WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Dec 12, 2016 – 03:43 PM EST

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

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

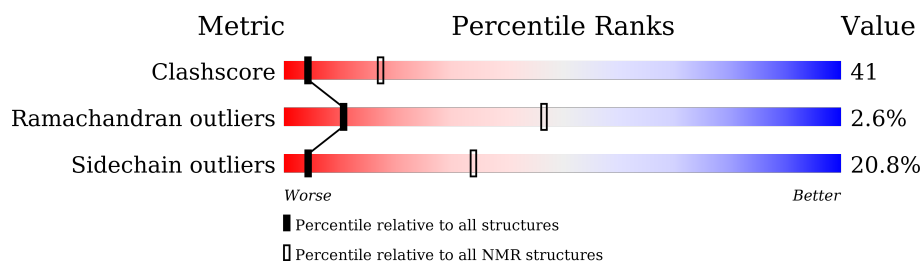|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20028442
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment 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	Percentile Ranks	Value
Clashscore		41
Ramachandran outliers		2.6%
Sidechain outliers		20.8%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	85	34% 64% •
2	B	256	30% 48% • 20%

2 Ensemble composition and analysis (i)

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.

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

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
			Total	C	H	N	O	S	
1	A	85	1298	402	653	108	130	5	0

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

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

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 (i)

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
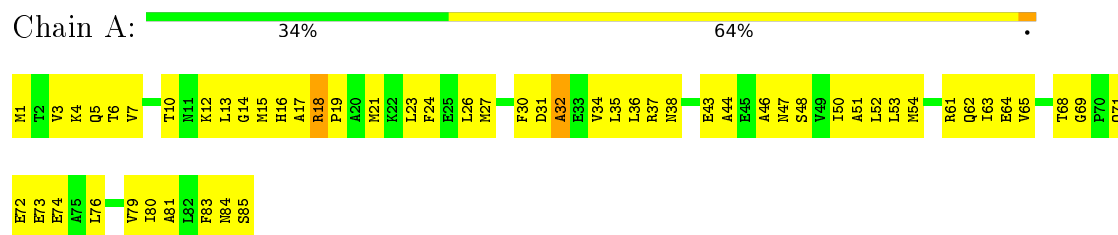
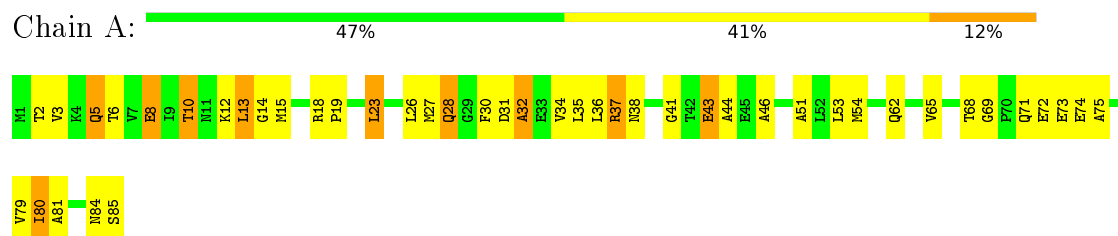• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
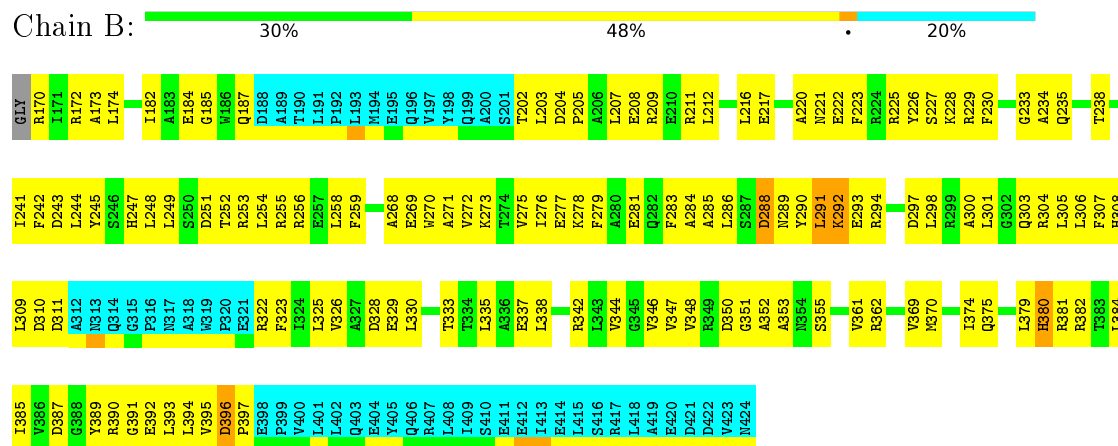
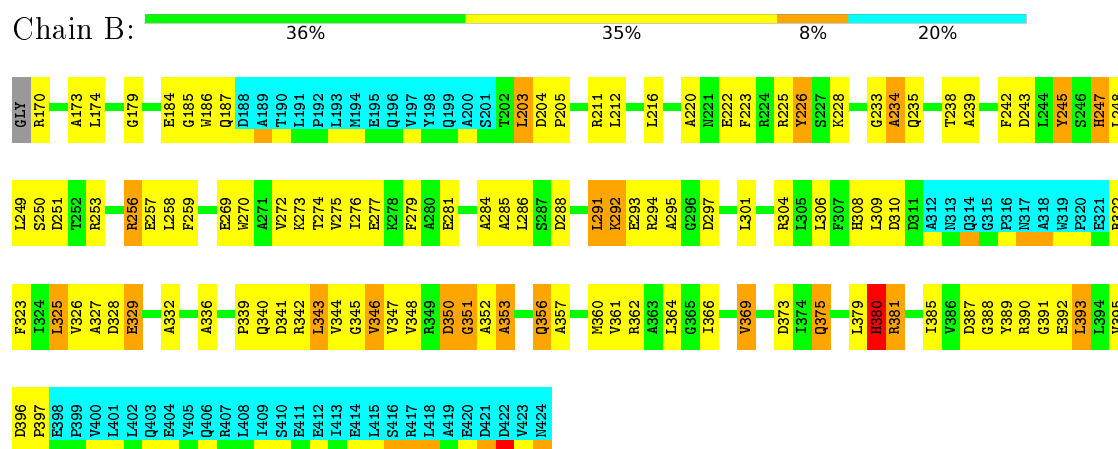## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

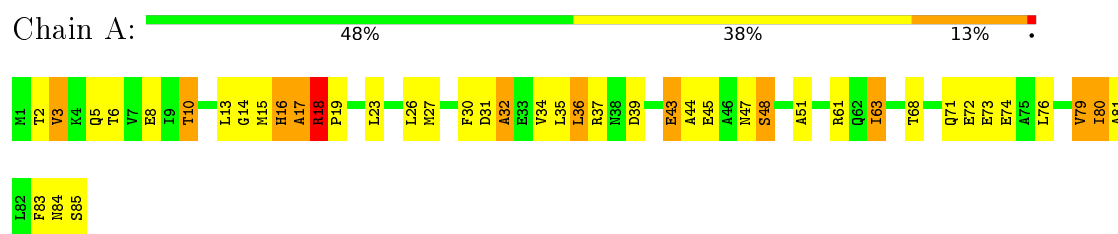• Molecule 1: Phosphocarrier protein NPr

Chain A: 47% 41% 12%

M1 T2 V3 K4 Q5 T6 V7 E8 I9 T10 N11 K12 L13 G14 M15 R18 P19 L23 L26 M27 Q28 G29 F30 D31 A32 E33 V34 L35 L36 R37 N38 G41 T42 E43 A44 E45 A46 A51 L52 L53 M54 Q62 V65 T68 G69 P70 Q71 E72 E73 E74 A75

