



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:31 AM UTC

PDB ID : 1BUQ / pdb_00001buq
Title : SOLUTION STRUCTURE OF DELTA-5-3-KETOSTEROID ISOMERASE
COMPLEXED WITH THE STEROID 19-NORTESTOSTERONE-HEMISU
CCINATE
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Deposited on : 1998-09-04

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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

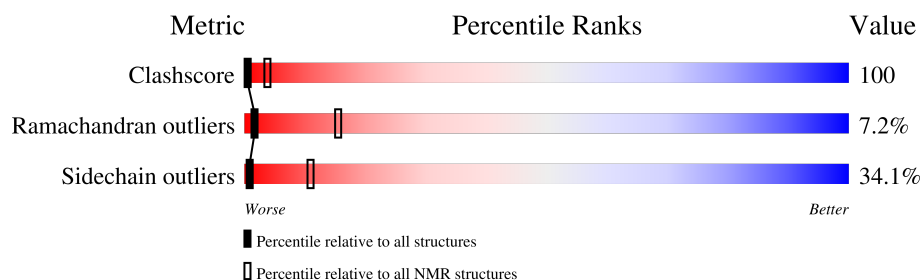
1 Overall quality at a glance

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	125	
1	B	125	

2 Ensemble composition and analysis

This entry contains 15 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:3-A:125, B:201-B:323 (246)	1.44	5

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 6, 7, 9, 10, 11, 12, 14
2	3, 8, 13
Single-model clusters	15

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3858 atoms, of which 1918 are hydrogens and 0 are deuteriums.

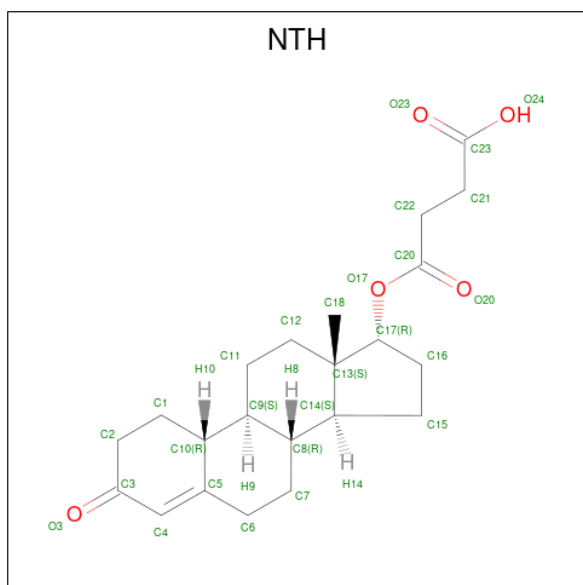
- Molecule 1 is a protein called PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMISUCCINATE).

Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			1873	597	930	165	178	3	
1	B	125	Total	C	H	N	O	S	0
			1873	597	930	165	178	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	PHE	TYR	engineered mutation	UNP P00947
A	88	PHE	TYR	engineered mutation	UNP P00947
B	255	PHE	TYR	engineered mutation	UNP P00947
B	288	PHE	TYR	engineered mutation	UNP P00947

- Molecule 2 is SUCCINIC ACID MONO-(13-METHYL-3-OXO-2,3,6,7,8,9,10,11,12,13,14,15,16,17-TETRADECAHYDRO-1H-CYCLOPENTA[A]PHENANTHREN-17-YL) ESTER (CCD ID: NTH) (formula: $C_{22}H_{30}O_5$).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	O
			56	22	29	5

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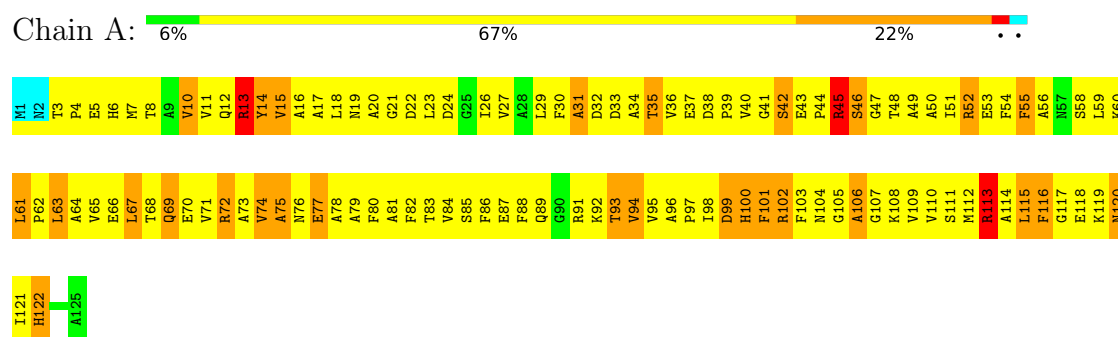
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	B	1	56	22	29	5

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 (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



4.2 Scores per residue for each member of the ensemble

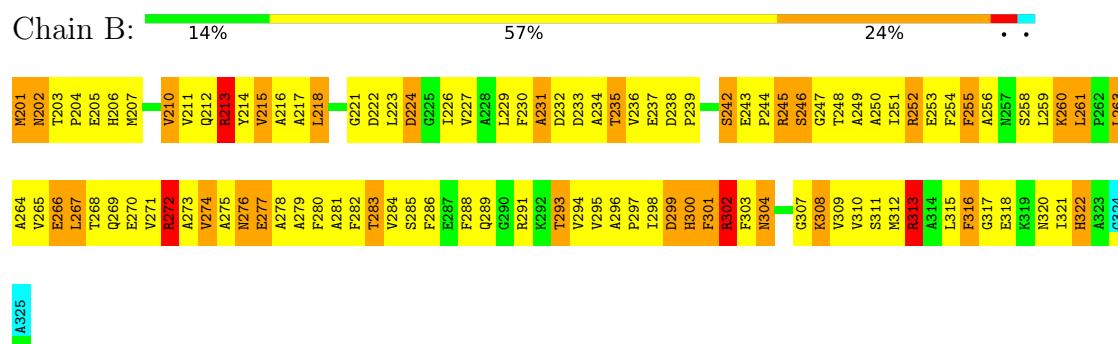
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

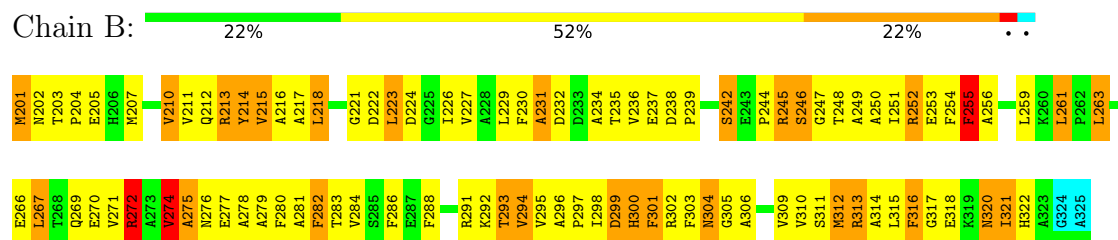


4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

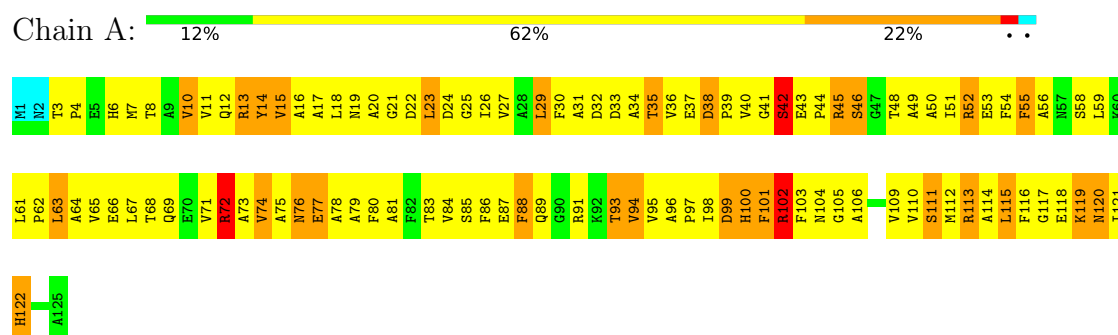


- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

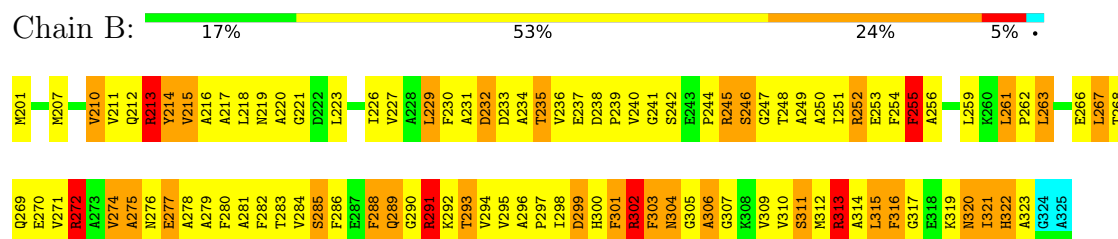


4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

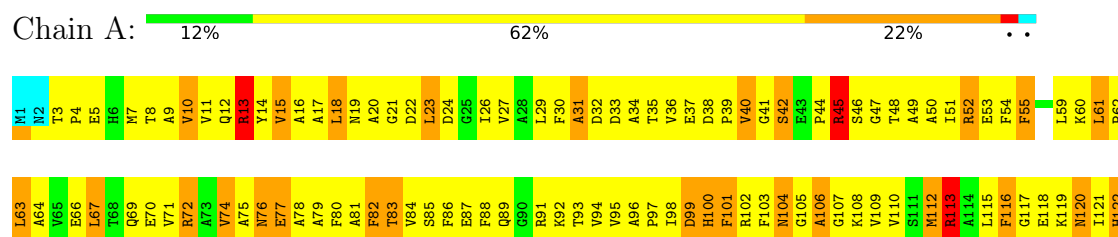


- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)





- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain B: 15% 58% 20% 5%



4.2.5 Score per residue for model 5 (medoid)

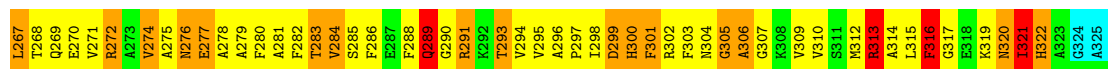
- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 20% 50% 25% 5%



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain B: 18% 52% 24% 5%



4.2.6 Score per residue for model 6

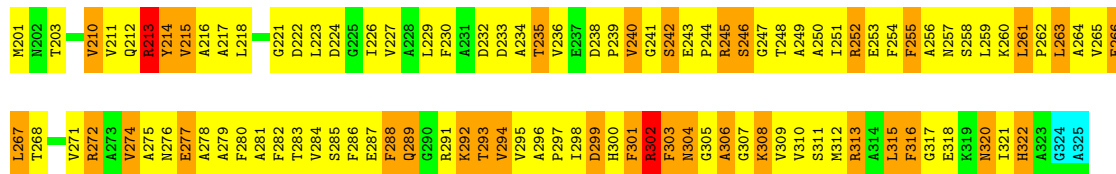
- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 18% 47% 29% 5%



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain B: 16% 54% 26% . .



4.2.7 Score per residue for model 7

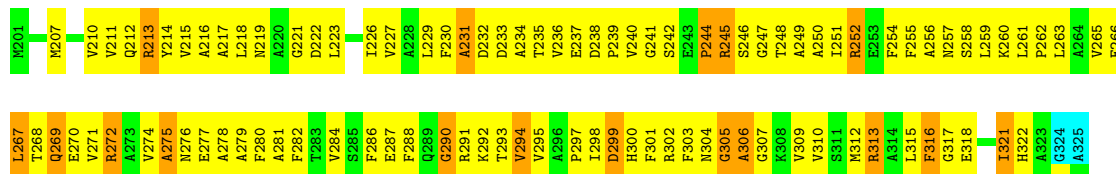
- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 21% 65% 13% .



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

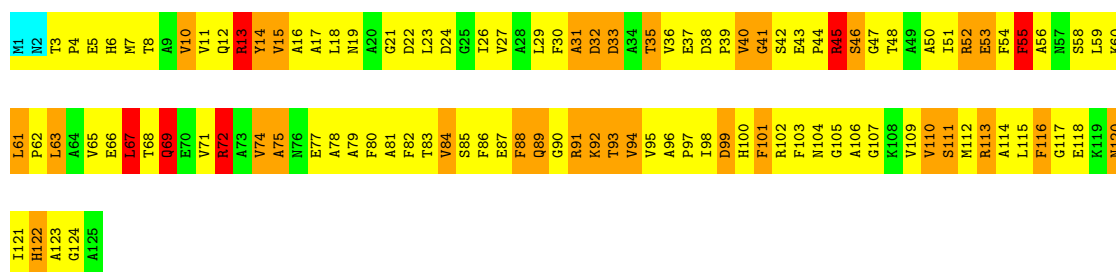
Chain B: 21% 64% 14% .



4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 11% 58% 25% 5% .



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

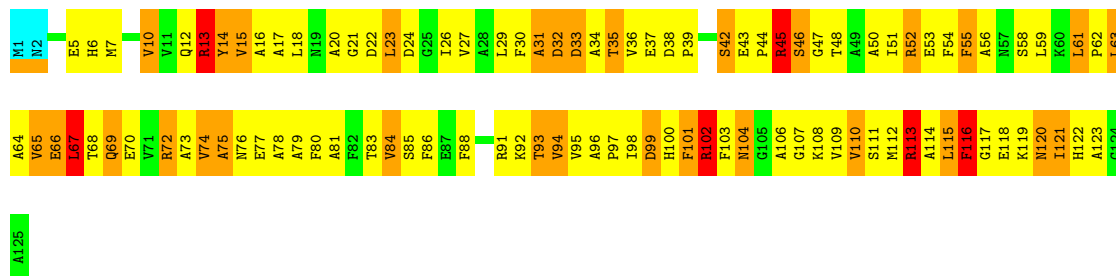
Chain B: 18% 54% 22% 5%



4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 17% 53% 24% 5%



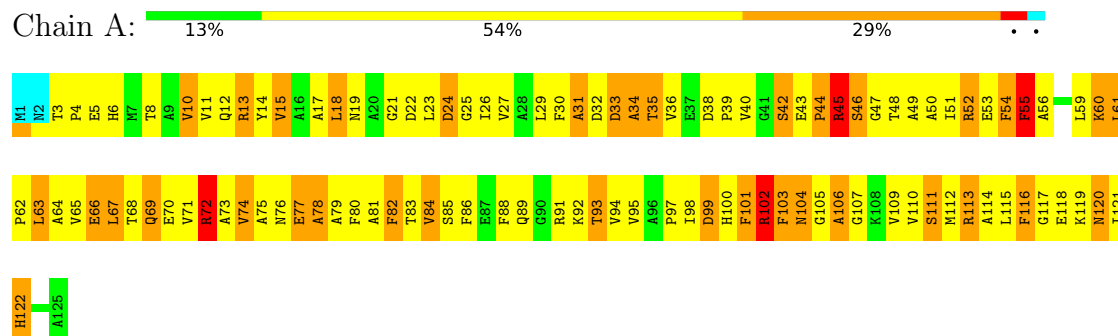
- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain B: 14% 52% 30% . .



4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

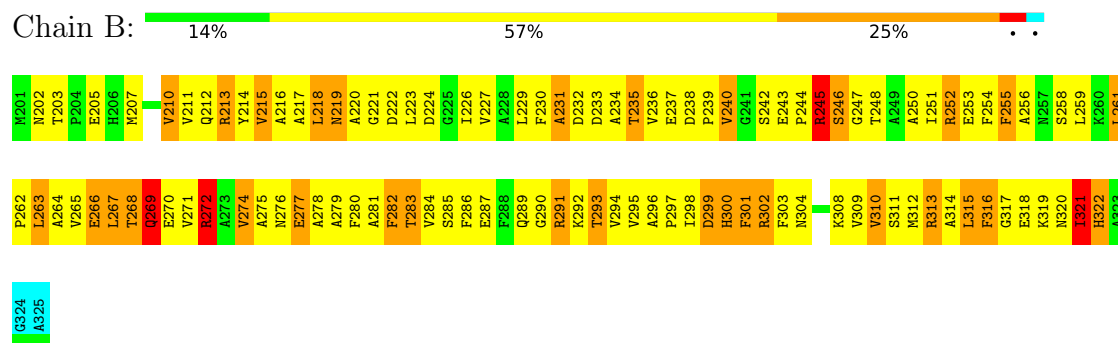


4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

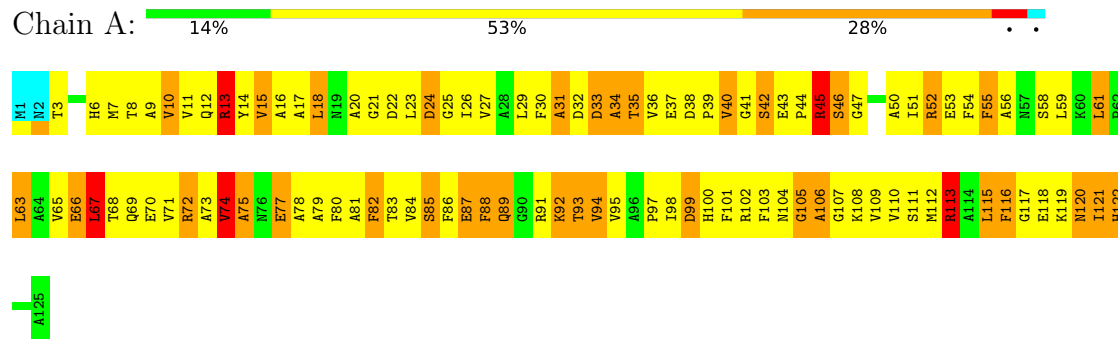


- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

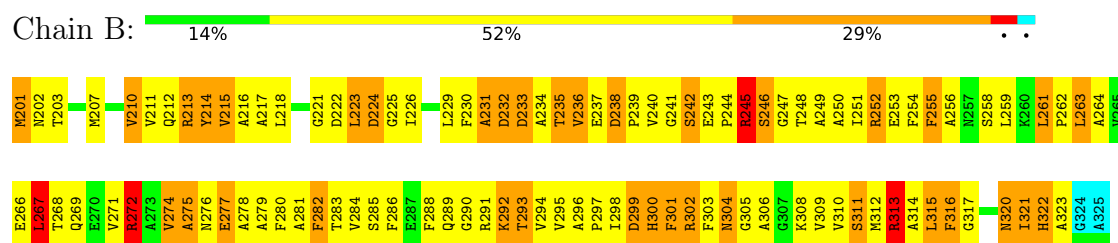


4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

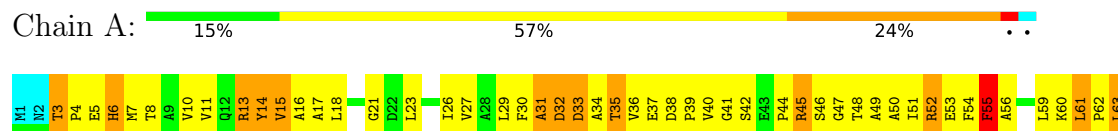


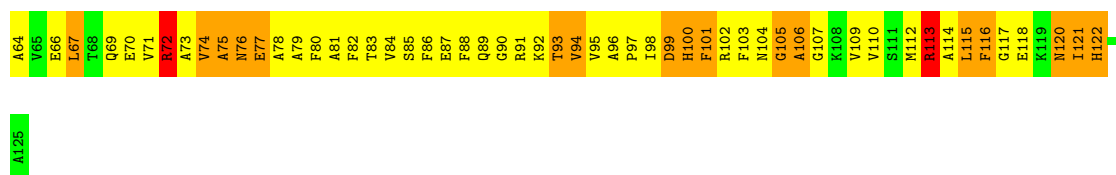
- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



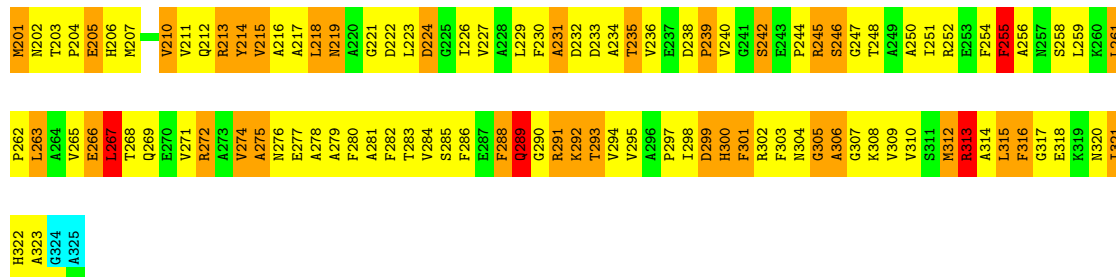
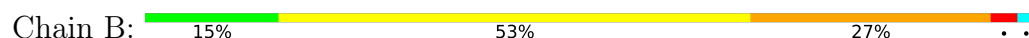
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)



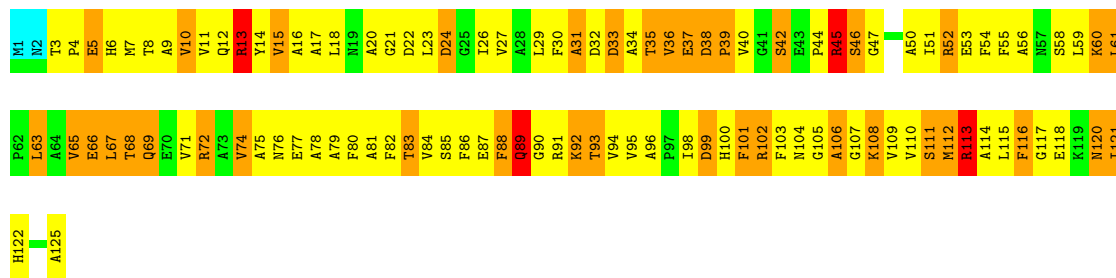
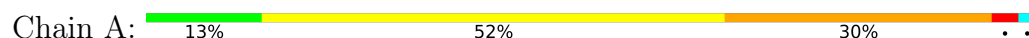


- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMISUCCINATE)

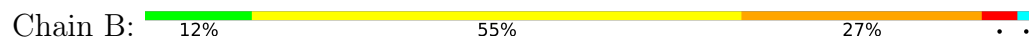


4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMISUCCINATE)



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMISUCCINATE)



4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain A: 8% 58% 28% 5% •



- Molecule 1: PROTEIN (3-KETOSTEROID ISOMERASE-19-NORTESTOSTERONE-HEMIS UCCINATE)

Chain B: 14% 58% 25% • •



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING AND REFINEMENT CALCULATIONS*.

