

Apr 23, 2024 - 03:17 pm BST

PDB ID	:	6ZQB
EMDB ID	:	EMD-11358
Title	:	Cryo-EM structure of the 90S pre-ribosome from Saccharomyces cerevisiae, state $\mathrm{B2}$
Authors	:	Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2020-07-09
Resolution	:	3.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.90 Å.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality	of chain	
1	UA	923	60%	27%	• 10%
2	UB	810	49%	13%	37%
3	UC	610	15% 6%	79%	
4	UD	776	57%	29%	• 13%
5	UE	643	53%	20% ·	26%
6	UF	440	48%	18% •	33%
7	UG	554	65%		29% • •

Continued on next page...



Continued from previous page... Chain Length Quality of chain Mol 8 UH 713 44% 17% 38% . 9 UI 57511% 6% 82% 10 UJ 176955% 7% 37% UK 11 25064% 30% • • 12UL 943 59% 30% 11% • 13UM 817 62% • 7% 30% UN 1414573% 25% • UO • • 1551368% 26% UP 16 21419% 72% 9% 17UQ 896 62% 29% • 7% 18 UR 59458% 20% 19% • US1955263% 23% 13% . 5% 20UT 2493 • 10% 88% UU 2193967% • 10% 21% UV 221237 64% 24% 13% 23UX 18961% 28% 8% • UΖ 2742410% 62% 28% CA25327 26% 57% 14% • CB25327 47% 22% 30% CD2650455% 19% 25% . CE 2751172% 15% 13% 28 CF . . 12673% 21% 28CG126•• 64% 32% 29 CH 57351% • 27% 21% CI 30 18362% 32% 5%•

Continued on next page...



Continued from previous page... Chain Length Quality of chain Mol CJ29031 66% 27% • • CK 3259326% 8% • 65% i 33 CL 1183 46% 19% 34% • CM367 3470% 28% . i 35CN29757% 21% 22% 36 JA 105657% 20% 23% 15% JB 36 1056 76% 21% . 37 JC 707 31% 19% 50% JE 38 357 24% 14% 62% . JF3925262% 24% 14% JG 39 25265% 25% • 9% 8% $_{\rm JH}$ 40 483 53% 46% 41 JJ27434% 47% 18% JK 425345%• 92% 43JM21746% 17% 38% 44JN346 42% 11% 46% • JO 4531659% 15% 25% JP 464897% 59% 30% • 47JQ20628% 69% • DA 2554869% 24% • 6% DE 4926159% • 6% 34% DF 5022575% 19% • 5% \mathbf{DG} 2365156% 36% 8% DH 190• • 5265% 31% DI 200 5312% 64% 24%

Continued on next page...



Mol	Chain	Length		Qua	lity of chain		
54	DJ	197		61%		27%	• 10%
55	DL	156	i	57%		33%	10%
56	DN	151	–	75%			23% •••
57	DO	137		69%		19%	12%
58	DQ	143		61%		24%	• 13%
59	DS	147	—	67%		•	29%
60	DW	130		74%			25% •
61	DX	145		49%	19%	•	29%
62	DY	135	38%		33%	•	28%
63	Db	82			96%		
64	Dc	67		9(0%		• 6%
65	D2	700	20%	33%	17%	•	25%
66	D3	1808	18%	29%	16% •	3	4%
67	D4	175	26%	3	9%	27%	8%

Continued from previous page...



2 Entry composition (i)

There are 69 unique types of molecules in this entry. The entry contains 223151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues		Α	AltConf	Trace			
1	UA	834	Total 6635	C 4223	N 1140	0 1253	S 19	0	0

• Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues		At	AltConf	Trace			
2	UB	508	Total 3743	C 2373	N 665	O 696	S 9	0	0

• Molecule 3 is a protein called Something about silencing protein 10.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
3	UC	128	Total 1026	C 633	N 204	O 189	0	0

• Molecule 4 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues		A	AltConf	Trace			
4	UD	675	Total 5361	C 3395	N 929	0 1015	$\frac{\mathrm{S}}{22}$	0	0

• Molecule 5 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues		At	AltConf	Trace			
5	UE	475	Total 3772	C 2400	N 649	0 710	S 13	0	0

• Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues		At	AltConf	Trace			
6	UF	293	Total 2487	C 1605	N 435	O 434	S 13	0	0



• Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues		At	AltConf	Trace			
7	UG	533	Total 4218	C 2646	N 758	0 802	S 12	0	0

• Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues		Ate		AltConf	Trace		
8	UH	441	Total 2690	C 1672	N 492	O 523	${ m S} { m 3}$	0	0

• Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	UI	102	Total 846	С 547	N 149	0 148	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues		Α	AltConf	Trace			
10	UJ	1117	Total 6857	C 4267	N 1252	O 1326	S 12	0	0

• Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues		At		AltConf	Trace		
11	UK	241	Total 2016	C 1251	N 388	O 370	S 7	0	0

• Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues		Α			AltConf	Trace	
12	UL	842	Total 6720	C 4300	N 1126	O 1267	S 27	0	0

• Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues		Α	AltConf	Trace			
13	UM	762	Total 5957	C 3779	N 1006	0 1144	S 28	0	0

• Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 14,U3 small nucleolar RNA-associated protein 14.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	UN	145	Total 1207	C 750	N 230	O 225	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues		At	AltConf	Trace			
15	UO	493	Total 3911	C 2462	N 702	O 735	S 12	0	0

• Molecule 16 is a protein called Bud site selection protein 21.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
16	UP	60	Total 495	C 310	N 101	0 84	0	0

• Molecule 17 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues		Α	toms			AltConf	Trace
17	UO	830	Total	С	Ν	Ο	\mathbf{S}	0	0
11	UQ	052	6662	4236	1124	1283	19	0	0

• Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	UR	481	Total 3791	C 2399	N 668	0 714	S 10	0	0

• Molecule 19 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	US	481	Total 3650	C 2355	N 611	O 672	S 12	0	0

• Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues		Ato		AltConf	Trace	
20	UT	2234	Total 11108	C 6640	N 2234	0 2234	0	0

• Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 21.



Mol	Chain	Residues		А	toms			AltConf	Trace
91	TIT	818	Total	С	Ν	Ο	\mathbf{S}	0	0
	00	040	6678	4241	1149	1267	21	0	0

• Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues		Α	AltConf	Trace			
22	UV	1080	Total 8725	C 5672	N 1/130	O 1590	S 24	0	0

• Molecule 23 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues		A	toms	AltConf	Trace		
23	UX	174	Total 1395	C 890	N 255	O 240	S 10	0	0

• Molecule 24 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
24	UZ	247	Total 2006	C 1284	N 356	O 358	S 8	0	0

• Molecule 25 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	CA	242	Total	С	Ν	0	S	0	0
2.0	UA	242	1881	1193	338	340	10	0	0
25	CP	228	Total	С	Ν	0	S	0	0
2.0		220	1782	1131	320	321	10	0	0

• Molecule 26 is a protein called Nucleolar protein 56.

Mol	Chain	Residues		Ate		AltConf	Trace		
26	CD	380	Total 2994	C 1898	N 513	0 574	S 9	0	0

• Molecule 27 is a protein called Nucleolar protein 58.

Mol	Chain	Residues		Ate		AltConf	Trace		
27	CE	435	Total 2985	C 1852	N 543	O 582	S 8	0	0

• Molecule 28 is a protein called 13 kDa ribonucleoprotein-associated protein.



Mol	Chain	Residues		At	oms			AltConf	Trace
<u> </u>	CE	192	Total	С	Ν	0	S	0	0
20	Or	123	931	594	160	173	4	0	0
<u> </u>	CC	192	Total	С	Ν	0	S	0	0
20	UG	123	928	591	160	173	4	0	0

• Molecule 29 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues		At	oms			AltConf	Trace
29	CH	454	Total 3634	C 2311	N 638	O 675	S 10	0	0

• Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues		At	oms		AltConf	Trace	
30	CI	182	Total 1530	C 967	N 287	O 269	S 7	0	0

• Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues		At		AltConf	Trace		
31	CJ	282	Total 2296	C 1441	N 430	0 418	${ m S} 7$	0	0

• Molecule 32 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues		Ate	AltConf	Trace			
32	СК	207	Total 1667	C 1034	N 297	O 332	$\frac{S}{4}$	0	0

• Molecule 33 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues		А	AltConf	Trace			
33	CL	781	Total 6332	C 4063	N 1122	0 1117	S 30	0	0

• Molecule 34 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues		At	AltConf	Trace			
34	СМ	360	Total 2781	C 1781	N 473	O 516	S 11	0	0

• Molecule 35 is a protein called Ribosomal RNA-processing protein 7.



Mol	Chain	Residues		At	AltConf	Trace			
35	CN	232	Total 1893	C 1213	N 322	0 351	${ m S} 7$	0	0

• Molecule 36 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms	AltConf	Trace
36	JA	812	Total C N O S 5892 3727 1041 1099 25	0	0
36	JB	835	Total C N O 4132 2462 835 835	0	0

• Molecule 37 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues		Ate	AltConf	Trace			
37	JC	354	Total 2845	C 1795	N 489	0 552	S 9	0	0

• Molecule 38 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	JE	136	Total 1125	C 674	N 231	0 217	${ m S} { m 3}$	0	0

• Molecule 39 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues		At	AltConf	Trace			
30	IF	216	Total	С	Ν	Ο	\mathbf{S}	0	0
- 00	51	210	1701	1079	296	315	11	0	0
30	IC	230	Total	С	Ν	Ο	\mathbf{S}	0	0
- 39	10	230	1799	1142	313	333	11	0	0

• Molecule 40 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues		Ato	\mathbf{ms}		AltConf	Trace
40	JH	261	Total 1295	C 773	N 261	O 261	0	0

• Molecule 41 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues		At	AltConf	Trace			
41	JJ	182	Total 1448	C 926	N 262	O 256	${S \over 4}$	0	0



• Molecule 42 is a protein called Protein BFR2.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
42	JK	42	Total 334	C 213	N 54	O 67	0	0

• Molecule 43 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues		At			AltConf	Trace	
43	JM	135	Total 1137	C 721	N 211	O 201	${S \over 4}$	0	0

• Molecule 44 is a protein called Protein FAF1.

Mol	Chain	Residues		At	oms		AltConf	Trace	
44	JN	186	Total 1428	C 879	N 287	O 259	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	JO	236	Total 1930	C 1231	N 342	0 345	S 12	0	0

• Molecule 46 is a protein called Protein SOF1.

Mol	Chain	Residues		At	AltConf	Trace			
46	JP	457	Total 3725	C 2328	N 679	0 702	S 16	0	0

• Molecule 47 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
47	JQ	63	Total 381	C 234	N 69	0 78	0	0

• Molecule 48 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
48	DA	240	Total 1912	C 1209	N 354	0 345	${S \atop 4}$	0	0

• Molecule 49 is a protein called 40S ribosomal protein S4-A.



Mol	Chain	Residues		At	AltConf	Trace			
49	DE	245	Total 1944	C 1245	N 360	O 336	${ m S} { m 3}$	0	0

• Molecule 50 is a protein called Rps5p.

Mol	Chain	Residues		Ate	AltConf	Trace			
50	DF	213	Total 1669	C 1045	N 307	0 314	${ m S} { m 3}$	0	0

• Molecule 51 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues		Ate		AltConf	Trace		
51	DG	218	Total 1755	C 1102	N 337	0 313	${ m S} { m 3}$	0	0

• Molecule 52 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
52	DH	184	Total	С	N	Ō	0	0
02	DII	104	1477	949	265	263	0	0

• Molecule 53 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
53	DI	177	Total 1399	C 869	N 279	O 249	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 54 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues		At	oms		AltConf	Trace	
54	DJ	177	Total 1428	C 902	N 275	O 250	S 1	0	0

• Molecule 55 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
55	DL	140	Total 1129	C 724	N 215	0 187	${ m S} { m 3}$	0	0

• Molecule 56 is a protein called 40S ribosomal protein S13.



Mol	Chain	Residues		At	oms	AltConf	Trace		
56	DN	150	Total 1192	C 759	N 224	O 207	${ m S} { m 2}$	0	0

• Molecule 57 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
57	DO	120	Total 881	С 544	N 167	0 167	${ m S} { m 3}$	0	0

• Molecule 58 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
58	DQ	125	Total 973	C 625	N 174	0 174	0	0

• Molecule 59 is a protein called 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
59	DS	104	Total 516	C 308	N 104	O 104	0	0

• Molecule 60 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues		At	oms		AltConf	Trace	
60	DW	129	Total 1021	C 650	N 188	O 180	${ m S} { m 3}$	0	0

• Molecule 61 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues		At	oms		AltConf	Trace	
61	DX	103	Total 786	$\begin{array}{c} \mathrm{C} \\ 503 \end{array}$	N 144	0 137	${ m S} { m 2}$	0	0

• Molecule 62 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
62	DY	97	Total 767	C 490	N 138	O 139	0	0

• Molecule 63 is a protein called 40S ribosomal protein S27-A.



Mol	Chain	Residues		At	oms	AltConf	Trace		
63	Db	81	Total 610	C 382	N 110	0 113	${ m S}{ m 5}$	0	0

• Molecule 64 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
64	Dc	63	Total 497	C 306	N 99	0 91	S 1	0	0

• Molecule 65 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues		A	toms			AltConf	Trace
65	D2	522	Total	С	Ν	Ο	Р	0	0
00	D^2	522	11138	4977	1976	3663	522	0	0

• Molecule 66 is a RNA chain called 18S rRNA.

Mol	Chain	Residues		A		AltConf	Trace		
66	D3	1198	Total 25549	C 11417	N 4548	O 8386	Р 1198	0	0

• Molecule 67 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues		А	toms			AltConf	Trace
67	D4	175	Total 3712	C 1661	N 648	O 1228	Р 175	0	0

• Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf				
68	UX	1	Total Zn 1 1	0				
68	Db	1	Total Zn 1 1	0				

• Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues	Residues Atoms								
60	CI	1	Total	С	Ν	0	Р	0			
09	CL	L	32	10	5	14	3	0			



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Periodic tryptophan protein 2



• Molecule 2: Nucleolar complex protein 14

Chain UB: 49%



13%

37%





L602 N610

• Molecule 4: U3 small nucleolar RNA-associated protein 4



• Molecule 5: U3 small nucleolar RNA-associated protein 5









Li390 Li396 C1396 C1366 C1366





HIS A SUN CONTREMENTATION CONT











• Molecule 12: U3 small nucleolar RNA-associated protein 12







• Molecule 14: U3 small nucleolar RNA-associated protein 14,U3 small nucleolar RNA-associated protein 14



С	hε	ir	11	U	N	•										739	%														2!	5%			•	•			
Q276	R277	<mark>q280</mark>		E294	K 297	W298	1 303	R306	R307	A308	D309	F313	K317	E320	H323	F327	0331	K837 K838	N839	L840	K841	1 64.2 0.84.3	8844 S844	<mark>S845</mark>	A846 Ve47	R854	L861	R862	M863 P864	•	E868	R872	<mark>0876</mark>	I879	K880	P881	M884	T885	
86	06	91	<mark>.</mark>	94 0 E	80 90	97																																	

• Molecule 15: U3 small nucleolar RNA-associated protein 15







• Molecule 19: Nucleolar complex protein 4







•••••

PRO THR GLY SER SER SER SER V283 V283

• Molecule 21: U3 small nucleolar RNA-associated protein 21



131 ALA GLN GLU GLU CLU GLU SER SER

DB





• Molecule 24: Ribosome biogenesis protein UTP30





• Molecule 25: rl	RNA 2'-O-methyltrans	ferase fibrillarin	
Chain CA:	57%	14%	• 26%
MET SER PHE ARG ARG CLY SER ARG CLY SER SER ARG	GLY GLY SER SER ARG GLY PHE GLY GLY GLY GLY GLY GLY ALA ARG GLY	ARG GLY SER ARG CLY CLY CLY CLY CLY CLY CLY CLY CLY	ABCA ABCA GLY ALA ALA ARA CLY SER ARC CLY SER CLY PHE CLY ARG GLY ARG GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C
SER ARG GLY GLY ALA ALA CLY SER ARG GLY GLY	GLY GLY GLY ALA ALA ALA ALA GLY GLY CIO E102 E102 E102 E103 M111 M111	G114 R122 V125 SER SER GLU ASP GLU	P135 P135 P136 P136 T137 V143 V143 V143 V143 V145 V168 V168 V168 V168 V171
6174 A175 A176 S177 C178 C192 C192 C193 V194 V193	F199 S200 S200 K212 M223 M223 R223 (228 K229 Y230 Y230 R231 Y231 Y231 Y233 Y233	0238 0239 0246 0246 0246 1252 1253 1253 1253 1253 1253	521 L301 L305 L305 E307 P309 P309 P309 P309 P309 P314 C314 C314 C314 C314 C314 C314 C312 C312 C312 C312 C312 C312 C312 C312
• Molecule 25: rl	RNA 2'-O-methyltrans	ferase fibrillarin	
Chain CB:	47%	22%	30%
MET SER PHE ARG CLY SER ARG GLY SER ARG	GLY GLY SER ARG GLY GLY PHE GLY GLY SER ARG GLY SER ARG GLY ALA	ARG GLY GLY SER ARG GLY GLY GLY GLY GLY GLY	ARG GLY GLY GLY ALA ALA ARG CLY SER ARG CLY PHE CLY ARG GLY GLY GLY GLY GLY
SER ARG GLY GLY ALA ARG GLY SER SER ARG GLY GLY	GLY GLY GLY ALLA ALLA ALLA ALLA ALLA ALL	V966 Y97 1987 1988 1988 110 1110 1117 1117 1117 1118	N125 N125 CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
Y141 Y144 W145 N145 F146 F146 R148 A152 L159	F163 1164 1164 1167 1171 1171 1171 1171 1172 1172 1172	E191 197 198 198 198 198 198 198 199 190 190 190 101 101 101 101 101 101	R214 R215 P215 1217 1217 1221 P227 P227 P227 C239 C239 C239 C239 C239 C239 F241
V244 (2249 (2249 (2262 (2263 (2264 (2264 (2264 (2264	K272 C275 C275 C275 C275 C275 C275 C275 C	H313 H313 C314 T315 V316 V316 V316 R319 Y320 Y320 S323 C324 LEU	S X1
• Molecule 26: N	ucleolar protein 56		
Chain CD:	55%	19%	• 25%
MET ALA 193 194 19 19 19 19 19 19 19	423 829 839 830 835 138 138 138 138 148 148 148 148 148 148 148 148	N67 370 770 178 178 178 178 178 183 183 183	196 106 101 101 101 117 117 1128 1128 1128 1128 1128 1128
H134 K137 L1422 Q1432 Q143 Q143 R149 R149	211 22 2166 2171 2180 2180 2180 2188 2188 2188 2188 218	M198 Y199 H202 H203 F203 F203 F205 L206 L221 L221	0231 1234 1237 1237 1234 1234 8245 8245 8245 8256 8256 8256 8256 8256 8256 8256 825
A255 R256 1257 8258 M259 1265 1265 M265 M265 M269	V271 V271 777 A775 0276 0276 1281 1281 1281 1281 1285 13321 13328	T322 T326 CLY CLY CLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LYS THR LYS GLY ASN ASN ASN THR TYR CLFU LEU LLEU LLEU LLEU LLEU STR SSR SSR SPHE
ILE SER LYS SER ALA SER ALA SER AIA K370 R372 R377	Kusa Kusa Kusa Kusa Kusa Kusa Kusa Kusa	V403 L404 L404 R411 A11 A11 A11 A11 A11 A11 A11 A11 C12 C12 F10 F10 F10	ASN ASN GLU LLE CLU LLE CLN GLU GLU GLU GLU CLN ALA ALA ALA ALA ALA ANP ASP ASP CNO ASP ASP ASP ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN
ALA ALA ALA GLU CLU GLU CLU CLU CLU CLU SER SER	LYS LYS LYS LYS LYS LYS CLU ASP ASP ASP ASP ASP CLU CLU CLYS CLU CYS CLU	GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	LY13 ASP ASP LY13 ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY ASP LY AS
LYS SER ASP ASP			



• Molecule 27: Nucleolar protein 58 Chain CE: 72% 13% 15% ASP GSU GSU GSU GSU GSU GSU GSU GSU CSSER ASP GSU CSSER CSSE • Molecule 28: 13 kDa ribonucleoprotein-associated protein Chain CF: 73% 21% MET SER ALA • Molecule 28: 13 kDa ribonucleoprotein-associated protein Chain CG: 64% 32% E E S • Molecule 29: Ribosomal RNA-processing protein 9 Chain CH: 51% 27% 21% LYS GLU ASP VAL ALA ALA GLU GLU GLN

V627 V626 V627 V627 V626 V627 V627 V627 V627 V627 V627 V627 V626 V644 V666 V646 V747 V666 V644 V666 V646 V747 V666 V646 V747 V666 V646 V747 V666 V646 V747 V666 V747 V746 V666 V617 V666 V617 V666 V617 V666 V617 V666 V747 V666 V747 V747

• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CI:	6	2%	32%	5%•
MET V2 K4 L5 E9 Q10	K11 L12 K14 K15 K15 K14 K15 K16 K15 C12 C10 C20 C25 C25 C25 C25 C25 C25 C25 C25 C25 C25	D29 730 731 732 733 733 733 733 733 733 733 733 733	X44 X47 C51 C51 L57 L57 L61 L61 L64 R71	L77 L78 L79 D80 K81 L82 L82
M85 G86 V87 L88 K91 I94	L97 E98 V103 V113 L118 L118 V128 V128 V136	V138 G139 L142 L142 D145 P146 P146 P146 V150 V150 V150 V150 V151 V151 V157 V157	W160 V161 D162 T166 K165 K166 K166 L171 L171 K171	11/3 5183
• Molecule	31: U3 small nucle	olar ribonucleoprotein p	protein IMP4	
Chain CJ:		66%	27%	•••
M1 R7 E8 R9 R10 E11 Y12	113 120 120 120 120 120 120 120 120 120 120	S51 L52 L52 K58 S61 K58 K63 K162 K63 K162 K10 K11 ALA ASP ASP ASP ASP	472 188 189 893 893 893 893 893 1100	P112 V115 R116 L117 N118 R119
6120 N121 Y122 V123 M124 P125 N126 L127	V128 V129 A130 C131 C131 C136 C135 C135 C136 C136 V140 V140 V140 V141 C144	T150 2151 2151 2155 2157 2158 2158 2158 2158 2158 2158 2178 2176	11/7 E184 V185 N186 P187 H188 L189 D192 D192 T195	K200 R201 V202 V203 C204 C204 F210
N211 A212 A212 P214 K215 E219 R220	V221 1222 1223 N226 N226 C228 D229 C228 C228 N234 N233 N235 H236 H236 H236 H236	G244 V250 C351 P253 R253 E260 L266 V273 Q276 R279	F 280 1281 R 282 N 285 Y 289 L 290	
• Molecule	32: U3 small nucle	olar RNA-associated pr	otein MPP10	
Chain CK:	26%	8% •	65%	
MET SER GLU CLU LEU PHE GLY VAL LEU	LYS SER ASN ASN ASN ALA CLZ LEU LEU LEU LYS ASP ASP ASA	THR LYS ASP ASP ASP ALA ALA ASP TTR ASP TTR ASP TTR ASP TTR CYS	ASN GLY SER THR LYS LYS ALA GLU CEU ASP GLU TLE	THR VAL ASP GLY LEU ASP ALA ASN
GLN VAL TRP TRP GLN VAL LYS LEU	VAL LEU ASP SER SER ASP GLY GLY GLN GLN GLN GLN	GLU LFSU LYS LYS ASP VAL VAL VAL THR PRO SER ASN LEU SER SER SER SER SER SER SER SER	ALEU ALEU SER SER SER SER GLU GLU GLU GLU GLU GLU	ALA GLU SER VAL PHE LYS GLU LYS LYS
GLN MET LEU SER ALA ASP VAL SER	GLU TILE CLU GLU GLU GLU GLU ASP SER SER SER SER GLU ASP ASP	OLU GLU PRO RET MET MET MET ASP CLU ALA ALA ALA ALA ALA ALC CLU CLU	PHE PHE ALA ALA GLU CTU CTV CTV SER SER SER CLN GLN ASP	GLU ARG HIS SER SER PRO ASP PRO
TYR GLY ILE ASN ASP LYS PHE PHE	ASP LEU CLU CLU CLU CLU ASP ASP ASP ASP ALA ALA ASP ASP	SER ALU GLU GLU GLU GLU GLU GLU ASP GLU ASP ASP ASP ASP ASP CLU CLN	MET MET PRO PRO PRO SER ASP GLU GLU GLU GLU GLU CLU TLE TYR	TYR GLU ASP PHE PHE ASP LYS PRO
THR LYS GLU PRO VAL LYS LYS HIS	SER VAL LYA LYA ASP PRO LYS GLU GLU ASP GLU ASP GLU GLU GLU	GLU GLU GLU ASP SER ALA ALA ASP LLEU LLEU LLEU LLEU ASP ALA ALA ALA	GLU ASP CLU CLU PRO ASN ALA ALA GLU GLV ALA	SER ASP N296 L297 I305







KI 026 P923 RR0 K1034 P929 RN0 L1034 F926 MR1 L1034 F929 MR1 L1034 F929 MR1 L1034 F929 MR1 L1067 V939 M1062 L1067 V936 M1063 K1066 V936 M1072 S1051 V936 M1073 K1072 K934 M1074 F1076 V1073 V1073 K1076 F946 V1074 F1076 K1116 K1116 K1116 F967 K1116 K1116 F967 K1116 K1116 F967 K1116 K1167 F967 K1116 K1168 K977 K1156 K1156 M997 K1156 K1156 M997 K1156 K1156 M997 K1156 K1169 F991 K1156 K160 F991

• Molecule 34: RNA 3'-terminal phosphate cyclase-like protein





W O R L D W I D E PROTEIN DATA BANK

LIEU SERIA SERIA CILIEU CILIEU

LYS PRO ARG LYS SER LYS LYS LYS ALA ASN

• Molecule 37: Ribosome biogenesis protein ENP2




• Molecule 39: Ribosomal RNA small subunit methyltransferase NEP1 Chain JF: 62% 24% 14% • Molecule 39: Ribosomal RNA small subunit methyltransferase NEP1 Chain JG: 65% 25% 9% SEH ASN GLY GLY GLY • Molecule 40: Essential nuclear protein 1 8% Chain JH: 53% 46% MET THR MET THR SERRA SERRA SERRA SERRA ARG CLVSS CLVS GLY TYR TYR COLUCTION COLU



• Molecule 41: Pre-rRNA-processing protein PNO1

Chain JJ: 47% 18% 34% • Molecule 42: Protein BFR2 Chain JK: 5% . 92% VAL VAL SERRA SERA LLEU LILEU LYSS LYSS SER ASN A ASN A ASN A ASN A ASN A ASN A ALA A ASN LLYS SER A SN A ASN • Molecule 43: rRNA-processing protein FCF2 Chain JM: 46% 17% 38%











• Molecule 47: Regulator of rDNA transcription protein 14

α · τ			
Chain JQ:	28%	•	69%

NET SER NET SE

• Molecule 48: 40S ribosomal protein S1-A



V244 T245 GLY DHE LYS ASP GLU VAL LEU GLU GLU THR VAL

• Molecule 49: 40S ribosomal protein S4-A





• Molecule 51: 40S ribosomal protein S6-A







22 7 111 112 113 413	8 8 9 1 8 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	88 887 SP SP SP SP SP SP SP SP SP SP SP SP SP	LY XS YR 99 102 103	118 119 LA Nuk Nuk Nuk	NNK NNK NNK NNK
		UN POPULATION		<u> </u>	
• Molecule 60	· 408 ribosomal 1	protein S22-A			
• Molecule 00	. 405 1100501181]	510000111 (522-74			
Chain DW:		74%		25%	·
MET T2 R3 S4 N15 K22 V25	R28 929 830 831 134 134 138 138 138 138 138 138 138 138 138	F50 E51 H56 H56 V63 G67 R667	L69 L69 C72 C72 S76 P77 R77 R78 R78	K82 M89 P95 P95	q98 K124 G127 Y130
• Molecule 61	: 40S ribosomal p	protein S23-A			
Chain DX:	49%		19%	• 29%	
MET GLY CLYS GLY GLY CLYS PRO ARG GLY CLEU ASN	ALA ARG LYS LYS LEU LEU ARG ARG ARG ARG ARG ARG	TRP ALA GLU ASN ASN TYR LYS LYS ARG	LEU LEU GLY ALA ALA ALA FHE LYS SER SER	F42 F43 A49 K50 G51 G51 E60 S61 S61 R62 R63	866 869 870 877 877 878
V87 P88 N89 C92 C92 L193 N94	D100 E101 E101 L103 L103 F107 F107 F107 F108 R109 K110 D116	K123 K123 L133 L133 A134 V136 K137 K137 F138	SER SER		
• Molecule 62	: 40S ribosomal p	protein S24-A			
Chain DY:	38%		33%	• 28%	
MET 82 83 84 13 17 17 17 17 17 17 19 110	V111 V12 S14 S14 N15 A19 C22 F23 C22 V24 V24	D256 V27 L28 H29 N34 L40 R41	L44 V47 D53 A54 V55 S56	F55 (559 (559 (559 (560 (568 (568 (568 (568 (568 (568) (568) (568) (568) (568) (568) (568) (568) (568) (568) (568) (569) (56	G71 F72 G73 L74 V75 A80
K83 198 191 192 193 193 194 194 198	VAL VAL GLU GLU CYS ALA SER ARG GLN GLN GLN GLN GLN CYS	LYS ASN ASP ASP LYS LYS LYS TLE PHE GLY THR	GLY LYS ARG LEU LEU LYS LYS VAL	ALA ARG ASN ALA ALA ASP	
• Molecule 63	: 40S ribosomal p	protein S27-A			
Chain Db:		96%			
NET V2 L13 V4 K82 K82					
• Molecule 64	: 40S ribosomal p	protein S28-A			
Chain Dc:		90%			• 6%
MET ASP ASN LVS LVS V12 V28 V28	750 1912				
• Molecule 65	: 5ETS RNA				















4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	I	Bond lengths		Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	UA	1.71	109/6780~(1.6%)	1.08	35/9175~(0.4%)
2	UB	0.51	0/3796	0.61	6/5137~(0.1%)
3	UC	1.03	1/1034~(0.1%)	0.86	2/1365~(0.1%)
4	UD	0.95	15/5461~(0.3%)	0.82	6/7395~(0.1%)
5	UE	1.07	8/3840~(0.2%)	0.88	6/5208~(0.1%)
6	UF	1.03	4/2538~(0.2%)	0.84	5/3405~(0.1%)
7	UG	1.60	70/4302~(1.6%)	1.11	26/5805~(0.4%)
8	UH	0.39	0/2703	0.68	11/3703~(0.3%)
9	UI	0.50	0/861	0.80	2/1156~(0.2%)
10	UJ	0.85	11/6903~(0.2%)	0.75	14/9474~(0.1%)
11	UK	1.26	14/2042~(0.7%)	0.96	1/2704~(0.0%)
12	UL	0.76	2/6851~(0.0%)	0.79	6/9246~(0.1%)
13	UM	0.71	5/6058~(0.1%)	0.80	6/8201~(0.1%)
14	UN	1.22	8/1231~(0.6%)	0.93	6/1661~(0.4%)
15	UO	1.10	12/3993~(0.3%)	0.90	10/5413~(0.2%)
16	UP	0.56	0/499	0.84	0/659
17	UQ	0.96	10/6794~(0.1%)	0.86	12/9203~(0.1%)
18	UR	1.50	36/3875~(0.9%)	1.02	17/5254~(0.3%)
19	US	0.61	0/3736	0.75	7/5086~(0.1%)
20	UT	0.28	0/11085	0.52	0/15445
21	UU	1.49	68/6815~(1.0%)	0.98	17/9213~(0.2%)
22	UV	0.50	0/8933	0.60	3/12081~(0.0%)
23	UX	1.50	16/1418~(1.1%)	1.07	5/1906~(0.3%)
24	UZ	0.70	1/2041~(0.0%)	0.74	1/2745~(0.0%)
25	CA	1.43	14/1917~(0.7%)	1.00	6/2588~(0.2%)
25	CB	0.73	0/1815	0.77	1/2448~(0.0%)
26	CD	0.96	3/3041~(0.1%)	0.85	7/4098~(0.2%)
27	CE	0.88	4/3012~(0.1%)	0.79	0/4091
28	CF	1.33	6/944~(0.6%)	0.97	5/1284~(0.4%)
28	CG	0.93	0/941	1.00	$\overline{5/1281}~(0.4\%)$
29	CH	0.61	1/3705~(0.0%)	0.68	1/4983~(0.0%)
30	CI	1.84	39/1559~(2.5%)	1.21	19/2097~(0.9%)



ЪД-1		I	Bond lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
31	CJ	1.36	21/2337~(0.9%)	1.04	13/3148~(0.4%)	
32	CK	1.06	2/1685~(0.1%)	0.98	6/2261~(0.3%)	
33	CL	1.18	27/6471~(0.4%)	0.92	19/8708~(0.2%)	
34	CM	0.85	0/2832	0.78	3/3825~(0.1%)	
35	CN	0.44	0/1934	0.59	1/2604~(0.0%)	
36	JA	0.48	0/5994	0.65	1/8139~(0.0%)	
36	JB	0.30	0/4128	0.57	0/5747	
37	JC	0.51	0/2908	0.71	1/3938~(0.0%)	
38	JE	0.55	0/1139	0.75	2/1512~(0.1%)	
39	$_{\mathrm{JF}}$	0.51	0/1727	0.70	1/2329~(0.0%)	
39	JG	0.82	0/1828	0.83	3/2470~(0.1%)	
40	JH	0.24	0/1293	0.37	0/1801	
41	JJ	0.65	1/1475~(0.1%)	0.77	4/1987~(0.2%)	
42	JK	0.49	0/342	0.71	1/462~(0.2%)	
43	JM	1.02	2/1156~(0.2%)	0.88	2/1536~(0.1%)	
44	JN	1.15	4/1435~(0.3%)	0.96	4/1907~(0.2%)	
45	JO	1.01	3/1961~(0.2%)	0.89	3/2631~(0.1%)	
46	JP	1.64	70/3802~(1.8%)	1.06	17/5118~(0.3%)	
47	JQ	0.41	0/385	0.57	0/529	
48	DA	1.00	2/1937~(0.1%)	0.90	2/2593~(0.1%)	
49	DE	0.46	0/1985	0.63	1/2675~(0.0%)	
50	DF	1.23	4/1690~(0.2%)	0.93	7/2285~(0.3%)	
51	DG	0.45	0/1779	0.62	0/2379	
52	DH	0.58	0/1502	0.74	2/2023~(0.1%)	
53	DI	0.46	0/1422	0.63	1/1899~(0.1%)	
54	DJ	1.14	5/1450~(0.3%)	0.92	1/1941~(0.1%)	
55	DL	0.40	0/1155	0.60	0/1557	
56	DN	0.82	0/1215	0.70	1/1638~(0.1%)	
57	DO	0.98	0/892	0.79	0/1202	
58	DQ	1.70	18/990~(1.8%)	1.04	2/1335~(0.1%)	
59	DS	0.31	0/513	0.59	0/711	
60	DW	1.18	3/1038~(0.3%)	0.93	1/1395~(0.1%)	
61	DX	1.27	1/798~(0.1%)	0.99	2/1065~(0.2%)	
62	DY	0.60	0/780	0.88	2/1049~(0.2%)	
63	Db	0.91	0/620	0.84	2/838~(0.2%)	
64	Dc	1.26	2/499~(0.4%)	1.05	2/670~(0.3%)	
65	D2	2.24	$658/12457~\overline{(5.3\%)}$	1.69	$374/19407~(\overline{1.9\%})$	
66	D3	1.84	889/28553~(3.1%)	1.49	518/44437~(1.2%)	
67	D4	2.61	329/4142~(7.9%)	1.84	155/6435~(2.4%)	
All	All	1.26	2498/230772~(1.1%)	1.04	$1402/321696~(0.4\overline{\%})$	

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



Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	4
4	UD	0	7
5	UE	0	1
6	UF	0	3
7	UG	0	4
10	UJ	0	3
12	UL	0	4
13	UM	0	2
14	UN	0	1
15	UO	0	1
17	UQ	0	4
18	UR	0	3
20	UT	0	7
21	UU	0	4
23	UX	0	1
26	CD	0	1
27	CE	0	1
30	CI	0	1
31	CJ	0	2
32	CK	0	1
34	CM	0	1
36	JA	0	1
36	JB	0	3
37	JC	0	2
38	JE	0	2
43	JM	0	1
44	JN	0	1
46	JP	0	4
48	DA	0	3
49	DE	0	1
52	DH	0	1
58	DQ	0	2
59	DS	0	1
60	DW	0	1
61	DX	0	3
All	All	0	82

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.

All (2498) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	CL	1081	SER	CA-CB	-16.22	1.28	1.52



001111	naca jion	i previe	ius puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	280	А	N9-C4	-13.97	1.29	1.37
67	D4	61	G	C5-C4	-12.91	1.29	1.38
66	D3	584	С	N1-C6	-12.87	1.29	1.37
67	D4	61	G	N7-C5	-12.51	1.31	1.39
65	D2	305	А	N9-C4	-12.39	1.30	1.37
13	UM	443	PRO	CG-CD	-12.23	1.10	1.50
65	D2	233	G	N9-C4	-11.98	1.28	1.38
7	UG	154	CYS	CB-SG	-11.87	1.62	1.82
65	D2	341	G	N7-C5	-11.84	1.32	1.39
66	D3	1606	С	N1-C6	-11.78	1.30	1.37
65	D2	280	А	N3-C4	-11.68	1.27	1.34
11	UK	223	GLU	CB-CG	-11.46	1.30	1.52
66	D3	1525	А	N9-C4	-11.45	1.30	1.37
67	D4	30	А	N7-C5	-11.36	1.32	1.39
67	D4	62	С	C4-C5	-11.31	1.33	1.43
65	D2	298	А	C5-C4	-11.29	1.30	1.38
66	D3	1603	U	N1-C2	-11.24	1.28	1.38
66	D3	1593	А	N9-C4	-11.23	1.31	1.37
18	UR	408	CYS	CB-SG	-11.18	1.63	1.82
65	D2	387	С	N3-C4	-11.13	1.26	1.33
66	D3	1166	А	N9-C4	-11.05	1.31	1.37
65	D2	473	А	N9-C4	-11.01	1.31	1.37
66	D3	1482	C	N1-C6	-11.00	1.30	1.37
66	D3	6	G	C5-C4	-10.98	1.30	1.38
67	D4	85	G	C5-C4	-10.93	1.30	1.38
66	D3	554	С	N1-C6	-10.88	1.30	1.37
65	D2	338	A	N3-C4	-10.78	1.28	1.34
66	D3	1525	A	C5-C4	-10.78	1.31	1.38
67	D4	331	A	N9-C4	-10.77	1.31	1.37
65	D2	233	G	N7-C5	-10.76	1.32	1.39
66	D3	1618	С	N1-C6	-10.76	1.30	1.37
67	D4	60	A	N3-C4	-10.70	1.28	1.34
65	D2	387	С	N1-C6	-10.67	1.30	1.37
67	D4	22	A	N9-C4	-10.62	1.31	1.37
65	D2	291	G	C5-C4	-10.58	1.30	1.38
66	D3	1596	С	N1-C6	-10.50	1.30	1.37
65	D2	473	A	C5-C4	-10.47	1.31	1.38
67	D4	22	A	N3-C4	-10.40	1.28	1.34
66	D3	590	C	N3-C4	-10.40	1.26	1.33
67	D4	54	C	N1-C6	-10.34	1.30	1.37
65	D2	293	U	N1-C2	-10.33	1.29	1.38
65	D2	296	C	N1-C6	-10.32	1.30	1.37



Continued fr	om previous	page

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	333	G	C5-C4	-10.30	1.31	1.38
66	D3	1604	U	N1-C2	-10.19	1.29	1.38
65	D2	309	А	N3-C4	-10.15	1.28	1.34
11	UK	223	GLU	CG-CD	-10.13	1.36	1.51
66	D3	1610	G	C6-N1	-10.13	1.32	1.39
66	D3	1604	U	C2-N3	-10.12	1.30	1.37
65	D2	301	U	N1-C2	-10.10	1.29	1.38
1	UA	617	VAL	CB-CG2	-10.09	1.31	1.52
65	D2	312	U	N3-C4	-9.97	1.29	1.38
66	D3	1584	G	N3-C4	-9.97	1.28	1.35
65	D2	311	С	N3-C4	-9.96	1.26	1.33
66	D3	1069	А	N7-C5	-9.90	1.33	1.39
46	JP	356	TYR	CE1-CZ	-9.88	1.25	1.38
65	D2	387	С	C4-C5	-9.89	1.35	1.43
65	D2	474	А	N3-C4	-9.88	1.28	1.34
66	D3	1163	А	N9-C4	-9.86	1.31	1.37
67	D4	62	С	N1-C6	-9.86	1.31	1.37
66	D3	1465	С	N1-C6	-9.83	1.31	1.37
67	D4	60	A	C6-N1	-9.83	1.28	1.35
67	D4	30	А	C5-C4	-9.81	1.31	1.38
65	D2	310	U	C2-N3	-9.80	1.30	1.37
66	D3	1158	С	N1-C6	-9.80	1.31	1.37
66	D3	564	G	N9-C4	-9.79	1.30	1.38
65	D2	380	A	N9-C4	-9.77	1.31	1.37
67	D4	26	C	N3-C4	-9.71	1.27	1.33
65	D2	398	А	N9-C4	-9.71	1.32	1.37
66	D3	1607	G	C5-C4	-9.69	1.31	1.38
66	D3	1585	U	C4-C5	-9.66	1.34	1.43
66	D3	565	С	N1-C6	-9.65	1.31	1.37
67	D4	61	G	N1-C2	-9.65	1.30	1.37
67	D4	85	G	N1-C2	-9.60	1.30	1.37
66	D3	572	С	N1-C6	-9.60	1.31	1.37
65	D2	299	G	C5-C4	-9.59	1.31	1.38
1	UA	102	VAL	CB-CG2	-9.56	1.32	1.52
66	D3	1610	G	N1-C2	-9.54	1.30	1.37
65	D2	295	А	N7-C5	-9.54	1.33	1.39
66	D3	550	A	N9-C4	-9.52	1.32	1.37
65	D2	275	A	N7-C5	-9.52	1.33	1.39
67	D4	57	A	N3-C4	-9.48	1.29	1.34
65	D2	143	A	N9-C4	-9.48	1.32	1.37
66	D3	590	C	N1-C6	-9.47	1.31	1.37
65	D2	298	A	N9-C4	-9.46	1.32	1.37



OOnu	nucu jion	i previe	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	291	G	N1-C2	-9.45	1.30	1.37
66	D3	1046	G	C5-C4	-9.41	1.31	1.38
66	D3	1605	G	C6-N1	-9.39	1.32	1.39
65	D2	386	А	N7-C5	-9.37	1.33	1.39
66	D3	1607	G	N3-C4	-9.37	1.28	1.35
66	D3	573	С	N1-C6	-9.36	1.31	1.37
67	D4	28	А	C5-C4	-9.35	1.32	1.38
66	D3	592	А	N9-C4	-9.34	1.32	1.37
65	D2	333	G	C2-N3	-9.34	1.25	1.32
67	D4	55	А	N7-C5	-9.31	1.33	1.39
65	D2	164	G	C5-C4	-9.30	1.31	1.38
65	D2	289	U	N1-C2	-9.29	1.30	1.38
65	D2	282	G	C5-C4	-9.29	1.31	1.38
65	D2	338	А	C6-N1	-9.28	1.29	1.35
67	D4	75	С	N1-C2	-9.27	1.30	1.40
66	D3	555	А	N9-C4	-9.26	1.32	1.37
65	D2	287	G	C5-C4	-9.26	1.31	1.38
65	D2	233	G	C5-C6	-9.24	1.33	1.42
65	D2	86	С	N1-C6	-9.24	1.31	1.37
65	D2	311	С	N1-C6	-9.22	1.31	1.37
67	D4	61	G	N9-C8	-9.22	1.31	1.37
65	D2	389	U	N1-C2	-9.19	1.30	1.38
67	D4	63	С	N3-C4	-9.16	1.27	1.33
66	D3	1599	С	N1-C6	-9.16	1.31	1.37
67	D4	330	A	N7-C5	-9.15	1.33	1.39
66	D3	1604	U	N3-C4	-9.13	1.30	1.38
67	D4	32	G	N1-C2	-9.13	1.30	1.37
67	D4	73	A	N9-C4	-9.13	1.32	1.37
65	D2	309	A	C6-N1	-9.13	1.29	1.35
67	D4	32	G	C5-C4	-9.13	1.31	1.38
65	D2	336	G	C5-C4	-9.12	1.31	1.38
46	JP	351	VAL	CB-CG1	-9.11	1.33	1.52
66	D3	1490	C	N1-C6	-9.11	1.31	1.37
1	UA	593	VAL	CB-CG2	-9.09	1.33	1.52
67	D4	61	G	C5-C6	-9.07	1.33	1.42
65	D2	282	G	N9-C8	-9.07	1.31	1.37
67	D4	70	U	C2-N3	-9.07	1.31	1.37
58	DQ	97	VAL	CB-CG2	-9.07	1.33	1.52
66	D3	1590	G	N7-C5	-9.05	1.33	1.39
66	D3	1602		N1-C6	-9.04	1.31	1.37
67	D4	60	A	N7-C5	-9.04	1.33	1.39
1 66	D3	559	$\mid C$	⊢ N1-C6	-9.03	1.31	1.37



001000	naca jion	" proore	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1527	С	N1-C6	-9.02	1.31	1.37
67	D4	73	A	N7-C5	-9.02	1.33	1.39
67	D4	326	U	C2-N3	-9.00	1.31	1.37
65	D2	341	G	C5-C6	-8.99	1.33	1.42
65	D2	291	G	C6-N1	-8.98	1.33	1.39
67	D4	27	U	N3-C4	-8.96	1.30	1.38
65	D2	291	G	N9-C8	-8.95	1.31	1.37
23	UX	13	VAL	CB-CG2	-8.94	1.34	1.52
65	D2	298	А	N3-C4	-8.94	1.29	1.34
65	D2	389	U	C2-N3	-8.94	1.31	1.37
65	D2	269	G	C6-N1	-8.89	1.33	1.39
67	D4	57	А	N9-C4	-8.88	1.32	1.37
66	D3	1483	А	C5-C6	-8.86	1.33	1.41
67	D4	26	С	N1-C6	-8.84	1.31	1.37
67	D4	65	С	N3-C4	-8.82	1.27	1.33
65	D2	309	А	C5-C4	-8.81	1.32	1.38
65	D2	237	А	C5-C4	-8.78	1.32	1.38
66	D3	6	G	N9-C8	-8.78	1.31	1.37
21	UU	443	TRP	CB-CG	-8.77	1.34	1.50
66	D3	10	G	N7-C5	-8.77	1.33	1.39
65	D2	336	G	N1-C2	-8.77	1.30	1.37
66	D3	1158	С	C4-C5	-8.77	1.35	1.43
66	D3	887	А	N9-C4	-8.74	1.32	1.37
65	D2	344	U	N1-C2	-8.73	1.30	1.38
65	D2	312	U	C2-N3	-8.72	1.31	1.37
65	D2	94	A	N9-C4	-8.72	1.32	1.37
65	D2	299	G	N1-C2	-8.72	1.30	1.37
67	D4	60	А	C5-C4	-8.71	1.32	1.38
67	D4	21	С	N1-C6	-8.71	1.31	1.37
66	D3	1524	А	N9-C4	-8.70	1.32	1.37
65	D2	301	U	C4-C5	-8.69	1.35	1.43
67	D4	27	U	C2-N3	-8.69	1.31	1.37
7	UG	159	TYR	CE1-CZ	-8.68	1.27	1.38
66	D3	1615	С	N1-C6	-8.67	1.31	1.37
65	D2	474	A	N9-C4	-8.67	1.32	1.37
28	CF	91	CYS	CB-SG	-8.65	1.67	1.82
65	D2	288	G	N7-C5	-8.65	1.34	1.39
66	D3	$1\overline{600}$	A	N7-C5	-8.65	1.34	1.39
67	D4	59	G	N3-C4	-8.64	1.29	1.35
66	D3	1047	G	N9-C8	-8.63	1.31	1.37
65	D2	323	A	C5-C6	-8.61	1.33	1.41
67	D4	69	A	N9-C4	-8.60	1.32	1.37



001000	naca jion	" preeve	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
64	Dc	12	VAL	CB-CG1	-8.59	1.34	1.52
66	D3	1607	G	N7-C5	-8.58	1.34	1.39
65	D2	309	А	N7-C5	-8.58	1.34	1.39
7	UG	216	TYR	CD2-CE2	-8.56	1.26	1.39
65	D2	234	А	N9-C4	-8.55	1.32	1.37
65	D2	472	А	N9-C4	-8.54	1.32	1.37
65	D2	474	А	C5-C6	-8.50	1.33	1.41
65	D2	386	А	C5-C4	-8.49	1.32	1.38
66	D3	557	G	N7-C5	-8.47	1.34	1.39
66	D3	1586	A	C5-C4	-8.47	1.32	1.38
30	CI	87	VAL	CB-CG2	-8.47	1.35	1.52
65	D2	240	С	N3-C4	-8.46	1.28	1.33
65	D2	291	G	N7-C5	-8.45	1.34	1.39
66	D3	1584	G	C5-C4	-8.45	1.32	1.38
66	D3	-1	G	N7-C5	-8.45	1.34	1.39
65	D2	391	С	C4-C5	-8.44	1.36	1.43
66	D3	1068	С	N1-C6	-8.43	1.32	1.37
65	D2	289	U	C2-N3	-8.40	1.31	1.37
30	CI	32	VAL	CB-CG1	-8.40	1.35	1.52
67	D4	63	С	N1-C2	-8.40	1.31	1.40
7	UG	168	VAL	CB-CG2	-8.40	1.35	1.52
66	D3	1605	G	N9-C8	-8.39	1.31	1.37
67	D4	32	G	C6-N1	-8.39	1.33	1.39
66	D3	1490	С	N3-C4	-8.37	1.28	1.33
66	D3	489	С	N1-C6	-8.37	1.32	1.37
65	D2	298	А	N7-C5	-8.36	1.34	1.39
66	D3	1584	G	N9-C4	-8.36	1.31	1.38
67	D4	64	A	C5-C4	-8.36	1.32	1.38
67	D4	63	С	C4-C5	-8.34	1.36	1.43
66	D3	6	G	N7-C5	-8.34	1.34	1.39
65	D2	306	G	C5-C4	-8.34	1.32	1.38
65	D2	388	С	N1-C6	-8.32	1.32	1.37
66	D3	1581	С	N1-C6	-8.32	1.32	1.37
66	D3	562	G	C5-C4	-8.29	1.32	1.38
67	D4	62	С	C5-C6	-8.29	1.27	1.34
67	D4	34	A	N9-C4	-8.28	1.32	1.37
65	D2	290	G	N7-C5	-8.28	1.34	1.39
66	D3	497	G	C5-C4	-8.28	1.32	1.38
67	D4	85	G	N7-C5	-8.27	1.34	1.39
66	D3	1465	C	N3-C4	-8.25	1.28	1.33
66	D3	1492	A	N7-C5	-8.25	1.34	1.39
18	UR	298	CYS	CB-SG	-8.25	1.68	$1.8\overline{2}$



001000	nucu jion	i precie	rus puye.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	-4	А	N9-C4	-8.24	1.32	1.37
67	D4	58	А	C5-C4	-8.24	1.32	1.38
67	D4	329	С	N1-C2	-8.24	1.31	1.40
67	D4	29	U	C2-N3	-8.22	1.31	1.37
65	D2	292	А	N7-C5	-8.22	1.34	1.39
66	D3	1614	А	N3-C4	-8.22	1.29	1.34
65	D2	282	G	N7-C5	-8.22	1.34	1.39
66	D3	1586	А	N7-C5	-8.22	1.34	1.39
65	D2	306	G	C2-N3	-8.21	1.26	1.32
66	D3	1490	С	C2-N3	-8.21	1.29	1.35
65	D2	237	А	N7-C5	-8.20	1.34	1.39
66	D3	1166	А	N3-C4	-8.20	1.29	1.34
67	D4	83	А	N9-C4	-8.19	1.32	1.37
67	D4	61	G	C8-N7	-8.19	1.26	1.30
65	D2	307	С	C4-C5	-8.18	1.36	1.43
66	D3	953	G	C5-C4	-8.18	1.32	1.38
66	D3	1586	A	C6-N1	-8.17	1.29	1.35
67	D4	33	A	C5-C4	-8.17	1.33	1.38
46	JP	59	VAL	CB-CG1	-8.16	1.35	1.52
1	UA	393	VAL	CB-CG1	-8.16	1.35	1.52
67	D4	64	A	N9-C8	-8.15	1.31	1.37
66	D3	567	A	N3-C4	-8.14	1.29	1.34
67	D4	326	U	N3-C4	-8.13	1.31	1.38
65	D2	338	A	N9-C4	-8.13	1.32	1.37
65	D2	283	A	N9-C4	-8.13	1.32	1.37
66	D3	955	A	C5-C6	-8.13	1.33	1.41
65	D2	161	A	N3-C4	-8.12	1.29	1.34
65	D2	299	G	C6-N1	-8.12	1.33	1.39
65	D2	92	C	N1-C6	-8.10	1.32	1.37
65	D2	335	G	C5-C4	-8.10	1.32	1.38
1	UA	585	TYR	CD1-CE1	-8.10	1.27	1.39
67	D4	75	C	N3-C4	-8.10	1.28	1.33
66	D3	1605	G	C5-C4	-8.09	1.32	1.38
65	D2	336	G	N7-C5	-8.08	1.34	1.39
67	D4	30	A	C5-C6	-8.08	1.33	1.41
67	D4	25	U	C4-C5	-8.07	1.36	1.43
21		323	VAL	CB-CG1	-8.07	1.35	1.52
66	D3	1613		C4-C5	-8.07	1.36	1.43
65	D2	341	G	<u>C8-N7</u>	-8.06	1.26	1.30
67	D4	39		NI-C6	-8.05	1.32	1.37
65	D2	280	A	N7-C5	-8.05	1.34	1.39
1 66	D3	955	I A	N7-C5	-8.05	1.34	1.39



001000	naca ji on	" proove	we page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1593	A	N7-C5	-8.05	1.34	1.39
67	D4	328	A	C5-C4	-8.04	1.33	1.38
67	D4	85	G	C6-N1	-8.03	1.33	1.39
66	D3	1590	G	C6-N1	-8.02	1.33	1.39
65	D2	307	С	N1-C2	-8.01	1.32	1.40
66	D3	1599	С	C4-C5	-8.01	1.36	1.43
65	D2	88	U	N1-C2	-8.01	1.31	1.38
65	D2	233	G	N3-C4	-8.01	1.29	1.35
65	D2	296	С	N3-C4	-8.00	1.28	1.33
66	D3	1607	G	N1-C2	-8.00	1.31	1.37
31	CJ	141	VAL	CB-CG1	-7.99	1.36	1.52
65	D2	241	U	N1-C2	-7.99	1.31	1.38
66	D3	10	G	C5-C4	-7.99	1.32	1.38
67	D4	329	С	N1-C6	-7.99	1.32	1.37
65	D2	292	А	N9-C4	-7.98	1.33	1.37
66	D3	-1	G	C5-C4	-7.96	1.32	1.38
65	D2	273	G	C6-N1	-7.96	1.33	1.39
66	D3	942	G	C5-C4	-7.96	1.32	1.38
66	D3	1633	А	N3-C4	-7.95	1.30	1.34
65	D2	248	G	C5-C4	-7.95	1.32	1.38
66	D3	8	U	C2-N3	-7.94	1.32	1.37
66	D3	478	А	N9-C4	-7.94	1.33	1.37
66	D3	1484	G	C5-C4	-7.94	1.32	1.38
65	D2	242	С	N3-C4	-7.94	1.28	1.33
65	D2	474	A	C6-N1	-7.94	1.29	1.35
66	D3	1488	G	N1-C2	-7.94	1.31	1.37
65	D2	477	G	N3-C4	-7.93	1.29	1.35
67	D4	21	С	C4-C5	-7.93	1.36	1.43
66	D3	951	A	N9-C4	-7.93	1.33	1.37
65	D2	300	С	N1-C6	-7.92	1.32	1.37
66	D3	1609	U	C4-C5	-7.92	1.36	1.43
65	D2	333	G	N7-C5	-7.91	1.34	1.39
58	DQ	90	VAL	CB-CG1	-7.91	1.36	1.52
65	D2	474	A	C5-C4	-7.90	1.33	1.38
67	D4	54	С	C4-C5	-7.90	1.36	1.43
58	DQ	69	VAL	CB-CG1	-7.89	1.36	1.52
65	D2	467	A	N9-C4	-7.89	1.33	1.37
65	D2	340	U	C4-C5	-7.89	1.36	1.43
65	D2	482	A	C5-C4	-7.89	1.33	1.38
65	D2	401	A	N7-C5	-7.89	1.34	1.39
66	D3	1592	A	N7-C5	-7.89	1.34	1.39
66	D3	1482	C	N3-C4	-7.88	1.28	1.33



001000	nucu jion	" precede	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CA	314	CYS	CB-SG	-7.88	1.68	1.82
67	D4	34	A	C5-C4	-7.88	1.33	1.38
66	D3	1069	А	C5-C6	-7.87	1.33	1.41
65	D2	278	G	C5-C4	-7.86	1.32	1.38
65	D2	476	А	N9-C4	-7.86	1.33	1.37
67	D4	67	G	C5-C4	-7.86	1.32	1.38
67	D4	75	С	C2-N3	-7.86	1.29	1.35
46	JP	308	VAL	CB-CG2	-7.85	1.36	1.52
65	D2	397	А	N7-C5	-7.85	1.34	1.39
66	D3	1466	G	N7-C5	-7.83	1.34	1.39
7	UG	206	VAL	CB-CG2	-7.82	1.36	1.52
66	D3	1605	G	N3-C4	-7.82	1.29	1.35
66	D3	500	С	N1-C2	-7.82	1.32	1.40
67	D4	82	G	C5-C4	-7.81	1.32	1.38
67	D4	26	С	N1-C2	-7.80	1.32	1.40
1	UA	263	VAL	CB-CG1	-7.80	1.36	1.52
66	D3	931	С	N1-C6	-7.80	1.32	1.37
66	D3	1485	C	N1-C6	-7.80	1.32	1.37
65	D2	269	G	N1-C2	-7.79	1.31	1.37
65	D2	272	A	N9-C4	-7.79	1.33	1.37
67	D4	331	A	N7-C5	-7.79	1.34	1.39
66	D3	1158	С	N3-C4	-7.79	1.28	1.33
66	D3	5	U	C2-N3	-7.78	1.32	1.37
66	D3	590	C	C2-N3	-7.78	1.29	1.35
66	D3	1586	A	N3-C4	-7.78	1.30	1.34
60	DW	25	VAL	CB-CG2	-7.78	1.36	1.52
66	D3	1074	G	N7-C5	-7.78	1.34	1.39
67	D4	18	G	C5-C4	-7.78	1.32	1.38
67	D4	68	A	N9-C4	-7.78	1.33	1.37
67	D4	85	G	N3-C4	-7.78	1.30	1.35
7	UG	256	VAL	CB-CG1	-7.77	1.36	1.52
67	D4	329	C	C4-C5	-7.77	1.36	1.43
21	UU	453	TRP	CB-CG	-7.76	1.36	1.50
65	D2	340	U	N1-C2	-7.76	1.31	1.38
66	D3	1076	A	N9-C4	-7.75	1.33	1.37
66	D3	1525	A	N3-C4	-7.75	1.30	1.34
65	D2	244	U	C2-N3	-7.74	1.32	1.37
65	D2	277	C	N3-C4	-7.74	1.28	1.33
65	D2	305	A	C6-N6	-7.74	1.27	1.33
65	D2	333	G	N9-C4	-7.73	1.31	1.38
65	D2	291	G	C2-N3	-7.72	1.26	1.32
66	D3	1037		C4-C5	-7.72	1.36	1.43



001000	naca jion	" procee	a page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	518	VAL	CB-CG2	-7.72	1.36	1.52
66	D3	1162	С	C4-C5	-7.72	1.36	1.43
66	D3	1584	G	C2-N3	-7.71	1.26	1.32
66	D3	551	G	C5-C4	-7.70	1.32	1.38
66	D3	1610	G	C5-C4	-7.70	1.32	1.38
66	D3	1081	А	N9-C4	-7.70	1.33	1.37
66	D3	887	А	N3-C4	-7.70	1.30	1.34
67	D4	325	С	N1-C6	-7.70	1.32	1.37
66	D3	545	А	N3-C4	-7.69	1.30	1.34
66	D3	937	С	N3-C4	-7.69	1.28	1.33
10	UJ	199	CYS	CB-SG	-7.69	1.69	1.82
65	D2	392	U	N1-C2	-7.69	1.31	1.38
65	D2	290	G	N1-C2	-7.69	1.31	1.37
66	D3	1047	G	C5-C4	-7.69	1.32	1.38
67	D4	77	U	C2-N3	-7.68	1.32	1.37
65	D2	292	А	N9-C8	-7.67	1.31	1.37
65	D2	387	С	C2-N3	-7.67	1.29	1.35
65	D2	301	U	N1-C6	-7.67	1.31	1.38
65	D2	473	А	N3-C4	-7.67	1.30	1.34
65	D2	345	U	C2-N3	-7.67	1.32	1.37
66	D3	554	С	N3-C4	-7.67	1.28	1.33
66	D3	1046	G	N9-C8	-7.67	1.32	1.37
66	D3	1607	G	C6-N1	-7.67	1.34	1.39
67	D4	32	G	C2-N3	-7.66	1.26	1.32
67	D4	24	U	N1-C6	-7.65	1.31	1.38
67	D4	65	С	N1-C2	-7.65	1.32	1.40
67	D4	330	A	N9-C4	-7.64	1.33	1.37
23	UX	65	VAL	CB-CG2	-7.64	1.36	1.52
65	D2	380	A	C5-C4	-7.64	1.33	1.38
65	D2	390	C	N1-C6	-7.64	1.32	1.37
67	D4	64	A	N9-C4	-7.64	1.33	1.37
46	JP	343	TYR	CD2-CE2	-7.63	1.27	1.39
66	D3	1072	С	C4-C5	-7.63	1.36	1.43
21	UU	487	TYR	CD2-CE2	-7.63	1.27	1.39
65	D2	278	G	N1-C2	-7.63	1.31	1.37
65	D2	308	A	C5-C4	-7.63	1.33	1.38
65	D2	349	G	N3-C4	-7.62	1.30	1.35
66	D3	1162	C	N1-C6	-7.62	1.32	1.37
65	D2	274	C	N1-C2	-7.61	1.32	1.40
17	UQ	320	VAL	CB-CG2	-7.61	1.36	1.52
67	D4	34	A	N3-C4	-7.60	1.30	1.34
66	D3	489	C	N3-C4	-7.60	1.28	1.33



OOnu	nucu fron	i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	34	A	C5-C6	-7.60	1.34	1.41
66	D3	416	А	N9-C4	-7.60	1.33	1.37
65	D2	303	А	C6-N1	-7.59	1.30	1.35
66	D3	1593	А	C5-C4	-7.59	1.33	1.38
66	D3	1045	С	N3-C4	-7.58	1.28	1.33
67	D4	331	А	N3-C4	-7.58	1.30	1.34
67	D4	55	А	N9-C8	-7.58	1.31	1.37
65	D2	292	А	C5-C4	-7.57	1.33	1.38
66	D3	1633	А	C5-C4	-7.56	1.33	1.38
67	D4	73	А	N3-C4	-7.56	1.30	1.34
67	D4	71	С	N1-C2	-7.56	1.32	1.40
1	UA	522	SER	CA-CB	-7.56	1.41	1.52
66	D3	590	С	C4-C5	-7.56	1.36	1.43
66	D3	1485	С	C4-C5	-7.56	1.36	1.43
46	JP	289	TYR	CD2-CE2	-7.55	1.28	1.39
30	CI	150	VAL	CB-CG1	-7.55	1.36	1.52
65	D2	296	С	C4-C5	-7.55	1.36	1.43
65	D2	245	С	N1-C6	-7.54	1.32	1.37
7	UG	203	TYR	CD2-CE2	-7.54	1.28	1.39
65	D2	339	A	N7-C5	-7.54	1.34	1.39
66	D3	1043	А	N7-C5	-7.53	1.34	1.39
65	D2	334	G	N7-C5	-7.53	1.34	1.39
65	D2	311	C	C2-N3	-7.53	1.29	1.35
65	D2	300	C	N1-C2	-7.53	1.32	1.40
67	D4	64	A	N7-C5	-7.53	1.34	1.39
18	UR	242	ASN	CB-CG	-7.52	1.33	1.51
66	D3	552	G	N7-C5	-7.51	1.34	1.39
30	CI	136	VAL	CB-CG1	-7.51	1.37	1.52
66	D3	550	A	N3-C4	-7.51	1.30	1.34
7	UG	384	VAL	CB-CG2	-7.51	1.37	1.52
66	D3	500	C	C2-N3	-7.50	1.29	1.35
66	D3	867	G	N7-C5	-7.50	1.34	1.39
66	D3	487	G	C5-C4	-7.50	1.33	1.38
65	D2	335	G	N9-C4	-7.49	1.31	1.38
66	D3	942	G	N7-C5	-7.49	1.34	1.39
66	D3	1592	A	C5-C4	-7.49	1.33	1.38
65	D2	406	U	N1-C2	-7.48	1.31	1.38
33	CL	919	VAL	CB-CG1	-7.48	1.37	1.52
67	D4	328	A	C6-N1	-7.48	1.30	1.35
46	JP	356	TYR	CG-CD2	-7.48	1.29	1.39
66	D3	1490	C	C4-C5	-7.47	1.36	1.43
30	CI	113	VAL	CB-CG1	-7.47	1.37	1.52



001111	nucu jion	" PICOUC	, as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	286	U	C2-N3	-7.47	1.32	1.37
65	D2	288	G	C5-C4	-7.47	1.33	1.38
66	D3	1157	А	N9-C4	-7.46	1.33	1.37
66	D3	1588	G	C5-C4	-7.46	1.33	1.38
66	D3	559	С	N1-C2	-7.46	1.32	1.40
65	D2	333	G	C5-C6	-7.45	1.34	1.42
66	D3	13	С	N1-C6	-7.45	1.32	1.37
67	D4	66	U	C2-N3	-7.44	1.32	1.37
66	D3	1613	U	N1-C2	-7.43	1.31	1.38
65	D2	86	С	C4-C5	-7.42	1.37	1.43
67	D4	34	А	N7-C5	-7.42	1.34	1.39
65	D2	273	G	N1-C2	-7.42	1.31	1.37
66	D3	1163	А	N3-C4	-7.42	1.30	1.34
65	D2	281	G	C5-C6	-7.42	1.34	1.42
65	D2	269	G	C5-C4	-7.42	1.33	1.38
65	D2	392	U	N1-C6	-7.42	1.31	1.38
66	D3	937	С	N1-C6	-7.42	1.32	1.37
64	Dc	28	VAL	CB-CG1	-7.42	1.37	1.52
67	D4	82	G	C6-N1	-7.42	1.34	1.39
65	D2	385	А	C6-N1	-7.41	1.30	1.35
66	D3	1633	А	C6-N1	-7.41	1.30	1.35
7	UG	268	VAL	CB-CG1	-7.40	1.37	1.52
65	D2	482	А	N3-C4	-7.40	1.30	1.34
65	D2	487	А	N7-C5	-7.39	1.34	1.39
65	D2	87	C	N1-C6	-7.39	1.32	1.37
65	D2	381	G	N3-C4	-7.39	1.30	1.35
65	D2	338	A	C5-C4	-7.39	1.33	1.38
67	D4	68	A	N7-C5	-7.39	1.34	1.39
65	D2	387	C	N1-C2	-7.38	1.32	1.40
65	D2	300	C	N3-C4	-7.38	1.28	1.33
21	UU	463	VAL	CB-CG2	-7.38	1.37	1.52
65	D2	388	C	N3-C4	-7.38	1.28	1.33
67	D4	22	A	C6-N1	-7.38	1.30	1.35
65	D2	320	A	C5-C4	-7.38	1.33	1.38
65	D2	471	C	N1-C6	-7.37	1.32	1.37
1	UA	266	VAL	CB-CG2	-7.37	1.37	1.52
21	UU	53	CYS	CB-SG	-7.37	1.69	1.82
7	UG	178	ASP	CB-CG	-7.36	1.36	1.51
65	D2	410	A	N9-C4	-7.35	1.33	1.37
46	JP	289	TYR	CD1-CE1	-7.35	1.28	1.39
65	D2	287	G	N1-C2	-7.34	1.31	1.37
66	D3	1635	A	C5-C4	-7.34	1.33	1.38



0011111	nucu jion	i previe	ius puye.	••			
Mol	Chain	Res	Type	Atoms	Ζ	Observed(A)	Ideal(Å)
65	D2	386	А	C5-C6	-7.34	1.34	1.41
66	D3	486	G	N3-C4	-7.34	1.30	1.35
66	D3	953	G	N7-C5	-7.34	1.34	1.39
1	UA	316	TRP	CB-CG	-7.33	1.37	1.50
66	D3	557	G	C5-C4	-7.33	1.33	1.38
65	D2	334	G	C5-C4	-7.33	1.33	1.38
66	D3	10	G	C5-C6	-7.32	1.35	1.42
66	D3	1604	U	C4-C5	-7.32	1.36	1.43
66	D3	589	C	N3-C4	-7.31	1.28	1.33
66	D3	930	A	N7-C5	-7.31	1.34	1.39
7	UG	177	TYR	CD2-CE2	-7.30	1.28	1.39
66	D3	490	С	N1-C6	-7.30	1.32	1.37
66	D3	497	G	N9-C4	-7.30	1.32	1.38
65	D2	397	A	C5-C6	-7.30	1.34	1.41
67	D4	72	С	N3-C4	-7.29	1.28	1.33
67	D4	84	U	C2-N3	-7.29	1.32	1.37
67	D4	329	С	N3-C4	-7.28	1.28	1.33
46	JP	308	VAL	CB-CG1	-7.28	1.37	1.52
58	DQ	7	VAL	CB-CG2	-7.28	1.37	1.52
65	D2	233	G	C2-N3	-7.28	1.26	1.32
66	D3	584	С	N3-C4	-7.26	1.28	1.33
18	UR	586	VAL	CB-CG2	-7.26	1.37	1.52
65	D2	234	A	N3-C4	-7.26	1.30	1.34
30	CI	32	VAL	CB-CG2	-7.25	1.37	1.52
66	D3	500	С	N3-C4	-7.25	1.28	1.33
65	D2	292	A	C5-C6	-7.25	1.34	1.41
67	D4	28	A	N7-C5	-7.25	1.34	1.39
65	D2	487	A	N3-C4	-7.25	1.30	1.34
67	D4	29	U	N3-C4	-7.25	1.31	1.38
46	JP	300	VAL	CB-CG1	-7.24	1.37	1.52
65	D2	388	С	C4-C5	-7.24	1.37	1.43
65	D2	472	A	C5-C4	-7.24	1.33	1.38
66	D3	489	С	C4-C5	-7.23	1.37	1.43
65	D2	293	U	C2-N3	-7.23	1.32	1.37
66	D3	952	A	N9-C4	-7.22	1.33	1.37
67	D4	55	A	C8-N7	-7.22	1.26	1.31
18	UR	582	GLU	CB-CG	-7.22	1.38	1.52
65	D2	310	U	N3-C4	-7.22	1.31	1.38
65	D2	234	A	N7-C5	-7.22	1.34	1.39
66	D3	-1	G	N3-C4	-7.21	1.30	1.35
66	D3	1042	G	C5-C4	-7.21	1.33	1.38
1	UA	530	VAL	CB-CG2	-7.20	1.37	1.52



OOnu		i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	UG	378	VAL	CB-CG2	-7.20	1.37	1.52
65	D2	293	U	N1-C6	-7.20	1.31	1.38
66	D3	1600	А	N9-C4	-7.20	1.33	1.37
14	UN	847	VAL	CB-CG2	-7.19	1.37	1.52
65	D2	306	G	N3-C4	-7.19	1.30	1.35
66	D3	552	G	C5-C4	-7.19	1.33	1.38
67	D4	25	U	C2-N3	-7.19	1.32	1.37
65	D2	246	G	C6-N1	-7.18	1.34	1.39
67	D4	31	G	C5-C4	-7.18	1.33	1.38
66	D3	1606	С	C4-C5	-7.18	1.37	1.43
66	D3	554	С	C2-N3	-7.17	1.30	1.35
67	D4	21	С	N1-C2	-7.17	1.32	1.40
66	D3	572	С	N1-C2	-7.17	1.32	1.40
66	D3	488	G	C5-C4	-7.17	1.33	1.38
66	D3	1634	С	N1-C6	-7.17	1.32	1.37
65	D2	305	А	N7-C5	-7.16	1.34	1.39
66	D3	1525	А	C6-N1	-7.16	1.30	1.35
1	UA	393	VAL	CB-CG2	-7.16	1.37	1.52
65	D2	306	G	N1-C2	-7.16	1.32	1.37
66	D3	497	G	N3-C4	-7.15	1.30	1.35
65	D2	474	A	N7-C5	-7.14	1.34	1.39
65	D2	235	A	N3-C4	-7.14	1.30	1.34
67	D4	63	C	N1-C6	-7.14	1.32	1.37
21	UU	487	TYR	CD1-CE1	-7.14	1.28	1.39
30	CI	47	TYR	CD2-CE2	-7.14	1.28	1.39
66	D3	569	C	C4-C5	-7.14	1.37	1.43
67	D4	79	G	N3-C4	-7.14	1.30	1.35
66	D3	477	A	N9-C4	-7.13	1.33	1.37
66	D3	567	A	C6-N1	-7.13	1.30	1.35
25	CA	172	TYR	CE1-CZ	-7.13	1.29	1.38
66	D3	498	G	N9-C8	-7.13	1.32	1.37
66	D3	572	C	C4-C5	-7.12	1.37	1.43
67	D4	322	A	N9-C4	-7.12	1.33	1.37
65	D2	266	U	C2-N3	-7.12	1.32	1.37
67	D4	86	A	N7-C5	-7.12	1.34	1.39
65	D2	274	C	C2-N3	-7.12	1.30	1.35
65	D2	273	G	C5-C4	-7.12	1.33	1.38
	UA	360	VAL	CB-CG2	-7.12	1.38	1.52
66	D3	574	G	C5-C4	-7.12	1.33	1.38
65	D2	278	G	N9-C8	-7.11	1.32	1.37
65	D2	303	A	C5-C6	-7.11	1.34	1.41
126	CD	34	VAL	ECB-CG1	-7.10	1.38	1.52



0011111	naca jion	i previe	ius puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	53	U	N1-C2	-7.10	1.32	1.38
65	D2	341	G	C5-C4	-7.10	1.33	1.38
67	D4	84	U	N3-C4	-7.10	1.32	1.38
66	D3	1043	А	N9-C4	-7.09	1.33	1.37
65	D2	458	А	N3-C4	-7.09	1.30	1.34
66	D3	1587	А	C5-C4	-7.09	1.33	1.38
67	D4	83	А	N7-C5	-7.09	1.34	1.39
66	D3	574	G	N9-C8	-7.09	1.32	1.37
66	D3	1174	С	C5-C6	-7.08	1.28	1.34
66	D3	1605	G	N1-C2	-7.08	1.32	1.37
4	UD	265	TRP	CB-CG	-7.08	1.37	1.50
17	UQ	318	GLU	CB-CG	-7.08	1.38	1.52
67	D4	32	G	N3-C4	-7.08	1.30	1.35
1	UA	89	VAL	CB-CG2	-7.08	1.38	1.52
1	UA	679	VAL	CB-CG1	-7.08	1.38	1.52
65	D2	409	С	N3-C4	-7.08	1.28	1.33
67	D4	85	G	C8-N7	-7.08	1.26	1.30
67	D4	325	C	C4-C5	-7.07	1.37	1.43
66	D3	1174	С	N1-C6	-7.07	1.32	1.37
67	D4	29	U	C4-C5	-7.07	1.37	1.43
46	JP	351	VAL	CB-CG2	-7.06	1.38	1.52
65	D2	400	С	N1-C2	-7.06	1.33	1.40
65	D2	296	C	N1-C2	-7.06	1.33	1.40
65	D2	411	A	N9-C4	-7.06	1.33	1.37
66	D3	1078	С	N1-C6	-7.06	1.32	1.37
67	D4	35	U	C2-N3	-7.06	1.32	1.37
65	D2	305	A	C6-N1	-7.06	1.30	1.35
66	D3	1071	U	C2-N3	-7.06	1.32	1.37
14	UN	879	ILE	CB-CG2	-7.05	1.30	1.52
66	D3	8	U	N3-C4	-7.05	1.32	1.38
66	D3	885	G	C6-N1	-7.05	1.34	1.39
66	D3	944	A	C5-C4	-7.05	1.33	1.38
65	D2	162	U	C2-N3	-7.04	1.32	1.37
66	D3	15	U	C2-N3	-7.04	1.32	1.37
66	D3	559	C	C4-C5	-7.04	1.37	1.43
7	UG	147	GLU	CB-CG	-7.04	1.38	1.52
67	D4	86	A	N9-C4	-7.04	1.33	1.37
66	D3	1588	G	N7-C5	-7.03	1.35	1.39
67	D4	84	U	N1-C2	-7.02	1.32	1.38
67	D4	85	G	N9-C8	-7.02	1.32	1.37
66	D3	1589	C	N3-C4	-7.01	1.29	1.33
66	D3	1590	G	C5-C4	-7.01	1.33	1.38



0011111	naca jion	i previe	rus puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1478	G	C6-N1	-7.00	1.34	1.39
67	D4	26	С	C2-N3	-7.00	1.30	1.35
66	D3	886	U	C2-N3	-7.00	1.32	1.37
66	D3	560	U	N1-C2	-7.00	1.32	1.38
66	D3	1073	G	N9-C8	-7.00	1.32	1.37
65	D2	273	G	N3-C4	-6.99	1.30	1.35
65	D2	386	А	C6-N1	-6.99	1.30	1.35
65	D2	392	U	C4-C5	-6.99	1.37	1.43
65	D2	296	С	C2-N3	-6.99	1.30	1.35
30	CI	103	VAL	CB-CG1	-6.98	1.38	1.52
66	D3	874	С	N1-C6	-6.98	1.32	1.37
65	D2	146	G	C2-N3	-6.98	1.27	1.32
66	D3	6	G	C5-C6	-6.98	1.35	1.42
67	D4	17	G	C5-C4	-6.98	1.33	1.38
28	CF	79	VAL	CB-CG2	-6.97	1.38	1.52
66	D3	552	G	C8-N7	-6.97	1.26	1.30
65	D2	383	G	C2-N3	-6.97	1.27	1.32
1	UA	585	TYR	CD2-CE2	-6.97	1.28	1.39
65	D2	336	G	C6-N1	-6.97	1.34	1.39
66	D3	477	А	N3-C4	-6.97	1.30	1.34
66	D3	1606	С	N3-C4	-6.97	1.29	1.33
7	UG	159	TYR	CD1-CE1	-6.96	1.28	1.39
66	D3	1483	А	N7-C5	-6.96	1.35	1.39
66	D3	548	G	C5-C4	-6.96	1.33	1.38
65	D2	279	A	N9-C4	-6.95	1.33	1.37
66	D3	1489	U	C4-C5	-6.95	1.37	1.43
66	D3	1590	G	C5-C6	-6.95	1.35	1.42
67	D4	55	A	C5-C6	-6.95	1.34	1.41
66	D3	1037	С	N1-C6	-6.94	1.32	1.37
66	D3	1607	G	N9-C8	-6.94	1.32	1.37
66	D3	635	A	N9-C4	-6.94	1.33	1.37
66	D3	1600	A	C6-N1	-6.94	1.30	1.35
67	D4	67	G	N7-C5	-6.93	1.35	1.39
67	D4	26	С	C4-C5	-6.93	1.37	1.43
21	UU	428	GLU	CB-CG	-6.93	1.39	1.52
65	D2	337	G	C5-C4	-6.93	1.33	1.38
1	UA	555	CYS	CB-SG	-6.92	1.70	1.82
65	D2	236	C	N1-C6	-6.92	1.32	1.37
66	D3	584	C	C4-C5	-6.92	1.37	1.43
66	D3	936	G	N9-C4	-6.92	1.32	1.38
67	D4	66	U	N1-C2	-6.92	1.32	1.38
5	UE	303	VAL	CB-CG1	-6.92	1.38	1.52



OOnu	nucu jion	i prevu	as page.	• • •			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	UU	487	TYR	CE1-CZ	-6.91	1.29	1.38
66	D3	553	G	N7-C5	-6.91	1.35	1.39
66	D3	1528	U	N1-C2	-6.91	1.32	1.38
67	D4	29	U	N1-C6	-6.90	1.31	1.38
65	D2	249	G	C5-C4	-6.90	1.33	1.38
21	UU	529	TYR	CD2-CE2	-6.89	1.29	1.39
67	D4	30	А	N9-C4	-6.89	1.33	1.37
66	D3	1607	G	C2-N3	-6.89	1.27	1.32
7	UG	134	VAL	CB-CG2	-6.89	1.38	1.52
65	D2	163	G	C5-C4	-6.89	1.33	1.38
66	D3	1047	G	N7-C5	-6.89	1.35	1.39
65	D2	244	U	N1-C2	-6.88	1.32	1.38
65	D2	402	G	C6-N1	-6.88	1.34	1.39
65	D2	164	G	N7-C5	-6.88	1.35	1.39
65	D2	162	U	N1-C6	-6.87	1.31	1.38
66	D3	1618	С	C4-C5	-6.87	1.37	1.43
67	D4	79	G	C5-C4	-6.87	1.33	1.38
7	UG	201	TYR	CD2-CE2	-6.87	1.29	1.39
13	UM	443	PRO	CB-CG	-6.87	1.15	1.50
18	UR	275	TYR	CD2-CE2	-6.87	1.29	1.39
65	D2	398	A	C6-N1	-6.86	1.30	1.35
1	UA	518	VAL	CB-CG1	-6.86	1.38	1.52
66	D3	1159	C	C4-C5	-6.85	1.37	1.43
65	D2	396	A	N9-C4	-6.85	1.33	1.37
7	UG	177	TYR	CE2-CZ	-6.84	1.29	1.38
1	UA	679	VAL	CB-CG2	-6.84	1.38	1.52
6	UF	7	TYR	CE1-CZ	-6.84	1.29	1.38
66	D3	545	A	C5-C4	-6.84	1.33	1.38
66	D3	13	C	N1-C2	-6.84	1.33	1.40
67	D4	30	A	N3-C4	-6.84	1.30	1.34
5	UE	454	GLU	CD-OE2	-6.83	1.18	1.25
65	D2	313	A	N7-C5	-6.83	1.35	1.39
66	D3	1609	U	C2-N3	-6.83	1.32	1.37
66	D3	557	G	C5-C6	-6.83	1.35	1.42
65	D2	283	A	N3-C4	-6.83	1.30	1.34
66	D3	1584	G	N1-C2	-6.83	1.32	1.37
65	D2	387	C	C5-C6	-6.83	1.28	1.34
66	D3	550	A	C5-C4	-6.83	1.33	1.38
67	D4	33	A	N9-C4	-6.83	1.33	1.37
66	D3	1492	A	C6-N1	-6.82	1.30	1.35
67	D4	34	A	N9-C8	-6.82	1.32	1.37
65	D2	245	$\mid C$	C4-C5	-6.82	1.37	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	421	ASN	CB-CG	-6.82	1.35	1.51
65	D2	243	A	C5-C4	-6.81	1.33	1.38
66	D3	555	A	C5-C4	-6.81	1.33	1.38
65	D2	290	G	C5-C4	-6.81	1.33	1.38
65	D2	482	A	C6-N1	-6.81	1.30	1.35
66	D3	1082	С	N3-C4	-6.80	1.29	1.33
21	UU	256	PHE	CB-CG	-6.80	1.39	1.51
46	JP	321	VAL	CB-CG2	-6.80	1.38	1.52
67	D4	69	А	N7-C5	-6.80	1.35	1.39
66	D3	1484	G	N9-C4	-6.79	1.32	1.38
66	D3	1167	G	N9-C4	-6.79	1.32	1.38
67	D4	333	U	N1-C2	-6.79	1.32	1.38
65	D2	235	А	C5-C4	-6.79	1.34	1.38
66	D3	7	G	C5-C4	-6.79	1.33	1.38
66	D3	956	С	C4-C5	-6.79	1.37	1.43
1	UA	82	VAL	CB-CG2	-6.78	1.38	1.52
66	D3	954	G	N9-C4	-6.78	1.32	1.38
67	D4	22	А	N7-C5	-6.78	1.35	1.39
65	D2	307	С	N1-C6	-6.78	1.33	1.37
21	UU	377	SER	CA-CB	-6.78	1.42	1.52
66	D3	1585	U	C4-O4	-6.78	1.18	1.23
65	D2	339	A	C5-C4	-6.78	1.34	1.38
65	D2	398	A	N3-C4	-6.78	1.30	1.34
65	D2	289	U	C4-C5	-6.77	1.37	1.43
66	D3	1586	A	C5-C6	-6.77	1.34	1.41
65	D2	237	A	N3-C4	-6.77	1.30	1.34
65	D2	298	A	N9-C8	-6.77	1.32	1.37
66	D3	1524	A	N3-C4	-6.77	1.30	1.34
67	D4	25	U	N1-C2	-6.77	1.32	1.38
67	D4	54	С	N1-C2	-6.77	1.33	1.40
23	UX	65	VAL	CB-CG1	-6.76	1.38	1.52
24	UZ	103	VAL	CB-CG2	-6.76	1.38	1.52
65	D2	160	C	N1-C6	-6.76	1.33	1.37
65	D2	292	A	P-O5'	-6.76	1.52	1.59
1	UA	37	VAL	CB-CG1	-6.76	1.38	1.52
1	UA	14	VAL	CB-CG1	-6.75	1.38	1.52
65	D2	237	A	C6-N1	-6.75	1.30	1.35
66	D3	551	G	N9-C4	-6.75	1.32	1.38
67	D4	69	A	C5-C4	-6.75	1.34	1.38
1	UA	353	TYR	CE2-CZ	-6.75	1.29	1.38
11	UK	96	VAL	CB-CG1	-6.75	1.38	1.52
67	D4	28	A	C6-N1	-6.75	1.30	1.35



001000	naca ji on	· procee	, ao pago.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	388	С	N1-C2	-6.75	1.33	1.40
66	D3	498	G	C6-N1	-6.74	1.34	1.39
65	D2	275	A	N3-C4	-6.74	1.30	1.34
66	D3	942	G	N9-C8	-6.74	1.33	1.37
66	D3	931	С	N1-C2	-6.74	1.33	1.40
1	UA	501	SER	CA-CB	-6.73	1.42	1.52
66	D3	1068	С	N3-C4	-6.73	1.29	1.33
67	D4	54	С	N3-C4	-6.73	1.29	1.33
67	D4	61	G	C2-N3	-6.73	1.27	1.32
65	D2	468	А	N9-C4	-6.73	1.33	1.37
65	D2	237	A	C5-C6	-6.72	1.34	1.41
66	D3	546	U	N1-C2	-6.72	1.32	1.38
67	D4	32	G	C5-C6	-6.72	1.35	1.42
65	D2	288	G	N9-C8	-6.72	1.33	1.37
65	D2	290	G	C8-N7	-6.72	1.26	1.30
65	D2	164	G	N9-C8	-6.72	1.33	1.37
66	D3	499	U	C2-N3	-6.72	1.33	1.37
65	D2	238	G	C5-C4	-6.72	1.33	1.38
65	D2	243	A	N9-C4	-6.72	1.33	1.37
65	D2	288	G	C8-N7	-6.72	1.26	1.30
30	CI	51	CYS	CB-SG	-6.71	1.70	1.82
67	D4	31	G	N3-C4	-6.71	1.30	1.35
67	D4	330	А	C5-C4	-6.71	1.34	1.38
67	D4	65	С	C4-C5	-6.71	1.37	1.43
66	D3	1483	A	N9-C4	-6.71	1.33	1.37
66	D3	551	G	N3-C4	-6.71	1.30	1.35
67	D4	31	G	N9-C4	-6.71	1.32	1.38
67	D4	45	U	N1-C2	-6.71	1.32	1.38
65	D2	275	A	N9-C4	-6.71	1.33	1.37
66	D3	1594	G	C5-C4	-6.71	1.33	1.38
65	D2	241	U	N1-C6	-6.70	1.31	1.38
65	D2	390	C	N1-C2	-6.70	1.33	1.40
66	D3	571	G	N9-C8	-6.70	1.33	1.37
66	D3	561	G	C5-C4	-6.70	1.33	1.38
66	D3	926	A	N9-C4	-6.70	1.33	1.37
66	D3	1633	A	N7-C5	-6.69	1.35	1.39
66	D3	9	U	N1-C2	-6.69	1.32	1.38
65	D2	380	A	N3-C4	-6.69	1.30	1.34
7	UG	429	GLU	CG-CD	-6.68	1.42	1.51
65	D2	242	C	C4-C5	-6.68	1.37	1.43
65	D2	397	A	N9-C4	-6.68	1.33	1.37
67	D4	326	U	N1-C6	-6.68	1.31	1.38



0 01000		~ <i>r</i> · · · · · · · · · · · · · · · · · · ·	r all page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	UK	64	TYR	CD2-CE2	-6.68	1.29	1.39
66	D3	488	G	N1-C2	-6.68	1.32	1.37
65	D2	323	А	N7-C5	-6.68	1.35	1.39
1	UA	305	VAL	CB-CG1	-6.67	1.38	1.52
65	D2	236	С	C4-C5	-6.67	1.37	1.43
65	D2	484	G	C2-N3	-6.67	1.27	1.32
65	D2	281	G	N7-C5	-6.67	1.35	1.39
67	D4	322	A	N3-C4	-6.67	1.30	1.34
65	D2	329	A	C5-C4	-6.67	1.34	1.38
66	D3	1072	C	N3-C4	-6.67	1.29	1.33
66	D3	1617	U	N3-C4	-6.67	1.32	1.38
65	D2	143	A	C5-C6	-6.66	1.35	1.41
65	D2	383	G	N3-C4	-6.66	1.30	1.35
67	D4	327	G	C6-N1	-6.66	1.34	1.39
18	UR	426	VAL	CB-CG2	-6.65	1.38	1.52
65	D2	466	A	N9-C4	-6.65	1.33	1.37
65	D2	241	U	C2-N3	-6.65	1.33	1.37
66	D3	1637	C	N1-C6	-6.65	1.33	1.37
18	UR	275	TYR	CE2-CZ	-6.65	1.29	1.38
66	D3	1	U	N1-C6	-6.65	1.31	1.38
66	D3	1584	G	N9-C8	-6.64	1.33	1.37
67	D4	328	A	C5-C6	-6.64	1.35	1.41
65	D2	242	C	N1-C2	-6.64	1.33	1.40
7	UG	180	GLU	CB-CG	-6.64	1.39	1.52
65	D2	291	G	C8-N7	-6.64	1.26	1.30
65	D2	445	U	N1-C2	-6.64	1.32	1.38
31	CJ	90	VAL	CB-CG1	-6.64	1.39	1.52
65	D2	376	U	N1-C2	-6.64	1.32	1.38
66	D3	1486	G	N7-C5	-6.64	1.35	1.39
1	UA	793	GLU	CB-CG	-6.63	1.39	1.52
21	UU	450	VAL	CB-CG2	-6.63	1.39	1.52
66	D3	862	A	N9-C4	-6.63	1.33	1.37
67	D4	58	A	N9-C8	-6.63	1.32	1.37
65	D2	161	A	C5-C4	-6.63	1.34	1.38
46	JP	40	GLU	CB-CG	-6.63	1.39	1.52
65	D2	391	C	N1-C6	-6.63	1.33	1.37
46	JP	332	TYR	CD2-CE2	-6.63	1.29	1.39
66	D3	562	G	C8-N7	-6.63	1.26	1.30
65	D2	349	G	N7-C5	-6.62	1.35	1.39
65	D2	336	G	C8-N7	-6.62	1.26	1.30
66	D3	6	G	N3-C4	-6.61	1.30	1.35
66	D3	591	A	N3-C4	-6.61	1.30	1.34



001000	naca jion	" precede	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
21	UU	529	TYR	CE2-CZ	-6.61	1.29	1.38
65	D2	235	А	C6-N1	-6.61	1.30	1.35
67	D4	25	U	N1-C6	-6.61	1.32	1.38
65	D2	380	А	N7-C5	-6.60	1.35	1.39
66	D3	1046	G	N7-C5	-6.60	1.35	1.39
65	D2	297	U	C2-N3	-6.60	1.33	1.37
67	D4	20	U	N1-C2	-6.60	1.32	1.38
67	D4	62	С	C2-N3	-6.60	1.30	1.35
65	D2	303	А	C6-N6	-6.60	1.28	1.33
66	D3	1160	A	C5-C6	-6.60	1.35	1.41
65	D2	309	А	N9-C4	-6.59	1.33	1.37
67	D4	32	G	C8-N7	-6.59	1.26	1.30
33	CL	1001	VAL	CB-CG2	-6.59	1.39	1.52
66	D3	1606	С	N1-C2	-6.59	1.33	1.40
66	D3	1614	А	N7-C5	-6.59	1.35	1.39
66	D3	1617	U	N1-C2	-6.59	1.32	1.38
11	UK	63	TYR	CD2-CE2	-6.58	1.29	1.39
65	D2	300	C	C2-N3	-6.58	1.30	1.35
66	D3	512	А	N9-C4	-6.58	1.33	1.37
67	D4	59	G	N9-C4	-6.58	1.32	1.38
67	D4	67	G	C6-N1	-6.58	1.34	1.39
66	D3	963	А	N9-C4	-6.58	1.33	1.37
65	D2	333	G	N3-C4	-6.58	1.30	1.35
65	D2	381	G	C2-N3	-6.58	1.27	1.32
7	UG	431	ARG	CB-CG	-6.57	1.34	1.52
65	D2	294	U	C2-N3	-6.57	1.33	1.37
46	JP	288	TYR	CD2-CE2	-6.57	1.29	1.39
65	D2	282	G	N9-C4	-6.57	1.32	1.38
30	CI	136	VAL	CB-CG2	-6.57	1.39	1.52
66	D3	1527	C	N3-C4	-6.57	1.29	1.33
14	UN	298	TRP	CB-CG	-6.57	1.38	1.50
30	CI	36	TYR	CD2-CE2	-6.57	1.29	1.39
66	D3	549	G	C2-N3	-6.57	1.27	1.32
65	D2	242	С	N1-C6	-6.56	1.33	1.37
66	D3	1028	C	N3-C4	-6.56	1.29	1.33
1	UA	831	VAL	CB-CG1	-6.56	1.39	1.52
66	D3	1074	G	C8-N7	-6.56	1.27	1.30
66	D3	1525	A	C5-C6	-6.56	1.35	1.41
66	D3	1638	G	N7-C5	-6.56	1.35	1.39
66	D3	1582	U	N1-C2	-6.56	1.32	1.38
66	D3	1151	A	N3-C4	-6.56	1.30	1.34
1	UA	681	VAL	CB-CG1	-6.55	1.39	1.52



COntro	naca jion	i previe	ius puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	284	U	C4-C5	-6.55	1.37	1.43
65	D2	307	С	N3-C4	-6.55	1.29	1.33
67	D4	72	С	N1-C6	-6.55	1.33	1.37
65	D2	248	G	N7-C5	-6.55	1.35	1.39
66	D3	1581	С	N3-C4	-6.55	1.29	1.33
65	D2	459	U	N1-C2	-6.55	1.32	1.38
66	D3	487	G	C5-C6	-6.54	1.35	1.42
66	D3	566	С	C4-C5	-6.54	1.37	1.43
65	D2	298	А	C5-C6	-6.54	1.35	1.41
46	JP	95	TRP	CB-CG	-6.53	1.38	1.50
17	UQ	472	TYR	CD1-CE1	-6.53	1.29	1.39
66	D3	565	С	N3-C4	-6.53	1.29	1.33
66	D3	1582	U	C2-N3	-6.53	1.33	1.37
65	D2	341	G	C6-N1	-6.53	1.34	1.39
65	D2	453	А	N9-C4	-6.52	1.33	1.37
33	CL	851	TRP	CB-CG	-6.52	1.38	1.50
65	D2	291	G	N3-C4	-6.52	1.30	1.35
65	D2	473	А	C6-N1	-6.52	1.30	1.35
65	D2	334	G	C5-C6	-6.52	1.35	1.42
21	UU	463	VAL	CB-CG1	-6.52	1.39	1.52
7	UG	177	TYR	CE1-CZ	-6.51	1.30	1.38
66	D3	953	G	N9-C8	-6.51	1.33	1.37
66	D3	1484	G	N7-C5	-6.51	1.35	1.39
65	D2	459	U	C2-N3	-6.51	1.33	1.37
66	D3	500	С	C4-C5	-6.51	1.37	1.43
7	UG	177	TYR	CD1-CE1	-6.51	1.29	1.39
65	D2	271	G	C2-N3	-6.51	1.27	1.32
66	D3	577	G	N3-C4	-6.51	1.30	1.35
30	CI	47	TYR	CD1-CE1	-6.51	1.29	1.39
65	D2	350	A	N3-C4	-6.51	1.30	1.34
66	D3	1074	G	N9-C8	-6.51	1.33	1.37
67	D4	78	G	N1-C2	-6.51	1.32	1.37
66	D3	953	G	N3-C4	-6.50	1.30	1.35
1	UA	89	VAL	CB-CG1	-6.50	1.39	1.52
13	UM	746	TRP	CB-CG	-6.50	1.38	1.50
66	D3	943	C	N1-C6	-6.50	1.33	1.37
67	D4	86	A	N3-C4	-6.50	1.30	1.34
66	D3	573	C	N1-C2	-6.50	1.33	1.40
11	UK	34	TYR	CD2-CE2	-6.50	1.29	1.39
66	D3	974	A	N9-C4	-6.50	1.33	1.37
1	UA	218	TRP	CB-CG	-6.49	1.38	1.50
66	D3	497	G	N7-C5	-6.49	1.35	1.39



001000	naca jion	" Proove	al page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	68	A	N9-C8	-6.49	1.32	1.37
65	D2	398	А	C5-C4	-6.49	1.34	1.38
65	D2	335	G	C5-C6	-6.48	1.35	1.42
67	D4	79	G	N7-C5	-6.48	1.35	1.39
66	D3	1635	A	N7-C5	-6.47	1.35	1.39
66	D3	1592	А	N9-C4	-6.47	1.33	1.37
67	D4	37	G	C5-C4	-6.47	1.33	1.38
65	D2	295	А	N9-C4	-6.47	1.33	1.37
65	D2	386	А	N3-C4	-6.47	1.30	1.34
66	D3	1594	G	C6-N1	-6.47	1.35	1.39
67	D4	18	G	N7-C5	-6.47	1.35	1.39
67	D4	62	С	N1-C2	-6.47	1.33	1.40
67	D4	52	U	C2-N3	-6.46	1.33	1.37
6	UF	127	LYS	CB-CG	-6.46	1.35	1.52
18	UR	481	TRP	CB-CG	-6.46	1.38	1.50
65	D2	269	G	N7-C5	-6.46	1.35	1.39
66	D3	1610	G	N3-C4	-6.46	1.30	1.35
7	UG	216	TYR	CE2-CZ	-6.46	1.30	1.38
65	D2	275	А	N9-C8	-6.46	1.32	1.37
4	UD	206	SER	CA-C	-6.46	1.36	1.52
65	D2	270	U	C2-N3	-6.46	1.33	1.37
66	D3	1587	А	N9-C4	-6.46	1.33	1.37
33	CL	929	VAL	CB-CG2	-6.45	1.39	1.52
65	D2	472	А	N3-C4	-6.45	1.30	1.34
66	D3	951	А	C5-C4	-6.45	1.34	1.38
65	D2	288	G	N1-C2	-6.45	1.32	1.37
66	D3	592	A	N3-C4	-6.45	1.30	1.34
66	D3	1075	C	N3-C4	-6.45	1.29	1.33
66	D3	560	U	N1-C6	-6.45	1.32	1.38
18	UR	586	VAL	CB-CG1	-6.44	1.39	1.52
58	DQ	96	TYR	CE2-CZ	-6.44	1.30	1.38
65	D2	329	A	C5-C6	-6.44	1.35	1.41
67	D4	18	G	C6-N1	-6.44	1.35	1.39
67	D4	58	А	N7-C5	-6.44	1.35	1.39
66	D3	1592	A	N3-C4	-6.43	1.30	1.34
46	JP	343	TYR	CE2-CZ	-6.43	1.30	1.38
65	D2	444	U	N1-C2	-6.43	1.32	1.38
67	D4	83	A	C5-C4	-6.43	1.34	1.38
67	D4	18	G	N9-C8	-6.43	1.33	1.37
66	D3	594	A	N9-C4	-6.43	1.33	1.37
66	D3	1077	C	N1-C6	-6.42	1.33	1.37
66	D3	1492	A	C5-C4	-6.42	1.34	1.38


OOnu	nucu jion	i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	585	TYR	CE2-CZ	-6.42	1.30	1.38
46	JP	40	GLU	CG-CD	-6.42	1.42	1.51
65	D2	237	A	N9-C4	-6.42	1.33	1.37
65	D2	288	G	C5-C6	-6.42	1.35	1.42
46	JP	313	PHE	CB-CG	-6.42	1.40	1.51
65	D2	245	С	N1-C2	-6.42	1.33	1.40
67	D4	82	G	C5-C6	-6.42	1.35	1.42
67	D4	72	С	C4-C5	-6.41	1.37	1.43
66	D3	1600	А	N3-C4	-6.41	1.31	1.34
65	D2	462	G	C5-C4	-6.41	1.33	1.38
66	D3	589	С	C2-N3	-6.41	1.30	1.35
66	D3	486	G	C6-N1	-6.40	1.35	1.39
66	D3	1584	G	C6-N1	-6.40	1.35	1.39
1	UA	411	VAL	CB-CG1	-6.40	1.39	1.52
65	D2	390	С	C4-C5	-6.40	1.37	1.43
33	CL	881	CYS	CB-SG	-6.40	1.71	1.82
66	D3	1167	G	N3-C4	-6.40	1.30	1.35
7	UG	244	ASN	CB-CG	-6.39	1.36	1.51
65	D2	463	А	N3-C4	-6.39	1.31	1.34
66	D3	7	G	N1-C2	-6.39	1.32	1.37
11	UK	64	TYR	CE2-CZ	-6.39	1.30	1.38
13	UM	743	CYS	CB-SG	-6.39	1.71	1.82
66	D3	627	C	N1-C6	-6.39	1.33	1.37
66	D3	952	A	N3-C4	-6.39	1.31	1.34
65	D2	452	A	N7-C5	-6.39	1.35	1.39
67	D4	332	G	N9-C4	-6.39	1.32	1.38
65	D2	237	A	N9-C8	-6.38	1.32	1.37
66	D3	-1	G	C5-C6	-6.38	1.35	1.42
65	D2	320	A	N3-C4	-6.38	1.31	1.34
67	D4	58	A	C6-N1	-6.38	1.31	1.35
66	D3	591	A	N9-C4	-6.38	1.34	1.37
7	UG	165	TYR	CD1-CE1	-6.38	1.29	1.39
67	D4	24	U	C2-N3	-6.38	1.33	1.37
67	D4	69	A	C5-C6	-6.38	1.35	1.41
66	D3	564	G	N3-C4	-6.38	1.30	1.35
66	D3	937	C	N1-C2	-6.37	1.33	1.40
66	D3	1525	A	N7-C5	-6.37	1.35	1.39
65	D2	240	C	N1-C2	-6.37	1.33	1.40
65	D2	289		C2-O2	-6.37	1.16	1.22
66	D3	10	G	N9-C8	-6.37	1.33	1.37
67	D4	78	G	C5-C4	-6.37	1.33	1.38
66	D3	8	U	C4-C5	6.37	1.37	1.43



001000	naca jion	" proove	al page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	599	А	N3-C4	-6.37	1.31	1.34
65	D2	481	U	N3-C4	-6.36	1.32	1.38
58	DQ	19	VAL	CB-CG1	-6.36	1.39	1.52
65	D2	339	А	C5-C6	-6.36	1.35	1.41
66	D3	1603	U	C4-C5	-6.36	1.37	1.43
65	D2	100	G	C5-C4	-6.35	1.33	1.38
66	D3	1157	А	N3-C4	-6.35	1.31	1.34
66	D3	1590	G	N3-C4	-6.35	1.31	1.35
18	UR	494	TYR	CD2-CE2	-6.35	1.29	1.39
66	D3	1040	G	N9-C4	-6.35	1.32	1.38
65	D2	461	А	C6-N1	-6.34	1.31	1.35
66	D3	562	G	N9-C8	-6.34	1.33	1.37
66	D3	1529	С	N1-C6	-6.34	1.33	1.37
46	JP	332	TYR	CD1-CE1	-6.34	1.29	1.39
66	D3	552	G	C6-N1	-6.34	1.35	1.39
67	D4	67	G	N1-C2	-6.34	1.32	1.37
30	CI	144	ASN	CB-CG	-6.34	1.36	1.51
66	D3	1156	С	C4-C5	-6.33	1.37	1.43
21	UU	428	GLU	CG-CD	-6.33	1.42	1.51
65	D2	391	С	N3-C4	-6.33	1.29	1.33
65	D2	277	С	N1-C6	-6.33	1.33	1.37
7	UG	384	VAL	CB-CG1	-6.33	1.39	1.52
66	D3	1065	А	N3-C4	-6.33	1.31	1.34
65	D2	385	А	N3-C4	-6.33	1.31	1.34
1	UA	458	TRP	CB-CG	-6.32	1.38	1.50
30	CI	21	TRP	CB-CG	-6.32	1.38	1.50
65	D2	452	А	N9-C4	-6.32	1.34	1.37
18	UR	535	ARG	CB-CG	-6.32	1.35	1.52
30	CI	148	TYR	CD2-CE2	-6.32	1.29	1.39
67	D4	33	А	N7-C5	-6.32	1.35	1.39
67	D4	70	U	N1-C2	-6.32	1.32	1.38
46	JP	117	CYS	CB-SG	-6.32	1.71	1.82
65	D2	385	А	C5-C4	-6.32	1.34	1.38
65	D2	243	А	N7-C5	-6.31	1.35	1.39
28	CF	93	VAL	CB-CG1	-6.31	1.39	1.52
65	D2	276	G	N9-C8	-6.31	1.33	1.37
66	D3	1599	С	N3-C4	-6.31	1.29	1.33
66	D3	473	A	N9-C4	-6.31	1.34	1.37
66	D3	497	G	N9-C8	-6.30	1.33	1.37
7	UG	114	TYR	CD1-CE1	-6.30	1.29	1.39
65	D2	397	A	C5-C4	-6.30	1.34	1.38
66	D3	928	U	N1-C2	-6.30	1.32	1.38



Ideal(Å)

Continued from previous page												
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)						
66	D3	1069	А	N9-C4	-6.30	1.34						
66	D3	557	G	N3-C4	-6.29	1.31						
65	D2	475	G	C8-N7	-6.29	1.27						
66	D3	9	U	C2-N3	-6.29	1.33						
66	D3	592	А	N7-C5	-6.29	1.35						
66	D3	1633	А	N9-C8	-6.29	1.32						
65	D2	340	U	C2-N3	-6.29	1.33						
65	D2	82	А	N7-C5	-6.29	1.35						
65	D2	246	G	C5-C4	-6.28	1.33						
66	D3	2	А	N9-C4	-6.28	1.34						
66	D3	940	А	N9-C4	-6.28	1.34						
4	UD	265	TRP	CE3-CZ3	-6.28	1.27						
1	UA	329	VAL	CB-CG2	-6.28	1.39						
66	D3	1482	C	$\overline{\text{C2-N3}}$	-6.28	1.30						

 α J fa n tin .

00	D3	1009	A	N9-C4	-0.30	1.34	1.37
66	D3	557	G	N3-C4	-6.29	1.31	1.35
65	D2	475	G	C8-N7	-6.29	1.27	1.30
66	D3	9	U	C2-N3	-6.29	1.33	1.37
66	D3	592	A	N7-C5	-6.29	1.35	1.39
66	D3	1633	А	N9-C8	-6.29	1.32	1.37
65	D2	340	U	C2-N3	-6.29	1.33	1.37
65	D2	82	А	N7-C5	-6.29	1.35	1.39
65	D2	246	G	C5-C4	-6.28	1.33	1.38
66	D3	2	А	N9-C4	-6.28	1.34	1.37
66	D3	940	А	N9-C4	-6.28	1.34	1.37
4	UD	265	TRP	CE3-CZ3	-6.28	1.27	1.38
1	UA	329	VAL	CB-CG2	-6.28	1.39	1.52
66	D3	1482	С	C2-N3	-6.28	1.30	1.35
1	UA	445	VAL	CB-CG2	-6.28	1.39	1.52
7	UG	440	ASP	CB-CG	-6.28	1.38	1.51
7	UG	203	TYR	CE2-CZ	-6.28	1.30	1.38
21	UU	61	TYR	CD1-CE1	-6.28	1.29	1.39
66	D3	1485	С	N1-C2	-6.27	1.33	1.40
66	D3	1488	G	C6-N1	-6.27	1.35	1.39
66	D3	558	U	C2-N3	-6.27	1.33	1.37
67	D4	65	С	N1-C6	-6.27	1.33	1.37
66	D3	562	G	C6-N1	-6.27	1.35	1.39
65	D2	331	U	N1-C2	-6.27	1.32	1.38
66	D3	1039	А	N7-C5	-6.27	1.35	1.39
1	UA	52	TYR	CE1-CZ	-6.26	1.30	1.38
65	D2	384	U	C2-N3	-6.26	1.33	1.37
66	D3	590	С	N1-C2	-6.26	1.33	1.40
15	UO	108	TYR	CD1-CE1	-6.26	1.29	1.39
30	CI	103	VAL	CB-CG2	-6.26	1.39	1.52
66	D3	12	U	N1-C2	-6.26	1.32	1.38
66	D3	548	G	N7-C5	-6.26	1.35	1.39
65	D2	240	C	C2-N3	-6.25	1.30	1.35
65	D2	240	С	N1-C6	-6.25	1.33	1.37
65	D2	397	A	N3-C4	-6.25	1.31	1.34
66	D3	1632	C	N1-C6	-6.25	1.33	1.37
58	DQ	7	VAL	CB-CG1	-6.25	1.39	1.52
65	D2	278	G	C6-N1	-6.25	1.35	1.39
7	UG	118	TYR	CD1-CE1	-6.25	1.29	1.39
21	UU	487	TYR	CE2-CZ	-6.25	1.30	1.38
65	D2	375	C	C4-C5	-6.25	1.38	1.43
67	D4	24	U	N3-C4	-6.25	1.32	1.38



N/[_]	Chain	Dar	T	A t a ma a	7	Oh a survey $d(\lambda)$	
	Chain	Res	Type	Atoms		Observed(A)	10eal(A)
66	D3	965		C2-N3	-6.24	1.33	1.37
1	UG	411	TYR	CEI-CZ	-6.24	1.30	1.38
66	D3	553	G	C5-C4	-6.24	1.33	1.38
67	D4	21	C	N3-C4	-6.24	1.29	1.33
67	D4	30	A	N9-C8	-6.24	1.32	1.37
46	JP	289	TYR	CE1-CZ	-6.24	1.30	1.38
65	D2	161	A	N9-C4	-6.24	1.34	1.37
65	D2	281	G	N9-C4	-6.23	1.32	1.38
67	D4	325	C	N3-C4	-6.23	1.29	1.33
65	D2	337	G	N1-C2	-6.23	1.32	1.37
66	D3	548	G	N9-C4	-6.23	1.32	1.38
31	CJ	157	PHE	CD1-CE1	-6.23	1.26	1.39
67	D4	92	A	N9-C4	-6.23	1.34	1.37
66	D3	562	G	N7-C5	-6.22	1.35	1.39
66	D3	1577	А	N7-C5	-6.22	1.35	1.39
66	D3	1047	G	N3-C4	-6.22	1.31	1.35
65	D2	247	U	N1-C2	-6.22	1.32	1.38
65	D2	90	G	C5-C4	-6.21	1.34	1.38
65	D2	291	G	C5-C6	-6.21	1.36	1.42
66	D3	1604	U	N1-C6	-6.21	1.32	1.38
66	D3	10	G	N9-C4	-6.21	1.32	1.38
66	D3	1077	С	N3-C4	-6.21	1.29	1.33
66	D3	1466	G	C5-C4	-6.21	1.34	1.38
25	CA	172	TYR	CD1-CE1	-6.21	1.30	1.39
46	JP	59	VAL	CB-CG2	-6.21	1.39	1.52
66	D3	575	С	C5-C6	-6.21	1.29	1.34
66	D3	1577	A	N9-C4	-6.21	1.34	1.37
66	D3	512	A	N7-C5	-6.20	1.35	1.39
66	D3	956	C	N1-C6	-6.20	1.33	1.37
65	D2	290	G	N9-C8	-6.20	1.33	1.37
65	D2	298	A	C6-N1	-6.20	1.31	1.35
1	UA	353	TYR	CD2-CE2	-6.20	1.30	1.39
66	D3	567	A	N9-C4	-6.20	1.34	1.37
66	 D3	485	A	N7-C5	-6.19	1.35	1.39
65	D2	384	U	C4-C5	-6.19	1.38	1.43
66	D3	1607	G	C5-C6	-6.19	1.36	1.13
1	UA	490	SER	CA-CB	-6,19	1.43	1.52
65	D2	482	A	C5-C6	-6.19	1.35	1.41
66	D3	156	A	N9-C4	-6.19	1.34	1.37
66	D3	870	C	N3-C4	-6.19	1 29	1 33
21	UU	487	TYR	CG-CD1	-6.18	1.20	1.30
66	D3	566	C	N3-C4	-6.18	1.01	1.33
00	1 10	1 000	\sim	1 10 01	1 0.10	1 1.40	1 1.00



001000	naca jion	" Proove	a page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	331	U	C4-C5	-6.18	1.38	1.43
65	D2	389	U	N1-C6	-6.18	1.32	1.38
65	D2	412	А	N9-C4	-6.18	1.34	1.37
21	UU	498	TYR	CE2-CZ	-6.18	1.30	1.38
33	CL	860	TYR	CE2-CZ	-6.18	1.30	1.38
65	D2	323	А	N3-C4	-6.18	1.31	1.34
67	D4	79	G	C5-C6	-6.18	1.36	1.42
65	D2	286	U	N3-C4	-6.17	1.32	1.38
66	D3	555	А	N7-C5	-6.17	1.35	1.39
66	D3	1116	А	N7-C5	-6.17	1.35	1.39
66	D3	1586	А	N9-C4	-6.17	1.34	1.37
66	D3	1151	A	N7-C5	-6.17	1.35	1.39
17	UQ	472	TYR	CD2-CE2	-6.17	1.30	1.39
65	D2	238	G	N1-C2	-6.17	1.32	1.37
1	UA	401	VAL	CB-CG2	-6.17	1.39	1.52
65	D2	381	G	N7-C5	-6.17	1.35	1.39
66	D3	497	G	C6-N1	-6.17	1.35	1.39
65	D2	451	G	N3-C4	-6.17	1.31	1.35
65	D2	82	А	C5-C6	-6.16	1.35	1.41
66	D3	549	G	N9-C4	-6.16	1.33	1.38
1	UA	684	VAL	CB-CG1	-6.16	1.40	1.52
18	UR	172	TYR	CD1-CE1	-6.16	1.30	1.39
66	D3	1	U	N1-C2	-6.16	1.33	1.38
66	D3	1525	A	N9-C8	-6.16	1.32	1.37
66	D3	1615	С	C4-C5	-6.16	1.38	1.43
66	D3	496	G	N7-C5	-6.16	1.35	1.39
66	D3	1609	U	N3-C4	-6.16	1.32	1.38
66	D3	500	С	N1-C6	-6.15	1.33	1.37
66	D3	550	A	C5-C6	-6.15	1.35	1.41
66	D3	1066	C	N1-C6	-6.15	1.33	1.37
66	D3	871	G	N9-C8	-6.15	1.33	1.37
27	CE	427	TYR	CD2-CE2	-6.15	1.30	1.39
66	D3	1587	А	N3-C4	-6.15	1.31	1.34
67	D4	60	А	N9-C8	-6.14	1.32	1.37
1	UA	37	VAL	CB-CG2	-6.14	1.40	1.52
65	D2	100	G	N7-C5	-6.14	1.35	1.39
65	D2	482	А	N1-C2	-6.14	1.28	1.34
66	D3	936	G	C5-C4	-6.14	1.34	1.38
7	UG	114	TYR	CE1-CZ	-6.14	1.30	1.38
66	D3	1484	G	N9-C8	-6.14	1.33	1.37
67	D4	86	A	C5-C4	-6.14	1.34	1.38
18	UR	494	TYR	CD1-CE1	-6.13	1.30	1.39



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1600	A	N9-C8	-6.13	1.32	1.37
66	D3	1481	С	C4-C5	-6.13	1.38	1.43
30	CI	161	VAL	CB-CG1	-6.13	1.40	1.52
65	D2	161	А	C5-C6	-6.13	1.35	1.41
66	D3	560	U	C2-N3	-6.13	1.33	1.37
25	CA	239	CYS	CB-SG	-6.13	1.71	1.82
65	D2	284	U	C5-C6	-6.13	1.28	1.34
67	D4	28	А	C5-C6	-6.13	1.35	1.41
65	D2	399	U	N1-C2	-6.13	1.33	1.38
46	JP	343	TYR	CE1-CZ	-6.12	1.30	1.38
65	D2	385	А	N7-C5	-6.12	1.35	1.39
66	D3	565	С	C2-N3	-6.12	1.30	1.35
67	D4	58	A	N9-C4	-6.12	1.34	1.37
66	D3	584	С	C2-N3	-6.12	1.30	1.35
67	D4	324	U	N1-C2	-6.12	1.33	1.38
21	UU	89	TYR	CD1-CE1	-6.12	1.30	1.39
65	D2	392	U	C2-N3	-6.12	1.33	1.37
65	D2	349	G	C6-N1	-6.12	1.35	1.39
66	D3	1046	G	N9-C4	-6.12	1.33	1.38
66	D3	1163	A	C6-N1	-6.12	1.31	1.35
21	UU	599	TRP	CB-CG	-6.11	1.39	1.50
67	D4	18	G	N3-C4	-6.11	1.31	1.35
66	D3	872	G	C5-C6	-6.11	1.36	1.42
4	UD	300	VAL	CB-CG1	-6.11	1.40	1.52
21	UU	441	ARG	CB-CG	-6.11	1.36	1.52
65	D2	309	A	N9-C8	-6.11	1.32	1.37
65	D2	344	U	C2-N3	-6.11	1.33	1.37
65	D2	334	G	C2-N3	-6.10	1.27	1.32
67	D4	22	A	C5-C4	-6.10	1.34	1.38
65	D2	381	G	C5-C4	-6.10	1.34	1.38
67	D4	78	G	C8-N7	-6.10	1.27	1.30
65	D2	268	G	C8-N7	-6.10	1.27	1.30
67	D4	20	U	C2-N3	-6.10	1.33	1.37
65	D2	409	С	N1-C6	-6.09	1.33	1.37
66	D3	931	С	N3-C4	-6.09	1.29	1.33
66	D3	560	U	N3-C4	-6.09	1.32	1.38
65	D2	402	G	N1-C2	-6.09	1.32	1.37
65	D2	411	A	C5-C4	-6.09	1.34	1.38
66	D3	878	G	C6-N1	-6.09	1.35	1.39
1	UA	419	TYR	CD2-CE2	-6.08	1.30	1.39
67	D4	78	G	N9-C8	-6.08	1.33	1.37
66	D3	572	C	N3-C4	-6.08	1.29	1.33

Continued from previous page...



001000	nucu jion	" proore	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1165	G	C5-C4	-6.08	1.34	1.38
66	D3	867	G	C5-C4	-6.08	1.34	1.38
66	D3	974	А	N3-C4	-6.08	1.31	1.34
65	D2	481	U	N1-C2	-6.08	1.33	1.38
66	D3	588	U	N1-C2	-6.07	1.33	1.38
17	UQ	506	TRP	CB-CG	-6.07	1.39	1.50
66	D3	577	G	N9-C4	-6.07	1.33	1.38
66	D3	591	А	C5-C4	-6.07	1.34	1.38
66	D3	1635	A	C5-C6	-6.07	1.35	1.41
65	D2	308	А	N9-C4	-6.07	1.34	1.37
66	D3	1482	С	C4-C5	-6.07	1.38	1.43
66	D3	1528	U	C2-N3	-6.07	1.33	1.37
21	UU	444	ASP	CB-CG	-6.07	1.39	1.51
23	UX	10	PHE	CD1-CE1	-6.07	1.27	1.39
67	D4	56	А	N3-C4	-6.07	1.31	1.34
66	D3	866	G	N9-C4	-6.06	1.33	1.38
65	D2	389	U	C4-C5	-6.06	1.38	1.43
66	D3	551	G	C6-N1	-6.06	1.35	1.39
7	UG	388	ASP	CB-CG	-6.06	1.39	1.51
65	D2	287	G	C6-N1	-6.06	1.35	1.39
66	D3	1042	G	N9-C4	-6.05	1.33	1.38
66	D3	1590	G	N1-C2	-6.05	1.32	1.37
7	UG	139	TRP	CB-CG	-6.05	1.39	1.50
66	D3	1067	С	N1-C6	-6.05	1.33	1.37
31	CJ	233	VAL	CB-CG1	-6.05	1.40	1.52
65	D2	89	C	C4-C5	-6.05	1.38	1.43
66	D3	955	A	C5-C4	-6.05	1.34	1.38
66	D3	1160	A	C6-N1	-6.05	1.31	1.35
65	D2	308	A	C6-N1	-6.04	1.31	1.35
66	D3	573	C	C4-C5	-6.04	1.38	1.43
30	CI	36	TYR	CB-CG	-6.04	1.42	1.51
66	D3	926	A	N3-C4	-6.04	1.31	1.34
7	UG	201	TYR	CE2-CZ	-6.04	1.30	1.38
66	D3	1072	С	C2-N3	-6.04	1.30	1.35
66	D3	878	G	C5-C4	-6.04	1.34	1.38
66	D3	1596	C	N3-C4	-6.04	1.29	1.33
1	UA	353	TYR	CE1-CZ	-6.03	1.30	1.38
65	D2	333	G	C6-N1	-6.03	1.35	1.39
66	D3	577	G	C5-C4	-6.03	1.34	1.38
66	D3	566	C	N1-C2	-6.03	1.34	1.40
66	D3	885	G	N1-C2	-6.03	1.32	1.37
65	D2	481	U	C2-N3	-6.02	1.33	1.37



Contro	naca jion	i previe	ius puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	234	А	C5-C6	-6.02	1.35	1.41
65	D2	484	G	C5-C4	-6.02	1.34	1.38
66	D3	558	U	N3-C4	-6.02	1.33	1.38
46	JP	270	ASN	CB-CG	-6.02	1.37	1.51
66	D3	557	G	C6-N1	-6.01	1.35	1.39
7	UG	449	ILE	CB-CG2	-6.01	1.34	1.52
67	D4	330	А	N9-C8	-6.01	1.32	1.37
65	D2	281	G	C5-C4	-6.01	1.34	1.38
65	D2	412	А	N3-C4	-6.01	1.31	1.34
18	UR	537	VAL	CB-CG1	-6.01	1.40	1.52
30	CI	173	TYR	CE1-CZ	-6.01	1.30	1.38
65	D2	161	A	C6-N1	-6.01	1.31	1.35
67	D4	68	А	C5-C4	-6.01	1.34	1.38
66	D3	599	A	N9-C4	-6.01	1.34	1.37
65	D2	396	А	N3-C4	-6.00	1.31	1.34
4	UD	213	TRP	CB-CG	-6.00	1.39	1.50
46	JP	113	VAL	CB-CG2	-6.00	1.40	1.52
65	D2	82	A	C6-N6	-6.00	1.29	1.33
65	D2	410	A	N3-C4	-6.00	1.31	1.34
66	D3	478	A	N7-C5	-6.00	1.35	1.39
67	D4	25	U	C5-C6	-6.00	1.28	1.34
65	D2	238	G	C2-N3	-6.00	1.27	1.32
67	D4	72	C	N1-C2	-6.00	1.34	1.40
67	D4	78	G	N7-C5	-6.00	1.35	1.39
15	UO	366	TYR	CE2-CZ	-6.00	1.30	1.38
25	CA	194	VAL	CB-CG1	-6.00	1.40	1.52
21	UU	505	VAL	CB-CG2	-6.00	1.40	1.52
66	D3	5	U	N3-C4	-6.00	1.33	1.38
66	D3	1589	С	N1-C6	-6.00	1.33	1.37
46	JP	321	VAL	CB-CG1	-5.99	1.40	1.52
65	D2	164	G	N9-C4	-5.99	1.33	1.38
67	D4	47	G	C5-C4	-5.99	1.34	1.38
65	D2	84	G	C5-C4	-5.99	1.34	1.38
65	D2	335	G	N1-C2	-5.99	1.32	1.37
66	D3	498	G	C5-C4	-5.99	1.34	1.38
66	D3	577	G	N7-C5	-5.99	1.35	1.39
66	D3	15	U	N3-C4	-5.99	1.33	1.38
67	D4	329	C	C2-N3	-5.99	1.30	1.35
66	D3	31	C	C4-C5	-5.98	1.38	1.43
18	UR	544	VAL	CB-CG1	-5.98	1.40	1.52
65	D2	246	G	N1-C2	-5.98	1.32	1.37
67	D4	79	G	N9-C4	-5.98	1.33	1.38



OOnu		i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	UO	361	MET	CA-CB	-5.98	1.40	1.53
21	UU	450	VAL	CB-CG1	-5.98	1.40	1.52
65	D2	250	G	C6-N1	-5.98	1.35	1.39
67	D4	40	A	N7-C5	-5.98	1.35	1.39
30	CI	160	TRP	CB-CG	-5.98	1.39	1.50
65	D2	407	А	C6-N1	-5.98	1.31	1.35
65	D2	477	G	N7-C5	-5.98	1.35	1.39
58	DQ	96	TYR	CE1-CZ	-5.97	1.30	1.38
66	D3	486	G	N9-C4	-5.97	1.33	1.38
66	D3	924	А	N9-C4	-5.97	1.34	1.37
66	D3	1073	G	N9-C4	-5.97	1.33	1.38
12	UL	148	TRP	CB-CG	-5.97	1.39	1.50
66	D3	1525	А	N1-C2	-5.97	1.28	1.34
65	D2	232	U	N1-C2	-5.97	1.33	1.38
66	D3	1603	U	N1-C6	-5.97	1.32	1.38
67	D4	30	А	C6-N1	-5.97	1.31	1.35
66	D3	514	G	C5-C4	-5.96	1.34	1.38
66	D3	1576	А	N9-C4	-5.96	1.34	1.37
67	D4	76	U	N3-C4	-5.96	1.33	1.38
30	CI	157	TYR	CE1-CZ	-5.96	1.30	1.38
1	UA	372	TRP	CE3-CZ3	-5.96	1.28	1.38
65	D2	389	U	N3-C4	-5.96	1.33	1.38
66	D3	512	А	C5-C6	-5.96	1.35	1.41
66	D3	1613	U	C2-N3	-5.96	1.33	1.37
67	D4	85	G	C2-N3	-5.96	1.27	1.32
7	UG	256	VAL	CB-CG2	-5.96	1.40	1.52
21	UU	612	TRP	CB-CG	-5.96	1.39	1.50
65	D2	381	G	N1-C2	-5.96	1.32	1.37
66	D3	1078	C	C4-C5	-5.96	1.38	1.43
66	D3	1597	A	N7-C5	-5.96	1.35	1.39
66	D3	1618	C	C5-C6	-5.96	1.29	1.34
23	UX	94	CYS	CB-SG	-5.95	1.72	1.81
66	D3	1465	C	C4-C5	-5.95	1.38	1.43
1	UA	529	GLU	CB-CG	-5.94	1.40	1.52
65	D2	411	A	C5-C6	-5.94	1.35	1.41
65	D2	477	G	N9-C4	-5.94	1.33	1.38
4	UD	241	VAL	CB-CG2	-5.94	1.40	1.52
10	UJ	119	GLU	CG-CD	-5.94	1.43	1.51
65	D2	103	G	N7-C5	-5.94	1.35	1.39
66	D3	560	U	C4-C5	-5.94	1.38	1.43
65	D2	338	A	N7-C5	-5.94	1.35	1.39
7	UG	411	TYR	$ $ CE2- \overline{CZ}	-5.93	1.30	1.38



00.000	naca ji on	" Procee	pago.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	UU	342	TYR	CE2-CZ	-5.93	1.30	1.38
65	D2	269	G	N9-C8	-5.93	1.33	1.37
1	UA	210	SER	CA-CB	-5.93	1.44	1.52
66	D3	564	G	C5-C4	-5.93	1.34	1.38
66	D3	872	G	N7-C5	-5.93	1.35	1.39
67	D4	51	С	N1-C6	-5.93	1.33	1.37
65	D2	308	А	N3-C4	-5.93	1.31	1.34
66	D3	915	А	N7-C5	-5.93	1.35	1.39
65	D2	99	U	N1-C6	-5.93	1.32	1.38
66	D3	591	А	C6-N1	-5.93	1.31	1.35
66	D3	1041	G	N9-C4	-5.93	1.33	1.38
66	D3	9	U	C4-C5	-5.92	1.38	1.43
67	D4	73	А	C6-N1	-5.92	1.31	1.35
67	D4	332	G	C5-C4	-5.92	1.34	1.38
21	UU	498	TYR	CE1-CZ	-5.92	1.30	1.38
65	D2	334	G	N3-C4	-5.92	1.31	1.35
66	D3	589	С	N1-C2	-5.92	1.34	1.40
65	D2	248	G	C8-N7	-5.92	1.27	1.30
66	D3	569	С	C2-N3	-5.92	1.31	1.35
66	D3	1590	G	N9-C8	-5.92	1.33	1.37
21	UU	101	TYR	CD2-CE2	-5.92	1.30	1.39
66	D3	1077	С	C4-C5	-5.92	1.38	1.43
1	UA	681	VAL	CB-CG2	-5.91	1.40	1.52
66	D3	1157	А	N7-C5	-5.91	1.35	1.39
65	D2	162	U	N1-C2	-5.91	1.33	1.38
66	D3	867	G	N3-C4	-5.91	1.31	1.35
66	D3	1612	U	N1-C2	-5.91	1.33	1.38
65	D2	281	G	N1-C2	-5.91	1.33	1.37
67	D4	325	C	C2-N3	-5.91	1.31	1.35
1	UA	530	VAL	CB-CG1	-5.91	1.40	1.52
21	UU	442	THR	CB-CG2	-5.91	1.32	1.52
5	UE	292	TYR	CE1-CZ	-5.90	1.30	1.38
67	D4	79	G	C6-N1	-5.90	1.35	1.39
65	D2	271	G	N3-C4	-5.90	1.31	1.35
65	D2	335	G	C2-N3	-5.90	1.28	1.32
66	D3	943	C	N1-C2	-5.90	1.34	1.40
65	D2	90	G	C6-N1	-5.90	1.35	1.39
25	CA	181	VAL	CB-CG2	-5.90	1.40	1.52
66	D3	1599	C	C2-N3	-5.90	1.31	1.35
23	UX	131	SER	CA-CB	-5.90	1.44	1.52
21	UU	90	VAL	CB-CG1	-5.89	1.40	1.52
65	D2	257	G _	C5-C4	-5.89	1.34	1.38



	itaea jien	r proore	page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	277	C	C2-N3	-5.89	1.31	1.35
21	UU	632	VAL	CB-CG1	-5.89	1.40	1.52
27	CE	427	TYR	CE2-CZ	-5.89	1.30	1.38
65	D2	243	А	N3-C4	-5.88	1.31	1.34
65	D2	385	А	C5-C6	-5.88	1.35	1.41
7	UG	201	TYR	CD1-CE1	-5.88	1.30	1.39
65	D2	271	G	C6-N1	-5.88	1.35	1.39
65	D2	248	G	C5-C6	-5.88	1.36	1.42
21	UU	27	PHE	CB-CG	-5.88	1.41	1.51
31	CJ	119	ARG	CG-CD	-5.88	1.37	1.51
66	D3	1466	G	C8-N7	-5.88	1.27	1.30
46	JP	113	VAL	CB-CG1	-5.88	1.40	1.52
18	UR	172	TYR	CE1-CZ	-5.88	1.30	1.38
66	D3	571	G	C5-C4	-5.87	1.34	1.38
66	D3	877	G	N7-C5	-5.87	1.35	1.39
66	D3	1038	U	C2-N3	-5.87	1.33	1.37
54	DJ	106	GLU	CB-CG	-5.87	1.41	1.52
65	D2	320	A	C5-C6	-5.87	1.35	1.41
65	D2	331	U	N1-C6	-5.87	1.32	1.38
31	CJ	58	TYR	CD2-CE2	-5.87	1.30	1.39
66	D3	875	G	C5-C4	-5.87	1.34	1.38
66	D3	930	A	N9-C8	-5.87	1.33	1.37
65	D2	287	G	N9-C8	-5.87	1.33	1.37
66	D3	1166	A	C5-C4	-5.87	1.34	1.38
65	D2	386	A	C6-N6	-5.87	1.29	1.33
66	D3	1604	U	C4-O4	-5.87	1.19	1.23
46	JP	311	VAL	CB-CG1	-5.86	1.40	1.52
58	DQ	90	VAL	CB-CG2	-5.86	1.40	1.52
67	D4	59	G	C2-N3	-5.86	1.28	1.32
21	UU	33	VAL	CB-CG2	-5.86	1.40	1.52
66	D3	11	A	N3-C4	-5.86	1.31	1.34
67	D4	70	U	N3-C4	-5.86	1.33	1.38
65	D2	331	U	C4-O4	-5.86	1.19	1.23
66	D3	547	U	C2-N3	-5.86	1.33	1.37
14	UN	891	ILE	C-N	-5.85	1.20	1.34
18	UR	411	TYR	CE2-CZ	-5.85	1.30	1.38
46	JP	81	ASN	CB-CG	-5.85	1.37	1.51
65	D2	384	U	N3-C4	-5.85	1.33	1.38
65	D2	386	A	N9-C8	-5.85	1.33	1.37
65	D2	471	C	N3-C4	-5.85	1.29	1.33
1	UA	476	VAL	CB-CG1	-5.85	1.40	1.52
23	UX	89	CYS	CB-SG	-5.85	1.72	1.81



001100	nucu jion	" PICOUC	we paye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	486	G	N1-C2	-5.85	1.33	1.37
7	UG	219	VAL	CB-CG1	-5.84	1.40	1.52
66	D3	1489	U	N1-C2	-5.84	1.33	1.38
7	UG	227	GLU	CB-CG	-5.84	1.41	1.52
30	CI	128	VAL	CB-CG2	-5.84	1.40	1.52
50	DF	162	VAL	CB-CG1	-5.84	1.40	1.52
46	JP	288	TYR	CE1-CZ	-5.84	1.30	1.38
65	D2	449	U	C2-N3	-5.84	1.33	1.37
66	D3	943	С	C4-C5	-5.84	1.38	1.43
66	D3	1574	G	C5-C4	-5.84	1.34	1.38
67	D4	33	А	C6-N1	-5.84	1.31	1.35
66	D3	1049	U	C2-N3	-5.84	1.33	1.37
67	D4	27	U	N1-C6	-5.84	1.32	1.38
5	UE	20	VAL	CB-CG1	-5.83	1.40	1.52
65	D2	336	G	N9-C4	-5.83	1.33	1.38
1	UA	331	GLU	CG-CD	-5.83	1.43	1.51
18	UR	268	TYR	CE2-CZ	-5.83	1.30	1.38
23	UX	136	TYR	CD2-CE2	-5.83	1.30	1.39
33	CL	825	VAL	CB-CG2	-5.83	1.40	1.52
1	UA	165	SER	CA-CB	-5.83	1.44	1.52
66	D3	1068	С	N1-C2	-5.83	1.34	1.40
7	UG	378	VAL	CB-CG1	-5.83	1.40	1.52
1	UA	575	GLU	CB-CG	-5.83	1.41	1.52
66	D3	1614	А	N9-C4	-5.83	1.34	1.37
21	UU	101	TYR	CD1-CE1	-5.83	1.30	1.39
65	D2	340	U	N1-C6	-5.83	1.32	1.38
66	D3	1485	С	N3-C4	-5.83	1.29	1.33
46	JP	288	TYR	CD1-CE1	-5.82	1.30	1.39
66	D3	510	G	C5-C4	-5.82	1.34	1.38
46	JP	325	TYR	CE1-CZ	-5.82	1.30	1.38
58	DQ	79	TYR	CE2-CZ	-5.82	1.30	1.38
66	D3	559	С	N3-C4	-5.82	1.29	1.33
66	D3	1043	A	C5-C4	-5.82	1.34	1.38
66	D3	1044	U	N3-C4	-5.82	1.33	1.38
46	JP	356	TYR	CD1-CE1	-5.82	1.30	1.39
65	D2	273	G	N9-C8	-5.82	1.33	1.37
67	D4	47	G	N3-C4	-5.82	1.31	1.35
17	UQ	354	TYR	CD2-CE2	-5.82	1.30	1.39
67	D4	22	A	C5-C6	-5.81	1.35	1.41
44	JN	234	VAL	CB-CG1	-5.81	1.40	1.52
65	D2	396	A	C5-C6	-5.81	1.35	1.41
66	D3	333	A	N9-C4	-5.81	1.34	1.37



00000	naca ji on	i precie	, uo page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
66	D3	478	A	N3-C4	-5.81	1.31	1.34
67	D4	81	U	N1-C2	-5.81	1.33	1.38
30	CI	31	GLN	CB-CG	-5.81	1.36	1.52
66	D3	486	G	C5-C4	-5.81	1.34	1.38
66	D3	1041	G	N7-C5	-5.81	1.35	1.39
66	D3	1490	C	C5-C6	-5.81	1.29	1.34
67	D4	72	C	C2-N3	-5.81	1.31	1.35
67	D4	332	G	N3-C4	-5.81	1.31	1.35
66	D3	29	U	N1-C2	-5.81	1.33	1.38
1	UA	494	ASP	CA-C	-5.80	1.37	1.52
66	D3	1609	U	N1-C6	-5.80	1.32	1.38
65	D2	82	А	C5-C4	-5.80	1.34	1.38
65	D2	292	А	C6-N1	-5.80	1.31	1.35
65	D2	329	А	N7-C5	-5.80	1.35	1.39
66	D3	1151	А	N9-C4	-5.80	1.34	1.37
66	D3	552	G	N1-C2	-5.80	1.33	1.37
67	D4	328	А	N9-C8	-5.80	1.33	1.37
66	D3	874	С	N3-C4	-5.80	1.29	1.33
66	D3	931	С	C4-C5	-5.80	1.38	1.43
66	D3	32	U	N1-C2	-5.80	1.33	1.38
31	CJ	157	PHE	CB-CG	-5.79	1.41	1.51
67	D4	84	U	C4-C5	-5.79	1.38	1.43
67	D4	330	А	C5-C6	-5.79	1.35	1.41
66	D3	1160	А	N7-C5	-5.79	1.35	1.39
66	D3	1173	С	C4-C5	-5.79	1.38	1.43
67	D4	37	G	N7-C5	-5.79	1.35	1.39
65	D2	443	G	C5-C4	-5.79	1.34	1.38
66	D3	498	G	N1-C2	-5.79	1.33	1.37
66	D3	15	U	N1-C6	-5.79	1.32	1.38
66	D3	599	А	C5-C4	-5.79	1.34	1.38
66	D3	1622	G	C5-C4	-5.79	1.34	1.38
67	D4	52	U	N1-C2	-5.79	1.33	1.38
1	UA	433	PHE	CD1-CE1	-5.78	1.27	1.39
65	D2	164	G	N3-C4	-5.78	1.31	1.35
15	UO	417	VAL	CB-CG1	-5.78	1.40	1.52
46	JP	13	TYR	CD2-CE2	-5.78	1.30	1.39
65	D2	311	С	C4-N4	-5.78	1.28	1.33
65	D2	337	G	N7-C5	-5.78	1.35	1.39
66	D3	1158	С	C2-N3	-5.78	1.31	1.35
7	UG	118	TYR	CE1-CZ	-5.78	1.31	1.38
66	D3	1638	G	C5-C6	-5.78	1.36	1.42
66	D3	571	G	C6-N1	-5.77	1.35	1.39



	j	- P					
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	704	TYR	CE1-CZ	-5.77	1.31	1.38
65	D2	320	A	N9-C4	-5.77	1.34	1.37
46	JP	58	PHE	CD1-CE1	-5.77	1.27	1.39
65	D2	307	С	C2-N3	-5.77	1.31	1.35
1	UA	457	VAL	CB-CG2	-5.77	1.40	1.52
11	UK	223	GLU	CD-OE2	-5.77	1.19	1.25
65	D2	290	G	C2-N3	-5.76	1.28	1.32
66	D3	512	A	C5-C4	-5.76	1.34	1.38
66	D3	928	U	C2-N3	-5.76	1.33	1.37
66	D3	9	U	N1-C6	-5.76	1.32	1.38
65	D2	345	U	N1-C2	-5.76	1.33	1.38
66	D3	584	С	C5-C6	-5.76	1.29	1.34
66	D3	1593	A	N3-C4	-5.76	1.31	1.34
67	D4	63	С	C2-N3	-5.76	1.31	1.35
67	D4	86	A	C6-N1	-5.76	1.31	1.35
65	D2	268	G	N7-C5	-5.76	1.35	1.39
66	D3	975	С	N3-C4	-5.76	1.29	1.33
67	D4	67	G	C8-N7	-5.75	1.27	1.30
67	D4	42	U	C2-N3	-5.75	1.33	1.37
17	UQ	317	TRP	CB-CG	-5.75	1.40	1.50
54	DJ	122	VAL	CB-CG1	-5.75	1.40	1.52
65	D2	452	А	N3-C4	-5.75	1.31	1.34
66	D3	867	G	C8-N7	-5.75	1.27	1.30
11	UK	106	TYR	CD1-CE1	-5.75	1.30	1.39
65	D2	293	U	N3-C4	-5.75	1.33	1.38
65	D2	471	С	C2-N3	-5.75	1.31	1.35
66	D3	578	U	C2-N3	-5.75	1.33	1.37
66	D3	1165	G	C2-N3	-5.75	1.28	1.32
65	D2	95	A	C5-C6	-5.74	1.35	1.41
67	D4	28	A	N1-C2	-5.74	1.29	1.34
65	D2	89	C	C5-C6	-5.74	1.29	1.34
66	D3	962	С	N1-C6	-5.74	1.33	1.37
66	D3	626	U	N1-C2	-5.74	1.33	1.38
66	D3	1043	A	N9-C8	-5.74	1.33	1.37
7	UG	165	TYR	CE1-CZ	-5.74	1.31	1.38
66	D3	6	G	N9-C4	-5.74	1.33	1.38
65	D2	272	A	C5-C4	-5.74	1.34	1.38
66	D3	1466	G	N9-C8	-5.73	1.33	1.37
7	UG	201	TYR	CG-CD2	-5.73	1.31	1.39
46	JP	48	THR	CB-CG2	-5.73	1.33	1.52
66	D3	939	A	N9-C4	-5.73	1.34	1.37
67	D4	324	U	C2-N3	-5.73	1.33	1.37



OOmit	писи јгоп	i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	DA	154	SER	CA-CB	-5.73	1.44	1.52
1	UA	509	VAL	CB-CG1	-5.73	1.40	1.52
66	D3	593	U	N1-C2	-5.72	1.33	1.38
67	D4	23	U	C2-N3	-5.72	1.33	1.37
67	D4	83	А	N3-C4	-5.72	1.31	1.34
66	D3	574	G	N1-C2	-5.72	1.33	1.37
66	D3	1169	G	N7-C5	-5.72	1.35	1.39
66	D3	936	G	N9-C8	-5.72	1.33	1.37
66	D3	962	С	N3-C4	-5.72	1.29	1.33
67	D4	19	А	C5-C4	-5.72	1.34	1.38
67	D4	41	С	N3-C4	-5.72	1.29	1.33
66	D3	576	G	C6-N1	-5.71	1.35	1.39
50	DF	17	VAL	CB-CG2	-5.71	1.40	1.52
65	D2	388	С	C2-N3	-5.71	1.31	1.35
65	D2	406	U	C4-C5	-5.71	1.38	1.43
21	UU	355	TYR	CD1-CE1	-5.71	1.30	1.39
21	UU	455	PHE	CD2-CE2	-5.71	1.27	1.39
67	D4	57	A	C6-N1	-5.71	1.31	1.35
65	D2	411	A	N3-C4	-5.71	1.31	1.34
65	D2	475	G	N7-C5	-5.71	1.35	1.39
66	D3	887	A	N7-C5	-5.71	1.35	1.39
66	D3	1587	A	C6-N1	-5.71	1.31	1.35
7	UG	159	TYR	CD2-CE2	-5.70	1.30	1.39
66	D3	924	A	N7-C5	-5.70	1.35	1.39
66	D3	1072	С	N1-C2	-5.70	1.34	1.40
66	D3	1072	С	N1-C6	-5.70	1.33	1.37
66	D3	1610	G	C2-N3	-5.70	1.28	1.32
67	D4	60	A	C5-C6	-5.70	1.35	1.41
65	D2	408	U	N1-C2	-5.70	1.33	1.38
14	UN	842	TYR	CD1-CE1	-5.70	1.30	1.39
21	UU	61	TYR	CD2-CE2	-5.70	1.30	1.39
65	D2	146	G	C6-N1	-5.70	1.35	1.39
66	D3	555	A	N9-C8	-5.70	1.33	1.37
21	00	426	GLU	CB-CG	-5.70	1.41	1.52
66	D3	942	G	C5-C6	-5.70	1.36	1.42
1	UA	515	TYR	CD2-CE2	-5.70	1.30	1.39
66	D3	13	C	C4-C5	-5.70	1.38	1.43
66	D3	1046	G	C8-N7	-5.70	1.27	1.30
66	D3	1622	G	C5-C6	-5.70	1.36	1.42
67	D4	65		C2-N3	-5.70	1.31	1.35
65	D2	453	A	N3-C4	-5.69	1.31	1.34
65	D2	487	A	C5-C6	-5.69	1.35	1.41



001111	nucu jion	i prevu	rus puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	577	G	C6-N1	-5.69	1.35	1.39
67	D4	55	А	N9-C4	-5.69	1.34	1.37
30	CI	150	VAL	CB-CG2	-5.69	1.41	1.52
66	D3	1592	A	N9-C8	-5.69	1.33	1.37
67	D4	79	G	N1-C2	-5.69	1.33	1.37
45	JO	146	VAL	CB-CG1	-5.68	1.41	1.52
66	D3	553	G	N3-C4	-5.68	1.31	1.35
66	D3	587	С	N1-C2	-5.68	1.34	1.40
67	D4	33	А	N3-C4	-5.68	1.31	1.34
67	D4	71	С	C4-C5	-5.68	1.38	1.43
65	D2	235	А	N9-C4	-5.68	1.34	1.37
66	D3	1152	А	N7-C5	-5.68	1.35	1.39
65	D2	254	С	N1-C6	-5.68	1.33	1.37
66	D3	1605	G	C2-N3	-5.68	1.28	1.32
65	D2	249	G	C6-N1	-5.68	1.35	1.39
66	D3	487	G	C8-N7	-5.68	1.27	1.30
66	D3	941	А	C5-C4	-5.68	1.34	1.38
67	D4	85	G	N9-C4	-5.68	1.33	1.38
65	D2	147	С	N1-C6	-5.67	1.33	1.37
66	D3	878	G	N7-C5	-5.67	1.35	1.39
66	D3	951	А	C5-C6	-5.67	1.35	1.41
66	D3	1588	G	C6-N1	-5.67	1.35	1.39
65	D2	278	G	C8-N7	-5.67	1.27	1.30
66	D3	1161	С	N3-C4	-5.67	1.29	1.33
66	D3	941	А	N3-C4	-5.67	1.31	1.34
66	D3	1080	U	C2-N3	-5.67	1.33	1.37
67	D4	327	G	N9-C8	-5.67	1.33	1.37
7	UG	206	VAL	CB-CG1	-5.67	1.41	1.52
66	D3	11	A	C6-N1	-5.67	1.31	1.35
67	D4	69	A	N3-C4	-5.67	1.31	1.34
21	UU	149	TYR	CD1-CE1	-5.67	1.30	1.39
65	D2	475	G	C5-C4	-5.67	1.34	1.38
66	D3	594	A	N3-C4	-5.67	1.31	1.34
66	D3	1588	G	C5-C6	-5.67	1.36	1.42
33	CL	899	VAL	CB-CG2	-5.66	1.41	1.52
65	D2	279	A	C6-N1	-5.66	1.31	1.35
65	D2	281	G	N3-C4	-5.66	1.31	1.35
65	D2	381	G	C5-C6	-5.66	1.36	1.42
65	D2	412	A	C5-C6	-5.66	1.35	1.41
66	D3	1068	C	C2-N3	-5.66	1.31	1.35
7	UG	86	VAL	CB-CG1	-5.66	1.41	1.52
21	UU	322	TYR	CE1-CZ	-5.66	1.31	1.38



	Chain	D ec	Trme	Atoma	7	Observed(Å)	Ideal(Å)
		nes	Type	Atoms		Observed(A)	$1 \frac{1}{20}$
60	D2 D2	233	G	C5-C4	-5.00	1.34	1.38
00 60	D3	496	G	C5-C6	-5.00	1.30	1.42
00	D3	1635	A	N3-C4	-5.00	1.31	1.34
67	D4	100	U	N3-C4	-5.66	1.33	1.38
43	JM	136	TYR	CD2-CE2	-5.66	1.30	1.39
23	UX	53	PHE	CD1-CE1	-5.65	1.27	1.39
46	JP	247	TYR	CD1-CE1	-5.65	1.30	1.39
66	D3	549	G	N7-C5	-5.65	1.35	1.39
13	UM	801	GLU	CB-CG	-5.65	1.41	1.52
65	D2	249	G	N3-C4	-5.65	1.31	1.35
66	D3	948	G	N7-C5	-5.65	1.35	1.39
18	UR	275	TYR	CD1-CE1	-5.64	1.30	1.39
66	D3	1082	C	N1-C6	-5.64	1.33	1.37
66	D3	1616	G	N9-C8	-5.64	1.33	1.37
65	D2	336	G	C5-C6	-5.64	1.36	1.42
1	UA	585	TYR	CE1-CZ	-5.64	1.31	1.38
66	D3	477	А	N7-C5	-5.64	1.35	1.39
66	D3	1157	А	C5-C6	-5.64	1.35	1.41
65	D2	392	U	C2-O2	-5.64	1.17	1.22
66	D3	1466	G	N3-C4	-5.64	1.31	1.35
67	D4	45	U	C2-N3	-5.64	1.33	1.37
46	JP	287	TYR	CD1-CE1	-5.64	1.30	1.39
66	D3	877	G	C5-C6	-5.64	1.36	1.42
67	D4	67	G	N9-C8	-5.64	1.33	1.37
65	D2	299	G	N9-C4	-5.63	1.33	1.38
67	D4	82	G	N1-C2	-5.63	1.33	1.37
66	D3	562	G	N1-C2	-5.63	1.33	1.37
66	D3	886	U	N1-C2	-5.63	1.33	1.38
66	D3	1039	А	C5-C4	-5.63	1.34	1.38
33	CL	991	PHE	CB-CG	-5.63	1.41	1.51
66	D3	1575	G	C6-N1	-5.63	1.35	1.39
66	D3	1620	С	N3-C4	-5.63	1.30	1.33
67	D4	17	G	N1-C2	-5.63	1.33	1.37
21	UU	342	TYR	CD1-CE1	-5.62	1.30	1.39
66	D3	1750	A	N9-C4	-5.62	1.34	1.37
33	CL	195	TRP	CB-CG	-5.62	1.40	1.50
65	D2	445	U	C4-C5	-5.62	1.38	1.43
66	D3	1589	C	C4-C5	-5.62	1.38	1.43
66	D3	1596	C	C4-C5	-5.62	1.38	1.43
25	CA	270	SER	CA-CB	-5.62	1.44	1.52
46	JP	13	TYR	CD1-CE1	-5.62	1.30	1.39
65	D2	299	G	C2-N3	-5.62	1.28	1.32



		-	ue page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	928	U	N1-C6	-5.62	1.32	1.38
66	D3	1082	С	N1-C2	-5.62	1.34	1.40
67	D4	55	A	C2'-C1'	-5.62	1.47	1.53
66	D3	1170	G	N1-C2	-5.62	1.33	1.37
66	D3	1174	С	C4-C5	-5.62	1.38	1.43
66	D3	488	G	C6-N1	-5.61	1.35	1.39
67	D4	28	A	N3-C4	-5.61	1.31	1.34
66	D3	1114	G	N1-C2	-5.61	1.33	1.37
65	D2	292	A	C4'-C3'	-5.61	1.47	1.52
1	UA	604	TYR	CB-CG	-5.61	1.43	1.51
21	UU	455	PHE	CE1-CZ	-5.61	1.26	1.37
67	D4	64	A	C8-N7	-5.61	1.27	1.31
67	D4	82	G	C6-O6	-5.61	1.19	1.24
18	UR	172	TYR	CE2-CZ	-5.61	1.31	1.38
18	UR	531	CYS	CB-SG	-5.61	1.72	1.81
66	D3	933	А	C5-C6	-5.61	1.36	1.41
66	D3	1161	С	N1-C6	-5.61	1.33	1.37
66	D3	1469	А	N7-C5	-5.61	1.35	1.39
66	D3	1051	G	N7-C5	-5.61	1.35	1.39
66	D3	1580	С	N3-C4	-5.61	1.30	1.33
66	D3	1594	G	N1-C2	-5.61	1.33	1.37
1	UA	167	ASP	CB-CG	-5.60	1.40	1.51
66	D3	1113	А	N3-C4	-5.60	1.31	1.34
66	D3	498	G	N7-C5	-5.60	1.35	1.39
66	D3	499	U	N1-C2	-5.60	1.33	1.38
66	D3	955	А	N3-C4	-5.60	1.31	1.34
65	D2	391	С	N1-C2	-5.60	1.34	1.40
65	D2	299	G	C8-N7	-5.60	1.27	1.30
33	CL	1073	VAL	CB-CG2	-5.60	1.41	1.52
66	D3	6	G	C6-N1	-5.60	1.35	1.39
66	D3	1614	А	C6-N1	-5.60	1.31	1.35
67	D4	49	С	N1-C2	-5.60	1.34	1.40
65	D2	234	А	C6-N1	-5.60	1.31	1.35
66	D3	1113	А	N9-C4	-5.60	1.34	1.37
7	UG	322	VAL	CB-CG2	-5.59	1.41	1.52
21	UU	593	PHE	CD1-CE1	-5.59	1.28	1.39
65	D2	319	А	N9-C4	-5.59	1.34	1.37
65	D2	349	G	C5-C4	-5.59	1.34	1.38
66	D3	514	G	N3-C4	-5.59	1.31	1.35
7	UG	408	GLU	CG-CD	-5.59	1.43	1.51
66	D3	548	G	N9-C8	-5.59	1.33	1.37
66	D3	553	G	C6-N1	-5.59	1.35	1.39



CONU	nucu jion	i prevu	rus puge.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	30	А	C8-N7	-5.59	1.27	1.31
66	D3	955	А	C6-N1	-5.59	1.31	1.35
66	D3	1526	А	N9-C4	-5.59	1.34	1.37
32	CK	477	GLU	CG-CD	-5.58	1.43	1.51
31	CJ	123	VAL	CB-CG1	-5.58	1.41	1.52
31	CJ	157	PHE	C-N	-5.58	1.23	1.34
66	D3	548	G	C5-C6	-5.58	1.36	1.42
66	D3	1482	С	N1-C2	-5.58	1.34	1.40
65	D2	298	А	N1-C2	-5.58	1.29	1.34
67	D4	82	G	N9-C8	-5.58	1.33	1.37
7	UG	168	VAL	CB-CG1	-5.58	1.41	1.52
65	D2	278	G	N9-C4	-5.58	1.33	1.38
67	D4	322	А	N7-C5	-5.58	1.35	1.39
66	D3	564	G	C5-C6	-5.58	1.36	1.42
66	D3	884	А	N7-C5	-5.58	1.35	1.39
1	UA	194	VAL	CB-CG1	-5.58	1.41	1.52
1	UA	604	TYR	CE2-CZ	-5.58	1.31	1.38
66	D3	1484	G	C6-N1	-5.58	1.35	1.39
67	D4	78	G	C6-N1	-5.58	1.35	1.39
18	UR	494	TYR	CE1-CZ	-5.57	1.31	1.38
30	CI	173	TYR	CD2-CE2	-5.57	1.30	1.39
66	D3	1075	С	C4-C5	-5.57	1.38	1.43
66	D3	1577	А	C5-C6	-5.57	1.36	1.41
65	D2	477	G	C5-C4	-5.57	1.34	1.38
21	UU	61	TYR	CE1-CZ	-5.57	1.31	1.38
65	D2	457	G	N7-C5	-5.57	1.35	1.39
65	D2	451	G	C5-C4	-5.57	1.34	1.38
1	UA	353	TYR	CD1-CE1	-5.57	1.30	1.39
66	D3	6	G	N1-C2	-5.57	1.33	1.37
66	D3	1074	G	C5-C4	-5.57	1.34	1.38
66	D3	1482	C	C5-C6	-5.57	1.29	1.34
66	D3	1616	G	N7-C5	-5.57	1.35	1.39
33	CL	947	PHE	CD2-CE2	-5.57	1.28	1.39
66	D3	591	A	N7-C5	-5.57	1.35	1.39
65	D2	271	G	C5-C4	-5.56	1.34	1.38
66	D3	565	C	N1-C2	-5.56	1.34	1.40
66	D3	1077	С	N1-C2	-5.56	1.34	1.40
33	CL	897	CYS	CB-SG	-5.56	1.72	1.81
65	D2	411	A	N7-C5	-5.56	1.35	1.39
66	D3	887	A	C5-C4	-5.56	1.34	1.38
66	D3	1604	U	C5-C6	-5.56	1.29	1.34
7	UG	159	TYR	CG-CD1	-5.56	1.31	1.39



	Chain	Res	$\frac{\mathbf{T}\mathbf{v}\mathbf{n}\mathbf{e}}{\mathbf{T}\mathbf{v}\mathbf{n}\mathbf{e}}$	Atoms	7.	Observed(Å)	Ideal(Å)
15	UO	237	TRP	CB-CG	-5.56	1 40	$1 \text{ future}(\mathbf{A})$
65	D2	472		C5 C6	-5.50	1.40	1.00
66	D2 D3	1044	II	C2-N3	-5.50	1.30	1.41
67	D_{4}	1044		N1 C6	-5.50	1.00	1.37
21		912		CB-CG	-5.50	1.55	1.57
30	CI	36	TVR	CE1-CZ	-5.50	1.40	1.30
31	CI	58	TYR	CD1-CE1	-5.56	1.31	1.30
50	DF	162	VAL	CB-CG2	-5.56	1.01	1.53
65	D2	480	C	N1-C6	-5.56	1.11	1.32
1	UA	7	PHE	CD1-CE1	-5.56	1.33	1.39
31	CJ	204	CYS	CB-SG	-5.56	1.72	1.81
65	D2	397	A	C6-N1	-5.56	1.31	1.35
18	UR	555	TRP	CZ3-CH2	-5.56	1.31	1.40
65	D2	381	G	C2-N2	-5.55	1.28	1.34
65	D2	481	U	C4-C5	-5.55	1.38	1.43
66	D3	871	G	C6-N1	-5.55	1.35	1.39
66	D3	1609	U	C5-C6	-5.55	1.29	1.34
66	D3	1614	A	C5-C6	-5.55	1.36	1.41
67	D4	46	U	C2-N3	-5.55	1.33	1.37
28	CF	50	GLU	CG-CD	-5.55	1.43	1.51
65	D2	334	G	C6-N1	-5.55	1.35	1.39
66	D3	567	A	C5-C6	-5.55	1.36	1.41
28	CF	39	GLU	CG-CD	-5.55	1.43	1.51
65	D2	146	G	C5-C4	-5.55	1.34	1.38
65	D2	297	U	C4-C5	-5.55	1.38	1.43
66	D3	1588	G	N3-C4	-5.54	1.31	1.35
67	D4	35	U	N1-C6	-5.54	1.32	1.38
65	D2	274	С	C2-O2	-5.54	1.19	1.24
65	D2	375	С	N3-C4	-5.54	1.30	1.33
66	D3	1047	G	C6-N1	-5.54	1.35	1.39
4	UD	195	TRP	CB-CG	-5.54	1.40	1.50
27	CE	362	VAL	CB-CG1	-5.54	1.41	1.52
66	D3	1613	U	C5-C6	-5.54	1.29	1.34
67	D4	80	U	P-O5'	-5.54	1.54	1.59
67	D4	56	A	N9-C4	-5.54	1.34	1.37
23	UX	145	VAL	CB-CG1	-5.54	1.41	1.52
66	D3	499	U	N3-C4	-5.53	1.33	1.38
66	D3	550	A	N7-C5	-5.53	1.35	1.39
67	D4	29	U	N1-C2	-5.53	1.33	1.38
66	D3	1049	U	N3-C4	-5.53	1.33	1.38
1	UA	476	VAL	CB-CG2	-5.53	1.41	1.52
66	D3	1048	G	N3-C4	-5.53	1.31	1.35



001000	nucu jion	v preced	rus puye.				
Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
67	D4	331	А	C5-C4	-5.53	1.34	1.38
66	D3	549	G	N3-C4	-5.53	1.31	1.35
66	D3	875	G	N1-C2	-5.53	1.33	1.37
1	UA	606	VAL	CB-CG2	-5.52	1.41	1.52
31	CJ	11	GLU	CB-CG	-5.52	1.41	1.52
65	D2	86	С	N1-C2	-5.52	1.34	1.40
66	D3	1083	G	N7-C5	-5.52	1.35	1.39
44	JN	253	TYR	CB-CG	-5.52	1.43	1.51
65	D2	281	G	C6-N1	-5.52	1.35	1.39
65	D2	333	G	N9-C8	-5.52	1.33	1.37
66	D3	1605	G	N9-C4	-5.52	1.33	1.38
66	D3	551	G	N9-C8	-5.52	1.33	1.37
65	D2	412	А	C5-C4	-5.52	1.34	1.38
66	D3	545	А	C6-N1	-5.52	1.31	1.35
66	D3	954	G	N7-C5	-5.52	1.35	1.39
66	D3	1642	G	N9-C4	-5.52	1.33	1.38
21	UU	466	VAL	CB-CG2	-5.51	1.41	1.52
66	D3	1485	С	C5-C6	-5.51	1.29	1.34
15	UO	30	TYR	CE2-CZ	-5.51	1.31	1.38
65	D2	243	A	C6-N1	-5.51	1.31	1.35
66	D3	867	G	N9-C8	-5.51	1.33	1.37
1	UA	84	PHE	CD1-CE1	-5.51	1.28	1.39
1	UA	308	VAL	CB-CG2	-5.51	1.41	1.52
58	DQ	97	VAL	CB-CG1	-5.51	1.41	1.52
66	D3	1071	U	N1-C2	-5.51	1.33	1.38
66	D3	1603	U	C2-N3	-5.51	1.33	1.37
65	D2	384	U	N1-C2	-5.50	1.33	1.38
66	D3	1588	G	N9-C8	-5.50	1.33	1.37
66	D3	568	G	C5-C6	-5.50	1.36	1.42
7	UG	216	TYR	CD1-CE1	-5.50	1.31	1.39
18	UR	320	TYR	CD2-CE2	-5.50	1.31	1.39
65	D2	238	G	N3-C4	-5.50	1.31	1.35
65	D2	391	C	C5-C6	-5.50	1.29	1.34
66	D3	1488	G	N7-C5	-5.50	1.35	1.39
67	D4	34	A	C6-N1	-5.50	1.31	1.35
66	D3	1	U	C2-N3	-5.50	1.33	1.37
65	D2	232	U	C4-C5	-5.50	1.38	1.43
65	D2	162	U	N3-C4	-5.49	1.33	1.38
31	CJ	11	GLU	CG-CD	-5.49	1.43	1.51
11	UK	106	TYR	CD2-CE2	-5.49	1.31	1.39
23	UX	136	TYR	CD1-CE1	-5.49	1.31	1.39
66	D3	1037	C	C5-C6	-5.49	1.29	1.34



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
65	D2	90	G	N1-C2	-5.49	1.33	1.37
65	D2	309	А	N1-C2	-5.49	1.29	1.34
66	D3	1157	А	C6-N1	-5.49	1.31	1.35
66	D3	1466	G	C5-C6	-5.49	1.36	1.42
1	UA	515	TYR	CD1-CE1	-5.49	1.31	1.39
65	D2	83	U	N3-C4	-5.49	1.33	1.38
65	D2	308	А	N9-C8	-5.48	1.33	1.37
65	D2	396	А	C5-C4	-5.48	1.34	1.38
66	D3	562	G	N3-C4	-5.48	1.31	1.35
66	D3	944	А	C6-N1	-5.48	1.31	1.35
65	D2	480	С	N1-C2	-5.48	1.34	1.40
18	UR	579	VAL	CB-CG2	-5.48	1.41	1.52
65	D2	291	G	P-O5'	-5.48	1.54	1.59
66	D3	1167	G	C5-C4	-5.48	1.34	1.38
66	D3	1484	G	N3-C4	-5.48	1.31	1.35
66	D3	5	U	N1-C6	-5.48	1.33	1.38
66	D3	863	А	N3-C4	-5.48	1.31	1.34
21	UU	378	PHE	CE1-CZ	-5.48	1.26	1.37
65	D2	378	С	N1-C6	-5.48	1.33	1.37
65	D2	401	A	C5-C4	-5.48	1.34	1.38
65	D2	398	A	C5-C6	-5.47	1.36	1.41
66	D3	543	С	N1-C6	-5.47	1.33	1.37
66	D3	927	С	N1-C2	-5.47	1.34	1.40
66	D3	939	A	N7-C5	-5.47	1.35	1.39
67	D4	19	A	C6-N1	-5.47	1.31	1.35
25	CA	320	TYR	CD1-CE1	-5.47	1.31	1.39
26	CD	131	VAL	CB-CG2	-5.47	1.41	1.52
65	D2	454	С	C4-C5	-5.47	1.38	1.43
66	D3	1618	С	N3-C4	-5.47	1.30	1.33
46	JP	289	TYR	CE2-CZ	-5.47	1.31	1.38
65	D2	287	G	N7-C5	-5.47	1.35	1.39
66	D3	876	G	N1-C2	-5.47	1.33	1.37
66	D3	952	A	C6-N1	-5.47	1.31	1.35
66	D3	1040	G	N3-C4	-5.47	1.31	1.35
66	D3	1083	G	C6-N1	-5.47	1.35	1.39
66	D3	1164	G	C5-C4	-5.47	1.34	1.38
67	D4	56	A	N7-C5	-5.47	1.35	1.39
1	UA	684	VAL	CB-CG2	-5.47	1.41	1.52
7	UG	165	TYR	CD2-CE2	-5.47	1.31	1.39
11	UK	63	TYR	CE2-CZ	-5.47	1.31	1.38
23	UX	100	ASP	CB-CG	-5.47	1.40	1.51
65	D2	230	I C	N1-C6	-5.47	1.33	1.37



OOnu	<i>nucu jron</i>	i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	282	G	C8-N7	-5.47	1.27	1.30
66	D3	546	U	C4-C5	-5.47	1.38	1.43
66	D3	1635	А	N9-C8	-5.46	1.33	1.37
1	UA	331	GLU	CB-CG	-5.46	1.41	1.52
54	DJ	96	VAL	CB-CG1	-5.46	1.41	1.52
65	D2	290	G	C5-C6	-5.46	1.36	1.42
65	D2	248	G	N9-C8	-5.46	1.34	1.37
1	UA	361	VAL	CB-CG1	-5.46	1.41	1.52
66	D3	938	G	N7-C5	-5.46	1.35	1.39
30	CI	36	TYR	CD1-CE1	-5.46	1.31	1.39
65	D2	409	С	C4-C5	-5.46	1.38	1.43
66	D3	561	G	C6-N1	-5.46	1.35	1.39
66	D3	578	U	N1-C2	-5.46	1.33	1.38
66	D3	877	G	C5-C4	-5.46	1.34	1.38
66	D3	1610	G	N9-C8	-5.46	1.34	1.37
66	D3	1484	G	C8-N7	-5.45	1.27	1.30
67	D4	42	U	N3-C4	-5.45	1.33	1.38
1	UA	509	VAL	CB-CG2	-5.45	1.41	1.52
18	UR	432	VAL	CB-CG2	-5.45	1.41	1.52
54	DJ	85	VAL	CB-CG2	-5.45	1.41	1.52
65	D2	299	G	N9-C8	-5.45	1.34	1.37
65	D2	396	A	N7-C5	-5.45	1.35	1.39
65	D2	310	U	N1-C6	-5.45	1.33	1.38
66	D3	590	С	C5-C6	-5.45	1.29	1.34
21	UU	423	ARG	CG-CD	-5.44	1.38	1.51
21	UU	601	VAL	CB-CG2	-5.44	1.41	1.52
46	JP	14	VAL	CB-CG2	-5.44	1.41	1.52
25	CA	96	VAL	CB-CG1	-5.44	1.41	1.52
46	JP	372	VAL	CB-CG1	-5.44	1.41	1.52
65	D2	268	G	N9-C8	-5.44	1.34	1.37
66	D3	939	A	C5-C6	-5.44	1.36	1.41
30	Cl	173	TYR	CE2-CZ	-5.44	1.31	1.38
46	JP	35	PHE	CD2-CE2	-5.44	1.28	1.39
65	D2	84	G	N7-C5	-5.44	1.35	1.39
66	D3	511	A	N9-C4	-5.44	1.34	1.37
66	D3	1041	G	NI-C2	-5.44	1.33	1.37
	UA	411	VAL	CB-CG2	-5.44	1.41	1.52
60	D2	275	A	C5-C4	-5.44	1.34	1.38
00		1041	G		-0.44	1.54	1.38
	D2 D2	295	A	C0 N0	-5.44	1.54	1.38
60	D3	513		CZ-N3	-5.44	1.33	1.37
1 07	$\downarrow D4$	06	A	1 00-00	-0.44	1.30	1.41



OOnu		i previe	as page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	57	А	C5-C4	-5.44	1.34	1.38
66	D3	1484	G	N1-C2	-5.43	1.33	1.37
66	D3	1597	А	C5-C4	-5.43	1.34	1.38
14	UN	313	PHE	CB-CG	-5.43	1.42	1.51
58	DQ	22	VAL	CB-CG2	-5.43	1.41	1.52
66	D3	31	С	N1-C2	-5.43	1.34	1.40
21	UU	342	TYR	CD2-CE2	-5.43	1.31	1.39
33	CL	935	VAL	CB-CG2	-5.43	1.41	1.52
66	D3	1591	С	N3-C4	-5.43	1.30	1.33
66	D3	478	А	C5-C4	-5.43	1.34	1.38
66	D3	1613	U	N3-C4	-5.43	1.33	1.38
46	JP	230	ASN	CB-CG	-5.42	1.38	1.51
66	D3	1156	С	N1-C2	-5.42	1.34	1.40
6	UF	7	TYR	CD1-CE1	-5.42	1.31	1.39
66	D3	416	А	N3-C4	-5.42	1.31	1.34
66	D3	588	U	C2-N3	-5.42	1.33	1.37
46	JP	54	PHE	CD2-CE2	-5.42	1.28	1.39
65	D2	162	U	C4-C5	-5.42	1.38	1.43
66	D3	1588	G	N9-C4	-5.42	1.33	1.38
10	UJ	129	VAL	CB-CG1	-5.42	1.41	1.52
14	UN	842	TYR	CE1-CZ	-5.42	1.31	1.38
30	CI	161	VAL	CB-CG2	-5.41	1.41	1.52
66	D3	1582	U	N1-C6	-5.41	1.33	1.38
67	D4	29	U	C4-O4	-5.41	1.19	1.23
66	D3	1592	A	C6-N1	-5.41	1.31	1.35
5	UE	29	VAL	CB-CG2	-5.41	1.41	1.52
66	D3	8	U	C4-O4	-5.41	1.19	1.23
66	D3	930	A	C5-C4	-5.41	1.34	1.38
66	D3	1750	A	N3-C4	-5.41	1.31	1.34
21	UU	441	ARG	CG-CD	-5.41	1.38	1.51
65	D2	302	A	C5-C4	-5.41	1.34	1.38
66	D3	936	G	N3-C4	-5.41	1.31	1.35
67	D4	51	С	N3-C4	-5.41	1.30	1.33
65	D2	412	A	N7-C5	-5.41	1.36	1.39
65	D2	476	A	N3-C4	-5.41	1.31	1.34
65	D2	250	G	C5-C4	-5.40	1.34	1.38
66	D3	-1	G	C6-N1	-5.40	1.35	1.39
66	D3	14	C	N1-C2	-5.40	1.34	1.40
18	UR	320	TYR	CE2-CZ	-5.40	1.31	1.38
65	D2	259	G	N7-C5	-5.40	1.36	1.39
65	D2	449	U	N1-C2	-5.40	1.33	1.38
66	D3	940	A	N3-C4	-5.40	1.31	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1064	G	N7-C5	-5.40	1.36	1.39
65	D2	447	G	N9-C4	-5.40	1.33	1.38
28	CF	97	VAL	CB-CG1	-5.40	1.41	1.52
30	CI	44	TYR	CE2-CZ	-5.40	1.31	1.38
67	D4	20	U	C4-C5	-5.40	1.38	1.43
66	D3	941	А	N9-C4	-5.40	1.34	1.37
66	D3	884	А	N9-C4	-5.39	1.34	1.37
1	UA	173	TRP	CB-CG	-5.39	1.40	1.50
15	UO	366	TYR	CD2-CE2	-5.39	1.31	1.39
65	D2	458	А	C6-N1	-5.39	1.31	1.35
65	D2	482	А	N7-C5	-5.39	1.36	1.39
30	CI	36	TYR	CE2-CZ	-5.39	1.31	1.38
65	D2	479	G	C5-C4	-5.39	1.34	1.38
66	D3	1632	С	N3-C4	-5.39	1.30	1.33
67	D4	83	А	N9-C8	-5.39	1.33	1.37
65	D2	248	G	N9-C4	-5.39	1.33	1.38
65	D2	273	G	N7-C5	-5.39	1.36	1.39
66	D3	1617	U	C4-C5	-5.39	1.38	1.43
30	CI	128	VAL	CB-CG1	-5.39	1.41	1.52
66	D3	956	С	N1-C2	-5.39	1.34	1.40
67	D4	62	С	N3-C4	-5.39	1.30	1.33
7	UG	139	TRP	CE3-CZ3	-5.38	1.29	1.38
50	DF	95	ASN	CB-CG	-5.38	1.38	1.51
58	DQ	92	TYR	CD1-CE1	-5.38	1.31	1.39
65	D2	476	А	N7-C5	-5.38	1.36	1.39
4	UD	321	VAL	CB-CG1	-5.38	1.41	1.52
67	D4	45	U	N3-C4	-5.38	1.33	1.38
7	UG	196	LEU	CG-CD2	-5.38	1.31	1.51
65	D2	88	U	C2-N3	-5.38	1.33	1.37
65	D2	244	U	N3-C4	-5.38	1.33	1.38
66	D3	559	С	C2-N3	-5.38	1.31	1.35
66	D3	566	С	N1-C6	-5.38	1.33	1.37
18	UR	555	TRP	CD2-CE2	-5.38	1.34	1.41
65	D2	320	A	N7-C5	-5.38	1.36	1.39
66	D3	1042	G	N9-C8	-5.38	1.34	1.37
12	UL	854	CYS	CB-SG	-5.38	1.73	1.81
65	D2	272	A	N3-C4	-5.38	1.31	1.34
65	D2	473	A	N7-C5	-5.38	1.36	1.39
18	UR	429	TYR	CE2-CZ	-5.38	1.31	1.38
66	D3	561	G	N7-C5	-5.37	1.36	1.39
66	D3	1494	С	N1-C6	-5.37	1.33	1.37
65	D2	160	l C	N1-C2	-5.37	1.34	1.40



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	944	A	N3-C4	-5.37	1.31	1.34
66	D3	1153	G	C5-C4	-5.37	1.34	1.38
66	D3	1471	А	C5-C6	-5.37	1.36	1.41
67	D4	333	U	C2-N3	-5.37	1.33	1.37
65	D2	273	G	C2-N3	-5.37	1.28	1.32
65	D2	446	U	C2-N3	-5.37	1.33	1.37
65	D2	459	U	C4-C5	-5.37	1.38	1.43
66	D3	575	С	N1-C2	-5.37	1.34	1.40
1	UA	577	SER	CA-CB	-5.36	1.45	1.52
66	D3	929	А	N3-C4	-5.36	1.31	1.34
66	D3	1038	U	N1-C6	-5.36	1.33	1.38
66	D3	1607	G	N9-C4	-5.36	1.33	1.38
66	D3	569	С	N3-C4	-5.36	1.30	1.33
66	D3	936	G	N7-C5	-5.36	1.36	1.39
65	D2	298	А	C6-N6	-5.36	1.29	1.33
65	D2	396	А	C6-N1	-5.36	1.31	1.35
65	D2	447	G	C2-N3	-5.36	1.28	1.32
46	JP	362	TYR	CD1-CE1	-5.36	1.31	1.39
66	D3	867	G	C6-N1	-5.35	1.35	1.39
25	CA	143	VAL	CB-CG1	-5.35	1.41	1.52
44	JN	221	VAL	CB-CG1	-5.35	1.41	1.52
1	UA	425	PHE	CD2-CE2	-5.35	1.28	1.39
21	UU	443	TRP	CE3-CZ3	-5.35	1.29	1.38
21	UU	149	TYR	CD2-CE2	-5.35	1.31	1.39
66	D3	553	G	N1-C2	-5.35	1.33	1.37
33	CL	939	TYR	CE1-CZ	-5.35	1.31	1.38
41	JJ	130	MET	CA-CB	5.35	1.65	1.53
66	D3	868	G	C5-C4	-5.35	1.34	1.38
65	D2	89	C	C2-N3	-5.34	1.31	1.35
66	D3	973	A	N9-C4	-5.34	1.34	1.37
67	D4	32	G	N7-C5	-5.34	1.36	1.39
67	D4	331	A	C5-C6	-5.34	1.36	1.41
21	UU	593	PHE	CE1-CZ	-5.34	1.27	1.37
1	UA	52	TYR	CE2-CZ	-5.34	1.31	1.38
10	UJ	101	TYR	CE2-CZ	-5.34	1.31	1.38
1	UA	207	TYR	CD1-CE1	-5.34	1.31	1.39
65	D2	390	C	N3-C4	-5.34	1.30	1.33
66	D3	1580	C	N1-C6	-5.34	1.33	1.37
31	CJ	58	TYR	CE2-CZ	-5.34	1.31	1.38
46	JP	58	PHE	CB-CG	-5.34	1.42	1.51
30	CI	87	VAL	CB-CG1	-5.33	1.41	1.52
46	JP	288	TYR	CE2-CZ	-5.33	1.31	1.38



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
66	D3	1066	C	N1-C2	-5.33	1.34	1.40
66	D3	1590	G	N9-C4	-5.33	1.33	1.38
3	UC	582	VAL	CB-CG2	-5.33	1.41	1.52
21	UU	443	TRP	CG-CD1	-5.33	1.29	1.36
65	D2	487	A	C6-N1	-5.33	1.31	1.35
65	D2	452	А	C6-N1	-5.33	1.31	1.35
66	D3	1072	С	C5-C6	-5.33	1.30	1.34
33	CL	1074	GLN	CB-CG	-5.33	1.38	1.52
18	UR	515	THR	CB-CG2	-5.32	1.34	1.52
65	D2	387	С	C4-N4	-5.32	1.29	1.33
66	D3	597	G	C6-N1	-5.32	1.35	1.39
21	UU	183	VAL	CB-CG2	-5.32	1.41	1.52
65	D2	341	G	N1-C2	-5.32	1.33	1.37
65	D2	345	U	N3-C4	-5.32	1.33	1.38
66	D3	953	G	N1-C2	-5.32	1.33	1.37
10	UJ	221	VAL	CB-CG1	-5.32	1.41	1.52
46	JP	362	TYR	CD2-CE2	-5.32	1.31	1.39
58	DQ	92	TYR	CE2-CZ	-5.32	1.31	1.38
21	UU	654	TRP	CE3-CZ3	-5.32	1.29	1.38
31	CJ	131	CYS	CB-SG	-5.32	1.73	1.81
65	D2	392	U	N3-C4	-5.32	1.33	1.38
66	D3	11	A	C5-C4	-5.32	1.35	1.38
67	D4	328	A	N3-C4	-5.32	1.31	1.34
25	CA	240	VAL	CB-CG2	-5.31	1.41	1.52
66	D3	1478	G	N7-C5	-5.31	1.36	1.39
65	D2	254	С	N1-C2	-5.31	1.34	1.40
65	D2	339	А	N9-C4	-5.31	1.34	1.37
67	D4	37	G	C2-N3	-5.31	1.28	1.32
66	D3	919	A	N3-C4	-5.31	1.31	1.34
15	UO	108	TYR	CE1-CZ	-5.30	1.31	1.38
65	D2	299	G	N3-C4	-5.30	1.31	1.35
66	D3	11	A	N9-C4	-5.30	1.34	1.37
66	D3	1466	G	C6-N1	-5.30	1.35	1.39
66	D3	1582	U	C4-C5	-5.30	1.38	1.43
66	D3	953	G	C6-N1	-5.30	1.35	1.39
66	D3	1613	U	C4-O4	-5.30	1.19	1.23
66	D3	552	G	C5-C6	-5.30	1.37	1.42
67	D4	31	G	C2-N3	-5.30	1.28	1.32
10	UJ	262	VAL	CB-CG1	-5.30	1.41	1.52
43	JM	136	TYR	CD1-CE1	-5.30	1.31	1.39
46	JP	332	TYR	CE2-CZ	-5.30	1.31	1.38
65	D2	100	G	C5-C6	-5.30	1.37	1.42



OOnu	<i>nucu jron</i>	i previe	ius puyc.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
65	D2	450	G	C6-N1	-5.30	1.35	1.39
65	D2	348	U	C2-N3	-5.29	1.34	1.37
4	UD	201	VAL	CB-CG1	-5.29	1.41	1.52
4	UD	244	VAL	CB-CG2	-5.29	1.41	1.52
67	D4	40	А	C5-C6	-5.29	1.36	1.41
30	CI	44	TYR	CE1-CZ	-5.29	1.31	1.38
1	UA	279	PHE	CD2-CE2	-5.29	1.28	1.39
1	UA	704	TYR	CD1-CE1	-5.29	1.31	1.39
65	D2	274	С	N3-C4	-5.29	1.30	1.33
67	D4	325	С	N1-C2	-5.29	1.34	1.40
46	JP	375	TRP	CD2-CE2	-5.28	1.35	1.41
65	D2	410	A	N7-C5	-5.28	1.36	1.39
66	D3	939	А	N3-C4	-5.28	1.31	1.34
1	UA	401	VAL	CB-CG1	-5.28	1.41	1.52
21	UU	101	TYR	CE2-CZ	-5.28	1.31	1.38
65	D2	271	G	N1-C2	-5.28	1.33	1.37
66	D3	929	А	N7-C5	-5.28	1.36	1.39
66	D3	1593	А	C6-N1	-5.28	1.31	1.35
7	UG	173	TYR	CD1-CE1	-5.28	1.31	1.39
66	D3	938	G	N9-C8	-5.28	1.34	1.37
66	D3	1488	G	N9-C8	-5.28	1.34	1.37
65	D2	246	G	N9-C8	-5.27	1.34	1.37
65	D2	276	G	C5-C4	-5.27	1.34	1.38
65	D2	473	A	C5-C6	-5.27	1.36	1.41
66	D3	1167	G	C2-N3	-5.27	1.28	1.32
65	D2	85	G	C5-C4	-5.27	1.34	1.38
66	D3	601	А	N9-C4	-5.27	1.34	1.37
66	D3	1042	G	C5-C6	-5.27	1.37	1.42
65	D2	270	U	C4-C5	-5.27	1.38	1.43
1	UA	601	ILE	CB-CG2	-5.27	1.36	1.52
66	D3	1069	А	N3-C4	-5.27	1.31	1.34
66	D3	866	G	N7-C5	-5.26	1.36	1.39
66	D3	1612	U	C2-N3	-5.26	1.34	1.37
65	D2	258	С	N3-C4	-5.26	1.30	1.33
1	UA	50	PHE	CB-CG	-5.26	1.42	1.51
18	UR	178	VAL	CB-CG2	-5.26	1.41	1.52
18	UR	352	GLN	CB-CG	-5.26	1.38	1.52
66	D3	556	A	C5-C4	-5.26	1.35	1.38
66	D3	584	C	N1-C2	-5.26	1.34	1.40
66	D3	976	G	N7-C5	-5.26	1.36	1.39
66	D3	574	G	N7-C5	-5.26	1.36	1.39
1	UA	617	VAL	CB-CG1	-5.26	1.41	1.52



001000	naca jion	" proore	a page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
66	D3	568	G	N7-C5	-5.26	1.36	1.39
66	D3	938	G	C6-N1	-5.26	1.35	1.39
66	D3	554	С	N1-C2	-5.25	1.34	1.40
66	D3	572	С	C2-N3	-5.25	1.31	1.35
66	D3	1047	G	N1-C2	-5.25	1.33	1.37
7	UG	452	VAL	CB-CG1	-5.25	1.41	1.52
65	D2	163	G	C5-C6	-5.25	1.37	1.42
65	D2	259	G	C5-C4	-5.25	1.34	1.38
66	D3	1465	С	N1-C2	-5.25	1.34	1.40
66	D3	935	U	C2-N3	-5.25	1.34	1.37
31	CJ	157	PHE	CD2-CE2	-5.25	1.28	1.39
46	JP	287	TYR	CE2-CZ	-5.25	1.31	1.38
65	D2	334	G	N9-C8	-5.25	1.34	1.37
66	D3	1026	A	N9-C4	-5.25	1.34	1.37
30	CI	148	TYR	CD1-CE1	-5.25	1.31	1.39
66	D3	878	G	N9-C8	-5.24	1.34	1.37
66	D3	1034	С	C4-C5	-5.24	1.38	1.43
66	D3	1067	С	N1-C2	-5.24	1.34	1.40
66	D3	1074	G	N9-C4	-5.24	1.33	1.38
67	D4	43	С	C4-C5	-5.24	1.38	1.43
67	D4	83	А	C5-C6	-5.24	1.36	1.41
44	JN	263	VAL	CB-CG2	-5.24	1.41	1.52
66	D3	1485	С	C2-N3	-5.24	1.31	1.35
15	UO	85	TYR	CD1-CE1	-5.24	1.31	1.39
65	D2	380	А	C5-C6	-5.24	1.36	1.41
67	D4	57	А	N7-C5	-5.24	1.36	1.39
15	UO	420	GLU	CB-CG	-5.24	1.42	1.52
66	D3	1170	G	C5-C4	-5.24	1.34	1.38
5	UE	204	SER	CA-CB	-5.23	1.45	1.52
65	D2	458	A	N9-C4	-5.23	1.34	1.37
66	D3	926	А	C5-C4	-5.23	1.35	1.38
66	D3	1153	G	N7-C5	-5.23	1.36	1.39
65	D2	308	А	N1-C2	-5.23	1.29	1.34
65	D2	335	G	N3-C4	-5.23	1.31	1.35
65	D2	381	G	N9-C4	-5.23	1.33	1.38
7	UG	149	PHE	CB-CG	-5.23	1.42	1.51
1	UA	438	VAL	CB-CG1	-5.23	1.41	1.52
65	D2	100	G	N9-C4	-5.23	1.33	1.38
65	D2	263	C	N1-C6	-5.23	1.34	1.37
66	D3	485	A	N3-C4	-5.22	1.31	1.34
66	D3	556	A	N7-C5	-5.22	1.36	1.39
66	D3	878	G	N1-C2	-5.22	1.33	1.37



Continued	from	previous	page
• • • • • • • • • • • •	J	P	F

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1151	А	C5-C6	-5.22	1.36	1.41
67	D4	63	С	C5-C6	-5.22	1.30	1.34
65	D2	87	С	N3-C4	-5.22	1.30	1.33
65	D2	332	U	N3-C4	-5.22	1.33	1.38
1	UA	372	TRP	CD2-CE2	-5.22	1.35	1.41
66	D3	28	А	N3-C4	-5.22	1.31	1.34
66	D3	1166	А	C2-N3	-5.22	1.28	1.33
66	D3	1632	С	N1-C2	-5.22	1.34	1.40
21	UU	474	PHE	CB-CG	-5.22	1.42	1.51
65	D2	246	G	N3-C4	-5.22	1.31	1.35
66	D3	576	G	N9-C8	-5.22	1.34	1.37
66	D3	594	А	C5-C6	-5.22	1.36	1.41
66	D3	11	А	C5-C6	-5.21	1.36	1.41
60	DW	49	GLU	CG-CD	-5.21	1.44	1.51
30	CI	160	TRP	CD2-CE2	-5.21	1.35	1.41
65	D2	146	G	N3-C4	-5.21	1.31	1.35
65	D2	253	U	N1-C2	-5.21	1.33	1.38
65	D2	268	G	C5-C4	-5.21	1.34	1.38
66	D3	957	G	N7-C5	-5.21	1.36	1.39
46	JP	94	TYR	CE2-CZ	-5.21	1.31	1.38
65	D2	246	G	C8-N7	-5.21	1.27	1.30
65	D2	266	U	N1-C2	-5.21	1.33	1.38
1	UA	315	GLU	CB-CG	-5.21	1.42	1.52
1	UA	567	ASP	CB-CG	-5.21	1.40	1.51
65	D2	242	С	C2-N3	-5.21	1.31	1.35
65	D2	302	А	N9-C4	-5.21	1.34	1.37
67	D4	69	А	N9-C8	-5.21	1.33	1.37
33	CL	987	TYR	CD2-CE2	-5.21	1.31	1.39
66	D3	957	G	N9-C8	-5.20	1.34	1.37
67	D4	323	G	C5-C4	-5.20	1.34	1.38
66	D3	1586	А	N1-C2	-5.20	1.29	1.34
66	D3	-4	A	C5-C6	-5.20	1.36	1.41
66	D3	1592	А	C5-C6	-5.20	1.36	1.41
46	JP	71	TYR	CE1-CZ	-5.20	1.31	1.38
66	D3	944	А	N9-C4	-5.20	1.34	1.37
65	D2	371	G	C5-C4	-5.19	1.34	1.38
1	UA	7	PHE	CD2-CE2	-5.19	1.28	1.39
66	D3	315	А	N9-C4	-5.19	1.34	1.37
67	D4	84	U	C4-O4	-5.19	1.19	1.23
1	UA	433	PHE	CD2-CE2	-5.19	1.28	1.39
4	UD	139	CYS	CB-SG	-5.19	1.73	1.81
65	D2	305	A	N3-C4	-5.19	1.31	1.34



$\alpha \cdot \cdot \cdot \cdot$	C		
Continued	trom	previous	page
		1	1 0

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	930	А	C8-N7	-5.19	1.27	1.31
21	UU	578	VAL	CB-CG2	-5.19	1.42	1.52
66	D3	1749	А	N9-C4	-5.19	1.34	1.37
67	D4	19	А	N9-C4	-5.19	1.34	1.37
66	D3	6	G	C2-N3	-5.19	1.28	1.32
46	JP	58	PHE	CD2-CE2	-5.18	1.28	1.39
65	D2	250	G	N7-C5	-5.18	1.36	1.39
66	D3	478	А	C5-C6	-5.18	1.36	1.41
66	D3	1527	С	C4-C5	-5.18	1.38	1.43
66	D3	1617	U	N1-C6	-5.18	1.33	1.38
67	D4	79	G	C2-N3	-5.18	1.28	1.32
7	UG	198	PHE	CE2-CZ	-5.18	1.27	1.37
23	UX	71	PHE	CB-CG	-5.18	1.42	1.51
46	JP	58	PHE	CG-CD2	-5.18	1.30	1.38
66	D3	1465	С	C2-N3	-5.18	1.31	1.35
67	D4	82	G	N7-C5	-5.18	1.36	1.39
31	CJ	123	VAL	CB-CG2	-5.18	1.42	1.52
21	UU	49	TYR	CE2-CZ	-5.18	1.31	1.38
33	CL	939	TYR	CD2-CE2	-5.18	1.31	1.39
65	D2	243	А	N9-C8	-5.18	1.33	1.37
65	D2	386	А	N9-C4	-5.18	1.34	1.37
66	D3	16	G	N3-C4	-5.18	1.31	1.35
66	D3	578	U	N3-C4	-5.18	1.33	1.38
66	D3	1480	G	C5-C4	-5.18	1.34	1.38
10	UJ	192	TYR	CE1-CZ	-5.17	1.31	1.38
65	D2	290	G	C6-N1	-5.17	1.35	1.39
66	D3	593	U	C4-C5	-5.17	1.38	1.43
46	JP	287	TYR	CG-CD1	-5.17	1.32	1.39
66	D3	1048	G	C6-N1	-5.17	1.35	1.39
21	UU	443	TRP	CD2-CE2	-5.17	1.35	1.41
66	D3	1083	G	N1-C2	-5.17	1.33	1.37
67	D4	18	G	N9-C4	-5.17	1.33	1.38
65	D2	164	G	C8-N7	-5.17	1.27	1.30
65	D2	303	A	N9-C4	-5.17	1.34	1.37
65	D2	334	G	N1-C2	-5.17	1.33	1.37
30	CI	36	TYR	CG-CD2	-5.16	1.32	1.39
65	D2	84	G	N3-C4	-5.16	1.31	1.35
65	D2	296	C	C4-N4	-5.16	1.29	1.33
66	D3	946	U	C2-N3	-5.16	1.34	1.37
67	D4	329	С	C5-C6	-5.16	1.30	1.34
10	UJ	220	VAL	CB-CG2	-5.16	1.42	1.52
66	D3	561	G	N9-C4	-5.16	1.33	1.38



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
66	D3	942	G	C8-N7	-5.16	1.27	1.30
65	D2	143	А	N7-C5	-5.16	1.36	1.39
66	D3	1598	U	C4-C5	-5.16	1.39	1.43
67	D4	29	U	C5-C6	-5.16	1.29	1.34
66	D3	574	G	C6-N1	-5.16	1.35	1.39
66	D3	1479	А	N9-C4	-5.16	1.34	1.37
1	UA	118	PHE	CD2-CE2	-5.16	1.28	1.39
45	JO	146	VAL	CB-CG2	-5.16	1.42	1.52
65	D2	287	G	C8-N7	-5.16	1.27	1.30
66	D3	1039	А	N3-C4	-5.15	1.31	1.34
29	CH	444	PRO	C-N	-5.15	1.22	1.34
46	JP	36	GLU	CB-CG	-5.15	1.42	1.52
65	D2	289	U	N3-C4	-5.15	1.33	1.38
66	D3	1082	С	C2-N3	-5.15	1.31	1.35
1	UA	587	PHE	CD2-CE2	-5.15	1.28	1.39
65	D2	160	С	C4-C5	-5.15	1.38	1.43
65	D2	392	U	C5-C6	-5.15	1.29	1.34
66	D3	488	G	N9-C8	-5.15	1.34	1.37
66	D3	940	A	N7-C5	-5.15	1.36	1.39
67	D4	23	U	N3-C4	-5.15	1.33	1.38
7	UG	95	VAL	CB-CG1	-5.15	1.42	1.52
33	CL	992	GLU	CB-CG	-5.15	1.42	1.52
4	UD	283	VAL	CB-CG1	-5.15	1.42	1.52
27	CE	428	ASN	CB-CG	-5.15	1.39	1.51
66	D3	490	С	N1-C2	-5.15	1.35	1.40
17	UQ	876	PHE	CD2-CE2	-5.15	1.28	1.39
18	UR	172	TYR	CD2-CE2	-5.15	1.31	1.39
31	CJ	122	TYR	CB-CG	-5.15	1.44	1.51
23	UX	10	PHE	CD2-CE2	-5.14	1.28	1.39
66	D3	874	С	C2-N3	-5.14	1.31	1.35
66	D3	1065	A	C5-C4	-5.14	1.35	1.38
7	UG	338	VAL	CB-CG2	-5.14	1.42	1.52
31	CJ	115	VAL	CB-CG1	-5.14	1.42	1.52
65	D2	244	U	N1-C6	-5.14	1.33	1.38
66	D3	1166	A	N7-C5	-5.14	1.36	1.39
33	CL	860	TYR	CD2-CE2	-5.14	1.31	1.39
66	D3	942	G	N9-C4	-5.14	1.33	1.38
1	UA	360	VAL	CB-CG1	-5.14	1.42	1.52
21	UU	27	PHE	CD2-CE2	-5.14	1.28	1.39
66	D3	1575	G	C5-C4	-5.14	1.34	1.38
$2\overline{6}$	CD	20	VAL	CB-CG2	-5.14	1.42	1.52
65	D2	473	A	N1-C2	-5.14	1.29	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	375	С	N1-C6	-5.14	1.34	1.37
4	UD	214	SER	CA-CB	-5.13	1.45	1.52
23	UX	13	VAL	CB-CG1	-5.13	1.42	1.52
1	UA	329	VAL	CB-CG1	-5.13	1.42	1.52
5	UE	292	TYR	CD1-CE1	-5.13	1.31	1.39
61	DX	136	TRP	CB-CG	-5.13	1.41	1.50
66	D3	553	G	C8-N7	-5.13	1.27	1.30
66	D3	587	С	N1-C6	-5.13	1.34	1.37
67	D4	28	А	N9-C4	-5.13	1.34	1.37
65	D2	99	U	C4-C5	-5.13	1.39	1.43
66	D3	940	А	C5-C4	-5.13	1.35	1.38
66	D3	1114	G	C6-N1	-5.13	1.35	1.39
67	D4	84	U	N1-C6	-5.13	1.33	1.38
46	JP	419	VAL	CB-CG2	-5.13	1.42	1.52
58	DQ	112	TYR	CE2-CZ	-5.13	1.31	1.38
65	D2	257	G	N7-C5	-5.13	1.36	1.39
66	D3	1157	A	C5-C4	-5.13	1.35	1.38
67	D4	21	С	C5-C6	-5.13	1.30	1.34
7	UG	255	THR	C-N	-5.13	1.22	1.34
46	JP	287	TYR	CD2-CE2	-5.13	1.31	1.39
65	D2	245	С	C5-C6	-5.13	1.30	1.34
67	D4	37	G	C5-C6	-5.13	1.37	1.42
67	D4	74	А	N7-C5	-5.13	1.36	1.39
66	D3	545	А	N9-C4	-5.12	1.34	1.37
67	D4	16	A	N9-C4	-5.12	1.34	1.37
11	UK	106	TYR	CE1-CZ	-5.12	1.31	1.38
46	JP	58	PHE	CE1-CZ	-5.12	1.27	1.37
65	D2	383	G	N9-C4	-5.12	1.33	1.38
66	D3	1468	U	N1-C2	-5.12	1.33	1.38
66	D3	1587	A	N1-C2	-5.12	1.29	1.34
5	UE	313	TYR	CD2-CE2	-5.12	1.31	1.39
66	D3	955	A	N9-C4	-5.12	1.34	1.37
67	D4	47	G	N9-C4	-5.12	1.33	1.38
11	UK	63	TYR	CD1-CE1	-5.12	1.31	1.39
17	UQ	876	PHE	CB-CG	-5.12	1.42	1.51
21	UU	529	TYR	CD1-CE1	-5.12	1.31	1.39
45	JO	57	TRP	CB-CG	-5.12	1.41	1.50
4	UD	267	PHE	CB-CG	-5.12	1.42	1.51
1	UA	644	ILE	CB-CG2	-5.12	1.36	1.52
18	UR	458	ILE	CB-CG2	-5.12	1.36	1.52
33	CL	899	VAL	CB-CG1	-5.12	1.42	1.52
66	D3	8	U	N1-C2	-5.12	1.33	1.38



OOnu	<i>nucu jron</i>	i previe	rus puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
66	D3	514	G	C6-N1	-5.12	1.35	1.39
67	D4	39	С	C4-C5	-5.12	1.38	1.43
10	UJ	262	VAL	CB-CG2	-5.11	1.42	1.52
46	JP	201	ILE	CB-CG2	-5.11	1.36	1.52
65	D2	285	U	C2-N3	-5.11	1.34	1.37
65	D2	309	А	C5-C6	-5.11	1.36	1.41
66	D3	1471	А	N7-C5	-5.11	1.36	1.39
67	D4	85	G	C5-C6	-5.11	1.37	1.42
67	D4	328	А	N7-C5	-5.11	1.36	1.39
46	JP	41	TYR	CD2-CE2	-5.11	1.31	1.39
46	JP	217	TRP	CB-CG	-5.11	1.41	1.50
65	D2	471	С	C4-C5	-5.11	1.38	1.43
66	D3	1617	U	C2-N3	-5.11	1.34	1.37
66	D3	1494	С	N3-C4	-5.11	1.30	1.33
67	D4	68	А	C8-N7	-5.11	1.27	1.31
65	D2	163	G	N7-C5	-5.11	1.36	1.39
66	D3	914	G	N9-C4	-5.11	1.33	1.38
66	D3	1480	G	N3-C4	-5.11	1.31	1.35
1	UA	532	VAL	CB-CG1	-5.11	1.42	1.52
33	CL	992	GLU	CG-CD	-5.11	1.44	1.51
65	D2	103	G	C8-N7	-5.11	1.27	1.30
66	D3	957	G	C5-C4	-5.11	1.34	1.38
14	UN	847	VAL	CB-CG1	-5.10	1.42	1.52
1	UA	141	VAL	CB-CG2	-5.10	1.42	1.52
1	UA	340	LYS	CA-CB	-5.10	1.42	1.53
1	UA	419	TYR	CD1-CE1	-5.10	1.31	1.39
65	D2	393	C	N3-C4	-5.10	1.30	1.33
66	D3	966	A	N7-C5	-5.10	1.36	1.39
66	D3	1634	C	C4-C5	-5.10	1.38	1.43
33	CL	969	VAL	CB-CG1	-5.10	1.42	1.52
60	DW	63	VAL	CB-CG2	-5.10	1.42	1.52
66	D3	931	C	C2-N3	-5.10	1.31	1.35
66	D3	1748	G	N7-C5	-5.10	1.36	1.39
67	D4	326	U	N1-C2	-5.10	1.33	1.38
25	CA	230	TYR	CD2-CE2	-5.10	1.31	1.39
65	D2	275	A	C8-N7	-5.10	1.27	1.31
66	D3	953	G	C8-N7	-5.10	1.27	1.30
66	D3	1615	C	N1-C2	-5.10	1.35	1.40
65	D2	328	A	C5-C4	-5.10	1.35	1.38
7	UG	73	TYR	CD2-CE2	-5.09	1.31	1.39
7	UG	408	GLU	CB-CG	-5.09	1.42	1.52
54	DJ	113	VAL	CB-CG1	-5.09	1.42	1.52



0011111	naca jion	i previe	ius puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
65	D2	311	С	C5-C6	-5.09	1.30	1.34
66	D3	635	А	C5-C4	-5.09	1.35	1.38
66	D3	923	А	N9-C4	-5.09	1.34	1.37
4	UD	276	PHE	CB-CG	-5.09	1.42	1.51
21	UU	582	TRP	CB-CG	-5.09	1.41	1.50
66	D3	548	G	C2-N3	-5.09	1.28	1.32
46	JP	385	VAL	CB-CG2	-5.09	1.42	1.52
65	D2	297	U	N3-C4	-5.09	1.33	1.38
66	D3	555	А	N3-C4	-5.09	1.31	1.34
66	D3	1083	G	C5-C4	-5.09	1.34	1.38
66	D3	1133	А	N7-C5	-5.09	1.36	1.39
25	CA	309	TYR	CD1-CE1	-5.09	1.31	1.39
65	D2	100	G	N9-C8	-5.09	1.34	1.37
11	UK	63	TYR	CE1-CZ	-5.09	1.31	1.38
65	D2	379	А	N9-C4	-5.09	1.34	1.37
66	D3	7	G	C2-N3	-5.09	1.28	1.32
66	D3	7	G	N9-C4	-5.09	1.33	1.38
66	D3	553	G	C5-C6	-5.08	1.37	1.42
10	UJ	142	TYR	CE2-CZ	-5.08	1.31	1.38
25	CA	193	VAL	CB-CG2	-5.08	1.42	1.52
46	JP	356	TYR	CD2-CE2	-5.08	1.31	1.39
66	D3	877	G	C2-N3	-5.08	1.28	1.32
67	D4	80	U	N1-C6	-5.08	1.33	1.38
7	UG	198	PHE	CG-CD1	-5.08	1.31	1.38
66	D3	545	A	N9-C8	-5.08	1.33	1.37
66	D3	937	С	C4-C5	-5.08	1.38	1.43
66	D3	1583	A	N7-C5	-5.08	1.36	1.39
65	D2	297	U	N1-C2	-5.07	1.33	1.38
66	D3	1598	U	C2-N3	-5.07	1.34	1.37
65	D2	305	A	N9-C8	-5.07	1.33	1.37
66	D3	578	U	N1-C6	-5.07	1.33	1.38
66	D3	1069	A	C8-N7	-5.07	1.28	1.31
67	D4	31	G	N9-C8	-5.07	1.34	1.37
1	UA	15	TYR	CD1-CE1	-5.07	1.31	1.39
67	D4	64	A	P-O5'	-5.07	1.54	1.59
1	UA	458	TRP	CE3-CZ3	-5.07	1.29	1.38
65	D2	235	A	C5-C6	-5.07	1.36	1.41
66	D3	1583	A	C5-C4	-5.07	1.35	1.38
67	D4	64	A	C6-N1	-5.07	1.32	1.35
15	UO	255	VAL	CB-CG2	-5.06	1.42	1.52
66	D3	1583	A	C6-N1	-5.06	1.32	1.35
65	D2	145	A	N3-C4	-5.06	1.31	1.34



00.000	itaca ji on	Procee	ac page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	D2	254	C	N3-C4	-5.06	1.30	1.33
65	D2	337	G	N9-C8	-5.06	1.34	1.37
66	D3	551	G	N1-C2	-5.06	1.33	1.37
66	D3	1067	С	N3-C4	-5.06	1.30	1.33
66	D3	1596	С	C2-N3	-5.06	1.31	1.35
66	D3	1589	С	C2-N3	-5.06	1.31	1.35
33	CL	811	VAL	CB-CG2	-5.06	1.42	1.52
66	D3	564	G	N7-C5	-5.06	1.36	1.39
66	D3	15	U	C5-C6	-5.06	1.29	1.34
66	D3	485	А	N9-C4	-5.06	1.34	1.37
67	D4	40	А	N9-C4	-5.06	1.34	1.37
1	UA	33	VAL	CB-CG1	-5.05	1.42	1.52
7	UG	185	HIS	CA-CB	-5.05	1.42	1.53
65	D2	85	G	C2-N3	-5.05	1.28	1.32
65	D2	338	А	N1-C2	-5.05	1.29	1.34
65	D2	453	А	N7-C5	-5.05	1.36	1.39
66	D3	568	G	N3-C4	-5.05	1.31	1.35
66	D3	1530	С	N3-C4	-5.05	1.30	1.33
67	D4	36	С	N1-C6	-5.05	1.34	1.37
1	UA	629	PHE	CD2-CE2	-5.05	1.29	1.39
6	UF	105	GLN	CB-CG	-5.05	1.39	1.52
17	UQ	311	TYR	CE1-CZ	-5.05	1.31	1.38
1	UA	287	TYR	CD2-CE2	-5.05	1.31	1.39
66	D3	31	С	N1-C6	-5.05	1.34	1.37
66	D3	969	С	N3-C4	-5.05	1.30	1.33
67	D4	37	G	N1-C2	-5.05	1.33	1.37
65	D2	336	G	C2-N3	-5.05	1.28	1.32
65	D2	337	G	C6-N1	-5.05	1.36	1.39
65	D2	353	A	C5-C6	-5.05	1.36	1.41
7	UG	147	GLU	CG-CD	-5.05	1.44	1.51
66	D3	1039	А	N9-C4	-5.05	1.34	1.37
7	UG	118	TYR	CD2-CE2	-5.05	1.31	1.39
66	D3	-4	А	N3-C4	-5.05	1.31	1.34
66	D3	30	G	N7-C5	-5.05	1.36	1.39
33	CL	991	PHE	CD1-CE1	-5.04	1.29	1.39
58	DQ	60	PHE	CD1-CE1	-5.04	1.29	1.39
65	D2	448	G	N7-C5	-5.04	1.36	1.39
58	DQ	96	TYR	CG-CD1	-5.04	1.32	1.39
66	D3	557	G	N9-C4	-5.04	1.33	1.38
65	D2	463	A	C6-N1	-5.04	1.32	1.35
30	CI	5	LEU	CG-CD1	-5.04	1.33	1.51
65	D2	294	U	N3-C4	-5.04	1.33	1.38


001000	naca ji cii	" procee	a page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	D4	56	A	C5-C4	-5.04	1.35	1.38
66	D3	927	С	N1-C6	-5.04	1.34	1.37
67	D4	44	U	N1-C2	-5.04	1.34	1.38
66	D3	589	С	C4-C5	-5.04	1.39	1.43
66	D3	915	А	C5-C6	-5.04	1.36	1.41
66	D3	1046	G	C6-N1	-5.04	1.36	1.39
46	JP	35	PHE	CD1-CE1	-5.03	1.29	1.39
66	D3	592	A	C5-C4	-5.03	1.35	1.38
66	D3	1078	С	C5-C6	-5.03	1.30	1.34
58	DQ	31	VAL	CB-CG1	-5.03	1.42	1.52
66	D3	926	А	C6-N1	-5.03	1.32	1.35
7	UG	134	VAL	CB-CG1	-5.03	1.42	1.52
30	CI	173	TYR	CD1-CE1	-5.03	1.31	1.39
65	D2	395	С	N3-C4	-5.03	1.30	1.33
65	D2	448	G	C2-N3	-5.03	1.28	1.32
65	D2	461	А	N3-C4	-5.03	1.31	1.34
65	D2	477	G	C2-N3	-5.03	1.28	1.32
65	D2	370	U	C2-N3	-5.03	1.34	1.37
66	D3	14	С	N1-C6	-5.03	1.34	1.37
66	D3	489	С	C2-N3	-5.03	1.31	1.35
66	D3	1586	А	N9-C8	-5.03	1.33	1.37
67	D4	326	U	C5-C6	-5.03	1.29	1.34
65	D2	306	G	C6-N1	-5.02	1.36	1.39
67	D4	25	U	N3-C4	-5.02	1.33	1.38
15	UO	283	VAL	CB-CG2	-5.02	1.42	1.52
31	CJ	273	VAL	CB-CG1	-5.02	1.42	1.52
33	CL	939	TYR	CD1-CE1	-5.02	1.31	1.39
66	D3	10	G	C8-N7	-5.02	1.27	1.30
66	D3	503	G	C6-N1	-5.02	1.36	1.39
67	D4	53	U	C2-N3	-5.02	1.34	1.37
65	D2	303	A	N7-C5	-5.02	1.36	1.39
21	UU	298	VAL	CB-CG1	-5.02	1.42	1.52
31	CJ	202	VAL	CB-CG1	-5.02	1.42	1.52
46	JP	362	TYR	CE1-CZ	-5.02	1.32	1.38
65	D2	485	G	N7-C5	-5.02	1.36	1.39
48	DA	155	TYR	CD1-CE1	-5.02	1.31	1.39
66	D3	941	A	N7-C5	-5.02	1.36	1.39
1	UA	677	PRO	CB-CG	-5.02	1.24	1.50
46	JP	57	PRO	CB-CG	-5.02	1.24	1.50
65	D2	285	U	N1-C2	-5.01	1.34	1.38
10	UJ	109	TRP	CB-CG	-5.01	1.41	1.50
66	D3	1622	G	C2-N3	-5.01	1.28	1.32

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
18	UR	268	TYR	CD2-CE2	-5.01	1.31	1.39
23	UX	10	PHE	CB-CG	-5.01	1.42	1.51
66	D3	868	G	N7-C5	-5.01	1.36	1.39
66	D3	567	А	N7-C5	-5.01	1.36	1.39
66	D3	1605	G	N7-C5	-5.01	1.36	1.39
67	D4	30	А	P-O5'	-5.01	1.54	1.59
65	D2	280	А	C5-C6	-5.01	1.36	1.41
67	D4	40	А	C6-N1	-5.01	1.32	1.35
66	D3	570	А	C5-C6	-5.01	1.36	1.41
1	UA	606	VAL	CB-CG1	-5.00	1.42	1.52
32	CK	477	GLU	CB-CG	-5.00	1.42	1.52
65	D2	327	А	N9-C4	-5.00	1.34	1.37
66	D3	1488	G	C5-C4	-5.00	1.34	1.38
65	D2	93	А	C5-C6	-5.00	1.36	1.41
66	D3	877	G	C6-N1	-5.00	1.36	1.39
66	D3	1075	С	N1-C6	-5.00	1.34	1.37
65	D2	244	U	C2-O2	-5.00	1.17	1.22
66	D3	551	G	C2-N3	-5.00	1.28	1.32
66	D3	1582	U	N3-C4	-5.00	1.33	1.38

Continued from previous page...

All (1402) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
65	D2	312	U	O4'-C1'-N1	19.10	123.48	108.20
13	UM	443	PRO	N-CD-CG	-16.65	78.23	103.20
67	D4	27	U	N3-C2-O2	-15.30	111.49	122.20
65	D2	233	G	N3-C4-C5	14.71	135.96	128.60
21	UU	494	LEU	CB-CG-CD2	-14.58	86.21	111.00
67	D4	62	С	C5-C6-N1	14.55	128.28	121.00
65	D2	233	G	N3-C4-N9	-14.18	117.49	126.00
66	D3	1527	С	C6-N1-C2	-13.97	114.71	120.30
7	UG	160	LEU	CA-CB-CG	13.86	147.18	115.30
65	D2	233	G	C2-N3-C4	-13.66	105.07	111.90
66	D3	1481	С	C5-C6-N1	13.58	127.79	121.00
67	D4	55	А	C6-C5-N7	-13.54	122.83	132.30
67	D4	55	А	N1-C6-N6	13.37	126.62	118.60
65	D2	341	G	C4-C5-N7	13.25	116.10	110.80
66	D3	1159	С	C5-C6-N1	13.24	127.62	121.00
65	D2	311	С	C2-N3-C4	-13.17	113.32	119.90
67	D4	55	А	N9-C4-C5	-13.10	100.56	105.80
65	D2	311	С	N3-C4-C5	12.78	127.01	121.90
66	D3	1527	С	N3-C2-O2	-12.61	113.08	121.90



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	61	G	C4-C5-N7	12.20	115.68	110.80
67	D4	61	G	C5-C6-O6	-12.09	121.34	128.60
13	UM	443	PRO	CA-CB-CG	-12.05	81.11	104.00
65	D2	341	G	C6-C5-N7	-12.01	123.20	130.40
65	D2	301	U	O5'-P-OP2	-11.89	95.00	105.70
66	D3	959	U	N3-C2-O2	-11.77	113.96	122.20
65	D2	310	U	N3-C2-O2	-11.64	114.05	122.20
65	D2	284	U	C5-C6-N1	11.59	128.49	122.70
66	D3	1602	С	O5'-P-OP1	-11.57	95.28	105.70
67	D4	55	А	C8-N9-C1'	-11.42	107.15	127.70
65	D2	312	U	N1-C1'-C2'	11.40	128.83	114.00
65	D2	89	С	N3-C4-C5	11.40	126.46	121.90
66	D3	564	G	C5-N7-C8	-11.31	98.64	104.30
13	UM	443	PRO	CB-CG-CD	11.19	150.14	106.50
65	D2	311	С	C5-C6-N1	-11.19	115.41	121.00
65	D2	311	С	P-O3'-C3'	10.98	132.88	119.70
65	D2	281	G	C4-C5-N7	10.96	115.18	110.80
66	D3	1490	C	N3-C4-C5	10.93	126.27	121.90
66	D3	564	G	C4-C5-N7	10.91	115.17	110.80
67	D4	27	U	N1-C2-O2	10.90	130.43	122.80
66	D3	575	С	N3-C4-C5	10.88	126.25	121.90
65	D2	233	G	C5-N7-C8	-10.86	98.87	104.30
67	D4	90	С	N1-C2-O2	10.75	125.35	118.90
65	D2	524	U	OP1-P-O3'	-10.74	81.57	105.20
67	D4	61	G	C2-N3-C4	10.73	117.27	111.90
66	D3	1605	G	O5'-P-OP1	-10.66	96.11	105.70
66	D3	1069	A	C5-N7-C8	-10.49	98.65	103.90
66	D3	1483	A	N1-C6-N6	10.49	124.89	118.60
66	D3	1069	A	N7-C8-N9	10.48	119.04	113.80
67	D4	63	С	C6-N1-C2	-10.47	116.11	120.30
28	CG	89	ARG	NE-CZ-NH2	-10.43	115.09	120.30
65	D2	388	С	C6-N1-C2	-10.39	116.14	120.30
65	D2	86	С	O5'-P-OP1	-10.35	96.39	105.70
66	D3	1069	A	C8-N9-C4	-10.34	101.67	105.80
66	D3	1585	U	C5-C6-N1	10.32	127.86	122.70
66	D3	487	G	C5-C6-O6	-10.30	122.42	128.60
66	D3	575	С	C4-C5-C6	-10.29	112.25	117.40
65	D2	305	A	N1-C6-N6	-10.24	112.46	118.60
65	D2	328	A	C8-N9-C4	10.21	109.89	105.80
7	UG	372	LEU	CA-CB-CG	10.20	138.76	115.30
67	D4	62	C	C6-N1-C2	-10.19	116.22	120.30
67	D4	62	C	C5-C4-N4	-10.19	113.07	120.20



α \cdot \cdot \cdot	C	•	
1 Continued	trom	nromanic	naae
Continucu	11011	preduous	puyc
		1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	55	А	C4-N9-C1'	10.18	144.63	126.30
66	D3	1159	С	C6-N1-C2	-10.10	116.26	120.30
1	UA	519	LEU	CA-CB-CG	10.05	138.41	115.30
46	JP	50	LEU	CB-CG-CD2	-10.02	93.96	111.00
66	D3	638	U	N3-C2-O2	-10.01	115.19	122.20
65	D2	239	U	C5-C6-N1	-9.92	117.74	122.70
66	D3	9	U	O5'-P-OP1	-9.92	96.78	105.70
65	D2	310	U	N1-C2-O2	9.91	129.74	122.80
67	D4	59	G	C5-N7-C8	-9.89	99.36	104.30
66	D3	268	С	N1-C2-O2	9.87	124.82	118.90
65	D2	332	U	N3-C2-O2	-9.78	115.36	122.20
66	D3	1481	С	C4-C5-C6	-9.77	112.52	117.40
67	D4	62	С	C4-C5-C6	-9.76	112.52	117.40
46	JP	201	ILE	CG1-CB-CG2	-9.74	89.96	111.40
67	D4	55	А	C4-C5-N7	9.72	115.56	110.70
66	D3	1483	A	C4-C5-N7	9.72	115.56	110.70
65	D2	314	U	N1-C2-O2	9.70	129.59	122.80
66	D3	489	С	C6-N1-C2	-9.70	116.42	120.30
67	D4	55	A	N3-C4-N9	9.64	135.12	127.40
66	D3	1084	А	C8-N9-C4	-9.64	101.94	105.80
66	D3	1527	С	C2-N1-C1'	9.61	129.37	118.80
10	UJ	234	LEU	CB-CG-CD2	-9.56	94.75	111.00
66	D3	1581	С	N3-C2-O2	-9.50	115.25	121.90
66	D3	1481	С	C6-N1-C2	-9.50	116.50	120.30
66	D3	1599	С	C6-N1-C2	-9.49	116.50	120.30
67	D4	57	A	C8-N9-C4	-9.45	102.02	105.80
65	D2	233	G	N1-C6-O6	9.42	125.55	119.90
66	D3	1174	С	N3-C2-O2	-9.38	115.33	121.90
65	D2	137	С	C6-N1-C2	-9.35	116.56	120.30
67	D4	24	U	N3-C2-O2	-9.35	115.66	122.20
66	D3	1633	A	N1-C6-N6	-9.34	112.99	118.60
65	D2	323	A	N1-C6-N6	9.29	124.17	118.60
65	D2	312	U	C6-N1-C1'	9.27	134.18	121.20
67	D4	61	G	N3-C4-N9	9.21	131.53	126.00
65	D2	393	С	O5'-P-OP2	-9.16	97.45	105.70
66	D3	374	U	C2-N1-C1'	9.16	128.69	117.70
67	D4	55	A	C4-C5-C6	9.16	121.58	117.00
66	D3	1174	C	N1-C2-O2	9.12	124.37	118.90
65	D2	341	G	N3-C4-N9	9.09	131.45	126.00
65	D2	323	A	C4-C5-N7	9.08	115.24	110.70
66	D3	496	G	C4-C5-N7	9.08	$114.4\overline{3}$	110.80
30	CI	77	LEU	CB-CG-CD2	-9.05	95.62	111.00



α \cdot \cdot \cdot	C	•	
Continued	trom	nremous	naae
Contentaca	JIONO	preciouo	pago

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	57	А	N9-C4-C5	9.02	109.41	105.80
65	D2	298	А	C5-C6-N1	9.01	122.21	117.70
65	D2	289	U	C5-C6-N1	9.00	127.20	122.70
43	JM	81	VAL	C-N-CA	8.99	144.17	121.70
65	D2	233	G	C4-C5-N7	8.97	114.39	110.80
67	D4	55	А	C5-C6-N6	-8.93	116.55	123.70
65	D2	341	G	C5-C6-O6	-8.93	123.24	128.60
67	D4	58	А	N1-C6-N6	-8.91	113.26	118.60
67	D4	24	U	C5-C6-N1	-8.90	118.25	122.70
65	D2	314	U	N3-C2-O2	-8.87	115.99	122.20
65	D2	280	А	C5-N7-C8	-8.83	99.48	103.90
32	CK	440	LEU	CA-CB-CG	8.81	135.56	115.30
67	D4	58	А	C5-C6-N1	8.81	122.10	117.70
66	D3	374	U	N1-C2-O2	8.79	128.96	122.80
65	D2	314	U	C2-N1-C1'	8.78	128.24	117.70
65	D2	312	U	C2-N1-C1'	-8.76	107.19	117.70
66	D3	638	U	N1-C2-O2	8.76	128.93	122.80
25	CA	306	LEU	CA-CB-CG	8.76	135.44	115.30
65	D2	309	А	O5'-P-OP2	-8.75	97.82	105.70
66	D3	583	С	N1-C2-O2	8.71	124.13	118.90
65	D2	524	U	OP2-P-O3'	-8.71	86.03	105.20
67	D4	75	С	O5'-P-OP2	-8.71	97.86	105.70
65	D2	233	G	N3-C2-N2	-8.70	113.81	119.90
46	JP	300	VAL	CG1-CB-CG2	-8.63	97.09	110.90
66	D3	1486	G	C8-N9-C4	-8.61	102.95	106.40
66	D3	1486	G	N7-C8-N9	8.61	117.41	113.10
67	D4	63	С	C5-C6-N1	8.61	125.31	121.00
66	D3	956	C	C5-C6-N1	8.61	125.30	121.00
65	D2	277	С	N3-C2-O2	-8.61	115.88	121.90
66	D3	1069	А	C4-C5-N7	8.61	115.00	110.70
66	D3	583	С	N3-C2-O2	-8.57	115.90	121.90
65	D2	323	A	C6-C5-N7	-8.55	126.32	132.30
66	D3	934	С	C6-N1-C2	-8.54	116.88	120.30
65	D2	273	G	N1-C6-O6	-8.53	114.78	119.90
65	D2	338	A	N9-C4-C5	8.52	109.21	105.80
67	D4	27	U	C2-N1-C1'	8.52	127.92	117.70
66	D3	1581	С	N1-C2-O2	8.51	124.01	118.90
67	D4	24	U	N1-C2-O2	8.51	128.75	122.80
65	D2	299	G	N1-C6-O6	-8.50	114.80	119.90
65	D2	338	A	N1-C6-N6	-8.49	113.51	118.60
21	UU	522	LEU	CA-CB-CG	8.49	134.82	115.30
65	D2	394	U	C2-N1-C1'	8.49	$1\overline{27.89}$	117.70



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
65	D2	312	U	C3'-C2'-C1'	-8.46	94.73	101.50
66	D3	1492	A	N1-C6-N6	-8.44	113.53	118.60
67	D4	59	G	N7-C8-N9	8.43	117.32	113.10
66	D3	1483	А	C5-C6-N6	-8.43	116.96	123.70
65	D2	312	U	N1-C2-N3	8.43	119.96	114.90
45	JO	116	ILE	CG1-CB-CG2	-8.41	92.89	111.40
66	D3	1037	С	C5-C4-N4	-8.41	114.31	120.20
65	D2	143	A	C4-C5-N7	8.40	114.90	110.70
66	D3	1040	G	O5'-P-OP2	-8.39	98.15	105.70
66	D3	489	C	N3-C2-O2	-8.39	116.03	121.90
67	D4	61	G	C4-N9-C1'	8.38	137.40	126.50
64	Dc	12	VAL	CG1-CB-CG2	-8.37	97.50	110.90
66	D3	1611	А	C8-N9-C4	8.37	109.15	105.80
65	D2	310	U	N3-C4-O4	-8.36	113.55	119.40
67	D4	55	А	O4'-C1'-N9	8.35	114.88	108.20
66	D3	1173	С	C5-C6-N1	8.35	125.17	121.00
65	D2	403	С	C6-N1-C2	-8.30	116.98	120.30
67	D4	30	А	O5'-P-OP2	-8.30	98.23	105.70
46	JP	400	LEU	CB-CG-CD2	-8.30	96.90	111.00
1	UA	560	ILE	CG1-CB-CG2	-8.29	93.16	111.40
66	D3	1628	U	C5-C4-O4	-8.28	120.94	125.90
65	D2	143	A	C5-N7-C8	-8.27	99.76	103.90
1	UA	110	LEU	CA-CB-CG	8.26	134.29	115.30
65	D2	341	G	N7-C8-N9	8.26	117.23	113.10
66	D3	1483	A	N9-C4-C5	-8.24	102.50	105.80
67	D4	59	G	C4-C5-N7	8.22	114.09	110.80
65	D2	278	G	C8-N9-C4	8.21	109.68	106.40
65	D2	280	A	C2-N3-C4	-8.21	106.49	110.60
65	D2	311	С	C6-N1-C2	8.21	123.58	120.30
66	D3	542	A	O4'-C1'-N9	8.20	114.76	108.20
66	D3	554	С	C2-N3-C4	-8.18	115.81	119.90
66	D3	487	G	C6-C5-N7	-8.18	125.49	130.40
31	CJ	157	PHE	N-CA-C	8.17	133.06	111.00
65	D2	525	U	OP1-P-OP2	8.17	131.85	119.60
66	D3	374	U	N3-C2-O2	-8.16	116.49	122.20
66	D3	1037	С	C5-C6-N1	8.16	125.08	121.00
65	D2	284	U	C4-C5-C6	-8.16	114.81	119.70
65	D2	333	G	N3-C2-N2	-8.16	114.19	119.90
66	D3	870	C	N3-C4-C5	8.15	125.16	121.90
66	D3	872	G	C4-C5-N7	8.14	114.06	110.80
66	D3	1069	A	C6-C5-N7	-8.13	126.61	132.30
66	D3	1589	C	C6-N1-C2	-8.12	117.05	120.30



Continued	from	nrevious	naae
Commute	jiom	previous	page

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	UG	224	LEU	CB-CG-CD2	-8.09	97.25	111.00
66	D3	487	G	N9-C4-C5	-8.07	102.17	105.40
65	D2	311	С	N3-C4-N4	-8.06	112.36	118.00
66	D3	632	U	C5-C6-N1	8.06	126.73	122.70
67	D4	75	С	C4-C5-C6	-8.06	113.37	117.40
66	D3	1527	С	C4-C5-C6	8.05	121.43	117.40
66	D3	1604	U	O5'-P-OP1	-8.05	98.45	105.70
65	D2	535	G	N3-C4-N9	-8.04	121.17	126.00
66	D3	1490	С	C2-N3-C4	-8.03	115.88	119.90
67	D4	90	С	N3-C2-O2	-8.03	116.28	121.90
65	D2	341	G	C5-N7-C8	-8.03	100.29	104.30
67	D4	77	U	N3-C2-O2	-8.03	116.58	122.20
65	D2	341	G	C4-N9-C1'	8.02	136.93	126.50
65	D2	264	С	C6-N1-C2	-8.02	117.09	120.30
17	UQ	343	ASP	CB-CG-OD1	8.01	125.51	118.30
65	D2	400	С	C4-C5-C6	-8.01	113.40	117.40
18	UR	404	ILE	CG1-CB-CG2	-8.00	93.80	111.40
66	D3	583	С	C2-N1-C1'	8.00	127.60	118.80
67	D4	64	A	O5'-P-OP1	-8.00	98.50	105.70
30	CI	19	LEU	CB-CG-CD2	-7.99	97.41	111.00
1	UA	113	LEU	CB-CG-CD1	-7.99	97.42	111.00
65	D2	312	U	C5-C4-O4	7.99	130.69	125.90
66	D3	642	G	N3-C2-N2	-7.97	114.32	119.90
65	D2	281	G	C5-N7-C8	-7.97	100.31	104.30
66	D3	1620	С	C6-N1-C2	-7.96	117.12	120.30
36	JA	753	ASP	CB-CG-OD1	7.93	125.44	118.30
31	CJ	9	ARG	NE-CZ-NH2	-7.92	116.34	120.30
10	UJ	182	LEU	CB-CG-CD2	-7.91	97.55	111.00
7	UG	199	LEU	CA-CB-CG	7.90	133.48	115.30
1	UA	439	ASP	CB-CG-OD1	7.88	125.39	118.30
66	D3	31	С	C6-N1-C2	-7.87	117.15	120.30
66	D3	584	C	O5'-P-OP1	-7.87	98.61	105.70
65	D2	394	U	C5-C6-N1	7.86	126.63	122.70
65	D2	240	C	O5'-P-OP1	-7.86	98.63	105.70
65	D2	280	A	C8-N9-C4	-7.86	102.66	105.80
66	D3	959	U	N1-C2-O2	7.85	128.30	122.80
65	D2	280	A	N3-C4-N9	-7.81	121.15	127.40
66	D3	1159	C	N3-C4-N4	7.78	123.45	118.00
65	D2	323	A	C5-N7-C8	-7.77	100.02	103.90
65	D2	333	G	O5'-P-OP2	-7.76	98.71	105.70
66	D3	1037	C	C4-C5-C6	-7.76	113.52	117.40
66	D3	596	C	C6-N1-C2	-7.76	117.19	120.30



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
• • • • • • • • • • • •	J	P	r ~g = · · ·

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1174	С	C2-N1-C1'	7.74	127.31	118.80
66	D3	1488	G	N1-C6-O6	-7.73	115.26	119.90
66	D3	13	C	O5'-P-OP1	-7.72	98.75	105.70
66	D3	554	С	C5-C6-N1	-7.70	117.15	121.00
65	D2	472	A	C8-N9-C4	7.69	108.88	105.80
7	UG	330	LEU	CB-CG-CD2	-7.69	97.92	111.00
65	D2	444	U	O5'-P-OP1	-7.69	98.78	105.70
14	UN	277	ARG	NE-CZ-NH2	7.68	124.14	120.30
6	UF	127	LYS	CD-CE-NZ	-7.67	94.06	111.70
67	D4	62	С	N3-C4-N4	7.67	123.37	118.00
66	D3	890	С	N1-C2-O2	7.65	123.49	118.90
65	D2	313	А	O5'-P-OP1	-7.65	98.81	105.70
66	D3	24	U	C5-C6-N1	7.65	126.52	122.70
66	D3	564	G	N3-C4-C5	7.63	132.42	128.60
65	D2	275	А	C8-N9-C4	-7.62	102.75	105.80
65	D2	291	G	O5'-P-OP1	-7.62	98.85	105.70
66	D3	495	С	C2-N1-C1'	7.60	127.16	118.80
66	D3	933	А	C4-C5-N7	7.58	114.49	110.70
66	D3	1599	С	C5-C6-N1	7.58	124.79	121.00
66	D3	1610	G	N1-C6-O6	-7.57	115.36	119.90
67	D4	41	С	C2-N1-C1'	-7.57	110.48	118.80
66	D3	566	С	C5-C6-N1	7.56	124.78	121.00
67	D4	52	U	O5'-P-OP1	-7.56	98.90	105.70
66	D3	487	G	N1-C6-O6	7.55	124.43	119.90
65	D2	341	G	C8-N9-C4	-7.53	103.39	106.40
7	UG	138	ASP	CB-CG-OD1	7.52	125.06	118.30
9	UI	507	ARG	CA-CB-CG	7.52	129.93	113.40
50	DF	162	VAL	C-N-CA	7.51	140.47	121.70
66	D3	933	A	N9-C4-C5	-7.51	102.80	105.80
18	UR	514	LEU	CB-CG-CD1	-7.51	98.24	111.00
65	D2	143	A	C2-N3-C4	-7.51	106.85	110.60
1	UA	465	LEU	CA-CB-CG	7.50	132.54	115.30
1	UA	611	LEU	CB-CG-CD2	-7.49	98.26	111.00
7	UG	125	LEU	CB-CG-CD2	-7.48	98.28	111.00
66	D3	1527	C	N3-C4-C5	-7.48	118.91	121.90
66	D3	1078	C	C6-N1-C2	-7.47	117.31	120.30
65	D2	375	С	C6-N1-C2	-7.45	117.32	120.30
66	D3	487	G	C4-C5-N7	7.45	113.78	110.80
66	D3	1594	G	N1-C6-O6	-7.44	115.43	119.90
66	D3	1042	G	C8-N9-C4	7.43	109.37	106.40
66	D3	579	A	P-O3'-C3'	7.42	128.61	119.70
67	D4	61	G	C6-C5-N7	-7.42	125.95	130.40



α \cdot 1	C		
Continued	trom	previous	page
	J	1	r J

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	UJ	261	LEU	CB-CG-CD2	-7.42	98.39	111.00
65	D2	418	С	C6-N1-C2	-7.41	117.33	120.30
66	D3	539	G	C4-C5-N7	7.40	113.76	110.80
7	UG	249	LEU	CB-CG-CD2	-7.40	98.42	111.00
65	D2	312	U	C5-C6-N1	-7.39	119.00	122.70
65	D2	488	U	N3-C2-O2	-7.38	117.03	122.20
66	D3	1084	A	N7-C8-N9	7.38	117.49	113.80
67	D4	65	C	C6-N1-C2	-7.37	117.35	120.30
67	D4	73	А	N7-C8-N9	7.36	117.48	113.80
67	D4	73	A	C5-N7-C8	-7.35	100.23	103.90
65	D2	314	U	C5-C6-N1	7.34	126.37	122.70
15	UO	273	ILE	CG1-CB-CG2	-7.33	95.29	111.40
66	D3	586	G	N1-C6-O6	-7.32	115.51	119.90
65	D2	303	А	C5-C6-N1	7.31	121.35	117.70
65	D2	284	U	O5'-P-OP1	-7.30	99.13	105.70
65	D2	335	G	C4-C5-N7	7.30	113.72	110.80
65	D2	89	C	C4-C5-C6	-7.29	113.75	117.40
65	D2	535	G	C8-N9-C1'	7.29	136.48	127.00
65	D2	82	А	C5-C6-N1	7.29	121.34	117.70
67	D4	260	U	N1-C2-O2	7.26	127.89	122.80
10	UJ	73	LEU	CA-CB-CG	7.26	132.00	115.30
65	D2	296	С	N3-C4-C5	7.25	124.80	121.90
66	D3	487	G	N3-C4-N9	7.25	130.35	126.00
67	D4	33	A	P-O3'-C3'	7.25	128.40	119.70
66	D3	1584	G	N3-C4-N9	-7.24	121.66	126.00
67	D4	73	A	C8-N9-C4	-7.24	102.91	105.80
66	D3	1070	C	O5'-P-OP1	-7.23	99.19	105.70
66	D3	489	С	C2-N1-C1'	7.23	126.75	118.80
67	D4	60	A	C8-N9-C4	-7.23	102.91	105.80
44	JN	109	PRO	N-CA-CB	7.22	111.97	103.30
66	D3	870	С	N3-C4-N4	-7.22	112.94	118.00
65	D2	295	A	C8-N9-C4	-7.22	102.91	105.80
25	CB	268	VAL	CG1-CB-CG2	-7.21	99.36	110.90
25	CA	171	LEU	CB-CG-CD2	7.19	123.22	111.00
65	D2	469	С	C6-N1-C2	-7.18	117.43	120.30
65	D2	395	С	N3-C2-O2	-7.17	116.88	121.90
65	D2	273	G	N9-C4-C5	7.16	108.26	105.40
67	D4	260	U	C2-N1-C1'	7.16	126.29	117.70
66	D3	1495	C	C6-N1-C2	-7.16	117.44	120.30
7	UG	466	LEU	CB-CG-CD2	-7.15	98.84	111.00
66	D3	966	A	C8-N9-C4	-7.15	102.94	105.80
66	D3	268	C	N3-C2-O2	-7.15	116.90	121.90



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
30	CI	64	LEU	CB-CG-CD2	-7.14	98.86	111.00
67	D4	59	G	C2-N3-C4	-7.14	108.33	111.90
26	CD	38	ILE	CG1-CB-CG2	-7.14	95.69	111.40
66	D3	496	G	N1-C6-O6	7.14	124.18	119.90
65	D2	143	A	N3-C4-C5	7.13	131.79	126.80
67	D4	61	G	C5-C6-N1	7.13	115.07	111.50
66	D3	1060	U	C2-N1-C1'	7.13	126.26	117.70
66	D3	1483	A	C5-N7-C8	-7.13	100.33	103.90
65	D2	333	G	N1-C2-N2	7.12	122.61	116.20
65	D2	482	A	C5-C6-N1	7.09	121.25	117.70
65	D2	289	U	C4-C5-C6	-7.09	115.45	119.70
4	UD	272	LEU	CB-CG-CD2	-7.08	98.96	111.00
17	UQ	356	LEU	CA-CB-CG	7.08	131.59	115.30
65	D2	431	А	N9-C4-C5	-7.07	102.97	105.80
65	D2	535	G	C4-N9-C1'	-7.06	117.32	126.50
65	D2	461	А	N1-C6-N6	-7.05	114.37	118.60
66	D3	1159	С	C5-C4-N4	-7.05	115.27	120.20
65	D2	328	А	N7-C8-N9	-7.05	110.28	113.80
67	D4	57	А	N1-C6-N6	-7.04	114.38	118.60
12	UL	809	LEU	CB-CG-CD2	-7.03	99.05	111.00
66	D3	1613	U	C5-C6-N1	7.03	126.22	122.70
67	D4	61	G	C8-N9-C1'	-7.03	117.86	127.00
65	D2	325	U	N1-C2-O2	7.03	127.72	122.80
65	D2	331	U	O5'-P-OP1	-7.03	99.38	105.70
67	D4	24	U	C4-C5-C6	7.03	123.92	119.70
46	JP	83	LEU	CA-CB-CG	7.02	131.45	115.30
66	D3	639	U	O4'-C1'-N1	7.02	113.82	108.20
66	D3	1486	G	C6-C5-N7	-7.00	126.20	130.40
67	D4	27	U	C5-C4-O4	6.99	130.10	125.90
66	D3	864	U	C2-N1-C1'	6.99	126.09	117.70
66	D3	583	С	C6-N1-C1'	-6.99	112.41	120.80
30	CI	61	LEU	CA-CB-CG	6.99	131.37	115.30
65	D2	302	A	C8-N9-C4	6.98	108.59	105.80
35	CN	201	ASP	CB-CG-OD1	6.97	124.58	118.30
65	D2	274	С	C4-C5-C6	-6.97	113.91	117.40
66	D3	638	U	C2-N1-C1'	6.97	126.07	117.70
65	D2	391	С	C5-C6-N1	6.97	124.49	121.00
65	D2	331	U	C5-C4-O4	-6.97	121.72	125.90
31	CJ	9	ARG	NE-CZ-NH1	6.94	$123.7\overline{7}$	120.30
66	D3	1654	G	C8-N9-C4	6.94	109.18	106.40
21	UU	417	LEU	CA-CB-CG	6.94	131.26	115.30
66	D3	1069	A	C5-C6-N6	-6.94	118.15	123.70



α \cdot \cdot \cdot	C		
(Continued	trom	nromanic	naae
Continucu	11011	preduous	puyc
		1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	65	С	C6-N1-C1'	6.94	129.12	120.80
66	D3	579	А	OP2-P-O3'	6.93	120.45	105.20
66	D3	948	G	C6-C5-N7	-6.93	126.24	130.40
67	D4	57	А	N7-C8-N9	6.92	117.26	113.80
65	D2	173	G	N3-C4-C5	6.92	132.06	128.60
66	D3	1629	G	C6-C5-N7	-6.92	126.25	130.40
67	D4	58	A	C6-N1-C2	-6.92	114.45	118.60
65	D2	309	A	N9-C4-C5	6.91	108.57	105.80
66	D3	1594	G	P-O3'-C3'	6.91	127.99	119.70
67	D4	22	A	C2-N3-C4	-6.91	107.14	110.60
66	D3	552	G	C4-C5-N7	6.91	113.56	110.80
65	D2	233	G	N7-C8-N9	6.90	116.55	113.10
65	D2	325	U	C5-C6-N1	6.90	126.15	122.70
65	D2	233	G	C8-N9-C4	-6.89	103.64	106.40
65	D2	220	U	N1-C2-O2	6.89	127.62	122.80
67	D4	26	С	C6-N1-C2	-6.89	117.54	120.30
65	D2	341	G	C5-C6-N1	6.89	114.94	111.50
66	D3	934	С	C5-C6-N1	6.89	124.44	121.00
65	D2	144	С	C6-N1-C2	-6.88	117.55	120.30
41	JJ	141	THR	C-N-CA	6.88	138.90	121.70
66	D3	1471	А	N1-C6-N6	6.88	122.73	118.60
66	D3	1628	U	C5-C6-N1	6.88	126.14	122.70
17	UQ	347	LEU	CA-CB-CG	6.87	131.10	115.30
22	UV	1139	LEU	CA-CB-CG	6.87	131.09	115.30
65	D2	242	C	O5'-P-OP1	-6.86	99.52	105.70
65	D2	278	G	C5-C6-N1	6.85	114.92	111.50
66	D3	1471	A	C5-C6-N6	-6.84	118.23	123.70
21	UU	493	ILE	CG1-CB-CG2	-6.83	96.38	111.40
66	D3	1527	С	N1-C2-O2	6.83	123.00	118.90
66	D3	1069	A	N1-C6-N6	6.83	122.70	118.60
67	D4	87	G	C4-N9-C1'	-6.82	117.63	126.50
33	CL	872	LEU	CA-CB-CG	6.82	130.99	115.30
66	D3	959	U	C2-N1-C1'	6.82	125.89	117.70
66	D3	1593	A	N3-C4-N9	-6.82	121.95	127.40
66	D3	8	U	N3-C2-O2	-6.81	117.43	122.20
65	D2	287	G	N3-C2-N2	6.80	124.66	119.90
66	D3	593	U	C5-C4-O4	-6.80	121.82	125.90
1	UA	617	VAL	CG1-CB-CG2	-6.79	100.03	110.90
18	UR	588	LEU	CB-CG-CD1	-6.77	99.49	111.00
66	D3	1159	C	C2-N1-C1'	6.77	126.24	118.80
23	UX	117	LEU	CA-CB-CG	6.76	130.86	115.30
7	UG	329	LEU	CA-CB-CG	6.76	130.85	115.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
66	D3	8	U	C6-N1-C2	-6.75	116.95	121.00
66	D3	1037	С	N1-C1'-C2'	-6.75	104.57	112.00
67	D4	59	G	C6-C5-N7	-6.75	126.35	130.40
8	UH	258	PRO	N-CA-CB	6.75	111.39	103.30
66	D3	54	С	N1-C2-O2	6.75	122.95	118.90
66	D3	1527	С	N1-C2-N3	6.75	123.92	119.20
65	D2	535	G	N3-C2-N2	-6.74	115.18	119.90
66	D3	1638	G	C8-N9-C4	-6.74	103.70	106.40
67	D4	73	А	O5'-P-OP1	-6.74	99.63	105.70
67	D4	326	U	C2-N3-C4	-6.73	122.96	127.00
65	D2	280	А	N7-C8-N9	6.72	117.16	113.80
66	D3	976	G	C4-N9-C1'	6.72	135.24	126.50
66	D3	1483	А	C6-C5-N7	-6.70	127.61	132.30
66	D3	548	G	C4-C5-N7	6.70	113.48	110.80
30	CI	94	ILE	CG1-CB-CG2	-6.70	96.67	111.40
65	D2	296	С	C6-N1-C2	6.70	122.98	120.30
10	UJ	182	LEU	CA-CB-CG	6.69	130.69	115.30
66	D3	976	G	N3-C4-N9	6.69	130.01	126.00
66	D3	1488	G	N1-C2-N2	-6.68	110.19	116.20
65	D2	244	U	N1-C2-N3	6.67	118.91	114.90
66	D3	1638	G	C6-C5-N7	-6.67	126.40	130.40
44	JN	94	PRO	N-CA-CB	6.67	111.30	103.30
65	D2	461	А	N9-C4-C5	6.66	108.46	105.80
66	D3	1611	А	N1-C2-N3	-6.66	125.97	129.30
66	D3	885	G	N3-C4-C5	-6.65	125.27	128.60
10	UJ	28	LEU	CB-CG-CD1	-6.65	99.69	111.00
46	JP	137	LEU	CB-CG-CD2	-6.65	99.69	111.00
5	UE	281	ILE	CG1-CB-CG2	-6.65	96.78	111.40
66	D3	543	С	C2-N3-C4	-6.64	116.58	119.90
67	D4	48	А	O5'-P-OP2	-6.64	99.72	105.70
65	D2	248	G	C4-C5-N7	6.64	113.46	110.80
13	UM	443	PRO	CA-N-CD	-6.63	102.21	111.50
65	D2	418	С	C5-C6-N1	6.63	124.32	121.00
65	D2	453	А	O5'-P-OP1	-6.63	99.73	105.70
67	D4	326	U	C5-C6-N1	-6.63	119.39	122.70
1	UA	493	TRP	C-N-CA	6.62	138.26	121.70
65	D2	346	G	C4-C5-N7	6.62	113.45	110.80
65	D2	312	U	C4-C5-C6	6.62	123.67	119.70
10	UJ	234	LEU	CA-CB-CG	6.62	130.53	115.30
65	D2	403	С	C5-C6-N1	6.62	124.31	121.00
65	D2	473	А	C4-C5-C6	-6.62	113.69	117.00
66	D3	489	C	N1-C2-O2	6.62	122.87	118.90



α \cdot \cdot \cdot	C	•	
Continued	from	previous	page
	5	1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	55	А	C5-N7-C8	-6.62	100.59	103.90
67	D4	59	G	N1-C2-N3	6.62	127.87	123.90
38	JE	254	ASP	CB-CG-OD1	6.61	124.25	118.30
8	UH	298	PRO	N-CA-CB	6.60	111.22	103.30
2	UB	400	PRO	N-CA-CB	6.60	111.22	103.30
1	UA	274	LEU	CA-CB-CG	6.59	130.46	115.30
66	D3	564	G	O5'-P-OP2	-6.59	99.77	105.70
66	D3	932	U	C2-N1-C1'	6.59	125.61	117.70
66	D3	1490	С	C5-C4-N4	-6.59	115.59	120.20
66	D3	1492	А	C8-N9-C4	-6.59	103.17	105.80
66	D3	1593	А	N1-C6-N6	-6.59	114.65	118.60
14	UN	309	ASP	CB-CG-OD1	6.58	124.23	118.30
65	D2	332	U	N1-C2-O2	6.58	127.41	122.80
66	D3	569	С	C4-C5-C6	-6.58	114.11	117.40
66	D3	542	А	OP1-P-O3'	6.58	119.67	105.20
66	D3	933	А	C5-C6-N6	-6.57	118.44	123.70
66	D3	1629	G	N1-C6-O6	6.57	123.84	119.90
66	D3	864	U	N1-C2-O2	6.56	127.39	122.80
67	D4	87	G	C6-C5-N7	6.55	134.33	130.40
65	D2	371	G	O5'-P-OP2	-6.55	99.80	105.70
66	D3	564	G	C2-N3-C4	-6.54	108.63	111.90
67	D4	61	G	N1-C2-N3	-6.54	119.97	123.90
46	JP	225	LEU	CB-CG-CD2	-6.54	99.88	111.00
65	D2	256	U	C5-C6-N1	-6.54	119.43	122.70
65	D2	296	С	C2-N1-C1'	-6.53	111.61	118.80
66	D3	552	G	C5-C6-N1	6.52	114.76	111.50
65	D2	340	U	C5-C6-N1	6.52	125.96	122.70
66	D3	1638	G	C4-C5-N7	6.52	113.41	110.80
65	D2	277	С	C6-N1-C2	-6.52	117.69	120.30
21	UU	494	LEU	CB-CG-CD1	6.51	122.07	111.00
62	DY	61	ARG	NE-CZ-NH2	-6.50	117.05	120.30
66	D3	1064	G	C6-C5-N7	-6.50	126.50	130.40
5	UE	111	ASP	CB-CG-OD1	6.49	124.14	118.30
30	CI	38	ILE	CG1-CB-CG2	-6.49	97.12	111.40
15	UO	277	LEU	CA-CB-CG	6.49	130.22	115.30
65	D2	220	U	C2-N1-C1'	6.48	125.48	117.70
66	D3	1785	U	N1-C2-O2	6.48	127.34	122.80
65	D2	298	A	C6-N1-C2	-6.48	114.71	118.60
66	D3	954	G	N3-C4-N9	-6.47	122.12	126.00
66	D3	584	С	C6-N1-C2	6.47	122.89	120.30
66	D3	1608	U	O5'-P-OP1	-6.46	99.89	105.70
66	D3	272	U	P-O3'-C3'	6.46	127.45	119.70



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	901	G	C4-C5-N7	6.45	113.38	110.80
66	D3	1159	С	C4-C5-C6	-6.44	114.18	117.40
21	UU	110	LEU	CB-CG-CD2	-6.44	100.05	111.00
65	D2	252	А	C8-N9-C4	6.44	108.38	105.80
66	D3	1162	С	C5-C6-N1	6.44	124.22	121.00
67	D4	41	С	C6-N1-C1'	6.44	128.53	120.80
21	UU	605	LEU	CB-CG-CD1	-6.44	100.05	111.00
65	D2	103	G	C4-C5-N7	6.44	113.38	110.80
66	D3	1638	G	C5-N7-C8	-6.44	101.08	104.30
65	D2	458	А	C8-N9-C4	-6.43	103.23	105.80
65	D2	281	G	C6-C5-N7	-6.43	126.54	130.40
33	CL	54	LEU	CB-CG-CD2	-6.43	100.07	111.00
65	D2	143	А	N1-C6-N6	6.43	122.46	118.60
19	US	326	LEU	CB-CG-CD1	-6.42	100.08	111.00
66	D3	948	G	C4-C5-N7	6.42	113.37	110.80
26	CD	7	LEU	CA-CB-CG	6.42	130.06	115.30
66	D3	1173	С	C6-N1-C2	-6.41	117.73	120.30
65	D2	312	U	C1'-O4'-C4'	-6.41	104.77	109.90
65	D2	336	G	C4-C5-N7	6.41	113.36	110.80
8	UH	325	PRO	N-CA-CB	6.40	110.98	103.30
66	D3	542	A	P-O3'-C3'	6.40	127.38	119.70
66	D3	1060	U	N1-C2-O2	6.40	127.28	122.80
65	D2	84	G	N3-C4-N9	6.39	129.84	126.00
21	UU	522	LEU	CB-CG-CD1	-6.39	100.14	111.00
50	DF	108	LEU	CA-CB-CG	-6.39	100.61	115.30
7	UG	434	LEU	CB-CG-CD1	-6.39	100.14	111.00
65	D2	459	U	C5-C4-O4	-6.38	122.07	125.90
65	D2	82	A	O5'-P-OP1	-6.38	99.96	105.70
12	UL	543	ASP	CB-CG-OD1	6.38	124.04	118.30
65	D2	103	G	C6-C5-N7	-6.38	126.57	130.40
28	CG	64	LEU	CB-CG-CD2	-6.38	100.16	111.00
26	CD	142	LEU	CB-CG-CD2	-6.37	100.17	111.00
67	D4	63	С	OP1-P-OP2	-6.37	110.04	119.60
46	JP	32	LEU	CB-CG-CD1	-6.36	100.18	111.00
7	UG	381	LEU	CB-CG-CD1	-6.35	100.20	111.00
66	D3	487	G	N9-C1'-C2'	-6.35	105.02	112.00
65	D2	290	G	C4-C5-N7	6.35	113.34	110.80
66	D3	34	G	N3-C4-C5	6.35	131.77	128.60
10	UJ	81	LEU	CA-CB-CG	6.34	129.88	115.30
66	D3	1525	A	N1-C2-N3	-6.34	126.13	129.30
66	D3	890	C	N3-C2-O2	-6.33	117.47	121.90
65	D2	90	G	N1-C6-O6	-6.33	116.10	119.90



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
• • • • • • • • • • • •	J	P	r ~g = · · ·

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1628	U	N3-C4-O4	6.33	123.83	119.40
18	UR	408	CYS	CA-CB-SG	-6.32	102.62	114.00
65	D2	312	U	N3-C2-O2	-6.32	117.77	122.20
66	D3	1581	С	C2-N1-C1'	6.32	125.75	118.80
67	D4	61	G	N9-C4-C5	-6.32	102.87	105.40
66	D3	1633	A	C2-N3-C4	6.32	113.76	110.60
65	D2	287	G	C5-C6-N1	6.31	114.66	111.50
66	D3	572	C	C6-N1-C2	6.31	122.83	120.30
65	D2	310	U	C5-C4-O4	6.31	129.69	125.90
66	D3	1530	С	N3-C4-N4	-6.31	113.58	118.00
65	D2	255	U	O5'-P-OP2	-6.31	100.03	105.70
65	D2	388	С	N3-C4-C5	-6.31	119.38	121.90
67	D4	29	U	OP2-P-O3'	6.31	119.07	105.20
66	D3	1072	С	C6-N1-C2	-6.30	117.78	120.30
66	D3	956	С	C6-N1-C2	-6.30	117.78	120.30
66	D3	591	А	N1-C6-N6	-6.29	114.83	118.60
1	UA	411	VAL	CG1-CB-CG2	-6.28	100.84	110.90
8	UH	70	PRO	N-CA-CB	6.28	110.84	103.30
66	D3	562	G	C6-N1-C2	-6.28	121.33	125.10
8	UH	235	PRO	N-CA-CB	6.27	110.83	103.30
65	D2	328	А	N9-C4-C5	-6.27	103.29	105.80
66	D3	1638	G	N7-C8-N9	6.27	116.24	113.10
66	D3	503	G	N1-C6-O6	-6.26	116.14	119.90
21	UU	110	LEU	CB-CG-CD1	-6.26	100.36	111.00
19	US	37	PRO	N-CA-CB	6.25	110.81	103.30
66	D3	1604	U	OP1-P-O3'	6.25	118.96	105.20
66	D3	1525	A	C4-C5-C6	-6.25	113.87	117.00
30	CI	142	LEU	CB-CG-CD2	-6.25	100.38	111.00
7	UG	433	LEU	CB-CG-CD1	-6.25	100.38	111.00
4	UD	191	LEU	CB-CG-CD1	-6.25	100.38	111.00
66	D3	965	U	N3-C2-O2	-6.24	117.83	122.20
34	CM	208	MET	CB-CG-SD	-6.23	93.71	112.40
65	D2	293	U	C2-N1-C1'	-6.23	110.22	117.70
66	D3	867	G	C4-N9-C1'	6.23	134.60	126.50
65	D2	315	U	C2-N1-C1'	6.22	125.16	117.70
67	D4	60	A	05'-P-OP2	-6.22	100.11	105.70
66	D3	1632	C	N3-C4-N4	-6.21	113.66	118.00
2	UB	285	PRO	N-CA-CB	6.20	110.74	103.30
66	D3	1153	G	C4-C5-N7	6.20	113.28	110.80
1	UA	339	LEU	CA-CB-CG	6.20	$129.5\overline{6}$	115.30
18	UR	345	LEU	CB-CG-CD1	-6.20	100.46	111.00
65	D2	386	A	O5'-P-OP1	-6.20	100.12	105.70



Continued	farear		
Commuea	jrom	previous	page

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
65	D2	447	G	N3-C4-N9	-6.20	122.28	126.00
66	D3	976	G	C6-C5-N7	-6.20	126.68	130.40
15	UO	421	LEU	CB-CG-CD1	-6.19	100.47	111.00
10	UJ	238	LEU	CB-CG-CD2	-6.19	100.47	111.00
14	UN	277	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	UA	702	LEU	CB-CG-CD1	-6.18	100.49	111.00
65	D2	335	G	O5'-P-OP1	-6.18	100.14	105.70
66	D3	1049	U	N3-C2-O2	-6.18	117.88	122.20
65	D2	452	А	C8-N9-C4	-6.17	103.33	105.80
33	CL	86	ILE	CG1-CB-CG2	-6.17	97.82	111.40
66	D3	864	U	N3-C2-O2	-6.17	117.88	122.20
66	D3	325	G	C8-N9-C4	6.17	108.87	106.40
65	D2	341	G	N9-C4-C5	-6.16	102.94	105.40
8	UH	61	PRO	N-CA-CB	6.15	110.68	103.30
28	CF	87	LEU	CB-CG-CD2	-6.15	100.55	111.00
65	D2	315	U	O5'-P-OP2	-6.15	100.17	105.70
67	D4	61	G	N1-C6-O6	6.15	123.59	119.90
31	CJ	20	LEU	CA-CB-CG	6.14	129.43	115.30
65	D2	294	U	N1-C2-N3	6.14	118.59	114.90
65	D2	387	С	C6-N1-C2	-6.14	117.84	120.30
66	D3	569	С	N3-C4-C5	6.14	124.36	121.90
65	D2	487	А	C8-N9-C4	-6.14	103.34	105.80
65	D2	535	G	N9-C4-C5	6.14	107.86	105.40
67	D4	67	G	N1-C6-O6	-6.14	116.22	119.90
65	D2	82	А	C4-C5-N7	6.13	113.77	110.70
65	D2	248	G	C5-C6-O6	-6.13	124.92	128.60
66	D3	471	А	C8-N9-C4	-6.13	103.35	105.80
21	UU	28	ARG	NE-CZ-NH1	-6.13	117.23	120.30
8	UH	59	PRO	N-CA-CB	6.13	110.66	103.30
66	D3	1036	A	C5-C6-N1	6.13	120.76	117.70
66	D3	487	G	C8-N9-C4	6.12	108.85	106.40
33	CL	988	ARG	NE-CZ-NH1	-6.12	117.24	120.30
66	D3	1609	U	N3-C2-O2	-6.12	117.92	122.20
8	UH	68	PRO	N-CA-CB	6.12	110.64	103.30
21	UU	367	LEU	CB-CG-CD2	-6.12	100.60	111.00
65	D2	311	С	C2-N1-C1'	-6.11	112.08	118.80
67	D4	90	С	C2-N1-C1'	6.11	125.52	118.80
65	D2	305	A	N3-C4-N9	-6.10	122.52	127.40
65	D2	331	U	N3-C2-O2	6.10	$1\overline{26.47}$	122.20
31	CJ	120	GLY	N-CA-C	-6.09	97.86	113.10
65	D2	309	A	N1-C6-N6	-6.09	114.94	118.60
65	D2	233	G	C8-N9-C1'	6.09	134.92	127.00



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
	J	1	1

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
65	D2	307	С	C5-C6-N1	6.09	124.04	121.00
18	UR	228	LEU	CB-CG-CD2	-6.09	100.65	111.00
66	D3	1604	U	C2-N1-C1'	-6.09	110.40	117.70
39	JF	124	VAL	C-N-CA	6.08	136.91	121.70
66	D3	1474	G	N3-C4-N9	-6.08	122.35	126.00
67	D4	82	G	C5-C6-N1	6.08	114.54	111.50
23	UX	141	LEU	CB-CG-CD2	-6.08	100.67	111.00
66	D3	1060	U	N3-C2-O2	-6.08	117.95	122.20
66	D3	6	G	C5-C6-O6	-6.07	124.96	128.60
2	UB	412	PRO	N-CA-CB	6.07	110.59	103.30
67	D4	25	U	C5-C4-O4	-6.07	122.26	125.90
18	UR	164	LEU	CB-CG-CD1	-6.07	100.68	111.00
66	D3	976	G	N3-C4-C5	-6.07	125.56	128.60
44	JN	108	PRO	N-CA-CB	6.07	110.58	103.30
66	D3	1062	А	C8-N9-C4	6.07	108.23	105.80
19	US	466	LEU	CB-CG-CD1	-6.06	100.70	111.00
46	JP	269	TRP	C-N-CA	-6.06	106.56	121.70
26	CD	40	ASP	CB-CG-OD1	6.05	123.75	118.30
66	D3	951	А	C4-C5-N7	6.05	113.73	110.70
66	D3	1123	С	N3-C2-O2	-6.05	117.67	121.90
66	D3	1167	G	N3-C4-N9	-6.05	122.37	126.00
65	D2	346	G	C6-C5-N7	-6.05	126.77	130.40
25	CA	223	ASP	CB-CG-OD1	6.05	123.74	118.30
50	DF	25	LEU	CA-CB-CG	6.05	129.21	115.30
66	D3	1513	G	C5-C6-O6	-6.05	124.97	128.60
66	D3	1616	G	C5-C6-N1	6.05	114.52	111.50
65	D2	283	А	N3-C4-C5	6.04	131.03	126.80
18	UR	272	LEU	CB-CG-CD2	-6.04	100.73	111.00
66	D3	1464	G	C6-C5-N7	-6.04	126.78	130.40
67	D4	39	С	C6-N1-C2	-6.04	117.89	120.30
65	D2	431	A	C5-C6-N6	-6.04	118.87	123.70
52	DH	143	LEU	CA-CB-CG	-6.04	101.42	115.30
66	D3	495	С	C5-C6-N1	6.04	124.02	121.00
66	D3	1114	G	C4-C5-N7	6.03	113.21	110.80
66	D3	1584	G	C6-C5-N7	6.03	134.02	130.40
65	D2	412	А	C5-N7-C8	-6.03	100.89	103.90
65	D2	305	А	C5-C6-N6	6.03	128.52	123.70
2	UB	201	PRO	N-CA-CB	6.03	110.53	103.30
65	D2	392	U	C5-C4-O4	-6.03	122.28	125.90
65	D2	238	G	C2-N3-C4	6.02	114.91	111.90
65	D2	383	G	C2-N3-C4	-6.02	108.89	111.90
66	D3	931	С	O5'-P-OP1	-6.02	100.28	105.70



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
	J	1	1 5

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
65	D2	172	С	N3-C2-O2	-6.01	117.69	121.90
67	D4	27	U	N3-C4-O4	-6.01	115.19	119.40
66	D3	572	С	N3-C4-C5	6.01	124.31	121.90
67	D4	35	U	C5-C4-O4	-6.01	122.29	125.90
67	D4	60	А	N1-C6-N6	-6.01	115.00	118.60
11	UK	48	LEU	CB-CG-CD2	-6.00	100.79	111.00
66	D3	1466	G	C6-C5-N7	-6.00	126.80	130.40
1	UA	592	ILE	CG1-CB-CG2	-6.00	98.19	111.40
65	D2	402	G	N3-C4-C5	-6.00	125.60	128.60
67	D4	61	G	N3-C4-C5	-6.00	125.60	128.60
48	DA	120	LEU	CB-CG-CD2	-6.00	100.80	111.00
15	UO	499	LYS	CA-CB-CG	6.00	126.59	113.40
66	D3	54	С	N3-C2-O2	-6.00	117.70	121.90
66	D3	1084	A	C5-C6-N1	-5.99	114.70	117.70
66	D3	1606	С	N3-C4-C5	-5.99	119.51	121.90
65	D2	341	G	N3-C4-C5	-5.98	125.61	128.60
66	D3	1084	А	C4-C5-C6	5.98	119.99	117.00
21	UU	223	LEU	CB-CG-CD2	-5.98	100.84	111.00
6	UF	12	ILE	CG1-CB-CG2	-5.98	98.25	111.40
67	D4	31	G	N3-C4-N9	-5.98	122.41	126.00
46	JP	83	LEU	CB-CG-CD2	-5.98	100.84	111.00
66	D3	1072	С	C5-C6-N1	5.98	123.99	121.00
22	UV	591	ASP	CB-CG-OD1	5.97	123.68	118.30
65	D2	348	U	C5-C6-N1	5.97	125.69	122.70
66	D3	564	G	N7-C8-N9	5.97	116.09	113.10
66	D3	1167	G	N3-C2-N2	-5.97	115.72	119.90
66	D3	638	U	C6-N1-C2	-5.97	117.42	121.00
66	D3	1510	U	N3-C2-O2	-5.97	118.02	122.20
1	UA	717	LEU	CB-CG-CD2	-5.96	100.86	111.00
19	US	296	MET	CG-SD-CE	-5.96	90.66	100.20
65	D2	284	U	N1-C2-N3	-5.96	111.32	114.90
30	CI	32	VAL	CG1-CB-CG2	-5.96	101.36	110.90
65	D2	467	A	N3-C4-C5	5.96	130.97	126.80
66	D3	471	A	N7-C8-N9	5.96	116.78	113.80
66	D3	494	U	C6-N1-C2	-5.96	117.43	121.00
66	D3	547	U	N3-C2-O2	-5.96	118.03	122.20
18	UR	353	ARG	NE-CZ-NH2	5.96	123.28	120.30
46	JP	259	VAL	CG1-CB-CG2	-5.96	101.37	110.90
65	D2	100	G	C4-C5-N7	5.95	113.18	110.80
46	JP	351	VAL	CG1-CB-CG2	-5.94	101.40	110.90
66	D3	566	C	C6-N1-C2	-5.93	117.93	120.30
66	D3	163	G	N3-C4-C5	5.93	131.56	128.60



$\alpha \cdot \cdot \cdot \cdot$	C		
Continued	from	previous	page
		1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1513	G	N1-C6-O6	5.93	123.46	119.90
66	D3	1603	U	C5-C6-N1	5.93	125.67	122.70
8	UH	316	PRO	N-CA-CB	5.93	110.41	103.30
66	D3	28	А	C8-N9-C4	-5.93	103.43	105.80
66	D3	542	А	C6-C5-N7	-5.92	128.15	132.30
65	D2	84	G	C8-N9-C1'	-5.92	119.30	127.00
65	D2	371	G	C8-N9-C4	5.92	108.77	106.40
66	D3	1064	G	C4-C5-N7	5.92	113.17	110.80
65	D2	286	U	N3-C2-O2	-5.92	118.06	122.20
66	D3	1177	С	C4-C5-C6	-5.92	114.44	117.40
44	JN	102	PRO	N-CA-CB	5.92	110.40	103.30
65	D2	392	U	N1-C2-N3	5.92	118.45	114.90
66	D3	591	А	N9-C4-C5	5.92	108.17	105.80
65	D2	449	U	C5-C6-N1	5.91	125.66	122.70
65	D2	171	G	C8-N9-C4	-5.91	104.03	106.40
32	CK	383	ARG	CA-CB-CG	-5.91	100.41	113.40
66	D3	495	С	C6-N1-C2	-5.91	117.94	120.30
65	D2	488	U	N1-C2-O2	5.90	126.93	122.80
66	D3	917	U	N3-C4-C5	-5.90	111.06	114.60
66	D3	1584	G	N9-C4-C5	5.90	107.76	105.40
32	CK	509	LEU	CA-CB-CG	-5.90	101.74	115.30
66	D3	374	U	C6-N1-C1'	-5.89	112.95	121.20
67	D4	36	С	C6-N1-C2	5.89	122.66	120.30
66	D3	1472	С	C6-N1-C2	-5.89	117.94	120.30
66	D3	1633	A	N9-C4-C5	5.89	108.16	105.80
66	D3	1620	С	P-O3'-C3'	5.89	126.77	119.70
34	CM	280	LEU	CB-CG-CD1	5.88	121.00	111.00
67	D4	86	A	C8-N9-C4	-5.88	103.45	105.80
46	JP	313	PHE	CB-CG-CD1	-5.88	116.69	120.80
66	D3	163	G	N3-C4-N9	-5.87	122.48	126.00
66	D3	1474	G	N3-C4-C5	5.87	131.53	128.60
8	UH	309	PRO	N-CA-CB	5.86	110.34	103.30
12	UL	898	LEU	CA-CB-CG	-5.86	101.82	115.30
65	D2	402	G	N1-C6-O6	-5.86	116.38	119.90
66	D3	1036	A	C6-N1-C2	-5.86	115.08	118.60
66	D3	1158	С	O5'-P-OP1	-5.86	100.43	105.70
66	D3	111	U	N1-C2-O2	5.85	126.90	122.80
65	D2	280	A	N9-C4-C5	5.85	108.14	105.80
65	D2	301	U	C5-C6-N1	5.85	125.62	122.70
65	D2	381	G	C4-C5-N7	5.85	113.14	110.80
66	D3	976	G	N7-C8-N9	5.85	116.03	113.10
66	D3	1472	С	C2-N1-C1'	5.85	125.23	118.80



α \cdot \cdot \cdot	C	•	
1 Continued	trom	nromanic	naae
Continucu	11011	preduous	puyc
		1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1589	С	C6-N1-C1'	5.84	127.81	120.80
65	D2	273	G	C5-C6-O6	5.84	132.10	128.60
65	D2	279	А	O5'-P-OP2	-5.84	100.45	105.70
65	D2	99	U	N1-C2-O2	5.83	126.88	122.80
66	D3	895	G	C5-C6-N1	-5.83	108.59	111.50
2	UB	598	LEU	CA-CB-CG	5.82	128.69	115.30
66	D3	1045	С	C2-N1-C1'	-5.82	112.39	118.80
65	D2	315	U	C5-C4-O4	-5.82	122.41	125.90
66	D3	1064	G	N3-C4-N9	5.82	129.49	126.00
67	D4	61	G	C5-N7-C8	-5.82	101.39	104.30
58	DQ	117	LEU	CB-CG-CD2	-5.82	101.11	111.00
67	D4	76	U	O5'-P-OP2	-5.82	100.47	105.70
65	D2	240	C	C2-N1-C1'	-5.81	112.41	118.80
65	D2	341	G	C8-N9-C1'	-5.81	119.44	127.00
65	D2	432	C	C6-N1-C2	5.81	122.62	120.30
65	D2	473	А	N1-C6-N6	-5.81	115.11	118.60
67	D4	59	G	C5-C6-N1	-5.81	108.59	111.50
1	UA	274	LEU	CB-CG-CD1	-5.81	101.12	111.00
67	D4	38	U	C2-N1-C1'	-5.81	110.73	117.70
7	UG	108	LEU	CA-CB-CG	5.81	128.66	115.30
7	UG	280	ILE	CG1-CB-CG2	-5.81	98.62	111.40
65	D2	433	C	N1-C2-O2	5.81	122.38	118.90
66	D3	575	C	C5-C6-N1	5.81	123.90	121.00
65	D2	288	G	N3-C2-N2	5.80	123.96	119.90
1	UA	152	LEU	CB-CG-CD2	-5.80	101.14	111.00
65	D2	431	A	N1-C6-N6	5.80	122.08	118.60
66	D3	867	G	C6-C5-N7	-5.80	126.92	130.40
67	D4	25	U	C5-C6-N1	5.80	125.60	122.70
65	D2	247	U	C2-N1-C1'	-5.79	110.75	117.70
65	D2	84	G	C4-C5-N7	5.79	113.12	110.80
65	D2	165	G	O5'-P-OP1	-5.79	100.49	105.70
65	D2	300	С	C6-N1-C1'	5.79	127.75	120.80
66	D3	1056	U	N3-C2-O2	-5.79	118.15	122.20
65	D2	303	A	C4-C5-C6	-5.79	114.11	117.00
65	D2	473	A	C5-C6-N1	5.79	120.59	117.70
65	D2	385	A	O4'-C1'-N9	-5.79	103.57	108.20
66	D3	111	U	C2-N1-C1'	5.79	124.65	117.70
66	D3	1624	C	C6-N1-C2	-5.79	117.98	120.30
65	D2	338	A	C8-N9-C4	-5.79	103.49	105.80
66	D3	1599	C	C5-C4-N4	-5.78	116.15	120.20
65	D2	288	G	C5-C6-N1	5.78	114.39	111.50
66	D3	538	A	C5-C6-N1	5.78	120.59	117.70



α \cdot \cdot \cdot	C	•	
Continued	trom	nremous	naae
Contentaca	JIONO	preciouo	pago

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1056	U	N1-C2-O2	5.77	126.84	122.80
65	D2	94	А	C8-N9-C4	5.77	108.11	105.80
1	UA	11	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	UA	517	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	UA	356	ASP	C-N-CA	-5.76	110.19	122.30
66	D3	1174	С	C6-N1-C1'	-5.76	113.88	120.80
66	D3	1061	А	O4'-C1'-N9	5.75	112.80	108.20
66	D3	1114	G	N3-C2-N2	5.75	123.93	119.90
66	D3	1510	U	C2-N1-C1'	5.75	124.60	117.70
66	D3	542	А	N9-C1'-C2'	5.75	121.47	114.00
67	D4	260	U	C5-C6-N1	5.75	125.57	122.70
28	CG	7	LYS	CD-CE-NZ	-5.74	98.49	111.70
13	UM	620	LEU	CA-CB-CG	5.74	128.50	115.30
65	D2	332	U	N3-C4-O4	-5.74	115.38	119.40
66	D3	1150	G	C8-N9-C4	5.74	108.69	106.40
65	D2	239	U	N1-C2-N3	5.73	118.34	114.90
66	D3	566	С	C4-C5-C6	-5.73	114.53	117.40
66	D3	965	U	N1-C2-O2	5.73	126.81	122.80
41	JJ	106	MET	CA-CB-CG	5.73	123.04	113.30
67	D4	87	G	N7-C8-N9	-5.73	110.24	113.10
66	D3	557	G	OP2-P-O3'	5.72	117.79	105.20
66	D3	1467	С	C2-N1-C1'	-5.72	112.50	118.80
50	DF	97	LEU	CB-CG-CD1	-5.72	101.28	111.00
54	DJ	99	LEU	CB-CG-CD2	-5.72	101.28	111.00
65	D2	381	G	C5-N7-C8	-5.72	101.44	104.30
66	D3	596	С	C6-N1-C1'	5.72	127.66	120.80
66	D3	1632	С	C6-N1-C2	5.72	122.59	120.30
15	UO	373	ILE	CG1-CB-CG2	-5.71	98.83	111.40
66	D3	573	С	N3-C4-N4	5.71	122.00	118.00
65	D2	399	U	C5-C6-N1	5.71	125.56	122.70
66	D3	496	G	C6-C5-N7	-5.71	126.97	130.40
65	D2	336	G	C5-C6-N1	5.71	114.35	111.50
66	D3	10	G	C4-C5-N7	5.71	113.08	110.80
66	D3	872	G	C2-N3-C4	-5.71	109.05	111.90
65	D2	318	A	C4-C5-N7	5.71	113.55	110.70
65	D2	239	U	C2-N3-C4	-5.70	123.58	127.00
67	D4	13	C	N3-C4-C5	5.70	124.18	121.90
66	D3	1605	G	N1-C6-O6	-5.70	116.48	119.90
67	D4	27	U	C6-N1-C1'	-5.70	113.22	121.20
65	D2	295	A	N7-C8-N9	5.70	116.65	113.80
66	D3	1078	С	N1-C2-O2	-5.70	115.48	118.90
66	D3	1616	G	C6-N1-C2	-5.70	121.68	125.10



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
	J	1	1 5

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
65	D2	392	U	N3-C4-O4	5.70	123.39	119.40
56	DN	72	MET	CB-CG-SD	-5.70	95.32	112.40
66	D3	543	С	N3-C4-C5	5.70	124.18	121.90
61	DX	87	VAL	N-CA-C	-5.69	95.63	111.00
65	D2	372	А	N1-C6-N6	-5.69	115.19	118.60
66	D3	1078	С	C5-C4-N4	-5.69	116.22	120.20
67	D4	41	С	OP2-P-O3'	5.68	117.70	105.20
66	D3	1657	U	P-O3'-C3'	5.68	126.51	119.70
65	D2	461	А	C8-N9-C4	-5.68	103.53	105.80
66	D3	690	G	C8-N9-C4	-5.68	104.13	106.40
67	D4	62	С	C2-N1-C1'	5.67	125.04	118.80
32	CK	426	LEU	CB-CG-CD2	-5.67	101.36	111.00
33	CL	834	TRP	CA-CB-CG	5.67	124.47	113.70
60	DW	55	ASP	CB-CG-OD1	5.67	123.40	118.30
66	D3	933	А	N1-C6-N6	5.67	122.00	118.60
66	D3	37	U	N1-C2-O2	5.67	126.77	122.80
65	D2	479	G	N1-C6-O6	-5.66	116.50	119.90
33	CL	872	LEU	CB-CG-CD1	-5.66	101.38	111.00
66	D3	583	С	P-O3'-C3'	5.66	126.49	119.70
66	D3	374	U	C5-C6-N1	5.66	125.53	122.70
66	D3	534	A	C5-N7-C8	-5.66	101.07	103.90
7	UG	390	LEU	CB-CG-CD2	-5.65	101.39	111.00
10	UJ	103	LEU	CB-CG-CD2	-5.65	101.39	111.00
65	D2	275	A	N7-C8-N9	5.65	116.63	113.80
66	D3	1466	G	C4-C5-N7	5.65	113.06	110.80
66	D3	426	G	N9-C4-C5	-5.65	103.14	105.40
65	D2	344	U	C2-N1-C1'	-5.65	110.92	117.70
66	D3	543	С	O5'-P-OP1	-5.65	100.62	105.70
32	CK	343	GLU	CA-CB-CG	5.64	125.82	113.40
65	D2	335	G	C5-N7-C8	-5.64	101.48	104.30
65	D2	409	С	N3-C4-C5	5.64	124.16	121.90
66	D3	1471	A	C4-C5-N7	5.64	113.52	110.70
7	UG	270	LEU	CB-CG-CD2	-5.64	101.41	111.00
67	D4	35	U	C2-N1-C1'	5.64	124.47	117.70
23	UX	119	LEU	CB-CG-CD1	-5.64	101.41	111.00
7	UG	390	LEU	CA-CB-CG	5.64	128.27	115.30
66	D3	1624	C	$C6-N1-\overline{C1'}$	5.64	127.56	120.80
65	D2	300	C	N3-C4-C5	-5.63	119.65	121.90
50	DF	108	LEU	CB-CG-CD2	-5.63	101.43	111.00
65	D2	319	A	C5-N7-C8	-5.63	101.09	103.90
65	D2	323	A	C5-C6-N6	-5.63	119.20	123.70
65	D2	319	A	C8-N9-C4	-5.62	103.55	105.80



α \cdot \cdot \cdot	C	•	
Continued	from	previous	page
	5	1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	549	G	C5-N7-C8	-5.62	101.49	104.30
66	D3	496	G	C5-N7-C8	-5.62	101.49	104.30
7	UG	442	ILE	CG1-CB-CG2	-5.62	99.03	111.40
65	D2	251	С	C6-N1-C2	-5.62	118.05	120.30
65	D2	288	G	C4-C5-N7	5.62	113.05	110.80
66	D3	864	U	C5-C6-N1	5.62	125.51	122.70
38	JE	334	LEU	CA-CB-CG	5.61	128.21	115.30
66	D3	539	G	C2-N3-C4	-5.61	109.09	111.90
65	D2	233	G	C6-C5-N7	-5.61	127.03	130.40
66	D3	1123	С	N1-C2-O2	5.61	122.27	118.90
18	UR	242	ASN	CB-CA-C	-5.61	99.18	110.40
17	UQ	315	GLY	N-CA-C	5.61	127.12	113.10
33	CL	932	LEU	CA-CB-CG	5.61	128.20	115.30
12	UL	752	LEU	CB-CG-CD2	5.61	120.53	111.00
67	D4	55	А	C8-N9-C4	5.61	108.04	105.80
65	D2	158	G	C8-N9-C4	5.60	108.64	106.40
66	D3	1616	G	N3-C4-C5	-5.60	125.80	128.60
23	UX	8	ARG	NE-CZ-NH2	5.60	123.10	120.30
26	CD	154	LEU	CB-CG-CD2	-5.60	101.48	111.00
65	D2	490	G	O4'-C1'-N9	5.60	112.68	108.20
65	D2	220	U	C5-C6-N1	5.60	125.50	122.70
67	D4	84	U	N3-C4-O4	-5.60	115.48	119.40
66	D3	34	G	N3-C4-N9	-5.59	122.64	126.00
48	DA	97	LEU	CA-CB-CG	-5.59	102.44	115.30
30	CI	77	LEU	CA-CB-CG	5.59	128.16	115.30
65	D2	305	А	C2-N3-C4	-5.59	107.80	110.60
66	D3	482	U	N3-C2-O2	-5.59	118.29	122.20
25	CA	251	ARG	CG-CD-NE	5.59	123.54	111.80
33	CL	829	LEU	CA-CB-CG	5.59	128.16	115.30
65	D2	246	G	C6-N1-C2	-5.59	121.75	125.10
7	UG	258	LEU	CB-CG-CD2	-5.58	101.51	111.00
65	D2	234	А	C2-N3-C4	-5.58	107.81	110.60
46	JP	147	LEU	CB-CG-CD2	-5.58	101.51	111.00
65	D2	490	G	C4-N9-C1'	-5.58	119.24	126.50
66	D3	513	U	C2-N1-C1'	-5.58	111.00	117.70
66	D3	1076	А	O5'-P-OP2	-5.58	100.67	105.70
66	D3	1584	G	C4-C5-N7	-5.58	108.57	110.80
67	D4	57	A	O5'-P-OP1	-5.58	100.68	105.70
67	D4	80	U	05'-P-OP2	-5.58	100.68	105.70
66	D3	24	U	N1-C2-O2	5.58	126.71	122.80
65	D2	280	А	N3-C4-C5	5.58	130.71	126.80
67	D4	260	U	N3-C2-O2	-5.57	118.30	122.20



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	UM	584	ILE	CG1-CB-CG2	5.57	123.65	111.40
66	D3	6	G	C5-C6-N1	5.57	114.28	111.50
33	CL	1135	ARG	CA-CB-CG	5.57	125.64	113.40
67	D4	59	G	N1-C6-O6	5.56	123.24	119.90
50	DF	29	ILE	CG1-CB-CG2	-5.56	99.16	111.40
33	CL	996	LEU	CA-CB-CG	5.56	128.09	115.30
65	D2	472	А	O5'-P-OP1	-5.56	100.70	105.70
66	D3	1114	G	N9-C4-C5	-5.56	103.18	105.40
66	D3	1611	А	C4-C5-C6	-5.55	114.22	117.00
65	D2	84	G	C6-C5-N7	-5.55	127.07	130.40
67	D4	67	G	O5'-P-OP2	-5.55	100.70	105.70
49	DE	87	MET	CA-CB-CG	5.55	122.73	113.30
65	D2	310	U	O5'-P-OP1	-5.55	100.71	105.70
7	UG	381	LEU	CA-CB-CG	5.55	128.06	115.30
66	D3	496	G	C5-C6-O6	-5.55	125.27	128.60
67	D4	58	А	C2-N3-C4	5.54	113.37	110.60
65	D2	423	С	C2-N1-C1'	5.54	124.90	118.80
66	D3	938	G	N1-C2-N2	-5.54	111.21	116.20
66	D3	1777	G	C4-C5-N7	5.54	113.02	110.80
67	D4	60	А	N9-C4-C5	5.54	108.02	105.80
21	UU	218	LEU	CB-CG-CD2	-5.54	101.58	111.00
65	D2	231	С	C6-N1-C1'	5.54	127.45	120.80
65	D2	314	U	C6-N1-C2	-5.54	117.68	121.00
66	D3	1491	U	O5'-P-OP1	-5.54	100.72	105.70
50	DF	97	LEU	CB-CG-CD2	-5.54	101.59	111.00
66	D3	1040	G	N3-C4-N9	-5.54	122.68	126.00
66	D3	1575	G	N1-C6-O6	-5.53	116.58	119.90
66	D3	1638	G	N1-C6-O6	5.53	123.22	119.90
28	CF	70	LEU	CB-CG-CD2	-5.53	101.60	111.00
30	CI	79	LEU	CB-CG-CD2	-5.53	101.60	111.00
66	D3	307	G	N3-C4-N9	5.53	129.32	126.00
66	D3	1471	A	C5-N7-C8	-5.53	101.14	103.90
67	D4	331	A	C5-N7-C8	-5.53	101.14	103.90
65	D2	324	U	N1-C2-O2	5.53	126.67	122.80
65	D2	289	U	C6-N1-C2	-5.53	117.68	121.00
66	D3	642	G	N1-C2-N2	5.53	121.17	116.20
66	D3	1487	A	C8-N9-C4	-5.52	103.59	105.80
1	UA	563	ARG	CG-CD-NE	5.52	123.39	111.80
41	JJ	100	MET	CA-CB-CG	5.52	122.68	113.30
65	D2	389	U	O5'-P-OP1	-5.52	100.73	105.70
65	D2	477	G	N3-C4-N9	-5.52	122.69	126.00
66	D3	1488	G	C5-C6-O6	5.52	131.91	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
31	CJ	129	ASP	CB-CG-OD1	5.52	123.27	118.30
65	D2	309	А	C8-N9-C4	-5.52	103.59	105.80
66	D3	10	G	C5-C6-O6	-5.52	125.29	128.60
66	D3	1618	С	C6-N1-C1'	-5.52	114.18	120.80
66	D3	1492	А	C2-N3-C4	5.51	113.36	110.60
65	D2	438	U	C5-C6-N1	5.51	125.45	122.70
65	D2	400	С	N3-C4-C5	5.51	124.10	121.90
67	D4	21	С	C5-C6-N1	5.51	123.75	121.00
66	D3	-2	А	O4'-C1'-N9	5.51	112.61	108.20
67	D4	70	U	O5'-P-OP1	-5.51	100.74	105.70
46	JP	62	LEU	CA-CB-CG	5.50	127.96	115.30
65	D2	535	G	O4'-C1'-N9	5.50	112.60	108.20
1	UA	275	LEU	CB-CG-CD1	-5.50	101.65	111.00
65	D2	287	G	N1-C2-N2	-5.50	111.25	116.20
65	D2	98	G	N3-C4-C5	-5.50	125.85	128.60
66	D3	1068	С	C2-N1-C1'	-5.50	112.75	118.80
65	D2	347	U	C5-C6-N1	5.50	125.45	122.70
66	D3	1037	С	N3-C4-C5	5.50	124.10	121.90
10	UJ	152	LEU	CB-CG-CD1	-5.49	101.67	111.00
65	D2	332	U	C5-C4-O4	5.49	129.19	125.90
6	UF	322	LEU	CA-CB-CG	5.49	127.92	115.30
65	D2	431	А	C4-C5-N7	5.49	113.44	110.70
66	D3	17	С	N1-C2-O2	5.49	122.19	118.90
66	D3	539	G	C6-C5-N7	-5.49	127.11	130.40
66	D3	557	G	C8-N9-C4	-5.49	104.21	106.40
66	D3	1063	U	C5-C6-N1	5.49	125.44	122.70
66	D3	1472	С	N3-C2-O2	-5.49	118.06	121.90
46	JP	374	LEU	CA-CB-CG	5.48	127.91	115.30
66	D3	867	G	C8-N9-C1'	-5.48	119.87	127.00
66	D3	494	U	N3-C2-O2	-5.48	118.36	122.20
66	D3	937	С	C6-N1-C1'	5.48	127.38	120.80
67	D4	332	G	O5'-P-OP1	-5.48	100.77	105.70
67	D4	55	А	C3'-C2'-C1'	-5.48	97.12	101.50
1	UA	588	ASP	CB-CG-OD1	5.48	123.23	118.30
65	D2	302	А	N7-C8-N9	-5.48	111.06	113.80
14	UN	313	PHE	N-CA-C	5.47	125.78	111.00
66	D3	500	С	C4-C5-C6	-5.47	114.66	117.40
66	D3	1612	U	O5'-P-OP1	-5.47	100.77	105.70
65	D2	348	U	C6-N1-C2	-5.47	117.72	121.00
33	CL	263	LEU	CA-CB-CG	5.47	127.87	115.30
65	D2	312	U	N3-C4-O4	-5.47	115.57	119.40
62	DY	40	LEU	CB-CG-CD1	-5.46	101.71	111.00

Continued from previous page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1057	U	P-O3'-C3'	5.46	126.26	119.70
5	UE	452	LEU	CB-CG-CD1	-5.46	101.71	111.00
21	UU	494	LEU	CD1-CG-CD2	-5.46	94.12	110.50
37	JC	350	PRO	C-N-CA	5.46	135.35	121.70
65	D2	137	С	N3-C2-O2	-5.46	118.08	121.90
17	UQ	264	ILE	CG1-CB-CG2	-5.46	99.40	111.40
67	D4	70	U	C2-N1-C1'	-5.46	111.16	117.70
65	D2	318	A	C5-C6-N6	-5.45	119.34	123.70
67	D4	22	A	N3-C4-N9	-5.45	123.04	127.40
21	UU	183	VAL	CG1-CB-CG2	-5.45	102.18	110.90
18	UR	212	LEU	CB-CG-CD1	-5.45	101.74	111.00
67	D4	57	A	C5-N7-C8	-5.45	101.17	103.90
28	CG	64	LEU	CB-CG-CD1	5.45	120.26	111.00
66	D3	883	С	C6-N1-C2	-5.45	118.12	120.30
66	D3	954	G	N3-C4-C5	5.45	131.32	128.60
65	D2	335	G	C5-C6-O6	-5.45	125.33	128.60
1	UA	30	LEU	CB-CG-CD2	-5.44	101.75	111.00
66	D3	577	G	N9-C4-C5	5.44	107.58	105.40
66	D3	1777	G	C6-C5-N7	-5.44	127.13	130.40
67	D4	85	G	N1-C6-O6	-5.44	116.64	119.90
67	D4	87	G	C8-N9-C1'	5.44	134.07	127.00
15	UO	164	LEU	CB-CG-CD2	-5.44	101.75	111.00
15	UO	431	LEU	CA-CB-CG	5.44	127.81	115.30
65	D2	319	A	N7-C8-N9	5.44	116.52	113.80
66	D3	1076	A	C2-N3-C4	-5.44	107.88	110.60
65	D2	89	С	C5-C4-N4	-5.44	116.39	120.20
65	D2	315	U	C6-N1-C1'	-5.44	113.59	121.20
65	D2	407	A	N1-C6-N6	-5.43	115.34	118.60
66	D3	1487	A	N1-C6-N6	-5.43	115.34	118.60
65	D2	444	U	C2-N1-C1'	-5.43	111.18	117.70
39	JG	97	LEU	CB-CG-CD1	-5.43	101.77	111.00
66	D3	901	G	C4-N9-C1'	5.43	133.56	126.50
66	D3	1038	U	N1-C2-N3	5.43	118.16	114.90
63	Db	4	VAL	CG1-CB-CG2	-5.43	102.22	110.90
66	D3	54	С	C6-N1-C2	-5.43	118.13	120.30
66	D3	499	U	C2-N1-C1'	-5.43	111.19	117.70
65	D2	240	C	C6-N1-C1'	5.42	127.31	120.80
66	D3	964	U	C5-C6-N1	-5.42	119.99	122.70
66	D3	32	U	C2-N1-C1'	-5.42	111.19	117.70
39	JG	99	LEU	CA-CB-CG	-5.42	102.84	115.30
65	D2	433	C	N3-C2-O2	-5.42	118.11	121.90
66	D3	564	G	C8-N9-C1'	5.42	134.04	127.00



$\alpha \cdot \cdot \cdot \cdot$	C	•	
Continued	from	previous	page
	9	1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	19	А	C8-N9-C4	5.41	107.97	105.80
66	D3	583	С	OP1-P-O3'	5.41	117.11	105.20
65	D2	231	С	C2-N1-C1'	-5.41	112.85	118.80
66	D3	569	С	C5-C6-N1	5.41	123.70	121.00
31	CJ	167	LEU	CA-CB-CG	5.41	127.73	115.30
66	D3	589	С	C6-N1-C1'	5.41	127.29	120.80
66	D3	1166	A	N3-C4-N9	-5.40	123.08	127.40
33	CL	919	VAL	CG1-CB-CG2	-5.40	102.26	110.90
17	UQ	529	LEU	CB-CG-CD2	-5.40	101.82	111.00
66	D3	639	U	P-O3'-C3'	5.40	126.18	119.70
66	D3	1488	G	N3-C2-N2	5.40	123.68	119.90
65	D2	265	A	N1-C6-N6	-5.39	115.36	118.60
66	D3	1478	G	N3-C4-C5	-5.39	125.90	128.60
66	D3	31	С	C5-C6-N1	5.39	123.69	121.00
66	D3	534	А	C4-C5-N7	5.39	113.39	110.70
66	D3	1165	G	C8-N9-C1'	5.39	134.00	127.00
67	D4	25	U	C4-C5-C6	-5.39	116.47	119.70
66	D3	1161	С	N3-C4-C5	5.38	124.05	121.90
67	D4	26	С	OP1-P-O3'	5.38	117.05	105.20
66	D3	1584	G	C5-C6-O6	5.38	131.83	128.60
1	UA	16	ARG	NE-CZ-NH2	5.38	122.99	120.30
5	UE	251	GLY	N-CA-C	-5.38	99.65	113.10
66	D3	144	U	O4'-C1'-N1	5.38	112.51	108.20
66	D3	1530	С	N3-C2-O2	-5.38	118.13	121.90
66	D3	1604	U	N3-C4-O4	-5.38	115.63	119.40
65	D2	271	G	N3-C2-N2	-5.38	116.14	119.90
66	D3	530	С	C6-N1-C2	-5.38	118.15	120.30
66	D3	1065	A	N1-C6-N6	-5.38	115.37	118.60
31	CJ	266	LEU	CB-CG-CD2	-5.38	101.86	111.00
33	CL	934	LEU	CB-CG-CD1	-5.37	101.86	111.00
65	D2	394	U	C6-N1-C1'	-5.37	113.68	121.20
66	D3	1618	С	C5-C4-N4	-5.37	116.44	120.20
66	D3	564	G	C6-C5-N7	-5.37	127.18	130.40
67	D4	80	U	C5-C6-N1	5.37	125.39	122.70
1	UA	643	LEU	CB-CG-CD1	-5.37	101.88	111.00
18	UR	543	LEU	CB-CG-CD1	-5.37	101.88	111.00
66	D3	948	G	C4-N9-C1'	5.37	133.47	126.50
66	D3	1611	A	N7-C8-N9	-5.37	111.12	113.80
7	UG	347	LEU	CB-CG-CD1	-5.36	101.88	111.00
17	UQ	37	LEU	CA-CB-CG	$5.3\overline{6}$	127.64	115.30
66	D3	547	U	N1-C2-O2	5.36	$1\overline{26.55}$	122.80
66	D3	539	G	C5-N7-C8	-5.36	101.62	104.30



α $\cdot \cdot$ \cdot	C		
Continued	from	previous	page
	9	1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
30	CI	56	ARG	NE-CZ-NH1	-5.36	117.62	120.30
63	Db	21	LEU	CA-CB-CG	5.36	127.62	115.30
65	D2	165	G	OP2-P-O3'	5.36	116.98	105.20
66	D3	866	G	C4-C5-N7	5.36	112.94	110.80
5	UE	301	LEU	CB-CG-CD2	-5.36	101.90	111.00
67	D4	10	С	C5-C4-N4	-5.36	116.45	120.20
67	D4	33	A	N1-C6-N6	-5.35	115.39	118.60
29	CH	320	GLY	N-CA-C	5.35	126.48	113.10
66	D3	951	А	C5-N7-C8	-5.35	101.23	103.90
65	D2	294	U	C6-N1-C1'	5.35	128.69	121.20
23	UX	12	LEU	CA-CB-CG	5.34	127.59	115.30
32	CK	326	LEU	CB-CG-CD1	-5.34	101.92	111.00
65	D2	344	U	C6-N1-C1'	5.34	128.68	121.20
65	D2	163	G	C4-C5-N7	5.34	112.94	110.80
65	D2	488	U	C6-N1-C2	-5.34	117.80	121.00
65	D2	283	А	N3-C4-N9	-5.34	123.13	127.40
65	D2	423	С	C6-N1-C2	-5.34	118.17	120.30
66	D3	1045	С	C6-N1-C1'	5.33	127.20	120.80
15	UO	303	LEU	CB-CG-CD1	-5.33	101.93	111.00
28	CG	89	ARG	NE-CZ-NH1	5.33	122.97	120.30
31	CJ	229	ASP	CB-CG-OD1	5.33	123.10	118.30
66	D3	914	G	N3-C4-C5	5.33	131.26	128.60
66	D3	1534	G	C8-N9-C4	-5.33	104.27	106.40
65	D2	300	С	C6-N1-C2	-5.33	118.17	120.30
65	D2	306	G	C5-C6-O6	5.33	131.80	128.60
66	D3	1604	U	C4-C5-C6	-5.33	116.50	119.70
17	UQ	596	LEU	CB-CG-CD2	-5.32	101.95	111.00
65	D2	336	G	C5-N7-C8	-5.32	101.64	104.30
65	D2	458	A	C2-N3-C4	-5.32	107.94	110.60
66	D3	534	A	N7-C8-N9	5.32	116.46	113.80
66	D3	1611	A	N9-C4-C5	-5.32	103.67	105.80
28	CF	44	LEU	CB-CG-CD1	-5.32	101.96	111.00
65	D2	281	G	N9-C4-C5	-5.32	103.27	105.40
65	D2	328	A	N1-C6-N6	5.32	121.79	118.60
67	D4	325	С	N3-C4-C5	5.32	124.03	121.90
19	US	470	MET	CA-CB-CG	5.31	122.33	113.30
66	D3	121	U	N3-C2-O2	-5.31	118.48	122.20
66	D3	959	U	C5-C4-O4	5.31	129.09	125.90
65	D2	254	C	N1-C2-O2	-5.31	115.71	118.90
66	D3	25	C	$C2-N1-\overline{C1'}$	5.31	124.64	118.80
66	D3	554	C	N1-C2-N3	5.31	122.92	119.20
66	D3	499	U	C5-C6-N1	-5.31	120.05	122.70



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
	J	1	I J

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	577	G	N3-C4-N9	-5.31	122.82	126.00
12	UL	581	ILE	CG1-CB-CG2	-5.31	99.73	111.40
17	UQ	473	LEU	CA-CB-CG	5.30	127.50	115.30
66	D3	1	U	C5-C6-N1	-5.30	120.05	122.70
66	D3	691	С	C2-N1-C1'	5.30	124.64	118.80
66	D3	959	U	C6-N1-C2	-5.30	117.82	121.00
66	D3	1080	U	C5-C6-N1	5.30	125.35	122.70
66	D3	528	U	C5-C6-N1	5.30	125.35	122.70
66	D3	494	U	C5-C6-N1	5.29	125.35	122.70
66	D3	928	U	C5-C6-N1	-5.29	120.05	122.70
66	D3	938	G	N3-C2-N2	5.29	123.61	119.90
66	D3	1151	А	C2-N3-C4	-5.29	107.95	110.60
66	D3	1070	С	O5'-P-OP2	-5.29	100.94	105.70
67	D4	27	U	N1-C2-N3	5.29	118.08	114.90
66	D3	1060	U	O4'-C1'-N1	5.29	112.43	108.20
18	UR	493	LEU	CB-CG-CD2	-5.29	102.01	111.00
66	D3	426	G	C4-C5-N7	5.29	112.92	110.80
1	UA	416	LEU	CA-CB-CG	5.29	127.46	115.30
65	D2	308	А	N1-C2-N3	-5.29	126.66	129.30
65	D2	492	G	P-O3'-C3'	5.29	126.04	119.70
66	D3	0	U	P-O3'-C3'	5.29	126.04	119.70
46	JP	116	LEU	CB-CG-CD2	-5.28	102.02	111.00
66	D3	502	U	O4'-C1'-N1	5.28	112.43	108.20
18	UR	426	VAL	CG1-CB-CG2	-5.28	102.45	110.90
30	CI	57	LEU	CB-CG-CD2	-5.28	102.02	111.00
67	D4	56	A	C5-N7-C8	-5.28	101.26	103.90
65	D2	391	С	C6-N1-C2	-5.28	118.19	120.30
30	CI	88	LEU	CA-CB-CG	5.28	127.44	115.30
66	D3	921	U	C2-N1-C1'	-5.28	111.37	117.70
1	UA	635	MET	CG-SD-CE	5.27	108.64	100.20
65	D2	378	С	C2-N1-C1'	5.27	124.60	118.80
66	D3	1629	G	C4-C5-N7	5.27	112.91	110.80
31	CJ	209	LEU	CB-CG-CD1	-5.27	102.04	111.00
65	D2	168	G	C5-C6-O6	5.27	131.76	128.60
66	D3	567	А	C2-N3-C4	-5.27	107.96	110.60
67	D4	59	G	O4'-C1'-N9	-5.27	103.98	108.20
6	UF	74	ILE	CG1-CB-CG2	-5.27	99.81	111.40
7	UG	433	LEU	CA-CB-CG	5.27	127.42	115.30
66	D3	1599	С	N3-C2-O2	-5.27	118.21	121.90
67	D4	326	U	N3-C2-O2	-5.27	118.51	122.20
33	CL	140	LEU	CB-CG-CD2	-5.26	102.05	111.00
66	D3	562	G	N1-C2-N3	5.26	127.06	123.90



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
• • • • • • • • • • • •	J	P	r ~g = · · ·

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1043	А	N1-C6-N6	-5.26	115.44	118.60
65	D2	383	G	N3-C4-C5	5.26	131.23	128.60
65	D2	173	G	C4-N9-C1'	-5.26	119.67	126.50
65	D2	290	G	N3-C2-N2	5.26	123.58	119.90
66	D3	22	А	C2-N3-C4	5.26	113.23	110.60
14	UN	861	LEU	CB-CG-CD1	-5.25	102.07	111.00
65	D2	447	G	C8-N9-C1'	5.25	133.83	127.00
15	UO	283	VAL	CG1-CB-CG2	-5.25	102.50	110.90
66	D3	104	А	N1-C2-N3	5.25	131.93	129.30
66	D3	579	A	O5'-P-OP2	-5.25	100.97	105.70
61	DX	43	PHE	CB-CG-CD1	5.25	124.47	120.80
10	UJ	102	LEU	CB-CG-CD1	-5.25	102.08	111.00
66	D3	554	C	N3-C2-O2	-5.25	118.23	121.90
2	UB	481	MET	CG-SD-CE	-5.24	91.81	100.20
18	UR	228	LEU	CA-CB-CG	5.24	127.36	115.30
22	UV	209	MET	CB-CG-SD	5.24	128.12	112.40
65	D2	388	C	C5-C6-N1	5.24	123.62	121.00
66	D3	500	C	C2-N1-C1'	-5.24	113.03	118.80
66	D3	885	G	N1-C2-N2	-5.24	111.48	116.20
66	D3	1657	U	OP2-P-O3'	5.24	116.73	105.20
66	D3	1491	U	OP1-P-O3'	5.24	116.72	105.20
30	CI	170	LEU	CB-CG-CD1	-5.24	102.10	111.00
30	CI	170	LEU	CB-CG-CD2	-5.24	102.10	111.00
45	JO	53	LEU	CB-CG-CD2	-5.24	102.10	111.00
65	D2	474	A	O5'-P-OP1	-5.24	100.99	105.70
66	D3	1166	A	N3-C4-C5	5.24	130.47	126.80
65	D2	305	A	N3-C4-C5	5.23	130.46	126.80
66	D3	976	G	C4-C5-N7	5.23	112.89	110.80
15	UO	108	TYR	CA-CB-CG	5.23	123.34	113.40
65	D2	84	G	C4-N9-C1'	5.23	133.30	126.50
65	D2	322	A	C8-N9-C4	5.23	107.89	105.80
66	D3	87	C	N1-C2-O2	5.23	122.04	118.90
67	D4	38	U	C5-C4-O4	5.23	129.04	125.90
65	D2	259	G	O5'-P-OP2	-5.23	100.99	105.70
66	D3	584	С	C2-N3-C4	-5.23	117.28	119.90
66	D3	496	G	N3-C4-C5	5.23	131.21	128.60
3	UC	602	LEU	CA-CB-CG	5.23	127.32	115.30
66	D3	555	A	N1-C6-N6	-5.22	115.47	118.60
65	D2	173	G	N3-C4-N9	-5.22	122.87	126.00
66	D3	1	U	C2-N3-C4	-5.22	123.87	127.00
53	DI	18	ARG	NE-CZ-NH1	5.22	122.91	120.30
66	D3	901	G	C6-C5-N7	-5.22	127.27	130.40



α \cdot \cdot	C		
Continued	from	previous	page

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
66	D3	1078	C	C2-N3-C4	-5.22	117.29	119.90
31	CJ	209	LEU	CB-CG-CD2	-5.21	102.14	111.00
66	D3	1581	C	C6-N1-C2	-5.21	118.22	120.30
65	D2	89	С	OP1-P-OP2	-5.21	111.78	119.60
66	D3	976	G	C8-N9-C4	-5.21	104.32	106.40
66	D3	8	U	C5-C6-N1	5.21	125.30	122.70
66	D3	475	A	N1-C6-N6	5.21	121.72	118.60
67	D4	60	A	C6-N1-C2	-5.21	115.48	118.60
65	D2	259	G	C6-C5-N7	-5.21	127.28	130.40
66	D3	536	C	N1-C2-O2	5.21	122.02	118.90
66	D3	956	С	N3-C4-N4	5.21	121.64	118.00
26	CD	234	LEU	CA-CB-CG	5.20	127.27	115.30
66	D3	1594	G	OP2-P-O3'	5.20	116.64	105.20
66	D3	1472	С	N1-C2-O2	5.20	122.02	118.90
41	JJ	270	LEU	CB-CG-CD2	-5.20	102.17	111.00
66	D3	1064	G	C8-N9-C1'	-5.20	120.25	127.00
67	D4	65	C	N3-C4-C5	-5.20	119.82	121.90
65	D2	287	G	C4-C5-N7	5.19	112.88	110.80
65	D2	459	U	N3-C4-O4	5.19	123.03	119.40
4	UD	774	LEU	CA-CB-CG	5.19	127.24	115.30
66	D3	542	A	C4-C5-C6	5.19	119.59	117.00
65	D2	441	С	C6-N1-C2	5.19	122.38	120.30
67	D4	85	G	C4-C5-N7	5.19	112.88	110.80
5	UE	540	LEU	CA-CB-CG	5.19	127.23	115.30
65	D2	233	G	C5-C6-N1	-5.18	108.91	111.50
67	D4	32	G	C4-C5-N7	5.18	112.87	110.80
66	D3	-4	A	C5-N7-C8	-5.18	101.31	103.90
66	D3	493	U	C5-C6-N1	5.18	125.29	122.70
7	UG	144	LEU	CA-CB-CG	5.18	127.21	115.30
65	D2	278	G	N9-C4-C5	-5.18	103.33	105.40
67	D4	28	A	C5-C6-N1	5.18	120.29	117.70
66	D3	307	G	N9-C4-C5	-5.17	103.33	105.40
65	D2	444	U	C6-N1-C1'	5.17	128.44	121.20
66	D3	1626	U	N1-C2-N3	5.17	118.00	114.90
1	UA	730	LEU	CB-CG-CD2	-5.17	102.21	111.00
66	D3	632	U	C2-N1-C1'	5.17	123.90	117.70
67	D4	56	A	O5'-P-OP2	-5.17	101.05	105.70
33	CL	1135	ARG	CB-CG-CD	-5.17	98.17	111.60
28	CF	79	VAL	CG1-CB-CG2	-5.16	102.64	110.90
66	D3	586	G	C6-C5-N7	$5.1\overline{6}$	133.50	130.40
19	US	344	ILE	CG1-CB-CG2	-5.16	100.05	111.40
65	D2	386	A	OP1-P-O3'	5.16	116.55	105.20



$\alpha \cdot \cdot$	ſ	•	
Continuea	Jrom	previous	page
	0	1	1 0

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	259	С	C2-N1-C1'	5.16	124.47	118.80
3	UC	602	LEU	CB-CG-CD2	-5.16	102.23	111.00
65	D2	394	U	N1-C2-O2	5.16	126.41	122.80
65	D2	98	G	C8-N9-C4	-5.15	104.34	106.40
66	D3	1580	С	C6-N1-C2	-5.15	118.24	120.30
30	CI	13	LEU	CB-CG-CD2	-5.15	102.24	111.00
42	JK	490	ILE	CG1-CB-CG2	-5.15	100.06	111.40
64	Dc	52	ASP	CB-CG-OD1	5.15	122.94	118.30
65	D2	307	С	C4-C5-C6	-5.15	114.83	117.40
67	D4	72	С	C6-N1-C2	-5.15	118.24	120.30
1	UA	298	LEU	CB-CG-CD1	-5.15	102.25	111.00
65	D2	81	А	OP1-P-O3'	5.15	116.52	105.20
65	D2	299	G	C5-C6-N1	5.15	114.07	111.50
66	D3	1600	А	C3'-C2'-C1'	5.15	105.62	101.50
1	UA	624	ASN	C-N-CA	-5.14	111.50	122.30
58	DQ	28	LEU	CA-CB-CG	5.14	127.13	115.30
65	D2	400	С	C2-N1-C1'	-5.14	113.14	118.80
66	D3	539	G	N9-C4-C5	-5.14	103.34	105.40
21	UU	423	ARG	NE-CZ-NH1	-5.14	117.73	120.30
66	D3	6	G	C6-N1-C2	-5.14	122.02	125.10
6	UF	75	LEU	CA-CB-CG	5.14	127.11	115.30
17	UQ	490	LEU	CB-CG-CD2	-5.14	102.27	111.00
67	D4	330	А	C5-C6-N6	-5.14	119.59	123.70
67	D4	33	А	C5-C6-N1	5.13	120.27	117.70
65	D2	323	А	N9-C4-C5	-5.13	103.75	105.80
65	D2	271	G	O5'-P-OP2	-5.13	101.08	105.70
28	CF	63	ILE	CG1-CB-CG2	-5.13	100.12	111.40
65	D2	314	U	C6-N1-C1'	-5.13	114.02	121.20
67	D4	85	G	C6-N1-C2	-5.13	122.02	125.10
66	D3	1037	С	N3-C4-N4	5.12	121.59	118.00
66	D3	1599	С	C2-N1-C1'	5.12	124.44	118.80
67	D4	42	U	N1-C2-N3	5.12	117.97	114.90
4	UD	422	LEU	CA-CB-CG	-5.12	103.52	115.30
65	D2	294	U	N3-C4-O4	-5.12	115.82	119.40
65	D2	329	А	C4-C5-N7	5.12	113.26	110.70
66	D3	548	G	C5-N7-C8	-5.12	101.74	104.30
67	D4	71	С	C4-C5-C6	-5.12	114.84	117.40
8	UH	531	LEU	CA-CB-CG	5.12	127.07	115.30
18	UR	178	VAL	CG1-CB-CG2	-5.12	102.71	110.90
19	US	469	LEU	CA-CB-CG	-5.12	103.53	115.30
66	D3	584	C	C5-C6-N1	-5.12	118.44	121.00
66	D3	541	А	C2-N3-C4	5.12	113.16	110.60



α \cdot \cdot \cdot	C	•	
Continued	trom	previous	<i>paae</i>
• • • • • • • • • • • • •	J	P	r ~g ····

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
67	D4	42	U	N3-C2-O2	-5.12	118.62	122.20
1	UA	568	ARG	CG-CD-NE	-5.12	101.06	111.80
30	CI	118	LEU	CA-CB-CG	5.12	127.06	115.30
66	D3	976	G	C8-N9-C1'	-5.12	120.35	127.00
66	D3	1618	С	C2-N1-C1'	5.12	124.43	118.80
66	D3	1620	С	N3-C2-O2	-5.12	118.32	121.90
66	D3	911	U	N1-C2-O2	5.11	126.38	122.80
65	D2	331	U	C6-N1-C2	5.11	124.07	121.00
67	D4	91	С	C5-C6-N1	5.11	123.56	121.00
1	UA	469	LEU	CA-CB-CG	5.11	127.05	115.30
65	D2	220	U	N3-C2-O2	-5.11	118.62	122.20
66	D3	34	G	C2-N3-C4	-5.11	109.34	111.90
65	D2	233	G	C5-C6-O6	-5.11	125.53	128.60
66	D3	1584	G	N7-C8-N9	-5.11	110.55	113.10
66	D3	545	А	N9-C1'-C2'	5.10	120.64	114.00
33	CL	1135	ARG	CG-CD-NE	5.10	122.52	111.80
1	UA	167	ASP	N-CA-CB	-5.10	101.42	110.60
4	UD	205	CYS	C-N-CA	5.10	134.45	121.70
25	CA	173	LEU	CA-CB-CG	5.10	127.03	115.30
66	D3	1585	U	C4-C5-C6	-5.10	116.64	119.70
66	D3	1076	A	C5-N7-C8	-5.10	101.35	103.90
65	D2	295	А	C5-N7-C8	-5.10	101.35	103.90
66	D3	594	А	N3-C4-N9	-5.10	123.32	127.40
4	UD	272	LEU	CA-CB-CG	5.10	127.02	115.30
65	D2	395	С	C2-N3-C4	-5.10	117.35	119.90
65	D2	337	G	C4-C5-N7	5.09	112.84	110.80
66	D3	1062	А	C4-C5-C6	-5.09	114.45	117.00
66	D3	1064	G	C4-N9-C1'	5.09	133.12	126.50
67	D4	318	U	C5-C6-N1	5.09	125.25	122.70
10	UJ	302	LEU	CB-CG-CD2	-5.09	102.35	111.00
12	UL	303	LEU	CA-CB-CG	5.09	127.00	115.30
65	D2	350	A	N9-C4-C5	5.09	107.84	105.80
66	D3	307	G	C5-C6-O6	-5.09	125.55	128.60
66	D3	1165	G	N3-C4-N9	-5.09	122.95	126.00
10	UJ	245	LEU	CB-CG-CD2	-5.08	102.36	111.00
65	D2	452	А	N7-C8-N9	5.08	116.34	113.80
66	D3	593	U	N3-C4-O4	5.08	122.96	119.40
9	UI	496	LEU	CA-CB-CG	5.08	126.98	115.30
30	CI	19	LEU	CB-CG-CD1	5.08	119.63	111.00
45	JO	146	VAL	CG1-CB-CG2	-5.08	102.78	110.90
65	D2	462	G	C5-C6-N1	5.08	114.04	111.50
31	CJ	279	ARG	NE-CZ-NH2	-5.08	117.76	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	CL	988	ARG	CG-CD-NE	-5.08	101.14	111.80
66	D3	1053	G	O4'-C1'-N9	5.08	112.26	108.20
66	D3	530	С	N1-C2-O2	5.07	121.94	118.90
66	D3	1614	А	C5-N7-C8	-5.07	101.36	103.90
1	UA	553	ILE	CG1-CB-CG2	-5.07	100.25	111.40
66	D3	416	А	C8-N9-C4	5.07	107.83	105.80
66	D3	1510	U	N1-C2-O2	5.07	126.35	122.80
33	CL	829	LEU	CB-CG-CD2	-5.07	102.38	111.00
66	D3	1149	G	C4-N9-C1'	5.07	133.09	126.50
66	D3	1062	А	N7-C8-N9	-5.07	111.27	113.80
31	CJ	46	LEU	CB-CG-CD2	-5.06	102.39	111.00
65	D2	323	А	N7-C8-N9	5.06	116.33	113.80
66	D3	872	G	N9-C4-C5	-5.06	103.38	105.40
66	D3	1593	А	N3-C4-C5	5.06	130.34	126.80
67	D4	57	А	C5-C6-N6	5.06	127.75	123.70
21	UU	542	LEU	CA-CB-CG	-5.06	103.67	115.30
66	D3	1080	U	N3-C2-O2	-5.06	118.66	122.20
66	D3	383	G	N3-C4-C5	5.05	131.13	128.60
52	DH	34	LEU	CA-CB-CG	5.05	126.92	115.30
66	D3	507	U	N1-C2-O2	5.05	126.34	122.80
66	D3	559	С	C5-C4-N4	-5.05	116.66	120.20
66	D3	695	U	C2-N1-C1'	5.05	123.76	117.70
66	D3	1039	А	C8-N9-C4	-5.05	103.78	105.80
66	D3	1584	G	C4-N9-C1'	-5.05	119.93	126.50
65	D2	239	U	C4-C5-C6	5.05	122.73	119.70
65	D2	259	G	C4-C5-N7	5.05	112.82	110.80
66	D3	1513	G	C4-C5-N7	5.05	112.82	110.80
65	D2	406	U	C4-C5-C6	-5.05	116.67	119.70
66	D3	1585	U	C2-N1-C1'	5.05	123.76	117.70
65	D2	290	G	C6-C5-N7	-5.05	127.37	130.40
66	D3	489	С	C5-C6-N1	5.05	123.52	121.00
65	D2	269	G	C4-N9-C1'	5.04	133.06	126.50
66	D3	937	С	C6-N1-C2	-5.04	118.28	120.30
67	D4	10	С	N3-C4-C5	5.04	123.92	121.90
14	UN	847	VAL	CG1-CB-CG2	-5.04	102.83	110.90
65	D2	298	А	C5-C6-N6	-5.04	119.67	123.70
66	D3	1531	G	C6-C5-N7	-5.04	127.38	130.40
66	D3	495	C	C6-N1-C1'	-5.04	114.75	120.80
7	UG	329	LEU	CB-CG-CD1	-5.03	102.44	111.00
66	D3	553	G	C6-C5-N7	-5.03	127.38	130.40
66	D3	1591	C	C5-C6-N1	$5.0\overline{3}$	$123.5\overline{2}$	121.00
26	CD	138	LEU	CB-CG-CD1	-5.03	102.44	111.00



α $\cdot \cdot$ \cdot	C		
Continued	from	previous	page
	5	1	1 5

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
18	UR	237	ARG	NE-CZ-NH1	5.03	122.81	120.30
65	D2	474	A	C2-N3-C4	-5.03	108.08	110.60
65	D2	489	G	C8-N9-C4	5.03	108.41	106.40
17	UQ	895	LEU	CA-CB-CG	-5.03	103.73	115.30
65	D2	82	A	C5-N7-C8	-5.03	101.39	103.90
65	D2	99	U	C2-N1-C1'	5.03	123.73	117.70
66	D3	872	G	N3-C4-C5	5.03	131.11	128.60
67	D4	53	U	C2-N1-C1'	-5.03	111.67	117.70
7	UG	229	ARG	NE-CZ-NH1	-5.03	117.79	120.30
65	D2	248	G	N9-C4-C5	-5.03	103.39	105.40
66	D3	1486	G	C4-N9-C1'	5.03	133.03	126.50
66	D3	468	А	C2-N3-C4	5.02	113.11	110.60
66	D3	872	G	C6-C5-N7	-5.02	127.39	130.40
33	CL	54	LEU	CA-CB-CG	5.02	126.85	115.30
67	D4	259	С	N3-C2-O2	-5.02	118.39	121.90
25	CA	301	LEU	CA-CB-CG	5.02	126.84	115.30
66	D3	381	С	C6-N1-C2	-5.02	118.29	120.30
66	D3	1638	G	C5-C6-O6	-5.02	125.59	128.60
39	JG	246	GLU	C-N-CA	-5.02	109.16	121.70
66	D3	307	G	C4-C5-N7	5.02	112.81	110.80
66	D3	417	A	P-O3'-C3'	5.02	125.72	119.70
66	D3	1492	А	C5-C6-N1	5.02	120.21	117.70
24	UZ	134	LEU	CA-CB-CG	5.01	126.83	115.30
65	D2	477	G	C2-N3-C4	-5.01	109.39	111.90
43	JM	211	GLU	N-CA-CB	5.01	119.62	110.60
65	D2	346	G	N9-C4-C5	-5.01	103.39	105.40
66	D3	885	G	C4-N9-C1'	5.01	133.02	126.50
65	D2	392	U	C6-N1-C2	-5.01	117.99	121.00
66	D3	1166	A	C5-N7-C8	-5.01	101.39	103.90
66	D3	1492	А	N3-C4-C5	-5.01	123.29	126.80
65	D2	338	A	C6-N1-C2	-5.01	115.60	118.60
66	D3	448	С	N3-C2-O2	-5.01	118.39	121.90
66	D3	1594	G	C5-C6-N1	5.01	114.00	111.50
17	UQ	613	LEU	CA-CB-CG	5.00	126.81	115.30
34	CM	19	LEU	CA-CB-CG	-5.00	103.79	115.30
30	CI	46	LYS	CA-CB-CG	5.00	124.40	113.40
66	D3	531	С	C6-N1-C2	-5.00	118.30	120.30
66	D3	549	G	C4-C5-N7	5.00	112.80	110.80
66	D3	1073	G	N3-C4-N9	-5.00	123.00	126.00

There are no chirality outliers.

All (82) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
26	CD	134	HIS	Peptide
27	CE	407	ARG	Peptide
30	CI	16	VAL	Peptide
31	CJ	167	LEU	Peptide
31	CJ	212	ALA	Peptide
32	CK	453	SER	Peptide
34	CM	365	LYS	Peptide
48	DA	11	LYS	Peptide
48	DA	208	GLN	Peptide
48	DA	24	PHE	Peptide
49	DE	66	MET	Peptide
52	DH	8	ILE	Peptide
58	DQ	13	LYS	Peptide
58	DQ	39	VAL	Peptide
59	DS	35	ILE	Peptide
60	DW	67	GLY	Peptide
61	DX	100	ASP	Peptide
61	DX	77	ILE	Peptide
61	DX	88	PRO	Peptide
36	JA	242	GLU	Peptide
36	JB	504	THR	Peptide
36	JB	739	ASN	Peptide
36	JB	859	ILE	Peptide
37	JC	132	HIS	Peptide
37	JC	77	TYR	Peptide
38	JE	242	MET	Peptide
38	JE	256	PRO	Peptide
43	JM	134	ARG	Peptide
44	JN	268	LYS	Peptide
46	JP	112	LEU	Peptide
46	JP	256	GLN	Peptide
46	JP	301	PHE	Peptide
46	JP	356	TYR	Peptide
1	UA	157	ASP	Peptide
1	UA	202	ASP	Peptide
1	UA	288	ASP	Peptide
1	UA	516	SER	Peptide
4	UD	117	ILE	Peptide
4	UD	161	ASP	Peptide
4	UD	198	ASP	Peptide
4	UD	251	ASP	Peptide
4	UD	266	ASP	Peptide
4	UD	279	HIS	Peptide
4	UD	279	HIS	Peptide


Mol	Chain	Res	Type	Group
4	UD	771	GLN	Peptide
5	UE	138	GLN	Peptide
6	UF	105	GLN	Peptide
6	UF	125	SER	Peptide
6	UF	142	THR	Peptide
7	UG	199	LEU	Peptide
7	UG	208	ALA	Peptide
7	UG	405	GLY	Peptide
7	UG	441	THR	Peptide
10	UJ	1695	MET	Peptide
10	UJ	554	ILE	Peptide
10	UJ	599	PHE	Peptide
12	UL	142	ASP	Peptide
12	UL	193	THR	Peptide
12	UL	194	HIS	Peptide
12	UL	243	THR	Peptide
13	UM	215	GLY	Peptide
13	UM	426	ILE	Peptide
14	UN	886	LYS	Peptide
15	UO	51	HIS	Peptide
17	UQ	317	TRP	Peptide
17	UQ	358	LEU	Peptide
17	UQ	394	SER	Peptide
17	UQ	780	GLU	Peptide
18	UR	347	GLY	Peptide
18	UR	468	CYS	Peptide
18	UR	503	SER	Peptide
20	UT	1357	ASN	Peptide
20	UT	1358	LYS	Peptide
20	UT	1714	SER	Peptide
20	UT	1925	ASP	Peptide
20	UT	323	PHE	Peptide
20	UT	706	LEU	Peptide
20	UT	707	PRO	Peptide
21	UU	637	ASN	Peptide
21	UU	757	PRO	Peptide
21	UU	855	PHE	Peptide
21	UU	901	LYS	Peptide
23	UX	109	LEU	Peptide

Continued from previous page...



5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	6635	0	6524	147	0
2	UB	3743	0	3445	80	0
3	UC	1026	0	1080	40	0
4	UD	5361	0	5364	141	0
5	UE	3772	0	3806	99	0
6	UF	2487	0	2533	59	0
7	UG	4218	0	4223	94	0
8	UH	2690	0	1931	69	0
9	UI	846	0	904	39	0
10	UJ	6857	0	5023	85	0
11	UK	2016	0	2093	59	0
12	UL	6720	0	6753	196	0
13	UM	5957	0	5992	182	0
14	UN	1207	0	1201	26	0
15	UO	3911	0	3906	119	0
16	UP	495	0	561	13	0
17	UQ	6662	0	6588	173	0
18	UR	3791	0	3772	89	0
19	US	3650	0	3365	102	0
20	UT	11108	0	4748	16	0
21	UU	6678	0	6652	131	0
22	UV	8725	0	8841	190	0
23	UX	1395	0	1474	40	0
24	UZ	2006	0	2118	54	0
25	CA	1881	0	1928	31	0
25	CB	1782	0	1826	54	0
26	CD	2994	0	3018	81	0
27	CE	2985	0	2703	59	0
28	CF	931	0	983	18	0
28	CG	928	0	976	34	0
29	CH	3634	0	3662	112	0
30	CI	1530	0	1572	36	0
31	CJ	2296	0	2325	64	0
32	CK	1667	0	1701	50	0
33	CL	6332	0	6516	190	0
34	CM	2781	0	2878	73	0
35	CN	1893	0	1875	37	0



Conti	nueu jron	<i>i previous</i>	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	JA	5892	0	5420	146	0
36	JB	4132	0	1819	17	0
37	JC	2845	0	2761	91	0
38	JE	1125	0	1101	46	0
39	JF	1701	0	1767	42	0
39	JG	1799	0	1872	48	0
40	JH	1295	0	570	2	0
41	JJ	1448	0	1524	43	0
42	JK	334	0	313	12	0
43	JM	1137	0	1187	28	0
44	JN	1428	0	1425	25	0
45	JO	1930	0	2025	38	0
46	JP	3725	0	3679	100	0
47	JQ	381	0	255	4	0
48	DA	1912	0	2023	53	0
49	DE	1944	0	2030	69	0
50	DF	1669	0	1724	31	0
51	DG	1755	0	1846	68	0
52	DH	1477	0	1568	49	0
53	DI	1399	0	1431	47	0
54	DJ	1428	0	1506	48	0
55	DL	1129	0	1196	35	0
56	DN	1192	0	1255	27	0
57	DO	881	0	910	21	0
58	DQ	973	0	1029	23	0
59	DS	516	0	222	12	0
60	DW	1021	0	1060	24	0
61	DX	786	0	843	20	0
62	DY	767	0	787	53	0
63	Db	610	0	629	0	0
64	Dc	497	0	535	0	0
65	D2	11138	0	5569	138	0
66	D3	25549	0	12882	423	0
67	D4	3712	0	1876	51	0
68	Db	1	0	0	0	0
68	UX	1	0	0	0	0
69	CL	32	0	12	3	0
All	All	223151	0	191511	4355	0

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 11.

All (4355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:CL:80:THR:CG2	33:CL:141:LEU:CD2	2.05	1.33
12:UL:349:SER:HA	12:UL:369:TYR:O	1.21	1.30
1:UA:315:GLU:OE1	41:JJ:273:ARG:HG3	1.34	1.28
7:UG:132:GLY:HA3	7:UG:150:LEU:O	1.24	1.26
13:UM:30:LYS:HA	13:UM:45:LEU:O	1.37	1.21
29:CH:162:CYS:HA	29:CH:186:PHE:O	1.38	1.20
33:CL:80:THR:HG22	33:CL:141:LEU:CD2	1.70	1.18
2:UB:740:MET:CE	59:DS:103:ASN:HA	1.74	1.17
17:UQ:332:GLN:NE2	18:UR:344:ARG:HD3	1.60	1.14
33:CL:80:THR:HG21	33:CL:141:LEU:CD2	1.73	1.12
33:CL:80:THR:HG21	33:CL:141:LEU:HD23	1.29	1.09
69:CL:2001:GTP:H5"	69:CL:2001:GTP:H8	1.05	1.07
33:CL:80:THR:CG2	33:CL:141:LEU:HD23	1.76	1.07
2:UB:740:MET:HE3	59:DS:103:ASN:HA	1.37	1.06
7:UG:132:GLY:CA	7:UG:150:LEU:O	2.07	1.02
33:CL:80:THR:CG2	33:CL:141:LEU:HD22	1.86	1.01
18:UR:382:GLY:HA3	18:UR:400:ILE:O	1.60	1.01
17:UQ:332:GLN:HE21	18:UR:344:ARG:HD3	0.86	1.01
33:CL:625:TRP:CZ2	34:CM:281:GLU:OE1	2.13	1.01
69:CL:2001:GTP:H5"	69:CL:2001:GTP:C8	1.95	1.01
62:DY:11:LYS:O	62:DY:23:PHE:HA	1.61	1.01
24:UZ:39:ILE:O	24:UZ:242:ILE:HA	1.62	1.00
12:UL:349:SER:CA	12:UL:369:TYR:O	2.10	0.99
52:DH:70:PHE:O	52:DH:74:GLN:HB2	1.62	0.98
21:UU:228:GLY:HA3	21:UU:246:ILE:O	1.64	0.97
62:DY:6:THR:HB	62:DY:28:LEU:O	1.64	0.97
4:UD:614:TRP:O	4:UD:618:ASN:HB2	1.63	0.97
17:UQ:332:GLN:HE21	18:UR:344:ARG:CD	1.77	0.96
13:UM:30:LYS:CA	13:UM:45:LEU:O	2.13	0.96
15:UO:279:GLY:CA	15:UO:298:PHE:O	2.15	0.94
24:UZ:38:ILE:O	24:UZ:198:SER:HA	1.68	0.94
1:UA:311:ASN:ND2	41:JJ:273:ARG:HH21	1.66	0.93
52:DH:81:LEU:O	52:DH:85:PHE:HD1	1.51	0.92
1:UA:315:GLU:OE1	41:JJ:273:ARG:CG	2.17	0.92
65:D2:502:G:H1	65:D2:535:G:H22	1.13	0.92
2:UB:740:MET:HE1	59:DS:103:ASN:HA	1.52	0.91
15:UO:191:GLY:CA	15:UO:211:HIS:O	2.19	0.91
15:UO:279:GLY:HA3	15:UO:298:PHE:O	1.72	0.90
8:UH:536:ARG:O	8:UH:540:LEU:HB3	1.71	0.89
33:CL:1138:ARG:HH11	66:D3:492:A:H62	1.19	0.89
18:UR:278:ASP:HB2	18:UR:281:THR:O	1.72	0.88
15:UO:191:GLY:HA3	15:UO:211:HIS:O	1.72	0.88



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
33:CL:625:TRP:CE2	34:CM:281:GLU:OE1	2.25	0.88
1:UA:77:GLY:HA3	1:UA:95:PHE:O	1.74	0.88
19:US:191:ILE:O	19:US:195:PHE:HB2	1.74	0.87
2:UB:740:MET:CE	59:DS:103:ASN:CA	2.53	0.86
41:JJ:103:PRO:HA	41:JJ:106:MET:HG2	1.57	0.86
15:UO:19:GLN:OE1	15:UO:19:GLN:N	2.08	0.85
1:UA:311:ASN:ND2	41:JJ:273:ARG:NH2	2.23	0.85
29:CH:160:ILE:HA	29:CH:188:TYR:O	1.77	0.85
19:US:215:ASN:HB3	19:US:218:LYS:HD3	1.59	0.85
33:CL:1138:ARG:NH1	66:D3:492:A:N7	2.24	0.84
21:UU:125:GLY:HA2	27:CE:430:ASP:HA	1.58	0.84
52:DH:84:LYS:HG3	52:DH:85:PHE:CE1	2.11	0.84
3:UC:545:LEU:O	3:UC:545:LEU:HD12	1.77	0.83
2:UB:740:MET:HE1	59:DS:103:ASN:CA	2.08	0.83
24:UZ:192:ASN:HD21	66:D3:1510:U:H5'	1.42	0.83
66:D3:1775:U:H3	66:D3:1786:G:H1	1.24	0.83
33:CL:80:THR:HG22	33:CL:141:LEU:HD21	1.58	0.83
33:CL:625:TRP:NE1	34:CM:281:GLU:OE1	2.11	0.83
46:JP:12:ASP:O	46:JP:23:GLN:NE2	2.11	0.82
39:JF:121:LEU:HB3	39:JF:163:ILE:O	1.80	0.82
33:CL:625:TRP:O	33:CL:627:SER:N	2.13	0.82
36:JA:282:THR:O	36:JA:469:SER:HA	1.79	0.82
13:UM:414:VAL:O	13:UM:428:ALA:HB3	1.80	0.81
31:CJ:9:ARG:HH22	31:CJ:12:TYR:HD2	1.27	0.81
15:UO:279:GLY:HA2	15:UO:298:PHE:O	1.79	0.81
43:JM:114:ARG:O	43:JM:118:GLN:HB2	1.81	0.81
66:D3:895:G:H1	66:D3:917:U:H3	1.26	0.81
65:D2:344:U:O2	65:D2:381:G:N2	2.15	0.80
33:CL:624:LYS:NZ	33:CL:625:TRP:HE1	1.80	0.80
37:JC:277:ILE:HA	37:JC:289:ILE:O	1.82	0.80
5:UE:101:THR:HG23	5:UE:103:ASN:H	1.46	0.79
33:CL:624:LYS:NZ	33:CL:625:TRP:NE1	2.29	0.79
30:CI:61:LEU:HD22	32:CK:437:ILE:HD11	1.65	0.79
29:CH:357:LEU:HD12	38:JE:256:PRO:HB2	1.65	0.79
52:DH:23:ALA:CB	52:DH:85:PHE:HZ	1.95	0.79
55:DL:124:THR:HB	55:DL:141:LYS:HB2	1.62	0.79
66:D3:1114:G:H1	67:D4:10:C:H42	1.31	0.79
15:UO:53:HIS:O	15:UO:68:SER:HB3	1.83	0.78
21:UU:488:ASN:ND2	58:DQ:98:ASP:OD2	2.16	0.78
62:DY:27:VAL:H	62:DY:69:SER:H	1.30	0.78
7:UG:502:ARG:NH1	65:D2:369:G:N7	2.26	0.78



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
48:DA:19:ARG:HH12	48:DA:22:ASP:H	1.32	0.77
17:UQ:96:ILE:HG12	17:UQ:108:THR:HG21	1.66	0.77
52:DH:84:LYS:CG	52:DH:85:PHE:CE1	2.67	0.77
15:UO:20:THR:HG21	15:UO:28:ARG:HH12	1.49	0.77
10:UJ:166:ASN:ND2	27:CE:408:THR:O	2.17	0.77
17:UQ:680:ALA:HB2	17:UQ:750:LEU:HD23	1.64	0.77
39:JF:151:ARG:HA	39:JF:158:LYS:HA	1.64	0.77
1:UA:666:ARG:NH2	1:UA:678:GLU:OE1	2.17	0.77
49:DE:87:MET:HA	49:DE:101:LEU:O	1.86	0.76
62:DY:63:GLN:HB2	62:DY:68:LYS:HB3	1.67	0.76
33:CL:1135:ARG:HH21	66:D3:495:C:H5'	1.50	0.76
52:DH:81:LEU:O	52:DH:85:PHE:CD1	2.39	0.76
12:UL:897:ASP:OD2	13:UM:758:ARG:NH1	2.17	0.76
33:CL:625:TRP:HZ2	34:CM:281:GLU:OE1	1.67	0.76
33:CL:80:THR:HG22	33:CL:141:LEU:HD22	1.54	0.76
26:CD:377:ARG:NH2	67:D4:111:G:N7	2.32	0.75
1:UA:412:ARG:HD3	1:UA:421:ASN:HD21	1.50	0.75
28:CG:14:ALA:HB1	29:CH:398:CYS:HB3	1.67	0.75
2:UB:740:MET:HE1	59:DS:103:ASN:N	2.02	0.75
22:UV:120:HIS:HB3	22:UV:288:THR:HG23	1.67	0.75
62:DY:26:ASP:HA	62:DY:69:SER:O	1.87	0.74
10:UJ:22:ARG:NH1	46:JP:20:GLN:O	2.20	0.74
21:UU:455:PHE:HB3	21:UU:477:ILE:HD12	1.69	0.74
38:JE:289:PHE:O	38:JE:293:ASN:HB2	1.87	0.74
36:JA:912:MET:HA	36:JA:915:LYS:HE2	1.70	0.74
66:D3:104:A:H61	66:D3:307:G:H3'	1.53	0.74
12:UL:448:GLY:HA3	12:UL:476:ILE:HD11	1.69	0.74
33:CL:267:ARG:HH12	33:CL:798:MET:HG2	1.51	0.74
49:DE:201:HIS:HB2	49:DE:205:PHE:O	1.87	0.74
38:JE:229:ASP:HB3	38:JE:232:GLU:HB2	1.70	0.74
65:D2:425:U:O4	65:D2:431:A:N6	2.20	0.74
1:UA:350:SER:OG	1:UA:351:LEU:N	2.20	0.74
13:UM:161:TRP:HB3	13:UM:177:LEU:HD12	1.69	0.74
23:UX:133:LYS:NZ	67:D4:33:A:OP1	2.19	0.74
3:UC:559:ARG:NH2	66:D3:544:A:O2'	2.21	0.73
7:UG:194:ARG:NH2	7:UG:210:GLU:OE2	2.21	0.73
22:UV:403:GLY:HA2	22:UV:410:LYS:HA	1.68	0.73
49:DE:210:ILE:O	49:DE:217:THR:HA	1.87	0.73
5:UE:490:ARG:NH2	65:D2:102:A:OP2	2.22	0.73
48:DA:19:ARG:HH22	48:DA:22:ASP:HA	1.53	0.73
66:D3:62:A:N1	66:D3:288:A:O2'	2.21	0.73



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:UG:464:LYS:NZ	66:D3:-2:A:N7	2.28	0.73
15:UO:77:PHE:HE2	15:UO:96:LEU:HD13	1.54	0.73
35:CN:97:GLU:HG3	35:CN:98:VAL:HG23	1.70	0.73
53:DI:65:PHE:HA	53:DI:181:GLY:O	1.89	0.73
66:D3:545:A:O2'	66:D3:546:U:O4'	2.07	0.73
17:UQ:458:GLN:HE21	17:UQ:467:GLN:HG3	1.54	0.73
32:CK:507:ILE:HD13	32:CK:528:LEU:HD23	1.71	0.73
5:UE:162:GLN:HA	5:UE:173:ILE:O	1.87	0.73
66:D3:642:G:N2	66:D3:692:C:O2	2.20	0.73
25:CB:210:MET:HA	25:CB:213:LYS:HD2	1.71	0.72
8:UH:643:ASP:OD1	9:UI:502:ARG:NH2	2.23	0.72
1:UA:586:SER:OG	1:UA:587:PHE:N	2.20	0.72
15:UO:83:VAL:HG13	15:UO:85:TYR:HE1	1.54	0.72
34:CM:114:PHE:O	34:CM:169:VAL:HA	1.89	0.72
53:DI:8:ARG:HH21	53:DI:21:PHE:H	1.37	0.72
6:UF:67:ARG:NH1	6:UF:84:SER:OG	2.23	0.72
43:JM:215:LYS:HG2	43:JM:216:ARG:HE	1.53	0.72
58:DQ:66:ARG:HH11	65:D2:267:U:H3	1.37	0.72
21:UU:455:PHE:HB3	21:UU:477:ILE:CD1	2.20	0.72
66:D3:1155:G:N2	66:D3:1624:C:O2	2.23	0.72
10:UJ:18:VAL:O	10:UJ:24:ARG:NH1	2.22	0.72
8:UH:552:LYS:HB2	8:UH:576:ARG:HH12	1.55	0.72
13:UM:313:LEU:HB3	13:UM:331:SER:HB3	1.72	0.72
15:UO:2:SER:OG	15:UO:3:THR:N	2.23	0.72
19:US:130:GLU:O	19:US:134:PHE:HB2	1.88	0.72
53:DI:116:HIS:O	53:DI:146:ARG:NH1	2.23	0.72
10:UJ:153:SER:O	10:UJ:169:ARG:NH1	2.23	0.72
18:UR:345:LEU:HD11	18:UR:352:GLN:HE21	1.54	0.72
23:UX:189:PHE:HE1	54:DJ:15:PRO:HB3	1.55	0.72
46:JP:440:ARG:NH2	66:D3:1042:G:OP1	2.23	0.72
29:CH:560:ARG:NH2	67:D4:249:G:N7	2.37	0.71
36:JA:16:ASN:HD21	36:JA:218:PRO:HA	1.55	0.71
1:UA:478:CYS:SG	1:UA:479:LEU:N	2.63	0.71
2:UB:740:MET:HE3	59:DS:103:ASN:CA	2.15	0.71
30:CI:143:ILE:HG22	30:CI:145:ASP:H	1.55	0.71
32:CK:335:ARG:NH2	33:CL:957:GLU:OE2	2.22	0.71
52:DH:19:GLN:OE1	52:DH:85:PHE:HE2	1.73	0.71
15:UO:211:HIS:CE1	15:UO:235:LYS:HE2	2.25	0.71
22:UV:270:ILE:HB	22:UV:292:ILE:HB	1.72	0.71
27:CE:231:ILE:HA	27:CE:234:ARG:HD2	1.72	0.71
66:D3:1115:U:H2'	66:D3:1116:A:H8	1.55	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:UC:560:ASN:HB3	3:UC:563:VAL:HG12	1.72	0.71
34:CM:306:GLU:HA	34:CM:356:GLY:O	1.90	0.71
48:DA:64:ARG:NH2	57:DO:37:GLU:OE1	2.23	0.71
13:UM:133:ASN:ND2	66:D3:1785:U:O2'	2.23	0.71
36:JA:887:ALA:HA	36:JA:891:GLN:HB2	1.73	0.71
1:UA:209:VAL:HG22	1:UA:215:VAL:HG22	1.73	0.71
33:CL:105:ILE:HG13	33:CL:356:ALA:HB2	1.71	0.71
9:UI:480:LYS:NZ	65:D2:11:A:OP2	2.23	0.71
12:UL:177:LEU:HD23	12:UL:191:LEU:HD21	1.73	0.71
29:CH:448:PHE:HB2	29:CH:460:ARG:HB3	1.72	0.71
26:CD:198:TRP:NE1	27:CE:165:GLN:OE1	2.23	0.70
4:UD:374:THR:HB	4:UD:757:ARG:HH12	1.57	0.70
22:UV:99:LYS:O	22:UV:103:PHE:HB2	1.90	0.70
9:UI:471:LYS:HE2	9:UI:475:THR:HG23	1.72	0.70
15:UO:51:HIS:O	15:UO:53:HIS:ND1	2.25	0.70
39:JG:112:VAL:HG23	39:JG:124:VAL:HB	1.74	0.70
11:UK:164:ASN:HB3	11:UK:166:LEU:HD23	1.72	0.70
51:DG:13:GLN:NE2	66:D3:151:G:N3	2.38	0.70
2:UB:213:GLU:HA	66:D3:1207:C:H1'	1.72	0.70
34:CM:200:VAL:HG12	34:CM:201:SER:H	1.57	0.70
36:JA:742:PHE:HB3	36:JA:762:MET:HB3	1.74	0.70
38:JE:266:ILE:HD11	54:DJ:139:GLN:HB2	1.74	0.70
38:JE:324:ASP:OD1	54:DJ:79:ARG:NH1	2.24	0.70
66:D3:523:G:H21	66:D3:529:A:H62	1.40	0.70
4:UD:370:ARG:NH2	4:UD:372:MET:SD	2.65	0.70
15:UO:277:LEU:HA	15:UO:302:VAL:H	1.55	0.70
1:UA:311:ASN:HD21	41:JJ:273:ARG:HH21	1.36	0.70
17:UQ:332:GLN:NE2	18:UR:344:ARG:CD	2.47	0.70
22:UV:173:ASN:HB2	66:D3:1700:C:H5'	1.74	0.70
39:JG:158:LYS:HE3	66:D3:1572:G:H21	1.57	0.70
19:US:189:ALA:HA	19:US:192:GLN:HG3	1.74	0.70
31:CJ:112:PRO:HB2	31:CJ:211:ASN:HD22	1.57	0.70
58:DQ:37:THR:O	58:DQ:45:ARG:NH1	2.25	0.70
12:UL:13:ALA:HA	12:UL:681:ILE:O	1.92	0.69
21:UU:625:VAL:HG12	21:UU:627:ASN:H	1.54	0.69
12:UL:581:ILE:HG22	12:UL:588:ILE:HG12	1.74	0.69
16:UP:190:LEU:HD12	16:UP:191:PRO:HD2	1.71	0.69
18:UR:564:LYS:HB2	18:UR:582:GLU:HG3	1.72	0.69
24:UZ:142:ARG:NH2	66:D3:1514:U:OP2	2.25	0.69
25:CB:267:VAL:HG11	25:CB:298:ILE:HD13	1.74	0.69
14:UN:890:VAL:HG23	46:JP:358:MET:HB3	1.74	0.69



A + a 1	A + ama - D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
36:JA:183:ARG:NH1	36:JA:557:SER:O	2.25	0.69
45:JO:288:GLN:OE1	45:JO:291:ARG:NH2	2.24	0.69
15:UO:16:LEU:HD13	15:UO:454:ARG:HH11	1.58	0.69
15:UO:191:GLY:HA2	15:UO:211:HIS:O	1.92	0.69
17:UQ:283:VAL:HG12	17:UQ:290:ILE:HG22	1.74	0.69
22:UV:186:ILE:HG12	22:UV:346:LEU:HD22	1.75	0.69
31:CJ:151:SER:OG	31:CJ:152:LEU:N	2.23	0.69
33:CL:72:VAL:HG22	33:CL:137:LEU:HB3	1.74	0.69
34:CM:113:LYS:HD2	34:CM:171:ASP:HA	1.75	0.69
15:UO:21:THR:OG1	15:UO:22:PRO:HD2	1.92	0.69
31:CJ:260:GLU:OE2	31:CJ:276:GLN:NE2	2.25	0.69
4:UD:32:ILE:HA	8:UH:720:TYR:HB3	1.73	0.69
7:UG:25:THR:OG1	14:UN:862:ARG:NH2	2.24	0.69
8:UH:599:MET:HG3	8:UH:644:SER:HB2	1.73	0.69
10:UJ:377:ARG:HE	10:UJ:414:LEU:HD12	1.57	0.69
10:UJ:407:PHE:O	10:UJ:410:ILE:O	2.11	0.69
13:UM:401:LEU:HD21	13:UM:416:ARG:HG3	1.73	0.69
25:CB:91:HIS:HB3	25:CB:96:VAL:O	1.93	0.69
33:CL:80:THR:HG21	33:CL:141:LEU:HD22	1.55	0.69
35:CN:88:LEU:HB2	35:CN:125:LEU:HB2	1.75	0.69
39:JF:232:LEU:HD13	39:JF:237:ALA:HB2	1.75	0.69
62:DY:93:ARG:NH2	66:D3:524:U:OP2	2.26	0.69
22:UV:1010:GLU:OE2	22:UV:1044:LYS:NZ	2.26	0.69
7:UG:183:GLU:OE2	30:CI:41:ARG:NH2	2.26	0.69
17:UQ:24:ASN:ND2	17:UQ:369:TYR:OH	2.25	0.69
54:DJ:133:HIS:ND1	54:DJ:162:SER:OG	2.24	0.69
13:UM:626:MET:HB3	13:UM:631:MET:HB3	1.75	0.68
36:JA:916:ILE:HA	36:JA:919:LYS:HD2	1.74	0.68
4:UD:83:ASN:ND2	4:UD:587:ALA:O	2.25	0.68
12:UL:134:THR:HB	12:UL:150:LEU:HB2	1.75	0.68
26:CD:393:SER:OG	26:CD:394:GLU:N	2.25	0.68
3:UC:503:GLN:HA	3:UC:506:LYS:HZ3	1.58	0.68
7:UG:498:ARG:HH22	7:UG:502:ARG:HH11	1.40	0.68
19:US:224:ASN:O	19:US:284:ARG:NH2	2.26	0.68
11:UK:22:ARG:NH1	33:CL:997:MET:O	2.26	0.68
13:UM:584:ILE:HG13	13:UM:586:LYS:H	1.58	0.68
33:CL:41:ARG:NH2	66:D3:27:U:OP1	2.25	0.68
34:CM:196:TYR:HA	34:CM:228:ASP:O	1.93	0.68
22:UV:1012:LEU:HD21	22:UV:1044:LYS:HB3	1.76	0.68
55:DL:73:GLY:HA3	55:DL:86:ILE:HD12	1.76	0.68
8:UH:535:SER:HA	8:UH:538:ARG:HH21	1.59	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
34:CM:315:LYS:HD3	34:CM:348:GLU:HB3	1.74	0.68
36:JA:133:ASN:OD1	36:JA:137:ARG:NH1	2.26	0.68
52:DH:144:VAL:HA	60:DW:42:GLN:HE22	1.56	0.68
66:D3:229:U:O2	66:D3:239:C:N4	2.26	0.68
14:UN:331:GLN:HA	26:CD:88:LYS:HE2	1.75	0.68
29:CH:160:ILE:O	29:CH:525:GLN:NE2	2.27	0.68
33:CL:551:LYS:O	33:CL:555:MET:HB2	1.94	0.68
46:JP:117:CYS:HG	46:JP:187:SER:HG	1.36	0.68
7:UG:164:GLN:HA	7:UG:179:HIS:HB3	1.74	0.68
26:CD:95:ASN:ND2	26:CD:117:ASP:OD2	2.27	0.68
31:CJ:176:ILE:HG22	31:CJ:177:ILE:HG12	1.75	0.68
10:UJ:166:ASN:HD21	27:CE:407:ARG:HD2	1.59	0.68
19:US:191:ILE:O	19:US:195:PHE:CB	2.41	0.68
21:UU:307:GLN:NE2	27:CE:422:THR:O	2.27	0.68
46:JP:327:LYS:HG2	46:JP:350:HIS:H	1.59	0.68
5:UE:489:ALA:HB1	15:UO:16:LEU:HD23	1.76	0.68
12:UL:412:GLY:HA3	12:UL:430:CYS:H	1.59	0.67
13:UM:787:PRO:HG3	32:CK:495:ILE:HD11	1.75	0.67
15:UO:31:THR:HG22	15:UO:32:SER:H	1.59	0.67
22:UV:865:ARG:NH2	66:D3:1060:U:OP2	2.27	0.67
29:CH:161:SER:H	29:CH:188:TYR:H	1.40	0.67
33:CL:841:THR:HG22	33:CL:860:TYR:HD2	1.58	0.67
37:JC:162:LEU:HB2	37:JC:176:PHE:HB2	1.76	0.67
37:JC:200:GLU:HA	37:JC:231:VAL:H	1.58	0.67
66:D3:694:U:O2'	66:D3:695:U:O2	2.12	0.67
66:D3:868:G:H1	66:D3:960:U:H3	1.41	0.67
15:UO:34:GLN:HG2	15:UO:71:ARG:HH21	1.59	0.67
18:UR:144:LYS:O	18:UR:147:ARG:NH1	2.27	0.67
6:UF:319:TYR:HA	6:UF:322:LEU:HD13	1.76	0.67
22:UV:1013:THR:HG23	22:UV:1016:GLN:H	1.59	0.67
22:UV:1108:LEU:O	22:UV:1112:CYS:HB2	1.94	0.67
33:CL:61:ARG:NH2	34:CM:306:GLU:O	2.28	0.67
37:JC:180:THR:HG22	37:JC:182:GLY:H	1.60	0.67
39:JG:31:LEU:HD13	39:JG:40:ARG:HE	1.59	0.67
49:DE:100:ARG:NH2	49:DE:121:TYR:O	2.27	0.67
53:DI:22:ARG:HD2	53:DI:25:ARG:HE	1.59	0.67
6:UF:191:ASN:HD22	43:JM:62:LEU:HG	1.59	0.67
13:UM:691:PRO:HB3	13:UM:742:ARG:HE	1.59	0.67
62:DY:27:VAL:HB	62:DY:69:SER:HB3	1.76	0.67
66:D3:88:U:H2'	66:D3:89:G:H8	1.60	0.67
15:UO:496:HIS:NE2	15:UO:500:GLU:OE1	2.28	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
51:DG:2:LYS:O	51:DG:108:VAL:HA	1.93	0.67
58:DQ:13:LYS:HG3	58:DQ:14:LYS:H	1.60	0.67
65:D2:477:G:N2	67:D4:42:U:O2	2.27	0.67
18:UR:453:VAL:HG21	28:CF:90:ALA:HB2	1.77	0.67
23:UX:121:ARG:NH2	46:JP:66:HIS:O	2.28	0.67
3:UC:554:ARG:NH1	66:D3:547:U:OP2	2.27	0.67
11:UK:100:LYS:NZ	11:UK:221:GLN:OE1	2.28	0.67
13:UM:667:GLN:NE2	13:UM:671:ASN:OD1	2.28	0.67
24:UZ:208:SER:OG	24:UZ:209:ILE:N	2.27	0.67
25:CB:264:GLN:HB3	25:CB:319:ARG:HH21	1.60	0.67
38:JE:291:GLU:HG3	62:DY:11:LYS:HE2	1.76	0.67
13:UM:15:ILE:HG13	13:UM:34:THR:HG21	1.77	0.67
17:UQ:678:LEU:HB2	17:UQ:694:LEU:HD11	1.77	0.67
48:DA:11:LYS:NZ	66:D3:912:U:OP2	2.28	0.67
50:DF:154:ALA:O	50:DF:156:ARG:NH1	2.28	0.67
51:DG:180:THR:HG23	51:DG:183:ARG:H	1.61	0.67
29:CH:159:CYS:SG	29:CH:523:LYS:NZ	2.65	0.66
33:CL:316:LYS:O	33:CL:320:PHE:HB2	1.95	0.66
46:JP:140:SER:OG	46:JP:141:ASP:N	2.28	0.66
66:D3:148:A:N6	66:D3:167:U:O4	2.28	0.66
66:D3:152:U:O2	66:D3:163:G:N2	2.28	0.66
5:UE:111:ASP:OD1	5:UE:112:LEU:N	2.27	0.66
22:UV:660:ASP:HB3	48:DA:93:GLY:HA2	1.77	0.66
36:JA:585:VAL:O	36:JA:639:ALA:HB3	1.95	0.66
8:UH:293:TYR:HA	8:UH:304:GLN:HA	1.76	0.66
12:UL:275:GLN:NE2	12:UL:276:ASN:O	2.27	0.66
29:CH:491:SER:OG	29:CH:492:TRP:N	2.27	0.66
30:CI:137:ARG:NH2	30:CI:139:GLY:O	2.28	0.66
66:D3:524:U:N3	66:D3:527:A:OP2	2.28	0.66
16:UP:200:ARG:HH12	65:D2:220:U:H5'	1.60	0.66
17:UQ:38:SER:OG	17:UQ:39:GLN:N	2.28	0.66
22:UV:586:VAL:O	22:UV:611:ASP:N	2.26	0.66
23:UX:103:MET:HG3	23:UX:127:ARG:HH21	1.59	0.66
34:CM:131:GLU:OE2	34:CM:156:ARG:NH2	2.29	0.66
54:DJ:127:VAL:O	54:DJ:131:GLN:HB2	1.95	0.66
33:CL:195:TRP:HB3	33:CL:200:GLN:HG3	1.76	0.66
33:CL:879:THR:OG1	66:D3:572:C:N4	2.29	0.66
60:DW:22:LYS:NZ	66:D3:1038:U:O2'	2.28	0.66
65:D2:182:G:H1	65:D2:215:U:H3	1.44	0.66
7:UG:152:GLU:HB3	7:UG:171:LYS:HB2	1.77	0.66
25:CB:197:VAL:HA	25:CB:220:ILE:O	1.96	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
49:DE:122:LYS:HB3	49:DE:164:LEU:HD21	1.78	0.66
50:DF:76:ARG:HE	58:DQ:122:ARG:HG2	1.59	0.66
52:DH:23:ALA:CB	52:DH:85:PHE:CZ	2.78	0.66
5:UE:444:ALA:O	5:UE:447:SER:O	2.13	0.66
46:JP:357:SER:OG	46:JP:358:MET:N	2.29	0.66
5:UE:553:LYS:NZ	9:UI:461:THR:O	2.22	0.66
7:UG:502:ARG:HD3	65:D2:370:U:H5	1.61	0.66
15:UO:20:THR:HG23	15:UO:28:ARG:HH22	1.59	0.66
21:UU:232:MET:HE1	21:UU:256:PHE:HZ	1.61	0.66
24:UZ:163:LYS:NZ	65:D2:256:U:OP1	2.28	0.66
18:UR:304:LEU:O	18:UR:307:GLN:NE2	2.29	0.66
25:CA:225:ARG:NH2	25:CA:246:GLN:OE1	2.28	0.66
61:DX:63:GLN:O	61:DX:66:SER:OG	2.09	0.66
6:UF:11:CYS:SG	6:UF:36:ARG:NH2	2.69	0.66
15:UO:301:PRO:HG2	15:UO:323:SER:HB3	1.76	0.66
36:JA:510:PRO:HB2	36:JA:652:ARG:HD3	1.77	0.66
36:JA:569:PRO:HD3	36:JA:583:LEU:HG	1.76	0.66
53:DI:10:LYS:O	53:DI:18:ARG:NH1	2.29	0.66
7:UG:274:ARG:NH1	65:D2:322:A:N7	2.44	0.65
11:UK:158:MET:SD	11:UK:161:ARG:NH2	2.68	0.65
17:UQ:561:LEU:HD12	17:UQ:562:PRO:HD2	1.78	0.65
19:US:467:ALA:HA	19:US:470:MET:HG2	1.78	0.65
17:UQ:375:ASN:ND2	18:UR:340:GLU:OE1	2.29	0.65
24:UZ:27:ASN:HB2	24:UZ:30:LEU:HB2	1.78	0.65
29:CH:201:ILE:HG22	29:CH:208:PRO:HB3	1.77	0.65
39:JG:32:THR:HG23	39:JG:34:LYS:H	1.61	0.65
58:DQ:58:ASP:OD1	58:DQ:58:ASP:N	2.27	0.65
62:DY:61:ARG:HH12	66:D3:523:G:H4'	1.61	0.65
65:D2:547:C:O2	65:D2:590:G:N2	2.29	0.65
19:US:461:SER:OG	19:US:462:SER:N	2.29	0.65
24:UZ:77:LYS:HG2	24:UZ:78:ASP:H	1.60	0.65
48:DA:214:LYS:NZ	66:D3:886:U:OP1	2.29	0.65
12:UL:171:CYS:SG	12:UL:172:GLN:N	2.69	0.65
18:UR:174:ARG:NH1	18:UR:179:ASP:OD1	2.27	0.65
29:CH:191:SER:O	29:CH:194:LEU:N	2.29	0.65
1:UA:33:VAL:HG12	1:UA:34:GLY:H	1.61	0.65
4:UD:124:THR:HG21	16:UP:191:PRO:HB3	1.78	0.65
7:UG:409:ALA:O	46:JP:8:ARG:NH2	2.27	0.65
12:UL:42:ILE:HG12	12:UL:51:ILE:HG22	1.76	0.65
13:UM:589:GLN:HA	13:UM:603:ASP:HA	1.78	0.65
31:CJ:112:PRO:HG2	31:CJ:211:ASN:HB2	1.78	0.65



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
57:DO:54:GLU:OE2	66:D3:901:G:N2	2.29	0.65
60:DW:3:ARG:NH2	66:D3:865:A:OP2	2.29	0.65
21:UU:894:ASP:OD1	21:UU:895:VAL:N	2.30	0.65
55:DL:129:ARG:NH1	66:D3:335:U:O2'	2.30	0.65
66:D3:1042:G:N2	66:D3:1077:C:O2	2.28	0.65
66:D3:1697:G:H1	66:D3:1704:U:H3	1.45	0.65
12:UL:349:SER:O	12:UL:368:PRO:HA	1.97	0.65
23:UX:81:ASP:HB3	23:UX:84:ARG:HB3	1.77	0.65
29:CH:457:GLU:OE2	29:CH:461:LYS:NZ	2.28	0.65
35:CN:80:THR:HB	35:CN:136:ASN:HB3	1.79	0.65
36:JA:861:MET:N	36:JA:861:MET:SD	2.66	0.65
11:UK:164:ASN:OD1	25:CB:91:HIS:ND1	2.26	0.65
15:UO:356:ASN:ND2	65:D2:236:C:OP1	2.30	0.65
20:UT:1921:LEU:O	20:UT:1924:LEU:C	2.35	0.65
43:JM:106:LEU:O	43:JM:146:ARG:NH1	2.29	0.65
5:UE:182:MET:HG2	5:UE:183:THR:N	2.11	0.65
11:UK:202:LYS:HD3	11:UK:206:GLN:HE21	1.62	0.65
18:UR:410:ASP:N	18:UR:410:ASP:OD1	2.25	0.65
33:CL:51:GLU:OE1	61:DX:50:LYS:N	2.20	0.65
4:UD:417:VAL:HG13	4:UD:460:LEU:HD13	1.79	0.65
4:UD:550:VAL:HG23	4:UD:563:LEU:HB2	1.78	0.65
11:UK:200:GLN:NE2	65:D2:424:G:OP1	2.27	0.65
22:UV:656:ARG:HD3	48:DA:243:LYS:H	1.61	0.65
23:UX:56:ASN:ND2	23:UX:169:GLY:O	2.28	0.65
51:DG:196:ARG:NH1	66:D3:285:G:OP1	2.30	0.65
62:DY:10:ARG:O	62:DY:24:VAL:N	2.24	0.65
3:UC:550:LEU:HD13	11:UK:6:HIS:CE1	2.33	0.64
18:UR:16:ASP:OD1	18:UR:17:GLU:N	2.30	0.64
36:JA:510:PRO:O	36:JA:652:ARG:NE	2.30	0.64
48:DA:216:LYS:NZ	66:D3:885:G:OP1	2.30	0.64
66:D3:1692:G:N2	66:D3:1710:U:O2	2.30	0.64
1:UA:582:THR:HG21	1:UA:683:SER:HA	1.79	0.64
27:CE:429:ALA:O	27:CE:432:ASP:N	2.30	0.64
31:CJ:94:ARG:NH2	66:D3:1606:C:OP2	2.30	0.64
33:CL:210:VAL:HG22	33:CL:215:TYR:HE1	1.60	0.64
33:CL:252:LEU:O	33:CL:268:LYS:HB2	1.97	0.64
36:JA:630:LEU:HB3	36:JA:722:TYR:HE2	1.62	0.64
15:UO:244:LYS:NZ	15:UO:247:GLU:OE2	2.30	0.64
39:JG:192:TYR:OH	39:JG:223:GLU:OE2	2.15	0.64
48:DA:71:ALA:HB2	48:DA:79:HIS:HA	1.79	0.64
8:UH:545:ARG:HH21	8:UH:569:GLU:HG2	1.62	0.64



Atom-1	Atom-2	Interatomic	Clash
1100111 1		distance (A)	overlap (A)
9:UI:439:LYS:O	9:UI:443:GLN:NE2	2.30	0.64
12:UL:938:VAL:HG12	32:CK:467:ILE:HG12	1.78	0.64
17:UQ:71:ASN:ND2	17:UQ:127:GLU:OE1	2.30	0.64
65:D2:174:U:H3	65:D2:222:G:H1	1.46	0.64
3:UC:568:LYS:NZ	66:D3:592:A:OP2	2.26	0.64
25:CA:171:LEU:HB2	25:CA:237:VAL:HG11	1.79	0.64
4:UD:385:ASN:HB3	4:UD:390:LEU:HB2	1.80	0.64
36:JA:725:VAL:HG22	36:JA:762:MET:HB2	1.78	0.64
53:DI:172:ARG:HE	53:DI:175:GLN:HG3	1.62	0.64
18:UR:449:ASP:OD1	18:UR:494:TYR:OH	2.16	0.64
21:UU:392:ARG:NH2	67:D4:64:A:OP2	2.30	0.64
24:UZ:228:LYS:O	24:UZ:232:GLY:N	2.26	0.64
30:CI:98:GLU:OE2	31:CJ:58:TYR:OH	2.16	0.64
39:JF:196:LEU:HD11	39:JF:202:ILE:HD13	1.78	0.64
51:DG:78:THR:HG22	51:DG:92:ARG:HG3	1.79	0.64
54:DJ:151:ASP:N	54:DJ:151:ASP:OD1	2.26	0.64
66:D3:445:A:H1'	66:D3:525:A:H5"	1.78	0.64
19:US:196:GLN:HA	19:US:199:PHE:HD2	1.63	0.64
25:CB:144:TRP:HE3	25:CB:152:ALA:HB2	1.63	0.64
27:CE:86:THR:HA	27:CE:106:ASN:O	1.97	0.64
39:JG:35:ASP:O	39:JG:40:ARG:NH2	2.22	0.64
2:UB:610:ARG:HE	2:UB:611:SER:H	1.46	0.64
11:UK:7:ASP:O	11:UK:10:LYS:N	2.31	0.64
19:US:466:LEU:HD13	19:US:469:LEU:HD12	1.79	0.64
8:UH:659:THR:HG21	9:UI:507:ARG:HH21	1.63	0.64
12:UL:424:CYS:SG	12:UL:425:ILE:N	2.71	0.64
29:CH:157:LEU:HD12	29:CH:189:THR:HB	1.78	0.64
33:CL:156:LEU:HD13	33:CL:197:GLU:HG2	1.80	0.64
51:DG:7:TYR:HB2	51:DG:113:ILE:HD12	1.79	0.64
58:DQ:50:GLU:OE2	58:DQ:82:ARG:NH2	2.31	0.64
1:UA:636:THR:OG1	1:UA:637:GLU:N	2.31	0.63
3:UC:560:ASN:OD1	3:UC:561:SER:N	2.30	0.63
4:UD:199:ASP:HA	4:UD:215:ALA:O	1.98	0.63
5:UE:532:ARG:HH22	15:UO:16:LEU:HD11	1.64	0.63
13:UM:30:LYS:CB	13:UM:45:LEU:O	2.47	0.63
18:UR:382:GLY:CA	18:UR:400:ILE:O	2.43	0.63
21:UU:309:ILE:HG12	21:UU:323:VAL:HG12	1.80	0.63
22:UV:138:ILE:HD11	22:UV:239:LEU:HD13	1.79	0.63
29:CH:304:ILE:HB	29:CH:318:LEU:HB2	1.80	0.63
53:DI:5:ARG:NH1	66:D3:332:U:O2'	2.31	0.63
7:UG:253:ASN:HB2	7:UG:255:THR:HG23	1.80	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:96:VAL:HG12	13:UM:97:ARG:HG3	1.79	0.63
15:UO:91:SER:OG	15:UO:92:ASP:N	2.32	0.63
19:US:495:MET:O	19:US:499:LEU:HB2	1.98	0.63
35:CN:218:LYS:NZ	66:D3:1064:G:O6	2.31	0.63
8:UH:31:VAL:HA	8:UH:354:GLU:HA	1.81	0.63
17:UQ:200:ASN:ND2	17:UQ:262:MET:O	2.27	0.63
21:UU:228:GLY:CA	21:UU:246:ILE:O	2.44	0.63
36:JA:198:CYS:SG	36:JA:199:LEU:N	2.72	0.63
50:DF:206:SER:O	50:DF:206:SER:OG	2.16	0.63
66:D3:75:U:O4	66:D3:80:A:N6	2.30	0.63
2:UB:383:THR:O	2:UB:431:ARG:NH2	2.32	0.63
13:UM:25:VAL:HG22	13:UM:294:LEU:HD23	1.81	0.63
22:UV:211:LYS:HB3	22:UV:299:PRO:HG2	1.80	0.63
28:CF:38:ASN:ND2	67:D4:82:G:N7	2.44	0.63
28:CG:24:VAL:HG12	28:CG:102:ILE:HD11	1.79	0.63
33:CL:1158:LYS:NZ	67:D4:12:U:O4	2.31	0.63
57:DO:25:ASP:OD1	57:DO:26:THR:N	2.28	0.63
4:UD:294:TYR:OH	4:UD:310:ASN:ND2	2.31	0.63
21:UU:170:LEU:O	21:UU:171:GLN:NE2	2.32	0.63
26:CD:198:TRP:HE3	26:CD:271:VAL:HG22	1.64	0.63
38:JE:277:LEU:O	38:JE:280:THR:OG1	2.17	0.63
46:JP:92:ILE:HD12	46:JP:136:MET:HE2	1.80	0.63
7:UG:74:LEU:HD12	46:JP:3:ILE:HG12	1.81	0.63
7:UG:483:ILE:HG23	7:UG:516:VAL:HG22	1.79	0.63
8:UH:665:GLN:HB3	9:UI:496:LEU:HD11	1.80	0.63
22:UV:603:THR:O	22:UV:606:ASN:ND2	2.32	0.63
23:UX:54:GLN:HG3	54:DJ:21:SER:HB3	1.79	0.63
24:UZ:148:LYS:HG3	24:UZ:149:LYS:HE2	1.81	0.63
33:CL:373:ILE:HB	36:JA:6:ILE:HD11	1.81	0.63
3:UC:438:ASP:O	39:JG:136:ARG:NH1	2.32	0.63
10:UJ:132:THR:HB	10:UJ:155:ILE:HD11	1.80	0.63
12:UL:449:THR:OG1	12:UL:451:ASN:O	2.16	0.63
17:UQ:747:ASP:OD1	17:UQ:748:SER:N	2.29	0.63
18:UR:415:SER:H	18:UR:418:LYS:HB2	1.62	0.63
22:UV:102:ILE:HA	22:UV:105:LEU:HD12	1.80	0.63
22:UV:707:PHE:O	22:UV:918:ARG:NH1	2.31	0.63
27:CE:324:LYS:NZ	67:D4:91:C:OP2	2.29	0.63
31:CJ:211:ASN:O	32:CK:383:ARG:NH1	2.31	0.63
54:DJ:152:SER:O	54:DJ:155:HIS:N	2.32	0.63
65:D2:426:G:C2	65:D2:428:A:H5"	2.33	0.63
12:UL:677:HIS:NE2	66:D3:1654:G:O2'	2.27	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
21:UU:626:ASP:N	21:UU:626:ASP:OD1	2.31	0.63
33:CL:1052:SER:O	66:D3:575:C:N4	2.31	0.63
36:JA:171:ARG:HH22	36:JA:525:SER:HA	1.63	0.63
57:DO:41:ARG:NH2	66:D3:916:U:O4	2.32	0.63
24:UZ:101:ILE:HG21	24:UZ:106:LEU:HD13	1.81	0.62
28:CF:28:ALA:O	28:CF:31:ARG:NH2	2.31	0.62
33:CL:624:LYS:NZ	34:CM:281:GLU:OE1	2.32	0.62
33:CL:944:ASN:HB3	66:D3:1595:U:H5"	1.80	0.62
48:DA:49:ASN:ND2	66:D3:895:G:OP1	2.32	0.62
6:UF:203:MET:O	6:UF:207:ASN:ND2	2.32	0.62
12:UL:51:ILE:HG13	12:UL:60:VAL:HB	1.81	0.62
12:UL:676:SER:OG	12:UL:678:ASP:OD1	2.15	0.62
22:UV:1221:HIS:NE2	35:CN:21:PRO:O	2.24	0.62
23:UX:88:ASP:OD1	54:DJ:57:ARG:NE	2.28	0.62
25:CA:231:ARG:NE	26:CD:10:GLU:OE2	2.31	0.62
59:DS:83:ALA:O	59:DS:86:LEU:C	2.38	0.62
5:UE:449:ASP:OD2	15:UO:280:HIS:NE2	2.29	0.62
22:UV:1103:ARG:HH11	22:UV:1232:ILE:HB	1.63	0.62
24:UZ:226:LYS:O	24:UZ:229:ARG:NH1	2.32	0.62
29:CH:364:GLU:HB3	29:CH:366:GLN:HG3	1.81	0.62
39:JF:214:ASP:O	39:JF:224:LYS:NZ	2.29	0.62
46:JP:365:SER:O	46:JP:365:SER:OG	2.14	0.62
32:CK:538:LYS:HG2	66:D3:1628:U:H3	1.64	0.62
33:CL:625:TRP:O	33:CL:626:LYS:C	2.35	0.62
65:D2:349:G:N2	65:D2:350:A:N3	2.47	0.62
11:UK:32:LYS:NZ	66:D3:555:A:OP1	2.32	0.62
17:UQ:403:ILE:HD11	17:UQ:414:ILE:HG13	1.81	0.62
18:UR:571:SER:HB3	18:UR:576:LEU:H	1.64	0.62
19:US:192:GLN:O	19:US:196:GLN:NE2	2.33	0.62
27:CE:290:LEU:O	27:CE:391:ARG:NH1	2.32	0.62
53:DI:32:GLN:O	53:DI:56:ARG:NH1	2.33	0.62
4:UD:543:ILE:O	4:UD:550:VAL:HA	2.00	0.62
6:UF:82:SER:OG	6:UF:83:LEU:N	2.33	0.62
13:UM:108:LEU:HD23	13:UM:119:VAL:HG12	1.82	0.62
29:CH:160:ILE:CA	29:CH:188:TYR:O	2.48	0.62
36:JB:899:ALA:HB1	36:JB:905:PRO:HA	1.82	0.62
49:DE:151:ASP:HB3	49:DE:154:ILE:HG13	1.80	0.62
52:DH:23:ALA:HB1	52:DH:85:PHE:HZ	1.63	0.62
10:UJ:81:LEU:O	10:UJ:124:ARG:NH1	2.33	0.62
22:UV:949:PHE:O	22:UV:960:LYS:NZ	2.32	0.62
33:CL:1004:ARG:NH2	66:D3:558:U:OP1	2.33	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
37:JC:77:TYR:OH	53:DI:56:ARG:NH1	2.32	0.62
38:JE:231:ARG:NH2	66:D3:368:U:OP2	2.33	0.62
39:JG:182:PHE:HE1	39:JG:231:PRO:HA	1.64	0.62
46:JP:324:SER:OG	46:JP:326:ASP:OD1	2.17	0.62
50:DF:118:LEU:HD22	50:DF:129:PRO:HB2	1.80	0.62
51:DG:134:GLY:N	66:D3:66:U:O4	2.32	0.62
12:UL:770:ASN:HA	12:UL:773:MET:HE3	1.82	0.62
17:UQ:662:VAL:HG12	17:UQ:672:VAL:HG22	1.80	0.62
22:UV:1175:GLU:OE2	22:UV:1176:LYS:NZ	2.32	0.62
49:DE:221:ARG:HG3	49:DE:223:ASN:H	1.64	0.62
66:D3:65:A:N6	66:D3:84:A:OP2	2.30	0.62
66:D3:442:C:O2'	66:D3:525:A:N1	2.28	0.62
5:UE:169:SER:HA	5:UE:186:GLY:HA3	1.81	0.62
5:UE:448:ASN:OD1	5:UE:483:ARG:NH2	2.32	0.62
17:UQ:113:ASN:O	17:UQ:133:LYS:NZ	2.32	0.62
17:UQ:730:ASP:O	17:UQ:734:VAL:N	2.33	0.62
41:JJ:94:PHE:HA	41:JJ:141:THR:O	1.98	0.62
52:DH:114:ARG:O	52:DH:117:THR:OG1	2.18	0.62
7:UG:364:ARG:NH2	65:D2:316:U:OP1	2.33	0.62
15:UO:60:SER:HA	15:UO:83:VAL:HG23	1.82	0.62
15:UO:435:ASP:H	15:UO:438:THR:HG1	1.45	0.62
31:CJ:212:ALA:HA	32:CK:383:ARG:CZ	2.30	0.62
51:DG:139:ASN:OD1	51:DG:142:ARG:NH1	2.32	0.62
66:D3:275:C:O2	66:D3:281:G:N2	2.33	0.62
1:UA:285:ARG:HG2	1:UA:297:GLN:HG3	1.82	0.61
1:UA:538:GLN:NE2	1:UA:554:ASP:OD1	2.33	0.61
13:UM:510:SER:HG	13:UM:514:THR:HG1	1.45	0.61
37:JC:121:ARG:NH1	66:D3:341:A:OP1	2.32	0.61
39:JG:74:GLN:HB3	39:JG:84:ILE:HD13	1.82	0.61
65:D2:415:U:H2'	65:D2:416:A:H8	1.64	0.61
66:D3:891:A:H2'	66:D3:892:A:H8	1.65	0.61
11:UK:139:SER:HB3	11:UK:142:LYS:HG2	1.82	0.61
22:UV:526:CYS:HA	22:UV:615:VAL:O	1.99	0.61
26:CD:4:ILE:HG22	26:CD:23:GLN:HE21	1.63	0.61
29:CH:560:ARG:NH2	67:D4:248:G:N7	2.47	0.61
35:CN:224:ASN:HA	35:CN:227:ARG:HD3	1.82	0.61
66:D3:104:A:OP2	66:D3:308:C:N4	2.33	0.61
2:UB:604:VAL:HG22	2:UB:606:PHE:H	1.65	0.61
4:UD:231:VAL:HG22	4:UD:265:TRP:HH2	1.65	0.61
4:UD:538:GLN:OE1	4:UD:539:ASN:ND2	2.33	0.61
8:UH:555:ILE:O	8:UH:585:ARG:NH2	2.32	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:40:ILE:HB	13:UM:56:ILE:HG23	1.83	0.61
22:UV:268:LEU:HB3	22:UV:294:LEU:HB2	1.82	0.61
22:UV:871:ARG:HE	22:UV:873:GLU:HB3	1.65	0.61
25:CB:268:VAL:HG12	25:CB:317:VAL:HG12	1.82	0.61
36:JA:769:ARG:NH2	36:JA:770:GLU:O	2.33	0.61
41:JJ:134:THR:HG23	41:JJ:136:SER:HB3	1.81	0.61
44:JN:224:HIS:NE2	67:D4:15:U:OP2	2.30	0.61
48:DA:106:THR:OG1	57:DO:116:GLU:OE2	2.18	0.61
50:DF:103:ASN:OD1	50:DF:180:ARG:NH1	2.32	0.61
51:DG:131:LYS:HE2	66:D3:166:C:H4'	1.81	0.61
58:DQ:122:ARG:NH2	66:D3:1583:A:O2'	2.30	0.61
6:UF:173:ARG:NH1	26:CD:83:ASP:OD2	2.32	0.61
12:UL:473:ASP:N	12:UL:494:ASP:OD2	2.33	0.61
20:UT:464:PHE:O	20:UT:468:ALA:HB2	1.99	0.61
51:DG:23:ARG:HB3	51:DG:41:VAL:HG23	1.82	0.61
53:DI:24:LYS:NZ	66:D3:400:A:N7	2.37	0.61
62:DY:61:ARG:O	62:DY:70:VAL:N	2.23	0.61
29:CH:69:GLN:NE2	38:JE:338:THR:O	2.33	0.61
33:CL:953:SER:OG	33:CL:957:GLU:OE1	2.17	0.61
65:D2:405:A:N6	65:D2:451:G:O2'	2.34	0.61
65:D2:506:G:N2	65:D2:531:C:O2	2.33	0.61
66:D3:655:G:N2	66:D3:679:U:O4'	2.33	0.61
3:UC:544:ILE:HG22	33:CL:834:TRP:CE2	2.36	0.61
12:UL:350:LYS:HA	12:UL:367:ILE:O	2.00	0.61
22:UV:99:LYS:NZ	22:UV:499:LEU:O	2.34	0.61
22:UV:897:ARG:NH1	48:DA:178:GLY:O	2.33	0.61
31:CJ:187:PRO:HB3	31:CJ:220:ARG:HE	1.65	0.61
4:UD:94:GLY:HA2	4:UD:428:ILE:HG13	1.82	0.61
5:UE:182:MET:HG2	5:UE:183:THR:H	1.63	0.61
8:UH:603:SER:OG	8:UH:604:LYS:N	2.33	0.61
12:UL:8:PHE:HA	12:UL:685:GLU:O	2.00	0.61
15:UO:200:SER:OG	15:UO:201:SER:N	2.33	0.61
19:US:245:GLN:HB3	19:US:248:GLU:HB3	1.82	0.61
25:CA:264:GLN:HA	25:CA:320:TYR:O	1.99	0.61
30:CI:56:ARG:HD2	32:CK:440:LEU:HD11	1.83	0.61
37:JC:328:MET:HA	37:JC:341:TYR:O	2.01	0.61
39:JG:55:ILE:O	39:JG:63:ASP:N	2.34	0.61
46:JP:228:ASN:ND2	46:JP:230:ASN:O	2.33	0.61
49:DE:11:ARG:NH1	49:DE:27:TYR:O	2.33	0.61
49:DE:212:ASP:O	49:DE:215:ASP:N	2.34	0.61
66:D3:1041:G:N2	66:D3:1078:C:O2	2.33	0.61



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
19:US:156:TRP:HE1	19:US:199:PHE:HE1	1.49	0.61
21:UU:397:GLN:NE2	21:UU:398:ASP:OD1	2.34	0.61
35:CN:105:SER:OG	35:CN:194:ARG:NH2	2.33	0.61
37:JC:164:ARG:HH22	37:JC:174:ASN:HB3	1.65	0.61
51:DG:42:GLY:HA3	51:DG:45:PHE:HD2	1.63	0.61
55:DL:8:GLN:NE2	55:DL:14:GLN:O	2.33	0.61
57:DO:116:GLU:OE1	57:DO:117:ASP:N	2.33	0.61
61:DX:116:ASP:OD1	61:DX:117:ILE:N	2.34	0.61
3:UC:550:LEU:HD13	11:UK:6:HIS:NE2	2.15	0.61
12:UL:302:ARG:HA	12:UL:305:GLU:HG2	1.83	0.61
12:UL:415:LYS:HG2	12:UL:427:THR:HG22	1.82	0.61
13:UM:43:ILE:HA	13:UM:53:LEU:H	1.66	0.61
24:UZ:50:ARG:NH2	66:D3:1510:U:OP1	2.33	0.61
39:JF:151:ARG:HG2	39:JF:158:LYS:HG2	1.83	0.61
6:UF:193:ILE:HG12	6:UF:266:ARG:HG3	1.83	0.61
12:UL:15:GLY:O	12:UL:360:ASN:ND2	2.32	0.61
33:CL:92:ARG:NH1	33:CL:92:ARG:O	2.33	0.61
5:UE:185:PRO:O	5:UE:215:TYR:OH	2.16	0.60
7:UG:527:ARG:HH12	65:D2:366:A:P	2.23	0.60
8:UH:80:ALA:HA	8:UH:88:ASP:HA	1.82	0.60
11:UK:149:GLU:O	11:UK:153:ASN:HA	2.01	0.60
12:UL:311:GLU:O	12:UL:315:LYS:NZ	2.29	0.60
13:UM:705:SER:O	13:UM:705:SER:OG	2.17	0.60
15:UO:92:ASP:N	15:UO:92:ASP:OD1	2.32	0.60
51:DG:142:ARG:HG3	51:DG:147:LEU:HB2	1.83	0.60
5:UE:434:THR:O	5:UE:463:ARG:NH2	2.34	0.60
8:UH:251:CYS:HA	8:UH:262:LEU:HA	1.81	0.60
24:UZ:224:THR:O	24:UZ:226:LYS:NZ	2.29	0.60
34:CM:251:GLN:HG2	34:CM:252:LYS:HG3	1.83	0.60
43:JM:79:LYS:NZ	43:JM:80:ASN:OD1	2.34	0.60
65:D2:177:U:H3	65:D2:220:U:H3	1.49	0.60
66:D3:628:G:N1	66:D3:970:A:OP2	2.29	0.60
17:UQ:118:VAL:HB	17:UQ:130:LYS:HB2	1.82	0.60
19:US:144:PRO:O	19:US:148:PHE:HB2	2.01	0.60
33:CL:775:GLU:OE1	33:CL:779:ARG:NH2	2.34	0.60
49:DE:105:VAL:HA	49:DE:190:GLY:HA3	1.84	0.60
53:DI:37:LYS:NZ	53:DI:93:THR:O	2.33	0.60
53:DI:98:LYS:NZ	66:D3:329:G:OP1	2.26	0.60
54:DJ:176:ASN:ND2	66:D3:511:A:OP2	2.33	0.60
4:UD:304:ILE:HD11	4:UD:329:HIS:HE1	1.66	0.60
22:UV:620:ASN:ND2	22:UV:623:GLU:OE2	2.35	0.60



A 4 a ma 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
26:CD:103:LYS:NZ	46:JP:158:LYS:O	2.29	0.60
48:DA:150:VAL:HG22	66:D3:1067:C:H5"	1.84	0.60
49:DE:188:ASN:OD1	49:DE:191:ARG:NE	2.31	0.60
55:DL:88:ARG:O	55:DL:104:HIS:HA	2.01	0.60
62:DY:13:ILE:HG13	62:DY:22:GLN:HB2	1.82	0.60
1:UA:760:ILE:HG21	21:UU:720:LEU:HD21	1.84	0.60
12:UL:24:VAL:HG21	12:UL:86:GLU:HA	1.83	0.60
12:UL:88:HIS:O	12:UL:92:ASP:N	2.34	0.60
13:UM:539:VAL:HA	13:UM:549:ALA:O	2.02	0.60
13:UM:702:LEU:HD21	13:UM:758:ARG:HD3	1.84	0.60
14:UN:320:GLU:OE1	14:UN:323:HIS:NE2	2.28	0.60
18:UR:344:ARG:HH21	65:D2:88:U:H3	1.49	0.60
23:UX:100:ASP:HA	23:UX:127:ARG:HH22	1.66	0.60
36:JA:80:GLU:OE2	36:JA:83:ARG:NH1	2.34	0.60
49:DE:153:ASN:OD1	51:DG:215:ARG:NH2	2.34	0.60
51:DG:185:GLN:OE1	66:D3:271:A:N6	2.31	0.60
55:DL:67:ARG:O	55:DL:127:GLN:NE2	2.34	0.60
2:UB:613:ILE:HG13	2:UB:614:ILE:H	1.66	0.60
17:UQ:404:SER:OG	17:UQ:405:ALA:N	2.35	0.60
39:JF:80:MET:SD	39:JF:82:ARG:NH1	2.74	0.60
66:D3:1744:A:H2'	66:D3:1745:G:H8	1.66	0.60
3:UC:591:TYR:CZ	3:UC:593:GLY:HA2	2.36	0.60
5:UE:494:ARG:NH2	65:D2:135:G:O3'	2.26	0.60
33:CL:621:LEU:O	33:CL:625:TRP:HD1	1.84	0.60
34:CM:87:THR:HG23	34:CM:117:LEU:HB3	1.82	0.60
36:JA:27:VAL:HG12	36:JA:150:ILE:HB	1.83	0.60
46:JP:144:THR:HG21	46:JP:146:LYS:HE3	1.83	0.60
62:DY:63:GLN:N	62:DY:68:LYS:O	2.31	0.60
65:D2:197:G:O2'	65:D2:200:A:N6	2.35	0.60
1:UA:730:LEU:HD21	1:UA:754:VAL:HG13	1.84	0.60
4:UD:249:ARG:NH2	4:UD:309:GLN:OE1	2.35	0.60
11:UK:73:ASP:HB3	11:UK:75:LYS:H	1.65	0.60
19:US:446:PHE:HB2	19:US:461:SER:HB2	1.83	0.60
21:UU:21:SER:HB3	21:UU:623:ILE:HG12	1.83	0.60
22:UV:412:LEU:HD12	22:UV:421:LEU:HD23	1.84	0.60
22:UV:1173:GLY:HA3	22:UV:1177:GLY:HA2	1.84	0.60
25:CA:155:ILE:HD11	25:CA:162:LEU:HD22	1.82	0.60
36:JA:737:TRP:HA	36:JA:740:ASN:HB2	1.84	0.60
39:JG:41:MET:O	39:JG:110:LEU:HA	2.02	0.60
49:DE:87:MET:CA	49:DE:101:LEU:O	2.50	0.60
52:DH:58:LEU:HB2	52:DH:90:VAL:HG12	1.83	0.60



A 4 a and 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
66:D3:57:G:H1	66:D3:90:C:H42	1.48	0.60
66:D3:367:A:H2	66:D3:378:A:H61	1.48	0.60
66:D3:683:C:H2'	66:D3:684:A:H8	1.65	0.60
3:UC:528:LEU:HD22	66:D3:579:A:H62	1.67	0.60
7:UG:388:ASP:OD1	7:UG:388:ASP:N	2.32	0.60
12:UL:115:LEU:HD22	12:UL:153:GLU:HB3	1.83	0.60
17:UQ:623:PHE:HE2	17:UQ:664:LEU:HD13	1.65	0.60
18:UR:557:THR:OG1	18:UR:558:SER:N	2.35	0.60
28:CG:54:MET:O	28:CG:80:PHE:HA	2.02	0.60
66:D3:645:C:O2	66:D3:690:G:N2	2.32	0.60
66:D3:1268:G:N2	66:D3:1442:U:O2	2.35	0.60
2:UB:802:GLU:OE2	2:UB:806:ARG:NH2	2.33	0.59
10:UJ:30:SER:HB3	10:UJ:41:ALA:HB2	1.83	0.59
15:UO:127:THR:HA	15:UO:144:SER:HA	1.83	0.59
21:UU:444:ASP:OD1	21:UU:445:MET:N	2.35	0.59
21:UU:470:GLN:OE1	21:UU:553:ARG:NH1	2.35	0.59
21:UU:477:ILE:O	21:UU:477:ILE:HG22	2.01	0.59
26:CD:166:SER:OG	26:CD:169:LYS:NZ	2.35	0.59
28:CG:84:ARG:NH1	67:D4:255:U:O4	2.35	0.59
36:JA:735:LYS:HA	36:JA:738:LYS:HE2	1.83	0.59
37:JC:277:ILE:HG22	37:JC:290:VAL:HG22	1.83	0.59
39:JG:40:ARG:NH1	39:JG:172:PRO:HG3	2.16	0.59
43:JM:108:LYS:HG3	43:JM:109:PRO:HD2	1.84	0.59
66:D3:1124:A:O2'	67:D4:1:G:N2	2.35	0.59
1:UA:671:SER:O	1:UA:671:SER:OG	2.19	0.59
3:UC:544:ILE:CG2	33:CL:834:TRP:CD2	2.85	0.59
8:UH:261:GLU:HA	8:UH:271:SER:HA	1.82	0.59
12:UL:414:LEU:HD22	12:UL:447:LEU:HD11	1.84	0.59
21:UU:370:SER:OG	21:UU:371:LYS:N	2.35	0.59
36:JA:635:ILE:HB	36:JA:725:VAL:HG12	1.83	0.59
36:JB:790:SER:HA	36:JB:794:HIS:HA	1.83	0.59
39:JF:31:LEU:HD22	39:JF:40:ARG:HH21	1.66	0.59
48:DA:88:VAL:HG22	48:DA:98:THR:HG22	1.83	0.59
62:DY:44:LEU:HA	62:DY:47:VAL:HG12	1.83	0.59
9:UI:444:ASN:HB3	9:UI:447:ASN:HB2	1.85	0.59
13:UM:343:MET:O	13:UM:624:SER:OG	2.20	0.59
21:UU:327:SER:OG	21:UU:328:LEU:N	2.32	0.59
33:CL:1020:SER:OG	33:CL:1021:LEU:N	2.30	0.59
34:CM:306:GLU:OE1	34:CM:355:LYS:NZ	2.27	0.59
49:DE:196:VAL:N	49:DE:209:HIS:O	2.33	0.59
53:DI:172:ARG:NH2	66:D3:331:A:N7	2.49	0.59



	A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
66:D3:1744:A:H2'	66:D3:1745:G:C8	2.37	0.59
7:UG:357:SER:O	7:UG:359:GLY:N	2.35	0.59
17:UQ:181:ALA:H	17:UQ:184:GLN:HB2	1.66	0.59
19:US:252:LYS:O	19:US:256:ASN:ND2	2.35	0.59
21:UU:282:SER:OG	21:UU:283:ARG:N	2.32	0.59
42:JK:466:TYR:HD2	45:JO:305:ALA:H	1.50	0.59
46:JP:256:GLN:HG2	46:JP:257:LYS:H	1.66	0.59
7:UG:211:THR:OG1	7:UG:212:GLY:N	2.35	0.59
13:UM:143:HIS:ND1	13:UM:167:ASP:OD1	2.35	0.59
13:UM:602:TRP:HB3	13:UM:610:LEU:H	1.68	0.59
18:UR:517:THR:O	18:UR:517:THR:OG1	2.19	0.59
21:UU:753:SER:OG	21:UU:754:GLU:N	2.36	0.59
34:CM:231:ARG:NH1	66:D3:1132:A:O2'	2.36	0.59
36:JA:852:TYR:HA	36:JA:855:ILE:HG22	1.84	0.59
1:UA:273:ARG:HD2	1:UA:290:PRO:HG2	1.83	0.59
11:UK:234:VAL:HG22	11:UK:240:ILE:HG22	1.84	0.59
13:UM:85:LEU:O	13:UM:98:SER:HA	2.03	0.59
17:UQ:156:THR:HG22	17:UQ:171:TYR:HE1	1.67	0.59
28:CF:64:LEU:HD23	28:CF:98:ILE:HD12	1.83	0.59
30:CI:152:ARG:NH1	31:CJ:11:GLU:OE2	2.36	0.59
33:CL:290:ILE:HD13	33:CL:296:PHE:HD2	1.68	0.59
37:JC:296:ILE:HD11	37:JC:310:SER:HB3	1.84	0.59
52:DH:84:LYS:HG3	52:DH:85:PHE:CD1	2.38	0.59
54:DJ:108:ARG:HH12	54:DJ:110:GLN:HE21	1.51	0.59
8:UH:253:SER:HA	8:UH:260:LYS:HA	1.83	0.59
17:UQ:176:LEU:HA	17:UQ:186:GLU:O	2.01	0.59
19:US:346:ASN:OD1	19:US:347:PRO:HD2	2.03	0.59
19:US:380:ILE:HG23	19:US:402:ILE:HD12	1.84	0.59
26:CD:382:LYS:NZ	67:D4:256:G:OP1	2.34	0.59
29:CH:68:LYS:HA	29:CH:71:LEU:HD12	1.85	0.59
39:JF:90:ASP:N	39:JF:90:ASP:OD1	2.32	0.59
2:UB:649:THR:HG23	2:UB:650:VAL:HG23	1.84	0.59
12:UL:396:SER:OG	12:UL:397:ILE:N	2.35	0.59
19:US:388:LEU:HD12	19:US:465:GLU:HG2	1.85	0.59
22:UV:919:TRP:HE3	22:UV:920:LEU:HD22	1.67	0.59
31:CJ:97:SER:OG	31:CJ:144:GLU:OE1	2.15	0.59
31:CJ:184:GLU:OE2	66:D3:1159:C:N4	2.35	0.59
36:JB:743:VAL:N	36:JB:763:LEU:O	2.27	0.59
55:DL:55:ASP:HB3	55:DL:58:CYS:HB2	1.83	0.59
65:D2:112:U:H2'	65:D2:113:A:C8	2.38	0.59
10:UJ:138:SER:OG	10:UJ:139:THR:N	2.34	0.59



Atom 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:338:ILE:HA	12:UL:357:THR:HA	1.85	0.59
23:UX:76:ILE:HD11	23:UX:119:LEU:HD22	1.83	0.59
36:JB:633:ALA:O	36:JB:723:LEU:HA	2.02	0.59
38:JE:238:ASN:OD1	38:JE:241:ARG:NH2	2.36	0.59
38:JE:296:ARG:NH2	62:DY:71:GLY:O	2.36	0.59
56:DN:69:ASN:OD1	56:DN:70:LYS:N	2.35	0.59
62:DY:7:ILE:HG13	62:DY:40:LEU:HD11	1.84	0.59
62:DY:27:VAL:HG12	62:DY:29:HIS:ND1	2.17	0.59
62:DY:62:THR:HA	62:DY:69:SER:HA	1.83	0.59
17:UQ:828:LYS:HD2	17:UQ:829:LEU:HG	1.83	0.59
33:CL:371:VAL:HG13	36:JA:6:ILE:HD12	1.84	0.59
38:JE:323:GLU:OE2	54:DJ:82:ARG:NE	2.31	0.59
67:D4:312:U:H2'	67:D4:313:A:H8	1.68	0.59
1:UA:782:ILE:O	1:UA:786:ALA:HB2	2.03	0.58
4:UD:436:ASP:O	4:UD:483:ASN:ND2	2.35	0.58
6:UF:85:ASP:OD1	6:UF:85:ASP:N	2.31	0.58
9:UI:429:HIS:HA	9:UI:432:LYS:HD2	1.85	0.58
13:UM:148:SER:OG	13:UM:194:ARG:NH2	2.35	0.58
18:UR:278:ASP:OD2	18:UR:281:THR:OG1	2.21	0.58
26:CD:110:LYS:NZ	26:CD:117:ASP:OD1	2.36	0.58
33:CL:945:THR:OG1	66:D3:1595:U:OP1	2.16	0.58
66:D3:325:G:H2'	66:D3:326:G:H8	1.68	0.58
4:UD:207:ASP:OD1	4:UD:211:ARG:NH2	2.36	0.58
5:UE:128:GLN:HB3	5:UE:138:GLN:HG2	1.85	0.58
5:UE:443:GLN:NE2	19:US:333:GLU:O	2.36	0.58
15:UO:285:ASP:OD1	15:UO:285:ASP:N	2.35	0.58
18:UR:359:LYS:HD3	18:UR:466:THR:HG21	1.85	0.58
29:CH:159:CYS:SG	29:CH:160:ILE:N	2.76	0.58
36:JA:790:SER:OG	36:JA:890:LEU:O	2.20	0.58
52:DH:84:LYS:CG	52:DH:85:PHE:CD1	2.85	0.58
53:DI:7:SER:O	53:DI:18:ARG:NH2	2.36	0.58
66:D3:683:C:H2'	66:D3:684:A:C8	2.38	0.58
66:D3:1153:G:N2	66:D3:1626:U:O2	2.36	0.58
6:UF:14:GLU:O	6:UF:18:LEU:HB2	2.03	0.58
11:UK:77:LEU:HD23	11:UK:77:LEU:H	1.68	0.58
15:UO:378:LYS:NZ	65:D2:90:G:OP1	2.29	0.58
17:UQ:393:ASN:ND2	17:UQ:435:ASP:OD1	2.35	0.58
17:UQ:426:ARG:NH1	65:D2:68:U:O2	2.36	0.58
25:CB:289:GLU:HA	25:CB:292:LYS:HG2	1.85	0.58
29:CH:146:LYS:NZ	29:CH:204:PHE:O	2.33	0.58
46:JP:188:HIS:ND1	46:JP:190:GLU:O	2.36	0.58



A 4 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
21:UU:290:ILE:O	21:UU:291:HIS:ND1	2.36	0.58
25:CA:269:ILE:O	25:CA:315:ILE:HA	2.03	0.58
26:CD:149:ARG:HH22	27:CE:242:SER:HA	1.68	0.58
27:CE:160:ASP:OD1	27:CE:160:ASP:N	2.35	0.58
33:CL:306:ASP:N	33:CL:306:ASP:OD1	2.33	0.58
36:JA:520:ARG:HH22	36:JA:560:PRO:HA	1.68	0.58
37:JC:242:THR:HG22	37:JC:256:ASP:HA	1.84	0.58
51:DG:14:LYS:HD2	51:DG:123:GLY:HA3	1.86	0.58
56:DN:114:ARG:NH2	66:D3:939:A:OP1	2.36	0.58
65:D2:192:G:H2'	65:D2:193:G:C8	2.38	0.58
11:UK:82:ARG:NH1	65:D2:248:G:OP2	2.29	0.58
16:UP:196:SER:HA	16:UP:199:ILE:HG22	1.85	0.58
22:UV:189:PHE:HB2	22:UV:203:ILE:HD13	1.84	0.58
22:UV:870:ALA:HB2	22:UV:878:LEU:HD12	1.84	0.58
25:CB:111:MET:SD	25:CB:216:ASN:ND2	2.76	0.58
36:JB:377:VAL:O	36:JB:381:ALA:HB2	2.03	0.58
37:JC:69:GLN:NE2	37:JC:85:ASP:OD1	2.37	0.58
38:JE:243:GLN:HB2	38:JE:327:ILE:HD11	1.84	0.58
45:JO:281:LEU:HD12	45:JO:284:GLN:HE21	1.68	0.58
49:DE:113:ARG:NH1	49:DE:114:ILE:O	2.37	0.58
7:UG:197:ASP:OD1	7:UG:198:PHE:N	2.37	0.58
12:UL:344:THR:HB	12:UL:352:GLU:HB2	1.84	0.58
13:UM:585:ASN:ND2	13:UM:627:ASN:O	2.36	0.58
14:UN:844:SER:OG	14:UN:845:SER:N	2.34	0.58
15:UO:175:SER:OG	15:UO:176:PHE:N	2.36	0.58
17:UQ:142:ALA:HB2	17:UQ:156:THR:HG23	1.84	0.58
29:CH:405:VAL:HG23	29:CH:415:THR:HG22	1.84	0.58
31:CJ:93:SER:OG	31:CJ:94:ARG:N	2.32	0.58
33:CL:824:ILE:HD11	33:CL:926:ILE:HG23	1.85	0.58
37:JC:97:THR:O	53:DI:32:GLN:NE2	2.36	0.58
37:JC:206:PHE:O	37:JC:215:VAL:N	2.27	0.58
37:JC:250:GLY:HA2	37:JC:274:ILE:HG13	1.85	0.58
49:DE:79:ASP:HB3	49:DE:82:TYR:HB2	1.85	0.58
55:DL:133:LYS:NZ	66:D3:324:U:OP1	2.27	0.58
1:UA:269:HIS:NE2	1:UA:312:GLN:O	2.34	0.58
3:UC:545:LEU:HD12	3:UC:545:LEU:C	2.21	0.58
7:UG:23:ARG:O	14:UN:862:ARG:NH1	2.37	0.58
25:CB:244:VAL:O	25:CB:249:GLN:NE2	2.37	0.58
26:CD:231:ASP:HA	26:CD:234:LEU:HD23	1.86	0.58
26:CD:377:ARG:NH1	67:D4:111:G:O6	2.37	0.58
33:CL:928:ILE:HG23	33:CL:1009:VAL:HG13	1.86	0.58



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
50:DF:203:LYS:HD2	50:DF:205:SER:HB2	1.86	0.58
52:DH:67:LEU:HD22	52:DH:94:ALA:HB2	1.85	0.58
1:UA:202:ASP:O	1:UA:204:GLU:N	2.37	0.58
2:UB:488:ASN:HB3	2:UB:491:ASP:HB2	1.85	0.58
4:UD:468:ASP:OD2	4:UD:472:ARG:NH1	2.37	0.58
5:UE:345:LEU:HB2	5:UE:346:HIS:HD2	1.69	0.58
5:UE:494:ARG:HH12	65:D2:136:U:H5'	1.68	0.58
12:UL:361:THR:HG22	12:UL:386:GLU:HB3	1.85	0.58
13:UM:120:GLY:HA3	13:UM:147:ILE:HG21	1.86	0.58
20:UT:156:ALA:O	20:UT:160:LYS:N	2.37	0.58
28:CG:49:SER:HA	28:CG:103:THR:HA	1.84	0.58
46:JP:69:GLY:HA2	46:JP:370:GLY:HA2	1.85	0.58
52:DH:162:ILE:HA	52:DH:165:LYS:HB2	1.83	0.58
4:UD:401:ILE:HD13	4:UD:418:CYS:HB3	1.86	0.58
4:UD:469:LEU:HD22	4:UD:472:ARG:HH12	1.68	0.58
9:UI:413:GLU:HB3	9:UI:416:ILE:HG12	1.85	0.58
17:UQ:367:SER:OG	17:UQ:367:SER:O	2.22	0.58
38:JE:339:SER:HB3	38:JE:342:GLY:HA2	1.86	0.58
45:JO:201:LYS:HE3	45:JO:205:ILE:HD11	1.86	0.58
46:JP:244:ILE:HD11	46:JP:264:THR:HG21	1.85	0.58
66:D3:1677:C:H42	66:D3:1724:U:H3	1.52	0.58
10:UJ:1535:TYR:O	10:UJ:1539:MET:CB	2.52	0.58
13:UM:192:ALA:HB3	13:UM:216:ARG:HD2	1.84	0.58
28:CG:49:SER:OG	28:CG:101:SER:OG	2.19	0.58
32:CK:517:LYS:O	32:CK:525:LYS:NZ	2.35	0.58
46:JP:225:LEU:HD22	46:JP:235:LEU:HD11	1.86	0.58
54:DJ:171:ARG:NH1	66:D3:538:A:OP2	2.33	0.58
1:UA:423:ARG:NH2	66:D3:1632:C:O2'	2.37	0.57
1:UA:650:ASN:HD22	1:UA:655:ASP:HB3	1.69	0.57
9:UI:477:LYS:HG3	9:UI:481:HIS:HE1	1.69	0.57
12:UL:165:SER:OG	12:UL:166:ILE:N	2.37	0.57
13:UM:294:LEU:HB2	13:UM:303:PHE:HB2	1.86	0.57
13:UM:538:ASP:OD2	13:UM:580:ARG:NE	2.36	0.57
22:UV:372:GLN:NE2	22:UV:511:PHE:O	2.31	0.57
24:UZ:115:LEU:HD21	24:UZ:140:GLY:HA3	1.86	0.57
27:CE:164:ILE:HG22	27:CE:301:ALA:HA	1.86	0.57
29:CH:232:THR:OG1	29:CH:259:LYS:NZ	2.36	0.57
33:CL:799:GLU:OE2	33:CL:799:GLU:N	2.37	0.57
35:CN:38:PHE:HB2	35:CN:56:VAL:HB	1.85	0.57
45:JO:291:ARG:NE	66:D3:316:A:OP2	2.25	0.57
55:DL:33:ARG:NH1	55:DL:53:TYR:O	2.37	0.57



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
8:UH:679:ILE:HD12	9:UI:483:LYS:HD3	1.87	0.57
17:UQ:181:ALA:HB3	17:UQ:184:GLN:HG3	1.85	0.57
22:UV:228:ARG:HH21	22:UV:296:ILE:H	1.51	0.57
26:CD:185:ASP:O	26:CD:189:ASN:ND2	2.37	0.57
37:JC:254:ILE:HB	37:JC:264:ILE:HB	1.84	0.57
48:DA:157:GLN:NE2	66:D3:1046:G:OP1	2.36	0.57
48:DA:243:LYS:NZ	48:DA:244:VAL:O	2.37	0.57
53:DI:172:ARG:NH1	66:D3:330:G:OP2	2.37	0.57
1:UA:623:LEU:HD13	1:UA:679:VAL:HG22	1.86	0.57
4:UD:72:SER:O	4:UD:72:SER:OG	2.22	0.57
5:UE:167:SER:OG	5:UE:168:HIS:N	2.37	0.57
36:JA:627:PHE:HA	36:JA:630:LEU:HD12	1.86	0.57
37:JC:56:SER:HA	37:JC:336:ILE:HG23	1.86	0.57
37:JC:189:ASN:HD22	37:JC:243:PHE:HE1	1.52	0.57
49:DE:104:ASP:OD2	49:DE:106:LYS:NZ	2.37	0.57
55:DL:132:SER:OG	55:DL:133:LYS:N	2.36	0.57
57:DO:124:ASP:OD2	66:D3:885:G:N2	2.31	0.57
62:DY:27:VAL:O	62:DY:68:LYS:CA	2.52	0.57
1:UA:852:THR:OG1	1:UA:853:ASP:N	2.37	0.57
5:UE:23:ALA:HB1	18:UR:261:PRO:HG3	1.84	0.57
11:UK:17:SER:OG	11:UK:18:GLN:N	2.28	0.57
17:UQ:429:ILE:HG13	17:UQ:737:ILE:HD11	1.85	0.57
17:UQ:690:ASN:OD1	17:UQ:751:SER:OG	2.22	0.57
18:UR:129:ASP:HA	18:UR:132:LYS:HG2	1.84	0.57
20:UT:1661:ILE:O	20:UT:1665:LEU:CB	2.53	0.57
33:CL:933:LYS:HA	33:CL:1003:LEU:O	2.04	0.57
52:DH:23:ALA:HB1	52:DH:85:PHE:CZ	2.39	0.57
52:DH:50:ASP:HA	52:DH:56:LYS:HG2	1.85	0.57
66:D3:319:U:H5'	66:D3:320:U:H5"	1.87	0.57
2:UB:514:TYR:OH	19:US:513:ARG:NH1	2.37	0.57
4:UD:612:THR:HG23	4:UD:615:SER:H	1.68	0.57
6:UF:79:LYS:NZ	65:D2:492:G:O6	2.35	0.57
12:UL:643:ASP:HB2	12:UL:650:ILE:HD11	1.85	0.57
22:UV:828:ASP:OD2	22:UV:853:ARG:NH1	2.35	0.57
29:CH:361:GLY:O	29:CH:431:LYS:NZ	2.24	0.57
49:DE:195:ILE:HA	49:DE:210:ILE:HA	1.85	0.57
66:D3:1629:G:O2'	66:D3:1631:A:N6	2.37	0.57
1:UA:27:LYS:NZ	41:JJ:274:TYR:OH	2.38	0.57
1:UA:351:LEU:HA	1:UA:361:VAL:O	2.04	0.57
4:UD:120:SER:OG	4:UD:121:THR:N	2.32	0.57
8:UH:593:ASP:OD1	8:UH:594:SER:N	2.38	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:UJ:145:THR:HB	10:UJ:147:VAL:HG12	1.87	0.57
12:UL:51:ILE:HD11	12:UL:61:SER:HB2	1.86	0.57
13:UM:180:ARG:NH1	66:D3:1778:G:OP1	2.37	0.57
15:UO:23:GLU:OE1	15:UO:293:LYS:HE2	2.03	0.57
33:CL:975:GLU:OE2	33:CL:977:LYS:NZ	2.31	0.57
36:JA:748:ARG:NH2	36:JA:750:THR:O	2.33	0.57
48:DA:97:LEU:HD22	48:DA:232:HIS:CG	2.39	0.57
60:DW:28:ARG:NH1	66:D3:865:A:OP1	2.35	0.57
66:D3:1219:A:H62	66:D3:1264:G:H21	1.51	0.57
2:UB:803:ARG:NH2	2:UB:806:ARG:O	2.36	0.57
6:UF:67:ARG:HH11	6:UF:84:SER:HG	1.50	0.57
13:UM:420:ASN:HB2	13:UM:423:LYS:HZ1	1.68	0.57
15:UO:27:TRP:NE1	15:UO:268:MET:SD	2.66	0.57
22:UV:592:PHE:HB3	22:UV:599:VAL:HG22	1.85	0.57
22:UV:871:ARG:NH2	22:UV:873:GLU:OE1	2.38	0.57
25:CA:175:ALA:HB1	25:CA:181:VAL:HG21	1.87	0.57
41:JJ:105:ARG:NH2	66:D3:1772:C:O2'	2.38	0.57
51:DG:2:LYS:NZ	66:D3:154:G:OP1	2.28	0.57
11:UK:111:ARG:NE	11:UK:208:GLU:OE2	2.38	0.57
12:UL:409:ALA:O	12:UL:412:GLY:N	2.32	0.57
17:UQ:381:SER:O	17:UQ:381:SER:OG	2.18	0.57
21:UU:859:ASP:N	21:UU:859:ASP:OD1	2.37	0.57
31:CJ:123:VAL:HG22	31:CJ:125:PRO:HD2	1.87	0.57
33:CL:282:SER:HB3	33:CL:782:GLY:HA2	1.86	0.57
39:JG:53:HIS:HB2	39:JG:68:LEU:HD11	1.85	0.57
60:DW:75:ILE:HG12	60:DW:127:GLY:HA2	1.87	0.57
65:D2:21:A:H2'	65:D2:22:A:C8	2.39	0.57
4:UD:248:PRO:HD2	4:UD:292:ASN:ND2	2.20	0.57
7:UG:214:LEU:HD22	7:UG:249:LEU:HD11	1.86	0.57
12:UL:26:ILE:HG23	12:UL:89:LYS:HE3	1.87	0.57
17:UQ:352:ASN:O	17:UQ:376:ALA:HB2	2.04	0.57
22:UV:286:TYR:O	22:UV:289:ARG:NH1	2.35	0.57
22:UV:1063:ARG:HH21	22:UV:1185:LEU:HD11	1.69	0.57
22:UV:1101:ASP:HB2	22:UV:1233:ASN:HB3	1.87	0.57
27:CE:207:ARG:HD2	27:CE:226:ILE:HG21	1.86	0.57
38:JE:227:ARG:O	49:DE:187:ARG:NH2	2.38	0.57
39:JG:76:LEU:HD12	39:JG:79:LYS:HB2	1.86	0.57
39:JG:124:VAL:HG22	39:JG:160:LEU:HD22	1.85	0.57
51:DG:160:ARG:NH2	66:D3:66:U:O2'	2.37	0.57
1:UA:380:LEU:HD13	32:CK:484:MET:HB3	1.85	0.57
1:UA:538:GLN:HG3	1:UA:554:ASP:HA	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
8:UH:562:PRO:O	8:UH:566:LEU:HB2	2.05	0.57
15:UO:67:SER:OG	15:UO:68:SER:N	2.37	0.57
23:UX:82:ILE:O	23:UX:86:MET:HB2	2.04	0.57
24:UZ:173:PRO:HA	24:UZ:176:VAL:HG12	1.86	0.57
31:CJ:235:GLN:HB3	31:CJ:250:VAL:O	2.05	0.57
48:DA:128:LYS:NZ	48:DA:132:ASP:OD1	2.27	0.57
1:UA:27:LYS:HD3	1:UA:43:ILE:HD12	1.86	0.56
2:UB:512:ASP:OD2	2:UB:515:HIS:ND1	2.32	0.56
4:UD:80:ASN:ND2	4:UD:88:GLU:OE2	2.33	0.56
5:UE:184:PHE:N	5:UE:184:PHE:CD2	2.73	0.56
7:UG:130:ARG:NH2	7:UG:379:GLU:OE2	2.38	0.56
8:UH:69:ILE:HA	8:UH:79:ASN:HA	1.87	0.56
15:UO:385:MET:SD	15:UO:393:ASN:ND2	2.73	0.56
22:UV:1087:LEU:O	22:UV:1090:THR:OG1	2.22	0.56
34:CM:156:ARG:HE	34:CM:230:TRP:HE1	1.53	0.56
37:JC:65:SER:OG	37:JC:109:ASP:O	2.20	0.56
53:DI:56:ARG:NH2	66:D3:332:U:OP1	2.38	0.56
66:D3:869:A:H61	66:D3:958:U:H3	1.51	0.56
66:D3:891:A:H2'	66:D3:892:A:C8	2.40	0.56
8:UH:675:LEU:HD12	9:UI:456:LEU:HD22	1.87	0.56
12:UL:549:SER:OG	12:UL:550:LEU:N	2.33	0.56
13:UM:314:ILE:HD13	13:UM:329:VAL:HA	1.86	0.56
17:UQ:278:GLY:HA2	17:UQ:300:VAL:HG23	1.87	0.56
17:UQ:306:SER:OG	17:UQ:307:HIS:N	2.36	0.56
17:UQ:618:ASP:OD1	17:UQ:618:ASP:N	2.38	0.56
22:UV:827:ARG:HH12	35:CN:175:LEU:HD11	1.69	0.56
36:JA:542:VAL:HA	36:JA:548:ASN:HD21	1.70	0.56
39:JF:100:LEU:O	39:JF:105:ASN:ND2	2.37	0.56
44:JN:108:PRO:O	44:JN:113:THR:N	2.27	0.56
1:UA:505:ARG:NH1	66:D3:1156:C:OP2	2.38	0.56
3:UC:493:ASP:OD2	3:UC:497:GLN:NE2	2.37	0.56
3:UC:544:ILE:HG23	33:CL:834:TRP:CD2	2.39	0.56
4:UD:561:LYS:HD3	4:UD:562:PRO:HD2	1.87	0.56
5:UE:342:ASP:OD1	5:UE:342:ASP:N	2.37	0.56
8:UH:632:THR:OG1	8:UH:633:GLN:N	2.37	0.56
9:UI:477:LYS:O	9:UI:481:HIS:ND1	2.39	0.56
10:UJ:362:LYS:HB3	10:UJ:365:ILE:HD12	1.86	0.56
12:UL:461:SER:OG	12:UL:462:SER:N	2.38	0.56
20:UT:1921:LEU:O	20:UT:1924:LEU:O	2.23	0.56
21:UU:717:ASP:HB2	21:UU:720:LEU:HD23	1.88	0.56
22:UV:1155:LEU:O	22:UV:1158:LYS:NZ	2.35	0.56



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:UX:113:TYR:HD1	44:JN:306:LEU:HD22	1.68	0.56
27:CE:288:THR:HG23	27:CE:293:GLU:HB3	1.87	0.56
33:CL:97:THR:OG1	33:CL:98:LEU:N	2.35	0.56
33:CL:293:VAL:HG13	33:CL:1022:LEU:HD21	1.87	0.56
33:CL:309:PRO:O	33:CL:314:GLN:NE2	2.27	0.56
33:CL:567:TRP:HH2	34:CM:315:LYS:HG3	1.69	0.56
34:CM:192:THR:HA	34:CM:224:ASN:O	2.04	0.56
38:JE:285:ARG:NH2	66:D3:371:G:O6	2.31	0.56
38:JE:330:SER:OG	66:D3:372:G:N3	2.37	0.56
39:JF:101:ASP:OD2	39:JF:132:ARG:NH1	2.34	0.56
41:JJ:129:ARG:NE	41:JJ:138:GLU:OE2	2.29	0.56
46:JP:201:ILE:HG22	46:JP:215:LEU:O	2.05	0.56
5:UE:163:LEU:HD23	5:UE:163:LEU:H	1.70	0.56
8:UH:604:LYS:HE2	8:UH:649:SER:HB3	1.86	0.56
26:CD:38:ILE:HD12	26:CD:126:ASP:OD1	2.05	0.56
29:CH:63:ARG:HD3	38:JE:248:TYR:CZ	2.40	0.56
29:CH:299:CYS:SG	29:CH:305:ARG:NH1	2.73	0.56
56:DN:72:MET:HA	56:DN:75:LEU:HB2	1.88	0.56
7:UG:324:ILE:HD12	7:UG:345:LEU:HD11	1.87	0.56
8:UH:678:LEU:HB3	9:UI:460:LEU:HD23	1.88	0.56
12:UL:223:ASP:N	12:UL:223:ASP:OD1	2.39	0.56
12:UL:237:LYS:HD2	13:UM:671:ASN:HD22	1.69	0.56
13:UM:616:HIS:NE2	13:UM:634:SER:OG	2.30	0.56
22:UV:288:THR:HG22	22:UV:290:PHE:HD2	1.70	0.56
30:CI:29:ASP:OD1	30:CI:30:THR:N	2.34	0.56
46:JP:311:VAL:HG23	46:JP:322:THR:HG22	1.88	0.56
1:UA:849:LEU:HD22	21:UU:897:HIS:HB2	1.86	0.56
8:UH:303:GLN:HA	8:UH:313:LYS:HA	1.87	0.56
12:UL:398:ASP:HB3	12:UL:406:LEU:HD12	1.88	0.56
18:UR:533:ALA:HA	18:UR:540:ALA:O	2.05	0.56
21:UU:476:PHE:N	21:UU:476:PHE:CD1	2.73	0.56
31:CJ:282:ARG:NH2	66:D3:560:U:OP2	2.39	0.56
33:CL:608:LEU:HB3	34:CM:16:ASN:HB3	1.87	0.56
36:JA:737:TRP:O	36:JA:740:ASN:C	2.43	0.56
37:JC:301:ASP:N	37:JC:306:LYS:O	2.32	0.56
38:JE:314:ASN:HA	38:JE:317:MET:HG2	1.88	0.56
39:JF:36:LYS:HB3	39:JF:172:PRO:HA	1.88	0.56
55:DL:57:LYS:NZ	66:D3:327:U:OP2	2.34	0.56
57:DO:79:VAL:O	57:DO:113:GLY:N	2.31	0.56
66:D3:460:A:H3'	66:D3:461:G:H8	1.69	0.56
4:UD:65:LEU:O	4:UD:66:ARG:NH1	2.31	0.56



A + a 1	A 4 a ma 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
11:UK:28:LEU:HD21	33:CL:969:VAL:HG11	1.87	0.56
12:UL:677:HIS:HE2	66:D3:1654:G:HO2'	1.52	0.56
13:UM:580:ARG:HG2	13:UM:623:LEU:HB3	1.88	0.56
17:UQ:522:SER:O	17:UQ:522:SER:OG	2.24	0.56
23:UX:109:LEU:HD12	23:UX:113:TYR:HE2	1.71	0.56
29:CH:421:ASN:HA	29:CH:436:GLU:O	2.06	0.56
31:CJ:244:GLY:HA2	32:CK:374:GLN:HE22	1.71	0.56
44:JN:317:ASN:OD1	60:DW:4:SER:OG	2.23	0.56
46:JP:367:SER:OG	46:JP:373:ARG:NH1	2.39	0.56
50:DF:151:GLY:HA3	50:DF:156:ARG:HH12	1.71	0.56
53:DI:99:ALA:N	53:DI:169:ILE:O	2.38	0.56
55:DL:10:GLU:HG3	55:DL:11:ARG:H	1.70	0.56
62:DY:34:ASN:O	66:D3:521:A:O2'	2.24	0.56
66:D3:153:G:H1	66:D3:161:U:H3	1.54	0.56
1:UA:311:ASN:HD21	41:JJ:273:ARG:NH2	1.96	0.56
12:UL:285:ARG:NH1	12:UL:371:LYS:O	2.39	0.56
12:UL:472:HIS:CG	12:UL:492:SER:HG	2.24	0.56
17:UQ:135:SER:OG	17:UQ:136:LEU:N	2.39	0.56
17:UQ:320:VAL:HG12	17:UQ:335:PRO:HA	1.86	0.56
21:UU:228:GLY:O	21:UU:245:LYS:HA	2.05	0.56
36:JA:72:LYS:NZ	66:D3:158:U:OP1	2.37	0.56
66:D3:1540:G:N2	66:D3:1571:C:O2	2.39	0.56
6:UF:169:GLN:NE2	6:UF:185:TYR:OH	2.39	0.56
20:UT:139:ALA:O	20:UT:142:PHE:C	2.44	0.56
22:UV:603:THR:OG1	22:UV:610:PHE:O	2.24	0.56
28:CF:7:LYS:HG3	28:CF:61:ILE:HG21	1.88	0.56
33:CL:135:ALA:O	33:CL:238:ARG:NH2	2.39	0.56
49:DE:174:LYS:O	49:DE:179:LYS:NZ	2.39	0.56
66:D3:1688:U:H3	66:D3:1713:G:H1	1.54	0.56
1:UA:222:LYS:HD2	1:UA:246:TYR:HB3	1.88	0.56
4:UD:742:LEU:N	4:UD:755:ILE:O	2.22	0.56
22:UV:529:VAL:HB	22:UV:613:VAL:HB	1.87	0.56
25:CA:114:GLY:O	25:CA:122:ARG:NH2	2.39	0.56
26:CD:101:SER:HB3	26:CD:128:ILE:HD13	1.88	0.56
44:JN:166:SER:HB2	45:JO:158:LEU:HD11	1.86	0.56
49:DE:45:ILE:HG13	49:DE:61:VAL:HG11	1.88	0.56
54:DJ:169:PRO:O	54:DJ:174:ARG:NH2	2.39	0.56
66:D3:148:A:N6	66:D3:166:C:N3	2.53	0.56
8:UH:189:ALA:HA	8:UH:196:ILE:HA	1.87	0.55
11:UK:164:ASN:HD21	25:CB:98:ILE:HD12	1.71	0.55
12:UL:101:GLY:HA2	12:UL:124:ILE:HG13	1.88	0.55



A 4 a 1	A t area 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:UX:117:LEU:O	23:UX:120:ALA:N	2.38	0.55
39:JG:41:MET:HG3	39:JG:202:ILE:HG23	1.88	0.55
51:DG:187:LYS:NZ	66:D3:140:A:OP2	2.38	0.55
66:D3:276:C:O2'	66:D3:278:U:OP2	2.23	0.55
66:D3:641:G:O6	66:D3:693:U:O2'	2.21	0.55
3:UC:562:ARG:HB3	54:DJ:37:LYS:HB3	1.88	0.55
4:UD:87:GLN:H	4:UD:378:TYR:HE2	1.52	0.55
4:UD:240:LEU:H	4:UD:258:SER:HB3	1.71	0.55
14:UN:894:LEU:O	46:JP:230:ASN:ND2	2.40	0.55
25:CB:109:LYS:HG2	25:CB:141:TYR:HE1	1.70	0.55
25:CB:144:TRP:CZ2	25:CB:183:HIS:HB3	2.41	0.55
26:CD:234:LEU:HD21	26:CD:252:ILE:HG13	1.87	0.55
34:CM:185:ARG:NH2	34:CM:349:ASP:OD2	2.32	0.55
41:JJ:216:ILE:O	41:JJ:220:THR:OG1	2.22	0.55
52:DH:41:LEU:HD11	52:DH:69:GLY:HA3	1.88	0.55
66:D3:50:C:H2'	66:D3:51:A:H8	1.71	0.55
4:UD:57:ILE:HA	4:UD:341:SER:HA	1.87	0.55
13:UM:344:ARG:NH1	13:UM:395:ASP:OD2	2.39	0.55
17:UQ:208:LEU:HD23	17:UQ:230:LEU:HD21	1.88	0.55
22:UV:920:LEU:HD12	22:UV:925:LEU:HB2	1.87	0.55
24:UZ:63:LYS:HG2	24:UZ:185:LYS:HE3	1.88	0.55
37:JC:147:ASN:ND2	37:JC:150:ASN:OD1	2.39	0.55
48:DA:179:SER:OG	48:DA:180:THR:O	2.23	0.55
1:UA:611:LEU:H	1:UA:611:LEU:HD23	1.72	0.55
12:UL:334:SER:OG	12:UL:335:LEU:N	2.36	0.55
12:UL:336:TYR:OH	12:UL:361:THR:OG1	2.14	0.55
17:UQ:258:TYR:CE2	17:UQ:414:ILE:HG12	2.41	0.55
21:UU:817:PHE:CE1	21:UU:833:LEU:HD11	2.42	0.55
22:UV:698:ASN:HB3	22:UV:701:ILE:HG22	1.88	0.55
33:CL:54:LEU:HD21	61:DX:77:ILE:HG13	1.87	0.55
33:CL:830:ARG:HB3	33:CL:880:TYR:HD1	1.71	0.55
53:DI:54:LYS:NZ	66:D3:333:A:OP2	2.33	0.55
1:UA:793:GLU:HG2	21:UU:721:LEU:HB2	1.88	0.55
4:UD:277:LYS:NZ	18:UR:347:GLY:O	2.39	0.55
4:UD:551:ASP:OD1	4:UD:561:LYS:N	2.39	0.55
5:UE:487:ARG:NH1	5:UE:487:ARG:HB2	2.21	0.55
10:UJ:286:LEU:O	10:UJ:326:LYS:NZ	2.34	0.55
12:UL:578:SER:OG	12:UL:591:SER:OG	2.21	0.55
15:UO:127:THR:O	15:UO:127:THR:OG1	2.24	0.55
17:UQ:26:SER:OG	17:UQ:27:SER:N	2.39	0.55
19:US:321:ASN:HB3	19:US:357:ARG:HH21	1.71	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
39:JF:73:HIS:HD2	39:JF:76:LEU:HB3	1.70	0.55
49:DE:185:GLY:H	49:DE:224:ASN:HB3	1.72	0.55
62:DY:60:PHE:CD1	62:DY:71:GLY:HA3	2.42	0.55
16:UP:182:SER:OG	16:UP:183:THR:N	2.40	0.55
38:JE:263:GLY:HA3	54:DJ:138:LYS:HB3	1.87	0.55
41:JJ:114:THR:HG23	41:JJ:115:LYS:HD3	1.88	0.55
49:DE:3:ARG:NH2	66:D3:94:U:OP2	2.40	0.55
11:UK:9:GLN:HE21	66:D3:572:C:H5	1.55	0.55
11:UK:59:ASN:ND2	30:CI:118:LEU:O	2.39	0.55
13:UM:593:CYS:HB2	13:UM:620:LEU:HG	1.89	0.55
15:UO:86:SER:O	15:UO:98:ALA:HA	2.06	0.55
15:UO:136:ASP:OD1	15:UO:137:ASN:N	2.39	0.55
18:UR:242:ASN:HD22	18:UR:585:LYS:HA	1.72	0.55
28:CG:59:GLU:OE2	28:CG:84:ARG:NH1	2.38	0.55
36:JA:840:LYS:NZ	36:JB:621:GLN:O	2.40	0.55
1:UA:334:SER:O	1:UA:334:SER:OG	2.20	0.55
8:UH:170:LYS:HA	8:UH:177:SER:HA	1.89	0.55
14:UN:277:ARG:HH11	52:DH:166:LEU:HB2	1.72	0.55
21:UU:51:VAL:HG22	21:UU:60:ILE:HG12	1.89	0.55
21:UU:188:VAL:H	21:UU:202:SER:HG	1.54	0.55
23:UX:70:ASN:ND2	23:UX:157:ASP:HB2	2.22	0.55
26:CD:388:ARG:NH1	28:CG:63:ILE:O	2.36	0.55
29:CH:187:ALA:HB2	29:CH:201:ILE:HD13	1.88	0.55
39:JF:70:CYS:N	39:JF:87:ALA:O	2.40	0.55
60:DW:98:GLN:N	60:DW:98:GLN:OE1	2.40	0.55
1:UA:200:SER:OG	1:UA:201:HIS:N	2.38	0.55
2:UB:737:ILE:HD12	59:DS:99:HIS:CB	2.36	0.55
5:UE:182:MET:CG	5:UE:183:THR:H	2.20	0.55
5:UE:231:ASP:HB2	5:UE:249:GLU:HG2	1.87	0.55
10:UJ:361:SER:HB3	10:UJ:362:LYS:HE3	1.88	0.55
13:UM:569:LYS:NZ	13:UM:604:CYS:O	2.37	0.55
21:UU:377:SER:O	21:UU:377:SER:OG	2.20	0.55
22:UV:182:ASP:O	22:UV:207:LEU:HA	2.07	0.55
25:CA:253:ILE:HD13	25:CA:269:ILE:HD12	1.89	0.55
25:CB:91:HIS:CB	25:CB:96:VAL:O	2.55	0.55
32:CK:533:LYS:O	32:CK:537:SER:HB3	2.07	0.55
34:CM:266:SER:OG	34:CM:267:ILE:N	2.39	0.55
46:JP:246:LEU:O	46:JP:255:THR:OG1	2.25	0.55
51:DG:136:LYS:HG2	51:DG:176:GLN:HB2	1.89	0.55
66:D3:1785:U:H2'	66:D3:1786:G:C8	2.42	0.55
2:UB:540:ILE:HD13	2:UB:575:PHE:HE1	1.72	0.55



A + a 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:209:LEU:HB3	13:UM:225:PHE:O	2.06	0.55
21:UU:600:ILE:HG13	21:UU:614:LEU:HD11	1.89	0.55
25:CA:168:LYS:O	25:CA:192:GLY:HA3	2.07	0.55
25:CB:172:TYR:HD2	25:CB:175:ALA:HB2	1.72	0.55
36:JA:851:ASP:HB3	36:JA:854:VAL:HG23	1.88	0.55
39:JG:190:GLN:NE2	39:JG:194:GLU:OE2	2.39	0.55
45:JO:291:ARG:CZ	66:D3:316:A:H5"	2.37	0.55
65:D2:426:G:N2	65:D2:429:A:OP2	2.40	0.55
66:D3:396:G:N1	66:D3:399:A:OP2	2.40	0.55
66:D3:1777:G:H2'	66:D3:1778:G:H8	1.72	0.55
1:UA:174:SER:OG	1:UA:175:VAL:N	2.38	0.54
7:UG:113:PRO:HA	7:UG:395:GLN:HA	1.88	0.54
12:UL:202:ALA:O	12:UL:227:LYS:NZ	2.28	0.54
13:UM:406:ALA:HB2	13:UM:440:VAL:HG13	1.88	0.54
17:UQ:73:LEU:HD13	17:UQ:129:PRO:HD2	1.88	0.54
18:UR:245:HIS:HB2	18:UR:284:LEU:HD21	1.87	0.54
19:US:156:TRP:CZ3	19:US:215:ASN:HB2	2.42	0.54
21:UU:295:TYR:OH	21:UU:351:GLN:OE1	2.21	0.54
22:UV:550:MET:HA	22:UV:553:VAL:HG12	1.89	0.54
25:CB:167:GLY:HA2	25:CB:191:GLU:HG2	1.89	0.54
33:CL:72:VAL:HA	33:CL:137:LEU:O	2.06	0.54
33:CL:775:GLU:OE2	33:CL:779:ARG:NE	2.39	0.54
44:JN:244:ASP:OD1	44:JN:248:LYS:NZ	2.39	0.54
50:DF:139:ASN:O	50:DF:214:LYS:NZ	2.37	0.54
2:UB:767:ILE:HD11	32:CK:349:ARG:HB2	1.88	0.54
4:UD:52:SER:HA	4:UD:104:TRP:CD1	2.42	0.54
4:UD:377:PRO:HD2	4:UD:634:VAL:HG21	1.90	0.54
6:UF:144:VAL:HG12	6:UF:181:LEU:HD22	1.89	0.54
6:UF:323:PHE:O	6:UF:331:ARG:NH1	2.40	0.54
7:UG:412:ASP:OD1	7:UG:413:ALA:N	2.41	0.54
8:UH:227:THR:HA	8:UH:244:LYS:H	1.72	0.54
10:UJ:65:LYS:HD2	18:UR:44:PHE:HD1	1.72	0.54
14:UN:881:PRO:HG2	14:UN:884:MET:HG2	1.90	0.54
22:UV:202:SER:HB2	22:UV:291:SER:HB3	1.89	0.54
28:CF:93:VAL:HG23	28:CF:95:ARG:H	1.72	0.54
29:CH:185:LEU:HD13	29:CH:527:VAL:HG11	1.89	0.54
31:CJ:195:THR:O	31:CJ:200:LYS:NZ	2.37	0.54
46:JP:244:ILE:O	46:JP:257:LYS:HA	2.07	0.54
49:DE:128:LYS:HA	49:DE:156:VAL:HG12	1.89	0.54
55:DL:140:VAL:HG23	55:DL:141:LYS:HG2	1.89	0.54
1:UA:47:SER:OG	1:UA:48:PHE:N	2.40	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:289:GLU:HA	12:UL:292:ILE:HD12	1.89	0.54
13:UM:421:SER:O	13:UM:423:LYS:N	2.40	0.54
13:UM:797:ASP:OD1	21:UU:927:LYS:NZ	2.30	0.54
15:UO:51:HIS:O	15:UO:53:HIS:N	2.37	0.54
19:US:230:SER:HB2	19:US:288:HIS:HD2	1.72	0.54
33:CL:251:ASP:OD1	33:CL:251:ASP:N	2.36	0.54
35:CN:35:HIS:CE1	35:CN:59:PRO:HG3	2.42	0.54
37:JC:232:THR:HG21	37:JC:273:ASP:HB2	1.88	0.54
46:JP:382:ARG:NE	67:D4:34:A:OP1	2.34	0.54
54:DJ:40:LYS:NZ	66:D3:473:A:OP2	2.40	0.54
66:D3:366:A:H2	66:D3:379:U:H3	1.53	0.54
4:UD:469:LEU:O	4:UD:473:THR:OG1	2.17	0.54
8:UH:639:SER:HB2	9:UI:499:ILE:HD11	1.90	0.54
12:UL:45:ALA:HB3	12:UL:48:ASP:HB3	1.88	0.54
26:CD:188:ILE:HD11	26:CD:281:LEU:HB3	1.88	0.54
27:CE:159:VAL:HG22	27:CE:279:ARG:HH22	1.72	0.54
31:CJ:222:ILE:HG12	31:CJ:235:GLN:HG3	1.90	0.54
33:CL:830:ARG:HD2	33:CL:880:TYR:HE1	1.73	0.54
49:DE:193:GLY:HA3	49:DE:212:ASP:HA	1.89	0.54
51:DG:87:ARG:NH2	66:D3:159:U:O3'	2.40	0.54
52:DH:23:ALA:HB3	52:DH:85:PHE:HZ	1.73	0.54
65:D2:6:A:N6	65:D2:8:A:N3	2.56	0.54
1:UA:300:MET:HG3	1:UA:328:LEU:HD13	1.88	0.54
2:UB:766:ARG:NE	32:CK:346:GLU:OE2	2.41	0.54
11:UK:196:LYS:NZ	65:D2:424:G:OP2	2.31	0.54
15:UO:32:SER:O	15:UO:32:SER:OG	2.23	0.54
31:CJ:188:HIS:HB2	31:CJ:221:VAL:HG12	1.90	0.54
36:JA:851:ASP:OD1	36:JA:853:HIS:ND1	2.41	0.54
66:D3:1650:U:H2'	66:D3:1651:A:C8	2.43	0.54
8:UH:28:TYR:O	17:UQ:685:ARG:NH1	2.32	0.54
13:UM:209:LEU:HD23	13:UM:225:PHE:HD2	1.73	0.54
13:UM:619:ARG:HB2	13:UM:637:ALA:HB2	1.89	0.54
13:UM:751:LYS:NZ	66:D3:1638:G:OP2	2.32	0.54
15:UO:23:GLU:HG2	15:UO:268:MET:CG	2.38	0.54
19:US:400:PRO:HB3	19:US:493:TYR:HD2	1.72	0.54
25:CA:223:ASP:OD1	25:CA:224:ALA:N	2.40	0.54
28:CG:50:GLU:N	28:CG:102:ILE:O	2.40	0.54
35:CN:16:VAL:HB	35:CN:37:MET:HB2	1.90	0.54
37:JC:74:THR:HG22	37:JC:81:ILE:HG22	1.90	0.54
37:JC:343:ILE:HG22	37:JC:346:LEU:H	1.73	0.54
45:JO:284:GLN:HA	45:JO:287:LYS:HG2	1.89	0.54



	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
49:DE:143:ASP:OD1	49:DE:143:ASP:N	2.41	0.54
62:DY:7:ILE:HG23	62:DY:27:VAL:HG22	1.89	0.54
1:UA:148:ASP:O	1:UA:165:SER:HB2	2.08	0.54
1:UA:524:ARG:NH2	1:UA:529:GLU:OE1	2.40	0.54
12:UL:537:VAL:HG22	12:UL:548:ILE:HG12	1.90	0.54
15:UO:20:THR:HG21	15:UO:28:ARG:NH1	2.20	0.54
17:UQ:64:LYS:NZ	17:UQ:123:GLY:O	2.40	0.54
17:UQ:743:ILE:HD11	17:UQ:757:PHE:HD2	1.73	0.54
24:UZ:71:ASN:ND2	24:UZ:123:ASP:OD2	2.39	0.54
25:CB:171:LEU:HB3	25:CB:240:VAL:HG22	1.90	0.54
29:CH:488:ILE:HG12	29:CH:498:VAL:HG22	1.90	0.54
34:CM:285:LYS:HG2	34:CM:316:GLU:HB3	1.90	0.54
37:JC:110:ASP:OD2	37:JC:112:THR:OG1	2.18	0.54
53:DI:10:LYS:NZ	66:D3:337:G:O3'	2.41	0.54
66:D3:104:A:N6	66:D3:308:C:OP2	2.41	0.54
2:UB:453:ASN:HA	2:UB:456:ILE:HD12	1.89	0.54
2:UB:701:ALA:HA	19:US:417:HIS:HB2	1.89	0.54
12:UL:148:TRP:CD1	12:UL:155:GLY:HA2	2.43	0.54
12:UL:854:CYS:SG	12:UL:855:LYS:N	2.80	0.54
17:UQ:511:GLU:OE2	17:UQ:530:LYS:NZ	2.28	0.54
19:US:419:PRO:HA	19:US:422:ILE:HG13	1.90	0.54
22:UV:435:CYS:SG	22:UV:436:HIS:N	2.80	0.54
22:UV:441:GLN:HE21	22:UV:456:LYS:HB3	1.72	0.54
22:UV:726:SER:OG	22:UV:768:PRO:O	2.25	0.54
26:CD:194:ARG:HG2	27:CE:169:LEU:HD12	1.89	0.54
36:JA:131:THR:HG22	36:JA:133:ASN:H	1.73	0.54
36:JA:387:ASP:HA	36:JA:409:ALA:HB3	1.89	0.54
48:DA:127:VAL:HG21	48:DA:176:VAL:HG11	1.89	0.54
53:DI:31:ARG:HH11	66:D3:332:U:H5"	1.71	0.54
17:UQ:745:ILE:O	17:UQ:754:LEU:N	2.41	0.54
26:CD:254:ASN:HA	26:CD:257:ILE:HG12	1.88	0.54
26:CD:277:ARG:HH12	27:CE:264:GLU:C	2.11	0.54
28:CF:50:GLU:HG3	28:CF:51:PHE:HD1	1.72	0.54
32:CK:321:GLU:OE2	32:CK:322:LYS:N	2.41	0.54
39:JF:49:SER:OG	39:JF:86:GLU:O	2.23	0.54
65:D2:323:A:H2'	65:D2:324:U:H4'	1.89	0.54
1:UA:441:SER:O	1:UA:443:GLU:N	2.40	0.54
4:UD:544:SER:HA	4:UD:549:VAL:O	2.07	0.54
8:UH:665:GLN:HA	8:UH:668:ILE:HG22	1.88	0.54
13:UM:433:HIS:HE1	13:UM:437:VAL:HB	1.72	0.54
17:UQ:352:ASN:O	17:UQ:376:ALA:CB	2.55	0.54



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
17:UQ:359:GLN:O	17:UQ:368:ASP:O	2.25	0.54
21:UU:455:PHE:CB	21:UU:477:ILE:CD1	2.85	0.54
21:UU:820:GLN:HE21	21:UU:832:SER:HB3	1.73	0.54
22:UV:530:GLN:HB2	22:UV:695:GLN:HB2	1.90	0.54
25:CB:314:CYS:SG	25:CB:315:ILE:N	2.81	0.54
39:JF:97:LEU:HD21	39:JF:132:ARG:HA	1.88	0.54
39:JG:174:LYS:NZ	50:DF:215:ASP:OD2	2.37	0.54
66:D3:188:A:N1	66:D3:197:A:O2'	2.34	0.54
66:D3:369:A:H2'	66:D3:370:A:H8	1.73	0.54
66:D3:553:G:N2	66:D3:584:C:N3	2.56	0.54
3:UC:547:ASN:ND2	33:CL:196:THR:HG21	2.23	0.53
4:UD:127:ASP:HB2	4:UD:134:LEU:HB2	1.90	0.53
6:UF:17:ASP:OD2	6:UF:82:SER:OG	2.24	0.53
6:UF:162:LYS:NZ	65:D2:533:G:OP2	2.41	0.53
7:UG:257:SER:HG	7:UG:259:TRP:HE1	1.57	0.53
13:UM:36:VAL:HG12	13:UM:37:LEU:H	1.72	0.53
17:UQ:710:LEU:HD12	17:UQ:722:LEU:HD23	1.89	0.53
29:CH:258:ARG:NH2	29:CH:279:ARG:O	2.37	0.53
30:CI:24:ASP:O	30:CI:26:GLY:N	2.41	0.53
38:JE:224:PHE:HZ	49:DE:207:LEU:HD21	1.71	0.53
39:JG:144:LEU:HD13	39:JG:150:ILE:HG12	1.91	0.53
66:D3:1272:U:H2'	66:D3:1273:G:H8	1.73	0.53
66:D3:1569:A:H2'	66:D3:1570:A:C8	2.43	0.53
2:UB:527:GLN:HG3	2:UB:531:GLN:HG3	1.90	0.53
2:UB:644:ASP:HA	2:UB:647:ILE:HD12	1.91	0.53
3:UC:544:ILE:CG2	33:CL:834:TRP:CE2	2.91	0.53
6:UF:191:ASN:ND2	43:JM:63:PRO:O	2.40	0.53
7:UG:163:GLU:OE2	7:UG:425:ARG:NH1	2.41	0.53
12:UL:358:SER:OG	12:UL:359:SER:N	2.41	0.53
16:UP:186:ASP:HA	16:UP:189:THR:HG22	1.89	0.53
17:UQ:146:HIS:ND1	17:UQ:147:SER:O	2.30	0.53
31:CJ:119:ARG:NH1	66:D3:1605:G:OP1	2.41	0.53
36:JA:10:ILE:HD13	36:JA:205:LEU:HD23	1.90	0.53
46:JP:84:ALA:HB1	46:JP:136:MET:HE3	1.89	0.53
48:DA:134:VAL:HB	48:DA:219:LYS:HB2	1.90	0.53
4:UD:265:TRP:HA	4:UD:272:LEU:HA	1.89	0.53
6:UF:3:LYS:HG3	65:D2:487:A:H62	1.73	0.53
7:UG:267:LEU:HD13	7:UG:444:LEU:HD12	1.90	0.53
17:UQ:610:SER:OG	17:UQ:659:ILE:O	2.25	0.53
22:UV:337:LEU:O	22:UV:340:SER:OG	2.22	0.53
27:CE:366:LYS:NZ	67:D4:82:G:OP1	2.35	0.53


Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
30:CI:15:LYS:HB2	67:D4:24:U:C5	2.43	0.53
31:CJ:87:ARG:NH2	31:CJ:135:GLY:O	2.30	0.53
36:JA:746:TYR:O	36:JA:760:CYS:HA	2.08	0.53
46:JP:71:TYR:OH	60:DW:68:ARG:NH1	2.39	0.53
50:DF:148:ARG:HH21	50:DF:157:ARG:HH22	1.55	0.53
51:DG:39:GLU:HG3	51:DG:46:LYS:HA	1.90	0.53
53:DI:8:ARG:HE	53:DI:21:PHE:HB3	1.72	0.53
66:D3:1496:U:H3	66:D3:1511:U:H3	1.55	0.53
4:UD:145:TRP:CD1	4:UD:161:ASP:HB3	2.44	0.53
5:UE:109:ASP:OD1	5:UE:110:ILE:N	2.38	0.53
12:UL:144:ASN:HB3	12:UL:160:ARG:HG3	1.90	0.53
21:UU:602:SER:O	21:UU:602:SER:OG	2.25	0.53
29:CH:557:SER:OG	29:CH:558:GLY:N	2.41	0.53
39:JG:99:LEU:O	39:JG:102:SER:OG	2.25	0.53
43:JM:62:LEU:HD12	43:JM:63:PRO:HD2	1.90	0.53
49:DE:141:THR:OG1	49:DE:143:ASP:OD1	2.20	0.53
5:UE:100:THR:OG1	5:UE:101:THR:O	2.19	0.53
13:UM:143:HIS:HD2	13:UM:175:TRP:HH2	1.57	0.53
13:UM:604:CYS:SG	13:UM:605:SER:N	2.82	0.53
15:UO:20:THR:CG2	15:UO:28:ARG:HH22	2.21	0.53
16:UP:181:LEU:HD13	25:CB:294:ARG:HD2	1.89	0.53
19:US:167:LYS:O	19:US:272:GLN:NE2	2.41	0.53
48:DA:32:ILE:HG22	48:DA:96:LEU:HD12	1.90	0.53
58:DQ:94:GLN:HB2	58:DQ:102:LYS:HG3	1.89	0.53
60:DW:38:LEU:O	60:DW:42:GLN:HB2	2.08	0.53
6:UF:145:ASP:OD1	43:JM:69:PHE:HB2	2.09	0.53
7:UG:358:MET:HA	65:D2:315:U:OP1	2.09	0.53
13:UM:464:LYS:HA	13:UM:486:THR:HA	1.89	0.53
17:UQ:335:PRO:HG2	65:D2:87:C:C5	2.44	0.53
17:UQ:716:ARG:HH21	17:UQ:772:THR:HB	1.73	0.53
22:UV:99:LYS:O	22:UV:103:PHE:CB	2.57	0.53
26:CD:237:LEU:HD22	26:CD:248:ALA:HB2	1.90	0.53
33:CL:299:ALA:HB2	33:CL:794:GLU:HG2	1.90	0.53
33:CL:1153:ASP:OD1	33:CL:1156:LYS:NZ	2.33	0.53
1:UA:27:LYS:HZ3	1:UA:43:ILE:CD1	2.21	0.53
1:UA:467:ASP:OD1	1:UA:468:ALA:N	2.41	0.53
2:UB:703:GLN:H	19:US:417:HIS:HB3	1.74	0.53
4:UD:355:THR:OG1	4:UD:356:LEU:N	2.41	0.53
12:UL:88:HIS:CE1	12:UL:90:ASP:HB2	2.43	0.53
15:UO:229:CYS:HB2	15:UO:258:LEU:HD22	1.90	0.53
22:UV:338:SER:O	22:UV:342:HIS:ND1	2.41	0.53



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
24:UZ:40:ILE:HG13	24:UZ:242:ILE:HG22	1.89	0.53
32:CK:454:VAL:O	32:CK:456:PHE:N	2.42	0.53
33:CL:118:LEU:HD22	33:CL:245:LEU:HD11	1.90	0.53
33:CL:246:ALA:HB3	33:CL:810:ILE:HG13	1.89	0.53
36:JA:167:ASP:OD2	36:JA:170:ALA:N	2.32	0.53
37:JC:168:GLU:HA	42:JK:477:ALA:HB2	1.91	0.53
37:JC:230:GLN:HB2	37:JC:248:SER:HB3	1.91	0.53
39:JF:111:GLN:OE1	39:JF:113:TYR:OH	2.22	0.53
46:JP:224:SER:OG	46:JP:225:LEU:N	2.40	0.53
46:JP:238:THR:HG1	46:JP:264:THR:HG1	1.57	0.53
51:DG:59:GLN:OE1	51:DG:72:ARG:NH1	2.42	0.53
65:D2:129:U:H4'	65:D2:130:G:H5"	1.89	0.53
66:D3:1665:U:OP2	66:D3:1665:U:H6	1.91	0.53
2:UB:600:LEU:HD12	2:UB:601:PRO:HD2	1.91	0.53
5:UE:451:SER:O	5:UE:454:GLU:HB3	2.09	0.53
10:UJ:29:HIS:O	10:UJ:123:ARG:NH2	2.41	0.53
13:UM:421:SER:O	13:UM:423:LYS:NZ	2.34	0.53
13:UM:518:TRP:HA	13:UM:526:GLU:HG2	1.91	0.53
17:UQ:229:SER:OG	17:UQ:230:LEU:N	2.42	0.53
17:UQ:778:ASP:OD1	17:UQ:779:ILE:N	2.41	0.53
18:UR:214:THR:HG22	21:UU:247:PRO:HG3	1.90	0.53
19:US:366:LEU:HD23	19:US:371:LEU:HD13	1.90	0.53
24:UZ:34:LYS:HA	24:UZ:204:ILE:HG12	1.91	0.53
25:CA:306:LEU:HD11	25:CA:313:HIS:HB2	1.89	0.53
26:CD:202:HIS:ND1	26:CD:203:PHE:HB2	2.23	0.53
29:CH:298:SER:OG	29:CH:325:VAL:O	2.27	0.53
29:CH:303:LYS:HE3	29:CH:319:TYR:HE2	1.73	0.53
38:JE:291:GLU:HA	62:DY:11:LYS:HD3	1.91	0.53
49:DE:42:LEU:HD12	49:DE:43:PRO:HD2	1.91	0.53
52:DH:111:LYS:HE2	66:D3:859:A:H5"	1.91	0.53
65:D2:194:G:H2'	65:D2:195:A:H8	1.73	0.53
1:UA:376:SER:O	1:UA:376:SER:OG	2.20	0.53
2:UB:562:PRO:HA	2:UB:565:VAL:HG12	1.90	0.53
6:UF:46:ARG:NH2	65:D2:480:C:O2	2.41	0.53
12:UL:176:TRP:CD1	12:UL:188:LEU:HD21	2.43	0.53
13:UM:636:ASP:OD1	13:UM:636:ASP:N	2.42	0.53
20:UT:969:SER:O	20:UT:972:LEU:C	2.47	0.53
34:CM:174:ILE:O	34:CM:361:ASN:ND2	2.42	0.53
34:CM:241:TRP:NE1	34:CM:262:GLY:HA3	2.24	0.53
36:JA:631:SER:O	36:JA:721:HIS:ND1	2.29	0.53
37:JC:171:ARG:HH11	42:JK:468:VAL:HG13	1.74	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
44:JN:328:ARG:HG3	44:JN:329:ILE:HG23	1.90	0.53
49:DE:99:PHE:HA	49:DE:112:HIS:O	2.09	0.53
52:DH:153:LEU:HD23	52:DH:186:PRO:HG3	1.91	0.53
54:DJ:107:ARG:NH1	54:DJ:153:GLU:OE2	2.33	0.53
65:D2:430:C:H41	65:D2:432:C:H41	1.57	0.53
66:D3:106:U:O4	66:D3:308:C:N4	2.41	0.53
66:D3:1511:U:H2'	66:D3:1512:G:C8	2.44	0.53
9:UI:497:LEU:HD22	15:UO:499:LYS:HZ3	1.74	0.53
11:UK:221:GLN:NE2	65:D2:244:U:OP1	2.42	0.53
12:UL:390:GLN:HG2	12:UL:394:VAL:HG22	1.91	0.53
13:UM:89:HIS:HE1	13:UM:91:LYS:HB2	1.74	0.53
15:UO:217:ASN:HD22	15:UO:257:CYS:HA	1.73	0.53
18:UR:407:PHE:HA	18:UR:424:ILE:O	2.08	0.53
19:US:210:ASP:HA	19:US:213:LEU:HD12	1.91	0.53
22:UV:443:HIS:HB2	22:UV:453:PRO:HA	1.91	0.53
24:UZ:192:ASN:ND2	66:D3:1509:C:O2'	2.42	0.53
29:CH:61:ASP:OD1	29:CH:64:ARG:NH1	2.42	0.53
33:CL:627:SER:OG	33:CL:628:VAL:N	2.41	0.53
34:CM:107:ALA:HA	34:CM:114:PHE:CE2	2.43	0.53
37:JC:323:VAL:HG21	37:JC:350:PRO:HG2	1.90	0.53
39:JF:99:LEU:HD21	39:JF:238:CYS:HB3	1.91	0.53
50:DF:146:THR:HG21	50:DF:220:VAL:HG12	1.91	0.53
54:DJ:105:LEU:HD23	54:DJ:108:ARG:HD2	1.91	0.53
58:DQ:22:VAL:HG22	58:DQ:65:ILE:HG12	1.90	0.53
66:D3:228:G:N2	66:D3:240:U:O4	2.41	0.53
5:UE:451:SER:HA	5:UE:454:GLU:OE1	2.09	0.52
5:UE:469:ILE:HG21	5:UE:505:CYS:HA	1.92	0.52
6:UF:145:ASP:OD2	43:JM:68:GLY:N	2.24	0.52
8:UH:670:GLU:O	8:UH:673:THR:OG1	2.20	0.52
13:UM:188:GLU:HG3	22:UV:657:ARG:HH22	1.74	0.52
13:UM:313:LEU:O	13:UM:330:THR:OG1	2.25	0.52
13:UM:512:ASP:OD1	13:UM:514:THR:OG1	2.27	0.52
17:UQ:332:GLN:NE2	18:UR:344:ARG:HB2	2.25	0.52
19:US:270:SER:O	19:US:274:TYR:HB2	2.08	0.52
21:UU:108:HIS:ND1	21:UU:109:LEU:O	2.33	0.52
22:UV:765:LEU:HD12	22:UV:917:LYS:HB3	1.91	0.52
24:UZ:243:PHE:CD1	24:UZ:253:PRO:HA	2.43	0.52
31:CJ:157:PHE:O	31:CJ:159:HIS:N	2.42	0.52
33:CL:359:SER:OG	33:CL:360:ASP:N	2.42	0.52
39:JF:44:VAL:HA	39:JF:113:TYR:O	2.08	0.52
39:JG:104:ILE:HG23	39:JG:110:LEU:HD22	1.91	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
51:DG:72:ARG:HG3	51:DG:98:ARG:HD3	1.91	0.52
65:D2:388:C:N4	65:D2:389:U:O4	2.41	0.52
66:D3:523:G:N1	66:D3:528:U:OP2	2.41	0.52
66:D3:1131:A:N3	66:D3:1136:U:N3	2.57	0.52
13:UM:45:LEU:HA	13:UM:50:ARG:HG2	1.91	0.52
13:UM:407:SER:OG	13:UM:408:LYS:N	2.42	0.52
17:UQ:727:GLN:HE22	17:UQ:740:LYS:HB3	1.74	0.52
33:CL:629:ASP:HA	33:CL:632:LYS:NZ	2.24	0.52
36:JA:907:ASN:HB2	36:JA:910:ILE:HG22	1.90	0.52
55:DL:132:SER:HB3	55:DL:135:VAL:HG22	1.90	0.52
56:DN:96:VAL:HG22	56:DN:100:LYS:HE3	1.90	0.52
66:D3:147:A:H62	66:D3:167:U:H3	1.57	0.52
66:D3:1155:G:N2	66:D3:1623:C:O2	2.36	0.52
66:D3:1268:G:O2'	66:D3:1270:G:O4'	2.27	0.52
1:UA:27:LYS:CG	1:UA:43:ILE:HD12	2.39	0.52
2:UB:426:THR:HA	2:UB:429:LEU:HD12	1.92	0.52
4:UD:287:THR:OG1	4:UD:288:THR:N	2.41	0.52
7:UG:18:GLN:O	7:UG:22:GLU:HB2	2.08	0.52
10:UJ:248:SER:OG	10:UJ:249:LYS:N	2.39	0.52
13:UM:746:TRP:O	13:UM:752:THR:OG1	2.26	0.52
15:UO:11:SER:O	15:UO:11:SER:OG	2.25	0.52
15:UO:114:ARG:NH2	66:D3:1532:U:OP2	2.33	0.52
17:UQ:407:ASN:HB2	17:UQ:413:SER:H	1.74	0.52
17:UQ:728:LEU:HB3	17:UQ:735:PRO:HA	1.90	0.52
21:UU:25:SER:OG	21:UU:655:THR:OG1	2.26	0.52
22:UV:975:LEU:HB3	22:UV:1041:VAL:HA	1.91	0.52
24:UZ:223:LEU:HD23	24:UZ:235:ILE:HD11	1.90	0.52
28:CG:89:ARG:HH11	29:CH:474:TRP:HH2	1.58	0.52
37:JC:299:ILE:O	37:JC:308:TYR:N	2.42	0.52
41:JJ:217:GLU:OE2	41:JJ:224:ILE:N	2.33	0.52
53:DI:86:SER:O	66:D3:341:A:O2'	2.21	0.52
54:DJ:58:ASP:O	54:DJ:61:THR:OG1	2.24	0.52
65:D2:174:U:H2'	65:D2:175:A:C8	2.44	0.52
66:D3:209:U:H2'	66:D3:210:A:C8	2.45	0.52
13:UM:439:ALA:HB3	13:UM:457:ALA:HB3	1.92	0.52
13:UM:665:GLN:HG3	13:UM:688:LEU:HD21	1.91	0.52
19:US:130:GLU:O	19:US:134:PHE:CB	2.57	0.52
21:UU:192:ASN:O	21:UU:196:GLY:N	2.42	0.52
22:UV:236:THR:HG21	22:UV:256:TYR:HE1	1.73	0.52
28:CF:46:ARG:NH1	67:D4:326:U:OP1	2.33	0.52
32:CK:295:LYS:NZ	32:CK:296:ASN:O	2.42	0.52



	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
38:JE:324:ASP:O	54:DJ:79:ARG:NH1	2.42	0.52
55:DL:103:ARG:NH1	66:D3:352:A:OP1	2.39	0.52
5:UE:533:ARG:O	15:UO:498:SER:OG	2.27	0.52
6:UF:198:ASN:OD1	6:UF:201:LYS:NZ	2.35	0.52
10:UJ:284:SER:OG	18:UR:203:GLY:O	2.18	0.52
12:UL:836:ILE:HG13	12:UL:857:LEU:HD13	1.90	0.52
22:UV:580:TYR:HB2	22:UV:618:ILE:HD13	1.91	0.52
26:CD:277:ARG:CZ	27:CE:264:GLU:HB3	2.40	0.52
31:CJ:162:THR:O	31:CJ:162:THR:OG1	2.25	0.52
33:CL:625:TRP:O	33:CL:627:SER:O	2.27	0.52
33:CL:829:LEU:HD11	33:CL:860:TYR:HE1	1.74	0.52
34:CM:46:LYS:N	34:CM:49:GLU:OE1	2.41	0.52
35:CN:148:HIS:HB2	35:CN:155:LEU:HD21	1.91	0.52
37:JC:128:LYS:NZ	66:D3:409:C:OP1	2.35	0.52
46:JP:280:ALA:HB2	46:JP:311:VAL:HB	1.90	0.52
50:DF:76:ARG:NE	58:DQ:122:ARG:HG2	2.25	0.52
65:D2:20:C:H2'	65:D2:21:A:H8	1.75	0.52
66:D3:1540:G:H2'	66:D3:1541:G:H8	1.74	0.52
66:D3:1662:G:H2'	66:D3:1663:G:H8	1.72	0.52
5:UE:495:GLN:O	5:UE:499:ASN:HB2	2.09	0.52
9:UI:480:LYS:O	9:UI:483:LYS:HB2	2.10	0.52
12:UL:365:TYR:OH	12:UL:381:LYS:NZ	2.43	0.52
17:UQ:343:ASP:OD1	17:UQ:344:CYS:N	2.42	0.52
19:US:327:MET:O	19:US:330:PHE:O	2.28	0.52
29:CH:357:LEU:HD13	38:JE:258:TRP:H	1.74	0.52
33:CL:54:LEU:O	33:CL:55:HIS:ND1	2.42	0.52
36:JA:12:SER:O	36:JA:16:ASN:ND2	2.42	0.52
39:JG:83:ASP:HB3	39:JG:86:GLU:HG3	1.91	0.52
57:DO:48:VAL:HG21	57:DO:53:ASP:HB2	1.91	0.52
66:D3:443:C:O2	66:D3:445:A:N6	2.38	0.52
66:D3:1689:A:H2'	66:D3:1690:G:C8	2.44	0.52
3:UC:496:GLN:NE2	3:UC:497:GLN:OE1	2.43	0.52
3:UC:556:LYS:HA	3:UC:559:ARG:HB2	1.90	0.52
5:UE:161:ALA:HA	5:UE:175:ILE:HD12	1.92	0.52
5:UE:346:HIS:ND1	5:UE:346:HIS:O	2.43	0.52
10:UJ:334:THR:HA	10:UJ:337:ASP:HB2	1.92	0.52
13:UM:24:THR:HG21	13:UM:68:LYS:HD2	1.91	0.52
13:UM:26:SER:OG	13:UM:28:ASN:OD1	2.28	0.52
22:UV:971:LYS:NZ	22:UV:1032:PRO:O	2.31	0.52
27:CE:247:ILE:HD11	27:CE:252:LEU:HD12	1.92	0.52
35:CN:168:PHE:HA	35:CN:171:PHE:CD2	2.44	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
52:DH:159:VAL:O	52:DH:163:ASP:HB2	2.09	0.52
55:DL:74:THR:OG1	55:DL:87:ARG:O	2.28	0.52
66:D3:527:A:H2'	66:D3:528:U:H6	1.75	0.52
1:UA:376:SER:O	1:UA:378:PHE:N	2.43	0.52
4:UD:207:ASP:HB2	4:UD:209:ARG:HG2	1.92	0.52
6:UF:126:TYR:O	6:UF:130:HIS:ND1	2.37	0.52
18:UR:29:ASP:OD2	18:UR:31:THR:N	2.43	0.52
21:UU:265:SER:O	21:UU:265:SER:OG	2.25	0.52
29:CH:504:ASN:HB2	29:CH:506:ARG:HH21	1.73	0.52
32:CK:452:SER:O	32:CK:452:SER:OG	2.21	0.52
34:CM:85:ALA:HA	34:CM:115:SER:O	2.10	0.52
35:CN:46:ASN:HB3	35:CN:49:GLU:HB2	1.92	0.52
36:JA:208:LEU:HB3	36:JA:210:LEU:HG	1.92	0.52
43:JM:114:ARG:HA	43:JM:117:VAL:HG12	1.92	0.52
53:DI:184:LEU:HD12	53:DI:188:GLU:HB3	1.91	0.52
4:UD:581:SER:OG	4:UD:582:VAL:N	2.43	0.52
10:UJ:21:ASP:OD1	10:UJ:22:ARG:N	2.42	0.52
12:UL:197:ILE:HG22	12:UL:198:GLU:HG3	1.91	0.52
17:UQ:665:ILE:HG22	17:UQ:669:ASN:HB2	1.91	0.52
18:UR:181:GLU:HB3	21:UU:281:ARG:HH21	1.75	0.52
21:UU:176:TYR:OH	21:UU:219:ASP:OD1	2.23	0.52
22:UV:1035:THR:HA	22:UV:1058:LEU:HD22	1.92	0.52
24:UZ:39:ILE:HD11	24:UZ:245:LYS:HE2	1.91	0.52
25:CB:116:SER:HB3	25:CB:122:ARG:HH21	1.75	0.52
29:CH:159:CYS:HB3	29:CH:242:VAL:HG12	1.91	0.52
33:CL:95:LYS:NZ	36:JA:89:ASN:OD1	2.31	0.52
36:JA:316:GLU:O	36:JA:318:LEU:N	2.36	0.52
39:JF:121:LEU:CB	39:JF:163:ILE:O	2.55	0.52
46:JP:260:GLN:OE1	46:JP:281:ASN:ND2	2.43	0.52
1:UA:157:ASP:OD1	1:UA:157:ASP:N	2.43	0.52
3:UC:552:PRO:HA	11:UK:7:ASP:OD2	2.10	0.52
5:UE:32:GLN:HG3	5:UE:33:PRO:HD2	1.92	0.52
8:UH:313:LYS:N	8:UH:323:PHE:O	2.42	0.52
19:US:98:PHE:O	19:US:102:LEU:N	2.43	0.52
30:CI:11:LYS:NZ	67:D4:26:C:OP1	2.41	0.52
36:JB:784:ARG:O	36:JB:788:LEU:CB	2.58	0.52
37:JC:287:ASN:ND2	37:JC:301:ASP:OD1	2.33	0.52
49:DE:60:GLU:OE1	49:DE:60:GLU:N	2.43	0.52
11:UK:125:LEU:HD12	11:UK:126:MET:H	1.74	0.51
15:UO:33:ALA:HA	15:UO:329:ILE:O	2.10	0.51
21:UU:285:HIS:ND1	21:UU:286:VAL:O	2.43	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
29:CH:241:THR:HG21	29:CH:285:SER:HA	1.92	0.51
37:JC:295:ARG:HH11	37:JC:315:VAL:HA	1.75	0.51
41:JJ:114:THR:HA	41:JJ:117:TYR:HE1	1.75	0.51
41:JJ:186:GLU:HB3	41:JJ:188:LYS:HG2	1.92	0.51
45:JO:130:ASN:HD21	57:DO:127:ARG:HH21	1.58	0.51
48:DA:155:TYR:OH	66:D3:932:U:OP2	2.23	0.51
62:DY:80:ALA:HA	62:DY:83:LYS:HG2	1.92	0.51
4:UD:441:VAL:HG11	4:UD:478:VAL:HG21	1.93	0.51
5:UE:116:GLN:OE1	5:UE:128:GLN:NE2	2.43	0.51
6:UF:320:ILE:HD11	6:UF:338:VAL:HG11	1.92	0.51
12:UL:760:ILE:HG13	12:UL:831:LYS:HB3	1.92	0.51
17:UQ:508:ILE:HG22	17:UQ:531:PHE:HD1	1.75	0.51
18:UR:349:GLU:O	18:UR:352:GLN:O	2.27	0.51
19:US:180:PHE:HD1	19:US:184:TYR:HD2	1.57	0.51
21:UU:544:ALA:HB1	21:UU:563:ASP:HB3	1.92	0.51
29:CH:120:ARG:HH22	62:DY:15:ASN:HA	1.75	0.51
33:CL:157:ASN:O	33:CL:161:HIS:ND1	2.43	0.51
34:CM:107:ALA:HB1	34:CM:170:VAL:HG11	1.92	0.51
39:JG:93:HIS:NE2	39:JG:132:ARG:O	2.44	0.51
43:JM:113:MET:O	43:JM:116:GLU:N	2.42	0.51
1:UA:555:CYS:O	1:UA:557:LYS:N	2.44	0.51
2:UB:515:HIS:CD2	2:UB:518:ILE:H	2.28	0.51
10:UJ:262:VAL:HG23	10:UJ:298:THR:HG23	1.92	0.51
12:UL:337:LYS:NZ	66:D3:1654:G:OP2	2.43	0.51
17:UQ:16:SER:HB2	17:UQ:783:LEU:HB2	1.92	0.51
51:DG:139:ASN:ND2	66:D3:143:G:OP2	2.40	0.51
51:DG:173:PRO:HA	66:D3:66:U:H5"	1.91	0.51
60:DW:56:HIS:O	66:D3:861:U:O2'	2.27	0.51
65:D2:430:C:H5"	65:D2:431:A:H5"	1.92	0.51
1:UA:134:ALA:HB1	65:D2:297:U:C4	2.45	0.51
2:UB:749:LYS:NZ	66:D3:1176:G:N7	2.50	0.51
10:UJ:194:SER:HB3	21:UU:335:VAL:HG11	1.93	0.51
12:UL:392:THR:O	12:UL:679:HIS:ND1	2.38	0.51
12:UL:837:ASP:OD1	12:UL:882:ARG:NH1	2.43	0.51
13:UM:236:THR:HB	48:DA:244:VAL:HG23	1.92	0.51
13:UM:546:LYS:HB3	13:UM:562:LEU:HD22	1.92	0.51
13:UM:642:GLN:HB2	13:UM:644:TRP:HE1	1.74	0.51
26:CD:328:GLN:HE21	26:CD:332:THR:HG23	1.74	0.51
36:JA:173:ARG:NH2	36:JA:186:GLU:OE1	2.43	0.51
36:JA:515:LEU:HB2	36:JA:712:LEU:HD22	1.92	0.51
39:JF:89:PRO:O	39:JF:92:THR:OG1	2.24	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:DI:50:GLY:HA2	66:D3:397:A:H4'	1.92	0.51
55:DL:26:LYS:HZ2	55:DL:30:ARG:HH22	1.57	0.51
56:DN:70:LYS:HB2	56:DN:73:ARG:HE	1.74	0.51
57:DO:47:LYS:NZ	57:DO:66:ASP:OD2	2.42	0.51
65:D2:21:A:H2'	65:D2:22:A:H8	1.73	0.51
66:D3:429:G:H2'	66:D3:430:G:C8	2.45	0.51
66:D3:1679:G:H2'	66:D3:1722:A:H61	1.76	0.51
4:UD:248:PRO:HD2	4:UD:292:ASN:HD21	1.76	0.51
4:UD:625:GLU:HG3	4:UD:734:PHE:HE2	1.74	0.51
5:UE:182:MET:CG	5:UE:183:THR:N	2.72	0.51
8:UH:574:ARG:HD2	8:UH:578:LEU:HD12	1.93	0.51
12:UL:162:HIS:ND1	12:UL:181:SER:OG	2.44	0.51
12:UL:270:SER:HB3	12:UL:286:ILE:HD11	1.92	0.51
12:UL:582:SER:OG	12:UL:583:PHE:N	2.43	0.51
13:UM:116:LEU:HD12	13:UM:128:VAL:HG22	1.93	0.51
13:UM:279:LYS:NZ	13:UM:317:GLU:O	2.44	0.51
13:UM:458:SER:OG	13:UM:460:ASP:O	2.27	0.51
17:UQ:768:TRP:CZ3	17:UQ:770:TYR:HA	2.46	0.51
18:UR:389:SER:O	18:UR:389:SER:OG	2.28	0.51
21:UU:632:VAL:HG13	21:UU:641:LEU:HD11	1.93	0.51
22:UV:1031:ASP:OD2	22:UV:1035:THR:N	2.43	0.51
34:CM:246:VAL:HA	34:CM:256:TYR:O	2.10	0.51
52:DH:44:LYS:HG3	52:DH:63:PRO:HD3	1.93	0.51
52:DH:161:GLN:HA	52:DH:164:TYR:CZ	2.46	0.51
62:DY:27:VAL:O	62:DY:68:LYS:N	2.43	0.51
66:D3:322:G:O6	66:D3:343:C:N4	2.43	0.51
66:D3:501:U:O2'	66:D3:502:U:OP2	2.28	0.51
4:UD:637:PHE:HE2	4:UD:744:VAL:HG12	1.75	0.51
5:UE:334:TRP:CD1	5:UE:335:ASN:HB2	2.46	0.51
10:UJ:550:TYR:O	10:UJ:553:SER:C	2.48	0.51
13:UM:235:LYS:NZ	13:UM:272:SER:O	2.40	0.51
13:UM:679:THR:HG21	13:UM:723:GLU:HB2	1.91	0.51
19:US:447:ASP:OD1	19:US:448:VAL:N	2.43	0.51
21:UU:264:LEU:O	21:UU:275:PHE:HA	2.11	0.51
29:CH:343:ASP:OD2	29:CH:345:THR:OG1	2.28	0.51
36:JA:567:LEU:HD22	36:JA:653:ALA:HB2	1.93	0.51
55:DL:75:VAL:HA	55:DL:86:ILE:HA	1.93	0.51
66:D3:90:C:H2'	66:D3:91:G:H8	1.75	0.51
2:UB:515:HIS:HD2	2:UB:518:ILE:H	1.58	0.51
6:UF:125:SER:HB2	6:UF:128:LYS:H	1.75	0.51
7:UG:511:GLU:OE1	7:UG:515:ARG:NH2	2.43	0.51



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
12:UL:129:PHE:HB3	12:UL:136:LEU:HD12	1.92	0.51
12:UL:574:LEU:HD12	12:UL:594:ASP:HB3	1.93	0.51
18:UR:334:SER:N	18:UR:335:GLN:OE1	2.44	0.51
22:UV:236:THR:HG22	22:UV:268:LEU:HD22	1.93	0.51
26:CD:185:ASP:OD2	26:CD:285:ARG:NH2	2.41	0.51
29:CH:194:LEU:HD11	29:CH:238:GLU:H	1.74	0.51
30:CI:82:LEU:HD22	30:CI:87:VAL:HG21	1.93	0.51
36:JA:862:LEU:O	36:JA:866:TYR:HB2	2.10	0.51
36:JB:427:ILE:O	36:JB:430:LEU:C	2.48	0.51
38:JE:296:ARG:HH22	62:DY:70:VAL:HG22	1.75	0.51
39:JF:41:MET:O	39:JF:110:LEU:HA	2.10	0.51
39:JG:45:LEU:HD12	39:JG:114:ILE:HG12	1.92	0.51
46:JP:436:SER:OG	46:JP:440:ARG:NH1	2.44	0.51
49:DE:183:VAL:HG13	49:DE:190:GLY:H	1.74	0.51
51:DG:48:TYR:OH	51:DG:119:GLN:O	2.24	0.51
60:DW:30:SER:OG	60:DW:31:SER:N	2.44	0.51
66:D3:575:C:O2'	66:D3:576:G:O5'	2.28	0.51
66:D3:1122:G:C2	66:D3:1123:C:H1'	2.46	0.51
5:UE:443:GLN:HE22	19:US:333:GLU:H	1.58	0.51
7:UG:106:LEU:O	7:UG:397:GLY:HA3	2.11	0.51
13:UM:487:ARG:HE	13:UM:523:GLY:HA3	1.76	0.51
13:UM:747:ASN:O	13:UM:747:ASN:ND2	2.44	0.51
15:UO:260:TYR:OH	15:UO:262:GLU:OE1	2.23	0.51
15:UO:375:HIS:NE2	15:UO:377:ASP:OD2	2.38	0.51
17:UQ:711:ILE:HG12	17:UQ:721:ALA:HA	1.92	0.51
22:UV:130:LYS:HE3	22:UV:134:ILE:HD11	1.92	0.51
22:UV:606:ASN:HB2	22:UV:608:PHE:HD2	1.75	0.51
22:UV:716:SER:O	22:UV:719:THR:OG1	2.23	0.51
22:UV:1220:PHE:HA	22:UV:1223:ILE:HD12	1.91	0.51
28:CG:7:LYS:NZ	29:CH:463:GLN:HE21	2.09	0.51
29:CH:485:ASN:HA	29:CH:501:ILE:HD12	1.93	0.51
33·CL·86·ILE·HD11	33·CL:117·PHE·HB3	1.00	0.51
36.1A.730.THB.HG23	36:1A:733:LEU:H	1.23	0.51
38. IE: 250: ABG: NH1	38. IE: 255: GLN·H	2.08	0.51
66·D3·1777·G·H2'	66·D3·1778·G·C8	2.00	0.51
67·D4·312·U·H2'	67:D4:313:A:C8	2.10	0.51
1.UA:16:ABC:NH2	$1 \cdot \text{II} \Delta \cdot 345 \cdot \text{PHE} \cdot \text{HB}2$	2.10	0.51
1.UA.311.ASN.HD99	41. II.273. ARC. NH2	2.25	0.51
7.U.G.189.THR.O	7.UC.182.THR.OC1	2.00	0.51
7.UC.240.LEU.HD12	7.UC.250.TRP.CD1	2.25	0.51
$13 \cdot \text{UM} \cdot 544 \cdot \text{TVR} \cdot \text{HR9}$	13·UM·587·CI N·HC2	1 03	0.51



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:621:TRP:HH2	48:DA:14:LYS:HA	1.76	0.51
15:UO:53:HIS:O	15:UO:68:SER:CB	2.57	0.51
22:UV:683:ASN:HA	22:UV:696:ILE:HG13	1.93	0.51
24:UZ:187:THR:OG1	24:UZ:188:SER:N	2.42	0.51
30:CI:137:ARG:HA	30:CI:142:LEU:HA	1.92	0.51
33:CL:1081:SER:O	33:CL:1081:SER:OG	2.21	0.51
46:JP:237:SER:OG	46:JP:238:THR:N	2.43	0.51
51:DG:5:ILE:HA	51:DG:111:LEU:O	2.11	0.51
1:UA:664:SER:OG	32:CK:450:VAL:O	2.20	0.51
12:UL:281:ILE:HG22	12:UL:332:ILE:HB	1.93	0.51
13:UM:561:SER:HB3	13:UM:564:THR:HG22	1.93	0.51
15:UO:220:ALA:HA	15:UO:226:ILE:HG22	1.93	0.51
19:US:251:SER:HA	19:US:254:LYS:HG2	1.93	0.51
21:UU:308:PRO:HB2	21:UU:324:PHE:HB2	1.93	0.51
23:UX:79:LYS:NZ	60:DW:94:LEU:O	2.32	0.51
28:CG:95:ARG:HG2	67:D4:254:A:OP2	2.10	0.51
30:CI:15:LYS:HB2	67:D4:24:U:H5	1.76	0.51
35:CN:11:ASN:O	35:CN:40:LYS:NZ	2.44	0.51
37:JC:278:ILE:O	37:JC:289:ILE:HB	2.10	0.51
41:JJ:112:SER:O	41:JJ:112:SER:OG	2.25	0.51
43:JM:127:ARG:HA	43:JM:130:LEU:HD23	1.92	0.51
48:DA:104:ASP:OD1	48:DA:105:PHE:N	2.44	0.51
53:DI:8:ARG:NH2	53:DI:22:ARG:H	2.09	0.51
55:DL:45:PRO:HB2	55:DL:47:THR:HG22	1.93	0.51
65:D2:210:U:H2'	65:D2:211:G:H8	1.75	0.51
1:UA:711:LEU:HD12	1:UA:712:PHE:H	1.76	0.50
4:UD:206:SER:O	4:UD:206:SER:OG	2.28	0.50
7:UG:23:ARG:NH2	46:JP:36:GLU:OE2	2.43	0.50
12:UL:149:ASP:OD1	12:UL:149:ASP:N	2.41	0.50
12:UL:263:THR:OG1	12:UL:264:ASN:N	2.44	0.50
13:UM:584:ILE:HG21	13:UM:589:GLN:N	2.26	0.50
17:UQ:330:SER:OG	17:UQ:331:GLN:N	2.44	0.50
17:UQ:722:LEU:HD13	17:UQ:743:ILE:HG22	1.93	0.50
18:UR:550:SER:O	18:UR:550:SER:OG	2.28	0.50
21:UU:382:LYS:NZ	65:D2:293:U:OP1	2.41	0.50
24:UZ:181:ARG:NH1	47:JQ:201:ASP:O	2.44	0.50
28:CG:37:ALA:HB2	28:CG:98:ILE:HD11	1.92	0.50
33:CL:313:TYR:O	33:CL:317:LEU:HB2	2.10	0.50
35:CN:144:TYR:OH	35:CN:156:PHE:N	2.37	0.50
36:JA:45:MET:O	36:JA:48:ASP:C	2.49	0.50
36:JA:55:VAL:HG23	36:JA:121:MET:HB3	1.93	0.50



A + a 1	A + ama - D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
38:JE:296:ARG:HH12	62:DY:70:VAL:HG22	1.76	0.50
44:JN:226:ASP:N	44:JN:226:ASP:OD1	2.44	0.50
48:DA:16:GLN:OE1	66:D3:912:U:N3	2.44	0.50
53:DI:34:ALA:HB2	53:DI:56:ARG:HD3	1.92	0.50
53:DI:62:THR:HA	53:DI:76:THR:O	2.10	0.50
54:DJ:35:GLY:O	54:DJ:110:GLN:NE2	2.43	0.50
55:DL:47:THR:HG23	55:DL:114:ALA:HB1	1.92	0.50
56:DN:49:GLN:HA	56:DN:52:VAL:HG12	1.93	0.50
4:UD:92:GLU:OE2	4:UD:430:THR:OG1	2.25	0.50
13:UM:197:ASP:OD1	13:UM:197:ASP:N	2.43	0.50
13:UM:291:ILE:HG23	13:UM:307:SER:HB2	1.94	0.50
17:UQ:265:ASP:OD2	17:UQ:270:GLN:N	2.44	0.50
17:UQ:371:PHE:HB2	17:UQ:385:ILE:HB	1.92	0.50
21:UU:414:ILE:HG12	21:UU:434:HIS:HD1	1.76	0.50
24:UZ:172:ASP:OD1	24:UZ:172:ASP:N	2.45	0.50
29:CH:116:ILE:O	29:CH:119:SER:OG	2.24	0.50
29:CH:549:LEU:HB2	29:CH:552:TRP:CZ3	2.46	0.50
32:CK:497:ASN:OD1	32:CK:497:ASN:N	2.45	0.50
36:JA:31:ASP:N	36:JA:203:ASP:OD2	2.44	0.50
36:JA:775:VAL:HG13	36:JA:812:GLN:HA	1.93	0.50
49:DE:188:ASN:HA	49:DE:191:ARG:HH21	1.77	0.50
52:DH:84:LYS:HG2	52:DH:85:PHE:CD1	2.46	0.50
62:DY:27:VAL:O	62:DY:68:LYS:HA	2.11	0.50
1:UA:310:VAL:HG12	1:UA:317:LEU:HG	1.93	0.50
2:UB:484:ARG:HB3	2:UB:492:ALA:HB1	1.93	0.50
4:UD:644:SER:OG	4:UD:658:ASP:OD1	2.17	0.50
12:UL:262:ILE:O	12:UL:270:SER:OG	2.26	0.50
17:UQ:459:ILE:HD12	17:UQ:469:ASN:HB3	1.93	0.50
19:US:296:MET:HG3	19:US:326:LEU:HD22	1.94	0.50
19:US:341:LEU:HD11	19:US:365:PHE:HD2	1.76	0.50
21:UU:611:THR:HB	21:UU:621:ASP:HB3	1.91	0.50
22:UV:803:LYS:NZ	22:UV:859:ASP:OD1	2.31	0.50
24:UZ:135:LEU:HD21	24:UZ:139:LEU:HD23	1.92	0.50
25:CA:110:ASN:OD1	25:CA:111:MET:N	2.45	0.50
33:CL:1025:GLU:OE1	33:CL:1025:GLU:N	2.45	0.50
34:CM:183:ILE:O	34:CM:312:ARG:NH1	2.44	0.50
36:JA:783:LYS:HA	36:JA:786:LEU:HD12	1.94	0.50
42:JK:474:ASN:HA	42:JK:477:ALA:HB3	1.92	0.50
52:DH:130:VAL:O	52:DH:133:THR:OG1	2.22	0.50
66:D3:107:C:H2'	66:D3:108:A:C8	2.46	0.50
2:UB:437:SER:O	2:UB:495:ASN:ND2	2.45	0.50



A 4 a 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:UD:149:ILE:HG22	4:UD:156:LEU:HB3	1.92	0.50
4:UD:565:ARG:HH12	10:UJ:635:TYR:H	1.60	0.50
8:UH:544:LEU:HB3	8:UH:551:PHE:HD1	1.76	0.50
13:UM:547:LEU:HD11	13:UM:568:MET:HG3	1.94	0.50
21:UU:51:VAL:HG11	21:UU:90:VAL:HG21	1.93	0.50
28:CG:95:ARG:HG3	28:CG:96:PRO:HD2	1.93	0.50
33:CL:830:ARG:HB3	33:CL:880:TYR:CD1	2.46	0.50
35:CN:20:LEU:HD12	35:CN:33:SER:HB2	1.92	0.50
61:DX:51:GLY:O	61:DX:101:GLU:HA	2.12	0.50
66:D3:505:A:N6	66:D3:585:A:O2'	2.44	0.50
67:D4:258:U:H2'	67:D4:259:C:C6	2.47	0.50
1:UA:758:ILE:HD11	1:UA:798:TRP:HZ2	1.76	0.50
2:UB:515:HIS:HB3	2:UB:518:ILE:HB	1.93	0.50
4:UD:116:SER:HB3	4:UD:126:TRP:HE1	1.77	0.50
4:UD:485:LYS:HD2	4:UD:499:ASP:HA	1.94	0.50
4:UD:535:GLU:O	4:UD:541:ALA:HA	2.11	0.50
5:UE:495:GLN:O	5:UE:499:ASN:CB	2.59	0.50
6:UF:198:ASN:HA	6:UF:201:LYS:HG2	1.91	0.50
12:UL:269:THR:OG1	12:UL:288:LYS:NZ	2.42	0.50
13:UM:269:LEU:HD23	13:UM:279:LYS:HD3	1.92	0.50
18:UR:436:ASP:O	18:UR:441:GLY:HA2	2.11	0.50
21:UU:459:ASP:N	21:UU:459:ASP:OD1	2.45	0.50
49:DE:151:ASP:OD2	51:DG:215:ARG:NH1	2.45	0.50
66:D3:300:A:H2'	66:D3:301:A:C8	2.47	0.50
66:D3:458:G:H2'	66:D3:460:A:C8	2.47	0.50
1:UA:130:ASP:N	1:UA:130:ASP:OD1	2.42	0.50
12:UL:245:MET:N	12:UL:245:MET:SD	2.85	0.50
15:UO:126:PRO:O	15:UO:145:ASP:N	2.44	0.50
17:UQ:295:TRP:CH2	17:UQ:320:VAL:HG21	2.47	0.50
21:UU:631:ASN:HB2	21:UU:644:THR:HG22	1.93	0.50
28:CG:50:GLU:OE2	28:CG:104:THR:HA	2.12	0.50
33:CL:553:ILE:HG12	34:CM:323:ILE:HD12	1.93	0.50
37:JC:147:ASN:HB3	37:JC:152:ASP:HB2	1.94	0.50
37:JC:238:ASN:HB2	37:JC:279:TRP:CZ2	2.47	0.50
44:JN:102:PRO:O	44:JN:106:TYR:N	2.43	0.50
46:JP:228:ASN:N	46:JP:228:ASN:OD1	2.41	0.50
1:UA:260:GLN:NE2	65:D2:330:C:C6	2.80	0.50
1:UA:309:SER:OG	1:UA:310:VAL:N	2.44	0.50
4:UD:71:ARG:HB2	4:UD:75:ASN:HB2	1.94	0.50
4:UD:92:GLU:HB2	4:UD:428:ILE:HB	1.93	0.50
4:UD:258:SER:O	4:UD:258:SER:OG	2.30	0.50



Atom-1	Atom-2	Interatomic	Clash
	1100m =	distance (Å)	overlap (Å)
10:UJ:407:PHE:O	10:UJ:410:ILE:C	2.50	0.50
12:UL:212:VAL:HG22	12:UL:217:LEU:HD13	1.94	0.50
12:UL:259:ILE:HA	12:UL:273:TYR:O	2.12	0.50
15:UO:319:VAL:HG12	15:UO:329:ILE:HG12	1.93	0.50
21:UU:639:ASP:OD1	21:UU:659:GLN:NE2	2.40	0.50
26:CD:48:ILE:HD11	26:CD:127:LEU:HD13	1.94	0.50
38:JE:247:GLU:OE2	54:DJ:78:ARG:NH1	2.34	0.50
45:JO:291:ARG:NH2	66:D3:316:A:H5"	2.27	0.50
66:D3:182:A:H2'	66:D3:183:U:C6	2.47	0.50
1:UA:730:LEU:HD11	1:UA:754:VAL:HG22	1.94	0.50
2:UB:554:GLN:HE22	2:UB:559:ARG:HD2	1.77	0.50
6:UF:197:ILE:HG22	6:UF:201:LYS:NZ	2.27	0.50
12:UL:641:TYR:O	12:UL:650:ILE:N	2.44	0.50
13:UM:308:ASP:OD2	13:UM:310:THR:OG1	2.29	0.50
17:UQ:244:ILE:HD12	17:UQ:283:VAL:HG11	1.94	0.50
17:UQ:360:MET:HB3	17:UQ:368:ASP:HB2	1.94	0.50
19:US:253:PHE:HA	19:US:256:ASN:HD22	1.77	0.50
22:UV:887:ALA:O	22:UV:892:SER:OG	2.29	0.50
24:UZ:228:LYS:HB2	24:UZ:232:GLY:HA3	1.94	0.50
27:CE:226:ILE:HG13	27:CE:227:LEU:HD12	1.92	0.50
30:CI:71:ARG:CZ	31:CJ:61:SER:HB2	2.42	0.50
33:CL:798:MET:SD	33:CL:802:LYS:NZ	2.75	0.50
48:DA:62:LYS:NZ	48:DA:89:ASP:O	2.39	0.50
50:DF:100:ASN:O	50:DF:103:ASN:N	2.41	0.50
51:DG:142:ARG:HA	51:DG:147:LEU:HD12	1.94	0.50
52:DH:99:LEU:HB2	52:DH:116:ARG:HB3	1.94	0.50
60:DW:77:PRO:O	60:DW:79:PHE:N	2.44	0.50
66:D3:153:G:H2'	66:D3:154:G:H8	1.77	0.50
66:D3:311:U:H3	66:D3:355:G:H1	1.60	0.50
1:UA:27:LYS:HG2	1:UA:43:ILE:CD1	2.42	0.50
7:UG:190:HIS:HD1	7:UG:207:THR:HG21	1.77	0.50
17:UQ:202:SER:OG	17:UQ:203:SER:N	2.44	0.50
17:UQ:583:LYS:HD3	17:UQ:596:LEU:HD21	1.93	0.50
29:CH:257:ASP:N	29:CH:257:ASP:OD1	2.37	0.50
37:JC:237:ARG:HD3	37:JC:288:LYS:NZ	2.27	0.50
37:JC:352:TRP:CE3	37:JC:353:CYS:HB2	2.46	0.50
51:DG:186:ARG:NH2	66:D3:269:G:OP2	2.45	0.50
66:D3:78:A:H2'	66:D3:79:C:C6	2.46	0.50
66:D3:107:C:H2'	66:D3:108:A:H8	1.77	0.50
8:UH:669:ALA:O	8:UH:673:THR:HG23	2.12	0.49
10:UJ:345:ASP:OD1	10:UJ:346:LYS:N	2.44	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:UJ:345:ASP:O	10:UJ:349:THR:HG22	2.11	0.49
12:UL:127:LEU:HD12	12:UL:136:LEU:HD11	1.93	0.49
13:UM:209:LEU:HD23	13:UM:225:PHE:CD2	2.46	0.49
43:JM:112:ASN:O	43:JM:114:ARG:NE	2.43	0.49
1:UA:344:HIS:NE2	1:UA:366:ASP:OD2	2.31	0.49
1:UA:735:PHE:HD2	1:UA:758:ILE:HG22	1.77	0.49
7:UG:127:ILE:HD13	7:UG:398:ILE:HD11	1.94	0.49
7:UG:498:ARG:HH22	7:UG:502:ARG:NH1	2.07	0.49
8:UH:272:PHE:HA	8:UH:280:GLN:H	1.76	0.49
10:UJ:353:ARG:NE	10:UJ:386:ASP:OD2	2.40	0.49
12:UL:335:LEU:HB3	12:UL:336:TYR:CD2	2.47	0.49
12:UL:400:SER:O	12:UL:404:LYS:HB3	2.11	0.49
12:UL:748:ALA:HB1	12:UL:812:ILE:HG13	1.94	0.49
13:UM:782:VAL:O	13:UM:786:ILE:HD12	2.11	0.49
17:UQ:438:THR:OG1	17:UQ:439:ASN:N	2.44	0.49
18:UR:391:SER:O	18:UR:391:SER:OG	2.26	0.49
22:UV:777:ASP:OD1	22:UV:777:ASP:N	2.40	0.49
23:UX:87:MET:HG3	23:UX:92:ALA:O	2.12	0.49
27:CE:385:ASP:N	27:CE:385:ASP:OD1	2.44	0.49
29:CH:285:SER:HB2	29:CH:298:SER:HB3	1.94	0.49
30:CI:33:MET:HG2	30:CI:38:ILE:HG13	1.93	0.49
33:CL:625:TRP:C	33:CL:627:SER:N	2.65	0.49
44:JN:195:ILE:HG13	44:JN:196:VAL:H	1.76	0.49
62:DY:57:VAL:O	62:DY:94:TYR:OH	2.29	0.49
66:D3:1735:U:O5'	66:D3:1735:U:H6	1.95	0.49
1:UA:192:ASP:HB2	1:UA:212:ASP:HB2	1.95	0.49
4:UD:231:VAL:HG22	4:UD:265:TRP:CH2	2.45	0.49
4:UD:760:LEU:HD11	4:UD:766:GLN:HB2	1.93	0.49
5:UE:460:ARG:NE	65:D2:112:U:O2'	2.45	0.49
10:UJ:167:PHE:HA	27:CE:407:ARG:HH12	1.76	0.49
12:UL:332:ILE:HG12	12:UL:379:PRO:HG3	1.93	0.49
13:UM:420:ASN:HB2	13:UM:423:LYS:NZ	2.28	0.49
13:UM:443:PRO:HD3	13:UM:499:VAL:HG11	1.94	0.49
14:UN:303:GLN:O	14:UN:307:ARG:HG2	2.12	0.49
18:UR:167:GLN:HG2	65:D2:309:A:C2	2.47	0.49
19:US:303:TYR:CZ	19:US:320:LEU:HD13	2.47	0.49
25:CA:228:GLN:O	25:CA:231:ARG:NH2	2.38	0.49
28:CG:26:GLN:HG3	54:DJ:154:LYS:HZ1	1.77	0.49
29:CH:180:LYS:O	29:CH:184:ARG:NH1	2.45	0.49
31:CJ:28:LYS:HG2	31:CJ:46:LEU:HD21	1.94	0.49
35:CN:178:ASP:OD1	35:CN:179:TYR:N	2.46	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
36:JA:187:ARG:NH1	36:JA:489:LEU:O	2.45	0.49
36:JA:826:THR:HG22	36:JA:828:THR:H	1.77	0.49
36:JA:894:ASN:HB3	36:JA:897:THR:HG23	1.93	0.49
37:JC:183:VAL:HG13	37:JC:199:THR:HG22	1.94	0.49
41:JJ:204:ARG:NH1	41:JJ:250:LEU:O	2.45	0.49
51:DG:102:VAL:HG21	51:DG:109:LEU:HD21	1.94	0.49
56:DN:48:SER:OG	56:DN:86:GLU:OE2	2.28	0.49
65:D2:123:C:H3'	65:D2:124:A:C8	2.47	0.49
4:UD:130:THR:HG23	4:UD:132:LEU:H	1.76	0.49
8:UH:561:LEU:HB3	8:UH:566:LEU:HD22	1.93	0.49
11:UK:64:TYR:CD2	33:CL:1079:PHE:HD2	2.30	0.49
12:UL:45:ALA:N	12:UL:48:ASP:O	2.45	0.49
12:UL:432:TYR:HB3	12:UL:450:ARG:HG2	1.93	0.49
12:UL:673:VAL:HG22	12:UL:683:ILE:HG12	1.95	0.49
13:UM:227:MET:N	13:UM:227:MET:SD	2.86	0.49
24:UZ:66:LYS:O	24:UZ:69:ASP:N	2.44	0.49
26:CD:8:LEU:HD11	26:CD:78:LEU:HD11	1.93	0.49
26:CD:67:ASN:O	26:CD:70:SER:OG	2.26	0.49
34:CM:118:PHE:HB2	34:CM:166:VAL:HG22	1.95	0.49
36:JA:614:ILE:HD13	36:JA:617:LEU:HD21	1.94	0.49
48:DA:53:GLY:HA3	48:DA:56:SER:HB2	1.93	0.49
65:D2:528:G:H2'	65:D2:529:A:C8	2.47	0.49
3:UC:592:GLU:HG2	3:UC:593:GLY:H	1.76	0.49
4:UD:61:THR:HG21	4:UD:681:ILE:HG21	1.93	0.49
7:UG:449:ILE:HD12	14:UN:842:TYR:HB3	1.93	0.49
8:UH:548:PRO:O	8:UH:576:ARG:NH2	2.45	0.49
12:UL:392:THR:HG22	12:UL:393:ASP:H	1.78	0.49
18:UR:404:ILE:H	18:UR:404:ILE:HD12	1.77	0.49
21:UU:455:PHE:CB	21:UU:477:ILE:HD11	2.42	0.49
23:UX:109:LEU:HB3	23:UX:113:TYR:CD2	2.48	0.49
34:CM:83:GLY:HA3	34:CM:114:PHE:HE1	1.78	0.49
36:JA:822:ASN:HD22	36:JA:869:ASP:H	1.60	0.49
46:JP:314:SER:HA	46:JP:356:TYR:CD2	2.48	0.49
49:DE:130:GLN:HB3	49:DE:138:TYR:CZ	2.48	0.49
58:DQ:38:LEU:HA	58:DQ:45:ARG:HH12	1.76	0.49
66:D3:1580:C:H2'	66:D3:1581:C:H6	1.76	0.49
1:UA:349:ASN:HA	1:UA:682:THR:HG21	1.93	0.49
1:UA:633:LYS:NZ	65:D2:293:U:O4	2.40	0.49
2:UB:578:GLU:OE1	2:UB:674:LYS:NZ	2.39	0.49
4:UD:579:ARG:NH1	4:UD:644:SER:OG	2.44	0.49
7:UG:456:SER:OG	7:UG:457:SER:N	2.46	0.49



	A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
19:US:195:PHE:HE2	19:US:222:LEU:HD21	1.78	0.49
23:UX:118:LYS:NZ	46:JP:68:ASP:OD1	2.44	0.49
24:UZ:65:PHE:HD2	24:UZ:70:LEU:HD21	1.76	0.49
24:UZ:77:LYS:O	24:UZ:102:SER:OG	2.29	0.49
28:CG:28:ALA:HB2	28:CG:33:LEU:HD23	1.94	0.49
34:CM:193:GLY:HA3	34:CM:245:LEU:HD13	1.93	0.49
37:JC:112:THR:HG23	37:JC:128:LYS:HB3	1.95	0.49
49:DE:179:LYS:H	49:DE:195:ILE:HG12	1.77	0.49
66:D3:450:U:H3	66:D3:456:A:H61	1.60	0.49
66:D3:1114:G:H1	67:D4:10:C:N4	2.05	0.49
66:D3:1671:A:H3'	66:D3:1672:G:H8	1.77	0.49
1:UA:782:ILE:O	1:UA:786:ALA:CB	2.61	0.49
2:UB:518:ILE:O	2:UB:522:LEU:N	2.42	0.49
5:UE:365:SER:OG	5:UE:366:GLY:N	2.45	0.49
6:UF:28:GLU:OE1	6:UF:28:GLU:N	2.46	0.49
12:UL:234:GLU:HB3	12:UL:240:GLY:HA3	1.94	0.49
13:UM:403:ILE:HB	13:UM:415:TRP:HB2	1.95	0.49
17:UQ:87:SER:O	17:UQ:112:ASN:N	2.46	0.49
19:US:487:PRO:HB2	39:JG:24:VAL:HG22	1.95	0.49
21:UU:523:ASP:OD1	21:UU:523:ASP:N	2.27	0.49
36:JA:662:GLU:HG2	36:JA:766:LEU:O	2.12	0.49
38:JE:324:ASP:OD1	38:JE:324:ASP:N	2.41	0.49
49:DE:103:TYR:O	49:DE:182:TYR:OH	2.29	0.49
53:DI:41:LYS:NZ	66:D3:260:U:OP1	2.37	0.49
55:DL:85:VAL:HG12	55:DL:108:PRO:HB3	1.95	0.49
55:DL:94:ILE:O	55:DL:98:ASN:N	2.45	0.49
65:D2:516:U:N3	65:D2:519:A:OP2	2.44	0.49
1:UA:27:LYS:CD	1:UA:43:ILE:HD12	2.43	0.49
4:UD:275:SER:O	4:UD:275:SER:OG	2.28	0.49
4:UD:614:TRP:O	4:UD:618:ASN:CB	2.50	0.49
7:UG:192:GLU:OE1	7:UG:194:ARG:NH1	2.46	0.49
9:UI:418:LYS:HA	9:UI:421:LEU:HD12	1.94	0.49
17:UQ:40:ASP:O	17:UQ:42:ARG:N	2.46	0.49
18:UR:41:ASN:O	18:UR:41:ASN:ND2	2.41	0.49
18:UR:350:SER:O	18:UR:380:ASN:ND2	2.45	0.49
23:UX:19:THR:O	23:UX:19:THR:OG1	2.28	0.49
25:CB:258:HIS:ND1	25:CB:320:TYR:OH	2.35	0.49
45:JO:295:ARG:HH12	66:D3:317:C:P	2.36	0.49
46:JP:244:ILE:HB	46:JP:258:ILE:HG22	1.94	0.49
61:DX:43:PHE:CD1	61:DX:49:ALA:HB2	2.47	0.49
66:D3:90:C:H2'	66:D3:91:G:C8	2.48	0.49



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
66:D3:1057:U:O2'	66:D3:1058:U:O5'	2.27	0.49
66:D3:1124:A:H1'	67:D4:1:G:H22	1.78	0.49
67:D4:199:G:H2'	67:D4:200:C:H6	1.78	0.49
13:UM:557:VAL:HB	13:UM:571:LEU:HB2	1.94	0.49
17:UQ:866:LEU:HD13	18:UR:231:LYS:HE3	1.94	0.49
30:CI:156:ASP:OD1	31:CJ:7:ARG:NH1	2.45	0.49
33:CL:837:LYS:NZ	66:D3:579:A:OP2	2.45	0.49
35:CN:17:PRO:HB3	35:CN:34:LEU:HB3	1.95	0.49
36:JA:659:ASP:O	36:JA:663:GLY:C	2.51	0.49
37:JC:63:LYS:HB3	37:JC:104:PHE:CE2	2.48	0.49
38:JE:341:ARG:HH22	38:JE:344:LYS:HE2	1.77	0.49
39:JF:123:GLU:HG3	39:JF:161:LYS:HB2	1.95	0.49
43:JM:60:LYS:NZ	65:D2:553:A:OP1	2.45	0.49
53:DI:83:TYR:HB3	53:DI:101:ILE:HB	1.94	0.49
54:DJ:38:ASN:HB3	54:DJ:40:LYS:H	1.76	0.49
58:DQ:94:GLN:HG3	58:DQ:102:LYS:HE2	1.95	0.49
65:D2:182:G:N2	65:D2:215:U:O2	2.35	0.49
66:D3:527:A:H2'	66:D3:528:U:C6	2.47	0.49
66:D3:679:U:H2'	66:D3:680:U:C2	2.48	0.49
66:D3:1782:A:OP2	66:D3:1783:C:N4	2.46	0.49
67:D4:199:G:H1	67:D4:250:C:H42	1.60	0.49
4:UD:769:PHE:HE1	16:UP:211:LEU:HD12	1.78	0.49
5:UE:92:ALA:O	5:UE:94:GLU:N	2.46	0.49
12:UL:553:ASN:OD1	12:UL:553:ASN:N	2.44	0.49
13:UM:209:LEU:CB	13:UM:225:PHE:O	2.61	0.49
13:UM:397:THR:HB	13:UM:402:TRP:HB2	1.95	0.49
13:UM:803:SER:O	13:UM:803:SER:OG	2.24	0.49
22:UV:186:ILE:HG23	22:UV:346:LEU:HD13	1.93	0.49
26:CD:270:ASN:OD1	27:CE:271:GLN:NE2	2.35	0.49
33:CL:629:ASP:HA	33:CL:632:LYS:HZ1	1.76	0.49
37:JC:300:TRP:HA	37:JC:307:ALA:HA	1.94	0.49
52:DH:114:ARG:HA	52:DH:117:THR:HG23	1.95	0.49
61:DX:89:ASN:O	61:DX:92:CYS:N	2.46	0.49
66:D3:50:C:H2'	66:D3:51:A:C8	2.48	0.49
66:D3:450:U:H2'	66:D3:451:A:C8	2.48	0.49
66:D3:502:U:H2'	66:D3:503:G:C8	2.48	0.49
66:D3:1211:A:H2'	66:D3:1212:G:C8	2.48	0.49
1:UA:73:ILE:HG22	1:UA:74:ASP:O	2.13	0.48
8:UH:680:ASP:OD1	9:UI:483:LYS:NZ	2.29	0.48
11:UK:166:LEU:HD21	25:CB:91:HIS:HA	1.95	0.48
15:UO:255:VAL:HA	15:UO:276:SER:HA	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
17:UQ:720:ILE:HG22	17:UQ:745:ILE:HG12	1.94	0.48
21:UU:438:LYS:HZ3	21:UU:462:PHE:HE1	1.59	0.48
27:CE:280:MET:HA	27:CE:283:ILE:HG22	1.95	0.48
29:CH:549:LEU:HB2	29:CH:552:TRP:HZ3	1.78	0.48
33:CL:114:ARG:HH11	33:CL:310:THR:HG23	1.78	0.48
36:JA:793:PHE:HB2	36:JA:796:PHE:CD1	2.48	0.48
51:DG:23:ARG:HG2	51:DG:41:VAL:HA	1.95	0.48
53:DI:65:PHE:O	53:DI:73:SER:HA	2.13	0.48
58:DQ:106:LYS:HG3	58:DQ:117:LEU:HD21	1.95	0.48
65:D2:141:A:H2	65:D2:143:A:H4'	1.78	0.48
1:UA:647:ALA:O	1:UA:656:ARG:HG2	2.13	0.48
2:UB:433:ILE:HG12	2:UB:455:LEU:HD13	1.95	0.48
5:UE:197:ILE:HG12	5:UE:241:ALA:HB2	1.94	0.48
6:UF:128:LYS:HE2	6:UF:128:LYS:HB2	1.61	0.48
7:UG:483:ILE:HD11	7:UG:515:ARG:HE	1.77	0.48
8:UH:585:ARG:NE	8:UH:589:ASP:OD2	2.37	0.48
10:UJ:85:VAL:HG13	46:JP:7:LYS:HB2	1.95	0.48
13:UM:464:LYS:NZ	13:UM:466:TRP:HB2	2.28	0.48
17:UQ:311:TYR:CE2	17:UQ:325:GLN:HB3	2.48	0.48
29:CH:188:TYR:HD2	29:CH:196:LEU:HD11	1.77	0.48
35:CN:130:ASP:OD1	35:CN:133:SER:N	2.39	0.48
39:JF:69:ASN:HB2	39:JF:72:ASP:HB2	1.95	0.48
40:JH:433:THR:HA	40:JH:465:SER:HA	1.94	0.48
54:DJ:93:LEU:HA	54:DJ:96:VAL:HG12	1.95	0.48
66:D3:113:U:H5"	66:D3:114:C:H5'	1.93	0.48
66:D3:1739:C:H2'	66:D3:1740:A:H8	1.78	0.48
1:UA:347:SER:OG	1:UA:365:GLU:HB2	2.13	0.48
1:UA:605:ASP:HB2	1:UA:612:LEU:HD11	1.95	0.48
4:UD:497:ILE:N	4:UD:509:GLN:O	2.43	0.48
8:UH:271:SER:N	8:UH:281:PHE:O	2.46	0.48
13:UM:290:ILE:HG22	13:UM:306:LEU:HG	1.95	0.48
19:US:179:GLU:O	19:US:183:LYS:HG2	2.13	0.48
27:CE:361:ARG:NH1	67:D4:83:A:OP2	2.46	0.48
29:CH:230:ASN:HB3	29:CH:275:PRO:HB3	1.94	0.48
31:CJ:212:ALA:HA	32:CK:383:ARG:NH1	2.28	0.48
36:JA:19:GLN:HE22	36:JA:219:LEU:HD12	1.78	0.48
39:JF:175:CYS:O	39:JF:177:LYS:NZ	2.47	0.48
39:JF:177:LYS:N	39:JF:222:ASP:OD2	2.40	0.48
46:JP:224:SER:HB3	46:JP:238:THR:HG22	1.95	0.48
50:DF:145:ASP:OD1	50:DF:146:THR:N	2.47	0.48
55:DL:68:GLY:HA3	55:DL:127:GLN:HE21	1.77	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:UA:563:ARG:NH2	67:D4:60:A:OP2	2.47	0.48
5:UE:105:TYR:HB2	5:UE:121:ASP:OD1	2.13	0.48
5:UE:128:GLN:OE1	5:UE:138:GLN:NE2	2.37	0.48
12:UL:655:ALA:HB3	12:UL:656:HIS:HD1	1.79	0.48
13:UM:130:ASP:OD2	13:UM:133:ASN:N	2.33	0.48
13:UM:409:ASP:HB3	13:UM:411:THR:HG22	1.96	0.48
18:UR:531:CYS:HB3	18:UR:543:LEU:HD23	1.95	0.48
29:CH:545:LYS:N	29:CH:561:ASN:OD1	2.42	0.48
34:CM:201:SER:HA	66:D3:1133:A:H2	1.78	0.48
39:JG:96:LEU:HD21	39:JG:114:ILE:HD11	1.94	0.48
49:DE:87:MET:N	49:DE:101:LEU:O	2.47	0.48
51:DG:50:PHE:HA	51:DG:112:VAL:O	2.13	0.48
1:UA:743:PHE:HZ	1:UA:778:ILE:HD13	1.77	0.48
24:UZ:83:TYR:OH	24:UZ:169:GLU:OE2	2.30	0.48
26:CD:186:LYS:HA	26:CD:189:ASN:HD21	1.79	0.48
27:CE:321:GLY:HA3	27:CE:341:LEU:HB2	1.96	0.48
29:CH:276:THR:HG21	29:CH:281:GLY:HA3	1.96	0.48
29:CH:344:ARG:HA	29:CH:402:ILE:HG13	1.96	0.48
31:CJ:219:GLU:O	31:CJ:237:VAL:HA	2.12	0.48
36:JA:77:ILE:HD11	36:JA:86:ARG:CZ	2.43	0.48
39:JG:152:SER:HB3	39:JG:159:LEU:HD21	1.95	0.48
65:D2:2:U:H2'	65:D2:3:G:C8	2.48	0.48
65:D2:210:U:H2'	65:D2:211:G:C8	2.48	0.48
1:UA:758:ILE:HD11	1:UA:798:TRP:CZ2	2.48	0.48
2:UB:419:LYS:HA	2:UB:422:LEU:HB2	1.95	0.48
10:UJ:329:THR:HA	10:UJ:332:ILE:HG22	1.95	0.48
13:UM:407:SER:OG	13:UM:409:ASP:N	2.39	0.48
15:UO:496:HIS:O	15:UO:499:LYS:HB3	2.13	0.48
17:UQ:88:ILE:HA	17:UQ:111:THR:HA	1.95	0.48
17:UQ:334:LEU:N	17:UQ:335:PRO:CD	2.76	0.48
22:UV:141:TRP:HZ3	22:UV:144:LYS:HB2	1.78	0.48
22:UV:181:PRO:HG2	22:UV:207:LEU:HD12	1.94	0.48
22:UV:345:TYR:OH	22:UV:472:THR:OG1	2.28	0.48
22:UV:649:TRP:HH2	22:UV:681:ILE:HD11	1.79	0.48
22:UV:1195:LYS:HZ2	22:UV:1197:ARG:HG2	1.77	0.48
25:CB:214:ARG:HB2	25:CB:217:ILE:HD12	1.95	0.48
29:CH:430:LYS:HB2	38:JE:256:PRO:HG3	1.96	0.48
31:CJ:150:THR:HA	31:CJ:167:LEU:O	2.13	0.48
36:JA:384:VAL:O	36:JA:406:VAL:HA	2.13	0.48
41:JJ:226:LEU:HD13	41:JJ:231:ILE:HG22	1.95	0.48
42:JK:487:ASP:HA	42:JK:490:ILE:HG12	1.95	0.48



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
48:DA:166:LYS:O	48:DA:170:GLU:HG2	2.13	0.48
66:D3:93:A:H61	66:D3:396:G:H1'	1.77	0.48
66:D3:539:G:N3	66:D3:540:G:N2	2.61	0.48
3:UC:504:ASP:HA	3:UC:507:ILE:HG12	1.96	0.48
4:UD:255:SER:O	4:UD:262:ILE:HA	2.13	0.48
12:UL:256:GLY:HA2	12:UL:276:ASN:HA	1.96	0.48
12:UL:406:LEU:HD11	12:UL:438:PHE:CD1	2.48	0.48
17:UQ:726:GLN:HB3	17:UQ:739:TYR:CE1	2.48	0.48
18:UR:415:SER:OG	18:UR:416:ARG:N	2.46	0.48
31:CJ:9:ARG:NH2	31:CJ:12:TYR:HD2	2.04	0.48
33:CL:548:ASN:OD1	33:CL:549:ILE:N	2.47	0.48
34:CM:188:ILE:HD11	34:CM:247:ALA:HB1	1.95	0.48
36:JA:660:TYR:OH	36:JA:715:GLN:O	2.30	0.48
39:JF:242:CYS:O	39:JF:245:ALA:N	2.45	0.48
45:JO:291:ARG:HH22	66:D3:316:A:H8	1.61	0.48
48:DA:88:VAL:HG11	48:DA:96:LEU:HD13	1.94	0.48
51:DG:73:ILE:O	51:DG:96:SER:HA	2.13	0.48
53:DI:22:ARG:HD2	53:DI:25:ARG:NE	2.26	0.48
55:DL:90:TYR:HE1	55:DL:105:LYS:HG3	1.79	0.48
66:D3:323:A:H61	66:D3:345:U:H3	1.62	0.48
66:D3:654:C:H42	66:D3:680:U:H3	1.61	0.48
1:UA:475:PRO:O	1:UA:492:SER:OG	2.32	0.48
4:UD:313:LYS:HZ2	4:UD:316:LYS:HD2	1.78	0.48
8:UH:571:PHE:HD2	8:UH:606:ASP:HB3	1.78	0.48
11:UK:46:SER:OG	11:UK:47:THR:N	2.47	0.48
13:UM:406:ALA:HB1	13:UM:437:VAL:HG13	1.96	0.48
13:UM:460:ASP:OD1	13:UM:460:ASP:N	2.39	0.48
17:UQ:105:HIS:ND1	17:UQ:122:LYS:HD2	2.28	0.48
19:US:194:TYR:O	19:US:197:SER:OG	2.27	0.48
33:CL:862:THR:HB	33:CL:872:LEU:HD11	1.94	0.48
36:JA:588:ILE:HG22	36:JA:635:ILE:HG13	1.96	0.48
37:JC:151:CYS:HB2	37:JC:167:LEU:HB2	1.95	0.48
41:JJ:148:ASP:N	41:JJ:148:ASP:OD1	2.44	0.48
46:JP:9:SER:OG	46:JP:11:ASP:OD1	2.28	0.48
46:JP:264:THR:HA	46:JP:281:ASN:HA	1.94	0.48
65:D2:502:G:H1	65:D2:535:G:N2	1.96	0.48
66:D3:514:G:N7	66:D3:537:G:N2	2.62	0.48
2:UB:515:HIS:HD2	2:UB:517:VAL:H	1.62	0.48
4:UD:545:ARG:O	4:UD:548:GLY:N	2.40	0.48
6:UF:197:ILE:HD13	6:UF:200:ARG:HD3	1.96	0.48
10:UJ:777:ASP:O	10:UJ:781:ASN:CB	2.61	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:159:LEU:HD23	12:UL:189:TRP:CD2	2.49	0.48
12:UL:531:THR:OG1	12:UL:532:ASP:OD1	2.20	0.48
19:US:333:GLU:OE2	19:US:334:TYR:N	2.46	0.48
19:US:386:LEU:O	19:US:390:SER:OG	2.19	0.48
21:UU:430:ILE:HB	21:UU:443:TRP:HB2	1.94	0.48
21:UU:456:ASP:OD1	21:UU:457:THR:N	2.47	0.48
28:CF:79:VAL:HG21	28:CF:121:ILE:HG12	1.96	0.48
33:CL:1072:ALA:O	33:CL:1076:GLU:HG2	2.13	0.48
37:JC:18:GLY:HA2	37:JC:337:PRO:HB2	1.96	0.48
37:JC:99:ALA:O	37:JC:118:GLN:NE2	2.45	0.48
38:JE:293:ASN:HA	49:DE:53:LYS:HE3	1.94	0.48
51:DG:35:GLU:OE2	51:DG:50:PHE:N	2.47	0.48
51:DG:83:CYS:SG	66:D3:162:A:H5"	2.53	0.48
62:DY:61:ARG:N	62:DY:70:VAL:O	2.40	0.48
2:UB:530:GLU:OE1	2:UB:531:GLN:NE2	2.36	0.48
2:UB:740:MET:HE1	59:DS:102:ALA:C	2.33	0.48
3:UC:547:ASN:HD22	33:CL:196:THR:HG21	1.78	0.48
10:UJ:19:ALA:HB1	10:UJ:25:ARG:HB2	1.96	0.48
12:UL:359:SER:OG	12:UL:391:ARG:O	2.31	0.48
13:UM:433:HIS:CD2	13:UM:435:ALA:H	2.32	0.48
13:UM:580:ARG:HB3	13:UM:593:CYS:SG	2.53	0.48
29:CH:217:GLY:H	29:CH:220:TYR:HE2	1.62	0.48
30:CI:168:LYS:HB3	30:CI:172:ARG:HH21	1.78	0.48
31:CJ:192:ASP:OD2	31:CJ:227:ARG:NH1	2.46	0.48
36:JA:789:LEU:HD23	36:JA:890:LEU:HG	1.95	0.48
37:JC:164:ARG:NH2	37:JC:174:ASN:HB3	2.29	0.48
51:DG:3:LEU:O	51:DG:15:THR:HA	2.14	0.48
51:DG:42:GLY:HA3	51:DG:45:PHE:CD2	2.47	0.48
53:DI:49:ARG:NH2	66:D3:398:G:O3'	2.46	0.48
56:DN:125:LEU:HD12	56:DN:125:LEU:HA	1.68	0.48
56:DN:146:ALA:HA	56:DN:149:LEU:HD12	1.95	0.48
7:UG:464:LYS:HZ1	66:D3:-2:A:H62	1.62	0.47
12:UL:98:TYR:O	12:UL:101:GLY:N	2.46	0.47
13:UM:281:THR:HG22	13:UM:327:ILE:HB	1.95	0.47
13:UM:571:LEU:HB3	13:UM:602:TRP:HZ2	1.79	0.47
15:UO:25:ARG:NH2	65:D2:100:G:N7	2.62	0.47
15:UO:69:ARG:HG3	15:UO:70:THR:HG23	1.95	0.47
17:UQ:661:THR:O	17:UQ:672:VAL:HA	2.14	0.47
21:UU:476:PHE:HD1	21:UU:476:PHE:H	1.62	0.47
21:UU:848:GLU:O	21:UU:851:SER:N	2.47	0.47
23:UX:121:ARG:NH1	46:JP:369:ASP:O	2.46	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
26:CD:399:VAL:O	26:CD:402:SER:OG	2.22	0.47
28:CG:10:PRO:HB2	28:CG:124:LEU:HD21	1.96	0.47
39:JG:90:ASP:OD1	39:JG:90:ASP:N	2.46	0.47
41:JJ:128:VAL:HG22	41:JJ:139:LEU:HG	1.96	0.47
41:JJ:196:ASP:OD1	41:JJ:196:ASP:N	2.47	0.47
47:JQ:184:TYR:OH	65:D2:254:C:OP2	2.28	0.47
49:DE:54:TYR:O	62:DY:15:ASN:ND2	2.45	0.47
51:DG:62:PRO:HG2	51:DG:97:VAL:HG23	1.94	0.47
1:UA:9:ASN:OD1	1:UA:10:LEU:N	2.46	0.47
4:UD:77:GLU:OE1	4:UD:79:TRP:NE1	2.37	0.47
4:UD:345:ASP:N	4:UD:345:ASP:OD1	2.47	0.47
5:UE:82:ASN:ND2	5:UE:84:GLU:OE2	2.47	0.47
7:UG:287:TYR:HD2	7:UG:288:TYR:CE1	2.32	0.47
13:UM:332:SER:OG	13:UM:381:VAL:O	2.31	0.47
17:UQ:487:GLU:HA	17:UQ:490:LEU:HD13	1.95	0.47
19:US:356:ALA:HA	19:US:499:LEU:HD21	1.96	0.47
27:CE:227:LEU:HD23	27:CE:231:ILE:HG22	1.95	0.47
33:CL:749:THR:OG1	61:DX:78:LYS:O	2.32	0.47
35:CN:218:LYS:HE3	35:CN:219:ASN:HD21	1.79	0.47
44:JN:329:ILE:HD11	60:DW:89:TRP:CZ3	2.49	0.47
45:JO:145:LEU:O	45:JO:152:THR:OG1	2.32	0.47
46:JP:247:TYR:HA	46:JP:254:PRO:HA	1.95	0.47
49:DE:181:VAL:HG23	49:DE:225:VAL:HG13	1.96	0.47
50:DF:157:ARG:HB2	50:DF:224:ASN:HD21	1.78	0.47
51:DG:10:ASN:HA	51:DG:128:THR:HG23	1.96	0.47
54:DJ:171:ARG:HA	54:DJ:174:ARG:HG2	1.96	0.47
55:DL:75:VAL:HG13	55:DL:119:VAL:HA	1.96	0.47
65:D2:550:C:H2'	65:D2:551:A:H8	1.79	0.47
66:D3:209:U:H2'	66:D3:210:A:H8	1.79	0.47
66:D3:376:C:O2'	66:D3:377:G:O4'	2.29	0.47
66:D3:539:G:H1'	66:D3:540:G:H21	1.79	0.47
4:UD:656:ARG:NH2	4:UD:731:HIS:O	2.47	0.47
6:UF:57:ILE:HD11	6:UF:95:ILE:HB	1.95	0.47
10:UJ:124:ARG:HA	10:UJ:124:ARG:HD2	1.76	0.47
11:UK:235:ASP:OD1	11:UK:236:SER:N	2.44	0.47
12:UL:455:GLN:HG2	12:UL:467:THR:HG23	1.97	0.47
15:UO:97:CYS:HB3	15:UO:132:PHE:CE2	2.49	0.47
15:UO:285:ASP:OD1	15:UO:293:LYS:NZ	2.48	0.47
20:UT:1340:SER:O	20:UT:1344:TRP:N	2.41	0.47
21:UU:184:THR:OG1	21:UU:187:ASN:OD1	2.31	0.47
21:UU:423:ARG:HG3	21:UU:427:TRP:CZ2	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
22:UV:529:VAL:HA	22:UV:695:GLN:O	2.14	0.47
25:CB:93:HIS:HE1	25:CB:162:LEU:H	1.60	0.47
29:CH:130:GLY:N	29:CH:483:TYR:HH	2.12	0.47
29:CH:256:ARG:HA	29:CH:282:GLU:HG3	1.95	0.47
33:CL:808:PHE:HE2	33:CL:1026:LYS:HB3	1.78	0.47
37:JC:79:PRO:O	37:JC:97:THR:OG1	2.27	0.47
37:JC:153:LEU:HD23	37:JC:167:LEU:HD13	1.95	0.47
40:JH:321:PHE:O	40:JH:325:LEU:N	2.41	0.47
41:JJ:266:VAL:O	41:JJ:270:LEU:HB2	2.14	0.47
44:JN:109:PRO:O	44:JN:114:GLN:N	2.48	0.47
48:DA:26:ARG:NH2	66:D3:896:U:OP1	2.47	0.47
48:DA:176:VAL:HG23	48:DA:184:LEU:HD12	1.96	0.47
49:DE:125:LYS:HB2	49:DE:226:PHE:HD1	1.78	0.47
51:DG:212:LEU:HD23	51:DG:216:LEU:HD23	1.95	0.47
56:DN:29:SER:OG	56:DN:32:SER:OG	2.21	0.47
58:DQ:15:SER:O	58:DQ:15:SER:OG	2.29	0.47
67:D4:313:A:H2'	67:D4:314:C:C6	2.49	0.47
8:UH:676:TRP:HB2	9:UI:486:LEU:HB3	1.96	0.47
12:UL:749:GLY:O	12:UL:753:MET:HG3	2.14	0.47
12:UL:769:TYR:CE2	12:UL:787:LYS:HG2	2.49	0.47
13:UM:501:PRO:HG2	13:UM:543:GLN:HB3	1.96	0.47
13:UM:552:SER:OG	13:UM:554:ASP:OD1	2.33	0.47
13:UM:552:SER:OG	13:UM:556:THR:O	2.30	0.47
18:UR:217:ASN:O	18:UR:217:ASN:ND2	2.47	0.47
18:UR:400:ILE:HD11	18:UR:404:ILE:HA	1.97	0.47
21:UU:743:ARG:HD3	32:CK:474:ILE:O	2.14	0.47
25:CB:93:HIS:NE2	25:CB:159:LEU:O	2.43	0.47
26:CD:171:ASP:N	26:CD:171:ASP:OD1	2.48	0.47
31:CJ:281:ILE:HG23	66:D3:562:G:C5	2.49	0.47
36:JA:9:ARG:NH1	36:JA:214:LYS:O	2.47	0.47
36:JB:283:ALA:O	36:JB:411:THR:HA	2.14	0.47
42:JK:488:ASP:OD1	42:JK:489:GLN:N	2.42	0.47
45:JO:273:LYS:HA	45:JO:276:LYS:HZ2	1.79	0.47
45:JO:285:LYS:O	45:JO:288:GLN:HB2	2.15	0.47
49:DE:208:VAL:O	49:DE:219:VAL:HA	2.14	0.47
55:DL:98:ASN:O	55:DL:99:ARG:NH1	2.47	0.47
65:D2:167:U:H2'	65:D2:168:G:O4'	2.14	0.47
65:D2:329:A:O2'	65:D2:331:U:OP2	2.31	0.47
66:D3:1216:C:H2'	66:D3:1217:A:H4'	1.95	0.47
66:D3:1715:G:H2'	66:D3:1716:C:C6	2.49	0.47
6:UF:34:LYS:O	6:UF:37:THR:OG1	2.32	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:UG:458:THR:HG23	14:UN:854:ARG:HG2	1.95	0.47
12:UL:496:THR:HG22	12:UL:529:GLU:HA	1.96	0.47
17:UQ:780:GLU:O	17:UQ:782:THR:N	2.48	0.47
33:CL:215:TYR:HB3	33:CL:216:PRO:HD2	1.95	0.47
36:JA:86:ARG:NH2	36:JA:90:GLU:O	2.48	0.47
41:JJ:119:PRO:HA	41:JJ:123:HIS:HB2	1.97	0.47
61:DX:132:LEU:HD23	61:DX:132:LEU:HA	1.71	0.47
65:D2:97:G:C2	65:D2:148:G:C2	3.03	0.47
66:D3:235:G:H2'	66:D3:236:A:C8	2.49	0.47
4:UD:192:THR:OG1	4:UD:242:TRP:O	2.28	0.47
4:UD:519:THR:N	4:UD:522:SER:OG	2.47	0.47
9:UI:477:LYS:HG3	9:UI:481:HIS:CE1	2.48	0.47
12:UL:387:LEU:O	12:UL:415:LYS:NZ	2.32	0.47
13:UM:265:ALA:HA	13:UM:290:ILE:HG23	1.95	0.47
13:UM:301:GLN:HB3	13:UM:313:LEU:HD11	1.97	0.47
13:UM:614:ASP:N	13:UM:614:ASP:OD1	2.47	0.47
18:UR:144:LYS:HD3	65:D2:311:C:N4	2.30	0.47
18:UR:372:HIS:ND1	18:UR:373:GLY:O	2.34	0.47
19:US:450:GLU:HG3	19:US:452:ASP:H	1.80	0.47
21:UU:834:LEU:HA	21:UU:834:LEU:HD23	1.68	0.47
25:CA:125:VAL:HG12	43:JM:150:GLY:HA3	1.95	0.47
30:CI:3:ARG:NH2	30:CI:9:GLU:OE2	2.47	0.47
34:CM:189:SER:OG	34:CM:248:GLN:O	2.27	0.47
35:CN:80:THR:HG21	35:CN:140:ALA:HB2	1.97	0.47
35:CN:131:ALA:HA	35:CN:134:ILE:HG22	1.96	0.47
37:JC:133:TYR:HE1	42:JK:472:ILE:HG12	1.80	0.47
56:DN:148:ALA:HA	56:DN:151:ASN:HB2	1.96	0.47
66:D3:363:G:H2'	66:D3:364:G:C8	2.50	0.47
66:D3:1270:G:O6	66:D3:1439:C:N4	2.47	0.47
66:D3:1680:G:H5'	66:D3:1722:A:H61	1.79	0.47
4:UD:107:VAL:HG23	4:UD:110:GLU:HB2	1.95	0.47
4:UD:288:THR:HG22	4:UD:295:VAL:HG22	1.97	0.47
4:UD:689:ASN:HD22	4:UD:689:ASN:C	2.17	0.47
10:UJ:404:PHE:O	10:UJ:408:ILE:HG12	2.15	0.47
12:UL:596:ASN:N	12:UL:596:ASN:OD1	2.45	0.47
12:UL:678:ASP:OD1	12:UL:678:ASP:N	2.46	0.47
13:UM:574:HIS:HE2	13:UM:594:GLY:HA3	1.79	0.47
17:UQ:167:SER:OG	65:D2:64:U:OP2	2.32	0.47
18:UR:228:LEU:O	18:UR:545:HIS:NE2	2.48	0.47
21:UU:64:ASN:O	21:UU:344:ARG:NH1	2.47	0.47
22:UV:242:LEU:HD12	22:UV:245:LYS:HZ3	1.79	0.47



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
29:CH:437:ARG:HD3	29:CH:437:ARG:HA	1.66	0.47
29:CH:523:LYS:O	29:CH:541:ALA:HA	2.15	0.47
33:CL:824:ILE:HD11	33:CL:926:ILE:HG12	1.97	0.47
33:CL:963:GLY:N	33:CL:976:ILE:O	2.46	0.47
36:JA:174:THR:HG22	36:JA:176:ALA:H	1.79	0.47
38:JE:288:SER:HA	38:JE:291:GLU:HB2	1.95	0.47
41:JJ:118:PRO:O	41:JJ:122:GLU:HG3	2.14	0.47
45:JO:130:ASN:ND2	57:DO:127:ARG:HH21	2.13	0.47
46:JP:221:ASN:OD1	46:JP:221:ASN:N	2.47	0.47
49:DE:47:PHE:HE2	49:DE:101:LEU:HD11	1.80	0.47
51:DG:10:ASN:HB3	51:DG:128:THR:HA	1.97	0.47
51:DG:22:HIS:HA	51:DG:25:ARG:NH1	2.30	0.47
51:DG:103:GLY:H	51:DG:106:LEU:HD23	1.80	0.47
62:DY:16:PRO:HA	62:DY:19:ALA:HA	1.97	0.47
1:UA:430:ARG:HG3	32:CK:460:PRO:O	2.15	0.47
1:UA:462:THR:O	1:UA:464:GLN:N	2.47	0.47
1:UA:539:ILE:HD12	1:UA:553:ILE:HD11	1.96	0.47
4:UD:106:ASN:H	4:UD:153:GLN:HG2	1.80	0.47
5:UE:187:HIS:CG	5:UE:206:ALA:HB2	2.50	0.47
8:UH:537:THR:HA	8:UH:540:LEU:HD23	1.97	0.47
8:UH:611:ILE:HD11	8:UH:654:LEU:HD21	1.96	0.47
10:UJ:268:LEU:HD11	18:UR:219:LYS:HD2	1.96	0.47
12:UL:136:LEU:HD23	12:UL:148:TRP:HE3	1.78	0.47
13:UM:105:SER:HA	13:UM:121:GLY:HA2	1.95	0.47
15:UO:128:HIS:CD2	15:UO:172:ARG:HE	2.33	0.47
17:UQ:678:LEU:O	17:UQ:691:SER:HA	2.14	0.47
17:UQ:685:ARG:HB2	17:UQ:687:GLN:HE22	1.80	0.47
17:UQ:722:LEU:HD22	17:UQ:766:ILE:HD11	1.96	0.47
21:UU:183:VAL:HG12	21:UU:188:VAL:HG22	1.97	0.47
22:UV:433:ASP:HB3	22:UV:437:ASP:HB2	1.96	0.47
23:UX:65:VAL:HA	23:UX:152:ILE:O	2.15	0.47
23:UX:86:MET:HB3	23:UX:86:MET:HE2	1.53	0.47
23:UX:182:ILE:HG21	23:UX:185:LEU:HD12	1.97	0.47
24:UZ:91:GLU:HA	24:UZ:94:SER:HB2	1.96	0.47
25:CB:323:SER:OG	25:CB:324:GLY:N	2.48	0.47
26:CD:221:LEU:HD11	26:CD:276:GLN:HA	1.97	0.47
36:JA:29:VAL:O	36:JA:202:ASP:HA	2.14	0.47
65:D2:262:U:H2'	65:D2:263:C:C6	2.50	0.47
66:D3:97:C:H2'	66:D3:98:U:C6	2.50	0.47
4:UD:277:LYS:NZ	18:UR:348:HIS:HB3	2.29	0.47
7:UG:116:ILE:HG23	7:UG:116:ILE:HD12	1.68	0.47



Atom-1	Atom-2	Interatomic	Clash
	2100HT 2	distance (Å)	overlap (Å)
17:UQ:319:LYS:HD3	17:UQ:339:GLY:H	1.79	0.47
17:UQ:334:LEU:HD23	17:UQ:334:LEU:HA	1.75	0.47
18:UR:458:ILE:HD11	18:UR:482:LEU:HD11	1.96	0.47
20:UT:248:HIS:H	20:UT:251:ALA:HB3	1.79	0.47
22:UV:205:THR:OG1	22:UV:293:ASN:O	2.23	0.47
23:UX:72:ILE:HD12	23:UX:72:ILE:HG23	1.70	0.47
26:CD:82:LEU:HA	26:CD:82:LEU:HD23	1.71	0.47
28:CF:50:GLU:N	28:CF:102:ILE:O	2.44	0.47
29:CH:424:LEU:HB3	29:CH:434:PHE:HB3	1.97	0.47
31:CJ:9:ARG:HD2	31:CJ:9:ARG:HA	1.51	0.47
33:CL:795:LYS:HE3	33:CL:795:LYS:HB2	1.73	0.47
35:CN:176:ASP:N	35:CN:176:ASP:OD1	2.47	0.47
36:JA:591:GLU:OE2	36:JA:614:ILE:N	2.35	0.47
36:JA:738:LYS:O	36:JA:810:LYS:NZ	2.48	0.47
46:JP:189:ARG:NH2	46:JP:229:GLN:OE1	2.48	0.47
46:JP:416:HIS:O	46:JP:417:ARG:NH2	2.45	0.47
49:DE:100:ARG:HH12	49:DE:122:LYS:HA	1.79	0.47
57:DO:20:TYR:HE1	57:DO:22:SER:HB3	1.79	0.47
66:D3:1650:U:H2'	66:D3:1651:A:H8	1.80	0.47
66:D3:1739:C:H2'	66:D3:1740:A:C8	2.50	0.47
67:D4:248:G:H2'	67:D4:249:G:C8	2.49	0.47
1:UA:296:GLN:NE2	1:UA:332:TRP:O	2.48	0.47
2:UB:709:SER:HB2	39:JG:106:LYS:HB3	1.96	0.47
4:UD:237:GLU:OE2	16:UP:208:ARG:NH2	2.42	0.47
13:UM:89:HIS:CE1	13:UM:91:LYS:HB2	2.50	0.47
18:UR:252:GLN:O	18:UR:567:SER:OG	2.32	0.47
21:UU:135:ASN:HD21	21:UU:166:GLU:HA	1.80	0.47
33:CL:59:VAL:HG12	33:CL:758:ILE:HD11	1.97	0.47
52:DH:84:LYS:HG3	52:DH:85:PHE:CZ	2.50	0.47
56:DN:54:LEU:HD23	56:DN:54:LEU:HA	1.68	0.47
56:DN:87:ASP:N	56:DN:87:ASP:OD1	2.44	0.47
65:D2:165:G:N2	65:D2:231:C:O2	2.48	0.47
66:D3:57:G:H1'	66:D3:91:G:H22	1.80	0.47
66:D3:1699:G:N2	66:D3:1702:A:OP2	2.45	0.47
1:UA:418:ARG:NH2	32:CK:488:SER:O	2.47	0.46
1:UA:458:TRP:CD1	1:UA:465:LEU:HB3	2.50	0.46
2:UB:805:LEU:HD22	2:UB:806:ARG:HD3	1.96	0.46
4:UD:680:THR:OG1	4:UD:681:ILE:N	2.49	0.46
5:UE:244:ILE:O	5:UE:255:ILE:HA	2.15	0.46
7:UG:286:GLY:O	7:UG:304:ARG:NH2	2.48	0.46
9:UI:419:PHE:O	9:UI:422:THR:OG1	2.30	0.46



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:341:ALA:HA	12:UL:354:VAL:O	2.14	0.46
15:UO:21:THR:HG23	15:UO:24:GLN:HB2	1.98	0.46
15:UO:75:LYS:HD3	15:UO:111:TYR:HA	1.96	0.46
17:UQ:291:ARG:NH1	17:UQ:329:ASN:OD1	2.44	0.46
18:UR:391:SER:O	18:UR:393:LEU:N	2.48	0.46
19:US:350:MET:SD	19:US:390:SER:OG	2.73	0.46
22:UV:1038:GLN:OE1	22:UV:1038:GLN:N	2.48	0.46
29:CH:242:VAL:HG23	29:CH:253:THR:HG22	1.97	0.46
33:CL:874:TYR:OH	66:D3:578:U:OP2	2.30	0.46
36:JA:520:ARG:NH1	36:JA:559:ALA:O	2.48	0.46
36:JA:579:ILE:HD12	36:JA:580:PRO:HD2	1.96	0.46
43:JM:135:HIS:CE1	66:D3:487:G:C5	3.03	0.46
43:JM:213:ARG:NH1	66:D3:1491:U:OP2	2.48	0.46
46:JP:314:SER:O	46:JP:317:GLY:N	2.46	0.46
49:DE:19:LEU:HB2	49:DE:108:ARG:HD2	1.97	0.46
53:DI:48:THR:HG21	53:DI:54:LYS:HE3	1.96	0.46
54:DJ:139:GLN:OE1	54:DJ:139:GLN:N	2.49	0.46
57:DO:24:ASN:ND2	66:D3:902:G:OP2	2.48	0.46
65:D2:238:G:N3	65:D2:238:G:H5'	2.30	0.46
66:D3:152:U:H3	66:D3:162:A:H61	1.62	0.46
4:UD:309:GLN:HE21	4:UD:318:ASN:HA	1.80	0.46
5:UE:54:GLU:HG2	5:UE:55:ASP:H	1.79	0.46
6:UF:144:VAL:O	6:UF:147:TRP:N	2.48	0.46
9:UI:470:ILE:HG22	9:UI:471:LYS:HB2	1.98	0.46
10:UJ:227:ASN:ND2	10:UJ:230:LYS:HZ3	2.13	0.46
11:UK:138:ASP:OD1	11:UK:139:SER:N	2.46	0.46
12:UL:581:ILE:HG21	12:UL:581:ILE:HD13	1.65	0.46
15:UO:142:THR:O	15:UO:149:THR:OG1	2.22	0.46
17:UQ:113:ASN:O	17:UQ:115:HIS:ND1	2.48	0.46
17:UQ:209:ALA:HB2	17:UQ:264:ILE:HD11	1.97	0.46
17:UQ:293:LEU:HD23	17:UQ:324:TRP:CE3	2.50	0.46
17:UQ:314:SER:HG	17:UQ:324:TRP:HE1	1.62	0.46
17:UQ:868:ASN:OD1	17:UQ:868:ASN:N	2.43	0.46
22:UV:242:LEU:HA	22:UV:245:LYS:HZ3	1.80	0.46
25:CB:184:VAL:HA	25:CB:187:VAL:HG12	1.98	0.46
27:CE:16:LYS:H	27:CE:45:ALA:HB2	1.80	0.46
29:CH:158:THR:HG21	29:CH:240:LEU:HD12	1.98	0.46
29:CH:181:ASN:OD1	29:CH:182:LYS:N	2.48	0.46
54:DJ:136:VAL:HG22	54:DJ:156:ILE:HG12	1.97	0.46
54:DJ:152:SER:HA	54:DJ:155:HIS:HB2	1.96	0.46
55:DL:125:VAL:HG12	55:DL:139:VAL:HA	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
62:DY:41:ARG:HD2	62:DY:94:TYR:CD2	2.50	0.46
66:D3:99:C:H2'	66:D3:100:A:C8	2.50	0.46
66:D3:151:G:H2'	66:D3:152:U:H6	1.81	0.46
66:D3:1704:U:H2'	66:D3:1705:C:C6	2.50	0.46
5:UE:436:THR:OG1	19:US:297:ASP:OD2	2.25	0.46
12:UL:88:HIS:ND1	12:UL:91:THR:OG1	2.35	0.46
12:UL:123:ALA:HB3	12:UL:141:LYS:HD2	1.98	0.46
13:UM:188:GLU:OE2	48:DA:242:LYS:NZ	2.32	0.46
13:UM:518:TRP:HB3	13:UM:525:LEU:HA	1.97	0.46
16:UP:163:LEU:HD23	16:UP:167:ARG:HH22	1.80	0.46
17:UQ:378:ASP:HB3	17:UQ:380:THR:HG22	1.95	0.46
18:UR:156:ASN:N	18:UR:156:ASN:OD1	2.41	0.46
18:UR:408:CYS:SG	18:UR:459:GLN:HA	2.54	0.46
19:US:260:ASN:O	19:US:263:SER:OG	2.31	0.46
22:UV:373:ARG:HG2	22:UV:515:ILE:HD11	1.98	0.46
24:UZ:253:PRO:HB2	24:UZ:256:GLN:NE2	2.30	0.46
29:CH:349:TRP:CZ3	29:CH:356:ARG:HB3	2.50	0.46
32:CK:470:GLU:HA	32:CK:490:LEU:HD23	1.98	0.46
34:CM:122:THR:HG21	34:CM:156:ARG:HG3	1.98	0.46
36:JA:815:SER:OG	36:JA:816:ASP:N	2.47	0.46
36:JA:881:GLN:HB2	36:JA:916:ILE:HG21	1.97	0.46
36:JB:515:LEU:HA	36:JB:566:VAL:O	2.15	0.46
37:JC:194:LEU:HD11	37:JC:243:PHE:HE2	1.79	0.46
55:DL:128:CYS:HB2	55:DL:131:ILE:HD11	1.97	0.46
57:DO:43:THR:HB	57:DO:46:MET:HG2	1.96	0.46
66:D3:315:A:N6	66:D3:349:U:HO2'	2.13	0.46
66:D3:904:G:H8	66:D3:905:A:C8	2.33	0.46
66:D3:1167:G:N2	66:D3:1579:U:O2	2.48	0.46
1:UA:115:SER:O	1:UA:115:SER:OG	2.29	0.46
5:UE:238:SER:HB3	5:UE:243:SER:HB2	1.96	0.46
11:UK:51:LEU:HD12	33:CL:1077:LEU:HD11	1.97	0.46
13:UM:461:LEU:HD21	13:UM:491:GLU:HA	1.96	0.46
17:UQ:111:THR:OG1	17:UQ:112:ASN:N	2.48	0.46
19:US:156:TRP:CZ3	19:US:212:LEU:HA	2.49	0.46
20:UT:2091:ASN:O	20:UT:2095:LEU:N	2.35	0.46
25:CA:171:LEU:HD22	25:CA:173:LEU:HD12	1.96	0.46
26:CD:203:PHE:HE1	26:CD:255:ALA:HA	1.80	0.46
29:CH:437:ARG:O	29:CH:439:ALA:N	2.36	0.46
33:CL:288:VAL:HG12	33:CL:814:GLY:HA2	1.96	0.46
33:CL:838:ILE:HD12	33:CL:874:TYR:HB3	1.98	0.46
37:JC:70:TYR:CZ	37:JC:111:TRP:HD1	2.33	0.46



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
45:JO:41:PHE:CD2	45:JO:98:ARG:HG3	2.51	0.46
62:DY:59:GLY:O	62:DY:71:GLY:HA2	2.16	0.46
66:D3:442:C:H42	66:D3:462:G:H1	1.63	0.46
4:UD:298:ALA:HB1	4:UD:333:ILE:HG21	1.97	0.46
4:UD:376:GLU:HA	4:UD:377:PRO:HD3	1.78	0.46
12:UL:224:SER:HA	12:UL:251:GLN:HE21	1.81	0.46
12:UL:898:LEU:HD23	12:UL:898:LEU:HA	1.66	0.46
13:UM:198:ILE:HG12	13:UM:211:LEU:HD13	1.96	0.46
13:UM:224:ASP:OD1	13:UM:225:PHE:N	2.49	0.46
16:UP:159:LYS:O	16:UP:162:THR:OG1	2.26	0.46
19:US:124:LEU:HD11	19:US:184:TYR:CZ	2.51	0.46
21:UU:564:ASP:N	21:UU:564:ASP:OD1	2.46	0.46
22:UV:241:ILE:HG22	22:UV:245:LYS:NZ	2.30	0.46
22:UV:1214:LEU:HD21	22:UV:1216:LYS:HE2	1.96	0.46
24:UZ:32:ASN:O	24:UZ:34:LYS:NZ	2.49	0.46
28:CF:95:ARG:NH1	67:D4:79:G:N7	2.63	0.46
28:CF:111:LYS:HB3	28:CF:111:LYS:HE2	1.66	0.46
34:CM:26:LEU:HD23	34:CM:26:LEU:HA	1.69	0.46
36:JA:61:LYS:HE3	36:JA:62:LYS:HE3	1.97	0.46
36:JA:862:LEU:O	36:JA:866:TYR:CB	2.64	0.46
39:JG:50:LEU:HD13	39:JG:116:THR:HG22	1.98	0.46
41:JJ:126:LEU:HD21	41:JJ:139:LEU:HB3	1.98	0.46
46:JP:66:HIS:ND1	46:JP:87:SER:HB3	2.30	0.46
46:JP:225:LEU:HD23	46:JP:225:LEU:HA	1.65	0.46
46:JP:449:LYS:NZ	66:D3:1053:G:OP1	2.28	0.46
50:DF:102:ARG:HD2	50:DF:102:ARG:N	2.30	0.46
53:DI:47:ARG:NH2	66:D3:396:G:N7	2.64	0.46
60:DW:82:LYS:H	60:DW:85:ASP:HB2	1.80	0.46
66:D3:538:A:H8	66:D3:543:C:N4	2.12	0.46
66:D3:1503:A:N1	66:D3:1504:G:N2	2.63	0.46
66:D3:1671:A:H3'	66:D3:1672:G:C8	2.51	0.46
4:UD:285:CYS:HB2	4:UD:298:ALA:HB3	1.98	0.46
10:UJ:139:THR:HG21	10:UJ:151:ILE:HD13	1.97	0.46
12:UL:50:ASN:HB3	12:UL:52:TRP:HZ3	1.81	0.46
22:UV:533:LEU:HD21	22:UV:539:LEU:HD12	1.97	0.46
22:UV:741:ILE:HA	22:UV:744:MET:HE2	1.97	0.46
22:UV:884:LYS:HA	22:UV:884:LYS:HD2	1.73	0.46
22:UV:1050:ILE:O	22:UV:1054:SER:HB3	2.15	0.46
23:UX:13:VAL:HG21	65:D2:461:A:N1	2.31	0.46
26:CD:149:ARG:NH2	27:CE:242:SER:HA	2.31	0.46
29:CH:485:ASN:O	29:CH:500:LYS:HA	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
36:JA:63:LEU:HA	36:JA:63:LEU:HD23	1.73	0.46
37:JC:281:ASP:OD1	37:JC:281:ASP:N	2.46	0.46
44:JN:308:ILE:HG21	60:DW:95:PRO:HG3	1.98	0.46
45:JO:283:GLU:O	45:JO:286:GLU:HG3	2.15	0.46
50:DF:84:LYS:O	50:DF:92:ARG:NH2	2.43	0.46
7:UG:548:GLU:OE1	35:CN:185:HIS:ND1	2.42	0.46
10:UJ:33:LEU:HB2	10:UJ:119:GLU:HG2	1.97	0.46
12:UL:671:PHE:HA	12:UL:684:TRP:O	2.16	0.46
13:UM:43:ILE:HG22	13:UM:52:ILE:HG22	1.97	0.46
15:UO:21:THR:O	15:UO:24:GLN:HB2	2.15	0.46
15:UO:284:PHE:CE1	15:UO:292:VAL:HG22	2.50	0.46
17:UQ:656:ASP:N	17:UQ:656:ASP:OD1	2.44	0.46
22:UV:408:SER:HB3	22:UV:456:LYS:HD2	1.98	0.46
26:CD:35:GLN:O	26:CD:38:ILE:HG22	2.15	0.46
29:CH:438:ILE:O	29:CH:441:GLY:N	2.30	0.46
36:JA:591:GLU:OE1	36:JA:634:ARG:NH1	2.49	0.46
41:JJ:103:PRO:O	41:JJ:106:MET:N	2.49	0.46
60:DW:15:ASN:ND2	60:DW:72:CYS:O	2.47	0.46
65:D2:2:U:H2'	65:D2:3:G:H8	1.81	0.46
4:UD:40:ASP:OD1	4:UD:40:ASP:N	2.43	0.46
11:UK:68:HIS:CE1	67:D4:56:A:H4'	2.51	0.46
12:UL:752:LEU:HD22	12:UL:824:MET:HE1	1.98	0.46
13:UM:76:LEU:HB3	13:UM:88:PHE:HD2	1.81	0.46
15:UO:452:ASP:OD1	15:UO:453:VAL:N	2.39	0.46
17:UQ:315:GLY:HA2	17:UQ:341:ILE:HD11	1.97	0.46
20:UT:139:ALA:O	20:UT:142:PHE:O	2.33	0.46
21:UU:627:ASN:ND2	21:UU:647:THR:OG1	2.31	0.46
22:UV:428:TYR:CZ	22:UV:432:MET:HG3	2.51	0.46
23:UX:96:PRO:HG2	23:UX:125:ILE:HD13	1.97	0.46
25:CB:272:LYS:HE2	25:CB:275:CYS:HB2	1.97	0.46
33:CL:976:ILE:HD13	33:CL:976:ILE:HG21	1.79	0.46
34:CM:287:ALA:HB2	34:CM:314:ASN:HB2	1.97	0.46
36:JA:496:LEU:HG	36:JA:536:LYS:HA	1.97	0.46
43:JM:177:LEU:HD12	43:JM:177:LEU:HA	1.75	0.46
50:DF:101:GLY:HA2	50:DF:104:ASN:OD1	2.15	0.46
53:DI:84:HIS:ND1	53:DI:85:PRO:HD2	2.31	0.46
54:DJ:20:GLU:HB3	54:DJ:23:ARG:HG2	1.98	0.46
66:D3:328:A:H2'	66:D3:329:G:C8	2.50	0.46
2:UB:646:THR:HA	2:UB:649:THR:HG22	1.96	0.46
2:UB:651:TRP:CD1	2:UB:661:ILE:HD13	2.51	0.46
5:UE:548:ASP:HA	5:UE:551:ILE:HG22	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:UJ:149:LYS:HE2	10:UJ:149:LYS:HB3	1.64	0.46
10:UJ:274:ILE:HG12	18:UR:211:ILE:HD12	1.97	0.46
13:UM:212:LEU:HG	13:UM:220:ILE:HD11	1.96	0.46
14:UN:868:GLU:HA	46:JP:26:ARG:HH12	1.81	0.46
15:UO:423:LYS:HB3	15:UO:423:LYS:HE2	1.72	0.46
15:UO:495:ILE:O	15:UO:499:LYS:HB2	2.16	0.46
17:UQ:458:GLN:NE2	17:UQ:467:GLN:HG3	2.28	0.46
17:UQ:533:THR:OG1	17:UQ:534:LYS:N	2.48	0.46
21:UU:60:ILE:HD12	21:UU:70:PHE:HB2	1.98	0.46
22:UV:577:ARG:NH2	22:UV:626:LYS:O	2.36	0.46
25:CB:172:TYR:HE1	25:CB:241:PHE:CD2	2.34	0.46
45:JO:291:ARG:HA	45:JO:294:GLU:HG3	1.97	0.46
46:JP:183:GLN:HE21	46:JP:183:GLN:HB2	1.55	0.46
48:DA:149:GLN:HG2	66:D3:1066:C:H4'	1.97	0.46
53:DI:105:ASP:N	53:DI:105:ASP:OD1	2.49	0.46
1:UA:157:ASP:O	1:UA:159:ARG:N	2.48	0.46
5:UE:362:ARG:NH1	17:UQ:591:GLU:OE2	2.34	0.46
6:UF:177:ASP:N	6:UF:177:ASP:OD1	2.48	0.46
7:UG:301:TRP:HA	7:UG:308:GLN:HA	1.98	0.46
8:UH:188:ILE:O	8:UH:197:GLU:N	2.48	0.46
12:UL:261:PHE:CD1	12:UL:272:PHE:HB3	2.51	0.46
20:UT:1662:SER:O	20:UT:1665:LEU:C	2.54	0.46
21:UU:187:ASN:OD1	21:UU:187:ASN:N	2.47	0.46
25:CB:280:VAL:HG22	25:CB:281:ASP:H	1.81	0.46
26:CD:329:ALA:HB3	26:CD:332:THR:HG22	1.98	0.46
28:CG:13:ASP:OD1	28:CG:14:ALA:N	2.49	0.46
28:CG:79:VAL:HG21	28:CG:121:ILE:HG12	1.98	0.46
33:CL:308:CYS:SG	33:CL:355:TYR:HB2	2.56	0.46
33:CL:808:PHE:CE2	33:CL:1026:LYS:HB3	2.51	0.46
36:JA:738:LYS:HE2	36:JA:738:LYS:HB3	1.76	0.46
37:JC:315:VAL:HG11	37:JC:335:SER:HB2	1.98	0.46
41:JJ:271:LYS:HB2	41:JJ:271:LYS:HE2	1.34	0.46
46:JP:109:HIS:HD2	46:JP:113:VAL:HG12	1.81	0.46
62:DY:61:ARG:HH22	66:D3:523:G:C4'	2.28	0.46
65:D2:123:C:H3'	65:D2:124:A:H8	1.81	0.46
66:D3:271:A:N1	66:D3:284:G:H2'	2.31	0.46
66:D3:469:C:H3'	66:D3:470:A:C8	2.51	0.46
1:UA:275:LEU:HB2	1:UA:289:LEU:HD22	1.97	0.45
2:UB:524:LEU:HD13	19:US:507:LEU:HD11	1.98	0.45
5:UE:198:THR:HG22	5:UE:199:ASN:H	1.81	0.45
6:UF:105:GLN:HE21	6:UF:105:GLN:HB3	1.53	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:UF:107:LEU:HD12	43:JM:69:PHE:HE1	1.81	0.45
8:UH:211:ILE:N	8:UH:220:LYS:O	2.40	0.45
10:UJ:1510:PHE:O	10:UJ:1514:SER:CB	2.63	0.45
19:US:467:ALA:O	19:US:470:MET:HB2	2.17	0.45
21:UU:530:ASP:OD1	21:UU:531:PHE:N	2.48	0.45
22:UV:313:ASN:HD22	22:UV:326:LEU:HB3	1.81	0.45
22:UV:652:LYS:HD2	22:UV:652:LYS:HA	1.72	0.45
27:CE:428:ASN:HB3	27:CE:430:ASP:OD1	2.15	0.45
39:JG:70:CYS:SG	39:JG:71:ASP:N	2.88	0.45
44:JN:298:LYS:NZ	66:D3:1033:C:OP2	2.49	0.45
48:DA:61:LEU:HD23	48:DA:61:LEU:HA	1.78	0.45
48:DA:79:HIS:O	48:DA:81:PHE:N	2.42	0.45
65:D2:217:C:H2'	65:D2:218:U:H6	1.80	0.45
2:UB:788:ILE:HD13	2:UB:788:ILE:HA	1.80	0.45
3:UC:493:ASP:HA	3:UC:496:GLN:HE22	1.81	0.45
4:UD:497:ILE:HB	4:UD:509:GLN:HB2	1.97	0.45
4:UD:581:SER:HG	4:UD:594:PHE:C	2.19	0.45
11:UK:11:LYS:HB2	11:UK:11:LYS:HE2	1.81	0.45
12:UL:284:PHE:CD1	12:UL:328:PRO:HA	2.51	0.45
12:UL:588:ILE:HG13	12:UL:602:LEU:HD12	1.98	0.45
22:UV:114:VAL:HG22	22:UV:195:ILE:HB	1.98	0.45
22:UV:668:VAL:HG21	48:DA:240:LYS:HZ2	1.81	0.45
33:CL:975:GLU:CD	33:CL:977:LYS:HZ3	2.17	0.45
39:JF:177:LYS:O	39:JF:222:ASP:N	2.32	0.45
39:JG:115:GLN:HG2	39:JG:121:LEU:HD13	1.98	0.45
45:JO:64:LEU:HA	45:JO:64:LEU:HD23	1.77	0.45
49:DE:6:LYS:O	49:DE:30:ARG:NH1	2.33	0.45
56:DN:61:THR:OG1	56:DN:62:GLN:N	2.49	0.45
56:DN:69:ASN:OD1	56:DN:73:ARG:HB2	2.16	0.45
62:DY:55:VAL:HA	62:DY:75:VAL:HG23	1.98	0.45
65:D2:498:G:H2'	65:D2:499:U:C6	2.51	0.45
66:D3:381:C:H2'	66:D3:382:C:H4'	1.98	0.45
66:D3:1124:A:H1'	67:D4:1:G:H1	1.81	0.45
67:D4:306:G:H2'	67:D4:307:G:H8	1.81	0.45
1:UA:262:LYS:H	1:UA:280:THR:HG22	1.82	0.45
3:UC:592:GLU:HG2	3:UC:593:GLY:N	2.31	0.45
5:UE:532:ARG:HE	5:UE:532:ARG:HB2	1.53	0.45
6:UF:137:LEU:HA	6:UF:137:LEU:HD23	1.77	0.45
7:UG:109:LYS:HB2	7:UG:109:LYS:HE3	1.67	0.45
7:UG:502:ARG:HD3	65:D2:370:U:C5	2.48	0.45
12:UL:88:HIS:HB2	12:UL:129:PHE:CZ	2.52	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:126:LEU:HB2	12:UL:169:PHE:HE1	1.81	0.45
12:UL:934:ALA:HB1	32:CK:470:GLU:HG3	1.98	0.45
17:UQ:140:LYS:HB2	17:UQ:156:THR:OG1	2.17	0.45
17:UQ:334:LEU:HA	17:UQ:335:PRO:HD2	1.71	0.45
22:UV:228:ARG:NH2	22:UV:296:ILE:H	2.13	0.45
24:UZ:103:VAL:HG21	24:UZ:131:VAL:HG11	1.98	0.45
27:CE:319:ILE:HD12	27:CE:319:ILE:HG23	1.76	0.45
32:CK:476:MET:HE1	32:CK:489:SER:HB2	1.97	0.45
33:CL:131:ILE:HA	33:CL:131:ILE:HD13	1.73	0.45
33:CL:824:ILE:HG21	33:CL:824:ILE:HD13	1.74	0.45
33:CL:890:CYS:O	33:CL:922:ILE:HD11	2.16	0.45
33:CL:980:LEU:H	33:CL:987:TYR:HA	1.81	0.45
36:JA:505:ARG:NE	36:JA:643:GLU:O	2.46	0.45
37:JC:191:VAL:HG22	42:JK:484:LYS:HE3	1.98	0.45
39:JG:31:LEU:HD13	39:JG:40:ARG:NE	2.28	0.45
46:JP:139:CYS:SG	46:JP:185:ILE:HB	2.56	0.45
48:DA:141:ALA:HA	48:DA:209:ASN:O	2.16	0.45
48:DA:190:PRO:HG2	48:DA:192:VAL:HG13	1.97	0.45
51:DG:25:ARG:HA	51:DG:28:PHE:CD2	2.52	0.45
59:DS:83:ALA:O	59:DS:86:LEU:O	2.33	0.45
61:DX:132:LEU:HD23	61:DX:135:LEU:HD12	1.97	0.45
66:D3:505:A:N6	66:D3:586:G:H2'	2.32	0.45
66:D3:1592:A:N3	66:D3:1605:G:N2	2.64	0.45
4:UD:87:GLN:HB3	4:UD:378:TYR:CD2	2.51	0.45
4:UD:149:ILE:HA	4:UD:156:LEU:HA	1.98	0.45
4:UD:527:TYR:HA	4:UD:530:ARG:HD3	1.99	0.45
4:UD:611:LEU:HD12	4:UD:615:SER:HB2	1.98	0.45
6:UF:21:LYS:NZ	6:UF:80:THR:OG1	2.34	0.45
6:UF:289:HIS:NE2	27:CE:216:SER:OG	2.42	0.45
9:UI:481:HIS:O	9:UI:484:SER:OG	2.23	0.45
10:UJ:59:LEU:HD23	10:UJ:59:LEU:HA	1.77	0.45
15:UO:229:CYS:SG	15:UO:258:LEU:HD13	2.57	0.45
15:UO:323:SER:O	15:UO:323:SER:OG	2.34	0.45
19:US:345:ILE:HD12	19:US:349:LEU:HD12	1.99	0.45
20:UT:896:LEU:O	20:UT:900:GLU:CB	2.64	0.45
22:UV:574:LEU:HD23	22:UV:574:LEU:HA	1.75	0.45
22:UV:744:MET:HE1	22:UV:810:ILE:HG23	1.98	0.45
22:UV:1096:TYR:HD2	22:UV:1099:VAL:HG22	1.82	0.45
26:CD:277:ARG:NH2	27:CE:264:GLU:HB3	2.32	0.45
31:CJ:173:ARG:HD2	31:CJ:251:GLY:HA2	1.97	0.45
33:CL:1115:LYS:O	33:CL:1119:ILE:HG12	2.17	0.45



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
33:CL:1118:THR:OG1	65:D2:445:U:O2'	2.33	0.45
36:JA:121:MET:HG3	36:JA:147:ILE:HB	1.99	0.45
36:JA:520:ARG:HA	36:JA:523:LEU:HB3	1.98	0.45
38:JE:319:VAL:HG22	38:JE:324:ASP:HB3	1.97	0.45
51:DG:137:ARG:HH12	66:D3:143:G:H8	1.65	0.45
61:DX:60:GLU:OE1	61:DX:60:GLU:N	2.49	0.45
62:DY:6:THR:HB	62:DY:28:LEU:HB2	1.97	0.45
65:D2:105:G:N2	65:D2:140:U:O2	2.48	0.45
66:D3:655:G:H1'	66:D3:656:G:N7	2.31	0.45
1:UA:705:SER:OG	1:UA:706:THR:N	2.49	0.45
2:UB:310:ARG:O	2:UB:314:MET:N	2.49	0.45
4:UD:404:MET:HA	4:UD:414:TYR:HA	1.99	0.45
7:UG:99:THR:OG1	7:UG:100:ALA:N	2.50	0.45
8:UH:537:THR:OG1	8:UH:538:ARG:N	2.49	0.45
12:UL:260:GLU:HB3	12:UL:273:TYR:CE1	2.51	0.45
12:UL:400:SER:HB2	12:UL:404:LYS:HB3	1.98	0.45
13:UM:490:HIS:NE2	13:UM:508:THR:OG1	2.44	0.45
22:UV:251:PHE:HE2	22:UV:284:ASN:HA	1.82	0.45
22:UV:1150:VAL:O	22:UV:1154:ASN:ND2	2.50	0.45
25:CA:198:GLU:OE2	25:CA:200:SER:N	2.47	0.45
25:CA:236:MET:HG3	26:CD:133:LEU:HA	1.98	0.45
25:CB:97:TYR:OH	25:CB:109:LYS:NZ	2.29	0.45
26:CD:221:LEU:HD21	26:CD:276:GLN:HB2	1.98	0.45
28:CG:56:ALA:HB2	28:CG:80:PHE:HD2	1.82	0.45
30:CI:162:ASP:OD1	30:CI:162:ASP:N	2.37	0.45
31:CJ:211:ASN:OD1	31:CJ:212:ALA:N	2.49	0.45
33:CL:190:LEU:HD23	33:CL:190:LEU:HA	1.66	0.45
48:DA:19:ARG:NH1	48:DA:22:ASP:H	2.07	0.45
48:DA:187:LYS:O	48:DA:190:PRO:HD2	2.17	0.45
51:DG:121:LEU:N	51:DG:125:THR:OG1	2.50	0.45
66:D3:235:G:H2'	66:D3:236:A:H8	1.82	0.45
66:D3:460:A:H3'	66:D3:461:G:C8	2.51	0.45
66:D3:1781:A:H3'	66:D3:1782:A:O4'	2.17	0.45
1:UA:167:ASP:OD2	1:UA:169:SER:OG	2.31	0.45
1:UA:732:GLU:HG3	1:UA:734:GLN:HE22	1.80	0.45
2:UB:385:ASP:O	2:UB:389:ASP:N	2.44	0.45
3:UC:434:PHE:HD1	39:JG:132:ARG:HH11	1.64	0.45
8:UH:271:SER:O	8:UH:281:PHE:N	2.46	0.45
12:UL:764:GLU:HG2	12:UL:834:LYS:HE2	1.98	0.45
13:UM:63:GLU:OE1	13:UM:64:ILE:N	2.49	0.45
13:UM:363:ARG:HG2	13:UM:383:ILE:HG22	1.98	0.45



A + a 1	Adam 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:810:LEU:HA	13:UM:810:LEU:HD23	1.73	0.45
15:UO:33:ALA:HB2	15:UO:330:ARG:HG2	1.98	0.45
15:UO:178:PRO:HD3	15:UO:220:ALA:HB1	1.99	0.45
17:UQ:332:GLN:HE22	18:UR:344:ARG:HB2	1.79	0.45
19:US:273:GLN:O	19:US:276:SER:N	2.49	0.45
21:UU:414:ILE:HG12	21:UU:434:HIS:ND1	2.32	0.45
25:CA:101:GLY:O	43:JM:127:ARG:NH1	2.50	0.45
28:CF:119:ASP:O	28:CF:122:GLU:HG3	2.16	0.45
33:CL:828:ARG:NH1	61:DX:94:ASN:OD1	2.49	0.45
33:CL:828:ARG:NH1	61:DX:94:ASN:O	2.50	0.45
37:JC:329:PHE:O	37:JC:340:THR:HA	2.16	0.45
66:D3:328:A:H2'	66:D3:329:G:H8	1.82	0.45
66:D3:538:A:H8	66:D3:543:C:H42	1.65	0.45
66:D3:1746:A:H2'	66:D3:1747:G:H8	1.80	0.45
6:UF:199:ARG:HA	6:UF:202:VAL:HG12	1.98	0.45
10:UJ:121:LEU:HD23	10:UJ:121:LEU:HA	1.71	0.45
13:UM:507:ALA:HA	13:UM:516:LYS:O	2.17	0.45
15:UO:217:ASN:ND2	15:UO:257:CYS:HA	2.32	0.45
15:UO:285:ASP:CG	15:UO:293:LYS:HZ3	2.20	0.45
15:UO:405:PHE:HE2	15:UO:442:LEU:HD12	1.81	0.45
17:UQ:237:LEU:HD21	17:UQ:285:LEU:HD12	1.99	0.45
17:UQ:284:SER:O	17:UQ:288:LEU:HA	2.17	0.45
17:UQ:415:THR:OG1	17:UQ:416:SER:N	2.50	0.45
17:UQ:488:LEU:HA	17:UQ:488:LEU:HD23	1.70	0.45
19:US:344:ILE:HG12	19:US:349:LEU:HD21	1.98	0.45
21:UU:378:PHE:HA	21:UU:386:SER:HB2	1.99	0.45
22:UV:160:VAL:HG11	22:UV:230:VAL:HG12	1.98	0.45
22:UV:763:THR:HG21	22:UV:935:GLU:HG2	1.98	0.45
22:UV:919:TRP:O	22:UV:922:THR:OG1	2.30	0.45
24:UZ:64:LEU:HB3	24:UZ:65:PHE:HD1	1.81	0.45
25:CB:212:LYS:HA	26:CD:259:MET:HE3	1.99	0.45
29:CH:249:LYS:HA	29:CH:249:LYS:HD2	1.75	0.45
29:CH:409:ASP:OD1	29:CH:412:HIS:N	2.46	0.45
31:CJ:23:SER:O	31:CJ:26:GLN:HB3	2.17	0.45
33:CL:80:THR:HG23	33:CL:172:THR:HG21	1.98	0.45
33:CL:1056:LYS:HA	33:CL:1056:LYS:HD3	1.75	0.45
36:JA:19:GLN:NE2	36:JA:219:LEU:HD12	2.31	0.45
36:JA:545:HIS:ND1	36:JA:547:LYS:O	2.50	0.45
38:JE:247:GLU:CD	54:DJ:78:ARG:HH11	2.19	0.45
44:JN:315:THR:HG21	44:JN:320:ILE:HD12	1.98	0.45
46:JP:96:ASN:OD1	46:JP:97:MET:N	2.50	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
51:DG:169:TYR:HE2	66:D3:73:U:C4	2.35	0.45
52:DH:28:GLU:O	52:DH:35:LYS:HB2	2.15	0.45
52:DH:70:PHE:O	52:DH:74:GLN:CB	2.50	0.45
66:D3:149:C:H2'	66:D3:150:U:H6	1.82	0.45
66:D3:364:G:H2'	66:D3:366:A:C8	2.52	0.45
66:D3:450:U:H2'	66:D3:451:A:H8	1.82	0.45
66:D3:1498:G:H2'	66:D3:1499:G:H8	1.81	0.45
66:D3:1688:U:H3	66:D3:1713:G:H22	1.65	0.45
2:UB:465:LYS:HG2	2:UB:466:TYR:CZ	2.52	0.45
4:UD:636:ILE:HG12	4:UD:648:PHE:CD1	2.51	0.45
6:UF:196:LEU:HD12	6:UF:196:LEU:HA	1.81	0.45
10:UJ:381:ARG:NH1	17:UQ:856:GLU:OE1	2.49	0.45
12:UL:436:CYS:HA	12:UL:447:LEU:HD23	1.99	0.45
13:UM:41:ASN:OD1	13:UM:55:LYS:HG2	2.17	0.45
17:UQ:215:VAL:HA	17:UQ:218:LYS:HB2	1.99	0.45
21:UU:428:GLU:HG2	21:UU:451:GLY:HA3	1.99	0.45
24:UZ:104:LYS:HE2	24:UZ:104:LYS:HB2	1.73	0.45
27:CE:149:ARG:HH21	27:CE:154:PHE:HB2	1.80	0.45
27:CE:193:PRO:HD2	27:CE:242:SER:HB2	1.98	0.45
28:CG:105:ASN:OD1	28:CG:106:ASP:N	2.50	0.45
31:CJ:139:LEU:HD23	31:CJ:266:LEU:HD21	1.98	0.45
33:CL:210:VAL:HG12	33:CL:213:GLY:H	1.82	0.45
33:CL:830:ARG:HG3	33:CL:831:ARG:O	2.16	0.45
37:JC:185:HIS:CD2	37:JC:233:THR:HA	2.52	0.45
51:DG:160:ARG:NH1	66:D3:68:A:OP1	2.30	0.45
52:DH:38:LEU:HA	52:DH:41:LEU:HB2	1.99	0.45
56:DN:20:ARG:NH2	66:D3:861:U:O3'	2.50	0.45
62:DY:88:THR:HA	62:DY:91:LEU:HB2	1.99	0.45
65:D2:377:U:H2'	65:D2:378:C:H6	1.81	0.45
66:D3:912:U:H4'	66:D3:913:G:H5'	1.98	0.45
66:D3:1216:C:O2'	66:D3:1218:G:N2	2.50	0.45
66:D3:1486:G:H8	66:D3:1486:G:H5"	1.81	0.45
1:UA:163:THR:O	1:UA:163:THR:OG1	2.35	0.45
2:UB:441:TYR:CE2	2:UB:619:LEU:HB2	2.52	0.45
6:UF:106:ASP:O	6:UF:109:PHE:N	2.49	0.45
11:UK:93:MET:HA	11:UK:96:VAL:HG12	1.97	0.45
11:UK:103:ASP:HB3	11:UK:218:MET:HE1	1.98	0.45
13:UM:77:THR:HG21	13:UM:117:LEU:HD22	1.98	0.45
15:UO:431:LEU:O	15:UO:434:ARG:HG2	2.17	0.45
17:UQ:64:LYS:HZ3	17:UQ:123:GLY:H	1.65	0.45
17:UQ:440:VAL:HB	17:UQ:765:TRP:CE2	2.51	0.45


		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
19:US:472:HIS:CG	19:US:473:TYR:H	2.34	0.45
21:UU:240:ARG:HH21	21:UU:243:THR:HB	1.81	0.45
22:UV:523:TYR:CD2	22:UV:616:LYS:HD2	2.52	0.45
22:UV:579:LYS:HB2	22:UV:618:ILE:HG22	1.99	0.45
28:CG:51:PHE:CZ	28:CG:102:ILE:HD13	2.52	0.45
29:CH:476:THR:OG1	29:CH:490:GLY:O	2.26	0.45
32:CK:340:LEU:HD12	32:CK:340:LEU:HA	1.73	0.45
32:CK:538:LYS:HG2	66:D3:1628:U:N3	2.31	0.45
34:CM:108:PRO:HB2	34:CM:174:ILE:HG12	1.99	0.45
37:JC:62:ILE:HG13	37:JC:332:ALA:HB2	1.98	0.45
39:JG:40:ARG:HH11	39:JG:172:PRO:HG3	1.79	0.45
39:JG:90:ASP:HA	39:JG:134:PHE:HE2	1.82	0.45
46:JP:196:THR:HG22	46:JP:204:TRP:HE1	1.82	0.45
51:DG:214:LYS:HA	51:DG:214:LYS:HD2	1.77	0.45
54:DJ:23:ARG:HH21	54:DJ:23:ARG:HD3	1.62	0.45
66:D3:914:G:H5'	66:D3:914:G:C8	2.51	0.45
66:D3:1708:U:H2'	66:D3:1709:C:C2	2.52	0.45
1:UA:592:ILE:HD13	1:UA:592:ILE:HG21	1.72	0.45
4:UD:235:LYS:HE3	4:UD:235:LYS:HB3	1.85	0.45
4:UD:479:LYS:HD3	4:UD:479:LYS:HA	1.86	0.45
16:UP:194:LYS:HB3	16:UP:194:LYS:HE2	1.57	0.45
17:UQ:216:SER:HA	17:UQ:222:HIS:HA	1.99	0.45
17:UQ:379:LEU:HD23	17:UQ:379:LEU:HA	1.67	0.45
18:UR:352:GLN:HE22	18:UR:377:LEU:HD13	1.82	0.45
25:CB:264:GLN:N	25:CB:320:TYR:O	2.50	0.45
26:CD:372:LYS:HD2	26:CD:372:LYS:H	1.82	0.45
31:CJ:281:ILE:HG23	66:D3:562:G:C6	2.51	0.45
32:CK:430:LEU:HD13	44:JN:203:ILE:HD12	1.99	0.45
34:CM:298:ILE:HD13	34:CM:298:ILE:HA	1.79	0.45
37:JC:180:THR:HG21	37:JC:199:THR:HB	1.99	0.45
37:JC:253:TYR:HB3	37:JC:255:TYR:CE1	2.52	0.45
41:JJ:96:SER:HA	41:JJ:139:LEU:O	2.17	0.45
49:DE:98:ASN:H	49:DE:113:ARG:NH1	2.15	0.45
50:DF:165:LEU:HA	50:DF:165:LEU:HD12	1.76	0.45
60:DW:3:ARG:HH21	66:D3:865:A:H4'	1.81	0.45
66:D3:1684:U:H3	66:D3:1717:G:H1	1.64	0.45
4:UD:488:ILE:HB	4:UD:496:PHE:HB2	1.99	0.44
4:UD:579:ARG:NH2	4:UD:659:PHE:HB2	2.32	0.44
4:UD:622:LEU:O	4:UD:627:LYS:NZ	2.50	0.44
5:UE:169:SER:O	5:UE:169:SER:OG	2.32	0.44
8:UH:161:ASP:O	8:UH:163:PHE:N	2.50	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:UI:487:ARG:NH1	65:D2:8:A:O2'	2.50	0.44
10:UJ:1544:PHE:O	10:UJ:1548:PHE:N	2.48	0.44
10:UJ:1588:GLY:HA2	10:UJ:1633:ASP:HA	1.99	0.44
11:UK:180:ASN:HB2	11:UK:186:PRO:HG3	1.98	0.44
12:UL:298:LYS:O	12:UL:301:LYS:HG2	2.17	0.44
13:UM:602:TRP:CG	13:UM:609:CYS:HA	2.52	0.44
15:UO:51:HIS:HB3	15:UO:53:HIS:CE1	2.52	0.44
17:UQ:586:SER:OG	17:UQ:587:PHE:N	2.49	0.44
18:UR:514:LEU:HD22	18:UR:540:ALA:HB1	1.99	0.44
19:US:456:THR:O	19:US:458:ALA:N	2.43	0.44
21:UU:177:LEU:O	21:UU:179:LYS:HG3	2.17	0.44
22:UV:519:ASP:N	22:UV:519:ASP:OD1	2.50	0.44
25:CB:145:ASN:HB2	25:CB:148:ARG:HB2	1.98	0.44
28:CF:32:GLN:O	28:CF:103:THR:HG22	2.17	0.44
29:CH:415:THR:HG1	29:CH:425:TRP:HE1	1.64	0.44
31:CJ:89:ILE:HD11	31:CJ:136:THR:HG21	1.99	0.44
31:CJ:186:ASN:HB3	31:CJ:214:PRO:HB3	1.99	0.44
33:CL:280:LEU:HD12	33:CL:281:PRO:HD2	1.97	0.44
37:JC:189:ASN:ND2	37:JC:236:PHE:HB2	2.33	0.44
51:DG:7:TYR:CE1	51:DG:9:VAL:HB	2.53	0.44
51:DG:37:ASP:N	51:DG:37:ASP:OD1	2.50	0.44
57:DO:47:LYS:HD3	57:DO:47:LYS:HA	1.77	0.44
65:D2:132:C:H2'	65:D2:133:U:C6	2.52	0.44
65:D2:180:G:H2'	65:D2:181:A:C8	2.51	0.44
5:UE:203:ILE:HG12	5:UE:214:VAL:HG22	1.98	0.44
6:UF:152:LYS:O	6:UF:156:GLU:HG2	2.18	0.44
7:UG:106:LEU:HA	7:UG:106:LEU:HD23	1.77	0.44
10:UJ:271:LYS:HA	18:UR:220:ASP:HB2	1.99	0.44
10:UJ:333:LEU:HD12	10:UJ:333:LEU:HA	1.73	0.44
11:UK:58:ARG:HD3	33:CL:1076:GLU:O	2.17	0.44
13:UM:111:ASP:OD1	13:UM:112:SER:N	2.50	0.44
13:UM:442:LEU:HD13	13:UM:445:ILE:HD11	1.99	0.44
17:UQ:210:HIS:CE1	17:UQ:226:SER:HB3	2.53	0.44
18:UR:408:CYS:SG	18:UR:458:ILE:HG23	2.57	0.44
18:UR:471:LEU:HD23	18:UR:471:LEU:HA	1.72	0.44
21:UU:21:SER:OG	21:UU:24:PHE:O	2.35	0.44
25:CA:212:LYS:HZ3	27:CE:243:MET:HG3	1.83	0.44
27:CE:245:THR:OG1	27:CE:246:GLU:N	2.50	0.44
29:CH:307:TYR:HD2	29:CH:314:GLN:HA	1.82	0.44
32:CK:453:SER:O	32:CK:453:SER:OG	2.31	0.44
33:CL:228:SER:O	33:CL:228:SER:OG	2.32	0.44



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
33:CL:753:LEU:HD12	33:CL:753:LEU:HA	1.69	0.44
33:CL:978:ARG:HE	33:CL:978:ARG:HB3	1.56	0.44
38:JE:320:ILE:HD11	54:DJ:48:GLN:OE1	2.17	0.44
46:JP:297:SER:OG	46:JP:299:ASN:O	2.33	0.44
51:DG:77:LEU:HB3	51:DG:84:TYR:CG	2.53	0.44
53:DI:101:ILE:HD13	53:DI:101:ILE:HA	1.82	0.44
66:D3:682:C:H2'	66:D3:683:C:C6	2.52	0.44
1:UA:663:GLY:HA3	30:CI:147:ALA:O	2.17	0.44
4:UD:525:VAL:HA	4:UD:526:PRO:HD3	1.80	0.44
5:UE:436:THR:C	19:US:294:LYS:HZ3	2.21	0.44
9:UI:417:LYS:O	9:UI:421:LEU:HG	2.18	0.44
11:UK:54:LYS:HE3	65:D2:453:A:H5"	1.98	0.44
12:UL:553:ASN:HA	12:UL:575:PRO:HA	2.00	0.44
15:UO:221:VAL:HG23	15:UO:260:TYR:CG	2.53	0.44
17:UQ:220:HIS:ND1	65:D2:21:A:H5"	2.33	0.44
17:UQ:744:ILE:HA	17:UQ:755:GLY:O	2.17	0.44
22:UV:310:PRO:HB3	22:UV:330:PRO:HA	1.98	0.44
22:UV:315:ILE:HB	22:UV:553:VAL:HG23	1.99	0.44
22:UV:378:ASN:N	22:UV:378:ASN:OD1	2.50	0.44
22:UV:1116:SER:O	22:UV:1116:SER:OG	2.33	0.44
23:UX:112:LYS:NZ	44:JN:303:GLU:O	2.51	0.44
25:CB:93:HIS:CE1	25:CB:162:LEU:H	2.35	0.44
25:CB:302:GLU:HB3	25:CB:317:VAL:HG22	1.99	0.44
26:CD:251:VAL:HA	26:CD:254:ASN:HB2	1.98	0.44
28:CG:33:LEU:HD11	28:CG:100:ALA:HB1	1.99	0.44
28:CG:58:CYS:HG	28:CG:61:ILE:HA	1.82	0.44
28:CG:65:LEU:O	28:CG:68:PRO:HD2	2.17	0.44
29:CH:295:LEU:O	29:CH:306:THR:HA	2.17	0.44
30:CI:38:ILE:HG21	30:CI:38:ILE:HD13	1.64	0.44
36:JA:737:TRP:O	36:JA:740:ASN:O	2.34	0.44
36:JA:827:ARG:HA	36:JA:830:LEU:HD12	1.98	0.44
44:JN:268:LYS:O	44:JN:270:GLY:N	2.50	0.44
46:JP:456:GLU:HA	46:JP:459:LYS:HE2	1.98	0.44
53:DI:74:LYS:HA	53:DI:74:LYS:HD3	1.81	0.44
56:DN:46:THR:O	56:DN:50:ILE:HG12	2.17	0.44
66:D3:406:U:H2'	66:D3:407:A:C8	2.53	0.44
66:D3:533:U:H2'	66:D3:534:A:H8	1.82	0.44
67:D4:310:G:H2'	67:D4:311:G:H8	1.81	0.44
1:UA:27:LYS:HG2	1:UA:43:ILE:HD12	1.99	0.44
1:UA:125:PRO:HD3	1:UA:136:PHE:HE1	1.83	0.44
1:UA:315:GLU:HA	1:UA:332:TRP:HE1	1.82	0.44



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:UD:279:HIS:HB3	4:UD:305:PHE:CE1	2.53	0.44
5:UE:252:SER:OG	5:UE:253:LEU:N	2.51	0.44
5:UE:492:THR:HB	5:UE:533:ARG:HH21	1.82	0.44
7:UG:48:LYS:O	7:UG:52:GLN:HG3	2.18	0.44
8:UH:168:LYS:HA	8:UH:179:LYS:HA	2.00	0.44
8:UH:659:THR:CG2	9:UI:507:ARG:HH21	2.30	0.44
11:UK:185:MET:HG3	11:UK:189:SER:HB3	2.00	0.44
12:UL:125:THR:OG1	12:UL:126:LEU:N	2.49	0.44
12:UL:446:ILE:HD13	12:UL:456:LEU:HB3	2.00	0.44
12:UL:860:ILE:HD12	12:UL:860:ILE:HA	1.75	0.44
13:UM:405:THR:HB	13:UM:413:ILE:HG23	1.99	0.44
17:UQ:259:VAL:HG23	17:UQ:273:VAL:HG13	2.00	0.44
19:US:254:LYS:HZ1	19:US:288:HIS:CD2	2.35	0.44
21:UU:367:LEU:HA	21:UU:367:LEU:HD23	1.81	0.44
22:UV:439:HIS:CE1	22:UV:458:ILE:HB	2.52	0.44
22:UV:459:ASP:OD1	22:UV:459:ASP:N	2.42	0.44
27:CE:348:VAL:HG22	27:CE:359:ILE:HG22	1.98	0.44
32:CK:509:LEU:HD23	32:CK:509:LEU:HA	1.74	0.44
32:CK:534:ARG:NH2	66:D3:1628:U:OP2	2.50	0.44
33:CL:830:ARG:HD2	33:CL:880:TYR:CE1	2.51	0.44
33:CL:1019:THR:O	33:CL:1019:THR:OG1	2.24	0.44
37:JC:225:ASP:OD2	37:JC:227:ARG:NH2	2.50	0.44
39:JG:182:PHE:CE1	39:JG:231:PRO:HA	2.47	0.44
42:JK:489:GLN:NE2	42:JK:490:ILE:HG22	2.33	0.44
65:D2:496:G:O6	65:D2:497:A:N6	2.51	0.44
66:D3:309:C:H2'	66:D3:310:C:H6	1.82	0.44
1:UA:106:PRO:HG2	1:UA:158:SER:HB3	2.00	0.44
4:UD:532:ASN:HB3	4:UD:533:HIS:CE1	2.52	0.44
5:UE:435:GLY:O	19:US:294:LYS:NZ	2.37	0.44
10:UJ:86:GLN:HB2	10:UJ:91:ILE:HD11	2.00	0.44
12:UL:279:LYS:HG2	12:UL:336:TYR:O	2.17	0.44
12:UL:661:TRP:NE1	12:UL:677:HIS:HB2	2.32	0.44
13:UM:16:TYR:HB3	13:UM:335:GLY:HA3	2.00	0.44
22:UV:518:PHE:CE2	22:UV:1075:LEU:HB3	2.53	0.44
22:UV:584:GLU:OE1	22:UV:614:ARG:NH1	2.50	0.44
22:UV:933:LEU:O	22:UV:937:ILE:HG12	2.17	0.44
24:UZ:73:LEU:HD13	24:UZ:99:GLU:HB3	1.98	0.44
26:CD:74:VAL:HG13	26:CD:78:LEU:HD23	1.98	0.44
26:CD:225:ASP:N	26:CD:225:ASP:OD1	2.51	0.44
31:CJ:51:SER:OG	31:CJ:52:LEU:N	2.51	0.44
34:CM:303:ILE:HD11	34:CM:359:PHE:CD1	2.52	0.44



A 4 1	A 4 a a a a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
36:JA:746:TYR:HB3	36:JA:761:VAL:HG12	1.98	0.44
45:JO:117:LEU:HD12	45:JO:117:LEU:HA	1.82	0.44
46:JP:290:ASP:OD1	46:JP:291:MET:N	2.51	0.44
66:D3:1174:C:O2'	66:D3:1175:U:O4'	2.36	0.44
66:D3:1274:C:H2'	66:D3:1275:A:C8	2.53	0.44
1:UA:745:LEU:HD12	1:UA:745:LEU:HA	1.80	0.44
2:UB:512:ASP:OD1	2:UB:512:ASP:N	2.50	0.44
5:UE:174:ASP:O	5:UE:178:LYS:HA	2.16	0.44
5:UE:245:ALA:HB2	5:UE:296:ILE:HD12	1.99	0.44
5:UE:469:ILE:O	5:UE:509:HIS:NE2	2.49	0.44
7:UG:485:ASP:OD1	7:UG:486:VAL:N	2.50	0.44
9:UI:439:LYS:HA	9:UI:442:THR:HG22	1.98	0.44
12:UL:137:ILE:HG23	12:UL:147:VAL:HG22	1.99	0.44
12:UL:488:LEU:HD23	12:UL:488:LEU:HA	1.80	0.44
15:UO:212:ASP:N	15:UO:212:ASP:OD1	2.50	0.44
15:UO:315:ASN:N	15:UO:315:ASN:OD1	2.50	0.44
17:UQ:175:ALA:O	17:UQ:187:VAL:HA	2.17	0.44
19:US:340:LYS:HA	19:US:340:LYS:HD2	1.70	0.44
21:UU:155:THR:OG1	21:UU:156:LYS:N	2.51	0.44
21:UU:735:LEU:HD23	21:UU:735:LEU:HA	1.74	0.44
22:UV:731:LYS:NZ	22:UV:735:ASP:OD1	2.47	0.44
24:UZ:85:GLU:OE2	24:UZ:86:THR:OG1	2.34	0.44
24:UZ:163:LYS:HA	24:UZ:163:LYS:HD2	1.82	0.44
26:CD:96:ILE:HA	26:CD:96:ILE:HD13	1.76	0.44
29:CH:522:THR:HG23	29:CH:548:ARG:HG2	1.99	0.44
34:CM:23:LEU:HD23	34:CM:23:LEU:HA	1.73	0.44
34:CM:53:LEU:HA	34:CM:53:LEU:HD23	1.73	0.44
36:JA:817:ASP:HB2	36:JA:820:HIS:HD1	1.82	0.44
37:JC:166:ASN:OD1	37:JC:167:LEU:N	2.51	0.44
37:JC:200:GLU:OE1	37:JC:230:GLN:NE2	2.48	0.44
39:JF:63:ASP:OD1	39:JF:63:ASP:N	2.50	0.44
46:JP:66:HIS:HD1	46:JP:87:SER:HB3	1.82	0.44
51:DG:30:LYS:H	51:DG:102:VAL:HG12	1.81	0.44
55:DL:115:PHE:HB3	55:DL:142:VAL:HG21	1.99	0.44
61:DX:61:SER:O	61:DX:69:ARG:HD3	2.17	0.44
66:D3:157:A:O2'	66:D3:158:U:O4'	2.27	0.44
66:D3:369:A:H2'	66:D3:370:A:C8	2.53	0.44
2:UB:428:VAL:O	2:UB:432:HIS:HB2	2.17	0.44
3:UC:502:LYS:NZ	66:D3:1499:G:OP1	2.50	0.44
3:UC:503:GLN:OE1	3:UC:506:LYS:NZ	2.49	0.44
4:UD:117:ILE:HD11	4:UD:147:ILE:HB	1.99	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:UE:487:ARG:HB2	5:UE:487:ARG:HH11	1.82	0.44
10:UJ:32:SER:OG	10:UJ:33:LEU:N	2.51	0.44
11:UK:166:LEU:HD12	11:UK:170:GLN:HB3	2.00	0.44
17:UQ:581:GLY:HA2	17:UQ:602:PRO:HD2	1.99	0.44
18:UR:562:LEU:HA	18:UR:562:LEU:HD23	1.77	0.44
19:US:1:MET:O	19:US:5:ILE:N	2.47	0.44
19:US:345:ILE:HG23	19:US:382:LYS:HE2	1.99	0.44
33:CL:64:GLU:N	33:CL:64:GLU:OE2	2.49	0.44
33:CL:815:LEU:HA	33:CL:815:LEU:HD23	1.72	0.44
36:JA:14:ILE:HD12	36:JA:43:LEU:HD22	2.00	0.44
36:JA:545:HIS:HB2	36:JA:637:ARG:NH2	2.33	0.44
39:JG:156:GLU:OE1	39:JG:157:GLU:HG2	2.17	0.44
43:JM:203:LYS:HE2	43:JM:203:LYS:HB2	1.78	0.44
45:JO:295:ARG:HH22	66:D3:317:C:P	2.41	0.44
48:DA:130:SER:HB2	48:DA:180:THR:HG22	2.00	0.44
52:DH:5:GLN:HG2	52:DH:6:ALA:H	1.82	0.44
65:D2:193:G:H2'	65:D2:194:G:H8	1.83	0.44
66:D3:1688:U:H2'	66:D3:1689:A:C8	2.53	0.44
4:UD:552:ILE:HB	4:UD:563:LEU:HD11	1.98	0.44
7:UG:230:THR:O	7:UG:230:THR:OG1	2.32	0.44
10:UJ:210:LEU:HD21	10:UJ:253:CYS:HA	1.99	0.44
12:UL:495:LYS:HE2	12:UL:495:LYS:HB2	1.74	0.44
12:UL:655:ALA:HB2	12:UL:684:TRP:CH2	2.53	0.44
13:UM:154:GLY:HA3	13:UM:161:TRP:CD1	2.52	0.44
15:UO:21:THR:HG22	15:UO:24:GLN:CD	2.38	0.44
15:UO:413:LEU:HD23	15:UO:413:LEU:HA	1.80	0.44
19:US:407:ARG:HE	19:US:491:LEU:HD13	1.83	0.44
21:UU:503:ARG:HD2	21:UU:523:ASP:HB3	1.98	0.44
21:UU:866:ASP:O	21:UU:869:THR:OG1	2.30	0.44
22:UV:800:GLU:O	22:UV:804:THR:HG23	2.18	0.44
22:UV:1160:SER:HA	22:UV:1190:PHE:HD2	1.83	0.44
25:CA:212:LYS:NZ	27:CE:243:MET:O	2.45	0.44
26:CD:52:SER:OG	26:CD:53:PHE:N	2.50	0.44
27:CE:371:LEU:HD23	27:CE:371:LEU:HA	1.66	0.44
28:CG:58:CYS:SG	28:CG:61:ILE:HA	2.58	0.44
31:CJ:171:VAL:HG21	31:CJ:253:ARG:HD3	1.99	0.44
33:CL:780:ILE:HG22	34:CM:336:GLU:HB3	1.99	0.44
33:CL:1113:ILE:HA	33:CL:1113:ILE:HD13	1.80	0.44
36:JA:45:MET:O	36:JA:48:ASP:O	2.36	0.44
37:JC:297:ALA:HB3	37:JC:311:MET:HG3	2.00	0.44
38:JE:263:GLY:HA3	54:DJ:138:LYS:HE3	1.99	0.44



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
41:JJ:120:LEU:HD11	41:JJ:159:ILE:HD11	2.00	0.44
43:JM:122:LEU:HD23	43:JM:122:LEU:HA	1.78	0.44
49:DE:71:LYS:HG2	49:DE:76:VAL:HG22	1.99	0.44
52:DH:98:ILE:HG13	52:DH:100:PRO:HD3	1.98	0.44
56:DN:3:ARG:HD3	56:DN:3:ARG:HA	1.84	0.44
62:DY:57:VAL:HG12	62:DY:73:GLY:HA3	2.00	0.44
66:D3:412:A:N3	66:D3:422:G:N2	2.65	0.44
66:D3:1266:U:H5"	66:D3:1267:G:H5'	1.99	0.44
2:UB:515:HIS:CD2	2:UB:517:VAL:H	2.36	0.44
5:UE:109:ASP:O	5:UE:119:CYS:HA	2.17	0.44
5:UE:210:ARG:HH21	5:UE:210:ARG:HD2	1.68	0.44
5:UE:481:LEU:HD22	5:UE:502:VAL:HG23	1.99	0.44
7:UG:142:GLY:O	10:UJ:8:LEU:HB3	2.18	0.44
9:UI:484:SER:HB3	65:D2:10:C:OP1	2.18	0.44
11:UK:94:ASP:OD1	11:UK:94:ASP:N	2.50	0.44
12:UL:530:LEU:HD13	12:UL:550:LEU:HD21	1.99	0.44
30:CI:40:ASN:HB3	30:CI:42:GLU:HG2	1.99	0.44
31:CJ:43:PRO:HD2	31:CJ:46:LEU:HD12	1.98	0.44
33:CL:623:LYS:HB3	33:CL:623:LYS:HE3	1.74	0.44
34:CM:14:SER:HB3	34:CM:36:ILE:HG23	1.99	0.44
37:JC:179:ASP:OD1	37:JC:179:ASP:N	2.37	0.44
60:DW:2:THR:OG1	66:D3:634:G:O2'	2.34	0.44
62:DY:2:SER:OG	62:DY:3:ASP:N	2.51	0.44
66:D3:1662:G:H2'	66:D3:1663:G:C8	2.51	0.44
1:UA:44:ASN:O	1:UA:46:LYS:HG2	2.18	0.43
5:UE:24:LEU:HD23	5:UE:24:LEU:HA	1.66	0.43
5:UE:131:LEU:HA	5:UE:131:LEU:HD23	1.76	0.43
6:UF:167:ILE:HD11	14:UN:327:PHE:CE1	2.53	0.43
10:UJ:63:GLU:HA	10:UJ:64:PRO:HD3	1.82	0.43
12:UL:537:VAL:HA	12:UL:547:ALA:O	2.17	0.43
15:UO:133:HIS:HB2	15:UO:139:ILE:HG13	1.99	0.43
17:UQ:363:ASN:ND2	17:UQ:368:ASP:OD2	2.43	0.43
22:UV:188:SER:HA	22:UV:191:LEU:HD12	1.99	0.43
22:UV:380:SER:OG	22:UV:479:LYS:O	2.26	0.43
22:UV:853:ARG:HD3	22:UV:889:TYR:CZ	2.53	0.43
22:UV:1213:ILE:HG12	22:UV:1214:LEU:HD23	1.99	0.43
29:CH:551:ARG:O	29:CH:553:ILE:N	2.51	0.43
30:CI:56:ARG:HH11	30:CI:56:ARG:HD3	1.61	0.43
33:CL:75:VAL:HG22	33:CL:120:CYS:SG	2.58	0.43
36:JA:879:SER:HB3	36:JA:881:GLN:HG2	2.00	0.43
39:JF:125:ASN:OD1	39:JF:125:ASN:N	2.49	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
43:JM:215:LYS:HG2	43:JM:216:ARG:HH11	1.83	0.43
45:JO:96:LYS:HA	45:JO:96:LYS:HD2	1.80	0.43
54:DJ:109:LEU:HB2	54:DJ:146:PHE:HB3	1.99	0.43
65:D2:194:G:H2'	65:D2:195:A:C8	2.52	0.43
66:D3:1034:C:O2	66:D3:1084:A:N6	2.51	0.43
66:D3:1272:U:H2'	66:D3:1273:G:C8	2.52	0.43
1:UA:424:THR:O	1:UA:424:THR:OG1	2.29	0.43
4:UD:199:ASP:CA	4:UD:215:ALA:O	2.65	0.43
4:UD:332:ASP:N	4:UD:332:ASP:OD1	2.51	0.43
12:UL:75:ARG:HE	12:UL:75:ARG:HB2	1.62	0.43
12:UL:656:HIS:HB3	12:UL:682:ARG:NH1	2.33	0.43
14:UN:294:GLU:O	14:UN:297:LYS:HB3	2.18	0.43
15:UO:278:ASP:HA	19:US:331:ASN:HD21	1.82	0.43
18:UR:22:LEU:HA	18:UR:22:LEU:HD23	1.76	0.43
19:US:201:GLN:O	19:US:204:GLU:HG3	2.18	0.43
21:UU:114:THR:OG1	21:UU:115:ASP:N	2.52	0.43
22:UV:864:LEU:HD23	22:UV:864:LEU:HA	1.87	0.43
23:UX:68:ASP:OD1	23:UX:69:THR:N	2.49	0.43
26:CD:248:ALA:O	26:CD:252:ILE:HG12	2.18	0.43
34:CM:118:PHE:O	34:CM:165:GLU:HA	2.18	0.43
35:CN:147:LEU:HD21	35:CN:154:GLU:HB2	2.00	0.43
36:JA:788:LEU:HB3	36:JA:793:PHE:CZ	2.53	0.43
37:JC:93:PHE:HE2	37:JC:95:ARG:HB2	1.83	0.43
38:JE:236:ARG:HB3	38:JE:239:LYS:HD3	1.99	0.43
39:JF:143:GLN:HE22	39:JF:150:ILE:HG13	1.83	0.43
44:JN:316:ARG:HD3	66:D3:1036:A:H1'	1.98	0.43
46:JP:49:LYS:NZ	67:D4:25:U:OP2	2.40	0.43
46:JP:263:ARG:HG2	46:JP:264:THR:O	2.18	0.43
51:DG:101:ILE:HD13	51:DG:101:ILE:HA	1.88	0.43
58:DQ:110:THR:HG23	58:DQ:114:ARG:HG3	1.99	0.43
66:D3:52:U:H2'	66:D3:53:G:C8	2.53	0.43
66:D3:105:A:H62	66:D3:308:C:N4	2.17	0.43
66:D3:355:G:H2'	66:D3:356:G:C8	2.53	0.43
66:D3:380:U:H2'	66:D3:381:C:C6	2.52	0.43
66:D3:1270:G:H2'	66:D3:1271:G:C8	2.53	0.43
3:UC:540:ILE:HD12	3:UC:540:ILE:HG23	1.79	0.43
7:UG:138:ASP:O	7:UG:140:ARG:N	2.49	0.43
7:UG:497:LEU:HD22	7:UG:516:VAL:HG13	2.00	0.43
10:UJ:136:LEU:O	10:UJ:140:LEU:HB2	2.18	0.43
10:UJ:270:LEU:HD23	10:UJ:270:LEU:HA	1.78	0.43
10:UJ:372:LYS:HD3	10:UJ:372:LYS:HA	1.83	0.43



A 4 amo 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:209:LEU:HD12	13:UM:209:LEU:HA	1.85	0.43
13:UM:343:MET:HG3	13:UM:353:LEU:HD21	1.99	0.43
13:UM:498:SER:HB3	13:UM:541:PHE:HD2	1.83	0.43
15:UO:21:THR:HG22	15:UO:24:GLN:NE2	2.33	0.43
15:UO:448:LYS:O	15:UO:451:GLU:HB3	2.18	0.43
17:UQ:712:THR:HG22	17:UQ:720:ILE:HD11	2.00	0.43
22:UV:174:TYR:HB3	22:UV:223:ARG:HH11	1.82	0.43
22:UV:708:LEU:HD12	22:UV:708:LEU:HA	1.72	0.43
26:CD:149:ARG:HH12	27:CE:242:SER:C	2.21	0.43
29:CH:545:LYS:HA	29:CH:545:LYS:HD3	1.85	0.43
30:CI:80:ASP:HA	30:CI:91:LYS:HD3	2.00	0.43
33:CL:204:LEU:HD23	33:CL:204:LEU:H	1.83	0.43
34:CM:155:LYS:O	34:CM:165:GLU:N	2.48	0.43
38:JE:304:GLU:O	38:JE:308:GLN:HB2	2.19	0.43
49:DE:59:ARG:NH2	66:D3:446:A:OP2	2.51	0.43
54:DJ:45:ILE:HD13	54:DJ:45:ILE:HA	1.87	0.43
55:DL:85:VAL:HA	55:DL:108:PRO:HA	2.01	0.43
56:DN:120:SER:OG	66:D3:628:G:OP1	2.36	0.43
65:D2:20:C:H2'	65:D2:21:A:C8	2.53	0.43
65:D2:376:U:H2'	65:D2:377:U:H6	1.84	0.43
66:D3:898:A:N1	66:D3:911:U:O2'	2.41	0.43
66:D3:1665:U:OP2	66:D3:1665:U:C6	2.70	0.43
4:UD:32:ILE:HD11	4:UD:751:GLU:HG2	1.99	0.43
5:UE:473:LYS:HA	5:UE:474:PRO:HD3	1.82	0.43
6:UF:167:ILE:HD11	14:UN:327:PHE:CD1	2.53	0.43
6:UF:339:LEU:HB2	6:UF:343:LYS:HZ3	1.83	0.43
12:UL:607:CYS:HB3	66:D3:1133:A:C8	2.53	0.43
17:UQ:143:ASN:OD1	17:UQ:144:VAL:N	2.51	0.43
25:CB:125:VAL:C	25:CB:139:VAL:H	2.21	0.43
25:CB:262:LYS:HB2	25:CB:262:LYS:HE3	1.81	0.43
26:CD:171:ASP:OD2	26:CD:321:SER:OG	2.34	0.43
26:CD:386:ALA:HB2	26:CD:404:LEU:HD22	2.01	0.43
29:CH:162:CYS:CA	29:CH:186:PHE:O	2.33	0.43
33:CL:1021:LEU:HB2	33:CL:1026:LYS:NZ	2.33	0.43
34:CM:274:LYS:O	34:CM:278:GLN:HG2	2.18	0.43
36:JA:72:LYS:HB2	36:JA:72:LYS:HE3	1.85	0.43
39:JF:174:LYS:HG2	39:JF:200:GLU:HG3	2.00	0.43
48:DA:181:LEU:HD12	48:DA:181:LEU:HA	1.69	0.43
49:DE:49:ARG:NH2	66:D3:448:C:OP1	2.51	0.43
50:DF:100:ASN:O	50:DF:102:ARG:N	2.51	0.43
52:DH:27:LEU:O	52:DH:31:SER:OG	2.26	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
53:DI:163:GLY:O	53:DI:164:ARG:NE	2.49	0.43
56:DN:128:TYR:OH	66:D3:964:U:OP1	2.23	0.43
65:D2:117:G:H2'	65:D2:118:A:C8	2.53	0.43
65:D2:215:U:H2'	65:D2:216:U:C6	2.53	0.43
66:D3:376:C:H2'	66:D3:377:G:H8	1.83	0.43
66:D3:575:C:O2'	66:D3:576:G:H8	2.00	0.43
66:D3:1666:U:H3'	66:D3:1666:U:C6	2.53	0.43
66:D3:1683:C:O2'	66:D3:1684:U:O5'	2.36	0.43
4:UD:53:HIS:NE2	4:UD:64:ASP:O	2.43	0.43
6:UF:104:PRO:HG2	26:CD:142:LEU:HD11	2.00	0.43
8:UH:558:CYS:O	8:UH:585:ARG:NH1	2.34	0.43
8:UH:631:SER:HA	8:UH:634:LEU:HD12	2.01	0.43
10:UJ:130:LYS:HD3	10:UJ:130:LYS:HA	1.65	0.43
10:UJ:136:LEU:HD23	10:UJ:136:LEU:HA	1.76	0.43
11:UK:6:HIS:O	11:UK:9:GLN:HB2	2.19	0.43
11:UK:40:ASP:OD2	11:UK:44:LYS:NZ	2.49	0.43
13:UM:672:TYR:HA	13:UM:675:LYS:HG2	1.99	0.43
22:UV:218:ASP:HB3	22:UV:224:CYS:HB3	2.00	0.43
22:UV:584:GLU:HB3	22:UV:614:ARG:HB3	1.99	0.43
22:UV:1188:PRO:HA	22:UV:1191:LYS:HB2	2.01	0.43
24:UZ:243:PHE:HA	24:UZ:252:LEU:O	2.18	0.43
29:CH:313:SER:HB2	62:DY:4:ALA:HA	2.00	0.43
29:CH:425:TRP:CH2	29:CH:432:PRO:HG3	2.53	0.43
31:CJ:123:VAL:HG23	66:D3:1606:C:OP1	2.18	0.43
33:CL:1063:HIS:NE2	43:JM:201:GLY:HA3	2.33	0.43
33:CL:1067:LEU:HD23	33:CL:1067:LEU:H	1.82	0.43
36:JA:590:LEU:HD21	36:JA:594:ILE:HG12	2.00	0.43
36:JB:642:PRO:O	36:JB:645:ALA:HB3	2.17	0.43
37:JC:279:TRP:HZ3	37:JC:281:ASP:HB3	1.83	0.43
41:JJ:105:ARG:HH22	66:D3:1772:C:H4'	1.83	0.43
44:JN:325:ASP:HA	44:JN:328:ARG:HG2	2.00	0.43
49:DE:91:THR:OG1	49:DE:92:LEU:N	2.51	0.43
49:DE:150:PRO:HB2	49:DE:154:ILE:HD12	2.00	0.43
50:DF:29:ILE:HD13	50:DF:29:ILE:HG21	1.76	0.43
54:DJ:30:LEU:HA	54:DJ:30:LEU:HD23	1.75	0.43
62:DY:6:THR:CB	62:DY:28:LEU:O	2.50	0.43
65:D2:522:C:H2'	65:D2:523:U:C6	2.54	0.43
66:D3:187:G:H1'	66:D3:198:A:H61	1.84	0.43
66:D3:327:U:H2'	66:D3:328:A:H8	1.84	0.43
67:D4:198:U:O2'	67:D4:200:C:OP2	2.29	0.43
1:UA:574:SER:O	1:UA:574:SER:OG	2.34	0.43



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:UL:661:TRP:HE1	12:UL:677:HIS:HB2	1.82	0.43
17:UQ:340:ILE:HG12	17:UQ:359:GLN:HB3	2.01	0.43
19:US:195:PHE:CZ	19:US:222:LEU:HD11	2.54	0.43
21:UU:179:LYS:HA	21:UU:191:PHE:O	2.19	0.43
25:CB:164:ILE:HG12	25:CB:170:VAL:HG21	2.00	0.43
27:CE:405:ASP:OD1	27:CE:405:ASP:N	2.50	0.43
28:CG:7:LYS:HD2	28:CG:65:LEU:HD21	2.01	0.43
29:CH:137:GLY:HA3	29:CH:500:LYS:HG3	1.99	0.43
33:CL:290:ILE:HG13	33:CL:812:MET:HG3	2.00	0.43
34:CM:135:TRP:HB3	34:CM:246:VAL:HG11	2.01	0.43
36:JA:219:LEU:O	36:JA:221:PRO:HD3	2.19	0.43
37:JC:358:SER:O	37:JC:361:GLU:HB3	2.19	0.43
41:JJ:216:ILE:HA	41:JJ:263:LEU:HD21	2.01	0.43
43:JM:114:ARG:NH2	43:JM:117:VAL:HG11	2.33	0.43
45:JO:295:ARG:NH1	66:D3:317:C:OP2	2.51	0.43
46:JP:201:ILE:HG21	46:JP:201:ILE:HD13	1.68	0.43
46:JP:228:ASN:HB3	46:JP:269:TRP:CD2	2.54	0.43
62:DY:26:ASP:OD1	62:DY:27:VAL:N	2.52	0.43
65:D2:197:G:N2	65:D2:200:A:OP2	2.51	0.43
66:D3:294:C:H2'	66:D3:295:A:H8	1.84	0.43
66:D3:1496:U:H2'	66:D3:1497:U:H6	1.82	0.43
2:UB:654:LEU:HA	19:US:471:GLU:OE2	2.19	0.43
3:UC:592:GLU:HB2	25:CA:103:GLU:OE2	2.18	0.43
5:UE:121:ASP:OD1	5:UE:122:SER:N	2.51	0.43
7:UG:333:SER:HB2	7:UG:378:VAL:HG21	1.99	0.43
10:UJ:83:ARG:NE	10:UJ:130:LYS:HG3	2.33	0.43
11:UK:246:LYS:HE2	11:UK:246:LYS:HB3	1.94	0.43
12:UL:457:PHE:HA	12:UL:463:SER:O	2.18	0.43
13:UM:53:LEU:HD23	13:UM:53:LEU:HA	1.73	0.43
14:UN:277:ARG:HA	14:UN:280:GLN:HB2	2.00	0.43
15:UO:234:PHE:HE2	15:UO:284:PHE:HE2	1.66	0.43
17:UQ:531:PHE:HD2	17:UQ:545:THR:HB	1.84	0.43
22:UV:307:LYS:HA	22:UV:307:LYS:HD3	1.85	0.43
22:UV:358:SER:O	22:UV:358:SER:OG	2.34	0.43
22:UV:926:LEU:HD23	22:UV:1167:LYS:HD3	2.01	0.43
24:UZ:149:LYS:HD3	24:UZ:149:LYS:HA	1.60	0.43
24:UZ:245:LYS:HB3	24:UZ:251:SER:HA	2.00	0.43
26:CD:137:LYS:NZ	65:D2:481:U:OP2	2.38	0.43
27:CE:159:VAL:HB	27:CE:161:VAL:HG12	2.00	0.43
28:CG:43:THR:HG22	28:CG:49:SER:HB2	2.00	0.43
29:CH:187:ALA:HB3	29:CH:199:TYR:HB2	2.00	0.43



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:CI:97:LEU:HD23	30:CI:97:LEU:HA	1.79	0.43
31:CJ:189:LEU:HB2	32:CK:379:ASP:O	2.19	0.43
33:CL:606:VAL:O	34:CM:15:GLN:NE2	2.50	0.43
33:CL:836:LYS:HB2	33:CL:836:LYS:HE2	1.83	0.43
36:JA:480:ASP:HB3	36:JA:483:GLU:HB3	2.00	0.43
36:JA:630:LEU:HB3	36:JA:722:TYR:CE2	2.50	0.43
39:JG:243:HIS:HA	39:JG:246:GLU:OE1	2.19	0.43
49:DE:92:LEU:HD12	49:DE:92:LEU:HA	1.75	0.43
53:DI:58:LEU:O	53:DI:59:ARG:NH1	2.47	0.43
65:D2:217:C:H2'	65:D2:218:U:C6	2.53	0.43
66:D3:153:G:H2'	66:D3:154:G:C8	2.53	0.43
66:D3:912:U:O2	66:D3:914:G:N1	2.51	0.43
4:UD:537:ASP:HB2	4:UD:575:ILE:HD13	2.01	0.43
5:UE:259:PRO:O	5:UE:273:LYS:NZ	2.39	0.43
5:UE:332:LEU:O	5:UE:334:TRP:N	2.52	0.43
5:UE:345:LEU:H	5:UE:345:LEU:HD12	1.84	0.43
5:UE:445:LEU:HB3	5:UE:476:LEU:HD12	2.01	0.43
7:UG:513:LYS:HE3	7:UG:513:LYS:HB2	1.65	0.43
8:UH:523:LEU:HD23	8:UH:526:LEU:HD12	2.01	0.43
10:UJ:135:LEU:O	10:UJ:139:THR:HG22	2.18	0.43
11:UK:29:GLU:OE2	33:CL:1062:ARG:NH1	2.50	0.43
14:UN:895:LYS:HE3	14:UN:895:LYS:HB2	1.81	0.43
18:UR:427:ASN:OD1	18:UR:428:ALA:N	2.52	0.43
19:US:281:LEU:HA	19:US:285:ILE:HD12	2.00	0.43
21:UU:179:LYS:HD3	21:UU:190:LEU:HD21	2.01	0.43
22:UV:179:LYS:O	22:UV:231:TYR:OH	2.36	0.43
22:UV:465:PRO:HD3	22:UV:482:VAL:HG22	1.99	0.43
26:CD:274:PHE:CE1	27:CE:169:LEU:HD11	2.54	0.43
31:CJ:223:THR:O	31:CJ:233:VAL:HA	2.18	0.43
33:CL:289:HIS:CE1	33:CL:291:ALA:HA	2.54	0.43
34:CM:282:GLU:O	34:CM:286:SER:HB3	2.18	0.43
35:CN:132:ALA:O	35:CN:136:ASN:ND2	2.52	0.43
36:JA:738:LYS:HG3	36:JA:807:SER:HB3	1.99	0.43
36:JA:776:GLU:HA	36:JA:779:LYS:HZ2	1.83	0.43
36:JB:566:VAL:HA	36:JB:584:CYS:O	2.19	0.43
37:JC:10:ASP:N	37:JC:10:ASP:OD1	2.51	0.43
41:JJ:217:GLU:OE1	41:JJ:223:ARG:HA	2.19	0.43
42:JK:462:ARG:HH21	66:D3:341:A:H5"	1.83	0.43
56:DN:35:GLU:HA	56:DN:38:VAL:HG22	2.01	0.43
58:DQ:25:GLY:HA3	58:DQ:64:ASP:OD2	2.19	0.43
65:D2:534:A:N3	65:D2:536:A:N6	2.67	0.43



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
66:D3:875:G:O2'	66:D3:877:G:OP2	2.32	0.43
66:D3:1733:C:H2'	66:D3:1734:U:C6	2.54	0.43
1:UA:361:VAL:HG22	1:UA:371:VAL:HG22	2.01	0.43
3:UC:436:GLY:HA3	39:JG:132:ARG:NH2	2.33	0.43
4:UD:97:ARG:NE	16:UP:193:LYS:HD2	2.34	0.43
4:UD:137:TYR:HB2	4:UD:177:LEU:HD13	1.99	0.43
5:UE:370:LYS:HE3	5:UE:370:LYS:HB2	1.82	0.43
6:UF:31:LEU:HD23	6:UF:31:LEU:HA	1.77	0.43
6:UF:300:MET:HA	6:UF:303:GLU:HB3	2.00	0.43
8:UH:658:LEU:HD23	9:UI:503:LEU:HD21	2.01	0.43
10:UJ:296:LEU:HD12	10:UJ:296:LEU:HA	1.74	0.43
10:UJ:390:LEU:HD12	10:UJ:390:LEU:HA	1.86	0.43
10:UJ:411:ASN:O	10:UJ:415:VAL:HG23	2.19	0.43
11:UK:161:ARG:HD3	11:UK:163:GLU:HG2	2.00	0.43
12:UL:255:ARG:NH1	12:UL:257:LEU:HD11	2.34	0.43
12:UL:326:LEU:HA	12:UL:326:LEU:HD23	1.74	0.43
15:UO:11:SER:OG	15:UO:412:GLU:OE2	2.30	0.43
15:UO:94:LYS:O	15:UO:110:SER:OG	2.21	0.43
17:UQ:225:ILE:HD11	17:UQ:241:LEU:HD12	2.00	0.43
19:US:459:LEU:HD12	19:US:459:LEU:HA	1.75	0.43
21:UU:498:TYR:HD1	50:DF:16:VAL:HG22	1.84	0.43
21:UU:585:SER:OG	21:UU:606:ASP:OD2	2.34	0.43
21:UU:604:SER:OG	21:UU:606:ASP:OD1	2.30	0.43
22:UV:254:LEU:HD11	22:UV:268:LEU:HD21	2.00	0.43
29:CH:144:GLU:N	29:CH:144:GLU:OE2	2.51	0.43
29:CH:548:ARG:H	29:CH:548:ARG:HG3	1.53	0.43
32:CK:297:LEU:HD12	32:CK:297:LEU:HA	1.84	0.43
32:CK:473:THR:OG1	32:CK:487:ALA:O	2.27	0.43
33:CL:1021:LEU:HD23	33:CL:1021:LEU:H	1.83	0.43
34:CM:143:LYS:HB2	34:CM:143:LYS:HE2	1.67	0.43
36:JA:532:ASN:O	36:JA:536:LYS:HG3	2.19	0.43
36:JA:745:VAL:HG21	36:JA:763:LEU:HB2	2.01	0.43
49:DE:201:HIS:CB	49:DE:205:PHE:O	2.62	0.43
51:DG:4:ASN:O	51:DG:110:ALA:HA	2.18	0.43
54:DJ:16:LYS:HB2	54:DJ:16:LYS:HE2	1.84	0.43
55:DL:8:GLN:OE1	55:DL:14:GLN:N	2.52	0.43
56:DN:62:GLN:HE21	56:DN:62:GLN:HB3	1.59	0.43
65:D2:168:G:C6	65:D2:169:A:H2	2.36	0.43
66:D3:382:C:H3'	66:D3:383:G:H8	1.83	0.43
66:D3:640:U:OP2	66:D3:640:U:H4'	2.15	0.43
66:D3:645:C:H2'	66:D3:646:C:C6	2.54	0.43



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
66:D3:1785:U:H2'	66:D3:1786:G:H8	1.81	0.43
1:UA:387:THR:OG1	1:UA:388:SER:N	2.52	0.43
1:UA:715:PHE:HD1	1:UA:716:ASP:HB2	1.84	0.43
4:UD:443:GLY:HA2	4:UD:448:THR:HG23	2.00	0.43
9:UI:417:LYS:HD2	9:UI:455:TRP:CD2	2.54	0.43
10:UJ:152:LEU:HA	10:UJ:152:LEU:HD23	1.86	0.43
12:UL:273:TYR:HB3	12:UL:343:TRP:CZ2	2.54	0.43
12:UL:538:ARG:HH11	12:UL:581:ILE:H	1.67	0.43
12:UL:836:ILE:HD12	12:UL:853:ILE:HG23	2.01	0.43
13:UM:44:ASP:OD1	13:UM:44:ASP:N	2.50	0.43
13:UM:465:LYS:HE2	13:UM:465:LYS:HB3	1.77	0.43
13:UM:529:LEU:HD12	13:UM:560:TRP:CZ3	2.54	0.43
17:UQ:19:LYS:HE2	17:UQ:19:LYS:HB3	1.82	0.43
17:UQ:156:THR:HG22	17:UQ:171:TYR:CE1	2.51	0.43
21:UU:606:ASP:OD1	21:UU:606:ASP:N	2.39	0.43
21:UU:734:LEU:HA	21:UU:734:LEU:HD23	1.73	0.43
26:CD:180:LEU:HD12	27:CE:183:ARG:HG2	2.00	0.43
26:CD:382:LYS:HD3	26:CD:382:LYS:HA	1.74	0.43
33:CL:65:ASP:OD1	33:CL:65:ASP:N	2.48	0.43
34:CM:303:ILE:HD12	34:CM:303:ILE:HA	1.76	0.43
36:JA:891:GLN:HB3	36:JA:893:LYS:HE3	2.01	0.43
37:JC:146:TYR:CZ	37:JC:148:LYS:HA	2.53	0.43
37:JC:236:PHE:HA	37:JC:243:PHE:CD1	2.54	0.43
44:JN:226:ASP:OD1	44:JN:227:LYS:N	2.52	0.43
45:JO:113:ALA:O	45:JO:116:ILE:N	2.51	0.43
46:JP:109:HIS:CD2	46:JP:140:SER:HB2	2.54	0.43
46:JP:210:LYS:HD3	46:JP:210:LYS:HA	1.66	0.43
46:JP:231:GLU:C	46:JP:233:ASP:H	2.21	0.43
46:JP:420:PRO:HD2	46:JP:423:ILE:HD12	2.01	0.43
51:DG:2:LYS:HA	51:DG:16:PHE:O	2.18	0.43
67:D4:99:U:H2'	67:D4:100:U:C6	2.54	0.43
67:D4:246:A:H2'	67:D4:247:U:H4'	2.01	0.43
1:UA:222:LYS:HG3	1:UA:223:ARG:H	1.84	0.42
1:UA:689:THR:O	1:UA:819:THR:OG1	2.36	0.42
7:UG:289:MET:HB2	7:UG:303:ILE:HD11	2.00	0.42
9:UI:417:LYS:NZ	9:UI:454:LEU:HG	2.34	0.42
14:UN:863:MET:HE3	14:UN:864:PRO:HD2	2.00	0.42
15:UO:404:ALA:HB1	15:UO:417:VAL:HG11	2.00	0.42
17:UQ:153:ILE:HB	17:UQ:174:TYR:HB2	2.01	0.42
17:UQ:328:THR:O	17:UQ:328:THR:OG1	2.32	0.42
19:US:341:LEU:HD11	19:US:365:PHE:CD2	2.53	0.42



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
22:UV:1229:ASP:OD1	22:UV:1229:ASP:N	2.52	0.42
23:UX:72:ILE:HA	23:UX:72:ILE:HD13	1.78	0.42
25:CB:144:TRP:CE2	25:CB:183:HIS:HB3	2.54	0.42
28:CG:59:GLU:HA	28:CG:60:PRO:HA	1.90	0.42
29:CH:235:HIS:ND1	29:CH:257:ASP:OD2	2.52	0.42
31:CJ:226:ASN:O	31:CJ:227:ARG:HD3	2.19	0.42
33:CL:140:LEU:HD12	33:CL:140:LEU:HA	1.82	0.42
33:CL:923:ASP:N	33:CL:923:ASP:OD1	2.52	0.42
33:CL:1135:ARG:HH21	66:D3:495:C:C5'	2.25	0.42
34:CM:176:GLN:HG3	34:CM:305:LYS:HB3	2.00	0.42
35:CN:18:PHE:H	35:CN:35:HIS:H	1.67	0.42
36:JA:201:VAL:HG23	36:JA:207:VAL:HA	1.99	0.42
39:JG:188:ARG:NH1	39:JG:190:GLN:OE1	2.52	0.42
49:DE:37:LYS:HG2	66:D3:297:U:H5"	2.00	0.42
65:D2:151:U:O2'	65:D2:152:U:O4'	2.36	0.42
66:D3:293:U:H2'	66:D3:294:C:C6	2.54	0.42
1:UA:430:ARG:O	32:CK:458:PRO:HD2	2.19	0.42
5:UE:84:GLU:OE1	5:UE:86:TRP:NE1	2.39	0.42
12:UL:791:ASN:OD1	12:UL:792:ALA:N	2.50	0.42
17:UQ:265:ASP:CG	17:UQ:270:GLN:H	2.22	0.42
25:CB:272:LYS:HG3	25:CB:275:CYS:HB3	2.01	0.42
26:CD:185:ASP:OD1	26:CD:285:ARG:NE	2.52	0.42
28:CG:95:ARG:HD3	29:CH:551:ARG:HB2	2.00	0.42
29:CH:486:VAL:HA	29:CH:499:TRP:O	2.19	0.42
36:JA:199:LEU:HA	36:JA:199:LEU:HD23	1.80	0.42
36:JA:827:ARG:HA	36:JA:830:LEU:HB2	2.00	0.42
39:JF:107:ALA:HB2	39:JG:230:TYR:HE2	1.83	0.42
39:JF:132:ARG:HD3	39:JG:88:ARG:HH22	1.83	0.42
45:JO:85:THR:OG1	45:JO:86:ARG:N	2.53	0.42
52:DH:84:LYS:HD3	52:DH:85:PHE:CE1	2.54	0.42
65:D2:125:G:H2'	65:D2:126:A:H8	1.83	0.42
66:D3:151:G:H2'	66:D3:152:U:C6	2.55	0.42
66:D3:355:G:H2'	66:D3:356:G:H8	1.84	0.42
66:D3:1634:C:H2'	66:D3:1635:A:O4'	2.19	0.42
1:UA:515:TYR:CD1	58:DQ:118:ILE:HD13	2.54	0.42
1:UA:802:LEU:HD23	1:UA:802:LEU:HA	1.84	0.42
6:UF:50:ILE:HD12	6:UF:50:ILE:HA	1.83	0.42
8:UH:571:PHE:CD2	8:UH:606:ASP:HB3	2.55	0.42
10:UJ:66:PHE:HZ	10:UJ:105:ALA:HB2	1.83	0.42
12:UL:284:PHE:HD1	12:UL:328:PRO:HA	1.84	0.42
13:UM:267:PHE:HB3	13:UM:281:THR:HG23	2.01	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
17:UQ:276:ALA:O	17:UQ:299:SER:OG	2.24	0.42
19:US:155:LEU:HD23	19:US:155:LEU:HA	1.80	0.42
19:US:254:LYS:HE3	19:US:288:HIS:O	2.20	0.42
21:UU:132:THR:OG1	21:UU:136:SER:OG	2.24	0.42
22:UV:518:PHE:HE2	22:UV:1075:LEU:HB3	1.84	0.42
22:UV:1094:LYS:HD3	22:UV:1094:LYS:HA	1.81	0.42
22:UV:1108:LEU:HD23	22:UV:1108:LEU:HA	1.89	0.42
23:UX:152:ILE:HG13	23:UX:171:PRO:HB2	2.02	0.42
25:CB:146:PRO:HA	25:CB:152:ALA:HB3	2.00	0.42
25:CB:227:PRO:HA	25:CB:230:TYR:CE1	2.54	0.42
33:CL:94:THR:HG21	33:CL:354:ILE:HG22	2.02	0.42
33:CL:848:SER:O	33:CL:848:SER:OG	2.35	0.42
34:CM:68:SER:HB3	34:CM:73:THR:HB	2.00	0.42
36:JA:25:ILE:HA	36:JA:148:VAL:O	2.19	0.42
36:JA:846:SER:HB3	36:JA:918:ARG:CZ	2.49	0.42
37:JC:26:PRO:HB2	37:JC:29:ILE:HG12	2.01	0.42
39:JF:130:ILE:HD11	39:JF:137:PHE:CE1	2.55	0.42
42:JK:497:LEU:HA	42:JK:497:LEU:HD23	1.78	0.42
46:JP:270:ASN:HB3	46:JP:313:PHE:CE1	2.53	0.42
50:DF:88:PRO:O	50:DF:91:GLU:N	2.48	0.42
53:DI:193:LEU:HA	53:DI:193:LEU:HD23	1.85	0.42
56:DN:64:ARG:HH11	56:DN:70:LYS:HE3	1.84	0.42
58:DQ:60:PHE:CZ	58:DQ:89:LEU:HD22	2.54	0.42
60:DW:34:ILE:HG21	60:DW:34:ILE:HD13	1.78	0.42
61:DX:103:LEU:HA	61:DX:103:LEU:HD12	1.82	0.42
66:D3:1666:U:C6	66:D3:1666:U:C3'	3.02	0.42
67:D4:30:A:O2'	67:D4:32:G:O6	2.38	0.42
67:D4:205:G:H1	67:D4:245:U:H1'	1.83	0.42
1:UA:494:ASP:OD2	1:UA:496:THR:OG1	2.37	0.42
2:UB:462:LEU:HD23	2:UB:462:LEU:HA	1.82	0.42
2:UB:469:GLU:O	2:UB:473:GLU:HG3	2.19	0.42
2:UB:548:ARG:HE	2:UB:642:SER:HB2	1.84	0.42
2:UB:798:LYS:HE2	2:UB:798:LYS:HB3	1.95	0.42
4:UD:375:VAL:HG12	4:UD:757:ARG:HH11	1.84	0.42
7:UG:13:LYS:HB2	7:UG:13:LYS:HE3	1.87	0.42
7:UG:42:LEU:HD12	7:UG:42:LEU:HA	1.74	0.42
9:UI:506:LEU:HD23	9:UI:506:LEU:HA	1.69	0.42
12:UL:349:SER:CB	12:UL:369:TYR:O	2.66	0.42
12:UL:611:LEU:HA	12:UL:611:LEU:HD23	1.78	0.42
12:UL:618:ILE:HA	12:UL:634:SER:HA	2.01	0.42
15:UO:21:THR:HG23	15:UO:24:GLN:H	1.85	0.42



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
17:UQ:490:LEU:HB3	17:UQ:491:GLN:H	1.70	0.42
18:UR:165:ARG:HA	21:UU:175:THR:HG21	2.02	0.42
18:UR:225:SER:O	18:UR:227:LEU:N	2.52	0.42
18:UR:503:SER:O	18:UR:504:THR:OG1	2.33	0.42
19:US:183:LYS:HG3	19:US:184:TYR:CD1	2.54	0.42
21:UU:30:ILE:HG21	21:UU:30:ILE:HD13	1.74	0.42
21:UU:131:SER:OG	21:UU:167:ILE:HD13	2.19	0.42
22:UV:126:LYS:HA	22:UV:126:LYS:HD2	1.74	0.42
22:UV:202:SER:OG	22:UV:203:ILE:N	2.53	0.42
26:CD:29:SER:O	26:CD:29:SER:OG	2.32	0.42
27:CE:363:LEU:HD12	27:CE:363:LEU:HA	1.79	0.42
30:CI:165:LYS:HB3	30:CI:165:LYS:HE3	1.74	0.42
33:CL:551:LYS:O	33:CL:555:MET:CB	2.65	0.42
35:CN:165:PHE:HA	35:CN:168:PHE:CD2	2.55	0.42
39:JF:31:LEU:HD13	39:JF:40:ARG:HE	1.84	0.42
39:JF:178:VAL:O	39:JF:204:VAL:HA	2.20	0.42
41:JJ:255:PRO:HA	41:JJ:256:PRO:HD3	1.82	0.42
45:JO:298:GLU:HA	45:JO:301:LYS:HZ2	1.85	0.42
48:DA:11:LYS:HZ1	66:D3:911:U:H3'	1.84	0.42
50:DF:133:VAL:HG22	50:DF:198:LEU:HD13	2.01	0.42
53:DI:69:SER:OG	53:DI:70:GLU:OE1	2.35	0.42
54:DJ:36:LEU:HD23	54:DJ:36:LEU:HA	1.80	0.42
60:DW:69:LEU:HD11	60:DW:72:CYS:HB3	2.01	0.42
65:D2:134:A:H2'	65:D2:135:G:H8	1.84	0.42
65:D2:193:G:H2'	65:D2:194:G:C8	2.54	0.42
1:UA:46:LYS:HB3	1:UA:46:LYS:HE2	1.81	0.42
2:UB:432:HIS:HA	2:UB:435:PHE:HB3	2.00	0.42
3:UC:559:ARG:NH2	66:D3:545:A:H5'	2.35	0.42
5:UE:461:ASP:O	5:UE:465:ILE:HG12	2.20	0.42
7:UG:185:HIS:HE1	30:CI:19:LEU:O	2.03	0.42
8:UH:212:SER:HA	8:UH:219:ALA:HA	2.01	0.42
12:UL:331:THR:OG1	12:UL:332:ILE:N	2.53	0.42
13:UM:593:CYS:HB3	13:UM:623:LEU:HD22	2.01	0.42
13:UM:669:LEU:HD22	13:UM:693:ARG:NH2	2.35	0.42
13:UM:683:LEU:HD23	13:UM:683:LEU:HA	1.81	0.42
15:UO:43:THR:HG22	15:UO:44:HIS:CE1	2.54	0.42
18:UR:140:THR:HG21	18:UR:142:LYS:HZ1	1.84	0.42
21:UU:605:LEU:HA	21:UU:605:LEU:HD12	1.83	0.42
21:UU:763:SER:O	21:UU:763:SER:OG	2.31	0.42
22:UV:801:LYS:NZ	22:UV:836:GLU:OE1	2.33	0.42
22:UV:975:LEU:HD12	22:UV:975:LEU:HA	1.84	0.42



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:UX:27:LYS:NZ	23:UX:28:ASN:OD1	2.52	0.42
23:UX:149:LYS:HG2	23:UX:170:ILE:HD11	2.00	0.42
24:UZ:226:LYS:HA	24:UZ:226:LYS:HD3	1.87	0.42
26:CD:199:TYR:O	26:CD:203:PHE:HB3	2.20	0.42
26:CD:205:GLU:HG3	26:CD:254:ASN:HB3	2.01	0.42
29:CH:161:SER:HB3	29:CH:188:TYR:HB2	2.02	0.42
31:CJ:279:ARG:HA	31:CJ:279:ARG:HD2	1.79	0.42
33:CL:1139:LEU:HD12	33:CL:1139:LEU:HA	1.70	0.42
69:CL:2001:GTP:C8	69:CL:2001:GTP:C5'	2.86	0.42
34:CM:263:ASP:OD1	34:CM:264:ALA:N	2.45	0.42
36:JA:747:LEU:HD11	36:JA:758:HIS:HB2	2.01	0.42
36:JA:879:SER:OG	36:JA:880:VAL:N	2.53	0.42
39:JG:88:ARG:HB3	39:JG:90:ASP:OD1	2.20	0.42
44:JN:235:PRO:HD2	44:JN:238:ILE:HD12	2.01	0.42
46:JP:270:ASN:HB3	46:JP:313:PHE:CD1	2.54	0.42
48:DA:17:LYS:HA	48:DA:17:LYS:HD3	1.89	0.42
49:DE:207:LEU:HD23	49:DE:207:LEU:HA	1.80	0.42
51:DG:135:PRO:HA	66:D3:167:U:H5'	2.02	0.42
51:DG:155:ASP:N	51:DG:155:ASP:OD1	2.35	0.42
51:DG:160:ARG:HH21	51:DG:171:LYS:HD2	1.84	0.42
52:DH:174:ASN:HD21	52:DH:180:GLN:HA	1.83	0.42
65:D2:439:A:N6	65:D2:441:C:N3	2.66	0.42
66:D3:1743:U:H2'	66:D3:1744:A:C8	2.55	0.42
1:UA:308:VAL:HG22	1:UA:319:PHE:CD1	2.55	0.42
1:UA:522:SER:HB2	1:UA:583:ILE:HG23	2.02	0.42
1:UA:844:TYR:CE2	12:UL:899:GLY:HA3	2.55	0.42
2:UB:530:GLU:HG2	2:UB:566:TYR:CE2	2.55	0.42
3:UC:553:LYS:HG2	66:D3:586:G:C2	2.54	0.42
4:UD:541:ALA:HB3	4:UD:553:LEU:HB2	2.02	0.42
6:UF:272:THR:O	6:UF:276:VAL:HG22	2.19	0.42
7:UG:333:SER:O	7:UG:333:SER:OG	2.37	0.42
8:UH:309:PRO:HA	8:UH:330:ARG:HA	2.02	0.42
11:UK:79:ILE:HG21	11:UK:79:ILE:HD13	1.81	0.42
11:UK:250:ARG:O	28:CF:94:SER:OG	2.34	0.42
15:UO:90:ARG:HG3	15:UO:132:PHE:CG	2.55	0.42
17:UQ:43:ASN:HA	17:UQ:57:VAL:HG23	2.02	0.42
17:UQ:604:PHE:HB3	17:UQ:606:HIS:CD2	2.54	0.42
17:UQ:750:LEU:HD12	17:UQ:750:LEU:HA	1.75	0.42
19:US:347:PRO:HB3	19:US:386:LEU:HD22	2.00	0.42
19:US:399:ILE:HG21	19:US:480:LEU:HB3	2.02	0.42
23:UX:30:GLU:H	23:UX:30:GLU:HG3	1.69	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
25:CB:200:SER:OG	25:CB:201:HIS:N	2.52	0.42
26:CD:237:LEU:HA	26:CD:240:LEU:HB2	2.02	0.42
26:CD:322:LEU:HD12	26:CD:322:LEU:HA	1.88	0.42
28:CF:125:LEU:HA	28:CF:125:LEU:HD23	1.84	0.42
30:CI:25:GLN:HE21	30:CI:25:GLN:HB2	1.50	0.42
32:CK:495:ILE:HG21	32:CK:495:ILE:HD13	1.82	0.42
34:CM:19:LEU:HD12	34:CM:19:LEU:HA	1.84	0.42
34:CM:271:LEU:HD12	34:CM:271:LEU:HA	1.85	0.42
36:JA:789:LEU:HD21	36:JA:891:GLN:HG3	2.02	0.42
36:JB:743:VAL:O	36:JB:763:LEU:N	2.48	0.42
42:JK:494:PHE:HA	42:JK:497:LEU:HG	2.01	0.42
45:JO:102:LYS:HE2	45:JO:102:LYS:HB2	1.67	0.42
51:DG:21:GLU:HG2	51:DG:25:ARG:HH12	1.85	0.42
51:DG:28:PHE:CZ	51:DG:104:PRO:HA	2.55	0.42
54:DJ:97:LEU:HA	54:DJ:97:LEU:HD23	1.81	0.42
65:D2:185:A:C6	65:D2:213:G:C6	3.07	0.42
66:D3:1128:C:H2'	66:D3:1129:U:H6	1.84	0.42
66:D3:1638:G:O2'	66:D3:1639:C:O5'	2.35	0.42
66:D3:1743:U:H2'	66:D3:1744:A:H8	1.84	0.42
1:UA:202:ASP:N	1:UA:202:ASP:OD1	2.43	0.42
1:UA:482:SER:O	1:UA:486:SER:HA	2.20	0.42
2:UB:572:LEU:HB2	2:UB:667:LEU:HD21	2.02	0.42
3:UC:551:THR:HA	3:UC:552:PRO:HD3	1.91	0.42
4:UD:233:LYS:HA	4:UD:239:THR:HG21	2.02	0.42
5:UE:335:ASN:ND2	15:UO:369:ASP:O	2.52	0.42
7:UG:196:LEU:HA	7:UG:196:LEU:HD23	1.78	0.42
7:UG:263:MET:HA	7:UG:264:PRO:HD2	1.91	0.42
12:UL:46:LEU:O	12:UL:47:GLU:HG2	2.20	0.42
12:UL:412:GLY:O	12:UL:414:LEU:N	2.52	0.42
12:UL:482:THR:OG1	12:UL:484:ASP:OD1	2.29	0.42
15:UO:450:ILE:HD12	15:UO:450:ILE:HG23	1.85	0.42
17:UQ:198:LEU:HD23	17:UQ:198:LEU:HA	1.84	0.42
19:US:3:LEU:O	19:US:7:GLU:N	2.52	0.42
20:UT:470:ILE:O	20:UT:472:ASP:N	2.45	0.42
22:UV:304:GLU:HB2	22:UV:307:LYS:HB2	1.99	0.42
26:CD:381:ASN:O	26:CD:384:SER:OG	2.35	0.42
29:CH:422:ILE:HD11	29:CH:475:ILE:HG21	2.01	0.42
36:JA:90:GLU:OE2	36:JA:91:MET:N	2.53	0.42
36:JB:737:TRP:O	36:JB:740:ASN:C	2.58	0.42
38:JE:355:ARG:HD2	38:JE:355:ARG:HA	1.83	0.42
39:JF:150:ILE:O	39:JF:159:LEU:N	2.50	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
51:DG:49:VAL:HB	51:DG:115:LYS:H	1.84	0.42
62:DY:88:THR:HA	62:DY:91:LEU:HD12	2.01	0.42
66:D3:267:U:H3	66:D3:288:A:H61	1.67	0.42
66:D3:476:U:OP1	66:D3:477:A:O2'	2.27	0.42
1:UA:666:ARG:HE	1:UA:666:ARG:HB2	1.69	0.42
1:UA:844:TYR:CD2	12:UL:899:GLY:HA3	2.54	0.42
2:UB:647:ILE:HA	2:UB:651:TRP:HB2	2.02	0.42
4:UD:157:SER:HB3	4:UD:195:TRP:HZ2	1.85	0.42
4:UD:183:LEU:HD22	4:UD:223:GLY:HA2	2.02	0.42
4:UD:353:GLU:O	4:UD:355:THR:N	2.51	0.42
4:UD:490:SER:OG	4:UD:494:ASP:HB2	2.19	0.42
5:UE:272:SER:O	5:UE:272:SER:OG	2.31	0.42
8:UH:563:LEU:HA	8:UH:563:LEU:HD23	1.76	0.42
9:UI:417:LYS:HG3	9:UI:455:TRP:CH2	2.55	0.42
11:UK:246:LYS:HE3	28:CF:29:ASN:HD21	1.85	0.42
12:UL:499:PHE:CD1	12:UL:526:THR:HG23	2.54	0.42
13:UM:513:LYS:HE2	13:UM:513:LYS:HB3	1.78	0.42
13:UM:584:ILE:HG13	13:UM:586:LYS:N	2.32	0.42
13:UM:702:LEU:HA	13:UM:702:LEU:HD23	1.68	0.42
17:UQ:623:PHE:CE2	17:UQ:664:LEU:HD13	2.51	0.42
18:UR:178:VAL:HG13	18:UR:179:ASP:HB2	2.01	0.42
21:UU:721:LEU:HD13	21:UU:721:LEU:HA	1.87	0.42
22:UV:490:GLU:OE1	22:UV:580:TYR:OH	2.35	0.42
25:CA:177:SER:HB3	25:CA:178:GLY:H	1.72	0.42
25:CA:264:GLN:CA	25:CA:320:TYR:O	2.66	0.42
25:CA:315:ILE:HG21	25:CA:315:ILE:HD13	1.66	0.42
25:CB:116:SER:OG	67:D4:318:U:O2'	2.36	0.42
29:CH:368:LEU:O	29:CH:371:ARG:HG3	2.20	0.42
31:CJ:236:HIS:CD2	32:CK:369:ILE:HD13	2.55	0.42
32:CK:357:ILE:HD13	32:CK:357:ILE:HA	1.72	0.42
33:CL:296:PHE:HZ	33:CL:797:PRO:HD3	1.84	0.42
33:CL:1033:ARG:H	33:CL:1033:ARG:HG3	1.61	0.42
36:JA:169:HIS:CE1	36:JA:705:LEU:HD11	2.54	0.42
36:JB:25:ILE:O	36:JB:198:CYS:HA	2.20	0.42
48:DA:64:ARG:HA	48:DA:64:ARG:HD3	1.91	0.42
50:DF:205:SER:O	50:DF:205:SER:OG	2.29	0.42
51:DG:22:HIS:CD2	51:DG:23:ARG:HG3	2.55	0.42
62:DY:25:VAL:HG11	62:DY:60:PHE:CZ	2.54	0.42
62:DY:61:ARG:HB2	62:DY:70:VAL:CG1	2.50	0.42
66:D3:1600:A:H4'	66:D3:1601:G:H5"	2.02	0.42
2:UB:542:PHE:O	2:UB:546:LEU:HD23	2.19	0.42



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:UB:604:VAL:HG13	2:UB:606:PHE:HD1	1.84	0.42
3:UC:566:ARG:NH1	66:D3:479:C:OP2	2.44	0.42
5:UE:3:SER:HA	5:UE:4:PRO:HD3	1.84	0.42
5:UE:123:SER:HB3	5:UE:141:ARG:NH2	2.35	0.42
5:UE:281:ILE:HG13	5:UE:328:VAL:HG13	2.01	0.42
5:UE:481:LEU:HD23	5:UE:481:LEU:HA	1.82	0.42
7:UG:38:LYS:HB3	7:UG:38:LYS:HE3	1.87	0.42
10:UJ:59:LEU:HD11	10:UJ:114:THR:HG22	2.02	0.42
10:UJ:275:ILE:HD12	10:UJ:306:LEU:HD23	2.01	0.42
12:UL:336:TYR:CE1	12:UL:359:SER:HB3	2.55	0.42
13:UM:217:ASP:OD1	13:UM:218:ASP:N	2.50	0.42
14:UN:277:ARG:HG3	14:UN:277:ARG:HH21	1.84	0.42
19:US:385:ARG:HA	19:US:465:GLU:OE2	2.19	0.42
21:UU:32:ASN:HB3	21:UU:54:VAL:HG11	2.02	0.42
21:UU:442:THR:OG1	21:UU:453:TRP:O	2.31	0.42
23:UX:69:THR:HG23	23:UX:106:LEU:HD22	2.02	0.42
23:UX:170:ILE:HA	23:UX:170:ILE:HD13	1.82	0.42
24:UZ:45:LYS:HD2	24:UZ:194:ASP:HA	2.00	0.42
29:CH:411:PHE:HA	29:CH:427:LEU:HD13	2.00	0.42
33:CL:187:LYS:HE2	33:CL:206:TYR:CD2	2.55	0.42
37:JC:116:HIS:CE1	37:JC:124:GLN:HB2	2.55	0.42
39:JF:31:LEU:HD23	39:JF:31:LEU:HA	1.82	0.42
41:JJ:117:TYR:CD1	41:JJ:118:PRO:HD3	2.55	0.42
41:JJ:227:ALA:HB3	41:JJ:230:LYS:H	1.85	0.42
44:JN:215:LEU:HA	44:JN:215:LEU:HD23	1.72	0.42
44:JN:264:LEU:HD23	44:JN:264:LEU:HA	1.82	0.42
46:JP:120:GLN:OE1	46:JP:120:GLN:N	2.53	0.42
46:JP:319:GLU:OE1	46:JP:340:ARG:NH2	2.42	0.42
46:JP:399:LYS:HA	46:JP:399:LYS:HD2	1.81	0.42
48:DA:111:ARG:HA	48:DA:111:ARG:HD3	1.84	0.42
49:DE:140:VAL:HA	49:DE:145:ARG:O	2.19	0.42
50:DF:84:LYS:HB3	50:DF:84:LYS:HE2	1.71	0.42
61:DX:97:ASP:HB2	61:DX:100:ASP:OD2	2.19	0.42
65:D2:136:U:H2'	65:D2:137:C:H6	1.85	0.42
65:D2:262:U:H2'	65:D2:263:C:H6	1.84	0.42
66:D3:53:G:H2'	66:D3:54:C:O4'	2.20	0.42
66:D3:376:C:H2'	66:D3:377:G:C8	2.54	0.42
66:D3:1035:G:H1	66:D3:1082:C:H42	1.67	0.42
1:UA:58:ILE:HA	1:UA:74:ASP:HA	2.02	0.42
1:UA:125:PRO:HD3	1:UA:136:PHE:CE1	2.55	0.42
1:UA:758:ILE:HG21	1:UA:758:ILE:HD13	1.78	0.42



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:UA:775:LEU:HD12	1:UA:775:LEU:HA	1.75	0.42
5:UE:476:LEU:HD13	5:UE:476:LEU:HA	1.87	0.42
7:UG:534:LYS:HA	7:UG:534:LYS:HD3	1.85	0.42
12:UL:50:ASN:HB3	12:UL:52:TRP:CZ3	2.55	0.42
13:UM:314:ILE:HD12	13:UM:330:THR:HG23	2.02	0.42
15:UO:149:THR:HG23	15:UO:164:LEU:HB2	2.02	0.42
18:UR:277:ILE:HD12	18:UR:277:ILE:HG23	1.84	0.42
21:UU:320:LYS:HA	21:UU:345:SER:OG	2.19	0.42
21:UU:925:LEU:HA	21:UU:925:LEU:HD23	1.70	0.42
24:UZ:80:SER:HB2	24:UZ:102:SER:HB2	2.01	0.42
29:CH:331:LEU:HA	29:CH:331:LEU:HD23	1.85	0.42
29:CH:350:LYS:HE3	29:CH:353:ASP:HB2	2.02	0.42
32:CK:305:ILE:HD13	32:CK:305:ILE:HA	1.88	0.42
33:CL:634:ARG:HH21	34:CM:185:ARG:NH1	2.17	0.42
33:CL:907:THR:OG1	33:CL:908:GLY:N	2.52	0.42
36:JA:73:ARG:NH1	36:JA:99:SER:OG	2.53	0.42
36:JA:217:LYS:HA	36:JA:217:LYS:HD3	1.55	0.42
36:JA:486:LEU:HD12	36:JA:486:LEU:HA	1.77	0.42
36:JA:656:LEU:HD23	36:JA:656:LEU:HA	1.85	0.42
36:JB:44:MET:O	36:JB:47:ALA:C	2.58	0.42
39:JG:246:GLU:HB2	39:JG:251:ILE:HB	2.00	0.42
41:JJ:263:LEU:HD12	41:JJ:263:LEU:HA	1.74	0.42
46:JP:96:ASN:ND2	46:JP:99:THR:HG22	2.34	0.42
46:JP:454:ILE:O	46:JP:459:LYS:NZ	2.48	0.42
49:DE:205:PHE:CD1	49:DE:207:LEU:HG	2.55	0.42
50:DF:217:LEU:HD23	50:DF:217:LEU:HA	1.68	0.42
52:DH:112:ARG:NH2	52:DH:117:THR:HG22	2.34	0.42
54:DJ:128:LEU:HD23	54:DJ:128:LEU:HA	1.68	0.42
54:DJ:134:ILE:HD13	54:DJ:134:ILE:HA	1.85	0.42
58:DQ:58:ASP:O	58:DQ:61:SER:N	2.49	0.42
65:D2:125:G:H2'	65:D2:126:A:C8	2.55	0.42
66:D3:1738:U:H2'	66:D3:1739:C:C6	2.55	0.42
67:D4:306:G:H2'	67:D4:307:G:C8	2.55	0.42
1:UA:73:ILE:HG12	1:UA:79:ALA:HB2	2.01	0.41
4:UD:74:GLY:HA2	4:UD:99:ILE:HG12	2.01	0.41
4:UD:556:LYS:HB3	4:UD:556:LYS:HE3	1.74	0.41
9:UI:411:TRP:HB3	9:UI:455:TRP:HE1	1.85	0.41
11:UK:231:LYS:HE2	11:UK:233:ILE:HG22	2.01	0.41
13:UM:69:LEU:HD12	13:UM:69:LEU:HA	1.88	0.41
13:UM:138:HIS:NE2	13:UM:177:LEU:HD22	2.35	0.41
13:UM:269:LEU:HB3	13:UM:279:LYS:HB2	2.01	0.41



A 4 a and 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:314:ILE:HD12	13:UM:314:ILE:HA	1.83	0.41
13:UM:806:LEU:HD23	13:UM:806:LEU:HA	1.85	0.41
15:UO:108:TYR:HB3	15:UO:117:LEU:H	1.85	0.41
15:UO:131:LYS:HB3	15:UO:131:LYS:HE3	1.89	0.41
17:UQ:657:SER:OG	17:UQ:675:ARG:N	2.51	0.41
19:US:262:LEU:HD13	19:US:262:LEU:HA	1.80	0.41
22:UV:337:LEU:O	22:UV:341:THR:HG22	2.19	0.41
22:UV:1216:LYS:HA	22:UV:1219:ILE:HD12	2.02	0.41
27:CE:175:LYS:HB2	27:CE:175:LYS:HE2	1.78	0.41
29:CH:156:ASN:HA	29:CH:544:ALA:HB1	2.00	0.41
29:CH:245:SER:HB2	29:CH:247:ASP:OD1	2.20	0.41
31:CJ:100:LEU:HD22	31:CJ:144:GLU:HB3	2.02	0.41
33:CL:833:ARG:NH2	61:DX:138:GLU:O	2.52	0.41
33:CL:928:ILE:HD13	33:CL:928:ILE:HG21	1.83	0.41
37:JC:93:PHE:CE2	37:JC:95:ARG:HB2	2.54	0.41
37:JC:166:ASN:H	37:JC:173:LEU:HD23	1.85	0.41
51:DG:211:LEU:O	51:DG:215:ARG:HG3	2.19	0.41
54:DJ:86:LEU:HD12	54:DJ:86:LEU:HA	1.70	0.41
66:D3:263:C:N4	66:D3:264:G:O6	2.53	0.41
66:D3:1025:A:H2'	66:D3:1026:A:C8	2.55	0.41
66:D3:1666:U:H5'	66:D3:1666:U:H6	1.84	0.41
1:UA:62:ASP:OD1	1:UA:63:LEU:N	2.53	0.41
1:UA:779:LEU:HD23	1:UA:779:LEU:HA	1.78	0.41
5:UE:332:LEU:HD12	5:UE:332:LEU:HA	1.90	0.41
7:UG:81:GLU:OE1	46:JP:1:MET:HB2	2.20	0.41
9:UI:466:GLU:O	9:UI:470:ILE:HG12	2.20	0.41
10:UJ:261:LEU:HA	10:UJ:261:LEU:HD23	1.82	0.41
15:UO:28:ARG:NH1	65:D2:142:U:O2	2.53	0.41
17:UQ:433:ARG:NE	65:D2:4:C:OP1	2.53	0.41
19:US:148:PHE:O	19:US:152:ILE:HG12	2.19	0.41
19:US:226:ASP:HB2	19:US:284:ARG:HD3	2.01	0.41
21:UU:327:SER:HG	21:UU:329:SER:H	1.65	0.41
21:UU:493:ILE:HG21	21:UU:493:ILE:HD13	1.78	0.41
22:UV:883:LEU:HD23	22:UV:883:LEU:HA	1.90	0.41
22:UV:1111:SER:HA	22:UV:1129:PRO:HG3	2.01	0.41
22:UV:1165:SER:OG	22:UV:1166:ARG:N	2.52	0.41
23:UX:135:THR:O	23:UX:135:THR:OG1	2.34	0.41
28:CG:59:GLU:OE2	28:CG:59:GLU:N	2.54	0.41
29:CH:74:LEU:HD12	29:CH:74:LEU:HA	1.80	0.41
33:CL:215:TYR:HB3	33:CL:216:PRO:CD	2.50	0.41
33:CL:235:LEU:HA	33:CL:235:LEU:HD23	1.85	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
33:CL:254:HIS:HB3	33:CL:256:GLU:OE1	2.19	0.41
34:CM:324:ILE:HD12	34:CM:324:ILE:HA	1.93	0.41
36:JB:802:LEU:O	36:JB:805:ILE:N	2.51	0.41
37:JC:14:TYR:HB2	37:JC:342:TYR:O	2.20	0.41
37:JC:141:GLY:HA2	37:JC:157:ALA:HA	2.01	0.41
37:JC:160:ASN:HB3	37:JC:180:THR:O	2.21	0.41
39:JF:116:THR:OG1	39:JF:119:GLY:N	2.54	0.41
45:JO:90:ASP:OD2	45:JO:93:ILE:HG12	2.20	0.41
45:JO:159:LEU:HA	45:JO:159:LEU:HD23	1.83	0.41
46:JP:450:ASP:OD1	46:JP:450:ASP:N	2.36	0.41
58:DQ:118:ILE:HD12	58:DQ:118:ILE:HA	1.88	0.41
65:D2:190:U:H2'	65:D2:191:U:C6	2.55	0.41
66:D3:1782:A:H8	66:D3:1782:A:O5'	2.02	0.41
1:UA:30:LEU:HG	1:UA:39:VAL:HG22	2.02	0.41
2:UB:561:ILE:HG12	19:US:473:TYR:CD2	2.55	0.41
3:UC:502:LYS:NZ	24:UZ:251:SER:OG	2.46	0.41
4:UD:758:ASN:HB3	4:UD:761:THR:OG1	2.20	0.41
7:UG:162:ASN:HB3	7:UG:164:GLN:H	1.85	0.41
7:UG:317:THR:HG23	7:UG:334:ARG:HB3	2.03	0.41
7:UG:440:ASP:OD1	14:UN:838:LYS:HB3	2.20	0.41
7:UG:527:ARG:NH1	65:D2:366:A:OP1	2.47	0.41
10:UJ:336:LEU:HD23	10:UJ:336:LEU:HA	1.87	0.41
12:UL:220:THR:HG23	12:UL:259:ILE:HD11	2.02	0.41
13:UM:35:PRO:HD3	13:UM:67:LEU:HD21	2.01	0.41
13:UM:302:MET:HB2	13:UM:314:ILE:HG22	2.02	0.41
15:UO:439:LEU:HD23	15:UO:439:LEU:HA	1.87	0.41
15:UO:509:GLN:HE21	15:UO:509:GLN:HB3	1.73	0.41
19:US:180:PHE:CD1	19:US:184:TYR:HD2	2.37	0.41
22:UV:1136:LEU:O	22:UV:1139:LEU:HB2	2.20	0.41
26:CD:237:LEU:O	26:CD:240:LEU:C	2.59	0.41
29:CH:336:CYS:SG	29:CH:349:TRP:HB2	2.59	0.41
29:CH:342:ARG:HE	29:CH:342:ARG:HB3	1.73	0.41
33:CL:369:ASP:OD1	33:CL:370:ALA:N	2.52	0.41
34:CM:337:VAL:HG13	34:CM:354:ILE:HG13	2.03	0.41
36:JA:59:TYR:OH	66:D3:416:A:N1	2.53	0.41
37:JC:152:ASP:OD1	37:JC:166:ASN:ND2	2.54	0.41
38:JE:300:THR:O	38:JE:304:GLU:HG2	2.21	0.41
45:JO:98:ARG:O	45:JO:101:ILE:HG12	2.20	0.41
49:DE:112:HIS:O	49:DE:114:ILE:HG12	2.19	0.41
52:DH:6:ALA:O	52:DH:9:LEU:C	2.59	0.41
65:D2:117:G:H2'	65:D2:118:A:H8	1.85	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
65:D2:273:G:N2	65:D2:274:C:O2	2.53	0.41
66:D3:417:A:H5'	66:D3:418:G:C4	2.55	0.41
1:UA:502:ILE:HD13	1:UA:502:ILE:HG21	1.83	0.41
2:UB:494:SER:HB2	2:UB:497:ASP:OD2	2.21	0.41
2:UB:548:ARG:NH1	2:UB:638:ASN:OD1	2.39	0.41
3:UC:596:THR:HG22	43:JM:137:LYS:HG3	2.02	0.41
4:UD:741:LEU:HA	4:UD:756:GLU:HA	2.02	0.41
7:UG:78:ASN:HB3	7:UG:80:LEU:H	1.85	0.41
7:UG:118:TYR:CE1	7:UG:125:LEU:HD12	2.55	0.41
7:UG:279:SER:O	7:UG:292:THR:HG22	2.21	0.41
12:UL:484:ASP:OD1	12:UL:485:GLY:N	2.54	0.41
12:UL:857:LEU:HD12	12:UL:857:LEU:HA	1.71	0.41
12:UL:926:GLN:HG3	41:JJ:264:ARG:NH1	2.36	0.41
13:UM:97:ARG:NH2	13:UM:133:ASN:HA	2.36	0.41
13:UM:265:ALA:HB3	13:UM:284:PRO:HG3	2.03	0.41
13:UM:537:TRP:CD1	13:UM:553:GLY:HA2	2.55	0.41
14:UN:837:LYS:O	14:UN:840:LEU:HB3	2.20	0.41
15:UO:101:ALA:HA	15:UO:126:PRO:HB3	2.03	0.41
15:UO:206:ILE:HD13	15:UO:206:ILE:HA	1.86	0.41
18:UR:16:ASP:O	18:UR:20:GLN:HB2	2.21	0.41
18:UR:344:ARG:NH2	65:D2:88:U:H3	2.14	0.41
19:US:124:LEU:HD11	19:US:184:TYR:OH	2.20	0.41
19:US:280:ILE:HG23	19:US:284:ARG:HD2	2.02	0.41
21:UU:190:LEU:HB3	21:UU:200:PHE:HB3	2.01	0.41
21:UU:229:GLU:HA	21:UU:244:ILE:O	2.20	0.41
22:UV:188:SER:HA	22:UV:191:LEU:HB2	2.03	0.41
22:UV:235:LEU:HD23	22:UV:235:LEU:HA	1.87	0.41
22:UV:1037:LEU:HD11	22:UV:1050:ILE:HG22	2.02	0.41
24:UZ:130:ARG:NH2	24:UZ:169:GLU:OE1	2.53	0.41
29:CH:449:ASN:OD1	29:CH:450:ASP:N	2.53	0.41
30:CI:143:ILE:HD12	30:CI:143:ILE:HG23	1.82	0.41
36:JA:870:LYS:H	36:JA:870:LYS:HG2	1.57	0.41
45:JO:94:ILE:HD12	45:JO:94:ILE:HA	1.91	0.41
46:JP:345:THR:OG1	46:JP:346:LYS:N	2.53	0.41
49:DE:149:TYR:HB3	51:DG:208:TYR:CG	2.55	0.41
57:DO:112:ILE:HD13	57:DO:112:ILE:HA	1.93	0.41
58:DQ:13:LYS:HG3	58:DQ:14:LYS:N	2.32	0.41
65:D2:188:A:H2	65:D2:209:G:H22	1.67	0.41
65:D2:312:U:O2'	65:D2:313:A:H5'	2.20	0.41
66:D3:208:U:H3	66:D3:257:A:H61	1.69	0.41
66:D3:529:A:H2'	66:D3:530:C:O4'	2.20	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
66:D3:1037:C:H6	66:D3:1037:C:O5'	2.03	0.41
66:D3:1699:G:H2'	66:D3:1701:A:N7	2.35	0.41
1:UA:474:GLY:O	1:UA:492:SER:OG	2.37	0.41
6:UF:14:GLU:OE2	6:UF:36:ARG:NH2	2.27	0.41
10:UJ:111:LEU:HD23	10:UJ:111:LEU:HA	1.85	0.41
12:UL:20:ASN:HA	12:UL:339:LYS:HE3	2.03	0.41
12:UL:48:ASP:OD2	12:UL:62:LYS:HD3	2.20	0.41
12:UL:268:LYS:N	12:UL:371:LYS:HZ3	2.18	0.41
12:UL:428:PHE:CD1	12:UL:463:SER:HB3	2.55	0.41
13:UM:237:LEU:HD13	13:UM:275:GLY:HA2	2.03	0.41
14:UN:306:ARG:HA	14:UN:306:ARG:HD3	1.94	0.41
15:UO:22:PRO:O	15:UO:25:ARG:HB2	2.21	0.41
15:UO:287:LEU:HD23	15:UO:287:LEU:HA	1.86	0.41
17:UQ:35:ALA:HB1	17:UQ:46:ILE:HD13	2.01	0.41
17:UQ:264:ILE:HG21	17:UQ:264:ILE:HD13	1.80	0.41
17:UQ:464:LYS:HB3	17:UQ:464:LYS:HE2	1.85	0.41
18:UR:395:LEU:HD23	18:UR:395:LEU:HA	1.81	0.41
19:US:407:ARG:HH11	19:US:491:LEU:HD22	1.84	0.41
24:UZ:209:ILE:HA	24:UZ:212:ILE:HG22	2.02	0.41
25:CA:252:ILE:HD13	25:CA:252:ILE:HG21	1.75	0.41
25:CB:272:LYS:HB3	25:CB:313:HIS:NE2	2.35	0.41
27:CE:320:LEU:HD12	27:CE:320:LEU:HA	1.83	0.41
29:CH:367:LYS:HD3	29:CH:367:LYS:HA	1.77	0.41
33:CL:635:PHE:HA	34:CM:188:ILE:HG23	2.02	0.41
38:JE:265:ASP:HB3	38:JE:274:ILE:HG23	2.02	0.41
39:JG:99:LEU:HD23	39:JG:99:LEU:HA	1.82	0.41
41:JJ:219:ALA:HB1	41:JJ:267:ALA:HB2	2.03	0.41
46:JP:298:LEU:HD23	46:JP:298:LEU:HA	1.88	0.41
51:DG:32:ILE:HD11	51:DG:63:MET:HG3	2.00	0.41
52:DH:49:ILE:HG12	52:DH:175:LYS:HG3	2.03	0.41
57:DO:76:ILE:HD13	57:DO:76:ILE:HA	1.89	0.41
65:D2:369:G:C2	65:D2:371:G:C8	3.08	0.41
65:D2:443:G:N2	65:D2:444:U:O2	2.54	0.41
66:D3:154:G:H1	66:D3:160:C:H42	1.67	0.41
66:D3:391:A:H2'	66:D3:392:G:H8	1.85	0.41
66:D3:1695:G:H2'	66:D3:1696:G:C8	2.55	0.41
2:UB:571:ILE:HD13	2:UB:571:ILE:HA	1.89	0.41
10:UJ:364:ASN:OD1	10:UJ:364:ASN:N	2.53	0.41
10:UJ:406:TYR:O	10:UJ:409:SER:OG	2.21	0.41
11:UK:115:LEU:O	11:UK:119:GLU:HG2	2.21	0.41
11:UK:195:LEU:HA	11:UK:195:LEU:HD23	1.82	0.41



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
17:UQ:386:ASN:OD1	17:UQ:387:GLY:N	2.54	0.41
17:UQ:823:ALA:HB1	17:UQ:827:HIS:NE2	2.35	0.41
19:US:397:THR:HG23	19:US:499:LEU:HA	2.02	0.41
21:UU:591:PHE:HA	21:UU:601:VAL:O	2.20	0.41
21:UU:837:LEU:HB3	21:UU:884:PHE:CE2	2.56	0.41
22:UV:207:LEU:HB2	22:UV:296:ILE:HD13	2.02	0.41
22:UV:261:ASN:HD21	22:UV:588:GLN:HE22	1.68	0.41
22:UV:329:THR:O	22:UV:333:ASN:HB2	2.21	0.41
25:CA:162:LEU:HA	25:CA:162:LEU:HD12	1.88	0.41
26:CD:143:GLN:OE1	26:CD:147:LEU:HB2	2.20	0.41
26:CD:194:ARG:HD3	26:CD:194:ARG:HA	1.98	0.41
29:CH:63:ARG:HB2	54:DJ:70:LEU:HD21	2.02	0.41
31:CJ:13:LEU:HD23	31:CJ:13:LEU:HA	1.71	0.41
31:CJ:117:LEU:HA	31:CJ:117:LEU:HD12	1.64	0.41
31:CJ:285:ASN:OD1	31:CJ:285:ASN:N	2.49	0.41
33:CL:607:ASP:OD1	33:CL:607:ASP:N	2.51	0.41
33:CL:1128:LYS:HD3	33:CL:1128:LYS:HA	1.84	0.41
34:CM:18:ARG:HD3	34:CM:98:TYR:CE1	2.56	0.41
34:CM:185:ARG:HA	34:CM:186:PRO:HD3	1.90	0.41
35:CN:23:HIS:HB3	35:CN:26:LEU:HD13	2.02	0.41
36:JA:361:ARG:O	36:JA:363:HIS:N	2.50	0.41
36:JA:865:LEU:HD12	36:JA:865:LEU:HA	1.87	0.41
37:JC:70:TYR:CZ	37:JC:111:TRP:CD1	3.09	0.41
38:JE:285:ARG:O	38:JE:288:SER:OG	2.26	0.41
45:JO:287:LYS:HA	45:JO:290:GLU:HG3	2.01	0.41
46:JP:201:ILE:CG2	46:JP:215:LEU:HB2	2.50	0.41
46:JP:248:ASP:OD2	46:JP:251:THR:OG1	2.27	0.41
48:DA:19:ARG:HH12	48:DA:22:ASP:N	2.10	0.41
49:DE:126:VAL:HB	49:DE:158:ASP:HB2	2.01	0.41
57:DO:15:GLY:O	57:DO:79:VAL:HA	2.20	0.41
65:D2:328:A:O2'	65:D2:329:A:H5"	2.20	0.41
66:D3:498:G:N2	66:D3:499:U:O2	2.54	0.41
67:D4:105:C:H42	67:D4:309:G:H1	1.69	0.41
1:UA:430:ARG:HB3	32:CK:458:PRO:HB2	2.02	0.41
1:UA:667:GLY:O	1:UA:673:ARG:NH2	2.53	0.41
2:UB:435:PHE:O	2:UB:439:GLN:HG2	2.21	0.41
4:UD:309:GLN:NE2	4:UD:318:ASN:HA	2.34	0.41
4:UD:332:ASP:O	4:UD:351:GLY:HA3	2.21	0.41
4:UD:638:SER:HA	4:UD:646:LEU:HD13	2.02	0.41
4:UD:657:ILE:HD13	4:UD:732:PHE:HB2	2.02	0.41
4:UD:735:THR:OG1	4:UD:737:LYS:HG2	2.21	0.41



	A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:UE:234:GLU:HB2	5:UE:247:THR:HB	2.02	0.41
7:UG:75:GLU:HA	7:UG:76:PRO:HD3	1.78	0.41
7:UG:303:ILE:HG21	7:UG:303:ILE:HD13	1.81	0.41
7:UG:508:VAL:HG22	45:JO:73:LEU:HD23	2.02	0.41
8:UH:262:LEU:N	8:UH:270:PHE:O	2.50	0.41
9:UI:503:LEU:O	9:UI:507:ARG:HD2	2.19	0.41
10:UJ:196:LEU:HD23	10:UJ:196:LEU:HA	1.86	0.41
10:UJ:373:ILE:HD12	10:UJ:373:ILE:HA	1.96	0.41
12:UL:292:ILE:HG23	12:UL:324:PHE:CZ	2.56	0.41
13:UM:133:ASN:HD22	13:UM:135:TYR:HD1	1.69	0.41
13:UM:303:PHE:HA	13:UM:312:GLN:O	2.20	0.41
19:US:452:ASP:HA	19:US:453:PRO:HD3	1.93	0.41
21:UU:110:LEU:HA	21:UU:110:LEU:HD12	1.89	0.41
21:UU:218:LEU:HA	21:UU:218:LEU:HD23	1.64	0.41
21:UU:497:LYS:HB3	50:DF:17:VAL:HG23	2.02	0.41
21:UU:900:ASN:O	21:UU:901:LYS:HG2	2.20	0.41
25:CA:142:ARG:HH11	25:CA:142:ARG:HD3	1.74	0.41
25:CB:117:VAL:HG13	25:CB:118:TYR:HD1	1.84	0.41
26:CD:263:ILE:HD11	26:CD:268:MET:HE2	2.03	0.41
29:CH:235:HIS:NE2	29:CH:253:THR:OG1	2.53	0.41
29:CH:409:ASP:CG	29:CH:411:PHE:H	2.23	0.41
32:CK:314:LEU:HD23	32:CK:314:LEU:HA	1.79	0.41
36:JA:8:SER:O	36:JA:12:SER:CB	2.69	0.41
36:JA:727:TYR:CE2	36:JA:729:LEU:HA	2.55	0.41
37:JC:192:ASN:O	37:JC:194:LEU:N	2.49	0.41
37:JC:239:ASP:OD1	37:JC:240:GLY:N	2.53	0.41
38:JE:228:PHE:CZ	49:DE:189:LEU:HD22	2.55	0.41
39:JG:117:SER:OG	39:JG:118:ARG:HD2	2.20	0.41
44:JN:323:LYS:HA	44:JN:323:LYS:HD2	1.85	0.41
46:JP:85:THR:HG21	46:JP:372:VAL:HG21	2.01	0.41
48:DA:172:LEU:HD23	48:DA:172:LEU:HA	1.85	0.41
49:DE:37:LYS:HE2	49:DE:37:LYS:HB3	1.97	0.41
49:DE:41:SER:OG	49:DE:84:ALA:O	2.34	0.41
54:DJ:63:ASP:OD1	54:DJ:63:ASP:N	2.53	0.41
56:DN:43:LYS:HE2	56:DN:43:LYS:HB3	1.95	0.41
66:D3:1480:G:N2	66:D3:1528:U:O2	2.54	0.41
66:D3:1675:C:H2'	66:D3:1676:U:O4'	2.20	0.41
1:UA:825:GLN:O	1:UA:829:VAL:HG22	2.21	0.41
5:UE:216:ASP:OD1	5:UE:217:ILE:N	2.54	0.41
6:UF:14:GLU:OE1	6:UF:87:SER:OG	2.20	0.41
7:UG:389:LEU:HD13	7:UG:400:ASN:HD22	1.86	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
10:UJ:66:PHE:CZ	10:UJ:105:ALA:HB2	2.55	0.41
12:UL:572:HIS:CD2	12:UL:598:LYS:HE2	2.56	0.41
12:UL:620:ASN:HD21	12:UL:663:LEU:N	2.19	0.41
12:UL:633:CYS:SG	12:UL:663:LEU:HD22	2.61	0.41
12:UL:855:LYS:HE2	12:UL:855:LYS:HB3	1.80	0.41
13:UM:154:GLY:HA3	13:UM:161:TRP:HD1	1.84	0.41
13:UM:355:LEU:HA	13:UM:355:LEU:HD23	1.85	0.41
13:UM:805:ILE:HG21	13:UM:805:ILE:HD13	1.86	0.41
17:UQ:96:ILE:HD12	17:UQ:151:TYR:CE2	2.55	0.41
17:UQ:524:ASP:OD1	17:UQ:524:ASP:N	2.45	0.41
22:UV:186:ILE:O	22:UV:204:ASP:HB2	2.21	0.41
24:UZ:109:ARG:HE	24:UZ:109:ARG:HB2	1.67	0.41
25:CB:204:GLY:HA3	25:CB:221:ILE:HD11	2.03	0.41
28:CG:53:ILE:HA	28:CG:53:ILE:HD13	1.77	0.41
29:CH:67:ALA:HB1	38:JE:249:ILE:HD13	2.02	0.41
29:CH:492:TRP:HB3	29:CH:520:VAL:HG22	2.03	0.41
30:CI:85:MET:HE1	32:CK:448:LEU:HB3	2.03	0.41
33:CL:133:LYS:NZ	33:CL:850:GLY:O	2.37	0.41
36:JA:8:SER:O	36:JA:12:SER:HB2	2.21	0.41
36:JA:80:GLU:OE1	36:JA:85:THR:OG1	2.25	0.41
36:JA:523:LEU:HD11	36:JA:534:LEU:HD13	2.02	0.41
37:JC:61:LYS:HA	37:JC:61:LYS:HD3	1.96	0.41
39:JF:80:MET:HB3	39:JF:82:ARG:NH2	2.36	0.41
62:DY:40:LEU:HA	62:DY:40:LEU:HD13	1.70	0.41
65:D2:519:A:H2'	65:D2:520:A:O4'	2.20	0.41
66:D3:88:U:H2'	66:D3:89:G:C8	2.48	0.41
66:D3:108:A:C6	66:D3:307:G:C6	3.09	0.41
66:D3:212:U:N3	66:D3:213:A:N7	2.69	0.41
66:D3:282:C:H2'	66:D3:283:U:O4'	2.21	0.41
66:D3:375:U:H5'	66:D3:376:C:OP1	2.20	0.41
66:D3:538:A:H5'	66:D3:543:C:C5	2.55	0.41
66:D3:688:G:H2'	66:D3:689:G:C8	2.55	0.41
1:UA:155:SER:OG	1:UA:160:PHE:HB2	2.21	0.41
1:UA:573:ASN:N	1:UA:573:ASN:OD1	2.52	0.41
1:UA:644:ILE:HD12	1:UA:644:ILE:HG23	1.84	0.41
2:UB:577:VAL:HG11	2:UB:596:TYR:HA	2.02	0.41
4:UD:524:LYS:HD2	4:UD:524:LYS:HA	1.81	0.41
4:UD:535:GLU:HG3	4:UD:573:VAL:HG23	2.03	0.41
5:UE:83:GLY:O	5:UE:101:THR:HG22	2.20	0.41
6:UF:87:SER:OG	6:UF:88:ILE:N	2.53	0.41
7:UG:150:LEU:HD11	7:UG:154:CYS:SG	2.61	0.41



A 4 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
8:UH:79:ASN:N	8:UH:89:GLY:O	2.53	0.41
8:UH:231:PHE:HA	8:UH:238:ASP:HA	2.02	0.41
8:UH:596:LYS:HD2	8:UH:643:ASP:HB3	2.03	0.41
10:UJ:166:ASN:CG	27:CE:407:ARG:HH11	2.24	0.41
10:UJ:231:LEU:HD23	10:UJ:231:LEU:HA	1.71	0.41
10:UJ:316:PRO:HD2	10:UJ:319:ILE:HD12	2.02	0.41
11:UK:48:LEU:HA	11:UK:48:LEU:HD12	1.70	0.41
12:UL:107:ASP:OD2	12:UL:110:SER:N	2.42	0.41
12:UL:299:ARG:NH1	12:UL:324:PHE:HB2	2.35	0.41
12:UL:352:GLU:OE1	12:UL:364:TYR:OH	2.28	0.41
12:UL:439:LEU:HB2	12:UL:444:LEU:O	2.20	0.41
12:UL:643:ASP:OD2	12:UL:646:LYS:N	2.34	0.41
12:UL:838:THR:O	12:UL:841:GLN:HB2	2.21	0.41
15:UO:83:VAL:HG13	15:UO:85:TYR:CE1	2.44	0.41
15:UO:273:ILE:HG21	15:UO:273:ILE:HD13	1.76	0.41
17:UQ:110:PHE:CD2	17:UQ:144:VAL:HG21	2.56	0.41
17:UQ:126:VAL:O	17:UQ:128:SER:N	2.46	0.41
17:UQ:177:THR:OG1	17:UQ:178:PHE:N	2.54	0.41
17:UQ:294:LYS:HD2	65:D2:83:U:H5'	2.03	0.41
17:UQ:301:LEU:HD23	17:UQ:301:LEU:HA	1.73	0.41
17:UQ:383:LEU:HD12	17:UQ:383:LEU:HA	1.83	0.41
17:UQ:426:ARG:NH1	65:D2:68:U:OP2	2.30	0.41
17:UQ:727:GLN:NE2	17:UQ:740:LYS:HB3	2.34	0.41
18:UR:155:ILE:HG23	18:UR:155:ILE:HD12	1.80	0.41
18:UR:456:THR:OG1	18:UR:457:LYS:N	2.54	0.41
19:US:324:PHE:HA	19:US:327:MET:HE2	2.03	0.41
19:US:366:LEU:HD11	19:US:379:PHE:CD2	2.56	0.41
21:UU:728:ARG:HA	21:UU:728:ARG:HD3	1.75	0.41
22:UV:111:LEU:O	22:UV:115:LYS:HB2	2.21	0.41
22:UV:221:ASN:HA	22:UV:315:ILE:HD13	2.02	0.41
22:UV:763:THR:HG22	22:UV:917:LYS:HE3	2.03	0.41
22:UV:828:ASP:HB2	22:UV:839:THR:HG23	2.02	0.41
22:UV:831:ILE:HD13	22:UV:831:ILE:HA	1.86	0.41
25:CA:305:THR:HA	25:CA:314:CYS:SG	2.61	0.41
25:CB:109:LYS:HG2	25:CB:141:TYR:CE1	2.53	0.41
26:CD:30:ARG:HA	26:CD:30:ARG:HD3	1.88	0.41
26:CD:206:LEU:HD21	26:CD:251:VAL:HG21	2.02	0.41
27:CE:157:ASP:OD1	27:CE:157:ASP:N	2.42	0.41
27:CE:252:LEU:O	27:CE:256:ASN:HB2	2.21	0.41
29:CH:146:LYS:O	29:CH:566:ALA:HA	2.19	0.41
30:CI:166:ILE:O	30:CI:170:LEU:HG	2.20	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
31:CJ:215:LYS:HA	31:CJ:215:LYS:HD2	1.82	0.41
31:CJ:279:ARG:HH21	31:CJ:279:ARG:HD3	1.65	0.41
31:CJ:281:ILE:HD13	31:CJ:281:ILE:HG21	1.80	0.41
32:CK:511:ASN:OD1	32:CK:511:ASN:N	2.46	0.41
33:CL:858:PRO:HA	33:CL:885:PHE:HB3	2.02	0.41
35:CN:180:LEU:O	35:CN:184:ILE:HG12	2.21	0.41
36:JA:918:ARG:O	36:JA:921:SER:OG	2.39	0.41
37:JC:144:LEU:HD21	37:JC:153:LEU:HD12	2.03	0.41
37:JC:194:LEU:HD11	37:JC:243:PHE:CE2	2.55	0.41
39:JF:175:CYS:HB2	39:JF:177:LYS:HZ2	1.86	0.41
45:JO:85:THR:HG23	45:JO:87:LYS:H	1.86	0.41
45:JO:104:LEU:HA	45:JO:104:LEU:HD23	1.88	0.41
46:JP:278:VAL:HG21	46:JP:320:ILE:HD13	2.03	0.41
49:DE:114:ILE:HD13	49:DE:114:ILE:HA	1.92	0.41
49:DE:131:LEU:HD12	49:DE:131:LEU:HA	1.87	0.41
52:DH:23:ALA:HA	52:DH:26:GLU:HG2	2.03	0.41
53:DI:169:ILE:HD13	53:DI:169:ILE:HA	1.97	0.41
54:DJ:106:GLU:OE1	54:DJ:115:LYS:HE3	2.19	0.41
55:DL:72:THR:O	55:DL:88:ARG:NE	2.34	0.41
56:DN:114:ARG:HD3	56:DN:114:ARG:HA	1.89	0.41
62:DY:27:VAL:CB	62:DY:69:SER:HB3	2.50	0.41
65:D2:338:A:O2'	65:D2:340:U:O4	2.26	0.41
66:D3:317:C:H2'	66:D3:318:U:C6	2.55	0.41
67:D4:35:U:H6	67:D4:35:U:H5"	1.86	0.41
1:UA:223:ARG:HA	1:UA:223:ARG:HD3	1.84	0.41
1:UA:722:THR:O	1:UA:726:THR:HG23	2.21	0.41
1:UA:790:GLN:O	1:UA:792:ILE:N	2.54	0.41
2:UB:710:ILE:HG22	2:UB:711:PRO:O	2.21	0.41
10:UJ:385:THR:HG1	10:UJ:418:CYS:HG	1.68	0.41
13:UM:219:ILE:HD13	13:UM:219:ILE:HA	1.83	0.41
13:UM:513:LYS:HG2	13:UM:535:GLY:N	2.35	0.41
14:UN:872:ARG:NE	14:UN:876:GLN:HE21	2.19	0.41
17:UQ:92:LEU:HD23	17:UQ:92:LEU:HA	1.78	0.41
17:UQ:200:ASN:HD22	17:UQ:263:ALA:HA	1.86	0.41
18:UR:445:ARG:NH2	18:UR:500:MET:O	2.41	0.41
22:UV:329:THR:HG22	22:UV:332:TYR:HB3	2.02	0.41
22:UV:596:LYS:HA	22:UV:596:LYS:HD3	1.88	0.41
22:UV:950:ILE:HA	22:UV:951:PRO:HD3	1.95	0.41
29:CH:154:GLU:OE1	29:CH:195:GLN:HB3	2.21	0.41
30:CI:33:MET:HA	30:CI:38:ILE:HG12	2.02	0.41
31:CJ:7:ARG:O	31:CJ:11:GLU:HG3	2.21	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
31:CJ:226:ASN:OD1	31:CJ:289:TYR:OH	2.27	0.41
31:CJ:236:HIS:HD2	32:CK:369:ILE:HD13	1.86	0.41
33:CL:71:ILE:HD13	33:CL:71:ILE:HG21	1.88	0.41
33:CL:98:LEU:HA	33:CL:98:LEU:HD12	1.78	0.41
33:CL:312:PHE:HD1	33:CL:312:PHE:HA	1.73	0.41
33:CL:312:PHE:HA	33:CL:315:GLN:HG3	2.03	0.41
34:CM:119:LYS:HG2	34:CM:165:GLU:HG2	2.03	0.41
35:CN:228:LYS:HG3	66:D3:1059:U:O4	2.21	0.41
35:CN:261:GLN:O	35:CN:264:GLU:HG3	2.21	0.41
37:JC:326:THR:HG21	37:JC:348:PRO:HD2	2.02	0.41
46:JP:139:CYS:HB3	46:JP:185:ILE:HD13	2.03	0.41
46:JP:191:ASN:HB3	46:JP:193:THR:OG1	2.20	0.41
46:JP:272:MET:HG3	46:JP:316:THR:O	2.21	0.41
46:JP:400:LEU:HD12	46:JP:400:LEU:HA	1.69	0.41
48:DA:83:LYS:HE2	48:DA:83:LYS:HB2	1.84	0.41
49:DE:88:ASP:O	49:DE:100:ARG:HA	2.21	0.41
52:DH:141:ARG:NH2	60:DW:51:GLU:OE2	2.54	0.41
52:DH:177:THR:HG23	52:DH:179:LYS:HG2	2.03	0.41
60:DW:2:THR:N	66:D3:966:A:HO2'	2.18	0.41
62:DY:53:ASP:OD1	62:DY:53:ASP:N	2.40	0.41
65:D2:550:C:H2'	65:D2:551:A:C8	2.55	0.41
66:D3:9:U:H2'	66:D3:10:G:O4'	2.20	0.41
66:D3:181:A:H2'	66:D3:182:A:C8	2.55	0.41
66:D3:186:C:H2'	66:D3:187:G:O4'	2.20	0.41
66:D3:410:A:H2'	66:D3:411:C:O4'	2.21	0.41
66:D3:630:A:C5	66:D3:631:G:C8	3.09	0.41
1:UA:23:SER:OG	1:UA:24:ASP:N	2.54	0.40
1:UA:315:GLU:O	1:UA:316:TRP:HD1	2.04	0.40
4:UD:212:ILE:HG21	4:UD:212:ILE:HD13	1.85	0.40
5:UE:123:SER:HB3	5:UE:141:ARG:HH22	1.86	0.40
5:UE:173:ILE:HG21	5:UE:173:ILE:HD13	1.88	0.40
6:UF:271:LEU:HD13	6:UF:337:HIS:HB3	2.03	0.40
6:UF:309:LEU:HD13	6:UF:312:LEU:HD11	2.03	0.40
7:UG:484:PRO:HG2	7:UG:497:LEU:HD23	2.03	0.40
10:UJ:59:LEU:HB3	10:UJ:66:PHE:CD2	2.56	0.40
10:UJ:349:THR:HG21	10:UJ:379:GLU:HG2	2.03	0.40
11:UK:190:LEU:O	11:UK:194:LYS:HG2	2.22	0.40
12:UL:23:CYS:HB2	12:UL:41:LEU:HD11	2.02	0.40
12:UL:143:SER:HB3	12:UL:162:HIS:HB2	2.04	0.40
12:UL:289:GLU:OE1	12:UL:289:GLU:N	2.52	0.40
13:UM:433:HIS:NE2	13:UM:435:ALA:O	2.54	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
13:UM:618:ASN:OD1	13:UM:618:ASN:N	2.51	0.40
15:UO:97:CYS:HB3	15:UO:132:PHE:HE2	1.85	0.40
15:UO:404:ALA:CB	15:UO:417:VAL:HG11	2.51	0.40
21:UU:419:ILE:HD13	21:UU:419:ILE:HG21	1.90	0.40
22:UV:115:LYS:HA	22:UV:115:LYS:HD2	1.93	0.40
22:UV:738:TYR:O	22:UV:742:PHE:HB2	2.20	0.40
23:UX:103:MET:CG	23:UX:127:ARG:HH21	2.32	0.40
23:UX:109:LEU:HB3	23:UX:113:TYR:CE2	2.56	0.40
27:CE:4:VAL:O	27:CE:14:LEU:HA	2.20	0.40
32:CK:489:SER:O	32:CK:489:SER:OG	2.37	0.40
33:CL:156:LEU:HD23	33:CL:156:LEU:HA	1.86	0.40
33:CL:1108:LYS:HB3	33:CL:1108:LYS:HE3	1.83	0.40
35:CN:70:PHE:HZ	35:CN:158:TRP:HA	1.86	0.40
35:CN:255:LYS:O	35:CN:261:GLN:HB3	2.21	0.40
36:JA:25:ILE:HG23	36:JA:198:CYS:SG	2.61	0.40
36:JA:32:ARG:N	36:JA:203:ASP:OD2	2.36	0.40
36:JA:71:LYS:HA	36:JA:71:LYS:HD3	1.86	0.40
36:JA:97:PHE:CE1	36:JA:101:GLN:HG3	2.56	0.40
36:JA:108:TYR:OH	36:JA:126:ASP:O	2.37	0.40
36:JA:117:ASN:O	36:JA:141:THR:OG1	2.39	0.40
36:JA:846:SER:HB3	36:JA:918:ARG:NH1	2.35	0.40
37:JC:55:PHE:CD1	37:JC:75:GLY:HA3	2.56	0.40
41:JJ:185:PHE:HB2	41:JJ:231:ILE:CG1	2.51	0.40
46:JP:21:GLU:H	46:JP:21:GLU:HG3	1.64	0.40
46:JP:202:HIS:HB3	46:JP:211:PRO:HB3	2.03	0.40
50:DF:143:ARG:O	50:DF:162:VAL:HG12	2.21	0.40
57:DO:62:LEU:HD23	57:DO:62:LEU:HA	1.71	0.40
58:DQ:98:ASP:N	58:DQ:98:ASP:OD1	2.47	0.40
61:DX:70:LYS:O	61:DX:87:VAL:HG12	2.21	0.40
62:DY:10:ARG:C	62:DY:24:VAL:HG12	2.41	0.40
62:DY:25:VAL:HB	62:DY:71:GLY:C	2.42	0.40
65:D2:246:G:H2'	65:D2:247:U:O4'	2.22	0.40
66:D3:8:U:O4	67:D4:27:U:H5	2.04	0.40
66:D3:314:C:H42	66:D3:354:C:H42	1.69	0.40
66:D3:353:A:OP2	66:D3:354:C:N4	2.51	0.40
66:D3:1676:U:H1'	66:D3:1726:G:N2	2.36	0.40
1:UA:63:LEU:HD12	1:UA:69:LEU:O	2.21	0.40
1:UA:336:SER:OG	21:UU:744:SER:OG	2.26	0.40
2:UB:548:ARG:HH11	2:UB:642:SER:HB2	1.86	0.40
2:UB:606:PHE:CZ	2:UB:677:ASP:HB3	2.56	0.40
4:UD:83:ASN:O	4:UD:85:TRP:N	2.47	0.40



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:UD:102:LEU:HD23	4:UD:102:LEU:HA	1.90	0.40
4:UD:383:LEU:HD23	4:UD:383:LEU:HA	1.94	0.40
6:UF:144:VAL:O	6:UF:148:ILE:HD12	2.21	0.40
8:UH:32:ALA:O	8:UH:353:ARG:N	2.50	0.40
10:UJ:266:THR:O	10:UJ:266:THR:OG1	2.34	0.40
12:UL:106:TRP:CZ3	12:UL:113:VAL:HB	2.56	0.40
12:UL:123:ALA:O	12:UL:141:LYS:N	2.48	0.40
12:UL:406:LEU:HA	12:UL:406:LEU:HD23	1.92	0.40
12:UL:760:ILE:HA	12:UL:760:ILE:HD13	1.86	0.40
13:UM:86:LYS:HZ2	13:UM:86:LYS:HG2	1.65	0.40
17:UQ:349:PRO:HB2	17:UQ:350:GLN:HG3	2.02	0.40
18:UR:158:VAL:O	18:UR:161:ILE:HG22	2.21	0.40
18:UR:181:GLU:HB3	21:UU:281:ARG:NH2	2.36	0.40
18:UR:545:HIS:HB2	18:UR:552:PHE:CZ	2.57	0.40
19:US:156:TRP:HZ3	19:US:215:ASN:HB2	1.86	0.40
19:US:314:VAL:HG11	19:US:352:VAL:HG11	2.02	0.40
19:US:341:LEU:O	19:US:344:ILE:HG22	2.20	0.40
21:UU:375:LEU:HD12	21:UU:414:ILE:HD12	2.03	0.40
21:UU:525:ILE:HG21	21:UU:525:ILE:HD13	1.83	0.40
22:UV:330:PRO:HG2	22:UV:331:LEU:HD12	2.03	0.40
22:UV:464:THR:HG23	22:UV:466:THR:HG23	2.02	0.40
22:UV:795:GLU:O	22:UV:799:LEU:HB2	2.21	0.40
22:UV:1098:PHE:CZ	22:UV:1184:GLY:HA3	2.56	0.40
25:CB:198:GLU:OE2	25:CB:200:SER:N	2.54	0.40
26:CD:411:ARG:HA	26:CD:411:ARG:HD3	1.91	0.40
28:CF:63:ILE:HG21	28:CF:63:ILE:HD13	1.80	0.40
31:CJ:127:LEU:HD12	31:CJ:127:LEU:HA	1.84	0.40
32:CK:447:LYS:HE2	32:CK:447:LYS:HB2	1.85	0.40
33:CL:176:LEU:HD22	33:CL:176:LEU:HA	1.93	0.40
33:CL:257:LEU:HD23	33:CL:257:LEU:HA	1.84	0.40
33:CL:863:THR:HA	33:CL:868:ARG:O	2.21	0.40
34:CM:7:LYS:N	34:CM:30:PRO:HB2	2.36	0.40
34:CM:48:TYR:CE2	34:CM:94:LYS:HE3	2.56	0.40
35:CN:100:LEU:HA	35:CN:100:LEU:HD12	1.88	0.40
36:JA:215:ASN:N	36:JA:215:ASN:OD1	2.53	0.40
37:JC:34:LYS:HE3	37:JC:34:LYS:HB3	1.93	0.40
39:JG:166:PRO:O	39:JG:169:ASP:HB3	2.21	0.40
43:JM:68:GLY:O	43:JM:72:LEU:HB2	2.22	0.40
46:JP:112:LEU:HB3	46:JP:113:VAL:O	2.22	0.40
48:DA:97:LEU:HD23	48:DA:97:LEU:HA	1.83	0.40
50:DF:40:ILE:HG12	50:DF:69:PHE:CE2	2.57	0.40



	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
52:DH:61:PHE:HA	52:DH:93:LEU:O	2.21	0.40
60:DW:78:ARG:O	60:DW:124:LYS:HD3	2.21	0.40
61:DX:107:PHE:HD1	61:DX:123:LYS:HB3	1.86	0.40
65:D2:509:A:H2'	65:D2:510:A:C8	2.57	0.40
66:D3:1122:G:H1	67:D4:3:C:H42	1.70	0.40
2:UB:740:MET:HE3	59:DS:103:ASN:CB	2.51	0.40
5:UE:56:SER:O	5:UE:56:SER:OG	2.31	0.40
5:UE:322:ILE:HD12	5:UE:322:ILE:HA	1.90	0.40
6:UF:281:LEU:HD23	6:UF:281:LEU:HA	1.80	0.40
7:UG:60:ALA:HA	7:UG:63:THR:HG22	2.03	0.40
7:UG:185:HIS:ND1	30:CI:24:ASP:OD2	2.55	0.40
7:UG:309:LEU:HD23	7:UG:309:LEU:HA	1.88	0.40
7:UG:448:SER:O	14:UN:843:GLN:HG2	2.21	0.40
8:UH:660:LEU:HD23	8:UH:660:LEU:HA	1.81	0.40
11:UK:135:ILE:HA	25:CB:302:GLU:OE2	2.21	0.40
12:UL:672:VAL:HG13	12:UL:684:TRP:HD1	1.86	0.40
13:UM:736:LEU:HD23	13:UM:736:LEU:HA	1.88	0.40
14:UN:317:LYS:HD2	14:UN:317:LYS:HA	1.92	0.40
15:UO:239:LEU:HA	15:UO:239:LEU:HD12	1.84	0.40
17:UQ:559:LYS:HB3	17:UQ:576:ALA:HB3	2.02	0.40
19:US:295:LEU:HD13	19:US:295:LEU:HA	1.95	0.40
19:US:399:ILE:HA	19:US:399:ILE:HD13	1.83	0.40
21:UU:511:ASP:OD1	21:UU:512:GLY:N	2.54	0.40
21:UU:630:THR:HG22	21:UU:644:THR:O	2.21	0.40
21:UU:847:LEU:HD12	21:UU:847:LEU:HA	1.81	0.40
22:UV:807:LEU:HD23	22:UV:807:LEU:HA	1.83	0.40
22:UV:814:LEU:O	22:UV:818:SER:HB2	2.21	0.40
22:UV:1102:LEU:HG	22:UV:1231:VAL:HA	2.03	0.40
23:UX:76:ILE:HD12	23:UX:76:ILE:HG23	1.83	0.40
24:UZ:155:ARG:NH2	47:JQ:179:VAL:HG21	2.37	0.40
24:UZ:179:GLN:HG2	47:JQ:192:ALA:HB3	2.03	0.40
25:CA:308:PRO:HG2	25:CA:309:TYR:CE2	2.56	0.40
25:CB:239:CYS:SG	25:CB:240:VAL:N	2.93	0.40
26:CD:245:SER:O	26:CD:250:ARG:NH2	2.54	0.40
26:CD:266:THR:O	26:CD:270:ASN:ND2	2.54	0.40
30:CI:94:ILE:HG21	30:CI:94:ILE:HD13	1.79	0.40
32:CK:365:LEU:HD12	32:CK:365:LEU:HA	1.91	0.40
33:CL:952:PHE:CD2	33:CL:958:VAL:HG22	2.56	0.40
34:CM:309:GLY:O	34:CM:353:THR:HA	2.22	0.40
46:JP:60:GLY:O	46:JP:374:LEU:HD23	2.21	0.40
46:JP:329:ILE:O	46:JP:342:ILE:HA	2.21	0.40



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:DI:84:HIS:CD2	53:DI:86:SER:H	2.39	0.40
55:DL:130:PRO:HA	55:DL:136:ARG:HG3	2.02	0.40
57:DO:48:VAL:HG22	57:DO:50:ALA:H	1.85	0.40
61:DX:133:LEU:HA	61:DX:133:LEU:HD23	1.77	0.40
65:D2:121:G:H1'	65:D2:124:A:H61	1.86	0.40
66:D3:143:G:H2'	66:D3:144:U:H4'	2.04	0.40
66:D3:640:U:O2'	66:D3:641:G:H8	2.04	0.40
1:UA:669:ASP:O	1:UA:672:THR:OG1	2.38	0.40
2:UB:210:VAL:HA	66:D3:1208:A:H61	1.86	0.40
2:UB:543:GLY:HA3	2:UB:567:PHE:HZ	1.87	0.40
4:UD:155:LYS:HA	4:UD:169:ASP:HA	2.04	0.40
5:UE:91:LEU:HD23	5:UE:91:LEU:HA	1.83	0.40
7:UG:174:THR:HB	7:UG:187:LEU:HB2	2.04	0.40
11:UK:120:LYS:NZ	67:D4:323:G:OP1	2.49	0.40
11:UK:149:GLU:OE2	11:UK:156:SER:OG	2.32	0.40
12:UL:746:LEU:HD23	12:UL:746:LEU:HA	1.81	0.40
13:UM:151:LYS:HD2	13:UM:151:LYS:HA	1.91	0.40
17:UQ:565:ARG:O	17:UQ:569:ASN:HA	2.22	0.40
18:UR:137:ILE:HG21	18:UR:137:ILE:HD13	1.81	0.40
20:UT:1334:ASP:HA	20:UT:1335:GLY:HA3	1.63	0.40
21:UU:752:LYS:HE2	21:UU:752:LYS:HB2	1.86	0.40
22:UV:282:ASP:OD1	22:UV:283:TYR:N	2.54	0.40
22:UV:441:GLN:NE2	22:UV:456:LYS:HB3	2.36	0.40
22:UV:1149:LEU:HD23	22:UV:1149:LEU:HA	1.88	0.40
25:CA:135:PRO:HA	25:CA:136:PRO:HD3	1.91	0.40
25:CB:244:VAL:HG23	25:CB:249:GLN:HG2	2.03	0.40
26:CD:202:HIS:CE1	26:CD:203:PHE:HB2	2.56	0.40
27:CE:328:ARG:O	27:CE:332:THR:HG22	2.22	0.40
27:CE:429:ALA:HA	27:CE:432:ASP:HB2	2.02	0.40
28:CG:87:LEU:HD12	28:CG:87:LEU:HA	1.91	0.40
29:CH:431:LYS:HE3	29:CH:431:LYS:HB3	1.91	0.40
31:CJ:42:LEU:HD23	31:CJ:42:LEU:HA	1.90	0.40
33:CL:831:ARG:HD3	33:CL:838:ILE:HA	2.02	0.40
33:CL:1034:LEU:O	33:CL:1038:ILE:HG23	2.20	0.40
34:CM:158:SER:H	34:CM:162:GLY:HA2	1.86	0.40
35:CN:199:GLN:HA	35:CN:202:VAL:HG12	2.02	0.40
36:JA:763:LEU:HD23	36:JA:774:LEU:HD13	2.02	0.40
36:JA:911:ALA:O	36:JA:915:LYS:HG3	2.22	0.40
37:JC:301:ASP:HB2	37:JC:306:LYS:HB3	2.02	0.40
45:JO:180:LEU:HA	45:JO:180:LEU:HD23	1.78	0.40
46:JP:91:VAL:HG23	46:JP:106:PHE:O	2.21	0.40


		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
48:DA:179:SER:OG	48:DA:180:THR:N	2.54	0.40
51:DG:77:LEU:HB3	51:DG:84:TYR:CD2	2.57	0.40
52:DH:84:LYS:CD	52:DH:85:PHE:CE1	3.04	0.40
52:DH:174:ASN:O	52:DH:178:GLY:HA2	2.22	0.40
55:DL:27:THR:OG1	55:DL:28:SER:N	2.55	0.40
55:DL:131:ILE:HB	55:DL:135:VAL:HG23	2.02	0.40
56:DN:84:ILE:HA	56:DN:85:PRO:HD3	1.81	0.40
56:DN:112:LYS:NZ	66:D3:974:A:O3'	2.45	0.40
62:DY:8:ARG:HE	62:DY:9:THR:H	1.69	0.40
66:D3:538:A:H5'	66:D3:543:C:H5	1.86	0.40
66:D3:1661:U:H2'	66:D3:1662:G:C8	2.56	0.40
4:UD:180:ASP:OD1	4:UD:181:THR:OG1	2.38	0.40
4:UD:219:ASP:OD1	4:UD:220:GLU:N	2.55	0.40
7:UG:136:SER:HG	7:UG:159:TYR:HH	1.69	0.40
7:UG:168:VAL:HG22	7:UG:177:TYR:HE2	1.87	0.40
8:UH:668:ILE:HD12	9:UI:448:GLU:HA	2.04	0.40
12:UL:536:CYS:SG	12:UL:537:VAL:N	2.94	0.40
12:UL:540:SER:HG	12:UL:544:ARG:H	1.67	0.40
13:UM:345:TYR:CZ	13:UM:626:MET:HB2	2.56	0.40
15:UO:21:THR:CG2	15:UO:24:GLN:HB2	2.51	0.40
17:UQ:22:LEU:HD21	17:UQ:32:LYS:HD3	2.03	0.40
18:UR:129:ASP:HA	18:UR:132:LYS:HE3	2.04	0.40
20:UT:1775:ALA:HB1	38:JE:353:ALA:HB1	2.04	0.40
21:UU:868:LEU:HA	21:UU:868:LEU:HD23	1.72	0.40
22:UV:468:PHE:CD2	22:UV:470:LYS:HG2	2.57	0.40
22:UV:626:LYS:HA	22:UV:626:LYS:HD2	1.88	0.40
22:UV:635:SER:OG	22:UV:636:GLU:N	2.55	0.40
26:CD:170:ASN:HD21	27:CE:190:TRP:HE1	1.68	0.40
26:CD:198:TRP:CE3	26:CD:271:VAL:HG22	2.49	0.40
27:CE:160:ASP:O	27:CE:164:ILE:HG12	2.21	0.40
27:CE:258:LEU:HA	27:CE:258:LEU:HD12	1.90	0.40
29:CH:289:ARG:HB3	29:CH:292:SER:HB3	2.03	0.40
36:JA:814:LEU:HD23	36:JA:814:LEU:HA	1.90	0.40
37:JC:178:LEU:HA	37:JC:214:ARG:HH22	1.86	0.40
37:JC:304:ASP:OD1	37:JC:304:ASP:N	2.50	0.40
41:JJ:182:ILE:HA	41:JJ:233:ILE:O	2.22	0.40
45:JO:167:GLN:O	45:JO:170:THR:N	2.48	0.40
46:JP:238:THR:OG1	46:JP:264:THR:OG1	2.29	0.40
46:JP:320:ILE:HD13	46:JP:320:ILE:HG21	1.83	0.40
49:DE:101:LEU:HD13	49:DE:101:LEU:HA	1.92	0.40
50:DF:80:LYS:HE3	50:DF:83:ARG:HH21	1.87	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
52:DH:143:LEU:HA	52:DH:143:LEU:HD23	1.88	0.40
53:DI:9:HIS:NE2	66:D3:339:C:OP1	2.52	0.40
53:DI:49:ARG:HH22	66:D3:399:A:P	2.45	0.40
54:DJ:104:PHE:HD1	54:DJ:104:PHE:HA	1.73	0.40
66:D3:57:G:H2'	66:D3:58:U:C6	2.56	0.40
66:D3:230:C:N3	66:D3:236:A:N6	2.69	0.40
66:D3:309:C:H2'	66:D3:310:C:C6	2.57	0.40
66:D3:892:A:C6	66:D3:893:U:C4	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	UA	830/923~(90%)	730 (88%)	99~(12%)	1 (0%)	51	84
2	UB	496/810~(61%)	458 (92%)	35 (7%)	3 (1%)	25	63
3	UC	124/610~(20%)	113 (91%)	10 (8%)	1 (1%)	19	57
4	UD	663/776~(85%)	585 (88%)	78 (12%)	0	100	100
5	UE	465/643~(72%)	401 (86%)	63 (14%)	1 (0%)	47	79
6	UF	283/440~(64%)	273 (96%)	10 (4%)	0	100	100
7	UG	529/554~(96%)	471 (89%)	58 (11%)	0	100	100
8	UH	423/713~(59%)	305 (72%)	94 (22%)	24 (6%)	1	21
9	UI	98/575~(17%)	92 (94%)	6 (6%)	0	100	100
10	UJ	1093/1769~(62%)	1038 (95%)	55 (5%)	0	100	100
11	UK	237/250~(95%)	217 (92%)	19 (8%)	1 (0%)	34	71
12	UL	828/943~(88%)	733 (88%)	94 (11%)	1 (0%)	51	84
13	UM	750/817~(92%)	666 (89%)	84 (11%)	0	100	100



α $\cdot \cdot$ \cdot	c		
Continued	from	previous	page

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
14	UN	141/145~(97%)	124 (88%)	16 (11%)	1 (1%)	22	60
15	UO	489/513~(95%)	433 (88%)	55~(11%)	1 (0%)	47	79
16	UP	58/214~(27%)	57~(98%)	1 (2%)	0	100	100
17	UQ	820/896~(92%)	720 (88%)	98~(12%)	2 (0%)	47	79
18	UR	473/594 (80%)	432 (91%)	40 (8%)	1 (0%)	47	79
19	US	471/552~(85%)	421 (89%)	49 (10%)	1 (0%)	47	79
20	UT	2189/2493~(88%)	2067 (94%)	122 (6%)	0	100	100
21	UU	842/939~(90%)	737 (88%)	105 (12%)	0	100	100
22	UV	1068/1237~(86%)	1006 (94%)	62 (6%)	0	100	100
23	UX	170/189~(90%)	151 (89%)	18 (11%)	1 (1%)	25	63
24	UZ	245/274~(89%)	217 (89%)	28 (11%)	0	100	100
25	CA	238/327~(73%)	220 (92%)	18 (8%)	0	100	100
25	CB	224/327~(68%)	197 (88%)	27 (12%)	0	100	100
26	CD	376/504~(75%)	351 (93%)	25 (7%)	0	100	100
27	CE	431/511 (84%)	394 (91%)	37~(9%)	0	100	100
28	CF	121/126~(96%)	112 (93%)	9~(7%)	0	100	100
28	CG	121/126~(96%)	111 (92%)	10 (8%)	0	100	100
29	CH	446/573~(78%)	399 (90%)	45 (10%)	2 (0%)	34	71
30	CI	180/183~(98%)	162 (90%)	18 (10%)	0	100	100
31	CJ	278/290~(96%)	247 (89%)	30 (11%)	1 (0%)	34	71
32	CK	203/593~(34%)	177 (87%)	25 (12%)	1 (0%)	29	67
33	CL	771/1183~(65%)	704 (91%)	63 (8%)	4 (0%)	29	67
34	CM	358/367~(98%)	334 (93%)	24 (7%)	0	100	100
35	CN	224/297~(75%)	210 (94%)	14 (6%)	0	100	100
36	JA	802/1056~(76%)	717 (89%)	85 (11%)	0	100	100
36	JB	827/1056~(78%)	736 (89%)	91 (11%)	0	100	100
37	JC	350/707~(50%)	308 (88%)	42 (12%)	0	100	100
38	JE	134/357~(38%)	119 (89%)	14 (10%)	1 (1%)	22	60
39	JF	212/252~(84%)	201 (95%)	11 (5%)	0	100	100
39	JG	226/252~(90%)	215 (95%)	11 (5%)	0	100	100
40	JH	257/483~(53%)	244 (95%)	13 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
41	JJ	180/274~(66%)	166~(92%)	13 (7%)	1 (1%)	25	63
42	JK	40/534~(8%)	30~(75%)	10~(25%)	0	100	100
43	JM	129/217~(59%)	113 (88%)	15 (12%)	1 (1%)	19	57
44	JN	178/346~(51%)	154 (86%)	19 (11%)	5(3%)	5	34
45	JO	232/316~(73%)	215 (93%)	17 (7%)	0	100	100
46	JP	453/489~(93%)	412 (91%)	41 (9%)	0	100	100
47	JQ	59/206~(29%)	49 (83%)	9 (15%)	1 (2%)	9	43
48	DA	236/255~(92%)	207 (88%)	29 (12%)	0	100	100
49	DE	243/261~(93%)	224 (92%)	19 (8%)	0	100	100
50	DF	211/225~(94%)	188 (89%)	23 (11%)	0	100	100
51	DG	216/236~(92%)	203 (94%)	13 (6%)	0	100	100
52	DH	182/190~(96%)	160 (88%)	22 (12%)	0	100	100
53	DI	173/200~(86%)	160 (92%)	13 (8%)	0	100	100
54	DJ	175/197~(89%)	160 (91%)	15 (9%)	0	100	100
55	DL	138/156~(88%)	125 (91%)	13 (9%)	0	100	100
56	DN	148/151~(98%)	127 (86%)	21 (14%)	0	100	100
57	DO	118/137~(86%)	107 (91%)	10 (8%)	1 (1%)	19	57
58	DQ	123/143~(86%)	114 (93%)	9~(7%)	0	100	100
59	DS	98/147~(67%)	89 (91%)	9 (9%)	0	100	100
60	DW	127/130~(98%)	106 (84%)	21 (16%)	0	100	100
61	DX	101/145~(70%)	89~(88%)	12 (12%)	0	100	100
62	DY	95/135~(70%)	79~(83%)	16 (17%)	0	100	100
63	Db	79/82~(96%)	66 (84%)	13 (16%)	0	100	100
64	Dc	61/67~(91%)	52 (85%)	9 (15%)	0	100	100
All	All	24359/32678 (74%)	22000 (90%)	2302 (10%)	57 (0%)	50	79

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	UB	399	HIS
8	UH	59	PRO
8	UH	61	PRO
8	UH	68	PRO
8	UH	127	TYR



Mol	Chain	Res	Type
8	UH	258	PRO
8	UH	309	PRO
15	UO	20	THR
17	UQ	335	PRO
29	СН	438	ILE
32	CK	454	VAL
33	CL	78	PRO
33	CL	626	LYS
41	JJ	273	ARG
44	JN	94	PRO
44	JN	97	ILE
8	UH	52	ILE
8	UH	162	GLU
8	UH	235	PRO
8	UH	316	PRO
8	UH	533	PRO
19	US	85	GLU
8	UH	29	VAL
8	UH	208	SER
8	UH	287	LEU
8	UH	297	LEU
43	JM	202	ARG
44	JN	107	VAL
44	JN	111	LYS
8	UH	245	LEU
23	UX	52	PHE
44	JN	93	GLN
3	UC	594	GLU
8	UH	53	SER
8	UH	308	PHE
17	UQ	318	GLU
31	CJ	93	SER
57	DO	129	LYS
2	UB	284	ALA
2	UB	395	ASP
8	UH	198	ILE
8	UH	298	PRO
11	UK	226	LYS
12	UL	336	TYR
18	UR	226	LYS
29	СН	439	ALA
33	CL	81	GLY



Mol	Chain	Res	Type
8	UH	292	ILE
1	UA	33	VAL
47	JQ	146	ILE
8	UH	70	PRO
14	UN	881	PRO
8	UH	56	ILE
8	UH	266	ILE
38	JE	274	ILE
5	UE	517	PRO
33	CL	774	PRO

5.3.2 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 EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{ntiles}
1	UA	730/812~(90%)	729 (100%)	1 (0%)	93	97
2	UB	345/732~(47%)	345~(100%)	0	100	100
3	UC	107/538~(20%)	103~(96%)	4 (4%)	34	60
4	UD	615/713~(86%)	612~(100%)	3~(0%)	88	93
5	UE	428/574~(75%)	426 (100%)	2 (0%)	88	93
6	UF	277/414~(67%)	275~(99%)	2 (1%)	84	90
7	UG	462/480~(96%)	462 (100%)	0	100	100
8	UH	150/657~(23%)	149~(99%)	1 (1%)	84	90
9	UI	97/533~(18%)	97 (100%)	0	100	100
10	UJ	390/1633~(24%)	388 (100%)	2 (0%)	88	93
11	UK	226/234~(97%)	223~(99%)	3 (1%)	69	82
12	UL	746/832~(90%)	745~(100%)	1 (0%)	93	97
13	UM	665/719~(92%)	663 (100%)	2 (0%)	92	95
14	UN	135/135~(100%)	135 (100%)	0	100	100
15	UO	437/454~(96%)	435 (100%)	2(0%)	88	93
16	UP	57/196~(29%)	56~(98%)	1 (2%)	59	77



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
17	UQ	769/826~(93%)	763~(99%)	6(1%)	81	89
18	UR	424/529~(80%)	421 (99%)	3 (1%)	84	90
19	US	360/506~(71%)	360~(100%)	0	100	100
21	UU	743/819~(91%)	740 (100%)	3~(0%)	91	94
22	UV	985/1125~(88%)	980 (100%)	5~(0%)	88	93
23	UX	156/169~(92%)	155~(99%)	1 (1%)	86	91
24	UZ	230/256~(90%)	228 (99%)	2 (1%)	78	87
25	CA	202/240~(84%)	200 (99%)	2 (1%)	76	86
25	CB	192/240~(80%)	191 (100%)	1 (0%)	88	93
26	CD	326/435~(75%)	325 (100%)	1 (0%)	92	95
27	CE	244/433~(56%)	244 (100%)	0	100	100
28	CF	102/104~(98%)	102 (100%)	0	100	100
28	CG	101/104~(97%)	100 (99%)	1 (1%)	76	86
29	CH	395/503~(78%)	393 (100%)	2 (0%)	88	93
30	CI	171/172~(99%)	170 (99%)	1 (1%)	86	91
31	CJ	251/258~(97%)	249 (99%)	2 (1%)	81	89
32	CK	187/535~(35%)	187 (100%)	0	100	100
33	CL	690/1039~(66%)	684 (99%)	6 (1%)	78	87
34	CM	307/312~(98%)	306 (100%)	1 (0%)	92	95
35	CN	212/274~(77%)	212 (100%)	0	100	100
36	JA	549/934~(59%)	545~(99%)	4 (1%)	84	90
37	JC	318/636~(50%)	318 (100%)	0	100	100
38	JE	119/315~(38%)	118~(99%)	1 (1%)	81	89
39	$_{ m JF}$	195/222~(88%)	195 (100%)	0	100	100
39	JG	206/222~(93%)	206 (100%)	0	100	100
41	JJ	159/238~(67%)	156 (98%)	3 (2%)	57	75
42	JK	35/482~(7%)	35 (100%)	0	100	100
43	JM	124/200~(62%)	123 (99%)	1 (1%)	81	89
44	JN	141/304~(46%)	141 (100%)	0	100	100
45	JO	215/289~(74%)	213 (99%)	2 (1%)	78	87
46	JP	412/443~(93%)	412 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
47	JQ	22/192~(12%)	21 (96%)	1 (4%)	27	56
48	DA	212/224~(95%)	209 (99%)	3 (1%)	67	81
49	DE	209/222~(94%)	206 (99%)	3 (1%)	67	81
50	DF	180/191~(94%)	180 (100%)	0	100	100
51	DG	187/201~(93%)	186 (100%)	1 (0%)	88	93
52	DH	164/170~(96%)	162 (99%)	2 (1%)	71	83
53	DI	142/161~(88%)	141 (99%)	1 (1%)	84	90
54	DJ	151/166~(91%)	150 (99%)	1 (1%)	84	90
55	DL	125/137~(91%)	125 (100%)	0	100	100
56	DN	127/128~(99%)	127 (100%)	0	100	100
57	DO	91/105~(87%)	91 (100%)	0	100	100
58	DQ	105/119~(88%)	105 (100%)	0	100	100
60	DW	$110/111 \ (99\%)$	110 (100%)	0	100	100
61	DX	85/120 (71%)	83~(98%)	2 (2%)	49	69
62	DY	81/113 (72%)	81 (100%)	0	100	100
63	Db	70/71~(99%)	70 (100%)	0	100	100
64	Dc	56/60~(93%)	56 (100%)	0	100	100
All	All	17504/25311~(69%)	17418 (100%)	86 (0%)	89	93

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	674	LYS
3	UC	544	ILE
3	UC	545	LEU
3	UC	548	LYS
3	UC	553	LYS
4	UD	472	ARG
4	UD	565	ARG
4	UD	689	ASN
5	UE	180	VAL
5	UE	184	PHE
6	UF	67	ARG
6	UF	266	ARG
8	UH	664	LYS
10	UJ	143	TYR



Mol	Chain	Res	Type
10	UJ	145	THR
11	UK	82	ARG
11	UK	150	LYS
11	UK	217	ARG
12	UL	255	ARG
13	UM	464	LYS
13	UM	747	ASN
15	UO	20	THR
15	UO	509	GLN
16	UP	160	ARG
17	UQ	333	PHE
17	UQ	334	LEU
17	UQ	432	ARG
17	UQ	433	ARG
17	UQ	446	ASN
17	UQ	828	LYS
18	UR	41	ASN
18	UR	217	ASN
18	UR	365	ASN
21	UU	19	LYS
21	UU	476	PHE
21	UU	587	ARG
22	UV	154	LYS
22	UV	269	ARG
22	UV	520	ASN
22	UV	712	ASN
22	UV	834	ASN
23	UX	60	LYS
24	UZ	117	GLN
24	UZ	120	LYS
25	CA	122	ARG
25	CA	138	LYS
25	CB	231	ARG
26	CD	391	ASN
28	CG	31	ARG
$\overline{29}$	CH	370	ARG
29	CH	506	ARG
30	CI	25	GLN
31	CJ	116	ARG
31	CJ	226	ASN
33	CL	45	ARG
33	CL	84	THR



Mol	Chain	Res	Type
33	CL	92	ARG
33	CL	119	GLU
33	CL	176	LEU
33	CL	960	ARG
34	CM	147	ARG
36	JA	9	ARG
36	JA	32	ARG
36	JA	829	HIS
36	JA	861	MET
38	JE	356	ARG
41	JJ	129	ARG
41	JJ	271	LYS
41	JJ	273	ARG
43	JM	77	LYS
45	JO	274	ARG
45	JO	280	LYS
47	JQ	183	ARG
48	DA	8	ARG
48	DA	11	LYS
48	DA	19	ARG
49	DE	3	ARG
49	DE	200	ARG
49	DE	233	LYS
51	DG	4	ASN
52	DH	19	GLN
52	DH	42	GLN
53	DI	24	LYS
54	DJ	57	ARG
61	DX	109	ARG
61	DX	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	UA	421	ASN
3	UC	496	GLN
4	UD	292	ASN
4	UD	310	ASN
4	UD	483	ASN
5	UE	346	HIS
5	UE	443	GLN
6	UF	169	GLN



Mol	Chain	Res	Type
6	UF	191	ASN
6	UF	207	ASN
9	UI	443	GLN
10	UJ	166	ASN
10	UJ	227	ASN
11	UK	206	GLN
12	UL	390	GLN
12	UL	901	ASN
13	UM	667	GLN
13	UM	671	ASN
13	UM	757	GLN
15	UO	24	GLN
15	UO	313	GLN
17	UQ	115	HIS
17	UQ	289	GLN
17	UQ	332	GLN
18	UR	41	ASN
18	UR	242	ASN
18	UR	365	ASN
19	US	196	GLN
19	US	200	ASN
19	US	256	ASN
22	UV	1154	ASN
23	UX	70	ASN
24	UZ	117	GLN
24	UZ	192	ASN
24	UZ	193	ASN
26	CD	23	GLN
26	CD	189	ASN
27	CE	145	HIS
28	CG	113	GLN
29	CH	463	GLN
33	CL	241	HIS
33	CL	315	GLN
36	JA	19	GLN
36	JA	548	ASN
36	JA	822	ASN
39	JF	73	HIS
39	JG	73	HIS
48	DA	16	GLN
52	DH	19	GLN
52	DH	170	GLN



Continued from previous page...

Mol	Chain	Res	Type
52	DH	174	ASN
55	DL	127	GLN
62	DY	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
65	D2	518/700~(74%)	166 (32%)	9(1%)
66	D3	1172/1808~(64%)	423~(36%)	28~(2%)
67	D4	169/175~(96%)	62~(36%)	2(1%)
All	All	1859/2683~(69%)	651 (35%)	39~(2%)

All (651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
65	D2	6	А
65	D2	7	А
65	D2	8	А
65	D2	9	G
65	D2	15	G
65	D2	63	G
65	D2	69	U
65	D2	70	А
65	D2	81	А
65	D2	82	А
65	D2	83	U
65	D2	86	С
65	D2	90	G
65	D2	97	G
65	D2	98	G
65	D2	103	G
65	D2	107	G
65	D2	109	С
65	D2	113	А
65	D2	122	U
65	D2	124	А
65	D2	125	G
65	D2	129	U
65	D2	130	G
65	D2	137	С
65	D2	141	А



Mol	Chain	Res	Type
65	D2	144	С
65	D2	150	G
65	D2	151	U
65	D2	152	U
65	D2	153	U
65	D2	162	U
65	D2	163	G
65	D2	166	U
65	D2	169	А
65	D2	170	U
65	D2	171	G
65	D2	176	U
65	D2	177	U
65	D2	184	U
65	D2	185	A
65	D2	193	G
65	D2	197	G
65	D2	200	А
65	D2	207	G
65	D2	220	U
65	D2	227	U
65	D2	234	А
65	D2	235	А
65	D2	236	С
65	D2	237	А
65	D2	238	G
65	D2	239	U
65	D2	240	С
65	D2	248	G
65	D2	252	A
65	D2	253	U
65	D2	256	U
65	D2	259	G
$\overline{65}$	D2	264	C
65	D2	266	U
65	D2	267	U
65	D2	268	G
65	D2	269	G
$\overline{65}$	D2	271	G
65	D2	278	G
65	D2	279	A
65	D2	280	A



Mol	Chain	Res	Type
65	D2	281	G
65	D2	284	U
65	D2	287	G
65	D2	292	А
65	D2	294	U
65	D2	302	А
65	D2	303	А
65	D2	304	U
65	D2	305	А
65	D2	306	G
65	D2	310	U
65	D2	311	C
65	D2	312	U
65	D2	313	A
65	D2	314	U
65	D2	315	U
65	D2	316	U
65	D2	320	А
65	D2	322	А
65	D2	323	А
65	D2	324	U
65	D2	325	U
65	D2	326	С
65	D2	327	А
65	D2	328	А
65	D2	331	U
65	D2	337	G
65	D2	341	G
65	D2	346	G
65	D2	354	G
65	D2	356	С
65	D2	358	G
65	D2	368	U
65	D2	370	U
65	D2	371	G
65	D2	372	A
65	D2	373	U
65	D2	374	U
65	D2	379	A
65	D2	384	U
65	D2	385	A
65	D2	386	A



Mol	Chain	Res	Type
65	D2	389	U
65	D2	395	С
65	D2	399	U
65	D2	407	А
65	D2	410	А
65	D2	418	С
65	D2	422	С
65	D2	425	U
65	D2	426	G
65	D2	427	А
65	D2	428	А
65	D2	430	С
65	D2	431	A
65	D2	432	С
65	D2	435	G
65	D2	441	С
65	D2	442	U
65	D2	443	G
65	D2	449	U
65	D2	451	G
65	D2	461	А
65	D2	462	G
65	D2	463	А
65	D2	465	G
65	D2	468	А
65	D2	469	С
65	D2	474	А
65	D2	475	G
65	D2	477	G
65	D2	478	U
65	D2	481	U
65	D2	482	А
65	D2	483	U
$\overline{65}$	D2	486	U
65	D2	487	А
65	D2	488	U
65	D2	489	G
65	D2	490	G
65	D2	491	U
65	D2	492	G
65	D2	493	A
65	D2	494	C



Mol	Chain	Res	Type
65	D2	518	А
65	D2	525	U
65	D2	526	U
65	D2	534	А
65	D2	535	G
65	D2	536	А
65	D2	538	С
65	D2	540	U
65	D2	541	U
65	D2	542	U
65	D2	546	G
65	D2	548	А
65	D2	584	U
65	D2	586	A
66	D3	-6	A
66	D3	-5	G
66	D3	-2	А
66	D3	-1	G
66	D3	0	U
66	D3	1	U
66	D3	2	А
66	D3	4	С
66	D3	6	G
66	D3	7	G
66	D3	9	U
66	D3	12	U
66	D3	14	С
66	D3	17	С
66	D3	23	G
66	D3	24	U
66	D3	25	C
66	D3	26	A
66	D3	36	C
66	D3	37	U
66	D3	38	C
66	D3	39	A
66	D3	51	А
66	D3	54	C
66	D3	55	A
66	D3	60	U
66	D3	65	A
66	D3	66	U



Mol	Chain	Res	Type
66	D3	69	G
66	D3	73	U
66	D3	74	U
66	D3	75	U
66	D3	76	А
66	D3	78	А
66	D3	81	G
66	D3	93	А
66	D3	94	U
66	D3	97	С
66	D3	99	С
66	D3	100	А
66	D3	104	А
66	D3	114	С
66	D3	116	U
66	D3	127	G
66	D3	128	U
66	D3	140	А
66	D3	141	U
66	D3	142	G
66	D3	143	G
66	D3	144	U
66	D3	145	А
66	D3	146	U
66	D3	153	G
66	D3	156	А
66	D3	158	U
66	D3	159	U
66	D3	162	А
66	D3	166	С
66	D3	167	U
66	D3	182	A
66	D3	184	С
66	D3	188	A
66	D3	190	C
66	D3	192	U
66	D3	193	U
66	D3	194	U
66	D3	195	G
66	D3	196	G
66	D3	197	A
66	D3	198	A



Mol	Chain	Res	Type
66	D3	200	А
66	D3	203	U
66	D3	204	G
66	D3	213	A
66	D3	227	U
66	D3	232	U
66	D3	234	G
66	D3	238	U
66	D3	241	U
66	D3	257	А
66	D3	260	U
66	D3	261	U
66	D3	262	U
66	D3	263	С
66	D3	265	A
66	D3	266	A
66	D3	271	A
66	D3	272	U
66	D3	273	G
66	D3	275	С
66	D3	276	С
66	D3	277	U
66	D3	278	U
66	D3	280	U
66	D3	298	С
66	D3	299	А
66	D3	302	U
66	D3	313	U
66	D3	314	С
66	D3	317	С
66	D3	319	U
66	D3	320	U
66	D3	321	C
66	D3	322	G
66	D3	337	G
66	D3	338	C
66	D3	350	U
66	D3	351	C
66	D3	352	A
66	D3	359	A
66	D3	360	A
66	D3	361	C



Mol	Chain	Res	Type
66	D3	366	А
66	D3	368	U
66	D3	369	А
66	D3	370	А
66	D3	371	G
66	D3	372	G
66	D3	373	G
66	D3	374	U
66	D3	376	С
66	D3	382	С
66	D3	383	G
66	D3	388	G
66	D3	400	A
66	D3	402	C
66	D3	403	G
66	D3	404	G
66	D3	411	С
66	D3	413	U
66	D3	416	А
66	D3	417	А
66	D3	418	G
66	D3	440	U
66	D3	441	А
66	D3	444	С
66	D3	446	А
66	D3	453	U
66	D3	454	U
66	D3	455	С
66	D3	459	G
66	D3	461	G
66	D3	466	U
66	D3	467	G
66	D3	468	A
66	D3	469	С
66	D3	470	A
66	D3	474	A
66	D3	477	A
66	D3	487	G
66	D3	488	G
66	D3	491	C
66	D3	494	U
66	D3	496	G



Mol	Chain	Res	Type
66	D3	501	U
66	D3	502	U
66	D3	503	G
66	D3	505	А
66	D3	506	А
66	D3	513	U
66	D3	514	G
66	D3	523	G
66	D3	524	U
66	D3	525	A
66	D3	531	С
66	D3	534	А
66	D3	539	G
66	D3	540	G
66	D3	543	С
66	D3	545	A
66	D3	546	U
66	D3	548	G
66	D3	557	G
66	D3	558	U
66	D3	562	G
66	D3	563	U
66	D3	564	G
66	D3	565	С
66	D3	566	С
66	D3	570	A
66	D3	572	С
66	D3	576	G
66	D3	579	A
66	D3	580	A
66	D3	582	U
66	D3	584	C
66	D3	585	A
66	D3	586	G
66	D3	587	С
66	D3	594	A
66	D3	595	G
66	D3	601	A
66	D3	602	U
66	D3	603	U
66	D3	625	С
66	D3	629	U



Mol	Chain	Res	Type
66	D3	634	G
66	D3	635	А
66	D3	639	U
66	D3	640	U
66	D3	642	G
66	D3	649	U
66	D3	650	U
66	D3	652	G
66	D3	654	С
66	D3	655	G
66	D3	656	G
66	D3	657	U
66	D3	658	С
66	D3	677	G
66	D3	679	U
66	D3	680	U
66	D3	682	С
66	D3	685	А
66	D3	691	С
66	D3	692	С
66	D3	693	U
66	D3	694	U
66	D3	695	U
66	D3	860	U
66	D3	861	U
66	D3	862	А
66	D3	863	А
66	D3	867	G
66	D3	873	U
66	D3	886	U
66	D3	895	G
66	D3	898	А
66	D3	900	A
66	D3	904	G
66	D3	906	А
66	D3	912	U
66	D3	913	G
66	D3	914	G
66	D3	915	A
66	D3	916	U
66	D3	921	U
66	D3	925	G



Mol	Chain	Res	Type
66	D3	926	А
66	D3	931	С
66	D3	932	U
66	D3	933	А
66	D3	935	U
66	D3	939	А
66	D3	940	А
66	D3	942	G
66	D3	951	А
66	D3	960	U
66	D3	964	U
66	D3	966	A
66	D3	970	А
66	D3	977	A
66	D3	978	A
66	D3	1029	U
66	D3	1031	U
66	D3	1032	G
66	D3	1033	С
66	D3	1036	А
66	D3	1037	С
66	D3	1038	U
66	D3	1039	A
66	D3	1040	G
66	D3	1042	G
66	D3	1043	А
66	D3	1044	U
66	D3	1050	G
66	D3	1053	G
66	D3	1058	U
66	D3	1061	A
66	D3	1062	A
66	D3	1063	U
66	D3	1064	G
66	D3	1065	A
66	D3	1070	С
66	D3	1072	С
66	D3	1076	A
66	D3	1079	U
66	D3	1081	A
66	D3	1082	С
66	D3	1084	А



Mol	Chain	Res	Type
66	D3	1118	G
66	D3	1119	G
66	D3	1123	С
66	D3	1126	G
66	D3	1128	С
66	D3	1132	А
66	D3	1133	А
66	D3	1134	С
66	D3	1135	U
66	D3	1136	U
66	D3	1140	G
66	D3	1143	A
66	D3	1144	U
66	D3	1145	U
66	D3	1146	G
66	D3	1149	G
66	D3	1152	А
66	D3	1154	G
66	D3	1156	С
66	D3	1158	С
66	D3	1159	С
66	D3	1160	А
66	D3	1161	С
66	D3	1167	G
66	D3	1176	G
66	D3	1177	С
66	D3	1178	G
66	D3	1179	G
66	D3	1204	А
66	D3	1206	U
66	D3	1207	С
66	D3	1208	A
66	D3	1214	U
66	D3	1217	A
66	D3	1218	G
66	D3	1219	A
66	D3	1223	A
66	D3	1226	A
66	D3	1264	G
66	D3	1267	G
66	D3	1268	G
66	D3	1269	U



Mol	Chain	Res	Type
66	D3	1270	G
66	D3	1271	G
66	D3	1273	G
66	D3	1434	U
66	D3	1436	А
66	D3	1437	U
66	D3	1442	U
66	D3	1471	А
66	D3	1472	С
66	D3	1473	U
66	D3	1474	G
66	D3	1475	А
66	D3	1478	G
66	D3	1480	G
66	D3	1485	С
66	D3	1486	G
66	D3	1488	G
66	D3	1489	U
66	D3	1490	С
66	D3	1491	U
66	D3	1492	A
66	D3	1493	А
66	D3	1498	G
66	D3	1504	G
66	D3	1506	G
66	D3	1509	С
66	D3	1512	G
66	D3	1514	U
66	D3	1525	А
66	D3	1526	A
66	D3	1542	G
66	D3	1570	A
66	D3	1571	С
66	D3	1572	G
66	D3	1573	A
66	D3	1574	G
66	D3	1575	G
66	D3	1582	U
66	D3	1583	A
66	D3	1584	G
66	D3	1590	G
66	D3	1591	С



Mol	Chain	Res	Type
66	D3	1593	А
66	D3	1594	G
66	D3	1595	U
66	D3	1596	С
66	D3	1600	A
66	D3	1601	G
66	D3	1602	С
66	D3	1607	G
66	D3	1609	U
66	D3	1618	С
66	D3	1619	С
66	D3	1620	С
66	D3	1621	U
66	D3	1624	С
66	D3	1627	U
66	D3	1628	U
66	D3	1629	G
66	D3	1630	U
66	D3	1631	А
66	D3	1633	А
66	D3	1638	G
66	D3	1639	С
66	D3	1640	С
66	D3	1651	А
66	D3	1654	G
66	D3	1658	G
66	D3	1665	U
66	D3	1666	U
66	D3	1670	G
66	D3	1680	G
66	D3	1681	A
66	D3	1682	U
66	D3	1683	С
66	D3	1684	U
66	D3	1695	G
66	D3	1697	G
66	D3	1698	G
66	D3	1699	G
66	D3	1703	С
66	D3	1709	С
66	D3	1710	U
66	D3	1711	С



Mol	Chain	Res	Type
66	D3	1712	А
66	D3	1716	С
66	D3	1717	G
66	D3	1726	G
66	D3	1727	G
66	D3	1730	А
66	D3	1734	U
66	D3	1736	G
66	D3	1742	U
66	D3	1746	А
66	D3	1747	G
66	D3	1769	U
66	D3	1780	G
66	D3	1781	A
66	D3	1782	A
66	D3	1783	С
66	D3	1786	G
67	D4	3	С
67	D4	4	G
67	D4	10	С
67	D4	13	С
67	D4	14	А
67	D4	15	U
67	D4	16	А
67	D4	20	U
67	D4	22	А
67	D4	24	U
67	D4	25	U
67	D4	28	А
67	D4	29	U
67	D4	30	A
67	D4	32	G
67	D4	33	A
67	D4	34	A
67	D4	35	U
67	D4	37	G
67	D4	38	U
67	D4	39	C
67	D4	40	A
67	D4	41	C
67	D4	42	U
67	D4	49	С



Mol	Chain	Res	Type
67	D4	51	C
67	D4	55	А
67	D4	56	А
67	D4	58	А
67	D4	60	А
67	D4	61	G
67	D4	63	С
67	D4	67	G
67	D4	73	А
67	D4	80	U
67	D4	82	G
67	D4	87	G
67	D4	90	С
67	D4	91	С
67	D4	92	А
67	D4	97	С
67	D4	115	G
67	D4	117	А
67	D4	118	А
67	D4	199	G
67	D4	205	G
67	D4	247	U
67	D4	248	G
67	D4	252	С
67	D4	256	G
67	D4	258	U
67	D4	259	С
67	D4	260	U
67	D4	267	А
67	D4	310	G
67	D4	312	U
67	D4	320	G
67	D4	322	А
67	D4	324	U
67	D4	325	С
67	D4	328	А
67	D4	329	С

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type	
65	D2	81	А	
Continued on next page				



Mol	Chain	Res	Type
65	D2	239	U
65	D2	311	С
65	D2	312	U
65	D2	314	U
65	D2	331	U
65	D2	370	U
65	D2	486	U
65	D2	492	G
66	D3	-6	А
66	D3	-2	А
66	D3	0	U
66	D3	127	G
66	D3	158	U
66	D3	187	G
66	D3	272	U
66	D3	375	U
66	D3	417	А
66	D3	542	А
66	D3	579	А
66	D3	583	С
66	D3	639	U
66	D3	691	С
66	D3	912	U
66	D3	959	U
66	D3	1037	С
66	D3	1057	U
66	D3	1486	G
66	D3	1572	G
66	D3	1573	А
66	D3	1594	G
66	D3	1600	А
66	D3	1620	С
66	D3	1638	G
66	D3	1657	U
66	D3	1746	А
66	D3	1768	G
67	D4	24	U
67	D4	33	А

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	B	ond ang	les
		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2									
69	GTP	CL	2001	-	26,34,34	0.93	1 (3%)	32,54,54	1.49	5 (15%)								

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
69	GTP	CL	2001	-	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
69	CL	2001	GTP	C6-N1	-2.56	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
69	CL	2001	GTP	PA-O3A-PB	-3.97	119.20	132.83
69	CL	2001	GTP	PB-O3B-PG	-3.56	120.62	132.83
69	CL	2001	GTP	C3'-C2'-C1'	3.11	105.67	100.98
69	CL	2001	GTP	C5-C6-N1	2.35	118.11	113.95
69	CL	2001	GTP	C8-N7-C5	2.26	107.29	102.99

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
69	CL	2001	GTP	C5'-O5'-PA-O1A
69	CL	2001	GTP	C3'-C4'-C5'-O5'
69	CL	2001	GTP	C4'-C5'-O5'-PA
69	CL	2001	GTP	C5'-O5'-PA-O3A

All (4) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	CL	2001	GTP	3	0

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.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	D4	5
14	UN	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UN	349:SER	С	827:GLN	N	110.52
1	D4	118:A	O3'	197:G	Р	24.98
1	D4	267:A	O3'	304:U	Р	18.78
1	D4	106:C	O3'	111:G	Р	16.51
1	D4	206:C	O3'	245:U	Р	14.23
1	D4	260:U	O3'	263:A	Р	9.82



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11358. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240



The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 270

Y Index: 225

Z Index: 182

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 4278 nm^3 ; this corresponds to an approximate mass of 3864 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.


7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.256 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.72	4.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11358 and PDB model 6ZQB. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	Q-score
All	0.9700	0.4180
CA	0.9850	0.5400
CB	0.9790	0.4490
CD	0.9810	0.4390
CE	0.9870	0.4440
CF	0.9880	0.5340
CG	0.9830	0.4950
CH	0.9690	0.4040
CI	0.9870	0.5690
CJ	0.9840	0.5330
CK	0.9830	0.4980
CL	0.9800	0.4960
\mathcal{CM}	0.9880	0.4760
CN	0.9400	0.2930
D2	0.9930	0.4430
D3	0.9800	0.3870
D4	0.9970	0.4560
DA	0.9620	0.4930
DE	0.9710	0.3350
DF	0.9870	0.5290
DG	0.9460	0.2890
DH	0.9570	0.3480
DI	0.9700	0.3140
DJ	0.9820	0.5030
DL	0.9690	0.3070
DN	0.9610	0.4690
DO	0.9940	0.5030
DQ	0.9920	0.5580
DS	0.8970	0.2850
DW	0.9810	0.5160
DX	0.9850	0.5290
DY	0.9410	0.2750
Db	0.9820	0.5160
Dc	0.9900	0.5280
JA	0.9490	0.2970

Continued on next page...



Continued from previous page...

Chain	Atom inclusion	Q-score
JB	0.7950	0.1190
JC	0.9370	0.3250
JE	0.9340	0.3590
JF	0.9640	0.3740
JG	0.9800	0.4690
JH	0.8460	0.1060
JJ	0.9770	0.4150
JK	0.9670	0.2650
JM	0.9750	0.4760
JN	0.9810	0.5150
JO	0.9840	0.4700
JP	0.9900	0.5540
JQ	0.9290	0.3940
UA	0.9910	0.5600
UB	0.9620	0.3210
UC	0.9800	0.4710
UD	0.9850	0.4520
UE	0.9900	0.4920
UF	0.9750	0.4290
UG	0.9890	0.5480
UH	0.9820	0.2700
UI	0.9810	0.3370
UJ	0.9280	0.3780
UK	0.9840	0.4860
UL	0.9820	0.4370
UM	0.9760	0.4100
UN	0.9850	0.5020
UO	0.9900	0.5010
UP	0.9650	0.4030
UQ	0.9900	0.4770
UR	0.9930	0.5470
US	0.9700	0.3530
UT	0.9300	0.2440
UU	0.9950	0.5490
UV	0.9510	0.3270
UX	0.9880	0.5520
UZ	0.9840	0.4270