V79 I80 A81 N84 S85

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 36% 35% 8% 20%

GLY R170 A173 L174 G179 E184 G185 W186 Q187 D188 A189 T190 L191 P192 L193 M194 E195 Q196 V197 Y198 Q199 A200 S201 T202 L203 D204 P205 R211 L212 L216 A220 N221 E222 F223 R224 R225 Y226 S227 K228 G233 A234 Q235 T238 A239 F242 D243 L244 Y245 S246 H247 L248

L249 S250 D251 T252 R253 R256 E257 L258 F259 E269 W270 A271 V272 K273 T274 V275 I276 E277 K278 F279 A280 E281 A284 A285 L286 S287 D288 L291 K292 E293 R294 A295 G296 D297 L301 R304 L305 L306 F307 H308 L309 D310 D311 A312 A318 W319 F320 E321 R322

F323 I324 L325 V326 A327 D328 E329 A332 A336 P339 Q340 D341 R342 L343 V344 G345 V346 V347 V348 R349 D350 G351 A352 A353 Q356 A357 M360 V361 R362 A363 L364 G365 I366 V369 D373 I374 Q375 L379 H380 R381 I385 V386 D387 G388 Y389 R390 G391 E392 L393 L394 V395

D396 F397 E398 P399 V400 L401 L402 Q403 E404 Y405 Q406 R407 L408 I409 S410 E411 F412 I413 E414 L415 S416 R417 L418 A419 E420 D421 D422 V423 N424

4.2.2 Score per residue for model 2

• Molecule 1: Phosphocarrier protein NPr

Chain A: 48% 38% 13% •

M1 T2 V3 K4 Q5 T6 V7 E8 I9 T10 L13 G14 M15 H16 A17 R18 P19 L23 L26 M27 F30 D31 A32 V34 L35 L36 R37 N38 D39 E43 A44 E45 A46 N47 S48 A51 R61 Q62 I63 T68 Q71 E72 E73 E74 A75 L76 V79 I80 A81

L82 F83 N84 S85

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 37% 31% 11% 20%

GLY R170 I171 R172 A173 L174 I182 G185 W186 Q187 D188 A189 T190 L191 P192 L193 M194 E195 Q196 V197 Y198 Q199 A200 S201 T202 L203 D204 P205 A206 L207 E208 L212 L216 E217 E218 A219 A220 N221 E222 Y226 S227 F230 G233 A234 Q235 E236 E237 T238 F242 D243 L248

L249 S250 D251 T252 R253 L254 R255 L258 F259 V262 D263 K264 A268 E269 W270 A271 V272 K273 T274 V275 I276 E277 K278 E281 Q282 F283 L286 S287 D288 N289 L291 K292 E293 R294 A295 G296 D297 L301 G302 Q303 R304 H308 D310 D311 A312 N313 Q314 G315 P316 N317 A318

W319 F320 E321 R322 F323 I324 L325 V326 A327 D328 E329 L330 S331 A332 T333 T334 L335 A336 E337 R342 L343 V346 V347 V348 R349 D350 G351 A352 A353 N354 S355 Q356 M360 V361 R362 V369 M370 Q375 V378 L379 H380 R381 T383 L384 I385 V386 D387 R390 G391 E392 L393 L394
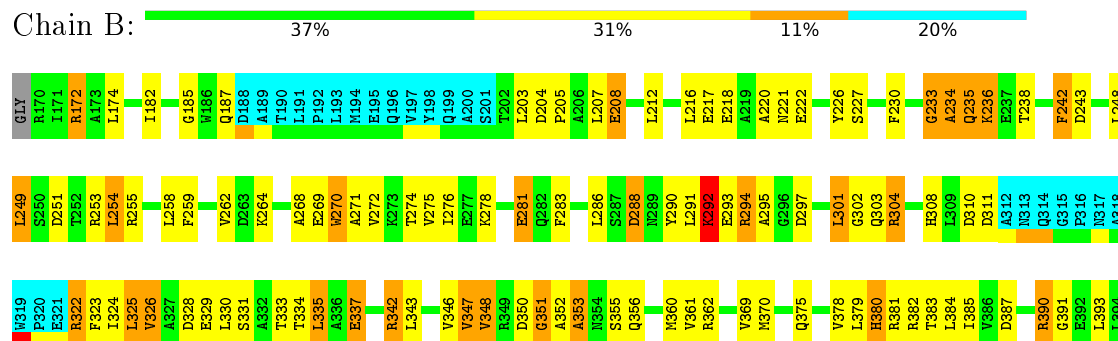
4.2.3 Score per residue for model 3

• Molecule 1: Phosphocarrier protein NPr

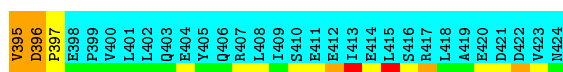• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

4.2.4 Score per residue for model 4

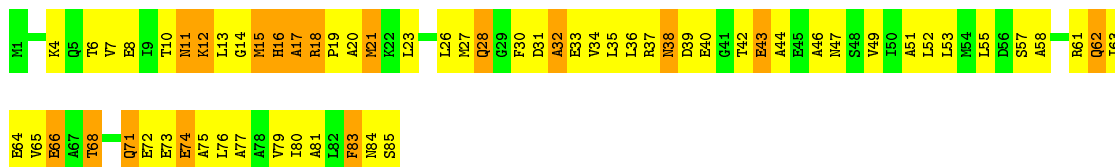• Molecule 1: Phosphocarrier protein NPr

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

4.2.5 Score per residue for model 5

- Molecule 1: Phosphocarrier protein NPr

Chain A: 46% 44% 11%

- Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 39% 34% 7% 20%
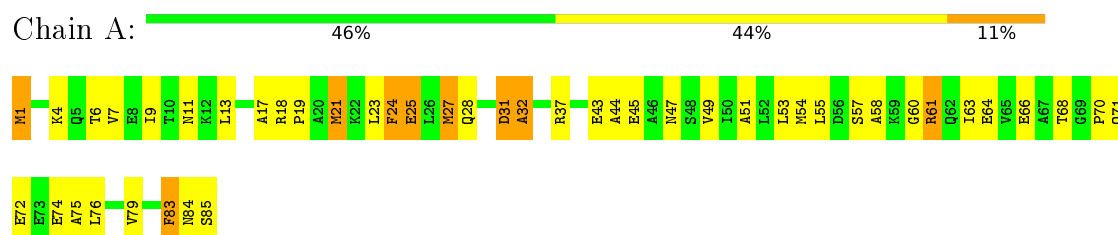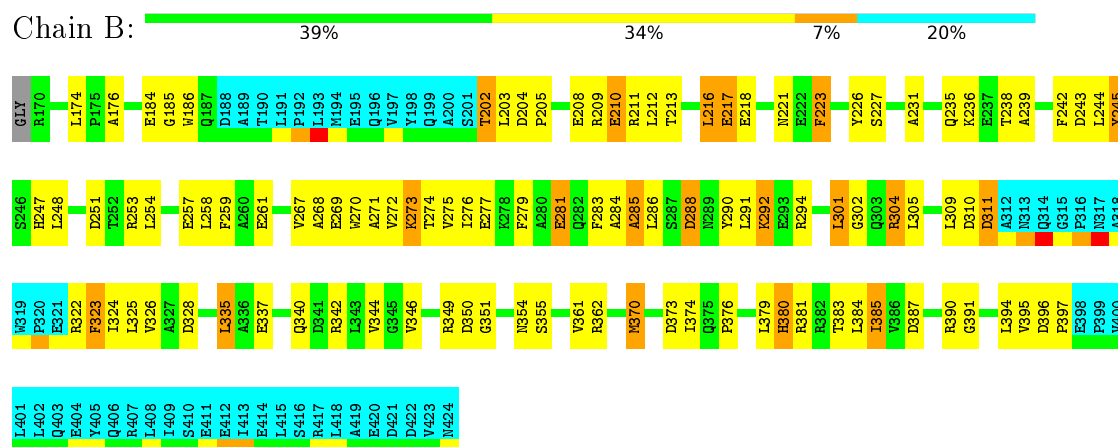
4.2.6 Score per residue for model 6

