

Full wwPDB NMR Structure Validation Report (i)

Oct 23, 2021 – 01:49 PM EDT

PDB ID : 1BUQ Title : SOLUTION STRUCTURE OF DELTA-5-3-KETOSTEROID ISOMERASE COMPLEXED WITH THE STEROID 19-NORTESTOSTERONE-HEMISU CCINATE Authors : Massiah, M.A.; Abeygunawardana, C.; Gittis, A.G.; Mildvan, A.S. Deposited on : 1998-09-04

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	$egin{array}{c} { m NMR} \ { m archive} \ (\#{ m Entries}) \end{array}$
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		Quality of chain		
1	А	125	9%	64%	24%	••
1	В	125	11%	62%	23%	••



2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

	Well-de	efined (core) p	protein residues	
Well-defined core	Residue ran	nge (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:125,	B:201-B:323	0.83	5
	(246)			

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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



3 Entry composition (i)

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

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

Mol	Chain	Residues			Aton	ns			Trace
1	Δ	195	Total	С	Η	Ν	0	S	0
	A	120	1873	597	930	165	178	3	0
1	В	195	Total	С	Η	Ν	0	S	0
	D	120	1873	597	930	165	178	3	

There are 4 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is SUCCINIC ACID MONO-(13-METHYL-3-OXO-2,3,6,7,8,9,10,11,12,13,14,1 5,16,17-TETRADECAHYDRO-1H-CYCLOPENTA[A]PHENANTHREN-17-YL) ESTER (three-letter code: NTH) (formula: $C_{22}H_{30}O_5$).



$\begin{bmatrix} 2 & A & 1 & \begin{bmatrix} Total & C & H & O \\ 56 & 22 & 29 & 5 \end{bmatrix}$	Mol	Chain	Residues	I	4ton	ns	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0	٨	1	Total	С	Η	0
	Ζ	А	1	56	22	29	5



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Mol	Chain	Residues	I	Aton	ns	
0	D	1	Total	С	Η	Ο
	D	1	56	22	29	5



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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



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



4.2 Scores per residue for each member of the ensemble

Colouring as in section $4.1\ {\rm above.}$



4.2.1 Score per residue for model 1

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



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



4.2.2 Score per residue for model 2

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





4.2.3 Score per residue for model 3

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



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



4.2.4 Score per residue for model 4





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



4.2.5 Score per residue for model 5 (medoid)

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



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



4.2.6 Score per residue for model 6





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



4.2.7 Score per residue for model 7

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





4.2.8 Score per residue for model 8





1121 H122 A123 G124 A125

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



4.2.9 Score per residue for model 9

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



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



4.2.10 Score per residue for model 10

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

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L63 L63 L65 L65 L65 L65 L65 L65 L65 L66 L67 L67 L66 L67 L67 L66 L67 L66 L67 L66 L67 L68 L69 L60 L60 L60 L610 L100 L100 L110 L115 L116 L115 L115 L112

H122 A125

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



4.2.11 Score per residue for model 11

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

Chain A:	15%	54%	28% ••
M1 N2 F4 H6 M7	V10 V11 Q12 Q12 V15 V15 A17 L18 V18	A20 621 621 123 123 124 123 123 123 123 123 123 133 133 133 133	D38 V40 V40 G41 542 543 746 746 647 151 151 151 155 756 756 756 756 756 756 756 756 756 7
P62 L63 A64 V65 E66 L67 T68 Q69	E70 V71 R72 R72 V74 A75 A75 A75 B779	481 F82 F83 F83 F84 F88 F88 F88 F88 F97 F93 F97 F97 F97 F97 F97 F97 F97 F97 F97 F97	H100 F101 R102 F103 F103 F103 R105 A105 A114 A115 A114 A115 C117 C117 C117 C117 C117 C117 C117 C

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



4.2.12 Score per residue for model 12



Mill Mill 13 13 14 14 17 14 17 14 17 14 14 14 14 14 14 14 14 14 15 12 14 12 15 12 125 125 126 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 128 129 128 129 128 129 128 129 128 129 128 129 128	F54 F55 A56 N57 S58 L59 L61
P82 P64 V65 V71	A114 L115 F116 G117 E118 K119 K119 N120 T121

H122 A125

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

Ch	aiı	n	В	: •		1	4%	ó												54	%														2	269	6					•	•					
M201 N202	T203	V210	V211	4212 7012	K213 Y214	V215	A216	A217	P718	G221	D222	L223	0224 0225	1226		L229	F230	A231	D232 D233	A234	T235	V236	E237 D238	P239	V240	G241	S242	543 D044	R 245	S246	G247	T248	A249 A250	1251	R252	E253 E254	F255	A256	N257	S258	L259	K260	P262	L263	A264	V265	E266	T.267
T268 Q269	E270 V271	R272	A273	V274	A275 N276	E277	A278	A279	F280 A281	F282	T283	V284	5285 F786	E287	F288	Q289	G290	R291	K292 T293	V294	V295	A296	1297 1298	D299	H300	F301	R302	F303	6305	A306	G307	K308	V309 V310	S311	M312	K313 A24A	1.315	F316	G317	-	N320	1321 1320	A323	G324	A325			

4.2.13 Score per residue for model 13

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







4.2.14 Score per residue for model 14

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



H122

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



4.2.15 Score per residue for model 15

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









5 Refinement protocol and experimental data overview (i)

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

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

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

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

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles		
WIOI	Unam	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$1.06 {\pm} 0.00$	$1{\pm}0/945~(~0.1{\pm}~0.0\%)$	$0.86 {\pm} 0.00$	$0{\pm}0/1281~(~0.0{\pm}~0.0\%)$	
1	В	1.06 ± 0.00	$1{\pm}0/952$ ($0.1{\pm}$ 0.0%)	$0.86 {\pm} 0.00$	$0{\pm}0/1293~(~0.0{\pm}~0.0\%)$	
All	All	1.06	30/28455~(~0.1%)	0.86	0/38610 ($0.0%$)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	А	$0.0{\pm}0.0$	$6.8 {\pm} 0.5$
1	В	$0.0{\pm}0.0$	6.7 ± 0.4
All	All	0	203

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

Mal	Chain	Dec	Turne	Atoma	Z Observed $(\hat{\lambda})$		Ideal(Å)	Moo	dels
	Unain	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	А	99	ASP	CG-OD2	5.81	1.38	1.25	7	15
1	В	299	ASP	CG-OD2	5.79	1.38	1.25	10	15

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	А	52	ARG	Sidechain	15
1	А	91	ARG	Sidechain	15



Contre	Continueu from precious page								
Mol	Chain	Res	Type	Group	Models (Total)				
1	А	102	ARG	Sidechain	15				
1	А	113	ARG	Sidechain	15				
1	В	213	ARG	Sidechain	15				
1	В	245	ARG	Sidechain	15				
1	В	291	ARG	Sidechain	15				
1	В	302	ARG	Sidechain	15				
1	А	13	ARG	Sidechain	14				
1	А	45	ARG	Sidechain	14				
1	А	72	ARG	Sidechain	14				
1	В	252	ARG	Sidechain	14				
1	В	272	ARG	Sidechain	14				
1	В	313	ARG	Sidechain	13				

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	927	913	912	$190{\pm}13$
1	В	933	922	918	187 ± 12
2	А	27	29	28	6 ± 3
2	В	27	29	28	6 ± 3
All	All	28710	28395	28290	5388

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 95.

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

Atom 1	Atom 2	$Clach(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A) Distance(A)		Worst	Total
1:B:261:LEU:HD23	1:B:263:LEU:HD21	1.12	1.15	13	1
1:B:295:VAL:HG22	1:B:321:ILE:HG23	1.11	1.18	3	10
1:B:261:LEU:HD21	1:B:263:LEU:HD21	1.03	1.21	8	1
1:A:63:LEU:HD13	1:A:84:VAL:HG13	1.03	1.23	14	1
1:A:74:VAL:HG11	1:B:240:VAL:HG21	1.03	1.28	5	3
1:A:79:ALA:HB2	1:B:315:LEU:HD11	1.02	1.26	9	5
1:B:281:ALA:HB2	1:B:298:ILE:HG23	1.02	1.26	14	11
1:A:95:VAL:HG22	1:A:121:ILE:HG23	1.01	1.31	9	12



			\mathbf{D}	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:75:ALA:HB3	1:B:240:VAL:HG12	1.00	1.29	10	2
1:B:261:LEU:HD22	2:B:326:NTH:H121	0.99	1.26	8	1
1:A:45:ARG:CG	1:A:50:ALA:HB1	0.99	1.88	2	6
1:A:81:ALA:HB2	1:A:98:ILE:HG23	0.98	1.33	7	14
1:B:211:VAL:HG11	1:B:271:VAL:HG21	0.98	1.29	15	13
1:A:23:LEU:CD2	1:A:59:LEU:HD22	0.98	1.88	10	7
1:A:61:LEU:HD22	1:A:63:LEU:HD21	0.98	1.31	10	9
1:A:14:TYR:CE1	1:A:18:LEU:HD11	0.98	1.94	7	15
1:A:21:GLY:CA	1:A:59:LEU:HD21	0.97	1.89	10	15
1:A:115:LEU:HD22	1:B:279:ALA:HB3	0.97	1.36	2	6
1:A:74:VAL:HG11	1:B:316:PHE:O	0.97	1.60	15	10
1:A:61:LEU:CD2	1:A:63:LEU:HD21	0.96	1.90	6	4
1:B:221:GLY:CA	1:B:259:LEU:HD21	0.96	1.91	15	13
1:B:223:LEU:CD2	1:B:259:LEU:HD22	0.96	1.89	15	6
1:A:61:LEU:HD21	1:A:63:LEU:CD2	0.96	1.90	6	1
1:B:281:ALA:CB	1:B:298:ILE:HD12	0.95	1.90	11	1
1:B:223:LEU:HD12	1:B:226:ILE:HD12	0.95	1.37	13	9
1:A:23:LEU:HD11	1:A:55:PHE:HB3	0.94	1.39	14	8
1:B:281:ALA:HB1	1:B:298:ILE:HD12	0.94	1.38	11	1
1:A:63:LEU:HD22	1:A:84:VAL:CG1	0.94	1.92	3	5
1:B:309:VAL:HG11	1:B:312:MET:CE	0.94	1.92	9	2
1:A:61:LEU:HD21	1:A:63:LEU:HD21	0.93	0.96	6	2
1:B:211:VAL:HG21	1:B:271:VAL:HG11	0.93	1.40	15	8
1:A:23:LEU:HD12	1:A:26:ILE:HD12	0.93	1.36	14	6
1:B:210:VAL:HA	1:B:229:LEU:HD21	0.93	1.41	12	15
1:B:215:VAL:HG11	1:B:267:LEU:HD11	0.93	1.38	8	2
1:A:40:VAL:HG21	1:B:274:VAL:HG11	0.92	1.39	5	3
1:B:297:PRO:O	1:B:298:ILE:HD13	0.92	1.64	11	1
1:B:261:LEU:HD22	1:B:263:LEU:HD21	0.92	1.40	5	9
1:A:11:VAL:HG11	1:A:71:VAL:HG21	0.92	1.40	15	13
1:A:75:ALA:CB	1:B:240:VAL:HG12	0.92	1.94	10	1
1:B:230:PHE:CD2	1:B:251:ILE:HG21	0.92	2.00	9	7
1:A:78:ALA:HB3	1:A:101:PHE:HB3	0.91	1.42	4	14
1:B:223:LEU:HD11	1:B:255:PHE:HB3	0.91	1.41	11	9
1:A:83:THR:HG22	1:A:95:VAL:O	0.91	1.64	14	4
1:B:295:VAL:HG12	1:B:297:PRO:HD3	0.91	1.43	13	15
1:B:226:ILE:HG21	1:B:255:PHE:CG	0.91	2.00	7	1
1:B:263:LEU:HD22	1:B:284:VAL:HG11	0.91	1.43	8	10
1:A:64:ALA:HB3	1:A:85:SER:OG	0.91	1.64	4	10
1:B:278:ALA:HB3	1:B:301:PHE:HB3	0.90	1.44	3	9
1:B:211:VAL:HG22	1:B:301:PHE:CE2	0.90	2.02	12	9



	A h		\mathbf{D}	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:61:LEU:HD13	2:A:126:NTH:H183	0.90	1.40	8	2
1:A:116:PHE:O	1:B:274:VAL:HG11	0.89	1.67	7	10
1:B:245:ARG:HG3	1:B:250:ALA:HB1	0.89	1.44	9	5
1:B:261:LEU:HD22	1:B:263:LEU:CD2	0.89	1.98	10	9
1:A:10:VAL:HA	1:A:29:LEU:HD21	0.89	1.44	14	14
1:A:72:ARG:CG	1:A:79:ALA:HB3	0.89	1.97	9	1
1:B:283:THR:HG22	1:B:295:VAL:O	0.88	1.68	11	4
1:A:34:ALA:HB3	1:A:51:ILE:CD1	0.88	1.99	7	2
1:B:271:VAL:HG13	1:B:280:PHE:HB3	0.88	1.44	4	14
1:A:23:LEU:HD13	1:A:26:ILE:HD12	0.88	1.44	1	6
1:A:45:ARG:HG3	1:A:50:ALA:HB1	0.88	1.45	2	7
1:B:264:ALA:HB3	1:B:285:SER:OG	0.88	1.68	1	9
1:B:223:LEU:HD13	1:B:226:ILE:HD12	0.88	1.46	2	6
1:B:263:LEU:HD13	1:B:284:VAL:HG13	0.88	1.45	1	1
1:A:71:VAL:HG13	1:A:80:PHE:HB3	0.87	1.45	3	10
1:A:95:VAL:HG12	1:A:97:PRO:HD3	0.87	1.45	6	13
1:A:34:ALA:N	1:A:51:ILE:HD11	0.87	1.83	5	3
1:B:263:LEU:HD23	1:B:286:PHE:CD1	0.87	2.04	14	5
1:A:34:ALA:O	1:A:51:ILE:HD11	0.87	1.70	7	5
1:B:221:GLY:HA2	1:B:259:LEU:HD21	0.86	1.46	9	10
1:A:26:ILE:HG22	1:A:30:PHE:CE2	0.86	2.05	1	1
1:A:20:ALA:HB3	1:A:22:ASP:OD2	0.86	1.68	4	1
1:A:115:LEU:HD22	1:B:279:ALA:CB	0.86	2.00	10	2
1:B:226:ILE:HD13	1:B:255:PHE:CD1	0.86	2.05	7	3
1:B:235:THR:HG23	1:B:246:SER:HB2	0.85	1.46	11	7
1:B:261:LEU:CD2	1:B:263:LEU:HD21	0.85	2.00	13	7
1:B:297:PRO:C	1:B:298:ILE:HD13	0.85	1.92	11	1
1:B:295:VAL:HG22	1:B:321:ILE:CG2	0.85	2.02	3	9
1:A:11:VAL:HG22	1:A:101:PHE:CE2	0.85	2.07	6	10
1:A:27:VAL:HG11	1:A:48:THR:HG23	0.84	1.48	10	1
1:A:63:LEU:HD13	1:A:84:VAL:CG1	0.84	2.02	14	3
1:B:215:VAL:CG1	1:B:267:LEU:HD11	0.84	2.02	8	1
1:A:78:ALA:HB3	1:A:101:PHE:CB	0.84	2.02	13	14
1:B:304:ASN:OD1	1:B:310:VAL:HG23	0.84	1.72	6	2
1:A:23:LEU:O	1:A:27:VAL:HG23	0.83	1.72	8	2
1:A:40:VAL:HG13	1:A:116:PHE:CE1	0.83	2.07	3	3
1:A:79:ALA:CB	1:B:315:LEU:HD11	0.83	2.03	9	5
1:A:104:ASN:OD1	1:A:110:VAL:HG23	0.83	1.72	6	3
1:A:63:LEU:HB2	1:A:84:VAL:HG12	0.83	1.47	9	2
1:A:61:LEU:HD22	1:A:63:LEU:CD2	0.83	2.04	8	8
1:A:7:MET:HB3	1:A:73:ALA:HB1	0.83	1.49	13	2



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			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:35:THR:HG23	1:A:46:SER:HB2	0.83	1.47	5	5
1:B:286:PHE:CZ	2:B:326:NTH:H221	0.83	2.09	6	6
1:B:263:LEU:HD23	1:B:286:PHE:CG	0.83	2.09	14	2
1:A:61:LEU:CD1	2:A:126:NTH:H183	0.83	2.04	8	2
1:B:213:ARG:HB3	1:B:229:LEU:HD22	0.83	1.48	7	8
1:A:34:ALA:C	1:A:51:ILE:HD11	0.82	1.95	7	2
1:B:263:LEU:HD22	1:B:284:VAL:CG1	0.82	2.04	8	7
1:A:13:ARG:HB3	1:A:29:LEU:HD22	0.82	1.48	9	6
1:B:278:ALA:HB3	1:B:301:PHE:CB	0.82	2.04	12	9
1:A:79:ALA:HB2	1:B:315:LEU:HD13	0.82	1.50	13	9
1:B:215:VAL:HA	1:B:218:LEU:HD12	0.82	1.52	7	15
1:B:263:LEU:HD22	1:B:284:VAL:HG12	0.81	1.52	13	2
1:A:95:VAL:HG21	2:A:126:NTH:O20	0.81	1.74	8	1
1:A:79:ALA:HB3	1:B:315:LEU:HD22	0.81	1.49	4	6
1:B:261:LEU:HD21	1:B:263:LEU:CD2	0.81	2.05	8	1
1:A:13:ARG:NH2	1:A:29:LEU:HD11	0.81	1.91	4	2
1:B:309:VAL:HG11	1:B:312:MET:HE1	0.81	1.51	13	2
1:B:245:ARG:CG	1:B:250:ALA:HB1	0.80	2.06	8	8
1:B:234:ALA:O	1:B:251:ILE:HD11	0.80	1.76	10	10
1:B:213:ARG:HD2	1:B:229:LEU:HD13	0.80	1.50	7	4
1:A:23:LEU:HD23	1:A:52:ARG:CG	0.80	2.05	11	7
1:B:286:PHE:CE2	2:B:326:NTH:H221	0.80	2.11	6	3
1:A:18:LEU:HB3	1:A:65:VAL:HG21	0.80	1.52	12	4
1:B:301:PHE:CE1	1:B:309:VAL:HG21	0.80	2.11	6	3
1:A:15:VAL:HA	1:A:18:LEU:HD12	0.79	1.54	5	15
1:A:86:PHE:CE1	2:A:126:NTH:H212	0.79	2.12	14	1
1:A:46:SER:O	1:A:50:ALA:HB3	0.79	1.75	14	7
1:A:104:ASN:HB3	1:A:110:VAL:HG21	0.79	1.54	15	9
1:A:21:GLY:HA2	1:A:59:LEU:HD21	0.79	1.52	11	13
1:A:79:ALA:HB2	1:B:315:LEU:CD1	0.79	2.07	12	7
1:A:93:THR:HG22	1:A:122:HIS:O	0.79	1.77	1	8
1:B:235:THR:HG23	1:B:246:SER:HB3	0.78	1.55	1	4
1:B:261:LEU:HD13	2:B:326:NTH:O17	0.78	1.78	5	4
1:A:63:LEU:HD22	1:A:84:VAL:HG11	0.78	1.54	6	8
1:A:79:ALA:CB	1:B:315:LEU:HD22	0.78	2.08	4	2
1:A:45:ARG:HB3	1:A:50:ALA:HB1	0.78	1.53	15	2
1:B:213:ARG:HD3	1:B:229:LEU:HD13	0.78	1.55	6	2
1:B:263:LEU:HB2	1:B:284:VAL:HG12	0.78	1.56	14	1
1:B:286:PHE:CZ	2:B:326:NTH:H212	0.78	2.13	8	1
1:A:86:PHE:CE2	2:A:126:NTH:H221	0.78	2.14	6	3
1:A:72:ARG:HG2	1:A:79:ALA:HB3	0.78	1.53	9	1