Of the 120 calculated structures, 15 were deposited, based on the following criterion: *NOE VIOLATION = < 0.35Å AND DIHEDRAL VIOLATION < 5 DEG..*

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

Software name	Classification	Version
X-PLOR	refinement	3.8
X-PLOR	structure solution	3.8

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NTH

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	1.46±0.01	1±0/945 (0.1± 0.0%)	1.26±0.01	0±1/1281 (0.0± 0.0%)
1	B	1.46±0.01	1±0/952 (0.1± 0.0%)	1.27±0.02	1±0/1293 (0.0± 0.0%)
All	All	1.46	31/28455 (0.1%)	1.27	15/38610 (0.0%)

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	6.8±0.5
1	B	0.0±0.0	6.7±0.4
All	All	0	203

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	A	99	ASP	CG-OD2	7.03	1.38	1.25	7	15
1	B	299	ASP	CG-OD2	7.01	1.38	1.25	10	15
1	A	42	SER	N-CA	5.12	1.49	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	B	255	PHE	CA-CB-CG	-5.50	108.30	113.80	5	8
1	A	55	PHE	CA-CB-CG	-5.46	108.34	113.80	10	5
1	A	75	ALA	CB-CA-C	-5.44	109.31	115.79	6	2

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	52	ARG	Sidechain	15
1	A	91	ARG	Sidechain	15
1	A	102	ARG	Sidechain	15
1	A	113	ARG	Sidechain	15
1	B	213	ARG	Sidechain	15
1	B	245	ARG	Sidechain	15
1	B	291	ARG	Sidechain	15
1	B	302	ARG	Sidechain	15
1	A	13	ARG	Sidechain	14
1	A	45	ARG	Sidechain	14
1	A	72	ARG	Sidechain	14
1	B	252	ARG	Sidechain	14
1	B	272	ARG	Sidechain	14
1	B	313	ARG	Sidechain	13

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	927	913	912	200±13
1	B	933	922	918	196±13
2	A	27	29	28	6±2
2	B	27	29	28	6±3
All	All	28710	28395	28290	5672

