

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2XDF
Title	:	Solution Structure of the Enzyme I Dimer Complexed with HPr Using Residual
		Dipolar Couplings and Small Angle X-Ray Scattering
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Deposited on	:	2010-04-30

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Qu	ality of chain		
1	А	573	38%	49%		12%
1	В	573	37%	51%		12%
2	С	85	65%		33%	••
2	D	85	64%		34%	••



2 Ensemble composition and analysis (i)

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20502 atoms, of which 10338 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHO-TRANSFERASE.

Mol	Chain	Residues	Atoms				Trace		
1	Λ	579	Total	С	Η	Ν	Ο	\mathbf{S}	0
	070	8956	2790	4514	757	874	21	0	
1	D	579	Total	С	Η	Ν	Ο	S	0
ГБ	575	8956	2790	4514	757	874	21		

• Molecule 2 is a protein called PHOSPHOCARRIER PROTEIN HPR.

Mol	Chain	Residues	Atoms					Trace	
0	C	95	Total	С	Η	Ν	Ο	S	0
	80	1295	401	655	107	130	2	0	
0	р	95	Total	С	Η	Ν	Ο	S	0
	D	00	1295	401	655	107	130	2	0



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: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE





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 (medoid)

• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE











4.2.2 Score per residue for model 2

• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE



• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE





1437 1438 1438 1438 1441 1456 1456 1456 1456 1456 1456 1456 1456 1456 1456 1457 1456 1457 1456 1457 1456 1457 1446 1446 1446 1447 1446 1446 1447 1446 1446 1446 1446 1446 1446 1446 1446 1446 1446 1446 1448 1448 1448 1448 1448 1448 1448 1448 1448 1448

R523 R523 R533 R549 R533 R534 R533 R533</t

Chain C: 72%	25%	•••
• Moloculo 2: PHOSPHOCABRIER PROTEIN HPR		
• Molecule 2. I HOST HOCARTIER I ROTEIN III R Chain D: 69%	28%	





5 Refinement protocol and experimental data overview (i)

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

Of the 120 calculated structures, 2 were deposited, based on the following criterion: *BEST EX-PERIMENT FIT, AND THEN LOWEST ENERGY.*

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

Software name	Classification	Version
Xplor-NIH	refinement	2.25
Xplor-NIH	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	А	4434	4510	4502	486 ± 7
1	В	4425	4497	4489	486 ± 5
2	С	640	655	650	38 ± 5
2	D	640	655	650	$38{\pm}4$
All	All	20278	20634	20582	1948

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 48.

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

Atom 1	Atom 2	$Clack(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:126:ARG:HH22	2:C:619:ALA:CB	1.61	1.04	1	1
1:B:126:ARG:HH22	2:D:619:ALA:CB	1.55	1.04	1	1
1:B:314:PHE:CE2	1:B:376:ALA:HA	1.49	1.41	1	1
1:A:314:PHE:CE2	1:A:376:ALA:HA	1.48	1.40	1	1
1:B:562:MET:SD	1:B:562:MET:CE	1.48	2.01	2	1
1:A:562:MET:CE	1:A:562:MET:SD	1.46	2.01	1	1
1:B:364:MET:SD	1:B:364:MET:CE	1.44	2.06	2	2



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:364:MET:CE	1:A:364:MET:SD	1.44	2.06	1	2
1:B:126:ARG:NH2	2:D:619:ALA:CB	1.39	1.84	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CD2	1.37	1.54	1	1
1:B:78:MET:CE	2:D:627:LYS:HD2	1.36	1.47	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CD2	1.36	1.55	1	1
1:A:469:MET:SD	1:A:469:MET:CE	1.36	2.14	2	1
1:B:469:MET:SD	1:B:469:MET:CE	1.36	2.13	1	1
1:B:469:MET:CE	1:B:469:MET:SD	1.36	2.13	2	1
1:A:126:ARG:NH2	2:C:619:ALA:CB	1.35	1.84	1	1
1:A:469:MET:CE	1:A:469:MET:SD	1.35	2.13	1	1
1:B:345:MET:SD	1:B:345:MET:CE	1.35	2.14	1	1
1:B:345:MET:CE	1:B:345:MET:SD	1.35	2.14	2	1
1:A:345:MET:SD	1:A:345:MET:CE	1.34	2.14	1	2
1:A:78:MET:CE	2:C:627:LYS:HD2	1.33	1.51	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CE2	1.33	1.58	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CE2	1.32	1.58	1	1
1:A:470:ILE:O	1:A:473:LEU:CD2	1.31	1.79	1	1
1:B:470:ILE:O	1:B:473:LEU:CD2	1.29	1.78	1	1
1:B:470:ILE:O	1:B:473:LEU:HD22	1.29	1.07	1	1
1:A:515:LEU:CA	1:A:520:LEU:HD21	1.28	1.58	2	1
1:B:515:LEU:CA	1:B:520:LEU:HD21	1.28	1.57	2	1
1:A:470:ILE:O	1:A:473:LEU:HD22	1.26	1.07	1	1
1:A:515:LEU:C	1:A:520:LEU:HD11	1.25	1.51	2	1
1:B:515:LEU:C	1:B:520:LEU:HD11	1.24	1.52	2	1
1:B:464:ASP:OD1	1:B:467:ASN:ND2	1.24	1.70	1	2
1:A:126:ARG:NH2	2:C:619:ALA:HB3	1.24	1.41	1	1
1:B:515:LEU:O	1:B:520:LEU:HG	1.24	1.30	2	1
1:A:515:LEU:O	1:A:520:LEU:HG	1.22	1.30	2	1
1:B:367:ARG:O	1:B:371:ARG:HG3	1.22	1.34	2	1
1:B:126:ARG:NH2	2:D:619:ALA:HB3	1.22	1.41	1	1
1:A:276:GLY:O	1:A:299:PHE:CD1	1.22	1.91	1	1
1:B:276:GLY:O	1:B:299:PHE:CD1	1.22	1.92	1	1
1:B:111:GLN:OE1	2:D:648:PHE:HB3	1.22	1.33	1	1
1:A:464:ASP:OD1	1:A:467:ASN:ND2	1.21	1.71	1	2
1:A:314:PHE:CE2	1:A:376:ALA:CA	1.21	2.23	1	1
1:A:449:PHE:CE2	1:A:499:THR:OG1	1.21	1.87	1	1
1:B:449:PHE:CE2	1:B:500:GLY:O	1.20	1.95	1	1
1:B:449:PHE:CE2	1:B:499:THR:OG1	1.20	1.87	1	1
1:A:431:GLU:HG3	1:A:452:GLY:O	1.20	1.34	1	1
1:B:314:PHE:CE2	1:B:376:ALA:CA	1.20	2.23	1	1
1:A:515:LEU:O	1:A:520:LEU:CG	1.19	1.90	2	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:272:CYS:SG	1:B:293:GLY:N	1.19	2.16	2	1
1:B:515:LEU:O	1:B:520:LEU:CG	1.18	1.90	2	1
1:A:449:PHE:CE2	1:A:500:GLY:O	1.18	1.94	1	1
1:A:272:CYS:SG	1:A:293:GLY:N	1.18	2.15	2	1
1:B:527:ALA:O	1:B:530:ILE:CG2	1.18	1.92	2	1
1:A:527:ALA:O	1:A:530:ILE:CG2	1.17	1.93	2	1
1:A:367:ARG:O	1:A:371:ARG:HG3	1.17	1.34	2	1
1:A:111:GLN:OE1	2:C:648:PHE:HB3	1.17	1.34	1	1
1:B:431:GLU:HG3	1:B:452:GLY:O	1.17	1.34	1	1
1:B:456:LEU:HD13	1:B:457:THR:N	1.13	1.59	1	1
1:B:314:PHE:CZ	1:B:376:ALA:HA	1.12	1.78	1	1
1:B:78:MET:CE	2:D:627:LYS:CD	1.12	2.28	1	1
1:A:314:PHE:CZ	1:A:376:ALA:HA	1.11	1.79	1	1
1:A:456:LEU:HD13	1:A:457:THR:N	1.11	1.59	1	1
1:B:463:VAL:HG11	1:B:473:LEU:HG	1.10	1.20	1	1
1:B:243:GLN:O	1:B:246:VAL:HG22	1.10	1.47	1	1
1:A:314:PHE:CD2	1:A:376:ALA:HA	1.09	1.81	1	1
1:A:243:GLN:O	1:A:246:VAL:HG22	1.09	1.47	1	1
1:B:314:PHE:CD2	1:B:376:ALA:HA	1.09	1.81	1	1
1:A:296:ARG:O	1:A:299:PHE:CE2	1.08	2.06	1	1
1:A:78:MET:HE1	2:C:627:LYS:HD2	1.08	1.18	1	1
1:A:78:MET:CE	2:C:627:LYS:CD	1.08	2.32	1	1
1:A:463:VAL:HG11	1:A:473:LEU:HG	1.07	1.20	1	1
1:B:296:ARG:O	1:B:299:PHE:CE2	1.07	2.07	1	1
1:A:464:ASP:OD1	1:B:355:LEU:O	1.06	1.72	1	2
1:B:78:MET:HE1	2:D:627:LYS:CD	1.06	1.77	1	1
1:A:360:ILE:HD12	1:A:391:PRO:O	1.05	1.52	2	1
1:B:360:ILE:HD12	1:B:391:PRO:O	1.04	1.53	2	1
1:A:515:LEU:C	1:A:520:LEU:CD1	1.03	2.27	2	1
1:A:296:ARG:O	1:A:299:PHE:CD2	1.03	2.12	1	1
1:A:527:ALA:O	1:A:530:ILE:HG22	1.02	1.48	2	1
1:B:269:VAL:HG11	1:B:523:PHE:CE2	1.02	1.88	2	1
1:A:269:VAL:HG11	1:A:523:PHE:CE2	1.02	1.88	2	1
1:A:276:GLY:CA	1:A:299:PHE:CD2	1.02	2.42	1	1
1:B:296:ARG:O	1:B:299:PHE:CD2	1.02	2.12	1	1
1:B:527:ALA:O	1:B:530:ILE:HG22	1.02	1.50	2	1
1:B:276:GLY:CA	1:B:299:PHE:CD2	1.02	2.42	1	1
1:B:296:ARG:O	1:B:299:PHE:CZ	1.02	2.13	1	1
1:B:367:ARG:O	1:B:371:ARG:CG	1.01	2.08	2	1
1:B:275:ILE:O	1:B:299:PHE:CE2	1.01	2.12	1	1
1:B:515:LEU:C	1:B:520:LEU:CD1	1.01	2.28	2	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:126:ARG:HH22	2:C:619:ALA:HB2	1.01	1.07	1	1
1:A:331:VAL:HG12	1:A:387:ARG:O	1.01	1.55	1	1
1:B:331:VAL:HG12	1:B:387:ARG:O	1.01	1.55	1	1
1:B:126:ARG:HH22	2:D:619:ALA:HB2	1.01	1.07	1	1
1:A:355:LEU:O	1:B:464:ASP:OD1	1.01	1.78	1	2
1:A:296:ARG:O	1:A:299:PHE:CZ	1.00	2.14	1	1
1:B:449:PHE:O	1:B:449:PHE:CD2	1.00	2.13	1	1
1:A:449:PHE:CD2	1:A:449:PHE:O	1.00	2.13	1	1
1:A:367:ARG:O	1:A:371:ARG:CG	1.00	2.08	2	1
1:B:232:THR:HG22	1:B:233:ASN:N	1.00	1.70	2	2
1:A:221:ASP:HA	1:A:239:MET:CE	1.00	1.87	1	2
1:B:232:THR:CG2	1:B:233:ASN:H	1.00	1.69	2	2
1:A:275:ILE:O	1:A:299:PHE:CE2	1.00	2.13	1	1
1:B:541:ASN:O	1:B:544:ASP:OD1	1.00	1.80	2	2
1:B:515:LEU:HA	1:B:520:LEU:HD21	0.99	1.02	2	1
1:A:232:THR:CG2	1:A:233:ASN:H	0.99	1.69	2	2
1:A:232:THR:HG22	1:A:233:ASN:N	0.99	1.71	1	2
1:B:221:ASP:HA	1:B:239:MET:CE	0.99	1.87	2	2
1:A:11:ILE:HD13	1:A:221:ASP:O	0.99	1.57	2	2
1:A:541:ASN:O	1:A:544:ASP:OD1	0.99	1.79	1	2
1:A:449:PHE:CZ	1:A:451:ILE:HB	0.99	1.93	1	1
1:A:232:THR:CG2	1:A:233:ASN:N	0.98	2.26	2	2
1:B:449:PHE:CZ	1:B:451:ILE:HB	0.98	1.93	1	1
1:A:515:LEU:HA	1:A:520:LEU:HD21	0.98	1.02	2	1
1:A:314:PHE:CE2	1:A:379:ARG:CB	0.98	2.46	1	1
1:B:11:ILE:HD13	1:B:221:ASP:O	0.98	1.57	2	2
1:A:78:MET:HE2	2:C:627:LYS:CD	0.98	1.88	1	1
1:B:314:PHE:CE2	1:B:379:ARG:CB	0.98	2.46	1	1
1:A:221:ASP:OD2	1:A:225:ASN:N	0.97	1.98	2	1
1:A:276:GLY:O	1:A:299:PHE:CE1	0.96	2.18	1	1
1:B:221:ASP:OD2	1:B:225:ASN:N	0.96	1.99	2	1
1:A:78:MET:HE2	2:C:627:LYS:HD2	0.96	1.36	1	1
1:B:533:ILE:O	1:B:537:ILE:HG23	0.95	1.61	2	1
1:B:232:THR:CG2	1:B:233:ASN:N	0.94	2.26	1	2
1:B:276:GLY:O	1:B:299:PHE:CE1	0.94	2.19	1	1
1:A:276:GLY:CA	1:A:299:PHE:CE2	0.94	2.51	1	1
1:B:515:LEU:CA	1:B:520:LEU:CD2	0.93	2.46	2	1
1:A:104:ALA:O	1:A:107:VAL:HG22	0.93	1.63	2	1
1:B:276:GLY:CA	1:B:299:PHE:CE2	0.93	2.51	1	1
1:B:292:VAL:CG1	1:B:329:VAL:HG22	0.93	1.94	1	1
1:B:314:PHE:CE2	1:B:379:ARG:HB2	0.93	1.99	1	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:292:VAL:CG1	1:A:329:VAL:HG22	0.93	1.93	1	1
1:A:533:ILE:O	1:A:537:ILE:HG23	0.92	1.61	2	1
1:A:314:PHE:CE2	1:A:379:ARG:HB2	0.92	1.99	1	1
1:A:515:LEU:CA	1:A:520:LEU:CD2	0.92	2.47	2	1
1:A:449:PHE:HE2	1:A:500:GLY:O	0.92	1.45	1	1
1:B:359:ALA:O	1:B:362:ILE:HG22	0.92	1.65	1	2
1:A:242:VAL:O	1:A:246:VAL:HG13	0.92	1.64	1	1
1:B:104:ALA:O	1:B:107:VAL:HG22	0.91	1.64	2	1
1:A:292:VAL:HG21	1:A:329:VAL:HG13	0.91	1.40	1	1
1:B:292:VAL:HG21	1:B:329:VAL:HG13	0.91	1.40	1	1
1:B:78:MET:HE1	2:D:627:LYS:HD2	0.91	0.94	1	1
1:B:449:PHE:O	1:B:449:PHE:HD2	0.91	1.48	1	1
1:B:54:LEU:HD12	1:B:55:GLU:N	0.91	1.81	2	1
1:B:242:VAL:O	1:B:246:VAL:HG13	0.90	1.64	1	1
1:A:464:ASP:CG	1:B:355:LEU:O	0.90	2.08	1	2
1:B:299:PHE:HD1	1:B:300:LEU:N	0.90	1.64	1	1
1:A:360:ILE:CD1	1:A:391:PRO:O	0.90	2.20	2	1
1:B:516:LEU:N	1:B:520:LEU:HD11	0.90	1.82	2	1
1:A:299:PHE:HD1	1:A:300:LEU:N	0.90	1.63	1	1
1:B:449:PHE:C	1:B:449:PHE:CD2	0.89	2.44	1	1
1:A:516:LEU:N	1:A:520:LEU:HD11	0.89	1.81	2	1
1:A:489:ILE:HA	1:A:499:THR:HG21	0.89	1.44	1	1
1:A:359:ALA:O	1:A:362:ILE:HG22	0.89	1.65	1	2
1:B:301:PHE:CG	1:B:342:LEU:HD22	0.89	2.03	2	1
1:A:269:VAL:HG13	1:A:521:ASP:O	0.89	1.66	2	1
1:B:269:VAL:HG13	1:B:521:ASP:O	0.89	1.66	2	1
1:A:54:LEU:HD12	1:A:55:GLU:N	0.88	1.81	2	1
1:A:449:PHE:HD2	1:A:449:PHE:O	0.88	1.48	1	1
1:B:449:PHE:HE2	1:B:500:GLY:O	0.88	1.45	1	1
1:A:301:PHE:CG	1:A:342:LEU:HD22	0.88	2.04	2	1
1:A:292:VAL:CG2	1:A:329:VAL:HG13	0.88	1.98	1	1
1:A:296:ARG:O	1:A:299:PHE:CE1	0.88	2.27	1	1
1:A:449:PHE:CD2	1:A:449:PHE:C	0.87	2.44	1	1
1:B:292:VAL:CG2	1:B:329:VAL:HG13	0.87	1.98	1	1
1:A:275:ILE:O	1:A:299:PHE:HE2	0.87	1.47	1	1
1:B:296:ARG:O	1:B:299:PHE:CE1	0.87	2.26	1	1
1:B:489:ILE:HG12	1:B:499:THR:HG21	0.87	1.44	2	1
1:B:360:ILE:CD1	1:B:391:PRO:O	0.87	2.22	2	1
1:B:263:THR:HG22	1:B:267:HIS:H	0.87	1.30	1	1
1:A:489:ILE:HG12	1:A:499:THR:HG21	0.86	1.44	2	1
1:B:431:GLU:HG2	1:B:455:ASP:CB	0.86	1.99	1	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:296:ARG:O	1:A:299:PHE:CG	0.86	2.28	1	1
1:A:12:ALA:HB1	1:A:177:LEU:HD13	0.86	1.47	2	1
1:A:175:LYS:CD	1:A:175:LYS:C	0.86	2.42	2	1
1:B:12:ALA:HB1	1:B:177:LEU:HD13	0.86	1.47	2	1
1:B:296:ARG:O	1:B:299:PHE:CG	0.86	2.28	1	1
1:A:269:VAL:HG11	1:A:523:PHE:CZ	0.86	2.06	2	1
1:B:489:ILE:HA	1:B:499:THR:HG21	0.86	1.44	1	1
1:B:515:LEU:HA	1:B:520:LEU:CD2	0.86	1.98	2	1
1:B:175:LYS:C	1:B:175:LYS:CD	0.86	2.43	2	1
1:B:269:VAL:HG11	1:B:523:PHE:CZ	0.86	2.06	2	1
1:A:221:ASP:CG	1:A:226:GLN:H	0.85	1.74	2	1
1:B:221:ASP:CG	1:B:226:GLN:H	0.85	1.74	2	1
1:A:431:GLU:HG2	1:A:455:ASP:CB	0.85	2.00	1	1
1:B:275:ILE:O	1:B:299:PHE:HE2	0.85	1.47	1	1
1:A:228:TYR:HB3	1:A:231:PRO:HG3	0.85	1.45	2	2
1:A:221:ASP:HA	1:A:239:MET:HE1	0.85	1.46	2	2
1:A:515:LEU:HB3	1:A:520:LEU:CD1	0.85	2.01	2	1
1:B:228:TYR:HB3	1:B:231:PRO:HG3	0.85	1.46	2	2
1:A:263:THR:HG22	1:A:267:HIS:H	0.85	1.30	1	1
1:B:50:ALA:O	1:B:54:LEU:HG	0.85	1.70	2	1
1:A:50:ALA:O	1:A:54:LEU:HG	0.85	1.70	2	1
1:B:115:LEU:HD11	2:D:651:GLN:HB3	0.85	1.48	2	1
1:B:544:ASP:OD1	1:B:545:ALA:N	0.85	2.10	2	2
1:B:527:ALA:O	1:B:530:ILE:HG23	0.85	1.69	2	1
1:A:544:ASP:OD1	1:A:545:ALA:N	0.85	2.10	2	2
1:A:115:LEU:HD11	2:C:651:GLN:HB3	0.84	1.48	2	1
1:B:278:VAL:O	1:B:281:VAL:HG22	0.84	1.73	2	1
1:B:51:SER:HA	1:B:54:LEU:HD21	0.84	1.49	2	1
1:B:515:LEU:HB3	1:B:520:LEU:CD1	0.84	2.01	2	1
1:A:302:MET:HB2	1:A:342:LEU:HD21	0.83	1.49	1	1
1:B:449:PHE:CD2	1:B:499:THR:CB	0.83	2.60	1	1
1:A:449:PHE:CD2	1:A:499:THR:CB	0.83	2.60	1	1
1:A:337:GLY:O	1:A:358:ARG:CZ	0.83	2.27	2	1
1:B:337:GLY:O	1:B:358:ARG:CZ	0.83	2.27	2	1
1:B:314:PHE:CZ	1:B:376:ALA:CA	0.83	2.56	1	1
1:A:336:ILE:HD12	1:A:336:ILE:H	0.83	1.34	2	1
1:A:372:ASP:OD1	1:A:372:ASP:C	0.83	2.17	2	1
1:A:314:PHE:CE2	1:A:379:ARG:HB3	0.83	2.09	1	1
1:A:304:ARG:O	1:A:344:TYR:CZ	0.83	2.32	1	1
1:B:314:PHE:CE2	1:B:379:ARG:HB3	0.83	2.08	1	1
1:A:355:LEU:O	1:B:464:ASP:CG	0.82	2.17	1	2