- Molecule 1: Phosphocarrier protein NPr

Chain A: 55% 35% 9%

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
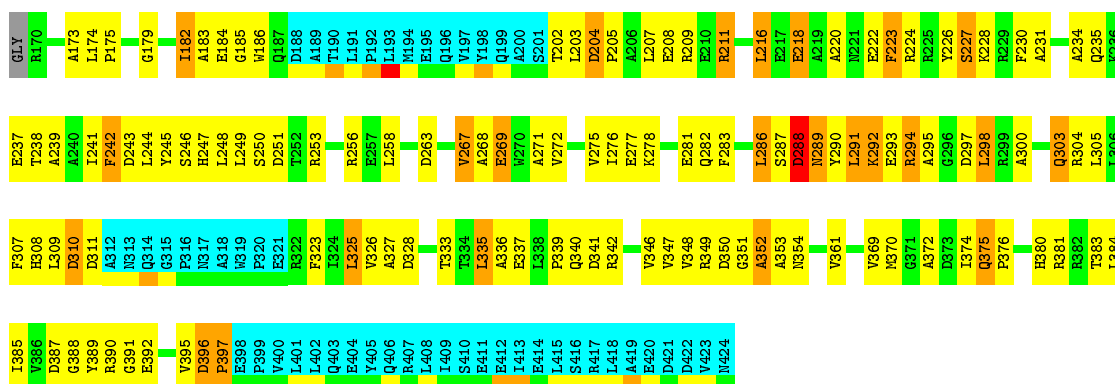
Chain B:
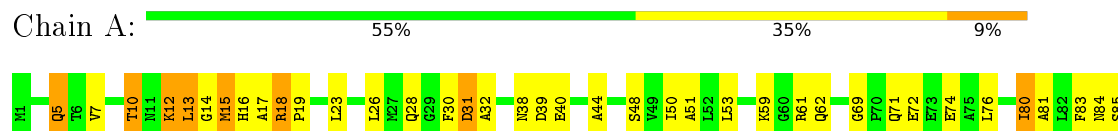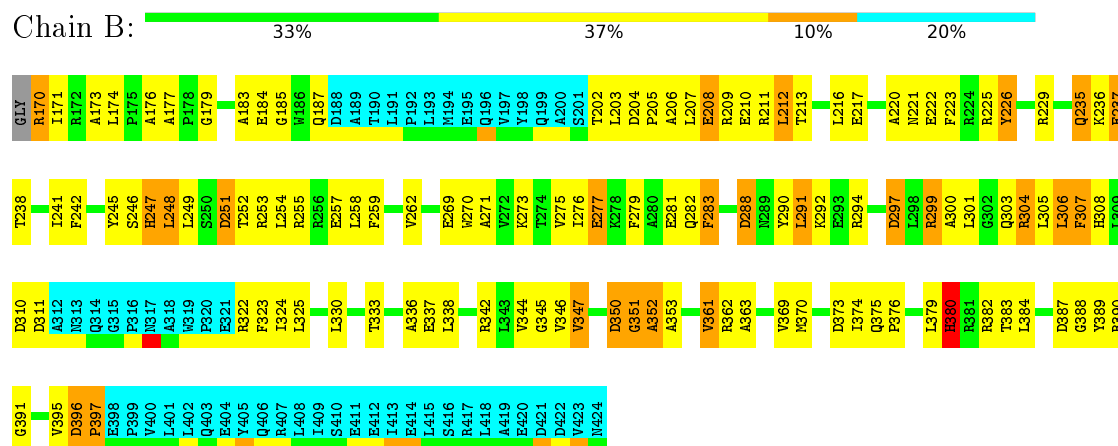
4.2.7 Score per residue for model 7

• Molecule 1: Phosphocarrier protein NPr

Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B:
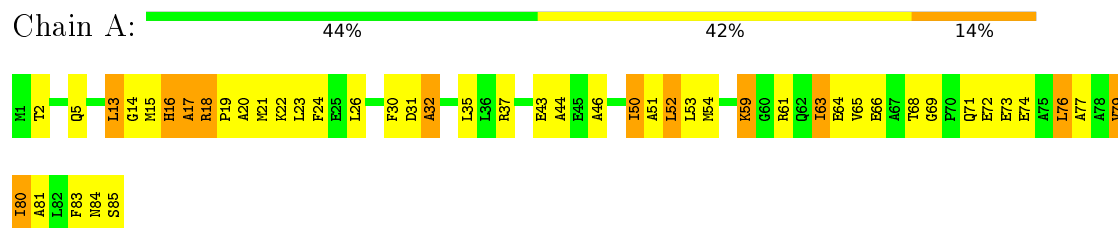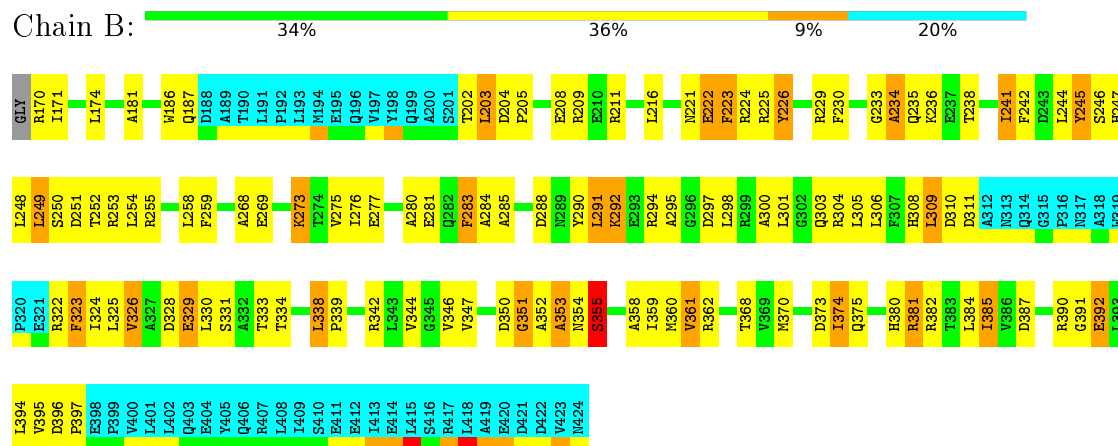
4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Phosphocarrier protein NPr

Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 37%   35%   8%   20%
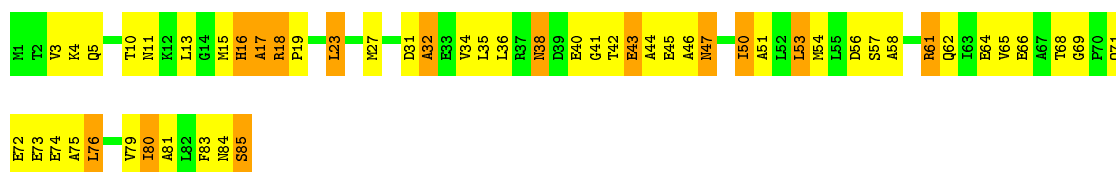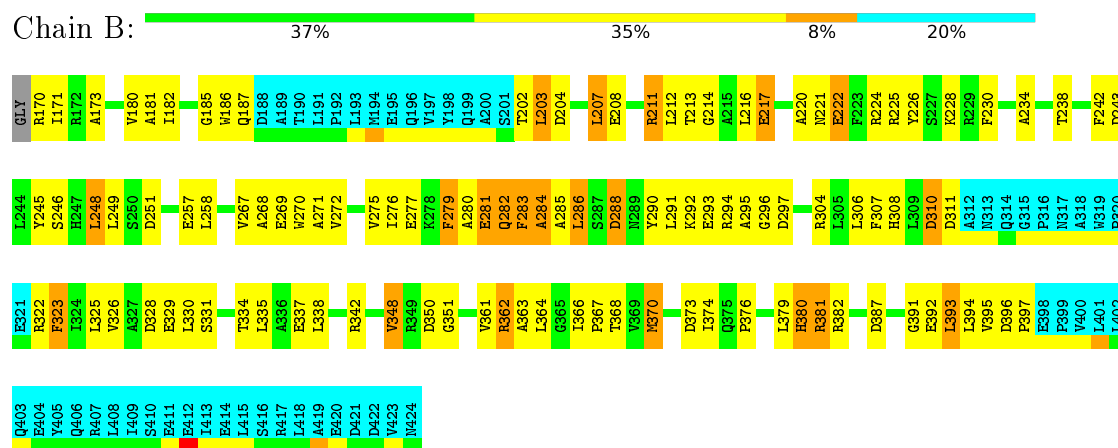
4.2.9 Score per residue for model 9

• Molecule 1: Phosphocarrier protein NPr

Chain A: 39%   48%   13%

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 35%   36%   9%   20%

4.2.10   Score per residue for model 10

• Molecule 1: Phosphocarrier protein NPr

Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B:

4.2.11   Score per residue for model 11
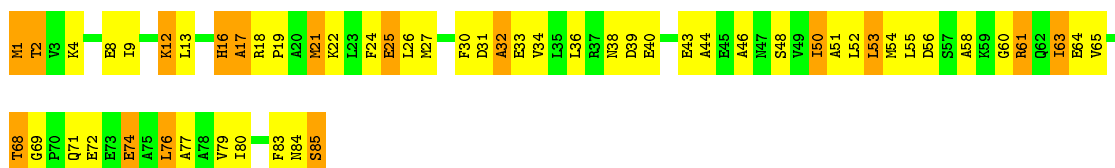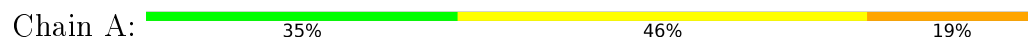
• Molecule 1: Phosphocarrier protein NPr

Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
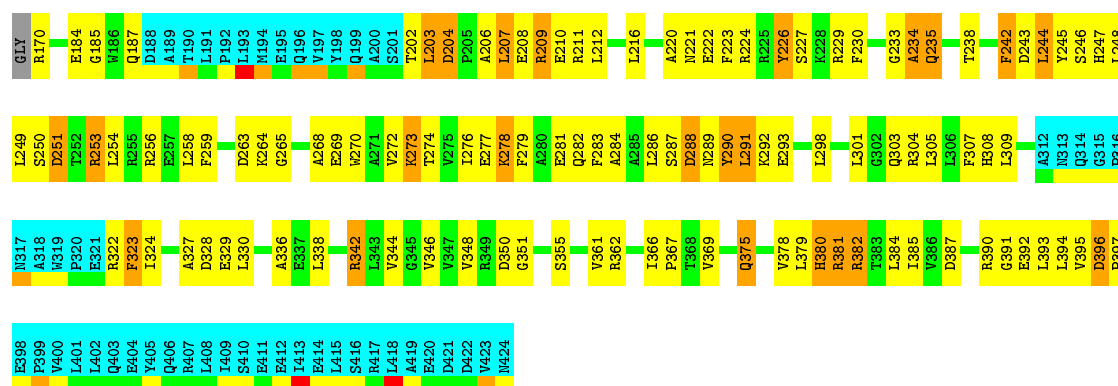
Chain B:

N317 A318 W319 P320 E321 R322 F323 I324 L325 V326 A327 D328 T333 T334 L335 A336 E337 L338 R342 R349 D350 G351 S355 M360 V361 R362 A363 L364 G365 I366 M370 Q375 P376 S377 V378 L379 H380 R381 R382 I385 V386 D387 G388 Y389 G391 E392 L393 L394 V395 D396 P397

E398 P399 V400 L401 L402 Q403 E404 Y405 Q406 R407 L408 I409 S410 E411 E412 I413 E414 L415 S416 R417 L418 A419 E420 D421 D422 V423 N424

4.2.12 Score per residue for model 12

• Molecule 1: Phosphocarrier protein NPr

Chain A: 42% 47% 11%

M1 T2 V3 T10 N11 K12 L13 G14 M15 H16 A17 R18 P19 A20 M21 K22 L23 L26 E25 L26 M27 Q28 G29 F30 D31 A32 E33 V34 L35 L36 R37 N38 D39 E40 A44 E45 A46 N47 S48 V49 I50 A51 L52 L53 M54 L55 V65 T68 G69 P70 Q71 E72 E73 E74 A75 L76

V79 I80 A81 L82 F83 N84 S85

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 29% 41% 10% 20%

GLY R170 I171 R172 A173 L174 P175 A176 G179 I182 A183 E184 G185 W186 Q187 D188 A189 T190 L191 P192 L193 M194 E195 Q196 V197 Y198 Q199 A200 S201 T202 L203 D204 P205 E208 R209 R210 R211 L212 T213 G214 A215 L216 E217 A220 N221 E222 R225 Y226 S227 K228 R229 F230 A231 Q235

K236 E237 T238 A239 A240 I241 F242 D243 L244 Y245 S246 H247 L248 L249 S250 D251 T252 R253 L254 R255 R256 E257 L258 F259 A260 E261 V262 D263 A268 E269 W270 A271 V272 K273 T274 V275 I276 E277 K278 F279 F283 A284 A285 L286 S287 D288 N289 Y290 L291 K292 E293 R294 A295 G296 D297 L298 R299 A300

L301 G302 Q303 R304 L305 L306 F307 H308 L309 A312 N313 Q314 G315 P316 N317 A318 W319 P320 E321 R322 F323 I324 L325 V326 A327 D328 E329 L330 T333 T334 L335 A336 E337 L338 R342 L343 V344 V348 R349 D350 G351 A352 A353 N354 S355 Q356 A357 V361 R362 A363 L364 G365 I366 P367 T368

V369 M370 Q375 L379 H380 R381 L384 I385 V386 D387 G388 Y389 R390 G391 V395 D396 P397 E398 P399 V400 L401 L402 Q403 E404 Y405 Q406 R407 L408 I409 S410 E411 E412 I413 E414 L415 S416 R417 L418 A419 E420 D421 D422 V423 N424