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 100.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:LEU:HD23	1:B:263:LEU:HD21	1.12	1.15	13	1
1:B:295:VAL:HG22	1:B:321:ILE:HG23	1.11	1.18	3	10
1:B:261:LEU:HD21	1:B:263:LEU:HD21	1.03	1.21	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD13	1:A:84:VAL:HG13	1.03	1.23	14	1
1:A:74:VAL:HG11	1:B:240:VAL:HG21	1.03	1.28	5	3
1:A:79:ALA:HB2	1:B:315:LEU:HD11	1.02	1.26	9	5
1:B:281:ALA:HB2	1:B:298:ILE:HG23	1.02	1.26	14	11
1:A:95:VAL:HG22	1:A:121:ILE:HG23	1.01	1.31	9	12
1:A:75:ALA:HB3	1:B:240:VAL:HG12	1.00	1.29	10	2
1:B:261:LEU:HD22	2:B:326:NTH:H121	0.99	1.26	8	1
1:A:45:ARG:CG	1:A:50:ALA:HB1	0.99	1.88	2	6
1:A:81:ALA:HB2	1:A:98:ILE:HG23	0.98	1.33	7	14
1:B:211:VAL:HG11	1:B:271:VAL:HG21	0.98	1.29	15	13
1:A:23:LEU:CD2	1:A:59:LEU:HD22	0.98	1.88	10	7
1:B:230:PHE:CE1	1:B:312:MET:HE1	0.98	1.94	2	1
1:A:61:LEU:HD22	1:A:63:LEU:HD21	0.98	1.31	10	9
1:A:14:TYR:CE1	1:A:18:LEU:HD11	0.98	1.94	7	15
1:A:21:GLY:CA	1:A:59:LEU:HD21	0.97	1.89	10	15
1:A:115:LEU:HD22	1:B:279:ALA:HB3	0.97	1.36	2	6
1:A:74:VAL:HG11	1:B:316:PHE:O	0.97	1.60	15	10
1:A:101:PHE:CE1	1:A:112:MET:HE2	0.96	1.95	10	4
1:A:61:LEU:CD2	1:A:63:LEU:HD21	0.96	1.90	6	4
1:B:221:GLY:CA	1:B:259:LEU:HD21	0.96	1.91	15	13
1:B:223:LEU:CD2	1:B:259:LEU:HD22	0.96	1.89	15	6
1:A:61:LEU:HD21	1:A:63:LEU:CD2	0.96	1.90	6	1
1:B:281:ALA:CB	1:B:298:ILE:HD12	0.95	1.90	11	1
1:B:223:LEU:HD12	1:B:226:ILE:HD12	0.95	1.37	13	9
1:A:23:LEU:HD11	1:A:55:PHE:HB3	0.94	1.39	14	8
1:B:281:ALA:HB1	1:B:298:ILE:HD12	0.94	1.38	11	1
1:A:63:LEU:HD22	1:A:84:VAL:CG1	0.94	1.92	3	5
1:B:214:TYR:CE2	1:B:312:MET:HE1	0.94	1.98	15	1
1:B:309:VAL:HG11	1:B:312:MET:CE	0.94	1.92	9	2
1:A:61:LEU:HD21	1:A:63:LEU:HD21	0.93	0.96	6	2
1:B:211:VAL:HG21	1:B:271:VAL:HG11	0.93	1.40	15	8
1:A:23:LEU:HD12	1:A:26:ILE:HD12	0.93	1.36	14	6
1:B:210:VAL:HA	1:B:229:LEU:HD21	0.93	1.41	12	15
1:B:215:VAL:HG11	1:B:267:LEU:HD11	0.93	1.38	8	2
1:A:40:VAL:HG21	1:B:274:VAL:HG11	0.92	1.39	5	3
1:B:297:PRO:O	1:B:298:ILE:HD13	0.92	1.64	11	1
1:B:261:LEU:HD22	1:B:263:LEU:HD21	0.92	1.40	5	9
1:A:11:VAL:HG11	1:A:71:VAL:HG21	0.92	1.40	15	13
1:A:75:ALA:CB	1:B:240:VAL:HG12	0.92	1.94	10	1
1:B:230:PHE:CD2	1:B:251:ILE:HG21	0.92	2.00	9	7
1:A:78:ALA:HB3	1:A:101:PHE:HB3	0.91	1.42	4	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:223:LEU:HD11	1:B:255:PHE:HB3	0.91	1.41	11	9
1:A:83:THR:HG22	1:A:95:VAL:O	0.91	1.64	14	4
1:B:295:VAL:HG12	1:B:297:PRO:HD3	0.91	1.43	13	15
1:B:226:ILE:HG21	1:B:255:PHE:CG	0.91	2.00	7	1
1:B:263:LEU:HD22	1:B:284:VAL:HG11	0.91	1.43	8	10
1:A:64:ALA:HB3	1:A:85:SER:OG	0.91	1.64	4	10
1:B:297:PRO:C	1:B:298:ILE:HD13	0.90	1.92	11	1
1:B:278:ALA:HB3	1:B:301:PHE:HB3	0.90	1.44	3	9
1:B:211:VAL:HG22	1:B:301:PHE:CE2	0.90	2.02	12	9
1:A:61:LEU:HD13	2:A:126:NTH:H183	0.90	1.40	8	2
1:A:116:PHE:O	1:B:274:VAL:HG11	0.89	1.67	7	10
1:B:245:ARG:HG3	1:B:250:ALA:HB1	0.89	1.44	9	5
1:B:261:LEU:HD22	1:B:263:LEU:CD2	0.89	1.98	10	9
1:A:10:VAL:HA	1:A:29:LEU:HD21	0.89	1.44	14	14
1:A:72:ARG:CG	1:A:79:ALA:HB3	0.89	1.97	9	1
1:B:309:VAL:HG11	1:B:312:MET:HE2	0.89	1.43	9	1
1:B:283:THR:HG22	1:B:295:VAL:O	0.88	1.68	11	4
1:A:34:ALA:HB3	1:A:51:ILE:CD1	0.88	1.99	7	2
1:B:271:VAL:HG13	1:B:280:PHE:HB3	0.88	1.44	4	14
1:A:23:LEU:HD13	1:A:26:ILE:HD12	0.88	1.44	1	6
1:A:45:ARG:HG3	1:A:50:ALA:HB1	0.88	1.45	2	7
1:B:264:ALA:HB3	1:B:285:SER:OG	0.88	1.68	1	9
1:B:223:LEU:HD13	1:B:226:ILE:HD12	0.88	1.46	2	6
1:B:263:LEU:HD13	1:B:284:VAL:HG13	0.88	1.45	1	1
1:A:71:VAL:HG13	1:A:80:PHE:HB3	0.87	1.45	3	10
1:A:95:VAL:HG12	1:A:97:PRO:HD3	0.87	1.45	6	13
1:A:34:ALA:C	1:A:51:ILE:HD11	0.87	1.95	7	2
1:A:34:ALA:N	1:A:51:ILE:HD11	0.87	1.83	5	3
1:B:263:LEU:HD23	1:B:286:PHE:CD1	0.87	2.04	14	5
1:A:34:ALA:O	1:A:51:ILE:HD11	0.87	1.70	7	5
1:B:221:GLY:HA2	1:B:259:LEU:HD21	0.86	1.46	9	10
1:A:26:ILE:HG22	1:A:30:PHE:CE2	0.86	2.05	1	1
1:A:20:ALA:HB3	1:A:22:ASP:OD2	0.86	1.68	4	1
1:A:115:LEU:HD22	1:B:279:ALA:CB	0.86	2.00	10	2
1:B:226:ILE:HD13	1:B:255:PHE:CD1	0.86	2.05	7	3
1:B:235:THR:HG23	1:B:246:SER:HB2	0.85	1.46	11	7
1:B:261:LEU:CD2	1:B:263:LEU:HD21	0.85	2.00	13	7
1:B:295:VAL:HG22	1:B:321:ILE:CG2	0.85	2.02	3	9
1:A:11:VAL:HG22	1:A:101:PHE:CE2	0.85	2.07	6	10
1:A:27:VAL:HG11	1:A:48:THR:HG23	0.84	1.48	10	1
1:A:63:LEU:HD13	1:A:84:VAL:CG1	0.84	2.02	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:215:VAL:CG1	1:B:267:LEU:HD11	0.84	2.02	8	1
1:A:78:ALA:HB3	1:A:101:PHE:CB	0.84	2.02	13	14
1:B:304:ASN:OD1	1:B:310:VAL:HG23	0.84	1.72	6	2
1:A:23:LEU:O	1:A:27:VAL:HG23	0.83	1.72	8	2
1:A:40:VAL:HG13	1:A:116:PHE:CE1	0.83	2.07	3	3
1:A:79:ALA:CB	1:B:315:LEU:HD11	0.83	2.03	9	5
1:A:104:ASN:OD1	1:A:110:VAL:HG23	0.83	1.72	6	3
1:A:63:LEU:HB2	1:A:84:VAL:HG12	0.83	1.47	9	2
1:A:61:LEU:HD22	1:A:63:LEU:CD2	0.83	2.04	8	8
1:A:7:MET:HB3	1:A:73:ALA:HB1	0.83	1.49	13	2
1:A:35:THR:HG23	1:A:46:SER:HB2	0.83	1.47	5	5
1:B:286:PHE:CZ	2:B:326:NTH:H221	0.83	2.09	6	6
1:B:263:LEU:HD23	1:B:286:PHE:CG	0.83	2.09	14	2
1:A:61:LEU:CD1	2:A:126:NTH:H183	0.83	2.04	8	2
1:B:213:ARG:HB3	1:B:229:LEU:HD22	0.83	1.48	7	8
1:B:263:LEU:HD22	1:B:284:VAL:CG1	0.82	2.04	8	7
1:A:13:ARG:HB3	1:A:29:LEU:HD22	0.82	1.48	9	6
1:B:278:ALA:HB3	1:B:301:PHE:CB	0.82	2.04	12	9
1:A:79:ALA:HB2	1:B:315:LEU:HD13	0.82	1.50	13	9
1:B:215:VAL:HA	1:B:218:LEU:HD12	0.82	1.52	7	15
1:B:263:LEU:HD22	1:B:284:VAL:HG12	0.81	1.52	13	2
1:A:95:VAL:HG21	2:A:126:NTH:O20	0.81	1.74	8	1
1:A:79:ALA:HB3	1:B:315:LEU:HD22	0.81	1.49	4	6
1:B:261:LEU:HD21	1:B:263:LEU:CD2	0.81	2.05	8	1
1:A:13:ARG:NH2	1:A:29:LEU:HD11	0.81	1.91	4	2
1:B:245:ARG:CG	1:B:250:ALA:HB1	0.80	2.06	8	8
1:A:30:PHE:CE1	1:A:112:MET:HE1	0.80	2.11	2	2
1:B:234:ALA:O	1:B:251:ILE:HD11	0.80	1.76	10	10
1:B:213:ARG:HD2	1:B:229:LEU:HD13	0.80	1.50	7	4
1:A:23:LEU:HD23	1:A:52:ARG:CG	0.80	2.05	11	7
1:B:286:PHE:CE2	2:B:326:NTH:H221	0.80	2.11	6	3
1:A:18:LEU:HB3	1:A:65:VAL:HG21	0.80	1.52	12	4
1:B:301:PHE:CE1	1:B:309:VAL:HG21	0.80	2.11	6	3
1:A:15:VAL:HA	1:A:18:LEU:HD12	0.79	1.54	5	15
1:A:99:ASP:CG	1:A:112:MET:HE3	0.79	2.02	15	1
1:A:86:PHE:CE1	2:A:126:NTH:H212	0.79	2.12	14	1
1:A:46:SER:O	1:A:50:ALA:HB3	0.79	1.75	14	7
1:A:104:ASN:HB3	1:A:110:VAL:HG21	0.79	1.54	15	9
1:A:21:GLY:HA2	1:A:59:LEU:HD21	0.79	1.52	11	13
1:A:79:ALA:HB2	1:B:315:LEU:CD1	0.79	2.07	12	7
1:A:93:THR:HG22	1:A:122:HIS:O	0.79	1.77	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:THR:HG23	1:B:246:SER:HB3	0.78	1.55	1	4
1:B:261:LEU:HD13	2:B:326:NTH:O17	0.78	1.78	5	4
1:A:63:LEU:HD22	1:A:84:VAL:HG11	0.78	1.54	6	8
1:A:79:ALA:CB	1:B:315:LEU:HD22	0.78	2.08	4	2
1:A:45:ARG:HB3	1:A:50:ALA:HB1	0.78	1.53	15	2
1:B:213:ARG:HD3	1:B:229:LEU:HD13	0.78	1.55	6	2
1:B:263:LEU:HB2	1:B:284:VAL:HG12	0.78	1.56	14	1
1:B:286:PHE:CZ	2:B:326:NTH:H212	0.78	2.13	8	1
1:A:86:PHE:CE2	2:A:126:NTH:H221	0.78	2.14	6	3
1:A:72:ARG:HG2	1:A:79:ALA:HB3	0.78	1.53	9	1
1:A:10:VAL:HG11	1:A:103:PHE:CE1	0.77	2.13	13	3
1:A:61:LEU:HD13	2:A:126:NTH:O17	0.77	1.79	10	3
1:A:40:VAL:HG21	1:B:274:VAL:CG1	0.77	2.10	5	4
1:B:286:PHE:CE1	2:B:326:NTH:H221	0.77	2.13	10	5
1:B:215:VAL:HG11	1:B:267:LEU:CD1	0.77	2.10	8	1
1:A:95:VAL:CG2	1:A:121:ILE:HG23	0.77	2.10	12	6
1:B:246:SER:O	1:B:250:ALA:HB3	0.77	1.79	2	10
1:A:11:VAL:HG11	1:A:71:VAL:CG2	0.77	2.10	12	14
1:B:281:ALA:CB	1:B:298:ILE:HG23	0.76	2.09	14	4
1:A:23:LEU:HD23	1:A:52:ARG:HG3	0.76	1.56	9	7
1:B:263:LEU:CB	1:B:284:VAL:HG13	0.76	2.09	9	10
1:A:27:VAL:CG1	1:A:48:THR:HG23	0.76	2.10	10	3
1:B:267:LEU:HD23	1:B:281:ALA:O	0.76	1.80	10	2
1:B:239:PRO:O	1:B:240:VAL:HG13	0.76	1.81	9	1
1:A:40:VAL:HG11	1:B:274:VAL:HG11	0.76	1.55	2	1
1:A:26:ILE:HG21	1:A:55:PHE:CD1	0.75	2.16	2	3
1:B:261:LEU:HD12	1:B:263:LEU:CG	0.75	2.12	14	1
1:B:223:LEU:HD23	1:B:252:ARG:CG	0.75	2.10	10	9
1:B:231:ALA:HB2	1:B:309:VAL:O	0.75	1.80	14	9
1:B:281:ALA:HB2	1:B:298:ILE:CG2	0.75	2.11	14	7
1:B:236:VAL:HG22	1:B:312:MET:HE2	0.75	1.56	7	2
1:A:79:ALA:HB3	1:B:315:LEU:HD21	0.75	1.55	8	1
1:B:211:VAL:HG11	1:B:271:VAL:CG2	0.75	2.11	12	14
1:A:74:VAL:CG1	1:B:240:VAL:HG21	0.75	2.10	5	3
1:B:234:ALA:N	1:B:251:ILE:HD11	0.75	1.96	1	6
1:B:245:ARG:HB3	1:B:250:ALA:HB1	0.75	1.56	13	4
1:A:81:ALA:CB	1:A:98:ILE:HG23	0.75	2.11	7	6
1:B:227:VAL:HG11	1:B:248:THR:HG23	0.75	1.57	2	5
1:A:63:LEU:HD23	1:A:86:PHE:CD1	0.74	2.17	10	5
1:A:10:VAL:HG11	1:A:103:PHE:CZ	0.74	2.17	13	8
1:A:7:MET:HE1	1:A:103:PHE:CD2	0.74	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:HG22	1:A:101:PHE:CD2	0.74	2.17	6	6
1:A:61:LEU:HB3	1:A:63:LEU:HD11	0.74	1.57	9	2
1:B:210:VAL:HG11	1:B:303:PHE:CE1	0.74	2.17	1	4
1:A:63:LEU:HB3	1:A:84:VAL:HG13	0.74	1.57	7	1
1:B:261:LEU:HD23	1:B:263:LEU:CD2	0.74	2.06	13	3
1:B:309:VAL:HG11	1:B:312:MET:HE1	0.74	1.59	13	2
1:A:63:LEU:CB	1:A:84:VAL:HG13	0.74	2.13	4	6
1:B:223:LEU:HD22	1:B:259:LEU:HD22	0.74	1.58	7	5
1:A:30:PHE:CZ	1:A:112:MET:HE1	0.74	2.18	2	4
1:B:263:LEU:HB2	1:B:284:VAL:HG13	0.74	1.60	8	8
1:A:115:LEU:HD13	1:B:279:ALA:HB2	0.73	1.59	11	11
1:A:14:TYR:CE2	1:A:112:MET:HE1	0.73	2.18	4	2
1:B:210:VAL:CG2	1:B:309:VAL:HG22	0.73	2.13	14	1
1:A:11:VAL:HG21	1:A:71:VAL:CG1	0.73	2.13	13	6
1:A:45:ARG:HG2	1:A:50:ALA:HB1	0.73	1.59	2	1
1:A:38:ASP:OD1	1:A:114:ALA:HB3	0.73	1.83	9	3
1:B:269:GLN:OE1	1:B:281:ALA:HB3	0.73	1.82	11	1
1:A:115:LEU:HD11	1:B:279:ALA:HB2	0.73	1.59	4	1
1:B:261:LEU:CD2	2:B:326:NTH:H121	0.72	2.13	8	1
1:A:11:VAL:HG21	1:A:71:VAL:HG11	0.72	1.61	3	6
1:A:13:ARG:HD2	1:A:29:LEU:HD13	0.72	1.61	4	3
1:B:234:ALA:HB3	1:B:251:ILE:HD13	0.72	1.61	9	1
1:B:223:LEU:HD23	1:B:252:ARG:HG3	0.72	1.61	13	9
1:A:116:PHE:O	1:B:274:VAL:HG21	0.72	1.85	8	8
1:B:263:LEU:HD13	1:B:284:VAL:CG1	0.71	2.14	1	3
1:A:34:ALA:HB3	1:A:51:ILE:HD13	0.71	1.62	7	2
1:A:10:VAL:HG12	1:A:101:PHE:CZ	0.71	2.20	13	10
1:A:31:ALA:HB2	1:A:109:VAL:O	0.71	1.85	10	10
1:A:61:LEU:HD13	2:A:126:NTH:C17	0.71	2.15	12	2
1:A:36:VAL:CG2	1:A:51:ILE:HD12	0.71	2.15	12	5
1:A:61:LEU:HD13	1:A:62:PRO:HD2	0.71	1.61	9	1
1:B:278:ALA:HB3	1:B:301:PHE:HB2	0.71	1.60	4	2
1:A:63:LEU:CB	1:A:84:VAL:HG12	0.71	2.16	9	6
1:A:74:VAL:HG21	1:B:316:PHE:O	0.71	1.86	11	9
1:A:95:VAL:HG13	1:A:120:ASN:ND2	0.71	2.01	11	2
1:A:27:VAL:HG21	1:A:52:ARG:HB2	0.70	1.63	2	6
1:B:293:THR:HG22	1:B:322:HIS:O	0.70	1.86	2	4
1:A:21:GLY:HA3	1:A:59:LEU:HD21	0.70	1.61	10	2
1:B:322:HIS:CD2	2:B:326:NTH:H212	0.70	2.21	13	1
1:A:58:SER:OG	2:A:126:NTH:H11	0.70	1.86	9	7
1:A:116:PHE:CZ	2:A:126:NTH:H62	0.70	2.22	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:PHE:CD2	1:A:51:ILE:HG21	0.70	2.20	8	4
1:B:210:VAL:HG11	1:B:303:PHE:CZ	0.70	2.21	4	11
1:A:94:VAL:HG12	1:A:122:HIS:CG	0.70	2.22	12	5
1:B:317:GLY:C	1:B:321:ILE:HD12	0.70	2.11	3	2
1:B:230:PHE:CG	1:B:251:ILE:HG21	0.70	2.22	4	2
1:B:293:THR:HG23	1:B:323:ALA:HA	0.70	1.61	15	1
1:A:26:ILE:HD13	1:A:55:PHE:CD1	0.70	2.22	2	4
1:A:79:ALA:HB3	1:B:315:LEU:CD2	0.70	2.16	4	3
1:A:80:PHE:CE1	1:A:101:PHE:CD2	0.70	2.80	7	5
1:B:210:VAL:HG21	1:B:309:VAL:HG22	0.70	1.64	14	1
1:A:7:MET:HE3	1:A:74:VAL:O	0.69	1.87	15	2
1:B:258:SER:OG	2:B:326:NTH:H11	0.69	1.86	7	9
1:B:316:PHE:CE2	2:B:326:NTH:H72	0.69	2.22	14	1
1:A:10:VAL:HG21	1:A:103:PHE:CE2	0.69	2.22	12	4
1:B:238:ASP:OD2	2:B:326:NTH:H61	0.69	1.87	13	1
1:B:234:ALA:C	1:B:251:ILE:HD11	0.69	2.12	9	1
1:A:75:ALA:HB2	1:B:240:VAL:O	0.69	1.88	6	1
1:A:40:VAL:HG21	1:B:274:VAL:HB	0.69	1.64	8	2
1:A:115:LEU:HD22	1:B:279:ALA:HB2	0.69	1.62	10	1
1:A:61:LEU:CD1	2:A:126:NTH:H122	0.69	2.17	2	1
1:B:211:VAL:HG21	1:B:271:VAL:CG1	0.69	2.18	15	6
1:A:68:THR:O	1:A:70:GLU:N	0.69	2.26	9	2
1:B:221:GLY:C	1:B:259:LEU:HD21	0.69	2.12	11	11
1:B:295:VAL:HG21	2:B:326:NTH:O20	0.69	1.88	8	2
1:A:115:LEU:HD11	1:B:300:HIS:CD2	0.69	2.23	4	1
1:A:80:PHE:CE1	1:A:101:PHE:CE2	0.69	2.82	14	5
1:A:36:VAL:HG23	1:A:51:ILE:HD12	0.68	1.64	12	6
1:A:94:VAL:HG13	1:A:122:HIS:CB	0.68	2.18	15	4
1:B:226:ILE:HD13	1:B:255:PHE:CE1	0.68	2.23	7	1
1:A:99:ASP:OD1	1:A:112:MET:HE3	0.68	1.89	15	1
1:A:10:VAL:HG21	1:A:103:PHE:CZ	0.68	2.23	2	6
1:B:295:VAL:HG13	1:B:321:ILE:HG23	0.68	1.65	5	3
1:A:86:PHE:CE2	2:A:126:NTH:H211	0.68	2.22	11	1
1:A:115:LEU:HD13	1:B:300:HIS:NE2	0.68	2.03	10	3
1:B:317:GLY:O	1:B:321:ILE:HD12	0.68	1.88	12	2
1:A:81:ALA:HB2	1:A:98:ILE:CG2	0.68	2.15	7	5
1:A:45:ARG:CD	1:A:50:ALA:HB1	0.68	2.19	1	2
1:B:304:ASN:HB3	1:B:310:VAL:HG21	0.68	1.66	15	7
1:B:203:THR:O	1:B:203:THR:HG23	0.68	1.88	15	8
1:A:72:ARG:HG3	1:A:79:ALA:HB3	0.68	1.66	9	1
1:B:315:LEU:O	1:B:316:PHE:CD1	0.68	2.47	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:281:ALA:HB1	1:B:298:ILE:CD1	0.68	2.17	11	1
1:B:261:LEU:HD13	2:B:326:NTH:H121	0.68	1.64	12	1
1:B:271:VAL:HG13	1:B:280:PHE:CB	0.68	2.19	14	9
1:A:93:THR:HG23	1:A:123:ALA:HA	0.68	1.65	4	1
1:A:116:PHE:O	1:B:274:VAL:HG22	0.68	1.89	4	1
1:A:3:THR:HG23	1:A:3:THR:O	0.67	1.89	15	5
1:B:210:VAL:CG2	1:B:309:VAL:HG23	0.67	2.19	10	2
1:B:261:LEU:HD22	1:B:263:LEU:HD23	0.67	1.65	12	4
1:B:295:VAL:CG2	1:B:321:ILE:HG23	0.67	2.18	2	7
1:B:210:VAL:CA	1:B:229:LEU:HD21	0.67	2.19	15	7
1:A:99:ASP:OD2	1:A:112:MET:HE3	0.67	1.88	3	4
1:B:261:LEU:HD23	1:B:263:LEU:HD23	0.67	1.67	15	2
1:A:63:LEU:CD1	1:A:84:VAL:HG13	0.67	2.12	14	1
1:A:14:TYR:CZ	1:A:18:LEU:HD11	0.67	2.24	7	3
1:B:268:THR:O	1:B:270:GLU:N	0.67	2.27	8	1
1:B:301:PHE:HE1	1:B:309:VAL:HG21	0.67	1.49	6	2
1:A:14:TYR:CE1	1:A:55:PHE:CE2	0.67	2.82	7	2
1:B:210:VAL:HG21	1:B:303:PHE:CE1	0.66	2.24	2	1
1:A:63:LEU:HB3	1:A:84:VAL:HG12	0.66	1.67	11	1
1:B:316:PHE:CG	1:B:317:GLY:N	0.66	2.64	5	4
1:A:61:LEU:HD12	2:A:126:NTH:H122	0.66	1.64	2	1
1:A:23:LEU:HD21	1:A:52:ARG:HA	0.66	1.67	3	3
1:A:71:VAL:HG13	1:A:80:PHE:CB	0.66	2.19	3	6
1:B:221:GLY:HA2	1:B:259:LEU:HD11	0.66	1.67	10	9
1:B:211:VAL:HG22	1:B:280:PHE:CD2	0.66	2.25	2	1
1:A:115:LEU:HD13	1:B:300:HIS:CE1	0.66	2.26	3	1
1:A:11:VAL:CG1	1:A:71:VAL:HG21	0.66	2.20	6	12
1:B:258:SER:OG	2:B:326:NTH:H112	0.66	1.91	15	4
1:A:40:VAL:HG23	1:A:40:VAL:O	0.66	1.90	15	5
1:A:72:ARG:CZ	1:A:74:VAL:CG2	0.66	2.73	9	1
1:B:236:VAL:HG23	1:B:251:ILE:CD1	0.66	2.20	12	1
1:A:21:GLY:C	1:A:59:LEU:HD21	0.66	2.16	7	14
1:B:298:ILE:HD12	1:B:320:ASN:OD1	0.66	1.91	3	2
1:A:105:GLY:O	1:A:106:ALA:HB2	0.66	1.91	11	9
1:A:40:VAL:O	1:B:275:ALA:HB2	0.66	1.90	14	1
1:A:21:GLY:HA2	1:A:59:LEU:HD11	0.65	1.69	2	6
1:B:316:PHE:CD1	1:B:316:PHE:C	0.65	2.74	5	2
1:B:261:LEU:O	1:B:263:LEU:HD23	0.65	1.91	1	1
1:B:305:GLY:O	1:B:306:ALA:HB2	0.65	1.91	9	7
1:A:61:LEU:HD23	1:A:63:LEU:HD23	0.65	1.68	12	3
1:A:115:LEU:O	1:A:116:PHE:CD1	0.65	2.49	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG23	1:A:46:SER:CB	0.65	2.22	5	1
1:B:286:PHE:CE2	1:B:293:THR:CG2	0.65	2.79	14	1
1:B:210:VAL:CG1	1:B:301:PHE:CE1	0.65	2.80	10	11
1:A:86:PHE:CZ	2:A:126:NTH:H221	0.65	2.26	13	8
1:A:10:VAL:CA	1:A:29:LEU:HD21	0.65	2.21	14	3
1:A:23:LEU:HD11	1:A:55:PHE:C	0.65	2.17	8	6
1:B:263:LEU:CB	1:B:284:VAL:HG12	0.65	2.20	14	4
1:A:67:LEU:HD22	1:A:71:VAL:CG2	0.65	2.22	10	1
1:B:223:LEU:HD11	1:B:255:PHE:C	0.65	2.17	15	5
1:A:14:TYR:CE1	1:A:18:LEU:CD1	0.64	2.80	1	14
1:A:105:GLY:O	1:A:106:ALA:HB3	0.64	1.91	15	3
1:A:10:VAL:CG1	1:A:101:PHE:CZ	0.64	2.79	7	11
1:B:305:GLY:O	1:B:306:ALA:HB3	0.64	1.92	8	4
1:A:63:LEU:HB2	1:A:84:VAL:HG13	0.64	1.69	12	5
1:B:317:GLY:O	1:B:321:ILE:HD11	0.64	1.92	9	9
1:B:226:ILE:HG21	1:B:255:PHE:CD2	0.64	2.27	3	5
1:A:15:VAL:HB	1:A:67:LEU:HD11	0.64	1.68	5	2
1:B:293:THR:HG23	1:B:323:ALA:CA	0.64	2.23	15	1
1:A:30:PHE:CD2	1:A:51:ILE:CG2	0.64	2.80	8	3
1:B:214:TYR:CE1	1:B:218:LEU:CD1	0.64	2.80	6	15
1:A:10:VAL:CG1	1:A:101:PHE:CE1	0.64	2.81	14	9
1:A:82:PHE:CD1	1:A:82:PHE:N	0.64	2.65	4	7
1:A:10:VAL:CG2	1:A:103:PHE:CZ	0.64	2.81	6	6
1:A:94:VAL:HG12	1:A:122:HIS:CB	0.64	2.22	9	9
1:A:58:SER:OG	2:A:126:NTH:H111	0.64	1.93	11	2
1:A:95:VAL:HG12	1:A:97:PRO:CD	0.64	2.22	6	11
1:A:61:LEU:HD12	1:A:63:LEU:CG	0.64	2.22	9	1
1:A:67:LEU:C	1:A:68:THR:HG22	0.64	2.18	5	1
1:B:210:VAL:CG1	1:B:301:PHE:CZ	0.64	2.81	7	10
1:B:282:PHE:CD1	1:B:282:PHE:N	0.63	2.66	13	8
1:B:223:LEU:CD2	1:B:256:ALA:HB2	0.63	2.24	4	7
1:B:296:ALA:HB3	1:B:320:ASN:O	0.63	1.92	12	4
1:A:115:LEU:HD11	1:B:279:ALA:CB	0.63	2.23	4	1
1:A:10:VAL:CG1	1:A:103:PHE:CZ	0.63	2.82	3	5
1:B:258:SER:OG	2:B:326:NTH:H111	0.63	1.94	9	3
1:B:286:PHE:N	1:B:286:PHE:CD1	0.63	2.66	8	3
1:B:277:GLU:O	1:B:278:ALA:HB2	0.63	1.92	15	7
1:A:104:ASN:HB3	1:A:110:VAL:HG11	0.63	1.70	8	1
1:A:88:PHE:N	1:A:88:PHE:CD1	0.63	2.66	15	2
1:B:286:PHE:CZ	1:B:293:THR:HG23	0.63	2.28	14	1
1:A:35:THR:O	1:A:36:VAL:HG23	0.63	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:SER:OG	2:A:126:NTH:H112	0.63	1.93	3	3
1:A:86:PHE:CD1	1:A:86:PHE:N	0.63	2.66	6	8
1:A:23:LEU:HD21	1:A:59:LEU:HD22	0.63	1.71	5	2
1:B:288:PHE:N	1:B:288:PHE:CD1	0.63	2.66	9	3
1:B:297:PRO:CB	1:B:316:PHE:CD1	0.63	2.82	7	2
1:A:40:VAL:HG23	1:A:41:GLY:N	0.63	2.08	2	2
1:A:18:LEU:HD21	1:A:55:PHE:CE1	0.63	2.27	10	1
1:A:116:PHE:CE2	2:A:126:NTH:H61	0.63	2.29	10	1
1:A:98:ILE:HD12	1:B:272:ARG:HH21	0.63	1.54	14	1
1:B:263:LEU:CD1	1:B:284:VAL:HG13	0.63	2.22	1	1
1:B:210:VAL:CG2	1:B:303:PHE:CZ	0.63	2.82	3	2
1:A:45:ARG:HD3	1:A:50:ALA:HB1	0.62	1.69	1	2
1:B:295:VAL:HG12	1:B:297:PRO:CD	0.62	2.24	2	13
1:A:7:MET:CE	1:A:103:PHE:CD2	0.62	2.81	3	1
1:A:67:LEU:HD23	1:A:81:ALA:O	0.62	1.94	5	2
1:B:286:PHE:CD1	1:B:286:PHE:N	0.62	2.65	14	1
1:B:226:ILE:HG22	1:B:230:PHE:CE2	0.62	2.28	2	1
1:B:230:PHE:CD2	1:B:251:ILE:CG2	0.62	2.83	4	6
1:A:23:LEU:HD22	1:A:59:LEU:HD22	0.62	1.71	2	6
1:A:115:LEU:CD1	1:B:279:ALA:HB2	0.62	2.24	1	6
1:A:30:PHE:CG	1:A:51:ILE:HG21	0.62	2.28	3	4
1:A:26:ILE:HG21	1:A:55:PHE:HD2	0.62	1.54	7	1
1:B:226:ILE:CG2	1:B:255:PHE:CD2	0.62	2.82	7	1
1:B:210:VAL:HG22	1:B:309:VAL:CG2	0.62	2.25	14	4
1:B:223:LEU:O	1:B:227:VAL:HG23	0.62	1.93	8	2
1:B:214:TYR:CE1	1:B:218:LEU:HD11	0.62	2.29	7	15
1:A:3:THR:O	1:A:7:MET:HE3	0.62	1.93	12	4
1:A:18:LEU:HB3	1:A:65:VAL:HG11	0.62	1.72	9	2
1:A:17:ALA:HB1	1:A:22:ASP:OD1	0.62	1.95	6	1
1:B:210:VAL:HG21	1:B:303:PHE:CE2	0.62	2.29	14	4
1:B:245:ARG:CD	1:B:254:PHE:CD1	0.62	2.82	9	1
1:A:74:VAL:HG13	1:B:316:PHE:O	0.62	1.95	8	3
1:A:61:LEU:HD23	1:A:61:LEU:O	0.62	1.94	6	1
1:B:223:LEU:HD21	1:B:259:LEU:HD22	0.62	1.70	3	3
1:B:245:ARG:HG2	1:B:250:ALA:HB1	0.62	1.71	5	1
1:A:75:ALA:HB3	1:B:240:VAL:CG1	0.62	2.16	10	1
1:B:211:VAL:CG1	1:B:271:VAL:HG21	0.61	2.24	10	11
1:A:95:VAL:HG22	1:A:121:ILE:CG2	0.61	2.24	14	8
1:A:40:VAL:HB	1:B:274:VAL:HG11	0.61	1.71	4	1
1:A:79:ALA:CB	1:B:315:LEU:HD21	0.61	2.25	8	2
1:B:322:HIS:NE2	2:B:326:NTH:H212	0.61	2.10	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:TYR:CE1	1:A:55:PHE:CZ	0.61	2.88	7	1
1:A:86:PHE:CE1	2:A:126:NTH:H221	0.61	2.30	7	2
1:A:21:GLY:O	1:A:59:LEU:HD21	0.61	1.95	4	4
1:A:94:VAL:HG13	1:A:95:VAL:N	0.61	2.08	12	7
1:B:210:VAL:CG1	1:B:303:PHE:CZ	0.61	2.84	10	9
1:A:26:ILE:HD13	1:A:55:PHE:CE1	0.61	2.31	2	1
1:B:240:VAL:HG23	1:B:240:VAL:O	0.61	1.94	12	4
1:A:71:VAL:HG22	1:A:80:PHE:HB2	0.61	1.72	6	2
1:A:113:ARG:NH2	1:B:300:HIS:CE1	0.61	2.69	9	1
1:B:286:PHE:CE2	1:B:293:THR:HG23	0.61	2.30	14	1
1:B:263:LEU:HD23	1:B:286:PHE:HB3	0.61	1.73	4	3
1:A:14:TYR:CD1	1:A:14:TYR:C	0.61	2.78	2	15
1:B:211:VAL:CG2	1:B:301:PHE:CE2	0.61	2.84	3	8
1:B:234:ALA:HB3	1:B:251:ILE:CD1	0.61	2.24	9	1
1:A:61:LEU:HD23	1:A:63:LEU:CD2	0.61	2.25	12	2
1:B:304:ASN:OD1	1:B:310:VAL:HG21	0.61	1.96	14	1
1:A:11:VAL:HG11	1:A:71:VAL:CG1	0.61	2.25	2	2
1:B:211:VAL:HG22	1:B:301:PHE:CD2	0.61	2.31	10	8
1:B:293:THR:HG22	1:B:323:ALA:HA	0.61	1.71	12	2
1:A:40:VAL:CB	1:B:274:VAL:HG11	0.61	2.25	4	1
1:B:227:VAL:HG21	1:B:252:ARG:HB2	0.61	1.73	5	7
1:B:277:GLU:HG2	1:B:278:ALA:N	0.61	2.11	14	1
1:B:234:ALA:HB1	1:B:310:VAL:O	0.61	1.96	8	8
1:B:295:VAL:HG13	1:B:320:ASN:ND2	0.61	2.10	4	1
1:B:294:VAL:HG13	1:B:322:HIS:HB2	0.60	1.72	10	3
1:A:85:SER:HA	1:A:94:VAL:HG23	0.60	1.72	2	5
1:B:226:ILE:HG21	1:B:255:PHE:CD1	0.60	2.31	7	1
1:B:263:LEU:CB	1:B:284:VAL:CG1	0.60	2.80	3	6
1:A:30:PHE:CZ	1:A:112:MET:CE	0.60	2.85	10	2
1:A:61:LEU:CD2	1:A:63:LEU:HD23	0.60	2.26	4	1
1:A:61:LEU:CD2	1:A:63:LEU:CD2	0.60	2.79	4	9
1:B:238:ASP:OD2	2:B:326:NTH:H62	0.60	1.96	7	5
1:A:86:PHE:CD1	1:A:86:PHE:C	0.60	2.79	4	1
1:B:214:TYR:CD1	1:B:214:TYR:C	0.60	2.79	7	15
1:B:261:LEU:CD2	1:B:263:LEU:CD2	0.60	2.80	7	10
1:A:61:LEU:HD23	1:A:63:LEU:HD11	0.60	1.73	3	1
1:B:210:VAL:HG21	1:B:303:PHE:CZ	0.60	2.31	3	2
1:B:226:ILE:HD13	1:B:255:PHE:CD2	0.60	2.32	8	3
1:B:315:LEU:O	1:B:316:PHE:CB	0.60	2.50	5	2
1:B:236:VAL:CG2	1:B:251:ILE:HG23	0.60	2.27	9	1
1:B:280:PHE:O	1:B:298:ILE:HG23	0.60	1.96	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:210:VAL:CG2	1:B:309:VAL:CG2	0.60	2.79	14	4
1:A:61:LEU:HD13	1:A:63:LEU:HD21	0.60	1.73	2	1
1:A:58:SER:HB2	2:A:126:NTH:H11	0.60	1.73	7	1
1:A:85:SER:CB	1:A:94:VAL:HG23	0.59	2.26	3	1
1:A:79:ALA:CB	1:B:315:LEU:CD1	0.59	2.80	7	3
1:A:10:VAL:HG22	1:A:109:VAL:CG2	0.59	2.27	2	2
1:B:213:ARG:CB	1:B:229:LEU:HD22	0.59	2.24	7	3
1:B:223:LEU:CD2	1:B:252:ARG:CG	0.59	2.81	13	9
1:B:223:LEU:HD21	1:B:259:LEU:HB2	0.59	1.74	7	1
1:A:100:HIS:NE2	1:B:300:HIS:CD2	0.59	2.70	15	1
1:A:75:ALA:HB1	1:B:241:GLY:HA3	0.59	1.73	3	1
1:A:7:MET:HE2	1:A:7:MET:HA	0.59	1.74	14	1
1:A:10:VAL:HG13	1:A:101:PHE:CE1	0.59	2.33	6	4
1:A:40:VAL:CG2	1:B:274:VAL:CG1	0.59	2.81	4	1
1:B:218:LEU:HB3	1:B:265:VAL:HG21	0.59	1.73	15	5
1:A:63:LEU:CB	1:A:84:VAL:CG1	0.59	2.81	11	3
1:A:7:MET:HE2	1:A:73:ALA:HB1	0.59	1.73	7	2
1:B:276:ASN:O	1:B:303:PHE:CD1	0.59	2.55	7	3
1:B:210:VAL:HG12	1:B:301:PHE:CZ	0.59	2.32	13	6
1:B:236:VAL:HG23	1:B:251:ILE:HD12	0.59	1.73	12	2
1:B:321:ILE:HG22	1:B:322:HIS:N	0.59	2.13	7	2
1:A:23:LEU:HD22	1:A:56:ALA:HB2	0.59	1.73	11	2
1:A:77:GLU:HG2	1:A:78:ALA:N	0.59	2.11	12	1
1:A:34:ALA:HB1	1:A:110:VAL:O	0.59	1.97	7	9
1:B:247:GLY:O	1:B:251:ILE:HD12	0.59	1.98	6	7
1:A:100:HIS:CG	1:A:101:PHE:N	0.59	2.71	9	3
1:A:72:ARG:CZ	1:A:74:VAL:HG22	0.58	2.28	5	1
1:B:238:ASP:O	1:B:254:PHE:CE2	0.58	2.56	15	3
1:A:80:PHE:CZ	1:A:99:ASP:HB3	0.58	2.34	11	14
1:B:288:PHE:CD2	1:B:293:THR:OG1	0.58	2.57	5	4
1:A:86:PHE:CE1	1:A:88:PHE:CE1	0.58	2.91	4	1
1:B:258:SER:OG	2:B:326:NTH:H10	0.58	1.98	9	2
1:A:26:ILE:CG2	1:A:30:PHE:CE2	0.58	2.83	1	1
1:A:11:VAL:HG11	1:A:71:VAL:HG22	0.58	1.74	12	2
1:B:245:ARG:NH1	1:B:251:ILE:CG1	0.58	2.66	7	1
1:B:294:VAL:O	1:B:321:ILE:O	0.58	2.20	7	2
1:B:236:VAL:CG1	1:B:237:GLU:N	0.58	2.65	12	3
1:B:273:ALA:C	1:B:274:VAL:HG22	0.58	2.23	14	3
1:B:261:LEU:HD12	1:B:263:LEU:HG	0.58	1.76	14	1
1:B:261:LEU:HD13	1:B:262:PRO:HD2	0.58	1.74	14	1
1:A:4:PRO:HA	1:A:7:MET:HE3	0.58	1.73	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ASP:O	1:A:54:PHE:CZ	0.58	2.56	15	7
1:A:63:LEU:HD23	1:A:86:PHE:CG	0.58	2.33	9	4
1:A:3:THR:O	1:A:3:THR:HG23	0.58	1.98	12	2
1:B:238:ASP:OD1	1:B:314:ALA:HB3	0.58	1.98	15	2
1:A:80:PHE:CE2	1:A:82:PHE:CE2	0.58	2.91	10	2
1:A:80:PHE:O	1:A:98:ILE:HG23	0.58	1.98	2	3
1:A:11:VAL:CG2	1:A:101:PHE:CE2	0.58	2.87	14	8
1:A:77:GLU:O	1:A:78:ALA:HB2	0.58	1.99	13	6
1:A:40:VAL:C	1:B:275:ALA:HB2	0.58	2.23	14	1
1:A:86:PHE:CZ	1:A:93:THR:OG1	0.58	2.57	14	1
1:A:36:VAL:CG1	1:A:37:GLU:N	0.58	2.67	11	5
1:A:88:PHE:CD2	1:A:93:THR:OG1	0.58	2.55	14	5
1:A:23:LEU:CD2	1:A:52:ARG:CG	0.58	2.81	9	7
1:A:63:LEU:CD2	1:A:84:VAL:CG1	0.58	2.81	7	2
1:B:230:PHE:HD2	1:B:251:ILE:HG21	0.58	1.58	6	1
1:B:226:ILE:CD1	1:B:255:PHE:CD1	0.58	2.86	7	1
1:A:3:THR:O	1:A:6:HIS:CE1	0.58	2.57	11	1
1:B:316:PHE:CD2	1:B:317:GLY:N	0.58	2.71	9	9
1:A:72:ARG:CZ	1:A:74:VAL:HG23	0.58	2.28	9	1
1:B:269:GLN:NE2	1:B:281:ALA:HB3	0.58	2.13	13	1
1:A:116:PHE:CD2	1:A:117:GLY:N	0.58	2.72	4	6
1:B:223:LEU:CD2	1:B:259:LEU:CD2	0.58	2.80	7	6
1:B:295:VAL:HG22	1:B:321:ILE:HA	0.58	1.75	4	1
1:B:316:PHE:CD2	1:B:320:ASN:OD1	0.58	2.57	4	1
1:A:94:VAL:CG1	1:A:122:HIS:CB	0.58	2.82	14	4
1:B:297:PRO:HB3	1:B:316:PHE:CD1	0.58	2.32	7	1
1:B:223:LEU:HD23	1:B:252:ARG:HG2	0.58	1.76	9	4
1:A:101:PHE:CE1	1:A:112:MET:CE	0.58	2.82	10	1
1:B:299:ASP:OD2	1:B:312:MET:HE3	0.58	1.98	3	3
1:B:236:VAL:HG13	1:B:312:MET:HE2	0.58	1.76	5	1
1:A:6:HIS:NE2	1:A:7:MET:CG	0.58	2.67	11	1
1:A:78:ALA:HB3	1:A:101:PHE:HB2	0.58	1.74	2	6
1:A:116:PHE:CE1	2:A:126:NTH:H62	0.58	2.34	2	1
1:B:236:VAL:CG2	1:B:251:ILE:CD1	0.58	2.81	12	1
1:B:286:PHE:CD1	1:B:293:THR:O	0.57	2.57	9	2
1:A:26:ILE:HG21	1:A:55:PHE:CD2	0.57	2.33	7	3
1:A:43:GLU:N	1:A:44:PRO:HD3	0.57	2.14	3	5
1:B:234:ALA:CB	1:B:310:VAL:O	0.57	2.52	8	8
1:A:37:GLU:O	1:A:114:ALA:HB3	0.57	1.99	2	1
1:A:41:GLY:O	1:A:42:SER:C	0.57	2.47	2	1
1:A:81:ALA:C	1:A:82:PHE:CD2	0.57	2.82	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:HD3	1:A:29:LEU:HD13	0.57	1.74	7	1
1:A:76:ASN:O	1:A:103:PHE:CG	0.57	2.57	13	1
1:A:64:ALA:HB3	1:A:85:SER:HG	0.57	1.59	15	3
1:B:211:VAL:HG11	1:B:271:VAL:HG22	0.57	1.76	2	3
1:A:72:ARG:NE	1:A:74:VAL:CG2	0.57	2.67	9	1
1:A:103:PHE:CE1	1:A:108:LYS:O	0.57	2.57	2	1
1:B:235:THR:HG23	1:B:246:SER:CB	0.57	2.25	11	3
1:A:117:GLY:O	1:A:121:ILE:HD11	0.57	1.99	5	10
1:A:33:ASP:C	1:A:51:ILE:HD11	0.57	2.25	5	1
1:A:23:LEU:HA	1:A:26:ILE:HD12	0.57	1.76	10	1
1:A:23:LEU:CD2	1:A:59:LEU:CD2	0.57	2.82	5	7
1:A:13:ARG:CB	1:A:29:LEU:HD22	0.57	2.25	9	2
1:A:15:VAL:HG13	1:A:65:VAL:CG1	0.57	2.29	8	1
1:A:27:VAL:HG21	1:A:52:ARG:HG3	0.57	1.77	8	1
1:A:10:VAL:HG11	1:A:109:VAL:CG2	0.57	2.30	9	1
1:A:23:LEU:HD23	1:A:52:ARG:HG2	0.57	1.73	11	2
1:B:304:ASN:N	1:B:310:VAL:HG21	0.57	2.14	13	1
1:B:322:HIS:O	1:B:322:HIS:ND1	0.57	2.37	13	1
1:A:115:LEU:CD1	1:B:279:ALA:CB	0.57	2.83	1	2
1:A:38:ASP:OD2	2:A:126:NTH:H10	0.57	2.00	2	1
1:B:288:PHE:C	1:B:289:GLN:CG	0.57	2.77	13	3
1:B:230:PHE:CZ	1:B:312:MET:CE	0.57	2.88	9	2
1:B:286:PHE:CE2	1:B:288:PHE:CE1	0.57	2.92	9	2
1:B:204:PRO:HA	1:B:207:MET:HE3	0.57	1.74	1	2
1:A:95:VAL:CG1	1:A:120:ASN:ND2	0.57	2.67	10	2
1:A:38:ASP:OD2	2:A:126:NTH:H62	0.57	2.00	9	5
1:B:301:PHE:CE1	1:B:312:MET:SD	0.57	2.98	13	2
1:B:304:ASN:N	1:B:304:ASN:ND2	0.57	2.53	10	2
1:A:67:LEU:CD2	1:A:71:VAL:CG2	0.57	2.83	10	1
1:A:88:PHE:CZ	1:A:93:THR:OG1	0.57	2.57	11	1
1:B:202:ASN:HB3	1:B:207:MET:HE1	0.57	1.75	11	1
1:A:63:LEU:HD13	1:A:84:VAL:HG11	0.56	1.76	9	2
1:B:304:ASN:HB3	1:B:310:VAL:HG11	0.56	1.77	11	1
1:B:206:HIS:CE1	1:B:207:MET:CG	0.56	2.88	13	1
1:B:274:VAL:O	1:B:275:ALA:C	0.56	2.48	2	11
1:A:61:LEU:HD22	1:A:63:LEU:HD23	0.56	1.77	13	2
1:A:77:GLU:CD	1:A:100:HIS:CE1	0.56	2.83	12	1
1:B:263:LEU:CD2	1:B:284:VAL:HG12	0.56	2.29	13	1
1:B:286:PHE:CZ	1:B:293:THR:OG1	0.56	2.57	5	6
1:B:235:THR:HG22	1:B:246:SER:HB2	0.56	1.74	2	2
1:A:74:VAL:CB	1:B:240:VAL:HG21	0.56	2.30	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:CG2	1:A:101:PHE:CD2	0.56	2.87	6	3
1:B:211:VAL:HG11	1:B:271:VAL:CG1	0.56	2.29	7	2
1:A:61:LEU:CD1	1:A:63:LEU:HD21	0.56	2.30	9	1
1:A:98:ILE:HD11	1:B:272:ARG:CZ	0.56	2.31	12	1
1:A:101:PHE:CE1	1:A:112:MET:SD	0.56	2.98	12	2
1:B:294:VAL:O	1:B:322:HIS:HB3	0.56	2.00	13	1
1:B:293:THR:HG22	1:B:294:VAL:N	0.56	2.16	15	1
1:B:294:VAL:HG13	1:B:322:HIS:CB	0.56	2.31	10	3
1:A:61:LEU:HD12	1:A:63:LEU:CD2	0.56	2.31	9	1
1:B:280:PHE:CZ	1:B:299:ASP:HB3	0.56	2.36	11	14
1:A:109:VAL:HG12	1:A:110:VAL:N	0.56	2.16	14	3
1:A:38:ASP:OD2	1:A:114:ALA:HB3	0.56	2.01	8	2
1:A:94:VAL:HG13	1:A:122:HIS:HB3	0.56	1.78	15	1
1:B:307:GLY:O	1:B:308:LYS:CB	0.56	2.53	1	2
1:B:294:VAL:HG12	1:B:322:HIS:CB	0.56	2.31	11	7
1:B:296:ALA:N	1:B:320:ASN:O	0.56	2.39	12	6
1:A:94:VAL:O	1:A:122:HIS:CB	0.56	2.54	14	6
1:B:297:PRO:CB	1:B:316:PHE:CG	0.56	2.89	9	1
1:B:301:PHE:CE1	1:B:312:MET:HE2	0.56	2.36	12	1
1:B:206:HIS:NE2	1:B:207:MET:HE2	0.56	2.16	13	1
1:B:279:ALA:HB2	1:B:300:HIS:CE1	0.56	2.36	14	1
1:A:36:VAL:O	1:A:44:PRO:CB	0.56	2.54	1	14
1:B:240:VAL:HG22	1:B:316:PHE:HE1	0.56	1.60	5	1
1:A:107:GLY:O	1:A:108:LYS:CB	0.56	2.53	14	2
1:A:43:GLU:O	1:A:54:PHE:CZ	0.56	2.59	8	2
1:B:321:ILE:HG21	2:B:326:NTH:H222	0.56	1.76	12	2
1:A:38:ASP:OD2	2:A:126:NTH:H61	0.56	2.01	12	1
1:A:76:ASN:O	1:A:103:PHE:CD2	0.56	2.59	13	1
1:A:72:ARG:CB	1:A:79:ALA:O	0.56	2.54	5	13
1:B:227:VAL:CG1	1:B:248:THR:HG23	0.56	2.30	11	5
1:A:10:VAL:CG2	1:A:109:VAL:CG2	0.56	2.83	2	3
1:A:11:VAL:HG22	1:A:101:PHE:HE2	0.56	1.60	3	5
1:B:211:VAL:HG22	1:B:301:PHE:HE2	0.56	1.57	3	5
1:B:317:GLY:C	1:B:321:ILE:CD1	0.56	2.79	3	2
1:A:68:THR:O	1:A:69:GLN:CG	0.56	2.54	5	2
1:B:294:VAL:O	1:B:322:HIS:CA	0.56	2.54	13	1
1:A:67:LEU:O	1:A:68:THR:CB	0.55	2.55	5	1
1:B:264:ALA:HB3	1:B:285:SER:HG	0.55	1.61	1	3
1:B:285:SER:OG	1:B:294:VAL:HG23	0.55	2.02	3	1
1:A:10:VAL:HG22	1:A:109:VAL:HG23	0.55	1.77	6	6
1:B:285:SER:HA	1:B:294:VAL:HG23	0.55	1.79	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:VAL:HG12	1:A:122:HIS:HB2	0.55	1.78	9	3
1:A:10:VAL:CG1	1:A:109:VAL:CG2	0.55	2.84	9	4
1:A:15:VAL:HG13	1:A:65:VAL:HG12	0.55	1.79	8	1
1:B:316:PHE:CE1	2:B:326:NTH:H61	0.55	2.37	8	1
1:A:34:ALA:CB	1:A:110:VAL:O	0.55	2.55	3	9
1:B:294:VAL:CG1	1:B:322:HIS:CD2	0.55	2.90	8	1
1:B:261:LEU:HD12	1:B:263:LEU:CD1	0.55	2.31	14	1
1:A:116:PHE:O	1:B:274:VAL:CG1	0.55	2.55	12	13
1:B:236:VAL:O	1:B:244:PRO:CB	0.55	2.55	1	14
1:A:73:ALA:C	1:A:74:VAL:HG22	0.55	2.27	10	4
1:B:309:VAL:CG1	1:B:310:VAL:N	0.55	2.69	13	3
1:A:100:HIS:CB	1:A:113:ARG:NE	0.55	2.70	9	1
1:B:297:PRO:HB3	1:B:316:PHE:CG	0.55	2.36	9	1
1:A:39:PRO:O	1:A:40:VAL:O	0.55	2.25	2	1
1:B:304:ASN:CB	1:B:310:VAL:HG21	0.55	2.32	12	4
1:A:14:TYR:HE2	1:A:112:MET:HE1	0.55	1.57	4	2
1:B:268:THR:O	1:B:269:GLN:CG	0.55	2.54	8	1
1:A:72:ARG:O	1:A:78:ALA:HB1	0.55	2.02	12	1
1:A:101:PHE:CD1	1:A:103:PHE:CE1	0.55	2.95	14	2
1:A:115:LEU:CD2	1:B:279:ALA:CB	0.55	2.83	10	2
1:A:11:VAL:CG2	1:A:71:VAL:HG11	0.55	2.32	13	1
1:A:74:VAL:O	1:A:75:ALA:C	0.55	2.50	15	12
1:B:304:ASN:OD1	1:B:310:VAL:HG22	0.55	2.00	1	1
1:A:34:ALA:N	1:A:51:ILE:CD1	0.55	2.67	5	2
1:A:23:LEU:CD2	1:A:56:ALA:HB2	0.55	2.32	14	5
1:B:238:ASP:O	1:B:254:PHE:CZ	0.55	2.59	8	6
1:B:238:ASP:OD2	1:B:314:ALA:CB	0.55	2.55	12	3
1:A:102:ARG:CB	1:A:111:SER:CB	0.55	2.84	10	2
1:B:288:PHE:CE2	1:B:291:ARG:HB3	0.55	2.37	9	1
1:A:10:VAL:O	1:A:14:TYR:CB	0.55	2.55	4	15
1:B:234:ALA:N	1:B:251:ILE:CD1	0.55	2.69	11	4
1:B:234:ALA:CA	1:B:310:VAL:O	0.55	2.55	12	9
