1	A	234	ARG	3
1	B	234	ARG	3
1	A	270	ILE	3
1	A	283	GLN	3
1	A	285	ILE	3
1	B	270	ILE	3
1	B	283	GLN	3
1	B	285	ILE	3
1	A	278	ASN	3
1	B	278	ASN	3
1	A	263	ASP	2
1	A	273	ASP	2
1	B	263	ASP	2
1	B	273	ASP	2
1	A	284	PHE	1
1	B	284	PHE	1
1	A	244	ASP	1
1	B	244	ASP	1
1	A	260	SER	1
1	B	260	SER	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 oligosaccharides 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