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:304:ARG:O	1:B:344:TYR:CZ	0.82	2.32	1	1
1:B:394:ILE:HD13	1:B:394:ILE:H	0.82	1.33	2	1
1:A:51:SER:HA	1:A:54:LEU:HD21	0.82	1.49	2	1
1:B:177:LEU:H	1:B:177:LEU:HD12	0.82	1.35	1	1
1:A:394:ILE:HD13	1:A:394:ILE:H	0.82	1.34	2	1
1:B:463:VAL:CG1	1:B:473:LEU:HG	0.81	2.04	1	1
1:B:372:ASP:OD1	1:B:372:ASP:C	0.81	2.17	2	1
1:A:177:LEU:H	1:A:177:LEU:HD12	0.81	1.34	1	1
1:A:474:TYR:CG	1:A:474:TYR:O	0.81	2.34	2	2
1:B:360:ILE:HD13	1:B:390:PHE:CD2	0.81	2.10	2	1
1:B:296:ARG:O	1:B:299:PHE:CD1	0.81	2.32	1	1
1:A:556:PRO:HB3	1:B:441:HIS:ND1	0.81	1.89	2	2
1:A:314:PHE:CZ	1:A:376:ALA:CA	0.81	2.56	1	1
1:B:449:PHE:CD2	1:B:499:THR:CA	0.81	2.63	1	1
1:A:356:GLY:O	1:A:358:ARG:HG2	0.81	1.75	2	1
1:A:527:ALA:O	1:A:530:ILE:HG23	0.81	1.72	2	1
1:B:78:MET:HE2	2:D:627:LYS:CD	0.81	2.01	1	1
1:B:534:LYS:O	1:B:537:ILE:HG13	0.81	1.76	2	1
1:A:449:PHE:CD2	1:A:499:THR:CA	0.81	2.63	1	1
1:B:221:ASP:HA	1:B:239:MET:HE1	0.81	1.52	2	2
1:A:463:VAL:CG1	1:A:473:LEU:HG	0.80	2.04	1	1
1:A:126:ARG:HD3	2:C:616:THR:OG1	0.80	1.76	2	1
1:A:296:ARG:O	1:A:299:PHE:CD1	0.80	2.34	1	1
1:B:464:ASP:N	1:B:464:ASP:OD1	0.80	2.15	1	1
1:B:356:GLY:O	1:B:358:ARG:HG2	0.80	1.74	2	1
1:A:299:PHE:CD1	1:A:300:LEU:N	0.80	2.49	1	1
1:B:456:LEU:HD11	1:B:481:VAL:CG1	0.80	2.07	1	1
1:B:449:PHE:CD2	1:B:499:THR:HA	0.80	2.11	1	1
1:B:177:LEU:O	1:B:177:LEU:HD12	0.80	1.77	2	1
1:A:177:LEU:HD12	1:A:177:LEU:O	0.80	1.77	2	1
1:B:474:TYR:O	1:B:474:TYR:CG	0.80	2.34	2	1
1:A:78:MET:HE1	2:C:627:LYS:CD	0.80	1.98	1	1
1:B:388:ILE:HD12	1:B:389:MET:N	0.80	1.92	2	1
1:A:74:GLU:OE1	2:C:624:LYS:NZ	0.80	2.15	1	1
1:B:336:ILE:HD12	1:B:336:ILE:H	0.80	1.34	2	1
1:A:175:LYS:C	1:A:175:LYS:HD3	0.79	1.97	2	1
1:B:175:LYS:C	1:B:175:LYS:HD3	0.79	1.96	2	1
1:B:515:LEU:C	1:B:520:LEU:CG	0.79	2.50	2	1
1:A:199:LEU:HD23	1:A:199:LEU:O	0.79	1.78	1	1
1:A:205:THR:OG1	1:A:208:VAL:HG22	0.79	1.76	1	1
1:A:449:PHE:CD2	1:A:499:THR:HA	0.79	2.11	1	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:126:ARG:HD3	2:D:616:THR:OG1	0.79	1.77	2	1
1:A:360:ILE:HD13	1:A:390:PHE:CD2	0.79	2.11	2	1
1:A:534:LYS:O	1:A:537:ILE:HG13	0.79	1.76	2	1
1:A:515:LEU:C	1:A:520:LEU:CG	0.79	2.50	2	1
1:A:431:GLU:HG2	1:A:455:ASP:HB3	0.79	1.54	1	1
1:B:199:LEU:HD23	1:B:199:LEU:O	0.79	1.78	1	1
1:B:299:PHE:CD1	1:B:300:LEU:N	0.79	2.50	1	1
1:B:74:GLU:OE1	2:D:624:LYS:NZ	0.78	2.16	1	1
1:A:456:LEU:HD11	1:A:481:VAL:CG1	0.78	2.07	1	1
1:B:431:GLU:HG2	1:B:455:ASP:HB3	0.78	1.53	1	1
1:B:449:PHE:CD1	1:B:488:VAL:HG11	0.78	2.14	1	1
1:A:302:MET:SD	1:A:342:LEU:HG	0.78	2.19	2	1
1:A:438:ILE:CG2	1:A:441:HIS:HB2	0.78	2.09	2	1
1:A:353:PRO:O	1:A:358:ARG:CD	0.78	2.32	2	1
1:A:301:PHE:CD2	1:A:342:LEU:HD22	0.78	2.14	2	1
1:A:350:GLU:N	1:A:350:GLU:CD	0.78	2.37	2	1
1:A:388:ILE:HD12	1:A:389:MET:N	0.78	1.94	2	1
1:B:438:ILE:CG2	1:B:441:HIS:HB2	0.78	2.08	2	1
1:A:449:PHE:CD1	1:A:488:VAL:HG11	0.78	2.14	1	1
1:B:205:THR:OG1	1:B:208:VAL:HG22	0.78	1.78	1	1
1:A:11:ILE:CD1	1:A:221:ASP:O	0.78	2.32	2	2
1:A:160:ALA:O	1:A:181:THR:HG23	0.78	1.79	1	1
1:A:515:LEU:HA	1:A:520:LEU:CD2	0.77	1.98	2	1
1:B:353:PRO:O	1:B:358:ARG:CD	0.77	2.32	2	1
1:B:13:PHE:CZ	1:B:240:ARG:HD2	0.77	2.15	2	2
1:B:515:LEU:O	1:B:520:LEU:CD1	0.77	2.31	2	1
1:B:11:ILE:CD1	1:B:221:ASP:O	0.77	2.33	2	2
1:B:350:GLU:N	1:B:350:GLU:CD	0.77	2.37	2	1
1:B:476:PRO:O	1:B:481:VAL:CG2	0.77	2.33	2	1
1:B:50:ALA:O	1:B:54:LEU:CG	0.77	2.33	2	1
1:B:160:ALA:O	1:B:181:THR:HG23	0.77	1.79	1	1
1:B:402:LEU:HD13	1:B:403:ARG:N	0.76	1.96	2	1
1:A:476:PRO:O	1:A:481:VAL:CG2	0.76	2.33	2	1
1:A:50:ALA:O	1:A:54:LEU:CG	0.76	2.33	2	1
1:B:175:LYS:HD3	1:B:176:VAL:N	0.76	1.96	2	1
1:B:221:ASP:HA	1:B:239:MET:HE2	0.76	1.55	1	2
1:B:301:PHE:CD2	1:B:342:LEU:HD22	0.76	2.14	2	1
1:A:13:PHE:CZ	1:A:240:ARG:HD2	0.76	2.15	1	2
1:B:79:LEU:HD13	2:D:647:LEU:HB3	0.76	1.56	1	2
1:A:317:TYR:OH	1:A:331:VAL:HB	0.76	1.80	1	1
1:B:337:GLY:O	1:B:358:ARG:NE	0.76	2.19	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:307:LEU:HD23	1:A:307:LEU:O	0.76	1.80	2	1
1:B:115:LEU:CD1	2:D:651:GLN:HB3	0.76	2.09	2	1
1:A:79:LEU:HD13	2:C:647:LEU:HB3	0.76	1.56	1	2
1:A:314:PHE:CD2	1:A:376:ALA:CA	0.76	2.61	1	1
1:B:314:PHE:CD2	1:B:376:ALA:CA	0.76	2.61	1	1
1:A:402:LEU:HD13	1:A:403:ARG:N	0.76	1.96	2	1
1:A:115:LEU:CD1	2:C:651:GLN:HB3	0.76	2.09	2	1
1:A:111:GLN:CD	2:C:648:PHE:HB3	0.76	2.01	1	2
1:A:449:PHE:CE2	1:A:499:THR:CB	0.75	2.70	1	1
1:A:278:VAL:O	1:A:281:VAL:HG22	0.75	1.80	2	1
1:A:449:PHE:HD2	1:A:499:THR:HA	0.75	1.42	1	1
1:B:431:GLU:CG	1:B:452:GLY:O	0.75	2.28	1	1
1:A:292:VAL:HG11	1:A:329:VAL:HG22	0.75	1.58	1	1
1:B:307:LEU:HD23	1:B:307:LEU:O	0.75	1.81	2	1
1:B:454:ASN:O	1:B:457:THR:HG22	0.75	1.82	2	1
1:B:296:ARG:N	1:B:299:PHE:CE2	0.75	2.55	1	1
1:B:449:PHE:CE2	1:B:499:THR:CB	0.75	2.69	1	1
1:B:304:ARG:NH1	1:B:342:LEU:HD23	0.75	1.97	2	1
1:A:449:PHE:CE1	1:A:451:ILE:HB	0.75	2.16	1	1
1:A:337:GLY:O	1:A:358:ARG:NE	0.75	2.19	2	1
1:A:515:LEU:O	1:A:520:LEU:CD1	0.75	2.30	2	1
1:B:162:ASP:HA	1:B:181:THR:HG21	0.75	1.57	1	1
1:B:449:PHE:CE1	1:B:451:ILE:HB	0.75	2.16	1	1
1:B:111:GLN:CD	2:D:648:PHE:HB3	0.74	2.01	1	2
1:B:317:TYR:OH	1:B:331:VAL:HB	0.74	1.82	1	1
1:A:464:ASP:N	1:A:464:ASP:OD1	0.74	2.14	1	2
1:A:454:ASN:O	1:A:457:THR:HG22	0.74	1.82	2	1
1:A:301:PHE:O	1:A:304:ARG:CD	0.74	2.36	2	1
1:B:362:ILE:CG2	1:B:363:ALA:N	0.74	2.50	2	2
1:A:162:ASP:HA	1:A:181:THR:HG21	0.74	1.57	1	1
1:B:449:PHE:HD2	1:B:499:THR:HA	0.74	1.42	1	1
1:A:175:LYS:HD3	1:A:176:VAL:N	0.74	1.96	2	1
1:A:449:PHE:CD1	1:A:488:VAL:CG1	0.74	2.71	1	1
1:B:292:VAL:HG11	1:B:329:VAL:HG22	0.74	1.59	1	1
1:A:296:ARG:N	1:A:299:PHE:CE2	0.73	2.55	1	1
1:A:362:ILE:CG2	1:A:363:ALA:N	0.73	2.50	2	2
1:A:512:THR:O	1:A:516:LEU:HG	0.73	1.83	2	1
1:B:126:ARG:HH11	2:D:651:GLN:NE2	0.73	1.81	2	1
1:A:314:PHE:CD2	1:A:376:ALA:O	0.73	2.40	1	1
1:A:463:VAL:HG21	1:A:473:LEU:CD2	0.73	2.12	1	1
1:B:314:PHE:CD2	1:B:376:ALA:O	0.73	2.40	1	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:449:PHE:CD1	1:B:488:VAL:CG1	0.73	2.71	1	1
1:B:272:CYS:SG	1:B:293:GLY:CA	0.73	2.76	2	1
1:A:317:TYR:CZ	1:A:331:VAL:HB	0.73	2.18	1	1
1:B:263:THR:OG1	1:B:540:THR:HG23	0.73	1.84	1	1
1:A:272:CYS:SG	1:A:273:ALA:N	0.73	2.62	2	1
1:B:353:PRO:O	1:B:358:ARG:HD3	0.73	1.84	2	1
1:A:10:GLY:O	1:A:11:ILE:HD13	0.73	1.82	1	2
1:B:362:ILE:HG23	1:B:363:ALA:N	0.73	1.99	1	2
1:A:221:ASP:HA	1:A:239:MET:HE2	0.73	1.58	1	2
1:B:232:THR:O	1:B:236:ILE:HG13	0.73	1.84	2	2
1:B:228:TYR:CD2	1:B:235:VAL:HG11	0.73	2.19	1	2
1:A:228:TYR:CD2	1:A:235:VAL:HG11	0.73	2.19	2	2
1:A:272:CYS:SG	1:A:293:GLY:CA	0.73	2.76	2	1
1:B:512:THR:O	1:B:516:LEU:HG	0.73	1.83	2	1
1:B:317:TYR:CZ	1:B:331:VAL:HB	0.73	2.19	1	1
1:B:485:ILE:HD11	1:B:501:MET:SD	0.72	2.24	2	1
1:B:74:GLU:HA	1:B:77:ILE:CG2	0.72	2.14	2	1
1:A:304:ARG:O	1:A:344:TYR:CE1	0.72	2.42	1	1
1:B:456:LEU:O	1:B:456:LEU:HD22	0.72	1.84	1	1
1:A:232:THR:O	1:A:236:ILE:HG13	0.72	1.84	1	2
1:B:530:ILE:O	1:B:530:ILE:HD12	0.72	1.84	2	1
1:A:485:ILE:HD11	1:A:501:MET:SD	0.72	2.24	2	1
1:A:434:ALA:O	1:A:437:THR:OG1	0.72	2.07	1	1
1:B:179:PHE:CZ	1:B:181:THR:OG1	0.72	2.40	1	1
1:B:302:MET:HB2	1:B:342:LEU:HD21	0.72	1.60	1	1
1:A:126:ARG:HD3	2:C:651:GLN:CG	0.72	2.14	1	1
1:A:456:LEU:O	1:A:456:LEU:HD22	0.72	1.84	1	1
1:A:441:HIS:ND1	1:B:556:PRO:HB3	0.72	1.99	2	2
1:B:463:VAL:HG21	1:B:473:LEU:CD2	0.72	2.14	1	1
1:B:10:GLY:O	1:B:11:ILE:HD13	0.72	1.85	1	2
1:A:353:PRO:O	1:A:358:ARG:HD3	0.72	1.84	2	1
1:A:74:GLU:HA	1:A:77:ILE:CG2	0.72	2.14	2	1
1:B:219:ILE:HD11	1:B:236:ILE:HG12	0.72	1.62	2	2
1:B:272:CYS:SG	1:B:273:ALA:N	0.72	2.62	2	1
1:B:80:LEU:HD13	1:B:80:LEU:O	0.72	1.84	2	1
1:B:228:TYR:CB	1:B:231:PRO:HG3	0.72	2.14	1	2
1:A:263:THR:OG1	1:A:540:THR:HG23	0.72	1.84	1	1
1:B:434:ALA:O	1:B:437:THR:OG1	0.72	2.07	1	1
1:A:80:LEU:HD13	1:A:80:LEU:O	0.72	1.84	2	1
1:A:228:TYR:CB	1:A:231:PRO:HG3	0.71	2.14	2	2
1:A:456:LEU:CD1	1:A:457:THR:N	0.71	2.50	1	1



	io ao page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:126:ARG:HD3	2:D:651:GLN:CG	0.71	2.14	1	1
1:A:428:VAL:HG12	1:A:429:MET:O	0.71	1.85	2	1
1:B:304:ARG:O	1:B:344:TYR:CE1	0.71	2.43	1	1
1:B:456:LEU:CD1	1:B:457:THR:N	0.71	2.50	1	1
1:A:362:ILE:HG23	1:A:363:ALA:N	0.71	1.99	1	2
1:A:354:PHE:H	1:B:352:ASN:HD21	0.71	1.27	1	2
1:A:294:LEU:HD11	1:A:332:ARG:NH2	0.71	2.00	2	1
1:A:530:ILE:HD12	1:A:530:ILE:O	0.71	1.85	2	1
1:A:314:PHE:CE2	1:A:376:ALA:C	0.71	2.63	1	1
1:B:314:PHE:CE2	1:B:376:ALA:C	0.71	2.63	1	1
1:A:476:PRO:O	1:A:481:VAL:HG21	0.71	1.85	2	1
1:A:177:LEU:HD12	1:A:177:LEU:C	0.71	2.06	2	1
1:A:431:GLU:CG	1:A:452:GLY:O	0.71	2.28	1	1
1:B:428:VAL:HG12	1:B:429:MET:O	0.71	1.85	2	1
1:A:567:LYS:O	1:A:571:GLU:HG3	0.70	1.87	2	2
1:A:126:ARG:HD3	2:C:651:GLN:HG3	0.70	1.62	1	1
1:A:73:PHE:O	1:A:77:ILE:HG22	0.70	1.87	2	1
1:B:301:PHE:O	1:B:304:ARG:CD	0.70	2.39	2	1
1:A:347:PHE:N	1:A:347:PHE:CD1	0.70	2.59	2	1
1:A:179:PHE:CZ	1:A:181:THR:OG1	0.70	2.40	1	1
1:B:456:LEU:HD11	1:B:481:VAL:HG13	0.70	1.63	1	1
1:B:177:LEU:HD12	1:B:177:LEU:C	0.70	2.06	2	1
1:A:126:ARG:HH11	2:C:651:GLN:NE2	0.70	1.84	2	1
1:B:431:GLU:CD	1:B:455:ASP:HB2	0.70	2.07	1	1
1:B:73:PHE:O	1:B:77:ILE:HG22	0.70	1.87	2	1
1:A:431:GLU:CD	1:A:455:ASP:HB2	0.70	2.07	1	1
1:B:304:ARG:CG	1:B:306:ALA:O	0.70	2.40	2	1
1:A:456:LEU:HD11	1:A:481:VAL:HG13	0.70	1.64	1	1
1:A:90:ILE:HD12	1:A:91:ALA:N	0.70	2.01	1	1
1:B:90:ILE:HD12	1:B:91:ALA:N	0.70	2.01	1	1
1:A:314:PHE:CZ	1:A:375:ARG:C	0.70	2.65	1	1
1:B:567:LYS:O	1:B:571:GLU:HG3	0.69	1.87	2	2
1:B:476:PRO:O	1:B:481:VAL:HG21	0.69	1.85	2	1
1:B:314:PHE:CZ	1:B:375:ARG:C	0.69	2.65	1	1
1:B:11:ILE:HD12	1:B:239:MET:CE	0.69	2.16	2	2
1:A:228:TYR:CG	1:A:235:VAL:HG11	0.69	2.22	2	2
1:B:228:TYR:CG	1:B:235:VAL:HG11	0.69	2.23	1	2
1:A:219:ILE:HD11	1:A:236:ILE:HG12	0.69	1.62	1	2
1:B:372:ASP:CG	1:B:373:GLN:N	0.69	2.45	1	1
1:B:431:GLU:HG3	1:B:452:GLY:C	0.69	2.07	1	1
1:A:11:ILE:HD12	1:A:239:MET:CE	0.69	2.17	2	2