1:B:305:GLY:O	1:B:306:ALA:CB	0.55	2.55	12	11
1:B:210:VAL:HG13	1:B:301:PHE:CE1	0.55	2.36	10	6
1:A:74:VAL:CG2	1:B:316:PHE:O	0.54	2.55	4	7
1:A:80:PHE:CD1	1:A:101:PHE:CD2	0.54	2.95	14	3
1:A:88:PHE:C	1:A:89:GLN:CG	0.54	2.80	12	2
1:B:203:THR:O	1:B:207:MET:HE3	0.54	2.01	12	2
1:A:74:VAL:CG1	1:B:316:PHE:O	0.54	2.55	4	11
1:A:115:LEU:HD13	1:B:279:ALA:CB	0.54	2.30	11	3
1:B:281:ALA:C	1:B:282:PHE:CD2	0.54	2.85	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:240:VAL:HG13	1:B:316:PHE:CE1	0.54	2.38	3	1
1:A:104:ASN:OD1	1:A:110:VAL:CG2	0.54	2.56	10	5
1:B:303:PHE:CD1	1:B:303:PHE:N	0.54	2.74	14	8
1:B:303:PHE:C	1:B:310:VAL:CG2	0.54	2.81	11	2
1:A:67:LEU:HD22	1:A:71:VAL:HG23	0.54	1.78	10	1
1:A:109:VAL:CG1	1:A:110:VAL:N	0.54	2.70	14	4
1:B:275:ALA:O	1:B:276:ASN:CB	0.54	2.54	5	1
1:A:104:ASN:HD21	1:A:106:ALA:HB3	0.54	1.63	7	1
1:A:86:PHE:CZ	2:A:126:NTH:H211	0.54	2.37	11	2
1:B:238:ASP:OD1	1:B:314:ALA:CB	0.54	2.55	15	2
1:B:271:VAL:HG22	1:B:280:PHE:HB2	0.54	1.78	10	1
1:A:94:VAL:CG1	1:A:95:VAL:N	0.54	2.70	9	6
1:B:272:ARG:CB	1:B:279:ALA:O	0.54	2.56	2	13
1:A:61:LEU:HB3	1:A:63:LEU:HD21	0.54	1.78	4	1
1:A:94:VAL:HG22	1:A:95:VAL:N	0.54	2.16	15	5
1:A:75:ALA:HB2	1:B:240:VAL:C	0.54	2.26	6	2
1:A:85:SER:HB3	1:A:94:VAL:HG23	0.54	1.78	7	1
1:A:14:TYR:CD1	1:A:14:TYR:O	0.54	2.60	10	1
1:B:206:HIS:CE1	1:B:207:MET:HG3	0.54	2.36	13	1
1:B:321:ILE:HG22	1:B:322:HIS:H	0.54	1.63	3	11
1:B:288:PHE:O	1:B:290:GLY:N	0.54	2.41	13	2
1:A:73:ALA:C	1:A:74:VAL:CG2	0.54	2.80	7	3
1:B:297:PRO:HB2	1:B:316:PHE:CD1	0.54	2.37	9	1
1:A:69:GLN:HG2	1:A:70:GLU:N	0.54	2.18	10	1
1:A:95:VAL:HG13	1:A:120:ASN:O	0.54	2.01	10	1
1:A:61:LEU:O	1:A:63:LEU:CD2	0.54	2.56	14	2
1:A:80:PHE:CD1	1:A:80:PHE:C	0.54	2.85	11	2
1:A:13:ARG:NH2	1:A:29:LEU:CD1	0.54	2.69	4	1
1:A:75:ALA:O	1:A:76:ASN:CB	0.54	2.55	4	1
1:B:294:VAL:HG22	1:B:295:VAL:H	0.54	1.63	13	3
1:B:284:VAL:HG12	1:B:286:PHE:HD1	0.54	1.63	6	1
1:B:281:ALA:HB2	1:B:298:ILE:CG1	0.54	2.33	15	3
1:A:100:HIS:O	1:A:112:MET:CG	0.54	2.56	13	14
1:A:116:PHE:O	1:B:274:VAL:CG2	0.54	2.56	10	13
1:A:79:ALA:CB	1:B:315:LEU:CD2	0.54	2.80	4	2
1:B:294:VAL:HG13	1:B:295:VAL:N	0.54	2.17	6	4
1:B:315:LEU:O	1:B:316:PHE:CG	0.54	2.60	7	3
1:B:236:VAL:HG12	1:B:237:GLU:N	0.54	2.17	9	2
1:B:261:LEU:CD1	1:B:263:LEU:HD21	0.54	2.33	14	1
1:A:61:LEU:O	1:A:63:LEU:CD1	0.54	2.56	1	7
1:B:210:VAL:O	1:B:214:TYR:CB	0.54	2.56	15	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:263:LEU:HB3	1:B:284:VAL:HG13	0.54	1.79	7	2
1:B:304:ASN:OD1	1:B:310:VAL:CG1	0.54	2.56	4	1
1:A:10:VAL:CG2	1:A:109:VAL:HG23	0.54	2.32	6	6
1:A:17:ALA:CA	1:A:22:ASP:OD1	0.54	2.56	6	1
1:B:236:VAL:CG2	1:B:251:ILE:HD12	0.54	2.33	12	1
1:A:49:ALA:O	1:A:53:GLU:CB	0.54	2.56	10	7
1:B:317:GLY:O	1:B:321:ILE:CD1	0.54	2.56	3	12
1:A:95:VAL:HG22	1:A:121:ILE:HA	0.54	1.80	2	2
1:B:261:LEU:O	1:B:263:LEU:CD1	0.54	2.56	5	8
1:A:86:PHE:CD2	1:A:87:GLU:O	0.54	2.60	12	3
1:B:300:HIS:O	1:B:312:MET:CG	0.54	2.56	11	11
1:A:61:LEU:O	1:A:63:LEU:HD23	0.54	2.02	14	1
1:B:273:ALA:C	1:B:274:VAL:CG2	0.54	2.81	14	1
1:A:100:HIS:CD2	1:B:300:HIS:NE2	0.54	2.76	15	1
1:B:304:ASN:OD1	1:B:310:VAL:CG2	0.53	2.56	1	6
1:A:88:PHE:O	1:A:90:GLY:N	0.53	2.42	14	2
1:B:210:VAL:HG13	1:B:301:PHE:CZ	0.53	2.37	2	6
1:B:286:PHE:CZ	1:B:293:THR:HB	0.53	2.38	11	4
1:A:36:VAL:HG23	1:A:51:ILE:CD1	0.53	2.33	8	3
1:B:245:ARG:NH1	1:B:245:ARG:O	0.53	2.40	7	1
1:A:40:VAL:O	1:B:275:ALA:HB3	0.53	2.03	8	1
1:A:86:PHE:CD1	1:A:93:THR:O	0.53	2.61	8	1
1:B:304:ASN:OD1	1:B:310:VAL:CB	0.53	2.56	14	1
1:B:285:SER:HB3	1:B:294:VAL:HG23	0.53	1.80	13	1
1:B:258:SER:OG	2:B:326:NTH:H8	0.53	2.04	4	1
1:B:245:ARG:NH1	1:B:251:ILE:HG13	0.53	2.19	7	1
1:A:86:PHE:CE1	1:A:93:THR:O	0.53	2.61	9	2
1:A:77:GLU:CG	1:A:102:ARG:HG3	0.53	2.34	1	3
1:B:261:LEU:O	1:B:263:LEU:CD2	0.53	2.57	1	2
1:B:296:ALA:O	1:B:320:ASN:ND2	0.53	2.42	5	6
1:A:61:LEU:HD12	1:A:63:LEU:HG	0.53	1.78	9	1
1:B:243:GLU:O	1:B:254:PHE:CZ	0.53	2.61	15	3
1:B:309:VAL:CG1	1:B:312:MET:HE1	0.53	2.33	13	1
1:B:249:ALA:O	1:B:253:GLU:CB	0.53	2.56	4	4
1:A:120:ASN:OD1	1:A:121:ILE:CD1	0.53	2.57	2	2
1:A:88:PHE:CE1	1:A:91:ARG:O	0.53	2.62	8	1
1:B:261:LEU:HD23	1:B:261:LEU:O	0.53	2.02	8	1
1:A:100:HIS:CB	1:A:113:ARG:O	0.53	2.57	14	2
1:A:119:LYS:NZ	1:B:270:GLU:CD	0.53	2.67	11	1
1:A:77:GLU:CD	1:A:100:HIS:NE2	0.53	2.67	12	1
1:B:293:THR:OG1	1:B:294:VAL:N	0.53	2.42	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:VAL:O	1:A:18:LEU:N	0.53	2.42	9	14
1:A:41:GLY:O	1:A:42:SER:CB	0.53	2.55	3	4
1:B:246:SER:O	1:B:250:ALA:CB	0.53	2.57	11	8
1:B:276:ASN:O	1:B:303:PHE:N	0.53	2.42	15	5
1:B:252:ARG:O	1:B:256:ALA:CB	0.53	2.56	15	8
1:A:38:ASP:O	1:A:54:PHE:CE2	0.53	2.62	10	3
1:B:280:PHE:CE1	1:B:301:PHE:CD2	0.53	2.97	6	2
1:A:34:ALA:CB	1:A:51:ILE:CD1	0.53	2.82	7	1
1:B:245:ARG:O	1:B:245:ARG:CZ	0.53	2.57	7	1
1:A:38:ASP:O	1:A:43:GLU:CB	0.53	2.56	3	3
1:B:247:GLY:O	1:B:251:ILE:CG1	0.53	2.57	14	7
1:A:62:PRO:O	1:A:86:PHE:CB	0.53	2.57	2	4
1:B:235:THR:O	1:B:236:VAL:HG23	0.53	2.04	2	1
1:A:23:LEU:O	1:A:26:ILE:N	0.53	2.42	9	7
1:B:294:VAL:O	1:B:295:VAL:HG23	0.53	2.04	7	2
1:B:239:PRO:O	1:B:240:VAL:CG1	0.53	2.56	9	1
1:A:7:MET:CB	1:A:73:ALA:HB1	0.53	2.29	13	1
1:A:38:ASP:OD2	1:A:114:ALA:CB	0.53	2.57	8	4
1:B:278:ALA:O	1:B:301:PHE:N	0.53	2.42	6	13
1:B:294:VAL:CG1	1:B:322:HIS:CB	0.53	2.87	8	5
1:B:299:ASP:OD1	1:B:300:HIS:N	0.53	2.42	1	4
1:A:45:ARG:O	1:A:51:ILE:CD1	0.53	2.57	3	4
1:B:221:GLY:HA3	1:B:259:LEU:HD21	0.53	1.78	15	2
1:B:245:ARG:HB2	1:B:254:PHE:CD2	0.53	2.39	3	3
1:A:72:ARG:NE	1:A:73:ALA:N	0.53	2.57	5	1
1:A:80:PHE:CE2	1:A:82:PHE:CE1	0.53	2.97	6	2
1:B:219:ASN:ND2	1:B:265:VAL:O	0.53	2.42	7	3
1:B:267:LEU:O	1:B:268:THR:CG2	0.53	2.57	12	1
1:A:88:PHE:CZ	2:A:126:NTH:O23	0.53	2.62	1	2
1:B:217:ALA:O	1:B:222:ASP:N	0.53	2.42	9	10
1:B:245:ARG:CB	1:B:250:ALA:HB1	0.53	2.33	14	4
1:B:298:ILE:HG22	1:B:299:ASP:N	0.53	2.19	12	4
1:A:118:GLU:OE1	1:B:201:MET:HE2	0.53	2.04	13	1
1:B:294:VAL:O	1:B:322:HIS:CB	0.53	2.57	14	2
1:A:34:ALA:CA	1:A:110:VAL:O	0.53	2.57	1	9
1:A:117:GLY:O	1:A:121:ILE:CD1	0.53	2.57	5	9
1:B:215:VAL:O	1:B:218:LEU:N	0.53	2.42	8	15
1:A:76:ASN:O	1:A:103:PHE:N	0.53	2.42	10	8
1:A:103:PHE:CD1	1:A:108:LYS:O	0.53	2.62	2	1
1:A:105:GLY:O	1:A:106:ALA:CB	0.53	2.57	5	10
1:B:247:GLY:O	1:B:251:ILE:CD1	0.53	2.57	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:O	1:A:51:ILE:HD11	0.53	2.03	11	3
1:B:232:ASP:O	1:B:248:THR:N	0.53	2.42	10	3
1:B:295:VAL:CG1	1:B:321:ILE:HG23	0.53	2.33	5	2
1:A:30:PHE:CZ	1:A:112:MET:HE3	0.53	2.39	6	1
1:B:293:THR:CB	1:B:322:HIS:HB2	0.53	2.34	13	2
1:B:315:LEU:C	1:B:316:PHE:CD1	0.53	2.87	9	2
1:B:215:VAL:HG21	1:B:267:LEU:HD21	0.53	1.80	8	1
1:A:47:GLY:O	1:A:51:ILE:CG1	0.52	2.56	14	4
1:B:201:MET:O	1:B:202:ASN:CB	0.52	2.57	2	2
1:A:45:ARG:HB2	1:A:54:PHE:CD2	0.52	2.38	2	2
1:A:86:PHE:CZ	1:A:93:THR:HB	0.52	2.39	7	6
1:B:276:ASN:ND2	1:B:303:PHE:O	0.52	2.43	2	1
1:A:17:ALA:O	1:A:22:ASP:N	0.52	2.43	9	7
1:B:294:VAL:HG12	1:B:322:HIS:HB3	0.52	1.79	14	4
1:B:298:ILE:CD1	1:B:320:ASN:OD1	0.52	2.57	3	2
1:B:300:HIS:CB	1:B:313:ARG:O	0.52	2.57	4	2
1:B:245:ARG:HD2	1:B:251:ILE:N	0.52	2.20	7	1
1:A:61:LEU:HB2	2:A:126:NTH:H183	0.52	1.78	12	1
1:A:36:VAL:O	1:A:44:PRO:CA	0.52	2.57	6	5
1:A:45:ARG:HG2	1:A:50:ALA:CB	0.52	2.34	2	1
1:A:52:ARG:O	1:A:56:ALA:CB	0.52	2.58	7	6
1:B:229:LEU:O	1:B:309:VAL:CG2	0.52	2.57	2	1
1:B:207:MET:HA	1:B:303:PHE:CZ	0.52	2.40	7	2
1:B:246:SER:C	1:B:250:ALA:HB3	0.52	2.30	3	1
1:A:34:ALA:O	1:A:51:ILE:CD1	0.52	2.57	15	2
1:B:286:PHE:CZ	1:B:293:THR:CB	0.52	2.92	5	4
1:B:237:GLU:O	1:B:314:ALA:CB	0.52	2.57	5	1
1:A:37:GLU:OE2	1:A:113:ARG:CD	0.52	2.58	14	1
1:A:102:ARG:O	1:A:110:VAL:HG23	0.52	2.04	1	2
1:A:4:PRO:O	1:A:8:THR:CB	0.52	2.57	3	3
1:A:10:VAL:CG1	1:A:109:VAL:HG22	0.52	2.35	3	1
1:B:217:ALA:HB3	1:B:226:ILE:HG12	0.52	1.81	3	6
1:A:98:ILE:HG22	1:A:99:ASP:N	0.52	2.20	12	4
1:B:284:VAL:HG12	1:B:286:PHE:CD1	0.52	2.38	6	1
1:A:96:ALA:O	1:A:120:ASN:ND2	0.52	2.42	14	3
1:A:39:PRO:O	1:A:41:GLY:N	0.52	2.42	8	1
1:A:74:VAL:HG12	1:B:240:VAL:HG21	0.52	1.82	8	1
1:B:203:THR:O	1:B:203:THR:CG2	0.52	2.57	15	2
1:A:102:ARG:CZ	1:B:313:ARG:CD	0.52	2.88	15	1
1:A:15:VAL:HA	1:A:18:LEU:CD1	0.52	2.34	10	15
1:A:61:LEU:HD12	1:A:63:LEU:HD21	0.52	1.81	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:HIS:CD2	1:A:101:PHE:N	0.52	2.78	9	1
1:B:304:ASN:CG	1:B:310:VAL:HG21	0.52	2.30	12	1
1:A:95:VAL:HG12	1:A:96:ALA:N	0.52	2.20	14	2
1:B:280:PHE:O	1:B:298:ILE:CG2	0.52	2.57	5	5
1:A:99:ASP:OD1	1:A:100:HIS:N	0.52	2.43	12	7
1:B:245:ARG:CD	1:B:250:ALA:C	0.52	2.83	7	1
1:A:36:VAL:HG12	1:A:37:GLU:N	0.52	2.18	8	4
1:A:39:PRO:O	1:A:40:VAL:HG13	0.52	2.04	1	1
1:B:227:VAL:HG11	1:B:248:THR:CG2	0.52	2.34	2	1
1:B:302:ARG:O	1:B:310:VAL:HG23	0.52	2.03	11	2
1:A:30:PHE:CE1	1:A:112:MET:HE3	0.52	2.40	6	2
1:A:80:PHE:CD1	1:A:80:PHE:N	0.52	2.77	7	1
1:B:286:PHE:CE1	1:B:293:THR:O	0.52	2.62	9	1
1:B:309:VAL:CG1	1:B:312:MET:HE2	0.52	2.26	9	1
1:A:46:SER:O	1:A:50:ALA:CB	0.52	2.57	12	2
1:A:35:THR:N	1:A:110:VAL:O	0.52	2.42	1	1
1:B:270:GLU:O	1:B:272:ARG:CZ	0.52	2.57	9	1
1:A:45:ARG:HD2	1:A:51:ILE:HD13	0.52	1.82	11	1
1:A:63:LEU:HB3	1:A:84:VAL:CG1	0.52	2.34	11	2
1:A:88:PHE:CZ	2:A:126:NTH:O24	0.52	2.63	11	1
1:A:120:ASN:OD1	1:B:272:ARG:NH2	0.52	2.42	14	2
1:A:109:VAL:HG11	1:A:112:MET:HE1	0.52	1.82	14	1
1:A:39:PRO:O	1:A:40:VAL:CG1	0.52	2.58	1	1
1:A:80:PHE:CE2	1:A:99:ASP:HB3	0.52	2.40	11	3
1:A:102:ARG:HB3	1:A:111:SER:CB	0.52	2.35	10	5
1:B:211:VAL:HG22	1:B:280:PHE:CD1	0.52	2.39	7	2
1:A:100:HIS:NE2	1:B:315:LEU:CD1	0.52	2.72	5	1
1:B:261:LEU:HD13	2:B:326:NTH:C20	0.52	2.34	7	1
1:A:3:THR:O	1:A:3:THR:CG2	0.52	2.58	15	6
1:A:40:VAL:O	1:A:42:SER:N	0.52	2.43	2	1
1:A:17:ALA:CB	1:A:22:ASP:OD1	0.52	2.57	6	2
1:A:37:GLU:OE1	1:A:113:ARG:CG	0.52	2.58	1	1
1:A:87:GLU:CG	1:A:88:PHE:N	0.52	2.73	8	2
1:B:210:VAL:HG12	1:B:301:PHE:CE2	0.52	2.40	4	3
1:A:77:GLU:OE1	1:B:313:ARG:NE	0.52	2.43	5	1
1:B:289:GLN:CG	1:B:289:GLN:O	0.52	2.56	6	1
1:B:261:LEU:HB3	1:B:263:LEU:HD21	0.52	1.81	15	1
1:B:223:LEU:O	1:B:226:ILE:N	0.51	2.43	11	8
1:B:247:GLY:C	1:B:251:ILE:HD12	0.51	2.30	2	2
1:B:231:ALA:CB	1:B:309:VAL:O	0.51	2.57	14	2
1:A:31:ALA:CB	1:A:109:VAL:O	0.51	2.56	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:HG3	1:A:54:PHE:CG	0.51	2.40	6	1
1:A:121:ILE:HG22	1:A:122:HIS:H	0.51	1.66	6	13
1:A:80:PHE:CE1	1:A:99:ASP:HB3	0.51	2.40	10	11
1:A:94:VAL:HG12	1:A:122:HIS:HB3	0.51	1.81	14	3
1:A:40:VAL:HG12	1:A:114:ALA:O	0.51	2.06	8	2
1:A:58:SER:OG	2:A:126:NTH:H10	0.51	2.05	8	3
1:B:297:PRO:HB3	1:B:316:PHE:CD2	0.51	2.40	9	1
1:B:207:MET:CB	1:B:273:ALA:HB1	0.51	2.36	8	2
1:A:10:VAL:HG13	1:A:101:PHE:CZ	0.51	2.41	2	4
1:A:92:LYS:CD	1:A:92:LYS:C	0.51	2.82	2	2
1:B:226:ILE:CG2	1:B:230:PHE:CE2	0.51	2.93	2	1
1:A:19:ASN:ND2	1:A:65:VAL:O	0.51	2.43	10	3
1:A:99:ASP:OD2	1:A:112:MET:CE	0.51	2.58	3	3
1:B:294:VAL:CG1	1:B:322:HIS:HB3	0.51	2.35	10	2
1:B:263:LEU:HB3	1:B:284:VAL:HG12	0.51	1.81	11	1
1:A:78:ALA:O	1:A:101:PHE:N	0.51	2.43	2	14
1:B:210:VAL:HG21	1:B:303:PHE:HE1	0.51	1.65	2	1
1:A:72:ARG:CD	1:B:315:LEU:CD2	0.51	2.88	7	1
1:B:316:PHE:CZ	2:B:326:NTH:H72	0.51	2.40	14	2
1:A:37:GLU:OE2	1:A:113:ARG:NH1	0.51	2.44	13	1
1:A:38:ASP:HA	1:A:39:PRO:C	0.51	2.30	9	11
1:B:223:LEU:CD2	1:B:252:ARG:HG2	0.51	2.36	9	8
1:B:223:LEU:CD2	1:B:252:ARG:HG3	0.51	2.34	10	5
1:A:10:VAL:HG12	1:A:101:PHE:CE2	0.51	2.41	5	2
1:B:281:ALA:C	1:B:282:PHE:CD1	0.51	2.89	7	3
1:A:75:ALA:CB	1:B:241:GLY:HA3	0.51	2.36	7	1
1:B:210:VAL:HG13	1:B:309:VAL:CG2	0.51	2.36	7	1
1:A:120:ASN:OD1	1:A:121:ILE:HD13	0.51	2.05	11	1
1:B:280:PHE:CE2	1:B:282:PHE:CE1	0.51	2.99	7	3
1:A:23:LEU:O	1:A:24:ASP:C	0.51	2.54	3	8
1:B:240:VAL:HG12	1:B:314:ALA:O	0.51	2.06	3	1
1:A:115:LEU:C	1:A:116:PHE:CD1	0.51	2.89	4	1
1:A:104:ASN:C	1:A:104:ASN:ND2	0.51	2.69	7	2
1:A:61:LEU:CB	1:A:63:LEU:HD11	0.51	2.33	9	1
1:B:261:LEU:HD12	1:B:263:LEU:HD11	0.51	1.82	14	1
1:B:294:VAL:HG22	1:B:295:VAL:N	0.51	2.21	1	6
1:A:117:GLY:O	1:A:120:ASN:OD1	0.51	2.28	11	3
1:B:309:VAL:HG12	1:B:310:VAL:N	0.51	2.19	13	3
1:A:40:VAL:HG22	1:A:116:PHE:CZ	0.51	2.40	3	1
1:A:86:PHE:CE1	1:A:93:THR:HB	0.51	2.40	14	4
1:A:23:LEU:CD2	1:A:52:ARG:HG2	0.51	2.35	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:300:HIS:CD2	1:B:301:PHE:N	0.51	2.79	7	1
1:A:45:ARG:NH1	1:A:51:ILE:O	0.51	2.43	11	1
1:A:79:ALA:CB	1:B:315:LEU:HD13	0.51	2.34	1	3
1:B:211:VAL:CG2	1:B:301:PHE:CD2	0.51	2.94	10	4
1:B:280:PHE:CE1	1:B:301:PHE:CE2	0.51	2.98	6	3
1:B:287:GLU:OE1	1:B:288:PHE:N	0.51	2.43	7	1
1:B:297:PRO:HB3	1:B:316:PHE:CE1	0.51	2.40	7	1
1:A:100:HIS:NE2	1:A:101:PHE:O	0.51	2.44	9	1
1:B:280:PHE:CE1	1:B:299:ASP:HB3	0.51	2.41	4	11
1:A:61:LEU:CG	1:A:63:LEU:HD21	0.51	2.36	3	1
1:B:217:ALA:CB	1:B:226:ILE:HG12	0.51	2.36	7	2
1:B:300:HIS:CG	1:B:301:PHE:N	0.51	2.79	7	3
1:A:72:ARG:HD3	1:B:315:LEU:CD2	0.51	2.35	7	1
1:A:104:ASN:OD1	1:A:107:GLY:N	0.51	2.43	14	1
1:A:40:VAL:O	1:B:275:ALA:CB	0.51	2.58	15	1
1:A:38:ASP:O	1:A:43:GLU:O	0.51	2.29	7	5
1:B:223:LEU:O	1:B:224:ASP:C	0.51	2.54	12	9
1:A:113:ARG:CG	1:A:114:ALA:N	0.51	2.73	7	1
1:B:230:PHE:CZ	1:B:312:MET:HE1	0.51	2.40	9	1
1:B:245:ARG:HD3	1:B:254:PHE:CD1	0.51	2.41	9	1
1:B:287:GLU:CG	1:B:291:ARG:O	0.51	2.59	9	1
1:B:245:ARG:HB2	1:B:254:PHE:CD1	0.51	2.41	14	1
1:B:235:THR:OG1	1:B:311:SER:CB	0.50	2.59	2	1
1:A:10:VAL:HB	1:A:103:PHE:CZ	0.50	2.40	15	3
1:B:263:LEU:CD2	1:B:284:VAL:CG1	0.50	2.87	8	2
1:B:286:PHE:CE1	1:B:293:THR:HB	0.50	2.41	4	6
1:A:14:TYR:CE2	1:A:80:PHE:CZ	0.50	3.00	10	2
1:B:261:LEU:HB3	1:B:263:LEU:HD11	0.50	1.83	14	1
1:B:215:VAL:HA	1:B:218:LEU:CD1	0.50	2.35	11	15
1:B:280:PHE:CE2	1:B:299:ASP:HB3	0.50	2.41	2	4
1:B:276:ASN:ND2	1:B:304:ASN:O	0.50	2.43	6	1
1:A:119:LYS:CE	1:B:270:GLU:OE2	0.50	2.59	9	1
1:A:35:THR:O	1:A:36:VAL:CG2	0.50	2.59	15	1
1:A:45:ARG:HG3	1:A:54:PHE:CD1	0.50	2.41	7	2
1:A:63:LEU:HB2	1:A:84:VAL:CG1	0.50	2.35	6	2
1:A:56:ALA:O	1:A:59:LEU:N	0.50	2.44	7	1
1:A:116:PHE:CG	1:A:117:GLY:N	0.50	2.75	9	2
1:B:288:PHE:CE2	1:B:291:ARG:CB	0.50	2.94	9	1
1:B:315:LEU:O	1:B:316:PHE:CD2	0.50	2.65	13	1
1:B:268:THR:OG1	1:B:269:GLN:N	0.50	2.43	14	1
1:A:14:TYR:CD1	1:A:15:VAL:HG23	0.50	2.42	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ALA:HB2	1:A:98:ILE:CG1	0.50	2.36	2	2
1:B:210:VAL:HB	1:B:303:PHE:CE2	0.50	2.41	6	4
1:B:277:GLU:OE2	1:B:302:ARG:NE	0.50	2.44	8	1
1:B:304:ASN:N	1:B:310:VAL:CG2	0.50	2.73	13	1
1:A:37:GLU:OE1	1:A:37:GLU:N	0.50	2.45	15	1
1:A:45:ARG:HG3	1:A:54:PHE:CD2	0.50	2.41	1	1
1:A:115:LEU:O	1:A:116:PHE:HB3	0.50	2.07	7	14
1:A:10:VAL:HB	1:A:103:PHE:CE2	0.50	2.42	15	4
1:A:45:ARG:CB	1:A:50:ALA:HB1	0.50	2.37	4	2
1:A:94:VAL:CG1	1:A:122:HIS:CD2	0.50	2.95	7	1
1:B:238:ASP:OD2	1:B:314:ALA:HB3	0.50	2.06	11	1
1:B:263:LEU:HB3	1:B:284:VAL:CG1	0.50	2.36	10	5
1:A:93:THR:HG22	1:A:94:VAL:N	0.50	2.22	4	1
1:B:204:PRO:O	1:B:208:THR:CB	0.50	2.59	15	2
1:B:285:SER:CB	1:B:294:VAL:HG23	0.50	2.37	13	2
1:A:23:LEU:CD2	1:A:52:ARG:HG3	0.50	2.36	7	5
1:B:284:VAL:O	1:B:295:VAL:N	0.50	2.44	3	4
1:B:201:MET:CG	1:B:201:MET:O	0.50	2.60	4	1
1:A:36:VAL:CG2	1:A:51:ILE:CD1	0.50	2.90	8	2
1:A:116:PHE:C	1:B:274:VAL:HG11	0.50	2.31	7	1
1:B:316:PHE:CD2	1:B:321:ILE:HD11	0.50	2.42	7	1
1:B:219:ASN:OD1	1:B:265:VAL:N	0.50	2.43	10	1
1:B:281:ALA:O	1:B:282:PHE:CB	0.50	2.59	10	2
1:B:258:SER:HB2	2:B:326:NTH:H10	0.50	1.82	13	1
1:B:261:LEU:CD2	1:B:263:LEU:HD23	0.50	2.36	15	1
1:A:72:ARG:CG	1:A:79:ALA:O	0.50	2.60	2	1
1:A:72:ARG:NH1	1:B:316:PHE:O	0.50	2.44	5	1
1:A:103:PHE:CD1	1:A:103:PHE:N	0.50	2.80	8	3
1:A:37:GLU:OE1	1:A:113:ARG:NE	0.50	2.43	15	2
1:B:214:TYR:CE2	1:B:255:PHE:CZ	0.50	2.99	7	15
1:B:237:GLU:OE1	1:B:313:ARG:CZ	0.50	2.59	2	1
1:B:258:SER:HG	2:B:326:NTH:H8	0.50	1.66	4	1
1:A:15:VAL:HG21	1:A:67:LEU:HG	0.50	1.84	5	1
1:B:213:ARG:HA	1:B:216:ALA:HB3	0.50	1.83	7	1
1:A:96:ALA:N	1:A:120:ASN:O	0.50	2.43	9	3
1:A:80:PHE:CZ	1:A:99:ASP:CB	0.50	2.95	11	1
1:A:8:THR:O	1:A:11:VAL:N	0.49	2.43	12	4
1:A:6:HIS:NE2	1:A:7:MET:HG3	0.49	2.22	11	1
1:A:88:PHE:O	1:A:89:GLN:C	0.49	2.55	12	2
1:A:11:VAL:HG11	1:A:71:VAL:HG13	0.49	1.85	2	1
1:A:70:GLU:O	1:A:72:ARG:NE	0.49	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ARG:HD3	1:A:54:PHE:CD1	0.49	2.41	8	3
1:A:94:VAL:CG1	1:A:122:HIS:CG	0.49	2.95	14	3
1:A:7:MET:HE2	1:A:73:ALA:CB	0.49	2.37	7	1
1:A:38:ASP:O	1:A:43:GLU:HB2	0.49	2.07	1	3
1:B:227:VAL:O	1:B:230:PHE:O	0.49	2.31	5	4
1:A:35:THR:HG23	1:A:46:SER:HB3	0.49	1.82	3	2
1:A:36:VAL:O	1:A:44:PRO:HA	0.49	2.07	12	5
1:B:210:VAL:CG1	1:B:309:VAL:CG2	0.49	2.91	7	4
1:B:223:LEU:HD22	1:B:256:ALA:HB2	0.49	1.83	9	4
1:A:72:ARG:CD	1:B:315:LEU:HD21	0.49	2.38	7	1
1:B:315:LEU:O	1:B:316:PHE:C	0.49	2.55	9	2
1:B:267:LEU:C	1:B:268:THR:HG23	0.49	2.31	12	1
1:B:286:PHE:CE2	1:B:288:PHE:CD1	0.49	3.01	13	1
1:B:307:GLY:C	1:B:308:LYS:CG	0.49	2.84	4	2
1:A:45:ARG:O	1:A:51:ILE:HD13	0.49	2.07	9	1
1:A:116:PHE:CD1	1:A:116:PHE:C	0.49	2.85	9	1
1:B:208:THR:O	1:B:211:VAL:N	0.49	2.43	15	2
1:B:263:LEU:HB2	1:B:284:VAL:CG1	0.49	2.36	11	2
1:A:118:GLU:HA	1:A:121:ILE:CG1	0.49	2.36	3	13
1:A:115:LEU:CD1	1:B:300:HIS:CD2	0.49	2.94	4	1
1:B:227:VAL:HG21	1:B:252:ARG:CB	0.49	2.37	15	3
1:B:261:LEU:CD2	1:B:263:LEU:HD11	0.49	2.37	8	1
1:B:281:ALA:CA	1:B:298:ILE:HD12	0.49	2.35	11	1
1:A:33:ASP:N	1:A:33:ASP:OD1	0.49	2.43	2	2
1:B:234:ALA:O	1:B:251:ILE:CD1	0.49	2.58	10	3
1:B:210:VAL:HB	1:B:303:PHE:CZ	0.49	2.42	6	5
1:A:115:LEU:CG	1:B:279:ALA:CB	0.49	2.90	4	1
1:A:40:VAL:O	1:A:40:VAL:CG2	0.49	2.60	13	2
1:B:315:LEU:C	1:B:316:PHE:CD2	0.49	2.90	13	1
1:A:47:GLY:C	1:A:51:ILE:HD12	0.49	2.32	14	1
1:B:315:LEU:O	1:B:316:PHE:HB3	0.49	2.08	8	12
1:A:80:PHE:O	1:A:98:ILE:CG2	0.49	2.61	10	5
1:A:115:LEU:O	1:A:116:PHE:C	0.49	2.55	4	1
1:A:103:PHE:C	1:A:110:VAL:CG2	0.49	2.86	8	1
1:B:211:VAL:CG2	1:B:271:VAL:HG11	0.49	2.30	12	2
1:A:36:VAL:HG13	1:A:37:GLU:N	0.49	2.21	14	1
1:A:96:ALA:O	1:A:120:ASN:CG	0.49	2.56	15	8
1:A:36:VAL:O	1:A:44:PRO:HB3	0.49	2.08	14	9
1:A:29:LEU:O	1:A:109:VAL:N	0.49	2.43	3	1
1:A:39:PRO:O	1:A:40:VAL:C	0.49	2.54	6	2
1:A:104:ASN:CB	1:A:110:VAL:HG21	0.49	2.33	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:262:PRO:O	1:B:286:PHE:CB	0.49	2.61	6	2
1:A:58:SER:CB	2:A:126:NTH:H11	0.49	2.37	7	1
1:A:77:GLU:OE2	1:A:100:HIS:CE1	0.49	2.66	9	1
1:A:23:LEU:HD23	1:A:59:LEU:HD22	0.49	1.81	10	1
1:B:293:THR:CG2	1:B:322:HIS:O	0.49	2.61	15	1
1:A:52:ARG:O	1:A:53:GLU:C	0.49	2.56	11	12
1:B:236:VAL:O	1:B:244:PRO:HB3	0.49	2.08	11	13
1:A:17:ALA:CB	1:A:26:ILE:HG12	0.49	2.38	2	1
1:B:272:ARG:O	1:B:279:ALA:N	0.49	2.44	4	4
1:B:317:GLY:O	1:B:320:ASN:OD1	0.49	2.31	4	1
1:B:207:MET:HB3	1:B:273:ALA:HB1	0.49	1.85	8	2
1:A:98:ILE:CD1	1:B:272:ARG:HD2	0.49	2.38	11	1
1:B:235:THR:N	1:B:310:VAL:O	0.49	2.45	12	3
1:A:94:VAL:HG22	1:A:95:VAL:H	0.49	1.68	14	1
1:B:296:ALA:O	1:B:320:ASN:CG	0.49	2.56	9	9
1:B:304:ASN:CG	1:B:310:VAL:CG2	0.49	2.86	12	2
1:A:59:LEU:O	1:A:60:LYS:C	0.49	2.56	10	4
1:B:292:LYS:CD	1:B:292:LYS:C	0.49	2.86	6	3
1:A:75:ALA:CB	1:B:241:GLY:CA	0.49	2.90	7	1
1:A:79:ALA:HB3	1:B:315:LEU:HD11	0.49	1.83	7	1
1:A:19:ASN:CG	1:A:65:VAL:O	0.49	2.56	11	2
1:B:268:THR:O	1:B:269:GLN:HG2	0.49	2.08	8	1
1:A:72:ARG:NH1	1:A:78:ALA:C	0.49	2.70	9	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.49	2.43	10	1
1:A:10:VAL:O	1:A:14:TYR:HB3	0.48	2.08	1	3
1:B:212:GLN:O	1:B:213:ARG:C	0.48	2.56	13	15
1:B:237:GLU:OE2	1:B:313:ARG:NE	0.48	2.43	1	1
1:B:252:ARG:O	1:B:256:ALA:N	0.48	2.44	3	12
1:B:295:VAL:CG1	1:B:297:PRO:HG3	0.48	2.38	7	8
1:A:10:VAL:CB	1:A:103:PHE:CE2	0.48	2.96	3	2
1:A:38:ASP:CG	1:A:114:ALA:CB	0.48	2.86	3	1
1:B:212:GLN:O	1:B:215:VAL:N	0.48	2.45	7	8
1:A:68:THR:C	1:A:69:GLN:HG2	0.48	2.33	9	2
1:B:237:GLU:O	1:B:314:ALA:HB2	0.48	2.08	5	1
1:B:231:ALA:N	1:B:309:VAL:O	0.48	2.42	10	2
1:A:72:ARG:C	1:A:72:ARG:CD	0.48	2.86	9	1
1:A:67:LEU:HD22	1:A:82:PHE:HB3	0.48	1.85	1	1
1:B:300:HIS:N	1:B:313:ARG:O	0.48	2.46	13	7
1:A:10:VAL:HG13	1:A:109:VAL:CG2	0.48	2.39	3	2
1:B:263:LEU:HD23	1:B:286:PHE:CB	0.48	2.37	4	1
1:A:68:THR:O	1:A:69:GLN:HG2	0.48	2.09	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:240:VAL:HG22	1:B:316:PHE:CE1	0.48	2.43	5	1
1:B:277:GLU:CG	1:B:301:PHE:O	0.48	2.61	10	1
1:A:47:GLY:O	1:A:51:ILE:CD1	0.48	2.61	1	4
1:B:215:VAL:O	1:B:216:ALA:C	0.48	2.56	4	15
1:B:236:VAL:O	1:B:244:PRO:CA	0.48	2.61	6	8
1:A:100:HIS:N	1:A:113:ARG:O	0.48	2.45	3	7
1:B:245:ARG:HG3	1:B:254:PHE:CD2	0.48	2.43	2	1
1:A:17:ALA:CB	1:A:26:ILE:HG13	0.48	2.37	11	5
1:A:102:ARG:CB	1:A:111:SER:HB3	0.48	2.39	10	2
1:B:245:ARG:NH1	1:B:246:SER:HA	0.48	2.23	7	1
1:B:268:THR:C	1:B:269:GLN:HG2	0.48	2.34	8	1
1:A:12:GLN:O	1:A:13:ARG:C	0.48	2.57	3	14
1:A:15:VAL:O	1:A:16:ALA:C	0.48	2.57	13	14
1:A:115:LEU:CD1	1:B:300:HIS:NE2	0.48	2.76	3	1
1:A:23:LEU:CD1	1:A:26:ILE:HD12	0.48	2.32	5	3
1:A:100:HIS:CD2	1:A:113:ARG:HG3	0.48	2.44	9	1
1:B:318:GLU:HA	1:B:321:ILE:HD12	0.48	1.84	11	1
1:A:37:GLU:OE2	1:A:113:ARG:NH2	0.48	2.46	15	1
1:B:237:GLU:HB2	1:B:313:ARG:CG	0.48	2.39	1	2
1:B:238:ASP:HA	1:B:239:PRO:C	0.48	2.34	2	14
1:B:277:GLU:CG	1:B:302:ARG:HG3	0.48	2.37	4	3
1:A:10:VAL:O	1:A:14:TYR:HB2	0.48	2.09	3	13
1:A:12:GLN:O	1:A:15:VAL:N	0.48	2.47	2	11
1:A:52:ARG:O	1:A:56:ALA:N	0.48	2.46	7	9
1:B:214:TYR:CD1	1:B:215:VAL:HG23	0.48	2.44	15	7
1:A:22:ASP:CG	1:A:22:ASP:O	0.48	2.57	7	2
1:B:294:VAL:O	1:B:322:HIS:HA	0.48	2.07	13	2
1:A:98:ILE:CD1	1:B:272:ARG:NH1	0.48	2.76	12	1
1:A:6:HIS:HD2	1:A:7:MET:HE3	0.48	1.69	14	1
1:A:47:GLY:O	1:A:51:ILE:HD12	0.48	2.08	1	4
1:B:300:HIS:O	1:B:312:MET:HG2	0.48	2.07	7	12
1:B:272:ARG:N	1:B:279:ALA:O	0.48	2.47	4	10
1:B:210:VAL:HG22	1:B:309:VAL:HG23	0.48	1.83	10	3
1:B:286:PHE:CZ	1:B:288:PHE:CE2	0.48	3.00	5	2
1:B:287:GLU:CD	1:B:288:PHE:N	0.48	2.71	7	2
1:A:38:ASP:HB3	1:A:54:PHE:CE2	0.48	2.44	7	1
1:A:74:VAL:HG11	1:B:240:VAL:HG11	0.48	1.86	8	1
1:A:77:GLU:CG	1:A:100:HIS:NE2	0.48	2.76	12	1
1:A:77:GLU:HG3	1:A:100:HIS:NE2	0.48	2.24	12	1
1:B:258:SER:HA	2:B:326:NTH:H111	0.48	1.86	13	1
1:A:7:MET:HE2	1:A:7:MET:CA	0.48	2.39	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:263:LEU:CD2	1:B:286:PHE:CD1	0.48	2.90	14	1
1:A:69:GLN:CG	1:A:70:GLU:N	0.48	2.73	15	4
1:A:72:ARG:CZ	1:A:72:ARG:HB3	0.48	2.38	5	1
1:B:286:PHE:CE2	1:B:288:PHE:CE2	0.48	3.02	5	1
1:B:239:PRO:O	1:B:241:GLY:N	0.48	2.46	6	1
1:A:72:ARG:HG3	1:A:79:ALA:CB	0.48	2.38	9	1
1:B:252:ARG:O	1:B:253:GLU:C	0.48	2.57	3	10
1:A:81:ALA:CB	1:A:98:ILE:HG13	0.48	2.39	2	1
1:A:115:LEU:HG	1:B:279:ALA:CB	0.48	2.39	4	1
1:B:222:ASP:CG	1:B:222:ASP:O	0.48	2.57	9	4
1:B:302:ARG:HB3	1:B:311:SER:CB	0.48	2.39	12	2
1:B:288:PHE:O	1:B:289:GLN:C	0.48	2.57	5	4
1:A:68:THR:O	1:A:69:GLN:O	0.48	2.32	8	5
1:A:63:LEU:HD21	2:A:126:NTH:O20	0.48	2.08	7	1
1:B:245:ARG:HD3	1:B:250:ALA:HB1	0.48	1.84	11	1
1:A:66:GLU:O	1:A:67:LEU:C	0.48	2.57	1	10
1:A:100:HIS:O	1:A:112:MET:HG2	0.48	2.09	9	13
1:B:202:ASN:O	1:B:203:THR:C	0.48	2.57	1	4
1:B:277:GLU:CG	1:B:302:ARG:CG	0.48	2.91	4	3
1:B:300:HIS:HB2	1:B:313:ARG:CB	0.48	2.39	12	2
1:B:210:VAL:O	1:B:214:TYR:HB2	0.48	2.09	3	11
1:A:50:ALA:O	1:A:51:ILE:C	0.48	2.56	10	4
1:A:86:PHE:CE2	1:A:93:THR:HB	0.48	2.43	6	1
2:B:326:NTH:H222	2:B:326:NTH:H161	0.48	1.85	13	2
1:B:206:HIS:NE2	1:B:207:MET:CE	0.48	2.76	13	1
1:A:33:ASP:HA	1:A:47:GLY:CA	0.48	2.39	5	6
1:A:66:GLU:O	1:A:67:LEU:O	0.48	2.32	9	13
1:A:67:LEU:HD23	1:A:67:LEU:N	0.48	2.23	1	1
1:A:85:SER:HB3	1:A:94:VAL:CG2	0.48	2.39	3	3
1:A:61:LEU:HD23	1:A:63:LEU:CD1	0.48	2.39	3	1
1:A:96:ALA:O	1:A:120:ASN:OD1	0.48	2.32	4	4
1:A:117:GLY:O	1:A:120:ASN:N	0.48	2.47	3	3
1:B:232:ASP:O	1:B:248:THR:OG1	0.48	2.32	9	7
1:A:63:LEU:HD23	1:A:86:PHE:CD2	0.48	2.44	5	1
1:A:102:ARG:CD	1:A:111:SER:HB2	0.48	2.38	6	3
1:B:238:ASP:O	1:B:243:GLU:O	0.48	2.32	6	2
1:B:257:ASN:ND2	1:B:260:LYS:HE2	0.48	2.23	6	1
1:B:245:ARG:CD	1:B:250:ALA:HB1	0.48	2.39	11	2
1:B:238:ASP:OD1	1:B:239:PRO:HA	0.48	2.08	9	5
1:A:86:PHE:CE2	1:A:88:PHE:CD1	0.48	3.02	12	1
1:A:27:VAL:O	1:A:30:PHE:O	0.47	2.32	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:GLU:CD	1:A:88:PHE:O	0.47	2.57	2	3
1:A:7:MET:HA	1:A:103:PHE:CE2	0.47	2.43	15	3
1:A:94:VAL:CG1	1:A:122:HIS:HB3	0.47	2.39	15	3
1:B:303:PHE:CE1	1:B:309:VAL:HG22	0.47	2.44	4	1
1:B:288:PHE:O	1:B:291:ARG:N	0.47	2.40	5	2
1:A:107:GLY:C	1:A:108:LYS:CG	0.47	2.86	14	2
1:A:26:ILE:O	1:A:29:LEU:N	0.47	2.47	7	1
1:A:61:LEU:CD2	1:A:63:LEU:HG	0.47	2.39	7	1
1:A:104:ASN:OD1	1:A:110:VAL:HG22	0.47	2.09	11	1
1:B:204:PRO:O	1:B:205:GLU:C	0.47	2.56	13	1
1:B:240:VAL:HG22	1:B:316:PHE:CZ	0.47	2.43	15	1
1:A:100:HIS:HB3	1:A:113:ARG:CB	0.47	2.39	1	1
1:A:115:LEU:CD2	1:B:279:ALA:HB3	0.47	2.39	10	3
1:B:217:ALA:O	1:B:221:GLY:N	0.47	2.47	7	14
1:A:13:ARG:O	1:A:14:TYR:C	0.47	2.57	2	2
1:A:42:SER:O	1:A:43:GLU:CB	0.47	2.62	2	1
1:A:87:GLU:C	1:A:87:GLU:OE1	0.47	2.57	2	1
1:A:39:PRO:HD2	1:A:42:SER:CB	0.47	2.39	14	7
1:B:201:MET:O	1:B:202:ASN:C	0.47	2.57	14	3
1:A:72:ARG:HD2	1:A:73:ALA:N	0.47	2.24	9	1
1:B:210:VAL:HG21	1:B:309:VAL:HG23	0.47	1.84	10	1
1:B:245:ARG:HG3	1:B:254:PHE:CD1	0.47	2.44	13	2
1:A:99:ASP:OD1	1:A:113:ARG:O	0.47	2.33	8	10
1:B:259:LEU:O	1:B:260:LYS:C	0.47	2.57	4	5
1:A:17:ALA:HB3	1:A:26:ILE:HG12	0.47	1.86	13	3
1:A:17:ALA:O	1:A:21:GLY:N	0.47	2.48	7	12
1:A:93:THR:CG2	1:A:122:HIS:O	0.47	2.60	8	1
1:A:104:ASN:N	1:A:110:VAL:CG2	0.47	2.77	9	1
1:A:6:HIS:CD2	1:A:7:MET:N	0.47	2.83	11	1
1:A:36:VAL:HG11	1:A:54:PHE:CD2	0.47	2.44	14	1
1:A:6:HIS:NE2	1:A:106:ALA:O	0.47	2.47	1	1
1:A:30:PHE:CE1	1:A:112:MET:CE	0.47	2.98	1	2
1:B:233:ASP:HA	1:B:247:GLY:CA	0.47	2.39	7	11
1:B:266:GLU:O	1:B:267:LEU:O	0.47	2.33	4	15
1:B:299:ASP:OD1	1:B:313:ARG:O	0.47	2.33	10	11
1:A:38:ASP:OD1	1:A:114:ALA:CB	0.47	2.58	3	1
1:B:277:GLU:O	1:B:278:ALA:CB	0.47	2.62	10	3
2:B:326:NTH:H222	2:B:326:NTH:C16	0.47	2.39	13	2
1:A:22:ASP:CG	1:A:24:ASP:OD1	0.47	2.58	10	1
1:A:77:GLU:HG3	1:A:101:PHE:O	0.47	2.10	12	1
1:A:45:ARG:HB2	1:A:54:PHE:CD1	0.47	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:LEU:HD12	1:B:263:LEU:CD2	0.47	2.40	14	1
1:A:102:ARG:NH1	1:A:113:ARG:HD2	0.47	2.25	15	1
1:A:38:ASP:HA	1:A:39:PRO:O	0.47	2.09	2	2
1:A:85:SER:CA	1:A:94:VAL:HG23	0.47	2.38	3	4
1:A:116:PHE:CZ	2:A:126:NTH:C6	0.47	2.98	7	2
1:A:98:ILE:O	1:A:115:LEU:O	0.47	2.33	3	1
1:A:27:VAL:HG21	1:A:52:ARG:CG	0.47	2.39	11	3
1:A:74:VAL:HG22	1:B:316:PHE:O	0.47	2.09	12	2
1:B:296:ALA:O	1:B:320:ASN:OD1	0.47	2.32	8	2
1:B:315:LEU:O	1:B:316:PHE:O	0.47	2.33	9	1
1:B:258:SER:CB	2:B:326:NTH:H10	0.47	2.38	13	1
1:B:285:SER:CA	1:B:294:VAL:HG23	0.47	2.40	15	2
1:A:77:GLU:CG	1:A:102:ARG:CG	0.47	2.92	1	2
1:B:210:VAL:O	1:B:214:TYR:HB3	0.47	2.09	1	6
1:B:230:PHE:O	1:B:231:ALA:O	0.47	2.33	14	13
1:A:36:VAL:HG13	1:A:112:MET:HE2	0.47	1.86	7	1
1:A:113:ARG:NH1	1:B:277:GLU:OE2	0.47	2.48	7	2
1:A:45:ARG:HD3	1:A:54:PHE:CB	0.47	2.40	11	1
1:B:274:VAL:O	1:B:277:GLU:O	0.47	2.32	14	1
1:A:30:PHE:HD2	1:A:34:ALA:HB3	0.47	1.70	15	1
1:A:21:GLY:O	1:A:59:LEU:CD2	0.47	2.62	6	3
1:A:30:PHE:O	1:A:31:ALA:O	0.47	2.33	14	12
1:A:94:VAL:O	1:A:122:HIS:HB2	0.47	2.10	4	11
1:B:250:ALA:O	1:B:251:ILE:C	0.47	2.58	9	8
1:B:269:GLN:HG3	1:B:270:GLU:N	0.47	2.25	10	7
1:A:97:PRO:CB	1:A:116:PHE:HB3	0.47	2.40	3	1
1:B:296:ALA:CB	1:B:320:ASN:O	0.47	2.63	12	2
1:A:14:TYR:CE1	1:A:80:PHE:CZ	0.47	3.02	4	2
1:A:72:ARG:O	1:A:79:ALA:O	0.47	2.33	4	1
1:B:226:ILE:HD13	1:B:255:PHE:CE2	0.47	2.44	4	1
1:A:71:VAL:HG12	1:A:72:ARG:N	0.47	2.24	5	1
1:A:39:PRO:O	1:A:40:VAL:HG22	0.47	2.10	6	1
1:A:113:ARG:HG2	1:A:114:ALA:N	0.47	2.25	7	1
1:A:92:LYS:O	1:A:124:GLY:O	0.47	2.33	8	1
1:B:238:ASP:OD1	1:B:239:PRO:O	0.47	2.32	9	1
1:A:22:ASP:CG	1:A:24:ASP:CG	0.47	2.82	10	1
1:A:55:PHE:CE1	2:A:126:NTH:C2	0.47	2.98	10	1
1:A:64:ALA:CB	1:A:85:SER:OG	0.47	2.58	10	1
1:A:115:LEU:HD13	1:B:300:HIS:CD2	0.47	2.45	10	1
1:A:45:ARG:HB3	1:A:54:PHE:CD2	0.47	2.44	11	1
1:A:45:ARG:NE	1:A:54:PHE:HB3	0.47	2.25	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CZ	2:A:126:NTH:C22	0.47	2.98	11	1
1:B:230:PHE:HD2	1:B:234:ALA:HB3	0.47	1.70	12	2
1:B:286:PHE:CD2	1:B:287:GLU:N	0.47	2.83	11	1
1:B:292:LYS:CD	1:B:292:LYS:O	0.47	2.63	12	1
1:A:88:PHE:O	1:A:89:GLN:O	0.47	2.33	15	1
1:B:214:TYR:CZ	1:B:312:MET:HE1	0.47	2.44	15	1
1:B:245:ARG:HB2	1:B:254:PHE:CG	0.47	2.45	15	1
1:A:41:GLY:O	1:A:42:SER:O	0.47	2.33	6	2
1:A:100:HIS:O	1:A:112:MET:HG3	0.47	2.09	14	2
1:B:295:VAL:CG1	1:B:320:ASN:ND2	0.47	2.78	4	1
1:B:234:ALA:H	1:B:251:ILE:HD11	0.47	1.64	7	1
1:B:245:ARG:HD2	1:B:250:ALA:C	0.47	2.34	7	1
1:A:35:THR:CG2	1:A:46:SER:HB2	0.47	2.40	12	4
1:B:286:PHE:CZ	1:B:293:THR:CG2	0.47	2.98	14	1
1:A:43:GLU:N	1:A:44:PRO:CD	0.47	2.78	3	5
1:B:230:PHE:O	1:B:231:ALA:C	0.47	2.57	11	4
1:B:247:GLY:O	1:B:251:ILE:HG13	0.47	2.10	9	8
1:A:78:ALA:N	1:A:101:PHE:O	0.47	2.48	4	1
1:B:222:ASP:O	1:B:222:ASP:CG	0.47	2.58	6	2
1:B:223:LEU:HG	1:B:256:ALA:HB2	0.47	1.87	8	2
1:B:321:ILE:CG2	2:B:326:NTH:H222	0.47	2.40	12	1
1:B:315:LEU:C	1:B:316:PHE:CG	0.47	2.93	13	1
1:A:62:PRO:O	1:A:86:PHE:HB2	0.47	2.10	11	8
1:A:72:ARG:N	1:A:79:ALA:O	0.47	2.46	10	7
1:A:26:ILE:HG21	1:A:55:PHE:CG	0.47	2.45	5	3
1:B:268:THR:O	1:B:269:GLN:O	0.47	2.33	7	4
1:A:100:HIS:NE2	1:B:315:LEU:HD13	0.47	2.25	5	1
1:B:243:GLU:N	1:B:244:PRO:HD3	0.47	2.24	6	2
1:B:202:ASN:ND2	1:B:207:MET:HE1	0.47	2.25	8	1
1:A:20:ALA:O	1:A:21:GLY:C	0.46	2.58	14	7
1:B:294:VAL:CG1	1:B:295:VAL:N	0.46	2.78	6	3
1:B:220:ALA:O	1:B:221:GLY:C	0.46	2.58	11	2
1:A:35:THR:OG1	1:A:111:SER:OG	0.46	2.33	12	4
1:B:304:ASN:CA	1:B:310:VAL:HG21	0.46	2.40	7	2
1:B:309:VAL:CG1	1:B:312:MET:CE	0.46	2.93	13	2
1:A:101:PHE:CD1	1:A:112:MET:HE2	0.46	2.42	10	1
1:A:94:VAL:CG2	1:A:95:VAL:N	0.46	2.77	15	1
1:A:33:ASP:O	1:A:34:ALA:O	0.46	2.33	10	3
1:B:302:ARG:CB	1:B:311:SER:CB	0.46	2.93	3	1
1:B:288:PHE:C	1:B:289:GLN:HG2	0.46	2.35	5	3
1:A:32:ASP:O	1:A:48:THR:OG1	0.46	2.33	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD11	1:A:55:PHE:O	0.46	2.10	8	1
1:A:6:HIS:CG	1:A:7:MET:N	0.46	2.83	11	1
1:A:15:VAL:HG22	1:A:65:VAL:HG11	0.46	1.87	12	1
1:B:293:THR:CG2	1:B:322:HIS:ND1	0.46	2.78	13	1
1:A:95:VAL:CG1	1:A:96:ALA:N	0.46	2.78	14	2