	A + - 0	(1,1)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:10:VAL:HG11	1:A:103:PHE:CE1	0.77	2.13	13	3
1:A:61:LEU:HD13	2:A:126:NTH:O17	0.77	1.79	10	3
1:A:40:VAL:HG21	1:B:274:VAL:CG1	0.77	2.10	5	4
1:B:286:PHE:CE1	2:B:326:NTH:H221	0.77	2.13	10	5
1:B:215:VAL:HG11	1:B:267:LEU:CD1	0.77	2.10	8	1
1:A:95:VAL:CG2	1:A:121:ILE:HG23	0.77	2.10	12	6
1:B:246:SER:O	1:B:250:ALA:HB3	0.77	1.79	2	10
1:A:11:VAL:HG11	1:A:71:VAL:CG2	0.77	2.10	12	14
1:B:281:ALA:CB	1:B:298:ILE:HG23	0.76	2.09	14	4
1:A:23:LEU:HD23	1:A:52:ARG:HG3	0.76	1.56	9	7
1:B:263:LEU:CB	1:B:284:VAL:HG13	0.76	2.09	9	10
1:A:27:VAL:CG1	1:A:48:THR:HG23	0.76	2.10	10	3
1:B:267:LEU:HD23	1:B:281:ALA:O	0.76	1.80	10	2
1:B:239:PRO:O	1:B:240:VAL:HG13	0.76	1.81	9	1
1:A:40:VAL:HG11	1:B:274:VAL:HG11	0.76	1.55	2	1
1:A:26:ILE:HG21	1:A:55:PHE:CD1	0.75	2.16	2	3
1:B:261:LEU:HD12	1:B:263:LEU:CG	0.75	2.12	14	1
1:B:223:LEU:HD23	1:B:252:ARG:CG	0.75	2.10	10	9
1:B:231:ALA:HB2	1:B:309:VAL:O	0.75	1.80	14	9
1:B:281:ALA:HB2	1:B:298:ILE:CG2	0.75	2.11	14	7
1:A:79:ALA:HB3	1:B:315:LEU:HD21	0.75	1.55	8	1
1:B:211:VAL:HG11	1:B:271:VAL:CG2	0.75	2.11	12	14
1:A:74:VAL:CG1	1:B:240:VAL:HG21	0.75	2.10	5	3
1:B:234:ALA:N	1:B:251:ILE:HD11	0.75	1.96	1	6
1:B:245:ARG:HB3	1:B:250:ALA:HB1	0.75	1.56	13	4
1:A:81:ALA:CB	1:A:98:ILE:HG23	0.75	2.11	7	6
1:B:227:VAL:HG11	1:B:248:THR:HG23	0.75	1.57	2	5
1:A:30:PHE:CZ	1:A:112:MET:HE3	0.74	2.17	6	3
1:A:63:LEU:HD23	1:A:86:PHE:CD1	0.74	2.17	10	5
1:A:10:VAL:HG11	1:A:103:PHE:CZ	0.74	2.17	13	8
1:A:11:VAL:HG22	1:A:101:PHE:CD2	0.74	2.17	6	6
1:A:61:LEU:HB3	1:A:63:LEU:HD11	0.74	1.57	9	2
1:B:210:VAL:HG11	1:B:303:PHE:CE1	0.74	2.17	1	4
1:A:63:LEU:HB3	1:A:84:VAL:HG13	0.74	1.57	7	1
1:B:261:LEU:HD23	1:B:263:LEU:CD2	0.74	2.06	13	3
1:B:309:VAL:HG11	1:B:312:MET:HE2	0.74	1.58	9	1
1:A:63:LEU:CB	1:A:84:VAL:HG13	0.74	2.13	4	6
1:B:223:LEU:HD22	1:B:259:LEU:HD22	0.74	1.58	7	5
1:B:263:LEU:HB2	1:B:284:VAL:HG13	0.74	1.60	8	8
1:A:115:LEU:HD13	1:B:279:ALA:HB2	0.73	1.59	11	11
1:B:210:VAL:CG2	1:B:309:VAL:HG22	0.73	2.13	14	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:11:VAL:HG21	1:A:71:VAL:CG1	0.73	2.13	13	6
1:A:45:ARG:HG2	1:A:50:ALA:HB1	0.73	1.59	2	1
1:A:38:ASP:OD1	1:A:114:ALA:HB3	0.73	1.83	9	3
1:B:269:GLN:OE1	1:B:281:ALA:HB3	0.73	1.82	11	1
1:A:115:LEU:HD11	1:B:279:ALA:HB2	0.73	1.59	4	1
1:B:261:LEU:CD2	2:B:326:NTH:H121	0.72	2.13	8	1
1:A:11:VAL:HG21	1:A:71:VAL:HG11	0.72	1.61	3	6
1:A:13:ARG:HD2	1:A:29:LEU:HD13	0.72	1.61	4	3
1:B:234:ALA:HB3	1:B:251:ILE:HD13	0.72	1.61	9	1
1:B:223:LEU:HD23	1:B:252:ARG:HG3	0.72	1.61	13	9
1:A:116:PHE:O	1:B:274:VAL:HG21	0.72	1.85	8	8
1:B:263:LEU:HD13	1:B:284:VAL:CG1	0.71	2.14	1	3
1:A:34:ALA:HB3	1:A:51:ILE:HD13	0.71	1.62	7	2
1:A:10:VAL:HG12	1:A:101:PHE:CZ	0.71	2.20	13	10
1:A:31:ALA:HB2	1:A:109:VAL:O	0.71	1.85	10	10
1:A:61:LEU:HD13	2:A:126:NTH:C17	0.71	2.15	12	2
1:A:36:VAL:CG2	1:A:51:ILE:HD12	0.71	2.15	12	5
1:A:61:LEU:HD13	1:A:62:PRO:HD2	0.71	1.61	9	1
1:B:278:ALA:HB3	1:B:301:PHE:HB2	0.71	1.60	4	2
1:A:63:LEU:CB	1:A:84:VAL:HG12	0.71	2.16	9	6
1:A:74:VAL:HG21	1:B:316:PHE:O	0.71	1.86	11	9
1:A:95:VAL:HG13	1:A:120:ASN:ND2	0.71	2.01	11	2
1:A:27:VAL:HG21	1:A:52:ARG:HB2	0.70	1.63	2	6
1:B:293:THR:HG22	1:B:322:HIS:O	0.70	1.86	2	4
1:A:21:GLY:HA3	1:A:59:LEU:HD21	0.70	1.61	10	2
1:B:322:HIS:CD2	2:B:326:NTH:H212	0.70	2.21	13	1
1:A:58:SER:OG	2:A:126:NTH:H11	0.70	1.86	9	7
1:A:116:PHE:CZ	2:A:126:NTH:H62	0.70	2.22	2	2
1:A:30:PHE:CD2	1:A:51:ILE:HG21	0.70	2.20	8	4
1:B:210:VAL:HG11	1:B:303:PHE:CZ	0.70	2.21	4	11
1:A:94:VAL:HG12	1:A:122:HIS:CG	0.70	2.22	12	5
1:B:230:PHE:CG	1:B:251:ILE:HG21	0.70	2.22	4	2
1:B:293:THR:HG23	1:B:323:ALA:HA	0.70	1.61	15	1
1:A:26:ILE:HD13	1:A:55:PHE:CD1	0.70	2.22	2	4
1:A:79:ALA:HB3	1:B:315:LEU:CD2	0.70	2.16	4	3
1:A:80:PHE:CE1	1:A:101:PHE:CD2	0.70	2.80	7	5
1:B:210:VAL:HG21	1:B:309:VAL:HG22	0.70	1.64	14	1
1:B:258:SER:OG	2:B:326:NTH:H11	0.69	1.86	7	9
1:B:316:PHE:CE2	2:B:326:NTH:H72	0.69	2.22	14	1
1:A:10:VAL:HG21	1:A:103:PHE:CE2	0.69	2.22	12	4
1:B:238:ASP:OD2	2:B:326:NTH:H61	0.69	1.87	13	1



	At. 0		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:75:ALA:HB2	1:B:240:VAL:O	0.69	1.88	6	1
1:A:40:VAL:HG21	1:B:274:VAL:HB	0.69	1.64	8	2
1:A:115:LEU:HD22	1:B:279:ALA:HB2	0.69	1.62	10	1
1:A:61:LEU:CD1	2:A:126:NTH:H122	0.69	2.17	2	1
1:B:211:VAL:HG21	1:B:271:VAL:CG1	0.69	2.18	15	6
1:A:68:THR:O	1:A:70:GLU:N	0.69	2.26	9	2
1:B:295:VAL:HG21	2:B:326:NTH:O20	0.69	1.88	8	2
1:A:115:LEU:HD11	1:B:300:HIS:CD2	0.69	2.23	4	1
1:A:80:PHE:CE1	1:A:101:PHE:CE2	0.69	2.82	14	5
1:A:36:VAL:HG23	1:A:51:ILE:HD12	0.68	1.64	12	6
1:A:94:VAL:HG13	1:A:122:HIS:CB	0.68	2.18	15	4
1:B:226:ILE:HD13	1:B:255:PHE:CE1	0.68	2.23	7	1
1:A:10:VAL:HG21	1:A:103:PHE:CZ	0.68	2.23	2	6
1:B:295:VAL:HG13	1:B:321:ILE:HG23	0.68	1.65	5	3
1:A:86:PHE:CE2	2:A:126:NTH:H211	0.68	2.22	11	1
1:A:115:LEU:HD13	1:B:300:HIS:NE2	0.68	2.03	10	3
1:B:317:GLY:O	1:B:321:ILE:HD12	0.68	1.88	12	2
1:A:81:ALA:HB2	1:A:98:ILE:CG2	0.68	2.15	7	5
1:A:45:ARG:CD	1:A:50:ALA:HB1	0.68	2.19	1	2
1:B:304:ASN:HB3	1:B:310:VAL:HG21	0.68	1.66	15	7
1:B:203:THR:O	1:B:203:THR:HG23	0.68	1.88	15	8
1:A:72:ARG:HG3	1:A:79:ALA:HB3	0.68	1.66	9	1
1:B:315:LEU:O	1:B:316:PHE:CD1	0.68	2.47	7	3
1:B:281:ALA:HB1	1:B:298:ILE:CD1	0.68	2.17	11	1
1:B:261:LEU:HD13	2:B:326:NTH:H121	0.68	1.64	12	1
1:B:271:VAL:HG13	1:B:280:PHE:CB	0.68	2.19	14	9
1:A:93:THR:HG23	1:A:123:ALA:HA	0.68	1.65	4	1
1:A:116:PHE:O	1:B:274:VAL:HG22	0.68	1.89	4	1
1:A:3:THR:HG23	1:A:3:THR:O	0.67	1.89	15	6
1:B:210:VAL:CG2	1:B:309:VAL:HG23	0.67	2.19	10	2
1:B:261:LEU:HD22	1:B:263:LEU:HD23	0.67	1.65	12	4
1:B:295:VAL:CG2	1:B:321:ILE:HG23	0.67	2.18	2	7
1:B:210:VAL:CA	1:B:229:LEU:HD21	0.67	2.19	15	7
1:B:261:LEU:HD23	1:B:263:LEU:HD23	0.67	1.67	15	2
1:A:63:LEU:CD1	1:A:84:VAL:HG13	0.67	2.12	14	1
1:A:14:TYR:CZ	1:A:18:LEU:HD11	0.67	2.24	7	3
1:B:268:THR:O	1:B:270:GLU:N	0.67	2.27	8	1
1:B:301:PHE:HE1	1:B:309:VAL:HG21	0.67	1.49	6	2
1:A:14:TYR:CE1	1:A:55:PHE:CE2	0.67	2.82	7	2
1:B:210:VAL:HG21	1:B:303:PHE:CE1	0.66	2.24	2	1
1:A:63:LEU:HB3	1:A:84:VAL:HG12	0.66	1.67	11	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:316:PHE:CG	1:B:317:GLY:N	0.66	2.64	5	5
1:A:61:LEU:HD12	2:A:126:NTH:H122	0.66	1.64	2	1
1:A:23:LEU:HD21	1:A:52:ARG:HA	0.66	1.67	3	3
1:A:71:VAL:HG13	1:A:80:PHE:CB	0.66	2.19	3	6
1:B:221:GLY:HA2	1:B:259:LEU:HD11	0.66	1.67	10	9
1:B:211:VAL:HG22	1:B:280:PHE:CD2	0.66	2.25	2	1
1:A:115:LEU:HD13	1:B:300:HIS:CE1	0.66	2.26	3	1
1:A:11:VAL:CG1	1:A:71:VAL:HG21	0.66	2.20	6	12
1:B:258:SER:OG	2:B:326:NTH:H112	0.66	1.91	15	4
1:A:40:VAL:HG23	1:A:40:VAL:O	0.66	1.90	15	5
1:B:305:GLY:O	1:B:306:ALA:HB2	0.66	1.91	14	7
1:A:72:ARG:CZ	1:A:74:VAL:CG2	0.66	2.73	9	1
1:B:236:VAL:HG23	1:B:251:ILE:CD1	0.66	2.20	12	1
1:B:298:ILE:HD12	1:B:320:ASN:OD1	0.66	1.91	3	2
1:A:105:GLY:O	1:A:106:ALA:HB2	0.66	1.91	11	9
1:A:40:VAL:O	1:B:275:ALA:HB2	0.66	1.90	14	1
1:A:21:GLY:HA2	1:A:59:LEU:HD11	0.65	1.69	2	6
1:B:317:GLY:C	1:B:321:ILE:HD12	0.65	2.11	3	2
1:B:261:LEU:O	1:B:263:LEU:HD23	0.65	1.91	1	1
1:A:61:LEU:HD23	1:A:63:LEU:HD23	0.65	1.68	12	3
1:A:115:LEU:O	1:A:116:PHE:CD1	0.65	2.49	4	1
1:A:35:THR:HG23	1:A:46:SER:CB	0.65	2.22	5	1
1:B:286:PHE:CE2	1:B:293:THR:CG2	0.65	2.79	14	1
1:B:264:ALA:HB3	1:B:285:SER:HG	0.65	1.51	14	3
1:B:210:VAL:CG1	1:B:301:PHE:CE1	0.65	2.80	10	11
1:A:86:PHE:CZ	2:A:126:NTH:H221	0.65	2.26	13	8
1:A:10:VAL:CA	1:A:29:LEU:HD21	0.65	2.21	14	3
1:B:263:LEU:CB	1:B:284:VAL:HG12	0.65	2.20	14	4
1:A:67:LEU:HD22	1:A:71:VAL:CG2	0.65	2.22	10	1
1:A:14:TYR:CE1	1:A:18:LEU:CD1	0.64	2.80	1	14
1:A:105:GLY:O	1:A:106:ALA:HB3	0.64	1.91	15	3
1:B:234:ALA:C	1:B:251:ILE:HD11	0.64	2.12	9	1
1:A:10:VAL:CG1	1:A:101:PHE:CZ	0.64	2.79	7	11
1:B:305:GLY:O	1:B:306:ALA:HB3	0.64	1.92	8	4
1:A:63:LEU:HB2	1:A:84:VAL:HG13	0.64	1.69	12	5
1:B:317:GLY:O	1:B:321:ILE:HD11	0.64	1.92	9	9
1:B:226:ILE:HG21	1:B:255:PHE:CD2	0.64	2.27	3	5
1:A:15:VAL:HB	1:A:67:LEU:HD11	0.64	1.68	5	2
1:B:293:THR:HG23	1:B:323:ALA:CA	0.64	2.23	15	1
1:A:30:PHE:CD2	1:A:51:ILE:CG2	0.64	2.80	8	3
1:B:214:TYR:CE1	1:B:218:LEU:CD1	0.64	2.80	6	15



	no uo puge		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:10:VAL:CG1	1:A:101:PHE:CE1	0.64	2.81	14	9
1:A:82:PHE:CD1	1:A:82:PHE:N	0.64	2.65	4	7
1:A:10:VAL:CG2	1:A:103:PHE:CZ	0.64	2.81	6	6
1:A:94:VAL:HG12	1:A:122:HIS:CB	0.64	2.22	9	9
1:A:58:SER:OG	2:A:126:NTH:H111	0.64	1.93	11	2
1:A:95:VAL:HG12	1:A:97:PRO:CD	0.64	2.22	6	11
1:A:61:LEU:HD12	1:A:63:LEU:CG	0.64	2.22	9	1
1:B:210:VAL:CG1	1:B:301:PHE:CZ	0.64	2.81	7	10
1:B:282:PHE:CD1	1:B:282:PHE:N	0.63	2.66	13	8
1:A:7:MET:CE	1:A:103:PHE:CD2	0.63	2.81	3	1
1:B:309:VAL:CG1	1:B:312:MET:HE1	0.63	2.21	13	1
1:B:223:LEU:CD2	1:B:256:ALA:HB2	0.63	2.24	4	7
1:B:296:ALA:HB3	1:B:320:ASN:O	0.63	1.92	12	4
1:A:115:LEU:HD11	1:B:279:ALA:CB	0.63	2.23	4	1
1:A:10:VAL:CG1	1:A:103:PHE:CZ	0.63	2.82	3	5
1:A:101:PHE:CE1	1:A:112:MET:CE	0.63	2.82	10	2
1:B:258:SER:OG	2:B:326:NTH:H111	0.63	1.94	9	3
1:B:286:PHE:N	1:B:286:PHE:CD1	0.63	2.66	8	3
1:B:277:GLU:O	1:B:278:ALA:HB2	0.63	1.92	15	7
1:A:104:ASN:HB3	1:A:110:VAL:HG11	0.63	1.70	8	1
1:B:221:GLY:C	1:B:259:LEU:HD21	0.63	2.12	11	8
1:A:88:PHE:N	1:A:88:PHE:CD1	0.63	2.66	15	2
1:B:286:PHE:CZ	1:B:293:THR:HG23	0.63	2.28	14	1
1:A:35:THR:O	1:A:36:VAL:HG23	0.63	1.92	15	1
1:A:58:SER:OG	2:A:126:NTH:H112	0.63	1.93	3	3
1:A:86:PHE:CD1	1:A:86:PHE:N	0.63	2.66	6	8
1:A:23:LEU:HD21	1:A:59:LEU:HD22	0.63	1.71	5	2
1:B:288:PHE:N	1:B:288:PHE:CD1	0.63	2.66	9	3
1:B:297:PRO:CB	1:B:316:PHE:CD1	0.63	2.82	7	2
1:A:40:VAL:HG23	1:A:41:GLY:N	0.63	2.08	2	2
1:A:18:LEU:HD21	1:A:55:PHE:CE1	0.63	2.27	10	1
1:A:116:PHE:CE2	2:A:126:NTH:H61	0.63	2.29	10	1
1:A:98:ILE:HD12	1:B:272:ARG:HH21	0.63	1.54	14	1
1:B:263:LEU:CD1	1:B:284:VAL:HG13	0.63	2.22	1	1
1:B:210:VAL:CG2	1:B:303:PHE:CZ	0.63	2.82	3	2
1:A:45:ARG:HD3	1:A:50:ALA:HB1	0.62	1.69	1	2
1:B:295:VAL:HG12	1:B:297:PRO:CD	0.62	2.24	2	13
1:A:67:LEU:HD23	1:A:81:ALA:O	0.62	1.94	5	2
1:B:286:PHE:CD1	1:B:286:PHE:N	0.62	2.65	14	1
1:A:94:VAL:HG13	1:A:95:VAL:N	0.62	2.08	12	7
1:B:226:ILE:HG22	1:B:230:PHE:CE2	0.62	2.28	2	1



	to us puge		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:230:PHE:CD2	1:B:251:ILE:CG2	0.62	2.83	4	6
1:A:23:LEU:HD22	1:A:59:LEU:HD22	0.62	1.71	2	6
1:A:115:LEU:CD1	1:B:279:ALA:HB2	0.62	2.24	1	6
1:A:30:PHE:CG	1:A:51:ILE:HG21	0.62	2.28	3	4
1:A:26:ILE:HG21	1:A:55:PHE:HD2	0.62	1.54	7	1
1:B:226:ILE:CG2	1:B:255:PHE:CD2	0.62	2.82	7	1
1:B:210:VAL:HG22	1:B:309:VAL:CG2	0.62	2.25	14	4
1:B:223:LEU:O	1:B:227:VAL:HG23	0.62	1.93	8	2
1:B:214:TYR:CE1	1:B:218:LEU:HD11	0.62	2.29	7	15
1:A:18:LEU:HB3	1:A:65:VAL:HG11	0.62	1.72	9	2
1:A:17:ALA:HB1	1:A:22:ASP:OD1	0.62	1.95	6	1
1:B:210:VAL:HG21	1:B:303:PHE:CE2	0.62	2.29	14	4
1:B:245:ARG:CD	1:B:254:PHE:CD1	0.62	2.82	9	1
1:A:74:VAL:HG13	1:B:316:PHE:O	0.62	1.95	8	3
1:A:61:LEU:HD23	1:A:61:LEU:O	0.62	1.94	6	1
1:B:223:LEU:HD21	1:B:259:LEU:HD22	0.62	1.70	3	3
1:B:245:ARG:HG2	1:B:250:ALA:HB1	0.62	1.71	5	1
1:A:75:ALA:HB3	1:B:240:VAL:CG1	0.62	2.16	10	1
1:B:211:VAL:CG1	1:B:271:VAL:HG21	0.61	2.24	10	11
1:A:95:VAL:HG22	1:A:121:ILE:CG2	0.61	2.24	14	8
1:A:40:VAL:HB	1:B:274:VAL:HG11	0.61	1.71	4	1
1:A:79:ALA:CB	1:B:315:LEU:HD21	0.61	2.25	8	2
1:B:322:HIS:NE2	2:B:326:NTH:H212	0.61	2.10	13	1
1:A:14:TYR:CE1	1:A:55:PHE:CZ	0.61	2.88	7	1
1:A:86:PHE:CE1	2:A:126:NTH:H221	0.61	2.30	7	2
1:A:21:GLY:O	1:A:59:LEU:HD21	0.61	1.95	4	4
1:B:210:VAL:CG1	1:B:303:PHE:CZ	0.61	2.84	10	9
1:A:26:ILE:HD13	1:A:55:PHE:CE1	0.61	2.31	2	1
1:B:240:VAL:HG23	1:B:240:VAL:O	0.61	1.94	12	4
1:A:71:VAL:HG22	1:A:80:PHE:HB2	0.61	1.72	6	2
1:A:113:ARG:NH2	1:B:300:HIS:CE1	0.61	2.69	9	1
1:B:286:PHE:CE2	1:B:293:THR:HG23	0.61	2.30	14	1
1:B:263:LEU:HD23	1:B:286:PHE:HB3	0.61	1.73	4	3
1:A:21:GLY:C	1:A:59:LEU:HD21	0.61	2.16	7	11
1:B:211:VAL:CG2	1:B:301:PHE:CE2	0.61	2.84	3	8
1:B:234:ALA:HB3	1:B:251:ILE:CD1	0.61	2.24	9	1
1:A:61:LEU:HD23	1:A:63:LEU:CD2	0.61	2.25	12	2
1:B:304:ASN:OD1	1:B:310:VAL:HG21	0.61	1.96	14	1
1:A:11:VAL:HG11	1:A:71:VAL:CG1	0.61	2.25	2	2
1:B:211:VAL:HG22	1:B:301:PHE:CD2	0.61	2.31	10	8
1:B:293:THR:HG22	1:B:323:ALA:HA	0.61	1.71	12	2



		(1, 1)	${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:40:VAL:CB	1:B:274:VAL:HG11	0.61	2.25	4	1
1:B:227:VAL:HG21	1:B:252:ARG:HB2	0.61	1.73	5	7
1:B:277:GLU:HG2	1:B:278:ALA:N	0.61	2.11	14	1
1:B:234:ALA:HB1	1:B:310:VAL:O	0.61	1.96	8	8
1:B:295:VAL:HG13	1:B:320:ASN:ND2	0.61	2.10	4	1
1:B:316:PHE:CD1	1:B:316:PHE:C	0.60	2.74	5	2
1:B:294:VAL:HG13	1:B:322:HIS:HB2	0.60	1.72	10	3
1:A:85:SER:HA	1:A:94:VAL:HG23	0.60	1.72	2	5
1:B:226:ILE:HG21	1:B:255:PHE:CD1	0.60	2.31	7	1
1:B:263:LEU:CB	1:B:284:VAL:CG1	0.60	2.80	3	6
1:A:30:PHE:CZ	1:A:112:MET:CE	0.60	2.85	10	2
1:A:61:LEU:CD2	1:A:63:LEU:HD23	0.60	2.26	4	1
1:A:23:LEU:HD11	1:A:55:PHE:C	0.60	2.17	8	6
1:A:61:LEU:CD2	1:A:63:LEU:CD2	0.60	2.79	4	9
1:B:238:ASP:OD2	2:B:326:NTH:H62	0.60	1.96	7	5
1:B:261:LEU:CD2	1:B:263:LEU:CD2	0.60	2.80	7	10
1:A:61:LEU:HD23	1:A:63:LEU:HD11	0.60	1.73	3	1
1:B:210:VAL:HG21	1:B:303:PHE:CZ	0.60	2.31	3	2
1:B:223:LEU:HD11	1:B:255:PHE:C	0.60	2.17	15	5
1:B:226:ILE:HD13	1:B:255:PHE:CD2	0.60	2.32	8	3
1:B:315:LEU:O	1:B:316:PHE:CB	0.60	2.50	5	2
1:B:236:VAL:CG2	1:B:251:ILE:HG23	0.60	2.27	9	1
1:B:280:PHE:O	1:B:298:ILE:HG23	0.60	1.96	15	5
1:B:210:VAL:CG2	1:B:309:VAL:CG2	0.60	2.79	14	4
1:A:30:PHE:CE1	1:A:112:MET:HE1	0.60	2.32	2	2
1:A:61:LEU:HD13	1:A:63:LEU:HD21	0.60	1.73	2	1
1:A:58:SER:HB2	2:A:126:NTH:H11	0.60	1.73	7	1
1:A:85:SER:CB	1:A:94:VAL:HG23	0.59	2.26	3	1
1:A:79:ALA:CB	1:B:315:LEU:CD1	0.59	2.80	7	3
1:A:10:VAL:HG22	1:A:109:VAL:CG2	0.59	2.27	2	2
1:B:213:ARG:CB	1:B:229:LEU:HD22	0.59	2.24	7	3
1:B:223:LEU:CD2	1:B:252:ARG:CG	0.59	2.81	13	9
1:B:223:LEU:HD21	1:B:259:LEU:HB2	0.59	1.74	7	1
1:A:100:HIS:NE2	1:B:300:HIS:CD2	0.59	2.70	15	1
1:B:230:PHE:CE1	1:B:312:MET:HE1	0.59	2.32	2	1
1:A:75:ALA:HB1	1:B:241:GLY:HA3	0.59	1.73	3	1
1:A:10:VAL:HG13	1:A:101:PHE:CE1	0.59	2.33	6	4
1:A:40:VAL:CG2	1:B:274:VAL:CG1	0.59	2.81	4	1
1:B:218:LEU:HB3	1:B:265:VAL:HG21	0.59	1.73	15	5
1:A:63:LEU:CB	1:A:84:VAL:CG1	0.59	2.81	11	3
1:B:276:ASN:O	1:B:303:PHE:CD1	0.59	2.55	7	3



	A L		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:88:PHE:CD2	1:A:93:THR:OG1	0.59	2.55	14	5
1:B:210:VAL:HG12	1:B:301:PHE:CZ	0.59	2.32	13	6
1:B:236:VAL:HG23	1:B:251:ILE:HD12	0.59	1.73	12	2
1:B:321:ILE:HG22	1:B:322:HIS:N	0.59	2.13	7	2
1:A:23:LEU:HD22	1:A:56:ALA:HB2	0.59	1.73	11	2
1:A:77:GLU:HG2	1:A:78:ALA:N	0.59	2.11	12	1
1:B:230:PHE:CZ	1:B:312:MET:HE3	0.59	2.33	12	1
1:A:34:ALA:HB1	1:A:110:VAL:O	0.59	1.97	7	9
1:B:247:GLY:O	1:B:251:ILE:HD12	0.59	1.98	6	7
1:A:100:HIS:CG	1:A:101:PHE:N	0.59	2.71	9	3
1:A:72:ARG:CZ	1:A:74:VAL:HG22	0.58	2.28	5	1
1:B:238:ASP:O	1:B:254:PHE:CE2	0.58	2.56	15	3
1:A:80:PHE:CZ	1:A:99:ASP:HB3	0.58	2.34	11	14
1:B:288:PHE:CD2	1:B:293:THR:OG1	0.58	2.57	5	3
1:A:86:PHE:CE1	1:A:88:PHE:CE1	0.58	2.91	4	1
1:B:258:SER:OG	2:B:326:NTH:H10	0.58	1.98	9	2
1:A:26:ILE:CG2	1:A:30:PHE:CE2	0.58	2.83	1	1
1:A:11:VAL:HG11	1:A:71:VAL:HG22	0.58	1.74	12	2
1:B:245:ARG:NH1	1:B:251:ILE:CG1	0.58	2.66	7	1
1:B:294:VAL:O	1:B:321:ILE:O	0.58	2.20	7	2
1:B:236:VAL:CG1	1:B:237:GLU:N	0.58	2.65	12	3
1:B:261:LEU:HD12	1:B:263:LEU:HG	0.58	1.76	14	1
1:B:261:LEU:HD13	1:B:262:PRO:HD2	0.58	1.74	14	1
1:A:38:ASP:O	1:A:54:PHE:CZ	0.58	2.56	15	7
1:A:63:LEU:HD23	1:A:86:PHE:CG	0.58	2.33	9	4
1:B:238:ASP:OD1	1:B:314:ALA:HB3	0.58	1.98	15	2
1:A:80:PHE:CE2	1:A:82:PHE:CE2	0.58	2.91	10	2
1:A:80:PHE:O	1:A:98:ILE:HG23	0.58	1.98	2	3
1:A:11:VAL:CG2	1:A:101:PHE:CE2	0.58	2.87	14	8
1:A:77:GLU:O	1:A:78:ALA:HB2	0.58	1.99	13	6
1:A:86:PHE:CZ	1:A:93:THR:OG1	0.58	2.57	14	1
1:A:36:VAL:CG1	1:A:37:GLU:N	0.58	2.67	11	5
1:A:23:LEU:CD2	1:A:52:ARG:CG	0.58	2.81	9	7
1:A:63:LEU:CD2	1:A:84:VAL:CG1	0.58	2.81	7	2
1:B:230:PHE:HD2	1:B:251:ILE:HG21	0.58	1.58	6	1
1:B:226:ILE:CD1	1:B:255:PHE:CD1	0.58	2.86	7	1
1:A:3:THR:O	1:A:6:HIS:CE1	0.58	2.57	11	1
1:B:316:PHE:CD2	1:B:317:GLY:N	0.58	2.71	9	9
1:B:230:PHE:CE1	1:B:312:MET:CE	0.58	2.86	2	1
1:A:72:ARG:CZ	1:A:74:VAL:HG23	0.58	2.28	9	1
1:B:269:GLN:NE2	1:B:281:ALA:HB3	0.58	2.13	13	1



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:116:PHE:CD2	1:A:117:GLY:N	0.58	2.72	4	6
1:B:223:LEU:CD2	1:B:259:LEU:CD2	0.58	2.80	7	6
1:B:295:VAL:HG22	1:B:321:ILE:HA	0.58	1.75	4	1
1:B:316:PHE:CD2	1:B:320:ASN:OD1	0.58	2.57	4	1
1:A:94:VAL:CG1	1:A:122:HIS:CB	0.58	2.82	14	4
1:B:297:PRO:HB3	1:B:316:PHE:CD1	0.58	2.32	7	1
1:B:223:LEU:HD23	1:B:252:ARG:HG2	0.58	1.76	9	4
1:A:6:HIS:NE2	1:A:7:MET:CG	0.58	2.67	11	1
1:A:78:ALA:HB3	1:A:101:PHE:HB2	0.58	1.74	2	6
1:A:116:PHE:CE1	2:A:126:NTH:H62	0.58	2.34	2	1
1:B:236:VAL:CG2	1:B:251:ILE:CD1	0.58	2.81	12	1
1:B:286:PHE:CD1	1:B:293:THR:O	0.57	2.57	9	2
1:A:26:ILE:HG21	1:A:55:PHE:CD2	0.57	2.33	7	3
1:A:101:PHE:CE1	1:A:112:MET:HE2	0.57	2.33	10	1
1:A:43:GLU:N	1:A:44:PRO:HD3	0.57	2.14	3	5
1:B:234:ALA:CB	1:B:310:VAL:O	0.57	2.52	8	8
1:A:37:GLU:O	1:A:114:ALA:HB3	0.57	1.99	2	1
1:A:13:ARG:HD3	1:A:29:LEU:HD13	0.57	1.74	7	1
1:A:76:ASN:O	1:A:103:PHE:CG	0.57	2.57	13	1
1:A:64:ALA:HB3	1:A:85:SER:HG	0.57	1.59	15	3
1:B:211:VAL:HG11	1:B:271:VAL:HG22	0.57	1.76	2	3
1:A:72:ARG:NE	1:A:74:VAL:CG2	0.57	2.67	9	1
1:A:103:PHE:CE1	1:A:108:LYS:O	0.57	2.57	2	1
1:B:235:THR:HG23	1:B:246:SER:CB	0.57	2.25	11	3
1:A:117:GLY:O	1:A:121:ILE:HD11	0.57	1.99	5	10
1:A:67:LEU:C	1:A:68:THR:HG22	0.57	2.18	5	1
1:A:23:LEU:HA	1:A:26:ILE:HD12	0.57	1.76	10	1
1:A:23:LEU:CD2	1:A:59:LEU:CD2	0.57	2.82	5	7
1:A:13:ARG:CB	1:A:29:LEU:HD22	0.57	2.25	9	2
1:A:15:VAL:HG13	1:A:65:VAL:CG1	0.57	2.29	8	1
1:A:27:VAL:HG21	1:A:52:ARG:HG3	0.57	1.77	8	1
1:A:10:VAL:HG11	1:A:109:VAL:CG2	0.57	2.30	9	1
1:A:23:LEU:HD23	1:A:52:ARG:HG2	0.57	1.73	11	2
1:B:304:ASN:N	1:B:310:VAL:HG21	0.57	2.14	13	1
1:B:322:HIS:O	1:B:322:HIS:ND1	0.57	2.37	13	1
1:A:115:LEU:CD1	1:B:279:ALA:CB	0.57	2.83	1	2
1:A:38:ASP:OD2	2:A:126:NTH:H10	0.57	2.00	2	1
1:B:230:PHE:CZ	1:B:312:MET:CE	0.57	2.88	9	2
1:B:286:PHE:CE2	1:B:288:PHE:CE1	0.57	2.92	9	2
1:A:95:VAL:CG1	1:A:120:ASN:ND2	0.57	2.67	10	2
1:A:38:ASP:OD2	2:A:126:NTH:H62	0.57	2.00	9	5



	A4		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:301:PHE:CE1	1:B:312:MET:SD	0.57	2.98	13	2
1:B:304:ASN:N	1:B:304:ASN:ND2	0.57	2.53	10	2
1:A:67:LEU:CD2	1:A:71:VAL:CG2	0.57	2.83	10	1
1:A:88:PHE:CZ	1:A:93:THR:OG1	0.57	2.57	11	1
1:A:63:LEU:HD13	1:A:84:VAL:HG11	0.56	1.76	9	2
1:B:304:ASN:HB3	1:B:310:VAL:HG11	0.56	1.77	11	1
1:B:206:HIS:CE1	1:B:207:MET:CG	0.56	2.88	13	1
1:A:61:LEU:HD22	1:A:63:LEU:HD23	0.56	1.77	13	2
1:B:263:LEU:CD2	1:B:284:VAL:HG12	0.56	2.29	13	1
1:A:14:TYR:CD1	1:A:14:TYR:C	0.56	2.78	2	15
1:B:286:PHE:CZ	1:B:293:THR:OG1	0.56	2.57	5	6
1:B:235:THR:HG22	1:B:246:SER:HB2	0.56	1.74	2	2
1:A:74:VAL:CB	1:B:240:VAL:HG21	0.56	2.30	4	2
1:A:11:VAL:CG2	1:A:101:PHE:CD2	0.56	2.87	6	3
1:B:211:VAL:HG11	1:B:271:VAL:CG1	0.56	2.29	7	2
1:A:61:LEU:CD1	1:A:63:LEU:HD21	0.56	2.30	9	1
1:A:98:ILE:HD11	1:B:272:ARG:CZ	0.56	2.31	12	1
1:A:101:PHE:CE1	1:A:112:MET:SD	0.56	2.98	12	2
1:B:294:VAL:O	1:B:322:HIS:HB3	0.56	2.00	13	1
1:B:293:THR:HG22	1:B:294:VAL:N	0.56	2.16	15	1
1:B:294:VAL:HG13	1:B:322:HIS:CB	0.56	2.31	10	3
1:A:61:LEU:HD12	1:A:63:LEU:CD2	0.56	2.31	9	1
1:B:280:PHE:CZ	1:B:299:ASP:HB3	0.56	2.36	11	14
1:A:109:VAL:HG12	1:A:110:VAL:N	0.56	2.16	14	3
1:A:38:ASP:OD2	1:A:114:ALA:HB3	0.56	2.01	8	2
1:A:30:PHE:CE1	1:A:112:MET:HE3	0.56	2.35	6	2
1:A:94:VAL:HG13	1:A:122:HIS:HB3	0.56	1.78	15	1
1:B:307:GLY:O	1:B:308:LYS:CB	0.56	2.53	1	2
1:B:294:VAL:HG12	1:B:322:HIS:CB	0.56	2.31	11	7
1:B:296:ALA:N	1:B:320:ASN:O	0.56	2.39	12	6
1:A:94:VAL:O	1:A:122:HIS:CB	0.56	2.54	14	6
1:B:297:PRO:CB	1:B:316:PHE:CG	0.56	2.89	9	1
1:B:279:ALA:HB2	1:B:300:HIS:CE1	0.56	2.36	14	1
1:A:36:VAL:O	1:A:44:PRO:CB	0.56	2.54	1	14
1:B:240:VAL:HG22	1:B:316:PHE:HE1	0.56	1.60	5	1
1:A:107:GLY:O	1:A:108:LYS:CB	0.56	2.53	14	2
1:A:43:GLU:O	1:A:54:PHE:CZ	0.56	2.59	8	2
1:B:321:ILE:HG21	2:B:326:NTH:H222	0.56	1.76	12	2
1:A:38:ASP:OD2	2:A:126:NTH:H61	0.56	2.01	12	1
1:A:76:ASN:O	1:A:103:PHE:CD2	0.56	2.59	13	1
1:A:72:ARG:CB	1:A:79:ALA:O	0.56	2.54	5	13



	h h		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:227:VAL:CG1	1:B:248:THR:HG23	0.56	2.30	11	5
1:A:10:VAL:CG2	1:A:109:VAL:CG2	0.56	2.83	2	3
1:A:11:VAL:HG22	1:A:101:PHE:HE2	0.56	1.60	3	5
1:B:211:VAL:HG22	1:B:301:PHE:HE2	0.56	1.57	3	5
1:A:68:THR:O	1:A:69:GLN:CG	0.56	2.54	5	2
1:B:294:VAL:O	1:B:322:HIS:CA	0.56	2.54	13	1
1:A:67:LEU:O	1:A:68:THR:CB	0.55	2.55	5	1
1:B:285:SER:OG	1:B:294:VAL:HG23	0.55	2.02	3	1
1:A:86:PHE:CD1	1:A:86:PHE:C	0.55	2.79	4	1
1:A:10:VAL:HG22	1:A:109:VAL:HG23	0.55	1.77	6	6
1:B:285:SER:HA	1:B:294:VAL:HG23	0.55	1.79	6	2
1:A:94:VAL:HG12	1:A:122:HIS:HB2	0.55	1.78	9	3
1:B:214:TYR:CD1	1:B:214:TYR:C	0.55	2.79	7	15
1:A:10:VAL:CG1	1:A:109:VAL:CG2	0.55	2.84	9	4
1:A:15:VAL:HG13	1:A:65:VAL:HG12	0.55	1.79	8	1
1:B:316:PHE:CE1	2:B:326:NTH:H61	0.55	2.37	8	1
1:A:34:ALA:CB	1:A:110:VAL:O	0.55	2.55	3	9
1:B:294:VAL:CG1	1:B:322:HIS:CD2	0.55	2.90	8	1
1:B:261:LEU:HD12	1:B:263:LEU:CD1	0.55	2.31	14	1
1:A:116:PHE:O	1:B:274:VAL:CG1	0.55	2.55	12	13
1:B:236:VAL:O	1:B:244:PRO:CB	0.55	2.55	1	14
1:B:294:VAL:HG13	1:B:295:VAL:N	0.55	2.17	6	4
1:B:309:VAL:CG1	1:B:310:VAL:N	0.55	2.69	13	3
1:A:100:HIS:CB	1:A:113:ARG:NE	0.55	2.70	9	1
1:B:297:PRO:HB3	1:B:316:PHE:CG	0.55	2.36	9	1
1:A:39:PRO:O	1:A:40:VAL:O	0.55	2.25	2	1
1:B:304:ASN:CB	1:B:310:VAL:HG21	0.55	2.32	12	4
1:B:268:THR:O	1:B:269:GLN:CG	0.55	2.54	8	1
1:A:72:ARG:O	1:A:78:ALA:HB1	0.55	2.02	12	1
1:A:101:PHE:CD1	1:A:103:PHE:CE1	0.55	2.95	14	2
1:A:115:LEU:CD2	1:B:279:ALA:CB	0.55	2.83	10	2
1:A:11:VAL:CG2	1:A:71:VAL:HG11	0.55	2.32	13	1
1:B:304:ASN:OD1	1:B:310:VAL:HG22	0.55	2.00	1	1
1:A:34:ALA:N	1:A:51:ILE:CD1	0.55	2.67	5	2
1:A:23:LEU:CD2	1:A:56:ALA:HB2	0.55	2.32	14	5
1:B:238:ASP:O	1:B:254:PHE:CZ	0.55	2.59	8	6
1:B:238:ASP:OD2	1:B:314:ALA:CB	0.55	2.55	12	3
1:A:102:ARG:CB	1:A:111:SER:CB	0.55	2.84	10	2
1:B:288:PHE:CE2	1:B:291:ARG:HB3	0.55	2.37	9	1
1:A:10:VAL:O	1:A:14:TYR:CB	0.55	2.55	4	15
1:B:234:ALA:N	1:B:251:ILE:CD1	0.55	2.69	11	4



	h h	(1,1)	${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:234:ALA:CA	1:B:310:VAL:O	0.55	2.55	12	9
1:B:305:GLY:O	1:B:306:ALA:CB	0.55	2.55	12	11
1:B:210:VAL:HG13	1:B:301:PHE:CE1	0.55	2.36	10	6
1:A:74:VAL:CG2	1:B:316:PHE:O	0.54	2.55	4	7
1:A:80:PHE:CD1	1:A:101:PHE:CD2	0.54	2.95	14	3
1:B:214:TYR:CE2	1:B:312:MET:CE	0.54	2.90	15	1
1:A:74:VAL:CG1	1:B:316:PHE:O	0.54	2.55	4	11
1:A:115:LEU:HD13	1:B:279:ALA:CB	0.54	2.30	11	3
1:B:240:VAL:HG13	1:B:316:PHE:CE1	0.54	2.38	3	1
1:A:104:ASN:OD1	1:A:110:VAL:CG2	0.54	2.56	10	5
1:B:303:PHE:CD1	1:B:303:PHE:N	0.54	2.74	14	8
1:A:67:LEU:HD22	1:A:71:VAL:HG23	0.54	1.78	10	1
1:A:109:VAL:CG1	1:A:110:VAL:N	0.54	2.70	14	4
1:B:275:ALA:O	1:B:276:ASN:CB	0.54	2.54	5	1
1:A:104:ASN:HD21	1:A:106:ALA:HB3	0.54	1.63	7	1
1:A:86:PHE:CZ	2:A:126:NTH:H211	0.54	2.37	11	2
1:B:238:ASP:OD1	1:B:314:ALA:CB	0.54	2.55	15	2
1:B:271:VAL:HG22	1:B:280:PHE:HB2	0.54	1.78	10	1
1:A:94:VAL:CG1	1:A:95:VAL:N	0.54	2.70	9	6
1:B:272:ARG:CB	1:B:279:ALA:O	0.54	2.56	2	13
1:A:61:LEU:HB3	1:A:63:LEU:HD21	0.54	1.78	4	1
1:A:94:VAL:HG22	1:A:95:VAL:N	0.54	2.16	15	5
1:A:85:SER:HB3	1:A:94:VAL:HG23	0.54	1.78	7	1
1:A:14:TYR:O	1:A:14:TYR:CD1	0.54	2.60	10	1
1:B:206:HIS:CE1	1:B:207:MET:HG3	0.54	2.36	13	1
1:B:321:ILE:HG22	1:B:322:HIS:H	0.54	1.63	3	11
1:B:288:PHE:O	1:B:290:GLY:N	0.54	2.41	13	2
1:B:236:VAL:HG12	1:B:237:GLU:N	0.54	2.17	9	2
1:B:297:PRO:HB2	1:B:316:PHE:CD1	0.54	2.37	9	1
1:A:69:GLN:HG2	1:A:70:GLU:N	0.54	2.18	10	1
1:A:95:VAL:HG13	1:A:120:ASN:O	0.54	2.01	10	1
1:A:61:LEU:O	1:A:63:LEU:CD2	0.54	2.56	14	2
1:A:13:ARG:NH2	1:A:29:LEU:CD1	0.54	2.69	4	1
1:A:75:ALA:O	1:A:76:ASN:CB	0.54	2.55	4	1
1:B:294:VAL:HG22	1:B:295:VAL:H	0.54	1.63	13	3
1:B:284:VAL:HG12	1:B:286:PHE:HD1	0.54	1.63	6	1
1:B:281:ALA:HB2	1:B:298:ILE:CG1	0.54	2.33	15	3
1:A:100:HIS:O	1:A:112:MET:CG	0.54	2.56	13	14
1:A:116:PHE:O	1:B:274:VAL:CG2	0.54	2.56	10	13
1:A:79:ALA:CB	1:B:315:LEU:CD2	0.54	2.80	4	2
1:B:315:LEU:O	1:B:316:PHE:CG	0.54	2.60	7	3



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:261:LEU:CD1	1:B:263:LEU:HD21	0.54	2.33	14	1
1:A:61:LEU:O	1:A:63:LEU:CD1	0.54	2.56	1	7
1:B:210:VAL:O	1:B:214:TYR:CB	0.54	2.56	15	14
1:B:263:LEU:HB3	1:B:284:VAL:HG13	0.54	1.79	7	2
1:B:304:ASN:OD1	1:B:310:VAL:CG1	0.54	2.56	4	1
1:A:10:VAL:CG2	1:A:109:VAL:HG23	0.54	2.32	6	6
1:A:17:ALA:CA	1:A:22:ASP:OD1	0.54	2.56	6	1
1:B:236:VAL:CG2	1:B:251:ILE:HD12	0.54	2.33	12	1
1:A:49:ALA:O	1:A:53:GLU:CB	0.54	2.56	10	7
1:B:317:GLY:O	1:B:321:ILE:CD1	0.54	2.56	3	12
1:A:95:VAL:HG22	1:A:121:ILE:HA	0.54	1.80	2	2
1:B:261:LEU:O	1:B:263:LEU:CD1	0.54	2.56	5	8
1:B:273:ALA:C	1:B:274:VAL:HG22	0.54	2.23	14	3
1:A:86:PHE:CD2	1:A:87:GLU:O	0.54	2.60	12	3
1:B:300:HIS:O	1:B:312:MET:CG	0.54	2.56	11	11
1:A:3:THR:O	1:A:7:MET:HE2	0.54	2.03	13	1
1:A:61:LEU:O	1:A:63:LEU:HD23	0.54	2.02	14	1
1:A:100:HIS:CD2	1:B:300:HIS:NE2	0.54	2.76	15	1
1:B:304:ASN:OD1	1:B:310:VAL:CG2	0.53	2.56	1	6
1:A:88:PHE:O	1:A:90:GLY:N	0.53	2.42	14	2
1:B:210:VAL:HG13	1:B:301:PHE:CZ	0.53	2.37	2	6
1:B:286:PHE:CZ	1:B:293:THR:HB	0.53	2.38	11	4
1:A:36:VAL:HG23	1:A:51:ILE:CD1	0.53	2.33	8	3
1:B:245:ARG:NH1	1:B:245:ARG:O	0.53	2.40	7	1
1:A:40:VAL:O	1:B:275:ALA:HB3	0.53	2.03	8	1
1:A:86:PHE:CD1	1:A:93:THR:O	0.53	2.61	8	1
1:B:304:ASN:OD1	1:B:310:VAL:CB	0.53	2.56	14	1
1:B:285:SER:HB3	1:B:294:VAL:HG23	0.53	1.80	13	1
1:B:258:SER:OG	2:B:326:NTH:H8	0.53	2.04	4	1
1:B:245:ARG:NH1	1:B:251:ILE:HG13	0.53	2.19	7	1
1:A:86:PHE:CE1	1:A:93:THR:O	0.53	2.61	9	2
1:A:77:GLU:CG	1:A:102:ARG:HG3	0.53	2.34	1	3
1:B:261:LEU:O	1:B:263:LEU:CD2	0.53	2.57	1	2
1:B:296:ALA:O	1:B:320:ASN:ND2	0.53	2.42	5	6
1:A:61:LEU:HD12	1:A:63:LEU:HG	0.53	1.78	9	1
1:B:243:GLU:O	1:B:254:PHE:CZ	0.53	2.61	15	3
1:B:249:ALA:O	1:B:253:GLU:CB	0.53	2.56	4	4
1:A:120:ASN:OD1	1:A:121:ILE:CD1	0.53	2.57	2	2
1:A:88:PHE:CE1	1:A:91:ARG:O	0.53	2.62	8	1
1:B:261:LEU:HD23	1:B:261:LEU:O	0.53	2.02	8	1
1:A:100:HIS:CB	1:A:113:ARG:O	0.53	2.57	14	2



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:293:THR:OG1	1:B:294:VAL:N	0.53	2.42	14	1
1:A:15:VAL:O	1:A:18:LEU:N	0.53	2.42	9	14
1:A:41:GLY:O	1:A:42:SER:CB	0.53	2.55	3	4
1:B:246:SER:O	1:B:250:ALA:CB	0.53	2.57	11	8
1:B:276:ASN:O	1:B:303:PHE:N	0.53	2.42	15	5
1:B:252:ARG:O	1:B:256:ALA:CB	0.53	2.56	15	8
1:A:38:ASP:O	1:A:54:PHE:CE2	0.53	2.62	10	3
1:B:280:PHE:CE1	1:B:301:PHE:CD2	0.53	2.97	6	2
1:A:34:ALA:CB	1:A:51:ILE:CD1	0.53	2.82	7	1
1:B:245:ARG:O	1:B:245:ARG:CZ	0.53	2.57	7	1
1:A:38:ASP:O	1:A:43:GLU:CB	0.53	2.56	3	3
1:B:247:GLY:O	1:B:251:ILE:CG1	0.53	2.57	14	7
1:A:62:PRO:O	1:A:86:PHE:CB	0.53	2.57	2	4
1:B:235:THR:O	1:B:236:VAL:HG23	0.53	2.04	2	1
1:A:23:LEU:O	1:A:26:ILE:N	0.53	2.42	9	7
1:B:294:VAL:O	1:B:295:VAL:HG23	0.53	2.04	7	2
1:B:239:PRO:O	1:B:240:VAL:CG1	0.53	2.56	9	1
1:A:7:MET:CB	1:A:73:ALA:HB1	0.53	2.29	13	1
1:A:40:VAL:C	1:B:275:ALA:HB2	0.53	2.23	14	1
1:A:38:ASP:OD2	1:A:114:ALA:CB	0.53	2.57	8	4
1:B:278:ALA:O	1:B:301:PHE:N	0.53	2.42	6	13
1:B:294:VAL:CG1	1:B:322:HIS:CB	0.53	2.87	8	5
1:B:299:ASP:OD1	1:B:300:HIS:N	0.53	2.42	1	4
1:A:81:ALA:C	1:A:82:PHE:CD2	0.53	2.82	14	5
1:A:45:ARG:O	1:A:51:ILE:CD1	0.53	2.57	3	4
1:B:221:GLY:HA3	1:B:259:LEU:HD21	0.53	1.78	15	2
1:B:245:ARG:HB2	1:B:254:PHE:CD2	0.53	2.39	3	3
1:A:72:ARG:NE	1:A:73:ALA:N	0.53	2.57	5	1
1:A:80:PHE:CE2	1:A:82:PHE:CE1	0.53	2.97	6	2
1:B:219:ASN:ND2	1:B:265:VAL:O	0.53	2.42	7	3
1:B:267:LEU:O	1:B:268:THR:CG2	0.53	2.57	12	1
1:A:36:VAL:HG12	1:A:37:GLU:N	0.53	2.18	8	4
1:A:88:PHE:CZ	2:A:126:NTH:O23	0.53	2.62	1	2
1:B:217:ALA:O	1:B:222:ASP:N	0.53	2.42	9	10
1:B:245:ARG:CB	1:B:250:ALA:HB1	0.53	2.33	14	4
1:B:298:ILE:HG22	1:B:299:ASP:N	0.53	2.19	12	4
1:A:41:GLY:O	1:A:42:SER:C	0.53	2.47	2	1
1:B:294:VAL:O	1:B:322:HIS:CB	0.53	2.57	14	2
1:A:34:ALA:CA	1:A:110:VAL:O	0.53	2.57	1	9
1:A:117:GLY:O	1:A:121:ILE:CD1	0.53	2.57	5	9
1:B:215:VAL:O	1:B:218:LEU:N	0.53	2.42	8	15



			${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:76:ASN:O	1:A:103:PHE:N	0.53	2.42	10	8
1:A:103:PHE:CD1	1:A:108:LYS:O	0.53	2.62	2	1
1:A:105:GLY:O	1:A:106:ALA:CB	0.53	2.57	5	10
1:B:247:GLY:O	1:B:251:ILE:CD1	0.53	2.57	6	6
1:A:45:ARG:O	1:A:51:ILE:HD11	0.53	2.03	11	3
1:B:232:ASP:O	1:B:248:THR:N	0.53	2.42	10	3
1:B:295:VAL:CG1	1:B:321:ILE:HG23	0.53	2.33	5	2
1:B:293:THR:CB	1:B:322:HIS:HB2	0.53	2.34	13	2
1:B:215:VAL:HG21	1:B:267:LEU:HD21	0.53	1.80	8	1
1:A:47:GLY:O	1:A:51:ILE:CG1	0.52	2.56	14	4
1:B:201:MET:O	1:B:202:ASN:CB	0.52	2.57	2	2
1:A:45:ARG:HB2	1:A:54:PHE:CD2	0.52	2.38	2	2
1:A:86:PHE:CZ	1:A:93:THR:HB	0.52	2.39	7	6
1:B:276:ASN:ND2	1:B:303:PHE:O	0.52	2.43	2	1
1:A:17:ALA:O	1:A:22:ASP:N	0.52	2.43	9	7
1:B:294:VAL:HG12	1:B:322:HIS:HB3	0.52	1.79	14	4
1:B:298:ILE:CD1	1:B:320:ASN:OD1	0.52	2.57	3	2
1:B:300:HIS:CB	1:B:313:ARG:O	0.52	2.57	4	2
1:B:245:ARG:HD2	1:B:251:ILE:N	0.52	2.20	7	1
1:A:61:LEU:HB2	2:A:126:NTH:H183	0.52	1.78	12	1
1:A:36:VAL:O	1:A:44:PRO:CA	0.52	2.57	6	5
1:A:45:ARG:HG2	1:A:50:ALA:CB	0.52	2.34	2	1
1:A:52:ARG:O	1:A:56:ALA:CB	0.52	2.58	7	6
1:B:229:LEU:O	1:B:309:VAL:CG2	0.52	2.57	2	1
1:B:207:MET:HA	1:B:303:PHE:CZ	0.52	2.40	7	2
1:A:34:ALA:O	1:A:51:ILE:CD1	0.52	2.57	15	2
1:B:286:PHE:CZ	1:B:293:THR:CB	0.52	2.92	5	4
1:B:237:GLU:O	1:B:314:ALA:CB	0.52	2.57	5	1
1:B:288:PHE:HZ	1:B:293:THR:HG1	0.52	1.45	7	1
1:A:37:GLU:OE2	1:A:113:ARG:CD	0.52	2.58	14	1
1:A:102:ARG:O	1:A:110:VAL:HG23	0.52	2.04	1	2
1:A:4:PRO:O	1:A:8:THR:CB	0.52	2.57	3	3
1:A:10:VAL:CG1	1:A:109:VAL:HG22	0.52	2.35	3	1
1:B:217:ALA:HB3	1:B:226:ILE:HG12	0.52	1.81	3	6
1:A:33:ASP:C	1:A:51:ILE:HD11	0.52	2.25	5	1
1:A:98:ILE:HG22	1:A:99:ASP:N	0.52	2.20	12	4
1:B:284:VAL:HG12	1:B:286:PHE:CD1	0.52	2.38	6	1
1:A:96:ALA:O	1:A:120:ASN:ND2	0.52	2.42	14	3
1:A:39:PRO:O	1:A:41:GLY:N	0.52	2.42	8	1
1:A:74:VAL:HG12	1:B:240:VAL:HG21	0.52	1.82	8	1
1:B:203:THR:O	1:B:203:THR:CG2	0.52	2.57	15	2



	to uo puge		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:102:ARG:CZ	1:B:313:ARG:CD	0.52	2.88	15	1
1:A:15:VAL:HA	1:A:18:LEU:CD1	0.52	2.34	10	15
1:A:61:LEU:HD12	1:A:63:LEU:HD21	0.52	1.81	9	1
1:A:100:HIS:CD2	1:A:101:PHE:N	0.52	2.78	9	1
1:A:95:VAL:HG12	1:A:96:ALA:N	0.52	2.20	14	2
1:B:280:PHE:O	1:B:298:ILE:CG2	0.52	2.57	5	5
1:A:99:ASP:OD1	1:A:100:HIS:N	0.52	2.43	12	7
1:B:288:PHE:C	1:B:289:GLN:CG	0.52	2.78	5	3
1:A:39:PRO:O	1:A:40:VAL:HG13	0.52	2.04	1	1
1:B:227:VAL:HG11	1:B:248:THR:CG2	0.52	2.34	2	1
1:B:302:ARG:O	1:B:310:VAL:HG23	0.52	2.03	11	2
1:A:80:PHE:CD1	1:A:80:PHE:N	0.52	2.77	7	1
1:B:286:PHE:CE1	1:B:293:THR:O	0.52	2.62	9	1
1:A:46:SER:O	1:A:50:ALA:CB	0.52	2.57	12	2
1:A:35:THR:N	1:A:110:VAL:O	0.52	2.42	1	1
1:B:270:GLU:O	1:B:272:ARG:CZ	0.52	2.57	9	1
1:A:45:ARG:HD2	1:A:51:ILE:HD13	0.52	1.82	11	1
1:A:63:LEU:HB3	1:A:84:VAL:CG1	0.52	2.34	11	2
1:A:88:PHE:CZ	2:A:126:NTH:O24	0.52	2.63	11	1
1:A:120:ASN:OD1	1:B:272:ARG:NH2	0.52	2.42	14	2
1:A:39:PRO:O	1:A:40:VAL:CG1	0.52	2.58	1	1
1:A:80:PHE:CE2	1:A:99:ASP:HB3	0.52	2.40	11	3
1:A:102:ARG:HB3	1:A:111:SER:CB	0.52	2.35	10	5
1:B:211:VAL:HG22	1:B:280:PHE:CD1	0.52	2.39	7	2
1:B:274:VAL:O	1:B:275:ALA:C	0.52	2.48	2	11
1:A:100:HIS:NE2	1:B:315:LEU:CD1	0.52	2.72	5	1
1:B:261:LEU:HD13	2:B:326:NTH:C20	0.52	2.34	7	1
1:A:77:GLU:CD	1:A:100:HIS:CE1	0.52	2.83	12	1
1:A:3:THR:O	1:A:3:THR:CG2	0.52	2.58	15	6
1:A:40:VAL:O	1:A:42:SER:N	0.52	2.43	2	1
1:A:17:ALA:CB	1:A:22:ASP:OD1	0.52	2.57	6	2
1:A:37:GLU:OE1	1:A:113:ARG:CG	0.52	2.58	1	1
1:A:87:GLU:CG	1:A:88:PHE:N	0.52	2.73	8	2
1:B:210:VAL:HG12	1:B:301:PHE:CE2	0.52	2.40	4	3
1:A:77:GLU:OE1	1:B:313:ARG:NE	0.52	2.43	5	1
1:B:289:GLN:CG	1:B:289:GLN:O	0.52	2.56	6	1
1:B:261:LEU:HB3	1:B:263:LEU:HD21	0.52	1.81	15	1
1:B:223:LEU:O	1:B:226:ILE:N	0.51	2.43	11	8
1:B:231:ALA:CB	1:B:309:VAL:O	0.51	2.57	14	2
1:A:31:ALA:CB	1:A:109:VAL:O	0.51	2.56	10	3
1:A:45:ARG:HG3	1:A:54:PHE:CG	0.51	2.40	6	1



	to us page		$\operatorname{Distance}(\operatorname{\AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:121:ILE:HG22	1:A:122:HIS:H	0.51	1.66	6	13
1:A:80:PHE:CE1	1:A:99:ASP:HB3	0.51	2.40	10	11
1:A:94:VAL:HG12	1:A:122:HIS:HB3	0.51	1.81	14	3
1:A:40:VAL:HG12	1:A:114:ALA:O	0.51	2.06	8	2
1:A:58:SER:OG	2:A:126:NTH:H10	0.51	2.05	8	3
1:B:297:PRO:HB3	1:B:316:PHE:CD2	0.51	2.40	9	1
1:B:207:MET:CB	1:B:273:ALA:HB1	0.51	2.36	8	2
1:A:10:VAL:HG13	1:A:101:PHE:CZ	0.51	2.41	2	4
1:B:226:ILE:CG2	1:B:230:PHE:CE2	0.51	2.93	2	1
1:A:19:ASN:ND2	1:A:65:VAL:O	0.51	2.43	10	3
1:A:99:ASP:OD2	1:A:112:MET:CE	0.51	2.58	3	3
1:B:294:VAL:CG1	1:B:322:HIS:HB3	0.51	2.35	10	2
1:B:263:LEU:HB3	1:B:284:VAL:HG12	0.51	1.81	11	1
1:A:78:ALA:O	1:A:101:PHE:N	0.51	2.43	2	14
1:B:210:VAL:HG21	1:B:303:PHE:HE1	0.51	1.65	2	1
1:A:72:ARG:CD	1:B:315:LEU:CD2	0.51	2.88	7	1
1:B:316:PHE:CZ	2:B:326:NTH:H72	0.51	2.40	14	2
1:A:37:GLU:OE2	1:A:113:ARG:NH1	0.51	2.44	13	1
1:B:223:LEU:CD2	1:B:252:ARG:HG2	0.51	2.36	9	8
1:B:223:LEU:CD2	1:B:252:ARG:HG3	0.51	2.34	10	5
1:A:10:VAL:HG12	1:A:101:PHE:CE2	0.51	2.41	5	2
1:A:75:ALA:CB	1:B:241:GLY:HA3	0.51	2.36	7	1
1:B:210:VAL:HG13	1:B:309:VAL:CG2	0.51	2.36	7	1
1:A:120:ASN:OD1	1:A:121:ILE:HD13	0.51	2.05	11	1
1:B:280:PHE:CE2	1:B:282:PHE:CE1	0.51	2.99	7	3
1:B:240:VAL:HG12	1:B:314:ALA:O	0.51	2.06	3	1
1:A:61:LEU:CB	1:A:63:LEU:HD11	0.51	2.33	9	1
1:B:261:LEU:HD12	1:B:263:LEU:HD11	0.51	1.82	14	1
1:B:294:VAL:HG22	1:B:295:VAL:N	0.51	2.21	1	6
1:A:117:GLY:O	1:A:120:ASN:OD1	0.51	2.28	11	3
1:B:309:VAL:HG12	1:B:310:VAL:N	0.51	2.19	13	3
1:A:40:VAL:HG22	1:A:116:PHE:CZ	0.51	2.40	3	1
1:A:86:PHE:CE1	1:A:93:THR:HB	0.51	2.40	14	4
1:A:23:LEU:CD2	1:A:52:ARG:HG2	0.51	2.35	15	3
1:B:300:HIS:CD2	1:B:301:PHE:N	0.51	2.79	7	1
1:A:45:ARG:NH1	1:A:51:ILE:O	0.51	2.43	11	1
1:A:79:ALA:CB	1:B:315:LEU:HD13	0.51	2.34	1	3
1:B:211:VAL:CG2	1:B:301:PHE:CD2	0.51	2.94	10	4
1:B:280:PHE:CE1	1:B:301:PHE:CE2	0.51	2.98	6	3
1:B:287:GLU:OE1	1:B:288:PHE:N	0.51	2.43	7	1
1:B:297:PRO:HB3	1:B:316:PHE:CE1	0.51	2.40	7	1



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:100:HIS:NE2	1:A:101:PHE:O	0.51	2.44	9	1
1:B:280:PHE:CE1	1:B:299:ASP:HB3	0.51	2.41	4	11
1:A:61:LEU:CG	1:A:63:LEU:HD21	0.51	2.36	3	1
1:B:217:ALA:CB	1:B:226:ILE:HG12	0.51	2.36	7	2
1:B:300:HIS:CG	1:B:301:PHE:N	0.51	2.79	7	3
1:A:72:ARG:HD3	1:B:315:LEU:CD2	0.51	2.35	7	1
1:A:104:ASN:OD1	1:A:107:GLY:N	0.51	2.43	14	1
1:A:40:VAL:O	1:B:275:ALA:CB	0.51	2.58	15	1
1:A:38:ASP:O	1:A:43:GLU:O	0.51	2.29	7	5
1:A:113:ARG:CG	1:A:114:ALA:N	0.51	2.73	7	1
1:B:245:ARG:HD3	1:B:254:PHE:CD1	0.51	2.41	9	1
1:B:287:GLU:CG	1:B:291:ARG:O	0.51	2.59	9	1
1:B:245:ARG:HB2	1:B:254:PHE:CD1	0.51	2.41	14	1
1:B:235:THR:OG1	1:B:311:SER:CB	0.50	2.59	2	1
1:A:10:VAL:HB	1:A:103:PHE:CZ	0.50	2.40	15	3
1:B:263:LEU:CD2	1:B:284:VAL:CG1	0.50	2.87	8	2
1:B:286:PHE:CE1	1:B:293:THR:HB	0.50	2.41	4	6
1:A:14:TYR:CE2	1:A:80:PHE:CZ	0.50	3.00	10	2
1:B:261:LEU:HB3	1:B:263:LEU:HD11	0.50	1.83	14	1
1:B:215:VAL:HA	1:B:218:LEU:CD1	0.50	2.35	11	15
1:B:280:PHE:CE2	1:B:299:ASP:HB3	0.50	2.41	2	4
1:A:73:ALA:C	1:A:74:VAL:HG22	0.50	2.27	10	2
1:B:276:ASN:ND2	1:B:304:ASN:O	0.50	2.43	6	1
1:A:119:LYS:CE	1:B:270:GLU:OE2	0.50	2.59	9	1
1:A:35:THR:O	1:A:36:VAL:CG2	0.50	2.59	15	1
1:A:45:ARG:HG3	1:A:54:PHE:CD1	0.50	2.41	7	2
1:A:63:LEU:HB2	1:A:84:VAL:CG1	0.50	2.35	6	2
1:A:56:ALA:O	1:A:59:LEU:N	0.50	2.44	7	1
1:A:116:PHE:CG	1:A:117:GLY:N	0.50	2.75	9	2
1:B:288:PHE:CE2	1:B:291:ARG:CB	0.50	2.94	9	1
1:B:315:LEU:O	1:B:316:PHE:CD2	0.50	2.65	13	1
1:B:268:THR:OG1	1:B:269:GLN:N	0.50	2.43	14	1
1:A:14:TYR:CD1	1:A:15:VAL:HG23	0.50	2.42	5	7
1:A:81:ALA:HB2	1:A:98:ILE:CG1	0.50	2.36	2	2
1:B:210:VAL:HB	1:B:303:PHE:CE2	0.50	2.41	6	4
1:B:277:GLU:OE2	1:B:302:ARG:NE	0.50	2.44	8	1
1:B:304:ASN:N	1:B:310:VAL:CG2	0.50	2.73	13	1
1:A:37:GLU:OE1	1:A:37:GLU:N	0.50	2.45	15	1
1:A:45:ARG:HG3	1:A:54:PHE:CD2	0.50	2.41	1	1
1:A:74:VAL:O	1:A:75:ALA:C	0.50	2.50	15	11
1:A:115:LEU:O	1:A:116:PHE:HB3	0.50	2.07	7	14



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:10:VAL:HB	1:A:103:PHE:CE2	0.50	2.42	15	4
1:B:317:GLY:C	1:B:321:ILE:CD1	0.50	2.79	3	1
1:A:45:ARG:CB	1:A:50:ALA:HB1	0.50	2.37	4	2
1:A:94:VAL:CG1	1:A:122:HIS:CD2	0.50	2.95	7	1
1:B:238:ASP:OD2	1:B:314:ALA:HB3	0.50	2.06	11	1
1:B:263:LEU:HB3	1:B:284:VAL:CG1	0.50	2.36	10	5
1:A:93:THR:HG22	1:A:94:VAL:N	0.50	2.22	4	1
1:B:204:PRO:O	1:B:208:THR:CB	0.50	2.59	15	2
1:B:285:SER:CB	1:B:294:VAL:HG23	0.50	2.37	13	2
1:A:23:LEU:CD2	1:A:52:ARG:HG3	0.50	2.36	7	5
1:B:284:VAL:O	1:B:295:VAL:N	0.50	2.44	3	4
1:B:201:MET:CG	1:B:201:MET:O	0.50	2.60	4	1
1:A:36:VAL:CG2	1:A:51:ILE:CD1	0.50	2.90	8	2
1:B:316:PHE:CD2	1:B:321:ILE:HD11	0.50	2.42	7	1
1:B:219:ASN:OD1	1:B:265:VAL:N	0.50	2.43	10	1
1:B:281:ALA:O	1:B:282:PHE:CB	0.50	2.59	10	2
1:B:258:SER:HB2	2:B:326:NTH:H10	0.50	1.82	13	1
1:A:36:VAL:HG13	1:A:37:GLU:N	0.50	2.21	14	1
1:B:261:LEU:CD2	1:B:263:LEU:HD23	0.50	2.36	15	1
1:A:72:ARG:CG	1:A:79:ALA:O	0.50	2.60	2	1
1:A:72:ARG:NH1	1:B:316:PHE:O	0.50	2.44	5	1
1:A:103:PHE:CD1	1:A:103:PHE:N	0.50	2.80	8	3
1:A:88:PHE:C	1:A:89:GLN:CG	0.50	2.80	12	2
1:A:37:GLU:OE1	1:A:113:ARG:NE	0.50	2.43	15	2
1:B:214:TYR:CE2	1:B:255:PHE:CZ	0.50	2.99	7	15
1:B:237:GLU:OE1	1:B:313:ARG:CZ	0.50	2.59	2	1
1:B:258:SER:HG	2:B:326:NTH:H8	0.50	1.66	4	1
1:A:15:VAL:HG21	1:A:67:LEU:HG	0.50	1.84	5	1
1:B:213:ARG:HA	1:B:216:ALA:HB3	0.50	1.83	7	1
1:B:303:PHE:C	1:B:310:VAL:CG2	0.50	2.81	11	2
1:A:96:ALA:N	1:A:120:ASN:O	0.50	2.43	9	3
1:A:80:PHE:CZ	1:A:99:ASP:CB	0.50	2.95	11	1
1:A:8:THR:O	1:A:11:VAL:N	0.49	2.43	12	4
1:A:6:HIS:NE2	1:A:7:MET:HG3	0.49	2.22	11	1
1:A:11:VAL:HG11	1:A:71:VAL:HG13	0.49	1.85	2	1
1:A:70:GLU:O	1:A:72:ARG:NE	0.49	2.45	2	1
1:A:45:ARG:HD3	1:A:54:PHE:CD1	0.49	2.41	8	3
1:A:75:ALA:HB2	1:B:240:VAL:C	0.49	2.26	6	1
1:A:94:VAL:CG1	1:A:122:HIS:CG	0.49	2.95	14	3
1:A:38:ASP:O	1:A:43:GLU:HB2	0.49	2.07	1	3
1:B:227:VAL:O	1:B:230:PHE:O	0.49	2.31	5	4



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:35:THR:HG23	1:A:46:SER:HB3	0.49	1.82	3	2
1:A:36:VAL:O	1:A:44:PRO:HA	0.49	2.07	12	5
1:B:210:VAL:CG1	1:B:309:VAL:CG2	0.49	2.91	7	4
1:B:223:LEU:HD22	1:B:256:ALA:HB2	0.49	1.83	9	4
1:A:73:ALA:C	1:A:74:VAL:CG2	0.49	2.80	7	2
1:A:72:ARG:CD	1:B:315:LEU:HD21	0.49	2.38	7	1
1:B:286:PHE:CE2	1:B:288:PHE:CD1	0.49	3.01	13	1
1:A:45:ARG:O	1:A:51:ILE:HD13	0.49	2.07	9	1
1:B:208:THR:O	1:B:211:VAL:N	0.49	2.43	15	2
1:A:80:PHE:CD1	1:A:80:PHE:C	0.49	2.85	11	1
1:B:263:LEU:HB2	1:B:284:VAL:CG1	0.49	2.36	11	2
1:A:118:GLU:HA	1:A:121:ILE:CG1	0.49	2.36	3	13
1:A:115:LEU:CD1	1:B:300:HIS:CD2	0.49	2.94	4	1
1:B:227:VAL:HG21	1:B:252:ARG:CB	0.49	2.37	15	3
1:B:261:LEU:CD2	1:B:263:LEU:HD11	0.49	2.37	8	1
1:B:281:ALA:CA	1:B:298:ILE:HD12	0.49	2.35	11	1
1:A:33:ASP:N	1:A:33:ASP:OD1	0.49	2.43	2	2
1:B:234:ALA:O	1:B:251:ILE:CD1	0.49	2.58	10	3
1:B:281:ALA:C	1:B:282:PHE:CD2	0.49	2.85	9	4
1:B:210:VAL:HB	1:B:303:PHE:CZ	0.49	2.42	6	5
1:A:115:LEU:CG	1:B:279:ALA:CB	0.49	2.90	4	1
1:A:40:VAL:O	1:A:40:VAL:CG2	0.49	2.60	13	2
1:B:315:LEU:O	1:B:316:PHE:HB3	0.49	2.08	8	12
1:A:80:PHE:O	1:A:98:ILE:CG2	0.49	2.61	10	5
1:A:99:ASP:OD2	1:A:112:MET:HE3	0.49	2.08	4	2
1:B:211:VAL:CG2	1:B:271:VAL:HG11	0.49	2.30	12	2
1:A:36:VAL:O	1:A:44:PRO:HB3	0.49	2.08	14	9
1:A:29:LEU:O	1:A:109:VAL:N	0.49	2.43	3	1
1:A:104:ASN:CB	1:A:110:VAL:HG21	0.49	2.33	11	3
1:B:262:PRO:O	1:B:286:PHE:CB	0.49	2.61	6	2
1:A:58:SER:CB	2:A:126:NTH:H11	0.49	2.37	7	1
1:A:77:GLU:OE2	1:A:100:HIS:CE1	0.49	2.66	9	1
1:A:23:LEU:HD23	1:A:59:LEU:HD22	0.49	1.81	10	1
1:B:206:HIS:NE2	1:B:207:MET:CE	0.49	2.76	13	1
1:B:293:THR:CG2	1:B:322:HIS:O	0.49	2.61	15	1
1:B:236:VAL:O	1:B:244:PRO:HB3	0.49	2.08	11	13
1:A:17:ALA:CB	1:A:26:ILE:HG12	0.49	2.38	2	1
1:B:272:ARG:O	1:B:279:ALA:N	0.49	2.44	4	4
1:B:317:GLY:O	1:B:320:ASN:OD1	0.49	2.31	4	1
1:B:207:MET:HB3	1:B:273:ALA:HB1	0.49	1.85	8	2
1:A:98:ILE:CD1	1:B:272:ARG:HD2	0.49	2.38	11	1



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:235:THR:N	1:B:310:VAL:O	0.49	2.45	12	3
1:A:94:VAL:HG22	1:A:95:VAL:H	0.49	1.68	14	1
1:A:75:ALA:CB	1:B:241:GLY:CA	0.49	2.90	7	1
1:A:79:ALA:HB3	1:B:315:LEU:HD11	0.49	1.83	7	1
1:B:268:THR:O	1:B:269:GLN:HG2	0.49	2.08	8	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.49	2.43	10	1
1:A:10:VAL:O	1:A:14:TYR:HB3	0.48	2.08	1	3
1:B:237:GLU:OE2	1:B:313:ARG:NE	0.48	2.43	1	1
1:B:252:ARG:O	1:B:256:ALA:N	0.48	2.44	3	12
1:B:295:VAL:CG1	1:B:297:PRO:HG3	0.48	2.38	7	8
1:A:10:VAL:CB	1:A:103:PHE:CE2	0.48	2.96	3	2
1:B:212:GLN:O	1:B:215:VAL:N	0.48	2.45	7	8
1:B:237:GLU:O	1:B:314:ALA:HB2	0.48	2.08	5	1
1:B:231:ALA:N	1:B:309:VAL:O	0.48	2.42	10	2
1:B:273:ALA:C	1:B:274:VAL:CG2	0.48	2.81	14	1
1:A:67:LEU:HD22	1:A:82:PHE:HB3	0.48	1.85	1	1
1:B:300:HIS:N	1:B:313:ARG:O	0.48	2.46	13	7
1:A:10:VAL:HG13	1:A:109:VAL:CG2	0.48	2.39	3	2
1:B:263:LEU:HD23	1:B:286:PHE:CB	0.48	2.37	4	1
1:A:68:THR:O	1:A:69:GLN:HG2	0.48	2.09	5	2
1:B:240:VAL:HG22	1:B:316:PHE:CE1	0.48	2.43	5	1
1:B:277:GLU:CG	1:B:301:PHE:O	0.48	2.61	10	1
1:A:47:GLY:O	1:A:51:ILE:CD1	0.48	2.61	1	4
1:B:236:VAL:O	1:B:244:PRO:CA	0.48	2.61	6	8
1:A:100:HIS:N	1:A:113:ARG:O	0.48	2.45	3	7
1:B:245:ARG:HG3	1:B:254:PHE:CD2	0.48	2.43	2	1
1:A:17:ALA:CB	1:A:26:ILE:HG13	0.48	2.37	11	5
1:A:102:ARG:CB	1:A:111:SER:HB3	0.48	2.39	10	2
1:B:245:ARG:NH1	1:B:246:SER:HA	0.48	2.23	7	1
1:A:119:LYS:NZ	1:B:270:GLU:CD	0.48	2.67	11	1
1:A:77:GLU:CD	1:A:100:HIS:NE2	0.48	2.67	12	1
1:A:115:LEU:CD1	1:B:300:HIS:NE2	0.48	2.76	3	1
1:A:23:LEU:CD1	1:A:26:ILE:HD12	0.48	2.32	5	3
1:A:100:HIS:CD2	1:A:113:ARG:HG3	0.48	2.44	9	1
1:B:318:GLU:HA	1:B:321:ILE:HD12	0.48	1.84	11	1
1:A:37:GLU:OE2	1:A:113:ARG:NH2	0.48	2.46	15	1
1:B:237:GLU:HB2	1:B:313:ARG:CG	0.48	2.39	1	2
1:B:277:GLU:CG	1:B:302:ARG:HG3	0.48	2.37	4	3
1:A:10:VAL:O	1:A:14:TYR:HB2	0.48	2.09	3	13
1:A:12:GLN:O	1:A:15:VAL:N	0.48	2.47	2	11
1:A:52:ARG:O	1:A:56:ALA:N	0.48	2.46	7	9



	to us page		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:214:TYR:CD1	1:B:215:VAL:HG23	0.48	2.44	15	7
1:B:294:VAL:O	1:B:322:HIS:HA	0.48	2.07	13	2
1:A:98:ILE:CD1	1:B:272:ARG:NH1	0.48	2.76	12	1
1:A:47:GLY:O	1:A:51:ILE:HD12	0.48	2.08	1	4
1:B:300:HIS:O	1:B:312:MET:HG2	0.48	2.07	7	12
1:B:272:ARG:N	1:B:279:ALA:O	0.48	2.47	4	10
1:B:210:VAL:HG22	1:B:309:VAL:HG23	0.48	1.83	10	3
1:B:286:PHE:CZ	1:B:288:PHE:CE2	0.48	3.00	5	2
1:A:38:ASP:HB3	1:A:54:PHE:CE2	0.48	2.44	7	1
1:A:74:VAL:HG11	1:B:240:VAL:HG11	0.48	1.86	8	1
1:A:77:GLU:HG3	1:A:100:HIS:NE2	0.48	2.24	12	1
1:A:77:GLU:CG	1:A:100:HIS:NE2	0.48	2.76	12	1
1:B:258:SER:HA	2:B:326:NTH:H111	0.48	1.86	13	1
1:B:263:LEU:CD2	1:B:286:PHE:CD1	0.48	2.90	14	1
1:A:69:GLN:CG	1:A:70:GLU:N	0.48	2.73	15	4
1:A:72:ARG:CZ	1:A:72:ARG:HB3	0.48	2.38	5	1
1:B:286:PHE:CE2	1:B:288:PHE:CE2	0.48	3.02	5	1
1:B:239:PRO:O	1:B:241:GLY:N	0.48	2.46	6	1
1:A:72:ARG:HG3	1:A:79:ALA:CB	0.48	2.38	9	1
1:A:81:ALA:CB	1:A:98:ILE:HG13	0.48	2.39	2	1
1:A:115:LEU:HG	1:B:279:ALA:CB	0.48	2.39	4	1
1:B:302:ARG:HB3	1:B:311:SER:CB	0.48	2.39	12	2
1:A:68:THR:O	1:A:69:GLN:O	0.48	2.32	8	5
1:A:63:LEU:HD21	2:A:126:NTH:O20	0.48	2.08	7	1
1:B:245:ARG:HD3	1:B:250:ALA:HB1	0.48	1.84	11	1
1:A:100:HIS:O	1:A:112:MET:HG2	0.48	2.09	9	13
1:B:277:GLU:CG	1:B:302:ARG:CG	0.48	2.91	4	3
1:B:300:HIS:HB2	1:B:313:ARG:CB	0.48	2.39	12	2
1:B:210:VAL:O	1:B:214:TYR:HB2	0.48	2.09	3	11
1:A:86:PHE:CE2	1:A:93:THR:HB	0.48	2.43	6	1
1:B:315:LEU:C	1:B:316:PHE:CD1	0.48	2.87	9	2
2:B:326:NTH:H222	2:B:326:NTH:H161	0.48	1.85	13	2
1:A:33:ASP:HA	1:A:47:GLY:CA	0.48	2.39	5	6
1:A:66:GLU:O	1:A:67:LEU:O	0.48	2.32	9	13
1:A:67:LEU:HD23	1:A:67:LEU:N	0.48	2.23	1	1
1:A:85:SER:HB3	1:A:94:VAL:CG2	0.48	2.39	3	3
1:A:61:LEU:HD23	1:A:63:LEU:CD1	0.48	2.39	3	1
1:A:96:ALA:O	1:A:120:ASN:OD1	0.48	2.32	4	4
1:A:117:GLY:O	1:A:120:ASN:N	0.48	2.47	3	3
1:B:246:SER:C	1:B:250:ALA:HB3	0.48	2.30	3	1
1:B:299:ASP:OD2	1:B:312:MET:CE	0.48	2.62	3	2



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:63:LEU:HD23	1:A:86:PHE:CD2	0.48	2.44	5	1
1:B:232:ASP:O	1:B:248:THR:OG1	0.48	2.32	9	7
1:A:102:ARG:CD	1:A:111:SER:HB2	0.48	2.38	6	3
1:B:238:ASP:O	1:B:243:GLU:O	0.48	2.32	6	2
1:B:257:ASN:ND2	1:B:260:LYS:HE2	0.48	2.23	6	1
1:B:245:ARG:CD	1:B:250:ALA:HB1	0.48	2.39	11	2
1:B:238:ASP:OD1	1:B:239:PRO:HA	0.48	2.08	9	5
1:A:86:PHE:CE2	1:A:88:PHE:CD1	0.48	3.02	12	1
1:A:27:VAL:O	1:A:30:PHE:O	0.47	2.32	10	6
1:A:7:MET:HA	1:A:103:PHE:CE2	0.47	2.43	15	3
1:A:94:VAL:CG1	1:A:122:HIS:HB3	0.47	2.39	15	3
1:B:303:PHE:CE1	1:B:309:VAL:HG22	0.47	2.44	4	1
1:B:288:PHE:O	1:B:291:ARG:N	0.47	2.40	5	2
1:A:26:ILE:O	1:A:29:LEU:N	0.47	2.47	7	1
1:A:61:LEU:CD2	1:A:63:LEU:HG	0.47	2.39	7	1
1:A:104:ASN:OD1	1:A:110:VAL:HG22	0.47	2.09	11	1
1:B:240:VAL:HG22	1:B:316:PHE:CZ	0.47	2.43	15	1
1:A:100:HIS:HB3	1:A:113:ARG:CB	0.47	2.39	1	1
1:A:115:LEU:CD2	1:B:279:ALA:HB3	0.47	2.39	10	3
1:B:217:ALA:O	1:B:221:GLY:N	0.47	2.47	7	14
1:A:42:SER:O	1:A:43:GLU:CB	0.47	2.62	2	1
1:A:39:PRO:HD2	1:A:42:SER:CB	0.47	2.39	14	7
1:A:72:ARG:HD2	1:A:73:ALA:N	0.47	2.24	9	1
1:B:210:VAL:HG21	1:B:309:VAL:HG23	0.47	1.84	10	1
1:B:245:ARG:HG3	1:B:254:PHE:CD1	0.47	2.44	13	2
1:B:304:ASN:CG	1:B:310:VAL:HG21	0.47	2.30	12	1
1:A:99:ASP:OD1	1:A:113:ARG:O	0.47	2.33	8	10
1:A:17:ALA:HB3	1:A:26:ILE:HG12	0.47	1.86	13	3
1:A:17:ALA:O	1:A:21:GLY:N	0.47	2.48	7	12
1:B:245:ARG:CD	1:B:250:ALA:C	0.47	2.83	7	1
1:A:93:THR:CG2	1:A:122:HIS:O	0.47	2.60	8	1
1:A:104:ASN:N	1:A:110:VAL:CG2	0.47	2.77	9	1
1:A:6:HIS:CD2	1:A:7:MET:N	0.47	2.83	11	1
1:A:36:VAL:HG11	1:A:54:PHE:CD2	0.47	2.44	14	1
1:A:6:HIS:NE2	1:A:106:ALA:O	0.47	2.47	1	1
1:A:30:PHE:CE1	1:A:112:MET:CE	0.47	2.98	1	2
1:B:233:ASP:HA	1:B:247:GLY:CA	0.47	2.39	7	11
1:B:266:GLU:O	1:B:267:LEU:O	0.47	2.33	4	15
1:B:299:ASP:OD1	1:B:313:ARG:O	0.47	2.33	10	11
1:A:38:ASP:OD1	1:A:114:ALA:CB	0.47	2.58	3	1
1:B:277:GLU:O	1:B:278:ALA:CB	0.47	2.62	10	3



	A L		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
2:B:326:NTH:H222	2:B:326:NTH:C16	0.47	2.39	13	2
1:A:77:GLU:HG3	1:A:101:PHE:O	0.47	2.10	12	1
1:A:45:ARG:HB2	1:A:54:PHE:CD1	0.47	2.44	14	1
1:B:261:LEU:HD12	1:B:263:LEU:CD2	0.47	2.40	14	1
1:A:102:ARG:NH1	1:A:113:ARG:HD2	0.47	2.25	15	1
1:A:38:ASP:HA	1:A:39:PRO:O	0.47	2.09	2	2
1:A:85:SER:CA	1:A:94:VAL:HG23	0.47	2.38	3	4
1:A:116:PHE:CZ	2:A:126:NTH:C6	0.47	2.98	7	2
1:A:98:ILE:O	1:A:115:LEU:O	0.47	2.33	3	1
1:A:27:VAL:HG21	1:A:52:ARG:CG	0.47	2.39	11	3
1:A:74:VAL:HG22	1:B:316:PHE:O	0.47	2.09	12	2
1:B:296:ALA:O	1:B:320:ASN:OD1	0.47	2.32	8	2
1:B:315:LEU:O	1:B:316:PHE:O	0.47	2.33	9	1
1:A:30:PHE:CE2	1:A:112:MET:HE3	0.47	2.44	10	1
1:B:258:SER:CB	2:B:326:NTH:H10	0.47	2.38	13	1
1:B:285:SER:CA	1:B:294:VAL:HG23	0.47	2.40	15	2
1:A:77:GLU:CG	1:A:102:ARG:CG	0.47	2.92	1	2
1:B:210:VAL:O	1:B:214:TYR:HB3	0.47	2.09	1	6
1:B:230:PHE:O	1:B:231:ALA:O	0.47	2.33	14	13
1:A:113:ARG:NH1	1:B:277:GLU:OE2	0.47	2.48	7	2
1:A:45:ARG:HD3	1:A:54:PHE:CB	0.47	2.40	11	1
1:B:274:VAL:O	1:B:277:GLU:O	0.47	2.32	14	1
1:A:30:PHE:HD2	1:A:34:ALA:HB3	0.47	1.70	15	1
1:A:21:GLY:O	1:A:59:LEU:CD2	0.47	2.62	6	3
1:A:30:PHE:O	1:A:31:ALA:O	0.47	2.33	14	12
1:A:94:VAL:O	1:A:122:HIS:HB2	0.47	2.10	4	11
1:B:269:GLN:HG3	1:B:270:GLU:N	0.47	2.25	10	7
1:A:97:PRO:CB	1:A:116:PHE:HB3	0.47	2.40	3	1
1:B:296:ALA:CB	1:B:320:ASN:O	0.47	2.63	12	2
1:A:14:TYR:CE1	1:A:80:PHE:CZ	0.47	3.02	4	2
1:A:72:ARG:O	1:A:79:ALA:O	0.47	2.33	4	1
1:B:226:ILE:HD13	1:B:255:PHE:CE2	0.47	2.44	4	1
1:A:71:VAL:HG12	1:A:72:ARG:N	0.47	2.24	5	1
1:A:39:PRO:O	1:A:40:VAL:HG22	0.47	2.10	6	1
1:A:113:ARG:HG2	1:A:114:ALA:N	0.47	2.25	7	1
1:A:92:LYS:O	1:A:124:GLY:O	0.47	2.33	8	1
1:B:238:ASP:OD1	1:B:239:PRO:O	0.47	2.32	9	1
1:A:55:PHE:CE1	2:A:126:NTH:C2	0.47	2.98	10	1
1:A:64:ALA:CB	1:A:85:SER:OG	0.47	2.58	10	1
1:A:115:LEU:HD13	1:B:300:HIS:CD2	0.47	2.45	10	1
1:A:45:ARG:HB3	1:A:54:PHE:CD2	0.47	2.44	11	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:45:ARG:NE	1:A:54:PHE:HB3	0.47	2.25	11	1
1:A:86:PHE:CZ	2:A:126:NTH:C22	0.47	2.98	11	1
1:B:230:PHE:HD2	1:B:234:ALA:HB3	0.47	1.70	12	2
1:B:286:PHE:CD2	1:B:287:GLU:N	0.47	2.83	11	1
1:B:292:LYS:CD	1:B:292:LYS:O	0.47	2.63	12	1
1:A:88:PHE:O	1:A:89:GLN:O	0.47	2.33	15	1
1:B:245:ARG:HB2	1:B:254:PHE:CG	0.47	2.45	15	1
1:A:41:GLY:O	1:A:42:SER:O	0.47	2.33	6	2
1:A:100:HIS:O	1:A:112:MET:HG3	0.47	2.09	14	2
1:B:247:GLY:C	1:B:251:ILE:HD12	0.47	2.30	2	2
1:B:295:VAL:CG1	1:B:320:ASN:ND2	0.47	2.78	4	1
1:B:234:ALA:H	1:B:251:ILE:HD11	0.47	1.64	7	1
1:A:35:THR:CG2	1:A:46:SER:HB2	0.47	2.40	12	4
1:B:286:PHE:CZ	1:B:293:THR:CG2	0.47	2.98	14	1
1:A:43:GLU:N	1:A:44:PRO:CD	0.47	2.78	3	5
1:B:247:GLY:O	1:B:251:ILE:HG13	0.47	2.10	9	8
1:A:78:ALA:N	1:A:101:PHE:O	0.47	2.48	4	1
1:B:223:LEU:HG	1:B:256:ALA:HB2	0.47	1.87	8	2
1:B:321:ILE:CG2	2:B:326:NTH:H222	0.47	2.40	12	1
1:A:62:PRO:O	1:A:86:PHE:HB2	0.47	2.10	11	8
1:A:72:ARG:N	1:A:79:ALA:O	0.47	2.46	10	7
1:A:26:ILE:HG21	1:A:55:PHE:CG	0.47	2.45	5	3
1:A:92:LYS:CD	1:A:92:LYS:C	0.47	2.82	2	2
1:B:268:THR:O	1:B:269:GLN:O	0.47	2.33	7	4
1:A:100:HIS:NE2	1:B:315:LEU:HD13	0.47	2.25	5	1
1:B:243:GLU:N	1:B:244:PRO:HD3	0.47	2.24	6	2
1:B:294:VAL:CG1	1:B:295:VAL:N	0.46	2.78	6	3
1:B:281:ALA:C	1:B:282:PHE:CD1	0.46	2.89	7	2
1:B:304:ASN:CA	1:B:310:VAL:HG21	0.46	2.40	7	2
1:B:309:VAL:CG1	1:B:312:MET:HE2	0.46	2.37	9	1
1:B:309:VAL:CG1	1:B:312:MET:CE	0.46	2.93	13	2
1:A:35:THR:OG1	1:A:111:SER:OG	0.46	2.33	12	1
1:A:94:VAL:CG2	1:A:95:VAL:N	0.46	2.77	15	1
1:A:33:ASP:O	1:A:34:ALA:O	0.46	2.33	10	3
1:B:302:ARG:CB	1:B:311:SER:CB	0.46	2.93	3	1
1:A:32:ASP:O	1:A:48:THR:OG1	0.46	2.33	6	6
1:A:23:LEU:HD11	1:A:55:PHE:O	0.46	2.10	8	1
1:A:6:HIS:CG	1:A:7:MET:N	0.46	2.83	11	1
1:A:15:VAL:HG22	1:A:65:VAL:HG11	0.46	1.87	12	1
1:B:293:THR:CG2	1:B:322:HIS:ND1	0.46	2.78	13	1
1:A:95:VAL:CG1	1:A:96:ALA:N	0.46	2.78	14	2



	to us puge		Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:104:ASN:HB3	1:A:110:VAL:CG2	0.46	2.40	4	4
1:B:274:VAL:O	1:B:275:ALA:O	0.46	2.33	12	2
1:A:110:VAL:HG12	1:A:110:VAL:O	0.46	2.10	6	1
1:A:25:GLY:O	1:A:28:ALA:HB3	0.46	2.10	7	1
1:A:104:ASN:C	1:A:104:ASN:ND2	0.46	2.69	7	2
1:A:38:ASP:OD1	2:A:126:NTH:H62	0.46	2.11	8	1
1:B:264:ALA:N	1:B:285:SER:O	0.46	2.48	12	1
1:A:72:ARG:HD3	1:B:298:ILE:CD1	0.46	2.41	12	2
1:B:272:ARG:O	1:B:279:ALA:O	0.46	2.33	14	2
1:B:307:GLY:C	1:B:308:LYS:CG	0.46	2.83	1	2
1:B:318:GLU:HA	1:B:321:ILE:CG1	0.46	2.41	6	10
1:A:35:THR:O	1:A:112:MET:N	0.46	2.48	12	6
1:A:23:LEU:O	1:A:24:ASP:C	0.46	2.54	3	7
1:A:37:GLU:HB3	1:A:113:ARG:NH1	0.46	2.25	3	1
1:B:302:ARG:CB	1:B:311:SER:HB2	0.46	2.41	3	4
1:B:210:VAL:O	1:B:229:LEU:CD2	0.46	2.63	15	2
1:A:100:HIS:HB2	1:A:113:ARG:O	0.46	2.11	10	2
1:A:61:LEU:HD13	2:A:126:NTH:C20	0.46	2.40	7	1
1:B:287:GLU:OE2	1:B:290:GLY:N	0.46	2.49	7	1
1:A:104:ASN:N	1:A:110:VAL:HG21	0.46	2.25	9	1
1:A:36:VAL:O	1:A:44:PRO:HB2	0.46	2.11	11	1
1:B:206:HIS:NE2	1:B:207:MET:HE3	0.46	2.25	13	1
1:A:19:ASN:OD1	1:A:65:VAL:O	0.46	2.33	15	1
1:A:38:ASP:HA	1:A:39:PRO:C	0.46	2.30	9	7
1:A:84:VAL:O	1:A:94:VAL:HA	0.46	2.11	1	7
1:B:236:VAL:O	1:B:244:PRO:HA	0.46	2.10	6	11
1:A:14:TYR:CE2	1:A:55:PHE:CZ	0.46	3.04	15	10
1:A:84:VAL:O	1:A:95:VAL:N	0.46	2.49	3	3
1:B:285:SER:HA	1:B:294:VAL:CG2	0.46	2.40	6	2
1:B:297:PRO:HA	1:B:316:PHE:CB	0.46	2.40	9	1
1:A:80:PHE:CE2	1:A:82:PHE:CD2	0.46	3.03	10	1
1:A:85:SER:HA	1:A:94:VAL:CG2	0.46	2.41	1	7
1:A:95:VAL:CG1	1:A:97:PRO:HG3	0.46	2.41	12	8
1:B:237:GLU:OE1	1:B:313:ARG:NE	0.46	2.49	2	1
1:A:103:PHE:N	1:A:103:PHE:CD1	0.46	2.83	15	3
1:B:214:TYR:CE1	1:B:280:PHE:CZ	0.46	3.03	4	4
1:A:79:ALA:HB1	1:B:315:LEU:HD21	0.46	1.86	5	1
1:A:39:PRO:O	1:A:40:VAL:CG2	0.46	2.64	6	1
1:A:73:ALA:O	1:A:74:VAL:HG22	0.46	2.10	7	1
1:B:261:LEU:CG	1:B:263:LEU:HD21	0.46	2.39	8	1
1:A:72:ARG:NH2	1:B:315:LEU:HD12	0.46	2.26	9	1



	to us page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:B:287:GLU:HG3	1:B:291:ARG:O	0.46	2.11	9	2
1:B:223:LEU:O	1:B:224:ASP:C	0.46	2.54	12	8
1:B:235:THR:O	1:B:312:MET:N	0.46	2.49	4	3
1:A:116:PHE:CE1	2:A:126:NTH:C6	0.46	2.98	2	2
1:A:85:SER:HA	1:A:94:VAL:HG22	0.46	1.85	9	1
1:A:22:ASP:OD1	1:A:24:ASP:OD1	0.46	2.34	10	1
1:A:22:ASP:OD2	1:A:24:ASP:OD2	0.46	2.34	10	1
1:B:227:VAL:CG2	1:B:252:ARG:HB2	0.46	2.41	5	8
1:A:35:THR:CG2	1:A:46:SER:HB3	0.46	2.41	14	4
1:B:207:MET:SD	1:B:274:VAL:O	0.46	2.74	13	2
1:A:115:LEU:O	1:A:116:PHE:O	0.46	2.33	4	1
1:A:115:LEU:C	1:A:116:PHE:CD1	0.46	2.89	4	1
1:B:217:ALA:CB	1:B:226:ILE:HG13	0.46	2.41	4	4
1:B:230:PHE:CZ	1:B:312:MET:SD	0.46	3.09	13	2
1:A:18:LEU:HD21	1:A:55:PHE:CZ	0.46	2.46	10	1
2:A:126:NTH:C16	2:A:126:NTH:H222	0.46	2.40	14	1
1:B:233:ASP:N	1:B:233:ASP:OD1	0.46	2.48	15	1
1:A:34:ALA:HA	1:A:110:VAL:O	0.46	2.11	7	9
1:A:39:PRO:HG2	1:A:42:SER:CB	0.46	2.41	2	2
1:A:117:GLY:O	1:A:121:ILE:HG12	0.46	2.11	15	4
1:A:14:TYR:CE2	1:A:112:MET:CE	0.46	2.99	15	2
1:A:120:ASN:OD1	1:B:272:ARG:NE	0.46	2.43	4	1
1:A:3:THR:O	1:A:7:MET:SD	0.46	2.74	7	1
1:B:245:ARG:HG2	1:B:246:SER:N	0.46	2.26	7	1
1:B:293:THR:CG2	1:B:322:HIS:HB2	0.46	2.40	13	2
1:B:219:ASN:OD1	1:B:265:VAL:O	0.46	2.33	9	4
1:A:102:ARG:NH1	1:A:113:ARG:CD	0.46	2.79	15	1
1:A:27:VAL:CG2	1:A:52:ARG:HB2	0.46	2.42	1	9
1:B:234:ALA:HA	1:B:310:VAL:O	0.46	2.11	11	14
1:B:294:VAL:O	1:B:322:HIS:HB2	0.46	2.11	6	7
1:B:304:ASN:HB3	1:B:310:VAL:CG2	0.46	2.41	7	2
1:A:23:LEU:CD2	1:A:52:ARG:HA	0.46	2.41	9	2
1:B:214:TYR:CZ	1:B:218:LEU:HD11	0.46	2.46	4	2
1:A:72:ARG:CZ	1:A:72:ARG:CB	0.46	2.94	5	1
1:A:74:VAL:O	1:A:75:ALA:O	0.46	2.34	7	3
2:A:126:NTH:C16	2:A:126:NTH:H221	0.46	2.41	8	2
1:A:14:TYR:N	1:A:29:LEU:HD22	0.45	2.25	1	1
1:A:15:VAL:HG21	1:A:67:LEU:HD21	0.45	1.88	1	1
1:B:207:MET:SD	1:B:275:ALA:O	0.45	2.74	3	4
1:B:221:GLY:O	1:B:259:LEU:HD21	0.45	2.11	11	3
1:B:317:GLY:O	1:B:321:ILE:HG12	0.45	2.12	2	6



	tions page		${ m Distance}({ m \AA})$	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:119:LYS:HE2	1:B:204:PRO:CG	0.45	2.42	4	1
1:A:71:VAL:CG1	1:A:72:ARG:N	0.45	2.78	5	2
1:A:39:PRO:O	1:A:42:SER:CB	0.45	2.64	6	1
1:B:301:PHE:CE1	1:B:309:VAL:CG2	0.45	2.99	7	1
1:A:39:PRO:CD	1:A:42:SER:CB	0.45	2.94	9	1
1:B:207:MET:HE1	1:B:306:ALA:HA	0.45	1.87	9	1
1:B:282:PHE:CE2	1:B:284:VAL:HG23	0.45	2.46	15	1
1:A:80:PHE:O	1:A:99:ASP:N	0.45	2.47	1	4
1:A:102:ARG:N	1:A:111:SER:O	0.45	2.50	14	2
1:A:103:PHE:CE1	1:A:109:VAL:HG22	0.45	2.46	1	1
1:B:288:PHE:CD1	1:B:288:PHE:N	0.45	2.84	3	2
1:A:104:ASN:N	1:A:104:ASN:ND2	0.45	2.65	10	2
1:B:237:GLU:OE1	1:B:313:ARG:NH1	0.45	2.48	7	1
1:B:240:VAL:HG21	1:B:317:GLY:HA2	0.45	1.89	7	1
1:A:67:LEU:O	1:A:68:THR:HG23	0.45	2.11	12	1
1:A:37:GLU:OE2	1:A:113:ARG:HD3	0.45	2.12	14	1
1:A:75:ALA:CB	1:B:240:VAL:O	0.45	2.64	15	1
1:A:33:ASP:CB	1:A:47:GLY:HA2	0.45	2.42	4	5
1:A:49:ALA:O	1:A:53:GLU:HB2	0.45	2.11	1	6
1:A:88:PHE:CE2	2:A:126:NTH:O23	0.45	2.69	3	1
1:B:272:ARG:CG	1:B:279:ALA:O	0.45	2.64	9	4
1:B:308:LYS:HD2	1:B:308:LYS:N	0.45	2.26	6	1
1:A:86:PHE:CZ	2:A:126:NTH:C23	0.45	3.00	7	1
1:A:17:ALA:HB1	1:A:26:ILE:HG13	0.45	1.89	9	4
1:B:315:LEU:C	1:B:316:PHE:CD2	0.45	2.90	13	1
1:B:214:TYR:CE2	1:B:312:MET:HE1	0.45	2.46	15	1
1:B:239:PRO:HD2	1:B:242:SER:CB	0.45	2.40	2	6
1:B:276:ASN:OD1	1:B:276:ASN:O	0.45	2.34	4	1
1:A:116:PHE:C	1:B:274:VAL:HG11	0.45	2.31	7	1
1:B:211:VAL:HG13	1:B:280:PHE:CG	0.45	2.46	7	1
1:A:87:GLU:HG2	1:A:88:PHE:N	0.45	2.26	15	3
1:B:303:PHE:N	1:B:303:PHE:CD1	0.45	2.85	15	2
1:B:222:ASP:O	1:B:222:ASP:OD2	0.45	2.33	10	1
1:A:40:VAL:HG21	1:B:274:VAL:CB	0.45	2.41	13	1
1:A:72:ARG:O	1:A:79:ALA:N	0.45	2.49	7	2
1:B:316:PHE:CD1	1:B:317:GLY:N	0.45	2.85	5	1
1:A:88:PHE:N	1:A:91:ARG:O	0.45	2.49	6	1
1:A:14:TYR:CD2	1:A:101:PHE:CZ	0.45	3.04	10	1
1:B:304:ASN:ND2	1:B:310:VAL:HB	0.45	2.26	10	1
1:A:92:LYS:HE3	1:A:125:ALA:OXT	0.45	2.11	14	1
1:A:102:ARG:CD	1:B:313:ARG:HD3	0.45	2.41	15	1



			Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)		Worst	Total
1:A:7:MET:SD	1:A:74:VAL:O	0.45	2.75	4	1
1:A:63:LEU:HD23	1:A:86:PHE:HB3	0.45	1.88	7	1
1:B:280:PHE:O	1:B:299:ASP:N	0.45	2.47	7	4
1:A:43:GLU:OE1	1:A:43:GLU:N	0.45	2.48	9	1
1:A:72:ARG:NH2	1:B:315:LEU:HA	0.45	2.26	9	1
1:B:286:PHE:CE2	1:B:288:PHE:CZ	0.45	3.05	12	1
1:A:102:ARG:NH2	1:B:313:ARG:CB	0.45	2.80	15	1
1:A:23:LEU:CD1	1:A:55:PHE:HB3	0.45	2.42	10	7
1:A:69:GLN:HG3	1:A:70:GLU:N	0.45	2.26	13	4
1:A:64:ALA:N	1:A:85:SER:O	0.45	2.47	10	4
1:B:292:LYS:O	1:B:292:LYS:HD3	0.45	2.12	4	1
1:A:11:VAL:HG22	1:A:80:PHE:CD1	0.45	2.47	5	1
1:A:88:PHE:O	1:A:89:GLN:C	0.45	2.55	12	2
1:A:41:GLY:O	1:A:42:SER:HB2	0.45	2.12	7	3
1:A:102:ARG:CB	1:A:111:SER:HB2	0.45	2.41	1	2
1:A:24:ASP:O	1:A:28:ALA:CB	0.45	2.65	2	1
1:A:27:VAL:HG21	1:A:52:ARG:CB	0.45	2.38	2	2
1:A:10:VAL:CB	1:A:103:PHE:CZ	0.45	3.00	3	2
1:B:277:GLU:HG2	1:B:301:PHE:O	0.45	2.11	10	6
1:A:34:ALA:CA	1:A:51:ILE:HD11	0.45	2.42	7	1
1:B:245:ARG:NH1	1:B:251:ILE:HG12	0.45	2.27	7	1
1:A:72:ARG:NH1	1:A:78:ALA:C	0.45	2.70	9	1
1:B:210:VAL:CG2	1:B:303:PHE:CE2	0.45	3.00	9	1
1:A:22:ASP:OD1	1:A:24:ASP:OD2	0.45	2.33	10	1
1:B:321:ILE:HG22	1:B:322:HIS:CD2	0.45	2.47	13	1
1:A:98:ILE:CD1	1:B:272:ARG:NE	0.45	2.79	14	1
1:A:102:ARG:CB	1:A:111:SER:O	0.45	2.65	6	5
1:B:210:VAL:CB	1:B:303:PHE:CZ	0.45	3.00	6	5
1:B:262:PRO:O	1:B:286:PHE:HB2	0.45	2.11	15	6
1:B:297:PRO:HA	1:B:320:ASN:OD1	0.45	2.11	3	1
1:B:261:LEU:HD21	1:B:286:PHE:CD2	0.45	2.47	7	1
1:A:100:HIS:CD2	1:B:315:LEU:CD1	0.45	3.00	8	1
1:B:315:LEU:O	1:B:316:PHE:C	0.45	2.55	9	1
1:A:45:ARG:HD2	1:A:51:ILE:CD1	0.45	2.41	11	1
1:A:85:SER:OG	1:A:85:SER:O	0.45	2.33	15	2
1:A:100:HIS:CD2	1:B:300:HIS:CD2	0.45	3.04	15	1
1:B:226:ILE:HG22	1:B:230:PHE:CD2	0.45	2.46	1	1
1:A:37:GLU:O	1:A:114:ALA:CB	0.45	2.64	2	1
1:A:10:VAL:CG2	1:A:103:PHE:CE2	0.45	2.99	8	2
1:A:67:LEU:O	1:A:68:THR:HB	0.45	2.12	5	1
1:B:272:ARG:O	1:B:278:ALA:HB1	0.45	2.12	15	2



	A h		\mathbf{D} (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:B:293:THR:HB	1:B:322:HIS:CB	0.45	2.42	7	1	
1:B:267:LEU:C	1:B:268:THR:HG23	0.45	2.31	12	1	
1:B:293:THR:HG22	1:B:322:HIS:HB2	0.45	1.87	13	1	
1:B:273:ALA:O	1:B:274:VAL:HG22	0.45	2.12	14	1	
1:B:249:ALA:O	1:B:253:GLU:HB2	0.44	2.12	4	9	
1:B:317:GLY:O	1:B:320:ASN:N	0.44	2.43	4	1	
1:A:107:GLY:O	1:A:108:LYS:HB2	0.44	2.11	6	2	
1:A:117:GLY:O	1:A:121:ILE:CG1	0.44	2.65	15	2	
1:A:3:THR:O	1:A:3:THR:HG23	0.44	2.12	7	1	
1:A:10:VAL:HG11	1:A:109:VAL:HG22	0.44	1.88	9	1	
1:A:61:LEU:CD2	2:A:126:NTH:O17	0.44	2.66	9	1	
1:A:116:PHE:CD1	1:A:116:PHE:C	0.44	2.85	9	1	
1:A:86:PHE:CZ	2:A:126:NTH:C20	0.44	2.99	11	1	
1:A:120:ASN:OD1	1:B:272:ARG:CZ	0.44	2.65	14	2	
1:B:274:VAL:O	1:B:276:ASN:N	0.44	2.49	7	2	
1:A:3:THR:O	1:A:6:HIS:CD2	0.44	2.71	13	1	
1:A:47:GLY:C	1:A:51:ILE:HD12	0.44	2.32	14	1	
1:A:99:ASP:CG	1:A:112:MET:HE3	0.44	2.33	15	1	
1:A:38:ASP:OD1	1:A:39:PRO:HA	0.44	2.11	1	2	
1:A:57:ASN:ND2	1:A:60:LYS:CE	0.44	2.81	1	1	
1:B:269:GLN:CG	1:B:270:GLU:N	0.44	2.78	1	4	
1:A:23:LEU:O	1:A:25:GLY:N	0.44	2.51	11	2	
1:A:26:ILE:HG22	1:A:30:PHE:CD2	0.44	2.48	3	2	
1:B:217:ALA:HB1	1:B:226:ILE:HG13	0.44	1.88	11	4	
1:B:296:ALA:N	1:B:297:PRO:HD3	0.44	2.27	11	2	
1:A:86:PHE:CE1	2:A:126:NTH:C21	0.44	3.00	7	1	
1:B:258:SER:CB	2:B:326:NTH:H11	0.44	2.42	7	1	
1:A:10:VAL:HG21	1:A:109:VAL:HG23	0.44	1.89	9	1	
1:A:109:VAL:HG11	1:A:112:MET:CE	0.44	2.42	10	1	
1:A:11:VAL:HG11	1:A:71:VAL:HG11	0.44	1.90	13	1	
1:A:74:VAL:HG11	1:B:317:GLY:HA2	0.44	1.88	13	1	
2:A:126:NTH:H222	2:A:126:NTH:H161	0.44	1.89	14	1	
1:A:92:LYS:CD	1:A:92:LYS:O	0.44	2.66	1	4	
1:A:11:VAL:CG1	1:A:71:VAL:CG2	0.44	2.94	2	1	
1:A:97:PRO:HB3	1:A:120:ASN:ND2	0.44	2.27	11	3	
1:A:100:HIS:CB	1:A:113:ARG:HB2	0.44	2.42	2	2	
1:A:39:PRO:O	1:A:40:VAL:C	0.44	2.54	6	2	
1:A:115:LEU:O	1:A:116:PHE:C	0.44	2.55	4	1	
1:B:217:ALA:HB3	1:B:226:ILE:CG1	0.44	2.42	12	2	
1:A:27:VAL:CG2	1:A:52:ARG:HG3	0.44	2.42	8	1	
1:A:103:PHE:C	1:A:110:VAL:CG2	0.44	2.86	8	1	



		(1, 1, (3))	D: (8)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:45:ARG:CG	1:A:50:ALA:CB	0.44	2.83	10	1
1:B:238:ASP:HA	1:B:239:PRO:O	0.44	2.12	13	1
1:B:316:PHE:CE1	2:B:326:NTH:C6	0.44	3.00	14	1
1:A:102:ARG:NH1	1:B:313:ARG:HD2	0.44	2.28	15	1
1:A:52:ARG:O	1:A:53:GLU:C	0.44	2.56	11	10
1:A:72:ARG:HB2	1:A:79:ALA:O	0.44	2.12	4	8
1:A:96:ALA:O	1:A:120:ASN:CG	0.44	2.56	5	8
1:B:272:ARG:HB2	1:B:279:ALA:O	0.44	2.13	8	10
1:A:76:ASN:O	1:A:103:PHE:HB2	0.44	2.13	6	2
1:B:292:LYS:O	1:B:292:LYS:CD	0.44	2.65	4	1
1:B:263:LEU:CB	1:B:286:PHE:HB3	0.44	2.42	5	3
1:B:237:GLU:O	1:B:238:ASP:CB	0.44	2.65	9	1
1:A:37:GLU:OE2	1:A:113:ARG:CG	0.44	2.65	12	1
1:B:206:HIS:NE2	1:B:207:MET:HG3	0.44	2.28	13	1
1:B:263:LEU:HD13	1:B:284:VAL:HG11	0.44	1.89	13	1
1:B:286:PHE:CZ	2:B:326:NTH:C21	0.44	2.99	14	1
1:A:37:GLU:OE1	1:A:113:ARG:HG2	0.44	2.13	1	1
1:B:296:ALA:O	1:B:320:ASN:CG	0.44	2.56	9	7
1:A:118:GLU:HA	1:A:121:ILE:HG12	0.44	1.88	3	2
1:A:59:LEU:O	1:A:60:LYS:C	0.44	2.56	10	2
1:B:292:LYS:CD	1:B:292:LYS:C	0.44	2.86	6	2
1:A:19:ASN:CG	1:A:65:VAL:O	0.44	2.56	11	2
1:B:238:ASP:CB	1:B:239:PRO:HA	0.44	2.43	9	1
1:A:55:PHE:CZ	2:A:126:NTH:C2	0.44	3.00	10	1
1:B:223:LEU:HD23	1:B:259:LEU:HD22	0.44	1.83	15	1
1:B:212:GLN:O	1:B:213:ARG:C	0.44	2.56	13	15
1:B:294:VAL:HG12	1:B:322:HIS:HB2	0.44	1.89	2	1
1:A:38:ASP:CG	1:A:114:ALA:CB	0.44	2.86	3	1
1:A:68:THR:C	1:A:69:GLN:HG2	0.44	2.33	9	2
1:B:243:GLU:N	1:B:244:PRO:CD	0.44	2.80	6	1
1:A:72:ARG:C	1:A:72:ARG:CD	0.44	2.86	9	1
1:A:17:ALA:HB3	1:A:26:ILE:CG1	0.44	2.42	11	2
1:B:317:GLY:O	1:B:321:ILE:CG1	0.44	2.66	2	4
1:A:63:LEU:HD22	1:A:84:VAL:HG12	0.44	1.85	3	1
1:B:261:LEU:O	1:B:263:LEU:HD11	0.44	2.12	5	3
1:B:286:PHE:CE2	1:B:293:THR:OG1	0.44	2.70	5	1
1:A:86:PHE:CE2	1:A:93:THR:OG1	0.44	2.70	7	1
1:B:297:PRO:CB	1:B:316:PHE:CE1	0.44	3.00	7	1
1:B:222:ASP:OD2	1:B:225:GLY:N	0.44	2.51	10	1
1:A:63:LEU:CB	1:A:86:PHE:HB3	0.44	2.43	15	6
1:B:215:VAL:O	1:B:216:ALA:C	0.44	2.56	4	13



	to us page			Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:293:THR:CG2	1:B:323:ALA:HA	0.44	2.43	3	2
1:A:67:LEU:HA	1:A:82:PHE:CB	0.44	2.43	5	1
1:A:61:LEU:HD23	1:A:63:LEU:HG	0.44	1.89	7	1
1:B:293:THR:HG21	1:B:322:HIS:HB2	0.44	1.88	7	1
1:B:316:PHE:HZ	2:B:326:NTH:H61	0.44	1.73	7	1
1:B:268:THR:C	1:B:269:GLN:HG2	0.44	2.34	8	1
1:A:103:PHE:HA	1:A:110:VAL:HG23	0.44	1.90	13	1
1:B:272:ARG:HA	1:B:272:ARG:NE	0.44	2.28	15	1
1:A:12:GLN:O	1:A:13:ARG:C	0.43	2.57	3	14
1:A:47:GLY:O	1:A:51:ILE:HG13	0.43	2.13	10	6
1:A:77:GLU:HG2	1:A:101:PHE:O	0.43	2.13	2	2
1:A:93:THR:HG22	1:A:94:VAL:H	0.43	1.73	4	1
1:A:102:ARG:HB2	1:A:111:SER:O	0.43	2.13	6	3
1:A:30:PHE:CE2	1:A:51:ILE:CG2	0.43	3.01	8	1
1:B:302:ARG:CD	1:B:311:SER:HB2	0.43	2.43	8	1
1:A:3:THR:HG23	1:A:6:HIS:NE2	0.43	2.27	14	1
1:B:210:VAL:CG1	1:B:301:PHE:CD1	0.43	3.01	14	1
1:A:7:MET:SD	1:A:75:ALA:O	0.43	2.76	1	2
1:A:15:VAL:O	1:A:16:ALA:C	0.43	2.57	13	13
1:B:237:GLU:HB2	1:B:313:ARG:HG2	0.43	1.89	1	1
1:B:237:GLU:O	1:B:238:ASP:HB2	0.43	2.12	15	8
1:A:101:PHE:CE1	1:A:112:MET:HE1	0.43	2.47	10	2
1:A:61:LEU:HB3	1:A:63:LEU:CD2	0.43	2.43	4	2
1:B:318:GLU:HA	1:B:321:ILE:HG12	0.43	1.90	7	3
1:A:22:ASP:O	1:A:22:ASP:CG	0.43	2.57	7	1
1:B:210:VAL:HA	1:B:229:LEU:CD2	0.43	2.41	7	2
1:B:273:ALA:HA	1:B:278:ALA:CB	0.43	2.43	8	2
1:A:22:ASP:O	1:A:22:ASP:OD2	0.43	2.36	9	1
1:B:275:ALA:O	1:B:276:ASN:HB2	0.43	2.13	10	1
1:B:245:ARG:HD3	1:B:250:ALA:CA	0.43	2.43	11	1
1:B:292:LYS:HG2	1:B:293:THR:N	0.43	2.28	11	1
1:B:304:ASN:CG	1:B:310:VAL:CG2	0.43	2.86	12	1
1:A:34:ALA:O	1:A:51:ILE:CG1	0.43	2.66	15	1
1:A:11:VAL:HG22	1:A:80:PHE:CD2	0.43	2.48	2	1
1:A:69:GLN:OE1	1:A:70:GLU:O	0.43	2.36	4	1
1:A:98:ILE:HD11	1:B:272:ARG:NE	0.43	2.29	4	1
1:B:263:LEU:CD2	1:B:286:PHE:HB3	0.43	2.42	4	2
1:B:263:LEU:HD11	2:B:326:NTH:H121	0.43	1.90	4	1
1:B:241:GLY:O	1:B:242:SER:HB2	0.43	2.13	12	2
1:B:287:GLU:CD	1:B:288:PHE:N	0.43	2.71	7	2
1:A:77:GLU:CG	1:A:102:ARG:HA	0.43	2.43	14	1



	to us page			Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:26:ILE:CD1	1:A:55:PHE:CD1	0.43	2.99	2	1
1:A:118:GLU:CA	1:A:121:ILE:HG12	0.43	2.44	3	1
1:B:297:PRO:HB3	1:B:320:ASN:ND2	0.43	2.29	4	1
1:A:104:ASN:OD1	1:A:108:LYS:O	0.43	2.36	6	1
1:A:93:THR:CG2	1:A:123:ALA:HA	0.43	2.43	8	1
1:B:252:ARG:O	1:B:253:GLU:C	0.43	2.57	3	8
1:A:61:LEU:HD21	2:A:126:NTH:O20	0.43	2.13	3	1
1:A:15:VAL:HB	1:A:67:LEU:CD1	0.43	2.39	5	1
1:B:222:ASP:O	1:B:222:ASP:CG	0.43	2.57	9	3
1:A:39:PRO:HB3	1:A:116:PHE:CZ	0.43	2.48	7	1
1:B:286:PHE:CE2	2:B:326:NTH:H212	0.43	2.47	8	1
1:A:74:VAL:HB	1:B:240:VAL:HG21	0.43	1.90	12	1
1:A:7:MET:HA	1:A:7:MET:CE	0.43	2.43	14	1
1:A:41:GLY:CA	1:B:275:ALA:HB1	0.43	2.43	15	1
1:A:66:GLU:O	1:A:67:LEU:C	0.43	2.57	1	3
1:A:67:LEU:CD2	1:A:82:PHE:HB3	0.43	2.43	1	1
1:B:233:ASP:CB	1:B:247:GLY:HA2	0.43	2.44	4	5
1:A:77:GLU:CG	1:A:101:PHE:O	0.43	2.67	2	1
1:B:235:THR:OG1	1:B:311:SER:OG	0.43	2.35	2	1
1:B:222:ASP:CG	1:B:222:ASP:O	0.43	2.57	14	3
1:B:288:PHE:O	1:B:289:GLN:C	0.43	2.57	5	3
1:A:22:ASP:OD1	1:A:22:ASP:O	0.43	2.36	6	1
1:A:22:ASP:OD1	1:A:24:ASP:CB	0.43	2.66	8	1
1:A:115:LEU:O	1:A:116:PHE:CB	0.43	2.66	8	2
1:B:223:LEU:HG	1:B:256:ALA:CB	0.43	2.43	8	2
1:B:245:ARG:HG3	1:B:250:ALA:CB	0.43	2.38	8	1
1:A:22:ASP:OD2	1:A:25:GLY:N	0.43	2.45	10	1
1:A:50:ALA:O	1:A:51:ILE:C	0.43	2.56	10	3
1:A:81:ALA:CA	1:A:98:ILE:HG23	0.43	2.44	10	1
1:A:45:ARG:CZ	1:A:54:PHE:HB3	0.43	2.43	11	1
1:A:86:PHE:CE2	1:A:87:GLU:O	0.43	2.71	12	1
1:A:72:ARG:HB3	1:A:79:ALA:O	0.43	2.14	14	1
1:B:202:ASN:O	1:B:203:THR:C	0.43	2.57	1	2
1:B:207:MET:HB2	1:B:273:ALA:HB1	0.43	1.90	1	1
1:B:223:LEU:CD1	1:B:255:PHE:HB3	0.43	2.43	15	6
1:A:117:GLY:O	1:A:119:LYS:N	0.43	2.52	3	1
1:A:17:ALA:HA	1:A:22:ASP:OD1	0.43	2.14	4	2
1:A:14:TYR:CE1	1:A:15:VAL:HG23	0.43	2.49	15	2
1:A:72:ARG:HB3	1:A:72:ARG:NH2	0.43	2.28	5	1
1:A:94:VAL:HG12	1:A:122:HIS:CD2	0.43	2.49	7	1
1:B:227:VAL:HG21	1:B:252:ARG:CG	0.43	2.43	7	1



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	to us page			Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:204:PRO:O	1:B:208:THR:HB	0.43	2.12	15	2
1:B:238:ASP:OD1	2:B:326:NTH:H62	0.43	2.14	13	2
1:A:85:SER:O	1:A:85:SER:OG	0.43	2.33	12	1
1:B:223:LEU:O	1:B:225:GLY:N	0.43	2.52	12	1
1:A:72:ARG:HA	1:A:72:ARG:NE	0.43	2.28	14	1
1:B:233:ASP:HA	1:B:247:GLY:HA2	0.43	1.90	6	5
1:A:74:VAL:O	1:A:76:ASN:N	0.43	2.51	2	1
1:A:87:GLU:CD	1:A:88:PHE:O	0.43	2.57	2	3
1:B:235:THR:O	1:B:236:VAL:CG2	0.43	2.67	2	1
1:A:4:PRO:O	1:A:8:THR:HB	0.43	2.14	10	3
1:B:237:GLU:HA	1:B:244:PRO:HB3	0.43	1.89	7	2
1:B:278:ALA:CB	1:B:301:PHE:HB2	0.43	2.40	4	1
1:A:86:PHE:CZ	1:A:93:THR:CB	0.43	3.01	7	1
1:B:243:GLU:O	1:B:243:GLU:OE1	0.43	2.37	10	1
1:B:233:ASP:OD1	1:B:233:ASP:O	0.43	2.37	11	1
1:B:281:ALA:CA	1:B:298:ILE:HG23	0.43	2.43	11	1
1:B:204:PRO:O	1:B:205:GLU:C	0.43	2.56	13	1
1:A:116:PHE:HA	1:B:272:ARG:NH2	0.43	2.28	14	1
1:B:293:THR:HG22	1:B:294:VAL:H	0.43	1.73	15	1
1:B:239:PRO:O	1:B:242:SER:HB2	0.43	2.14	7	4
1:A:13:ARG:O	1:A:14:TYR:C	0.43	2.57	2	1
1:A:87:GLU:C	1:A:87:GLU:OE1	0.43	2.57	2	1
1:B:201:MET:O	1:B:202:ASN:C	0.43	2.57	14	2
1:B:293:THR:HB	1:B:322:HIS:HB2	0.43	1.89	13	2
1:B:210:VAL:CB	1:B:303:PHE:CE2	0.43	3.02	9	2
1:B:270:GLU:O	1:B:272:ARG:NH2	0.43	2.51	9	1
1:A:95:VAL:HG13	1:A:120:ASN:HD21	0.43	1.72	11	1
1:B:304:ASN:HB3	1:B:310:VAL:CG1	0.43	2.43	11	1
1:B:235:THR:CG2	1:B:246:SER:HB2	0.43	2.41	13	1
1:A:107:GLY:C	1:A:108:LYS:CG	0.43	2.86	14	1
1:B:267:LEU:HD22	1:B:271:VAL:CG2	0.43	2.44	14	1
1:B:278:ALA:O	1:B:300:HIS:ND1	0.43	2.51	14	1
1:B:238:ASP:HA	1:B:239:PRO:C	0.43	2.34	2	7
1:B:240:VAL:CG1	1:B:315:LEU:HA	0.43	2.44	3	1
1:B:259:LEU:O	1:B:260:LYS:C	0.43	2.57	4	2
1:B:284:VAL:O	1:B:294:VAL:HA	0.43	2.14	4	5
1:B:272:ARG:HG3	1:B:279:ALA:O	0.43	2.14	13	4
1:A:100:HIS:CB	1:A:113:ARG:HB3	0.43	2.43	7	1
1:A:84:VAL:O	1:A:94:VAL:HG22	0.43	2.13	9	1
1:A:61:LEU:O	1:A:63:LEU:HD11	0.43	2.14	15	2
1:B:300:HIS:CB	1:B:313:ARG:HB2	0.43	2.44	11	1



	to us page			Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:45:ARG:HD3	1:A:50:ALA:CA	0.43	2.44	12	1
1:B:322:HIS:NE2	2:B:326:NTH:C23	0.43	2.82	13	1
1:A:37:GLU:O	1:A:38:ASP:CB	0.43	2.66	14	1
1:A:73:ALA:HA	1:A:78:ALA:CB	0.42	2.44	1	2
1:B:300:HIS:CB	1:B:313:ARG:CB	0.42	2.97	12	2
1:A:40:VAL:HG11	1:B:274:VAL:CG1	0.42	2.36	2	1
1:B:281:ALA:O	1:B:282:PHE:HB3	0.42	2.14	14	3
1:A:68:THR:O	1:A:68:THR:OG1	0.42	2.33	5	1
1:A:108:LYS:HD2	1:A:108:LYS:N	0.42	2.28	6	1
1:B:256:ALA:O	1:B:259:LEU:N	0.42	2.52	7	1
1:B:321:ILE:CG2	1:B:322:HIS:N	0.42	2.79	7	1
1:B:322:HIS:O	1:B:322:HIS:CD2	0.42	2.72	7	1
1:A:61:LEU:HD13	2:A:126:NTH:C18	0.42	2.27	8	1
1:A:74:VAL:CG1	1:B:317:GLY:HA3	0.42	2.44	9	1
1:A:22:ASP:CG	1:A:24:ASP:OD1	0.42	2.58	10	1
1:A:65:VAL:HG13	1:A:82:PHE:CD2	0.42	2.49	1	1
1:B:307:GLY:O	1:B:308:LYS:HG3	0.42	2.14	1	1
1:A:37:GLU:HA	1:A:44:PRO:HB3	0.42	1.91	11	3
1:A:68:THR:HG23	1:A:69:GLN:N	0.42	2.29	3	2
1:A:23:LEU:HD21	1:A:59:LEU:CD2	0.42	2.42	5	1
1:B:263:LEU:CG	1:B:286:PHE:HB3	0.42	2.44	13	2
1:A:21:GLY:HA2	1:A:59:LEU:CD2	0.42	2.38	7	2
1:A:31:ALA:N	1:A:109:VAL:O	0.42	2.51	8	2
1:A:100:HIS:ND1	1:A:101:PHE:N	0.42	2.68	8	1
1:B:287:GLU:HG2	1:B:288:PHE:N	0.42	2.29	9	2
1:A:3:THR:O	1:A:6:HIS:ND1	0.42	2.52	11	1
1:B:286:PHE:CZ	1:B:288:PHE:CZ	0.42	3.07	12	1
1:A:72:ARG:CZ	1:B:298:ILE:HD11	0.42	2.44	1	1
1:B:237:GLU:CB	1:B:313:ARG:HG2	0.42	2.44	1	1
1:A:100:HIS:CE1	1:B:315:LEU:HD13	0.42	2.50	4	1
1:B:203:THR:CG2	1:B:205:GLU:HB2	0.42	2.44	5	1
1:A:39:PRO:O	1:A:42:SER:HB2	0.42	2.14	9	2
1:A:33:ASP:HA	1:A:47:GLY:HA2	0.42	1.91	9	6
1:A:120:ASN:OD1	1:B:272:ARG:NH1	0.42	2.52	12	1
1:B:314:ALA:HB1	1:B:316:PHE:HE2	0.42	1.74	13	1
1:A:100:HIS:HB3	1:A:113:ARG:O	0.42	2.14	14	1
1:B:316:PHE:CZ	2:B:326:NTH:C6	0.42	3.01	14	1
1:A:40:VAL:HG11	1:A:115:LEU:HA	0.42	1.89	15	1
1:A:86:PHE:HE2	2:A:126:NTH:H221	0.42	1.70	15	1
1:A:13:ARG:HD2	1:A:29:LEU:CD1	0.42	2.43	2	1
1:A:29:LEU:O	1:A:109:VAL:HB	0.42	2.14	3	2



		(1,1)		Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:14:TYR:CD1	1:A:15:VAL:N	0.42	2.87	4	1	
1:A:37:GLU:O	1:A:38:ASP:HB2	0.42	2.14	11	5	
1:B:261:LEU:CD2	1:B:263:LEU:CG	0.42	2.98	4	1	
1:A:102:ARG:HD2	1:A:111:SER:CB	0.42	2.44	6	1	
1:A:104:ASN:ND2	1:A:108:LYS:O	0.42	2.52	6	1	
1:B:213:ARG:O	1:B:214:TYR:C	0.42	2.57	7	1	
1:B:250:ALA:O	1:B:251:ILE:C	0.42	2.58	9	3	
2:B:326:NTH:H161	2:B:326:NTH:C21	0.42	2.44	13	2	
1:B:261:LEU:HB3	1:B:263:LEU:CD2	0.42	2.44	1	2	
1:A:61:LEU:CD1	2:A:126:NTH:C12	0.42	2.96	2	1	
1:A:63:LEU:HD22	1:A:86:PHE:CD1	0.42	2.50	2	1	
1:B:217:ALA:HB1	1:B:222:ASP:O	0.42	2.15	2	1	
1:A:23:LEU:HG	1:A:56:ALA:CB	0.42	2.44	6	2	
1:A:10:VAL:HA	1:A:29:LEU:CD2	0.42	2.43	7	1	
1:A:29:LEU:HD12	1:A:29:LEU:HA	0.42	1.74	9	1	
1:A:122:HIS:CG	1:A:123:ALA:N	0.42	2.88	9	1	
1:A:77:GLU:O	1:A:78:ALA:CB	0.42	2.64	13	2	
1:B:302:ARG:O	02:ARG:O 1:B:304:ASN:ND2		2.52	10	1	
1:B:316:PHE:HA	16:PHE:HA 1:B:320:ASN:ND2		2.29	11	1	
1:A:92:LYS:HG2	A:92:LYS:HG2 1:A:93:THR:N		2.29	12	1	
1:A:64:ALA:CB	1:A:85:SER:HG	0.42	2.28	15	1	
1:B:295:VAL:HG12	1:B:296:ALA:N	0.42	2.29	11	3	
1:A:110:VAL:O	1:A:110:VAL:CG1	0.42	2.68	6	1	
1:B:207:MET:HA	1:B:303:PHE:CE2	0.42	2.49	7	1	
1:B:245:ARG:HD2	1:B:250:ALA:C	0.42	2.34	7	1	
1:A:3:THR:O	1:A:6:HIS:NE2	0.42	2.53	13	1	
1:B:288:PHE:O	1:B:289:GLN:HG3	0.42	2.15	13	1	
1:B:307:GLY:O	1:B:308:LYS:HB2	0.42	2.14	4	2	
1:A:101:PHE:CE1	1:A:109:VAL:HG11	0.42	2.50	2	1	
1:A:72:ARG:NH2	1:A:74:VAL:HG22	0.42	2.28	5	1	
1:B:230:PHE:O	1:B:231:ALA:C	0.42	2.57	11	2	
1:B:295:VAL:HG13	1:B:321:ILE:HA	0.42	1.91	5	1	
1:B:207:MET:SD	1:B:303:PHE:CD2	0.42	3.13	9	1	
1:A:50:ALA:O	1:A:54:PHE:N	0.42	2.50	10	1	
1:B:211:VAL:HG11	1:B:271:VAL:HG11	0.42	1.92	10	1	
1:B:222:ASP:OD2	1:B:225:GLY:HA3	0.42	2.13	10	1	
1:B:288:PHE:CE2	1:B:293:THR:OG1	0.42	2.72	12	1	
1:A:15:VAL:HA	1:A:18:LEU:HB2	0.42	1.92	15	12	
1:A:4:PRO:O	1:A:8:THR:N	0.42	2.48	15	4	
1:B:301:PHE:CD2	1:B:303:PHE:CZ	0.42	3.08	4	1	
1:B:249:ALA:O	1:B:253:GLU:CG	0.42	2.68	6	2	



	A + - 0	(1,1)		Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:89:GLN:HG2	1:A:90:GLY:N	0.42	2.29	15	2
1:A:61:LEU:HD13	1:A:62:PRO:CD	0.42	2.41	9	1
1:A:55:PHE:CE1	2:A:126:NTH:H21	0.42	2.50	10	1
2:A:126:NTH:H161	2:A:126:NTH:C21	0.42	2.45	14	1
1:B:283:THR:HA	1:B:295:VAL:O	0.42	2.15	15	1
1:A:21:GLY:HA2	1:A:59:LEU:CD1	0.42	2.42	2	1
1:A:40:VAL:CG2	1:A:41:GLY:N	0.42	2.75	2	1
1:B:229:LEU:HD12	1:B:229:LEU:HA	0.42	1.74	5	3
1:B:286:PHE:HZ	2:B:326:NTH:H221	0.42	1.69	2	1
1:A:61:LEU:CD2	1:A:61:LEU:O	0.42	2.65	6	1
1:B:220:ALA:O	1:B:221:GLY:C	0.42	2.58	11	1
1:A:76:ASN:O	1:A:103:PHE:CB	0.42	2.67	13	1
1:A:7:MET:O	1:A:103:PHE:CZ	0.42	2.73	15	1
1:B:215:VAL:HA	1:B:218:LEU:HB2	0.42	1.92	7	13
1:B:301:PHE:CD1	1:B:303:PHE:CE1	0.42	3.08	1	1
1:B:307:GLY:O	1:B:308:LYS:CG	0.42	2.68	1	2
1:B:240:VAL:O	1:B:240:VAL:HG23	0.42	2.14	5	1
1:A:61:LEU:HB3	EU:HB3 1:A:63:LEU:CD1		2.45	7	1
1:A:10:VAL:HG22	1:A:29:LEU:HG	0.42	1.92	9	1
1:B:277:GLU:CG	:277:GLU:CG 1:B:302:ARG:HG2		2.45	9	1
1:A:23:LEU:HD21	1:A:59:LEU:HB2	0.42	1.90	10	1
1:A:20:ALA:O	1:A:21:GLY:C	0.42	2.58	14	2
1:B:267:LEU:O	1:B:268:THR:HG23	0.42	2.14	12	1
1:A:100:HIS:CE1	1:B:300:HIS:CD2	0.42	3.08	13	1
1:A:30:PHE:CG	1:A:51:ILE:CG2	0.42	3.01	14	1
1:B:304:ASN:OD1	1:B:310:VAL:HB	0.42	2.14	14	1
1:B:229:LEU:O	1:B:309:VAL:HB	0.41	2.15	2	1
1:A:34:ALA:HB3	1:A:51:ILE:HG13	0.41	1.91	3	1
1:B:296:ALA:O	1:B:320:ASN:CB	0.41	2.68	3	1
1:B:272:ARG:CA	1:B:279:ALA:O	0.41	2.68	4	1
1:B:288:PHE:C	1:B:289:GLN:HG2	0.41	2.35	5	2
1:B:276:ASN:O	1:B:303:PHE:HB2	0.41	2.15	6	4
1:A:61:LEU:HD11	2:A:126:NTH:H212	0.41	1.92	7	1
1:B:207:MET:CE	1:B:306:ALA:HA	0.41	2.45	9	1
1:B:278:ALA:O	1:B:301:PHE:HB2	0.41	2.15	10	2
1:B:281:ALA:CB	1:B:298:ILE:HG13	0.41	2.45	9	2
1:A:59:LEU:O	1:A:61:LEU:N	0.41	2.53	10	1
1:A:95:VAL:CG2	1:A:121:ILE:CG2	0.41	2.94	12	1
1:A:22:ASP:CG	1:A:22:ASP:O	0.41	2.56	15	1
1:A:81:ALA:O	1:A:82:PHE:CB	0.41	2.68	15	1
1:B:266:GLU:O 1:B:267:LEU:C		0.41	2.59	14	3



		(1,1)	D . (8)	Models	
Atom-1	Atom-2	Atom-2 Clash(A)		Worst	Total
1:B:219:ASN:ND2	1:B:266:GLU:OE1	0.41	2.53	4	1
1:A:47:GLY:O	1:A:51:ILE:HG12	0.41	2.16	13	2
1:B:235:THR:CG2	1:B:246:SER:HB3	0.41	2.45	6	1
1:A:6:HIS:NE2	1:A:7:MET:HG2	0.41	2.29	11	1
1:A:32:ASP:O	1:A:33:ASP:OD1	0.41	2.37	11	1
1:B:241:GLY:O	1:B:242:SER:CB	0.41	2.67	12	1
1:A:10:VAL:O	1:A:29:LEU:HD21	0.41	2.14	1	1
1:A:54:PHE:O	1:A:55:PHE:C	0.41	2.58	3	2
1:B:236:VAL:HG22	1:B:312:MET:CE	0.41	2.45	7	1
1:A:87:GLU:CD	1:A:90:GLY:O	0.41	2.59	8	1
1:B:236:VAL:HG23	1:B:251:ILE:HG12	0.41	1.91	9	1
1:A:14:TYR:OH	1:A:55:PHE:CZ	0.41	2.67	10	1
1:A:36:VAL:HG11	1:A:45:ARG:NE	0.41	2.31	11	1
1:A:101:PHE:CE1	1:A:109:VAL:HG21	0.41	2.51	12	1
1:A:36:VAL:O	1:A:37:GLU:HG2	0.41	2.16	1	1
1:A:7:MET:HE1	1:A:103:PHE:CD2	0.41	2.48	3	1
1:A:23:LEU:HD12	1:A:55:PHE:HB3	0.41	1.90	5	1
1:B:261:LEU:HD13	2:B:326:NTH:C17	0.41	2.45	5	1
1:A:113:ARG:NH1	1:B:313:ARG:NH1	0.41	2.68	8	1
1:B:243:GLU:O	1:B:243:GLU:CD	0.41	2.58	10	1
1:A:77:GLU:OE2	1:A:102:ARG:CZ	0.41	2.69	14	1
1:B:267:LEU:HA	1:B:282:PHE:CB	0.41	2.46	14	1
1:B:251:ILE:HD13	1:B:251:ILE:HA	0.41	1.74	15	1
1:A:39:PRO:C	1:A:40:VAL:HG13	0.41	2.36	1	1
1:A:39:PRO:HG2	1:A:42:SER:OG	0.41	2.15	2	2
1:A:42:SER:O	1:A:43:GLU:HB2	0.41	2.15	3	1
1:A:68:THR:CG2	1:A:69:GLN:N	0.41	2.84	3	1
1:A:113:ARG:NH2	1:B:277:GLU:HG3	0.41	2.30	3	1
1:A:40:VAL:CG1	1:A:115:LEU:HA	0.41	2.45	8	1
1:B:223:LEU:HD13	1:B:223:LEU:HA	0.41	1.76	8	1
1:A:110:VAL:O	1:A:110:VAL:HG12	0.41	2.14	12	1
1:A:23:LEU:HD13	1:A:23:LEU:HA	0.41	1.77	13	1
1:A:7:MET:CA	1:A:7:MET:HE2	0.41	2.45	14	1
1:A:100:HIS:CB	1:A:113:ARG:CB	0.41	2.98	2	1
1:B:235:THR:OG1	1:B:311:SER:HA	0.41	2.16	2	1
1:A:85:SER:CB	1:A:94:VAL:CG2	0.41	2.98	3	1
1:B:214:TYR:CE1	1:B:215:VAL:HG23	0.41	2.50	15	2
1:A:14:TYR:N	1:A:29:LEU:CD2	0.41	2.84	5	1
1:A:81:ALA:CB	1:A:98:ILE:CG1	0.41	2.99	8	1
1:B:315:LEU:C	1:B:316:PHE:CG	0.41	2.93	13	1
1:A:102:ARG:CZ	A:102:ARG:CZ 1:B:313:ARG:HD2		2.45	15	1



	At a		D1 / 8)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:100:HIS:HB2	1:A:113:ARG:CB 0.41 2.45		2	1	
1:A:97:PRO:HA	1:A:116:PHE:CB 0.41 2.45		4	1	
1:A:30:PHE:HZ	1:A:112:MET:HE3	0.41	1.68	6	1
1:B:248:THR:O	1:B:249:ALA:C	0.41	2.58	7	1
1:A:52:ARG:O	1:A:54:PHE:N	0.41	2.54	8	1
1:A:87:GLU:HB2	1:A:92:LYS:CB	0.41	2.45	8	1
1:A:40:VAL:CG1	1:A:114:ALA:O	0.41	2.68	11	1
1:A:88:PHE:CE2	1:A:93:THR:OG1	0.41	2.74	13	1
1:A:109:VAL:HG11	1:A:112:MET:HE1	0.41	1.92	14	1
1:A:115:LEU:HD21	1:B:272:ARG:HB3	0.41	1.91	14	1
1:B:304:ASN:ND2	1:B:304:ASN:N	0.41	2.66	1	2
1:A:14:TYR:CE2	1:A:112:MET:SD	0.41	3.14	6	1
1:A:102:ARG:HD2	1:A:111:SER:HB2	0.41	1.92	6	1
1:B:302:ARG:HD3	1:B:311:SER:OG	0.41	2.16	6	1
1:B:222:ASP:O	1:B:223:LEU:C	0.41	2.59	9	1
1:B:247:GLY:O	1:B:251:ILE:HG12	0.41	2.16	10	1
1:B:217:ALA:CB	1:B:226:ILE:CG1 0.41 2.98		2.98	11	1
1:A:38:ASP:OD2	2:A:126:NTH:C6	0.41	2.69	14	1
1:B:302:ARG:C	2:ARG:C 1:B:303:PHE:CD1		2.94	14	1
1:B:244:PRO:O	1:B:244:PRO:O 1:B:245:ARG:HD2		2.16	1	1
1:A:63:LEU:HA	:63:LEU:HA 1:A:86:PHE:HB3		1.93	2	1
1:A:22:ASP:O	1:A:23:LEU:C	0.41	2.59	3	1
1:A:26:ILE:HG22	1:A:30:PHE:HD2	0.41	1.76	3	1
1:A:15:VAL:CB	1:A:67:LEU:HD11	0.41	2.42	5	1
1:A:60:LYS:O	1:A:62:PRO:HD3	0.41	2.15	6	1
1:A:54:PHE:C	1:A:56:ALA:N	0.41	2.75	7	1
1:B:245:ARG:HD2	1:B:250:ALA:CB	0.41	2.46	7	1
1:B:261:LEU:HD11	2:B:326:NTH:H212	0.41	1.93	7	1
1:A:27:VAL:O	1:A:30:PHE:N	0.41	2.53	8	1
1:B:260:LYS:O	1:B:262:PRO:HD3	0.41	2.16	8	1
1:A:72:ARG:HD2	1:A:72:ARG:C	0.41	2.36	9	1
1:A:14:TYR:HH	1:A:55:PHE:HE2	0.41	1.49	10	1
1:A:59:LEU:C	1:A:61:LEU:N	0.41	2.74	10	1
1:A:78:ALA:O	1:A:101:PHE:HB2	0.41	2.15	10	1
1:A:86:PHE:CZ	2:A:126:NTH:O20	0.41	2.74	11	1
1:A:116:PHE:N	1:A:116:PHE:CD1	0.41	2.89	11	1
1:B:280:PHE:CZ	1:B:299:ASP:OD2	0.41	2.74	12	1
1:A:41:GLY:HA2	1:B:276:ASN:ND2	0.41	2.31	13	1
1:A:7:MET:HE2	1:A:7:MET:N	0.41	2.30	14	1
1:B:280:PHE:CZ	1:B:299:ASP:CB	0.41	3.04	2	1
1:A:10:VAL:HG13	1:A:10:VAL:HG13 1:A:109:VAL:HG22		1.93	3	1



	A t and D	$Cl_{\alpha} = l_{\alpha}(\hat{\lambda})$		Models	
Atom-1	Atom-2	Atom-2 Clash(A)		Worst	Total
1:A:23:LEU:C	1:A:25:GLY:N 0.41 2.7		2.73	3	1
1:A:48:THR:C	1:A:50:ALA:N	0.41	2.75	3	1
1:B:254:PHE:O	1:B:255:PHE:C	0.41	2.58	14	1
1:A:81:ALA:O	1:A:82:PHE:HB3	0.41	2.16	15	1
1:A:120:ASN:OD1	1:A:121:ILE:HD11	0.40	2.15	2	1
1:A:61:LEU:HD21	2:A:126:NTH:C20	0.40	2.46	3	1
1:B:247:GLY:O	1:B:251:ILE:N	0.40	2.55	3	1
1:A:23:LEU:HG	1:A:56:ALA:HB2	0.40	1.93	6	1
1:B:271:VAL:CG1	1:B:272:ARG:N	0.40	2.84	7	1
1:A:104:ASN:HB3	1:A:110:VAL:CG1	0.40	2.44	8	1
1:B:244:PRO:O	1:B:245:ARG:NE	0.40	2.54	9	1
1:A:26:ILE:O	1:A:30:PHE:CD1	0.40	2.74	13	1
1:A:79:ALA:HB2	1:A:100:HIS:CD2	0.40	2.51	13	1
1:B:322:HIS:NE2	2:B:326:NTH:C22	0.40	2.84	13	1
1:A:57:ASN:CG	1:A:60:LYS:CE	0.40	2.90	1	1
1:A:92:LYS:O	1:A:92:LYS:HD2	0.40	2.16	7	2
1:A:32:ASP:C	1:A:48:THR:HG1	0.40	2.19	8	1
1:B:215:VAL:CB	:215:VAL:CB 1:B:267:LEU:HD11		2.46	8	1
1:A:119:LYS:HE3	S:HE3 1:B:270:GLU:OE2		2.16	9	1
1:A:13:ARG:HH21	13:ARG:HH21 1:A:29:LEU:HD11		1.75	10	1
1:A:99:ASP:OD1	SP:OD1 1:A:114:ALA:HA		2.16	10	1
1:A:52:ARG:C	1:A:54:PHE:N	0.40	2.74	12	1
1:A:40:VAL:C	1:A:42:SER:N	0.40	2.74	2	1
1:A:117:GLY:O	1:A:118:GLU:C	0.40	2.59	3	1
1:A:117:GLY:CA	Y:CA 1:B:274:VAL:HG13		2.47	3	1
1:A:21:GLY:CA	1:A:59:LEU:CD2	0.40	2.82	10	1
1:B:201:MET:O	1:B:202:ASN:HB2	0.40	2.17	12	1
1:A:118:GLU:OE1	1:B:201:MET:CE	0.40	2.69	13	1
1:B:208:THR:O	1:B:211:VAL:HB	0.40	2.17	15	1
1:B:300:HIS:O	1:B:312:MET:HG3	0.40	2.17	15	1
1:B:295:VAL:CG1	1:B:296:ALA:N	0.40	2.84	1	1
1:A:29:LEU:O	1:A:109:VAL:CB	0.40	2.69	3	1
1:B:302:ARG:HB2	1:B:311:SER:O	0.40	2.16	3	1
1:A:119:LYS:HE2	1:B:204:PRO:HG2	0.40	1.92	4	1
1:A:4:PRO:O	1:A:8:THR:OG1	0.40	2.34	8	1
1:B:277:GLU:HG3	1:B:302:ARG:HG2	0.40	1.93	8	1
1:B:236:VAL:O	1:B:244:PRO:HB2	0.40	2.16	9	1
1:A:15:VAL:O	1:A:18:LEU:HB2	0.40	2.16	10	1
1:B:302:ARG:HD2	1:B:304:ASN:OD1	0.40	2.16	10	1
1:B:242:SER:O	1:B:243:GLU:HG2	0.40	2.17	11	1
1:A:3:THR:HB	1:A:3:THR:HB 1:A:6:HIS:NE2		2.31	13	1



A 4 1	A + 0	$C_{1} = c_{1} \begin{pmatrix} \lambda \\ \lambda \end{pmatrix}$	\mathbf{D}	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:B:272:ARG:NH1	1:B:272:ARG:HG2	0.40	2.31	14	1
1:A:83:THR:HA	1:A:95:VAL:O	0.40	2.16	15	1
1:B:276:ASN:ND2	1:B:276:ASN:N	0.40	2.69	1	1
1:B:276:ASN:OD1	1:B:303:PHE:HB2	0.40	2.15	2	1
1:B:289:GLN:O	1:B:290:GLY:C	0.40	2.59	3	1
1:A:56:ALA:O	1:A:57:ASN:C	0.40	2.57	7	1
1:A:86:PHE:CZ	1:A:88:PHE:CE1	0.40	3.10	12	1
1:A:98:ILE:CD1	1:B:272:ARG:CZ	0.40	2.99	12	1
1:A:107:GLY:O	1:A:108:LYS:CG	0.40	2.70	14	1
1:A:116:PHE:HA	1:B:272:ARG:CZ	0.40	2.45	14	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	iers Percentil	
1	А	122/125~(98%)	$92\pm3~(75\pm2\%)$	20 ± 3 (17 $\pm3\%$)	$10\pm2~(8\pm2\%)$	2	14
1	В	122/125~(98%)	$92\pm3~(75\pm2\%)$	22 ± 3 (18 $\pm2\%$)	$8\pm2~(6\pm2\%)$	3	19
All	All	3660/3750~(98%)	2757~(75%)	644 (18%)	259~(7%)	2	16

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

Mol	Chain	Res	Type	Models (Total)
1	А	31	ALA	15
1	А	116	PHE	15
1	В	267	LEU	15
1	В	316	PHE	15
1	А	67	LEU	14
1	В	231	ALA	14
1	А	106	ALA	13
1	А	107	GLY	10
1	А	75	ALA	9
1	В	275	ALA	9
1	B	306	ALA	9



Mol	Chain	Res	Type	Models (Total)
1	В	307	GLY	8
1	А	40	VAL	7
1	А	105	GLY	7
1	А	121	ILE	7
1	А	69	GLN	7
1	В	305	GLY	6
1	А	34	ALA	5
1	В	282	PHE	5
1	В	321	ILE	5
1	В	269	GLN	5
1	А	41	GLY	4
1	A	82	PHE	4
1	В	240	VAL	4
1	В	290	GLY	4
1	А	39	PRO	3
1	А	90	GLY	3
1	А	42	SER	3
1	А	89	GLN	3
1	А	74	VAL	3
1	А	78	ALA	3
1	В	308	LYS	2
1	А	68	THR	2
1	В	289	GLN	2
1	А	108	LYS	2
1	В	234	ALA	2
1	A	44	PRO	2
1	В	278	ALA	2
1	A	5	GLU	2
1	В	239	PRO	2
1	А	43	GLU	1
1	В	274	VAL	1
1	В	241	GLY	1
1	В	276	ASN	1
1	B	244	PRO	1
1	В	294	VAL	1
1	А	36	VAL	1

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6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	93/95~(98%)	$61 \pm 4 \ (65 \pm 4\%)$	$32 \pm 4 (35 \pm 4\%)$	1	10
1	В	95/95~(100%)	65 ± 3 (68 $\pm3\%$)	$30\pm3(32\pm3\%)$	1	14
All	All	2820/2850 (99%)	1884 (67%)	936~(33%)	1	11

All 126 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

\mathbf{Mol}	Chain	\mathbf{Res}	Type	Models (Total)
1	А	14	TYR	15
1	А	32	ASP	15
1	А	35	THR	15
1	А	46	SER	15
1	А	55	PHE	15
1	А	74	VAL	15
1	А	83	THR	15
1	А	101	PHE	15
1	В	232	ASP	15
1	В	255	PHE	15
1	В	263	LEU	15
1	В	274	VAL	15
1	В	283	THR	15
1	В	301	PHE	15
1	А	45	ARG	14
1	А	61	LEU	14
1	А	63	LEU	14
1	А	92	LYS	14
1	А	93	THR	14
1	В	235	THR	14
1	В	246	SER	14
1	В	254	PHE	14
1	В	261	LEU	14
1	В	293	THR	13
1	А	54	PHE	12
1	А	122	HIS	12
1	В	214	TYR	12
1	В	322	HIS	12
1	В	320	ASN	12
1	А	42	SER	11
1	А	88	PHE	11
1	В	245	ARG	11
1	В	288	PHE	11
1	В	304	ASN	11



Mol	Chain	Res	Type	Models (Total)
1	А	115	LEU	11
1	В	277	GLU	11
1	А	77	GLU	10
1	А	89	GLN	10
1	А	113	ARG	10
1	В	213	ARG	10
1	В	215	VAL	10
1	В	289	GLN	10
1	В	302	ARG	10
1	А	120	ASN	10
1	В	292	LYS	10
1	А	6	HIS	9
1	А	15	VAL	9
1	А	111	SER	9
1	А	100	HIS	9
1	А	102	ARG	9
1	А	33	ASP	9
1	В	315	LEU	9
1	В	272	ARG	8
1	В	311	SER	8
1	В	313	ARG	8
1	А	72	ARG	8
1	А	94	VAL	8
1	В	210	VAL	8
1	А	13	ARG	8
1	В	201	MET	7
1	В	242	SER	7
1	В	300	HIS	7
1	А	66	GLU	7
1	А	67	LEU	7
1	А	119	LYS	7
1	А	104	ASN	7
1	В	308	LYS	7
1	А	3	THR	6
1	А	24	ASP	6
1	А	68	THR	6
1	В	205	GLU	6
1	В	206	HIS	6
1	В	267	LEU	6
1	А	5	GLU	6
1	А	103	PHE	6
1	В	268	THR	6

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IVIOI	Unam	nes	Type	Models (10tal)
1	А	69	GLN	5
1	А	84	VAL	5
1	В	224	ASP	5
1	А	108	LYS	5
1	В	294	VAL	4
1	В	219	ASN	4
1	В	319	LYS	4
1	А	10	VAL	4
1	А	19	ASN	4
1	А	60	LYS	4
1	В	266	GLU	4
1	В	233	ASP	4
1	А	38	ASP	3
1	A	110	VAL	3
1	A	87	GLU	3
1	В	203	THR	3
1	A	23	LEU	3
1	А	76	ASN	3
1	В	257	ASN	3
1	В	310	VAL	3
1	А	85	SER	3
1	В	260	LYS	3
1	В	321	ILE	3
1	В	238	ASP	3
1	В	202	ASN	2
1	В	243	GLU	2
1	В	269	GLN	2
1	В	285	SER	2
1	В	303	PHE	2
1	A	82	PHE	2
1	А	112	MET	2
1	В	312	MET	2
1	В	316	PHE	2
1	В	284	VAL	2
1	A	7	MET	2
1	В	291	ARG	2
1	В	286	PHE	2
1	A	116	PHE	2
1	В	282	PHE	2
1	A	37	GLU	2
1	В	218	LEU	2

Continued from previous page... Mol | Chain | Res | Type | Models (Total) |

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1

GLU

43

1

А



Mol	Chain	Res	Type	Models (Total)
1	А	29	LEU	1
1	А	18	LEU	1
1	А	52	ARG	1
1	В	230	PHE	1
1	В	287	GLU	1
1	А	86	PHE	1
1	А	91	ARG	1
1	В	237	GLU	1

Continued from previous page...

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mal	Turne	Chain	Dec	Tink		Bond leng	gths
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	#Z>2
2	NTH	В	326	-	27,30,30	3.04 ± 0.02	8±0 (29±1%)
2	NTH	А	126	-	27,30,30	3.04 ± 0.02	8±0 (29±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles



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

Mal	Trune	Type Chain		Link	Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	#Z>2	
2	NTH	В	326	-	42,45,45	2.46 ± 0.01	11 ± 0 (26 $\pm1\%$)	
2	NTH	А	126	-	42,45,45	2.46 ± 0.01	11 ± 0 (26 $\pm1\%$)	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NTH	А	126	-	-	$0\pm0,7,62,62$	$0\pm0,4,4,4$
2	NTH	В	326	-	-	$0\pm0,7,62,62$	$0\pm0,4,4,4$

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

Mal	Chain	Dog	Tuno	Atoms	7	$Observed(\lambda)$	Ideal(Å)	Moo	dels
	Ullaili	nes	туре	Atoms		Observeu(A)	Iueai(A)	Worst	Total
2	А	126	NTH	O17-C17	12.31	1.25	1.46	2	15
2	В	326	NTH	O17-C17	12.29	1.25	1.46	1	15
2	В	326	NTH	C10-C5	4.76	1.60	1.52	1	15
2	А	126	NTH	C10-C5	4.73	1.60	1.52	11	15
2	А	126	NTH	C4-C3	4.57	1.55	1.45	10	15
2	В	326	NTH	C4-C3	4.52	1.55	1.45	7	15
2	А	126	NTH	C10-C9	4.38	1.61	1.54	10	15
2	В	326	NTH	C10-C9	4.27	1.61	1.54	7	15
2	В	326	NTH	C13-C17	3.11	1.48	1.53	10	15
2	А	126	NTH	C13-C17	3.09	1.48	1.53	13	15
2	А	126	NTH	C1-C10	2.57	1.58	1.53	2	15
2	В	326	NTH	C1-C10	2.49	1.58	1.53	6	15
2	А	126	NTH	C4-C5	2.25	1.37	1.34	11	15
2	В	326	NTH	C4-C5	2.25	1.37	1.34	4	15
2	А	126	NTH	C12-C11	2.13	1.57	1.53	15	15
2	В	326	NTH	C12-C11	2.13	1.57	1.53	6	12
2	В	326	NTH	C13-C14	2.01	1.58	1.55	5	1
2	А	126	NTH	C13-C14	2.01	1.58	1.55	8	1

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



Mal	l Chain Res Type Atoms		Atoma	7	Observed(0)		Models		
IVIOI	Unam	nes	туре	Atoms	L	Observed()	Ideal()	Worst	Total
2	А	126	NTH	C18-C13-C14	8.53	127.61	111.71	7	15
2	В	326	NTH	C18-C13-C14	8.50	127.56	111.71	7	15
2	А	126	NTH	C16-C17-C13	6.85	112.39	105.21	8	15
2	В	326	NTH	C16-C17-C13	6.82	112.36	105.21	10	15
2	В	326	NTH	O17-C17-C16	5.38	124.47	111.07	8	15
2	А	126	NTH	O17-C17-C16	5.36	124.41	111.07	14	15
2	В	326	NTH	C18-C13-C12	4.39	103.66	110.59	2	15
2	А	126	NTH	C18-C13-C12	4.36	103.70	110.59	5	15
2	А	126	NTH	O17-C20-C22	3.75	119.58	111.50	8	15
2	В	326	NTH	O17-C20-C22	3.52	119.08	111.50	7	15
2	В	326	NTH	O17-C17-C13	3.23	118.78	111.09	11	15
2	А	126	NTH	O17-C17-C13	3.21	118.75	111.09	15	15
2	А	126	NTH	C6-C5-C10	3.20	120.52	115.63	3	15
2	В	326	NTH	C6-C5-C10	3.17	120.48	115.63	10	15
2	А	126	NTH	C1-C10-C9	3.10	104.86	111.91	3	15
2	В	326	NTH	C1-C10-C9	3.09	104.89	111.91	1	15
2	В	326	NTH	C18-C13-C17	2.69	105.81	109.90	11	15
2	А	126	NTH	C18-C13-C17	2.68	105.83	109.90	10	15
2	В	326	NTH	C7-C6-C5	2.66	107.71	112.33	6	15
2	А	126	NTH	C7-C6-C5	2.65	107.72	112.33	7	15
2	В	326	NTH	C5-C4-C3	2.29	119.88	123.08	2	15
2	А	126	NTH	C5-C4-C3	2.22	119.99	123.08	4	15
2	А	126	NTH	C9-C10-C5	2.03	106.32	110.43	6	4
2	В	326	NTH	C9-C10-C5	2.01	106.36	110.43	14	5

occurrence in the ensemble.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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





6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