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:304:ARG:NH1	1:A:342:LEU:HD23	0.69	2.03	2	1
1:B:13:PHE:CE2	1:B:240:ARG:HD2	0.69	2.23	1	2
1:A:377:ILE:HD12	1:A:377:ILE:O	0.69	1.87	1	1
1:B:377:ILE:HD12	1:B:377:ILE:O	0.69	1.87	1	1
1:B:6:LEU:HD22	1:B:6:LEU:N	0.69	2.03	2	1
1:A:296:ARG:C	1:A:299:PHE:CE2	0.69	2.66	1	1
1:A:232:THR:HG23	1:A:233:ASN:H	0.69	1.47	1	2
1:B:181:THR:O	1:B:205:THR:CG2	0.69	2.41	1	1
1:B:126:ARG:HD3	2:D:651:GLN:HG3	0.69	1.62	1	1
1:A:556:PRO:HB3	1:B:441:HIS:CG	0.69	2.23	2	2
1:A:456:LEU:C	1:A:456:LEU:HD22	0.69	2.09	1	1
1:B:294:LEU:HD11	1:B:332:ARG:NH2	0.68	2.03	2	1
1:A:181:THR:O	1:A:205:THR:CG2	0.68	2.41	1	1
1:B:107:VAL:HG23	1:B:108:ILE:N	0.68	2.03	2	1
1:B:296:ARG:C	1:B:299:PHE:CE2	0.68	2.66	1	1
1:A:6:LEU:N	1:A:6:LEU:HD22	0.68	2.03	2	1
1:A:467:ASN:ND2	1:A:470:ILE:CG1	0.68	2.56	1	1
1:A:13:PHE:CE2	1:A:240:ARG:HD2	0.68	2.23	2	2
1:A:372:ASP:CG	1:A:373:GLN:N	0.68	2.45	1	1
1:A:464:ASP:CG	1:A:467:ASN:ND2	0.68	2.46	1	1
1:B:314:PHE:CE2	1:B:376:ALA:O	0.68	2.47	1	1
1:A:304:ARG:CG	1:A:306:ALA:O	0.68	2.41	2	1
1:B:301:PHE:O	1:B:304:ARG:NH1	0.68	2.26	2	1
1:A:431:GLU:HG3	1:A:452:GLY:C	0.68	2.06	1	1
1:B:317:TYR:CE2	1:B:386:LEU:HD22	0.68	2.24	1	1
1:B:464:ASP:CG	1:B:467:ASN:ND2	0.68	2.46	1	1
1:B:467:ASN:ND2	1:B:470:ILE:CG1	0.68	2.56	1	1
1:A:314:PHE:CE2	1:A:376:ALA:O	0.68	2.47	1	1
1:A:515:LEU:CB	1:A:520:LEU:CD2	0.68	2.72	2	1
1:A:177:LEU:N	1:A:177:LEU:HD12	0.68	2.03	1	1
1:A:317:TYR:CE1	1:A:331:VAL:HG21	0.68	2.24	1	1
1:B:177:LEU:HD12	1:B:177:LEU:N	0.68	2.03	1	1
1:A:107:VAL:HG23	1:A:108:ILE:N	0.67	2.04	2	1
1:B:456:LEU:C	1:B:456:LEU:HD22	0.67	2.09	1	1
1:A:13:PHE:CG	1:A:240:ARG:NH1	0.67	2.63	2	2
1:A:336:ILE:N	1:A:336:ILE:HD12	0.67	2.05	2	1
1:A:355:LEU:N	1:A:355:LEU:CD2	0.67	2.58	2	1
1:B:13:PHE:CG	1:B:240:ARG:NH1	0.67	2.63	2	2
1:A:515:LEU:CB	1:A:520:LEU:HD21	0.67	2.20	2	1
1:B:157:ILE:CG1	1:B:177:LEU:HD21	0.67	2.19	2	1
1:B:515:LEU:O	1:B:520:LEU:CD2	0.67	2.42	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:352:ASN:HD21	1:B:354:PHE:H	0.67	1.30	2	2
1:B:232:THR:HG23	1:B:233:ASN:H	0.67	1.48	1	2
1:B:296:ARG:CA	1:B:299:PHE:CE2	0.67	2.77	1	1
1:B:263:THR:OG1	1:B:540:THR:O	0.67	2.11	1	1
1:A:304:ARG:O	1:A:344:TYR:OH	0.67	2.12	1	1
1:A:304:ARG:NE	1:A:306:ALA:O	0.67	2.28	2	1
1:B:515:LEU:CB	1:B:520:LEU:CD2	0.67	2.72	2	1
1:B:296:ARG:CB	1:B:299:PHE:CD2	0.67	2.78	1	1
1:A:515:LEU:HB3	1:A:520:LEU:HD13	0.67	1.66	2	1
1:A:314:PHE:CZ	1:A:376:ALA:N	0.67	2.63	1	1
1:A:127:ALA:O	1:A:130:VAL:HG22	0.67	1.90	1	1
1:A:157:ILE:CG1	1:A:177:LEU:HD21	0.67	2.19	2	1
1:B:336:ILE:N	1:B:336:ILE:HD12	0.67	2.05	2	1
1:A:179:PHE:CE1	1:A:190:THR:HG21	0.67	2.25	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CG	0.67	2.21	1	1
1:A:296:ARG:CB	1:A:299:PHE:CD2	0.66	2.79	1	1
1:B:304:ARG:O	1:B:344:TYR:OH	0.66	2.13	1	1
1:A:230:ASN:N	1:A:231:PRO:CD	0.66	2.59	1	2
1:A:296:ARG:CA	1:A:299:PHE:CE2	0.66	2.78	1	1
1:A:292:VAL:HG21	1:A:329:VAL:CG1	0.66	2.18	1	1
1:B:179:PHE:CE1	1:B:190:THR:HG21	0.66	2.26	1	1
1:B:314:PHE:CZ	1:B:376:ALA:N	0.66	2.62	1	1
1:B:230:ASN:N	1:B:231:PRO:CD	0.66	2.59	1	2
1:A:232:THR:HG22	1:A:234:GLU:H	0.66	1.50	1	2
1:B:126:ARG:NH1	2:D:651:GLN:NE2	0.66	2.43	2	1
1:B:515:LEU:C	1:B:520:LEU:HD21	0.66	2.09	2	1
1:B:292:VAL:HG21	1:B:329:VAL:CG1	0.66	2.19	1	1
1:B:296:ARG:CB	1:B:299:PHE:CE2	0.66	2.79	1	1
1:A:175:LYS:CD	1:A:176:VAL:N	0.66	2.59	2	1
1:A:377:ILE:C	1:A:377:ILE:HD12	0.66	2.11	1	1
1:A:70:GLU:CD	1:A:70:GLU:C	0.66	2.55	1	2
1:A:314:PHE:CD2	1:A:379:ARG:HB3	0.66	2.25	1	1
1:B:515:LEU:HB3	1:B:520:LEU:HD13	0.65	1.67	2	1
1:B:515:LEU:CB	1:B:520:LEU:HD21	0.65	2.19	2	1
1:A:263:THR:OG1	1:A:540:THR:O	0.65	2.12	1	1
1:B:259:LEU:HB2	1:B:262:ILE:CG1	0.65	2.21	2	1
1:A:317:TYR:CE2	1:A:386:LEU:HD22	0.65	2.26	1	1
1:B:314:PHE:CD2	1:B:379:ARG:HB3	0.65	2.25	1	1
1:A:515:LEU:O	1:A:520:LEU:CD2	0.65	2.43	2	1
1:A:230:ASN:N	1:A:231:PRO:HD3	0.65	2.07	1	2
1:B:317:TYR:CE1	1:B:331:VAL:HG21	0.65	2.27	1	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:377:ILE:HD12	1:B:377:ILE:C	0.65	2.11	1	1
1:B:355:LEU:N	1:B:355:LEU:CD2	0.65	2.60	2	1
1:A:276:GLY:CA	1:A:299:PHE:CG	0.65	2.80	1	1
1:A:198:GLU:O	1:A:199:LEU:HD22	0.65	1.91	2	1
1:A:10:GLY:O	1:A:222:ALA:HB3	0.65	1.92	1	2
1:A:406:ILE:HD13	1:A:426:ILE:HD13	0.65	1.68	2	2
1:A:476:PRO:C	1:A:481:VAL:HG21	0.65	2.12	2	1
1:B:406:ILE:HD13	1:B:426:ILE:HD13	0.65	1.68	2	2
1:B:438:ILE:O	1:B:438:ILE:HG23	0.65	1.92	1	1
1:A:515:LEU:C	1:A:520:LEU:HD21	0.65	2.11	2	1
1:B:232:THR:HG22	1:B:234:GLU:H	0.65	1.51	2	2
1:B:269:VAL:CG1	1:B:523:PHE:CZ	0.65	2.80	2	1
1:B:70:GLU:CD	1:B:70:GLU:C	0.65	2.55	1	2
1:B:10:GLY:O	1:B:222:ALA:HB3	0.65	1.92	2	2
1:A:331:VAL:HG13	1:A:331:VAL:O	0.65	1.91	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CG	0.65	2.21	1	1
1:A:464:ASP:OD1	1:A:467:ASN:CG	0.65	2.35	2	2
1:B:295:TYR:OH	1:B:300:LEU:HD22	0.65	1.92	1	1
1:A:314:PHE:CE2	1:A:375:ARG:O	0.65	2.50	1	1
1:A:438:ILE:HG22	1:A:441:HIS:HB2	0.64	1.67	2	1
1:A:72:ILE:HD11	2:C:616:THR:HG21	0.64	1.69	2	1
1:B:198:GLU:O	1:B:199:LEU:HD22	0.64	1.91	2	1
1:B:476:PRO:C	1:B:481:VAL:HG21	0.64	2.12	2	1
1:B:374:LEU:HA	1:B:377:ILE:CG2	0.64	2.22	1	1
1:B:230:ASN:N	1:B:231:PRO:HD3	0.64	2.07	1	2
1:A:126:ARG:NH1	2:C:651:GLN:NE2	0.64	2.46	2	1
1:A:295:TYR:OH	1:A:300:LEU:HD22	0.64	1.92	1	1
1:A:357:TRP:CD1	1:A:358:ARG:NH2	0.64	2.66	2	1
1:A:449:PHE:CE1	1:A:488:VAL:HG11	0.64	2.27	1	1
1:B:314:PHE:CE2	1:B:375:ARG:O	0.64	2.50	1	1
1:B:317:TYR:OH	1:B:373:GLN:NE2	0.64	2.30	2	1
1:B:347:PHE:CD1	1:B:347:PHE:N	0.64	2.59	2	1
1:B:175:LYS:CD	1:B:176:VAL:N	0.64	2.59	2	1
1:B:464:ASP:OD1	1:B:467:ASN:CG	0.64	2.36	2	2
1:A:374:LEU:HA	1:A:377:ILE:CG2	0.64	2.22	1	1
1:A:449:PHE:HZ	1:A:451:ILE:HB	0.64	1.50	1	1
1:B:276:GLY:CA	1:B:299:PHE:CG	0.64	2.80	1	1
1:B:525:MET:HG3	1:B:526:SER:N	0.64	2.08	1	1
1:B:451:ILE:CG2	1:B:451:ILE:O	0.64	2.46	1	1
1:B:449:PHE:CE1	1:B:488:VAL:HG11	0.64	2.26	1	1
1:B:70:GLU:CG	1:B:71:ALA:N	0.64	2.61	1	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:438:ILE:O	1:A:438:ILE:HG23	0.64	1.92	1	1
1:A:451:ILE:CG2	1:A:451:ILE:O	0.64	2.46	1	1
1:A:304:ARG:O	1:A:304:ARG:NH1	0.63	2.31	2	1
1:B:464:ASP:OD1	1:B:464:ASP:N	0.63	2.29	2	1
1:B:72:ILE:HD11	2:D:616:THR:HG21	0.63	1.69	2	1
1:B:453:THR:HG22	1:B:503:GLY:HA3	0.63	1.70	1	1
1:B:394:ILE:HD13	1:B:394:ILE:N	0.63	2.00	2	1
1:A:296:ARG:CB	1:A:299:PHE:CE2	0.63	2.80	1	1
1:A:463:VAL:CG2	1:A:473:LEU:HD21	0.63	2.23	1	1
1:A:126:ARG:CD	2:C:616:THR:OG1	0.63	2.46	2	1
1:B:127:ALA:O	1:B:130:VAL:HG22	0.63	1.93	1	1
1:A:301:PHE:O	1:A:304:ARG:NH1	0.63	2.32	2	1
1:B:264:LEU:C	1:B:264:LEU:HD23	0.63	2.13	2	1
1:B:304:ARG:NH1	1:B:304:ARG:O	0.63	2.32	2	1
1:B:357:TRP:CD1	1:B:358:ARG:NH2	0.63	2.66	2	1
1:B:530:ILE:HD12	1:B:530:ILE:C	0.63	2.14	2	1
1:B:11:ILE:HG23	1:B:239:MET:CE	0.63	2.24	1	2
1:A:537:ILE:O	1:A:540:THR:HG22	0.63	1.94	1	1
1:B:342:LEU:HD12	1:B:344:TYR:CE1	0.63	2.29	1	1
1:A:264:LEU:HD23	1:A:264:LEU:C	0.63	2.13	2	1
1:B:537:ILE:O	1:B:540:THR:HG22	0.63	1.93	1	1
1:B:350:GLU:N	1:B:350:GLU:OE2	0.62	2.32	2	1
1:A:525:MET:HG3	1:A:526:SER:N	0.62	2.08	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CZ	0.62	2.24	1	1
1:A:11:ILE:HG23	1:A:239:MET:CE	0.62	2.24	2	2
1:A:441:HIS:CG	1:B:556:PRO:HB3	0.62	2.28	2	2
1:B:331:VAL:O	1:B:331:VAL:HG13	0.62	1.92	1	1
1:B:4:GLY:HA3	1:B:202:ILE:HD11	0.62	1.71	1	1
1:A:304:ARG:HG2	1:A:306:ALA:H	0.62	1.55	2	1
1:B:296:ARG:C	1:B:299:PHE:CZ	0.62	2.72	1	1
1:B:525:MET:CG	1:B:526:SER:N	0.62	2.62	1	1
1:B:50:ALA:O	1:B:54:LEU:CD2	0.62	2.47	2	1
1:A:70:GLU:CG	1:A:71:ALA:N	0.62	2.62	1	1
1:A:394:ILE:HD13	1:A:394:ILE:N	0.62	2.00	2	1
1:B:115:LEU:HD11	2:D:651:GLN:CB	0.62	2.23	2	1
1:B:126:ARG:CD	2:D:616:THR:OG1	0.62	2.47	2	1
1:A:342:LEU:HD12	1:A:344:TYR:CE1	0.62	2.30	1	1
1:A:317:TYR:OH	1:A:373:GLN:NE2	0.62	2.33	2	1
1:B:304:ARG:HG2	1:B:306:ALA:H	0.62	1.54	2	1
1:A:269:VAL:CG1	1:A:523:PHE:CZ	0.62	2.81	2	1
1:B:304:ARG:NE	1:B:306:ALA:O	0.61	2.33	2	1



			$Distance(\text{\AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:173:LEU:N	1:A:173:LEU:HD22	0.61	2.10	1	1
1:A:525:MET:CG	1:A:526:SER:N	0.61	2.62	1	1
1:A:367:ARG:C	1:A:371:ARG:HG3	0.61	2.15	2	1
1:A:115:LEU:HD11	2:C:651:GLN:CB	0.61	2.23	2	1
1:A:296:ARG:C	1:A:299:PHE:CZ	0.61	2.73	1	1
1:A:453:THR:HG22	1:A:503:GLY:HA3	0.61	1.70	1	1
1:A:513:LEU:HD22	1:A:513:LEU:H	0.61	1.53	1	1
1:A:337:GLY:O	1:A:358:ARG:CD	0.61	2.49	2	1
1:A:489:ILE:O	1:A:492:SER:HB2	0.61	1.95	2	2
1:A:530:ILE:HD12	1:A:530:ILE:C	0.61	2.16	2	1
1:A:58:LYS:HB2	1:A:73:PHE:CG	0.61	2.30	2	1
1:B:72:ILE:O	1:B:72:ILE:HD13	0.61	1.95	2	1
1:A:50:ALA:O	1:A:54:LEU:CD2	0.61	2.48	2	1
1:A:73:PHE:CD2	1:A:73:PHE:C	0.61	2.73	2	1
1:B:350:GLU:HB3	1:B:357:TRP:CZ2	0.61	2.31	2	1
1:B:438:ILE:HG22	1:B:441:HIS:HB2	0.61	1.70	2	1
1:A:238:LYS:O	1:A:242:VAL:HG23	0.61	1.95	2	2
1:B:238:LYS:O	1:B:242:VAL:HG23	0.61	1.96	2	2
1:B:58:LYS:HB2	1:B:73:PHE:CG	0.61	2.30	2	1
1:A:111:GLN:NE2	2:C:648:PHE:HB3	0.61	2.10	2	1
1:A:228:TYR:HB3	1:A:231:PRO:CG	0.61	2.25	1	2
2:D:679:LYS:NZ	2:D:683:GLU:OE1	0.61	2.30	2	1
1:B:463:VAL:CG2	1:B:473:LEU:HD21	0.61	2.25	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CZ	0.61	2.25	1	1
1:A:394:ILE:CD1	1:A:394:ILE:N	0.61	2.64	2	1
1:B:111:GLN:NE2	2:D:648:PHE:HB3	0.61	2.10	2	1
1:A:181:THR:O	1:A:205:THR:HG23	0.61	1.95	1	1
1:B:431:GLU:CG	1:B:455:ASP:CB	0.61	2.78	1	1
1:A:78:MET:HE2	2:C:627:LYS:HD3	0.61	1.68	1	1
1:B:337:GLY:O	1:B:358:ARG:CD	0.61	2.49	2	1
1:B:73:PHE:CD2	1:B:73:PHE:C	0.61	2.74	2	1
1:B:228:TYR:HB3	1:B:231:PRO:CG	0.60	2.25	2	2
1:B:360:ILE:CD1	1:B:390:PHE:CD2	0.60	2.84	2	1
1:A:342:LEU:O	1:A:347:PHE:CZ	0.60	2.54	2	1
1:A:402:LEU:C	1:A:402:LEU:HD13	0.60	2.17	2	1
1:A:515:LEU:CB	1:A:520:LEU:CD1	0.60	2.78	2	1
1:A:453:THR:HA	1:A:456:LEU:HD12	0.60	1.73	1	1
1:A:456:LEU:HD13	1:A:457:THR:CA	0.60	2.26	1	1
1:A:350:GLU:N	1:A:350:GLU:OE2	0.60	2.33	2	1
1:B:107:VAL:CG2	1:B:108:ILE:N	0.60	2.64	2	1
1:B:309:THR:OG1	1:B:310:GLU:N	0.60	2.32	2	1



	ious puge		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:513:LEU:H	1:B:513:LEU:HD22	0.60	1.54	1	1
1:A:221:ASP:OD2	1:A:226:GLN:N	0.60	2.34	2	1
1:B:342:LEU:O	1:B:347:PHE:CZ	0.60	2.55	2	1
1:B:394:ILE:CD1	1:B:394:ILE:N	0.60	2.64	2	1
1:A:304:ARG:NH2	1:A:312:GLU:OE2	0.60	2.33	1	1
1:B:179:PHE:CE1	1:B:181:THR:OG1	0.60	2.51	1	1
1:A:73:PHE:CD2	1:A:74:GLU:N	0.60	2.69	2	1
1:A:4:GLY:HA3	1:A:202:ILE:HD11	0.60	1.72	1	1
1:B:173:LEU:N	1:B:173:LEU:HD22	0.60	2.10	1	1
1:B:292:VAL:HG13	1:B:329:VAL:HG22	0.60	1.71	1	1
1:A:269:VAL:HG13	1:A:521:ASP:C	0.60	2.17	2	1
1:B:489:ILE:O	1:B:492:SER:HB2	0.60	1.95	2	2
1:A:350:GLU:HB3	1:A:357:TRP:CZ2	0.60	2.32	2	1
1:A:221:ASP:CA	1:A:239:MET:HE1	0.60	2.27	1	2
1:A:292:VAL:HG13	1:A:329:VAL:HG22	0.60	1.71	1	1
1:B:259:LEU:O	1:B:260:PRO:O	0.60	2.20	1	1
1:A:172:ASN:O	1:A:176:VAL:HG12	0.60	1.97	2	2
1:A:72:ILE:O	1:A:72:ILE:HD13	0.60	1.95	2	1
1:B:221:ASP:OD2	1:B:226:GLN:N	0.60	2.33	2	1
1:B:402:LEU:C	1:B:402:LEU:HD13	0.60	2.16	2	1
1:A:467:ASN:ND2	1:A:470:ILE:HG12	0.60	2.12	1	1
1:B:367:ARG:CZ	1:B:371:ARG:NH2	0.60	2.65	1	1
1:A:302:MET:N	1:A:342:LEU:HD21	0.60	2.12	2	1
1:B:269:VAL:HG13	1:B:521:ASP:C	0.60	2.16	2	1
1:B:515:LEU:CB	1:B:520:LEU:CD1	0.60	2.79	2	1
1:A:262:ILE:N	1:A:537:ILE:CD1	0.59	2.65	2	1
1:A:515:LEU:C	1:A:520:LEU:CD2	0.59	2.70	2	1
1:B:152:ILE:HG21	1:B:175:LYS:CG	0.59	2.27	2	1
1:B:301:PHE:C	1:B:342:LEU:HD21	0.59	2.18	2	1
1:B:73:PHE:CD2	1:B:74:GLU:N	0.59	2.70	2	1
1:A:179:PHE:CE1	1:A:181:THR:OG1	0.59	2.51	1	1
1:B:367:ARG:C	1:B:371:ARG:HG3	0.59	2.15	2	1
2:D:618:PRO:HB3	2:D:684:LEU:HD13	0.59	1.73	2	1
1:B:70:GLU:HG3	1:B:71:ALA:N	0.59	2.13	1	1
1:A:367:ARG:CZ	1:A:371:ARG:NH2	0.59	2.65	1	1
1:B:181:THR:O	1:B:205:THR:HG23	0.59	1.96	1	1
1:A:309:THR:OG1	1:A:310:GLU:N	0.59	2.33	2	1
1:B:259:LEU:CB	1:B:262:ILE:HG12	0.59	2.26	2	1
1:B:262:ILE:N	1:B:537:ILE:CD1	0.59	2.65	2	1
1:A:352:ASN:ND2	1:B:354:PHE:H	0.59	1.96	2	1
1:B:438:ILE:HG22	1:B:438:ILE:O	0.59	1.98	2	1



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:53:GLN:O	1:B:56:THR:OG1	0.59	2.20	2	2
1:A:152:ILE:HG21	1:A:175:LYS:CG	0.59	2.27	2	1
1:A:261:ALA:HA	1:A:537:ILE:HD11	0.59	1.74	2	1
1:B:152:ILE:CG2	1:B:175:LYS:HG3	0.59	2.28	2	1
1:B:302:MET:N	1:B:342:LEU:HD21	0.59	2.12	2	1
1:A:261:ALA:C	1:A:537:ILE:HD13	0.59	2.18	2	1
1:B:172:ASN:O	1:B:176:VAL:HG12	0.59	1.98	2	2
1:A:394:ILE:HG22	1:A:432:THR:HG21	0.59	1.73	1	1
1:B:467:ASN:ND2	1:B:470:ILE:HG12	0.59	2.13	1	1
1:A:221:ASP:OD2	1:A:224:ASN:C	0.58	2.40	2	1
1:A:530:ILE:HG23	1:A:531:PRO:HD3	0.58	1.74	2	1
1:B:221:ASP:OD2	1:B:224:ASN:C	0.58	2.40	2	1
1:B:350:GLU:OE1	1:B:357:TRP:NE1	0.58	2.36	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CD2	0.58	2.33	2	1
1:B:192:ILE:C	1:B:192:ILE:HD12	0.58	2.19	1	1
1:B:453:THR:HA	1:B:456:LEU:HD12	0.58	1.74	1	1
1:A:302:MET:HG2	1:A:342:LEU:CG	0.58	2.28	2	1
1:A:431:GLU:CG	1:A:455:ASP:CB	0.58	2.78	1	1
1:A:449:PHE:CE1	1:A:451:ILE:CB	0.58	2.86	1	1
1:A:107:VAL:CG2	1:A:108:ILE:N	0.58	2.66	2	1
1:A:82:ASP:OD1	1:A:82:ASP:N	0.58	2.35	2	1
1:A:152:ILE:CG2	1:A:175:LYS:HG3	0.58	2.28	2	1
1:A:301:PHE:C	1:A:342:LEU:HD21	0.58	2.18	2	1
1:A:354:PHE:H	1:B:352:ASN:ND2	0.58	1.97	2	1
1:A:53:GLN:O	1:A:56:THR:OG1	0.58	2.21	2	2
1:B:72:ILE:HD11	2:D:616:THR:CG2	0.58	2.28	2	1
1:B:79:LEU:HD11	2:D:648:PHE:CE1	0.58	2.32	2	2
1:A:89:ILE:CD1	1:A:90:ILE:HG23	0.58	2.29	1	1
1:A:79:LEU:HD11	2:C:648:PHE:CE1	0.58	2.34	2	2
1:A:301:PHE:CE1	1:A:304:ARG:CZ	0.58	2.86	2	1
1:B:50:ALA:HB2	1:B:140:ASN:ND2	0.58	2.14	2	1
1:A:126:ARG:HD3	2:C:651:GLN:CD	0.58	2.19	1	1
1:A:421:ASP:OD1	1:A:423:SER:HB2	0.58	1.99	2	2
1:B:449:PHE:CE1	1:B:451:ILE:CB	0.58	2.87	1	1
1:B:456:LEU:HD13	1:B:457:THR:CA	0.58	2.26	1	1
1:B:304:ARG:HE	1:B:306:ALA:C	0.58	2.01	2	1
1:B:358:ARG:CA	1:B:358:ARG:HE	0.58	2.09	2	1
1:B:180:ILE:HD13	1:B:202:ILE:H	0.58	1.59	2	1
1:B:331:VAL:HG11	1:B:377:ILE:HG12	0.58	1.76	2	1
1:B:353:PRO:O	1:B:358:ARG:HD2	0.58	1.98	2	1
1:B:421:ASP:OD1	1:B:423:SER:HB2	0.58	1.99	2	2



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:310:GLU:N	1:B:372:ASP:OD2	0.58	2.37	2	1
1:B:345:MET:HB3	1:B:347:PHE:CE2	0.58	2.34	2	1
1:B:126:ARG:HD3	2:D:651:GLN:CD	0.58	2.19	1	1
1:A:192:ILE:HD12	1:A:192:ILE:C	0.57	2.20	1	1
1:A:276:GLY:O	1:A:299:PHE:CG	0.57	2.55	1	1
1:B:282:GLU:O	1:B:285:GLU:HG2	0.57	1.99	1	1
1:A:50:ALA:HB2	1:A:140:ASN:ND2	0.57	2.14	2	1
1:A:331:VAL:HG11	1:A:377:ILE:HG12	0.57	1.76	2	1
1:A:350:GLU:OE1	1:A:357:TRP:NE1	0.57	2.37	2	1
1:B:515:LEU:C	1:B:520:LEU:CD2	0.57	2.69	2	1
1:B:79:LEU:HD21	2:D:648:PHE:CE2	0.57	2.34	1	2
1:B:470:ILE:HG22	1:B:473:LEU:HB2	0.57	1.76	2	1
1:B:374:LEU:O	1:B:377:ILE:HG23	0.57	1.98	1	1
1:A:357:TRP:HD1	1:A:358:ARG:NH2	0.57	1.98	2	1
1:B:279:ARG:NH2	2:D:685:GLU:OE2	0.57	2.37	2	1
1:B:126:ARG:NH2	2:D:619:ALA:HB1	0.57	2.04	1	1
1:B:115:LEU:HD21	2:D:651:GLN:CB	0.57	2.30	1	1
1:A:180:ILE:HD13	1:A:202:ILE:H	0.57	1.60	2	1
1:B:541:ASN:O	1:B:544:ASP:CG	0.57	2.43	1	2
1:A:232:THR:HG22	1:A:233:ASN:H	0.57	1.35	1	2
1:A:374:LEU:O	1:A:377:ILE:HG23	0.57	1.99	1	1
1:B:520:LEU:CD2	1:B:521:ASP:N	0.57	2.68	1	1
1:A:345:MET:HB3	1:A:347:PHE:CE2	0.57	2.34	2	1
1:A:358:ARG:HE	1:A:358:ARG:CA	0.57	2.09	2	1
1:B:13:PHE:CD2	1:B:240:ARG:NH1	0.57	2.73	2	2
1:B:428:VAL:CG1	1:B:429:MET:O	0.57	2.52	2	1
1:B:82:ASP:OD1	1:B:82:ASP:N	0.57	2.36	2	1
1:A:428:VAL:CG1	1:A:429:MET:O	0.57	2.52	2	1
1:A:79:LEU:HD21	2:C:648:PHE:CE2	0.57	2.35	1	2
1:A:13:PHE:CD2	1:A:240:ARG:NH1	0.57	2.73	2	2
1:A:310:GLU:N	1:A:372:ASP:OD2	0.57	2.36	2	1
1:B:261:ALA:C	1:B:537:ILE:HD13	0.57	2.19	2	1
1:A:221:ASP:CG	1:A:239:MET:SD	0.57	2.83	1	1
1:A:260:PRO:CB	1:A:290:GLU:HG3	0.57	2.30	1	1
1:A:520:LEU:HD22	1:A:522:GLU:H	0.57	1.60	1	1
1:B:89:ILE:CD1	1:B:90:ILE:HG23	0.57	2.30	1	1
1:A:89:ILE:CG2	1:A:90:ILE:N	0.57	2.67	2	1
1:B:252:GLU:OE1	1:B:255:LYS:NZ	0.57	2.32	2	1
1:B:314:PHE:CZ	1:B:375:ARG:O	0.57	2.57	1	1
1:B:394:ILE:HG22	1:B:432:THR:HG21	0.57	1.76	1	1
1:A:520:LEU:CD2	1:A:521:ASP:N	0.56	2.68	1	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:486:LYS:HD2	1:A:553:LEU:HD13	0.56	1.76	2	2
1:A:314:PHE:CZ	1:A:375:ARG:O	0.56	2.57	1	1
1:B:520:LEU:HD22	1:B:522:GLU:H	0.56	1.60	1	1
1:B:486:LYS:HD2	1:B:553:LEU:HD13	0.56	1.75	2	2
1:A:336:ILE:N	1:A:336:ILE:CD1	0.56	2.68	2	1
1:A:515:LEU:CB	1:A:520:LEU:HD11	0.56	2.29	2	1
1:A:541:ASN:O	1:A:544:ASP:CG	0.56	2.43	1	2
1:B:255:LYS:O	1:B:256:LEU:O	0.56	2.23	1	1
1:A:221:ASP:OD1	1:A:222:ALA:N	0.56	2.38	2	1
1:A:353:PRO:O	1:A:358:ARG:HD2	0.56	1.98	2	1
1:A:438:ILE:O	1:A:438:ILE:HG22	0.56	2.00	2	1
1:A:467:ASN:O	1:A:467:ASN:OD1	0.56	2.23	1	2
1:B:221:ASP:CG	1:B:239:MET:SD	0.56	2.84	1	1
1:A:271:VAL:CG2	1:A:271:VAL:O	0.56	2.54	2	1
1:B:89:ILE:CG2	1:B:90:ILE:N	0.56	2.68	2	1
1:A:72:ILE:HD11	2:C:616:THR:CG2	0.56	2.28	2	1
1:B:176:VAL:HG13	1:B:176:VAL:O	0.56	2.00	1	2
1:B:429:MET:SD	1:B:450:SER:OG	0.56	2.64	2	1
1:B:515:LEU:CB	1:B:520:LEU:HD11	0.56	2.30	2	1
1:B:467:ASN:ND2	1:B:470:ILE:HG13	0.56	2.15	1	1
1:A:301:PHE:O	1:A:342:LEU:CD2	0.56	2.54	2	1
1:B:412:GLU:O	1:B:416:GLU:HG3	0.56	2.01	2	2
1:B:464:ASP:O	1:B:467:ASN:OD1	0.56	2.23	1	2
1:A:360:ILE:CD1	1:A:390:PHE:CD2	0.56	2.86	2	1
1:A:470:ILE:HG22	1:A:473:LEU:HB2	0.56	1.77	2	1
1:A:515:LEU:CA	1:A:520:LEU:HD11	0.56	2.30	2	1
1:A:58:LYS:HB2	1:A:73:PHE:CD2	0.56	2.35	2	1
1:A:451:ILE:HD13	1:A:485:ILE:HG12	0.56	1.76	1	1
1:B:78:MET:HE2	2:D:627:LYS:HD3	0.56	1.78	1	1
1:A:176:VAL:O	1:A:176:VAL:HG13	0.56	2.01	1	1
1:B:451:ILE:HD13	1:B:485:ILE:HG12	0.56	1.76	1	1
1:A:115:LEU:HD21	2:C:651:GLN:CB	0.56	2.31	1	1
1:A:352:ASN:HD21	1:B:354:PHE:N	0.56	1.97	1	1
1:A:70:GLU:HG3	1:A:71:ALA:N	0.56	2.14	1	1
1:B:431:GLU:CG	1:B:455:ASP:HB2	0.56	2.31	1	1
1:B:463:VAL:HG21	1:B:473:LEU:HD21	0.56	1.77	1	1
1:A:13:PHE:N	1:A:13:PHE:CD1	0.55	2.74	2	1
1:A:302:MET:CG	1:A:342:LEU:HG	0.55	2.31	2	1
1:B:530:ILE:HG23	1:B:531:PRO:HD3	0.55	1.76	2	1
1:B:467:ASN:O	1:B:467:ASN:OD1	0.55	2.23	1	2
1:A:464:ASP:O	1:A:467:ASN:OD1	0.55	2.24	1	2



		$Olash(\lambda)$	${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:429:MET:SD	1:A:450:SER:OG	0.55	2.64	2	1
1:B:157:ILE:HG12	1:B:177:LEU:HD11	0.55	1.78	2	1
1:B:221:ASP:OD1	1:B:222:ALA:N	0.55	2.38	2	1
1:A:292:VAL:CG2	1:A:329:VAL:CG1	0.55	2.81	1	1
1:B:398:GLU:OE1	1:B:398:GLU:N	0.55	2.39	1	1
1:A:412:GLU:O	1:A:416:GLU:HG3	0.55	2.01	2	2
1:B:117:GLU:N	1:B:117:GLU:OE1	0.55	2.39	2	1
1:B:221:ASP:CA	1:B:239:MET:HE1	0.55	2.30	2	2
1:B:271:VAL:CG2	1:B:271:VAL:O	0.55	2.54	2	1
1:B:357:TRP:HD1	1:B:358:ARG:NH2	0.55	1.98	2	1
1:B:261:ALA:HA	1:B:537:ILE:HD11	0.55	1.77	2	1
1:A:474:TYR:CD2	1:A:474:TYR:O	0.55	2.59	2	2
1:B:58:LYS:CG	1:B:73:PHE:CD2	0.55	2.90	2	1
1:A:167:GLU:OE1	1:A:167:GLU:N	0.55	2.40	1	1
1:B:449:PHE:HZ	1:B:451:ILE:HB	0.55	1.50	1	1
1:B:125:GLU:OE1	1:B:125:GLU:N	0.55	2.38	2	1
1:B:11:ILE:HD12	1:B:239:MET:HE1	0.55	1.77	1	2
1:A:451:ILE:HG22	1:A:501:MET:HG2	0.55	1.79	1	1
1:B:455:ASP:OD1	1:B:459:TYR:CE1	0.55	2.59	1	1
1:A:355:LEU:HD13	1:B:462:ALA:HA	0.55	1.78	2	1
1:A:79:LEU:O	1:A:82:ASP:CG	0.55	2.45	2	1
1:B:474:TYR:O	1:B:474:TYR:CD2	0.55	2.60	2	1
2:D:650:LEU:O	2:D:652:THR:N	0.55	2.40	1	2
1:A:484:LEU:HD23	1:A:485:ILE:N	0.55	2.16	1	1
1:A:68:GLU:N	1:A:68:GLU:CD	0.55	2.60	1	1
1:B:339:ASP:OD2	1:B:465:ARG:NH2	0.55	2.39	1	1
1:A:157:ILE:HG12	1:A:177:LEU:HD11	0.55	1.78	2	1
1:A:253:LEU:O	1:A:257:LYS:NZ	0.55	2.35	2	1
1:A:389:MET:SD	1:A:450:SER:OG	0.55	2.65	2	1
1:A:522:GLU:OE1	1:A:523:PHE:N	0.55	2.39	2	1
1:A:467:ASN:ND2	1:A:470:ILE:HG13	0.55	2.16	1	1
1:A:117:GLU:N	1:A:117:GLU:OE1	0.55	2.40	2	1
1:B:271:VAL:O	1:B:271:VAL:HG23	0.55	2.02	2	1
1:B:272:CYS:SG	1:B:293:GLY:HA3	0.55	2.42	2	1
1:A:354:PHE:N	1:B:352:ASN:HD21	0.55	1.96	1	1
1:A:431:GLU:CG	1:A:455:ASP:HB2	0.55	2.32	1	1
1:B:276:GLY:O	1:B:299:PHE:CG	0.55	2.55	1	1
1:B:451:ILE:HG22	1:B:501:MET:HG2	0.55	1.77	1	1
1:B:79:LEU:O	1:B:82:ASP:CG	0.55	2.46	2	1
2:C:650:LEU:O	2:C:652:THR:N	0.55	2.40	2	2
1:A:456:LEU:HD13	1:A:457:THR:H	0.55	1.58	1	1



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:520:LEU:HD23	1:B:521:ASP:N	0.55	2.17	1	1
1:B:68:GLU:N	1:B:68:GLU:CD	0.55	2.61	1	1
1:B:301:PHE:O	1:B:342:LEU:CD2	0.54	2.54	2	1
1:A:125:GLU:OE1	1:A:125:GLU:N	0.54	2.39	2	1
1:A:58:LYS:CG	1:A:73:PHE:CD2	0.54	2.91	2	1
1:B:13:PHE:CD1	1:B:13:PHE:N	0.54	2.75	1	2
1:A:11:ILE:HD12	1:A:239:MET:HE1	0.54	1.79	1	2
1:A:302:MET:CA	1:A:342:LEU:HD21	0.54	2.32	2	1
1:B:522:GLU:OE1	1:B:523:PHE:N	0.54	2.40	2	1
1:A:520:LEU:HD23	1:A:521:ASP:N	0.54	2.18	1	1
1:B:292:VAL:CG1	1:B:329:VAL:HG13	0.54	2.32	1	1
1:A:152:ILE:HG21	1:A:175:LYS:HG3	0.54	1.79	2	1
1:A:126:ARG:NH2	2:C:619:ALA:HB1	0.54	2.05	1	1
1:A:339:ASP:OD2	1:A:465:ARG:NH2	0.54	2.40	1	1
1:A:271:VAL:HG23	1:A:271:VAL:O	0.54	2.02	2	1
1:B:363:ALA:HB1	1:B:370:LEU:HB2	0.54	1.79	2	2
1:A:68:GLU:CD	1:A:68:GLU:H	0.54	2.06	1	1
1:B:484:LEU:HD23	1:B:485:ILE:N	0.54	2.17	1	1
1:A:476:PRO:O	1:A:481:VAL:HG23	0.54	2.03	2	1
1:B:74:GLU:OE1	1:B:78:MET:SD	0.54	2.65	2	1
1:B:456:LEU:HD13	1:B:456:LEU:C	0.54	2.21	1	1
1:A:304:ARG:HE	1:A:306:ALA:C	0.54	2.05	2	1
1:A:345:MET:CB	1:A:347:PHE:CE2	0.54	2.90	2	1
1:A:405:GLU:HG3	1:A:409:TYR:CE1	0.54	2.38	2	2
1:B:292:VAL:CG2	1:B:329:VAL:CG1	0.54	2.82	1	1
1:B:449:PHE:CD2	1:B:499:THR:HB	0.54	2.38	1	1
1:B:126:ARG:HH21	2:D:619:ALA:HB3	0.54	1.49	1	1
1:A:374:LEU:HA	1:A:377:ILE:HG23	0.54	1.80	1	1
1:B:167:GLU:OE1	1:B:167:GLU:N	0.54	2.40	1	1
1:B:197:LEU:HD13	1:B:197:LEU:O	0.54	2.03	1	1
2:C:679:LYS:NZ	2:C:683:GLU:OE1	0.54	2.36	2	1
1:A:456:LEU:HD13	1:A:456:LEU:C	0.54	2.21	1	1
1:B:372:ASP:OD1	1:B:373:GLN:N	0.54	2.41	1	1
1:A:485:ILE:CG2	1:A:518:MET:SD	0.54	2.96	2	1
1:B:152:ILE:HG21	1:B:175:LYS:HG3	0.54	1.80	2	1
1:B:485:ILE:CG2	1:B:518:MET:SD	0.54	2.96	2	1
1:A:13:PHE:CD1	1:A:13:PHE:N	0.54	2.74	1	1
1:B:456:LEU:HD11	1:B:481:VAL:HG11	0.54	1.78	1	1
1:A:46:GLY:O	1:A:140:ASN:ND2	0.53	2.41	1	1
1:B:474:TYR:CD2	1:B:474:TYR:O	0.53	2.60	1	1
1:B:105:HIS:NE2	1:B:109:GLU:OE1	0.53	2.42	1	2



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:162:ASP:OD1	1:B:163:LEU:N	0.53	2.41	1	1
1:B:296:ARG:HB3	1:B:299:PHE:CD2	0.53	2.37	1	1
1:A:74:GLU:HA	1:A:77:ILE:HG22	0.53	1.80	2	1
1:B:259:LEU:HB2	1:B:262:ILE:HG12	0.53	1.80	2	1
1:B:5:ILE:HD13	1:B:5:ILE:O	0.53	2.03	2	1
1:A:221:ASP:CA	1:A:239:MET:CE	0.53	2.78	1	2
1:A:161:ALA:O	1:A:181:THR:CG2	0.53	2.56	1	1
1:A:197:LEU:HD13	1:A:197:LEU:O	0.53	2.03	1	1
1:B:345:MET:CB	1:B:347:PHE:CE2	0.53	2.91	2	1
1:B:309:THR:C	1:B:372:ASP:OD2	0.53	2.47	2	1
1:B:457:THR:CG2	1:B:458:GLN:N	0.53	2.71	2	1
1:A:221:ASP:OD2	1:A:239:MET:SD	0.53	2.67	1	1
1:A:537:ILE:HG13	1:A:538:ARG:N	0.53	2.19	2	1
1:B:302:MET:CA	1:B:342:LEU:HD21	0.53	2.33	2	1
1:B:336:ILE:CD1	1:B:336:ILE:N	0.53	2.68	2	1
1:B:405:GLU:HG3	1:B:409:TYR:CE1	0.53	2.38	2	2
1:A:296:ARG:HB3	1:A:299:PHE:CD2	0.53	2.38	1	1
1:A:272:CYS:SG	1:A:293:GLY:HA3	0.53	2.43	2	1
1:A:287:ASN:HB3	1:A:530:ILE:HG23	0.53	1.81	2	1
1:A:309:THR:C	1:A:372:ASP:OD2	0.53	2.47	2	1
1:A:363:ALA:HB1	1:A:370:LEU:HB2	0.53	1.79	2	2
1:A:74:GLU:OE1	1:A:78:MET:SD	0.53	2.67	2	1
1:B:358:ARG:HE	1:B:358:ARG:HA	0.53	1.64	2	1
1:A:279:ARG:NH2	2:C:685:GLU:OE2	0.53	2.36	2	1
1:A:292:VAL:CG1	1:A:329:VAL:HG13	0.53	2.33	1	1
1:A:455:ASP:OD1	1:A:459:TYR:CE1	0.53	2.62	1	1
1:A:456:LEU:C	1:A:456:LEU:CD2	0.53	2.77	1	1
1:A:463:VAL:HG11	1:A:473:LEU:CG	0.53	2.14	1	1
1:B:296:ARG:HB2	1:B:299:PHE:CE2	0.53	2.37	1	1
1:B:317:TYR:CZ	1:B:386:LEU:HD13	0.53	2.39	1	1
1:B:454:ASN:O	1:B:458:GLN:OE1	0.53	2.27	1	1
1:A:51:SER:O	1:A:54:LEU:HG	0.53	2.04	2	1
1:B:389:MET:SD	1:B:450:SER:OG	0.53	2.65	2	1
1:A:449:PHE:CD2	1:A:499:THR:HB	0.53	2.39	1	1
1:B:161:ALA:O	1:B:181:THR:CG2	0.53	2.56	1	1
1:A:511:ALA:HB1	1:A:515:LEU:HD13	0.53	1.81	2	1
1:A:296:ARG:HB2	1:A:299:PHE:CE2	0.53	2.38	1	1
1:B:470:ILE:HB	1:B:473:LEU:CD2	0.53	2.34	1	1
1:A:301:PHE:O	1:A:304:ARG:HD2	0.53	2.04	2	1
1:A:457:THR:CG2	1:A:458:GLN:N	0.53	2.72	2	1
1:B:51:SER:O	1:B:54:LEU:HG	0.53	2.04	2	1



	io ao page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:5:ILE:C	1:B:6:LEU:HD22	0.53	2.24	2	1
1:A:246:VAL:CG2	1:A:247:ALA:N	0.53	2.72	1	1
1:B:221:ASP:OD2	1:B:239:MET:SD	0.53	2.67	1	1
1:B:68:GLU:H	1:B:68:GLU:CD	0.53	2.06	1	1
1:A:5:ILE:C	1:A:6:LEU:HD22	0.53	2.25	2	1
1:A:161:ALA:O	1:A:181:THR:HG22	0.53	2.04	1	1
1:B:105:HIS:CE1	1:B:109:GLU:OE1	0.53	2.62	1	1
1:B:199:LEU:O	1:B:199:LEU:CD2	0.53	2.55	1	1
1:A:302:MET:HG2	1:A:342:LEU:HG	0.52	1.80	2	1
1:A:355:LEU:N	1:A:355:LEU:HD23	0.52	2.18	2	1
1:A:511:ALA:HB1	1:A:515:LEU:CD1	0.52	2.34	2	1
1:B:58:LYS:CD	1:B:58:LYS:C	0.52	2.78	2	1
1:A:88:GLU:N	1:A:88:GLU:OE1	0.52	2.42	1	1
1:B:276:GLY:C	1:B:299:PHE:CE1	0.52	2.82	1	1
1:A:79:LEU:O	1:A:82:ASP:OD1	0.52	2.26	2	2
1:B:287:ASN:HB3	1:B:530:ILE:HG23	0.52	1.80	2	1
1:B:476:PRO:O	1:B:481:VAL:HG23	0.52	2.03	2	1
1:B:74:GLU:CA	1:B:77:ILE:HG22	0.52	2.34	2	1
1:A:105:HIS:NE2	1:A:109:GLU:OE1	0.52	2.42	1	2
1:A:70:GLU:CD	1:A:71:ALA:N	0.52	2.62	1	1
1:B:263:THR:HG21	1:B:542:PHE:HB3	0.52	1.80	1	1
1:A:176:VAL:HG13	1:A:176:VAL:O	0.52	2.03	2	1
1:A:58:LYS:CD	1:A:58:LYS:C	0.52	2.78	2	1
1:B:116:GLU:OE2	1:B:131:ARG:NH2	0.52	2.42	2	2
1:A:162:ASP:OD1	1:A:163:LEU:N	0.52	2.42	1	1
1:A:199:LEU:O	1:A:199:LEU:CD2	0.52	2.54	1	1
1:A:205:THR:OG1	1:A:208:VAL:HG13	0.52	2.04	1	1
1:A:276:GLY:C	1:A:299:PHE:CE1	0.52	2.82	1	1
1:A:292:VAL:HG13	1:A:329:VAL:HA	0.52	1.81	1	1
1:A:372:ASP:OD1	1:A:373:GLN:N	0.52	2.42	1	1
1:A:5:ILE:HD13	1:A:5:ILE:O	0.52	2.04	2	1
1:A:449:PHE:CZ	1:A:451:ILE:CB	0.52	2.84	1	1
1:B:88:GLU:OE1	1:B:88:GLU:N	0.52	2.42	1	1
1:A:229:VAL:C	1:A:231:PRO:HD3	0.52	2.25	1	2
1:B:173:LEU:CD2	1:B:173:LEU:N	0.52	2.73	1	1
1:B:205:THR:OG1	1:B:208:VAL:HG13	0.52	2.04	1	1
1:B:303:ASP:OD1	1:B:303:ASP:C	0.52	2.48	1	1
1:B:292:VAL:HG13	1:B:329:VAL:HA	0.52	1.80	1	1
1:B:78:MET:HE1	2:D:627:LYS:CG	0.52	2.34	1	1
1:B:451:ILE:HD11	1:B:488:VAL:HG21	0.52	1.81	2	1
1:B:515:LEU:CA	1:B:520:LEU:HD11	0.52	2.31	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:105:HIS:CE1	1:A:109:GLU:OE1	0.52	2.62	1	1
1:A:470:ILE:C	1:A:473:LEU:HD22	0.52	2.10	1	1
1:A:58:LYS:HG3	1:A:73:PHE:CD2	0.52	2.40	2	1
1:A:74:GLU:CA	1:A:77:ILE:HG22	0.52	2.34	2	1
1:B:301:PHE:CD1	1:B:342:LEU:HD22	0.52	2.39	2	1
1:A:173:LEU:N	1:A:173:LEU:CD2	0.52	2.73	1	1
1:A:255:LYS:O	1:A:256:LEU:HB2	0.52	2.04	1	1
1:A:373:GLN:O	1:A:377:ILE:HG22	0.52	2.04	1	1
1:B:58:LYS:HG3	1:B:73:PHE:CD2	0.52	2.39	2	1
1:A:473:LEU:HD23	1:A:474:TYR:N	0.52	2.20	1	1
1:B:373:GLN:O	1:B:377:ILE:HG22	0.52	2.04	1	1
2:C:675:GLU:O	2:C:678:VAL:HG12	0.52	2.05	1	1
1:A:261:ALA:C	1:A:537:ILE:CD1	0.52	2.78	2	1
1:A:263:THR:HG21	1:A:542:PHE:HB3	0.52	1.80	1	1
1:A:492:SER:HA	1:A:497:LYS:CG	0.52	2.35	1	1
2:D:651:GLN:OE1	2:D:651:GLN:N	0.52	2.43	1	1
1:A:337:GLY:O	1:A:358:ARG:HD3	0.52	2.04	2	1
1:B:337:GLY:O	1:B:358:ARG:HD3	0.52	2.04	2	1
1:B:301:PHE:C	1:B:342:LEU:CD2	0.52	2.78	2	1
1:B:304:ARG:NH2	1:B:344:TYR:HB3	0.52	2.20	2	1
1:B:438:ILE:HG23	1:B:441:HIS:HB2	0.52	1.81	2	1
1:A:357:TRP:HB3	1:B:470:ILE:HD11	0.52	1.82	2	1
1:B:261:ALA:C	1:B:537:ILE:CD1	0.52	2.79	2	1
1:A:438:ILE:O	1:A:438:ILE:CG2	0.52	2.58	1	2
1:B:161:ALA:O	1:B:181:THR:HG22	0.52	2.04	1	1
1:B:456:LEU:HD13	1:B:457:THR:H	0.52	1.58	1	1
1:A:126:ARG:HH21	2:C:619:ALA:HB3	0.52	1.49	1	1
1:B:511:ALA:HB1	1:B:515:LEU:CD1	0.51	2.34	2	1
1:B:492:SER:HA	1:B:497:LYS:CG	0.51	2.35	1	1
1:A:451:ILE:HD11	1:A:488:VAL:HG21	0.51	1.81	2	1
1:B:342:LEU:O	1:B:347:PHE:CE1	0.51	2.63	2	1
1:A:454:ASN:O	1:A:458:GLN:OE1	0.51	2.27	1	1
1:A:342:LEU:O	1:A:347:PHE:CE1	0.51	2.62	2	1
1:B:157:ILE:HG13	1:B:177:LEU:HD21	0.51	1.82	2	1
1:B:305:ASP:O	1:B:344:TYR:CD1	0.51	2.63	2	1
1:B:537:ILE:HG13	1:B:538:ARG:N	0.51	2.19	2	1
1:B:557:THR:HB	1:B:560:GLU:OE1	0.51	2.05	1	2
1:A:156:VAL:O	1:A:177:LEU:HD12	0.51	2.05	1	1
1:A:520:LEU:CD2	1:A:522:GLU:H	0.51	2.19	1	1
1:B:192:ILE:HG13	1:B:193:MET:N	0.51	2.21	1	1
1:B:377:ILE:C	1:B:377:ILE:CD1	0.51	2.77	1	1



	<u> </u>	$Cleat (\lambda)$	${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:70:GLU:CD	1:B:71:ALA:N	0.51	2.63	1	1
1:A:305:ASP:O	1:A:344:TYR:CD1	0.51	2.63	2	1
1:B:511:ALA:HB1	1:B:515:LEU:HD13	0.51	1.81	2	1
1:A:177:LEU:CD1	1:A:177:LEU:H	0.51	2.15	1	1
1:A:317:TYR:CZ	1:A:386:LEU:HD13	0.51	2.40	1	1
1:B:473:LEU:HD23	1:B:474:TYR:N	0.51	2.21	1	1
1:B:520:LEU:CD2	1:B:522:GLU:H	0.51	2.18	1	1
1:A:341:GLU:H	1:A:341:GLU:CD	0.51	2.09	2	1
1:B:157:ILE:HG12	1:B:177:LEU:CG	0.51	2.36	2	1
1:B:394:ILE:H	1:B:394:ILE:CD1	0.51	2.12	2	1
2:C:612:ASN:O	2:C:615:HIS:CE1	0.51	2.64	2	1
1:B:246:VAL:CG2	1:B:247:ALA:N	0.51	2.73	1	1
1:B:456:LEU:CD2	1:B:456:LEU:C	0.51	2.78	1	1
1:A:334:MET:HB2	1:A:336:ILE:HD11	0.51	1.82	2	1
2:C:651:GLN:N	2:C:651:GLN:OE1	0.51	2.43	1	2
1:B:438:ILE:CG2	1:B:438:ILE:O	0.51	2.58	1	2
1:A:192:ILE:HG13	1:A:193:MET:N	0.51	2.20	1	1
1:A:456:LEU:HD11	1:A:481:VAL:HG11	0.51	1.79	1	1
1:B:156:VAL:O	1:B:177:LEU:HD12	0.51	2.05	1	1
1:B:304:ARG:NH2	1:B:312:GLU:OE2	0.51	2.38	1	1
1:A:301:PHE:CD1	1:A:342:LEU:HD22	0.51	2.41	2	1
1:A:449:PHE:CZ	1:A:451:ILE:N	0.51	2.78	1	1
1:A:116:GLU:OE2	1:A:131:ARG:NH2	0.51	2.42	2	2
1:A:304:ARG:O	1:A:304:ARG:HD3	0.51	2.05	2	1
1:A:18:LEU:CD1	1:A:209:THR:OG1	0.51	2.59	1	1
1:B:18:LEU:CD1	1:B:209:THR:OG1	0.51	2.59	1	1
1:B:354:PHE:O	1:B:358:ARG:CZ	0.51	2.59	1	1
2:D:675:GLU:O	2:D:678:VAL:HG12	0.51	2.05	1	1
1:B:229:VAL:C	1:B:231:PRO:HD3	0.51	2.25	2	2
1:B:51:SER:HA	1:B:54:LEU:CD2	0.51	2.31	2	1
1:B:74:GLU:HA	1:B:77:ILE:HG22	0.51	1.80	2	1
1:A:377:ILE:CD1	1:A:377:ILE:C	0.51	2.77	1	1
1:B:158:LEU:O	1:B:180:ILE:HG23	0.51	2.06	1	1
1:B:126:ARG:HG2	2:D:651:GLN:CG	0.51	2.36	2	1
1:A:46:GLY:O	1:A:140:ASN:OD1	0.51	2.29	1	1
1:A:470:ILE:HB	1:A:473:LEU:CD2	0.51	2.35	1	1
1:B:337:GLY:C	1:B:358:ARG:HG2	0.51	2.27	1	1
1:A:358:ARG:HA	1:A:358:ARG:HE	0.50	1.64	2	1
1:B:275:ILE:HG22	1:B:280:ASP:CB	0.50	2.35	2	1
2:D:612:ASN:O	2:D:615:HIS:CE1	0.50	2.64	2	1
2:D:651:GLN:N	2:D:651:GLN:OE1	0.50	2.43	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:331:VAL:O	1:B:331:VAL:CG1	0.50	2.59	1	1
1:B:520:LEU:HD23	1:B:521:ASP:H	0.50	1.65	1	1
1:A:157:ILE:HG12	1:A:177:LEU:CG	0.50	2.36	2	1
1:A:297:THR:HG23	1:A:332:ARG:O	0.50	2.07	2	1
1:A:301:PHE:C	1:A:342:LEU:CD2	0.50	2.79	2	1
1:A:354:PHE:O	1:A:358:ARG:CZ	0.50	2.59	1	1
1:B:374:LEU:HA	1:B:377:ILE:HG23	0.50	1.81	1	1
1:A:272:CYS:HG	1:A:273:ALA:N	0.50	2.04	2	1
1:A:331:VAL:CG1	1:A:331:VAL:O	0.50	2.59	1	1
1:B:449:PHE:CZ	1:B:451:ILE:N	0.50	2.79	1	1
1:B:449:PHE:CZ	1:B:451:ILE:CB	0.50	2.84	1	1
1:B:341:GLU:H	1:B:341:GLU:CD	0.50	2.09	2	1
1:A:556:PRO:HB3	1:B:441:HIS:CE1	0.50	2.41	2	2
1:B:105:HIS:CD2	1:B:109:GLU:OE1	0.50	2.65	2	1
1:B:275:ILE:HG22	1:B:280:ASP:HB3	0.50	1.83	2	1
1:B:463:VAL:CG2	1:B:473:LEU:CD2	0.50	2.87	1	1
1:A:301:PHE:CE1	1:A:304:ARG:NH2	0.50	2.79	2	1
1:A:467:ASN:O	1:A:467:ASN:CG	0.50	2.50	2	1
1:B:79:LEU:O	1:B:82:ASP:OD1	0.50	2.28	2	2
1:A:177:LEU:CD1	1:A:177:LEU:C	0.50	2.78	2	1
1:A:557:THR:HB	1:A:560:GLU:OE1	0.50	2.05	2	2
1:B:350:GLU:OE1	1:B:357:TRP:CZ2	0.50	2.65	2	1
1:A:520:LEU:HD23	1:A:521:ASP:H	0.50	1.65	1	1
1:B:448:PHE:C	1:B:497:LYS:NZ	0.50	2.66	1	1
1:A:226:GLN:OE1	1:A:228:TYR:CZ	0.49	2.65	2	1
1:B:355:LEU:N	1:B:355:LEU:HD23	0.49	2.22	2	1
1:A:337:GLY:C	1:A:358:ARG:HG2	0.49	2.26	1	1
1:B:449:PHE:CE2	1:B:500:GLY:N	0.49	2.80	1	1
1:A:157:ILE:HG13	1:A:177:LEU:HD21	0.49	1.82	2	1
1:A:205:THR:OG1	1:A:208:VAL:CG2	0.49	2.57	1	1
1:A:314:PHE:CG	1:A:376:ALA:HA	0.49	2.37	1	1
1:A:448:PHE:C	1:A:497:LYS:NZ	0.49	2.66	1	1
1:B:46:GLY:O	1:B:140:ASN:ND2	0.49	2.43	1	1
1:A:459:TYR:HB3	1:B:459:TYR:O	0.49	2.07	1	2
1:A:350:GLU:OE1	1:A:357:TRP:CZ2	0.49	2.65	2	1
1:A:358:ARG:CA	1:A:358:ARG:NE	0.49	2.76	2	1
1:B:297:THR:HG23	1:B:332:ARG:O	0.49	2.07	2	1
1:B:511:ALA:O	1:B:515:LEU:HD13	0.49	2.07	2	1
1:B:54:LEU:O	1:B:73:PHE:CE1	0.49	2.66	2	1
1:A:126:ARG:HG2	2:C:651:GLN:CG	0.49	2.37	2	1
1:B:221:ASP:CA	1:B:239:MET:CE	0.49	2.78	1	2



	t i o		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:314:PHE:HE2	1:A:379:ARG:CB	0.49	2.12	1	1
1:B:78:MET:CE	2:D:627:LYS:HB2	0.49	2.38	1	1
1:A:105:HIS:CD2	1:A:109:GLU:OE1	0.49	2.66	2	1
1:B:298:GLU:OE2	1:B:342:LEU:HD11	0.49	2.07	2	1
1:B:356:GLY:C	1:B:358:ARG:HG2	0.49	2.28	2	1
1:B:467:ASN:O	1:B:467:ASN:CG	0.49	2.50	2	1
1:B:51:SER:O	1:B:54:LEU:CD1	0.49	2.61	2	1
1:A:295:TYR:CD2	1:A:331:VAL:HG23	0.49	2.42	1	1
1:B:232:THR:HG22	1:B:233:ASN:H	0.49	1.34	1	1
1:B:89:ILE:HD11	1:B:90:ILE:HG23	0.49	1.85	1	1
1:A:51:SER:O	1:A:54:LEU:CD1	0.49	2.61	2	1
1:A:54:LEU:CD1	1:A:55:GLU:N	0.49	2.69	2	1
1:A:317:TYR:CE1	1:A:331:VAL:CG2	0.49	2.96	1	1
1:A:463:VAL:CG2	1:A:473:LEU:CD2	0.49	2.86	1	1
1:B:317:TYR:OH	1:B:386:LEU:HB3	0.49	2.07	1	1
1:A:275:ILE:HG22	1:A:280:ASP:CB	0.49	2.36	2	1
1:A:511:ALA:O	1:A:515:LEU:HD13	0.49	2.08	2	1
1:B:221:ASP:C	1:B:223:VAL:N	0.49	2.66	2	2
1:A:347:PHE:CD2	1:A:347:PHE:C	0.49	2.86	1	1
1:A:302:MET:HG2	1:A:342:LEU:CD1	0.49	2.37	2	1
1:B:358:ARG:CA	1:B:358:ARG:NE	0.49	2.76	2	1
1:A:86:GLU:O	1:A:90:ILE:CG1	0.49	2.61	1	1
1:B:101:ASP:HB2	1:B:138:LEU:HD21	0.49	1.85	1	1
1:B:263:THR:CG2	1:B:267:HIS:H	0.49	2.14	1	1
1:A:189:HIS:O	1:A:193:MET:SD	0.49	2.70	2	1
1:A:337:GLY:HA3	1:A:358:ARG:NH2	0.49	2.23	2	1
1:A:470:ILE:HD11	1:B:357:TRP:HB3	0.49	1.84	2	1
1:A:233:ASN:O	1:A:237:ASP:OD2	0.49	2.31	1	2
1:A:101:ASP:HB2	1:A:138:LEU:HD21	0.49	1.84	1	1
1:A:342:LEU:HD13	1:A:343:PRO:HD2	0.49	1.85	1	1
1:B:285:GLU:HG3	1:B:286:ARG:N	0.49	2.23	1	1
1:B:295:TYR:CD2	1:B:331:VAL:HG23	0.49	2.43	1	1
1:B:342:LEU:HD13	1:B:343:PRO:HD2	0.49	1.84	1	1
1:B:46:GLY:O	1:B:140:ASN:OD1	0.49	2.30	1	1
1:B:530:ILE:O	1:B:533:ILE:HG12	0.49	2.07	1	1
1:A:54:LEU:O	1:A:73:PHE:CE1	0.48	2.66	2	1
1:B:304:ARG:HD3	1:B:304:ARG:O	0.48	2.08	2	1
1:B:54:LEU:CD1	1:B:55:GLU:N	0.48	2.69	2	1
1:B:74:GLU:CA	1:B:77:ILE:CG2	0.48	2.90	2	1
1:A:78:MET:CE	2:C:627:LYS:HB2	0.48	2.38	1	1
1:B:140:ASN:O	1:B:140:ASN:ND2	0.48	2.46	1	1



		$Ol_{2} = l_{2} \begin{pmatrix} k \\ k \end{pmatrix}$	${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:451:ILE:HG23	1:B:451:ILE:O	0.48	2.08	1	1
1:A:449:PHE:CE2	1:A:500:GLY:N	0.48	2.80	1	1
1:A:89:ILE:HD11	1:A:90:ILE:HG23	0.48	1.83	1	1
1:B:86:GLU:O	1:B:90:ILE:CG1	0.48	2.61	1	1
1:A:345:MET:HB3	1:A:347:PHE:CZ	0.48	2.44	2	1
1:B:350:GLU:OE1	1:B:357:TRP:CE2	0.48	2.67	2	1
1:A:530:ILE:O	1:A:533:ILE:HG12	0.48	2.07	1	1
1:B:177:LEU:H	1:B:177:LEU:CD1	0.48	2.16	1	1
1:B:314:PHE:HE2	1:B:379:ARG:CB	0.48	2.12	1	1
1:A:126:ARG:CD	2:C:651:GLN:NE2	0.48	2.77	1	1
1:A:269:VAL:HG12	1:A:270:GLU:N	0.48	2.23	2	1
1:B:226:GLN:OE1	1:B:228:TYR:CZ	0.48	2.66	2	1
1:B:334:MET:HB2	1:B:336:ILE:HD11	0.48	1.83	2	1
1:B:111:GLN:OE1	2:D:648:PHE:CB	0.48	2.30	1	1
1:A:221:ASP:C	1:A:223:VAL:N	0.48	2.66	2	2
1:A:557:THR:HG22	1:A:560:GLU:H	0.48	1.69	2	2
1:B:189:HIS:O	1:B:193:MET:SD	0.48	2.71	2	1
1:B:233:ASN:O	1:B:237:ASP:OD2	0.48	2.31	2	2
1:B:314:PHE:CE1	1:B:376:ALA:HA	0.48	2.38	1	1
1:B:389:MET:CE	1:B:429:MET:SD	0.48	3.02	2	1
1:A:451:ILE:HG23	1:A:451:ILE:O	0.48	2.08	1	1
1:A:501:MET:CG	1:A:520:LEU:HD11	0.48	2.38	1	1
1:A:85:LEU:HD23	1:A:85:LEU:O	0.48	2.09	2	1
1:B:254:ALA:O	1:B:256:LEU:HD12	0.48	2.09	1	1
1:B:489:ILE:CA	1:B:499:THR:HG21	0.48	2.30	1	1
1:A:219:ILE:CD1	1:A:236:ILE:HG12	0.48	2.36	2	2
1:A:51:SER:HA	1:A:54:LEU:CD2	0.48	2.31	2	1
1:A:158:LEU:HD21	1:A:163:LEU:HD11	0.48	1.85	1	1
1:A:367:ARG:C	1:A:371:ARG:CG	0.48	2.78	2	1
1:A:537:ILE:CG1	1:A:538:ARG:N	0.48	2.77	2	1
1:B:11:ILE:CG2	1:B:239:MET:HE3	0.48	2.39	2	2
1:B:337:GLY:HA3	1:B:358:ARG:NH2	0.48	2.24	2	1
1:A:462:ALA:HA	1:B:355:LEU:HD13	0.48	1.85	2	1
1:B:301:PHE:O	1:B:304:ARG:HD2	0.48	2.06	2	1
1:B:557:THR:HG22	1:B:560:GLU:H	0.48	1.69	1	2
1:A:130:VAL:CG2	1:A:131:ARG:N	0.48	2.77	1	1
1:A:260:PRO:CG	1:A:290:GLU:HG3	0.48	2.39	1	1
1:A:292:VAL:HG11	1:A:329:VAL:HG13	0.48	1.85	1	1
1:A:317:TYR:CZ	1:A:331:VAL:CB	0.48	2.96	1	1
1:A:317:TYR:HD2	1:A:317:TYR:O	0.48	1.91	1	1
1:B:181:THR:HG22	1:B:182:ASP:N	0.48	2.24	1	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:292:VAL:HG11	1:B:329:VAL:HG13	0.48	1.84	1	1
1:B:182:ASP:N	1:B:182:ASP:OD1	0.47	2.47	2	1
1:B:219:ILE:CD1	1:B:236:ILE:HG12	0.47	2.36	2	2
1:B:269:VAL:HG12	1:B:270:GLU:N	0.47	2.23	2	1
1:B:367:ARG:C	1:B:371:ARG:CG	0.47	2.79	2	1
1:A:10:GLY:O	1:A:221:ASP:O	0.47	2.32	1	2
1:A:562:MET:CE	1:A:562:MET:CG	0.47	2.92	1	1
1:B:126:ARG:CD	2:D:651:GLN:NE2	0.47	2.77	1	1
1:B:470:ILE:C	1:B:473:LEU:HD22	0.47	2.09	1	1
1:A:356:GLY:C	1:A:358:ARG:HG2	0.47	2.28	2	1
1:A:58:LYS:HB2	1:A:73:PHE:CD1	0.47	2.43	2	1
1:B:10:GLY:O	1:B:221:ASP:O	0.47	2.32	2	2
1:B:537:ILE:CG1	1:B:538:ARG:N	0.47	2.77	2	1
1:A:317:TYR:OH	1:A:386:LEU:HB3	0.47	2.08	1	1
1:B:177:LEU:N	1:B:177:LEU:CD1	0.47	2.74	1	1
1:B:292:VAL:HG11	1:B:329:VAL:CG2	0.47	2.36	1	1
1:A:256:LEU:O	1:A:257:LYS:C	0.47	2.52	2	1
1:A:360:ILE:HD11	1:A:391:PRO:HD2	0.47	1.86	2	1
1:A:513:LEU:HD22	1:A:513:LEU:N	0.47	2.22	1	1
1:A:501:MET:SD	1:A:515:LEU:HD22	0.47	2.50	1	1
1:A:345:MET:CB	1:A:347:PHE:CZ	0.47	2.97	2	1
1:A:438:ILE:HG23	1:A:441:HIS:HB2	0.47	1.86	2	1
1:B:345:MET:HB3	1:B:347:PHE:CZ	0.47	2.44	2	1
1:B:50:ALA:O	1:B:54:LEU:HD23	0.47	2.09	2	1
1:B:347:PHE:C	1:B:347:PHE:CD2	0.47	2.85	1	1
1:A:58:LYS:HG3	1:A:73:PHE:CE2	0.47	2.44	2	1
1:B:146:ILE:HD13	1:B:146:ILE:N	0.47	2.25	2	1
1:B:301:PHE:CD1	1:B:301:PHE:O	0.47	2.67	2	1
1:B:58:LYS:HG3	1:B:73:PHE:CE2	0.47	2.44	2	1
1:B:158:LEU:HD21	1:B:163:LEU:HD11	0.47	1.85	1	1
1:A:535:LYS:O	1:A:539:ASN:ND2	0.47	2.48	2	1
1:A:74:GLU:O	1:A:77:ILE:CG2	0.47	2.63	2	1
1:B:562:MET:CE	1:B:562:MET:CG	0.47	2.92	2	1
1:A:158:LEU:O	1:A:180:ILE:HG23	0.47	2.09	1	1
1:A:463:VAL:HG21	1:A:473:LEU:HD21	0.47	1.75	1	1
1:A:51:SER:OG	1:A:52:ALA:N	0.47	2.47	1	1
1:B:317:TYR:O	1:B:317:TYR:HD2	0.47	1.91	1	1
1:B:501:MET:CG	1:B:520:LEU:HD11	0.47	2.40	1	1
1:A:182:ASP:N	1:A:182:ASP:OD1	0.47	2.47	2	1
1:A:301:PHE:O	1:A:301:PHE:CD1	0.47	2.68	2	1
1:A:304:ARG:HG2	1:A:306:ALA:O	0.47	2.09	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:287:ASN:O	1:B:530:ILE:CG1	0.47	2.63	2	1
1:B:345:MET:CB	1:B:347:PHE:CZ	0.47	2.98	2	1
1:B:360:ILE:CD1	1:B:390:PHE:CG	0.47	2.98	2	1
2:C:674:VAL:O	2:C:678:VAL:HG23	0.47	2.09	2	1
2:C:679:LYS:HZ1	2:C:683:GLU:CD	0.47	2.13	2	1
1:B:126:ARG:NH1	2:D:651:GLN:CD	0.47	2.68	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CD1	0.47	2.45	2	1
2:D:674:VAL:O	2:D:678:VAL:HG23	0.47	2.10	2	1
1:A:10:GLY:O	1:A:11:ILE:CD1	0.47	2.59	1	2
1:A:11:ILE:CG2	1:A:239:MET:HE3	0.47	2.40	1	2
1:A:126:ARG:O	1:A:130:VAL:HG13	0.47	2.09	1	1
1:B:474:TYR:CG	1:B:474:TYR:O	0.47	2.67	1	1
1:B:489:ILE:HA	1:B:499:THR:CG2	0.47	2.29	1	1
1:B:492:SER:O	1:B:497:LYS:HG2	0.47	2.10	1	1
1:B:259:LEU:CB	1:B:260:PRO:CD	0.47	2.93	1	1
1:B:314:PHE:CG	1:B:376:ALA:HA	0.47	2.37	1	1
1:B:43:PHE:CZ	1:B:47:ARG:NE	0.47	2.82	1	1
1:B:269:VAL:HG12	1:B:270:GLU:O	0.47	2.10	2	1
2:C:679:LYS:NZ	2:C:683:GLU:CD	0.47	2.68	2	1
1:A:398:GLU:OE1	1:A:398:GLU:N	0.47	2.47	1	1
1:A:389:MET:CE	1:A:429:MET:SD	0.47	3.02	2	1
1:B:157:ILE:HG12	1:B:177:LEU:CD1	0.47	2.40	2	1
1:B:470:ILE:O	1:B:470:ILE:HG22	0.47	2.10	2	1
1:B:515:LEU:CD1	1:B:515:LEU:N	0.47	2.78	2	1
1:A:449:PHE:CE1	1:A:488:VAL:CG1	0.47	2.97	1	1
1:A:463:VAL:CG1	1:A:473:LEU:CG	0.47	2.88	1	1
1:A:123:LEU:CD1	1:A:123:LEU:N	0.47	2.78	2	1
1:A:221:ASP:O	1:A:223:VAL:N	0.47	2.48	2	2
1:A:84:GLU:OE2	2:C:648:PHE:CD1	0.47	2.68	2	1
1:B:108:ILE:HG23	1:B:109:GLU:N	0.47	2.25	2	1
1:B:221:ASP:O	1:B:223:VAL:N	0.47	2.48	2	2
1:A:181:THR:HG22	1:A:182:ASP:N	0.47	2.24	1	1
1:B:149:LEU:N	1:B:149:LEU:HD12	0.47	2.25	1	1
1:A:146:ILE:HD13	1:A:146:ILE:N	0.46	2.24	2	1
1:A:350:GLU:OE1	1:A:357:TRP:CE2	0.46	2.68	2	1
1:A:457:THR:HG23	1:A:458:GLN:N	0.46	2.25	2	1
1:A:5:ILE:CD1	1:A:5:ILE:O	0.46	2.63	2	1
1:B:177:LEU:CD1	1:B:177:LEU:C	0.46	2.78	2	1
1:B:515:LEU:HB3	1:B:520:LEU:CD2	0.46	2.40	2	1
1:B:6:LEU:CD2	1:B:6:LEU:N	0.46	2.75	2	1
1:A:140:ASN:O	1:A:140:ASN:ND2	0.46	2.48	1	1



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:149:LEU:N	1:A:149:LEU:HD12	0.46	2.25	1	1
1:A:164:THR:OG1	1:A:167:GLU:OE1	0.46	2.33	1	1
1:A:255:LYS:O	1:A:256:LEU:CB	0.46	2.62	1	1
1:A:369:ILE:O	1:A:372:ASP:OD2	0.46	2.33	1	1
1:B:140:ASN:ND2	1:B:140:ASN:C	0.46	2.68	1	1
1:B:369:ILE:O	1:B:372:ASP:OD2	0.46	2.33	1	1
1:B:51:SER:OG	1:B:52:ALA:N	0.46	2.47	1	1
1:A:515:LEU:N	1:A:515:LEU:CD1	0.46	2.79	2	1
1:B:304:ARG:CZ	1:B:304:ARG:O	0.46	2.63	2	1
1:B:457:THR:HG23	1:B:458:GLN:N	0.46	2.26	2	1
1:A:260:PRO:HG2	1:A:268:GLN:HE21	0.46	1.69	1	1
1:A:330:ILE:N	1:A:330:ILE:CD1	0.46	2.78	1	1
1:A:314:PHE:CE1	1:A:376:ALA:HA	0.46	2.38	1	1
1:A:390:PHE:CD2	1:A:390:PHE:N	0.46	2.80	1	1
1:A:492:SER:O	1:A:497:LYS:HG2	0.46	2.10	1	1
1:A:43:PHE:CE2	1:A:89:ILE:HD13	0.46	2.46	1	1
1:B:304:ARG:NH2	1:B:312:GLU:CD	0.46	2.69	1	1
1:B:501:MET:SD	1:B:515:LEU:HD22	0.46	2.50	1	1
1:A:272:CYS:SG	1:A:273:ALA:O	0.46	2.73	2	1
1:B:74:GLU:O	1:B:77:ILE:CG2	0.46	2.63	2	1
1:A:260:PRO:HG3	1:A:290:GLU:HG3	0.46	1.86	1	1
1:B:147:ILE:HG23	1:B:148:ASP:N	0.46	2.25	1	1
1:B:330:ILE:CD1	1:B:330:ILE:N	0.46	2.78	1	1
1:B:126:ARG:HD3	2:D:651:GLN:NE2	0.46	2.25	1	1
1:A:50:ALA:O	1:A:54:LEU:HD23	0.46	2.09	2	1
1:B:304:ARG:CD	1:B:304:ARG:C	0.46	2.84	2	1
2:C:617:ARG:HB3	2:C:618:PRO:HD3	0.46	1.87	2	1
1:B:5:ILE:O	1:B:6:LEU:O	0.46	2.34	1	2
1:A:43:PHE:CZ	1:A:47:ARG:NE	0.46	2.83	1	1
1:A:113:SER:O	1:A:117:GLU:OE2	0.46	2.34	2	1
1:A:157:ILE:HG12	1:A:177:LEU:CD1	0.46	2.40	2	1
1:A:5:ILE:O	1:A:6:LEU:O	0.46	2.34	1	2
1:A:147:ILE:HG23	1:A:148:ASP:N	0.46	2.25	1	1
1:A:179:PHE:CD2	1:A:179:PHE:C	0.46	2.89	1	1
1:B:179:PHE:CD2	1:B:179:PHE:C	0.46	2.89	1	1
1:B:390:PHE:N	1:B:390:PHE:CD2	0.46	2.79	1	1
1:B:66:GLY:CA	1:B:68:GLU:OE2	0.46	2.64	1	1
1:A:264:LEU:CD2	1:A:264:LEU:C	0.46	2.84	2	1
1:A:269:VAL:HG12	1:A:270:GLU:O	0.46	2.09	2	1
1:B:485:ILE:CG2	1:B:486:LYS:N	0.46	2.79	2	1
1:B:522:GLU:OE1	1:B:523:PHE:O	0.46	2.34	2	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:74:GLU:CA	1:A:77:ILE:CG2	0.46	2.90	2	1
1:B:27:ASP:N	1:B:27:ASP:OD1	0.46	2.48	2	2
1:B:294:LEU:HD23	1:B:294:LEU:C	0.46	2.30	2	1
1:B:85:LEU:O	1:B:85:LEU:HD23	0.46	2.10	2	1
1:A:27:ASP:N	1:A:27:ASP:OD1	0.46	2.49	1	2
1:A:520:LEU:CD2	1:A:520:LEU:C	0.46	2.84	1	1
1:A:333:THR:OG1	1:A:390:PHE:CD1	0.46	2.64	2	1
1:A:470:ILE:HG22	1:A:470:ILE:O	0.46	2.10	2	1
1:B:360:ILE:HD11	1:B:391:PRO:HD2	0.46	1.86	2	1
1:A:11:ILE:CG2	1:A:239:MET:CE	0.46	2.93	1	2
1:A:459:TYR:O	1:B:459:TYR:HB3	0.46	2.10	1	2
1:A:276:GLY:CA	1:A:299:PHE:CZ	0.46	2.95	1	1
1:A:66:GLY:CA	1:A:68:GLU:OE2	0.46	2.64	1	1
1:B:332:ARG:NH1	1:B:335:ASP:N	0.46	2.64	1	1
1:B:520:LEU:CD2	1:B:520:LEU:C	0.46	2.83	1	1
1:A:108:ILE:HG23	1:A:109:GLU:N	0.46	2.25	2	1
1:A:298:GLU:OE2	1:A:342:LEU:HD11	0.46	2.11	2	1
1:B:12:ALA:CB	1:B:177:LEU:HD13	0.46	2.33	2	1
1:B:5:ILE:O	1:B:5:ILE:CD1	0.46	2.63	2	1
1:B:11:ILE:CG2	1:B:239:MET:CE	0.46	2.94	1	2
1:B:130:VAL:CG2	1:B:131:ARG:N	0.46	2.79	1	1
1:B:455:ASP:OD1	1:B:459:TYR:CZ	0.46	2.68	1	1
1:A:6:LEU:CD2	1:A:6:LEU:N	0.46	2.76	2	1
1:B:107:VAL:CG2	1:B:108:ILE:H	0.46	2.24	2	1
1:B:110:GLY:O	1:B:113:SER:OG	0.46	2.31	2	1
1:B:272:CYS:SG	1:B:273:ALA:O	0.46	2.73	2	1
1:B:277:THR:O	1:B:278:VAL:C	0.46	2.54	2	2
1:A:123:LEU:N	1:A:123:LEU:HD12	0.46	2.26	1	2
1:B:449:PHE:CE1	1:B:488:VAL:CG1	0.46	2.97	1	1
1:B:470:ILE:HB	1:B:473:LEU:HD22	0.46	1.86	1	1
1:A:294:LEU:HD23	1:A:294:LEU:C	0.45	2.31	2	1
1:B:259:LEU:CB	1:B:262:ILE:CG1	0.45	2.90	2	1
1:B:10:GLY:O	1:B:11:ILE:CD1	0.45	2.61	1	2
1:A:161:ALA:O	1:A:182:ASP:OD1	0.45	2.34	1	1
1:A:292:VAL:HG11	1:A:329:VAL:CG2	0.45	2.35	1	1
1:B:317:TYR:CE1	1:B:331:VAL:CG2	0.45	2.98	1	1
1:B:66:GLY:N	1:B:68:GLU:OE2	0.45	2.49	1	1
1:A:126:ARG:HD3	2:C:651:GLN:NE2	0.45	2.25	1	1
1:A:177:LEU:CD1	1:A:177:LEU:O	0.45	2.60	2	1
1:A:522:GLU:OE1	1:A:523:PHE:O	0.45	2.35	2	1
1:A:261:ALA:HA	1:A:537:ILE:CD1	0.45	2.41	2	1



	A 4 a 0		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:277:THR:O	1:B:279:ARG:N	0.45	2.49	2	2
1:B:535:LYS:O	1:B:539:ASN:ND2	0.45	2.49	2	1
1:A:470:ILE:HB	1:A:473:LEU:HD22	0.45	1.87	1	1
1:A:4:GLY:HA3	1:A:202:ILE:CD1	0.45	2.42	1	1
1:B:164:THR:OG1	1:B:167:GLU:OE1	0.45	2.33	1	1
1:B:43:PHE:CE2	1:B:89:ILE:HD13	0.45	2.46	1	1
1:A:278:VAL:O	1:A:281:VAL:HG13	0.45	2.10	2	1
1:A:360:ILE:CD1	1:A:390:PHE:CG	0.45	3.00	2	1
1:B:123:LEU:CD1	1:B:123:LEU:N	0.45	2.79	2	1
1:A:126:ARG:NH2	2:C:616:THR:HA	0.45	2.27	1	1
1:B:123:LEU:N	1:B:123:LEU:HD12	0.45	2.26	1	1
1:B:317:TYR:CZ	1:B:331:VAL:CB	0.45	2.97	1	1
2:C:678:VAL:HG13	2:C:679:LYS:N	0.45	2.27	1	1
2:D:617:ARG:HB3	2:D:618:PRO:HD3	0.45	1.87	2	1
1:A:277:THR:O	1:A:279:ARG:N	0.45	2.49	1	2
1:B:87:GLN:O	1:B:90:ILE:HG13	0.45	2.11	1	1
1:A:126:ARG:NE	2:C:651:GLN:NE2	0.45	2.64	1	1
1:B:268:GLN:OE1	1:B:268:GLN:O	0.45	2.35	2	1
1:B:118:LEU:CD2	1:B:118:LEU:N	0.45	2.79	1	1
1:B:513:LEU:HD22	1:B:513:LEU:N	0.45	2.22	1	1
1:B:521:ASP:O	1:B:521:ASP:OD1	0.45	2.35	1	1
1:A:309:THR:HG23	1:A:312:GLU:H	0.45	1.72	2	1
1:B:255:LYS:O	1:B:256:LEU:HB3	0.45	2.12	2	1
1:B:478:SER:HB3	1:B:481:VAL:HG22	0.45	1.88	2	1
1:A:161:ALA:C	1:A:181:THR:CG2	0.45	2.85	1	1
1:B:161:ALA:C	1:B:181:THR:CG2	0.45	2.85	1	1
1:A:11:ILE:HG23	1:A:239:MET:HE2	0.45	1.89	2	2
1:A:12:ALA:HB1	1:A:177:LEU:CD1	0.45	2.34	2	1
1:A:287:ASN:O	1:A:530:ILE:CG1	0.45	2.64	2	1
1:B:264:LEU:C	1:B:264:LEU:CD2	0.45	2.84	2	1
1:B:294:LEU:HD23	1:B:295:TYR:N	0.45	2.27	2	1
1:B:80:LEU:HD13	1:B:80:LEU:C	0.45	2.32	2	1
1:A:118:LEU:N	1:A:118:LEU:CD2	0.45	2.79	1	1
1:A:192:ILE:CD1	1:A:192:ILE:C	0.45	2.85	1	1
1:A:203:VAL:HG22	1:A:203:VAL:O	0.45	2.12	1	1
1:B:161:ALA:O	1:B:182:ASP:OD1	0.45	2.35	1	1
1:B:301:PHE:HD2	1:B:342:LEU:HG	0.45	1.72	1	1
1:B:436:ALA:HB1	1:B:484:LEU:HG	0.45	1.89	1	1
1:A:485:ILE:CG2	1:A:486:LYS:N	0.45	2.79	2	1
1:B:123:LEU:HD12	1:B:123:LEU:N	0.45	2.27	2	1
1:B:301:PHE:O	1:B:304:ARG:HD3	0.45	2.09	2	1



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:162:ASP:HA	1:A:181:THR:CG2	0.45	2.36	1	1
1:A:66:GLY:N	1:A:68:GLU:OE2	0.45	2.49	1	1
1:B:85:LEU:O	1:B:89:ILE:HG23	0.45	2.12	1	1
1:B:78:MET:HE2	2:D:627:LYS:HD2	0.45	1.51	1	1
1:A:121:GLU:O	1:A:125:GLU:OE2	0.45	2.35	2	1
1:A:268:GLN:O	1:A:268:GLN:OE1	0.45	2.35	2	1
1:B:51:SER:O	1:B:54:LEU:CG	0.45	2.65	2	1
1:A:126:ARG:NH1	2:C:651:GLN:CD	0.45	2.71	2	1
1:A:140:ASN:C	1:A:140:ASN:ND2	0.45	2.70	1	1
1:A:301:PHE:HD2	1:A:342:LEU:HG	0.45	1.72	1	1
1:A:317:TYR:OH	1:A:331:VAL:CB	0.45	2.59	1	1
1:A:470:ILE:O	1:A:473:LEU:HD23	0.45	1.94	1	1
1:B:205:THR:OG1	1:B:208:VAL:CG2	0.45	2.58	1	1
1:B:317:TYR:OH	1:B:331:VAL:CB	0.45	2.61	1	1
2:D:678:VAL:HG13	2:D:679:LYS:N	0.45	2.26	1	1
1:A:89:ILE:HD13	1:A:89:ILE:O	0.44	2.12	2	1
1:A:89:ILE:HG13	1:A:90:ILE:H	0.44	1.73	1	1
1:B:463:VAL:HG11	1:B:473:LEU:CG	0.44	2.14	1	1
1:B:90:ILE:CD1	1:B:91:ALA:N	0.44	2.77	1	1
1:B:126:ARG:NE	2:D:651:GLN:NE2	0.44	2.64	1	1
1:A:277:THR:O	1:A:278:VAL:C	0.44	2.54	2	2
1:A:51:SER:O	1:A:54:LEU:CG	0.44	2.65	2	1
1:B:113:SER:O	1:B:117:GLU:OE2	0.44	2.34	2	1
1:B:357:TRP:O	1:B:358:ARG:NH2	0.44	2.50	2	1
1:A:332:ARG:NH1	1:A:335:ASP:N	0.44	2.64	1	1
1:A:90:ILE:CD1	1:A:91:ALA:N	0.44	2.78	1	1
1:B:203:VAL:O	1:B:203:VAL:HG22	0.44	2.12	1	1
1:A:556:PRO:O	1:B:396:VAL:CG2	0.44	2.65	2	2
1:B:121:GLU:O	1:B:125:GLU:OE2	0.44	2.36	2	1
1:B:484:LEU:O	1:B:488:VAL:HG23	0.44	2.12	2	2
1:A:110:GLY:O	1:A:113:SER:OG	0.44	2.32	2	1
1:B:269:VAL:CB	1:B:523:PHE:CZ	0.44	3.00	2	1
1:B:431:GLU:OE1	1:B:431:GLU:O	0.44	2.36	2	1
1:A:489:ILE:CA	1:A:499:THR:HG21	0.44	2.30	1	1
1:A:484:LEU:O	1:A:488:VAL:HG23	0.44	2.12	2	2
1:B:172:ASN:O	1:B:175:LYS:HD2	0.44	2.13	2	1
1:B:521:ASP:OD1	1:B:521:ASP:O	0.44	2.35	2	1
1:A:521:ASP:O	1:A:521:ASP:OD1	0.44	2.34	1	2
1:A:448:PHE:C	1:A:497:LYS:HZ1	0.44	2.15	1	1
1:A:85:LEU:O	1:A:89:ILE:HG23	0.44	2.12	1	1
1:B:138:LEU:O	1:B:141:ILE:CG2	0.44	2.65	1	1



) Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:332:ARG:HH12	1:B:334:MET:HA	0.44	1.72	1	1
1:B:470:ILE:O	1:B:473:LEU:HD23	0.44	1.93	1	1
1:A:225:ASN:OD1	1:A:225:ASN:N	0.44	2.51	2	1
1:A:294:LEU:HD23	1:A:295:TYR:N	0.44	2.27	2	1
1:A:295:TYR:HB3	1:A:331:VAL:HA	0.44	1.90	2	2
1:A:80:LEU:HD13	1:A:80:LEU:C	0.44	2.32	2	1
1:B:54:LEU:HD22	1:B:77:ILE:HD13	0.44	1.90	2	1
2:D:679:LYS:NZ	2:D:683:GLU:CD	0.44	2.71	2	1
1:B:463:VAL:CG1	1:B:473:LEU:CG	0.44	2.89	1	1
2:C:680:LEU:O	2:C:684:LEU:HG	0.44	2.13	1	1
1:A:357:TRP:O	1:A:358:ARG:NH2	0.44	2.50	2	1
1:B:84:GLU:OE2	2:D:648:PHE:CD1	0.44	2.71	2	1
2:C:650:LEU:C	2:C:652:THR:N	0.44	2.71	1	2
1:A:101:ASP:N	1:A:101:ASP:OD1	0.44	2.50	1	1
1:A:455:ASP:OD1	1:A:459:TYR:CZ	0.44	2.70	1	1
1:B:192:ILE:CG1	1:B:193:MET:N	0.44	2.80	1	1
1:B:23:GLU:N	1:B:23:GLU:OE1	0.44	2.45	1	1
1:B:449:PHE:CZ	1:B:500:GLY:O	0.44	2.62	1	1
1:A:302:MET:HG2	1:A:342:LEU:HD11	0.44	1.88	2	1
1:A:515:LEU:HB3	1:A:520:LEU:CD2	0.44	2.41	2	1
1:B:295:TYR:HB3	1:B:331:VAL:HA	0.44	1.90	2	2
1:B:74:GLU:O	1:B:77:ILE:HG23	0.44	2.13	2	1
2:D:650:LEU:C	2:D:652:THR:N	0.44	2.72	2	2
1:A:302:MET:HA	1:A:342:LEU:HD11	0.44	1.90	1	1
1:B:314:PHE:CD2	1:B:376:ALA:C	0.44	2.88	1	1
1:B:126:ARG:NH2	2:D:616:THR:HA	0.44	2.27	1	1
1:A:172:ASN:O	1:A:175:LYS:HD2	0.44	2.13	2	1
1:A:357:TRP:CD1	1:A:358:ARG:CZ	0.44	3.01	2	1
1:B:225:ASN:OD1	1:B:225:ASN:N	0.44	2.50	2	1
1:A:138:LEU:O	1:A:141:ILE:CG2	0.44	2.66	1	1
1:A:85:LEU:O	1:A:89:ILE:CG1	0.44	2.66	1	1
1:B:126:ARG:O	1:B:130:VAL:HG13	0.44	2.12	1	1
1:A:172:ASN:HB2	1:A:175:LYS:CE	0.43	2.43	2	1
1:A:301:PHE:O	1:A:304:ARG:HD3	0.43	2.10	2	1
1:A:50:ALA:HB2	1:A:140:ASN:HD22	0.43	1.73	2	1
1:A:92:LEU:O	1:A:96:LYS:N	0.43	2.50	2	2
1:B:333:THR:OG1	1:B:390:PHE:CD1	0.43	2.63	2	1
1:B:101:ASP:OD1	1:B:101:ASP:N	0.43	2.49	1	2
1:A:263:THR:CG2	1:A:267:HIS:H	0.43	2.14	1	1
1:B:542:PHE:CD1	1:B:543:GLU:N	0.43	2.87	1	1
1:A:301:PHE:CE1	1:A:304:ARG:NE	0.43	2.86	2	1



	A.L. 0		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:516:LEU:CD2	1:A:523:PHE:CZ	0.43	3.01	2	1
1:A:261:ALA:CA	1:A:537:ILE:CD1	0.43	2.96	2	1
1:B:264:LEU:O	1:B:264:LEU:HD23	0.43	2.13	2	1
1:B:515:LEU:N	1:B:515:LEU:HD12	0.43	2.27	2	1
1:A:304:ARG:NH2	1:A:344:TYR:HB3	0.43	2.28	2	1
1:A:530:ILE:C	1:A:530:ILE:CD1	0.43	2.78	2	1
2:C:647:LEU:O	2:C:651:GLN:OE1	0.43	2.36	2	2
1:A:310:GLU:CG	1:A:311:GLU:N	0.43	2.81	1	1
1:A:47:ARG:NH2	1:A:85:LEU:CD2	0.43	2.81	1	1
1:A:87:GLN:O	1:A:90:ILE:HG13	0.43	2.12	1	1
1:B:453:THR:CA	1:B:456:LEU:HD12	0.43	2.42	1	1
1:B:47:ARG:NH2	1:B:85:LEU:CD2	0.43	2.81	1	1
1:B:4:GLY:HA3	1:B:202:ILE:CD1	0.43	2.41	1	1
1:B:84:GLU:O	1:B:88:GLU:OE2	0.43	2.35	1	1
1:A:478:SER:HB3	1:A:481:VAL:HG22	0.43	1.88	2	1
1:B:80:LEU:HD23	1:B:133:ILE:CG2	0.43	2.44	2	1
1:B:89:ILE:O	1:B:89:ILE:HD13	0.43	2.13	2	1
1:A:396:VAL:CG2	1:B:556:PRO:O	0.43	2.66	2	2
1:A:464:ASP:CG	1:A:467:ASN:HB3	0.43	2.33	2	1
1:A:515:LEU:N	1:A:515:LEU:HD12	0.43	2.28	2	1
1:A:192:ILE:CG1	1:A:193:MET:N	0.43	2.80	1	1
1:A:314:PHE:CD2	1:A:376:ALA:C	0.43	2.88	1	1
1:A:332:ARG:HH12	1:A:334:MET:HA	0.43	1.72	1	1
1:A:436:ALA:HB1	1:A:484:LEU:HG	0.43	1.89	1	1
1:B:259:LEU:HB3	1:B:260:PRO:HD2	0.43	1.90	1	1
1:B:310:GLU:CG	1:B:311:GLU:N	0.43	2.81	1	1
1:B:317:TYR:CE1	1:B:377:ILE:HD13	0.43	2.49	1	1
1:A:451:ILE:HB	1:A:501:MET:SD	0.43	2.54	2	1
1:A:473:LEU:CD2	1:B:361:ARG:NE	0.43	2.82	2	1
1:B:516:LEU:CD2	1:B:523:PHE:CZ	0.43	3.02	2	1
1:B:82:ASP:OD2	2:D:648:PHE:HE1	0.43	1.97	2	1
1:A:296:ARG:HB2	1:A:299:PHE:CD2	0.43	2.46	1	1
1:B:276:GLY:CA	1:B:299:PHE:CZ	0.43	2.95	1	1
1:B:448:PHE:C	1:B:497:LYS:HZ1	0.43	2.17	1	1
1:A:107:VAL:CG2	1:A:108:ILE:H	0.43	2.25	2	1
1:A:115:LEU:O	1:A:118:LEU:HB2	0.43	2.14	2	2
1:A:74:GLU:O	1:A:78:MET:HB2	0.43	2.13	2	1
1:A:80:LEU:HD23	1:A:133:ILE:CG2	0.43	2.43	2	1
1:B:126:ARG:NH2	2:D:619:ALA:HB2	0.43	1.88	1	1
1:B:78:MET:CE	2:D:627:LYS:CB	0.43	2.97	1	1
1:A:182:ASP:O	1:A:183:ALA:O	0.43	2.37	2	2



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:264:LEU:HD23	1:A:264:LEU:O	0.43	2.13	2	1
1:A:269:VAL:CB	1:A:523:PHE:CZ	0.43	3.01	2	1
1:A:74:GLU:O	1:A:77:ILE:HG23	0.43	2.13	2	1
1:B:32:SER:OG	1:B:33:ALA:N	0.43	2.52	2	2
1:B:50:ALA:HB2	1:B:140:ASN:HD22	0.43	1.72	2	1
1:B:58:LYS:CB	1:B:73:PHE:CD2	0.43	3.01	2	1
2:D:610:ALA:O	2:D:657:GLN:HB2	0.43	2.14	2	1
1:B:463:VAL:HB	1:B:473:LEU:HD11	0.43	1.90	1	1
1:B:449:PHE:CZ	1:B:499:THR:OG1	0.43	2.52	1	1
1:B:152:ILE:CG2	1:B:175:LYS:CG	0.43	2.95	2	1
1:B:301:PHE:CG	1:B:342:LEU:CD2	0.43	2.91	2	1
1:B:360:ILE:HD11	1:B:390:PHE:CG	0.43	2.49	2	1
1:B:464:ASP:CG	1:B:467:ASN:HB3	0.43	2.34	2	1
1:B:287:ASN:O	1:B:530:ILE:HG12	0.43	2.14	2	1
2:D:647:LEU:O	2:D:651:GLN:OE1	0.43	2.36	1	2
1:A:101:ASP:CB	1:A:138:LEU:HD21	0.43	2.44	1	1
1:A:453:THR:CA	1:A:456:LEU:HD12	0.43	2.42	1	1
1:A:84:GLU:O	1:A:88:GLU:OE2	0.43	2.36	1	1
1:B:243:GLN:C	1:B:243:GLN:CD	0.43	2.78	1	1
1:B:300:LEU:O	1:B:303:ASP:OD1	0.43	2.37	1	1
1:B:11:ILE:HD12	1:B:239:MET:HE3	0.43	1.91	2	1
1:B:547:VAL:O	1:B:551:GLN:HG3	0.43	2.14	2	2
1:B:74:GLU:O	1:B:78:MET:HB2	0.43	2.13	2	1
1:B:182:ASP:O	1:B:183:ALA:O	0.43	2.37	1	2
1:B:8:SER:OG	1:B:199:LEU:O	0.43	2.36	1	2
1:A:243:GLN:C	1:A:243:GLN:CD	0.43	2.77	1	1
1:A:287:ASN:ND2	1:A:528:ILE:HA	0.43	2.28	1	1
1:B:513:LEU:H	1:B:513:LEU:CD2	0.43	2.26	1	1
1:A:485:ILE:HG22	1:A:518:MET:SD	0.42	2.54	2	1
1:B:177:LEU:O	1:B:177:LEU:CD1	0.42	2.60	2	1
1:B:8:SER:CB	1:B:199:LEU:O	0.42	2.67	2	2
1:B:92:LEU:O	1:B:96:LYS:N	0.42	2.50	2	2
1:A:194:ALA:HA	1:A:199:LEU:CD2	0.42	2.45	1	1
1:A:321:ALA:HB2	1:A:386:LEU:HD21	0.42	1.91	1	1
1:A:431:GLU:HG3	1:A:452:GLY:CA	0.42	2.43	1	1
1:A:463:VAL:HB	1:A:473:LEU:HD11	0.42	1.90	1	1
1:B:85:LEU:O	1:B:89:ILE:CG1	0.42	2.66	1	1
1:B:272:CYS:HG	1:B:273:ALA:N	0.42	2.08	2	1
1:B:302:MET:SD	1:B:342:LEU:HG	0.42	2.54	2	1
1:B:357:TRP:CD1	1:B:358:ARG:CZ	0.42	3.02	2	1
1:A:441:HIS:CE1	1:B:556:PRO:HB3	0.42	2.48	2	2



		(1 - 1)		Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:84:GLU:CG	1:B:85:LEU:N	0.42	2.82	2	1
1:A:179:PHE:CZ	HE:CZ 1:A:181:THR:CB		3.02	1	1
1:A:296:ARG:H	1:A:299:PHE:HE2	0.42	1.56	1	1
1:A:431:GLU:CD	1:A:452:GLY:HA3	0.42	2.35	1	1
1:B:296:ARG:H	:ARG:H 1:B:299:PHE:HE2		1.55	1	1
1:B:431:GLU:CD	1:B:452:GLY:HA3	0.42	2.35	1	1
1:B:47:ARG:NH2	1:B:85:LEU:HD21	0.42	2.29		
1:B:285:GLU:CG	1:B:286:ARG:N	0.42	2.82	2	1
1:B:451:ILE:HB	1:B:501:MET:SD	0.42	2.54	2	1
1:A:49:LYS:O	1:A:50:ALA:C	0.42	2.57	1	2
1:A:47:ARG:NH2	1:A:85:LEU:HD21	0.42	2.30	1	1
1:A:542:PHE:CD1	1:A:543:GLU:N	0.42	2.87	1	1
1:B:101:ASP:CB	1:B:138:LEU:HD21	0.42	2.44	1	1
1:A:221:ASP:OD1	1:A:226:GLN:N	0.42	2.52	2	1
1:A:498:TRP:CD1	1:A:498:TRP:N	0.42	2.88	2	1
1:B:172:ASN:HB2	1:B:175:LYS:CE	0.42	2.44	2	1
1:B:309:THR:HG23	1:B:312:GLU:H	0.42	1.74	2	1
2:D:623:VAL:HG13	2:D:644:ALA:O	0.42	2.14	2	2
1:A:32:SER:OG	1:A:33:ALA:N	0.42	2.52	1	2
1:A:449:PHE:CZ 1:A:499:THR:C		0.42	2.52	1	1
1:B:179:PHE:CZ 1:B:181:THR:CB		0.42	3.02	1	1
1:B:371:ARG:O	1:B:371:ARG:O 1:B:375:ARG:HB2		2.15	1	1
1:B:542:PHE:C	1:B:542:PHE:C 1:B:542:PHE:CD1		2.93	1	1
1:A:74:GLU:OE1	:A:74:GLU:OE1 2:C:624:LYS:CE		2.66	1	1
1:A:54:LEU:CD2	1:A:77:ILE:HD13	0.42	2.44	2	1
1:B:157:ILE:HG12	1:B:177:LEU:HD21	0.42	1.89	2	1
1:B:243:GLN:OE1	1:B:243:GLN:C	0.42	2.58	2	1
1:A:8:SER:CB	1:A:199:LEU:O	0.42	2.67	1	2
1:A:449:PHE:CD2	1:A:500:GLY:N	0.42	2.87	1	1
1:A:78:MET:HE1	2:C:627:LYS:CG	0.42	2.43	1	1
1:A:108:ILE:CG2	1:A:109:GLU:N	0.42	2.82	2	1
1:A:84:GLU:CG	1:A:85:LEU:N	0.42	2.82	2	1
1:B:179:PHE:O	1:B:201:ALA:HB1	0.42	2.15	1	2
1:A:371:ARG:O	1:A:375:ARG:HB2	0.42	2.15	1	1
1:A:542:PHE:CD1	1:A:542:PHE:C	0.42	2.93	1	1
1:B:449:PHE:CD2	1:B:500:GLY:N	0.42	2.88	1	1
1:A:504:GLU:O	1:A:504:GLU:OE1	0.42	2.38	2	1
1:A:54:LEU:HD22	1:A:77:ILE:HD13	0.42	1.90	2	1
1:B:115:LEU:O	1:B:118:LEU:HB2	0.42	2.14	2	2
1:B:252:GLU:O	1:B:255:LYS:HG3	0.42	2.14	2	1
1:B:262:ILE:O	1:B:262:ILE:O 1:B:262:ILE:HD12		2.15	2	1



				Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:B:269:VAL:CG1	1:B:270:GLU:N	0.42	2.83	2	1	
1:B:498:TRP:CD1	1:B:498:TRP:N	0.42	2.88	2	1	
1:B:54:LEU:CD2	1:B:77:ILE:HD13	0.42	2.44	2	1	
1:A:8:SER:OG	A:8:SER:OG 1:A:199:LEU:O		2.37	1	2	
1:A:455:ASP:O	1:A:458:GLN:HB2	0.42	2.14	1	1	
1:A:5:ILE:HG22	.:5:ILE:HG22 1:A:5:ILE:O		2.15	1	1	
1:A:72:ILE:HG13	1:A:73:PHE:N	0.42	2.30	1	1	
1:A:547:VAL:O	1:A:551:GLN:HG3	0.42	2.14	2	2	
2:C:623:VAL:HG13	2:C:644:ALA:O	0.42	2.14	1	2	
1:A:449:PHE:CZ	1:A:500:GLY:O	0.42	2.62	1	1	
1:B:520:LEU:HD22	1:B:522:GLU:N	0.42	2.29	1	1	
1:B:72:ILE:HG13	1:B:73:PHE:N	0.42	2.29	1	1	
1:A:301:PHE:CG	1:A:342:LEU:CD2	0.42	2.92	2	1	
1:A:298:GLU:O	1:A:301:PHE:HB3	0.42	2.15	2	1	
1:A:304:ARG:C	1:A:304:ARG:HD3	0.42	2.34	2	1	
1:A:489:ILE:CG1	1:A:499:THR:HG21	0.42	2.32	2	1	
1:B:298:GLU:O	1:B:301:PHE:HB3	0.42	2.14	2	1	
1:B:485:ILE:HG22 1:B:518:MET:SD		0.42	2.54	2	1	
1:B:194:ALA:HA	1:B:194:ALA:HA 1:B:199:LEU:CD2		2.45	1	1	
1:B:455:ASP:O 1:B:458:GLN:HB2		0.42	2.14	1	1	
1:A:243:GLN:OE1	1:A:243:GLN:OE1 1:A:243:GLN:C		2.59	2	1	
1:A:305:ASP:N 1:A:305:ASP:OD1		0.42	2.53	2	1	
1:A:58:LYS:CB	1:A:73:PHE:CD2	0.42	3.03	2	1	
1:B:171:LEU:HD23	1:B:171:LEU:HD23 1:B:175:LYS:NZ		2.30	2	1	
1:B:337:GLY:O	1:B:358:ARG:NH1	0.42	2.52	2	1	
1:B:49:LYS:O	1:B:50:ALA:C	0.42	2.57	2	2	
1:B:302:MET:HA	1:B:342:LEU:HD11	0.42	1.91	1	1	
2:D:649:LYS:O	2:D:652:THR:OG1	0.42	2.36	1	1	
2:D:678:VAL:CG1	2:D:679:LYS:N	0.42	2.82	1	1	
1:A:304:ARG:CD	1:A:304:ARG:C	0.41	2.87	2	1	
1:B:108:ILE:CG2	1:B:109:GLU:N	0.41	2.83	2	1	
1:A:317:TYR:CE1	1:A:331:VAL:CB	0.41	3.02	1	1	
1:B:296:ARG:HB2	1:B:299:PHE:CD2	0.41	2.46	1	1	
1:A:361:ARG:NE	1:B:473:LEU:CD2	0.41	2.84	2	1	
1:B:11:ILE:HG23	1:B:239:MET:HE2	0.41	1.92	1	2	
1:A:456:LEU:CD1	1:A:456:LEU:C	0.41	2.86	1	1	
1:A:513:LEU:CD2	1:A:513:LEU:H	0.41	2.26	1	1	
1:A:78:MET:CE	2:C:627:LYS:CB	0.41	2.98	1	1	
1:B:192:ILE:C	1:B:192:ILE:CD1	0.41	2.84	1	1	
1:B:431:GLU:HG3	1:B:452:GLY:CA	0.41	2.45	1	1	
1:B:89:ILE:HG13 1:B:90:ILE:H		0.41	1.73	1	1	



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:90:ILE:HD12	1:B:90:ILE:C	0.41	2.36	1	1
2:C:678:VAL:CG1	2:C:679:LYS:N	0.41	2.82	1	1
1:A:262:ILE:O	1:A:262:ILE:HD12	0.41	2.15	2	1
1:A:337:GLY:CA	37:GLY:CA 1:A:358:ARG:NH2		2.83	2	1
1:A:337:GLY:O	1:A:358:ARG:NH1	0.41	2.52	2	1
1:B:270:GLU:N	0:GLU:N 1:B:270:GLU:OE1		2.54	2	1
1:B:350:GLU:HB3	1:B:357:TRP:CH2	0.41	2.50	2	1
1:B:72:ILE:CG2	1:B:73:PHE:N	0.41	2.83	2	1
1:A:111:GLN:OE1	2:C:648:PHE:CB	0.41	2.31	1	1
1:A:181:THR:C	1:A:205:THR:CG2	0.41	2.88	1	1
1:B:221:ASP:C	1:B:223:VAL:H	0.41	2.19	1	1
1:B:453:THR:HG21	1:B:505:LEU:HB2	0.41	1.92	1	1
1:B:304:ARG:HG2	1:B:306:ALA:O	0.41	2.10	2	1
1:A:257:LYS:O	1:A:257:LYS:HG3	0.41	2.14	1	1
1:A:78:MET:HE1	2:C:627:LYS:HB2	0.41	1.92	1	1
1:B:181:THR:C	1:B:205:THR:CG2	0.41	2.88	1	1
1:B:302:MET:CB	1:B:342:LEU:HD21	0.41	2.37	1	1
1:B:347:PHE:CE1	1:B:347:PHE:CE1 1:B:348:PRO:O		2.74	1	1
1:B:74:GLU:OE1	1:B:74:GLU:OE1 2:D:624:LYS:CE		2.68	1	1
1:A:221:ASP:C	1:A:221:ASP:C 1:A:223:VAL:H		2.19	2	2
1:A:269:VAL:CG1	1:A:269:VAL:CG1 1:A:270:GLU:N		2.83	2	1
1:A:431:GLU:OE1	A:431:GLU:OE1 1:A:431:GLU:O		2.39	2	1
1:B:307:LEU:HD23	1:B:307:LEU:HD23 1:B:307:LEU:C		2.35	2	1
1:B:337:GLY:CA	337:GLY:CA 1:B:358:ARG:NH2		2.84	2	1
1:B:372:ASP:O	1:B:372:ASP:OD1	0.41	2.38	2	1
1:A:23:GLU:N	1:A:23:GLU:OE1	0.41	2.44	1	1
1:A:393:ILE:O	1:A:393:ILE:CG2	0.41	2.68	1	1
1:A:489:ILE:HA	1:A:499:THR:CG2	0.41	2.30	1	1
1:A:171:LEU:HD23	1:A:175:LYS:NZ	0.41	2.30	2	1
1:A:179:PHE:O	1:A:201:ALA:HB1	0.41	2.15	2	2
1:A:455:ASP:O	1:A:458:GLN:HB3	0.41	2.15	2	1
1:A:484:LEU:CD1	1:B:437:THR:CG2	0.41	2.97	2	1
1:B:12:ALA:HB1	1:B:177:LEU:CD1	0.41	2.33	2	1
1:A:79:LEU:HD22	2:C:647:LEU:HD23	0.41	1.93	2	1
1:A:316:ALA:O	1:A:320:VAL:HG23	0.41	2.16	1	1
1:B:321:ALA:HB2	1:B:386:LEU:HD21	0.41	1.91	1	1
1:A:157:ILE:HG12	1:A:177:LEU:HD21	0.41	1.89	2	1
1:A:307:LEU:HD23	1:A:307:LEU:C	0.41	2.35	2	1
1:A:77:ILE:HG23	1:A:78:MET:N	0.41	2.30	2	1
1:B:357:TRP:C	1:B:358:ARG:NE	0.41	2.74	2	1
1:B:388:ILE:HD12	1:B:388:ILE:HD12 1:B:388:ILE:C		2.34	2	1



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:82:ASP:OD2	2:C:648:PHE:HE1	0.41	1.98	2	1
2:D:679:LYS:O	2:D:683:GLU:N	0.41	2.54	1	2
1:A:181:THR:C	1:A:205:THR:HG23	0.41	2.35	1	1
1:A:310:GLU:CD	A:310:GLU:CD 1:A:310:GLU:N		2.74	1	1
1:A:118:LEU:CD2	1:A:118:LEU:N	0.41	2.84	2	1
1:A:121:GLU:O	GLU:O 1:A:125:GLU:CD		2.59	2	1
1:A:198:GLU:C	1:A:199:LEU:HD22	0.41	2.36	2	1
1:A:214:ASN:OD1	1:A:214:ASN:O	0.41	2.38	2	1
1:A:287:ASN:O	1:A:530:ILE:HG12	0.41	2.15	2	1
1:A:354:PHE:C	1:A:355:LEU:CD2	0.41	2.88	2	1
2:D:617:ARG:CB	2:D:618:PRO:HD3	0.41	2.46	2	1
1:A:197:LEU:O	1:A:197:LEU:CD1	0.41	2.68	1	1
1:A:556:PRO:O	1:B:396:VAL:CG1	0.41	2.68	1	1
1:B:320:VAL:O	1:B:324:CYS:SG	0.41	2.72	1	1
1:A:270:GLU:OE1	1:A:270:GLU:N	0.41	2.54	2	1
1:B:261:ALA:CA	1:B:537:ILE:CD1	0.41	2.98	2	1
1:B:455:ASP:O	1:B:458:GLN:HB3	0.41	2.16	2	1
2:D:618:PRO:HB3 2:D:684:LEU:HD22		0.41	1.92	2	1
1:A:499:THR:O	1:A:499:THR:O 1:A:499:THR:HG23		2.16	2	1
1:B:214:ASN:OD1 1:B:214:ASN:O		0.41	2.38	2	2
1:B:271:VAL:HG12	1:B:271:VAL:HG12 1:B:523:PHE:CD1		2.50	2	1
2:C:679:LYS:O	2:C:679:LYS:O 2:C:683:GLU:N		2.54	2	2
1:A:214:ASN:O	1:A:214:ASN:O 1:A:214:ASN:OD1		2.38	1	1
1:B:197:LEU:O	1:B:197:LEU:O 1:B:197:LEU:CD1		2.68	1	1
1:B:387:ARG:NH1	1:B:425:GLU:OE2	0.41	2.54	1	1
1:B:118:LEU:N	1:B:118:LEU:CD2	0.41	2.84	2	1
1:B:121:GLU:O	1:B:125:GLU:CD	0.41	2.60	2	1
1:B:198:GLU:C	1:B:199:LEU:HD22	0.41	2.36	2	1
1:B:388:ILE:C	1:B:388:ILE:CD1	0.41	2.89	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CE2	0.41	2.51	2	1
1:A:123:LEU:N	1:A:123:LEU:CD1	0.41	2.84	1	1
1:B:162:ASP:HA	1:B:181:THR:CG2	0.41	2.36	1	1
1:B:181:THR:C	1:B:205:THR:HG23	0.41	2.35	1	1
1:B:260:PRO:HG3	1:B:290:GLU:HG3	0.41	1.92	1	1
1:B:317:TYR:CE1	1:B:331:VAL:CB	0.41	3.04	1	1
1:A:232:THR:HG22	:232:THR:HG22 1:A:234:GLU:N		2.27	2	1
1:A:252:GLU:O	1:A:255:LYS:HG2	0.40	2.16	2	1
1:A:367:ARG:O	1:A:368:GLU:C	0.40	2.60	2	2
1:A:485:ILE:HG22	1:A:486:LYS:N	0.40	2.31	2	1
1:A:515:LEU:CA	1:A:520:LEU:CD1	0.40	2.97	2	1
1:B:283:GLY:O 1:B:287:ASN:ND2		0.40	2.53	2	1



				Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:388:ILE:O	1:B:388:ILE:HG13	0.40	2.15	2	1
1:A:204:GLY:O	1:A:205:THR:C	0.40	2.60	1	1
1:A:90:ILE:HD12	1:A:90:ILE:C	0.40	2.36	1	1
1:B:182:ASP:C	1:B:182:ASP:OD1	0.40	2.59	1	1
1:B:316:ALA:O	1:B:320:VAL:HG23	0.40	2.16	1	1
1:A:350:GLU:HB3	1:A:357:TRP:CH2	0.40	2.50	2	1
1:A:365:ASP:OD1	1:A:365:ASP:C	0.40	2.60	2	1
1:B:476:PRO:CA	1:B:481:VAL:HG21	0.40	2.46	2	1
1:B:485:ILE:HG22	1:B:486:LYS:N	0.40	2.31	2	1
1:A:314:PHE:CZ	1:A:379:ARG:HB2	0.40	2.49	1	1
1:A:453:THR:HG21	1:A:505:LEU:HB2	0.40	1.92	1	1
1:B:243:GLN:O	1:B:246:VAL:CG2	0.40	2.42	1	1
1:A:357:TRP:C	1:A:358:ARG:NE	0.40	2.74	2	1
1:B:175:LYS:HD3	1:B:176:VAL:CA	0.40	2.46	2	1
1:B:294:LEU:HD23	1:B:296:ARG:N	0.40	2.31	2	1
1:A:180:ILE:HD11	1:A:208:VAL:HG21	0.40	1.92	1	1
1:A:292:VAL:CG1	1:A:329:VAL:CG2	0.40	2.83	1	1
1:A:11:ILE:HD12 1:A:239:MET:HE3		0.40	1.88	2	1
1:A:360:ILE:HD11	0:ILE:HD11 1:A:390:PHE:CG		2.52	2	1
1:A:354:PHE:CG	1:A:354:PHE:CG 1:A:458:GLN:OE1		2.75	2	1
1:A:72:ILE:CG2	1:A:72:ILE:CG2 1:A:73:PHE:N		2.84	2	1
1:B:186:ARG:C	1:B:188:SER:H	0.40	2.19	2	2
1:B:204:GLY:O	GLY:O 1:B:205:THR:C		2.59	2	1
1:B:304:ARG:HD3	1:B:304:ARG:C	0.40	2.36	2	1
1:B:367:ARG:O	1:B:368:GLU:C	0.40	2.60	2	2
1:B:67:GLU:OE1	1:B:70:GLU:OE1	0.40	2.39	2	1
1:A:130:VAL:HG23	1:A:131:ARG:N	0.40	2.32	1	1
1:A:145:LYS:HG3	1:A:146:ILE:N	0.40	2.32	1	1
1:A:246:VAL:HG23	1:A:247:ALA:N	0.40	2.31	1	1
1:A:276:GLY:C	1:A:299:PHE:CD1	0.40	2.83	1	1
1:A:337:GLY:C	1:A:358:ARG:CG	0.40	2.90	1	1
1:B:305:ASP:HA	1:B:344:TYR:CZ	0.40	2.52	1	1
1:B:393:ILE:O	1:B:393:ILE:CG2	0.40	2.68	1	1
1:A:388:ILE:O	1:A:388:ILE:HG13	0.40	2.15	2	1
1:B:302:MET:HG3	1:B:302:MET:O	0.40	2.16	2	1
1:B:354:PHE:CG	1:B:458:GLN:OE1	0.40	2.75	2	1
2:C:657:GLN:O	2:C:657:GLN:HG3	0.40	2.17	2	1
1:A:182:ASP:C	1:A:182:ASP:OD1	0.40	2.59	1	1
1:A:347:PHE:CE1	1:A:348:PRO:O	0.40	2.75	1	1
1:A:470:ILE:CG2	1:A:473:LEU:HD13	0.40	2.46	1	1
1:B:173:LEU:CD2	173:LEU:CD2 1:B:173:LEU:H		2.29	1	1



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Atom-1	Atom-2	$\mathrm{Clash}(\mathrm{\AA})$	$\operatorname{Distance}(\operatorname{\AA})$	Models	
				Worst	Total
1:B:310:GLU:N	1:B:310:GLU:CD	0.40	2.74	1	1

5.2 Torsion angles (i)

5.2.1 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	Perce	ntiles
1	А	570/573~(99%)	$538 \pm 1 \ (94 \pm 0\%)$	$26 \pm 1 \ (4 \pm 0 \%)$	7±0 (1±0%)	17	64
1	В	569/573~(99%)	$536 \pm 1 \ (94 \pm 0\%)$	$26 \pm 1 \ (5 \pm 0 \%)$	7±0 (1±0%)	17	64
2	С	83/85~(98%)	76 ± 0 (92 $\pm0\%$)	$6{\pm}0~(7{\pm}0\%)$	1±0 (1±0%)	17	64
2	D	83/85~(98%)	76 ± 0 (92 $\pm0\%$)	$6{\pm}0~(7{\pm}0\%)$	1±0 (1±0%)	17	64
All	All	2610/2632~(99%)	2451~(94%)	127~(5%)	32~(1%)	17	64

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	183	ALA	2
1	В	183	ALA	2
1	А	260	PRO	2
1	А	6	LEU	2
2	D	651	GLN	2
1	В	232	THR	2
1	А	232	THR	2
1	В	6	LEU	2
1	А	148	ASP	2
1	А	278	VAL	2
1	В	148	ASP	2
1	В	278	VAL	2
2	С	651	GLN	2
1	В	255	LYS	1
1	В	256	LEU	1
1	В	254	ALA	1
1	А	256	LEU	1



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Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	А	257	LYS	1
1	В	260	PRO	1

5.2.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	473/474~(100%)	$409\pm5~(86\pm1\%)$	$65\pm5(14\pm1\%)$	7	47
1	В	472/474~(100%)	$406 \pm 4 \ (86 \pm 1\%)$	$66 \pm 4 (14 \pm 1\%)$	6	46
2	С	70/70~(100%)	63 ± 2 (90 $\pm3\%$)	$7\pm2~(10\pm3\%)$	11	56
2	D	70/70~(100%)	64 ± 2 (91 $\pm2\%$)	$7\pm2(9\pm2\%)$	12	59
All	All	2170/2176~(100%)	1882 (87%)	288 (13%)	7	48

All 227 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	В	404	LYS	2
1	А	58	LYS	2
1	А	27	ASP	2
1	В	307	LEU	2
1	А	474	TYR	2
1	В	396	VAL	2
1	А	520	LEU	2
1	А	80	LEU	2
1	А	388	ILE	2
1	В	240	ARG	2
1	А	402	LEU	2
1	В	347	PHE	2
1	В	215	ASP	2
1	В	464	ASP	2
1	А	396	VAL	2
1	А	32	SER	2
1	В	402	LEU	2
2	С	641	SER	2
1	А	240	ARG	2



			us puye	
Mol	Chain	Res	Type	Models (Total)
2	D	630	THR	2
1	В	455	ASP	2
1	А	411	GLN	2
1	А	455	ASP	2
1	В	423	SER	2
2	С	630	THR	2
1	В	28	ARG	2
1	В	372	ASP	2
1	А	215	ASP	2
1	А	372	ASP	2
1	В	213	LYS	2
1	В	27	ASP	2
1	В	334	MET	2
1	А	28	ARG	2
1	А	561	LEU	2
1	В	411	GLN	2
1	А	557	THR	2
1	А	404	LYS	2
1	А	464	ASP	2
2	D	651	GLN	2
1	В	520	LEU	2
2	С	651	GLN	2
1	А	209	THR	2
1	В	557	THR	2
2	D	643	SER	2
1	A	213	LYS	2
1	А	423	SER	2
1	А	216	ASP	2
1	А	334	MET	2
1	А	347	PHE	2
1	В	80	LEU	2
1	В	32	SER	2
2	С	643	SER	2
1	А	299	PHE	2
1	В	58	LYS	2
1	В	299	PHE	2
1	В	474	TYR	2
1	В	388	ILE	2
1	В	561	LEU	2
1	В	216	ASP	2
1	A	307	LEU	2
2	D	641	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	В	470	ILE	1
2	D	676	HIS	1
1	В	262	ILE	1
1	В	85	LEU	1
1	А	189	HIS	1
1	В	182	ASP	1
1	В	89	ILE	1
1	А	179	PHE	1
1	В	125	GLU	1
1	А	199	LEU	1
1	В	350	GLU	1
1	А	317	TYR	1
1	В	281	VAL	1
1	В	355	LEU	1
1	А	192	ILE	1
1	В	137	LEU	1
1	В	140	ASN	1
1	В	317	TYR	1
1	В	205	THR	1
1	А	163	LEU	1
1	А	392	MET	1
1	А	140	ASN	1
1	А	125	GLU	1
1	В	398	GLU	1
1	В	146	ILE	1
1	В	73	PHE	1
1	А	137	LEU	1
1	В	72	ILE	1
1	В	47	ARG	1
1	В	332	ARG	1
1	В	209	THR	1
1	А	484	LEU	1
1	В	367	ARG	1
1	A	523	PHE	1
1	В	360	ILE	1
1	В	77	ILE	1
1	A	473	LEU	1
1	А	379	ARG	1
1	А	431	GLU	1
1	А	78	MET	1
1	А	77	ILE	1
1	А	449	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	В	189	HIS	1
1	В	530	ILE	1
1	А	72	ILE	1
1	А	180	ILE	1
1	А	277	THR	1
1	А	205	THR	1
1	А	360	ILE	1
1	В	390	PHE	1
1	А	88	GLU	1
1	А	70	GLU	1
1	В	499	THR	1
2	D	607	THR	1
1	А	286	ARG	1
2	D	614	LEU	1
1	А	350	GLU	1
1	А	309	THR	1
1	А	73	PHE	1
1	А	281	VAL	1
1	А	268	GLN	1
2	С	615	HIS	1
1	А	197	LEU	1
1	В	310	GLU	1
1	В	529	SER	1
1	В	117	GLU	1
1	А	513	LEU	1
1	А	304	ARG	1
1	В	76	HIS	1
1	В	456	LEU	1
1	В	272	CYS	1
1	В	256	LEU	1
1	A	529	SER	1
1	В	473	LEU	1
1	A	272	CYS	1
1	В	88	GLU	1
1	A	355	LEU	1
1	В	70	GLU	1
2	С	683	GLU	1
1	В	523	PHE	1
1	В	199	LEU	1
1	В	431	GLU	1
1	В	171	LEU	1
1	В	5	ILE	1



2X	DF

Mol	Chain	Res	Type	Models (Total)
1	А	451	ILE	1
1	А	138	LEU	1
1	А	146	ILE	1
2	С	614	LEU	1
1	В	326	SER	1
1	В	309	THR	1
1	В	197	LEU	1
1	В	484	LEU	1
1	А	480	SER	1
1	А	499	THR	1
1	В	150	SER	1
1	В	502	CYS	1
1	А	501	MET	1
1	В	192	ILE	1
2	С	607	THR	1
1	А	470	ILE	1
1	В	379	ARG	1
1	А	175	LYS	1
1	А	117	GLU	1
1	А	377	ILE	1
1	А	187	THR	1
1	В	268	GLN	1
1	В	336	ILE	1
1	В	485	ILE	1
1	В	78	MET	1
1	В	193	MET	1
1	А	182	ASP	1
1	В	138	LEU	1
1	В	330	ILE	1
1	В	144	LEU	1
1	В	513	LEU	1
1	А	344	TYR	1
1	В	303	ASP	1
1	В	175	LYS	1
1	А	336	ILE	1
2	C	$6\overline{12}$	ASN	1
1	В	292	VAL	1
1	A	485	ILE	1
1	B	$39\overline{4}$	ILE	1
1	А	313	GLN	1
1	A	502	CYS	1
1	А	332	ARG	1



Mol	Chain	Res	Type	Models (Total)
1	В	344	TYR	1
1	В	451	ILE	1
1	А	367	ARG	1
1	В	377	ILE	1
1	В	541	ASN	1
1	В	304	ARG	1
1	В	302	MET	1
1	А	171	LEU	1
1	А	398	GLU	1
1	А	530	ILE	1
1	В	313	GLN	1
1	А	330	ILE	1
2	С	676	HIS	1
1	А	456	LEU	1
1	А	310	GLU	1
1	В	180	ILE	1
1	А	144	LEU	1
1	В	501	MET	1
1	В	163	LEU	1
1	А	89	ILE	1
1	В	179	PHE	1
1	А	193	MET	1
1	А	262	ILE	1
1	А	150	SER	1
1	В	480	SER	1
1	А	358	ARG	1
1	В	449	PHE	1
1	А	47	ARG	1
1	В	392	MET	1
1	A	394	ILE	1
1	A	5	ILE	1
2	D	683	GLU	1
1	A	390	PHE	1
1	A	85	LEU	1
1	В	259	LEU	1
2	D	615	HIS	1
1	A	292	VAL	1
1	В	187	THR	1
1	A	76	HIS	1
1	В	358	ARG	1

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5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

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

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

No chemical shift data were provided