4.2.13 Score per residue for model 13

• Molecule 1: Phosphocarrier protein NPr

Chain A: 45% 40% 14% •

M1 T2 V3 T6 K12 L13 G14 M15 H16 A17 R18 P19 A20 M21 K22 L23 F24 E25 L26 M27 Q28 G29 F30 D31 A32 L35 L36 R37 E43 A44 E45 A46 N47 S48 V49 I50 A51 L52 L53 M54 Q62 I63 E64 T68 G69 P70 Q71 E72 E73 E74 A75 L76 V79

I80 A81 N84 S85

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 40% 32% 8% 20%
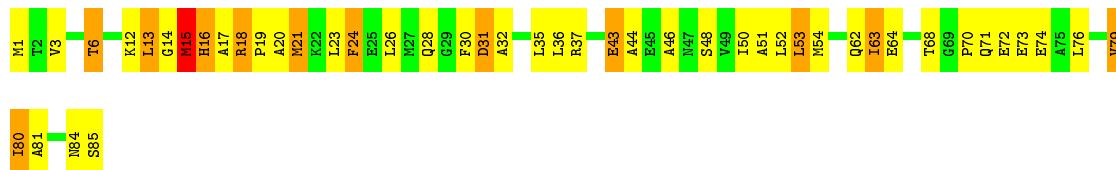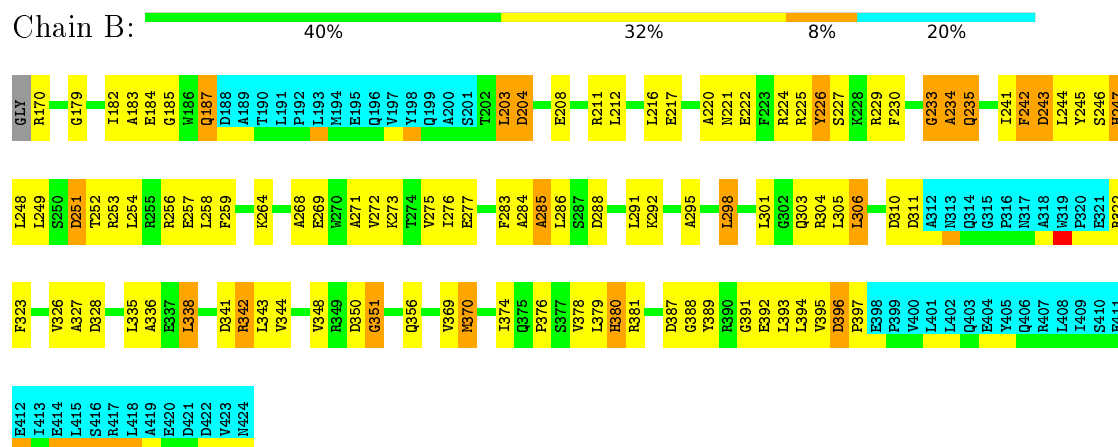
4.2.14 Score per residue for model 14

• Molecule 1: Phosphocarrier protein NPr

Chain A: 35% 48% 16%

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B: 36% 34% 9% 20%
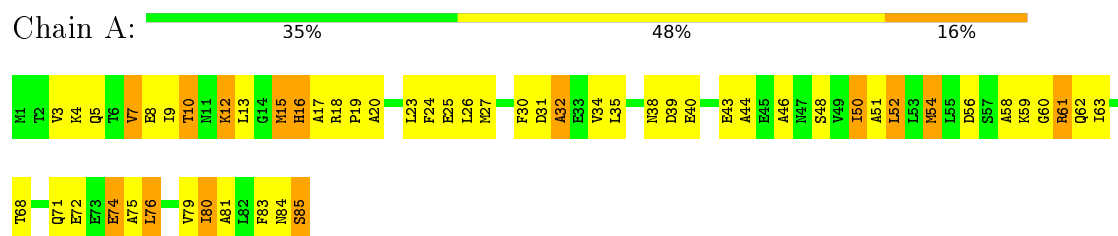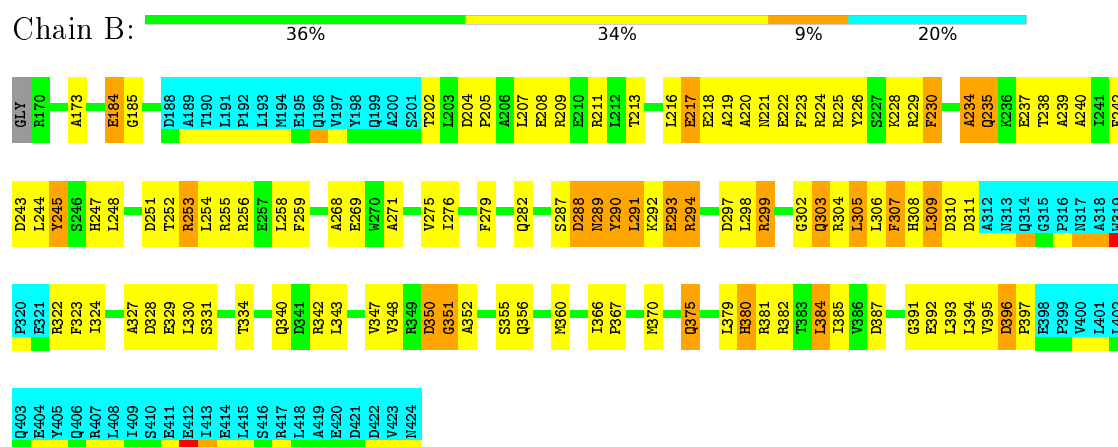
4.2.15 Score per residue for model 15

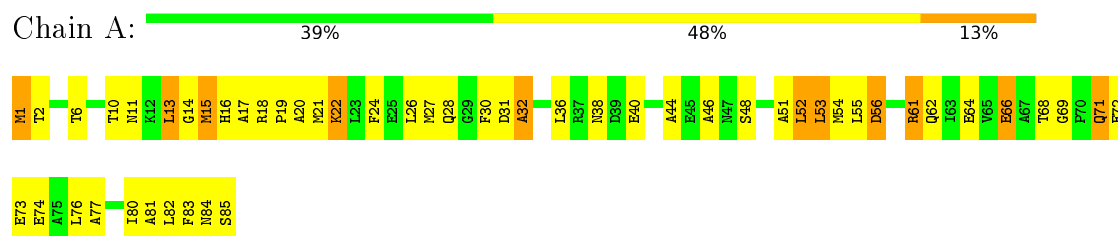• Molecule 1: Phosphocarrier protein NPr
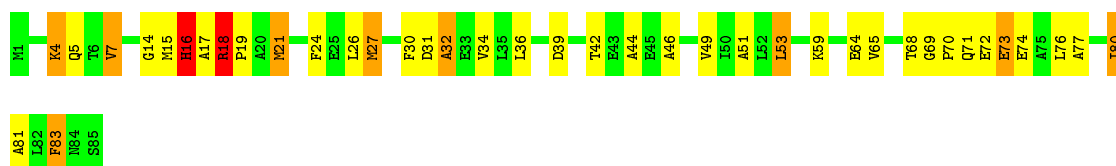
Chain A: 53% 34% 11% ·

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
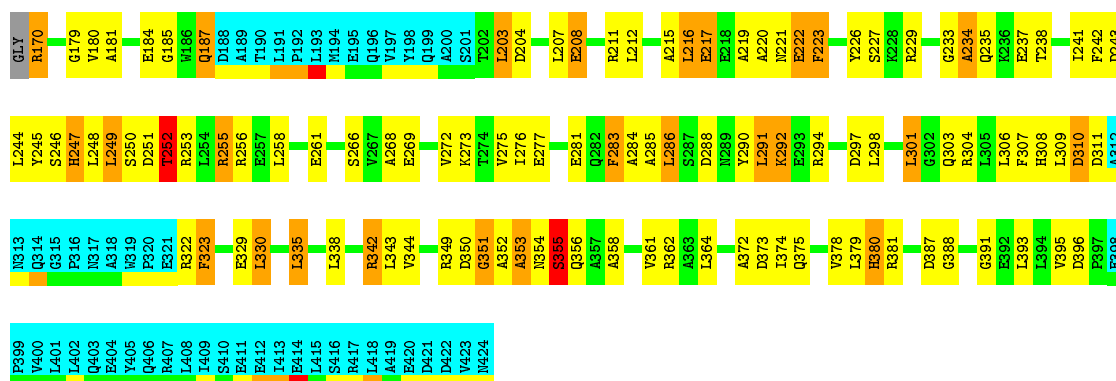
Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: Phosphocarrier protein NPr
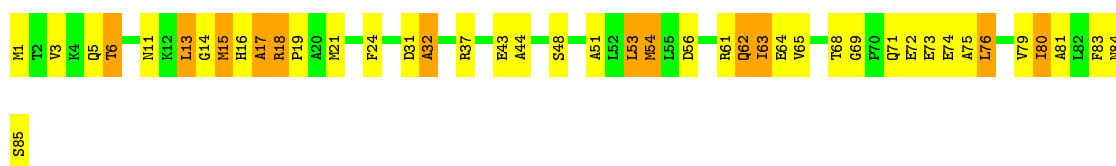
Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
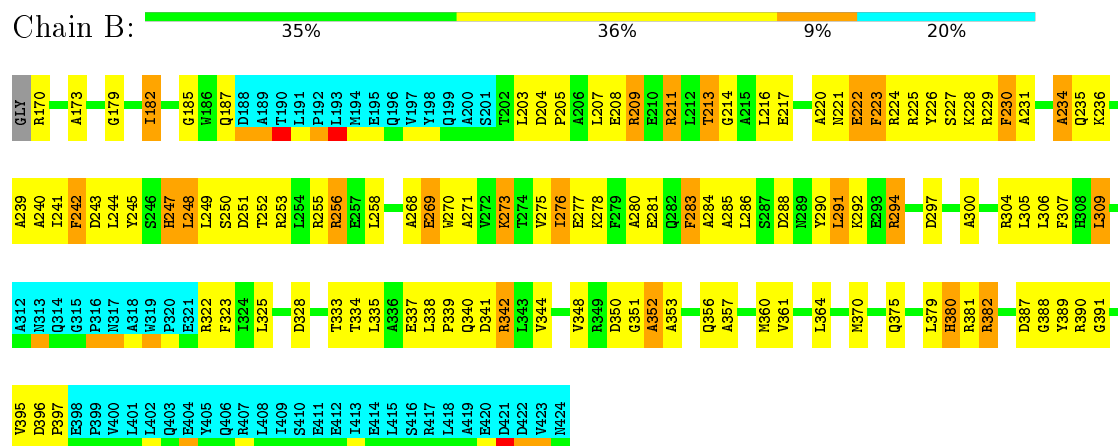
Chain B:
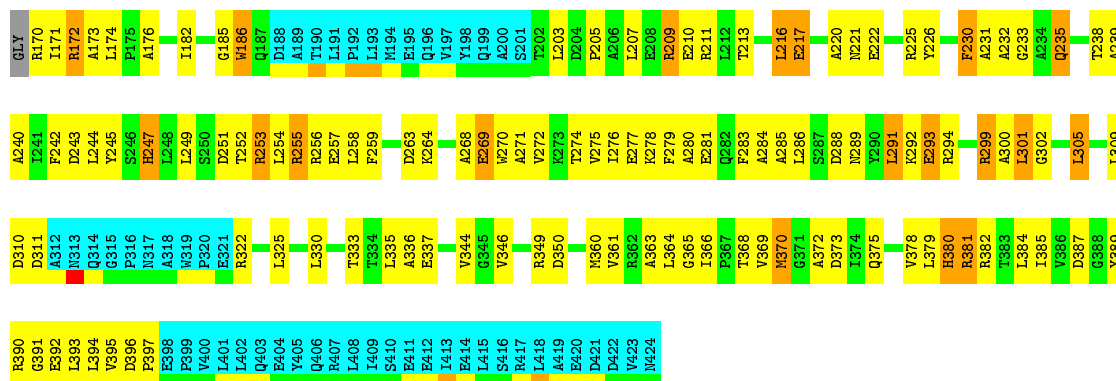
4.2.17 Score per residue for model 17

• Molecule 1: Phosphocarrier protein NPr
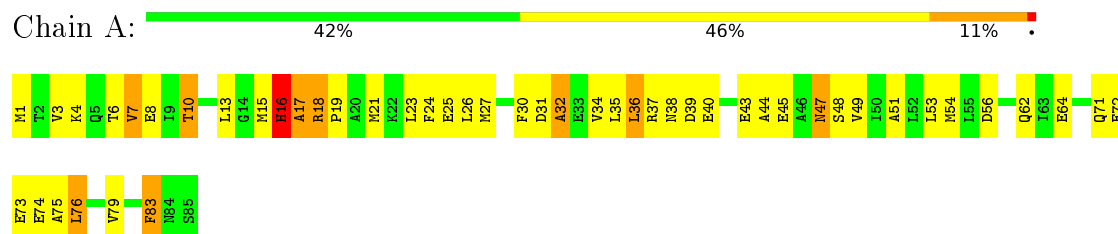
• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
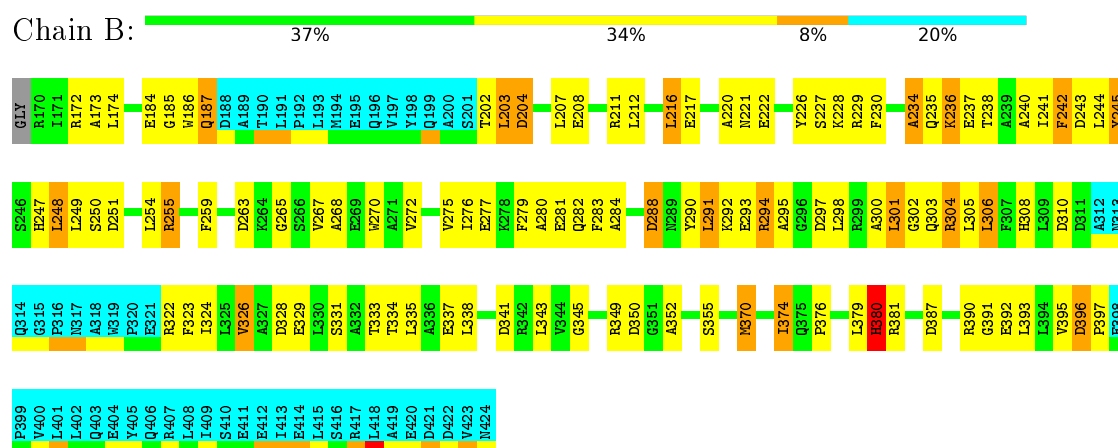
4.2.18 Score per residue for model 18

• Molecule 1: Phosphocarrier protein NPr
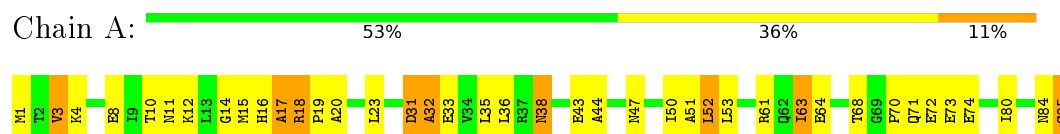
• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP
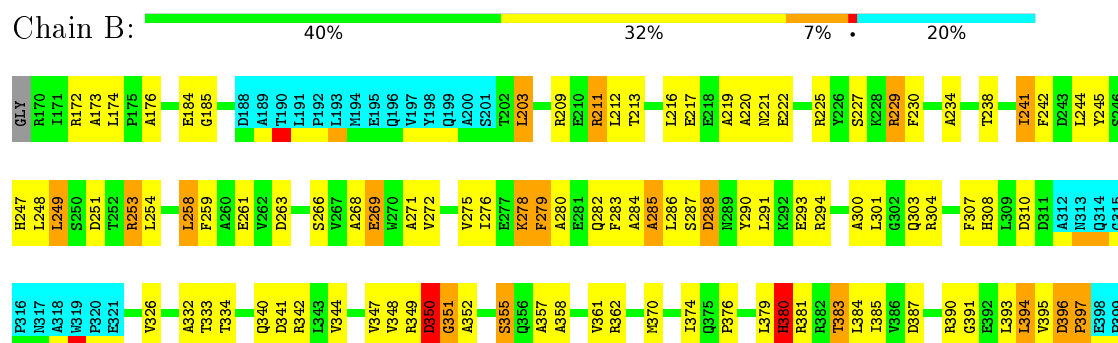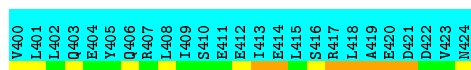
4.2.19 Score per residue for model 19
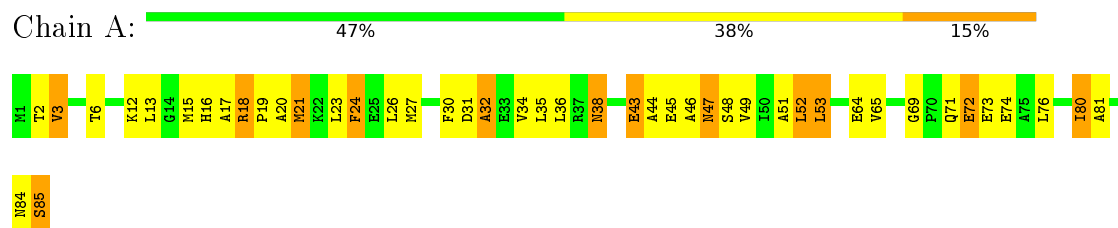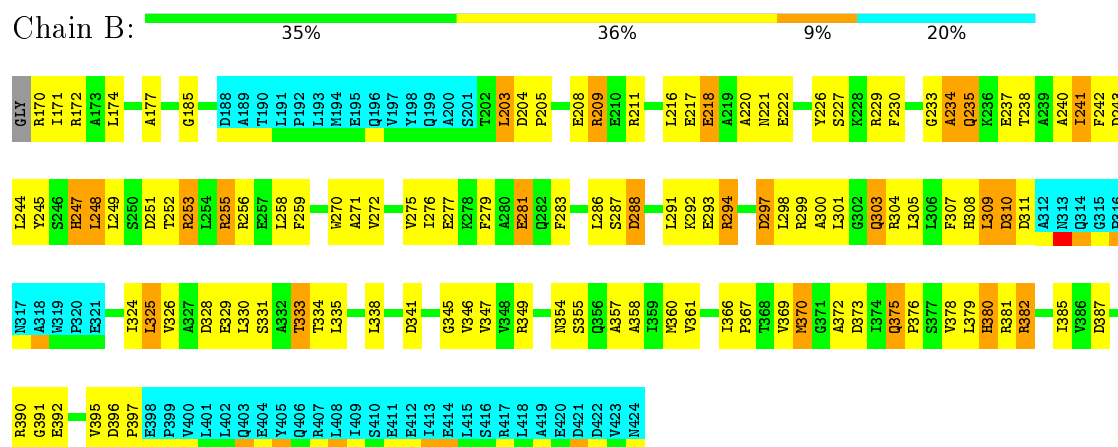
• Molecule 1: Phosphocarrier protein NPr

Chain A:

• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B:
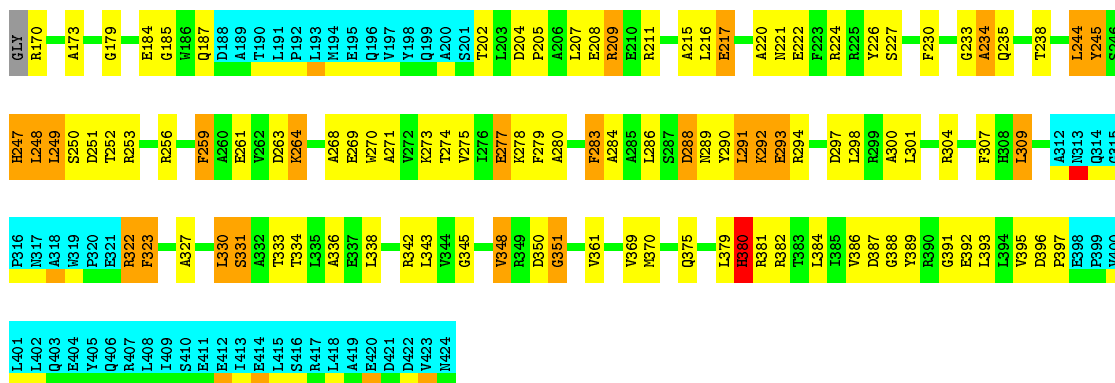
4.2.20 Score per residue for model 20

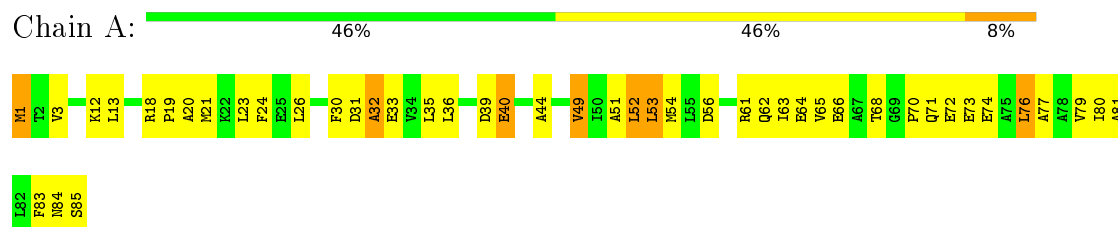• Molecule 1: Phosphocarrier protein NPr

Chain A:

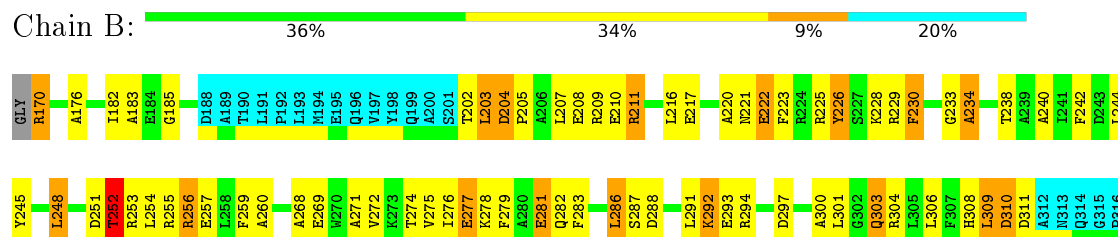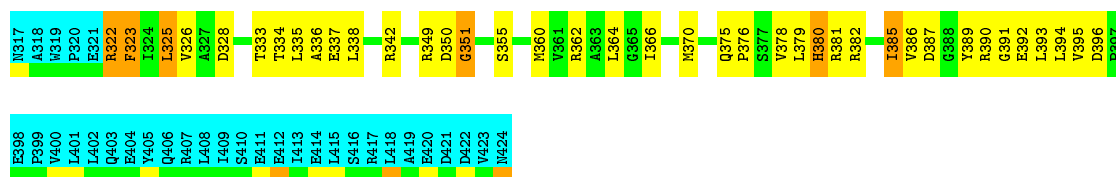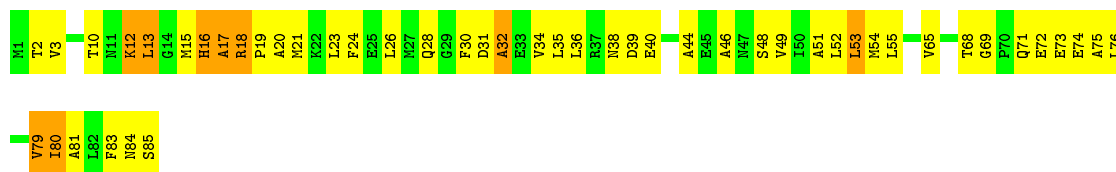• Molecule 2: Phosphoenolpyruvate-protein phosphotransferase PtsP

Chain B:

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: *STRUC-TURES 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)	5t1o_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 (i)

6.1 Standard geometry (i)

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 (i)

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	Models 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	Models 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	Models 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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Full wwPDB NMR Structure Validation Report

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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:288:ASP:HB3	2:B:291:LEU:HD21	0.60	1.73	7	1
2:B:244:LEU:HD23	2:B:294:ARG:NH2	0.60	2.11	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:211:ARG:NH2	2:B:269:GLU:OE1	0.59	2.36	6	3
2:B:237:GLU:OE1	2:B:238:THR:N	0.59	2.36	6	1
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:187:GLN:OE1	2:B:326:VAL:O	0.55	2.25	7	1
2:B:209:ARG:NH2	2:B:259:PHE:CZ	0.55	2.75	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:213:THR:OG1	2:B:255:ARG:CZ	0.50	2.60	6	2
2:B:235:GLN:NE2	2:B:238:THR:OG1	0.50	2.44	6	1

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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:36:LEU:O	1:A:43:GLU:OE1	0.47	2.32	2	1
1:A:16:HIS:CE1	2:B:291:LEU:HD11	0.47	2.44	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:38:ASN:HA	1:A:63:ILE:HG22	0.47	1.86	14	2
1:A:5:GLN:OE1	1:A:7:VAL:HG23	0.47	2.09	14	1
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:HD21	1:A:40:GLU:C	0.46	2.13	8	1
1:A:38:ASN:CG	1:A:40:GLU:H	0.46	2.14	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:279:PHE:CE2	2:B:298:LEU:HB3	0.46	2.46	20	1
2:B:297:ASP:OD2	2:B:333:THR:HG23	0.46	2.10	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:286:LEU:HB2	2:B:291:LEU:HD22	0.43	1.91	15	1
2:B:283:PHE:O	2:B:291:LEU:HD21	0.43	2.14	15	1
2:B:349:ARG:HE	2:B:374:ILE:N	0.43	2.12	15	1
2:B:349:ARG:HE	2:B:373:ASP:C	0.43	2.17	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:185:GLY:O	2:B:381:ARG:HA	0.41	2.15	13	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: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 (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	83/85 (98%)	73±1 (88±1%)	8±1 (9±1%)	2±1 (3±1%)	9	43
2	B	203/256 (79%)	181±4 (89±2%)	17±4 (8±2%)	5±2 (2±1%)	12	49
All	All	5720/6820 (84%)	5078 (89%)	496 (9%)	146 (3%)	11	47

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%)	4	33
2	B	160/205 (78%)	127±4 (79±3%)	33±4 (21±3%)	4	34
All	All	4560/5460 (84%)	3610 (79%)	950 (21%)	4	34

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 (i)

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: 5t1o_cs.cif

Chemical shift list name: *EIN_NPr_Complex.str*

7.1.1 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	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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	249	0.13 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	229	1.10 ± 0.07	Should be applied
$^{13}C'$	250	-0.23 ± 0.09	None needed (< 0.5 ppm)
^{15}N	232	0.70 ± 0.22	Should be applied

7.1.3 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 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	^{1}H	^{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.

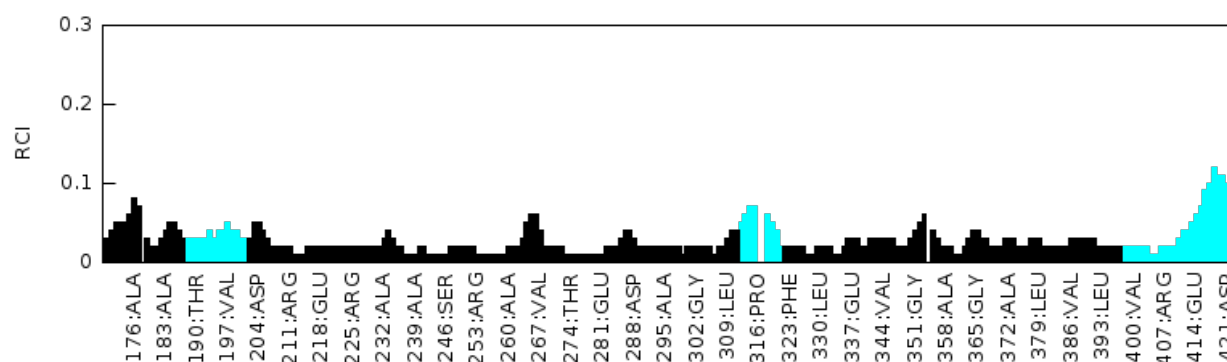|	Total	^{1}H	^{13}C	^{15}N
Backbone	963/1674 (58%)	232/667 (35%)	499/680 (73%)	232/327 (71%)
Sidechain	229/2261 (10%)	0/1310 (0%)	229/840 (27%)	0/111 (0%)
Aromatic	2/211 (1%)	1/113 (1%)	0/91 (0%)	1/7 (14%)
Overall	1194/4146 (29%)	233/2090 (11%)	728/1611 (45%)	233/445 (52%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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: 5t1o_cs.cif

Chemical shift list name: *NPr_ EIN_ Complex.str*

7.2.1 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	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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	51	0.61 ± 0.31	None needed (imprecise)
$^{13}C_\beta$	42	0.70 ± 0.08	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	52	0.17 ± 0.40	None needed (< 0.5 ppm)

7.2.3 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 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: