



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 08:29 am BST

PDB ID : 5T1O
Title : Solution-state NMR and SAXS structural ensemble of NPr (1-85) in complex with EIN-Ntr (170-424)
Authors : Strickland, M.; Stanley, A.M.; Wang, G.; Schwieters, C.D.; Buchanan, S.; Peterkofsky, A.; Tjandra, N.
Deposited on : 2016-08-19

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

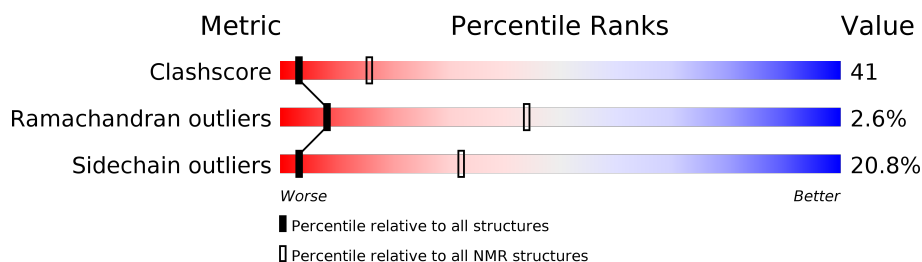
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 33%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	85	
2	B	256	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:85, B:170-B:187, B:202-B:311, B:322-B:397 (289)	0.49	8

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 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5287 atoms, of which 2646 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phosphocarrier protein NPr.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1298	402	653	108	130	5	

- Molecule 2 is a protein called Phosphoenolpyruvate-protein phosphotransferase PtsP.

Mol	Chain	Residues	Atoms						Trace
2	B	255	Total	C	H	N	O	S	0
			3989	1256	1993	354	383	3	

There are 2 discrepancies between the modelled and reference sequences:

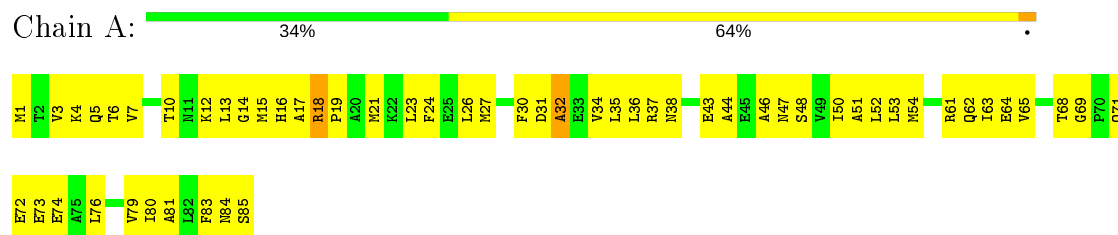
Chain	Residue	Modelled	Actual	Comment	Reference
B	169	GLY	-	expression tag	UNP P37177
B	356	GLN	HIS	engineered mutation	UNP P37177

4 Residue-property plots

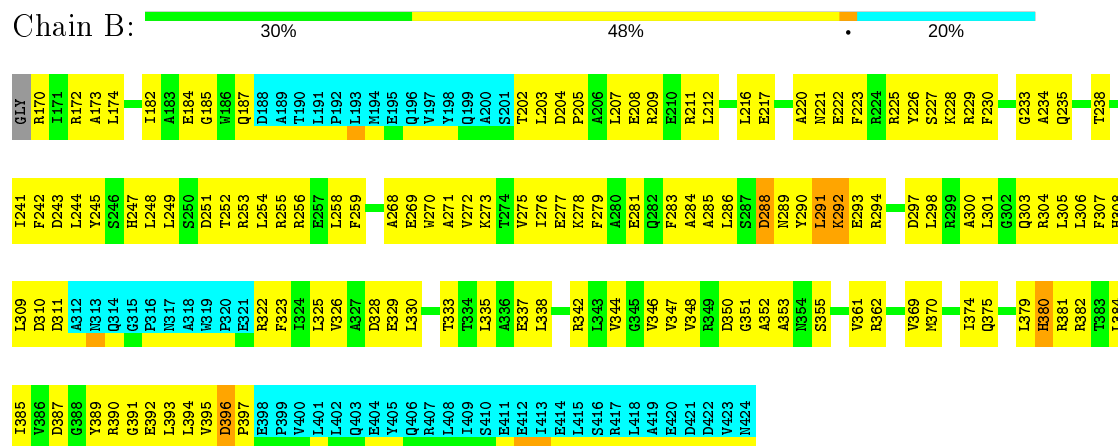
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Phosphocarrier protein NPr



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

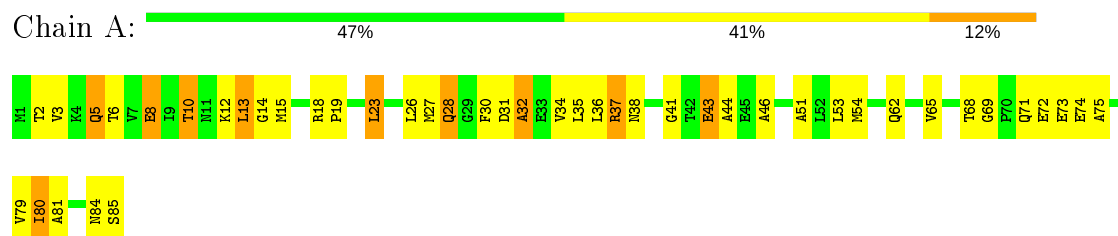


4.2 Scores per residue for each member of the ensemble

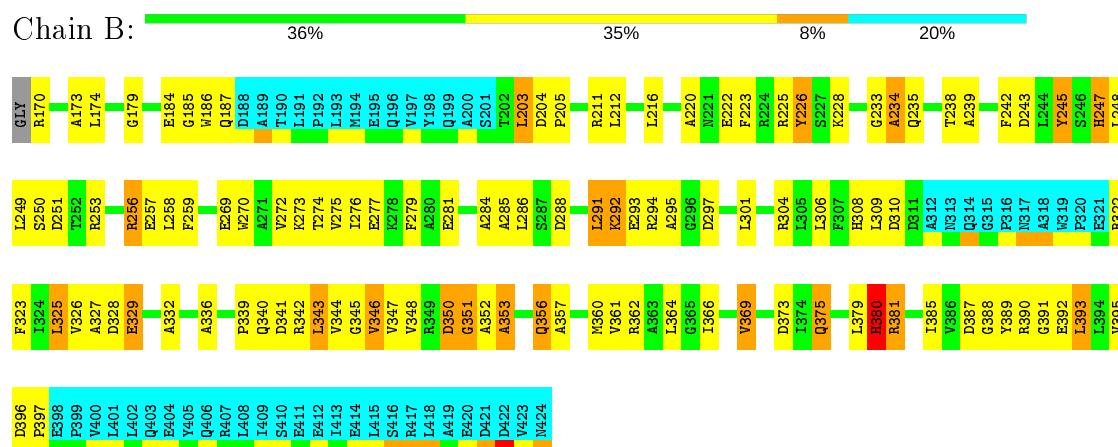
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Phosphocarrier protein NPr

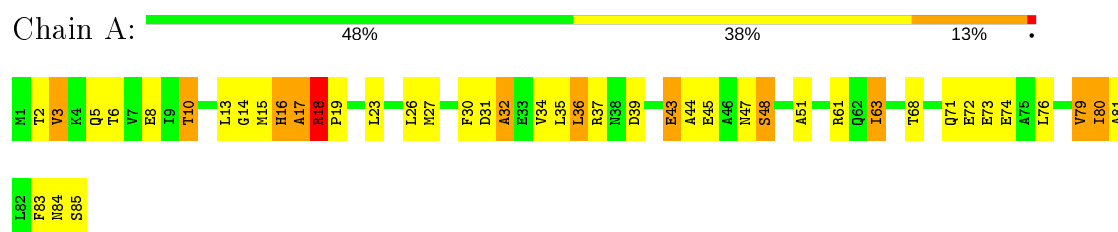


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

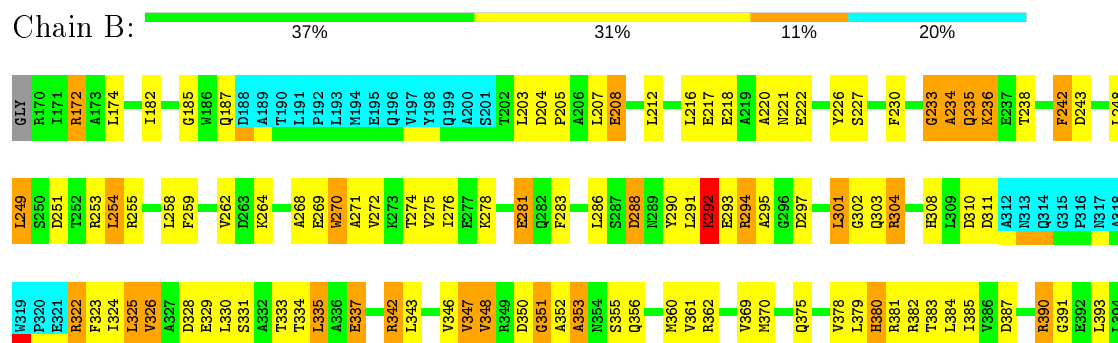


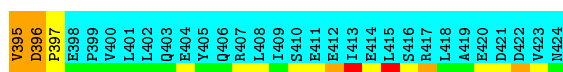
4.2.2 Score per residue for model 2

- Molecule 1: Phosphocarrier protein NPr



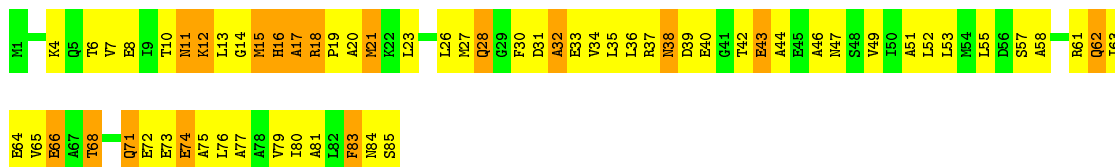
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



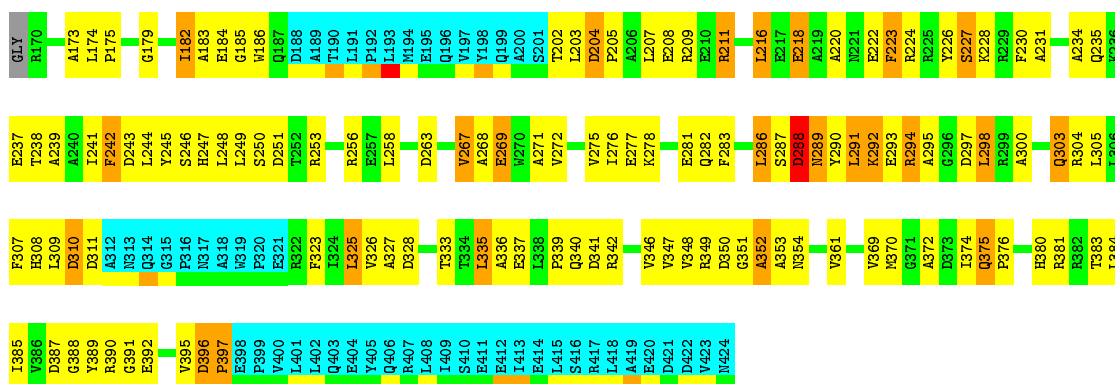


4.2.3 Score per residue for model 3

- Molecule 1: Phosphocarrier protein NPr

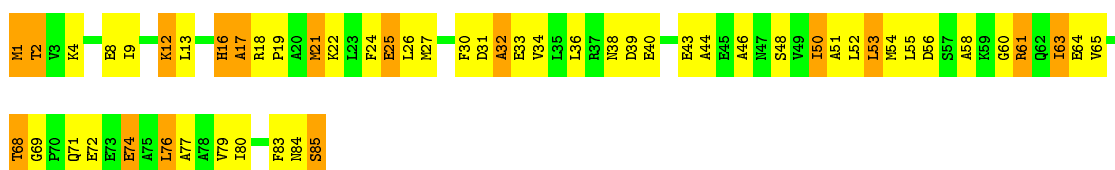
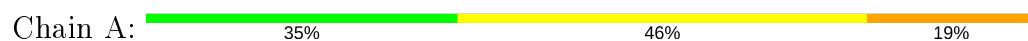


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



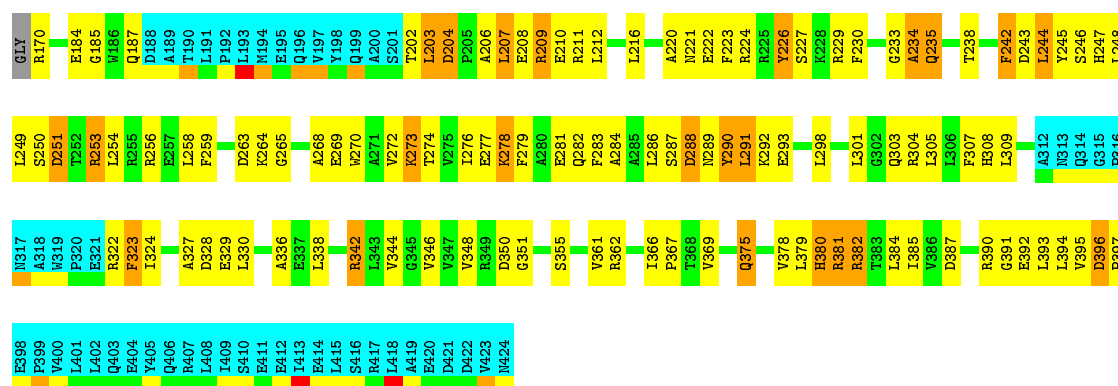
4.2.4 Score per residue for model 4

- Molecule 1: Phosphocarrier protein NPr



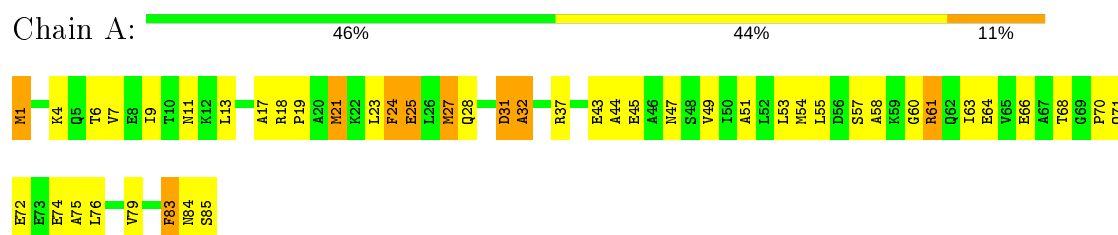
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



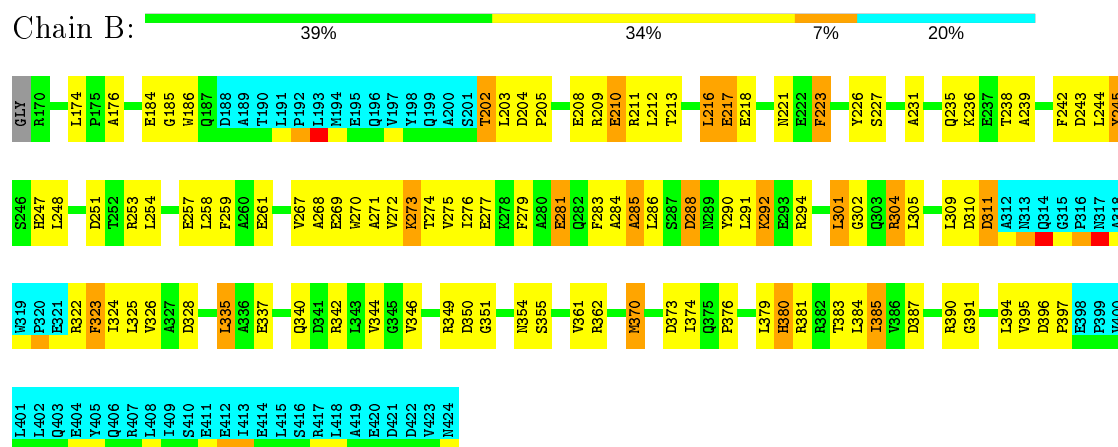


4.2.5 Score per residue for model 5

- Molecule 1: Phosphocarrier protein NPr

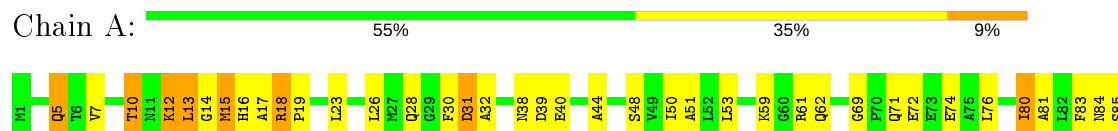


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

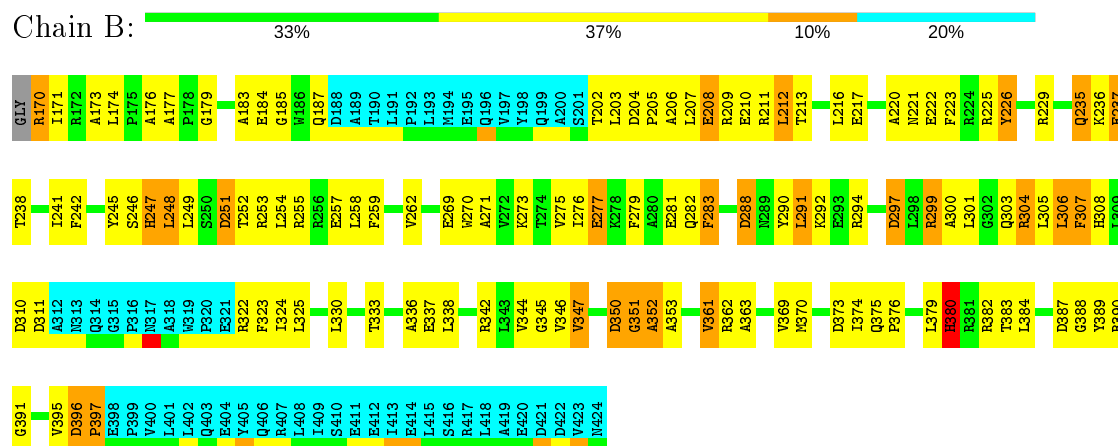


4.2.6 Score per residue for model 6

- Molecule 1: Phosphocarrier protein NPr

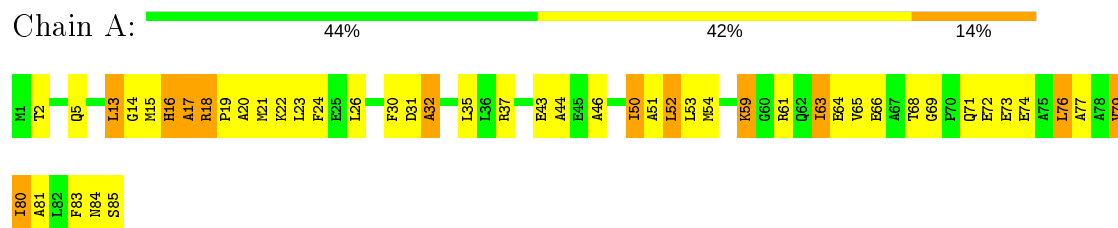


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

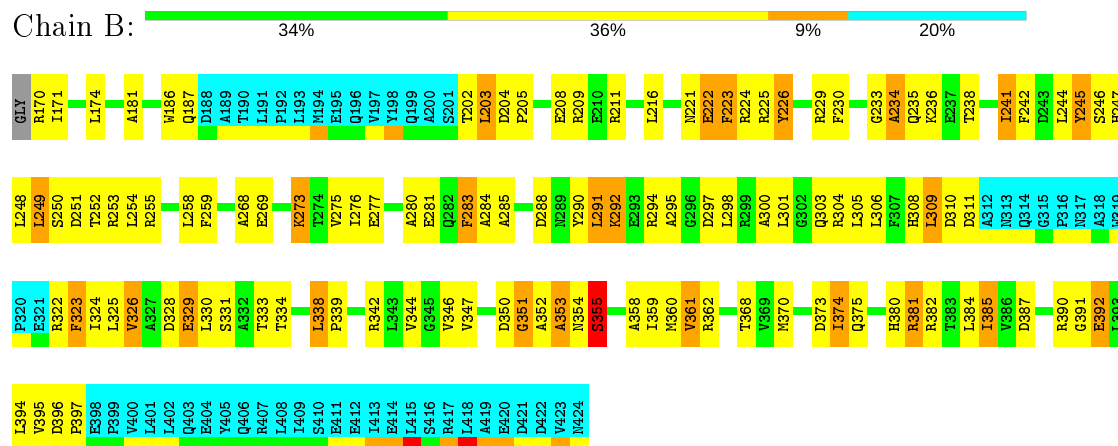


4.2.7 Score per residue for model 7

- Molecule 1: Phosphocarrier protein NPr



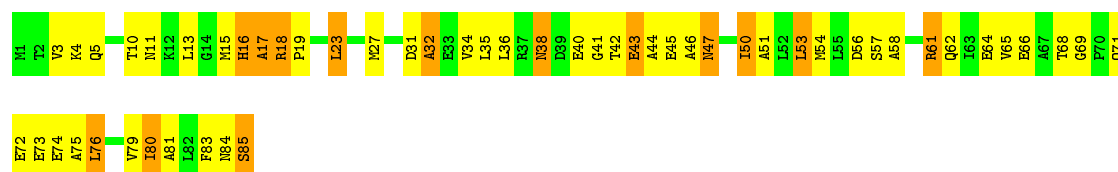
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



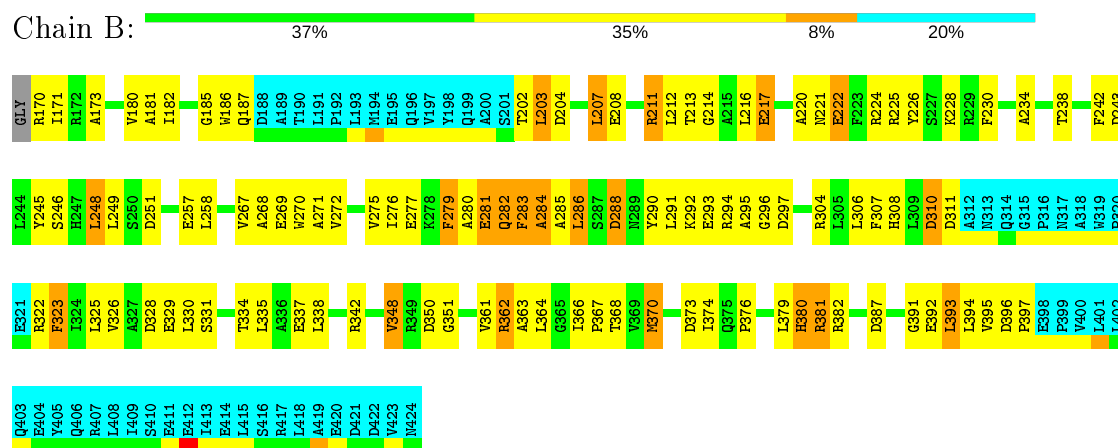
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Phosphocarrier protein NPr



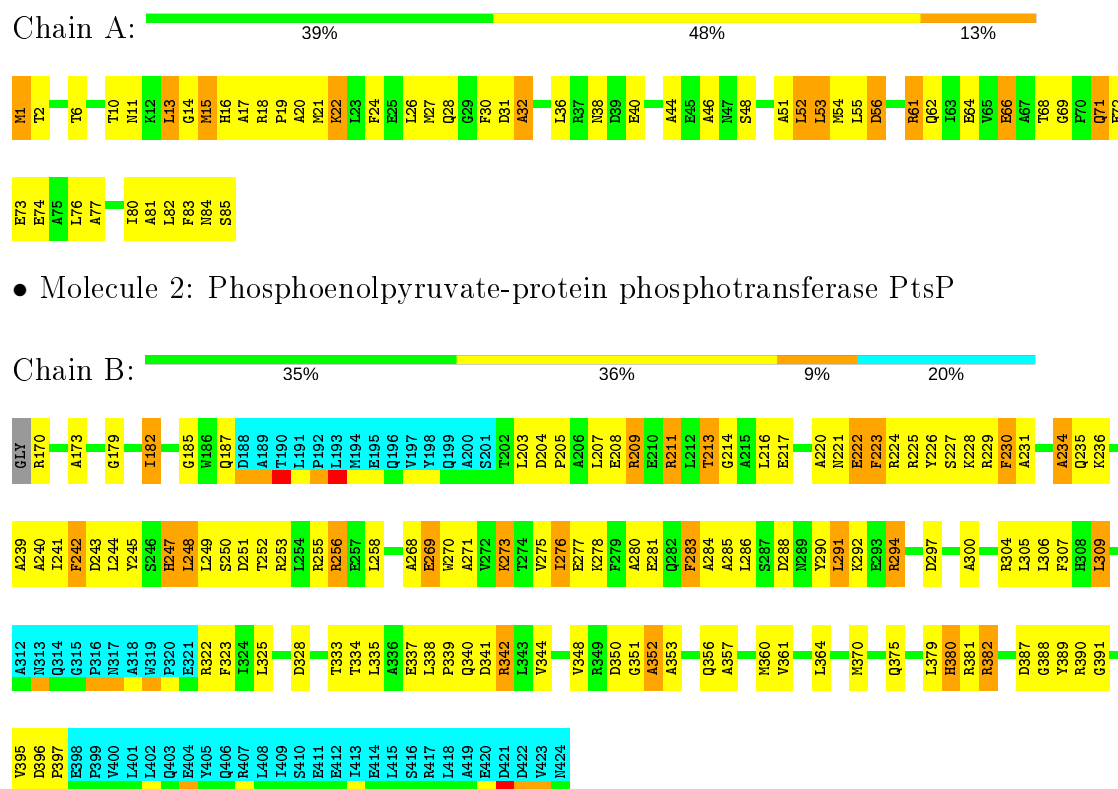


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



4.2.9 Score per residue for model 9

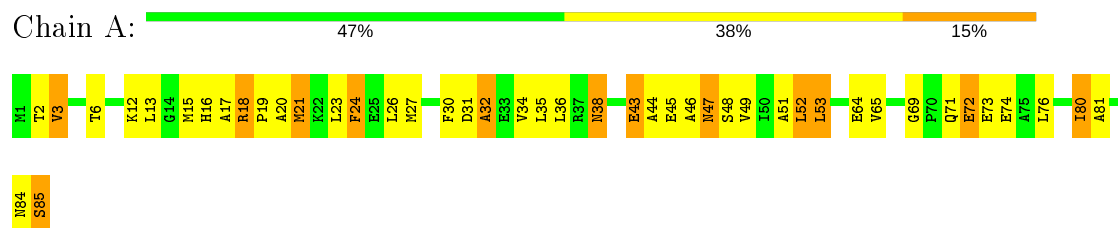
- Molecule 1: Phosphocarrier protein NPr

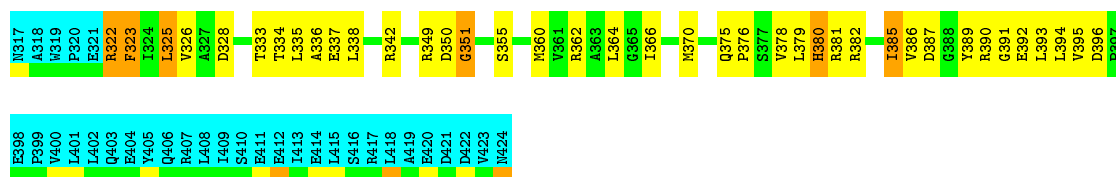


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

4.2.10 Score per residue for model 10

- Molecule 1: Phosphocarrier protein NPr

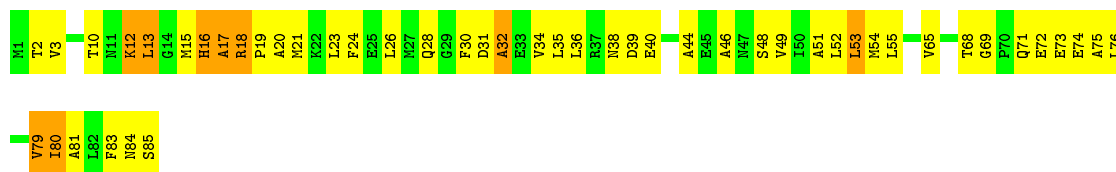




4.2.12 Score per residue for model 12

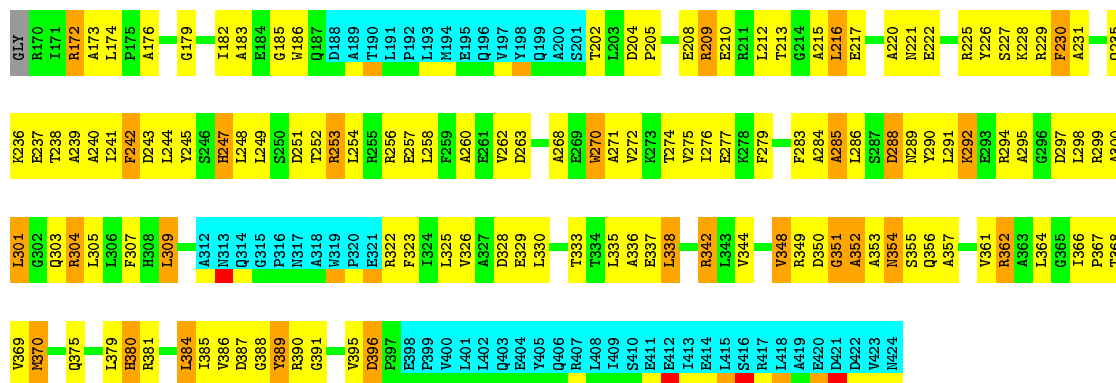
- Molecule 1: Phosphocarrier protein NPr

Chain A: 42% 47% 11%



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

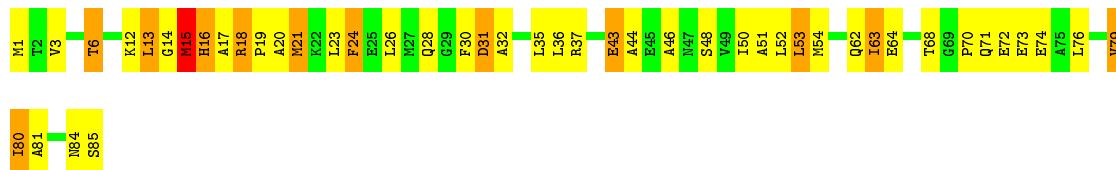
Chain B: 29% 41% 10% 20%



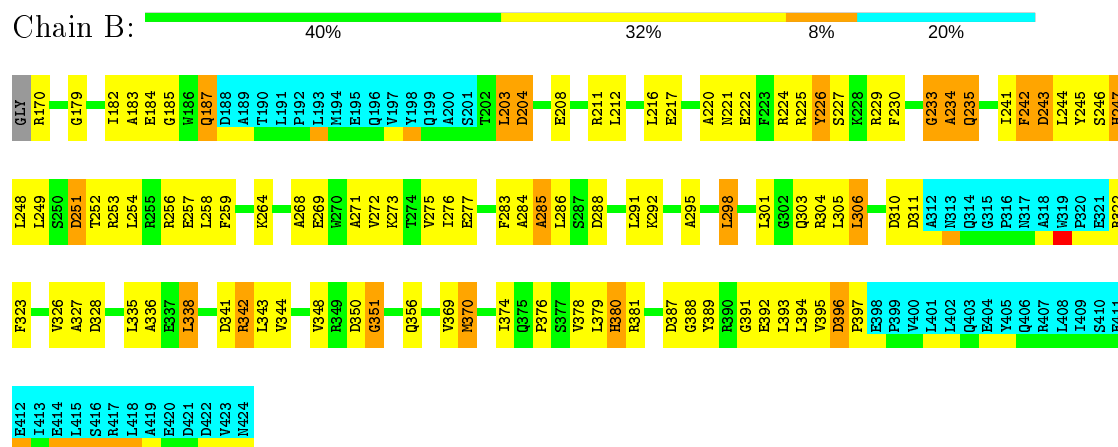
4.2.13 Score per residue for model 13

- Molecule 1: Phosphocarrier protein NPr

Chain A: 45% 40% 14%

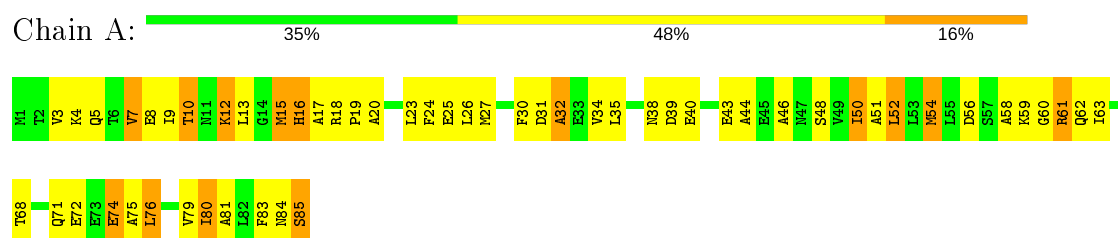


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

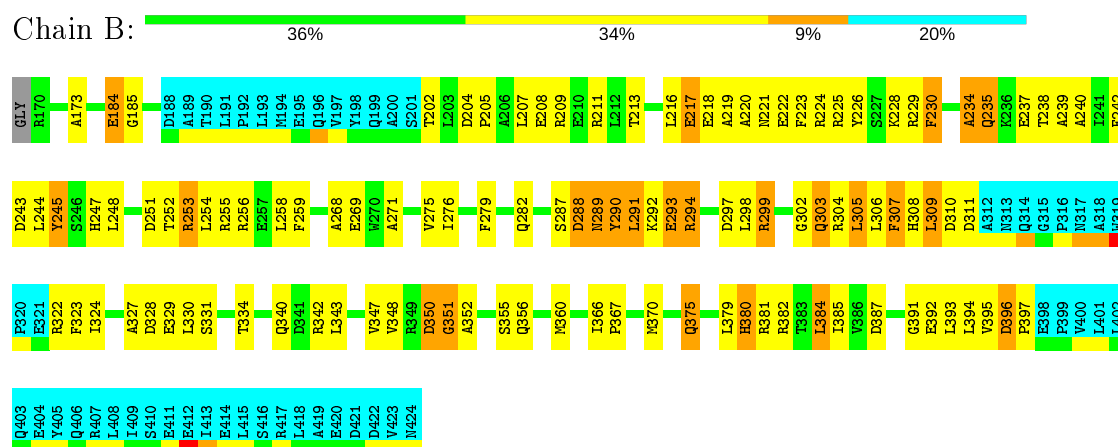


4.2.14 Score per residue for model 14

- Molecule 1: Phosphocarrier protein NPr



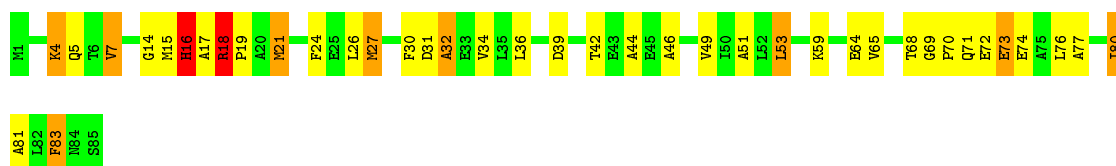
- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



4.2.15 Score per residue for model 15

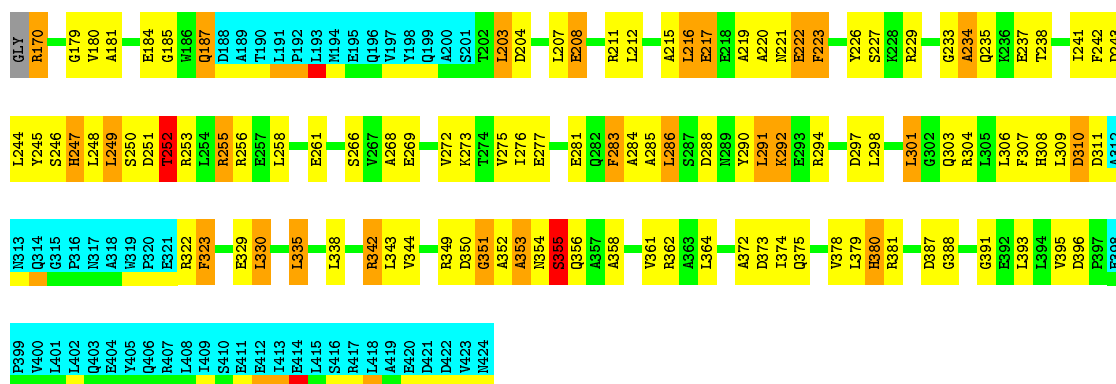
- Molecule 1: Phosphocarrier protein NPr





• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

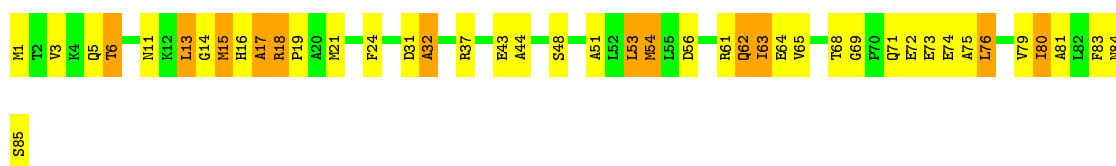
Chain B: 37% 32% 10% 20%



4.2.16 Score per residue for model 16

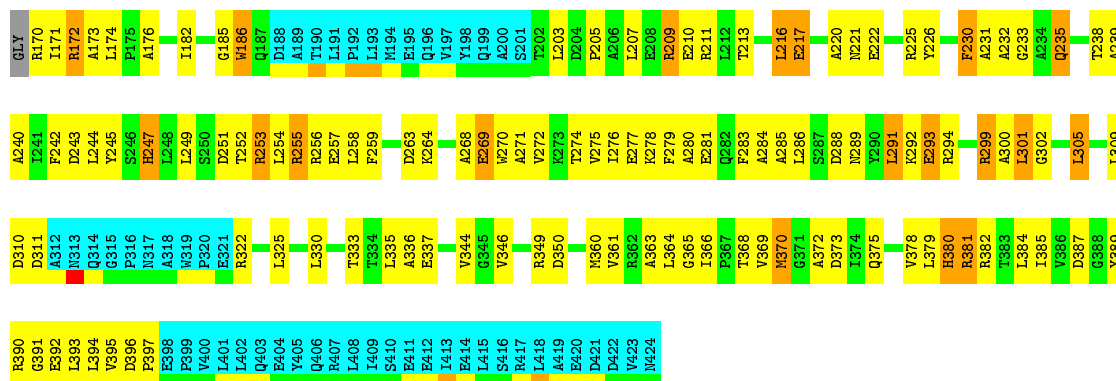
• Molecule 1: Phosphocarrier protein NPr

Chain A: 49% 36% 14%



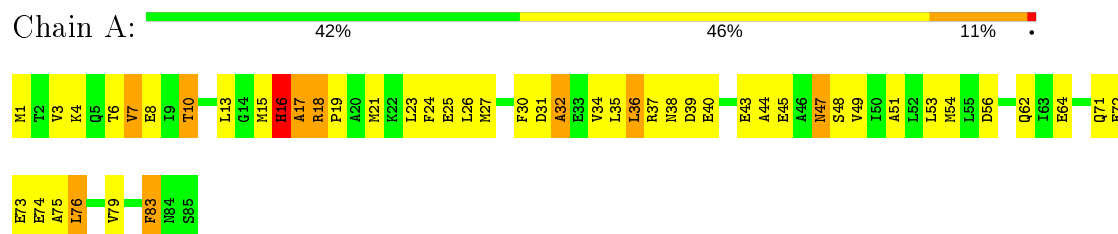
• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 33% 39% 7% 20%

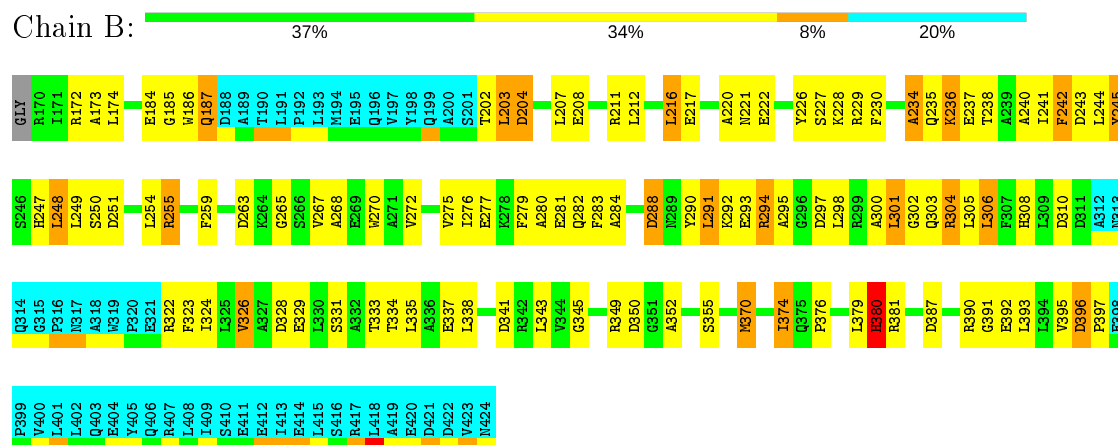


4.2.17 Score per residue for model 17

- Molecule 1: Phosphocarrier protein NPr

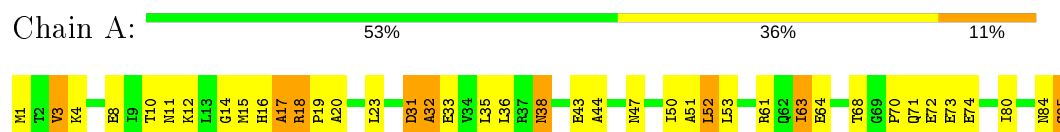


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

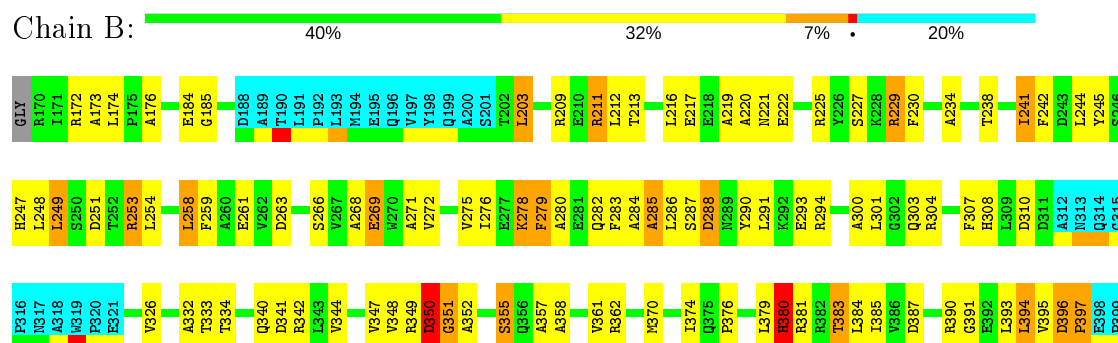


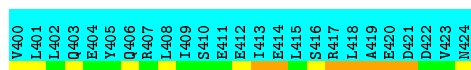
4.2.18 Score per residue for model 18

- Molecule 1: Phosphocarrier protein NPr



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



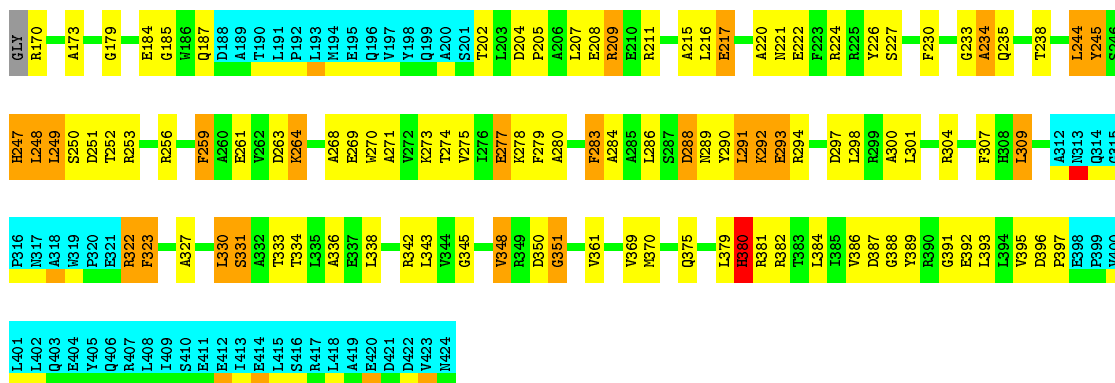
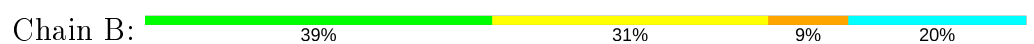


4.2.19 Score per residue for model 19

- Molecule 1: Phosphocarrier protein NPr

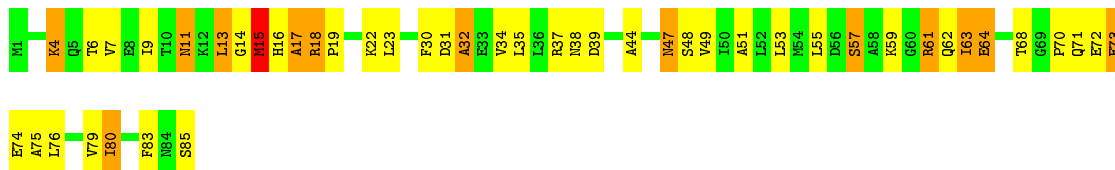


- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



4.2.20 Score per residue for model 20

- Molecule 1: Phosphocarrier protein NPr



- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP



G391	G314	L244
E392	G315	Y245
L393	P316	S246
L394	N317	H247
V395	A318	L248
D396	N319	L249
P397	P320	S250
E398	E321	D251
P399	R322	T252
V400	V326	R253
L401	A327	L254
L402	D328	L258
Q403	E329	F259
E404	L330	
Y405	T333	V262
Q406	T334	D263
R407	L335	
L408	L336	V267
I409	A337	A268
S410	E338	E269
E411	L339	W270
E412		A271
I413	V346	V272
E414	V347	K273
I415	V348	T274
S416	R349	V275
R417		L276
L418	S355	E277
A419	Q356	K278
E420	A357	F279
D421	A358	A280
D422	I359	E281
V423	M360	Q282
N424	V361	F283
	R362	A284
	A363	A285
	L364	L286
	G365	S287
	I366	D288
	P367	N289
		Y290
	M370	L291
		K292
	D373	E293
	L374	R294
	Q375	
		D297
	L379	L298
	H380	
	R381	Q303
	R382	R304
	T383	L305
	L384	L306
	I385	
	V386	L309
	D387	D310
	G388	D311
	Y389	A312
	R390	N313

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.37.7
ANALYSIS	structure solution	2.4.2
TopSpin	structure solution	3.0
Gaussian	structure solution	9
NMRPipe	structure solution	8.2
TALOS-N	structure solution	4.12

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	1391
Number of shifts mapped to atoms	1391
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	645	653	653	65±15
2	B	1587	1608	1607	123±14
All	All	44640	45220	45200	3678

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:CA	1:A:19:PRO:HG2	1.27	1.60	18	1
1:A:15:MET:HA	1:A:19:PRO:CD	1.27	1.56	18	1
1:A:10:THR:O	1:A:11:ASN:OD1	1.24	1.55	8	3
1:A:53:LEU:O	1:A:53:LEU:HD22	1.23	1.32	16	2
1:A:15:MET:HA	1:A:19:PRO:CG	1.20	1.67	18	1
2:B:338:LEU:O	2:B:338:LEU:HD22	1.13	1.42	7	1
1:A:15:MET:CA	1:A:19:PRO:CG	1.12	2.26	18	1
1:A:20:ALA:CB	1:A:52:LEU:HD21	1.11	1.74	18	1
1:A:9:ILE:HG22	1:A:61:ARG:O	1.11	1.44	5	3
1:A:53:LEU:HD13	1:A:54:MET:N	1.11	1.59	16	2
1:A:76:LEU:O	1:A:80:ILE:HG23	1.11	1.46	11	3
1:A:15:MET:O	1:A:17:ALA:N	1.09	1.86	15	6
2:B:395:VAL:O	2:B:397:PRO:CD	1.08	2.00	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:H	1:A:19:PRO:HD2	1.08	1.04	20	3
1:A:10:THR:C	1:A:11:ASN:OD1	1.07	1.94	3	1
1:A:15:MET:CA	1:A:19:PRO:CD	1.06	2.33	18	1
2:B:393:LEU:N	2:B:393:LEU:HD22	1.05	1.65	8	1
2:B:203:LEU:N	2:B:203:LEU:HD13	1.05	1.61	17	1
2:B:395:VAL:O	2:B:397:PRO:HD3	1.05	1.48	18	1
2:B:203:LEU:HD13	2:B:203:LEU:N	1.05	1.53	8	1
1:A:14:GLY:O	1:A:19:PRO:CG	1.04	2.05	18	4
1:A:17:ALA:HB3	1:A:18:ARG:HH11	1.04	1.11	17	2
1:A:3:VAL:HG21	1:A:72:GLU:OE1	1.03	1.53	1	1
1:A:9:ILE:HG21	1:A:58:ALA:O	1.02	1.54	14	3
2:B:330:LEU:H	2:B:330:LEU:HD23	1.02	1.10	14	2
1:A:15:MET:HB3	1:A:19:PRO:CB	1.02	1.85	18	1
2:B:233:GLY:O	2:B:234:ALA:O	1.02	1.77	10	9
1:A:10:THR:O	1:A:11:ASN:CG	1.01	1.98	3	3
1:A:15:MET:CA	1:A:19:PRO:HD2	1.01	1.84	18	1
2:B:286:LEU:HD12	2:B:288:ASP:OD1	1.00	1.56	2	1
1:A:53:LEU:O	2:B:291:LEU:HD21	1.00	1.55	18	1
1:A:74:GLU:OE1	1:A:75:ALA:N	1.00	1.94	12	1
2:B:384:LEU:HD22	2:B:384:LEU:O	1.00	1.56	20	1
1:A:71:GLN:O	1:A:74:GLU:HG3	0.99	1.56	12	1
1:A:16:HIS:O	1:A:19:PRO:HD2	0.99	1.57	7	1
2:B:338:LEU:C	2:B:338:LEU:HD22	0.99	1.78	7	1
1:A:15:MET:HB3	1:A:19:PRO:HB2	0.99	1.35	18	1
1:A:37:ARG:O	1:A:63:ILE:HG23	0.98	1.58	5	3
2:B:176:ALA:HB2	2:B:370:MET:SD	0.98	1.97	16	3
2:B:244:LEU:C	2:B:244:LEU:HD13	0.98	1.78	19	1
2:B:173:ALA:HB1	2:B:370:MET:O	0.97	1.59	18	11
2:B:286:LEU:HD23	2:B:287:SER:N	0.97	1.73	4	1
1:A:14:GLY:O	1:A:19:PRO:HG3	0.96	1.58	18	2
2:B:395:VAL:O	2:B:397:PRO:N	0.96	1.98	18	13
2:B:248:LEU:HD23	2:B:249:LEU:N	0.96	1.75	10	3
1:A:15:MET:HB3	1:A:19:PRO:CG	0.96	1.91	18	1
1:A:53:LEU:C	1:A:53:LEU:HD13	0.96	1.81	16	1
2:B:244:LEU:HD12	2:B:245:TYR:N	0.95	1.76	17	1
2:B:203:LEU:HD23	2:B:203:LEU:H	0.95	1.14	11	1
1:A:71:GLN:HB3	1:A:74:GLU:HG2	0.95	1.38	12	1
2:B:204:ASP:O	2:B:208:GLU:HB2	0.94	1.61	5	8
2:B:395:VAL:C	2:B:397:PRO:HD3	0.94	1.83	3	14
2:B:251:ASP:O	2:B:253:ARG:N	0.94	2.00	11	9
2:B:251:ASP:O	2:B:251:ASP:OD1	0.94	1.84	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:204:ASP:O	2:B:208:GLU:CB	0.94	2.16	13	9
1:A:53:LEU:HD13	1:A:53:LEU:C	0.94	1.82	8	1
1:A:34:VAL:C	1:A:35:LEU:HD22	0.94	1.84	12	3
1:A:15:MET:CB	1:A:19:PRO:CG	0.93	2.45	18	1
1:A:26:LEU:O	1:A:30:PHE:CD2	0.93	2.21	10	8
1:A:53:LEU:HB2	2:B:291:LEU:HD13	0.93	1.40	16	1
1:A:75:ALA:O	1:A:79:VAL:HG13	0.92	1.64	16	3
2:B:182:ILE:H	2:B:182:ILE:HD13	0.92	1.21	3	1
2:B:251:ASP:OD1	2:B:251:ASP:O	0.91	1.88	4	8
1:A:18:ARG:H	1:A:19:PRO:CD	0.91	1.78	20	3
2:B:203:LEU:H	2:B:203:LEU:HD22	0.91	1.25	17	2
1:A:53:LEU:HD23	1:A:54:MET:N	0.91	1.81	9	2
1:A:15:MET:SD	1:A:19:PRO:HD3	0.91	2.05	20	1
1:A:13:LEU:H	1:A:13:LEU:HD13	0.91	1.26	1	1
2:B:242:PHE:CG	2:B:243:ASP:N	0.90	2.39	12	6
2:B:392:GLU:C	2:B:393:LEU:HD13	0.90	1.85	8	1
2:B:395:VAL:O	2:B:396:ASP:OD1	0.90	1.89	8	2
2:B:244:LEU:O	2:B:244:LEU:HD23	0.90	1.65	15	2
2:B:351:GLY:O	2:B:352:ALA:O	0.90	1.89	9	3
2:B:286:LEU:HD21	2:B:288:ASP:O	0.90	1.67	11	1
1:A:13:LEU:HD22	1:A:13:LEU:N	0.90	1.80	16	2
2:B:184:GLU:O	2:B:324:ILE:HG22	0.90	1.66	4	1
2:B:203:LEU:CD1	2:B:203:LEU:N	0.90	2.30	8	1
2:B:286:LEU:HD12	2:B:288:ASP:OD2	0.90	1.67	3	1
1:A:50:ILE:O	1:A:53:LEU:HG	0.89	1.64	7	2
2:B:322:ARG:O	2:B:323:PHE:CG	0.89	2.25	6	6
2:B:350:ASP:O	2:B:352:ALA:N	0.89	2.05	3	4
2:B:216:LEU:HD23	2:B:217:GLU:N	0.89	1.83	17	1
2:B:394:LEU:N	2:B:394:LEU:HD22	0.88	1.83	7	1
2:B:286:LEU:O	2:B:286:LEU:HD23	0.88	1.68	11	1
2:B:380:HIS:CD2	2:B:381:ARG:H	0.88	1.86	16	2
2:B:217:GLU:O	2:B:221:ASN:HB3	0.88	1.67	2	1
1:A:13:LEU:HD13	1:A:13:LEU:N	0.88	1.84	1	1
1:A:5:GLN:OE1	1:A:76:LEU:HD21	0.88	1.68	15	2
1:A:30:PHE:O	1:A:30:PHE:CD1	0.88	2.27	14	5
1:A:71:GLN:HB3	1:A:74:GLU:CG	0.87	1.99	12	1
1:A:15:MET:HA	1:A:19:PRO:HD2	0.87	1.38	18	1
2:B:244:LEU:HD23	2:B:244:LEU:C	0.87	1.90	5	4
1:A:13:LEU:HA	1:A:83:PHE:CZ	0.87	2.04	5	1
2:B:380:HIS:ND1	2:B:381:ARG:N	0.87	2.23	10	2
2:B:241:ILE:HG23	2:B:242:PHE:N	0.86	1.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLU:CD	1:A:75:ALA:N	0.86	2.27	12	1
1:A:15:MET:N	1:A:19:PRO:HG2	0.86	1.84	18	1
1:A:77:ALA:O	1:A:80:ILE:HG13	0.86	1.71	4	2
2:B:361:VAL:O	2:B:366:ILE:HG22	0.86	1.71	16	1
2:B:291:LEU:HD13	2:B:292:LYS:N	0.86	1.84	12	1
1:A:20:ALA:HB2	1:A:52:LEU:HD21	0.86	1.44	18	1
1:A:18:ARG:N	1:A:19:PRO:HD2	0.86	1.86	20	12
2:B:393:LEU:HD22	2:B:393:LEU:H	0.86	1.19	8	1
1:A:72:GLU:CD	1:A:73:GLU:N	0.85	2.29	1	8
1:A:76:LEU:O	1:A:79:VAL:HG22	0.85	1.71	16	3
1:A:23:LEU:HD11	1:A:79:VAL:HG22	0.85	1.49	5	2
1:A:13:LEU:N	1:A:13:LEU:HD13	0.85	1.86	16	1
1:A:15:MET:CB	1:A:19:PRO:HG2	0.85	1.98	18	1
1:A:13:LEU:HD23	1:A:13:LEU:H	0.85	1.31	4	3
2:B:286:LEU:HB2	2:B:291:LEU:HD21	0.85	1.47	20	1
2:B:379:LEU:O	2:B:381:ARG:N	0.85	2.10	16	15
2:B:248:LEU:O	2:B:251:ASP:OD2	0.85	1.94	7	7
2:B:357:ALA:O	2:B:361:VAL:HG23	0.85	1.71	10	3
2:B:271:ALA:O	2:B:275:VAL:HG22	0.85	1.72	9	4
1:A:53:LEU:HD11	2:B:286:LEU:HD22	0.85	1.47	8	1
1:A:14:GLY:C	1:A:19:PRO:HG2	0.84	1.91	18	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.84	1.88	19	2
2:B:279:PHE:O	2:B:283:PHE:CD2	0.84	2.30	17	1
2:B:248:LEU:HD13	2:B:248:LEU:C	0.84	1.91	3	1
2:B:366:ILE:HG13	2:B:367:PRO:HD2	0.84	1.48	10	2
2:B:322:ARG:O	2:B:323:PHE:CD2	0.84	2.31	6	1
1:A:17:ALA:HB3	1:A:18:ARG:NH1	0.84	1.87	17	1
1:A:13:LEU:HD13	1:A:13:LEU:H	0.84	1.33	16	1
1:A:53:LEU:C	1:A:53:LEU:HD22	0.83	1.91	16	2
1:A:76:LEU:O	1:A:79:VAL:HG12	0.83	1.73	4	4
1:A:34:VAL:O	1:A:35:LEU:HD13	0.83	1.73	19	3
1:A:53:LEU:HD12	1:A:53:LEU:C	0.83	1.94	11	2
1:A:71:GLN:O	1:A:74:GLU:CG	0.83	2.25	12	1
2:B:279:PHE:O	2:B:283:PHE:CE2	0.83	2.31	17	1
2:B:207:LEU:O	2:B:211:ARG:HB3	0.82	1.74	8	1
2:B:290:TYR:O	2:B:293:GLU:OE2	0.82	1.97	14	1
2:B:272:VAL:O	2:B:276:ILE:HG23	0.82	1.75	20	6
2:B:344:VAL:HG13	2:B:345:GLY:N	0.82	1.88	1	1
2:B:301:LEU:HD12	2:B:301:LEU:O	0.82	1.74	2	3
2:B:286:LEU:CB	2:B:291:LEU:HD21	0.82	2.02	20	1
2:B:344:VAL:HG13	2:B:345:GLY:H	0.82	1.34	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:251:ASP:C	2:B:253:ARG:H	0.82	1.78	11	14
1:A:53:LEU:C	1:A:53:LEU:HD12	0.82	1.94	7	1
2:B:280:ALA:O	2:B:284:ALA:CB	0.82	2.28	17	5
1:A:56:ASP:OD2	2:B:291:LEU:HD11	0.82	1.74	9	1
1:A:15:MET:CE	1:A:19:PRO:CD	0.82	2.57	20	1
2:B:241:ILE:O	2:B:244:LEU:HG	0.82	1.75	17	1
1:A:36:LEU:HD22	1:A:36:LEU:N	0.81	1.90	10	1
1:A:74:GLU:CD	1:A:75:ALA:H	0.81	1.77	12	1
2:B:322:ARG:O	2:B:323:PHE:CD1	0.81	2.33	17	10
1:A:36:LEU:N	1:A:36:LEU:HD22	0.81	1.91	3	1
1:A:21:MET:SD	1:A:21:MET:N	0.81	2.53	10	1
2:B:223:PHE:CD1	2:B:224:ARG:N	0.81	2.49	4	1
2:B:338:LEU:HD13	2:B:342:ARG:NH1	0.81	1.90	12	1
2:B:338:LEU:CD2	2:B:338:LEU:O	0.81	2.29	7	1
1:A:18:ARG:HE	1:A:18:ARG:N	0.81	1.74	16	2
1:A:30:PHE:CD1	1:A:30:PHE:O	0.81	2.34	1	3
2:B:350:ASP:O	2:B:351:GLY:O	0.81	1.99	14	4
1:A:9:ILE:HG12	1:A:63:ILE:HD11	0.81	1.53	20	1
2:B:275:VAL:HG23	2:B:276:ILE:N	0.81	1.91	6	5
2:B:271:ALA:O	2:B:275:VAL:HG12	0.80	1.76	13	1
2:B:384:LEU:N	2:B:384:LEU:CD1	0.80	2.43	20	1
2:B:385:ILE:HD12	2:B:385:ILE:N	0.80	1.92	1	3
2:B:280:ALA:O	2:B:284:ALA:HB2	0.80	1.77	19	3
1:A:53:LEU:O	1:A:53:LEU:HD12	0.80	1.77	11	1
1:A:20:ALA:CB	1:A:52:LEU:CD2	0.80	2.60	18	1
1:A:30:PHE:HB2	1:A:71:GLN:CD	0.80	1.97	3	1
1:A:20:ALA:HB1	1:A:52:LEU:HD21	0.80	1.51	18	1
1:A:38:ASN:ND2	1:A:42:THR:H	0.79	1.74	8	1
2:B:393:LEU:N	2:B:393:LEU:CD2	0.79	2.40	8	1
2:B:361:VAL:HA	2:B:364:LEU:HD21	0.79	1.53	16	1
2:B:255:ARG:HE	2:B:255:ARG:N	0.79	1.75	17	1
2:B:257:GLU:OE2	2:B:279:PHE:CE1	0.79	2.35	5	2
2:B:330:LEU:H	2:B:330:LEU:CD2	0.79	1.90	14	1
1:A:62:GLN:C	1:A:63:ILE:HD13	0.79	1.98	20	1
2:B:253:ARG:O	2:B:256:ARG:HG3	0.79	1.77	1	2
2:B:258:LEU:HD21	2:B:272:VAL:HG23	0.79	1.55	1	1
2:B:241:ILE:CG2	2:B:242:PHE:N	0.79	2.45	10	4
2:B:203:LEU:N	2:B:203:LEU:HD23	0.79	1.93	4	3
1:A:15:MET:CB	1:A:19:PRO:HD2	0.79	2.08	18	1
1:A:77:ALA:O	1:A:80:ILE:HG12	0.79	1.78	9	2
2:B:244:LEU:O	2:B:244:LEU:HD22	0.79	1.76	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:341:ASP:OD1	2:B:342:ARG:N	0.79	2.16	9	4
1:A:14:GLY:O	1:A:19:PRO:HG2	0.79	1.75	18	4
2:B:288:ASP:O	2:B:292:LYS:CB	0.79	2.31	17	6
1:A:63:ILE:O	1:A:63:ILE:HD13	0.78	1.77	7	2
2:B:242:PHE:CD1	2:B:242:PHE:C	0.78	2.55	4	3
2:B:249:LEU:HD13	2:B:249:LEU:C	0.78	1.99	17	1
2:B:338:LEU:HD13	2:B:338:LEU:H	0.78	1.36	7	1
2:B:379:LEU:HD22	2:B:379:LEU:N	0.78	1.93	5	1
2:B:395:VAL:C	2:B:396:ASP:OD1	0.78	2.22	8	4
2:B:226:TYR:CE2	2:B:336:ALA:O	0.78	2.37	19	5
1:A:53:LEU:HD23	2:B:291:LEU:HB3	0.78	1.56	8	1
2:B:354:ASN:O	2:B:355:SER:O	0.78	2.01	15	2
2:B:182:ILE:N	2:B:182:ILE:HD13	0.78	1.91	3	1
1:A:15:MET:CB	1:A:19:PRO:CD	0.78	2.61	18	1
1:A:72:GLU:OE1	1:A:73:GLU:N	0.78	2.17	1	6
2:B:185:GLY:O	2:B:380:HIS:O	0.78	2.02	6	19
2:B:290:TYR:O	2:B:293:GLU:CD	0.78	2.22	14	1
2:B:216:LEU:C	2:B:216:LEU:HD12	0.77	2.00	5	1
1:A:31:ASP:O	1:A:70:PRO:HD2	0.77	1.78	13	5
1:A:30:PHE:CD1	1:A:74:GLU:OE1	0.77	2.37	12	1
1:A:15:MET:N	1:A:15:MET:SD	0.77	2.58	20	1
1:A:13:LEU:HD22	1:A:13:LEU:H	0.77	1.36	16	1
2:B:379:LEU:N	2:B:379:LEU:HD22	0.77	1.94	9	2
1:A:53:LEU:HD13	2:B:291:LEU:HD13	0.77	1.54	7	1
1:A:10:THR:HG22	1:A:10:THR:O	0.77	1.76	19	3
2:B:288:ASP:HB2	2:B:291:LEU:HD22	0.77	1.57	18	1
1:A:10:THR:C	1:A:11:ASN:CG	0.77	2.41	3	2
1:A:53:LEU:HG	2:B:291:LEU:HD22	0.77	1.57	16	1
2:B:303:GLN:HG3	2:B:304:ARG:N	0.77	1.95	14	3
1:A:23:LEU:HD11	1:A:79:VAL:HG23	0.76	1.56	12	1
1:A:63:ILE:HD13	1:A:63:ILE:N	0.76	1.96	20	1
2:B:393:LEU:O	2:B:393:LEU:HD12	0.76	1.79	16	1
2:B:322:ARG:C	2:B:323:PHE:CD1	0.76	2.59	17	2
2:B:212:LEU:C	2:B:212:LEU:HD13	0.76	2.00	17	1
2:B:338:LEU:HD22	2:B:338:LEU:N	0.76	1.93	8	1
2:B:384:LEU:HD13	2:B:384:LEU:H	0.76	1.39	20	1
1:A:27:MET:HA	1:A:30:PHE:CZ	0.76	2.16	3	8
2:B:184:GLU:O	2:B:324:ILE:CG2	0.76	2.33	4	1
2:B:291:LEU:HG	2:B:292:LYS:N	0.76	1.95	19	2
2:B:248:LEU:O	2:B:248:LEU:HD12	0.76	1.79	8	1
2:B:380:HIS:CG	2:B:381:ARG:H	0.76	1.98	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LEU:HD21	1:A:37:ARG:NE	0.76	1.96	13	1
2:B:338:LEU:CD2	2:B:338:LEU:C	0.76	2.54	7	1
1:A:23:LEU:HD21	1:A:79:VAL:HG22	0.76	1.56	1	1
2:B:275:VAL:HG23	2:B:276:ILE:H	0.76	1.40	6	3
2:B:304:ARG:O	2:B:308:HIS:ND1	0.76	2.19	14	3
1:A:69:GLY:O	1:A:72:GLU:HG3	0.75	1.81	1	2
1:A:53:LEU:CD2	1:A:53:LEU:O	0.75	2.25	16	2
1:A:53:LEU:CG	2:B:291:LEU:HD22	0.75	2.11	16	1
2:B:203:LEU:O	2:B:204:ASP:OD1	0.75	2.05	5	6
1:A:9:ILE:O	1:A:9:ILE:HG23	0.75	1.81	14	2
1:A:72:GLU:OE1	1:A:72:GLU:N	0.75	2.19	11	2
2:B:254:LEU:O	2:B:258:LEU:HD12	0.75	1.79	13	2
1:A:34:VAL:O	1:A:35:LEU:HD12	0.75	1.81	20	5
2:B:230:PHE:CE2	2:B:239:ALA:HB2	0.75	2.16	16	1
1:A:30:PHE:CD1	1:A:30:PHE:C	0.75	2.60	14	5
2:B:288:ASP:O	2:B:292:LYS:N	0.75	2.18	17	6
1:A:18:ARG:N	1:A:19:PRO:CD	0.74	2.50	10	17
1:A:18:ARG:N	1:A:19:PRO:HD3	0.74	1.97	6	1
2:B:216:LEU:O	2:B:220:ALA:N	0.74	2.20	6	18
1:A:13:LEU:CD2	1:A:13:LEU:H	0.74	1.92	16	3
2:B:241:ILE:CG2	2:B:242:PHE:H	0.74	1.94	10	1
1:A:16:HIS:O	1:A:17:ALA:HB2	0.74	1.83	18	5
2:B:330:LEU:CD2	2:B:330:LEU:H	0.74	1.95	10	1
1:A:72:GLU:CD	1:A:73:GLU:H	0.74	1.83	1	4
2:B:332:ALA:N	2:B:357:ALA:HB2	0.74	1.97	18	2
2:B:286:LEU:CD2	2:B:288:ASP:N	0.74	2.50	4	1
2:B:216:LEU:HG	2:B:217:GLU:N	0.74	1.97	5	1
2:B:374:ILE:O	2:B:376:PRO:HD3	0.74	1.82	5	4
1:A:80:ILE:O	1:A:84:ASN:OD1	0.74	2.06	11	2
2:B:244:LEU:C	2:B:244:LEU:CD1	0.74	2.54	19	1
2:B:378:VAL:O	2:B:380:HIS:CD2	0.74	2.40	10	1
1:A:35:LEU:N	1:A:35:LEU:HD22	0.74	1.97	12	1
2:B:364:LEU:HD11	2:B:366:ILE:CG2	0.74	2.12	16	1
2:B:204:ASP:O	2:B:208:GLU:HB3	0.74	1.82	13	1
1:A:16:HIS:O	1:A:17:ALA:CB	0.74	2.36	18	5
2:B:343:LEU:HD11	2:B:345:GLY:O	0.74	1.82	17	1
2:B:352:ALA:O	2:B:353:ALA:HB3	0.74	1.83	15	5
1:A:30:PHE:CD1	1:A:71:GLN:NE2	0.74	2.56	3	1
2:B:301:LEU:HD13	2:B:301:LEU:O	0.74	1.82	6	2
2:B:289:ASN:HD22	2:B:290:TYR:N	0.74	1.80	20	1
2:B:244:LEU:HD23	2:B:244:LEU:O	0.73	1.83	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PRO:O	1:A:23:LEU:HD13	0.73	1.82	17	3
1:A:15:MET:HE1	1:A:19:PRO:CG	0.73	2.13	20	1
2:B:204:ASP:O	2:B:208:GLU:HG2	0.73	1.81	7	6
1:A:83:PHE:CD1	1:A:83:PHE:O	0.73	2.41	17	2
2:B:330:LEU:N	2:B:330:LEU:HD23	0.73	1.93	14	2
1:A:30:PHE:C	1:A:30:PHE:CD1	0.73	2.62	2	3
1:A:16:HIS:O	1:A:21:MET:SD	0.73	2.46	15	1
1:A:15:MET:CE	1:A:19:PRO:CG	0.73	2.66	20	1
2:B:208:GLU:OE1	2:B:268:ALA:N	0.73	2.21	20	1
1:A:49:VAL:O	1:A:53:LEU:HD12	0.73	1.82	17	2
2:B:174:LEU:O	2:B:370:MET:SD	0.73	2.47	12	1
1:A:9:ILE:HG23	1:A:9:ILE:O	0.73	1.82	4	1
2:B:354:ASN:O	2:B:358:ALA:HB3	0.73	1.84	15	2
2:B:387:ASP:O	2:B:391:GLY:N	0.72	2.21	19	20
1:A:18:ARG:CB	1:A:19:PRO:HD3	0.72	2.14	2	7
1:A:30:PHE:HE1	1:A:32:ALA:O	0.72	1.67	17	8
1:A:15:MET:SD	1:A:19:PRO:CD	0.72	2.76	20	1
2:B:275:VAL:HG13	2:B:276:ILE:N	0.72	1.99	17	4
2:B:170:ARG:C	2:B:171:ILE:HD12	0.72	2.04	6	2
1:A:53:LEU:CD1	1:A:53:LEU:C	0.72	2.56	8	3
2:B:392:GLU:N	2:B:392:GLU:OE1	0.72	2.22	8	1
2:B:249:LEU:HD23	2:B:250:SER:N	0.72	1.98	19	2
2:B:251:ASP:OD1	2:B:253:ARG:N	0.72	2.23	6	3
2:B:286:LEU:C	2:B:286:LEU:HD23	0.72	2.04	11	2
2:B:258:LEU:HD12	2:B:258:LEU:C	0.72	2.05	18	1
2:B:184:GLU:CB	2:B:323:PHE:CE2	0.72	2.73	4	2
1:A:10:THR:O	1:A:10:THR:OG1	0.72	2.03	14	4
2:B:174:LEU:HD22	2:B:174:LEU:N	0.72	1.99	7	3
1:A:36:LEU:HD12	1:A:36:LEU:N	0.72	1.99	8	3
2:B:395:VAL:C	2:B:397:PRO:CD	0.71	2.57	3	9
2:B:247:HIS:O	2:B:251:ASP:HB3	0.71	1.84	4	4
1:A:83:PHE:O	1:A:83:PHE:CD1	0.71	2.42	15	2
2:B:249:LEU:HG	2:B:250:SER:N	0.71	1.99	7	2
2:B:248:LEU:C	2:B:248:LEU:HD13	0.71	2.05	12	1
2:B:290:TYR:O	2:B:293:GLU:OE1	0.71	2.07	14	1
2:B:379:LEU:O	2:B:380:HIS:O	0.71	2.09	11	2
2:B:248:LEU:HD23	2:B:248:LEU:C	0.71	2.05	6	3
2:B:289:ASN:ND2	2:B:290:TYR:H	0.71	1.82	20	2
2:B:203:LEU:HD23	2:B:203:LEU:N	0.71	1.95	11	1
2:B:204:ASP:OD1	2:B:208:GLU:OE2	0.71	2.07	15	2
2:B:248:LEU:O	2:B:251:ASP:CG	0.71	2.29	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD12	1:A:30:PHE:CE1	0.71	2.21	7	2
2:B:384:LEU:O	2:B:384:LEU:CD2	0.71	2.38	20	1
2:B:203:LEU:H	2:B:203:LEU:HD13	0.71	1.43	8	2
2:B:379:LEU:H	2:B:379:LEU:HD22	0.71	1.46	9	1
2:B:339:PRO:HB2	2:B:341:ASP:OD1	0.71	1.85	1	3
1:A:69:GLY:O	1:A:72:GLU:HB3	0.71	1.86	9	7
1:A:53:LEU:N	1:A:53:LEU:CD1	0.71	2.54	15	1
1:A:14:GLY:C	1:A:15:MET:SD	0.71	2.68	20	1
2:B:223:PHE:C	2:B:223:PHE:CD1	0.71	2.64	4	2
1:A:5:GLN:NE2	1:A:5:GLN:C	0.71	2.44	6	1
2:B:380:HIS:O	2:B:380:HIS:CG	0.71	2.44	7	1
2:B:382:ARG:HH22	2:B:396:ASP:CG	0.70	1.89	6	1
2:B:249:LEU:HD12	2:B:301:LEU:HD11	0.70	1.63	19	1
1:A:13:LEU:CD2	1:A:13:LEU:N	0.70	2.52	1	1
2:B:242:PHE:CD2	2:B:243:ASP:N	0.70	2.58	12	2
2:B:300:ALA:CB	2:B:333:THR:HG21	0.70	2.16	11	2
1:A:5:GLN:OE1	1:A:80:ILE:HD12	0.70	1.86	7	2
1:A:13:LEU:H	1:A:13:LEU:CD1	0.70	1.85	1	2
1:A:9:ILE:HG23	1:A:60:GLY:H	0.70	1.46	14	3
2:B:291:LEU:C	2:B:291:LEU:HD12	0.70	2.07	20	2
1:A:31:ASP:O	1:A:32:ALA:HB2	0.70	1.86	10	20
2:B:251:ASP:OD1	2:B:254:LEU:N	0.70	2.23	6	3
2:B:299:ARG:HG3	2:B:300:ALA:N	0.70	2.01	6	1
2:B:272:VAL:O	2:B:276:ILE:CG2	0.70	2.40	18	3
2:B:379:LEU:HD22	2:B:379:LEU:H	0.70	1.44	5	1
1:A:5:GLN:CD	1:A:5:GLN:O	0.70	2.30	14	1
2:B:384:LEU:HD22	2:B:384:LEU:C	0.70	2.06	20	1
2:B:212:LEU:HD13	2:B:212:LEU:C	0.70	2.06	5	1
1:A:75:ALA:O	1:A:79:VAL:HG23	0.70	1.86	1	5
2:B:244:LEU:HD13	2:B:245:TYR:N	0.70	2.00	19	1
2:B:288:ASP:N	2:B:288:ASP:OD1	0.70	2.25	20	1
2:B:291:LEU:HD13	2:B:291:LEU:C	0.70	2.07	12	1
1:A:71:GLN:HG2	1:A:74:GLU:HB2	0.69	1.62	3	1
2:B:258:LEU:HD21	2:B:275:VAL:HG21	0.69	1.64	3	1
2:B:184:GLU:HB2	2:B:323:PHE:CE2	0.69	2.22	4	2
2:B:258:LEU:HD13	2:B:258:LEU:C	0.69	2.08	5	1
2:B:379:LEU:O	2:B:380:HIS:C	0.69	2.30	6	16
2:B:174:LEU:HD12	2:B:174:LEU:N	0.69	2.02	12	1
1:A:16:HIS:O	1:A:17:ALA:HB3	0.69	1.88	2	4
1:A:63:ILE:C	1:A:63:ILE:HD13	0.69	2.08	7	1
2:B:289:ASN:ND2	2:B:290:TYR:N	0.69	2.40	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:338:LEU:H	2:B:338:LEU:CD1	0.69	2.00	7	1
2:B:288:ASP:CG	2:B:291:LEU:HD23	0.69	2.07	20	1
2:B:222:GLU:O	2:B:226:TYR:CD1	0.69	2.46	17	6
1:A:17:ALA:C	1:A:19:PRO:HD2	0.69	2.07	10	3
1:A:12:LYS:CD	1:A:12:LYS:O	0.69	2.41	14	1
2:B:233:GLY:O	2:B:234:ALA:C	0.69	2.30	10	8
2:B:203:LEU:N	2:B:203:LEU:CD1	0.69	2.36	17	2
2:B:172:ARG:N	2:B:172:ARG:HE	0.69	1.86	16	2
2:B:204:ASP:O	2:B:208:GLU:CG	0.69	2.41	10	7
2:B:338:LEU:HB2	2:B:342:ARG:NE	0.69	2.03	12	1
2:B:330:LEU:HD23	2:B:348:VAL:HG22	0.69	1.64	20	1
1:A:32:ALA:HB1	1:A:68:THR:O	0.69	1.87	13	12
1:A:15:MET:O	1:A:16:HIS:C	0.69	2.30	12	4
1:A:15:MET:O	1:A:16:HIS:O	0.69	2.11	7	1
2:B:288:ASP:O	2:B:292:LYS:HB3	0.69	1.88	2	6
2:B:270:TRP:CZ2	2:B:274:THR:OG1	0.69	2.45	5	1
1:A:64:GLU:O	1:A:66:GLU:OE1	0.68	2.11	8	1
1:A:14:GLY:O	1:A:15:MET:SD	0.68	2.51	16	1
2:B:230:PHE:O	2:B:234:ALA:N	0.68	2.26	17	10
2:B:240:ALA:O	2:B:243:ASP:OD1	0.68	2.11	14	1
2:B:384:LEU:CD1	2:B:384:LEU:H	0.68	1.99	20	1
1:A:36:LEU:C	1:A:37:ARG:HG2	0.68	2.09	1	1
2:B:378:VAL:O	2:B:380:HIS:ND1	0.68	2.25	16	1
2:B:395:VAL:O	2:B:396:ASP:C	0.68	2.30	3	20
1:A:16:HIS:O	1:A:18:ARG:N	0.68	2.26	7	4
2:B:394:LEU:N	2:B:394:LEU:CD2	0.68	2.57	7	2
2:B:395:VAL:HG13	2:B:395:VAL:O	0.68	1.89	8	3
1:A:14:GLY:O	1:A:15:MET:CB	0.68	2.42	3	4
1:A:76:LEU:O	1:A:76:LEU:HD13	0.68	1.89	8	2
2:B:300:ALA:CB	2:B:333:THR:OG1	0.68	2.42	18	4
1:A:18:ARG:NE	1:A:18:ARG:N	0.68	2.41	16	2
1:A:50:ILE:HD12	2:B:283:PHE:CE1	0.68	2.24	18	1
2:B:227:SER:OG	2:B:242:PHE:HB2	0.68	1.88	3	2
2:B:275:VAL:HG13	2:B:276:ILE:H	0.68	1.49	5	3
1:A:26:LEU:C	1:A:30:PHE:CD2	0.68	2.66	1	8
2:B:344:VAL:CG1	2:B:345:GLY:H	0.68	2.01	1	1
1:A:12:LYS:O	1:A:12:LYS:CG	0.68	2.40	12	3
1:A:13:LEU:HD12	1:A:13:LEU:N	0.68	2.04	9	1
1:A:76:LEU:HD12	1:A:76:LEU:O	0.68	1.89	10	1
2:B:301:LEU:HD12	2:B:301:LEU:C	0.68	2.10	16	2
1:A:9:ILE:CG2	1:A:61:ARG:O	0.67	2.36	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:374:ILE:HD13	2:B:374:ILE:N	0.67	2.04	7	1
1:A:20:ALA:HB1	1:A:52:LEU:CD2	0.67	2.18	18	3
2:B:279:PHE:CD2	2:B:282:GLN:NE2	0.67	2.62	4	3
1:A:16:HIS:C	1:A:19:PRO:HD2	0.67	2.09	7	1
2:B:275:VAL:CG2	2:B:276:ILE:N	0.67	2.57	16	3
2:B:307:PHE:O	2:B:307:PHE:CD1	0.67	2.48	14	1
2:B:323:PHE:CE2	2:B:342:ARG:NE	0.67	2.62	3	1
1:A:13:LEU:CD1	1:A:13:LEU:H	0.67	1.90	16	1
2:B:249:LEU:O	2:B:249:LEU:HD13	0.67	1.88	17	1
2:B:384:LEU:C	2:B:385:ILE:HD13	0.67	2.10	7	1
1:A:70:PRO:O	1:A:73:GLU:OE2	0.67	2.11	15	2
1:A:15:MET:HE3	1:A:19:PRO:CD	0.67	2.19	20	1
1:A:13:LEU:H	1:A:13:LEU:HD22	0.67	1.45	1	1
2:B:202:THR:C	2:B:203:LEU:HD13	0.67	2.10	17	2
2:B:344:VAL:CG1	2:B:345:GLY:N	0.67	2.58	1	1
2:B:207:LEU:O	2:B:211:ARG:CB	0.67	2.41	8	5
1:A:11:ASN:O	1:A:11:ASN:ND2	0.67	2.28	18	1
1:A:35:LEU:HD21	1:A:37:ARG:HE	0.67	1.49	13	1
2:B:230:PHE:CD2	2:B:239:ALA:HB2	0.67	2.24	16	1
2:B:384:LEU:HD13	2:B:384:LEU:O	0.67	1.90	20	1
1:A:13:LEU:O	1:A:83:PHE:CD1	0.67	2.48	11	8
2:B:366:ILE:CG2	2:B:367:PRO:HD2	0.67	2.20	4	3
2:B:242:PHE:CZ	2:B:336:ALA:HB2	0.67	2.25	20	2
1:A:38:ASN:ND2	1:A:54:MET:SD	0.66	2.68	17	2
2:B:272:VAL:O	2:B:276:ILE:CG1	0.66	2.43	18	4
2:B:288:ASP:O	2:B:292:LYS:HB2	0.66	1.90	8	3
1:A:24:PHE:CZ	2:B:247:HIS:CE1	0.66	2.83	10	2
2:B:226:TYR:OH	2:B:336:ALA:O	0.66	2.09	6	1
2:B:272:VAL:O	2:B:276:ILE:HG12	0.66	1.90	16	6
2:B:238:THR:O	2:B:241:ILE:CG1	0.66	2.43	17	3
1:A:63:ILE:HD11	1:A:65:VAL:HG23	0.66	1.64	7	1
2:B:244:LEU:CD1	2:B:245:TYR:N	0.66	2.57	17	1
2:B:352:ALA:O	2:B:353:ALA:CB	0.66	2.43	2	5
1:A:53:LEU:HD12	1:A:54:MET:N	0.66	2.05	7	1
1:A:17:ALA:CB	1:A:18:ARG:HH11	0.66	1.97	17	1
2:B:230:PHE:O	2:B:234:ALA:HB3	0.66	1.89	18	1
2:B:172:ARG:NE	2:B:172:ARG:N	0.66	2.43	2	1
1:A:71:GLN:OE1	1:A:75:ALA:N	0.66	2.28	3	1
2:B:283:PHE:CE2	2:B:298:LEU:CD1	0.66	2.79	3	1
2:B:258:LEU:HD23	2:B:259:PHE:N	0.66	2.05	7	1
1:A:38:ASN:HD22	1:A:38:ASN:N	0.66	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:325:LEU:HD13	2:B:325:LEU:C	0.66	2.10	12	2
1:A:53:LEU:C	1:A:53:LEU:CD2	0.66	2.60	16	2
1:A:15:MET:HE1	1:A:19:PRO:HG3	0.66	1.66	20	1
2:B:223:PHE:CD1	2:B:304:ARG:NH1	0.66	2.63	5	1
2:B:352:ALA:HB3	2:B:355:SER:OG	0.66	1.90	18	2
2:B:248:LEU:C	2:B:248:LEU:HD23	0.66	2.11	10	3
1:A:53:LEU:HD13	1:A:54:MET:CA	0.66	2.21	16	2
1:A:23:LEU:HD22	1:A:34:VAL:HG11	0.66	1.68	10	1
2:B:385:ILE:HG23	2:B:385:ILE:O	0.66	1.89	10	1
2:B:380:HIS:CD2	2:B:381:ARG:N	0.66	2.63	16	1
2:B:301:LEU:C	2:B:301:LEU:HD12	0.66	2.11	2	2
2:B:284:ALA:O	2:B:286:LEU:O	0.66	2.14	12	5
2:B:249:LEU:HD11	2:B:301:LEU:HD11	0.66	1.68	6	1
2:B:280:ALA:O	2:B:284:ALA:HB3	0.66	1.91	9	5
2:B:211:ARG:NE	2:B:309:LEU:CD1	0.66	2.58	14	1
2:B:286:LEU:HD22	2:B:288:ASP:O	0.66	1.90	4	1
2:B:283:PHE:O	2:B:291:LEU:HD11	0.66	1.91	12	2
2:B:227:SER:CB	2:B:242:PHE:CB	0.65	2.73	4	5
1:A:13:LEU:HD13	1:A:13:LEU:O	0.65	1.91	8	1
2:B:385:ILE:O	2:B:385:ILE:HG22	0.65	1.92	2	1
2:B:230:PHE:CD2	2:B:238:THR:HG21	0.65	2.26	11	3
2:B:304:ARG:O	2:B:308:HIS:CD2	0.65	2.49	2	7
2:B:182:ILE:N	2:B:182:ILE:CD1	0.65	2.60	3	1
1:A:9:ILE:CG2	1:A:58:ALA:O	0.65	2.39	14	3
1:A:23:LEU:HD21	1:A:79:VAL:HG12	0.65	1.68	8	1
2:B:338:LEU:CD2	2:B:338:LEU:N	0.65	2.60	8	1
2:B:227:SER:HB3	2:B:242:PHE:CD2	0.65	2.26	9	1
2:B:384:LEU:HD13	2:B:385:ILE:N	0.65	2.06	14	2
2:B:204:ASP:N	2:B:205:PRO:HD3	0.65	2.07	2	5
2:B:277:GLU:O	2:B:281:GLU:OE1	0.65	2.15	15	8
2:B:227:SER:CB	2:B:242:PHE:HB2	0.65	2.22	4	4
2:B:242:PHE:C	2:B:242:PHE:CD1	0.65	2.70	13	2
1:A:24:PHE:O	1:A:28:GLN:OE1	0.65	2.14	13	2
1:A:9:ILE:CG1	1:A:63:ILE:HD11	0.65	2.21	20	1
2:B:353:ALA:HB1	2:B:362:ARG:NH1	0.65	2.07	12	2
1:A:16:HIS:NE2	2:B:290:TYR:CE2	0.65	2.64	9	2
1:A:76:LEU:C	1:A:76:LEU:HD23	0.65	2.11	15	1
2:B:254:LEU:HD23	2:B:254:LEU:O	0.65	1.90	18	1
2:B:207:LEU:O	2:B:211:ARG:HB2	0.65	1.91	19	5
2:B:375:GLN:O	2:B:378:VAL:HG22	0.65	1.92	16	2
2:B:301:LEU:HG	2:B:302:GLY:N	0.65	2.07	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:N	1:A:21:MET:SD	0.65	2.70	3	2
2:B:273:LYS:O	2:B:277:GLU:HB2	0.65	1.92	6	3
2:B:338:LEU:N	2:B:338:LEU:CD1	0.65	2.60	7	1
2:B:338:LEU:N	2:B:338:LEU:HD22	0.65	2.07	9	1
1:A:38:ASN:HD21	1:A:58:ALA:HB2	0.65	1.51	3	1
1:A:12:LYS:CG	1:A:12:LYS:O	0.65	2.43	6	2
1:A:4:LYS:N	1:A:4:LYS:CD	0.65	2.60	15	1
2:B:288:ASP:O	2:B:291:LEU:HD23	0.65	1.92	19	1
1:A:18:ARG:CB	1:A:19:PRO:CD	0.64	2.75	2	5
2:B:283:PHE:CD2	2:B:283:PHE:N	0.64	2.62	8	2
2:B:227:SER:OG	2:B:242:PHE:HB3	0.64	1.92	5	1
1:A:15:MET:O	1:A:19:PRO:HD2	0.64	1.91	15	1
1:A:13:LEU:HD12	1:A:13:LEU:O	0.64	1.91	17	1
1:A:20:ALA:HB1	1:A:52:LEU:HD11	0.64	1.67	18	1
2:B:241:ILE:HG13	2:B:242:PHE:H	0.64	1.51	12	3
2:B:335:LEU:C	2:B:335:LEU:HD23	0.64	2.13	17	1
2:B:294:ARG:HH11	2:B:297:ASP:CG	0.64	1.96	2	1
2:B:211:ARG:NH2	2:B:269:GLU:OE2	0.64	2.30	6	3
2:B:307:PHE:C	2:B:307:PHE:CD1	0.64	2.71	14	1
2:B:283:PHE:N	2:B:283:PHE:CD1	0.64	2.60	18	3
2:B:215:ALA:HB1	2:B:309:LEU:HD22	0.64	1.69	12	1
2:B:249:LEU:HD12	2:B:250:SER:N	0.64	2.06	1	1
2:B:326:VAL:HG13	2:B:326:VAL:O	0.64	1.92	20	2
2:B:211:ARG:NH1	2:B:269:GLU:OE2	0.64	2.30	7	3
2:B:275:VAL:CG2	2:B:276:ILE:H	0.64	2.06	6	2
1:A:15:MET:C	1:A:17:ALA:N	0.64	2.49	15	1
2:B:259:PHE:O	2:B:262:VAL:HG22	0.64	1.93	2	3
2:B:174:LEU:CD2	2:B:174:LEU:N	0.64	2.59	7	2
2:B:366:ILE:HG23	2:B:367:PRO:HD2	0.64	1.70	4	4
1:A:21:MET:HG3	1:A:22:LYS:N	0.64	2.07	4	1
2:B:244:LEU:CD2	2:B:244:LEU:C	0.64	2.64	5	3
2:B:349:ARG:HH11	2:B:374:ILE:N	0.64	1.90	5	1
1:A:5:GLN:C	1:A:5:GLN:HE21	0.64	1.97	6	1
1:A:53:LEU:HB2	2:B:291:LEU:CD1	0.64	2.21	16	1
1:A:16:HIS:O	1:A:16:HIS:ND1	0.64	2.31	3	1
1:A:49:VAL:O	1:A:53:LEU:HD13	0.64	1.93	5	3
2:B:259:PHE:N	2:B:259:PHE:CD1	0.64	2.64	11	1
1:A:34:VAL:C	1:A:35:LEU:HD12	0.64	2.14	17	3
2:B:286:LEU:N	2:B:286:LEU:HD12	0.64	2.06	5	1
1:A:17:ALA:O	1:A:18:ARG:HB2	0.64	1.91	6	1
2:B:227:SER:CB	2:B:242:PHE:CG	0.64	2.81	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:251:ASP:C	2:B:253:ARG:N	0.63	2.45	11	16
2:B:338:LEU:CD2	2:B:339:PRO:O	0.63	2.46	7	1
1:A:1:MET:SD	1:A:1:MET:N	0.63	2.70	9	1
2:B:350:ASP:O	2:B:351:GLY:C	0.63	2.37	1	6
1:A:26:LEU:C	1:A:30:PHE:CE2	0.63	2.72	3	8
2:B:251:ASP:O	2:B:251:ASP:CG	0.63	2.35	4	1
2:B:306:LEU:O	2:B:310:ASP:OD2	0.63	2.15	11	1
1:A:15:MET:HE3	1:A:19:PRO:HD2	0.63	1.68	20	1
2:B:238:THR:O	2:B:241:ILE:HG12	0.63	1.94	17	3
1:A:35:LEU:N	1:A:35:LEU:CD2	0.63	2.61	19	1
2:B:384:LEU:N	2:B:384:LEU:HD13	0.63	2.01	20	1
2:B:205:PRO:O	2:B:209:ARG:N	0.63	2.31	10	5
2:B:243:ASP:OD1	2:B:244:LEU:N	0.63	2.31	14	1
1:A:13:LEU:CD1	1:A:19:PRO:HG2	0.63	2.23	14	1
2:B:267:VAL:O	2:B:271:ALA:CB	0.63	2.46	5	2
2:B:244:LEU:HD23	2:B:245:TYR:N	0.63	2.09	5	1
1:A:63:ILE:HD13	1:A:63:ILE:C	0.63	2.13	16	1
2:B:380:HIS:CG	2:B:381:ARG:N	0.63	2.63	16	1
1:A:15:MET:HG2	1:A:16:HIS:N	0.63	2.07	20	1
1:A:30:PHE:CE1	1:A:32:ALA:O	0.63	2.51	17	8
2:B:301:LEU:O	2:B:301:LEU:HD12	0.63	1.93	5	1
1:A:23:LEU:HD22	1:A:34:VAL:HG21	0.63	1.69	20	1
2:B:223:PHE:CZ	2:B:304:ARG:NH1	0.63	2.67	3	2
1:A:64:GLU:CD	1:A:64:GLU:O	0.63	2.37	10	1
1:A:71:GLN:O	1:A:74:GLU:CD	0.63	2.37	12	1
2:B:183:ALA:O	2:B:384:LEU:CD1	0.63	2.47	20	1
1:A:63:ILE:HG13	1:A:64:GLU:N	0.63	2.08	13	3
1:A:5:GLN:NE2	1:A:5:GLN:O	0.63	2.31	6	1
2:B:288:ASP:CB	2:B:291:LEU:HD23	0.63	2.24	20	1
1:A:84:ASN:O	1:A:85:SER:HB2	0.62	1.94	6	4
1:A:56:ASP:OD1	2:B:288:ASP:OD2	0.62	2.16	9	1
1:A:3:VAL:CG1	1:A:3:VAL:O	0.62	2.47	10	2
2:B:204:ASP:N	2:B:205:PRO:CD	0.62	2.63	2	5
2:B:361:VAL:CG1	2:B:362:ARG:N	0.62	2.62	6	3
2:B:251:ASP:OD1	2:B:251:ASP:C	0.62	2.36	4	3
2:B:223:PHE:CG	2:B:224:ARG:N	0.62	2.67	7	2
2:B:203:LEU:H	2:B:203:LEU:CD2	0.62	2.01	8	3
2:B:252:THR:OG1	2:B:253:ARG:NH1	0.62	2.30	16	1
1:A:38:ASN:N	1:A:38:ASN:OD1	0.62	2.30	18	1
1:A:77:ALA:HA	1:A:80:ILE:HG12	0.62	1.70	4	1
2:B:286:LEU:N	2:B:286:LEU:CD1	0.62	2.63	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:353:ALA:HB1	2:B:362:ARG:HH12	0.62	1.54	6	1
2:B:392:GLU:O	2:B:393:LEU:HD13	0.62	1.93	8	1
2:B:242:PHE:O	2:B:245:TYR:N	0.62	2.32	10	10
1:A:18:ARG:HB2	1:A:19:PRO:HD3	0.62	1.71	11	4
1:A:13:LEU:HD23	1:A:13:LEU:N	0.62	2.10	7	2
2:B:222:GLU:HG3	2:B:226:TYR:CE1	0.62	2.30	12	1
1:A:9:ILE:CG2	1:A:9:ILE:O	0.62	2.48	14	1
2:B:279:PHE:CD2	2:B:280:ALA:N	0.62	2.68	18	1
2:B:291:LEU:O	2:B:294:ARG:N	0.62	2.32	14	10
2:B:286:LEU:C	2:B:286:LEU:CD2	0.62	2.67	11	2
2:B:349:ARG:NE	2:B:372:ALA:O	0.62	2.32	10	2
2:B:226:TYR:CE1	2:B:304:ARG:NH1	0.62	2.68	11	1
2:B:251:ASP:C	2:B:251:ASP:OD1	0.62	2.37	17	2
1:A:24:PHE:CZ	1:A:46:ALA:O	0.62	2.52	15	4
2:B:231:ALA:CB	2:B:239:ALA:HB2	0.62	2.25	12	2
1:A:24:PHE:CE1	1:A:46:ALA:O	0.62	2.52	15	2
1:A:53:LEU:CB	2:B:291:LEU:HD13	0.62	2.23	16	1
2:B:203:LEU:HD12	2:B:203:LEU:H	0.61	1.55	1	1
1:A:71:GLN:HG2	1:A:74:GLU:CB	0.61	2.24	3	1
2:B:227:SER:OG	2:B:242:PHE:CB	0.61	2.48	5	3
1:A:20:ALA:CB	1:A:52:LEU:HD11	0.61	2.25	14	5
2:B:203:LEU:HD12	2:B:265:GLY:O	0.61	1.95	17	1
1:A:77:ALA:HA	1:A:80:ILE:CG1	0.61	2.25	4	1
2:B:225:ARG:O	2:B:229:ARG:HG2	0.61	1.94	7	1
1:A:38:ASN:N	1:A:38:ASN:ND2	0.61	2.46	10	2
1:A:49:VAL:O	1:A:53:LEU:HG	0.61	1.95	12	2
1:A:71:GLN:CB	1:A:74:GLU:CG	0.61	2.78	12	1
2:B:230:PHE:O	2:B:234:ALA:CB	0.61	2.48	18	1
1:A:33:GLU:OE1	1:A:35:LEU:HD13	0.61	1.95	3	1
2:B:222:GLU:OE2	2:B:226:TYR:CD2	0.61	2.52	3	1
2:B:306:LEU:O	2:B:310:ASP:OD1	0.61	2.17	6	4
2:B:300:ALA:HB1	2:B:333:THR:HG21	0.61	1.71	17	2
2:B:366:ILE:HG13	2:B:367:PRO:CD	0.61	2.23	10	2
2:B:215:ALA:CB	2:B:309:LEU:HD22	0.61	2.25	20	3
2:B:330:LEU:HD13	2:B:348:VAL:HG22	0.61	1.72	2	1
2:B:383:THR:O	2:B:384:LEU:HD12	0.61	1.94	5	1
2:B:286:LEU:HD13	2:B:292:LYS:N	0.61	2.10	4	1
2:B:283:PHE:N	2:B:283:PHE:CD2	0.61	2.64	6	1
2:B:203:LEU:HD23	2:B:203:LEU:O	0.61	1.95	18	1
2:B:286:LEU:CD2	2:B:288:ASP:H	0.61	2.08	4	1
2:B:223:PHE:CD1	2:B:246:SER:OG	0.61	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:389:TYR:C	2:B:389:TYR:CD1	0.61	2.74	12	1
2:B:374:ILE:O	2:B:374:ILE:HD13	0.61	1.96	17	1
1:A:36:LEU:CD2	1:A:36:LEU:N	0.61	2.63	10	3
1:A:36:LEU:CD2	1:A:46:ALA:HB2	0.61	2.26	3	2
2:B:222:GLU:OE2	2:B:226:TYR:CD1	0.61	2.54	13	2
1:A:38:ASN:ND2	1:A:41:GLY:N	0.61	2.48	8	1
1:A:27:MET:CE	1:A:32:ALA:O	0.61	2.48	15	1
1:A:53:LEU:HD23	2:B:291:LEU:CB	0.61	2.24	8	1
2:B:273:LYS:O	2:B:276:ILE:HG13	0.61	1.95	20	1
1:A:80:ILE:HD12	1:A:80:ILE:C	0.61	2.15	3	1
2:B:205:PRO:O	2:B:209:ARG:CB	0.61	2.49	14	8
2:B:385:ILE:HG23	2:B:394:LEU:HB2	0.61	1.72	5	1
2:B:275:VAL:CG1	2:B:276:ILE:N	0.61	2.63	17	4
2:B:251:ASP:OD1	2:B:253:ARG:CB	0.61	2.48	6	1
1:A:16:HIS:C	1:A:18:ARG:H	0.61	1.99	8	3
1:A:71:GLN:O	1:A:74:GLU:OE2	0.61	2.19	12	1
2:B:309:LEU:O	2:B:309:LEU:HD12	0.61	1.94	14	1
2:B:183:ALA:O	2:B:384:LEU:HD13	0.61	1.96	20	1
2:B:203:LEU:HD13	2:B:265:GLY:HA2	0.61	1.71	4	1
1:A:13:LEU:HD23	1:A:13:LEU:C	0.61	2.16	5	1
2:B:227:SER:HG	2:B:242:PHE:CB	0.61	2.09	5	1
2:B:253:ARG:HE	2:B:254:LEU:N	0.61	1.94	5	2
2:B:274:THR:O	2:B:278:LYS:N	0.61	2.31	11	3
1:A:62:GLN:NE2	1:A:63:ILE:O	0.61	2.34	16	1
2:B:226:TYR:CD2	2:B:336:ALA:O	0.60	2.54	13	2
2:B:227:SER:HB3	2:B:242:PHE:HB2	0.60	1.72	4	4
1:A:24:PHE:CE2	2:B:247:HIS:NE2	0.60	2.68	16	3
2:B:173:ALA:CB	2:B:370:MET:O	0.60	2.46	18	2
2:B:186:TRP:CD1	2:B:186:TRP:C	0.60	2.74	16	1
2:B:331:SER:OG	2:B:334:THR:OG1	0.60	2.18	17	2
2:B:325:LEU:HD13	2:B:326:VAL:N	0.60	2.11	11	4
1:A:72:GLU:N	1:A:72:GLU:OE1	0.60	2.34	3	2
2:B:271:ALA:O	2:B:275:VAL:HG13	0.60	1.95	6	1
2:B:244:LEU:HD23	2:B:294:ARG:NH2	0.60	2.11	7	1
2:B:288:ASP:HB3	2:B:291:LEU:HD21	0.60	1.73	7	1
1:A:3:VAL:HG21	1:A:72:GLU:OE2	0.60	1.96	12	3
2:B:213:THR:CG2	2:B:214:GLY:N	0.60	2.63	9	2
1:A:7:VAL:HG23	1:A:83:PHE:CZ	0.60	2.31	15	2
2:B:219:ALA:O	2:B:222:GLU:HG3	0.60	1.96	15	1
2:B:258:LEU:HG	2:B:259:PHE:N	0.60	2.11	18	1
1:A:71:GLN:HE22	1:A:75:ALA:HB2	0.60	1.56	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:HG	2:B:291:LEU:HD12	0.60	1.73	3	1
2:B:241:ILE:HG22	2:B:242:PHE:N	0.60	2.11	9	7
2:B:278:LYS:O	2:B:281:GLU:CD	0.60	2.39	20	1
1:A:36:LEU:N	1:A:36:LEU:CD2	0.60	2.64	3	1
1:A:31:ASP:O	1:A:32:ALA:CB	0.60	2.49	10	16
1:A:21:MET:C	1:A:21:MET:SD	0.60	2.80	4	3
1:A:13:LEU:O	1:A:13:LEU:HD23	0.60	1.96	5	1
2:B:286:LEU:HD23	2:B:292:LYS:N	0.60	2.11	10	1
1:A:35:LEU:O	1:A:66:GLU:OE1	0.60	2.20	11	1
1:A:23:LEU:HD12	1:A:34:VAL:HG11	0.60	1.73	8	2
2:B:286:LEU:CD1	2:B:288:ASP:OD2	0.60	2.49	3	1
2:B:221:ASN:O	2:B:225:ARG:NE	0.60	2.34	6	1
1:A:47:ASN:C	1:A:47:ASN:HD22	0.60	1.98	8	1
2:B:224:ARG:NE	2:B:246:SER:OG	0.60	2.34	13	1
1:A:36:LEU:HD23	1:A:36:LEU:N	0.60	2.12	2	2
1:A:53:LEU:CD1	2:B:283:PHE:O	0.60	2.50	9	1
1:A:27:MET:HA	1:A:30:PHE:CE2	0.60	2.32	10	7
1:A:9:ILE:O	1:A:9:ILE:CG2	0.60	2.50	4	2
2:B:338:LEU:CD1	2:B:342:ARG:NH1	0.60	2.64	12	1
2:B:184:GLU:O	2:B:324:ILE:HG12	0.60	1.97	6	2
2:B:213:THR:O	2:B:217:GLU:OE1	0.60	2.19	12	2
2:B:290:TYR:OH	2:B:294:ARG:NH1	0.60	2.35	19	2
1:A:49:VAL:HG13	2:B:248:LEU:HD21	0.60	1.72	11	1
2:B:358:ALA:HB1	2:B:362:ARG:HH11	0.60	1.57	18	1
2:B:179:GLY:O	2:B:388:GLY:N	0.60	2.35	1	8
2:B:327:ALA:O	2:B:348:VAL:HA	0.60	1.97	1	5
2:B:392:GLU:C	2:B:393:LEU:HD23	0.60	2.16	1	1
2:B:172:ARG:HE	2:B:172:ARG:CA	0.60	2.08	2	2
1:A:54:MET:O	1:A:54:MET:SD	0.60	2.59	7	1
2:B:226:TYR:CD1	2:B:304:ARG:NH1	0.60	2.70	11	1
2:B:286:LEU:CB	2:B:291:LEU:CD2	0.60	2.80	20	1
2:B:231:ALA:HB2	2:B:239:ALA:HB2	0.59	1.72	12	4
1:A:8:GLU:CD	1:A:8:GLU:O	0.59	2.40	17	1
2:B:257:GLU:OE2	2:B:279:PHE:CZ	0.59	2.55	8	4
2:B:301:LEU:CD1	2:B:301:LEU:C	0.59	2.71	17	3
2:B:385:ILE:O	2:B:385:ILE:HG13	0.59	1.95	11	1
2:B:375:GLN:CD	2:B:375:GLN:H	0.59	2.00	3	6
1:A:36:LEU:CD1	1:A:46:ALA:HB2	0.59	2.27	8	5
2:B:174:LEU:N	2:B:370:MET:O	0.59	2.35	6	11
2:B:216:LEU:HD12	2:B:216:LEU:O	0.59	1.97	5	1
2:B:216:LEU:CG	2:B:217:GLU:N	0.59	2.65	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:MET:SD	1:A:54:MET:O	0.59	2.60	14	1
2:B:278:LYS:O	2:B:281:GLU:OE2	0.59	2.20	20	1
2:B:328:ASP:OD1	2:B:328:ASP:N	0.59	2.36	7	3
1:A:2:THR:HG23	1:A:68:THR:HG23	0.59	1.74	4	1
1:A:53:LEU:C	1:A:53:LEU:CD1	0.59	2.67	7	2
1:A:28:GLN:HE21	1:A:28:GLN:N	0.59	1.95	1	1
2:B:292:LYS:HG3	2:B:293:GLU:N	0.59	2.13	2	2
2:B:248:LEU:CD1	2:B:248:LEU:C	0.59	2.66	3	2
1:A:15:MET:SD	1:A:18:ARG:HD2	0.59	2.38	7	1
2:B:218:GLU:O	2:B:222:GLU:CB	0.59	2.51	2	2
1:A:2:THR:CG2	1:A:68:THR:OG1	0.59	2.51	4	1
2:B:284:ALA:HB2	2:B:295:ALA:CB	0.59	2.28	8	1
2:B:322:ARG:O	2:B:323:PHE:HD1	0.59	1.79	8	1
1:A:13:LEU:O	1:A:83:PHE:CD2	0.59	2.55	16	2
2:B:366:ILE:CG1	2:B:367:PRO:HD2	0.59	2.24	10	2
2:B:241:ILE:HG13	2:B:242:PHE:N	0.59	2.13	15	3
1:A:3:VAL:O	1:A:3:VAL:HG13	0.59	1.98	14	1
1:A:15:MET:CE	1:A:19:PRO:HG3	0.59	2.24	20	1
1:A:36:LEU:HD21	1:A:46:ALA:HB2	0.59	1.74	3	2
1:A:6:THR:OG1	1:A:62:GLN:NE2	0.59	2.36	13	2
2:B:304:ARG:NH2	2:B:337:GLU:OE1	0.59	2.36	17	1
2:B:284:ALA:O	2:B:286:LEU:N	0.59	2.35	13	5
2:B:340:GLN:CD	2:B:340:GLN:O	0.59	2.41	14	2
2:B:237:GLU:OE1	2:B:238:THR:N	0.59	2.36	6	1
2:B:211:ARG:NH2	2:B:269:GLU:OE1	0.59	2.36	6	3
2:B:256:ARG:NH1	2:B:259:PHE:CD2	0.59	2.71	10	1
2:B:378:VAL:O	2:B:378:VAL:HG12	0.59	1.97	15	2
2:B:255:ARG:N	2:B:255:ARG:NE	0.59	2.51	17	1
1:A:5:GLN:NE2	1:A:6:THR:O	0.59	2.35	2	2
2:B:382:ARG:NH2	2:B:396:ASP:CG	0.59	2.56	6	1
2:B:396:ASP:CG	2:B:396:ASP:O	0.59	2.42	6	1
1:A:38:ASN:C	1:A:38:ASN:ND2	0.59	2.54	8	1
1:A:72:GLU:C	1:A:72:GLU:OE1	0.59	2.41	8	3
2:B:273:LYS:O	2:B:277:GLU:CG	0.59	2.51	13	1
1:A:5:GLN:CD	1:A:5:GLN:C	0.59	2.62	14	1
1:A:62:GLN:NE2	1:A:64:GLU:OE1	0.59	2.35	20	1
2:B:385:ILE:HD12	2:B:385:ILE:H	0.58	1.57	1	1
2:B:174:LEU:N	2:B:174:LEU:CD2	0.58	2.65	5	2
2:B:383:THR:HG22	2:B:385:ILE:CD1	0.58	2.28	2	1
2:B:223:PHE:O	2:B:227:SER:OG	0.58	2.21	3	1
1:A:24:PHE:CD2	1:A:24:PHE:N	0.58	2.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:250:SER:O	2:B:255:ARG:NH2	0.58	2.36	9	1
2:B:369:VAL:O	2:B:370:MET:SD	0.58	2.61	13	1
2:B:384:LEU:HD12	2:B:394:LEU:O	0.58	1.98	18	2
2:B:248:LEU:HD12	2:B:248:LEU:C	0.58	2.18	8	2
1:A:36:LEU:HD12	1:A:65:VAL:HG22	0.58	1.75	3	1
2:B:235:GLN:O	2:B:238:THR:OG1	0.58	2.21	7	4
2:B:270:TRP:CE2	2:B:274:THR:OG1	0.58	2.56	5	1
2:B:337:GLU:C	2:B:338:LEU:HD22	0.58	2.17	8	2
2:B:291:LEU:HD22	2:B:291:LEU:C	0.58	2.18	12	1
2:B:212:LEU:HG	2:B:213:THR:N	0.58	2.13	18	1
1:A:77:ALA:O	1:A:80:ILE:CG1	0.58	2.48	4	1
1:A:37:ARG:O	1:A:63:ILE:CG2	0.58	2.46	5	1
2:B:328:ASP:OD1	2:B:329:GLU:N	0.58	2.37	12	6
2:B:271:ALA:O	2:B:275:VAL:HG23	0.58	1.99	2	5
2:B:245:TYR:OH	2:B:297:ASP:CG	0.58	2.41	11	3
1:A:13:LEU:H	1:A:13:LEU:CD2	0.58	2.08	4	2
2:B:184:GLU:O	2:B:324:ILE:CG1	0.58	2.51	6	2
2:B:325:LEU:HD23	2:B:325:LEU:C	0.58	2.19	8	1
2:B:344:VAL:HG12	2:B:344:VAL:O	0.58	1.97	13	2
2:B:237:GLU:CG	2:B:238:THR:N	0.58	2.65	17	1
2:B:291:LEU:CG	2:B:292:LYS:N	0.58	2.65	19	4
2:B:222:GLU:O	2:B:226:TYR:HB2	0.58	1.99	12	3
1:A:36:LEU:N	1:A:36:LEU:HD12	0.58	2.14	11	1
2:B:259:PHE:N	2:B:259:PHE:CD2	0.58	2.69	13	2
2:B:364:LEU:HD11	2:B:366:ILE:HG22	0.58	1.75	16	1
2:B:396:ASP:OD1	2:B:396:ASP:N	0.58	2.34	12	3
1:A:71:GLN:OE1	1:A:74:GLU:HB3	0.58	1.98	3	1
1:A:18:ARG:O	1:A:22:LYS:CG	0.58	2.52	7	1
2:B:281:GLU:O	2:B:285:ALA:HB2	0.58	1.99	16	3
1:A:38:ASN:ND2	1:A:40:GLU:N	0.58	2.52	8	1
2:B:222:GLU:OE2	2:B:304:ARG:NH1	0.58	2.37	2	10
2:B:301:LEU:C	2:B:301:LEU:HD13	0.58	2.19	6	1
2:B:283:PHE:CD2	2:B:284:ALA:N	0.58	2.72	7	2
2:B:235:GLN:NE2	2:B:238:THR:HG23	0.58	2.13	10	1
2:B:291:LEU:O	2:B:291:LEU:HD22	0.58	1.99	12	1
2:B:393:LEU:O	2:B:393:LEU:CD1	0.58	2.52	16	1
1:A:47:ASN:O	1:A:47:ASN:CG	0.58	2.42	20	1
1:A:19:PRO:O	1:A:23:LEU:HD23	0.58	1.99	13	3
2:B:251:ASP:OD1	2:B:253:ARG:CA	0.58	2.52	6	1
1:A:20:ALA:HB2	1:A:52:LEU:HD11	0.58	1.75	14	5
1:A:3:VAL:HG13	1:A:3:VAL:O	0.58	1.99	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:249:LEU:O	2:B:255:ARG:NH2	0.58	2.37	16	1
2:B:249:LEU:CD1	2:B:249:LEU:C	0.58	2.72	17	1
1:A:35:LEU:C	1:A:36:LEU:HD23	0.58	2.19	2	2
2:B:209:ARG:CG	2:B:210:GLU:N	0.58	2.67	12	2
1:A:53:LEU:CD1	1:A:54:MET:N	0.58	2.52	16	2
2:B:290:TYR:CD2	2:B:291:LEU:CD2	0.58	2.86	8	1
2:B:223:PHE:CE2	2:B:242:PHE:CE2	0.58	2.92	9	1
2:B:268:ALA:O	2:B:272:VAL:HG22	0.57	1.99	3	6
1:A:63:ILE:C	1:A:63:ILE:CD1	0.57	2.70	7	1
1:A:13:LEU:H	1:A:13:LEU:HD12	0.57	1.56	9	1
1:A:28:GLN:N	1:A:28:GLN:OE1	0.57	2.36	3	1
1:A:63:ILE:CG2	1:A:64:GLU:N	0.57	2.67	19	3
2:B:204:ASP:HB2	2:B:208:GLU:HG2	0.57	1.75	8	2
2:B:259:PHE:CD2	2:B:259:PHE:N	0.57	2.71	20	1
2:B:384:LEU:O	2:B:385:ILE:HD13	0.57	1.99	7	1
2:B:291:LEU:CD1	2:B:292:LYS:N	0.57	2.65	12	2
1:A:35:LEU:CD2	1:A:35:LEU:N	0.57	2.68	14	2
2:B:375:GLN:N	2:B:375:GLN:OE1	0.57	2.38	4	2
2:B:217:GLU:O	2:B:221:ASN:ND2	0.57	2.38	12	11
1:A:26:LEU:HD22	1:A:30:PHE:CE1	0.57	2.34	11	4
2:B:172:ARG:N	2:B:172:ARG:NE	0.57	2.52	16	1
2:B:364:LEU:HD12	2:B:365:GLY:N	0.57	2.14	16	1
2:B:286:LEU:CB	2:B:291:LEU:HD22	0.57	2.30	19	1
2:B:330:LEU:HD13	2:B:348:VAL:CG2	0.57	2.29	2	1
1:A:24:PHE:CZ	2:B:247:HIS:NE2	0.57	2.73	16	3
2:B:247:HIS:ND1	2:B:247:HIS:C	0.57	2.55	10	4
2:B:227:SER:OG	2:B:242:PHE:CD1	0.57	2.57	12	1
2:B:283:PHE:CD1	2:B:283:PHE:N	0.57	2.71	16	2
2:B:288:ASP:O	2:B:291:LEU:CD2	0.57	2.53	19	1
2:B:330:LEU:HD23	2:B:348:VAL:CG2	0.57	2.29	20	1
2:B:248:LEU:HD13	2:B:249:LEU:N	0.57	2.14	3	2
2:B:375:GLN:CD	2:B:375:GLN:N	0.57	2.58	10	6
1:A:56:ASP:OD2	2:B:291:LEU:HD22	0.57	2.00	11	1
2:B:301:LEU:C	2:B:301:LEU:HD23	0.57	2.20	18	1
2:B:288:ASP:HB2	2:B:291:LEU:HD23	0.57	1.76	20	1
1:A:13:LEU:N	1:A:13:LEU:CD1	0.57	2.67	9	2
2:B:396:ASP:N	2:B:397:PRO:CD	0.57	2.68	20	13
1:A:2:THR:HG23	1:A:68:THR:CG2	0.57	2.29	4	1
2:B:376:PRO:HA	2:B:379:LEU:HD23	0.57	1.76	5	1
1:A:16:HIS:NE2	2:B:290:TYR:CD2	0.57	2.72	9	1
2:B:182:ILE:HD13	2:B:182:ILE:N	0.57	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:211:ARG:NH2	2:B:269:GLU:CD	0.56	2.59	6	1
2:B:379:LEU:HD13	2:B:384:LEU:HD22	0.56	1.75	6	1
2:B:176:ALA:O	2:B:362:ARG:NH2	0.56	2.38	11	2
2:B:245:TYR:O	2:B:248:LEU:N	0.56	2.34	7	4
2:B:258:LEU:HD11	2:B:275:VAL:HG21	0.56	1.76	9	1
1:A:3:VAL:O	1:A:3:VAL:CG1	0.56	2.53	14	1
2:B:246:SER:O	2:B:249:LEU:HD23	0.56	2.00	15	1
2:B:212:LEU:C	2:B:212:LEU:CD1	0.56	2.74	17	1
1:A:76:LEU:HD23	1:A:76:LEU:C	0.56	2.21	6	1
2:B:338:LEU:N	2:B:338:LEU:CD2	0.56	2.68	9	1
2:B:289:ASN:CG	2:B:290:TYR:N	0.56	2.58	12	2
1:A:18:ARG:HE	1:A:18:ARG:H	0.56	1.42	16	1
2:B:202:THR:O	2:B:204:ASP:OD2	0.56	2.24	5	1
2:B:251:ASP:OD2	2:B:253:ARG:HB2	0.56	2.00	6	1
2:B:374:ILE:CD1	2:B:374:ILE:N	0.56	2.67	7	1
1:A:63:ILE:CD1	1:A:63:ILE:C	0.56	2.73	16	1
1:A:53:LEU:HD11	2:B:286:LEU:HG	0.56	1.76	16	1
2:B:335:LEU:C	2:B:337:GLU:H	0.56	2.03	3	7
1:A:56:ASP:CG	2:B:288:ASP:OD2	0.56	2.44	9	1
2:B:291:LEU:C	2:B:291:LEU:CD1	0.56	2.72	20	3
1:A:12:LYS:HD3	1:A:12:LYS:O	0.56	2.00	14	1
2:B:293:GLU:OE1	2:B:294:ARG:N	0.56	2.34	14	1
2:B:384:LEU:C	2:B:384:LEU:HD13	0.56	2.21	14	1
1:A:53:LEU:HD13	1:A:53:LEU:N	0.56	2.15	15	1
2:B:230:PHE:CE2	2:B:238:THR:HG21	0.56	2.36	19	1
2:B:269:GLU:CD	2:B:269:GLU:H	0.56	2.04	9	1
1:A:13:LEU:H	1:A:13:LEU:HD23	0.56	1.60	12	2
2:B:364:LEU:CD1	2:B:366:ILE:HB	0.56	2.31	16	1
2:B:249:LEU:HG	2:B:301:LEU:HD11	0.56	1.77	18	1
2:B:283:PHE:CD1	2:B:283:PHE:C	0.56	2.79	19	1
1:A:69:GLY:O	1:A:72:GLU:CG	0.56	2.52	1	4
2:B:361:VAL:HA	2:B:364:LEU:CD2	0.56	2.29	16	1
2:B:246:SER:O	2:B:250:SER:OG	0.56	2.23	3	2
1:A:63:ILE:CG1	1:A:64:GLU:N	0.56	2.67	13	2
2:B:258:LEU:CD1	2:B:258:LEU:C	0.56	2.72	18	2
2:B:306:LEU:HD23	2:B:306:LEU:O	0.56	2.01	11	2
1:A:18:ARG:N	1:A:18:ARG:HE	0.56	1.99	10	1
2:B:302:GLY:O	2:B:306:LEU:HD12	0.56	2.01	14	1
2:B:286:LEU:HD13	2:B:291:LEU:HD13	0.56	1.78	15	1
1:A:31:ASP:N	1:A:71:GLN:OE1	0.56	2.37	20	1
1:A:18:ARG:HB3	1:A:19:PRO:HD3	0.56	1.78	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:174:LEU:N	2:B:174:LEU:HD22	0.56	2.16	2	1
2:B:213:THR:HG23	2:B:214:GLY:N	0.56	2.15	8	1
2:B:222:GLU:HG2	2:B:226:TYR:CE1	0.56	2.35	9	1
2:B:375:GLN:OE1	2:B:375:GLN:N	0.56	2.38	14	2
1:A:83:PHE:CD1	1:A:83:PHE:C	0.56	2.77	17	3
2:B:203:LEU:O	2:B:203:LEU:CD2	0.56	2.54	18	1
2:B:290:TYR:O	2:B:293:GLU:HG3	0.56	2.01	19	1
1:A:49:VAL:HG21	2:B:248:LEU:HD23	0.56	1.76	3	1
1:A:16:HIS:CG	1:A:17:ALA:N	0.56	2.70	13	2
1:A:13:LEU:C	1:A:13:LEU:HD12	0.56	2.20	17	1
2:B:279:PHE:C	2:B:279:PHE:CD1	0.56	2.79	20	1
2:B:247:HIS:O	2:B:251:ASP:HB2	0.56	2.01	3	1
2:B:222:GLU:O	2:B:226:TYR:CG	0.56	2.59	15	4
1:A:18:ARG:O	1:A:22:LYS:HG2	0.56	2.02	7	1
2:B:268:ALA:O	2:B:271:ALA:N	0.56	2.38	9	1
2:B:209:ARG:HG2	2:B:210:GLU:N	0.56	2.15	12	1
2:B:333:THR:HG23	2:B:334:THR:N	0.55	2.16	9	4
1:A:24:PHE:CE1	2:B:247:HIS:NE2	0.55	2.74	10	1
1:A:38:ASN:OD1	1:A:54:MET:SD	0.55	2.64	12	1
2:B:244:LEU:O	2:B:244:LEU:HD13	0.55	2.01	19	1
1:A:79:VAL:CG1	1:A:80:ILE:N	0.55	2.70	11	6
2:B:396:ASP:O	2:B:397:PRO:O	0.55	2.24	3	1
2:B:220:ALA:O	2:B:223:PHE:CE2	0.55	2.59	4	1
2:B:291:LEU:HD12	2:B:292:LYS:N	0.55	2.16	5	1
2:B:393:LEU:N	2:B:393:LEU:HD13	0.55	2.13	8	1
1:A:37:ARG:NE	1:A:43:GLU:OE2	0.55	2.39	7	1
2:B:361:VAL:HG11	2:B:368:THR:OG1	0.55	2.01	8	2
2:B:223:PHE:CE2	2:B:242:PHE:CZ	0.55	2.95	9	1
1:A:20:ALA:HB1	1:A:52:LEU:CD1	0.55	2.30	18	1
2:B:349:ARG:NH2	2:B:374:ILE:O	0.55	2.39	18	1
1:A:72:GLU:CG	1:A:73:GLU:N	0.55	2.69	3	7
2:B:382:ARG:NH1	2:B:383:THR:O	0.55	2.39	6	1
2:B:209:ARG:NH2	2:B:259:PHE:CZ	0.55	2.75	7	1
2:B:187:GLN:OE1	2:B:326:VAL:O	0.55	2.25	7	1
1:A:3:VAL:HG12	1:A:3:VAL:O	0.55	2.02	2	1
2:B:279:PHE:O	2:B:283:PHE:CE1	0.55	2.60	8	2
1:A:63:ILE:HG12	1:A:64:GLU:N	0.55	2.15	7	2
1:A:38:ASN:HD21	1:A:40:GLU:CA	0.55	2.15	8	1
2:B:379:LEU:CD2	2:B:379:LEU:N	0.55	2.67	9	1
2:B:360:MET:CG	2:B:361:VAL:N	0.55	2.70	1	1
2:B:237:GLU:O	2:B:241:ILE:HD13	0.55	2.01	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:294:ARG:O	2:B:297:ASP:N	0.55	2.39	3	2
2:B:346:VAL:HG13	2:B:368:THR:HG23	0.55	1.79	7	1
2:B:204:ASP:N	2:B:204:ASP:OD1	0.55	2.38	9	2
2:B:213:THR:O	2:B:217:GLU:OE2	0.55	2.24	16	1
2:B:283:PHE:CD1	2:B:284:ALA:N	0.55	2.74	17	1
2:B:303:GLN:CG	2:B:304:ARG:N	0.55	2.70	14	3
2:B:220:ALA:O	2:B:223:PHE:CD2	0.55	2.59	4	1
2:B:360:MET:O	2:B:364:LEU:HD13	0.55	2.01	20	2
2:B:211:ARG:CZ	2:B:309:LEU:HD21	0.55	2.32	11	1
2:B:344:VAL:O	2:B:366:ILE:HG23	0.55	2.01	1	1
2:B:299:ARG:NH1	2:B:303:GLN:N	0.55	2.55	12	1
2:B:221:ASN:O	2:B:225:ARG:CG	0.55	2.55	14	1
2:B:364:LEU:HD11	2:B:366:ILE:CB	0.55	2.31	16	1
1:A:53:LEU:O	2:B:286:LEU:HD13	0.55	2.02	1	1
2:B:286:LEU:O	2:B:292:LYS:HD2	0.55	2.01	1	1
2:B:390:ARG:NH1	2:B:392:GLU:OE2	0.55	2.40	1	1
2:B:392:GLU:O	2:B:393:LEU:HD23	0.55	2.02	1	2
1:A:44:ALA:CA	1:A:51:ALA:HB1	0.55	2.32	19	20
1:A:30:PHE:HB2	1:A:71:GLN:CG	0.55	2.32	3	1
1:A:47:ASN:CG	1:A:47:ASN:O	0.55	2.45	10	2
2:B:187:GLN:O	2:B:187:GLN:NE2	0.55	2.39	15	1
1:A:37:ARG:O	1:A:63:ILE:HG22	0.55	2.01	20	1
2:B:333:THR:CG2	2:B:334:THR:N	0.55	2.70	2	4
2:B:203:LEU:N	2:B:203:LEU:HD22	0.55	2.05	17	2
2:B:212:LEU:CG	2:B:213:THR:N	0.55	2.70	18	1
1:A:30:PHE:CB	1:A:71:GLN:CD	0.54	2.72	3	1
1:A:84:ASN:O	1:A:84:ASN:OD1	0.54	2.26	3	1
2:B:338:LEU:HD23	2:B:338:LEU:N	0.54	2.16	13	1
2:B:231:ALA:HB2	2:B:239:ALA:CB	0.54	2.32	20	1
1:A:37:ARG:HH11	1:A:66:GLU:CD	0.54	2.06	5	1
2:B:379:LEU:N	2:B:379:LEU:CD2	0.54	2.66	5	2
1:A:40:GLU:OE2	1:A:61:ARG:NH2	0.54	2.39	6	2
2:B:245:TYR:CZ	2:B:297:ASP:CB	0.54	2.90	9	1
1:A:27:MET:HE2	1:A:32:ALA:O	0.54	2.01	15	1
1:A:18:ARG:NE	1:A:18:ARG:HA	0.54	2.16	1	1
2:B:307:PHE:O	2:B:310:ASP:OD1	0.54	2.26	8	3
1:A:50:ILE:HA	1:A:53:LEU:HD23	0.54	1.79	4	2
2:B:279:PHE:CD2	2:B:282:GLN:OE1	0.54	2.59	17	1
2:B:258:LEU:CG	2:B:259:PHE:N	0.54	2.71	18	1
2:B:203:LEU:CD1	2:B:203:LEU:H	0.54	2.13	1	1
2:B:288:ASP:OD1	2:B:288:ASP:N	0.54	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:208:GLU:CD	2:B:268:ALA:H	0.54	2.05	20	1
1:A:21:MET:CG	1:A:22:LYS:N	0.54	2.71	4	1
2:B:222:GLU:N	2:B:225:ARG:HH11	0.54	2.00	6	1
1:A:38:ASN:ND2	1:A:38:ASN:O	0.54	2.41	8	1
2:B:256:ARG:NE	2:B:256:ARG:CA	0.54	2.68	9	1
2:B:251:ASP:OD2	2:B:253:ARG:NH2	0.54	2.41	12	2
2:B:330:LEU:O	2:B:330:LEU:HD12	0.54	2.01	15	1
2:B:276:ILE:O	2:B:280:ALA:HB2	0.54	2.02	18	1
1:A:15:MET:SD	1:A:19:PRO:HG3	0.54	2.42	20	1
1:A:39:ASP:OD1	1:A:40:GLU:N	0.54	2.40	11	4
1:A:13:LEU:N	1:A:13:LEU:CD2	0.54	2.71	7	2
2:B:245:TYR:OH	2:B:297:ASP:OD2	0.54	2.24	11	2
2:B:379:LEU:CD2	2:B:379:LEU:H	0.54	2.14	9	1
2:B:346:VAL:HG23	2:B:368:THR:HG23	0.54	1.77	16	1
2:B:235:GLN:HG2	2:B:236:LYS:H	0.54	1.62	2	2
1:A:7:VAL:HB	1:A:83:PHE:CE2	0.54	2.38	19	2
2:B:203:LEU:CD2	2:B:203:LEU:N	0.54	2.60	4	2
2:B:235:GLN:NE2	2:B:238:THR:H	0.54	2.01	6	1
2:B:211:ARG:HG3	2:B:212:LEU:N	0.54	2.17	8	1
2:B:242:PHE:N	2:B:242:PHE:CD1	0.54	2.75	11	2
2:B:282:GLN:CG	2:B:283:PHE:N	0.54	2.71	11	1
2:B:222:GLU:OE2	2:B:226:TYR:CE1	0.54	2.60	13	1
2:B:184:GLU:H	2:B:184:GLU:CD	0.54	2.06	15	1
1:A:61:ARG:NH2	1:A:62:GLN:H	0.54	2.00	20	1
1:A:11:ASN:OD1	1:A:11:ASN:N	0.54	2.41	3	1
2:B:331:SER:O	2:B:334:THR:OG1	0.54	2.25	2	3
2:B:172:ARG:N	2:B:172:ARG:CD	0.54	2.71	2	2
2:B:221:ASN:OD1	2:B:224:ARG:NH1	0.54	2.41	8	2
2:B:187:GLN:NE2	2:B:187:GLN:O	0.54	2.39	13	2
2:B:215:ALA:HB2	2:B:309:LEU:HD12	0.54	1.80	15	1
2:B:218:GLU:O	2:B:222:GLU:HB3	0.53	2.03	2	1
2:B:172:ARG:H	2:B:172:ARG:CD	0.53	2.16	20	2
1:A:32:ALA:CB	1:A:68:THR:O	0.53	2.57	11	6
2:B:291:LEU:O	2:B:294:ARG:HB2	0.53	2.03	8	2
2:B:212:LEU:HG	2:B:213:THR:H	0.53	1.62	18	1
2:B:303:GLN:HG2	2:B:304:ARG:N	0.53	2.18	3	2
2:B:253:ARG:HE	2:B:253:ARG:C	0.53	2.06	18	2
2:B:223:PHE:CZ	2:B:242:PHE:CZ	0.53	2.97	9	1
1:A:23:LEU:HD21	1:A:79:VAL:HG23	0.53	1.79	13	2
1:A:73:GLU:CG	1:A:74:GLU:N	0.53	2.70	9	3
2:B:172:ARG:CZ	2:B:392:GLU:OE2	0.53	2.56	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLY:O	1:A:15:MET:HB2	0.53	2.03	13	2
2:B:245:TYR:O	2:B:248:LEU:HB2	0.53	2.02	14	1
1:A:62:GLN:CD	1:A:63:ILE:N	0.53	2.61	16	1
2:B:288:ASP:O	2:B:291:LEU:CG	0.53	2.56	19	1
1:A:48:SER:OG	2:B:253:ARG:NE	0.53	2.42	2	1
2:B:350:ASP:OD1	2:B:351:GLY:N	0.53	2.41	2	3
2:B:291:LEU:HG	2:B:292:LYS:H	0.53	1.62	19	2
1:A:16:HIS:C	1:A:18:ARG:N	0.53	2.62	8	2
2:B:351:GLY:C	2:B:352:ALA:O	0.53	2.47	9	1
2:B:241:ILE:HG23	2:B:242:PHE:H	0.53	1.48	10	1
2:B:290:TYR:OH	2:B:294:ARG:NH2	0.53	2.39	12	1
2:B:309:LEU:O	2:B:309:LEU:CD1	0.53	2.56	14	1
2:B:338:LEU:CB	2:B:342:ARG:HE	0.53	2.17	12	1
1:A:56:ASP:OD2	2:B:291:LEU:HD23	0.53	2.02	4	1
2:B:222:GLU:CD	2:B:304:ARG:HH11	0.53	2.07	7	3
2:B:329:GLU:OE2	2:B:330:LEU:O	0.53	2.27	8	2
2:B:395:VAL:HG22	2:B:396:ASP:OD1	0.53	2.02	8	3
2:B:211:ARG:HH21	2:B:211:ARG:CB	0.53	2.16	9	1
2:B:326:VAL:HG22	2:B:347:VAL:CG2	0.53	2.33	10	1
1:A:74:GLU:OE1	1:A:75:ALA:CA	0.53	2.56	12	1
1:A:53:LEU:CB	2:B:291:LEU:HD22	0.53	2.33	16	1
2:B:261:GLU:O	2:B:264:LYS:CG	0.53	2.57	19	1
1:A:8:GLU:CD	1:A:8:GLU:H	0.53	2.06	1	2
2:B:242:PHE:CD1	2:B:243:ASP:N	0.53	2.77	3	2
2:B:286:LEU:CD2	2:B:287:SER:N	0.53	2.64	4	1
2:B:373:ASP:C	2:B:374:ILE:HD13	0.53	2.24	7	1
2:B:288:ASP:HB3	2:B:291:LEU:HD11	0.53	1.81	14	2
1:A:53:LEU:HD23	1:A:53:LEU:C	0.53	2.24	9	2
1:A:19:PRO:O	1:A:23:LEU:CD1	0.53	2.57	17	1
1:A:63:ILE:N	1:A:63:ILE:CD1	0.53	2.62	20	1
2:B:290:TYR:C	2:B:291:LEU:HD12	0.53	2.24	2	1
2:B:273:LYS:CG	2:B:274:THR:N	0.53	2.71	4	1
2:B:184:GLU:HB2	2:B:323:PHE:CD2	0.53	2.38	17	1
2:B:249:LEU:C	2:B:249:LEU:HD23	0.53	2.24	19	1
1:A:23:LEU:HD11	1:A:79:VAL:CG2	0.53	2.34	2	2
2:B:292:LYS:CD	2:B:292:LYS:C	0.53	2.77	2	1
1:A:10:THR:O	1:A:11:ASN:ND2	0.53	2.41	3	1
2:B:247:HIS:ND1	2:B:247:HIS:O	0.53	2.42	3	1
2:B:183:ALA:HB3	2:B:324:ILE:HG23	0.53	1.80	6	1
1:A:24:PHE:O	1:A:28:GLN:CD	0.53	2.47	13	1
2:B:288:ASP:OD2	2:B:291:LEU:HD23	0.53	2.04	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:276:ILE:HG13	2:B:277:GLU:N	0.53	2.19	8	6
1:A:21:MET:SD	2:B:240:ALA:O	0.53	2.67	16	1
2:B:383:THR:OG1	2:B:396:ASP:HB3	0.53	2.03	18	1
2:B:204:ASP:O	2:B:208:GLU:N	0.52	2.38	3	2
2:B:211:ARG:NH1	2:B:269:GLU:OE1	0.52	2.39	3	1
2:B:207:LEU:O	2:B:211:ARG:CG	0.52	2.57	8	5
2:B:361:VAL:HG12	2:B:362:ARG:N	0.52	2.18	6	2
2:B:364:LEU:HD23	2:B:366:ILE:HD12	0.52	1.81	11	1
1:A:4:LYS:H	1:A:4:LYS:CD	0.52	2.17	15	1
2:B:216:LEU:O	2:B:220:ALA:CB	0.52	2.57	15	1
2:B:244:LEU:O	2:B:248:LEU:N	0.52	2.42	17	1
2:B:208:GLU:OE2	2:B:268:ALA:HB2	0.52	2.04	20	1
2:B:323:PHE:CD1	2:B:324:ILE:N	0.52	2.77	5	1
1:A:38:ASN:HD22	1:A:42:THR:H	0.52	1.42	8	1
2:B:384:LEU:C	2:B:384:LEU:CD1	0.52	2.78	14	1
2:B:259:PHE:CD1	2:B:259:PHE:O	0.52	2.62	19	2
2:B:250:SER:O	2:B:255:ARG:NE	0.52	2.42	15	1
2:B:273:LYS:CD	2:B:273:LYS:C	0.52	2.78	7	1
1:A:28:GLN:HE22	2:B:247:HIS:CE1	0.52	2.22	9	1
2:B:204:ASP:OD1	2:B:208:GLU:HG2	0.52	2.04	20	2
2:B:385:ILE:C	2:B:385:ILE:HD12	0.52	2.24	11	1
2:B:184:GLU:CD	2:B:184:GLU:N	0.52	2.61	14	2
1:A:8:GLU:OE1	1:A:62:GLN:OE1	0.52	2.26	14	1
2:B:305:LEU:O	2:B:309:LEU:HD12	0.52	2.03	16	1
2:B:253:ARG:NE	2:B:253:ARG:C	0.52	2.63	18	2
2:B:221:ASN:OD1	2:B:224:ARG:CZ	0.52	2.58	14	1
2:B:212:LEU:HD11	2:B:255:ARG:NH2	0.52	2.19	17	1
1:A:53:LEU:HD13	2:B:283:PHE:CD1	0.52	2.40	19	1
2:B:283:PHE:CD2	2:B:298:LEU:HD13	0.52	2.40	3	1
1:A:43:GLU:H	1:A:43:GLU:CD	0.52	2.07	13	3
1:A:27:MET:HG3	1:A:28:GLN:N	0.52	2.19	5	1
1:A:14:GLY:O	1:A:15:MET:C	0.52	2.47	6	1
1:A:14:GLY:O	1:A:15:MET:O	0.52	2.28	6	1
2:B:335:LEU:O	2:B:335:LEU:HD23	0.52	2.04	13	1
2:B:291:LEU:N	2:B:291:LEU:CD1	0.52	2.71	18	1
2:B:239:ALA:O	2:B:243:ASP:CB	0.52	2.58	9	3
1:A:80:ILE:CG2	1:A:81:ALA:N	0.52	2.73	15	8
2:B:270:TRP:O	2:B:273:LYS:HG3	0.52	2.03	4	2
2:B:277:GLU:O	2:B:281:GLU:OE2	0.52	2.28	5	2
1:A:38:ASN:OD1	1:A:40:GLU:CB	0.52	2.58	8	1
2:B:203:LEU:O	2:B:203:LEU:CG	0.52	2.57	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:253:ARG:O	2:B:256:ARG:CG	0.52	2.55	1	1
2:B:297:ASP:OD2	2:B:356:GLN:NE2	0.52	2.42	1	1
1:A:77:ALA:C	1:A:80:ILE:HG13	0.52	2.24	4	1
2:B:286:LEU:HD23	2:B:288:ASP:OD1	0.52	2.04	8	1
2:B:364:LEU:HD11	2:B:366:ILE:HB	0.52	1.82	16	1
2:B:258:LEU:HA	2:B:275:VAL:HG11	0.52	1.80	18	1
2:B:289:ASN:CG	2:B:290:TYR:H	0.52	2.08	12	1
2:B:283:PHE:HD1	2:B:283:PHE:N	0.52	2.01	18	2
2:B:208:GLU:N	2:B:208:GLU:CD	0.52	2.63	2	1
2:B:227:SER:OG	2:B:242:PHE:CG	0.52	2.59	2	3
2:B:245:TYR:N	2:B:245:TYR:CD1	0.52	2.77	20	2
1:A:43:GLU:OE1	1:A:45:GLU:N	0.52	2.42	17	2
2:B:243:ASP:O	2:B:247:HIS:CD2	0.52	2.63	17	1
1:A:12:LYS:CG	1:A:14:GLY:O	0.52	2.58	1	1
1:A:2:THR:HG22	1:A:68:THR:OG1	0.52	2.05	1	3
2:B:286:LEU:HD23	2:B:292:LYS:CA	0.52	2.35	1	1
2:B:249:LEU:HB3	2:B:301:LEU:HD21	0.52	1.82	1	1
2:B:347:VAL:HG22	2:B:369:VAL:HG23	0.52	1.82	1	1
1:A:80:ILE:O	1:A:84:ASN:ND2	0.52	2.43	14	3
1:A:57:SER:O	1:A:61:ARG:CZ	0.52	2.58	3	1
1:A:38:ASN:HD21	1:A:55:LEU:HD12	0.52	1.65	4	2
2:B:310:ASP:N	2:B:310:ASP:OD1	0.52	2.43	5	1
2:B:275:VAL:CG1	2:B:276:ILE:H	0.52	2.17	17	3
2:B:248:LEU:HG	2:B:249:LEU:N	0.52	2.19	8	1
2:B:255:ARG:NH1	2:B:258:LEU:CD1	0.52	2.73	10	1
1:A:26:LEU:HG	1:A:30:PHE:HD1	0.52	1.65	12	1
2:B:205:PRO:O	2:B:209:ARG:HB2	0.52	2.04	16	2
2:B:186:TRP:CH2	2:B:381:ARG:NH1	0.52	2.78	17	1
2:B:258:LEU:CD1	2:B:275:VAL:HG11	0.51	2.35	1	1
1:A:8:GLU:CD	1:A:8:GLU:N	0.51	2.64	4	2
2:B:382:ARG:HH12	2:B:396:ASP:CB	0.51	2.17	6	1
2:B:222:GLU:OE1	2:B:304:ARG:NE	0.51	2.43	12	1
1:A:72:GLU:OE1	1:A:72:GLU:C	0.51	2.49	13	1
2:B:217:GLU:HG2	2:B:221:ASN:ND2	0.51	2.20	15	3
2:B:217:GLU:O	2:B:221:ASN:HB2	0.51	2.03	10	10
2:B:248:LEU:CD1	2:B:253:ARG:NH2	0.51	2.73	11	1
2:B:270:TRP:N	2:B:270:TRP:CD1	0.51	2.75	1	1
2:B:246:SER:O	2:B:250:SER:CB	0.51	2.58	3	2
2:B:184:GLU:HB3	2:B:323:PHE:CE2	0.51	2.39	4	1
2:B:394:LEU:HB3	2:B:397:PRO:HG3	0.51	1.83	4	3
1:A:13:LEU:O	1:A:13:LEU:CD2	0.51	2.57	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:269:GLU:N	2:B:269:GLU:OE1	0.51	2.44	9	4
2:B:273:LYS:CD	2:B:274:THR:N	0.51	2.73	4	1
1:A:1:MET:N	1:A:1:MET:SD	0.51	2.73	11	2
2:B:205:PRO:O	2:B:209:ARG:NE	0.51	2.42	6	1
2:B:276:ILE:CG2	2:B:277:GLU:N	0.51	2.73	6	2
2:B:258:LEU:CD2	2:B:275:VAL:HG21	0.51	2.36	15	3
2:B:284:ALA:O	2:B:285:ALA:C	0.51	2.48	12	7
2:B:291:LEU:O	2:B:292:LYS:C	0.51	2.49	2	10
1:A:37:ARG:O	1:A:63:ILE:HD12	0.51	2.06	2	1
2:B:326:VAL:O	2:B:326:VAL:HG13	0.51	2.05	5	1
1:A:69:GLY:O	1:A:72:GLU:OE1	0.51	2.29	9	1
2:B:249:LEU:HD11	2:B:305:LEU:HD11	0.51	1.82	9	1
1:A:2:THR:CG2	1:A:3:VAL:N	0.51	2.73	10	1
1:A:53:LEU:HB3	2:B:286:LEU:HD22	0.51	1.82	10	1
2:B:301:LEU:HD23	2:B:301:LEU:C	0.51	2.26	13	1
2:B:223:PHE:CE1	2:B:304:ARG:NH1	0.51	2.79	3	1
1:A:2:THR:HG23	1:A:68:THR:OG1	0.51	2.06	4	1
2:B:181:ALA:HB1	2:B:344:VAL:O	0.51	2.06	7	1
2:B:286:LEU:HG	2:B:287:SER:N	0.51	2.21	10	2
2:B:174:LEU:N	2:B:174:LEU:CD1	0.51	2.73	12	1
2:B:304:ARG:CZ	2:B:337:GLU:OE1	0.51	2.59	17	1
2:B:283:PHE:CE2	2:B:298:LEU:HD13	0.51	2.40	3	1
2:B:248:LEU:CD2	2:B:248:LEU:C	0.51	2.74	6	3
2:B:245:TYR:CZ	2:B:297:ASP:HB3	0.51	2.40	12	3
1:A:4:LYS:O	1:A:5:GLN:CG	0.51	2.59	8	1
1:A:13:LEU:CD1	1:A:13:LEU:N	0.51	2.54	16	1
2:B:276:ILE:C	2:B:276:ILE:HD12	0.51	2.26	18	1
2:B:288:ASP:N	2:B:291:LEU:HD23	0.51	2.21	19	1
1:A:71:GLN:O	1:A:71:GLN:CD	0.51	2.48	3	1
2:B:226:TYR:CZ	2:B:336:ALA:O	0.51	2.63	19	4
2:B:379:LEU:O	2:B:382:ARG:N	0.51	2.32	9	3
2:B:325:LEU:CD1	2:B:325:LEU:C	0.51	2.79	12	3
2:B:293:GLU:C	2:B:293:GLU:OE1	0.51	2.49	16	1
1:A:47:ASN:ND2	1:A:47:ASN:O	0.51	2.43	17	1
1:A:84:ASN:O	1:A:85:SER:CB	0.51	2.59	7	15
2:B:175:PRO:HB3	2:B:388:GLY:O	0.51	2.06	3	1
1:A:80:ILE:CG1	1:A:81:ALA:N	0.51	2.74	9	3
2:B:245:TYR:OH	2:B:297:ASP:HB2	0.51	2.07	6	3
1:A:16:HIS:O	1:A:19:PRO:CD	0.51	2.48	7	1
1:A:17:ALA:O	1:A:21:MET:N	0.51	2.35	7	1
1:A:79:VAL:CG2	1:A:80:ILE:N	0.51	2.73	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:O	1:A:20:ALA:N	0.51	2.44	9	1
2:B:238:THR:O	2:B:241:ILE:HG22	0.51	2.06	10	1
2:B:338:LEU:HD13	2:B:342:ARG:HH11	0.51	1.64	12	1
2:B:253:ARG:NH1	2:B:279:PHE:CE2	0.50	2.79	1	1
1:A:13:LEU:HA	1:A:83:PHE:CE2	0.50	2.40	5	1
2:B:202:THR:O	2:B:202:THR:HG23	0.50	2.06	11	1
2:B:386:VAL:HG22	2:B:393:LEU:HD12	0.50	1.81	11	1
1:A:5:GLN:OE1	1:A:5:GLN:C	0.50	2.49	14	1
1:A:7:VAL:CG2	1:A:83:PHE:CE2	0.50	2.94	15	1
2:B:211:ARG:NH2	2:B:268:ALA:HB3	0.50	2.21	20	1
1:A:44:ALA:HA	1:A:51:ALA:HB1	0.50	1.84	11	20
2:B:173:ALA:O	2:B:391:GLY:O	0.50	2.29	9	5
2:B:212:LEU:CD1	2:B:212:LEU:C	0.50	2.79	5	1
2:B:338:LEU:HD13	2:B:338:LEU:O	0.50	2.06	7	1
2:B:222:GLU:OE2	2:B:223:PHE:N	0.50	2.44	15	1
1:A:53:LEU:O	2:B:288:ASP:OD2	0.50	2.29	12	2
1:A:58:ALA:HB2	1:A:61:ARG:HH11	0.50	1.67	8	1
2:B:248:LEU:C	2:B:248:LEU:CD1	0.50	2.77	8	1
1:A:5:GLN:CD	1:A:76:LEU:HD21	0.50	2.25	15	1
2:B:293:GLU:HG3	2:B:294:ARG:N	0.50	2.21	16	1
1:A:23:LEU:O	1:A:23:LEU:HD23	0.50	2.06	18	1
1:A:38:ASN:HD21	1:A:40:GLU:CB	0.50	2.19	8	1
1:A:74:GLU:OE1	1:A:74:GLU:C	0.50	2.48	12	1
2:B:294:ARG:NH1	2:B:297:ASP:OD2	0.50	2.42	2	1
2:B:182:ILE:HG22	2:B:385:ILE:HG23	0.50	1.83	3	1
1:A:53:LEU:HB2	2:B:286:LEU:HD12	0.50	1.82	4	1
2:B:203:LEU:H	2:B:203:LEU:CD1	0.50	2.19	17	2
2:B:350:ASP:N	2:B:350:ASP:OD1	0.50	2.43	11	1
2:B:245:TYR:OH	2:B:297:ASP:O	0.50	2.30	17	1
2:B:186:TRP:CZ3	2:B:381:ARG:NH1	0.50	2.79	17	1
1:A:16:HIS:ND1	1:A:17:ALA:N	0.50	2.60	4	2
2:B:224:ARG:O	2:B:228:LYS:HB2	0.50	2.06	3	2
2:B:203:LEU:HD12	2:B:204:ASP:N	0.50	2.22	6	1
2:B:283:PHE:C	2:B:285:ALA:H	0.50	2.10	8	1
2:B:326:VAL:HG22	2:B:347:VAL:CG1	0.50	2.37	18	1
2:B:185:GLY:CA	2:B:380:HIS:O	0.50	2.59	3	1
2:B:208:GLU:OE1	2:B:268:ALA:HB2	0.50	2.06	7	2
1:A:25:GLU:OE1	1:A:25:GLU:N	0.50	2.45	5	1
2:B:211:ARG:HH12	2:B:269:GLU:CD	0.50	2.10	5	3
2:B:235:GLN:NE2	2:B:238:THR:OG1	0.50	2.44	6	1
2:B:213:THR:OG1	2:B:255:ARG:CZ	0.50	2.60	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:279:PHE:O	2:B:283:PHE:CD1	0.50	2.65	6	4
2:B:385:ILE:CG2	2:B:385:ILE:O	0.50	2.59	10	1
2:B:238:THR:HG22	2:B:360:MET:SD	0.50	2.46	14	1
2:B:216:LEU:O	2:B:220:ALA:HB3	0.50	2.07	15	1
2:B:254:LEU:HD23	2:B:255:ARG:HH22	0.50	1.66	16	1
2:B:255:ARG:CA	2:B:255:ARG:NE	0.50	2.73	17	1
2:B:279:PHE:CD2	2:B:279:PHE:C	0.50	2.83	18	1
2:B:248:LEU:HD23	2:B:249:LEU:CA	0.50	2.35	10	2
1:A:62:GLN:OE1	1:A:63:ILE:N	0.50	2.45	16	1
2:B:172:ARG:H	2:B:172:ARG:HD3	0.50	1.65	20	1
2:B:270:TRP:CE3	2:B:274:THR:OG1	0.50	2.64	2	1
2:B:247:HIS:O	2:B:247:HIS:ND1	0.50	2.44	10	2
2:B:211:ARG:HH21	2:B:211:ARG:CG	0.50	2.20	9	1
2:B:225:ARG:HE	2:B:229:ARG:HH12	0.50	1.50	14	1
2:B:349:ARG:CD	2:B:372:ALA:O	0.50	2.59	15	1
2:B:276:ILE:O	2:B:279:PHE:CD2	0.50	2.65	20	1
2:B:242:PHE:O	2:B:243:ASP:C	0.49	2.50	10	11
1:A:64:GLU:O	1:A:66:GLU:OE2	0.49	2.29	9	2
2:B:288:ASP:OD2	2:B:290:TYR:CB	0.49	2.60	4	1
2:B:203:LEU:C	2:B:204:ASP:OD1	0.49	2.51	13	2
1:A:77:ALA:O	1:A:80:ILE:HG22	0.49	2.07	15	2
2:B:268:ALA:O	2:B:269:GLU:C	0.49	2.50	8	5
2:B:258:LEU:HD23	2:B:275:VAL:HG21	0.49	1.84	15	4
2:B:338:LEU:CB	2:B:342:ARG:NE	0.49	2.75	12	1
1:A:27:MET:N	1:A:30:PHE:CE2	0.49	2.80	1	8
2:B:256:ARG:CD	2:B:257:GLU:N	0.49	2.75	1	1
2:B:375:GLN:N	2:B:375:GLN:CD	0.49	2.65	16	3
2:B:251:ASP:OD1	2:B:253:ARG:HB3	0.49	2.07	6	1
1:A:53:LEU:HD23	1:A:53:LEU:N	0.49	2.22	10	2
1:A:53:LEU:HD22	2:B:291:LEU:HD12	0.49	1.83	10	1
1:A:27:MET:CE	1:A:34:VAL:HG23	0.49	2.37	15	1
1:A:15:MET:HB3	1:A:19:PRO:CD	0.49	2.31	18	1
2:B:291:LEU:HD12	2:B:291:LEU:O	0.49	2.07	20	1
2:B:184:GLU:N	2:B:184:GLU:OE1	0.49	2.46	4	2
1:A:71:GLN:O	1:A:71:GLN:CG	0.49	2.60	3	1
2:B:187:GLN:CD	2:B:187:GLN:N	0.49	2.65	4	1
2:B:251:ASP:CG	2:B:253:ARG:H	0.49	2.09	6	1
1:A:50:ILE:HD12	2:B:282:GLN:OE1	0.49	2.07	14	1
2:B:292:LYS:CG	2:B:293:GLU:N	0.49	2.75	2	1
2:B:395:VAL:O	2:B:395:VAL:HG23	0.49	2.08	5	2
2:B:245:TYR:C	2:B:245:TYR:CD1	0.49	2.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ASN:OD1	1:A:40:GLU:HB2	0.49	2.06	8	1
2:B:362:ARG:HG2	2:B:363:ALA:N	0.49	2.23	8	1
2:B:325:LEU:CD1	2:B:342:ARG:HH11	0.49	2.21	9	1
2:B:286:LEU:CD1	2:B:288:ASP:OD1	0.49	2.48	2	1
2:B:182:ILE:O	2:B:182:ILE:HG23	0.49	2.05	8	2
1:A:36:LEU:HD11	1:A:46:ALA:HB2	0.49	1.82	8	3
2:B:379:LEU:H	2:B:379:LEU:CD2	0.49	2.17	5	1
2:B:245:TYR:OH	2:B:297:ASP:CB	0.49	2.60	6	2
2:B:342:ARG:HE	2:B:342:ARG:HA	0.49	1.67	6	1
2:B:373:ASP:OD1	2:B:374:ILE:HD13	0.49	2.07	7	1
1:A:56:ASP:CG	2:B:291:LEU:HD11	0.49	2.26	9	1
2:B:294:ARG:O	2:B:297:ASP:HB2	0.49	2.06	10	1
2:B:393:LEU:HD23	2:B:393:LEU:C	0.49	2.28	17	1
1:A:57:SER:HB3	2:B:288:ASP:OD2	0.49	2.08	20	1
2:B:283:PHE:CE2	2:B:298:LEU:HD11	0.49	2.42	3	1
2:B:203:LEU:HD13	2:B:265:GLY:CA	0.49	2.36	4	1
2:B:288:ASP:HB3	2:B:291:LEU:CD2	0.49	2.38	5	2
2:B:395:VAL:HG23	2:B:395:VAL:O	0.49	2.07	7	1
2:B:252:THR:HG22	2:B:255:ARG:NH1	0.49	2.22	9	1
2:B:172:ARG:NH2	2:B:392:GLU:OE2	0.49	2.46	10	1
2:B:211:ARG:CZ	2:B:309:LEU:HD11	0.49	2.38	14	1
1:A:15:MET:N	1:A:15:MET:CE	0.49	2.75	20	1
1:A:4:LYS:N	1:A:4:LYS:HD3	0.49	2.23	20	1
2:B:281:GLU:OE2	2:B:281:GLU:N	0.49	2.46	2	1
2:B:338:LEU:HD22	2:B:339:PRO:O	0.49	2.06	7	1
2:B:208:GLU:OE1	2:B:268:ALA:CB	0.49	2.60	17	3
1:A:38:ASN:HD21	1:A:41:GLY:N	0.49	2.06	8	1
2:B:249:LEU:HD21	2:B:301:LEU:HD21	0.49	1.84	13	1
1:A:52:LEU:O	1:A:56:ASP:OD1	0.49	2.31	4	1
1:A:13:LEU:O	1:A:13:LEU:CG	0.49	2.61	5	1
1:A:31:ASP:N	1:A:31:ASP:OD1	0.49	2.46	5	1
2:B:171:ILE:O	2:B:392:GLU:OE1	0.49	2.31	10	2
1:A:38:ASN:HD21	1:A:40:GLU:HB3	0.49	1.67	8	1
1:A:43:GLU:OE1	1:A:45:GLU:CG	0.49	2.61	8	1
2:B:395:VAL:O	2:B:395:VAL:CG1	0.49	2.60	8	2
1:A:18:ARG:CA	1:A:18:ARG:NE	0.49	2.76	10	1
2:B:235:GLN:HG3	2:B:238:THR:OG1	0.49	2.08	10	1
2:B:325:LEU:C	2:B:325:LEU:HD13	0.49	2.27	11	1
1:A:7:VAL:HG23	1:A:83:PHE:CE2	0.49	2.42	15	1
2:B:230:PHE:O	2:B:232:ALA:N	0.49	2.46	16	1
2:B:235:GLN:HE21	2:B:237:GLU:CD	0.49	2.11	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG11	2:B:248:LEU:HD12	0.49	1.84	20	1
1:A:18:ARG:NE	1:A:18:ARG:CA	0.49	2.76	1	1
2:B:245:TYR:O	2:B:248:LEU:HB3	0.49	2.07	10	4
2:B:258:LEU:HD23	2:B:258:LEU:C	0.49	2.28	7	1
2:B:338:LEU:HD13	2:B:338:LEU:N	0.49	2.06	7	1
2:B:375:GLN:H	2:B:375:GLN:CD	0.49	2.10	15	2
1:A:23:LEU:C	1:A:23:LEU:HD23	0.49	2.28	18	1
2:B:396:ASP:O	2:B:396:ASP:CG	0.49	2.51	18	1
1:A:43:GLU:CD	1:A:43:GLU:N	0.49	2.63	1	1
2:B:273:LYS:HG3	2:B:274:THR:N	0.49	2.23	4	1
2:B:328:ASP:O	2:B:350:ASP:OD1	0.49	2.31	13	2
2:B:395:VAL:O	2:B:395:VAL:HG13	0.49	2.06	19	1
1:A:3:VAL:CG2	1:A:72:GLU:HB2	0.48	2.37	1	1
1:A:71:GLN:O	1:A:74:GLU:N	0.48	2.46	7	19
2:B:268:ALA:HA	2:B:271:ALA:HB3	0.48	1.83	8	6
2:B:202:THR:HG23	2:B:204:ASP:OD1	0.48	2.08	3	1
2:B:396:ASP:N	2:B:397:PRO:HD3	0.48	2.21	3	6
2:B:273:LYS:C	2:B:273:LYS:CD	0.48	2.82	4	1
2:B:305:LEU:O	2:B:309:LEU:HD23	0.48	2.08	7	2
2:B:290:TYR:O	2:B:290:TYR:CD1	0.48	2.66	8	1
2:B:227:SER:HB3	2:B:242:PHE:CB	0.48	2.38	9	2
2:B:230:PHE:O	2:B:233:GLY:N	0.48	2.45	16	2
2:B:256:ARG:O	2:B:260:ALA:HB2	0.48	2.07	12	1
2:B:385:ILE:CD1	2:B:385:ILE:N	0.48	2.65	1	1
1:A:30:PHE:CG	1:A:74:GLU:CD	0.48	2.86	12	1
1:A:15:MET:SD	1:A:19:PRO:CG	0.48	3.01	20	1
1:A:16:HIS:CG	2:B:291:LEU:HD11	0.48	2.44	2	1
2:B:290:TYR:C	2:B:293:GLU:CD	0.48	2.72	14	1
2:B:249:LEU:HD23	2:B:250:SER:H	0.48	1.68	15	1
1:A:7:VAL:O	1:A:7:VAL:HG22	0.48	2.09	17	2
2:B:322:ARG:O	2:B:322:ARG:CG	0.48	2.61	17	1
2:B:357:ALA:O	2:B:361:VAL:HG22	0.48	2.08	9	1
2:B:384:LEU:HD12	2:B:386:VAL:HG13	0.48	1.84	12	1
2:B:244:LEU:O	2:B:247:HIS:ND1	0.48	2.44	13	1
1:A:5:GLN:O	1:A:65:VAL:HG22	0.48	2.09	19	2
1:A:15:MET:HB3	1:A:19:PRO:HD3	0.48	1.84	19	1
1:A:43:GLU:N	1:A:43:GLU:CD	0.48	2.67	3	2
2:B:344:VAL:O	2:B:344:VAL:HG12	0.48	2.08	4	5
2:B:385:ILE:CD1	2:B:397:PRO:HD2	0.48	2.38	4	1
2:B:177:ALA:O	2:B:388:GLY:HA3	0.48	2.08	6	1
2:B:238:THR:O	2:B:242:PHE:CD1	0.48	2.66	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:273:LYS:O	2:B:277:GLU:CB	0.48	2.62	13	1
2:B:244:LEU:HD13	2:B:294:ARG:HH22	0.48	1.68	17	1
2:B:208:GLU:OE1	2:B:208:GLU:N	0.48	2.46	6	2
2:B:209:ARG:CG	2:B:259:PHE:CD1	0.48	2.97	4	1
2:B:186:TRP:CE3	2:B:187:GLN:O	0.48	2.66	8	1
2:B:330:LEU:N	2:B:330:LEU:CD2	0.48	2.69	10	1
2:B:186:TRP:CD1	2:B:186:TRP:O	0.48	2.67	16	1
2:B:361:VAL:HG13	2:B:362:ARG:N	0.48	2.23	1	1
1:A:71:GLN:O	1:A:72:GLU:C	0.48	2.50	3	20
2:B:382:ARG:NH2	2:B:396:ASP:OD2	0.48	2.47	19	5
2:B:291:LEU:HD13	2:B:292:LYS:CA	0.48	2.38	12	1
1:A:56:ASP:C	2:B:288:ASP:OD2	0.48	2.52	14	1
2:B:244:LEU:HD12	2:B:244:LEU:C	0.48	2.29	17	1
1:A:79:VAL:HG13	1:A:80:ILE:N	0.48	2.23	4	2
2:B:244:LEU:CD2	2:B:294:ARG:HH11	0.48	2.20	5	1
2:B:241:ILE:HG22	2:B:242:PHE:H	0.48	1.68	9	1
1:A:21:MET:HB3	2:B:244:LEU:HD13	0.48	1.85	10	1
2:B:325:LEU:HB3	2:B:346:VAL:HG13	0.48	1.85	10	1
2:B:343:LEU:CD1	2:B:345:GLY:O	0.48	2.59	17	1
1:A:8:GLU:OE1	1:A:8:GLU:N	0.48	2.45	18	1
1:A:10:THR:O	1:A:10:THR:CG2	0.48	2.50	19	1
2:B:360:MET:SD	2:B:364:LEU:HD22	0.48	2.49	20	1
1:A:24:PHE:CE2	2:B:247:HIS:CE1	0.48	3.01	10	2
1:A:1:MET:C	1:A:1:MET:SD	0.48	2.91	11	1
2:B:326:VAL:HG12	2:B:376:PRO:HG3	0.48	1.84	11	1
2:B:184:GLU:OE1	2:B:381:ARG:O	0.48	2.32	18	1
2:B:252:THR:O	2:B:256:ARG:CG	0.48	2.62	19	1
1:A:28:GLN:CA	1:A:28:GLN:HE21	0.48	2.22	1	1
2:B:258:LEU:HD12	2:B:275:VAL:HG11	0.48	1.86	1	1
1:A:14:GLY:O	1:A:15:MET:HB3	0.48	2.09	7	3
2:B:251:ASP:OD2	2:B:253:ARG:CB	0.48	2.61	6	1
2:B:277:GLU:O	2:B:281:GLU:CD	0.48	2.52	6	2
1:A:50:ILE:HD12	2:B:283:PHE:CE2	0.48	2.44	6	1
2:B:222:GLU:OE2	2:B:304:ARG:CZ	0.48	2.62	8	1
2:B:222:GLU:OE1	2:B:304:ARG:NH1	0.48	2.47	19	2
2:B:308:HIS:ND1	2:B:308:HIS:N	0.48	2.61	11	1
2:B:253:ARG:CB	2:B:253:ARG:CZ	0.48	2.91	12	1
2:B:305:LEU:O	2:B:305:LEU:HD23	0.48	2.08	14	1
2:B:340:GLN:CD	2:B:340:GLN:N	0.48	2.68	18	1
1:A:16:HIS:CE1	2:B:291:LEU:HD11	0.47	2.44	2	1
1:A:36:LEU:O	1:A:43:GLU:OE1	0.47	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:324:ILE:CG2	2:B:325:LEU:N	0.47	2.76	7	2
2:B:284:ALA:O	2:B:292:LYS:NZ	0.47	2.43	4	4
2:B:350:ASP:O	2:B:350:ASP:OD1	0.47	2.32	5	2
2:B:351:GLY:O	2:B:352:ALA:C	0.47	2.50	9	2
2:B:221:ASN:C	2:B:225:ARG:HE	0.47	2.12	8	3
2:B:381:ARG:C	2:B:382:ARG:HG2	0.47	2.28	7	1
1:A:83:PHE:N	1:A:83:PHE:CD2	0.47	2.77	8	2
2:B:211:ARG:CG	2:B:211:ARG:NH2	0.47	2.75	9	1
1:A:15:MET:O	1:A:18:ARG:N	0.47	2.47	15	1
2:B:212:LEU:HD13	2:B:212:LEU:O	0.47	2.08	17	1
2:B:286:LEU:HB2	2:B:291:LEU:CD2	0.47	2.28	20	1
2:B:291:LEU:O	2:B:293:GLU:N	0.47	2.48	2	2
2:B:244:LEU:O	2:B:244:LEU:HD12	0.47	2.09	3	1
2:B:340:GLN:CG	2:B:340:GLN:O	0.47	2.62	5	1
2:B:373:ASP:N	2:B:373:ASP:OD1	0.47	2.46	8	1
1:A:53:LEU:CD2	1:A:53:LEU:C	0.47	2.82	9	1
1:A:12:LYS:O	1:A:12:LYS:CD	0.47	2.61	3	2
1:A:43:GLU:N	1:A:43:GLU:OE1	0.47	2.47	3	2
1:A:80:ILE:HD12	1:A:81:ALA:N	0.47	2.24	3	1
2:B:222:GLU:O	2:B:226:TYR:CB	0.47	2.62	12	2
1:A:79:VAL:HG22	1:A:83:PHE:CZ	0.47	2.43	11	1
2:B:236:LYS:O	2:B:240:ALA:N	0.47	2.39	17	2
1:A:56:ASP:O	2:B:288:ASP:OD2	0.47	2.32	14	1
1:A:15:MET:C	1:A:19:PRO:HD2	0.47	2.29	15	1
2:B:251:ASP:OD1	2:B:253:ARG:CZ	0.47	2.62	16	1
2:B:235:GLN:OE1	2:B:363:ALA:HB3	0.47	2.09	16	1
1:A:80:ILE:HG22	1:A:81:ALA:N	0.47	2.24	16	9
1:A:71:GLN:CG	1:A:74:GLU:CB	0.47	2.91	3	1
2:B:349:ARG:CB	2:B:372:ALA:O	0.47	2.63	3	2
1:A:76:LEU:O	1:A:80:ILE:CG2	0.47	2.41	9	2
1:A:38:ASN:N	1:A:38:ASN:HD22	0.47	2.06	12	1
1:A:5:GLN:OE1	1:A:7:VAL:HG23	0.47	2.09	14	1
1:A:38:ASN:HA	1:A:63:ILE:HG22	0.47	1.86	14	2
2:B:230:PHE:CE2	2:B:239:ALA:CB	0.47	2.95	16	1
2:B:293:GLU:O	2:B:295:ALA:N	0.47	2.48	2	3
2:B:187:GLN:CD	2:B:187:GLN:H	0.47	2.13	4	2
1:A:53:LEU:HG	1:A:54:MET:N	0.47	2.22	11	2
1:A:25:GLU:CD	1:A:25:GLU:N	0.47	2.68	5	2
2:B:247:HIS:HA	2:B:250:SER:OG	0.47	2.09	7	2
2:B:226:TYR:O	2:B:229:ARG:CG	0.47	2.63	12	2
1:A:50:ILE:HG12	1:A:51:ALA:N	0.47	2.25	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:221:ASN:OD1	2:B:224:ARG:NH2	0.47	2.48	14	1
2:B:180:VAL:HG22	2:B:181:ALA:N	0.47	2.25	15	1
2:B:187:GLN:C	2:B:187:GLN:NE2	0.47	2.68	15	1
1:A:49:VAL:CG2	2:B:248:LEU:HD11	0.47	2.39	19	1
2:B:374:ILE:O	2:B:374:ILE:HG23	0.47	2.08	3	1
2:B:376:PRO:O	2:B:380:HIS:ND1	0.47	2.48	3	1
2:B:223:PHE:CZ	2:B:304:ARG:CZ	0.47	2.97	20	2
2:B:284:ALA:C	2:B:286:LEU:N	0.47	2.68	18	3
2:B:171:ILE:O	2:B:392:GLU:CD	0.47	2.53	7	1
2:B:171:ILE:C	2:B:392:GLU:OE2	0.47	2.52	7	1
2:B:288:ASP:OD2	2:B:291:LEU:HB2	0.47	2.10	12	1
2:B:384:LEU:O	2:B:384:LEU:CD1	0.47	2.61	20	1
1:A:43:GLU:CA	1:A:43:GLU:OE1	0.47	2.60	1	1
2:B:170:ARG:N	2:B:393:LEU:O	0.47	2.47	19	4
2:B:328:ASP:N	2:B:328:ASP:OD1	0.47	2.43	9	3
2:B:335:LEU:O	2:B:337:GLU:N	0.47	2.48	3	1
2:B:245:TYR:O	2:B:245:TYR:CD1	0.47	2.68	5	1
2:B:301:LEU:C	2:B:301:LEU:CD1	0.47	2.77	5	2
2:B:393:LEU:H	2:B:393:LEU:CD2	0.47	2.05	8	1
2:B:218:GLU:CD	2:B:218:GLU:O	0.47	2.53	10	1
2:B:176:ALA:CB	2:B:370:MET:SD	0.47	2.92	12	1
2:B:245:TYR:HA	2:B:248:LEU:HD22	0.47	1.86	14	1
2:B:244:LEU:HD12	2:B:245:TYR:CA	0.47	2.39	17	1
2:B:340:GLN:CD	2:B:340:GLN:H	0.47	2.12	18	1
1:A:30:PHE:HA	1:A:71:GLN:OE1	0.47	2.10	20	1
2:B:335:LEU:HD21	2:B:343:LEU:CD1	0.47	2.40	2	1
1:A:64:GLU:C	1:A:66:GLU:OE2	0.47	2.53	3	1
2:B:335:LEU:C	2:B:337:GLU:N	0.47	2.69	3	2
2:B:349:ARG:HB2	2:B:372:ALA:O	0.47	2.09	3	2
2:B:272:VAL:HG23	2:B:273:LYS:N	0.47	2.25	4	1
1:A:63:ILE:HG22	1:A:64:GLU:N	0.47	2.23	5	2
2:B:392:GLU:CD	2:B:392:GLU:C	0.47	2.74	8	1
2:B:281:GLU:OE1	2:B:281:GLU:N	0.47	2.48	10	1
2:B:203:LEU:H	2:B:203:LEU:HD23	0.47	1.60	15	2
2:B:248:LEU:O	2:B:248:LEU:HD23	0.47	2.10	15	1
1:A:16:HIS:CG	1:A:16:HIS:O	0.47	2.67	19	1
2:B:383:THR:O	2:B:396:ASP:OD1	0.47	2.33	20	1
1:A:79:VAL:HG12	1:A:80:ILE:N	0.47	2.25	2	2
1:A:79:VAL:HG23	1:A:80:ILE:N	0.47	2.24	8	3
2:B:203:LEU:CD2	2:B:203:LEU:H	0.47	1.96	11	1
2:B:235:GLN:NE2	2:B:237:GLU:OE1	0.47	2.48	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:366:ILE:O	2:B:366:ILE:HG23	0.47	2.10	16	1
2:B:288:ASP:O	2:B:291:LEU:HG	0.47	2.09	20	2
2:B:349:ARG:HH11	2:B:373:ASP:C	0.47	2.12	5	1
1:A:53:LEU:HD13	2:B:286:LEU:HB2	0.47	1.87	11	1
2:B:293:GLU:CG	2:B:294:ARG:N	0.47	2.78	16	1
2:B:272:VAL:O	2:B:276:ILE:HD13	0.46	2.10	1	2
2:B:251:ASP:OD1	2:B:253:ARG:HB2	0.46	2.10	4	1
2:B:381:ARG:H	2:B:381:ARG:HD3	0.46	1.70	4	1
1:A:40:GLU:OE2	1:A:61:ARG:CZ	0.46	2.63	6	1
2:B:226:TYR:CE1	2:B:229:ARG:NH1	0.46	2.83	6	1
1:A:12:LYS:HG3	1:A:12:LYS:O	0.46	2.10	12	2
1:A:18:ARG:O	1:A:22:LYS:HB2	0.46	2.10	9	2
2:B:257:GLU:OE1	2:B:279:PHE:CE1	0.46	2.68	11	2
2:B:299:ARG:O	2:B:299:ARG:HD2	0.46	2.10	14	1
2:B:335:LEU:HD21	2:B:343:LEU:HD22	0.46	1.87	15	1
1:A:38:ASN:HA	1:A:63:ILE:CG2	0.46	2.40	20	1
2:B:249:LEU:HD21	2:B:301:LEU:HD13	0.46	1.86	2	1
2:B:271:ALA:O	2:B:275:VAL:CG2	0.46	2.63	11	4
1:A:71:GLN:C	1:A:71:GLN:NE2	0.46	2.69	3	1
2:B:185:GLY:C	2:B:380:HIS:O	0.46	2.52	3	1
2:B:245:TYR:OH	2:B:301:LEU:HD13	0.46	2.10	4	1
2:B:329:GLU:O	2:B:329:GLU:CD	0.46	2.54	4	1
1:A:6:THR:HG23	1:A:6:THR:O	0.46	2.11	5	1
1:A:7:VAL:HG23	1:A:7:VAL:O	0.46	2.11	5	1
2:B:269:GLU:OE1	2:B:269:GLU:N	0.46	2.48	5	1
2:B:323:PHE:C	2:B:323:PHE:CD1	0.46	2.86	5	1
1:A:24:PHE:O	1:A:28:GLN:NE2	0.46	2.49	13	1
2:B:259:PHE:CE2	2:B:263:ASP:OD2	0.46	2.68	16	1
2:B:393:LEU:C	2:B:393:LEU:HD12	0.46	2.30	16	1
2:B:340:GLN:O	2:B:343:LEU:O	0.46	2.33	1	1
1:A:83:PHE:C	1:A:83:PHE:CD1	0.46	2.86	3	1
2:B:227:SER:CB	2:B:242:PHE:HB3	0.46	2.41	3	2
1:A:53:LEU:HB2	2:B:291:LEU:HD22	0.46	1.87	16	2
1:A:38:ASN:CG	1:A:40:GLU:H	0.46	2.14	8	1
1:A:38:ASN:HD21	1:A:40:GLU:C	0.46	2.13	8	1
2:B:330:LEU:HD21	2:B:348:VAL:CG1	0.46	2.41	8	1
1:A:35:LEU:C	1:A:36:LEU:HD12	0.46	2.31	18	3
2:B:289:ASN:O	2:B:291:LEU:N	0.46	2.49	14	1
2:B:182:ILE:O	2:B:322:ARG:NH2	0.46	2.49	16	1
1:A:37:ARG:H	1:A:63:ILE:HD12	0.46	1.71	2	1
2:B:361:VAL:HG23	2:B:362:ARG:N	0.46	2.25	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:294:ARG:O	2:B:295:ALA:C	0.46	2.54	3	3
2:B:186:TRP:O	2:B:326:VAL:CG2	0.46	2.63	7	1
2:B:276:ILE:HG22	2:B:277:GLU:N	0.46	2.25	9	1
2:B:273:LYS:O	2:B:277:GLU:HG2	0.46	2.09	13	1
2:B:343:LEU:HD23	2:B:344:VAL:N	0.46	2.26	1	1
2:B:233:GLY:C	2:B:234:ALA:O	0.46	2.53	2	3
2:B:288:ASP:OD2	2:B:290:TYR:HB2	0.46	2.10	4	1
2:B:359:ILE:CG2	2:B:360:MET:N	0.46	2.78	7	1
2:B:349:ARG:NH2	2:B:376:PRO:HD3	0.46	2.25	10	1
2:B:386:VAL:HG22	2:B:393:LEU:CD1	0.46	2.41	11	1
2:B:297:ASP:OD1	2:B:356:GLN:NE2	0.46	2.49	14	1
1:A:27:MET:CA	1:A:30:PHE:CE2	0.46	2.99	10	3
1:A:18:ARG:O	1:A:21:MET:HG3	0.46	2.11	4	1
2:B:187:GLN:N	2:B:187:GLN:OE1	0.46	2.41	4	1
1:A:27:MET:SD	1:A:27:MET:C	0.46	2.93	5	1
2:B:293:GLU:HA	2:B:293:GLU:OE1	0.46	2.11	11	1
2:B:254:LEU:HD23	2:B:254:LEU:C	0.46	2.31	18	1
2:B:244:LEU:O	2:B:248:LEU:HG	0.46	2.11	4	1
2:B:245:TYR:CZ	2:B:297:ASP:HB2	0.46	2.45	9	1
1:A:76:LEU:C	1:A:76:LEU:HD12	0.46	2.31	10	1
2:B:262:VAL:CG2	2:B:263:ASP:N	0.46	2.78	20	1
2:B:325:LEU:HD23	2:B:326:VAL:N	0.46	2.26	8	3
2:B:390:ARG:O	2:B:391:GLY:C	0.46	2.54	2	4
2:B:256:ARG:O	2:B:260:ALA:CB	0.46	2.64	12	1
2:B:394:LEU:HD22	2:B:397:PRO:HB3	0.46	1.86	13	1
2:B:297:ASP:OD2	2:B:333:THR:HG23	0.46	2.10	20	1
2:B:279:PHE:CE2	2:B:298:LEU:HB3	0.46	2.46	20	1
2:B:235:GLN:HG2	2:B:236:LYS:N	0.46	2.26	2	2
2:B:342:ARG:C	2:B:342:ARG:CD	0.46	2.84	2	2
2:B:322:ARG:C	2:B:323:PHE:CG	0.46	2.89	17	2
2:B:288:ASP:CB	2:B:291:LEU:HD21	0.46	2.39	7	1
2:B:355:SER:OG	2:B:358:ALA:CB	0.46	2.64	10	1
2:B:171:ILE:HD12	2:B:393:LEU:HD11	0.46	1.87	16	1
1:A:54:MET:C	1:A:54:MET:SD	0.46	2.94	4	1
2:B:329:GLU:O	2:B:329:GLU:OE1	0.46	2.33	7	1
1:A:17:ALA:C	1:A:19:PRO:CD	0.46	2.82	9	1
1:A:65:VAL:O	1:A:65:VAL:HG23	0.46	2.11	10	1
2:B:304:ARG:HH22	2:B:336:ALA:C	0.46	2.15	11	1
2:B:338:LEU:HD23	2:B:338:LEU:H	0.46	1.71	13	1
2:B:297:ASP:CG	2:B:356:GLN:NE2	0.46	2.70	14	1
2:B:349:ARG:CG	2:B:350:ASP:N	0.46	2.79	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:MET:HG2	1:A:16:HIS:H	0.46	1.69	20	1
2:B:379:LEU:HA	2:B:382:ARG:HB2	0.45	1.89	4	1
1:A:5:GLN:CD	1:A:80:ILE:HD11	0.45	2.31	6	1
1:A:76:LEU:C	1:A:76:LEU:HD13	0.45	2.32	8	1
2:B:281:GLU:N	2:B:281:GLU:OE1	0.45	2.49	8	2
2:B:376:PRO:HA	2:B:379:LEU:HD12	0.45	1.88	8	1
2:B:222:GLU:CD	2:B:222:GLU:C	0.45	2.75	9	1
2:B:217:GLU:CD	2:B:217:GLU:C	0.45	2.74	14	1
2:B:210:GLU:CG	2:B:211:ARG:N	0.45	2.79	16	1
2:B:343:LEU:HD23	2:B:345:GLY:H	0.45	1.71	19	1
2:B:268:ALA:O	2:B:272:VAL:N	0.45	2.38	5	1
1:A:65:VAL:O	1:A:65:VAL:CG2	0.45	2.64	10	1
2:B:248:LEU:CD2	2:B:253:ARG:HH11	0.45	2.23	12	1
2:B:301:LEU:HD23	2:B:301:LEU:O	0.45	2.11	13	1
2:B:288:ASP:CB	2:B:291:LEU:HD11	0.45	2.42	14	1
2:B:283:PHE:CE1	2:B:298:LEU:HD12	0.45	2.46	15	1
2:B:384:LEU:C	2:B:384:LEU:CD2	0.45	2.79	20	1
2:B:352:ALA:C	2:B:354:ASN:H	0.45	2.14	3	1
2:B:307:PHE:O	2:B:310:ASP:CG	0.45	2.55	15	2
2:B:182:ILE:O	2:B:183:ALA:HB2	0.45	2.10	13	4
2:B:308:HIS:C	2:B:310:ASP:N	0.45	2.68	8	3
2:B:286:LEU:CD1	2:B:291:LEU:HB3	0.45	2.41	4	1
1:A:36:LEU:CD1	1:A:36:LEU:N	0.45	2.72	8	2
2:B:224:ARG:CZ	2:B:225:ARG:HH22	0.45	2.24	9	1
2:B:244:LEU:O	2:B:248:LEU:HD13	0.45	2.12	14	1
2:B:394:LEU:HD12	2:B:397:PRO:HG3	0.45	1.89	5	1
2:B:212:LEU:HB3	2:B:255:ARG:NH2	0.45	2.27	6	1
2:B:394:LEU:HD23	2:B:397:PRO:HG3	0.45	1.87	8	1
1:A:17:ALA:O	1:A:18:ARG:C	0.45	2.52	9	1
2:B:256:ARG:NH2	2:B:260:ALA:CB	0.45	2.79	11	1
1:A:71:GLN:HB2	1:A:74:GLU:OE2	0.45	2.11	12	1
2:B:300:ALA:HB1	2:B:333:THR:OG1	0.45	2.10	12	1
2:B:395:VAL:CG1	2:B:395:VAL:O	0.45	2.64	14	2
2:B:287:SER:O	2:B:288:ASP:C	0.45	2.55	18	1
2:B:247:HIS:O	2:B:251:ASP:N	0.45	2.50	14	3
1:A:15:MET:C	1:A:16:HIS:O	0.45	2.55	7	1
1:A:50:ILE:O	1:A:53:LEU:CG	0.45	2.52	7	1
2:B:177:ALA:CB	2:B:366:ILE:O	0.45	2.64	10	1
2:B:378:VAL:O	2:B:380:HIS:CE1	0.45	2.69	11	1
1:A:6:THR:N	1:A:64:GLU:OE2	0.45	2.50	13	1
1:A:84:ASN:C	1:A:85:SER:OG	0.45	2.53	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:HA	1:A:18:ARG:HE	0.45	1.72	1	1
2:B:249:LEU:HD21	2:B:301:LEU:HD22	0.45	1.87	2	1
2:B:394:LEU:H	2:B:394:LEU:HD22	0.45	1.62	7	1
1:A:21:MET:CB	2:B:244:LEU:HD13	0.45	2.42	10	1
2:B:235:GLN:NE2	2:B:237:GLU:CG	0.45	2.79	14	1
2:B:203:LEU:O	2:B:203:LEU:HG	0.45	2.11	18	1
2:B:244:LEU:HD23	2:B:294:ARG:HH11	0.45	1.72	18	1
2:B:247:HIS:CG	2:B:248:LEU:N	0.45	2.83	19	1
2:B:286:LEU:HB3	2:B:291:LEU:HD21	0.45	1.83	20	1
2:B:171:ILE:HD13	2:B:373:ASP:OD1	0.45	2.12	20	1
2:B:184:GLU:HB2	2:B:323:PHE:CZ	0.45	2.46	4	1
2:B:288:ASP:OD2	2:B:291:LEU:N	0.45	2.45	5	1
1:A:53:LEU:HA	2:B:291:LEU:HD13	0.45	1.89	9	1
2:B:235:GLN:N	2:B:235:GLN:OE1	0.45	2.49	13	1
2:B:276:ILE:HD13	2:B:302:GLY:HA2	0.45	1.89	14	1
1:A:5:GLN:N	1:A:64:GLU:OE2	0.45	2.50	15	1
1:A:80:ILE:HG13	1:A:81:ALA:N	0.45	2.27	11	3
2:B:205:PRO:O	2:B:209:ARG:HB3	0.45	2.12	7	2
2:B:171:ILE:N	2:B:171:ILE:HD12	0.45	2.27	6	1
1:A:53:LEU:HD13	2:B:291:LEU:HD12	0.45	1.86	6	1
2:B:227:SER:HB3	2:B:242:PHE:CG	0.45	2.46	9	1
2:B:248:LEU:C	2:B:248:LEU:CD2	0.45	2.75	10	1
1:A:40:GLU:N	1:A:40:GLU:OE2	0.45	2.49	12	1
1:A:18:ARG:CA	1:A:18:ARG:HE	0.45	2.24	17	1
1:A:10:THR:CG2	1:A:10:THR:O	0.45	2.60	18	1
2:B:244:LEU:CD2	2:B:244:LEU:O	0.45	2.60	19	1
2:B:204:ASP:OD1	2:B:204:ASP:N	0.45	2.49	1	1
2:B:245:TYR:CE2	2:B:249:LEU:HD12	0.45	2.46	4	1
2:B:212:LEU:O	2:B:212:LEU:HD13	0.45	2.10	5	1
2:B:225:ARG:O	2:B:229:ARG:HG3	0.45	2.12	11	1
1:A:26:LEU:HG	1:A:30:PHE:CD1	0.45	2.46	12	1
1:A:30:PHE:CG	1:A:74:GLU:OE1	0.45	2.69	12	1
2:B:217:GLU:HG3	2:B:218:GLU:N	0.45	2.27	14	1
1:A:36:LEU:HD22	1:A:65:VAL:HG22	0.45	1.88	15	1
2:B:250:SER:O	2:B:255:ARG:NH1	0.45	2.50	15	1
2:B:259:PHE:C	2:B:259:PHE:CD1	0.45	2.87	19	1
2:B:354:ASN:OD1	2:B:355:SER:N	0.45	2.50	5	1
2:B:385:ILE:HG23	2:B:394:LEU:CB	0.45	2.42	5	1
2:B:369:VAL:C	2:B:370:MET:SD	0.45	2.95	6	2
2:B:256:ARG:CG	2:B:257:GLU:N	0.45	2.79	12	2
1:A:4:LYS:N	1:A:4:LYS:HD2	0.45	2.26	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:NH1	1:A:21:MET:CE	0.45	2.80	16	1
2:B:394:LEU:HD22	2:B:394:LEU:N	0.45	2.27	16	1
1:A:48:SER:OG	2:B:253:ARG:CZ	0.44	2.65	2	1
2:B:235:GLN:HG3	2:B:237:GLU:H	0.44	1.72	3	1
2:B:270:TRP:O	2:B:274:THR:CB	0.44	2.66	4	1
2:B:206:ALA:O	2:B:210:GLU:HB2	0.44	2.13	6	2
1:A:13:LEU:CD2	1:A:13:LEU:C	0.44	2.84	5	1
2:B:216:LEU:CD1	2:B:216:LEU:C	0.44	2.65	5	1
2:B:205:PRO:O	2:B:209:ARG:CG	0.44	2.66	6	1
1:A:30:PHE:HA	1:A:71:GLN:NE2	0.44	2.27	7	1
1:A:56:ASP:OD1	2:B:288:ASP:CG	0.44	2.55	9	1
2:B:272:VAL:O	2:B:276:ILE:HG22	0.44	2.12	11	1
2:B:217:GLU:O	2:B:221:ASN:CG	0.44	2.55	18	2
1:A:76:LEU:CD2	1:A:76:LEU:O	0.44	2.65	14	1
2:B:342:ARG:O	2:B:344:VAL:HG23	0.44	2.13	15	1
2:B:349:ARG:CZ	2:B:374:ILE:O	0.44	2.65	17	1
1:A:3:VAL:O	1:A:3:VAL:HG12	0.44	2.12	18	1
1:A:9:ILE:HD12	1:A:13:LEU:HA	0.44	1.89	20	1
2:B:382:ARG:HH12	2:B:396:ASP:CG	0.44	2.16	6	1
2:B:216:LEU:CD1	2:B:255:ARG:NH2	0.44	2.80	10	1
2:B:256:ARG:CZ	2:B:259:PHE:CD2	0.44	3.01	10	1
2:B:187:GLN:NE2	2:B:187:GLN:C	0.44	2.71	13	1
2:B:309:LEU:O	2:B:309:LEU:CG	0.44	2.62	14	1
2:B:355:SER:O	2:B:358:ALA:N	0.44	2.50	15	1
2:B:230:PHE:C	2:B:232:ALA:N	0.44	2.70	16	1
1:A:49:VAL:HG23	2:B:248:LEU:HD11	0.44	1.89	19	1
2:B:272:VAL:CG1	2:B:273:LYS:N	0.44	2.80	1	1
2:B:212:LEU:HD21	2:B:258:LEU:CB	0.44	2.42	4	1
1:A:18:ARG:N	1:A:18:ARG:NE	0.44	2.64	10	1
1:A:72:GLU:HG2	1:A:73:GLU:N	0.44	2.26	10	1
2:B:259:PHE:HD1	2:B:259:PHE:N	0.44	2.06	11	1
2:B:245:TYR:CE1	2:B:297:ASP:HB3	0.44	2.48	19	2
1:A:36:LEU:O	1:A:43:GLU:OE2	0.44	2.35	17	1
2:B:288:ASP:CB	2:B:291:LEU:HD22	0.44	2.37	18	1
1:A:2:THR:HG22	1:A:3:VAL:N	0.44	2.27	10	2
1:A:59:LYS:O	1:A:59:LYS:CG	0.44	2.65	20	2
1:A:84:ASN:O	1:A:85:SER:HB3	0.44	2.12	9	1
2:B:338:LEU:HD12	2:B:342:ARG:NH2	0.44	2.28	9	1
2:B:279:PHE:O	2:B:282:GLN:HG2	0.44	2.12	11	1
1:A:16:HIS:C	1:A:16:HIS:CD2	0.44	2.91	12	1
2:B:297:ASP:O	2:B:301:LEU:HD12	0.44	2.13	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:261:GLU:C	2:B:266:SER:OG	0.44	2.55	18	2
2:B:392:GLU:HG2	2:B:393:LEU:N	0.44	2.28	17	2
1:A:11:ASN:ND2	1:A:11:ASN:O	0.44	2.50	20	1
2:B:248:LEU:O	2:B:248:LEU:HD22	0.44	2.13	3	1
1:A:12:LYS:HG2	1:A:12:LYS:O	0.44	2.13	12	2
2:B:308:HIS:O	2:B:310:ASP:N	0.44	2.51	8	2
2:B:385:ILE:CD1	2:B:385:ILE:C	0.44	2.84	11	1
2:B:267:VAL:O	2:B:271:ALA:N	0.44	2.40	5	2
1:A:33:GLU:OE2	1:A:34:VAL:N	0.44	2.50	4	1
2:B:270:TRP:CH2	2:B:274:THR:OG1	0.44	2.66	5	1
2:B:207:LEU:O	2:B:211:ARG:N	0.44	2.43	15	2
1:A:76:LEU:CD1	1:A:76:LEU:C	0.44	2.86	8	1
2:B:209:ARG:HH22	2:B:256:ARG:HH22	0.44	1.56	9	1
2:B:256:ARG:HE	2:B:256:ARG:HA	0.44	1.71	14	2
2:B:273:LYS:O	2:B:276:ILE:HG12	0.44	2.13	15	1
1:A:18:ARG:H	1:A:18:ARG:NE	0.44	2.08	16	1
2:B:247:HIS:HA	2:B:250:SER:HG	0.44	1.73	17	1
2:B:244:LEU:C	2:B:244:LEU:HD22	0.44	2.27	19	1
1:A:6:THR:HG23	1:A:62:GLN:CD	0.44	2.33	3	1
1:A:23:LEU:HD23	1:A:46:ALA:HB1	0.44	1.88	7	1
2:B:331:SER:HB3	2:B:333:THR:HG22	0.44	1.90	7	1
2:B:240:ALA:O	2:B:244:LEU:HD12	0.44	2.13	10	1
1:A:49:VAL:HG21	2:B:248:LEU:CD1	0.44	2.43	15	1
2:B:374:ILE:HG23	2:B:374:ILE:O	0.44	2.12	15	1
2:B:346:VAL:CG2	2:B:368:THR:HG23	0.44	2.42	16	1
2:B:301:LEU:HD12	2:B:305:LEU:HD23	0.44	1.88	17	1
1:A:55:LEU:O	1:A:55:LEU:HD23	0.44	2.12	20	1
2:B:360:MET:HG2	2:B:361:VAL:N	0.44	2.27	1	1
2:B:396:ASP:N	2:B:396:ASP:OD1	0.44	2.50	4	1
2:B:223:PHE:CZ	2:B:301:LEU:CD2	0.44	3.00	6	1
2:B:248:LEU:O	2:B:251:ASP:HB3	0.44	2.13	6	2
1:A:65:VAL:HG11	1:A:79:VAL:HG11	0.44	1.89	12	3
2:B:374:ILE:HG21	2:B:379:LEU:HD21	0.44	1.90	8	1
2:B:182:ILE:CD1	2:B:182:ILE:N	0.44	2.79	9	1
1:A:18:ARG:NH1	2:B:240:ALA:CB	0.44	2.81	9	2
1:A:69:GLY:O	1:A:72:GLU:CD	0.44	2.56	10	1
2:B:342:ARG:HG3	2:B:343:LEU:N	0.44	2.28	15	2
2:B:216:LEU:CD2	2:B:217:GLU:N	0.44	2.71	17	1
1:A:12:LYS:C	1:A:14:GLY:H	0.44	2.16	18	1
2:B:348:VAL:HG22	2:B:349:ARG:N	0.44	2.28	18	1
2:B:385:ILE:N	2:B:385:ILE:HD12	0.44	2.27	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:VAL:C	1:A:66:GLU:OE2	0.44	2.57	3	1
1:A:1:MET:SD	1:A:1:MET:C	0.44	2.96	4	1
2:B:288:ASP:O	2:B:291:LEU:HB3	0.44	2.13	12	2
2:B:283:PHE:C	2:B:285:ALA:N	0.44	2.71	8	1
2:B:187:GLN:HE21	2:B:187:GLN:C	0.44	2.16	13	1
2:B:270:TRP:CD2	2:B:274:THR:OG1	0.44	2.70	19	1
2:B:270:TRP:O	2:B:274:THR:HG23	0.43	2.12	1	1
1:A:17:ALA:O	1:A:18:ARG:CZ	0.43	2.66	2	1
2:B:218:GLU:O	2:B:222:GLU:HB2	0.43	2.13	3	2
1:A:20:ALA:O	1:A:24:PHE:CZ	0.43	2.71	7	1
2:B:237:GLU:HG2	2:B:238:THR:N	0.43	2.28	17	1
2:B:382:ARG:NH1	2:B:396:ASP:OD1	0.43	2.52	6	1
1:A:26:LEU:HD12	1:A:30:PHE:CD1	0.43	2.48	7	1
1:A:30:PHE:HB3	1:A:74:GLU:OE2	0.43	2.13	12	1
2:B:240:ALA:C	2:B:243:ASP:OD1	0.43	2.56	14	1
2:B:249:LEU:C	2:B:249:LEU:CD2	0.43	2.86	19	1
2:B:208:GLU:HG3	2:B:268:ALA:HB2	0.43	1.88	19	1
2:B:342:ARG:O	2:B:342:ARG:CD	0.43	2.66	2	1
1:A:37:ARG:NH1	1:A:66:GLU:CD	0.43	2.71	5	1
2:B:229:ARG:CG	2:B:230:PHE:N	0.43	2.80	9	1
1:A:36:LEU:O	1:A:37:ARG:HG2	0.43	2.13	13	1
2:B:251:ASP:CG	2:B:251:ASP:O	0.43	2.56	13	1
2:B:219:ALA:HB2	2:B:308:HIS:ND1	0.43	2.28	14	2
2:B:326:VAL:O	2:B:326:VAL:CG1	0.43	2.64	20	1
2:B:292:LYS:HG2	2:B:293:GLU:N	0.43	2.28	1	2
1:A:10:THR:OG1	1:A:10:THR:O	0.43	2.27	2	1
2:B:227:SER:O	2:B:230:PHE:N	0.43	2.51	4	1
1:A:21:MET:SD	2:B:244:LEU:HD12	0.43	2.53	5	1
2:B:362:ARG:CG	2:B:363:ALA:N	0.43	2.81	6	2
2:B:277:GLU:OE2	2:B:281:GLU:OE2	0.43	2.36	8	1
2:B:291:LEU:O	2:B:294:ARG:CB	0.43	2.67	8	1
2:B:299:ARG:HG2	2:B:300:ALA:N	0.43	2.28	16	1
2:B:288:ASP:OD1	2:B:288:ASP:O	0.43	2.37	17	1
2:B:223:PHE:CE2	2:B:304:ARG:NH1	0.43	2.87	20	1
2:B:203:LEU:HD12	2:B:203:LEU:N	0.43	2.26	1	1
2:B:173:ALA:HB2	2:B:393:LEU:HD11	0.43	1.90	19	2
2:B:281:GLU:CD	2:B:281:GLU:N	0.43	2.72	2	1
2:B:184:GLU:OE1	2:B:381:ARG:CG	0.43	2.66	3	1
2:B:221:ASN:O	2:B:225:ARG:HD3	0.43	2.13	7	2
2:B:286:LEU:O	2:B:292:LYS:NZ	0.43	2.50	9	2
2:B:345:GLY:C	2:B:346:VAL:HG23	0.43	2.34	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:N	1:A:36:LEU:CD1	0.43	2.81	11	1
1:A:62:GLN:CD	1:A:62:GLN:N	0.43	2.71	11	1
2:B:375:GLN:OE1	2:B:375:GLN:CA	0.43	2.67	14	1
1:A:6:THR:HG23	1:A:62:GLN:OE1	0.43	2.14	3	1
2:B:208:GLU:CD	2:B:208:GLU:N	0.43	2.70	6	1
2:B:216:LEU:HD22	2:B:255:ARG:CZ	0.43	2.44	7	1
2:B:281:GLU:O	2:B:285:ALA:N	0.43	2.52	7	1
2:B:245:TYR:HH	2:B:297:ASP:CG	0.43	2.17	8	1
2:B:322:ARG:O	2:B:323:PHE:HB3	0.43	2.13	12	1
2:B:212:LEU:CD1	2:B:258:LEU:HD13	0.43	2.43	15	1
1:A:15:MET:CE	1:A:20:ALA:HB2	0.43	2.43	18	1
2:B:278:LYS:O	2:B:282:GLN:CG	0.43	2.66	18	1
2:B:286:LEU:N	2:B:286:LEU:CD2	0.43	2.82	18	1
2:B:269:GLU:N	2:B:269:GLU:CD	0.43	2.71	1	2
2:B:209:ARG:HG3	2:B:210:GLU:N	0.43	2.28	6	1
2:B:359:ILE:HG23	2:B:360:MET:N	0.43	2.28	7	1
1:A:50:ILE:CG1	1:A:51:ALA:N	0.43	2.80	8	1
2:B:222:GLU:HG2	2:B:226:TYR:CD1	0.43	2.49	9	1
2:B:249:LEU:CD1	2:B:305:LEU:HD11	0.43	2.44	9	1
1:A:45:GLU:OE2	1:A:47:ASN:OD1	0.43	2.37	17	1
2:B:384:LEU:HD12	2:B:384:LEU:N	0.43	2.25	20	1
1:A:38:ASN:ND2	1:A:55:LEU:HD23	0.43	2.28	3	1
2:B:171:ILE:O	2:B:393:LEU:HD22	0.43	2.14	8	1
1:A:3:VAL:O	1:A:76:LEU:HD12	0.43	2.14	11	2
2:B:238:THR:O	2:B:241:ILE:HG13	0.43	2.13	17	2
2:B:395:VAL:HG12	2:B:396:ASP:OD1	0.43	2.13	13	1
2:B:212:LEU:C	2:B:212:LEU:HD12	0.43	2.34	18	1
1:A:73:GLU:HG2	1:A:74:GLU:H	0.43	1.74	19	1
2:B:293:GLU:OE2	2:B:356:GLN:CD	0.43	2.57	20	1
2:B:293:GLU:C	2:B:295:ALA:N	0.43	2.70	2	2
2:B:273:LYS:HG3	2:B:274:THR:H	0.43	1.74	4	1
1:A:15:MET:O	1:A:16:HIS:CB	0.43	2.67	9	1
1:A:6:THR:CG2	1:A:62:GLN:CD	0.43	2.87	9	1
2:B:256:ARG:NE	2:B:256:ARG:HA	0.43	2.29	9	1
2:B:305:LEU:O	2:B:309:LEU:HB2	0.43	2.14	9	1
2:B:248:LEU:HD12	2:B:253:ARG:HH22	0.43	1.72	11	1
2:B:172:ARG:CD	2:B:172:ARG:H	0.43	2.25	12	1
1:A:20:ALA:HB1	1:A:52:LEU:HD22	0.43	1.90	13	1
1:A:62:GLN:N	1:A:62:GLN:CD	0.43	2.69	14	1
2:B:184:GLU:N	2:B:184:GLU:CD	0.43	2.71	15	1
1:A:39:ASP:OD1	1:A:39:ASP:O	0.43	2.37	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:325:LEU:O	2:B:346:VAL:HG23	0.43	2.14	1	1
2:B:384:LEU:HD11	2:B:393:LEU:HD11	0.43	1.90	2	2
2:B:387:ASP:C	2:B:387:ASP:OD1	0.43	2.57	5	2
2:B:186:TRP:O	2:B:326:VAL:HG22	0.43	2.14	7	1
1:A:21:MET:SD	1:A:21:MET:C	0.43	2.97	9	1
2:B:349:ARG:NH1	2:B:375:GLN:OE1	0.43	2.51	11	2
1:A:35:LEU:CD2	1:A:37:ARG:HE	0.43	2.22	13	1
2:B:289:ASN:C	2:B:291:LEU:N	0.43	2.72	14	1
1:A:15:MET:C	1:A:17:ALA:H	0.43	2.10	15	1
2:B:219:ALA:HA	2:B:222:GLU:HG2	0.43	1.90	15	1
2:B:283:PHE:O	2:B:291:LEU:HD21	0.43	2.14	15	1
2:B:286:LEU:HB2	2:B:291:LEU:HD22	0.43	1.91	15	1
2:B:349:ARG:HE	2:B:373:ASP:C	0.43	2.17	15	1
2:B:349:ARG:HE	2:B:374:ILE:N	0.43	2.12	15	1
1:A:69:GLY:O	1:A:72:GLU:HG2	0.43	2.14	16	1
1:A:71:GLN:NE2	1:A:74:GLU:HG3	0.43	2.28	18	1
2:B:390:ARG:O	2:B:390:ARG:HG3	0.43	2.14	20	1
2:B:272:VAL:HG13	2:B:273:LYS:N	0.42	2.29	1	1
1:A:80:ILE:C	1:A:80:ILE:CD1	0.42	2.84	3	1
1:A:22:LYS:O	1:A:26:LEU:HD23	0.42	2.14	4	1
2:B:347:VAL:HG22	2:B:347:VAL:O	0.42	2.13	6	1
2:B:293:GLU:O	2:B:296:GLY:N	0.42	2.51	8	1
1:A:35:LEU:HD21	1:A:37:ARG:CZ	0.42	2.42	13	1
2:B:249:LEU:CG	2:B:250:SER:N	0.42	2.81	15	1
1:A:56:ASP:OD2	2:B:291:LEU:CG	0.42	2.67	17	1
2:B:324:ILE:CD1	2:B:326:VAL:HG13	0.42	2.44	17	1
1:A:12:LYS:C	1:A:14:GLY:N	0.42	2.73	18	1
2:B:238:THR:OG1	2:B:360:MET:SD	0.42	2.70	2	1
1:A:8:GLU:O	1:A:83:PHE:CE1	0.42	2.72	3	1
2:B:293:GLU:O	2:B:294:ARG:C	0.42	2.58	17	2
2:B:288:ASP:OD1	2:B:291:LEU:N	0.42	2.47	4	1
1:A:26:LEU:HB3	1:A:30:PHE:CE2	0.42	2.49	9	2
2:B:348:VAL:CG2	2:B:350:ASP:O	0.42	2.68	8	1
2:B:355:SER:OG	2:B:358:ALA:HB2	0.42	2.14	10	2
2:B:245:TYR:CZ	2:B:294:ARG:NE	0.42	2.86	12	1
1:A:35:LEU:HD12	1:A:36:LEU:N	0.42	2.29	13	1
2:B:239:ALA:O	2:B:243:ASP:CG	0.42	2.58	14	1
2:B:176:ALA:O	2:B:362:ARG:HD3	0.42	2.14	18	1
2:B:385:ILE:O	2:B:385:ILE:HG23	0.42	2.13	18	1
1:A:23:LEU:HD13	1:A:79:VAL:HG23	0.42	1.91	7	1
2:B:288:ASP:HB3	2:B:291:LEU:CG	0.42	2.44	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:245:TYR:CE2	2:B:294:ARG:NH2	0.42	2.87	9	1
2:B:283:PHE:HB3	2:B:295:ALA:HB2	0.42	1.91	12	1
1:A:56:ASP:OD2	2:B:288:ASP:OD2	0.42	2.36	16	1
2:B:209:ARG:O	2:B:212:LEU:HG	0.42	2.15	18	1
1:A:45:GLU:CD	1:A:47:ASN:HD21	0.42	2.17	2	1
2:B:258:LEU:CD1	2:B:272:VAL:HG12	0.42	2.45	2	1
1:A:5:GLN:HE22	1:A:80:ILE:HB	0.42	1.75	15	2
2:B:289:ASN:OD1	2:B:290:TYR:N	0.42	2.42	12	1
2:B:348:VAL:HG22	2:B:370:MET:SD	0.42	2.54	13	1
1:A:27:MET:HE1	1:A:34:VAL:N	0.42	2.28	15	1
2:B:374:ILE:O	2:B:374:ILE:CG2	0.42	2.66	15	1
1:A:13:LEU:C	1:A:13:LEU:CD1	0.42	2.87	17	1
2:B:290:TYR:OH	2:B:294:ARG:CZ	0.42	2.66	18	1
2:B:267:VAL:O	2:B:268:ALA:C	0.42	2.57	20	1
2:B:281:GLU:HG2	2:B:282:GLN:N	0.42	2.29	20	1
1:A:47:ASN:C	1:A:47:ASN:OD1	0.42	2.57	3	2
2:B:227:SER:O	2:B:228:LYS:C	0.42	2.57	3	1
1:A:23:LEU:CD1	1:A:79:VAL:HG22	0.42	2.35	5	1
2:B:171:ILE:HD12	2:B:171:ILE:N	0.42	2.29	10	1
2:B:237:GLU:O	2:B:241:ILE:N	0.42	2.45	10	1
2:B:286:LEU:HD11	2:B:288:ASP:HB3	0.42	1.92	11	1
1:A:71:GLN:C	1:A:74:GLU:HG3	0.42	2.31	12	1
2:B:268:ALA:O	2:B:272:VAL:HG13	0.42	2.13	12	1
2:B:299:ARG:HH11	2:B:303:GLN:N	0.42	2.13	12	1
2:B:343:LEU:C	2:B:343:LEU:HD23	0.42	2.35	13	1
1:A:20:ALA:CB	1:A:52:LEU:CD1	0.42	2.98	14	1
1:A:84:ASN:O	1:A:85:SER:OG	0.42	2.37	14	1
2:B:268:ALA:O	2:B:272:VAL:HG23	0.42	2.14	18	1
2:B:395:VAL:C	2:B:397:PRO:N	0.42	2.71	3	1
2:B:208:GLU:O	2:B:212:LEU:HB2	0.42	2.15	8	1
1:A:43:GLU:OE1	1:A:45:GLU:OE1	0.42	2.37	10	1
2:B:300:ALA:HB3	2:B:333:THR:HG21	0.42	1.90	10	1
2:B:216:LEU:HD11	2:B:249:LEU:O	0.42	2.13	12	1
2:B:186:TRP:CB	2:B:323:PHE:CD1	0.42	3.03	12	1
2:B:295:ALA:O	2:B:298:LEU:HB2	0.42	2.15	13	1
2:B:283:PHE:CZ	2:B:298:LEU:HD12	0.42	2.49	15	1
1:A:11:ASN:O	1:A:11:ASN:CG	0.42	2.57	16	1
2:B:279:PHE:CD2	2:B:283:PHE:CZ	0.42	3.07	16	1
1:A:6:THR:O	1:A:6:THR:HG23	0.42	2.14	1	2
2:B:209:ARG:NE	2:B:209:ARG:O	0.42	2.53	4	1
2:B:210:GLU:O	2:B:210:GLU:OE1	0.42	2.38	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:253:ARG:CD	2:B:253:ARG:C	0.42	2.88	5	1
2:B:251:ASP:CG	2:B:253:ARG:CB	0.42	2.88	6	1
2:B:213:THR:HG22	2:B:214:GLY:N	0.42	2.30	9	1
1:A:53:LEU:HD13	2:B:291:LEU:HD23	0.42	1.92	12	1
2:B:348:VAL:HG23	2:B:349:ARG:N	0.42	2.30	12	1
2:B:353:ALA:O	2:B:355:SER:N	0.42	2.53	12	1
2:B:211:ARG:HH22	2:B:269:GLU:CD	0.42	2.18	13	1
1:A:26:LEU:O	1:A:30:PHE:CG	0.42	2.72	14	1
1:A:24:PHE:CD1	2:B:247:HIS:CE1	0.42	3.08	19	1
2:B:258:LEU:HD13	2:B:259:PHE:N	0.42	2.30	5	1
2:B:203:LEU:HD12	2:B:204:ASP:H	0.42	1.74	6	1
2:B:235:GLN:CD	2:B:238:THR:OG1	0.42	2.58	6	1
2:B:208:GLU:HG2	2:B:262:VAL:HG21	0.42	1.90	12	1
2:B:326:VAL:O	2:B:376:PRO:HB3	0.42	2.14	13	1
2:B:335:LEU:CD2	2:B:335:LEU:C	0.42	2.85	17	1
2:B:228:LYS:HD2	2:B:228:LYS:H	0.42	1.73	20	1
1:A:30:PHE:CG	1:A:71:GLN:CD	0.42	2.93	3	1
2:B:330:LEU:HD11	2:B:346:VAL:HG11	0.42	1.90	6	1
2:B:350:ASP:OD2	2:B:351:GLY:N	0.42	2.52	8	1
2:B:242:PHE:CE2	2:B:336:ALA:HB2	0.42	2.50	11	1
2:B:353:ALA:O	2:B:354:ASN:C	0.42	2.58	12	1
1:A:76:LEU:CD2	1:A:76:LEU:C	0.42	2.89	14	1
2:B:269:GLU:OE1	2:B:269:GLU:CA	0.42	2.64	16	1
2:B:281:GLU:O	2:B:285:ALA:CB	0.42	2.67	16	1
2:B:225:ARG:C	2:B:229:ARG:NH2	0.42	2.74	18	1
2:B:279:PHE:CZ	2:B:298:LEU:CB	0.42	3.03	20	1
2:B:248:LEU:CD1	2:B:253:ARG:HH22	0.42	2.27	11	2
2:B:342:ARG:O	2:B:342:ARG:HG2	0.42	2.11	12	2
1:A:53:LEU:CD1	1:A:53:LEU:N	0.42	2.83	5	1
1:A:17:ALA:O	1:A:21:MET:CB	0.42	2.68	7	1
2:B:392:GLU:CA	2:B:392:GLU:OE1	0.42	2.62	8	1
1:A:16:HIS:CD2	2:B:290:TYR:CE2	0.42	3.08	9	1
2:B:209:ARG:NE	2:B:255:ARG:NH1	0.42	2.68	14	1
2:B:228:LYS:HD2	2:B:228:LYS:N	0.42	2.30	20	1
2:B:248:LEU:HD13	2:B:248:LEU:O	0.41	2.14	3	1
2:B:287:SER:O	2:B:289:ASN:N	0.41	2.54	3	1
2:B:378:VAL:HG12	2:B:378:VAL:O	0.41	2.15	4	1
2:B:282:GLN:HB3	2:B:283:PHE:CE2	0.41	2.50	8	1
2:B:392:GLU:O	2:B:392:GLU:CD	0.41	2.59	8	1
1:A:53:LEU:CD2	1:A:53:LEU:N	0.41	2.83	10	1
2:B:326:VAL:CG1	2:B:376:PRO:HG3	0.41	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:288:ASP:HB3	2:B:291:LEU:CD1	0.41	2.44	14	1
2:B:355:SER:O	2:B:356:GLN:C	0.41	2.58	15	1
1:A:38:ASN:ND2	1:A:63:ILE:CG2	0.41	2.83	20	1
1:A:40:GLU:HG2	1:A:40:GLU:O	0.41	2.15	4	1
1:A:49:VAL:CG1	2:B:248:LEU:HD21	0.41	2.45	11	1
2:B:291:LEU:C	2:B:293:GLU:OE1	0.41	2.58	14	1
1:A:49:VAL:HG21	2:B:248:LEU:HD11	0.41	1.90	15	1
2:B:217:GLU:OE2	2:B:221:ASN:ND2	0.41	2.53	17	1
2:B:348:VAL:HG22	2:B:350:ASP:H	0.41	1.75	18	1
2:B:335:LEU:HD13	2:B:335:LEU:O	0.41	2.15	2	1
1:A:53:LEU:CG	1:A:54:MET:N	0.41	2.83	4	2
2:B:245:TYR:O	2:B:248:LEU:CB	0.41	2.68	7	1
2:B:217:GLU:O	2:B:221:ASN:CB	0.41	2.69	10	2
2:B:170:ARG:N	2:B:394:LEU:HD23	0.41	2.30	11	1
2:B:243:ASP:OD1	2:B:243:ASP:C	0.41	2.58	13	1
1:A:32:ALA:CB	1:A:69:GLY:HA3	0.41	2.45	15	1
2:B:238:THR:CG2	2:B:360:MET:SD	0.41	3.08	16	1
2:B:288:ASP:OD1	2:B:292:LYS:HB2	0.41	2.15	17	1
2:B:293:GLU:OE2	2:B:356:GLN:NE2	0.41	2.54	20	1
1:A:28:GLN:NE2	1:A:28:GLN:N	0.41	2.64	1	1
1:A:5:GLN:OE1	1:A:6:THR:O	0.41	2.38	2	1
2:B:204:ASP:OD2	2:B:207:LEU:HD12	0.41	2.15	3	1
1:A:39:ASP:OD2	1:A:62:GLN:OE1	0.41	2.38	6	1
2:B:342:ARG:NE	2:B:342:ARG:HA	0.41	2.29	6	1
2:B:345:GLY:O	2:B:346:VAL:CG2	0.41	2.68	10	1
1:A:83:PHE:N	1:A:83:PHE:CD1	0.41	2.88	14	2
2:B:299:ARG:O	2:B:299:ARG:NE	0.41	2.54	12	1
2:B:350:ASP:C	2:B:350:ASP:OD1	0.41	2.58	12	1
1:A:3:VAL:HB	1:A:72:GLU:OE1	0.41	2.16	13	1
2:B:211:ARG:NE	2:B:309:LEU:HD12	0.41	2.28	14	1
2:B:325:LEU:HD22	2:B:335:LEU:HD21	0.41	1.92	16	1
2:B:290:TYR:O	2:B:293:GLU:HG2	0.41	2.15	18	1
1:A:15:MET:CG	1:A:16:HIS:H	0.41	2.27	20	1
2:B:291:LEU:O	2:B:294:ARG:CG	0.41	2.68	1	2
2:B:208:GLU:HB3	2:B:262:VAL:HG11	0.41	1.93	2	1
1:A:71:GLN:CG	1:A:74:GLU:HB3	0.41	2.44	3	1
1:A:80:ILE:CD1	1:A:81:ALA:N	0.41	2.84	3	1
2:B:209:ARG:HG2	2:B:259:PHE:CD1	0.41	2.49	4	1
2:B:278:LYS:CB	2:B:278:LYS:NZ	0.41	2.83	4	1
1:A:64:GLU:N	1:A:64:GLU:OE1	0.41	2.53	7	1
2:B:223:PHE:CD2	2:B:242:PHE:CE2	0.41	3.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:387:ASP:OD1	2:B:387:ASP:C	0.41	2.58	11	2
2:B:255:ARG:HG2	2:B:259:PHE:CE2	0.41	2.51	11	1
2:B:276:ILE:HG23	2:B:277:GLU:N	0.41	2.31	11	1
1:A:49:VAL:O	1:A:53:LEU:CG	0.41	2.67	12	1
2:B:279:PHE:O	2:B:283:PHE:CG	0.41	2.73	16	1
1:A:16:HIS:ND1	2:B:290:TYR:CZ	0.41	2.89	17	1
2:B:288:ASP:OD1	2:B:290:TYR:N	0.41	2.54	19	1
1:A:9:ILE:HG12	1:A:63:ILE:CD1	0.41	2.35	20	1
1:A:53:LEU:HD12	1:A:53:LEU:N	0.41	2.30	5	1
1:A:13:LEU:O	1:A:83:PHE:CG	0.41	2.73	6	2
1:A:16:HIS:ND1	1:A:17:ALA:HB2	0.41	2.31	7	1
2:B:276:ILE:CG1	2:B:277:GLU:N	0.41	2.83	8	2
1:A:70:PRO:HG2	1:A:71:GLN:NE2	0.41	2.31	11	1
2:B:295:ALA:O	2:B:298:LEU:N	0.41	2.51	13	1
2:B:344:VAL:CG1	2:B:344:VAL:O	0.41	2.69	13	1
2:B:185:GLY:O	2:B:381:ARG:HA	0.41	2.15	13	1
2:B:258:LEU:HD23	2:B:275:VAL:CG2	0.41	2.44	15	1
2:B:354:ASN:O	2:B:355:SER:C	0.41	2.55	15	1
2:B:346:VAL:CG2	2:B:347:VAL:N	0.41	2.83	3	1
2:B:328:ASP:O	2:B:351:GLY:N	0.41	2.50	5	1
2:B:324:ILE:HG22	2:B:345:GLY:HA3	0.41	1.92	6	1
1:A:14:GLY:C	1:A:16:HIS:H	0.41	2.19	9	1
2:B:209:ARG:NE	2:B:255:ARG:HH12	0.41	2.14	14	1
2:B:297:ASP:CG	2:B:356:GLN:HE22	0.41	2.19	14	1
1:A:5:GLN:O	1:A:5:GLN:HG2	0.41	2.14	15	1
2:B:222:GLU:HG3	2:B:223:PHE:N	0.41	2.29	15	1
1:A:73:GLU:HG3	1:A:74:GLU:N	0.41	2.30	9	1
1:A:53:LEU:HD21	2:B:286:LEU:HG	0.41	1.91	13	1
2:B:347:VAL:HG13	2:B:347:VAL:O	0.41	2.15	14	1
2:B:222:GLU:OE2	2:B:223:PHE:CA	0.41	2.68	15	1
1:A:17:ALA:CB	1:A:18:ARG:NH1	0.41	2.73	17	1
2:B:341:ASP:OD1	2:B:342:ARG:HG2	0.41	2.16	1	1
2:B:254:LEU:O	2:B:254:LEU:HD13	0.41	2.15	2	1
2:B:294:ARG:NH1	2:B:297:ASP:CG	0.41	2.72	2	1
1:A:38:ASN:HD21	1:A:58:ALA:CB	0.41	2.25	3	1
1:A:38:ASN:ND2	1:A:58:ALA:HB2	0.41	2.27	3	1
1:A:36:LEU:CD1	1:A:65:VAL:HG13	0.41	2.46	3	1
1:A:30:PHE:CG	1:A:71:GLN:NE2	0.41	2.87	3	1
2:B:388:GLY:O	2:B:389:TYR:C	0.41	2.59	3	1
1:A:77:ALA:CA	1:A:80:ILE:CG1	0.41	2.97	4	1
2:B:203:LEU:HD13	2:B:262:VAL:O	0.41	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:O	1:A:24:PHE:CE2	0.41	2.74	7	1
2:B:226:TYR:CD1	2:B:229:ARG:NH1	0.41	2.89	15	2
1:A:79:VAL:O	1:A:83:PHE:CG	0.41	2.74	8	1
1:A:45:GLU:HB3	1:A:47:ASN:HD22	0.41	1.76	10	1
2:B:389:TYR:CG	2:B:390:ARG:N	0.41	2.86	12	1
2:B:235:GLN:OE1	2:B:235:GLN:O	0.41	2.37	13	1
1:A:37:ARG:O	1:A:64:GLU:OE1	0.41	2.38	16	1
2:B:245:TYR:OH	2:B:301:LEU:CB	0.41	2.69	16	1
1:A:76:LEU:O	1:A:76:LEU:HD23	0.41	2.15	17	1
2:B:216:LEU:HD12	2:B:249:LEU:CD1	0.41	2.46	17	1
2:B:330:LEU:H	2:B:330:LEU:HD12	0.41	1.76	19	1
1:A:15:MET:CG	1:A:16:HIS:N	0.41	2.72	20	1
2:B:245:TYR:OH	2:B:294:ARG:NE	0.41	2.54	20	1
2:B:310:ASP:O	2:B:311:ASP:C	0.41	2.59	5	1
2:B:387:ASP:OD2	2:B:390:ARG:CZ	0.41	2.69	6	1
2:B:209:ARG:HD2	2:B:259:PHE:CE2	0.41	2.51	7	1
1:A:66:GLU:OE1	1:A:66:GLU:N	0.41	2.54	8	1
2:B:211:ARG:HH21	2:B:211:ARG:HB3	0.41	1.75	9	1
2:B:348:VAL:O	2:B:370:MET:HA	0.41	2.16	9	1
2:B:252:THR:OG1	2:B:252:THR:O	0.41	2.38	11	1
2:B:384:LEU:HD22	2:B:394:LEU:O	0.41	2.16	14	1
2:B:237:GLU:HG2	2:B:238:THR:H	0.41	1.76	17	1
2:B:273:LYS:O	2:B:277:GLU:OE1	0.41	2.39	19	1
2:B:208:GLU:OE2	2:B:267:VAL:HG12	0.40	2.16	3	1
2:B:270:TRP:CE3	2:B:270:TRP:O	0.40	2.74	5	1
1:A:38:ASN:ND2	1:A:41:GLY:H	0.40	2.10	8	1
1:A:64:GLU:CD	1:A:64:GLU:C	0.40	2.79	10	1
2:B:235:GLN:HE21	2:B:238:THR:HG23	0.40	1.76	10	1
2:B:326:VAL:HG11	2:B:379:LEU:HD12	0.40	1.94	12	1
2:B:330:LEU:HG	2:B:330:LEU:O	0.40	2.15	14	1
1:A:27:MET:HE1	1:A:34:VAL:HG23	0.40	1.91	15	1
2:B:252:THR:O	2:B:256:ARG:HB2	0.40	2.16	15	1
2:B:216:LEU:HD11	2:B:255:ARG:NE	0.40	2.32	16	1
2:B:332:ALA:H	2:B:357:ALA:HB2	0.40	1.75	18	1
1:A:15:MET:HE2	1:A:15:MET:N	0.40	2.31	20	1
1:A:7:VAL:O	1:A:7:VAL:HG13	0.40	2.15	20	1
2:B:384:LEU:C	2:B:385:ILE:HD12	0.40	2.36	2	1
1:A:53:LEU:CD1	2:B:291:LEU:HD13	0.40	2.39	7	1
2:B:180:VAL:HG12	2:B:181:ALA:N	0.40	2.31	8	1
2:B:393:LEU:N	2:B:393:LEU:CD1	0.40	2.75	8	1
2:B:204:ASP:OD1	2:B:208:GLU:CG	0.40	2.69	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:282:GLN:HG2	2:B:283:PHE:N	0.40	2.30	11	1
2:B:174:LEU:HD12	2:B:174:LEU:H	0.40	1.71	12	1
2:B:290:TYR:C	2:B:293:GLU:OE1	0.40	2.59	14	1
1:A:53:LEU:HD13	1:A:53:LEU:H	0.40	1.76	15	1
2:B:202:THR:O	2:B:267:VAL:HG22	0.40	2.17	17	1
2:B:244:LEU:HD23	2:B:294:ARG:NH1	0.40	2.31	18	1
1:A:16:HIS:ND1	2:B:291:LEU:HD11	0.40	2.31	2	1
2:B:326:VAL:CG1	2:B:347:VAL:HG13	0.40	2.46	2	1
1:A:38:ASN:ND2	1:A:55:LEU:HD12	0.40	2.32	4	1
1:A:13:LEU:O	1:A:13:LEU:HG	0.40	2.17	5	1
2:B:235:GLN:OE1	2:B:235:GLN:N	0.40	2.54	5	1
1:A:38:ASN:ND2	1:A:40:GLU:CA	0.40	2.84	8	1
1:A:61:ARG:C	1:A:62:GLN:NE2	0.40	2.74	11	1
2:B:292:LYS:NZ	2:B:292:LYS:HB2	0.40	2.31	11	1
2:B:352:ALA:HB3	2:B:355:SER:HB3	0.40	1.93	14	1
2:B:241:ILE:CG1	2:B:242:PHE:N	0.40	2.84	15	1
1:A:41:GLY:O	1:A:43:GLU:OE2	0.40	2.40	1	1
1:A:49:VAL:O	1:A:53:LEU:CD1	0.40	2.69	3	1
2:B:382:ARG:HH12	2:B:396:ASP:HB3	0.40	1.75	6	1
2:B:356:GLN:CG	2:B:357:ALA:N	0.40	2.84	9	1
2:B:270:TRP:O	2:B:274:THR:N	0.40	2.37	12	1
2:B:245:TYR:CD2	2:B:294:ARG:NH1	0.40	2.89	12	1
2:B:221:ASN:O	2:B:225:ARG:HG3	0.40	2.16	14	1
2:B:289:ASN:O	2:B:290:TYR:C	0.40	2.60	14	1
2:B:385:ILE:HG13	2:B:385:ILE:O	0.40	2.16	14	1
2:B:207:LEU:O	2:B:211:ARG:HG3	0.40	2.17	15	1
2:B:279:PHE:CE2	2:B:282:GLN:OE1	0.40	2.74	17	1
2:B:251:ASP:OD2	2:B:253:ARG:NH1	0.40	2.54	19	1
2:B:248:LEU:HD23	2:B:249:LEU:HD23	0.40	1.93	20	1
2:B:326:VAL:CG1	2:B:326:VAL:O	0.40	2.66	1	1
1:A:45:GLU:CD	1:A:47:ASN:OD1	0.40	2.60	2	1
1:A:5:GLN:NE2	1:A:76:LEU:HG	0.40	2.32	7	1
2:B:350:ASP:OD1	2:B:350:ASP:C	0.40	2.60	7	1
1:A:43:GLU:CD	1:A:43:GLU:O	0.40	2.59	8	1
2:B:283:PHE:CE2	2:B:294:ARG:NH1	0.40	2.89	11	1
2:B:395:VAL:HG12	2:B:396:ASP:CG	0.40	2.37	13	1
2:B:358:ALA:O	2:B:361:VAL:CG2	0.40	2.70	15	1
2:B:358:ALA:HB1	2:B:362:ARG:NH1	0.40	2.31	15	1
2:B:378:VAL:CG1	2:B:378:VAL:O	0.40	2.69	15	1
2:B:212:LEU:HD21	2:B:272:VAL:CG2	0.40	2.47	20	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	83/85 (98%)	73±1 (88±1%)	8±1 (9±1%)	2±1 (3±1%)	7	41
2	B	203/256 (79%)	181±4 (89±2%)	17±4 (8±2%)	5±2 (2±1%)	9	46
All	All	5720/6820 (84%)	5078 (89%)	496 (9%)	146 (3%)	8	44

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	380	HIS	18
1	A	32	ALA	18
2	B	234	ALA	13
2	B	351	GLY	12
1	A	17	ALA	11
1	A	16	HIS	9
2	B	311	ASP	9
2	B	353	ALA	5
1	A	18	ARG	5
1	A	15	MET	5
2	B	252	THR	5
2	B	288	ASP	4
2	B	285	ALA	4
2	B	396	ASP	4
2	B	352	ALA	4
2	B	336	ALA	3
2	B	397	PRO	3
2	B	350	ASP	2
2	B	355	SER	2
2	B	233	GLY	2
2	B	294	ARG	2
2	B	284	ALA	1
2	B	309	LEU	1
2	B	290	TYR	1
2	B	231	ALA	1
2	B	292	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	237	GLU	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	68/68 (100%)	54±3 (79±4%)	14±3 (21±4%)	3	32
2	B	160/205 (78%)	127±4 (79±3%)	33±4 (21±3%)	3	32
All	All	4560/5460 (84%)	3610 (79%)	950 (21%)	3	32

All 195 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)
2	B	203	LEU	13
2	B	291	LEU	13
1	A	48	SER	12
1	A	80	ILE	12
2	B	303	GLN	12
2	B	309	LEU	12
1	A	13	LEU	11
2	B	288	ASP	11
2	B	226	TYR	11
2	B	342	ARG	11
1	A	61	ARG	11
2	B	292	LYS	10
2	B	235	GLN	10
1	A	18	ARG	10
2	B	247	HIS	10
2	B	301	LEU	9
2	B	170	ARG	9
1	A	76	LEU	9
1	A	53	LEU	9
1	A	1	MET	9
2	B	298	LEU	9
2	B	338	LEU	9
2	B	389	TYR	8

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Mol	Chain	Res	Type	Models (Total)
2	B	305	LEU	8
1	A	63	ILE	8
1	A	4	LYS	8
1	A	43	GLU	8
2	B	269	GLU	8
1	A	12	LYS	8
1	A	21	MET	8
2	B	223	PHE	8
2	B	370	MET	8
2	B	369	VAL	8
2	B	306	LEU	8
2	B	228	LYS	7
2	B	323	PHE	7
2	B	253	ARG	7
2	B	202	THR	7
2	B	211	ARG	7
1	A	24	PHE	7
2	B	392	GLU	7
2	B	335	LEU	7
2	B	390	ARG	7
2	B	310	ASP	7
2	B	245	TYR	7
2	B	242	PHE	7
2	B	248	LEU	7
1	A	15	MET	7
2	B	325	LEU	7
2	B	283	PHE	7
2	B	187	GLN	6
2	B	330	LEU	6
2	B	222	GLU	6
2	B	216	LEU	6
2	B	382	ARG	6
2	B	396	ASP	6
1	A	47	ASN	6
2	B	204	ASP	6
2	B	263	ASP	6
2	B	172	ARG	6
2	B	381	ARG	6
2	B	270	TRP	6
1	A	52	LEU	6
2	B	384	LEU	6
2	B	212	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	85	SER	6
1	A	10	THR	6
2	B	254	LEU	6
2	B	209	ARG	6
2	B	217	GLU	6
2	B	293	GLU	6
2	B	355	SER	6
2	B	227	SER	5
2	B	304	ARG	5
1	A	16	HIS	5
2	B	281	GLU	5
2	B	279	PHE	5
1	A	62	GLN	5
2	B	289	ASN	5
2	B	375	GLN	5
1	A	38	ASN	5
2	B	249	LEU	5
1	A	50	ILE	5
2	B	264	LYS	5
2	B	380	HIS	5
1	A	23	LEU	5
1	A	6	THR	5
2	B	329	GLU	5
2	B	255	ARG	5
2	B	236	LYS	5
2	B	238	THR	5
2	B	278	LYS	5
2	B	230	PHE	5
1	A	83	PHE	5
2	B	229	ARG	5
2	B	256	ARG	5
2	B	322	ARG	5
2	B	346	VAL	5
2	B	252	THR	5
2	B	294	ARG	5
2	B	348	VAL	4
2	B	361	VAL	4
1	A	79	VAL	4
2	B	299	ARG	4
2	B	244	LEU	4
1	A	31	ASP	4
2	B	307	PHE	4

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Mol	Chain	Res	Type	Models (Total)
2	B	207	LEU	4
1	A	39	ASP	4
2	B	350	ASP	4
2	B	393	LEU	4
1	A	25	GLU	4
2	B	286	LEU	4
2	B	373	ASP	4
2	B	277	GLU	4
2	B	356	GLN	4
1	A	59	LYS	4
1	A	7	VAL	4
1	A	73	GLU	4
2	B	364	LEU	4
2	B	273	LYS	4
1	A	37	ARG	3
1	A	65	VAL	3
1	A	66	GLU	3
1	A	11	ASN	3
2	B	326	VAL	3
2	B	258	LEU	3
2	B	347	VAL	3
2	B	374	ILE	3
1	A	27	MET	3
1	A	35	LEU	3
2	B	297	ASP	3
1	A	74	GLU	3
2	B	385	ILE	3
2	B	290	TYR	3
2	B	186	TRP	3
1	A	28	GLN	3
1	A	3	VAL	3
1	A	57	SER	3
2	B	241	ILE	3
2	B	208	GLU	3
2	B	341	ASP	3
1	A	54	MET	3
1	A	68	THR	3
2	B	251	ASP	3
1	A	64	GLU	3
1	A	56	ASP	2
2	B	344	VAL	2
2	B	383	THR	2

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Mol	Chain	Res	Type	Models (Total)
2	B	360	MET	2
2	B	259	PHE	2
1	A	33	GLU	2
2	B	225	ARG	2
2	B	218	GLU	2
2	B	395	VAL	2
1	A	42	THR	2
1	A	36	LEU	2
2	B	210	GLU	2
1	A	55	LEU	2
1	A	22	LYS	2
2	B	340	GLN	2
2	B	324	ILE	2
2	B	267	VAL	2
2	B	333	THR	2
2	B	182	ILE	2
1	A	2	THR	2
2	B	362	ARG	2
2	B	331	SER	2
1	A	5	GLN	2
2	B	343	LEU	2
2	B	246	SER	2
1	A	8	GLU	2
2	B	282	GLN	2
2	B	243	ASP	2
1	A	71	GLN	2
2	B	354	ASN	2
2	B	257	GLU	1
2	B	334	THR	1
2	B	386	VAL	1
2	B	328	ASP	1
2	B	184	GLU	1
1	A	40	GLU	1
2	B	276	ILE	1
1	A	49	VAL	1
1	A	72	GLU	1
2	B	311	ASP	1
1	A	82	LEU	1
2	B	337	GLU	1
2	B	287	SER	1
2	B	224	ARG	1
2	B	174	LEU	1

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Mol	Chain	Res	Type	Models (Total)
2	B	221	ASN	1
2	B	394	LEU	1
2	B	213	THR	1
2	B	261	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 34% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *EIN_NPr_Complex.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1194
Number of shifts mapped to atoms	1194
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	249	0.14 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	229	1.10 ± 0.10	Should be applied
$^{13}\text{C}'$	250	-0.23 ± 0.11	None needed (< 0.5 ppm)
^{15}N	232	0.69 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 27%, i.e. 962 atoms were assigned a chemical shift out of a possible 3521. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	778/1427 (55%)	188/569 (33%)	402/578 (70%)	188/280 (67%)
Sidechain	182/1911 (10%)	0/1106 (0%)	182/708 (26%)	0/97 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/183 (1%)	1/99 (1%)	0/78 (0%)	1/6 (17%)
Overall	962/3521 (27%)	189/1774 (11%)	584/1364 (43%)	189/383 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 29%, i.e. 1194 atoms were assigned a chemical shift out of a possible 4146. 0 out of 68 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	963/1674 (58%)	232/667 (35%)	499/680 (73%)	232/327 (71%)
Sidechain	229/2261 (10%)	0/1310 (0%)	229/840 (27%)	0/111 (0%)
Aromatic	2/211 (1%)	1/113 (1%)	0/91 (0%)	1/7 (14%)
Overall	1194/4146 (29%)	233/2090 (11%)	728/1611 (45%)	233/445 (52%)

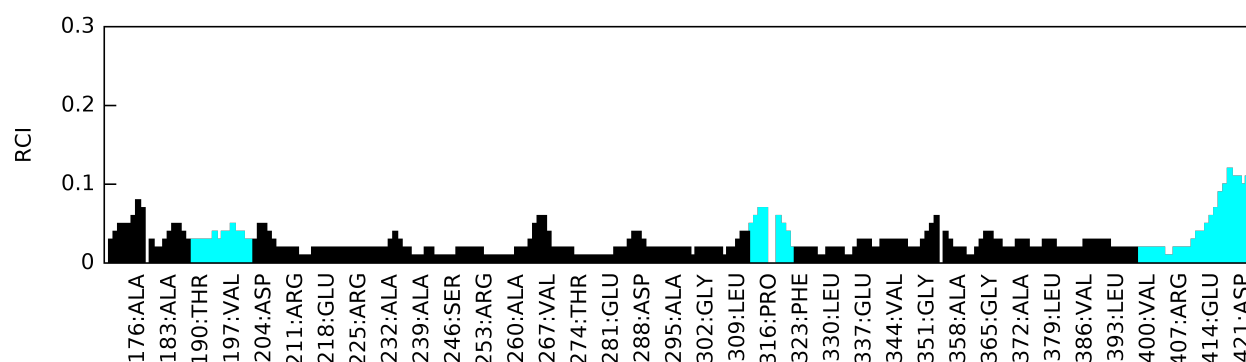
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:



7.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *NPr_EIN_Complex.str*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	197
Number of shifts mapped to atoms	197
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	51	0.65 ± 0.08	Should be applied
$^{13}\text{C}_\beta$	42	0.70 ± 0.15	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	52	0.16 ± 0.39	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 197 atoms were assigned a chemical shift out of a possible 3521. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	155/1427 (11%)	52/569 (9%)	51/578 (9%)	52/280 (19%)
Sidechain	42/1911 (2%)	0/1106 (0%)	42/708 (6%)	0/97 (0%)
Aromatic	0/183 (0%)	0/99 (0%)	0/78 (0%)	0/6 (0%)
Overall	197/3521 (6%)	52/1774 (3%)	93/1364 (7%)	52/383 (14%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 197 atoms were assigned a chemical shift out of a possible 4146. 0 out of 68 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	155/1674 (9%)	52/667 (8%)	51/680 (8%)	52/327 (16%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	42/2261 (2%)	0/1310 (0%)	42/840 (5%)	0/111 (0%)
Aromatic	0/211 (0%)	0/113 (0%)	0/91 (0%)	0/7 (0%)
Overall	197/4146 (5%)	52/2090 (2%)	93/1611 (6%)	52/445 (12%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