1:A:104:ASN:HB3	1:A:110:VAL:CG2	0.46	2.40	4	4
1:B:299:ASP:OD2	1:B:312:MET:CE	0.46	2.62	3	2
1:B:274:VAL:O	1:B:275:ALA:O	0.46	2.33	12	2
1:A:110:VAL:HG12	1:A:110:VAL:O	0.46	2.10	6	1
1:A:25:GLY:O	1:A:28:ALA:HB3	0.46	2.10	7	1
1:A:38:ASP:OD1	2:A:126:NTH:H62	0.46	2.11	8	1
1:B:264:ALA:N	1:B:285:SER:O	0.46	2.48	12	1
1:A:72:ARG:HD3	1:B:298:ILE:CD1	0.46	2.41	12	2
1:B:266:GLU:O	1:B:267:LEU:C	0.46	2.59	14	11
1:B:272:ARG:O	1:B:279:ALA:O	0.46	2.33	14	2
1:B:318:GLU:HA	1:B:321:ILE:CG1	0.46	2.41	6	10
1:A:35:THR:O	1:A:112:MET:N	0.46	2.48	12	6
1:A:37:GLU:HB3	1:A:113:ARG:NH1	0.46	2.25	3	1
1:B:302:ARG:CB	1:B:311:SER:HB2	0.46	2.41	3	4
1:B:210:VAL:O	1:B:229:LEU:CD2	0.46	2.63	15	2
1:A:100:HIS:HB2	1:A:113:ARG:O	0.46	2.11	10	2
1:B:213:ARG:O	1:B:214:TYR:C	0.46	2.57	7	2
1:A:61:LEU:HD13	2:A:126:NTH:C20	0.46	2.40	7	1
1:B:287:GLU:OE2	1:B:290:GLY:N	0.46	2.49	7	1
1:A:104:ASN:N	1:A:110:VAL:HG21	0.46	2.25	9	1
1:A:36:VAL:O	1:A:44:PRO:HB2	0.46	2.11	11	1
1:A:19:ASN:OD1	1:A:65:VAL:O	0.46	2.33	15	1
1:A:54:PHE:O	1:A:55:PHE:C	0.46	2.58	3	8
1:A:84:VAL:O	1:A:94:VAL:HA	0.46	2.11	1	7
1:B:236:VAL:O	1:B:244:PRO:HA	0.46	2.10	6	11
1:A:14:TYR:CE2	1:A:55:PHE:CZ	0.46	3.04	15	10
1:A:84:VAL:O	1:A:95:VAL:N	0.46	2.49	3	3
1:B:285:SER:HA	1:B:294:VAL:CG2	0.46	2.40	6	2
1:A:87:GLU:CD	1:A:90:GLY:O	0.46	2.59	8	1
1:B:297:PRO:HA	1:B:316:PHE:CB	0.46	2.40	9	1
1:A:80:PHE:CE2	1:A:82:PHE:CD2	0.46	3.03	10	1
1:B:243:GLU:O	1:B:243:GLU:CD	0.46	2.58	10	1
1:A:85:SER:HA	1:A:94:VAL:CG2	0.46	2.41	1	7
1:A:95:VAL:CG1	1:A:97:PRO:HG3	0.46	2.41	12	8
1:B:237:GLU:OE1	1:B:313:ARG:NE	0.46	2.49	2	1
1:A:103:PHE:N	1:A:103:PHE:CD1	0.46	2.83	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:214:TYR:CE1	1:B:280:PHE:CZ	0.46	3.03	4	4
1:A:79:ALA:HB1	1:B:315:LEU:HD21	0.46	1.86	5	1
1:A:39:PRO:O	1:A:40:VAL:CG2	0.46	2.64	6	1
1:A:73:ALA:O	1:A:74:VAL:HG22	0.46	2.10	7	1
1:B:261:LEU:CG	1:B:263:LEU:HD21	0.46	2.39	8	1
1:A:72:ARG:NH2	1:B:315:LEU:HD12	0.46	2.26	9	1
1:B:287:GLU:HG3	1:B:291:ARG:O	0.46	2.11	9	2
1:A:39:PRO:C	1:A:40:VAL:HG13	0.46	2.36	1	1
1:B:235:THR:O	1:B:312:MET:N	0.46	2.49	4	3
1:A:116:PHE:CE1	2:A:126:NTH:C6	0.46	2.98	2	2
1:A:85:SER:HA	1:A:94:VAL:HG22	0.46	1.85	9	1
1:A:22:ASP:OD1	1:A:24:ASP:OD1	0.46	2.34	10	1
1:A:22:ASP:OD2	1:A:24:ASP:OD2	0.46	2.34	10	1
1:B:227:VAL:CG2	1:B:252:ARG:HB2	0.46	2.41	5	8
1:A:35:THR:CG2	1:A:46:SER:HB3	0.46	2.41	14	4
1:B:207:MET:SD	1:B:274:VAL:O	0.46	2.74	13	2
1:A:115:LEU:O	1:A:116:PHE:O	0.46	2.33	4	1
1:B:217:ALA:CB	1:B:226:ILE:HG13	0.46	2.41	4	4
1:B:230:PHE:CZ	1:B:312:MET:SD	0.46	3.09	13	2
1:A:18:LEU:HD21	1:A:55:PHE:CZ	0.46	2.46	10	1
2:A:126:NTH:C16	2:A:126:NTH:H222	0.46	2.40	14	1
1:B:233:ASP:N	1:B:233:ASP:OD1	0.46	2.48	15	1
1:A:34:ALA:HA	1:A:110:VAL:O	0.46	2.11	7	9
1:A:39:PRO:HG2	1:A:42:SER:CB	0.46	2.41	2	2
1:A:117:GLY:O	1:A:121:ILE:HG12	0.46	2.11	15	4
1:A:120:ASN:OD1	1:B:272:ARG:NE	0.46	2.43	4	1
1:A:3:THR:O	1:A:7:MET:SD	0.46	2.74	7	1
1:B:245:ARG:HG2	1:B:246:SER:N	0.46	2.26	7	1
1:B:293:THR:CG2	1:B:322:HIS:HB2	0.46	2.40	13	2
1:B:219:ASN:OD1	1:B:265:VAL:O	0.46	2.33	9	4
1:A:102:ARG:NH1	1:A:113:ARG:CD	0.46	2.79	15	1
1:A:27:VAL:CG2	1:A:52:ARG:HB2	0.46	2.42	1	9
1:B:222:ASP:O	1:B:223:LEU:C	0.46	2.59	9	8
1:B:234:ALA:HA	1:B:310:VAL:O	0.46	2.11	11	14
1:B:294:VAL:O	1:B:322:HIS:HB2	0.46	2.11	6	7
1:B:304:ASN:HB3	1:B:310:VAL:CG2	0.46	2.41	7	2
1:A:23:LEU:CD2	1:A:52:ARG:HA	0.46	2.41	9	2
1:B:214:TYR:CZ	1:B:218:LEU:HD11	0.46	2.46	4	2
1:A:72:ARG:CZ	1:A:72:ARG:CB	0.46	2.94	5	1
1:A:74:VAL:O	1:A:75:ALA:O	0.46	2.34	7	3
2:A:126:NTH:C16	2:A:126:NTH:H221	0.46	2.41	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:302:ARG:C	1:B:303:PHE:CD1	0.46	2.94	14	1
1:A:14:TYR:N	1:A:29:LEU:HD22	0.45	2.25	1	1
1:A:15:VAL:HG21	1:A:67:LEU:HD21	0.45	1.88	1	1
1:B:207:MET:SD	1:B:275:ALA:O	0.45	2.74	3	4
1:B:221:GLY:O	1:B:259:LEU:HD21	0.45	2.11	11	3
1:B:317:GLY:O	1:B:321:ILE:HG12	0.45	2.12	2	6
1:A:22:ASP:O	1:A:23:LEU:C	0.45	2.59	3	5
1:A:119:LYS:HE2	1:B:204:PRO:CG	0.45	2.42	4	1
1:A:71:VAL:CG1	1:A:72:ARG:N	0.45	2.78	5	2
1:A:39:PRO:O	1:A:42:SER:CB	0.45	2.64	6	1
1:B:301:PHE:CE1	1:B:309:VAL:CG2	0.45	2.99	7	1
1:A:39:PRO:CD	1:A:42:SER:CB	0.45	2.94	9	1
1:A:59:LEU:C	1:A:61:LEU:N	0.45	2.74	10	1
1:B:282:PHE:CE2	1:B:284:VAL:HG23	0.45	2.46	15	1
1:A:80:PHE:O	1:A:99:ASP:N	0.45	2.47	1	4
1:A:102:ARG:N	1:A:111:SER:O	0.45	2.50	14	2
1:A:103:PHE:CE1	1:A:109:VAL:HG22	0.45	2.46	1	1
1:B:288:PHE:CD1	1:B:288:PHE:N	0.45	2.84	3	2
1:B:237:GLU:OE1	1:B:313:ARG:NH1	0.45	2.48	7	1
1:B:240:VAL:HG21	1:B:317:GLY:HA2	0.45	1.89	7	1
1:A:104:ASN:N	1:A:104:ASN:ND2	0.45	2.65	10	1
1:A:67:LEU:O	1:A:68:THR:HG23	0.45	2.11	12	1
1:A:37:GLU:OE2	1:A:113:ARG:HD3	0.45	2.12	14	1
1:A:75:ALA:CB	1:B:240:VAL:O	0.45	2.64	15	1
1:A:33:ASP:CB	1:A:47:GLY:HA2	0.45	2.42	4	5
1:A:49:ALA:O	1:A:53:GLU:HB2	0.45	2.11	1	6
1:B:254:PHE:O	1:B:255:PHE:C	0.45	2.58	14	7
1:A:23:LEU:C	1:A:25:GLY:N	0.45	2.73	3	3
1:A:88:PHE:CE2	2:A:126:NTH:O23	0.45	2.69	3	1
1:B:272:ARG:CG	1:B:279:ALA:O	0.45	2.64	9	4
1:B:308:LYS:HD2	1:B:308:LYS:N	0.45	2.26	6	1
1:A:86:PHE:CZ	2:A:126:NTH:C23	0.45	3.00	7	1
1:A:17:ALA:HB1	1:A:26:ILE:HG13	0.45	1.89	9	4
1:A:72:ARG:C	1:A:72:ARG:HD2	0.45	2.36	9	1
1:B:239:PRO:HD2	1:B:242:SER:CB	0.45	2.40	2	6
1:B:276:ASN:OD1	1:B:276:ASN:O	0.45	2.34	4	1
1:B:211:VAL:HG13	1:B:280:PHE:CG	0.45	2.46	7	1
1:A:87:GLU:HG2	1:A:88:PHE:N	0.45	2.26	15	3
1:B:303:PHE:N	1:B:303:PHE:CD1	0.45	2.85	15	2
1:B:222:ASP:O	1:B:222:ASP:OD2	0.45	2.33	10	1
1:A:40:VAL:HG21	1:B:274:VAL:CB	0.45	2.41	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ASN:CG	1:A:60:LYS:CE	0.45	2.90	1	1
1:A:72:ARG:O	1:A:79:ALA:N	0.45	2.49	7	2
1:A:52:ARG:C	1:A:54:PHE:N	0.45	2.74	8	8
1:A:88:PHE:N	1:A:91:ARG:O	0.45	2.49	6	1
1:A:32:ASP:C	1:A:48:THR:HG1	0.45	2.19	8	1
1:A:14:TYR:CD2	1:A:101:PHE:CZ	0.45	3.04	10	1
1:B:304:ASN:ND2	1:B:310:VAL:HB	0.45	2.26	10	1
1:A:92:LYS:HE3	1:A:125:ALA:OXT	0.45	2.11	14	1
1:A:102:ARG:CD	1:B:313:ARG:HD3	0.45	2.41	15	1
1:A:7:MET:SD	1:A:74:VAL:O	0.45	2.75	4	1
1:A:63:LEU:HD23	1:A:86:PHE:HB3	0.45	1.88	7	1
1:B:280:PHE:O	1:B:299:ASP:N	0.45	2.47	7	4
1:A:43:GLU:OE1	1:A:43:GLU:N	0.45	2.48	9	1
1:A:72:ARG:NH2	1:B:315:LEU:HA	0.45	2.26	9	1
1:B:286:PHE:CE2	1:B:288:PHE:CZ	0.45	3.05	12	1
1:A:102:ARG:NH2	1:B:313:ARG:CB	0.45	2.80	15	1
1:A:23:LEU:CD1	1:A:55:PHE:HB3	0.45	2.42	10	7
1:A:69:GLN:HG3	1:A:70:GLU:N	0.45	2.26	13	4
1:A:64:ALA:N	1:A:85:SER:O	0.45	2.47	10	4
1:B:292:LYS:O	1:B:292:LYS:HD3	0.45	2.12	4	1
1:A:11:VAL:HG22	1:A:80:PHE:CD1	0.45	2.47	5	1
1:A:36:VAL:HG22	1:A:112:MET:HE2	0.45	1.89	5	1
1:A:41:GLY:O	1:A:42:SER:HB2	0.45	2.12	7	3
1:A:102:ARG:CB	1:A:111:SER:HB2	0.45	2.41	1	2
1:A:24:ASP:O	1:A:28:ALA:CB	0.45	2.65	2	1
1:A:27:VAL:HG21	1:A:52:ARG:CB	0.45	2.38	2	2
1:A:10:VAL:CB	1:A:103:PHE:CZ	0.45	3.00	3	2
1:B:289:GLN:O	1:B:290:GLY:C	0.45	2.59	3	1
1:B:277:GLU:HG2	1:B:301:PHE:O	0.45	2.11	10	6
1:A:34:ALA:CA	1:A:51:ILE:HD11	0.45	2.42	7	1
1:B:245:ARG:NH1	1:B:251:ILE:HG12	0.45	2.27	7	1
1:B:210:VAL:CG2	1:B:303:PHE:CE2	0.45	3.00	9	1
1:A:22:ASP:OD1	1:A:24:ASP:OD2	0.45	2.33	10	1
1:B:321:ILE:HG22	1:B:322:HIS:CD2	0.45	2.47	13	1
1:A:98:ILE:CD1	1:B:272:ARG:NE	0.45	2.79	14	1
1:A:102:ARG:CB	1:A:111:SER:O	0.45	2.65	6	5
1:B:210:VAL:CB	1:B:303:PHE:CZ	0.45	3.00	6	5
1:B:262:PRO:O	1:B:286:PHE:HB2	0.45	2.11	15	6
1:B:297:PRO:HA	1:B:320:ASN:OD1	0.45	2.11	3	1
1:B:256:ALA:O	1:B:257:ASN:C	0.45	2.60	7	1
1:B:261:LEU:HD21	1:B:286:PHE:CD2	0.45	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:HIS:CD2	1:B:315:LEU:CD1	0.45	3.00	8	1
1:A:45:ARG:HD2	1:A:51:ILE:CD1	0.45	2.41	11	1
1:A:85:SER:OG	1:A:85:SER:O	0.45	2.33	15	2
1:A:100:HIS:CD2	1:B:300:HIS:CD2	0.45	3.04	15	1
1:B:226:ILE:HG22	1:B:230:PHE:CD2	0.45	2.46	1	1
1:A:37:GLU:O	1:A:114:ALA:CB	0.45	2.64	2	1
1:A:10:VAL:CG2	1:A:103:PHE:CE2	0.45	2.99	8	2
1:B:233:ASP:O	1:B:233:ASP:CG	0.45	2.60	4	1
1:A:67:LEU:O	1:A:68:THR:HB	0.45	2.12	5	1
1:B:275:ALA:O	1:B:276:ASN:CG	0.45	2.60	5	1
1:B:272:ARG:O	1:B:278:ALA:HB1	0.45	2.12	15	2
1:B:293:THR:HB	1:B:322:HIS:CB	0.45	2.42	7	1
1:B:293:THR:HG22	1:B:322:HIS:HB2	0.45	1.87	13	1
1:B:273:ALA:O	1:B:274:VAL:HG22	0.45	2.12	14	1
1:A:42:SER:C	1:A:43:GLU:CG	0.44	2.89	2	1
1:B:249:ALA:O	1:B:253:GLU:HB2	0.44	2.12	4	9
1:B:317:GLY:O	1:B:320:ASN:N	0.44	2.43	4	1
1:A:107:GLY:O	1:A:108:LYS:HB2	0.44	2.11	6	2
1:A:117:GLY:O	1:A:121:ILE:CG1	0.44	2.65	15	2
1:A:10:VAL:HG11	1:A:109:VAL:HG22	0.44	1.88	9	1
1:A:61:LEU:CD2	2:A:126:NTH:O17	0.44	2.66	9	1
1:A:86:PHE:CZ	2:A:126:NTH:C20	0.44	2.99	11	1
1:A:120:ASN:OD1	1:B:272:ARG:CZ	0.44	2.65	14	2
1:B:238:ASP:CG	1:B:239:PRO:HA	0.44	2.37	13	11
1:B:274:VAL:O	1:B:276:ASN:N	0.44	2.49	7	2
1:A:3:THR:O	1:A:6:HIS:CD2	0.44	2.71	13	1
1:A:38:ASP:OD1	1:A:39:PRO:HA	0.44	2.11	1	2
1:A:57:ASN:ND2	1:A:60:LYS:CE	0.44	2.81	1	1
1:B:269:GLN:CG	1:B:270:GLU:N	0.44	2.78	1	3
1:A:23:LEU:O	1:A:25:GLY:N	0.44	2.51	11	2
1:A:26:ILE:HG22	1:A:30:PHE:CD2	0.44	2.48	3	2
1:B:217:ALA:HB1	1:B:226:ILE:HG13	0.44	1.88	11	4
1:B:296:ALA:N	1:B:297:PRO:HD3	0.44	2.27	11	2
1:A:86:PHE:CE1	2:A:126:NTH:C21	0.44	3.00	7	1
1:B:258:SER:CB	2:B:326:NTH:H11	0.44	2.42	7	1
1:A:10:VAL:HG21	1:A:109:VAL:HG23	0.44	1.89	9	1
1:A:109:VAL:HG11	1:A:112:MET:CE	0.44	2.42	10	1
1:A:11:VAL:HG11	1:A:71:VAL:HG11	0.44	1.90	13	1
1:A:74:VAL:HG11	1:B:317:GLY:HA2	0.44	1.88	13	1
2:A:126:NTH:H222	2:A:126:NTH:H161	0.44	1.89	14	1
1:A:92:LYS:CD	1:A:92:LYS:O	0.44	2.66	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:CG1	1:A:71:VAL:CG2	0.44	2.94	2	1
1:A:97:PRO:HB3	1:A:120:ASN:ND2	0.44	2.27	11	3
1:A:100:HIS:CB	1:A:113:ARG:HB2	0.44	2.42	2	2
1:A:48:THR:C	1:A:50:ALA:N	0.44	2.75	3	1
1:B:217:ALA:HB3	1:B:226:ILE:CG1	0.44	2.42	12	2
1:A:107:GLY:C	1:A:108:LYS:HG2	0.44	2.38	6	2
1:A:54:PHE:C	1:A:56:ALA:N	0.44	2.75	7	5
1:A:27:VAL:CG2	1:A:52:ARG:HG3	0.44	2.42	8	1
1:A:45:ARG:CG	1:A:50:ALA:CB	0.44	2.83	10	1
1:B:238:ASP:HA	1:B:239:PRO:O	0.44	2.12	13	1
1:B:316:PHE:CE1	2:B:326:NTH:C6	0.44	3.00	14	1
1:A:102:ARG:NH1	1:B:313:ARG:HD2	0.44	2.28	15	1
1:A:72:ARG:HB2	1:A:79:ALA:O	0.44	2.12	4	8
1:B:272:ARG:HB2	1:B:279:ALA:O	0.44	2.13	8	10
1:A:76:ASN:O	1:A:103:PHE:HB2	0.44	2.13	6	2
1:B:292:LYS:O	1:B:292:LYS:CD	0.44	2.65	4	1
1:B:263:LEU:CB	1:B:286:PHE:HB3	0.44	2.42	5	3
1:B:237:GLU:O	1:B:238:ASP:CB	0.44	2.65	9	1
1:A:37:GLU:OE2	1:A:113:ARG:CG	0.44	2.65	12	1
1:B:206:HIS:NE2	1:B:207:MET:HG3	0.44	2.28	13	1
1:B:263:LEU:HD13	1:B:284:VAL:HG11	0.44	1.89	13	1
1:B:286:PHE:CZ	2:B:326:NTH:C21	0.44	2.99	14	1
1:A:37:GLU:OE1	1:A:113:ARG:HG2	0.44	2.13	1	1
1:A:102:ARG:HB2	1:A:111:SER:C	0.44	2.38	6	4
1:A:118:GLU:HA	1:A:121:ILE:HG12	0.44	1.88	3	2
1:B:207:MET:HE1	1:B:306:ALA:HA	0.44	1.90	9	1
1:B:238:ASP:CB	1:B:239:PRO:HA	0.44	2.43	9	1
1:A:55:PHE:CZ	2:A:126:NTH:C2	0.44	3.00	10	1
1:A:5:GLU:O	1:A:6:HIS:C	0.44	2.59	13	1
1:B:223:LEU:HD23	1:B:259:LEU:HD22	0.44	1.83	15	1
1:B:294:VAL:HG12	1:B:322:HIS:HB2	0.44	1.89	2	1
1:A:30:PHE:O	1:A:31:ALA:C	0.44	2.61	14	4
1:B:270:GLU:O	1:B:271:VAL:C	0.44	2.60	4	2
1:B:316:PHE:CD1	1:B:317:GLY:N	0.44	2.85	5	1
1:B:243:GLU:N	1:B:244:PRO:CD	0.44	2.80	6	1
1:A:17:ALA:HB3	1:A:26:ILE:CG1	0.44	2.42	11	2
1:B:317:GLY:O	1:B:321:ILE:CG1	0.44	2.66	2	4
1:A:63:LEU:HD22	1:A:84:VAL:HG12	0.44	1.85	3	1
1:B:261:LEU:O	1:B:263:LEU:HD11	0.44	2.12	5	3
1:B:286:PHE:CE2	1:B:293:THR:OG1	0.44	2.70	5	1
1:A:38:ASP:CG	2:A:126:NTH:H62	0.44	2.37	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CE2	1:A:93:THR:OG1	0.44	2.70	7	1
1:B:287:GLU:C	1:B:288:PHE:CD1	0.44	2.96	7	1
1:B:297:PRO:CB	1:B:316:PHE:CE1	0.44	3.00	7	1
1:B:222:ASP:OD2	1:B:225:GLY:N	0.44	2.51	10	1
1:A:4:PRO:O	1:A:5:GLU:C	0.44	2.60	15	1
1:A:63:LEU:CB	1:A:86:PHE:HB3	0.44	2.43	15	6
1:A:9:ALA:O	1:A:10:VAL:C	0.44	2.60	6	4
1:B:293:THR:CG2	1:B:323:ALA:HA	0.44	2.43	3	2
1:A:38:ASP:CG	1:A:39:PRO:HA	0.44	2.37	4	7
1:A:67:LEU:HA	1:A:82:PHE:CB	0.44	2.43	5	1
1:A:61:LEU:HD23	1:A:63:LEU:HG	0.44	1.89	7	1
1:B:293:THR:HG21	1:B:322:HIS:HB2	0.44	1.88	7	1
1:B:316:PHE:HZ	2:B:326:NTH:H61	0.44	1.73	7	1
1:A:103:PHE:HA	1:A:110:VAL:HG23	0.44	1.90	13	1
1:B:272:ARG:HA	1:B:272:ARG:NE	0.44	2.28	15	1
1:A:47:GLY:O	1:A:51:ILE:HG13	0.43	2.13	10	6
1:A:77:GLU:HG2	1:A:101:PHE:O	0.43	2.13	2	2
1:A:116:PHE:HB2	1:A:120:ASN:CG	0.43	2.38	2	2
1:A:93:THR:HG22	1:A:94:VAL:H	0.43	1.73	4	1
1:B:276:ASN:OD1	1:B:276:ASN:C	0.43	2.60	4	1
1:A:102:ARG:HB2	1:A:111:SER:O	0.43	2.13	6	3
1:A:26:ILE:O	1:A:27:VAL:C	0.43	2.61	7	1
1:B:248:THR:O	1:B:249:ALA:C	0.43	2.58	7	1
1:A:30:PHE:CE2	1:A:51:ILE:CG2	0.43	3.01	8	1
1:B:302:ARG:CD	1:B:311:SER:HB2	0.43	2.43	8	1
1:A:3:THR:HG23	1:A:6:HIS:NE2	0.43	2.27	14	1
1:B:210:VAL:CG1	1:B:301:PHE:CD1	0.43	3.01	14	1
1:A:7:MET:SD	1:A:75:ALA:O	0.43	2.76	1	2
1:B:237:GLU:HB2	1:B:313:ARG:HG2	0.43	1.89	1	1
1:B:237:GLU:O	1:B:238:ASP:HB2	0.43	2.12	15	7
1:A:40:VAL:O	1:A:41:GLY:C	0.43	2.60	2	1
1:A:61:LEU:HB3	1:A:63:LEU:CD2	0.43	2.43	4	2
1:B:318:GLU:HA	1:B:321:ILE:HG12	0.43	1.90	7	3
1:A:67:LEU:C	1:A:68:THR:CG2	0.43	2.87	5	1
1:B:280:PHE:CD1	1:B:280:PHE:C	0.43	2.96	5	2
1:B:210:VAL:HA	1:B:229:LEU:CD2	0.43	2.41	7	2
1:B:273:ALA:HA	1:B:278:ALA:CB	0.43	2.43	8	2
1:A:22:ASP:O	1:A:22:ASP:OD2	0.43	2.36	9	1
1:B:275:ALA:O	1:B:276:ASN:HB2	0.43	2.13	10	1
1:B:245:ARG:HD3	1:B:250:ALA:CA	0.43	2.43	11	1
1:B:292:LYS:HG2	1:B:293:THR:N	0.43	2.28	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ALA:O	1:A:51:ILE:CG1	0.43	2.66	15	1
1:B:252:ARG:C	1:B:254:PHE:N	0.43	2.74	1	7
1:A:11:VAL:HG22	1:A:80:PHE:CD2	0.43	2.48	2	1
1:A:117:GLY:C	1:A:119:LYS:N	0.43	2.74	3	4
1:A:117:GLY:O	1:A:118:GLU:C	0.43	2.59	3	1
1:A:69:GLN:OE1	1:A:70:GLU:O	0.43	2.36	4	1
1:A:98:ILE:HD11	1:B:272:ARG:NE	0.43	2.29	4	1
1:B:263:LEU:CD2	1:B:286:PHE:HB3	0.43	2.42	4	2
1:B:263:LEU:HD11	2:B:326:NTH:H121	0.43	1.90	4	1
1:A:104:ASN:ND2	1:A:104:ASN:N	0.43	2.64	6	1
1:B:241:GLY:O	1:B:242:SER:HB2	0.43	2.13	12	2
1:A:56:ALA:O	1:A:57:ASN:C	0.43	2.57	7	1
1:A:77:GLU:CG	1:A:102:ARG:HA	0.43	2.43	14	1
1:A:26:ILE:CD1	1:A:55:PHE:CD1	0.43	2.99	2	1
1:A:118:GLU:CA	1:A:121:ILE:HG12	0.43	2.44	3	1
1:B:259:LEU:C	1:B:261:LEU:N	0.43	2.76	9	3
1:B:297:PRO:HB3	1:B:320:ASN:ND2	0.43	2.29	4	1
1:A:104:ASN:OD1	1:A:108:LYS:O	0.43	2.36	6	1
1:A:93:THR:CG2	1:A:123:ALA:HA	0.43	2.43	8	1
1:A:61:LEU:HD21	2:A:126:NTH:O20	0.43	2.13	3	1
1:A:15:VAL:HB	1:A:67:LEU:CD1	0.43	2.39	5	1
1:A:39:PRO:HB3	1:A:116:PHE:CZ	0.43	2.48	7	1
1:B:286:PHE:CE2	2:B:326:NTH:H212	0.43	2.47	8	1
1:A:74:VAL:HB	1:B:240:VAL:HG21	0.43	1.90	12	1
1:A:7:MET:HA	1:A:7:MET:CE	0.43	2.43	14	1
1:A:41:GLY:CA	1:B:275:ALA:HB1	0.43	2.43	15	1
1:A:67:LEU:CD2	1:A:82:PHE:HB3	0.43	2.43	1	1
1:B:233:ASP:CB	1:B:247:GLY:HA2	0.43	2.44	4	5
1:A:40:VAL:C	1:A:42:SER:N	0.43	2.74	2	1
1:A:77:GLU:CG	1:A:101:PHE:O	0.43	2.67	2	1
1:B:235:THR:OG1	1:B:311:SER:OG	0.43	2.35	2	1
1:B:262:PRO:C	1:B:263:LEU:HG	0.43	2.37	8	6
1:A:22:ASP:OD1	1:A:22:ASP:O	0.43	2.36	6	1
1:A:22:ASP:OD1	1:A:24:ASP:CB	0.43	2.66	8	1
1:A:115:LEU:O	1:A:116:PHE:CB	0.43	2.66	8	2
1:B:223:LEU:HG	1:B:256:ALA:CB	0.43	2.43	8	2
1:B:245:ARG:HG3	1:B:250:ALA:CB	0.43	2.38	8	1
1:A:22:ASP:OD2	1:A:25:GLY:N	0.43	2.45	10	1
1:A:81:ALA:CA	1:A:98:ILE:HG23	0.43	2.44	10	1
1:A:45:ARG:CZ	1:A:54:PHE:HB3	0.43	2.43	11	1
1:A:86:PHE:CE2	1:A:87:GLU:O	0.43	2.71	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:HB3	1:A:79:ALA:O	0.43	2.14	14	1
1:B:207:MET:HB2	1:B:273:ALA:HB1	0.43	1.90	1	1
1:B:223:LEU:CD1	1:B:255:PHE:HB3	0.43	2.43	15	6
1:A:38:ASP:CG	1:A:114:ALA:HB3	0.43	2.38	3	1
1:A:117:GLY:O	1:A:119:LYS:N	0.43	2.52	3	1
1:A:17:ALA:HA	1:A:22:ASP:OD1	0.43	2.14	4	2
1:A:14:TYR:CE1	1:A:15:VAL:HG23	0.43	2.49	15	2
1:A:72:ARG:HB3	1:A:72:ARG:NH2	0.43	2.28	5	1
1:B:242:SER:C	1:B:244:PRO:HD3	0.43	2.39	6	2
1:A:94:VAL:HG12	1:A:122:HIS:CD2	0.43	2.49	7	1
1:B:227:VAL:HG21	1:B:252:ARG:CG	0.43	2.43	7	1
1:B:204:PRO:O	1:B:208:THR:HB	0.43	2.12	15	2
1:B:238:ASP:OD1	2:B:326:NTH:H62	0.43	2.14	13	2
1:A:85:SER:O	1:A:85:SER:OG	0.43	2.33	12	1
1:B:223:LEU:O	1:B:225:GLY:N	0.43	2.52	12	1
1:A:72:ARG:HA	1:A:72:ARG:NE	0.43	2.28	14	1
1:A:42:SER:C	1:A:44:PRO:HD3	0.43	2.39	1	3
1:B:233:ASP:HA	1:B:247:GLY:HA2	0.43	1.90	6	5
1:A:48:THR:O	1:A:49:ALA:C	0.43	2.60	13	3
1:A:74:VAL:O	1:A:76:ASN:N	0.43	2.51	2	1
1:B:235:THR:O	1:B:236:VAL:CG2	0.43	2.67	2	1
1:A:4:PRO:O	1:A:8:THR:HB	0.43	2.14	10	3
1:B:237:GLU:HA	1:B:244:PRO:HB3	0.43	1.89	7	2
1:B:278:ALA:CB	1:B:301:PHE:HB2	0.43	2.40	4	1
1:A:86:PHE:CZ	1:A:93:THR:CB	0.43	3.01	7	1
1:B:243:GLU:O	1:B:243:GLU:OE1	0.43	2.37	10	1
1:B:233:ASP:OD1	1:B:233:ASP:O	0.43	2.37	11	1
1:B:281:ALA:CA	1:B:298:ILE:HG23	0.43	2.43	11	1
1:A:116:PHE:HA	1:B:272:ARG:NH2	0.43	2.28	14	1
1:B:293:THR:HG22	1:B:294:VAL:H	0.43	1.73	15	1
1:B:239:PRO:O	1:B:242:SER:HB2	0.43	2.14	7	4
1:B:293:THR:HB	1:B:322:HIS:HB2	0.43	1.89	13	2
1:B:210:VAL:CB	1:B:303:PHE:CE2	0.43	3.02	9	2
1:B:270:GLU:O	1:B:272:ARG:NH2	0.43	2.51	9	1
1:B:281:ALA:C	1:B:282:PHE:CG	0.43	2.94	10	1
1:A:95:VAL:HG13	1:A:120:ASN:HD21	0.43	1.72	11	1
1:B:304:ASN:HB3	1:B:310:VAL:CG1	0.43	2.43	11	1
1:B:235:THR:CG2	1:B:246:SER:HB2	0.43	2.41	13	1
1:B:267:LEU:HD22	1:B:271:VAL:CG2	0.43	2.44	14	1
1:B:278:ALA:O	1:B:300:HIS:ND1	0.43	2.51	14	1
1:B:240:VAL:CG1	1:B:315:LEU:HA	0.43	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:289:GLN:C	1:B:291:ARG:N	0.43	2.76	3	1
1:B:284:VAL:O	1:B:294:VAL:HA	0.43	2.14	4	5
1:B:272:ARG:HG3	1:B:279:ALA:O	0.43	2.14	13	4
1:A:100:HIS:CB	1:A:113:ARG:HB3	0.43	2.43	7	1
1:B:303:PHE:C	1:B:310:VAL:HG23	0.43	2.39	7	1
1:A:84:VAL:O	1:A:94:VAL:HG22	0.43	2.13	9	1
1:A:61:LEU:O	1:A:63:LEU:HD11	0.43	2.14	15	2
1:B:300:HIS:CB	1:B:313:ARG:HB2	0.43	2.44	11	1
1:A:45:ARG:HD3	1:A:50:ALA:CA	0.43	2.44	12	1
1:B:223:LEU:C	1:B:225:GLY:N	0.43	2.75	12	1
1:B:322:HIS:NE2	2:B:326:NTH:C23	0.43	2.82	13	1
1:A:37:GLU:O	1:A:38:ASP:CB	0.43	2.66	14	1
1:A:73:ALA:HA	1:A:78:ALA:CB	0.42	2.44	1	2
1:B:300:HIS:CB	1:B:313:ARG:CB	0.42	2.97	12	2
1:A:40:VAL:HG11	1:B:274:VAL:CG1	0.42	2.36	2	1
1:B:281:ALA:O	1:B:282:PHE:HB3	0.42	2.14	14	3
1:A:68:THR:O	1:A:68:THR:OG1	0.42	2.33	5	1
1:A:108:LYS:HD2	1:A:108:LYS:N	0.42	2.28	6	1
1:B:256:ALA:O	1:B:259:LEU:N	0.42	2.52	7	1
1:B:322:HIS:O	1:B:322:HIS:CD2	0.42	2.72	7	1
1:A:61:LEU:HD13	2:A:126:NTH:C18	0.42	2.27	8	1
1:A:74:VAL:CG1	1:B:317:GLY:HA3	0.42	2.44	9	1
1:A:65:VAL:HG13	1:A:82:PHE:CD2	0.42	2.49	1	1
1:B:307:GLY:O	1:B:308:LYS:HG3	0.42	2.14	1	1
1:A:37:GLU:HA	1:A:44:PRO:HB3	0.42	1.91	11	3
1:A:68:THR:HG23	1:A:69:GLN:N	0.42	2.29	3	2
1:A:23:LEU:HD21	1:A:59:LEU:CD2	0.42	2.42	5	1
1:B:263:LEU:CG	1:B:286:PHE:HB3	0.42	2.44	13	2
1:A:21:GLY:HA2	1:A:59:LEU:CD2	0.42	2.38	7	2
1:A:31:ALA:N	1:A:109:VAL:O	0.42	2.51	8	2
1:A:100:HIS:ND1	1:A:101:PHE:N	0.42	2.68	8	1
1:B:287:GLU:HG2	1:B:288:PHE:N	0.42	2.29	9	2
1:A:3:THR:O	1:A:6:HIS:ND1	0.42	2.52	11	1
1:B:286:PHE:CZ	1:B:288:PHE:CZ	0.42	3.07	12	1
1:A:72:ARG:CZ	1:B:298:ILE:HD11	0.42	2.44	1	1
1:B:237:GLU:CB	1:B:313:ARG:HG2	0.42	2.44	1	1
1:A:100:HIS:CE1	1:B:315:LEU:HD13	0.42	2.50	4	1
1:B:203:THR:CG2	1:B:205:GLU:HB2	0.42	2.44	5	1
1:A:39:PRO:O	1:A:42:SER:HB2	0.42	2.14	9	2
1:A:33:ASP:HA	1:A:47:GLY:HA2	0.42	1.91	9	6
1:B:269:GLN:CD	1:B:281:ALA:HB3	0.42	2.39	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ASN:OD1	1:B:272:ARG:NH1	0.42	2.52	12	1
1:B:314:ALA:HB1	1:B:316:PHE:HE2	0.42	1.74	13	1
1:A:100:HIS:HB3	1:A:113:ARG:O	0.42	2.14	14	1
1:B:316:PHE:CZ	2:B:326:NTH:C6	0.42	3.01	14	1
1:A:40:VAL:HG11	1:A:115:LEU:HA	0.42	1.89	15	1
1:A:86:PHE:HE2	2:A:126:NTH:H221	0.42	1.70	15	1
1:A:13:ARG:HD2	1:A:29:LEU:CD1	0.42	2.43	2	1
1:A:29:LEU:O	1:A:109:VAL:HB	0.42	2.14	3	2
1:A:14:TYR:CD1	1:A:15:VAL:N	0.42	2.87	4	1
1:A:37:GLU:O	1:A:38:ASP:HB2	0.42	2.14	11	5
1:B:254:PHE:C	1:B:256:ALA:N	0.42	2.75	14	6
1:B:261:LEU:CD2	1:B:263:LEU:CG	0.42	2.98	4	1
1:A:102:ARG:HD2	1:A:111:SER:CB	0.42	2.44	6	1
1:A:104:ASN:ND2	1:A:108:LYS:O	0.42	2.52	6	1
2:B:326:NTH:H161	2:B:326:NTH:C21	0.42	2.44	13	2
1:A:88:PHE:C	1:A:89:GLN:HG2	0.42	2.38	14	1
1:A:8:THR:O	1:A:9:ALA:C	0.42	2.61	12	2
1:B:261:LEU:HB3	1:B:263:LEU:CD2	0.42	2.44	1	2
1:A:61:LEU:CD1	2:A:126:NTH:C12	0.42	2.96	2	1
1:A:63:LEU:HD22	1:A:86:PHE:CD1	0.42	2.50	2	1
1:B:217:ALA:HB1	1:B:222:ASP:O	0.42	2.15	2	1
1:A:23:LEU:HG	1:A:56:ALA:CB	0.42	2.44	6	2
1:A:10:VAL:HA	1:A:29:LEU:CD2	0.42	2.43	7	1
1:A:115:LEU:C	1:A:116:PHE:CD2	0.42	2.97	8	1
1:A:29:LEU:HD12	1:A:29:LEU:HA	0.42	1.74	9	1
1:A:77:GLU:O	1:A:78:ALA:CB	0.42	2.64	13	2
1:B:302:ARG:O	1:B:304:ASN:ND2	0.42	2.52	10	1
1:B:316:PHE:HA	1:B:320:ASN:ND2	0.42	2.29	11	1
1:A:92:LYS:HG2	1:A:93:THR:N	0.42	2.29	12	1
1:A:64:ALA:CB	1:A:85:SER:HG	0.42	2.28	15	1
1:B:267:LEU:C	1:B:268:THR:CG2	0.42	2.92	1	2
1:B:295:VAL:HG12	1:B:296:ALA:N	0.42	2.29	11	3
1:A:110:VAL:O	1:A:110:VAL:CG1	0.42	2.68	6	1
1:B:207:MET:HA	1:B:303:PHE:CE2	0.42	2.49	7	1
1:A:3:THR:O	1:A:6:HIS:NE2	0.42	2.53	13	1
1:B:288:PHE:O	1:B:289:GLN:HG3	0.42	2.15	13	1
1:B:307:GLY:O	1:B:308:LYS:HB2	0.42	2.14	4	2
1:A:101:PHE:CE1	1:A:109:VAL:HG11	0.42	2.50	2	1
1:A:72:ARG:NH2	1:A:74:VAL:HG22	0.42	2.28	5	1
1:B:295:VAL:HG13	1:B:321:ILE:HA	0.42	1.91	5	1
1:B:207:MET:SD	1:B:303:PHE:CD2	0.42	3.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ALA:O	1:A:54:PHE:N	0.42	2.50	10	1
1:B:211:VAL:HG11	1:B:271:VAL:HG11	0.42	1.92	10	1
1:B:222:ASP:OD2	1:B:225:GLY:HA3	0.42	2.13	10	1
1:B:238:ASP:C	1:B:243:GLU:HB2	0.42	2.40	12	1
1:B:288:PHE:CE2	1:B:293:THR:OG1	0.42	2.72	12	1
1:A:15:VAL:HA	1:A:18:LEU:HB2	0.42	1.92	15	12
1:A:4:PRO:O	1:A:8:THR:N	0.42	2.48	15	4
1:A:62:PRO:C	1:A:63:LEU:HG	0.42	2.38	3	4
1:B:301:PHE:CD2	1:B:303:PHE:CZ	0.42	3.08	4	1
1:B:249:ALA:O	1:B:253:GLU:CG	0.42	2.68	6	2
1:A:4:PRO:O	1:A:8:THR:OG1	0.42	2.34	8	1
1:A:89:GLN:HG2	1:A:90:GLY:N	0.42	2.29	15	2
1:A:61:LEU:HD13	1:A:62:PRO:CD	0.42	2.41	9	1
1:A:55:PHE:CE1	2:A:126:NTH:H21	0.42	2.50	10	1
2:A:126:NTH:H161	2:A:126:NTH:C21	0.42	2.45	14	1
1:B:283:THR:HA	1:B:295:VAL:O	0.42	2.15	15	1
1:A:21:GLY:HA2	1:A:59:LEU:CD1	0.42	2.42	2	1
1:A:40:VAL:CG2	1:A:41:GLY:N	0.42	2.75	2	1
1:B:229:LEU:HD12	1:B:229:LEU:HA	0.42	1.74	5	3
1:B:286:PHE:HZ	2:B:326:NTH:H221	0.42	1.69	2	1
1:B:255:PHE:CE1	1:B:312:MET:HE1	0.42	2.50	3	2
1:A:61:LEU:CD2	1:A:61:LEU:O	0.42	2.65	6	1
1:A:122:HIS:CG	1:A:123:ALA:N	0.42	2.88	9	1
1:A:22:ASP:CG	1:A:24:ASP:OD2	0.42	2.63	10	1
1:A:22:ASP:OD2	1:A:24:ASP:CG	0.42	2.63	10	1
1:A:76:ASN:O	1:A:103:PHE:CB	0.42	2.67	13	1
1:A:7:MET:O	1:A:103:PHE:CZ	0.42	2.73	15	1
1:B:215:VAL:HA	1:B:218:LEU:HB2	0.42	1.92	7	13
1:B:301:PHE:CD1	1:B:303:PHE:CE1	0.42	3.08	1	1
1:B:307:GLY:O	1:B:308:LYS:CG	0.42	2.68	1	2
1:B:240:VAL:O	1:B:240:VAL:HG23	0.42	2.14	5	1
1:A:61:LEU:HB3	1:A:63:LEU:CD1	0.42	2.45	7	1
1:A:10:VAL:HG22	1:A:29:LEU:HG	0.42	1.92	9	1
1:B:277:GLU:CG	1:B:302:ARG:HG2	0.42	2.45	9	1
1:A:23:LEU:HD21	1:A:59:LEU:HB2	0.42	1.90	10	1
1:B:267:LEU:O	1:B:268:THR:HG23	0.42	2.14	12	1
1:A:100:HIS:CE1	1:B:300:HIS:CD2	0.42	3.08	13	1
1:A:30:PHE:CG	1:A:51:ILE:CG2	0.42	3.01	14	1
1:B:304:ASN:OD1	1:B:310:VAL:HB	0.42	2.14	14	1
1:B:229:LEU:O	1:B:309:VAL:HB	0.41	2.15	2	1
1:A:34:ALA:HB3	1:A:51:ILE:HG13	0.41	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:296:ALA:O	1:B:320:ASN:CB	0.41	2.68	3	1
1:A:118:GLU:C	1:A:121:ILE:HG12	0.41	2.40	4	3
1:B:272:ARG:CA	1:B:279:ALA:O	0.41	2.68	4	1
1:A:39:PRO:C	1:A:40:VAL:HG22	0.41	2.40	6	1
1:B:276:ASN:O	1:B:303:PHE:HB2	0.41	2.15	6	4
1:B:318:GLU:C	1:B:321:ILE:HG12	0.41	2.40	14	2
1:A:61:LEU:HD11	2:A:126:NTH:H212	0.41	1.92	7	1
1:B:207:MET:CE	1:B:306:ALA:HA	0.41	2.45	9	1
1:B:278:ALA:O	1:B:301:PHE:HB2	0.41	2.15	10	2
1:B:281:ALA:CB	1:B:298:ILE:HG13	0.41	2.45	9	2
1:A:59:LEU:O	1:A:61:LEU:N	0.41	2.53	10	1
1:A:78:ALA:C	1:A:101:PHE:HB2	0.41	2.40	10	1
1:A:95:VAL:CG2	1:A:121:ILE:CG2	0.41	2.94	12	1
1:A:76:ASN:CG	1:A:105:GLY:HA2	0.41	2.40	14	1
1:A:81:ALA:O	1:A:82:PHE:CB	0.41	2.68	15	1
1:B:219:ASN:ND2	1:B:266:GLU:OE1	0.41	2.53	4	1
1:A:47:GLY:O	1:A:51:ILE:HG12	0.41	2.16	13	2
1:B:235:THR:CG2	1:B:246:SER:HB3	0.41	2.45	6	1
1:A:6:HIS:NE2	1:A:7:MET:HG2	0.41	2.29	11	1
1:A:32:ASP:O	1:A:33:ASP:OD1	0.41	2.37	11	1
1:B:241:GLY:O	1:B:242:SER:CB	0.41	2.67	12	1
1:A:10:VAL:O	1:A:29:LEU:HD21	0.41	2.14	1	1
1:B:214:TYR:HE2	1:B:312:MET:HE1	0.41	1.76	7	2
1:B:236:VAL:HG23	1:B:251:ILE:HG12	0.41	1.91	9	1
1:A:14:TYR:OH	1:A:55:PHE:CZ	0.41	2.67	10	1
1:A:22:ASP:OD1	1:A:24:ASP:CG	0.41	2.64	10	1
1:A:36:VAL:HG11	1:A:45:ARG:NE	0.41	2.31	11	1
1:A:101:PHE:CE1	1:A:109:VAL:HG21	0.41	2.51	12	1
1:A:36:VAL:O	1:A:37:GLU:HG2	0.41	2.16	1	1
1:A:23:LEU:HD12	1:A:55:PHE:HB3	0.41	1.90	5	1
1:B:261:LEU:HD13	2:B:326:NTH:C17	0.41	2.45	5	1
1:A:113:ARG:NH1	1:B:313:ARG:NH1	0.41	2.68	8	1
1:A:20:ALA:C	1:A:22:ASP:N	0.41	2.78	11	1
1:A:77:GLU:OE2	1:A:102:ARG:CZ	0.41	2.69	14	1
1:B:267:LEU:HA	1:B:282:PHE:CB	0.41	2.46	14	1
1:B:251:ILE:HD13	1:B:251:ILE:HA	0.41	1.74	15	1
1:B:255:PHE:HE2	1:B:312:MET:HE1	0.41	1.75	1	1
1:A:39:PRO:HG2	1:A:42:SER:OG	0.41	2.15	2	2
1:A:42:SER:O	1:A:43:GLU:HB2	0.41	2.15	3	1
1:A:68:THR:CG2	1:A:69:GLN:N	0.41	2.84	3	1
1:A:113:ARG:NH2	1:B:277:GLU:HG3	0.41	2.30	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:THR:C	1:A:69:GLN:CG	0.41	2.94	5	2
1:A:40:VAL:CG1	1:A:115:LEU:HA	0.41	2.45	8	1
1:B:223:LEU:HD13	1:B:223:LEU:HA	0.41	1.76	8	1
1:A:110:VAL:O	1:A:110:VAL:HG12	0.41	2.14	12	1
1:A:23:LEU:HD13	1:A:23:LEU:HA	0.41	1.77	13	1
1:A:100:HIS:CB	1:A:113:ARG:CB	0.41	2.98	2	1
1:B:235:THR:OG1	1:B:311:SER:HA	0.41	2.16	2	1
1:A:85:SER:CB	1:A:94:VAL:CG2	0.41	2.98	3	1
1:B:214:TYR:CE1	1:B:215:VAL:HG23	0.41	2.50	15	2
1:A:9:ALA:C	1:A:11:VAL:N	0.41	2.77	4	1
1:A:14:TYR:N	1:A:29:LEU:CD2	0.41	2.84	5	1
1:A:81:ALA:CB	1:A:98:ILE:CG1	0.41	2.99	8	1
1:A:75:ALA:HB3	1:B:240:VAL:C	0.41	2.41	15	1
1:A:102:ARG:CZ	1:B:313:ARG:HD2	0.41	2.45	15	1
1:A:100:HIS:HB2	1:A:113:ARG:CB	0.41	2.45	2	1
1:A:97:PRO:HA	1:A:116:PHE:CB	0.41	2.45	4	1
1:A:52:ARG:O	1:A:54:PHE:N	0.41	2.54	8	1
1:A:87:GLU:HB2	1:A:92:LYS:CB	0.41	2.45	8	1
1:B:268:THR:C	1:B:269:GLN:CG	0.41	2.94	8	1
1:A:40:VAL:CG1	1:A:114:ALA:O	0.41	2.68	11	1
1:A:88:PHE:CE2	1:A:93:THR:OG1	0.41	2.74	13	1
1:A:115:LEU:HD21	1:B:272:ARG:HB3	0.41	1.91	14	1
1:B:304:ASN:ND2	1:B:304:ASN:N	0.41	2.66	1	2
1:A:14:TYR:CE2	1:A:112:MET:SD	0.41	3.14	6	1
1:A:102:ARG:HD2	1:A:111:SER:HB2	0.41	1.92	6	1
1:B:302:ARG:HD3	1:B:311:SER:OG	0.41	2.16	6	1
1:B:247:GLY:O	1:B:251:ILE:HG12	0.41	2.16	10	1
1:B:217:ALA:CB	1:B:226:ILE:CG1	0.41	2.98	11	1
1:A:38:ASP:OD2	2:A:126:NTH:C6	0.41	2.69	14	1
1:B:244:PRO:O	1:B:245:ARG:HD2	0.41	2.16	1	1
1:A:63:LEU:HA	1:A:86:PHE:HB3	0.41	1.93	2	1
1:B:230:PHE:CD1	1:B:312:MET:HE1	0.41	2.45	2	1
1:A:26:ILE:HG22	1:A:30:PHE:HD2	0.41	1.76	3	1
1:A:15:VAL:CB	1:A:67:LEU:HD11	0.41	2.42	5	1
1:A:60:LYS:O	1:A:62:PRO:HD3	0.41	2.15	6	1
1:B:245:ARG:HD2	1:B:250:ALA:CB	0.41	2.46	7	1
1:B:248:THR:C	1:B:250:ALA:N	0.41	2.75	7	1
1:B:261:LEU:HD11	2:B:326:NTH:H212	0.41	1.93	7	1
1:A:27:VAL:O	1:A:30:PHE:N	0.41	2.53	8	1
1:B:260:LYS:O	1:B:262:PRO:HD3	0.41	2.16	8	1
1:A:14:TYR:HH	1:A:55:PHE:HE2	0.41	1.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ALA:O	1:A:101:PHE:HB2	0.41	2.15	10	1
1:A:86:PHE:CZ	2:A:126:NTH:O20	0.41	2.74	11	1
1:A:116:PHE:N	1:A:116:PHE:CD1	0.41	2.89	11	1
1:A:104:ASN:CG	1:A:105:GLY:N	0.41	2.79	12	1
1:B:280:PHE:CZ	1:B:299:ASP:OD2	0.41	2.74	12	1
1:A:41:GLY:HA2	1:B:276:ASN:ND2	0.41	2.31	13	1
1:B:208:THR:O	1:B:209:ALA:C	0.41	2.63	15	1
1:B:280:PHE:CZ	1:B:299:ASP:CB	0.41	3.04	2	1
1:A:10:VAL:HG13	1:A:109:VAL:HG22	0.41	1.93	3	1
1:A:81:ALA:O	1:A:82:PHE:HB3	0.41	2.16	15	1
1:A:120:ASN:OD1	1:A:121:ILE:HD11	0.40	2.15	2	1
1:A:61:LEU:HD21	2:A:126:NTH:C20	0.40	2.46	3	1
1:B:247:GLY:O	1:B:251:ILE:N	0.40	2.55	3	1
1:A:23:LEU:HG	1:A:56:ALA:HB2	0.40	1.93	6	1
1:B:271:VAL:CG1	1:B:272:ARG:N	0.40	2.84	7	1
1:A:22:ASP:C	1:A:24:ASP:N	0.40	2.78	8	1
1:A:104:ASN:HB3	1:A:110:VAL:CG1	0.40	2.44	8	1
1:B:244:PRO:O	1:B:245:ARG:NE	0.40	2.54	9	1
1:A:26:ILE:O	1:A:30:PHE:CD1	0.40	2.74	13	1
1:A:79:ALA:HB2	1:A:100:HIS:CD2	0.40	2.51	13	1
1:B:322:HIS:NE2	2:B:326:NTH:C22	0.40	2.84	13	1
1:A:92:LYS:O	1:A:92:LYS:HD2	0.40	2.16	7	2
1:A:17:ALA:HA	1:A:22:ASP:CG	0.40	2.41	4	1
1:A:37:GLU:CD	1:A:113:ARG:HD2	0.40	2.41	5	1
1:B:215:VAL:CB	1:B:267:LEU:HD11	0.40	2.46	8	1
1:A:22:ASP:O	1:A:22:ASP:CG	0.40	2.62	9	1
1:A:119:LYS:HE3	1:B:270:GLU:OE2	0.40	2.16	9	1
1:A:13:ARG:HH21	1:A:29:LEU:HD11	0.40	1.75	10	1
1:A:99:ASP:OD1	1:A:114:ALA:HA	0.40	2.16	10	1
1:A:117:GLY:CA	1:B:274:VAL:HG13	0.40	2.47	3	1
1:A:21:GLY:CA	1:A:59:LEU:CD2	0.40	2.82	10	1
1:B:201:MET:O	1:B:202:ASN:HB2	0.40	2.17	12	1
1:A:118:GLU:OE1	1:B:201:MET:CE	0.40	2.69	13	1
1:B:208:THR:O	1:B:211:VAL:HB	0.40	2.17	15	1
1:B:300:HIS:O	1:B:312:MET:HG3	0.40	2.17	15	1
1:B:295:VAL:CG1	1:B:296:ALA:N	0.40	2.84	1	1
1:A:29:LEU:O	1:A:109:VAL:CB	0.40	2.69	3	1
1:B:302:ARG:HB2	1:B:311:SER:O	0.40	2.16	3	1
1:B:302:ARG:HB2	1:B:311:SER:C	0.40	2.41	3	1
1:A:81:ALA:C	1:A:82:PHE:CG	0.40	2.99	4	1
1:A:119:LYS:HE2	1:B:204:PRO:HG2	0.40	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:277:GLU:HG3	1:B:302:ARG:HG2	0.40	1.93	8	1
1:B:236:VAL:O	1:B:244:PRO:HB2	0.40	2.16	9	1
1:A:15:VAL:O	1:A:18:LEU:HB2	0.40	2.16	10	1
1:A:109:VAL:HG11	1:A:112:MET:HE3	0.40	1.93	10	1
1:B:302:ARG:HD2	1:B:304:ASN:OD1	0.40	2.16	10	1
1:B:242:SER:O	1:B:243:GLU:HG2	0.40	2.17	11	1
1:A:3:THR:HB	1:A:6:HIS:NE2	0.40	2.31	13	1
1:B:272:ARG:NH1	1:B:272:ARG:HG2	0.40	2.31	14	1
1:A:83:THR:HA	1:A:95:VAL:O	0.40	2.16	15	1
1:B:276:ASN:ND2	1:B:276:ASN:N	0.40	2.69	1	1
1:B:276:ASN:OD1	1:B:303:PHE:HB2	0.40	2.15	2	1
1:B:316:PHE:HB2	1:B:320:ASN:CG	0.40	2.41	4	1
1:A:86:PHE:CZ	1:A:88:PHE:CE1	0.40	3.10	12	1
1:A:98:ILE:CD1	1:B:272:ARG:CZ	0.40	2.99	12	1
1:A:107:GLY:O	1:A:108:LYS:CG	0.40	2.70	14	1
1:A:116:PHE:HA	1:B:272:ARG:CZ	0.40	2.45	14	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/125 (98%)	85±21 (70±17%)	19±5 (16±4%)	9±3 (7±2%)	1	15
1	B	122/125 (98%)	90±8 (74±6%)	22±3 (18±3%)	8±2 (6±2%)	2	19
All	All	3491/3750 (93%)	2627 (75%)	614 (18%)	250 (7%)	2	15

All 47 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	267	LEU	15
1	B	316	PHE	15
1	A	31	ALA	14
1	A	116	PHE	14
1	A	67	LEU	13

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Mol	Chain	Res	Type	Models (Total)
1	B	231	ALA	13
1	A	106	ALA	12
1	A	107	GLY	9
1	B	275	ALA	9
1	B	306	ALA	9
1	A	75	ALA	8
1	B	307	GLY	8
1	A	40	VAL	7
1	A	121	ILE	7
1	A	69	GLN	7
1	A	105	GLY	6
1	B	305	GLY	6
1	A	34	ALA	5
1	B	282	PHE	5
1	B	321	ILE	5
1	B	269	GLN	5
1	A	41	GLY	4
1	A	82	PHE	4
1	B	240	VAL	4
1	B	290	GLY	4
1	A	39	PRO	3
1	A	90	GLY	3
1	A	42	SER	3
1	A	89	GLN	3
1	A	74	VAL	3
1	A	78	ALA	3
1	B	308	LYS	2
1	A	68	THR	2
1	B	289	GLN	2
1	A	108	LYS	2
1	B	234	ALA	2
1	A	44	PRO	2
1	B	278	ALA	2
1	B	239	PRO	2
1	A	43	GLU	1
1	B	274	VAL	1
1	B	241	GLY	1
1	B	276	ASN	1
1	B	244	PRO	1
1	B	294	VAL	1
1	A	5	GLU	1
1	A	36	VAL	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	93/95 (98%)	56±15 (60±16%)	30±9 (33±9%)	1	13
1	B	95/95 (100%)	59±16 (63±17%)	29±8 (31±9%)	1	15
All	All	2626/2850 (92%)	1731 (66%)	895 (34%)	1	11

All 132 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	VAL	14
1	A	32	ASP	14
1	A	35	THR	14
1	A	63	LEU	14
1	A	74	VAL	14
1	A	83	THR	14
1	B	210	VAL	14
1	B	215	VAL	14
1	B	232	ASP	14
1	B	255	PHE	14
1	B	263	LEU	14
1	B	274	VAL	14
1	B	283	THR	14
1	A	46	SER	13
1	A	55	PHE	13
1	A	61	LEU	13
1	A	92	LYS	13
1	A	93	THR	13
1	A	101	PHE	13
1	B	235	THR	13
1	B	246	SER	13
1	B	261	LEU	13
1	B	301	PHE	13
1	A	122	HIS	12
1	B	293	THR	12
1	B	322	HIS	12
1	A	10	VAL	12
1	B	320	ASN	12

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Mol	Chain	Res	Type	Models (Total)
1	A	89	GLN	11
1	B	277	GLU	11
1	B	289	GLN	11
1	A	45	ARG	11
1	A	42	SER	10
1	A	77	GLU	10
1	A	111	SER	10
1	A	120	ASN	10
1	B	214	TYR	10
1	B	292	LYS	10
1	A	94	VAL	9
1	A	113	ARG	9
1	B	205	GLU	9
1	B	304	ASN	9
1	B	313	ARG	9
1	A	13	ARG	9
1	B	315	LEU	9
1	A	6	HIS	8
1	A	66	GLU	8
1	A	88	PHE	8
1	B	201	MET	8
1	B	213	ARG	8
1	B	266	GLU	8
1	B	302	ARG	8
1	B	311	SER	8
1	A	14	TYR	8
1	A	100	HIS	8
1	A	102	ARG	8
1	A	115	LEU	8
1	A	33	ASP	8
1	B	245	ARG	8
1	B	272	ARG	7
1	B	300	HIS	7
1	A	5	GLU	7
1	A	3	THR	6
1	A	84	VAL	6
1	B	218	LEU	6
1	B	242	SER	6
1	A	67	LEU	6
1	A	119	LYS	6
1	A	72	ARG	6
1	B	268	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	B	288	PHE	6
1	B	319	LYS	6
1	A	18	LEU	6
1	A	60	LYS	6
1	A	104	ASN	6
1	B	308	LYS	6
1	A	68	THR	5
1	B	206	HIS	5
1	B	224	ASP	5
1	B	260	LYS	5
1	A	24	ASP	5
1	A	69	GLN	4
1	B	294	VAL	4
1	B	312	MET	4
1	B	321	ILE	4
1	A	19	ASN	4
1	A	108	LYS	4
1	B	233	ASP	4
1	A	38	ASP	3
1	A	110	VAL	3
1	A	87	GLU	3
1	B	203	THR	3
1	A	23	LEU	3
1	A	76	ASN	3
1	B	219	ASN	3
1	B	291	ARG	3
1	A	85	SER	3
1	B	267	LEU	3
1	B	243	GLU	2
1	A	43	GLU	2
1	B	223	LEU	2
1	A	29	LEU	2
1	B	303	PHE	2
1	A	82	PHE	2
1	A	112	MET	2
1	B	257	ASN	2
1	B	287	GLU	2
1	B	310	VAL	2
1	B	316	PHE	2
1	B	284	VAL	2
1	A	103	PHE	2
1	B	286	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	65	VAL	2
1	B	238	ASP	2
1	B	254	PHE	2
1	B	282	PHE	2
1	A	36	VAL	2
1	A	37	GLU	2
1	B	240	VAL	2
1	B	269	GLN	2
1	B	202	ASN	1
1	B	276	ASN	1
1	B	229	LEU	1
1	B	285	SER	1
1	A	86	PHE	1
1	A	91	ARG	1
1	A	53	GLU	1
1	A	116	PHE	1
1	B	237	GLU	1
1	A	54	PHE	1
1	B	236	VAL	1
1	A	7	MET	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard

deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NTH	B	326	-	30,30,30	2.99±0.02	9±0 (28±1%)
2	NTH	A	126	-	30,30,30	3.00±0.02	9±0 (29±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NTH	B	326	-	45,45,45	2.43±0.01	11±0 (24±0%)
2	NTH	A	126	-	45,45,45	2.43±0.01	11±0 (24±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NTH	B	326	-	-	0±0,9,62,62	0±0,4,4,4
2	NTH	A	126	-	-	0±0,9,62,62	0±0,4,4,4

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
2	A	126	NTH	O17-C17	12.82	1.25	1.46	2	15
2	B	326	NTH	O17-C17	12.81	1.25	1.46	1	15
2	A	126	NTH	C4-C3	4.70	1.55	1.45	10	15
2	B	326	NTH	C4-C3	4.64	1.55	1.45	7	15
2	B	326	NTH	C10-C5	4.63	1.60	1.52	1	15
2	A	126	NTH	C10-C5	4.61	1.60	1.52	11	15
2	A	126	NTH	C10-C9	4.44	1.61	1.54	10	15
2	B	326	NTH	C10-C9	4.33	1.61	1.54	7	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	326	NTH	C13-C17	3.27	1.48	1.53	10	15
2	A	126	NTH	C13-C17	3.25	1.48	1.53	13	15
2	A	126	NTH	C1-C10	2.57	1.58	1.53	2	15
2	B	326	NTH	C1-C10	2.48	1.58	1.53	6	15
2	A	126	NTH	C12-C11	2.28	1.57	1.53	15	15
2	B	326	NTH	C12-C11	2.27	1.57	1.53	6	15
2	A	126	NTH	C4-C5	2.12	1.37	1.34	11	14
2	B	326	NTH	C4-C5	2.11	1.37	1.34	4	13
2	B	326	NTH	C13-C14	2.09	1.58	1.55	5	10
2	A	126	NTH	C13-C14	2.09	1.58	1.55	8	13

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

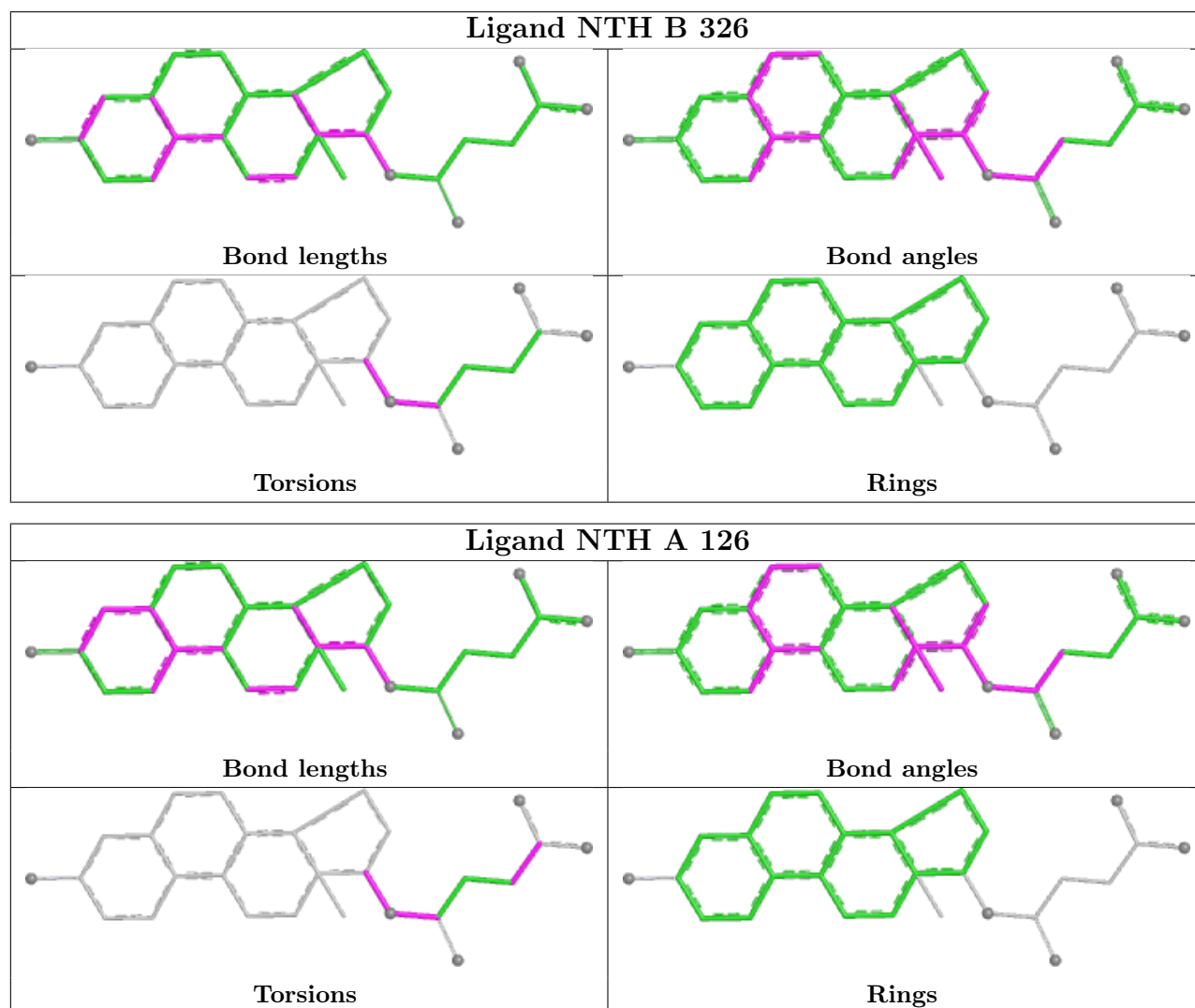
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	126	NTH	C18-C13-C14	8.79	127.61	111.68	7	15
2	B	326	NTH	C18-C13-C14	8.76	127.56	111.68	7	15
2	A	126	NTH	C16-C17-C13	7.13	112.39	105.18	8	15
2	B	326	NTH	C16-C17-C13	7.11	112.36	105.18	10	15
2	B	326	NTH	O17-C17-C16	5.45	124.47	111.06	8	15
2	A	126	NTH	O17-C17-C16	5.43	124.41	111.06	14	15
2	B	326	NTH	C18-C13-C12	4.71	103.66	110.61	2	15
2	A	126	NTH	C18-C13-C12	4.68	103.70	110.61	5	15
2	A	126	NTH	O17-C20-C22	3.74	119.58	111.48	8	15
2	B	326	NTH	O17-C20-C22	3.51	119.08	111.48	7	15
2	A	126	NTH	C1-C10-C9	3.29	104.86	111.96	3	15
2	B	326	NTH	C1-C10-C9	3.28	104.89	111.96	1	15
2	B	326	NTH	O17-C17-C13	3.24	118.78	111.20	11	15
2	A	126	NTH	O17-C17-C13	3.22	118.75	111.20	15	15
2	A	126	NTH	C6-C5-C10	2.88	120.52	115.78	3	15
2	B	326	NTH	C6-C5-C10	2.86	120.48	115.78	10	15
2	B	326	NTH	C7-C6-C5	2.78	107.71	112.47	6	15
2	A	126	NTH	C7-C6-C5	2.78	107.72	112.47	7	15
2	B	326	NTH	C18-C13-C17	2.72	105.81	109.84	11	15
2	A	126	NTH	C18-C13-C17	2.71	105.83	109.84	10	15
2	A	126	NTH	C9-C10-C5	2.15	106.32	110.63	6	15
2	B	326	NTH	C9-C10-C5	2.13	106.36	110.63	14	15
2	B	326	NTH	C14-C13-C17	2.01	95.99	98.69	15	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided