

Aug 7, 2023 – 05:43 PM EDT

PDB ID	:	7SUK
EMDB ID	:	EMD-25441
Title	:	Structure of Bfr2-Lcp5 Complex Observed in the Small Subunit Processome
		Isolated from R2TP-depleted Yeast Cells
Authors	:	Rai, J.; Zhao, Y.; Li, H.
Deposited on	:	2021-11-17
Resolution	:	3.99 Å(reported)
This is	a I	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:

:	0.0.1. dev 50
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35
	: : : : :

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 3.99 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${ m EM~structures}\ (\#{ m Entries})$
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		Qu	ality of c	hain		
1	NA	245	•	65%		18%	•	16%
2	SA	413		74%			15%	• 10%
3	NB	180	•	62%		17%		21%
4	L0	700	35%		28%	7%	30%	
5	L2	333	25%	21%	5%	499	%	
6	L3	127		71%			18%	11%
7	L4	228		70%			26%	•





Mol	Chain	Length	Quality of chain	
8	L5	213	• 82%	17%
9	L7	190	53% 31%	• 13%
10	L8	200	6 3% 20%	· 15%
11	L9	175	71%	27% •
12	LC	125	74%	26%
13	LD	156	56% 23%	• 19%
14	LE	127	67%	32% •
15	LF	90	60%	36% •
16	LG	63	84%	16%
17	LH	896	76%	17% 7%
18	LJ	513	75%	20% •
19	LK	123	88%	11% •
20	LL	555	70%	15% 14%
21	LM	431	86%	14%
22	LN	748	6 8%	22% • 9%
23	LO	855	75%	23% •
24	LP	420	77%	8% 15%
25	LQ	939	● 71%	18% • 10%
26	LS	594	66% 159	% 19%
27	LT	921	76%	16% 8%
28	LU	465	72%	25% ••
29	LV	362	• 71%	27% •
30	LW	438	82%	18%
31	LZ	182	79%	21% •
32	NG	111	5%	5%

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Mol	Chain	Length	Quality of chain							
33	NK	175	97%	. .						
34	\mathbf{SC}	247	81%	16% ••						
34	SD	247	67%	23% • 8%						
35	SE	121	• 73%	26% •						
35	SF	121	78%	21% •						
36	SG	464	68%	24% 8%						
37	SH	360	75%	24% •						
38	SI	1123	55% 16%	• 29%						
39	SJ	236	72%	19% 8%						
39	SK	236	79%	18% •						
40	SL	183	68%	26% 5%						
41	SM	290	790/	10%						
42	SN	230	7070	25%						
42	510	170	/5%	25%						
43	50	179	98%	•						
44	SQ	167	62% 1	7% • 19%						
45	SR	104	74%	23% •						
46	\mathbf{SS}	197	86%	13% •						
47	ST	806	63% 119	% 26%						
48	SY	248	83%	14% •						
49	SZ	261	99%	.						
50	NJ	265	99%							
51	NH	1141	33%	• 5%						
52	NI	187	60%	• 10%						
53	8	1807	25% 30% 10%	34%						
54	SU	513	82%	12% 6%						

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Mol	Chain	Length	Quality of cl	hain		
55	LI	687	56%	8%	36%	
56	ND	60	68%		30%	•
57	LR	811	9%		21%	• 6%
58	NE	240	9%	12%	32%	
59	SB	436	• 89%			11%
60	SV	92	59%	10%	32%	
61	SP	2418	92%			8%
62	LX	923	71%		16% •	12%
62	LY	923	9%		·	10%
63	L6	219	5%	18%	• 24%	
64	NF	124	51% 96%			•
65	5	534	46% 9% •		45%	
66	6	357	64%	13%	• 22%	

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2 Entry composition (i)

There are 66 unique types of molecules in this entry. The entry contains 213241 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 U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	NA	207	Total 1667	C 1034	N 297	O 332	${S \atop 4}$	0	0

• Molecule 2 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	370	Total 2854	C 1815	N 490	0 541	S 8	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	NB	142	Total 1098	C 677	N 218	O 203	0	0

• Molecule 4 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LO	488	Total 10405	C 4650	N 1838	O 3429	Р 488	0	0

• Molecule 5 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L2	169	Total 3585	C 1605	N 629	O 1182	Р 169	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L2	200	С	G	conflict	GB 751247007

• Molecule 6 is a protein called 40S ribosomal protein S18-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
6	L3	113	Total 901	$\begin{array}{c} \mathrm{C} \\ 569 \end{array}$	N 168	O 162	${ m S} { m 2}$	0	0

• Molecule 7 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
7	L4	228	Total 1810	C 1158	N 330	0 319	${ m S} { m 3}$	0	0

• Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues		Ate	AltConf	Trace			
8	L5	213	Total 1669	C 1045	N 307	0 314	$\frac{S}{3}$	0	0

• Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
9	L7	165	Total 1321	C 854	N 227	O 240	0	0

• Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	L8	170	Total 1349	C 839	N 267	0 241	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	L9	175	Total 1415	C 895	N 273	0 246	S 1	0	0

• Molecule 12 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
12	LC	125	Total 973	$\begin{array}{c} \mathrm{C} \\ 625 \end{array}$	N 174	О 174	0	0

• Molecule 13 is a protein called 40S ribosomal protein S11-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	LD	127	Total 1027	C 660	N 194	O 170	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
14	LE	127	Total 1003	C 640	N 183	0 177	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
15	\mathbf{LF}	90	Total 715	C 458	N 131	O 126	0	0

• Molecule 16 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
16	IC	63	Total	С	Ν	0	S	0	0
10	LG	03	497	306	99	91	1	0	0

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

Mol	Chain	Residues		Α	AltConf	Trace			
17	LH	834	Total 6633	C 4215	N 1121	O 1278	S 19	0	0

• Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues		At	AltConf	Trace			
18	LJ	493	Total 3911	C 2462	N 702	0 735	S 12	0	0

• Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	LK	123	Total 898	C 567	N 166	O 163	${S \over 2}$	0	0

• Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.



Mol	Chain	Residues		At	oms			AltConf	Trace
20	LL	475	Total 3772	C 2400	N 649	O 710	S 13	0	0

• Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues		At	AltConf	Trace			
21	LM	431	Total 3443	C 2224	N 566	O 641	S 12	0	0

• Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues		A	AltConf	Trace			
22	LN	678	Total 5344	C 3384	N 930	O 1009	S 21	0	0

• Molecule 23 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues		Α	AltConf	Trace			
22	ΙO	834	Total	С	Ν	Ο	\mathbf{S}	0	0
23	LO	034	6635	4223	1140	1253	19	0	0

• Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	LP	359	Total 2709	C 1723	N 486	0 488	S 12	0	0

• Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues		Α	AltConf	Trace			
25	ΙO	848	Total	С	Ν	Ο	\mathbf{S}	0	0
20	ЪQ	040	6640	4244	1116	1253	27	0	0

• Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues		At	AltConf	Trace			
26	LS	481	Total 3791	C 2399	N 668	0 714	S 10	0	0

• Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 21.



Mol	Chain	Residues		Α	toms			AltConf	Trace
27	LT	850	Total	С	Ν	0	\mathbf{S}	0	0
1	11	000	6697	4253	1154	1269	21		U

• Molecule 28 is a protein called Protein SOF1.

Mol	Chain	Residues		At	AltConf	Trace			
28	LU	457	Total 3725	C 2328	N 679	O 702	S 16	0	0

• Molecule 29 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues		At	AltConf	Trace			
29	LV	362	Total 2840	C 1789	N 487	0 555	S 9	0	0

• Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues		At	AltConf	Trace			
30	LW	438	Total 3428	C 2163	N 601	O 652	S 12	0	0

• Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues		At	AltConf	Trace			
31	LZ	182	Total 1530	C 967	N 287	O 269	S 7	0	0

• Molecule 32 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
32	NG	111	Total 543	C 321	N 111	0 111	0	0

• Molecule 33 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
33	NK	175	Total 868	C 518	N 175	0 175	0	0

• Molecule 34 is a protein called rRNA 2'-O-methyltransferase fibrillarin.



Mol	Chain	Residues		At		AltConf	Trace		
24	SC	242	Total	С	Ν	0	\mathbf{S}	0	0
04	50	242	1881	1193	338	340	10	0	0
24	SD	226	Total	С	Ν	0	S	0	0
04	JUG	220	1782	1131	320	321	10	0	U

• Molecule 35 is a protein called Ribonucloprotein.

Mol	Chain	Residues		At	oms		AltConf	Trace	
25	СĿ	191	Total	С	Ν	0	S	0	0
55	SE	121	916	583	158	171	4	0	0
25	SE	191	Total	С	Ν	0	S	0	0
00	SF	121	916	583	158	171	4	0	0

• Molecule 36 is a protein called RRP9 isoform 1.

Mol	Chain	Residues		At	AltConf	Trace			
36	SG	429	Total 3428	C 2185	N 596	O 637	S 10	0	0

• Molecule 37 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues		At	AltConf	Trace			
37	SH	360	Total 2781	C 1781	N 473	0 516	S 11	0	0

• Molecule 38 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues		Α	AltConf	Trace			
38	SI	802	Total 6412	C 4108	N 1142	0 1133	S 29	0	0

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

Mol	Chain	Residues		At		AltConf	Trace		
30	SI	216	Total	С	Ν	Ο	S	0	0
59	53	210	1701	1079	296	315	11	0	0
30	SK	230	Total	С	Ν	Ο	S	0	Ο
- 39		230	1799	1142	313	333	11	U	0

• Molecule 40 is a protein called rRNA-processing protein FCF1.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
40	SL	174	Total 1395	C 890	N 255	O 240	S 10	0	0

• Molecule 41 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues		At	AltConf	Trace			
41	SM	282	Total 2296	C 1441	N 430	0 418	${f S}{7}$	0	0

• Molecule 42 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues		Ate	AltConf	Trace			
42	SN	247	Total 2006	C 1284	N 356	0 358	S 8	0	0

• Molecule 43 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues		At	oms			AltConf	Trace
43	SO	179	Total 998	C 606	N 199	0 192	S 1	0	0

• Molecule 44 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
44	SQ	135	Total 1137	C 721	N 211	0 201	S 4	0	0

• Molecule 45 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	SR	104	Total 792	C 506	N 145	O 139	${S \over 2}$	0	0

• Molecule 46 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	SS	197	Total 1466	C 905	N 282	0 277	${S \over 2}$	0	0

• Molecule 47 is a protein called Nucleolar complex protein 14.



Mol	Chain	Residues		At	AltConf	Trace			
47	ST	599	Total 4473	C 2830	N 809	O 823	S 11	0	0

• Molecule 48 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues		At	AltConf	Trace			
48	SY	241	Total 2016	C 1251	N 388	O 370	${ m S} 7$	0	0

• Molecule 49 is a protein called Essential nuclear protein 1.

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

• Molecule 50 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
50	NJ	265	Total 1314	C 784	N 265	O 265	0	0

• Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues		Ato	AltConf	Trace		
51	NH	1082	Total 5362	C 3198	N 1082	O 1082	0	0

• Molecule 52 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
52	NI	169	Total 841	C 503	N 169	O 169	0	0

• Molecule 53 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
53	8	1192	Total 25439	C 11367	N 4542	O 8338	Р 1192	0	0

• Molecule 54 is a protein called Nucleolar complex protein 4.



Mol	Chain	Residues		At	AltConf	Trace			
54	SU	481	Total 3650	$\begin{array}{c} \mathrm{C} \\ 2355 \end{array}$	N 611	O 672	S 12	0	0

• Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues		At	AltConf	Trace			
55	LI	441	Total 2690	C 1672	N 492	O 523	${ m S} { m 3}$	0	0

• Molecule 56 is a protein called Bud site selection protein 21.

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

• Molecule 57 is a protein called U3 small nucleolar RNA-associated protein 13.

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

• Molecule 58 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	NE	163	Total 1235	C 759	N 252	0 221	${ m S} { m 3}$	0	0

• Molecule 59 is a protein called Nucleolar protein 58.

Mol	Chain	Residues		At	AltConf	Trace			
59	SB	435	Total 2985	C 1852	N 543	O 582	S 8	0	0

• Molecule 60 is a protein called Regulator of rDNA transcription protein 14.

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

• Molecule 61 is a protein called U3 small nucleolar RNA-associated protein 20.



Mol	Chain	Residues		Ato	AltConf	Trace		
61	SP	2234	Total 11108	C 6640	N 2234	O 2234	0	0

• Molecule 62 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms	AltConf	Trace
62	LY	835	Total C N O 4132 2462 835 835	0	0
62	LX	812	Total C N O S 5892 3727 1041 1099 25	0	0

• Molecule 63 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	L6	167	Total 1327	C 834	N 256	0 235	$\frac{S}{2}$	0	0

• Molecule 64 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
64	NF	124	Total 614	C 367	N 123	O 124	0	0

• Molecule 65 is a protein called Protein BFR2.

Mol	Chain	Residues		AltConf	f Trace					
65	5	296	Total 2389	C 1496	N 422	0 467	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0	

• Molecule 66 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	AltConf	f Trace					
66	6	277	Total 2244	C 1371	N 426	0 438	S 9	0	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: U3 small nucleolar RNA-associated protein MPP10



• Molecule 4: 5' ETS Chain L0: 35% 28% 30% 7% ⊃ບບ< AGOAGDD 53 **4**000 A315 U314 V315 ບບ < 0 0 D 0 0 0 0 una sa sa sa conconce a conconce a conconce a conconce a conconce a conconce a conce a conce a conce a conce a • Molecule 5: U3 snoRNA Chain L2: 25% 21% 49% 5% U88 C89 4 U U U U D рор u u u v u u DOODADO c c c c c c c c c c N N N N N - - - -







 \bullet Molecule 10: 40S ribosomal protein S8-A





I53 D54

• Molecule 15: 40S ribosomal protein S24-A

Ch	air	ı I	LF	·:								60	0%																	36	%							•				
A4 V5	R10		016 D16	L17	L18	A19	F23	D26	H29	N31	R32	D38	E39 140	R41	E42	K43	L44	C+P	A50	E51	K52	D53	A54 V55	G59	100	105	F72	G73	L74	677 776	N77	S78	079	A80 F84	402 V02	K84	F85	-	Y89	R90 101	TAT	761
R93																																										

• Molecule 16: 40S ribosomal protein S28-A

Chain LG:		84%	16%
T5 P6 A10 S21 V25	D52 D52 L54 L54 E60 R61 E63 R64 R64 R64		

• Molecule 17: NET1-associated nuclear protein 1



• Molecule 18: U3 small nucleolar RNA-associated protein 15

Chain LJ:

75%

20%







 \bullet Molecule 20: U3 small nucleolar RNA-associated protein 5



• Molecule 22: U3 small nucleolar RNA-associated protein 4







• Molecule 24: U3 small nucleolar RNA-associated protein 6



Chain LS: 66% 15% 19%









• Molecule 33: KRR1 small subunit processome component





• Molecule 34: rRNA 2'-O-methyltransferase fibrillarin









 \bullet Molecule 42: Ribosome biogenesis protein UTP30

Chain SN: 75% 25%

 \bullet Molecule 43: Pre-rRNA-processing protein PNO1

Chain SO: 98% • Molecule 44: rRNA-processing protein FCF2 Chain SQ: 62% 17% 19% VAL GLU GLU GLU GLU CGLU CGLU SCD ASP PRO ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP Ĕ ASP LYS SER GLU PHE TYR SER SER ARG ASN ASN ASN ASN ASN CLYS CLU • Molecule 45: 40S ribosomal protein S23-A Chain SR: 74% 23% L94 F9E D90 **V9** 6N • Molecule 46: U3 small nucleolar RNA-associated protein 14 Chain SS: 86% 13%

• Molecule 47: Nucleolar complex protein 14













• Molecule 51: U3 small nucleolar RNA-associated protein 22



10%

.

60%

86%

Chain NI:









• Molecule 57: U3 small nucleolar RNA-associated protein 13














• Molecule 62: RNA cytidine acetyltransferase



DB

 \bullet Molecule 63: 40S ribosomal protein S6-A











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199534	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 $(e^-/\text{\AA}^2)$	1.074	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	463.968, 463.968, 463.968	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	Bond lengths		Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	NA	0.28	0/1685	0.62	2/2261~(0.1%)
2	SA	0.27	0/2769	0.51	2/3728~(0.1%)
3	NB	0.31	0/1042	0.68	1/1377~(0.1%)
4	LO	0.39	0/11634	1.11	71/18120~(0.4%)
5	L2	0.39	0/4001	1.11	22/6215~(0.4%)
6	L3	0.27	0/871	0.61	0/1171
7	L4	0.32	0/1849	0.68	1/2497~(0.0%)
8	L5	0.29	0/1690	0.65	1/2285~(0.0%)
9	L7	0.32	0/1342	0.78	2/1807~(0.1%)
10	L8	0.33	0/1372	0.81	4/1834~(0.2%)
11	L9	0.37	0/1437	0.91	7/1924~(0.4%)
12	LC	0.39	0/990	0.81	2/1335~(0.1%)
13	LD	0.31	0/1050	0.76	3/1415~(0.2%)
14	LE	0.33	0/1020	0.77	1/1371~(0.1%)
15	LF	0.37	0/727	1.01	8/977~(0.8%)
16	LG	0.43	0/499	0.97	2/670~(0.3%)
17	LH	0.28	0/6694	0.57	6/9070~(0.1%)
18	LJ	0.29	0/3993	0.59	2/5413~(0.0%)
19	LK	0.25	0/735	0.55	0/987
20	LL	0.27	0/3840	0.56	0/5208
21	LM	0.28	0/3470	0.53	2/4694~(0.0%)
22	LN	0.28	0/5369	0.60	4/7272~(0.1%)
23	LO	0.33	0/6780	0.60	3/9175~(0.0%)
24	LP	0.29	0/2281	0.52	0/3059
25	LQ	0.27	0/6574	0.58	7/8881~(0.1%)
26	LS	0.30	0/3875	0.54	0/5254
27	LT	0.30	0/6834	0.59	5/9238~(0.1%)
28	LU	0.30	0/3802	0.63	2/5118~(0.0%)
29	LV	0.31	0/2902	0.68	2/3941~(0.1%)
30	LW	0.30	0/3505	0.57	2/4748~(0.0%)
31	LZ	0.38	0/1559	0.76	4/2097~(0.2%)
32	NG	0.26	0/542	0.48	0/750
33	NK	0.24	0/867	0.41	0/1208
34	\mathbf{SC}	0.33	0/1917	0.64	1/2588~(0.0%)



Mal	Chain	Bo	ond lengths	Bond angles	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
34	SD	0.31	0/1815	0.69	3/2448~(0.1%)
35	SE	0.38	0/928	0.73	1/1262~(0.1%)
35	SF	0.38	0/928	0.75	2/1262~(0.2%)
36	SG	0.27	0/3498	0.60	3/4712~(0.1%)
37	SH	0.29	0/2832	0.58	1/3825~(0.0%)
38	SI	0.30	0/6403	0.66	9/8616~(0.1%)
39	SJ	0.27	0/1727	0.58	0/2329
39	SK	0.30	0/1828	0.59	0/2470
40	SL	0.32	0/1418	0.70	3/1906~(0.2%)
41	SM	0.32	0/2337	0.69	4/3148~(0.1%)
42	SN	0.33	0/2041	0.67	2/2745~(0.1%)
43	SO	0.26	0/1003	0.55	0/1381
44	SQ	0.31	0/1156	0.71	4/1536~(0.3%)
45	SR	0.36	0/804	0.79	4/1074~(0.4%)
46	\mathbf{SS}	0.28	0/1230	0.69	3/1660~(0.2%)
47	ST	0.26	0/3826	0.57	3/5125~(0.1%)
48	SY	0.29	0/2042	0.59	0/2704
49	SZ	0.23	0/1294	0.38	0/1804
50	NJ	0.23	0/1313	0.33	0/1830
51	NH	0.24	0/5357	0.41	0/7463
52	NI	0.23	0/838	0.43	0/1166
53	8	2.20	5/28439~(0.0%)	1.13	168/44273~(0.4%)
54	SU	0.27	0/3736	0.53	2/5086~(0.0%)
55	LI	0.26	0/2703	0.58	3/3703~(0.1%)
56	ND	0.32	0/499	0.76	1/659~(0.2%)
57	LR	0.28	1/6058~(0.0%)	0.58	3/8201~(0.0%)
58	NE	0.27	0/1240	0.65	1/1645~(0.1%)
59	SB	0.27	0/3012	0.55	2/4091~(0.0%)
60	SV	0.36	0/385	0.66	2/529~(0.4%)
61	SP	0.23	0/11085	0.34	0/15445
62	LX	0.28	0/5994	0.58	$\overline{6/8139}\ (0.1\%)$
62	LY	0.24	0/4128	0.41	0/5747
63	L6	1.96	1/1341~(0.1%)	0.91	5/1789~(0.3%)
64	NF	0.24	0/613	0.47	0/853
65	5	0.27	0/2422	0.57	2/3257~(0.1%)
66	6	0.29	0/2271	0.66	$\overline{2/3029}(0.1\%)$
All	All	0.86	7/218061~(0.0%)	0.75	$40\overline{8}/304600~(0.1\%)$

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



Mol	Chain	#Chirality outliers	#Planarity outliers
1	NA	0	1
7	L4	0	2
9	L7	0	1
11	L9	0	1
15	LF	0	2
22	LN	0	1
29	LV	0	2
34	SD	0	1
35	SE	0	2
35	\mathbf{SF}	0	1
38	SI	0	1
55	LI	0	1
57	LR	0	1
63	L6	0	1
65	5	0	1
66	6	0	1
All	All	0	20

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
53	8	140	A	N7-C5	187.02	2.51	1.39
53	8	140	A	N9-C4	185.66	2.49	1.37
53	8	140	А	C8-N7	156.00	2.40	1.31
53	8	140	A	N9-C8	150.09	2.57	1.37
53	8	140	А	C5-C4	135.64	2.33	1.38
63	L6	184	LEU	CA-CB	70.71	3.16	1.53
57	LR	104	PRO	CG-CD	-5.93	1.31	1.50

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	140	А	N7-C8-N9	-24.47	101.57	113.80
53	8	140	А	N1-C2-N3	22.84	140.72	129.30
53	8	140	А	C6-N1-C2	20.60	130.96	118.60
53	8	140	A	C4-C5-C6	-18.93	107.53	117.00
53	8	140	A	C5-N7-C8	17.31	112.56	103.90
53	8	140	А	C6-C5-N7	17.27	144.39	132.30
63	L6	184	LEU	CA-CB-CG	17.07	154.55	115.30
53	8	140	А	N3-C4-C5	-15.55	115.91	126.80
57	LR	104	PRO	CA-N-CD	-11.81	94.96	111.50
53	8	140	A	N3-C4-N9	11.53	136.62	127.40
53	8	140	A	C8-N9-C4	11.37	110.35	105.80



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
27	LT	460	ASP	CB-CG-OD1	11.30	128.47	118.30
38	SI	348	ASP	CB-CG-OD1	10.64	127.88	118.30
16	LG	6	PRO	CA-N-CD	-10.39	96.95	111.50
15	m LF	53	ASP	CB-CG-OD2	10.01	127.31	118.30
53	8	1215	С	N1-C2-O2	10.00	124.90	118.90
53	8	1619	С	N1-C2-O2	9.84	124.81	118.90
5	L2	200	С	N1-C2-O2	9.76	124.76	118.90
53	8	1215	С	C2-N1-C1'	9.63	129.39	118.80
11	L9	18	PRO	CA-N-CD	-9.54	98.14	111.50
53	8	519	С	C2-N1-C1'	9.23	128.96	118.80
57	LR	104	PRO	N-CD-CG	-9.21	89.38	103.20
11	L9	25	ASP	CB-CG-OD1	9.16	126.55	118.30
53	8	1220	С	N1-C2-O2	9.07	124.34	118.90
11	L9	89	ASP	CB-CG-OD2	9.07	126.46	118.30
3	NB	550	LEU	CA-CB-CG	9.01	136.03	115.30
53	8	241	U	C2-N1-C1'	8.97	128.47	117.70
53	8	1619	С	C2-N1-C1'	8.97	128.67	118.80
12	LC	64	ASP	CB-CG-OD2	8.87	126.28	118.30
53	8	1123	С	N3-C2-O2	-8.87	115.69	121.90
15	m LF	18	LEU	CA-CB-CG	8.82	135.58	115.30
53	8	1215	С	N3-C2-O2	-8.77	115.76	121.90
10	L8	193	LEU	CA-CB-CG	8.75	135.43	115.30
23	LO	720	ASP	CB-CG-OD2	8.69	126.12	118.30
40	SL	68	ASP	CB-CG-OD2	8.67	126.10	118.30
53	8	241	U	N1-C2-O2	8.64	128.85	122.80
13	LD	71	LEU	CA-CB-CG	8.61	135.10	115.30
11	L9	63	ASP	CB-CG-OD2	8.57	126.01	118.30
53	8	258	С	N1-C2-O2	8.54	124.02	118.90
41	SM	41	PRO	CA-N-CD	-8.53	99.56	111.50
4	LO	216	U	N1-C2-O2	8.50	128.75	122.80
5	L2	201	С	N1-C2-O2	8.43	123.96	118.90
53	8	99	С	C5-C6-N1	8.40	125.20	121.00
63	L6	184	LEU	CB-CA-C	8.39	126.14	110.20
53	8	954	G	C4-N9-C1'	8.35	137.36	126.50
4	LO	203	С	N1-C2-O2	8.33	123.90	118.90
4	LO	216	U	N3-C2-O2	-8.30	116.39	122.20
53	8	519	С	N1-C2-O2	8.29	123.88	118.90
4	L0	284	U	N1-C2-O2	8.25	128.57	122.80
4	LO	347	U	N1-C2-O2	8.24	128.57	122.80
55	LI	589	ASP	CB-CG-OD2	8.15	125.64	118.30
53	8	1123	С	N1-C2-O2	8.14	123.79	118.90
36	SG	115	ASP	CB-CG-OD1	8.14	125.62	118.30



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	241	U	N3-C2-O2	-8.12	116.52	122.20
4	LO	284	U	N3-C2-O2	-8.10	116.53	122.20
4	LO	347	U	N3-C2-O2	-8.09	116.54	122.20
53	8	99	С	C6-N1-C2	-7.92	117.13	120.30
53	8	1619	С	N3-C2-O2	-7.89	116.37	121.90
62	LX	762	MET	CB-CG-SD	7.82	135.86	112.40
4	LO	332	U	N1-C2-O2	7.75	128.22	122.80
63	L6	57	ASP	CB-CG-OD2	7.71	125.24	118.30
4	L0	91	U	C5-C6-N1	7.70	126.55	122.70
27	LT	436	ASP	CB-CG-OD2	7.69	125.22	118.30
53	8	1220	С	N3-C2-O2	-7.68	116.53	121.90
4	LO	543	С	C2-N1-C1'	7.65	127.22	118.80
5	L2	200	С	C2-N1-C1'	7.62	127.19	118.80
53	8	1215	С	C6-N1-C2	-7.61	117.25	120.30
46	\mathbf{SS}	878	LEU	CA-CB-CG	7.58	132.72	115.30
23	LO	741	MET	CA-CB-CG	7.57	126.18	113.30
5	L2	200	С	N3-C2-O2	-7.56	116.61	121.90
4	LO	399	U	C2-N1-C1'	7.52	126.72	117.70
4	LO	332	U	C2-N1-C1'	7.50	126.69	117.70
5	L2	201	С	N3-C2-O2	-7.48	116.66	121.90
53	8	954	G	N3-C4-N9	7.48	130.49	126.00
4	LO	241	U	C2-N1-C1'	7.45	126.64	117.70
22	LN	598	LEU	CA-CB-CG	7.41	132.34	115.30
4	LO	531	С	C2-N1-C1'	7.39	126.93	118.80
15	LF	17	LEU	CA-CB-CG	7.38	132.27	115.30
53	8	954	G	C8-N9-C1'	-7.37	117.42	127.00
53	8	1066	С	N3-C2-O2	-7.35	116.75	121.90
5	L2	312	U	N3-C2-O2	-7.34	117.06	122.20
53	8	1066	С	N1-C2-O2	7.33	123.30	118.90
41	SM	41	PRO	C-N-CA	7.32	139.99	121.70
47	ST	9	LEU	CA-CB-CG	7.32	132.13	115.30
23	LO	642	ASP	CB-CG-OD2	7.28	124.86	118.30
4	LO	215	U	N1-C2-O2	7.28	127.90	122.80
4	L0	110	G	C4-N9-C1'	7.25	135.92	126.50
17	LH	383	LEU	CA-CB-CG	7.23	131.93	115.30
29	LV	286	GLU	CA-CB-CG	7.23	129.31	113.40
4	LO	332	U	N3-C2-O2	-7.23	117.14	122.20
4	LO	215	U	N3-C2-O2	-7.21	117.16	122.20
53	8	975	C	N3-C2-O2	-7.19	116.87	121.90
4	LO	215	U	C2-N1-C1'	7.16	126.29	117.70
53	8	1773	С	N1-C2-O2	7.15	123.19	118.90
34	SC	306	LEU	CA-CB-CG	7.11	131.66	115.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	975	С	C6-N1-C2	-7.10	117.46	120.30
38	SI	263	LEU	CA-CB-CG	7.09	131.61	115.30
4	LO	216	U	C2-N1-C1'	7.05	126.16	117.70
8	L5	55	ASP	CB-CG-OD2	7.05	124.64	118.30
4	LO	110	G	N3-C4-N9	7.04	130.22	126.00
25	LQ	67	LEU	CA-CB-CG	7.04	131.49	115.30
53	8	190	С	O4'-C1'-N1	7.04	113.83	108.20
63	L6	20	ASP	CB-CG-OD2	7.03	124.63	118.30
4	LO	455	С	C2-N1-C1'	7.01	126.51	118.80
53	8	975	C	N1-C2-O2	6.92	123.05	118.90
4	LO	399	U	N1-C2-O2	6.90	127.63	122.80
53	8	482	U	N3-C2-O2	-6.89	117.37	122.20
44	SQ	180	ASP	CB-CG-OD2	6.89	124.50	118.30
10	L8	96	LEU	CA-CB-CG	6.88	131.12	115.30
53	8	343	C	N1-C2-O2	6.87	123.02	118.90
5	L2	200	С	C6-N1-C2	-6.84	117.56	120.30
53	8	482	U	N1-C2-O2	6.84	127.59	122.80
53	8	1115	U	N3-C2-O2	-6.84	117.42	122.20
4	LO	203	С	N3-C2-O2	-6.83	117.12	121.90
47	ST	740	MET	CA-CB-CG	6.83	124.91	113.30
53	8	1115	U	N1-C2-O2	6.82	127.58	122.80
53	8	38	С	N1-C2-O2	6.81	122.99	118.90
11	L9	157	ASP	CB-CG-OD2	6.79	124.41	118.30
5	L2	100	U	N3-C2-O2	-6.78	117.45	122.20
5	L2	312	U	N1-C2-O2	6.76	127.53	122.80
53	8	1220	С	C6-N1-C2	-6.76	117.59	120.30
53	8	54	С	C6-N1-C2	-6.75	117.60	120.30
53	8	517	U	C2-N1-C1'	6.74	125.79	117.70
4	LO	64	U	C2-N1-C1'	6.73	125.78	117.70
53	8	150	U	C2-N1-C1'	6.73	125.78	117.70
53	8	1773	С	C2-N1-C1'	6.72	126.19	118.80
53	8	536	С	C2-N1-C1'	6.68	126.15	118.80
53	8	1571	С	N3-C2-O2	-6.67	117.23	121.90
53	8	1573	A	P-O3'-C3'	6.67	127.70	119.70
31	LZ	88	LEU	CA-CB-CG	6.63	130.55	115.30
4	LO	110	G	N3-C4-C5	-6.62	125.29	128.60
44	SQ	72	LEU	CA-CB-CG	6.61	130.49	115.30
53	8	519	C	C6-N1-C1'	-6.61	112.87	120.80
4	LO	64	U	N3-C2-O2	-6.56	117.61	122.20
53	8	482	U	C2-N1-C1'	6.55	125.56	117.70
53	8	282	C	N1-C2-O2	6.54	122.83	118.90
55	LI	721	LEU	CA-CB-CG	6.52	130.30	115.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	LO	284	U	C2-N1-C1'	6.51	125.51	117.70
53	8	1262	U	N3-C2-O2	-6.47	117.67	122.20
53	8	1773	С	N3-C2-O2	-6.46	117.38	121.90
53	8	990	С	N1-C2-O2	6.44	122.77	118.90
27	LT	489	MET	CB-CG-SD	6.44	131.72	112.40
53	8	343	С	N3-C2-O2	-6.44	117.39	121.90
53	8	1057	U	P-O3'-C3'	6.43	127.42	119.70
25	LQ	752	LEU	CA-CB-CG	6.43	130.09	115.30
53	8	975	С	C2-N1-C1'	6.43	125.87	118.80
53	8	1571	С	N1-C2-O2	6.42	122.75	118.90
53	8	258	C	N3-C2-O2	-6.40	117.42	121.90
28	LU	374	LEU	CA-CB-CG	6.40	130.01	115.30
35	SE	65	LEU	CA-CB-CG	6.39	130.00	115.30
5	L2	100	U	N1-C2-O2	6.38	127.26	122.80
4	LO	543	С	C6-N1-C2	-6.36	117.75	120.30
53	8	532	U	O5'-P-OP1	6.36	118.33	110.70
53	8	885	G	N1-C6-O6	-6.36	116.09	119.90
4	LO	399	U	C5-C6-N1	6.35	125.88	122.70
21	LM	367	LEU	CA-CB-CG	6.35	129.91	115.30
4	LO	64	U	N1-C2-O2	6.35	127.24	122.80
4	LO	317	С	N1-C2-O2	6.34	122.70	118.90
4	LO	399	U	N3-C2-O2	-6.33	117.77	122.20
53	8	377	G	C4-N9-C1'	6.33	134.73	126.50
54	SU	499	LEU	CA-CB-CG	6.33	129.85	115.30
53	8	880	С	C6-N1-C2	-6.31	117.77	120.30
53	8	917	U	C2-N1-C1'	6.31	125.27	117.70
22	LN	225	LEU	CA-CB-CG	6.30	129.80	115.30
53	8	1215	С	C6-N1-C1'	-6.30	113.24	120.80
18	LJ	313	GLN	CA-CB-CG	6.30	127.26	113.40
53	8	517	U	N1-C2-O2	6.28	127.19	122.80
53	8	1123	С	C6-N1-C2	-6.26	117.80	120.30
53	8	54	С	N1-C2-O2	6.24	122.64	118.90
15	LF	91	LEU	CA-CB-CG	6.23	129.63	115.30
58	NE	215	LEU	CA-CB-CG	6.23	129.62	115.30
4	LO	110	G	C8-N9-C1'	-6.22	118.92	127.00
5	L2	49	С	N1-C2-O2	6.20	122.62	118.90
27	LT	537	LEU	CA-CB-CG	6.19	129.55	115.30
4	LO	241	U	N3-C2-O2	-6.18	117.87	122.20
7	L4	87	MET	CA-CB-CG	6.18	123.81	113.30
45	SR	98	GLU	CA-CB-CG	6.18	127.00	113.40
4	LO	144	C	C2-N1-C1'	6.17	125.59	118.80
53	8	589	C	C2-N1-C1'	6.17	125.58	118.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	L2	201	С	C6-N1-C2	-6.16	117.83	120.30
53	8	954	G	N3-C4-C5	-6.15	125.52	128.60
53	8	258	С	C2-N1-C1'	6.15	125.57	118.80
53	8	50	С	C2-N1-C1'	6.14	125.56	118.80
40	SL	117	LEU	CA-CB-CG	6.13	129.41	115.30
38	SI	1145	MET	CA-CB-CG	6.12	123.70	113.30
53	8	1619	С	C6-N1-C1'	-6.12	113.46	120.80
53	8	343	С	C2-N1-C1'	6.11	125.52	118.80
53	8	1773	С	C6-N1-C2	-6.10	117.86	120.30
53	8	1619	С	C6-N1-C2	-6.09	117.86	120.30
53	8	519	С	N3-C2-O2	-6.08	117.64	121.90
56	ND	203	ASP	CB-CG-OD2	6.07	123.76	118.30
4	LO	340	U	C2-N1-C1'	6.07	124.98	117.70
53	8	354	С	C6-N1-C2	-6.05	117.88	120.30
63	L6	63	MET	CB-CG-SD	6.03	130.49	112.40
53	8	199	G	P-O3'-C3'	6.02	126.93	119.70
5	L2	200	С	C5-C6-N1	6.02	124.01	121.00
28	LU	358	MET	CA-CB-CG	6.02	123.53	113.30
53	8	99	С	C2-N1-C1'	6.02	125.42	118.80
66	6	77	MET	CB-CG-SD	6.01	130.44	112.40
62	LX	209	PRO	CA-N-CD	-6.01	103.08	111.50
53	8	1220	С	C2-N1-C1'	5.99	125.39	118.80
11	L9	147	MET	CB-CG-SD	5.99	130.36	112.40
4	L0	190	U	N3-C2-O2	-5.97	118.02	122.20
53	8	880	С	C5-C6-N1	5.97	123.99	121.00
4	LO	543	С	C5-C6-N1	5.97	123.98	121.00
53	8	517	U	N3-C2-O2	-5.96	118.02	122.20
38	SI	555	MET	CB-CG-SD	5.96	130.28	112.40
42	SN	156	MET	CB-CG-SD	5.95	130.24	112.40
53	8	937	С	N1-C2-O2	5.94	122.46	118.90
30	LW	160	LEU	CA-CB-CG	5.93	128.94	115.30
53	8	0	U	P-O3'-C3'	5.93	126.81	119.70
21	LM	234	LEU	CA-CB-CG	5.92	128.92	115.30
53	8	106	U	N1-C2-O2	5.92	126.94	122.80
53	8	-3	U	P-O3'-C3'	5.91	126.79	119.70
4	LO	394	U	C2-N1-C1'	5.90	124.78	117.70
4	LO	340	U	N1-C2-O2	5.90	126.93	122.80
14	LE	94	LEU	CA-CB-CG	5.88	128.83	115.30
53	8	282	C	C5-C6-N1	5.87	123.93	121.00
53	8	354	C	N1-C2-O2	5.85	122.41	118.90
4	LO	190	U	N1-C2-O2	5.84	126.89	122.80
15	LF	40	LEU	CA-CB-CG	5.83	128.71	115.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	1638	G	P-O3'-C3'	5.83	126.70	119.70
53	8	294	С	N1-C2-O2	5.83	122.40	118.90
53	8	448	С	N1-C2-O2	5.82	122.39	118.90
15	LF	85	PHE	CB-CG-CD1	5.81	124.87	120.80
53	8	1262	U	N1-C2-O2	5.81	126.86	122.80
53	8	208	U	C2-N1-C1'	5.80	124.66	117.70
53	8	354	С	C5-C6-N1	5.79	123.90	121.00
45	SR	93	LEU	CA-CB-CG	5.79	128.61	115.30
53	8	211	U	N3-C2-O2	-5.79	118.15	122.20
53	8	1115	U	C2-N1-C1'	5.79	124.64	117.70
4	LO	241	U	N1-C2-O2	5.78	126.85	122.80
53	8	54	С	N3-C2-O2	-5.78	117.85	121.90
5	L2	312	U	C2-N1-C1'	5.78	124.63	117.70
1	NA	515	MET	CA-CB-CG	5.77	123.11	113.30
53	8	1215	C	C5-C6-N1	5.77	123.88	121.00
31	LZ	170	LEU	CA-CB-CG	5.76	128.54	115.30
53	8	448	С	C2-N1-C1'	5.76	125.13	118.80
53	8	294	C	C2-N1-C1'	5.75	125.13	118.80
38	SI	608	LEU	CA-CB-CG	5.75	128.53	115.30
4	LO	203	C	C6-N1-C2	-5.75	118.00	120.30
41	SM	124	MET	CB-CG-SD	5.75	129.64	112.40
30	LW	125	LEU	CA-CB-CG	5.74	128.49	115.30
34	SD	232	MET	CA-CB-CG	5.71	123.02	113.30
53	8	241	U	C6-N1-C1'	-5.71	113.20	121.20
60	SV	185	PRO	CA-N-CD	-5.70	103.51	111.50
53	8	917	U	N1-C2-O2	5.70	126.79	122.80
4	LO	20	С	N1-C2-O2	5.69	122.31	118.90
53	8	106	U	N3-C2-O2	-5.69	118.22	122.20
35	SF	31	ARG	CA-CB-CG	5.69	125.91	113.40
4	LO	203	С	C2-N1-C1'	5.69	125.05	118.80
53	8	885	G	C5-C6-O6	5.67	132.00	128.60
17	LH	288	LEU	CA-CB-CG	5.67	128.34	115.30
25	LQ	810	LEU	CA-CB-CG	5.67	128.34	115.30
53	8	207	U	N3-C2-O2	-5.67	118.23	122.20
57	LR	631	MET	CA-CB-CG	5.67	122.93	113.30
4	LO	91	U	C2-N1-C1'	5.66	124.49	117.70
2	SA	7	LEU	CA-CB-CG	5.65	128.29	115.30
17	LH	664	LEU	CA-CB-CG	5.64	128.28	115.30
55	LI	534	LEU	CA-CB-CG	5.64	128.28	115.30
53	8	519	C	C5-C6-N1	5.62	123.81	121.00
31	LZ	97	LEU	CA-CB-CG	5.62	128.22	115.30
38	SI	812	MET	CA-CB-CG	5.61	122.83	113.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	38	С	N3-C2-O2	-5.60	117.98	121.90
15	LF	44	LEU	CA-CB-CG	5.60	128.17	115.30
37	SH	350	MET	CB-CG-SD	5.59	129.18	112.40
53	8	1686	С	C2-N1-C1'	5.58	124.94	118.80
53	8	347	G	C4-N9-C1'	5.58	133.75	126.50
62	LX	164	MET	CG-SD-CE	5.57	109.11	100.20
53	8	990	С	N3-C2-O2	-5.57	118.00	121.90
53	8	211	U	N1-C2-O2	5.56	126.69	122.80
65	5	337	MET	CA-CB-CG	5.56	122.75	113.30
46	SS	892	ASP	CB-CG-OD2	5.55	123.30	118.30
35	SF	50	GLU	CA-CB-CG	5.55	125.61	113.40
53	8	347	G	C8-N9-C1'	-5.55	119.79	127.00
66	6	71	TYR	CB-CG-CD1	-5.54	117.68	121.00
60	SV	185	PRO	N-CD-CG	-5.54	94.89	103.20
22	LN	272	LEU	CA-CB-CG	5.54	128.03	115.30
44	SQ	110	ASP	CB-CG-OD1	5.54	123.28	118.30
47	ST	104	MET	CB-CG-SD	5.52	128.96	112.40
34	SD	210	MET	CA-CB-CG	5.51	122.68	113.30
45	SR	133	LEU	CA-CB-CG	5.49	127.93	115.30
4	LO	531	С	N1-C2-O2	5.48	122.19	118.90
4	LO	543	С	N1-C2-O2	5.47	122.19	118.90
53	8	519	С	C6-N1-C2	-5.47	118.11	120.30
5	L2	72	С	N1-C2-O2	5.47	122.18	118.90
62	LX	15	ARG	CA-CB-CG	5.46	125.42	113.40
4	LO	264	С	C2-N1-C1'	5.46	124.80	118.80
38	SI	956	MET	CB-CG-SD	5.45	128.76	112.40
27	LT	494	LEU	CA-CB-CG	5.45	127.83	115.30
53	8	1620	С	N1-C2-O2	5.45	122.17	118.90
4	LO	347	U	C2-N1-C1'	5.43	124.22	117.70
17	LH	208	LEU	CA-CB-CG	5.43	127.78	115.30
5	L2	72	С	N3-C2-O2	-5.41	118.11	121.90
53	8	1148	С	C2-N1-C1'	5.41	124.75	118.80
53	8	465	G	C4-N9-C1'	5.41	133.53	126.50
25	LQ	479	LEU	CA-CB-CG	5.41	127.74	115.30
29	LV	328	MET	CA-CB-CG	5.40	122.49	113.30
53	8	294	С	C6-N1-C2	-5.39	118.14	120.30
17	LH	507	MET	CB-CG-SD	5.39	128.56	112.40
4	LO	455	C	N1-C2-O2	5.38	122.13	118.90
65	5	472	ILE	CG1-CB-CG2	-5.37	99.58	111.40
53	8	943	С	N1-C2-O2	5.37	122.12	118.90
53	8	1220	С	C5-C6-N1	5.37	123.69	121.00
53	8	207	U	N1-C2-O2	5.36	126.56	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	372	G	P-O3'-C3'	5.36	126.13	119.70
53	8	377	G	C8-N9-C1'	-5.33	120.06	127.00
53	8	880	С	C2-N1-C1'	5.33	124.66	118.80
53	8	1533	С	N1-C2-O2	5.33	122.10	118.90
34	SD	259	MET	CA-CB-CG	5.33	122.35	113.30
53	8	1066	С	C6-N1-C2	-5.30	118.18	120.30
53	8	937	С	N3-C2-O2	-5.29	118.19	121.90
53	8	1448	G	N3-C4-C5	-5.29	125.95	128.60
4	LO	394	U	N3-C2-O2	-5.28	118.50	122.20
25	LQ	185	MET	CB-CG-SD	5.27	128.22	112.40
44	SQ	216	ARG	CA-CB-CG	5.27	124.99	113.40
53	8	226	А	C2-N3-C4	5.27	113.23	110.60
53	8	954	G	C6-C5-N7	-5.27	127.24	130.40
53	8	305	С	C6-N1-C2	-5.27	118.19	120.30
1	NA	382	GLN	CA-CB-CG	5.26	124.98	113.40
25	LQ	752	LEU	CB-CG-CD2	5.26	119.95	111.00
10	L8	184	LEU	CB-CG-CD2	5.26	119.95	111.00
53	8	140	А	C4-C5-N7	-5.26	108.07	110.70
53	8	1175	U	N1-C2-O2	5.26	126.48	122.80
16	LG	6	PRO	N-CD-CG	-5.25	95.32	103.20
53	8	347	G	N3-C4-N9	5.25	129.15	126.00
4	LO	443	G	O4'-C1'-N9	5.25	112.40	108.20
53	8	917	U	N3-C2-O2	-5.25	118.53	122.20
4	LO	374	U	C2-N1-C1'	5.24	123.99	117.70
53	8	941	А	C4-N9-C1'	5.24	135.74	126.30
53	8	208	U	N3-C2-O2	-5.24	118.53	122.20
59	SB	162	MET	CA-CB-CG	5.24	122.20	113.30
53	8	1200	G	C4-N9-C1'	5.23	133.30	126.50
9	L7	8	ILE	CG1-CB-CG2	-5.23	99.90	111.40
53	8	962	С	C6-N1-C2	-5.22	118.21	120.30
53	8	484	С	N1-C2-O2	5.22	122.03	118.90
5	L2	39	С	C5-C6-N1	5.21	123.61	121.00
13	LD	80	MET	CB-CG-SD	5.21	128.03	112.40
53	8	1448	G	C4-N9-C1'	5.20	133.25	126.50
38	SI	347	LEU	CA-CB-CG	5.19	127.25	115.30
53	8	1199	G	C4-N9-C1'	5.19	133.24	126.50
53	8	1645	G	C4-N9-C1'	5.19	133.24	126.50
2	SA	193	MET	CA-CB-CG	5.18	122.11	113.30
4	LO	394	U	N1-C2-O2	5.18	126.43	122.80
4	LO	531	С	C6-N1-C1'	-5.18	114.58	120.80
4	LO	340	U	C5-C6-N1	5.17	125.28	122.70
53	8	377	G	N3-C4-N9	5.17	129.10	126.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	8	448	С	C5-C6-N1	5.17	123.58	121.00
38	SI	230	MET	CB-CG-SD	5.16	127.88	112.40
59	SB	421	MET	CB-CG-SD	5.15	127.86	112.40
62	LX	164	MET	CA-CB-CG	5.15	122.06	113.30
4	LO	537	G	N3-C4-N9	5.15	129.09	126.00
22	LN	240	LEU	CA-CB-CG	5.15	127.14	115.30
53	8	241	U	C5-C6-N1	5.14	125.27	122.70
53	8	343	С	C6-N1-C2	-5.14	118.24	120.30
5	L2	201	С	C2-N1-C1'	5.14	124.45	118.80
4	LO	541	U	N1-C2-O2	5.14	126.40	122.80
4	LO	144	С	N1-C2-O2	5.13	121.98	118.90
41	SM	42	LEU	CA-CB-CG	5.13	127.11	115.30
4	LO	212	U	C5-C6-N1	5.13	125.27	122.70
31	LZ	63	LEU	CA-CB-CG	5.13	127.10	115.30
53	8	1653	С	C6-N1-C2	-5.13	118.25	120.30
53	8	1057	U	OP1-P-O3'	5.13	116.48	105.20
53	8	1191	U	C2-N1-C1'	5.12	123.84	117.70
46	SS	894	LEU	CA-CB-CG	5.11	127.06	115.30
53	8	97	С	N1-C2-O2	5.11	121.97	118.90
4	LO	91	U	C5-C4-O4	-5.11	122.83	125.90
53	8	50	С	C6-N1-C2	-5.11	118.26	120.30
53	8	990	С	C6-N1-C2	-5.11	118.26	120.30
5	L2	39	С	C6-N1-C2	-5.11	118.26	120.30
9	L7	27	LEU	CA-CB-CG	5.11	127.05	115.30
5	L2	49	С	N3-C2-O2	-5.10	118.33	121.90
53	8	415	С	N1-C2-O2	5.10	121.96	118.90
62	LX	44	MET	CA-CB-CG	5.09	121.96	113.30
4	LO	317	С	N3-C2-O2	-5.09	118.34	121.90
4	LO	347	U	C5-C6-N1	5.09	125.25	122.70
11	L9	25	ASP	CB-CG-OD2	-5.09	113.72	118.30
4	LO	389	U	N1-C2-O2	5.09	126.36	122.80
4	LO	455	С	C5-C6-N1	5.09	123.55	121.00
25	LQ	175	ASP	CB-CG-OD1	5.09	122.88	118.30
4	LO	455	С	C6-N1-C2	-5.09	118.27	120.30
12	LC	107	LYS	CB-CG-CD	5.08	124.81	111.60
53	8	937	С	C6-N1-C2	-5.08	118.27	120.30
13	LD	80	MET	CB-CA-C	5.08	120.56	110.40
15	LF	74	LEU	CA-CB-CG	5.08	126.98	115.30
54	SU	413	MET	CB-CG-SD	5.08	127.63	112.40
18	LJ	360	MET	CA-CB-CG	5.07	121.92	113.30
53	8	98	U	C5-C6-N1	5.07	125.23	122.70
5	L2	27	U	N1-C2-O2	5.07	126.35	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	L2	102	U	N1-C2-O2	5.06	126.34	122.80
53	8	1448	G	N3-C4-N9	5.06	129.03	126.00
42	SN	156	MET	CG-SD-CE	5.06	108.29	100.20
40	SL	97	LEU	CA-CB-CG	5.05	126.92	115.30
53	8	448	С	C6-N1-C2	-5.05	118.28	120.30
53	8	589	C	N1-C2-O2	5.04	121.92	118.90
53	8	1646	С	N1-C2-O2	5.04	121.92	118.90
17	LH	498	LEU	CA-CB-CG	5.03	126.88	115.30
36	SG	333	MET	CA-CB-CG	5.03	121.85	113.30
4	LO	502	G	C4-N9-C1'	5.03	133.03	126.50
45	SR	101	GLU	CA-CB-CG	5.02	124.44	113.40
10	L8	61	GLU	CA-CB-CG	5.02	124.44	113.40
53	8	305	C	C2-N1-C1'	5.02	124.32	118.80
53	8	377	G	N3-C4-C5	-5.01	126.09	128.60
53	8	1200	G	N3-C4-C5	-5.01	126.09	128.60
4	LO	542	U	C2-N1-C1'	5.01	123.71	117.70
53	8	37	U	N1-C2-O2	5.00	126.30	122.80
4	LO	241	U	C6-N1-C1'	-5.00	114.20	121.20
36	SG	114	LYS	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
65	5	450	LEU	Peptide
66	6	338	THR	Peptide
7	L4	193	GLY	Peptide
7	L4	195	ILE	Peptide
63	L6	68	LEU	Peptide
9	L7	12	ALA	Peptide
11	L9	57	ARG	Sidechain
15	LF	31	ASN	Peptide
15	LF	51	GLU	Peptide
55	LI	257	SER	Peptide
22	LN	30	ARG	Sidechain
57	LR	626	MET	Peptide
29	LV	51	GLN	Peptide
29	LV	57	GLU	Peptide
1	NA	453	SER	Peptide
34	SD	321	MET	Peptide
35	SE	89	ARG	Sidechain
35	SE	9	PHE	Peptide



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Mol	Chain	Res	Type	Group
35	SF	9	PHE	Peptide
38	SI	198	VAL	Peptide

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	NA	1667	0	1701	37	0
2	SA	2854	0	2792	42	0
3	NB	1098	0	1102	24	0
4	LO	10405	0	5231	90	0
5	L2	3585	0	1819	34	0
6	L3	901	0	907	15	0
7	L4	1810	0	1865	42	0
8	L5	1669	0	1724	24	0
9	L7	1321	0	1390	42	0
10	L8	1349	0	1372	26	0
11	L9	1415	0	1497	31	0
12	LC	973	0	1029	25	0
13	LD	1027	0	1084	24	0
14	LE	1003	0	1040	27	0
15	LF	715	0	744	14	0
16	LG	497	0	535	6	0
17	LH	6633	0	6510	99	0
18	LJ	3911	0	3906	68	0
19	LK	898	0	811	10	0
20	LL	3772	0	3806	55	0
21	LM	3443	0	3559	41	0
22	LN	5344	0	5301	100	0
23	LO	6635	0	6525	118	0
24	LP	2709	0	2371	26	0
25	LQ	6640	0	6503	108	0
26	LS	3791	0	3772	55	0
27	LT	6697	0	6676	99	0
28	LU	3725	0	3679	93	0
29	LV	2840	0	2685	68	0
30	LW	3428	0	3407	53	0
31	LZ	1530	0	1572	24	0



Continued from previous page						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	NG	543	0	277	3	0
33	NK	868	0	379	3	0
34	SC	1881	0	1928	28	0
34	SD	1782	0	1826	35	0
35	SE	916	0	964	19	0
35	SF	916	0	964	20	0
36	SG	3428	0	3446	76	0
37	SH	2781	0	2878	60	0
38	SI	6412	0	6498	127	0
39	SJ	1701	0	1767	29	0
39	SK	1799	0	1872	33	0
40	SL	1395	0	1476	29	0
41	SM	2296	0	2325	42	0
42	SN	2006	0	2118	39	0
43	SO	998	0	631	3	0
44	SQ	1137	0	1188	20	0
45	SR	792	0	847	23	0
46	SS	1466	0	1257	22	0
47	ST	4473	0	4057	53	0
48	SY	2016	0	2093	28	0
49	SZ	1295	0	571	2	0
50	NJ	1314	0	610	1	0
51	NH	5362	0	2295	13	0
52	NI	841	0	365	4	0
53	8	25439	0	12823	271	0
54	SU	3650	0	3365	37	0
55	LI	2690	0	1931	33	0
56	ND	495	0	561	13	0
57	LR	5957	0	5992	109	0
58	NE	1235	0	1243	20	0
59	SB	2985	0	2703	32	0
60	SV	381	0	255	6	0
61	SP	11108	0	4748	4	0
62	LX	5892	0	5420	87	0
62	LY	4132	0	1819	5	0
63	L6	1327	0	1403	38	0
64	NF	614	0	279	7	0
65	5	2389	0	2411	36	0
66	6	2244	0	2245	38	0
All	All	213241	0	176745	2553	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 7.



Atom-1	Atom-2	Interatomic	Clash
E2.0.140.4.04	52.0.140. A.OF	distance (A)	$\frac{\text{overlap}(\mathbf{A})}{1.17}$
53:8:140:A:C4	05:8:140:A:C0	2.33	1.17
05:8:140:A:U4	03:L0:184:LEU:HA	1.94	1.02
45:SR:41:SER:N	53:8:600:U:HO2	1.68	0.91
53:8:140:A:C8	53:8:140:A:N7	2.40	0.88
53:8:140:A:C8	63:L6:184:LEU:CB	2.59	0.86
53:8:140:A:C5	63:L6:184:LEU:HB2	2.10	0.85
53:8:140:A:N9	63:L6:184:LEU:HB3	1.92	0.83
53:8:140:A:C5	63:L6:184:LEU:CB	2.64	0.81
53:8:140:A:C4	53:8:140:A:N9	2.49	0.80
53:8:140:A:C4	63:L6:184:LEU:CB	2.65	0.80
27:LT:432:THR:HG1	27:LT:443:TRP:HE1	1.29	0.79
53:8:140:A:C5	53:8:140:A:N7	2.51	0.79
53:8:140:A:N9	63:L6:184:LEU:CB	2.48	0.76
53:8:140:A:C8	63:L6:184:LEU:CA	2.70	0.74
53:8:1695:G:N2	53:8:1706:C:C2	2.56	0.74
53:8:140:A:N7	63:L6:184:LEU:CB	2.51	0.73
53:8:140:A:C4	63:L6:184:LEU:CA	2.72	0.73
53:8:140:A:C8	53:8:140:A:N9	2.57	0.73
53:8:984:G:H1	53:8:1017:U:H3	1.36	0.72
53:8:1588:G:H1	53:8:1608:U:H3	1.39	0.70
53:8:140:A:C5	63:L6:184:LEU:CA	2.74	0.70
28:LU:85:THR:HG1	28:LU:95:TRP:HE1	1.37	0.70
27:LT:584:HIS:HE2	27:LT:602:SER:HG	1.39	0.70
5:L2:85:G:N7	59:SB:361:ARG:NH1	2.41	0.68
46:SS:316:ASN:HD21	46:SS:895:LYS:H	1.42	0.68
29:LV:64:VAL:HG11	29:LV:323:VAL:HG22	1.76	0.67
31:LZ:109:ARG:HH22	31:LZ:155:GLU:HB2	1.59	0.67
62:LX:60:LYS:HG3	62:LX:61:LYS:HG2	1.76	0.67
25:LQ:137:ILE:HG23	25:LQ:147:VAL:HG22	1.75	0.66
53:8:140:A:N9	63:L6:184:LEU:CA	2.59	0.66
18:LJ:108:TYR:HB3	18:LJ:117:LEU:H	1.60	0.66
17:LH:630:LEU:HB2	17:LH:653:PHE:HB2	1.77	0.66
37:SH:315:LYS:HD2	37:SH:348:GLU:HB2	1.77	0.66
2:SA:191:PHE:HB3	2:SA:278:VAL:HG22	1.78	0.66
17:LH:17:GLY:HA2	17:LH:50:ASN:HD21	1.59	0.66
53:8:314:C:H42	53:8:354:C:H42	1.44	0.66
7:L4:71:LYS:HG2	7:L4:91:THR:HB	1.77	0.66
22:LN:265:TRP:HA	22:LN:272:LEU:HA	1.78	0.66
62:LX:27:VAL:HG23	62:LX:150:ILE:HB	1.78	0.66
27:LT:723:LEU:HD22	27:LT:879:GLU:HB2	1.76	0.65

All (2553) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:8:140:A:C4	63:L6:184:LEU:HB2	2.30	0.65
39:SJ:44:VAL:HG12	39:SJ:113:TYR:HB2	1.78	0.65
57:LR:495:ASN:H	57:LR:510:SER:HA	1.61	0.65
9:L7:43:PHE:HB2	9:L7:60:ILE:HD11	1.77	0.65
25:LQ:588:ILE:HB	25:LQ:600:TRP:HB2	1.77	0.65
25:LQ:594:ASP:HB2	53:8:1137:A:H1'	1.78	0.65
37:SH:141:MET:HA	37:SH:144:PHE:HB2	1.78	0.65
37:SH:181:HIS:HB3	37:SH:310:ARG:HH21	1.61	0.65
39:SK:51:GLU:HG2	39:SK:68:LEU:HD23	1.79	0.65
1:NA:516:SER:HB2	57:LR:691:PRO:HD2	1.79	0.65
10:L8:22:ARG:HH12	53:8:384:G:H5"	1.62	0.65
42:SN:63:LYS:HG2	42:SN:185:LYS:HB2	1.79	0.65
41:SM:100:LEU:HA	41:SM:103:PHE:HB3	1.79	0.65
7:L4:151:ASP:HA	63:L6:215:ARG:HH12	1.62	0.64
53:8:151:G:H22	53:8:163:G:H1	1.44	0.64
14:LE:51:GLU:HB2	14:LE:62:VAL:HB	1.79	0.64
25:LQ:392:THR:HG21	25:LQ:411:ASN:H	1.61	0.64
22:LN:482:ASP:HB2	22:LN:485:LYS:HB2	1.78	0.64
47:ST:647:ILE:HA	47:ST:651:TRP:HB2	1.80	0.64
35:SE:58:CYS:HA	35:SE:84:ARG:HD3	1.80	0.64
34:SD:171:LEU:HB2	34:SD:237:VAL:HG11	1.78	0.64
10:L8:44:HIS:HB3	10:L8:56:ARG:HB2	1.81	0.63
38:SI:828:ARG:NH1	45:SR:94:ASN:O	2.28	0.63
1:NA:484:MET:SD	23:LO:359:ARG:NH1	2.71	0.63
53:8:273:G:H1	53:8:284:G:H1'	1.64	0.63
53:8:1711:C:N4	53:8:1713:G:N7	2.46	0.63
5:L2:12:U:H3	53:8:1112:G:H1	1.46	0.63
39:SK:44:VAL:HG22	39:SK:113:TYR:HB2	1.78	0.63
20:LL:281:ILE:HG12	20:LL:328:VAL:HB	1.80	0.63
23:LO:717:LEU:HD23	23:LO:744:ARG:HG2	1.80	0.63
38:SI:924:VAL:O	47:ST:109:ARG:NH1	2.30	0.63
30:LW:434:LEU:HD11	31:LZ:9:GLU:HB2	1.80	0.63
34:SC:149:SER:HB2	34:SC:180:SER:HB2	1.80	0.63
62:LX:641:ASN:HB3	62:LX:644:TYR:HB2	1.81	0.63
7:L4:206:ASP:HB2	7:L4:222:LEU:HB3	1.78	0.63
23:LO:20:ILE:H	23:LO:307:THR:HG21	1.62	0.63
65:5:337:MET:SD	65:5:341:LYS:NZ	2.72	0.63
55:LI:604:LYS:HG3	55:LI:608:GLN:HE22	1.64	0.63
28:LU:315:PRO:HB2	46:SS:891:ILE:HD11	1.80	0.63
9:L7:140:VAL:HG12	9:L7:150:GLN:HB3	1.81	0.62
11:L9:60:LEU:HD21	11:L9:93:LEU:HB3	1.80	0.62



A + 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
38:SI:52:ARG:HH22	53:8:28:A:H4'	1.64	0.62
9:L7:150:GLN:HE22	9:L7:181:ILE:HD13	1.64	0.62
57:LR:395:ASP:HB3	57:LR:404:ALA:HB3	1.81	0.62
29:LV:50:ILE:HG22	29:LV:51:GLN:HG3	1.81	0.62
36:SG:333:MET:HG3	36:SG:335:ARG:HG2	1.80	0.62
45:SR:98:GLU:OE2	45:SR:99:ASN:ND2	2.33	0.62
53:8:140:A:N7	63:L6:184:LEU:CA	2.63	0.62
4:L0:551:A:N1	4:L0:586:A:N6	2.47	0.61
22:LN:139:CYS:SG	22:LN:140:ASN:N	2.72	0.61
27:LT:885:MET:HA	27:LT:888:LEU:HB2	1.83	0.61
48:SY:10:LYS:NZ	53:8:552:G:N7	2.48	0.61
57:LR:548:LEU:HB3	57:LR:560:TRP:HB2	1.81	0.61
57:LR:728:ILE:HA	57:LR:731:LEU:HD12	1.82	0.61
63:L6:72:ARG:HA	63:L6:98:ARG:HA	1.80	0.61
1:NA:346:GLU:HB2	47:ST:766:ARG:HH12	1.65	0.61
6:L3:14:ILE:HG22	6:L3:23:ASP:HA	1.80	0.61
23:LO:162:LEU:HB3	23:LO:172:ILE:HG12	1.83	0.61
27:LT:587:ARG:HH21	27:LT:605:LEU:HD11	1.65	0.61
30:LW:190:HIS:HD1	30:LW:207:THR:HG1	1.44	0.61
38:SI:944:ASN:ND2	38:SI:991:PHE:O	2.33	0.61
42:SN:42:THR:H	42:SN:195:ASN:HB2	1.64	0.61
14:LE:41:MET:HG2	14:LE:47:ILE:HG12	1.83	0.61
62:LX:786:LEU:HA	62:LX:890:LEU:HD21	1.82	0.61
18:LJ:213:GLN:NE2	18:LJ:233:ASN:OD1	2.34	0.61
40:SL:27:LYS:NZ	40:SL:28:ASN:OD1	2.33	0.61
62:LY:899:ALA:HB1	62:LY:905:PRO:HA	1.83	0.61
2:SA:155:GLY:HA2	34:SC:233:LEU:HD23	1.83	0.61
4:L0:123:C:N4	54:SU:134:PHE:O	2.34	0.61
22:LN:247:LEU:HD23	22:LN:292:ASN:HB3	1.83	0.61
27:LT:28:ARG:HH11	27:LT:30:ILE:HD13	1.66	0.61
27:LT:509:SER:OG	27:LT:510:LEU:N	2.34	0.61
22:LN:186:GLN:NE2	22:LN:205:CYS:SG	2.74	0.61
25:LQ:26:ILE:HB	25:LQ:40:GLN:HB2	1.83	0.61
39:SK:24:VAL:HG12	54:SU:487:PRO:HB2	1.81	0.61
4:L0:135:G:O2'	20:LL:494:ARG:NH1	2.33	0.60
9:L7:162:ILE:HA	9:L7:165:LYS:HG2	1.83	0.60
35:SE:17:THR:HA	35:SE:20:ILE:HG22	1.83	0.60
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.84	0.60
21:LM:194:SER:HB2	27:LT:335:VAL:HG11	1.81	0.60
27:LT:311:VAL:HG22	27:LT:321:GLU:HG2	1.83	0.60
29:LV:288:LYS:HB3	29:LV:299:ILE:HD11	1.83	0.60



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:L7:166:LEU:HD13	9:L7:183:PHE:HB2	1.82	0.60
23:LO:673:ARG:HG3	23:LO:675:MET:H	1.67	0.60
53:8:185:U:H3'	53:8:186:C:H4'	1.83	0.60
57:LR:64:ILE:HA	57:LR:80:SER:HA	1.82	0.60
29:LV:263:SER:OG	29:LV:264:ILE:N	2.35	0.60
66:6:238:ASN:OD1	66:6:241:ARG:NH2	2.35	0.60
4:L0:219:U:H5'	56:ND:204:ARG:HH12	1.66	0.60
12:LC:98:ASP:OD2	27:LT:488:ASN:ND2	2.35	0.60
23:LO:440:PRO:HG3	23:LO:483:GLN:HA	1.84	0.60
42:SN:103:VAL:HG11	42:SN:131:VAL:HG21	1.82	0.60
21:LM:366:ILE:HA	21:LM:369:LEU:HB2	1.84	0.60
62:LX:621:GLN:HB3	62:LX:784:ARG:HH12	1.66	0.60
47:ST:700:LEU:HD21	54:SU:467:ALA:HB2	1.84	0.60
57:LR:171:MET:HB3	57:LR:187:GLN:HA	1.84	0.60
17:LH:497:ASP:HB2	17:LH:510:TYR:HB3	1.83	0.59
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	1.84	0.59
57:LR:540:SER:HB2	57:LR:549:ALA:HB3	1.84	0.59
2:SA:385:MET:HG2	35:SF:63:ILE:HB	1.83	0.59
57:LR:290:ILE:HA	57:LR:306:LEU:HA	1.84	0.59
4:L0:174:U:O2'	4:L0:222:G:N2	2.35	0.59
36:SG:368:LEU:HD23	36:SG:371:ARG:HD3	1.83	0.59
36:SG:481:ILE:HD13	36:SG:486:VAL:HG13	1.84	0.59
36:SG:541:ALA:HB3	36:SG:564:TYR:HB3	1.84	0.59
38:SI:925:ASN:OD1	47:ST:109:ARG:NH1	2.35	0.59
15:LF:83:LYS:HE3	15:LF:91:LEU:HD12	1.85	0.59
44:SQ:131:ASP:HB3	44:SQ:134:ARG:HG2	1.85	0.59
5:L2:82:G:N7	35:SE:38:ASN:ND2	2.47	0.59
12:LC:121:SER:OG	12:LC:123:ARG:NH1	2.36	0.59
28:LU:226:LYS:HG2	28:LU:268:CYS:HA	1.85	0.59
28:LU:332:TYR:HB3	28:LU:339:SER:HA	1.83	0.59
38:SI:1122:ALA:HB2	44:SQ:194:ILE:HD12	1.83	0.59
13:LD:87:ARG:HH21	13:LD:106:ASN:HD21	1.50	0.59
28:LU:133:GLN:HE22	28:LU:169:GLU:HG2	1.67	0.59
4:L0:87:C:O2	17:LH:332:GLN:NE2	2.36	0.59
13:LD:33:ARG:NH2	13:LD:53:TYR:O	2.36	0.59
18:LJ:275:SER:HB3	18:LJ:305:CYS:HB3	1.84	0.59
22:LN:470:LEU:HD11	22:LN:498:VAL:HG11	1.85	0.59
23:LO:347:SER:HB2	23:LO:365:GLU:H	1.68	0.59
15:LF:54:ALA:HB2	15:LF:79:VAL:HG12	1.84	0.58
23:LO:79:ALA:HB3	23:LO:93:PHE:HB3	1.85	0.58
29:LV:121:ARG:HH12	53:8:340:U:H5"	1.66	0.58



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:NA:370:ARG:HH22	47:ST:52:ARG:HD3	1.69	0.58
2:SA:185:ASP:O	2:SA:189:ASN:ND2	2.36	0.58
4:L0:335:G:H1	4:L0:389:U:H3	1.51	0.58
5:L2:256:G:N7	35:SF:38:ASN:ND2	2.51	0.58
22:LN:489:CYS:HB2	22:LN:534:LEU:HD11	1.85	0.58
27:LT:128:LEU:HB3	27:LT:140:TYR:HB2	1.85	0.58
36:SG:198:LYS:HE2	36:SG:212:LYS:HB2	1.84	0.58
2:SA:277:ARG:NH2	59:SB:261:GLN:OE1	2.36	0.58
17:LH:320:VAL:HG22	17:LH:335:PRO:HA	1.84	0.58
22:LN:166:VAL:HG22	22:LN:182:ILE:HG12	1.85	0.58
57:LR:439:ALA:HB3	57:LR:457:ALA:HB3	1.85	0.58
63:L6:67:VAL:H	63:L6:100:ALA:HB2	1.68	0.58
11:L9:57:ARG:NH2	40:SL:87:MET:O	2.36	0.58
35:SF:22:ASP:O	35:SF:26:GLN:NE2	2.36	0.58
62:LX:585:VAL:HB	62:LX:639:ALA:HB3	1.85	0.58
9:L7:163:ASP:OD1	9:L7:163:ASP:N	2.34	0.58
28:LU:114:THR:HG1	28:LU:139:CYS:HG	1.51	0.58
36:SG:333:MET:SD	36:SG:350:LYS:NZ	2.76	0.58
36:SG:442:ILE:HA	36:SG:472:PRO:HA	1.84	0.58
41:SM:123:VAL:HG23	41:SM:126:ASN:HB2	1.86	0.58
63:L6:105:ASP:OD2	63:L6:105:ASP:N	2.35	0.58
10:L8:98:LYS:HD2	10:L8:172:ARG:HG2	1.84	0.58
29:LV:162:LEU:HB3	29:LV:176:PHE:HB2	1.85	0.58
1:NA:366:GLU:HA	1:NA:369:ILE:HD12	1.86	0.58
38:SI:1059:ARG:NH1	48:SY:33:ASP:OD2	2.35	0.58
62:LX:12:SER:O	62:LX:16:ASN:ND2	2.37	0.58
66:6:64:LYS:HB2	66:6:110:VAL:HG11	1.85	0.58
4:L0:471:C:OP1	21:LM:27:LYS:NZ	2.37	0.58
22:LN:384:VAL:HG23	22:LN:391:VAL:HG12	1.86	0.58
30:LW:354:CYS:SG	30:LW:364:ARG:NH2	2.77	0.58
37:SH:289:VAL:O	37:SH:317:GLN:NE2	2.36	0.58
1:NA:470:GLU:HG3	1:NA:490:LEU:HB2	1.86	0.58
25:LQ:447:LEU:HB3	25:LQ:455:GLN:HB2	1.86	0.58
54:SU:350:MET:O	54:SU:355:ARG:NH1	2.37	0.58
65:5:337:MET:O	66:6:96:ARG:NH2	2.37	0.58
8:L5:76:ARG:NH1	12:LC:120:ASP:OD2	2.37	0.58
26:LS:254:LEU:HD22	26:LS:263:LEU:HD11	1.86	0.58
42:SN:93:THR:HG22	42:SN:177:ARG:HB2	1.86	0.58
57:LR:440:VAL:HG12	57:LR:456:THR:HG22	1.85	0.58
34:SD:105:LEU:HD21	48:SY:124:GLN:HA	1.86	0.57
53:8:538:A:H5'	53:8:543:C:H41	1.68	0.57



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
9:L7:74:GLN:HG2	9:L7:92:PHE:HD2	1.68	0.57
26:LS:568:VAL:HG23	26:LS:579:VAL:HG22	1.87	0.57
45:SR:41:SER:N	53:8:600:U:O2'	2.36	0.57
53:8:376:C:O2'	53:8:378:A:N7	2.36	0.57
53:8:965:U:H5"	64:NF:126:ALA:HB2	1.86	0.57
65:5:193:ARG:HH11	66:6:75:LEU:HD13	1.69	0.57
1:NA:483:TYR:OH	27:LT:736:HIS:ND1	2.37	0.57
25:LQ:196:CYS:SG	25:LQ:197:ILE:N	2.76	0.57
36:SG:402:ILE:HA	36:SG:417:SER:HA	1.86	0.57
38:SI:761:GLN:O	38:SI:765:ASN:ND2	2.38	0.57
44:SQ:110:ASP:O	44:SQ:114:ARG:NH2	2.38	0.57
48:SY:140:ARG:NH1	56:ND:166:LEU:O	2.37	0.57
48:SY:154:THR:HA	48:SY:168:LYS:HG3	1.86	0.57
53:8:1161:C:H1'	53:8:1619:C:H41	1.69	0.57
9:L7:151:LYS:HE2	9:L7:184:GLU:HB3	1.86	0.57
22:LN:583:VAL:HG22	22:LN:593:GLU:HG3	1.86	0.57
27:LT:28:ARG:HH21	27:LT:71:VAL:HG11	1.69	0.57
37:SH:123:ALA:HB1	37:SH:261:ILE:HG21	1.85	0.57
44:SQ:202:ARG:O	53:8:1489:U:N3	2.37	0.57
47:ST:478:ILE:HG12	47:ST:524:LEU:HD13	1.86	0.57
61:SP:1475:GLN:HA	61:SP:1517:HIS:HA	1.85	0.57
10:L8:98:LYS:HB3	53:8:329:G:H5"	1.87	0.57
17:LH:602:PRO:HB3	55:LI:591:THR:HB	1.87	0.57
26:LS:312:ILE:HB	26:LS:324:TRP:HB3	1.87	0.57
29:LV:56:SER:HA	29:LV:336:ILE:HA	1.86	0.57
35:SF:22:ASP:OD2	36:SG:342:ARG:NH2	2.37	0.57
40:SL:171:PRO:HA	40:SL:184:LYS:HB2	1.86	0.57
57:LR:786:ILE:HG13	57:LR:787:PRO:HD3	1.86	0.57
65:5:444:ALA:O	65:5:448:ASN:ND2	2.38	0.57
1:NA:326:LEU:O	38:SI:930:LYS:NZ	2.32	0.57
18:LJ:48:ASN:ND2	18:LJ:51:HIS:O	2.38	0.57
21:LM:123:ARG:O	21:LM:126:GLN:NE2	2.37	0.57
25:LQ:760:ILE:HA	25:LQ:763:ILE:HB	1.85	0.57
53:8:966:A:OP2	64:NF:126:ALA:N	2.26	0.57
3:NB:507:ILE:HG22	3:NB:510:LYS:HE3	1.87	0.57
4:L0:337:G:OP1	58:NE:209:ARG:NH2	2.38	0.57
8:L5:60:ASP:HA	8:L5:65:ARG:HH22	1.70	0.57
26:LS:538:LYS:HE2	26:LS:563:GLY:HA2	1.87	0.57
41:SM:282:ARG:NH2	53:8:560:U:OP2	2.37	0.57
57:LR:313:LEU:HB3	57:LR:331:SER:HB3	1.86	0.57
28:LU:298:LEU:O	28:LU:457:ARG:NH1	2.38	0.57



	A 4 arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:8:579:A:H4'	53:8:580:A:H5'	1.87	0.57
55:LI:165:SER:HA	55:LI:181:ASP:HA	1.85	0.57
7:L4:200:ARG:NH1	7:L4:206:ASP:OD1	2.37	0.57
17:LH:867:VAL:HG22	17:LH:895:LEU:HD21	1.87	0.57
25:LQ:114:LEU:HG	25:LQ:115:LEU:HG	1.85	0.57
62:LX:104:ARG:NH1	62:LX:105:TYR:O	2.38	0.57
20:LL:516:ILE:HD12	20:LL:517:PRO:HD2	1.87	0.56
38:SI:1062:ARG:NH2	53:8:1490:C:OP1	2.38	0.56
14:LE:15:ASN:ND2	14:LE:72:CYS:O	2.38	0.56
25:LQ:433:ALA:HA	25:LQ:449:THR:HA	1.87	0.56
29:LV:66:ARG:HH12	29:LV:108:SER:HB2	1.68	0.56
35:SE:24:VAL:HG12	35:SE:102:ILE:HD11	1.85	0.56
39:SK:190:GLN:NE2	39:SK:244:GLY:O	2.38	0.56
4:L0:293:U:H3	23:LO:632:SER:HB3	1.70	0.56
22:LN:481:ILE:HA	22:LN:536:VAL:HG21	1.87	0.56
26:LS:448:LYS:NZ	26:LS:449:ASP:O	2.34	0.56
28:LU:344:HIS:NE2	28:LU:418:HIS:O	2.39	0.56
37:SH:281:GLU:OE1	38:SI:625:TRP:NE1	2.38	0.56
41:SM:93:SER:O	41:SM:119:ARG:NH1	2.39	0.56
53:8:111:U:HO2'	53:8:112:A:H8	1.53	0.56
53:8:140:A:C5	63:L6:184:LEU:HA	2.41	0.56
53:8:312:A:H2	53:8:315:A:H5'	1.71	0.56
63:L6:10:ASN:ND2	63:L6:127:THR:O	2.37	0.56
1:NA:480:GLN:O	27:LT:743:ARG:NH2	2.39	0.56
4:L0:274:C:H2'	4:L0:275:A:H8	1.70	0.56
11:L9:77:ILE:HG21	11:L9:91:LYS:HA	1.87	0.56
15:LF:15:ASN:HB3	15:LF:20:ARG:HB2	1.87	0.56
17:LH:536:ASP:N	17:LH:536:ASP:OD1	2.38	0.56
28:LU:258:ILE:HD12	28:LU:294:LEU:HB3	1.86	0.56
53:8:877:G:O2'	53:8:942:G:N2	2.39	0.56
9:L7:20:VAL:HA	9:L7:23:ALA:HB3	1.86	0.56
17:LH:559:LYS:HG2	17:LH:612:SER:HA	1.86	0.56
31:LZ:151:THR:HB	31:LZ:154:MET:HB2	1.87	0.56
42:SN:74:LEU:HD23	42:SN:100:ILE:HD12	1.88	0.56
45:SR:65:ASN:HB3	45:SR:90:ASP:HB2	1.88	0.56
28:LU:262:MET:O	28:LU:281:ASN:ND2	2.39	0.56
30:LW:178:ASP:HB2	30:LW:184:LEU:HD21	1.87	0.56
36:SG:523:LYS:NZ	36:SG:524:ILE:O	2.38	0.56
55:LI:555:ILE:O	55:LI:585:ARG:NH1	2.39	0.56
4:L0:375:C:OP2	46:SS:834:LYS:NZ	2.39	0.56
7:L4:24:SER:HB2	66:6:289:PHE:HZ	1.69	0.56



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
11:L9:79:ARG:HD2	66:6:323:GLU:HB3	1.87	0.56
17:LH:682:ASN:HB2	17:LH:689:ILE:HD11	1.88	0.56
39:SK:83:ASP:N	39:SK:83:ASP:OD1	2.39	0.56
40:SL:163:ARG:HD2	53:8:15:U:H4'	1.88	0.56
9:L7:150:GLN:NE2	9:L7:180:GLN:O	2.38	0.56
10:L8:67:TRP:HA	10:L8:183:ILE:HG22	1.88	0.56
26:LS:272:LEU:HD12	26:LS:288:LEU:HD23	1.87	0.56
27:LT:510:LEU:O	27:LT:553:ARG:NH1	2.39	0.56
37:SH:256:TYR:HD1	37:SH:283:ILE:HG12	1.69	0.56
42:SN:56:ILE:HD13	42:SN:183:ILE:HG13	1.88	0.56
53:8:1468:U:H2'	53:8:1469:A:H8	1.71	0.56
5:L2:34:A:N7	31:LZ:7:HIS:ND1	2.51	0.56
9:L7:164:TYR:HD2	46:SS:278:ILE:HD13	1.69	0.56
29:LV:126:GLN:NE2	29:LV:129:GLY:O	2.39	0.56
37:SH:111:LYS:NZ	38:SI:921:GLU:OE2	2.37	0.56
57:LR:416:ARG:H	57:LR:425:ASP:HB2	1.71	0.56
17:LH:690:ASN:HD22	17:LH:750:LEU:HB2	1.70	0.56
36:SG:356:ARG:NH1	66:6:260:ALA:O	2.38	0.56
37:SH:330:LYS:NZ	38:SI:554:TYR:O	2.39	0.56
41:SM:42:LEU:HD12	58:NE:218:LEU:HB3	1.88	0.56
15:LF:5:VAL:O	15:LF:43:LYS:NZ	2.38	0.55
20:LL:167:SER:O	20:LL:168:HIS:ND1	2.39	0.55
47:ST:616:LEU:HB3	47:ST:619:LEU:HB2	1.86	0.55
4:L0:169:A:N7	22:LN:236:LYS:NZ	2.53	0.55
11:L9:17:ARG:NH2	53:8:22:A:OP1	2.40	0.55
14:LE:41:MET:SD	14:LE:41:MET:N	2.70	0.55
28:LU:90:GLY:HA2	28:LU:113:VAL:HG23	1.89	0.55
28:LU:457:ARG:NH2	53:8:1:U:O4	2.39	0.55
34:SD:320:TYR:OH	34:SD:323:SER:OG	2.24	0.55
57:LR:513:LYS:HG2	57:LR:535:GLY:HA2	1.88	0.55
57:LR:596:ASP:OD1	57:LR:596:ASP:N	2.39	0.55
23:LO:88:ASN:ND2	27:LT:659:GLN:O	2.40	0.55
47:ST:482:GLN:HB2	47:ST:524:LEU:HD11	1.87	0.55
53:8:235:G:N2	53:8:236:A:N7	2.53	0.55
57:LR:296:ILE:HG22	57:LR:298:SER:H	1.71	0.55
57:LR:679:THR:OG1	57:LR:680:ASN:N	2.39	0.55
39:SK:70:CYS:SG	53:8:1192:C:N4	2.79	0.55
57:LR:227:MET:N	57:LR:227:MET:SD	2.78	0.55
4:L0:89:C:OP1	26:LS:319:ARG:NH1	2.39	0.55
23:LO:411:VAL:HG23	23:LO:425:PHE:HB2	1.89	0.55
23:LO:624:ASN:ND2	23:LO:676:ARG:O	2.39	0.55



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
34:SD:314:CYS:SG	34:SD:315:ILE:N	2.79	0.55
53:8:911:U:OP1	57:LR:534:ARG:NE	2.38	0.55
1:NA:534:ARG:NH2	53:8:1641:C:OP2	2.39	0.55
3:NB:544:ILE:O	38:SI:193:ARG:NH2	2.40	0.55
17:LH:71:ASN:HD22	17:LH:74:LEU:HG	1.70	0.55
17:LH:368:ASP:HB3	17:LH:389:LEU:HD13	1.88	0.55
20:LL:110:ILE:HD12	20:LL:119:CYS:HB3	1.88	0.55
34:SC:171:LEU:HB2	34:SC:237:VAL:HG11	1.88	0.55
47:ST:422:LEU:HA	47:ST:425:PHE:HB3	1.87	0.55
19:LK:496:LEU:HA	19:LK:499:ILE:HD12	1.89	0.55
22:LN:542:VAL:HG23	22:LN:552:ILE:HG13	1.88	0.55
30:LW:40:LYS:HA	30:LW:43:ARG:HG2	1.89	0.55
36:SG:164:GLN:NE2	36:SG:528:GLU:O	2.40	0.55
39:SJ:100:LEU:O	39:SJ:105:ASN:ND2	2.38	0.55
39:SK:144:LEU:HB2	39:SK:150:ILE:HD11	1.88	0.55
47:ST:548:ARG:NH2	47:ST:638:ASN:OD1	2.39	0.55
58:NE:265:SER:O	58:NE:273:ARG:NH1	2.40	0.55
10:L8:81:VAL:HA	10:L8:102:VAL:HA	1.87	0.55
12:LC:31:VAL:HG22	12:LC:67:VAL:HB	1.88	0.55
29:LV:152:ASP:OD1	29:LV:152:ASP:N	2.40	0.55
38:SI:855:GLN:HE21	38:SI:1016:ASN:HD22	1.55	0.55
47:ST:734:ARG:O	47:ST:738:ASN:ND2	2.39	0.55
5:L2:15:U:OP2	58:NE:224:HIS:NE2	2.38	0.55
9:L7:162:ILE:O	9:L7:166:LEU:N	2.39	0.55
14:LE:11:LEU:HD21	14:LE:37:PHE:HE1	1.72	0.55
21:LM:196:LEU:HD11	21:LM:213:THR:HG21	1.89	0.55
23:LO:556:ARG:NH2	23:LO:575:GLU:OE1	2.40	0.55
28:LU:228:ASN:ND2	28:LU:230:ASN:O	2.39	0.55
39:SJ:168:THR:HA	39:SJ:171:LEU:HB2	1.89	0.55
4:L0:391:C:O2	31:LZ:55:ARG:NH1	2.40	0.55
8:L5:92:ARG:NH2	8:L5:169:ASN:OD1	2.40	0.55
20:LL:203:ILE:HD11	20:LL:212:LEU:HB3	1.89	0.55
21:LM:166:ASN:ND2	59:SB:408:THR:O	2.40	0.55
25:LQ:338:ILE:HG22	25:LQ:355:LEU:HD21	1.87	0.55
34:SD:242:ALA:HB2	34:SD:253:ILE:HD11	1.89	0.55
36:SG:460:ARG:HA	36:SG:463:GLN:HB2	1.89	0.55
48:SY:140:ARG:NH2	56:ND:169:ASP:OD1	2.40	0.55
4:L0:489:G:O6	24:LP:120:ARG:NH1	2.40	0.54
9:L7:64:VAL:HG13	9:L7:67:LEU:HB2	1.89	0.54
14:LE:27:ILE:HB	14:LE:61:ILE:HB	1.89	0.54
14:LE:78:ARG:HH21	14:LE:124:LYS:HG3	1.71	0.54



Atom-1	Atom-2	Interatomic	Clash
	1100m =	distance (Å)	overlap (Å)
18:LJ:90:ARG:HH21	18:LJ:137:ASN:HB3	1.72	0.54
19:LK:456:LEU:HD23	55:LI:675:LEU:HD22	1.89	0.54
20:LL:469:ILE:HG21	20:LL:505:CYS:HA	1.89	0.54
21:LM:245:LEU:HB3	21:LM:257:ALA:HB2	1.89	0.54
28:LU:265:ASN:ND2	28:LU:308:VAL:O	2.39	0.54
28:LU:438:LYS:NZ	53:8:0:U:OP1	2.40	0.54
48:SY:234:VAL:HG22	48:SY:240:ILE:HG22	1.89	0.54
18:LJ:90:ARG:NH2	18:LJ:137:ASN:O	2.40	0.54
28:LU:450:ASP:OD1	28:LU:450:ASP:N	2.40	0.54
30:LW:115:HIS:HB3	30:LW:128:THR:HB	1.89	0.54
31:LZ:62:SER:O	58:NE:207:ARG:NH1	2.40	0.54
53:8:523:G:H21	53:8:529:A:H62	1.54	0.54
53:8:966:A:OP2	64:NF:125:LEU:N	2.40	0.54
7:L4:43:PRO:HB3	7:L4:81:THR:HA	1.90	0.54
38:SI:60:ASP:O	38:SI:239:ASN:ND2	2.40	0.54
54:SU:181:THR:HB	54:SU:225:HIS:HE1	1.71	0.54
55:LI:301:GLN:HA	55:LI:315:SER:HA	1.89	0.54
57:LR:15:ILE:HG12	57:LR:43:ILE:HD13	1.89	0.54
17:LH:19:LYS:HE2	17:LH:366:ASN:HD21	1.71	0.54
34:SD:91:HIS:NE2	48:SY:163:GLU:O	2.37	0.54
35:SF:13:ASP:O	35:SF:17:THR:OG1	2.24	0.54
53:8:1670:G:O2'	53:8:1731:A:N6	2.39	0.54
55:LI:207:HIS:HA	55:LI:223:THR:HA	1.89	0.54
4:L0:238:G:N2	4:L0:274:C:O2	2.37	0.54
26:LS:556:PRO:HB2	26:LS:560:THR:HG21	1.90	0.54
36:SG:137:GLY:HA3	36:SG:500:LYS:HD2	1.89	0.54
36:SG:498:VAL:HG23	36:SG:511:LEU:HB2	1.90	0.54
47:ST:488:ASN:HB2	47:ST:492:ALA:HB2	1.90	0.54
53:8:126:A:H61	53:8:290:G:H1	1.55	0.54
57:LR:593:CYS:HB2	57:LR:620:LEU:HG	1.89	0.54
10:L8:88:ASN:OD1	10:L8:88:ASN:N	2.41	0.54
17:LH:529:LEU:HB3	17:LH:547:VAL:HB	1.89	0.54
20:LL:189:SER:HB2	20:LL:206:ALA:HB1	1.89	0.54
26:LS:128:SER:O	26:LS:132:LYS:NZ	2.40	0.54
34:SD:173:LEU:HB3	34:SD:242:ALA:HA	1.90	0.54
37:SH:156:ARG:HH21	37:SH:230:TRP:HE1	1.54	0.54
57:LR:763:ILE:HG23	57:LR:772:LEU:HD13	1.90	0.54
17:LH:437:THR:OG1	17:LH:706:HIS:ND1	2.41	0.54
21:LM:59:LEU:HD21	21:LM:114:THR:HG22	1.90	0.54
28:LU:123:PHE:HA	28:LU:207:ASN:HD21	1.73	0.54
29:LV:67:ASP:OD1	29:LV:67:ASP:N	2.40	0.54



Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
29:LV:112:THR:HA	29:LV:128:LYS:HD3	1.89	0.54
29:LV:353:CYS:HB3	29:LV:356:LEU:HB2	1.89	0.54
30:LW:289:MET:HG2	30:LW:301:TRP:HB2	1.90	0.54
38:SI:344:ARG:NH1	53:8:426:G:O6	2.41	0.54
39:SJ:116:THR:HG22	39:SJ:118:ARG:H	1.72	0.54
39:SK:88:ARG:NH1	53:8:1191:U:O2	2.40	0.54
39:SK:199:ASP:N	39:SK:199:ASP:OD1	2.39	0.54
4:L0:146:G:N2	20:LL:360:ASN:OD1	2.38	0.54
11:L9:53:ARG:NH2	11:L9:99:LEU:O	2.40	0.54
23:LO:99:CYS:HB3	23:LO:113:LEU:HD11	1.90	0.54
23:LO:112:ALA:HB1	23:LO:119:LEU:HD11	1.88	0.54
28:LU:82:LYS:NZ	28:LU:154:ASP:OD2	2.40	0.54
39:SJ:63:ASP:N	39:SJ:63:ASP:OD1	2.40	0.54
4:L0:83:U:H2'	22:LN:327:LEU:HD22	1.90	0.54
10:L8:31:ARG:HH21	10:L8:48:THR:HG22	1.73	0.54
17:LH:664:LEU:HB3	17:LH:670:LEU:HD12	1.88	0.54
22:LN:122:VAL:HB	56:ND:192:PRO:HG3	1.90	0.54
22:LN:590:LYS:NZ	22:LN:619:THR:O	2.41	0.54
25:LQ:109:MET:N	25:LQ:109:MET:SD	2.80	0.54
30:LW:451:SER:OG	30:LW:452:VAL:N	2.41	0.54
39:SJ:35:ASP:N	39:SJ:35:ASP:OD1	2.41	0.54
66:6:336:ASP:OD1	66:6:336:ASP:N	2.40	0.54
7:L4:221:ARG:NH1	53:8:111:U:OP1	2.41	0.54
8:L5:51:VAL:HG11	8:L5:130:ILE:HG12	1.90	0.54
9:L7:138:LYS:NZ	9:L7:139:ARG:O	2.41	0.54
17:LH:404:SER:OG	17:LH:405:ALA:N	2.40	0.54
21:LM:124:ARG:NH1	21:LM:124:ARG:O	2.41	0.54
28:LU:340:ARG:NH1	28:LU:341:GLU:OE1	2.41	0.54
34:SD:122:ARG:NH1	34:SD:140:GLU:OE2	2.41	0.54
39:SJ:183:ASP:N	39:SJ:183:ASP:OD1	2.41	0.54
7:L4:57:ASN:ND2	53:8:446:A:OP1	2.41	0.53
26:LS:148:THR:OG1	26:LS:163:ARG:NH2	2.41	0.53
27:LT:342:TYR:HH	27:LT:345:SER:HG	1.56	0.53
36:SG:305:ARG:HG2	36:SG:317:ILE:HG23	1.90	0.53
37:SH:155:LYS:NZ	37:SH:163:GLY:O	2.40	0.53
42:SN:181:ARG:NH1	60:SV:203:SER:O	2.41	0.53
62:LX:131:THR:HG22	62:LX:134:LEU:H	1.73	0.53
1:NA:530:ARG:HH12	53:8:1642:G:H5"	1.73	0.53
7:L4:182:TYR:N	7:L4:226:PHE:O	2.40	0.53
17:LH:708:ASP:OD1	17:LH:708:ASP:N	2.41	0.53
22:LN:345:ASP:HB2	22:LN:361:LEU:HB2	1.89	0.53



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
26:LS:204:ASP:OD1	26:LS:204:ASP:N	2.41	0.53
27:LT:392:ARG:HE	27:LT:449:ARG:HH22	1.55	0.53
53:8:627:C:N4	53:8:970:A:OP2	2.41	0.53
54:SU:407:ARG:NH2	54:SU:490:LYS:O	2.41	0.53
15:LF:10:ARG:HH22	15:LF:26:ASP:HB2	1.73	0.53
20:LL:112:LEU:HD11	20:LL:131:LEU:HD11	1.89	0.53
23:LO:828:ILE:HG21	27:LT:930:MET:HB2	1.89	0.53
26:LS:436:ASP:OD1	26:LS:436:ASP:N	2.40	0.53
30:LW:258:LEU:HB2	30:LW:268:VAL:HG22	1.90	0.53
35:SF:58:CYS:HA	35:SF:84:ARG:HD3	1.91	0.53
38:SI:828:ARG:NH1	45:SR:94:ASN:OD1	2.41	0.53
41:SM:220:ARG:NH1	41:SM:235:GLN:OE1	2.42	0.53
54:SU:466:LEU:HA	54:SU:469:LEU:HD12	1.90	0.53
55:LI:567:LEU:HD21	55:LI:595:ILE:HD11	1.90	0.53
62:LX:736:PHE:O	62:LX:740:ASN:ND2	2.42	0.53
4:L0:334:G:OP1	31:LZ:56:ARG:NH2	2.41	0.53
8:L5:57:SER:OG	8:L5:167:ARG:NH1	2.39	0.53
14:LE:87:GLU:OE1	14:LE:117:ARG:NH2	2.37	0.53
18:LJ:134:THR:OG1	18:LJ:135:GLN:OE1	2.25	0.53
23:LO:36:ARG:NH2	23:LO:53:GLU:OE1	2.39	0.53
23:LO:597:ASN:HA	23:LO:680:ARG:HB2	1.90	0.53
26:LS:465:THR:HG23	26:LS:468:CYS:H	1.72	0.53
37:SH:340:LYS:HG3	37:SH:351:ILE:HB	1.90	0.53
45:SR:97:ASP:N	45:SR:97:ASP:OD1	2.40	0.53
6:L3:110:ARG:HH22	6:L3:113:LEU:HD12	1.73	0.53
7:L4:87:MET:O	7:L4:122:LYS:NZ	2.42	0.53
23:LO:567:ASP:OD1	23:LO:576:ARG:NH2	2.40	0.53
23:LO:598:ASN:ND2	23:LO:600:SER:OG	2.41	0.53
27:LT:346:ARG:NH1	27:LT:384:ALA:O	2.42	0.53
38:SI:67:PRO:O	38:SI:114:ARG:NH2	2.41	0.53
62:LX:635:ILE:HB	62:LX:725:VAL:HG12	1.90	0.53
63:L6:98:ARG:NH2	63:L6:105:ASP:OD2	2.34	0.53
1:NA:311:ILE:HB	38:SI:1032:LEU:HD13	1.90	0.53
4:L0:313:A:N6	30:LW:79:GLU:OE1	2.40	0.53
12:LC:42:GLU:OE2	12:LC:45:ARG:NH1	2.41	0.53
17:LH:461:ASP:OD1	17:LH:461:ASP:N	2.41	0.53
23:LO:834:GLU:HA	23:LO:837:ASN:HB2	1.89	0.53
29:LV:109:ASP:OD1	29:LV:109:ASP:N	2.41	0.53
29:LV:189:ASN:HB3	29:LV:194:LEU:H	1.73	0.53
29:LV:205:GLU:OE1	29:LV:207:TRP:NE1	2.41	0.53
34:SD:166:PRO:HA	34:SD:188:VAL:HA	1.91	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
35:SF:6:PRO:HB3	36:SG:465:GLN:HE21	1.72	0.53
38:SI:870:ARG:NH2	53:8:573:C:O2'	2.41	0.53
42:SN:58:PRO:HA	42:SN:186:ASN:HD22	1.74	0.53
47:ST:314:UNK:O	47:ST:559:ARG:NH2	2.42	0.53
54:SU:245:GLN:HB3	54:SU:248:GLU:HG2	1.90	0.53
4:L0:490:G:HO2'	4:L0:494:C:HO2'	1.55	0.53
28:LU:183:GLN:N	28:LU:197:GLY:O	2.38	0.53
36:SG:484:SER:OG	36:SG:485:ASN:N	2.42	0.53
38:SI:124:ASP:OD1	38:SI:124:ASP:N	2.35	0.53
41:SM:281:ILE:HD11	53:8:564:G:H4'	1.90	0.53
53:8:378:A:O2'	66:6:306:ARG:NH2	2.42	0.53
53:8:1052:U:H3	53:8:1066:C:H42	1.55	0.53
57:LR:325:ASP:OD1	57:LR:325:ASP:N	2.41	0.53
17:LH:297:ILE:O	17:LH:485:ARG:NH2	2.42	0.53
23:LO:828:ILE:HA	23:LO:832:ALA:HB3	1.91	0.53
27:LT:230:VAL:HB	27:LT:244:ILE:HB	1.91	0.53
28:LU:357:SER:OG	28:LU:358:MET:N	2.42	0.53
31:LZ:137:ARG:HA	31:LZ:142:LEU:HA	1.91	0.53
42:SN:33:ASP:OD1	42:SN:33:ASP:N	2.42	0.53
53:8:110:U:H4'	66:6:227:ARG:HH21	1.74	0.53
53:8:364:G:H1	53:8:380:U:H3	1.57	0.53
53:8:964:U:O2'	64:NF:125:LEU:O	2.27	0.53
20:LL:448:ASN:OD1	20:LL:483:ARG:NH1	2.42	0.53
22:LN:589:ASN:OD1	22:LN:632:ASN:ND2	2.42	0.53
24:LP:12:ILE:HG21	30:LW:62:ALA:HB1	1.90	0.53
53:8:956:C:H2'	53:8:957:G:C8	2.44	0.53
55:LI:261:GLU:HA	55:LI:271:SER:HA	1.90	0.53
62:LX:879:SER:OG	62:LX:880:VAL:N	2.42	0.53
3:NB:433:ARG:O	39:SJ:211:ARG:NH1	2.42	0.53
14:LE:92:ASN:O	40:SL:79:LYS:NZ	2.42	0.53
23:LO:156:GLN:NE2	23:LO:200:SER:O	2.42	0.53
30:LW:266:PRO:O	46:SS:832:ASN:ND2	2.41	0.53
31:LZ:145:ASP:OD1	31:LZ:145:ASP:N	2.38	0.53
39:SK:165:ASN:ND2	53:8:1576:A:OP1	2.42	0.53
47:ST:434:ILE:HD11	47:ST:500:PHE:HB2	1.91	0.53
54:SU:281:LEU:HA	54:SU:285:ILE:HB	1.91	0.53
55:LI:558:CYS:O	55:LI:585:ARG:NH2	2.41	0.53
57:LR:631:MET:HB2	57:LR:645:LYS:HG3	1.91	0.53
11:L9:59:LEU:HD21	11:L9:73:GLY:HA2	1.90	0.52
17:LH:16:SER:HB3	17:LH:783:LEU:HB2	1.91	0.52
17:LH:55:TYR:HB3	17:LH:383:LEU:HD11	1.90	0.52



	At and 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
20:LL:56:SER:O	20:LL:59:LYS:NZ	2.41	0.52
22:LN:66:ARG:NH1	22:LN:80:ASN:OD1	2.42	0.52
25:LQ:480:ASP:HB3	25:LQ:539:VAL:HG23	1.91	0.52
28:LU:330:ARG:NH1	28:LU:339:SER:OG	2.39	0.52
29:LV:46:ARG:NH1	29:LV:46:ARG:O	2.42	0.52
30:LW:144:LEU:HD21	30:LW:147:GLU:HB2	1.91	0.52
40:SL:157:ASP:OD2	40:SL:157:ASP:N	2.40	0.52
53:8:1083:G:N2	53:8:1095:U:OP2	2.41	0.52
53:8:1484:G:N2	53:8:1606:C:O2	2.42	0.52
62:LX:166:MET:N	62:LX:166:MET:SD	2.82	0.52
66:6:77:MET:HG2	66:6:95:ALA:HB2	1.90	0.52
6:L3:104:ASN:OD1	6:L3:104:ASN:N	2.40	0.52
11:L9:57:ARG:HH12	40:SL:88:ASP:HA	1.75	0.52
23:LO:491:ALA:HB2	23:LO:521:LEU:HB2	1.92	0.52
25:LQ:100:ASP:OD2	25:LQ:100:ASP:N	2.37	0.52
25:LQ:165:SER:OG	25:LQ:166:ILE:N	2.42	0.52
28:LU:26:ARG:HH21	46:SS:868:GLU:HA	1.74	0.52
35:SE:29:ASN:ND2	48:SY:244:TRP:O	2.42	0.52
37:SH:37:ARG:NH2	37:SH:49:GLU:OE2	2.37	0.52
53:8:364:G:N2	53:8:380:U:O2	2.40	0.52
53:8:1044:U:H3	53:8:1074:G:H1	1.57	0.52
6:L3:20:THR:HG21	6:L3:35:ILE:HG23	1.91	0.52
8:L5:63:GLN:HE22	8:L5:66:GLN:HE21	1.58	0.52
18:LJ:415:LEU:HD11	18:LJ:458:ILE:HD13	1.91	0.52
22:LN:585:ILE:HG12	22:LN:633:CYS:HB3	1.92	0.52
25:LQ:595:LYS:HA	25:LQ:618:ILE:HG13	1.90	0.52
28:LU:146:LYS:HG2	28:LU:175:THR:HG22	1.91	0.52
30:LW:116:ILE:O	30:LW:380:ASN:ND2	2.42	0.52
38:SI:287:ARG:HH21	38:SI:297:SER:HB2	1.73	0.52
42:SN:177:ARG:NH2	60:SV:201:ASP:O	2.39	0.52
53:8:23:G:H1	53:8:602:U:H2'	1.74	0.52
7:L4:183:VAL:HG21	7:L4:220:THR:HG21	1.92	0.52
13:LD:91:LEU:HB3	13:LD:100:TYR:HB3	1.91	0.52
24:LP:120:ARG:HH21	24:LP:123:GLN:HB3	1.75	0.52
25:LQ:172:GLN:HE22	25:LQ:178:ILE:HG13	1.74	0.52
25:LQ:807:ASP:HA	25:LQ:810:LEU:HD13	1.91	0.52
36:SG:335:ARG:HD3	36:SG:348:LEU:HD21	1.91	0.52
53:8:183:U:O2	53:8:203:U:N3	2.41	0.52
53:8:884:A:H61	53:8:927:C:H42	1.58	0.52
53:8:929:A:OP2	53:8:931:C:N4	2.42	0.52
54:SU:317:ILE:HD11	54:SU:349:LEU:HD22	1.90	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:NA:496:TYR:O	57:LR:788:TYR:OH	2.28	0.52
18:LJ:229:CYS:HB2	18:LJ:258:LEU:HD13	1.92	0.52
23:LO:29:LEU:HD21	23:LO:327:LEU:HD21	1.92	0.52
23:LO:453:PHE:HB3	23:LO:475:PRO:HA	1.92	0.52
34:SD:281:ASP:HB2	34:SD:284:THR:HG23	1.92	0.52
36:SG:286:LEU:HD23	36:SG:295:LEU:HD11	1.91	0.52
45:SR:95:PHE:O	45:SR:142:LYS:NZ	2.39	0.52
45:SR:103:LEU:HB2	45:SR:126:LYS:HB2	1.92	0.52
53:8:593:U:H5"	53:8:594:A:H5'	1.90	0.52
53:8:1274:C:H2'	53:8:1275:A:H8	1.75	0.52
57:LR:568:MET:N	57:LR:568:MET:SD	2.82	0.52
65:5:345:ARG:NH2	65:5:411:GLU:OE1	2.41	0.52
3:NB:580:ARG:NH1	40:SL:51:LEU:O	2.42	0.52
3:NB:588:SER:O	35:SF:46:ARG:NH1	2.42	0.52
9:L7:118:LEU:O	9:L7:122:HIS:ND1	2.42	0.52
11:L9:19:TYR:OH	53:8:20:G:N1	2.42	0.52
12:LC:16:ALA:HB2	12:LC:72:GLY:HA3	1.91	0.52
18:LJ:356:ASN:OD1	18:LJ:359:ARG:NH2	2.43	0.52
20:LL:155:PRO:HD3	20:LL:196:VAL:HG11	1.92	0.52
22:LN:345:ASP:OD1	22:LN:345:ASP:N	2.42	0.52
25:LQ:359:SER:HG	25:LQ:361:THR:HG1	1.55	0.52
26:LS:137:ILE:HD12	26:LS:155:ILE:HD12	1.92	0.52
35:SF:25:GLN:NE2	36:SG:323:ASP:OD1	2.40	0.52
37:SH:207:ARG:HE	37:SH:268:PRO:HG2	1.73	0.52
41:SM:49:ASP:OD1	41:SM:49:ASP:N	2.42	0.52
45:SR:49:ALA:HB3	45:SR:104:LEU:HB2	1.90	0.52
4:L0:491:U:H4'	24:LP:83:LEU:HD13	1.92	0.52
8:L5:156:ARG:NH1	8:L5:157:ARG:O	2.43	0.52
11:L9:100:LYS:NZ	40:SL:59:ILE:O	2.43	0.52
27:LT:274:ILE:HG12	27:LT:286:VAL:HG12	1.92	0.52
28:LU:145:VAL:HB	28:LU:176:PHE:HB2	1.92	0.52
28:LU:254:PRO:HG2	46:SS:284:ARG:HE	1.74	0.52
38:SI:160:GLN:NE2	38:SI:197:GLU:O	2.42	0.52
39:SJ:102:SER:HA	39:SK:236:VAL:HG21	1.91	0.52
39:SJ:188:ARG:HG2	39:SJ:191:ASP:H	1.75	0.52
62:LX:91:MET:SD	62:LX:91:MET:N	2.83	0.52
1:NA:496:TYR:OH	1:NA:508:ARG:NH2	2.41	0.52
4:L0:68:U:OP2	17:LH:426:ARG:NH1	2.42	0.52
13:LD:6:THR:OG1	13:LD:7:VAL:N	2.42	0.52
22:LN:520:LYS:O	22:LN:524:LYS:NZ	2.43	0.52
23:LO:303:ASN:HD21	23:LO:324:LEU:HD12	1.75	0.52



Atom-1	Atom-2	Interatomic	Clash
1100111 1	1100111-2	distance (Å)	overlap (Å)
23:LO:471:GLY:O	23:LO:498:ARG:NH2	2.39	0.52
25:LQ:479:LEU:HD22	25:LQ:490:THR:HG22	1.92	0.52
29:LV:116:HIS:HB2	29:LV:124:GLN:HB2	1.92	0.52
36:SG:242:VAL:HG23	36:SG:253:THR:HG22	1.92	0.52
47:ST:573:LEU:HB3	47:ST:593:LEU:HD11	1.91	0.52
47:ST:612:THR:OG1	47:ST:613:ILE:N	2.40	0.52
53:8:505:A:H61	53:8:585:A:H2'	1.75	0.52
53:8:992:A:OP2	53:8:993:A:N6	2.37	0.52
53:8:1170:G:N2	53:8:1571:C:O3'	2.42	0.52
62:LX:193:GLY:HA2	62:LX:212:GLY:H	1.75	0.52
2:SA:21:LYS:NZ	2:SA:45:THR:O	2.42	0.52
2:SA:210:VAL:HG11	2:SA:219:LEU:HD12	1.92	0.52
26:LS:464:THR:HG21	26:LS:476:ILE:HA	1.92	0.52
27:LT:93:ALA:HB2	27:LT:121:LEU:HD22	1.91	0.52
27:LT:430:ILE:HB	27:LT:443:TRP:HB2	1.91	0.52
30:LW:135:ALA:HB1	30:LW:144:LEU:HD11	1.91	0.52
30:LW:244:ASN:HB3	30:LW:246:VAL:HG22	1.91	0.52
36:SG:241:THR:HG21	36:SG:285:SER:HA	1.91	0.52
39:SK:96:LEU:HD11	39:SK:114:ILE:HD11	1.91	0.52
65:5:412:ASP:N	65:5:412:ASP:OD1	2.42	0.52
66:6:268:ASN:HD21	66:6:271:ARG:HB2	1.75	0.52
3:NB:562:ARG:NH1	53:8:476:U:OP2	2.42	0.52
4:L0:323:A:OP1	23:LO:191:ARG:NH1	2.43	0.52
22:LN:589:ASN:ND2	22:LN:629:LEU:O	2.42	0.52
26:LS:161:ILE:HD13	27:LT:177:LEU:HB2	1.92	0.52
27:LT:460:ASP:O	27:LT:481:ASN:ND2	2.43	0.52
38:SI:923:ASP:N	38:SI:923:ASP:OD1	2.43	0.52
47:ST:510:THR:HA	47:ST:518:ILE:HD13	1.91	0.52
47:ST:515:HIS:O	47:ST:519:THR:OG1	2.28	0.52
47:ST:678:PHE:HB3	47:ST:681:PRO:HD2	1.91	0.52
57:LR:699:LYS:HD3	57:LR:755:ILE:HD11	1.92	0.52
62:LX:326:PHE:HA	62:LX:360:LYS:HA	1.92	0.52
5:L2:314:C:H2'	5:L2:315:A:H8	1.75	0.51
21:LM:262:VAL:HG13	21:LM:301:LYS:HG2	1.93	0.51
36:SG:203:ASP:O	36:SG:538:ARG:NH2	2.43	0.51
36:SG:308:SER:HB3	36:SG:315:LEU:HD21	1.92	0.51
38:SI:366:MET:SD	38:SI:366:MET:N	2.83	0.51
40:SL:138:ASP:HB3	40:SL:160:LEU:HD13	1.92	0.51
42:SN:76:THR:OG1	42:SN:77:LYS:N	2.43	0.51
53:8:538:A:N3	53:8:540:G:N2	2.59	0.51
1:NA:370:ARG:NH2	41:SM:246:GLU:OE1	2.43	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
11:L9:36:LEU:HD11	11:L9:105:LEU:HD21	1.92	0.51
15:LF:29:HIS:HB2	15:LF:67:GLY:HA2	1.91	0.51
25:LQ:15:GLY:O	25:LQ:360:ASN:ND2	2.43	0.51
25:LQ:393:ASP:N	25:LQ:393:ASP:OD1	2.44	0.51
28:LU:85:THR:OG1	28:LU:95:TRP:NE1	2.35	0.51
41:SM:36:LEU:O	58:NE:214:ARG:NH2	2.43	0.51
53:8:598:U:H2'	53:8:599:A:H8	1.74	0.51
62:LX:9:ARG:HH22	62:LX:214:LYS:HA	1.75	0.51
6:L3:57:ARG:NH1	18:LJ:61:THR:OG1	2.41	0.51
7:L4:181:VAL:HA	7:L4:227:VAL:HA	1.93	0.51
23:LO:27:LYS:HD3	23:LO:43:ILE:HG13	1.91	0.51
23:LO:269:HIS:NE2	23:LO:312:GLN:O	2.43	0.51
23:LO:434:ASN:HD21	23:LO:450:LEU:HD23	1.74	0.51
28:LU:292:ARG:NH1	46:SS:296:SER:OG	2.44	0.51
31:LZ:66:PRO:HA	31:LZ:71:ARG:HH11	1.76	0.51
34:SC:310:GLU:OE1	34:SC:313:HIS:ND1	2.44	0.51
35:SE:33:LEU:HD11	35:SE:100:ALA:HB1	1.91	0.51
38:SI:1156:LYS:HD2	53:8:18:C:H5'	1.92	0.51
39:SK:90:ASP:N	39:SK:90:ASP:OD1	2.43	0.51
41:SM:19:GLU:HA	41:SM:22:ASP:HB2	1.91	0.51
47:ST:616:LEU:HD13	47:ST:619:LEU:HD12	1.93	0.51
51:NH:862:LEU:HA	51:NH:866:ALA:HB3	1.93	0.51
53:8:887:A:C2	53:8:925:G:N1	2.79	0.51
59:SB:404:ARG:NH1	59:SB:405:ASP:O	2.43	0.51
62:LX:802:LEU:HD23	62:LX:805:ILE:HD11	1.92	0.51
65:5:450:LEU:O	65:5:453:ASN:N	2.41	0.51
18:LJ:212:ASP:OD1	18:LJ:212:ASP:N	2.43	0.51
20:LL:440:ILE:HG12	20:LL:452:LEU:HD21	1.93	0.51
25:LQ:635:LYS:HA	25:LQ:659:GLU:HG2	1.92	0.51
27:LT:730:LYS:NZ	27:LT:838:ILE:O	2.41	0.51
28:LU:140:SER:OG	28:LU:141:ASP:N	2.43	0.51
42:SN:242:ILE:HG13	42:SN:254:ILE:HG13	1.93	0.51
53:8:1208:A:N6	53:8:1454:G:N1	2.58	0.51
53:8:1220:C:H42	53:8:1263:G:H1	1.58	0.51
55:LI:606:ASP:N	55:LI:606:ASP:OD1	2.42	0.51
57:LR:34:THR:HG23	57:LR:41:ASN:HB2	1.91	0.51
57:LR:42:ILE:HG21	57:LR:90:LEU:HD11	1.91	0.51
62:LX:62:LYS:O	62:LX:125:GLN:NE2	2.43	0.51
5:L2:326:U:OP1	35:SE:46:ARG:NH2	2.37	0.51
9:L7:51:VAL:HG23	9:L7:53:GLY:H	1.76	0.51
17:LH:709:ARG:HB2	17:LH:765:TRP:HD1	1.76	0.51


		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
18:LJ:266:SER:OG	18:LJ:268:MET:O	2.28	0.51
22:LN:232:ASP:OD1	22:LN:232:ASP:N	2.44	0.51
22:LN:597:ASN:N	22:LN:597:ASN:OD1	2.43	0.51
23:LO:300:MET:SD	23:LO:326:GLN:NE2	2.83	0.51
25:LQ:337:LYS:HB3	25:LQ:358:SER:HB3	1.91	0.51
26:LS:133:ILE:HD12	27:LT:194:ARG:HH12	1.75	0.51
26:LS:511:LEU:HD13	26:LS:544:VAL:HG11	1.92	0.51
27:LT:125:GLY:HA2	59:SB:430:ASP:HA	1.92	0.51
34:SC:284:THR:HG22	40:SL:64:GLN:HE22	1.75	0.51
40:SL:18:ASN:HB3	40:SL:21:LYS:HB3	1.92	0.51
57:LR:498:SER:OG	57:LR:539:VAL:O	2.29	0.51
3:NB:438:ASP:OD1	3:NB:438:ASP:N	2.42	0.51
4:L0:163:G:H4'	26:LS:354:SER:HB2	1.92	0.51
6:L3:56:LYS:HE2	6:L3:61:LEU:HG	1.93	0.51
20:LL:443:GLN:NE2	54:SU:333:GLU:O	2.43	0.51
23:LO:849:LEU:HD22	27:LT:897:HIS:HB2	1.93	0.51
25:LQ:922:ASP:OD1	25:LQ:922:ASP:N	2.40	0.51
26:LS:412:GLN:OE1	26:LS:420:ARG:NH2	2.44	0.51
26:LS:473:ILE:HA	26:LS:476:ILE:HD12	1.92	0.51
27:LT:627:ASN:ND2	27:LT:647:THR:OG1	2.37	0.51
28:LU:67:ARG:HH21	40:SL:122:ASP:HA	1.75	0.51
38:SI:1089:GLN:HB3	48:SY:82:ARG:HH21	1.75	0.51
38:SI:1150:SER:OG	38:SI:1154:LYS:NZ	2.44	0.51
47:ST:605:ASP:OD1	47:ST:605:ASP:N	2.44	0.51
50:NJ:1574:ALA:HA	50:NJ:1578:GLY:HA3	1.93	0.51
57:LR:563:ASP:OD1	57:LR:563:ASP:N	2.42	0.51
62:LX:753:ASP:OD1	62:LX:753:ASP:N	2.43	0.51
66:6:353:ALA:O	66:6:356:ARG:NH1	2.43	0.51
4:L0:183:A:N6	4:L0:213:G:O6	2.44	0.51
35:SE:42:LYS:HD2	35:SE:46:ARG:HH12	1.74	0.51
36:SG:185:LEU:HD21	36:SG:527:VAL:HG11	1.92	0.51
38:SI:288:VAL:HG23	38:SI:814:GLY:HA2	1.91	0.51
38:SI:767:ILE:O	38:SI:770:GLN:NE2	2.42	0.51
38:SI:968:THR:HG22	38:SI:1001:VAL:HG12	1.92	0.51
38:SI:974:GLY:HA3	38:SI:991:PHE:HD1	1.75	0.51
52:NI:15:VAL:HA	52:NI:38:PHE:HA	1.92	0.51
57:LR:505:ILE:HB	57:LR:517:ILE:HD11	1.92	0.51
1:NA:341:LEU:O	6:L3:120:ARG:NH2	2.44	0.51
2:SA:172:ASN:HA	2:SA:175:ILE:HD12	1.92	0.51
4:L0:467:A:H61	5:L2:49:C:H42	1.59	0.51
26:LS:493:LEU:HD21	26:LS:530:LEU:HD22	1.92	0.51



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
29:LV:57:GLU:O	29:LV:76:THR:OG1	2.29	0.51
31:LZ:120:MET:HA	48:SY:62:GLU:HA	1.92	0.51
34:SC:89:GLU:OE1	44:SQ:141:TRP:NE1	2.41	0.51
34:SD:110:ASN:ND2	34:SD:141:TYR:O	2.44	0.51
37:SH:119:LYS:HB3	37:SH:165:GLU:HB3	1.92	0.51
37:SH:201:SER:HB3	37:SH:204:LEU:HD13	1.93	0.51
37:SH:361:ASN:HD22	37:SH:364:LYS:HD2	1.76	0.51
2:SA:86:LEU:HD13	2:SA:116:VAL:HG21	1.93	0.51
4:L0:248:G:OP2	48:SY:82:ARG:NH2	2.44	0.51
23:LO:450:LEU:HA	23:LO:475:PRO:HB3	1.92	0.51
23:LO:525:PRO:HG2	23:LO:587:PHE:HA	1.92	0.51
25:LQ:488:LEU:HB3	25:LQ:500:TRP:HB2	1.91	0.51
28:LU:367:SER:HB3	28:LU:373:ARG:HH12	1.75	0.51
34:SD:301:LEU:HD23	34:SD:302:GLU:HB2	1.93	0.51
36:SG:525:GLN:HB2	36:SG:540:LEU:HB2	1.93	0.51
36:SG:546:GLU:OE2	36:SG:551:ARG:NH1	2.44	0.51
38:SI:846:VAL:HG22	38:SI:855:GLN:HB3	1.93	0.51
54:SU:167:LYS:O	54:SU:272:GLN:NE2	2.43	0.51
9:L7:50:ASP:HA	9:L7:56:LYS:HG3	1.92	0.51
10:L8:9:HIS:NE2	53:8:321:C:N3	2.50	0.51
11:L9:87:SER:HB3	11:L9:90:LYS:HG3	1.92	0.51
13:LD:64:VAL:HG12	13:LD:129:ARG:HH11	1.76	0.51
22:LN:370:ARG:NH2	22:LN:630:LYS:O	2.44	0.51
27:LT:307:GLN:NE2	59:SB:422:THR:O	2.39	0.51
27:LT:590:ALA:HB3	27:LT:631:ASN:HA	1.92	0.51
28:LU:403:ARG:NH2	46:SS:860:SER:O	2.44	0.51
29:LV:300:TRP:HA	29:LV:308:TYR:H	1.76	0.51
30:LW:113:PRO:HA	30:LW:395:GLN:HA	1.93	0.51
34:SD:257:SER:HA	34:SD:261:LEU:HD23	1.92	0.51
39:SJ:167:ILE:HG13	39:SJ:171:LEU:HG	1.92	0.51
39:SK:151:ARG:HB2	47:ST:716:LYS:HE3	1.93	0.51
53:8:883:C:O2	53:8:946:U:N3	2.44	0.51
57:LR:580:ARG:HG2	57:LR:623:LEU:HB3	1.93	0.51
5:L2:59:G:H5'	23:LO:570:THR:HG23	1.93	0.50
7:L4:140:VAL:HG12	7:L4:146:THR:HG22	1.92	0.50
11:L9:110:GLN:OE1	11:L9:126:ARG:NH1	2.41	0.50
11:L9:155:HIS:NE2	36:SG:321:HIS:O	2.45	0.50
11:L9:157:ASP:OD2	11:L9:158:PHE:N	2.44	0.50
13:LD:11:ARG:NH2	53:8:342:C:O2'	2.43	0.50
17:LH:490:LEU:HD11	18:LJ:426:LYS:HD2	1.93	0.50
23:LO:660:SER:HA	23:LO:672:THR:HA	1.93	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
24:LP:297:ASP:OD1	24:LP:297:ASP:N	2.43	0.50
36:SG:262:VAL:HG13	36:SG:271:VAL:HG23	1.91	0.50
38:SI:125:LEU:HD21	38:SI:899:VAL:HG21	1.93	0.50
38:SI:826:LYS:NZ	38:SI:923:ASP:OD2	2.44	0.50
39:SJ:239:SER:HG	39:SK:239:SER:HG	1.58	0.50
41:SM:187:PRO:HB3	41:SM:220:ARG:HE	1.75	0.50
2:SA:158:TYR:OH	34:SC:222:GLU:OE1	2.28	0.50
17:LH:531:PHE:HD2	17:LH:545:THR:HB	1.76	0.50
20:LL:64:LYS:HB3	20:LL:77:ILE:HD12	1.92	0.50
23:LO:78:ARG:NH1	23:LO:94:ASN:OD1	2.43	0.50
25:LQ:137:ILE:HG12	25:LQ:147:VAL:HG13	1.92	0.50
25:LQ:336:TYR:HB2	25:LQ:357:THR:HB	1.93	0.50
25:LQ:350:LYS:HD2	25:LQ:366:SER:HB3	1.91	0.50
38:SI:248:ARG:HG2	38:SI:272:TYR:HB2	1.93	0.50
57:LR:26:SER:OG	57:LR:28:ASN:OD1	2.30	0.50
9:L7:143:LEU:O	14:LE:42:GLN:NE2	2.45	0.50
14:LE:54:ASP:OD1	14:LE:54:ASP:N	2.45	0.50
18:LJ:40:ASN:HB2	18:LJ:60:SER:HB3	1.94	0.50
20:LL:231:ASP:N	20:LL:231:ASP:OD1	2.43	0.50
23:LO:30:LEU:HD11	23:LO:63:LEU:HD22	1.93	0.50
26:LS:257:HIS:HB2	26:LS:262:LEU:HB2	1.94	0.50
57:LR:18:GLY:HA2	57:LR:37:LEU:HG	1.92	0.50
62:LX:877:LEU:HD21	62:LX:919:LYS:HD3	1.93	0.50
10:L8:108:PRO:HA	10:L8:111:GLN:HB2	1.93	0.50
17:LH:136:LEU:HD13	17:LH:187:VAL:HB	1.93	0.50
17:LH:215:VAL:HG21	17:LH:224:SER:HB3	1.92	0.50
18:LJ:217:ASN:HB3	18:LJ:229:CYS:HB3	1.93	0.50
22:LN:417:VAL:HG11	22:LN:460:LEU:HD13	1.94	0.50
25:LQ:426:ARG:NH2	25:LQ:459:LEU:O	2.44	0.50
27:LT:738:ASP:OD1	27:LT:738:ASP:N	2.44	0.50
27:LT:851:SER:OG	43:SO:241:ARG:NH2	2.43	0.50
29:LV:184:ASN:ND2	29:LV:198:GLY:O	2.43	0.50
53:8:1491:U:H4'	53:8:1492:A:H5'	1.93	0.50
57:LR:96:VAL:HG12	57:LR:97:ARG:HD2	1.92	0.50
62:LX:215:ASN:N	62:LX:215:ASN:OD1	2.42	0.50
2:SA:330:ALA:HB1	2:SA:381:ASN:HA	1.94	0.50
19:LK:453:PRO:HB3	55:LI:675:LEU:HD11	1.94	0.50
28:LU:8:ARG:HH22	30:LW:409:ALA:HA	1.76	0.50
37:SH:283:ILE:O	38:SI:634:ARG:NH1	2.45	0.50
38:SI:285:GLY:H	38:SI:298:VAL:HG23	1.75	0.50
40:SL:165:ARG:NH1	53:8:19:A:N1	2.60	0.50



At any 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:8:992:A:H3'	53:8:993:A:C8	2.47	0.50
57:LR:44:ASP:N	57:LR:44:ASP:OD1	2.39	0.50
59:SB:299:LEU:HD22	59:SB:320:LEU:HD23	1.94	0.50
4:L0:316:U:OP1	30:LW:364:ARG:NH2	2.44	0.50
5:L2:306:G:H2'	5:L2:307:G:C8	2.47	0.50
9:L7:139:ARG:NH2	14:LE:52:TYR:O	2.44	0.50
10:L8:77:ARG:NH1	10:L8:78:ILE:O	2.44	0.50
22:LN:466:ASP:OD1	22:LN:466:ASP:N	2.42	0.50
25:LQ:65:ASP:HB2	25:LQ:67:LEU:HD22	1.94	0.50
34:SD:199:PHE:HE2	34:SD:223:ASP:HB2	1.75	0.50
56:ND:185:GLN:NE2	56:ND:186:ASP:OD2	2.45	0.50
57:LR:446:VAL:HG13	57:LR:448:LYS:H	1.76	0.50
1:NA:453:SER:O	1:NA:455:HIS:N	2.45	0.50
10:L8:193:LEU:HA	10:L8:196:LEU:HB2	1.93	0.50
25:LQ:7:ARG:NH2	25:LQ:70:GLY:O	2.45	0.50
25:LQ:655:ALA:HB2	25:LQ:684:TRP:HZ2	1.75	0.50
25:LQ:760:ILE:HD11	25:LQ:835:PHE:HB2	1.94	0.50
29:LV:89:LEU:HD12	63:L6:73:ILE:HG12	1.93	0.50
38:SI:287:ARG:HD2	38:SI:820:ILE:HD13	1.92	0.50
42:SN:39:ILE:HG12	42:SN:243:PHE:HB2	1.93	0.50
66:6:71:TYR:HD1	66:6:75:LEU:HD11	1.76	0.50
7:L4:16:HIS:HE2	66:6:230:ALA:HA	1.77	0.50
20:LL:438:THR:HG21	20:LL:471:ARG:HB3	1.93	0.50
22:LN:226:LEU:O	22:LN:227:HIS:ND1	2.45	0.50
23:LO:853:ASP:N	23:LO:853:ASP:OD1	2.44	0.50
24:LP:166:ASN:HD22	46:SS:328:THR:HA	1.77	0.50
25:LQ:102:VAL:HG12	25:LQ:118:ASN:HB3	1.94	0.50
25:LQ:547:ALA:HA	25:LQ:557:VAL:HA	1.93	0.50
27:LT:573:VAL:HG13	27:LT:574:THR:HG23	1.93	0.50
37:SH:184:ASP:N	37:SH:184:ASP:OD1	2.45	0.50
39:SJ:129:ARG:O	53:8:1194:A:N6	2.41	0.50
62:LX:920:MET:HA	62:LX:923:TYR:HB3	1.93	0.50
1:NA:479:ALA:O	23:LO:341:GLN:NE2	2.44	0.50
5:L2:253:G:OP2	35:SF:95:ARG:NH1	2.45	0.50
8:L5:189:THR:OG1	8:L5:192:GLU:OE1	2.30	0.50
13:LD:14:GLN:OE1	13:LD:14:GLN:N	2.45	0.50
20:LL:439:VAL:HG11	54:SU:300:THR:HG21	1.92	0.50
25:LQ:880:ILE:HA	25:LQ:883:VAL:HG12	1.93	0.50
25:LQ:917:ASN:ND2	25:LQ:919:GLU:OE2	2.44	0.50
28:LU:200:LYS:HE3	28:LU:214:ASP:HB3	1.94	0.50
36:SG:539:ILE:HB	36:SG:566:ALA:HB3	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
37:SH:327:ARG:NH2	38:SI:555:MET:O	2.36	0.50
38:SI:120:CYS:HB2	38:SI:131:ILE:HD13	1.92	0.50
47:ST:798:LYS:O	47:ST:801:ARG:NH2	2.45	0.50
57:LR:571:LEU:HD11	57:LR:590:LEU:HD23	1.94	0.50
57:LR:584:ILE:HG13	57:LR:586:LYS:H	1.77	0.50
62:LX:743:VAL:HG11	62:LX:774:LEU:HG	1.94	0.50
66:6:85:ASP:OD1	66:6:85:ASP:N	2.45	0.50
2:SA:129:ARG:NH1	34:SC:261:LEU:O	2.44	0.49
3:NB:554:ARG:NH2	53:8:547:U:OP2	2.44	0.49
4:L0:485:G:H1	28:LU:386:LYS:H	1.61	0.49
14:LE:76:SER:HB2	58:NE:320:ILE:HG12	1.94	0.49
17:LH:22:LEU:HD21	17:LH:32:LYS:HD3	1.93	0.49
18:LJ:285:ASP:OD1	18:LJ:285:ASP:N	2.42	0.49
22:LN:35:ARG:HA	22:LN:754:ILE:HB	1.94	0.49
22:LN:529:ASN:O	22:LN:545:ARG:NH1	2.39	0.49
28:LU:40:GLU:OE2	46:SS:865:ILE:N	2.43	0.49
28:LU:273:GLU:HA	46:SS:302:VAL:HG21	1.94	0.49
41:SM:281:ILE:HB	41:SM:284:ALA:HB2	1.94	0.49
51:NH:443:HIS:HA	51:NH:471:SER:H	1.76	0.49
57:LR:344:ARG:NH2	57:LR:395:ASP:OD1	2.42	0.49
4:L0:499:U:H2'	4:L0:500:G:H8	1.77	0.49
17:LH:214:ASP:N	17:LH:214:ASP:OD1	2.43	0.49
18:LJ:453:VAL:HG11	20:LL:532:ARG:HE	1.76	0.49
21:LM:12:ALA:HB2	30:LW:142:GLY:HA3	1.94	0.49
23:LO:528:LYS:O	23:LO:543:ASN:ND2	2.44	0.49
23:LO:650:ASN:ND2	23:LO:655:ASP:OD2	2.42	0.49
25:LQ:634:SER:OG	25:LQ:635:LYS:N	2.44	0.49
29:LV:187:SER:HB3	29:LV:196:ALA:HB3	1.93	0.49
29:LV:200:GLU:HA	29:LV:230:GLN:HB3	1.92	0.49
30:LW:177:TYR:HE1	30:LW:183:GLU:HG2	1.77	0.49
34:SD:249:GLN:HB3	34:SD:269:ILE:HD11	1.94	0.49
36:SG:348:LEU:HB3	36:SG:357:LEU:HB2	1.93	0.49
42:SN:126:VAL:HG22	42:SN:154:ILE:HG12	1.95	0.49
42:SN:148:LYS:HG2	42:SN:149:LYS:HD2	1.94	0.49
53:8:223:U:H3	53:8:243:G:H22	1.59	0.49
55:LI:295:TYR:HA	55:LI:302:LEU:HA	1.94	0.49
1:NA:527:ARG:NH1	53:8:1641:C:OP1	2.39	0.49
4:L0:331:U:H2'	30:LW:191:ILE:HD12	1.93	0.49
4:L0:348:U:OP2	4:L0:377:U:N3	2.45	0.49
14:LE:53:ILE:N	14:LE:60:LYS:O	2.43	0.49
17:LH:520:LEU:HD11	20:LL:542:ALA:HB1	1.93	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:LO:303:ASN:HA	23:LO:323:LYS:HE3	1.93	0.49
24:LP:2:SER:OG	24:LP:3:LYS:N	2.45	0.49
34:SD:100:ARG:NH2	60:SV:129:TRP:O	2.45	0.49
38:SI:279:PRO:HB3	38:SI:784:LYS:HA	1.94	0.49
41:SM:118:ASN:OD1	41:SM:118:ASN:N	2.45	0.49
53:8:140:A:C8	63:L6:184:LEU:N	2.80	0.49
53:8:863:A:H8	53:8:865:A:H4'	1.77	0.49
5:L2:64:A:OP2	27:LT:392:ARG:NH1	2.46	0.49
7:L4:116:ASP:OD1	7:L4:116:ASP:N	2.46	0.49
9:L7:44:LYS:HZ3	9:L7:61:PHE:HB3	1.77	0.49
21:LM:281:THR:HG21	26:LS:208:LEU:HB2	1.93	0.49
22:LN:102:LEU:HD23	22:LN:116:SER:HB2	1.94	0.49
22:LN:383:LEU:HD22	22:LN:394:TRP:HZ3	1.78	0.49
25:LQ:215:ASP:OD1	25:LQ:215:ASP:N	2.38	0.49
26:LS:345:LEU:HD11	26:LS:352:GLN:HE21	1.77	0.49
29:LV:85:ASP:OD1	29:LV:85:ASP:N	2.41	0.49
36:SG:256:ARG:NH1	36:SG:282:GLU:OE1	2.45	0.49
41:SM:193:ASN:HB3	41:SM:226:ASN:HB3	1.95	0.49
42:SN:71:ASN:HB2	42:SN:123:ASP:H	1.77	0.49
53:8:965:U:H3'	64:NF:125:LEU:H	1.77	0.49
58:NE:224:HIS:ND1	58:NE:226:ASP:OD1	2.46	0.49
65:5:194:ILE:O	65:5:197:GLN:NE2	2.45	0.49
24:LP:187:LYS:HE2	44:SQ:63:PRO:HB2	1.95	0.49
25:LQ:807:ASP:N	25:LQ:807:ASP:OD1	2.41	0.49
27:LT:53:CYS:HA	27:LT:58:PHE:HA	1.94	0.49
29:LV:291:THR:HG23	29:LV:300:TRP:HE1	1.77	0.49
34:SC:109:LYS:NZ	44:SQ:103:TRP:O	2.40	0.49
36:SG:252:VAL:HA	36:SG:262:VAL:HA	1.94	0.49
37:SH:329:ILE:HG23	37:SH:333:PHE:HD2	1.78	0.49
38:SI:867:THR:OG1	38:SI:868:ARG:NH1	2.45	0.49
42:SN:243:PHE:HB3	42:SN:251:SER:HB2	1.93	0.49
53:8:487:G:H2'	53:8:488:G:H8	1.76	0.49
57:LR:537:TRP:HD1	57:LR:553:GLY:HA2	1.76	0.49
61:SP:1120:GLN:O	61:SP:1124:TYR:N	2.45	0.49
5:L2:76:U:OP2	26:LS:513:GLN:NE2	2.45	0.49
18:LJ:431:LEU:HD21	18:LJ:466:VAL:HG22	1.93	0.49
22:LN:302:ARG:NH1	22:LN:330:GLY:O	2.45	0.49
42:SN:60:THR:HG23	42:SN:61:LYS:HG2	1.94	0.49
53:8:479:C:O2	53:8:510:G:N2	2.45	0.49
53:8:1057:U:O2'	53:8:1058:U:O2	2.31	0.49
55:LI:271:SER:O	55:LI:281:PHE:N	2.44	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
7:L4:163:ASP:OD2	7:L4:166:SER:OG	2.31	0.49
25:LQ:836:ILE:HA	25:LQ:839:VAL:HG12	1.94	0.49
26:LS:576:LEU:HD13	26:LS:588:LEU:HD21	1.94	0.49
36:SG:443:LEU:HD12	36:SG:471:GLN:HB2	1.93	0.49
36:SG:491:SER:OG	36:SG:492:TRP:N	2.46	0.49
37:SH:29:LYS:NZ	37:SH:332:ILE:O	2.42	0.49
37:SH:312:ARG:NH2	37:SH:349:ASP:OD2	2.46	0.49
38:SI:45:ARG:NE	53:8:28:A:OP1	2.44	0.49
45:SR:89:ASN:HD22	48:SY:4:LEU:HB3	1.76	0.49
53:8:1506:G:H2'	53:8:1507:G:H8	1.78	0.49
7:L4:117:GLU:O	7:L4:120:SER:OG	2.31	0.49
13:LD:92:HIS:N	13:LD:101:GLU:O	2.43	0.49
17:LH:524:ASP:OD1	17:LH:524:ASP:N	2.42	0.49
21:LM:130:LYS:HA	21:LM:130:LYS:HD2	1.66	0.49
22:LN:490:SER:OG	22:LN:491:CYS:N	2.46	0.49
23:LO:258:ALA:HB1	23:LO:261:ALA:HB3	1.94	0.49
29:LV:3:LEU:HD22	29:LV:15:GLN:H	1.78	0.49
36:SG:285:SER:N	36:SG:298:SER:OG	2.44	0.49
41:SM:183:SER:HB3	41:SM:220:ARG:HD3	1.95	0.49
62:LX:827:ARG:HA	62:LX:830:LEU:HD12	1.94	0.49
3:NB:493:ASP:OD1	3:NB:496:GLN:NE2	2.45	0.49
14:LE:103:ILE:HB	14:LE:110:ILE:HD11	1.93	0.49
18:LJ:411:LYS:NZ	18:LJ:448:LYS:O	2.42	0.49
20:LL:78:LEU:HB2	20:LL:86:TRP:HB2	1.95	0.49
22:LN:574:HIS:HE2	22:LN:638:SER:HG	1.61	0.49
38:SI:1049:ASN:OD1	38:SI:1049:ASN:N	2.42	0.49
38:SI:1113:ILE:HG13	44:SQ:119:ARG:HD2	1.95	0.49
53:8:901:G:H3'	53:8:902:G:H8	1.77	0.49
54:SU:350:MET:HA	54:SU:355:ARG:HB3	1.95	0.49
1:NA:372:ARG:NH2	1:NA:377:ASN:O	2.41	0.49
1:NA:484:MET:HB3	23:LO:359:ARG:HH12	1.78	0.49
8:L5:97:LEU:HD23	8:L5:176:THR:HG23	1.95	0.49
27:LT:24:PHE:HB3	27:LT:654:TRP:HB3	1.94	0.49
27:LT:569:VAL:HB	27:LT:579:ARG:HB2	1.94	0.49
28:LU:140:SER:OG	28:LU:142:ASP:OD1	2.30	0.49
29:LV:287:ASN:HB3	29:LV:302:ARG:HG2	1.95	0.49
31:LZ:78:LEU:HD22	31:LZ:97:LEU:HD11	1.95	0.49
34:SC:155:ILE:HD11	34:SC:162:LEU:HD13	1.92	0.49
36:SG:256:ARG:NH2	36:SG:549:LEU:O	2.46	0.49
53:8:199:G:O2'	53:8:201:G:N2	2.45	0.49
53:8:1049:U:O4	53:8:1067:C:N4	2.46	0.49



A + 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
57:LR:515:CYS:HB2	57:LR:536:LEU:HD22	1.95	0.49
6:L3:6:GLN:OE1	6:L3:6:GLN:N	2.46	0.48
10:L8:5:ARG:NH2	10:L8:27:PHE:O	2.46	0.48
17:LH:101:GLN:OE1	17:LH:104:ALA:N	2.46	0.48
18:LJ:453:VAL:HG21	20:LL:532:ARG:HG2	1.95	0.48
27:LT:188:VAL:H	27:LT:202:SER:HB3	1.78	0.48
27:LT:476:PHE:HD1	27:LT:486:ILE:HG12	1.78	0.48
30:LW:201:TYR:HB3	30:LW:437:LEU:HD23	1.95	0.48
38:SI:255:PRO:HA	38:SI:258:ILE:HD12	1.95	0.48
41:SM:143:HIS:HB2	41:SM:151:SER:HB3	1.94	0.48
53:8:897:C:H2'	53:8:914:G:H22	1.76	0.48
53:8:1193:A:OP2	53:8:1195:C:N4	2.45	0.48
57:LR:686:MET:HG2	57:LR:735:GLN:HB3	1.94	0.48
62:LX:9:ARG:NH1	62:LX:214:LYS:O	2.46	0.48
3:NB:574:LYS:HZ3	53:8:502:U:H5"	1.78	0.48
27:LT:62:ASP:HB2	27:LT:69:LEU:HD21	1.95	0.48
28:LU:76:ASN:HA	28:LU:118:VAL:HG21	1.94	0.48
30:LW:160:LEU:HD22	30:LW:219:VAL:HG11	1.96	0.48
30:LW:358:MET:N	30:LW:358:MET:SD	2.86	0.48
34:SD:309:TYR:OH	48:SY:127:PHE:O	2.27	0.48
36:SG:467:LYS:HA	36:SG:470:LEU:HD12	1.95	0.48
37:SH:156:ARG:NH2	37:SH:228:ASP:OD2	2.44	0.48
37:SH:323:ILE:HG23	38:SI:553:ILE:HG23	1.95	0.48
3:NB:556:LYS:HD3	3:NB:559:ARG:HD3	1.94	0.48
5:L2:201:C:O2	5:L2:249:G:N1	2.43	0.48
22:LN:156:LEU:HG	22:LN:170:ILE:HD11	1.96	0.48
23:LO:367:GLY:HA2	23:LO:390:VAL:HG23	1.95	0.48
24:LP:187:LYS:NZ	44:SQ:66:GLU:OE2	2.46	0.48
25:LQ:476:ILE:HD12	25:LQ:479:LEU:HD21	1.94	0.48
35:SF:11:LEU:HA	35:SF:80:PHE:HB2	1.94	0.48
38:SI:87:ARG:NE	38:SI:98:LEU:O	2.42	0.48
38:SI:176:LEU:HD23	38:SI:177:PHE:HB3	1.94	0.48
38:SI:827:ALA:O	38:SI:883:ALA:N	2.38	0.48
39:SJ:31:LEU:HD12	39:SJ:109:LYS:HA	1.95	0.48
47:ST:508:PHE:HB3	47:ST:518:ILE:HD11	1.95	0.48
53:8:461:G:H2'	53:8:462:G:H8	1.78	0.48
62:LX:776:GLU:OE2	62:LX:820:HIS:NE2	2.46	0.48
65:5:417:LEU:O	65:5:421:LEU:N	2.45	0.48
1:NA:350:THR:HG21	38:SI:975:GLU:HG2	1.95	0.48
10:L8:58:LEU:O	10:L8:59:ARG:NH1	2.41	0.48
13:LD:123:VAL:HG12	13:LD:142:VAL:HA	1.95	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
23:LO:559:ILE:HG21	23:LO:578:LYS:HA	1.95	0.48
25:LQ:805:ILE:O	25:LQ:808:THR:OG1	2.31	0.48
25:LQ:836:ILE:HD12	25:LQ:857:LEU:HD13	1.95	0.48
27:LT:721:LEU:HD13	27:LT:922:LEU:HD23	1.95	0.48
29:LV:191:VAL:HG23	65:5:484:LYS:HE2	1.96	0.48
34:SC:207:LEU:HG	34:SC:219:PRO:HB3	1.94	0.48
34:SD:208:ILE:HD12	59:SB:152:LEU:HD22	1.96	0.48
46:SS:300:ASP:OD2	46:SS:300:ASP:N	2.45	0.48
47:ST:63:ALA:HB1	53:8:1463:C:H4'	1.95	0.48
47:ST:64:ARG:HA	47:ST:78:ARG:HG2	1.95	0.48
51:NH:257:SER:HA	51:NH:592:PHE:H	1.78	0.48
51:NH:976:ILE:HA	51:NH:1042:ALA:HB3	1.95	0.48
53:8:875:G:N2	53:8:953:G:N3	2.61	0.48
54:SU:104:ALA:HB1	54:SU:115:LEU:HD21	1.95	0.48
62:LX:789:LEU:HD23	62:LX:890:LEU:HD23	1.95	0.48
5:L2:47:G:O2'	30:LW:180:GLU:OE1	2.30	0.48
11:L9:58:ASP:N	11:L9:58:ASP:OD1	2.45	0.48
22:LN:282:ASP:OD1	22:LN:282:ASP:N	2.37	0.48
25:LQ:273:TYR:OH	25:LQ:341:ALA:O	2.32	0.48
25:LQ:549:SER:HB3	25:LQ:579:ILE:HD11	1.96	0.48
27:LT:176:TYR:HB3	27:LT:179:LYS:HB2	1.93	0.48
28:LU:89:ASP:HB2	28:LU:91:VAL:HG12	1.96	0.48
30:LW:388:ASP:OD1	30:LW:388:ASP:N	2.40	0.48
41:SM:42:LEU:HD23	41:SM:43:PRO:HD2	1.94	0.48
62:LX:487:ASN:HD21	62:LX:493:ASP:HB2	1.78	0.48
63:L6:39:GLU:HG3	63:L6:46:LYS:HG3	1.94	0.48
28:LU:138:SER:OG	28:LU:139:CYS:N	2.47	0.48
29:LV:118:GLN:OE1	29:LV:124:GLN:NE2	2.47	0.48
38:SI:126:ASN:N	38:SI:126:ASN:OD1	2.47	0.48
42:SN:87:LEU:O	42:SN:93:THR:OG1	2.31	0.48
52:NI:39:ALA:HA	52:NI:55:LEU:HA	1.95	0.48
57:LR:619:ARG:O	57:LR:637:ALA:N	2.42	0.48
62:LX:537:MET:O	62:LX:541:TYR:N	2.46	0.48
2:SA:306:LEU:HD13	2:SA:404:LEU:HB3	1.96	0.48
9:L7:174:ASN:N	9:L7:174:ASN:OD1	2.46	0.48
11:L9:38:ASN:N	11:L9:38:ASN:OD1	2.47	0.48
18:LJ:168:THR:OG1	18:LJ:194:ARG:NH2	2.47	0.48
23:LO:470:SER:OG	41:SM:134:SER:O	2.29	0.48
25:LQ:565:PHE:O	37:SH:207:ARG:NH2	2.46	0.48
25:LQ:597:ILE:HD13	25:LQ:630:PHE:HE2	1.79	0.48
38:SI:826:LYS:HE3	38:SI:926:ILE:HG22	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
48:SY:241:SER:OG	48:SY:242:PHE:N	2.46	0.48
53:8:1514:U:H2'	53:8:1515:A:H8	1.78	0.48
53:8:1541:G:H21	53:8:1569:A:H62	1.60	0.48
62:LX:34:ARG:NH1	62:LX:64:LEU:O	2.46	0.48
62:LX:769:ARG:NH1	62:LX:770:GLU:O	2.47	0.48
65:5:290:ARG:HH12	66:6:101:GLN:HE21	1.61	0.48
65:5:471:PRO:HD2	65:5:472:ILE:HD12	1.94	0.48
7:L4:191:ARG:HH22	7:L4:218:PHE:HB3	1.78	0.48
8:L5:124:LEU:HD11	18:LJ:117:LEU:HD21	1.96	0.48
15:LF:55:VAL:HG23	15:LF:75:VAL:HB	1.96	0.48
18:LJ:35:LEU:HD23	18:LJ:326:LEU:HD13	1.96	0.48
23:LO:23:SER:OG	23:LO:24:ASP:N	2.46	0.48
25:LQ:745:SER:OG	25:LQ:746:LEU:N	2.46	0.48
29:LV:338:MET:N	29:LV:338:MET:SD	2.86	0.48
36:SG:259:LYS:HB2	36:SG:259:LYS:HE3	1.71	0.48
56:ND:190:LEU:HD12	56:ND:191:PRO:HD2	1.95	0.48
59:SB:227:LEU:HD23	59:SB:231:ILE:HG22	1.95	0.48
65:5:480:THR:OG1	65:5:481:SER:N	2.44	0.48
2:SA:25:ASP:OD1	2:SA:25:ASP:N	2.47	0.48
8:L5:72:HIS:O	12:LC:79:TYR:OH	2.32	0.48
17:LH:656:ASP:OD1	17:LH:656:ASP:N	2.43	0.48
18:LJ:220:ALA:HA	18:LJ:226:ILE:HG22	1.94	0.48
22:LN:106:ASN:H	22:LN:153:GLN:HG2	1.79	0.48
23:LO:130:ASP:N	23:LO:130:ASP:OD1	2.42	0.48
23:LO:296:GLN:NE2	23:LO:332:TRP:O	2.47	0.48
28:LU:329:ILE:HD11	28:LU:351:VAL:HG21	1.95	0.48
37:SH:228:ASP:OD2	37:SH:230:TRP:NE1	2.47	0.48
40:SL:130:CYS:HB2	40:SL:132:HIS:CE1	2.49	0.48
48:SY:168:LYS:HA	48:SY:171:LEU:HG	1.96	0.48
53:8:1003:A:H1'	53:8:1005:A:H62	1.79	0.48
53:8:1512:G:H2'	53:8:1513:G:H8	1.79	0.48
59:SB:162:MET:SD	59:SB:275:TYR:OH	2.66	0.48
59:SB:217:LYS:O	59:SB:221:THR:OG1	2.31	0.48
62:LX:723:LEU:O	62:LX:764:ASN:N	2.47	0.48
1:NA:322:LYS:HE3	1:NA:327:LYS:HG2	1.96	0.48
2:SA:306:LEU:HD21	2:SA:382:LYS:HB3	1.96	0.48
8:L5:16:VAL:HG21	27:LT:534:SER:HB3	1.95	0.48
17:LH:849:ASP:H	17:LH:852:ASP:HB2	1.78	0.48
17:LH:864:ASP:OD1	17:LH:864:ASP:N	2.47	0.48
18:LJ:125:HIS:NE2	39:SK:19:LEU:O	2.45	0.48
20:LL:66:VAL:HG22	20:LL:112:LEU:HD22	1.96	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
21:LM:275:ILE:HG22	21:LM:279:MET:HE1	1.96	0.48
23:LO:252:LYS:NZ	23:LO:253:LYS:O	2.44	0.48
31:LZ:138:VAL:HG22	31:LZ:158:VAL:HG12	1.96	0.48
36:SG:417:SER:HB3	36:SG:421:ASN:HB2	1.95	0.48
40:SL:22:ASP:OD1	40:SL:22:ASP:N	2.40	0.48
41:SM:268:ASN:OD1	48:SY:56:LYS:NZ	2.44	0.48
53:8:261:U:O2'	53:8:262:U:O4'	2.31	0.48
53:8:375:U:H5"	53:8:376:C:H5'	1.95	0.48
57:LR:279:LYS:NZ	57:LR:317:GLU:O	2.47	0.48
57:LR:619:ARG:NH1	57:LR:620:LEU:O	2.47	0.48
57:LR:630:ASP:HB3	57:LR:646:ASP:HB2	1.96	0.48
62:LX:771:SER:HB2	62:LX:773:TRP:CE2	2.49	0.48
7:L4:110:ALA:HB1	36:SG:112:LEU:HD23	1.96	0.47
17:LH:479:ASN:HD22	18:LJ:3:THR:HG21	1.79	0.47
25:LQ:72:SER:HA	25:LQ:75:ARG:HH22	1.79	0.47
26:LS:334:SER:OG	26:LS:335:GLN:N	2.47	0.47
29:LV:95:ARG:NH2	29:LV:129:GLY:O	2.47	0.47
33:NK:70:ALA:HB3	33:NK:83:LYS:H	1.78	0.47
34:SC:110:ASN:ND2	34:SC:112:ALA:O	2.47	0.47
35:SE:102:ILE:HG21	35:SE:114:ILE:HD11	1.96	0.47
39:SK:119:GLY:O	39:SK:165:ASN:ND2	2.44	0.47
53:8:513:U:H2'	53:8:514:G:C8	2.49	0.47
62:LX:29:VAL:HA	62:LX:152:LEU:HB3	1.96	0.47
62:LX:157:SER:HA	62:LX:160:GLN:HB2	1.96	0.47
1:NA:301:GLU:OE2	1:NA:304:GLN:NE2	2.47	0.47
8:L5:26:ALA:N	12:LC:27:GLY:O	2.44	0.47
17:LH:435:ASP:OD1	17:LH:435:ASP:N	2.41	0.47
21:LM:81:LEU:O	21:LM:124:ARG:NH2	2.47	0.47
26:LS:272:LEU:HD11	26:LS:314:THR:HG21	1.96	0.47
27:LT:128:LEU:HB2	27:LT:150:PRO:HG2	1.96	0.47
29:LV:154:TYR:HB3	29:LV:164:ARG:HA	1.94	0.47
36:SG:346:ALA:HB3	36:SG:359:PHE:HB2	1.95	0.47
37:SH:208:MET:HB3	37:SH:243:ILE:HD12	1.96	0.47
47:ST:726:LYS:NZ	53:8:1461:C:OP2	2.44	0.47
57:LR:21:ALA:HB3	57:LR:35:PRO:HG3	1.96	0.47
2:SA:26:ASP:OD2	28:LU:81:ASN:ND2	2.43	0.47
2:SA:126:ASP:OD1	34:SC:322:ARG:NH2	2.47	0.47
2:SA:142:LEU:HA	24:LP:105:GLN:HE21	1.79	0.47
2:SA:169:LYS:HA	2:SA:299:VAL:HG22	1.96	0.47
4:L0:490:G:H21	4:L0:495:G:H1'	1.78	0.47
18:LJ:191:GLY:H	18:LJ:214:PRO:HA	1.78	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
18:LJ:227:VAL:HG23	18:LJ:236:VAL:HG12	1.95	0.47
20:LL:488:ILE:HG13	20:LL:529:THR:HG21	1.96	0.47
22:LN:66:ARG:HH21	22:LN:528:ILE:HD11	1.79	0.47
22:LN:468:ASP:OD1	22:LN:468:ASP:N	2.45	0.47
22:LN:510:GLU:O	22:LN:558:ARG:NH1	2.42	0.47
27:LT:21:SER:HB2	27:LT:623:ILE:HG12	1.97	0.47
28:LU:125:ASP:OD1	28:LU:125:ASP:N	2.46	0.47
28:LU:380:TRP:NE1	28:LU:398:GLU:OE2	2.46	0.47
38:SI:125:LEU:HD22	38:SI:912:ARG:HD2	1.96	0.47
42:SN:41:ASN:ND2	53:8:1499:G:O2'	2.47	0.47
45:SR:126:LYS:HG2	45:SR:131:SER:HA	1.96	0.47
65:5:488:ASP:OD1	65:5:488:ASP:N	2.42	0.47
3:NB:531:ASN:O	38:SI:909:ASN:ND2	2.47	0.47
3:NB:555:ASN:OD1	3:NB:555:ASN:N	2.48	0.47
7:L4:138:TYR:HA	7:L4:148:ARG:HA	1.96	0.47
9:L7:144:VAL:HG23	28:LU:181:ALA:HB3	1.95	0.47
13:LD:68:GLY:HA3	13:LD:127:GLN:HE21	1.79	0.47
13:LD:134:THR:OG1	53:8:325:G:OP1	2.32	0.47
23:LO:496:THR:HA	23:LO:513:GLU:HA	1.96	0.47
23:LO:713:ASP:OD1	23:LO:713:ASP:N	2.40	0.47
27:LT:51:VAL:HG21	27:LT:90:VAL:HG21	1.97	0.47
51:NH:755:PRO:HA	51:NH:782:VAL:HA	1.95	0.47
57:LR:190:THR:OG1	57:LR:217:ASP:OD2	2.32	0.47
64:NF:114:ARG:O	64:NF:118:ILE:N	2.48	0.47
5:L2:115:G:O2'	5:L2:257:A:N3	2.44	0.47
12:LC:42:GLU:HA	12:LC:45:ARG:HH12	1.79	0.47
13:LD:65:SER:OG	53:8:115:G:OP2	2.33	0.47
14:LE:41:MET:HB2	14:LE:46:TYR:HB2	1.96	0.47
17:LH:195:ASN:N	17:LH:195:ASN:OD1	2.47	0.47
18:LJ:32:SER:O	18:LJ:71:ARG:NH2	2.39	0.47
22:LN:149:ILE:HD12	22:LN:153:GLN:HG3	1.95	0.47
28:LU:308:VAL:HA	28:LU:324:SER:HA	1.94	0.47
36:SG:348:LEU:HD22	36:SG:357:LEU:HD12	1.95	0.47
38:SI:56:VAL:HG23	45:SR:52:ILE:HD11	1.97	0.47
42:SN:190:ILE:HD12	42:SN:191:PRO:HD2	1.96	0.47
51:NH:631:GLY:N	51:NH:665:HIS:O	2.46	0.47
53:8:1203:A:O2'	53:8:1209:C:O2'	2.27	0.47
55:LI:594:SER:HA	55:LI:597:GLN:HE22	1.79	0.47
57:LR:344:ARG:HE	57:LR:395:ASP:HA	1.78	0.47
57:LR:746:TRP:O	57:LR:752:THR:OG1	2.32	0.47
58:NE:323:LYS:HA	58:NE:326:ILE:HD12	1.96	0.47



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
59:SB:160:ASP:N	59:SB:160:ASP:OD1	2.43	0.47
3:NB:602:LEU:HG	3:NB:604:ARG:HG2	1.96	0.47
7:L4:71:LYS:HB2	7:L4:76:VAL:HA	1.97	0.47
18:LJ:398:SER:O	18:LJ:434:ARG:NH2	2.39	0.47
20:LL:338:ASN:OD1	26:LS:337:ALA:N	2.48	0.47
20:LL:513:LEU:HD21	20:LL:523:LEU:HD11	1.97	0.47
25:LQ:41:LEU:HD23	25:LQ:52:TRP:HE1	1.80	0.47
27:LT:458:THR:OG1	27:LT:497:LYS:NZ	2.41	0.47
27:LT:849:ILE:HD12	27:LT:887:LEU:HD23	1.97	0.47
34:SD:145:ASN:OD1	34:SD:148:ARG:NH1	2.47	0.47
34:SD:308:PRO:HG3	48:SY:129:SER:HA	1.96	0.47
38:SI:54:LEU:HD21	45:SR:77:ILE:HB	1.95	0.47
38:SI:1024:LYS:O	38:SI:1026:LYS:NZ	2.45	0.47
53:8:9:U:O2'	58:NE:239:ARG:NH1	2.47	0.47
53:8:300:A:H2'	53:8:301:A:C8	2.49	0.47
53:8:897:C:OP2	53:8:914:G:N2	2.47	0.47
57:LR:290:ILE:HG22	57:LR:306:LEU:HG	1.97	0.47
1:NA:464:SER:OG	1:NA:465:LEU:N	2.48	0.47
3:NB:540:ILE:HD13	38:SI:150:MET:HG3	1.97	0.47
4:L0:503:C:H2'	4:L0:504:U:H6	1.79	0.47
7:L4:42:LEU:HD21	7:L4:47:PHE:HB2	1.96	0.47
8:L5:26:ALA:HB3	12:LC:28:LEU:HB3	1.97	0.47
10:L8:67:TRP:HE1	10:L8:69:SER:HG	1.63	0.47
12:LC:55:VAL:HG21	12:LC:89:LEU:HD21	1.97	0.47
16:LG:62:GLU:HB3	16:LG:64:ARG:HH21	1.80	0.47
19:LK:475:THR:HA	19:LK:478:ASN:HB2	1.97	0.47
22:LN:566:LEU:HD23	22:LN:570:ILE:HG12	1.96	0.47
22:LN:594:PHE:HA	22:LN:611:LEU:HA	1.95	0.47
23:LO:296:GLN:OE1	23:LO:330:TYR:OH	2.32	0.47
23:LO:412:ARG:NH2	25:LQ:942:VAL:O	2.48	0.47
23:LO:541:ILE:HD13	23:LO:606:VAL:HG13	1.97	0.47
25:LQ:476:ILE:HA	25:LQ:492:SER:HA	1.96	0.47
25:LQ:603:ASP:N	25:LQ:603:ASP:OD1	2.44	0.47
27:LT:194:ARG:HD3	59:SB:436:ALA:HB2	1.96	0.47
28:LU:185:ILE:HD11	28:LU:194:PHE:HD2	1.79	0.47
29:LV:277:ILE:HG12	29:LV:291:THR:HG22	1.97	0.47
30:LW:329:LEU:HD11	30:LW:340:LEU:HB3	1.96	0.47
38:SI:978:ARG:NH1	53:8:1600:A:OP1	2.48	0.47
38:SI:1034:LEU:HB2	38:SI:1037:GLN:HG3	1.97	0.47
39:SJ:90:ASP:N	39:SJ:90:ASP:OD1	2.47	0.47
41:SM:149:PRO:HG2	41:SM:170:VAL:HG21	1.95	0.47



	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
42:SN:128:ASP:OD1	42:SN:128:ASP:N	2.47	0.47
48:SY:135:ILE:HG23	56:ND:178:VAL:HG22	1.97	0.47
53:8:239:C:O2'	53:8:241:U:OP1	2.32	0.47
57:LR:337:HIS:HB3	57:LR:340:ILE:HD11	1.96	0.47
59:SB:351:ALA:HB1	59:SB:355:ASN:HB3	1.97	0.47
4:L0:293:U:H2'	23:LO:631:ASN:HA	1.97	0.47
18:LJ:222:SER:HB3	18:LJ:225:GLN:HB2	1.96	0.47
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	1.97	0.47
20:LL:58:LEU:HB2	20:LL:80:MET:HE1	1.96	0.47
25:LQ:24:VAL:HG12	25:LQ:42:ILE:HB	1.95	0.47
25:LQ:629:ASN:HD22	25:LQ:643:ASP:HA	1.80	0.47
27:LT:510:LEU:HD21	27:LT:514:ASN:HA	1.95	0.47
27:LT:601:VAL:HG12	27:LT:611:THR:HG22	1.96	0.47
29:LV:191:VAL:HG23	65:5:484:LYS:HB2	1.97	0.47
36:SG:333:MET:SD	36:SG:334:GLU:N	2.88	0.47
37:SH:327:ARG:NH2	38:SI:558:ILE:O	2.36	0.47
38:SI:300:GLN:HG3	38:SI:792:VAL:HG22	1.96	0.47
38:SI:1042:MET:HG3	38:SI:1044:LEU:HD13	1.95	0.47
42:SN:153:MET:HG3	60:SV:191:LEU:HD22	1.96	0.47
54:SU:317:ILE:HG23	54:SU:358:PHE:HB2	1.97	0.47
62:LX:569:PRO:HD3	62:LX:583:LEU:HG	1.97	0.47
1:NA:295:LYS:HB3	1:NA:296:ASN:H	1.52	0.47
4:L0:267:U:H3	12:LC:21:HIS:CG	2.32	0.47
7:L4:151:ASP:OD1	63:L6:215:ARG:NH2	2.48	0.47
14:LE:106:THR:HG23	14:LE:108:ALA:H	1.79	0.47
20:LL:151:LEU:HD11	20:LL:163:LEU:HD22	1.97	0.47
22:LN:288:THR:HG22	22:LN:295:VAL:HG23	1.96	0.47
22:LN:620:ASP:OD1	22:LN:620:ASP:N	2.48	0.47
23:LO:273:ARG:NH1	27:LT:763:SER:O	2.45	0.47
27:LT:414:ILE:HA	27:LT:434:HIS:HA	1.97	0.47
29:LV:85:ASP:O	29:LV:89:LEU:N	2.42	0.47
36:SG:186:PHE:HE1	36:SG:211:LEU:HD13	1.79	0.47
38:SI:1135:ARG:NH1	53:8:495:C:OP2	2.48	0.47
51:NH:186:ILE:HA	51:NH:190:ALA:HB2	1.96	0.47
54:SU:279:LEU:HA	54:SU:357:ARG:HH12	1.79	0.47
59:SB:379:ASP:OD1	59:SB:379:ASP:N	2.40	0.47
62:LX:45:MET:SD	62:LX:45:MET:N	2.88	0.47
62:LX:87:GLU:HB3	62:LX:90:GLU:HB2	1.96	0.47
1:NA:526:ASN:OD1	1:NA:529:ARG:NH2	2.47	0.47
8:L5:157:ARG:HB2	8:L5:224:ASN:HD21	1.80	0.47
9:L7:27:LEU:HG	9:L7:38:LEU:HD11	1.97	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
17:LH:233:ASP:OD1	17:LH:236:ASN:ND2	2.47	0.47
17:LH:510:TYR:HE1	17:LH:527:HIS:HB3	1.80	0.47
20:LL:281:ILE:HB	20:LL:291:ILE:HD11	1.97	0.47
22:LN:429:SER:OG	22:LN:430:THR:N	2.46	0.47
23:LO:159:ARG:NH1	23:LO:179:GLU:OE2	2.48	0.47
24:LP:278:MET:HB2	24:LP:312:LEU:HD13	1.96	0.47
30:LW:327:THR:OG1	30:LW:405:GLY:O	2.32	0.47
53:8:894:U:O2'	53:8:919:A:N6	2.48	0.47
53:8:1743:U:H2'	53:8:1744:A:H8	1.79	0.47
54:SU:399:ILE:HG21	54:SU:480:LEU:HB3	1.96	0.47
62:LX:817:ASP:OD1	62:LX:817:ASP:N	2.48	0.47
62:LX:894:ASN:O	62:LX:897:THR:OG1	2.30	0.47
4:L0:145:A:H2'	4:L0:146:G:H8	1.80	0.46
4:L0:413:C:H2'	4:L0:414:G:H8	1.79	0.46
16:LG:10:ALA:HB1	16:LG:30:VAL:HB	1.97	0.46
17:LH:408:THR:HG21	17:LH:488:LEU:HB2	1.97	0.46
18:LJ:376:ASN:OD1	18:LJ:376:ASN:N	2.47	0.46
19:LK:462:LEU:HD11	20:LL:556:THR:HG21	1.96	0.46
22:LN:624:LYS:HD3	22:LN:624:LYS:HA	1.72	0.46
24:LP:268:ASP:N	24:LP:268:ASP:OD1	2.48	0.46
30:LW:178:ASP:OD2	40:SL:24:ARG:NH1	2.48	0.46
36:SG:488:ILE:HG12	36:SG:498:VAL:HG12	1.96	0.46
37:SH:105:TYR:HE2	37:SH:296:LEU:HA	1.80	0.46
37:SH:298:ILE:HG13	37:SH:322:PHE:HE1	1.79	0.46
37:SH:366:ILE:HD11	38:SI:920:GLU:HA	1.96	0.46
38:SI:248:ARG:HB3	38:SI:357:PRO:HG2	1.98	0.46
39:SJ:113:TYR:HB3	39:SJ:121:LEU:HD11	1.96	0.46
40:SL:101:CYS:SG	40:SL:102:VAL:N	2.89	0.46
53:8:239:C:O2	53:8:244:A:N6	2.49	0.46
57:LR:332:SER:OG	57:LR:381:VAL:O	2.32	0.46
57:LR:464:LYS:HA	57:LR:487:ARG:H	1.80	0.46
2:SA:203:PHE:HB3	2:SA:206:LEU:HD13	1.97	0.46
4:L0:125:G:H2'	4:L0:126:A:H8	1.80	0.46
10:L8:6:ASP:HB2	10:L8:28:GLU:HG3	1.97	0.46
11:L9:34:PHE:HD2	11:L9:111:THR:HG21	1.80	0.46
11:L9:58:ASP:HA	11:L9:61:THR:HG22	1.97	0.46
13:LD:130:PRO:HB3	13:LD:136:ARG:HA	1.97	0.46
17:LH:215:VAL:HA	17:LH:218:LYS:HB2	1.96	0.46
17:LH:367:SER:O	17:LH:367:SER:OG	2.34	0.46
18:LJ:172:ARG:HH12	54:SU:370:HIS:HA	1.79	0.46
20:LL:191:VAL:HA	20:LL:206:ALA:HA	1.97	0.46



A + 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
22:LN:82:ARG:NH1	22:LN:726:UNK:O	2.48	0.46
22:LN:550:VAL:HG23	22:LN:563:LEU:HB2	1.98	0.46
23:LO:805:ALA:HA	57:LR:815:LYS:HE2	1.97	0.46
26:LS:534:SER:HB3	26:LS:540:ALA:HB1	1.96	0.46
27:LT:416:ALA:HB3	27:LT:433:ALA:HB3	1.96	0.46
28:LU:439:ARG:O	28:LU:443:ASN:ND2	2.48	0.46
32:NG:45:GLY:N	53:8:900:A:OP1	2.47	0.46
37:SH:59:VAL:HG23	37:SH:60:THR:HG23	1.95	0.46
39:SK:100:LEU:HD11	39:SK:112:VAL:HG11	1.96	0.46
48:SY:5:VAL:HG21	48:SY:10:LYS:HE3	1.96	0.46
57:LR:97:ARG:HH22	57:LR:133:ASN:HA	1.80	0.46
62:LX:725:VAL:HG22	62:LX:762:MET:HB2	1.97	0.46
62:LX:807:SER:HA	62:LX:810:LYS:HE2	1.96	0.46
63:L6:48:TYR:OH	63:L6:119:GLN:O	2.33	0.46
3:NB:608:PHE:HE2	34:SC:303:GLN:HB3	1.79	0.46
4:L0:90:G:OP1	18:LJ:378:LYS:NZ	2.42	0.46
4:L0:220:U:H5"	56:ND:200:ARG:HH21	1.80	0.46
22:LN:476:LYS:HG3	22:LN:491:CYS:HA	1.96	0.46
24:LP:278:MET:SD	24:LP:278:MET:N	2.81	0.46
25:LQ:259:ILE:HG12	25:LQ:274:ILE:HG23	1.97	0.46
26:LS:454:GLY:O	26:LS:487:GLU:N	2.48	0.46
28:LU:2:LYS:HB2	30:LW:75:GLU:HB2	1.98	0.46
29:LV:333:ASN:OD1	29:LV:333:ASN:N	2.43	0.46
38:SI:355:TYR:OH	38:SI:788:TYR:OH	2.29	0.46
38:SI:1148:GLU:HB3	38:SI:1152:ARG:HH12	1.80	0.46
39:SJ:228:SER:HB3	39:SJ:232:LEU:HD21	1.96	0.46
39:SK:100:LEU:HD13	39:SK:130:ILE:HD11	1.97	0.46
39:SK:178:VAL:HG23	39:SK:204:VAL:HG22	1.97	0.46
53:8:35:U:H1'	53:8:474:A:H61	1.80	0.46
53:8:1695:G:H2'	53:8:1696:G:C8	2.50	0.46
54:SU:196:GLN:OE1	54:SU:260:ASN:ND2	2.47	0.46
57:LR:510:SER:OG	57:LR:514:THR:OG1	2.31	0.46
58:NE:268:LYS:HD2	58:NE:298:LYS:HZ1	1.79	0.46
4:L0:93:A:OP2	18:LJ:384:ARG:NH2	2.42	0.46
5:L2:254:A:C8	35:SF:35:LYS:HE2	2.50	0.46
12:LC:103:ASN:HD21	23:LO:554:ASP:HB2	1.80	0.46
25:LQ:489:VAL:HG21	25:LQ:546:LEU:HD11	1.96	0.46
32:NG:15:GLY:N	32:NG:78:ALA:O	2.48	0.46
34:SC:293:LEU:HD22	34:SC:298:ILE:HD12	1.98	0.46
39:SK:155:SER:O	39:SK:155:SER:OG	2.32	0.46
57:LR:738:LEU:HA	57:LR:741:LYS:HE2	1.97	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
61:SP:248:HIS:H	61:SP:251:ALA:HB3	1.80	0.46
65:5:446:SER:HA	65:5:449:LYS:HZ1	1.81	0.46
2:SA:6:TYR:HD2	2:SA:86:LEU:HD23	1.80	0.46
2:SA:283:ASP:OD1	2:SA:286:ARG:NH2	2.47	0.46
4:L0:348:U:N3	4:L0:376:U:O2	2.49	0.46
6:L3:82:PRO:HB3	42:SN:68:ARG:HB2	1.97	0.46
19:LK:505:MET:O	19:LK:509:GLN:N	2.34	0.46
22:LN:649:TRP:NE1	22:LN:744:VAL:O	2.49	0.46
24:LP:67:ARG:NH2	24:LP:84:SER:OG	2.49	0.46
26:LS:519:SER:HB3	26:LS:535:ARG:HG2	1.98	0.46
27:LT:918:LYS:O	27:LT:921:ARG:NE	2.45	0.46
29:LV:282:ASN:OD1	29:LV:325:GLY:N	2.36	0.46
35:SE:32:GLN:NE2	35:SE:103:THR:O	2.41	0.46
35:SF:35:LYS:HD2	35:SF:91:CYS:SG	2.55	0.46
53:8:1684:U:H2'	53:8:1685:G:H8	1.79	0.46
62:LX:871:MET:N	62:LX:871:MET:SD	2.89	0.46
63:L6:98:ARG:NH1	63:L6:101:ILE:O	2.49	0.46
17:LH:508:ILE:HD11	17:LH:560:ILE:HG21	1.97	0.46
22:LN:251:ASP:OD1	22:LN:251:ASP:N	2.48	0.46
22:LN:330:GLY:HA3	22:LN:353:GLU:HG3	1.98	0.46
25:LQ:392:THR:OG1	25:LQ:393:ASP:N	2.48	0.46
34:SD:271:ILE:HG12	34:SD:289:GLU:HG3	1.97	0.46
36:SG:198:LYS:HD3	36:SG:268:LEU:HD13	1.97	0.46
39:SK:180:LEU:HD23	39:SK:237:ALA:HB1	1.97	0.46
53:8:329:G:H2'	53:8:330:G:H8	1.80	0.46
56:ND:160:ARG:HA	56:ND:163:LEU:HB3	1.97	0.46
57:LR:72:ASP:OD1	57:LR:72:ASP:N	2.46	0.46
57:LR:299:ASN:HB2	57:LR:301:GLN:HG2	1.98	0.46
65:5:241:ARG:NH2	66:6:19:SER:O	2.49	0.46
3:NB:559:ARG:HA	53:8:545:A:H62	1.79	0.46
17:LH:334:LEU:HD22	18:LJ:2:SER:HB2	1.97	0.46
23:LO:530:VAL:HG23	23:LO:544:ILE:HG12	1.97	0.46
25:LQ:165:SER:HB3	25:LQ:182:LYS:HB2	1.98	0.46
25:LQ:198:GLU:OE1	25:LQ:200:HIS:ND1	2.42	0.46
25:LQ:592:SER:OG	25:LQ:593:ALA:N	2.47	0.46
26:LS:233:LEU:O	26:LS:554:ASN:ND2	2.41	0.46
28:LU:387:THR:HG23	28:LU:390:GLU:H	1.81	0.46
34:SD:228:GLN:HA	34:SD:231:ARG:HB2	1.98	0.46
36:SG:131:ARG:HE	36:SG:411:PHE:HE2	1.62	0.46
36:SG:447:SER:OG	36:SG:449:ASN:OD1	2.34	0.46
37:SH:65:ILE:HG12	37:SH:76:TYR:HD1	1.80	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
37:SH:221:CYS:SG	37:SH:222:GLU:N	2.88	0.46
38:SI:861:THR:N	38:SI:882:ASN:O	2.44	0.46
38:SI:1051:ASP:OD1	38:SI:1051:ASP:N	2.48	0.46
48:SY:207:ARG:NH1	48:SY:210:GLN:OE1	2.49	0.46
66:6:306:ARG:O	66:6:310:GLN:NE2	2.49	0.46
4:L0:226:U:C2	22:LN:236:LYS:HE3	2.51	0.46
7:L4:233:LYS:HB3	7:L4:233:LYS:HE2	1.80	0.46
13:LD:125:VAL:HB	13:LD:137:PHE:HB3	1.97	0.46
18:LJ:104:LEU:HB2	18:LJ:121:ASN:HA	1.98	0.46
21:LM:387:LEU:HD12	21:LM:407:PHE:HE2	1.79	0.46
25:LQ:118:ASN:N	25:LQ:118:ASN:OD1	2.48	0.46
27:LT:76:THR:OG1	27:LT:78:SER:O	2.34	0.46
31:LZ:29:ASP:OD1	31:LZ:29:ASP:N	2.45	0.46
34:SD:224:ALA:O	34:SD:256:ASN:ND2	2.39	0.46
36:SG:263:TRP:HA	36:SG:270:PRO:HA	1.98	0.46
36:SG:417:SER:OG	36:SG:418:ASP:N	2.48	0.46
37:SH:183:ILE:HD13	37:SH:310:ARG:HH12	1.81	0.46
53:8:362:G:H2'	53:8:363:G:H8	1.80	0.46
54:SU:366:LEU:HB3	54:SU:405:LEU:HD21	1.97	0.46
57:LR:216:ARG:NE	57:LR:243:VAL:O	2.43	0.46
65:5:205:LYS:HA	65:5:349:PRO:HA	1.98	0.46
4:L0:411:A:H2'	4:L0:412:A:H8	1.81	0.46
10:L8:7:SER:OG	53:8:336:G:N2	2.49	0.46
10:L8:36:THR:OG1	10:L8:37:LYS:N	2.49	0.46
12:LC:36:ILE:HG23	12:LC:49:TYR:HE1	1.80	0.46
13:LD:35:TYR:OH	53:8:247:A:O3'	2.33	0.46
17:LH:200:ASN:HD22	17:LH:263:ALA:HA	1.80	0.46
17:LH:720:ILE:HD11	17:LH:766:ILE:HG21	1.98	0.46
17:LH:868:ASN:O	17:LH:871:SER:OG	2.33	0.46
18:LJ:52:PRO:HB3	18:LJ:309:PRO:HD2	1.97	0.46
20:LL:333:ASN:OD1	20:LL:333:ASN:N	2.49	0.46
20:LL:441:LEU:HB2	20:LL:456:VAL:HG11	1.98	0.46
25:LQ:331:THR:OG1	25:LQ:333:ARG:NH1	2.48	0.46
27:LT:163:GLN:O	27:LT:187:ASN:ND2	2.44	0.46
27:LT:359:ALA:HA	27:LT:419:ILE:HD13	1.98	0.46
35:SE:70:LEU:HD13	59:SB:311:LYS:HD2	1.98	0.46
36:SG:137:GLY:H	36:SG:485:ASN:HD21	1.63	0.46
51:NH:268:LEU:H	51:NH:294:LEU:H	1.64	0.46
53:8:1576:A:H3'	53:8:1577:A:H8	1.81	0.46
55:LI:537:THR:HB	55:LI:560:ASN:HB2	1.97	0.46
56:ND:183:THR:OG1	56:ND:186:ASP:OD2	2.33	0.46



Atom-1	Atom-2	Interatomic	Clash
	1100111 =	distance (Å)	overlap (Å)
8:L5:218:GLU:O	8:L5:222:LYS:N	2.46	0.46
12:LC:58:ASP:O	12:LC:61:SER:OG	2.31	0.46
14:LE:106:THR:OG1	14:LE:107:SER:N	2.49	0.46
17:LH:762:TYR:HB3	17:LH:779:ILE:HG12	1.98	0.46
18:LJ:273:ILE:HG22	18:LJ:283:VAL:HG23	1.98	0.46
20:LL:166:ALA:HB2	20:LL:170:ILE:HG23	1.98	0.46
25:LQ:145:ILE:HB	25:LQ:159:LEU:HB2	1.98	0.46
27:LT:546:ILE:HG23	27:LT:560:LEU:HB3	1.98	0.46
31:LZ:173:TYR:OH	38:SI:1082:GLN:OE1	2.33	0.46
34:SC:306:LEU:HD23	34:SC:315:ILE:HG12	1.96	0.46
35:SE:62:GLU:HG2	59:SB:373:TYR:HA	1.97	0.46
37:SH:347:ASN:ND2	37:SH:349:ASP:OD2	2.49	0.46
38:SI:295:ASP:OD2	38:SI:852:ARG:NH2	2.49	0.46
42:SN:181:ARG:NH1	60:SV:201:ASP:O	2.48	0.46
55:LI:55:TYR:HA	55:LI:72:THR:HA	1.98	0.46
55:LI:185:SER:HA	55:LI:201:PHE:HA	1.97	0.46
57:LR:302:MET:N	57:LR:302:MET:SD	2.89	0.46
62:LX:660:TYR:HB2	62:LX:712:LEU:HD21	1.97	0.46
66:6:235:ASP:OD1	66:6:235:ASP:N	2.48	0.46
16:LG:10:ALA:N	16:LG:54:LEU:O	2.49	0.45
18:LJ:440:GLU:O	18:LJ:444:ASN:ND2	2.45	0.45
25:LQ:124:ILE:HA	25:LQ:140:SER:HA	1.98	0.45
28:LU:58:PHE:HA	28:LU:375:TRP:CD1	2.51	0.45
28:LU:359:ASP:OD1	28:LU:359:ASP:N	2.49	0.45
34:SC:273:ALA:HA	34:SC:285:VAL:HG11	1.97	0.45
40:SL:149:LYS:HG2	40:SL:170:ILE:HD11	1.97	0.45
41:SM:7:ARG:NH1	41:SM:11:GLU:OE2	2.49	0.45
41:SM:72:GLN:NE2	41:SM:73:VAL:O	2.48	0.45
55:LI:257:SER:O	55:LI:259:ILE:N	2.49	0.45
9:L7:137:GLY:HA3	9:L7:153:LEU:HD23	1.97	0.45
17:LH:875:MET:N	17:LH:875:MET:SD	2.89	0.45
20:LL:252:SER:OG	20:LL:253:LEU:N	2.50	0.45
24:LP:44:ASN:OD1	24:LP:98:ARG:NH1	2.50	0.45
25:LQ:400:SER:OG	25:LQ:401:ASP:N	2.47	0.45
29:LV:207:TRP:CE2	29:LV:214:ARG:HB3	2.51	0.45
30:LW:340:LEU:O	30:LW:368:TYR:N	2.45	0.45
31:LZ:30:THR:HG23	31:LZ:34:ARG:HH21	1.82	0.45
36:SG:261:ILE:HG23	36:SG:273:VAL:HG12	1.99	0.45
38:SI:372:TYR:HD1	62:LX:5:ALA:HA	1.80	0.45
39:SK:112:VAL:HG13	39:SK:124:VAL:HB	1.98	0.45
53:8:1486:G:O6	53:8:1487:A:N6	2.49	0.45



	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:8:1662:G:H2'	53:8:1663:G:H8	1.81	0.45
57:LR:340:ILE:HD12	57:LR:355:LEU:HD22	1.98	0.45
57:LR:786:ILE:O	57:LR:789:THR:OG1	2.30	0.45
65:5:413:PHE:O	65:5:417:LEU:N	2.43	0.45
17:LH:96:ILE:H	17:LH:108:THR:HG21	1.81	0.45
22:LN:55:SER:HB2	22:LN:290:THR:HB	1.98	0.45
26:LS:426:VAL:HG23	26:LS:432:VAL:HG22	1.98	0.45
27:LT:49:TYR:OH	27:LT:86:HIS:O	2.30	0.45
27:LT:192:ASN:O	27:LT:196:GLY:N	2.49	0.45
27:LT:639:ASP:OD1	27:LT:639:ASP:N	2.47	0.45
28:LU:321:VAL:HG23	28:LU:331:ILE:HG12	1.98	0.45
29:LV:63:LYS:HD2	29:LV:63:LYS:HA	1.80	0.45
34:SC:268:VAL:HG22	34:SC:317:VAL:HG13	1.98	0.45
44:SQ:54:GLU:O	44:SQ:58:ASN:ND2	2.49	0.45
45:SR:89:ASN:O	45:SR:91:GLY:N	2.49	0.45
54:SU:430:ASP:OD1	54:SU:430:ASP:N	2.49	0.45
57:LR:191:SER:HB3	57:LR:216:ARG:H	1.82	0.45
57:LR:281:THR:HG22	57:LR:327:ILE:HB	1.97	0.45
58:NE:274:LYS:HA	58:NE:274:LYS:HD3	1.79	0.45
4:L0:253:U:H3	42:SN:78:ASP:HB2	1.81	0.45
10:L8:57:ALA:HB2	10:L8:177:GLY:HA2	1.98	0.45
15:LF:78:SER:OG	15:LF:81:GLU:OE2	2.34	0.45
22:LN:579:ARG:NH1	22:LN:593:GLU:OE2	2.41	0.45
28:LU:273:GLU:OE1	28:LU:288:TYR:OH	2.34	0.45
38:SI:900:GLN:HG2	38:SI:914:ALA:HB2	1.97	0.45
42:SN:189:TYR:OH	42:SN:231:GLN:O	2.32	0.45
42:SN:228:LYS:HE3	42:SN:228:LYS:HB3	1.68	0.45
53:8:312:A:H62	53:8:352:A:H1'	1.82	0.45
53:8:1511:U:H2'	53:8:1512:G:C8	2.52	0.45
53:8:1541:G:N2	53:8:1569:A:N7	2.64	0.45
4:L0:487:A:H62	24:LP:3:LYS:HG3	1.80	0.45
5:L2:105:C:O2'	5:L2:106:C:O4'	2.32	0.45
11:L9:134:ILE:HA	11:L9:158:PHE:HA	1.98	0.45
17:LH:397:LYS:NZ	17:LH:738:ASN:OD1	2.50	0.45
17:LH:719:ASN:OD1	17:LH:719:ASN:N	2.50	0.45
22:LN:120:SER:OG	22:LN:121:THR:N	2.40	0.45
22:LN:298:ALA:HB2	22:LN:336:ILE:HG13	1.99	0.45
22:LN:495:VAL:HB	22:LN:511:VAL:HB	1.98	0.45
23:LO:221:THR:OG1	23:LO:222:LYS:N	2.48	0.45
23:LO:356:ASP:OD1	23:LO:356:ASP:N	2.39	$0.\overline{45}$
23:LO:568:ARG:HD3	23:LO:568:ARG:HA	1.71	0.45



A 4 amo 1	A + amp 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:LO:777:ARG:HA	23:LO:777:ARG:HD2	1.80	0.45
25:LQ:17:ILE:HB	25:LQ:360:ASN:HB3	1.99	0.45
25:LQ:125:THR:N	25:LQ:139:GLY:O	2.50	0.45
27:LT:594:SER:HB2	27:LT:599:TRP:HB2	1.98	0.45
28:LU:329:ILE:HG13	28:LU:375:TRP:HZ3	1.80	0.45
29:LV:24:SER:O	29:LV:44:GLN:NE2	2.50	0.45
29:LV:62:ILE:HG23	29:LV:321:GLU:HB2	1.97	0.45
34:SD:223:ASP:OD2	34:SD:226:HIS:ND1	2.47	0.45
39:SK:25:PRO:HB2	47:ST:708:VAL:HG23	1.99	0.45
39:SK:96:LEU:HB3	39:SK:130:ILE:HD13	1.99	0.45
47:ST:546:LEU:HD23	47:ST:549:ILE:HD12	1.99	0.45
49:SZ:347:VAL:N	53:8:1220:C:OP1	2.50	0.45
53:8:327:U:H2'	53:8:328:A:H8	1.82	0.45
53:8:590:C:H2'	53:8:591:A:H8	1.82	0.45
59:SB:298:ARG:HB3	59:SB:341:LEU:HD21	1.98	0.45
62:LX:857:ASP:N	62:LX:857:ASP:OD1	2.50	0.45
2:SA:81:ILE:O	2:SA:85:ASN:ND2	2.50	0.45
2:SA:259:UNK:O	2:SA:264:SER:N	2.49	0.45
5:L2:8:U:H2'	5:L2:9:A:H8	1.82	0.45
6:L3:28:ILE:HA	6:L3:31:ALA:HB3	1.97	0.45
8:L5:224:ASN:OD1	8:L5:224:ASN:N	2.48	0.45
9:L7:49:ILE:HG23	9:L7:175:LYS:HD3	1.98	0.45
18:LJ:165:THR:OG1	18:LJ:166:GLY:N	2.49	0.45
18:LJ:378:LYS:HZ3	18:LJ:378:LYS:HG2	1.50	0.45
22:LN:240:LEU:H	22:LN:258:SER:HB3	1.80	0.45
24:LP:40:GLU:OE2	24:LP:91:ARG:NH2	2.45	0.45
24:LP:92:ILE:HA	24:LP:95:ILE:HD12	1.98	0.45
25:LQ:85:LEU:HB2	25:LQ:94:LEU:HD11	1.98	0.45
28:LU:225:LEU:HA	28:LU:237:SER:HA	1.98	0.45
28:LU:357:SER:OG	28:LU:359:ASP:OD1	2.27	0.45
29:LV:117:LEU:HD12	29:LV:123:ILE:HD11	1.99	0.45
34:SC:242:ALA:HB2	34:SC:253:ILE:HD11	1.98	0.45
34:SD:236:MET:SD	34:SD:236:MET:N	2.90	0.45
36:SG:229:GLU:HB2	36:SG:231:THR:HG23	1.99	0.45
38:SI:306:ASP:OD1	38:SI:306:ASP:N	2.42	0.45
51:NH:765:LEU:HA	51:NH:914:ARG:HA	1.99	0.45
53:8:319:U:H1'	53:8:323:A:C8	2.51	0.45
53:8:396:G:H21	53:8:398:G:H3'	1.81	0.45
53:8:1629:G:O2'	53:8:1630:U:O4'	2.33	0.45
57:LR:620:LEU:HA	57:LR:636:ASP:HA	1.99	$0.\overline{45}$
57:LR:744:ARG:HG3	57:LR:785:ILE:HG12	1.98	0.45



	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
62:LY:58:ALA:HB3	62:LY:125:GLN:H	1.82	0.45
62:LX:851:ASP:HB3	62:LX:854:VAL:HG23	1.99	0.45
65:5:216:ALA:HB1	66:6:4:LEU:HD22	1.99	0.45
9:L7:35:LYS:O	9:L7:39:ARG:NH1	2.50	0.45
17:LH:592:SER:O	17:LH:592:SER:OG	2.31	0.45
22:LN:399:VAL:HB	22:LN:420:LEU:HD12	1.98	0.45
23:LO:446:CYS:HB3	23:LO:457:VAL:HG12	1.98	0.45
23:LO:563:ARG:HH11	23:LO:630:LEU:HD12	1.82	0.45
25:LQ:614:HIS:HB2	25:LQ:618:ILE:HG12	1.98	0.45
27:LT:360:ASP:N	27:LT:360:ASP:OD1	2.49	0.45
28:LU:46:ASN:ND2	30:LW:434:LEU:O	2.45	0.45
28:LU:58:PHE:HD1	28:LU:375:TRP:HE1	1.65	0.45
30:LW:99:THR:HA	30:LW:102:LYS:HB2	1.99	0.45
36:SG:292:SER:OG	36:SG:293:ASP:N	2.50	0.45
38:SI:996:LEU:HB3	38:SI:998:SER:H	1.81	0.45
39:SK:124:VAL:HG22	39:SK:160:LEU:HD22	1.98	0.45
39:SK:181:SER:OG	39:SK:182:PHE:N	2.49	0.45
41:SM:144:GLU:OE1	41:SM:147:GLY:N	2.47	0.45
51:NH:403:GLY:HA2	51:NH:411:ILE:H	1.82	0.45
53:8:878:G:H2'	53:8:879:G:H8	1.81	0.45
3:NB:533:SER:OG	3:NB:534:GLY:N	2.49	0.45
4:L0:472:A:OP1	30:LW:145:ARG:NH1	2.48	0.45
7:L4:26:CYS:SG	7:L4:27:TYR:N	2.89	0.45
25:LQ:80:ALA:HB1	25:LQ:98:TYR:HB3	1.99	0.45
28:LU:225:LEU:HD12	28:LU:235:LEU:HD11	1.99	0.45
31:LZ:113:VAL:HG22	31:LZ:124:ILE:HD11	1.99	0.45
37:SH:68:SER:OG	37:SH:69:TYR:N	2.49	0.45
37:SH:234:ASN:OD1	37:SH:234:ASN:N	2.49	0.45
53:8:1157:A:O2'	53:8:1159:C:OP2	2.30	0.45
53:8:1693:A:H2'	53:8:1694:A:C4	2.52	0.45
57:LR:510:SER:OG	57:LR:512:ASP:OD1	2.33	0.45
66:6:88:LYS:HA	66:6:88:LYS:HD3	1.75	0.45
4:L0:100:G:N7	18:LJ:25:ARG:NH1	2.56	0.45
4:L0:548:A:H2'	4:L0:549:G:C8	2.52	0.45
5:L2:114:A:H61	5:L2:256:G:H1'	1.81	0.45
8:L5:95:ASN:O	53:8:1611:A:O2'	2.30	0.45
14:LE:11:LEU:O	14:LE:15:ASN:ND2	2.49	0.45
17:LH:437:THR:HB	17:LH:709:ARG:HD2	1.98	0.45
18:LJ:255:VAL:HG12	18:LJ:276:SER:HA	1.99	0.45
21:LM:250:SER:OG	$21:LM:25\overline{3:CYS:SG}$	2.69	$0.\overline{45}$
22:LN:303:LYS:HD3	22:LN:305:PHE:HE1	1.82	0.45



A + amo 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
25:LQ:81:GLU:OE1	25:LQ:657:GLN:NE2	2.50	0.45
28:LU:67:ARG:NH1	28:LU:89:ASP:OD2	2.41	0.45
28:LU:347:ARG:O	28:LU:373:ARG:NH2	2.50	0.45
36:SG:235:HIS:HA	36:SG:259:LYS:HZ1	1.81	0.45
38:SI:196:THR:HG23	38:SI:197:GLU:HG3	1.98	0.45
41:SM:285:ASN:HD22	47:ST:767:ILE:HD12	1.82	0.45
47:ST:511:SER:HA	47:ST:557:SER:HB3	1.98	0.45
54:SU:252:LYS:O	54:SU:256:ASN:ND2	2.50	0.45
63:L6:4:ASN:O	63:L6:111:LEU:N	2.46	0.45
4:L0:86:C:H5'	17:LH:295:TRP:HZ2	1.82	0.45
5:L2:62:C:O2'	27:LT:447:ASN:O	2.35	0.45
9:L7:127:GLU:HA	9:L7:130:VAL:HG22	1.98	0.45
17:LH:31:ASN:HD21	17:LH:201:ILE:HD12	1.81	0.45
17:LH:60:ARG:NH1	17:LH:381:SER:O	2.45	0.45
17:LH:283:VAL:HB	17:LH:290:ILE:HG22	1.98	0.45
17:LH:403:ILE:HG12	17:LH:417:LEU:HD21	1.99	0.45
26:LS:271:THR:OG1	26:LS:273:ARG:NH1	2.50	0.45
26:LS:351:THR:OG1	26:LS:352:GLN:N	2.50	0.45
26:LS:514:LEU:O	48:SY:248:ARG:NH2	2.50	0.45
30:LW:237:ALA:HB1	30:LW:280:ILE:HG12	1.99	0.45
7:L4:39:ARG:HA	7:L4:39:ARG:HD3	1.87	0.44
13:LD:71:LEU:HD21	13:LD:88:ARG:HG3	1.99	0.44
17:LH:707:MET:N	17:LH:707:MET:SD	2.91	0.44
17:LH:729:THR:O	17:LH:734:VAL:N	2.50	0.44
18:LJ:13:ALA:HB2	18:LJ:454:ARG:HG3	1.99	0.44
27:LT:66:LEU:HD12	27:LT:344:ARG:HB3	1.98	0.44
28:LU:230:ASN:ND2	28:LU:271:PRO:O	2.50	0.44
36:SG:206:LYS:HD2	36:SG:206:LYS:HA	1.77	0.44
38:SI:826:LYS:HB2	38:SI:921:GLU:HB3	1.98	0.44
38:SI:906:ASP:OD1	38:SI:906:ASP:N	2.43	0.44
41:SM:188:HIS:HB2	41:SM:221:VAL:HG12	1.99	0.44
53:8:29:U:H2'	53:8:30:G:H8	1.82	0.44
53:8:1502:G:N2	53:8:1505:A:OP2	2.42	0.44
57:LR:312:GLN:HB3	57:LR:329:VAL:HG21	1.99	0.44
62:LX:55:VAL:HG13	62:LX:103:ILE:HG23	1.99	0.44
17:LH:876:PHE:HZ	21:LM:180:ILE:HD11	1.82	0.44
19:LK:507:ARG:HB3	55:LI:655:LEU:HD23	1.99	0.44
23:LO:5:PHE:HA	23:LO:706:THR:HG22	1.99	0.44
23:LO:7:PHE:HD2	23:LO:51:GLU:HA	1.82	0.44
23:LO:825:GLN:HA	23:LO:828:ILE:HG22	1.98	0.44
27:LT:139:ILE:HD11	27:LT:157:LEU:HD12	1.99	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
29:LV:16:VAL:HG23	29:LV:340:THR:HG23	1.99	0.44
29:LV:106:ILE:HD11	29:LV:111:TRP:HA	1.98	0.44
38:SI:195:TRP:NE1	38:SI:202:ALA:O	2.38	0.44
39:SJ:232:LEU:HB3	39:SJ:237:ALA:HB2	2.00	0.44
41:SM:217:ASP:OD1	41:SM:217:ASP:N	2.45	0.44
42:SN:223:LEU:HB3	42:SN:235:ILE:HD12	1.98	0.44
48:SY:6:HIS:H	48:SY:9:GLN:HB3	1.82	0.44
54:SU:222:LEU:O	54:SU:225:HIS:NE2	2.46	0.44
57:LR:113:THR:OG1	57:LR:114:SER:N	2.49	0.44
57:LR:465:LYS:H	57:LR:486:THR:HA	1.82	0.44
59:SB:430:ASP:N	59:SB:430:ASP:OD1	2.49	0.44
61:SP:1398:LEU:O	61:SP:1402:ILE:N	2.48	0.44
62:LY:567:LEU:O	62:LY:583:LEU:N	2.49	0.44
66:6:265:ASP:HB2	66:6:275:LYS:HB2	1.99	0.44
7:L4:212:ASP:OD1	7:L4:212:ASP:N	2.45	0.44
8:L5:71:ALA:HB1	8:L5:91:GLU:HA	2.00	0.44
13:LD:78:THR:HA	13:LD:84:ILE:HG22	1.98	0.44
17:LH:550:PRO:HA	20:LL:366:GLY:HA3	2.00	0.44
17:LH:561:LEU:HD21	17:LH:615:TRP:HB2	1.99	0.44
18:LJ:95:LEU:HD11	18:LJ:117:LEU:HD22	1.99	0.44
22:LN:258:SER:HA	22:LN:282:ASP:HB3	1.98	0.44
22:LN:258:SER:HB2	56:ND:205:TRP:HZ2	1.83	0.44
23:LO:311:ASN:HD22	23:LO:316:TRP:HB2	1.81	0.44
26:LS:181:GLU:HB3	27:LT:281:ARG:HH21	1.82	0.44
27:LT:114:THR:HG22	27:LT:116:ALA:H	1.82	0.44
34:SC:244:VAL:HG22	34:SC:246:GLN:HG2	1.99	0.44
38:SI:90:VAL:HG11	38:SI:105:ILE:HD12	2.00	0.44
38:SI:833:ARG:NH2	45:SR:141:GLU:OE2	2.51	0.44
42:SN:74:LEU:HD13	42:SN:154:ILE:HD11	2.00	0.44
53:8:473:A:H1'	66:6:271:ARG:HD2	1.99	0.44
62:LX:36:GLN:HE21	62:LX:204:GLU:H	1.64	0.44
62:LX:162:TYR:O	62:LX:165:THR:OG1	2.32	0.44
66:6:266:ILE:HG22	66:6:274:ILE:HA	1.99	0.44
15:LF:38:ASP:OD1	15:LF:41:ARG:NH1	2.50	0.44
17:LH:71:ASN:HB3	17:LH:74:LEU:HB2	1.99	0.44
17:LH:597:LYS:HA	17:LH:597:LYS:HD3	1.71	0.44
17:LH:661:THR:HB	17:LH:673:ALA:HB3	2.00	0.44
20:LL:370:LYS:H	20:LL:372:VAL:HG23	1.82	0.44
21:LM:317:SER:OG	21:LM:321:LYS:NZ	2.50	0.44
22:LN:530:ARG:HD3	22:LN:530:ARG:HA	1.76	0.44
23:LO:593:VAL:HG11	23:LO:684:VAL:HG11	1.98	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
23:LO:760:ILE:HA	23:LO:763:ILE:HD12	1.99	0.44
28:LU:158:LYS:HA	28:LU:158:LYS:HD3	1.71	0.44
29:LV:143:SER:HB3	29:LV:186:VAL:HG12	1.98	0.44
34:SD:108:THR:OG1	34:SD:144:TRP:NE1	2.48	0.44
37:SH:323:ILE:HG12	38:SI:553:ILE:HG12	1.99	0.44
38:SI:843:ASP:OD1	38:SI:1035:THR:OG1	2.36	0.44
47:ST:731:ASP:HB3	47:ST:734:ARG:HB2	1.99	0.44
48:SY:3:LYS:HA	48:SY:3:LYS:HD2	1.81	0.44
48:SY:29:GLU:OE2	48:SY:37:ARG:NH1	2.50	0.44
53:8:327:U:H2'	53:8:328:A:C8	2.52	0.44
54:SU:277:ILE:HA	54:SU:280:ILE:HD12	1.99	0.44
54:SU:340:LYS:HD2	54:SU:340:LYS:HA	1.79	0.44
58:NE:234:VAL:HG23	58:NE:239:ARG:HB2	2.00	0.44
63:L6:54:GLY:O	63:L6:110:ALA:N	2.39	0.44
2:SA:101:SER:HB3	2:SA:128:ILE:HG21	1.99	0.44
4:L0:289:U:H2'	4:L0:290:G:H8	1.81	0.44
11:L9:19:TYR:HH	53:8:20:G:H1	1.64	0.44
13:LD:133:LYS:NZ	53:8:324:U:OP1	2.45	0.44
23:LO:624:ASN:HB2	23:LO:678:GLU:HA	1.99	0.44
30:LW:460:ARG:HB3	46:SS:847:VAL:HB	1.99	0.44
30:LW:462:ASN:HB2	30:LW:465:ASP:H	1.82	0.44
31:LZ:30:THR:HA	31:LZ:33:MET:HB2	1.99	0.44
34:SD:241:PHE:HA	34:SD:268:VAL:HB	2.00	0.44
37:SH:42:ASN:OD1	37:SH:42:ASN:N	2.50	0.44
53:8:468:A:H2	53:8:471:A:H62	1.64	0.44
53:8:1726:G:H2'	53:8:1727:G:C8	2.53	0.44
57:LR:14:PRO:HG3	57:LR:639:GLY:HA3	2.00	0.44
60:SV:181:ASP:HB2	60:SV:187:LEU:HD22	2.00	0.44
62:LX:861:MET:HA	62:LX:864:LEU:HD12	2.00	0.44
1:NA:364:SER:HB2	41:SM:227:ARG:HH22	1.82	0.44
2:SA:30:ARG:NH1	2:SA:122:GLU:OE2	2.50	0.44
4:L0:494:C:H2'	4:L0:495:G:H8	1.81	0.44
6:L3:67:GLU:HA	6:L3:70:VAL:HG12	2.00	0.44
14:LE:78:ARG:NH2	14:LE:125:ILE:O	2.51	0.44
16:LG:60:GLU:N	16:LG:60:GLU:OE2	2.50	0.44
21:LM:2:SER:OG	21:LM:3:SER:N	2.51	0.44
22:LN:116:SER:HB3	22:LN:126:TRP:HE1	1.82	0.44
23:LO:61:ILE:HG23	23:LO:70:LEU:HD11	2.00	0.44
23:LO:295:ILE:HG22	23:LO:296:GLN:HG3	2.00	0.44
30:LW:381:LEU:HD12	30:LW:390:LEU:HD12	2.00	0.44
35:SE:34:LYS:HD3	35:SE:34:LYS:HA	1.84	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
37:SH:107:ALA:HB1	37:SH:170:VAL:HG21	2.00	0.44
38:SI:889:LEU:HD22	38:SI:922:ILE:HG23	1.98	0.44
41:SM:219:GLU:HB3	47:ST:6:LEU:HD13	2.00	0.44
47:ST:698:ILE:HG12	54:SU:439:LYS:HD2	2.00	0.44
53:8:101:U:O5'	53:8:383:G:N2	2.51	0.44
57:LR:617:ASN:OD1	57:LR:617:ASN:N	2.51	0.44
58:NE:225:GLN:HA	58:NE:228:ILE:HG12	1.98	0.44
59:SB:245:THR:OG1	59:SB:246:GLU:N	2.51	0.44
62:LX:16:ASN:HD21	62:LX:218:PRO:HA	1.81	0.44
62:LX:771:SER:OG	62:LX:772:ASN:N	2.49	0.44
1:NA:342:THR:HG22	6:L3:119:ILE:HG21	1.99	0.44
4:L0:499:U:H2'	4:L0:500:G:C8	2.52	0.44
5:L2:77:U:H2'	5:L2:78:G:H8	1.83	0.44
7:L4:51:ARG:HH22	7:L4:110:ALA:HA	1.82	0.44
7:L4:102:VAL:N	7:L4:110:ALA:O	2.47	0.44
17:LH:55:TYR:HA	17:LH:62:CYS:HA	1.98	0.44
17:LH:364:ASN:ND2	17:LH:410:ASN:OD1	2.46	0.44
17:LH:483:LYS:HD3	17:LH:488:LEU:HA	1.98	0.44
18:LJ:38:GLU:N	18:LJ:325:GLY:O	2.45	0.44
18:LJ:449:GLY:O	18:LJ:455:SER:OG	2.36	0.44
21:LM:364:ASN:OD1	21:LM:364:ASN:N	2.49	0.44
23:LO:266:VAL:HG12	23:LO:277:VAL:HA	2.00	0.44
25:LQ:355:LEU:HB3	25:LQ:363:GLU:HB2	1.99	0.44
27:LT:305:ASN:ND2	59:SB:425:ARG:O	2.46	0.44
28:LU:300:VAL:HG22	53:8:-1:G:C6	2.53	0.44
29:LV:20:ASN:N	29:LV:20:ASN:OD1	2.50	0.44
29:LV:182:GLY:HA3	29:LV:199:THR:HA	1.99	0.44
38:SI:893:ASN:HD21	45:SR:98:GLU:HB3	1.83	0.44
44:SQ:56:GLU:O	44:SQ:60:LYS:NZ	2.45	0.44
47:ST:776:ASP:OD1	47:ST:780:LYS:NZ	2.48	0.44
51:NH:780:GLN:H	51:NH:850:PHE:HA	1.83	0.44
53:8:1592:A:H2'	53:8:1593:A:H8	1.82	0.44
63:L6:115:LYS:HE3	63:L6:115:LYS:HB2	1.84	0.44
66:6:84:ASP:HB3	66:6:87:CYS:HB2	1.99	0.44
5:L2:17:G:H2'	5:L2:18:G:C8	2.52	0.44
11:L9:139:GLN:HB3	66:6:266:ILE:HD11	2.00	0.44
12:LC:94:GLN:HB3	12:LC:102:LYS:HG3	2.00	0.44
16:LG:52:ASP:OD1	16:LG:52:ASP:N	2.51	0.44
18:LJ:5:ARG:NH1	18:LJ:393:ASN:OD1	2.51	0.44
18:LJ:500:GLU:OE2	18:LJ:503:ARG:NH1	2.51	0.44
21:LM:122:VAL:HA	21:LM:127:ILE:HG12	1.99	0.44



A 4 amo 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
22:LN:57:ILE:HG22	22:LN:340:GLN:HB3	2.00	0.44
22:LN:561:LYS:HD3	22:LN:561:LYS:HA	1.88	0.44
25:LQ:42:ILE:HG12	25:LQ:51:ILE:HB	1.98	0.44
25:LQ:455:GLN:HG2	25:LQ:467:THR:HB	2.00	0.44
29:LV:356:LEU:HD23	29:LV:359:ILE:HD11	1.99	0.44
34:SD:86:VAL:HG11	34:SD:123:ILE:HG21	2.00	0.44
37:SH:108:PRO:HB2	37:SH:174:ILE:HG12	2.00	0.44
37:SH:320:GLU:HA	37:SH:323:ILE:HD12	2.00	0.44
53:8:148:A:N6	53:8:166:C:N3	2.66	0.44
53:8:225:A:H2'	53:8:226:A:H4'	1.99	0.44
53:8:1592:A:H2'	53:8:1593:A:C8	2.53	0.44
53:8:1702:A:N6	53:8:1703:C:O2	2.51	0.44
54:SU:309:ASN:HB3	54:SU:312:ALA:HB3	1.98	0.44
54:SU:504:ASP:N	54:SU:504:ASP:OD1	2.51	0.44
55:LI:228:GLU:O	55:LI:242:CYS:N	2.51	0.44
57:LR:293:VAL:HG12	57:LR:304:LEU:HG	2.00	0.44
62:LX:779:LYS:HA	62:LX:782:ARG:HE	1.83	0.44
65:5:193:ARG:O	65:5:193:ARG:NE	2.49	0.44
5:L2:1:G:N2	53:8:1124:A:H1'	2.33	0.44
8:L5:89:ILE:HD12	8:L5:137:ILE:HD12	2.00	0.44
9:L7:75:THR:O	9:L7:79:ARG:NH1	2.51	0.44
11:L9:78:ARG:HH12	66:6:251:GLU:HG2	1.82	0.44
12:LC:99:GLU:HB2	12:LC:102:LYS:HE3	2.00	0.44
20:LL:253:LEU:HD21	20:LL:301:LEU:HD11	2.00	0.44
25:LQ:452:GLY:O	25:LQ:471:ALA:N	2.51	0.44
25:LQ:588:ILE:O	25:LQ:600:TRP:N	2.46	0.44
29:LV:71:CYS:SG	29:LV:72:MET:N	2.91	0.44
29:LV:250:GLY:HA3	29:LV:271:GLY:HA2	2.00	0.44
47:ST:604:VAL:HG13	47:ST:606:PHE:H	1.82	0.44
53:8:153:G:OP1	63:L6:15:THR:OG1	2.33	0.44
53:8:933:A:H4'	53:8:934:C:H5'	1.99	0.44
53:8:1506:G:H2'	53:8:1507:G:C8	2.53	0.44
57:LR:242:GLN:HE21	57:LR:263:GLY:HA3	1.83	0.44
6:L3:2:SER:OG	54:SU:370:HIS:O	2.36	0.43
7:L4:201:HIS:HB2	7:L4:207:LEU:HG	2.00	0.43
10:L8:7:SER:O	10:L8:10:LYS:NZ	2.38	0.43
14:LE:30:SER:HA	14:LE:34:ILE:HD11	2.00	0.43
18:LJ:426:LYS:HB2	18:LJ:429:VAL:HG23	1.99	0.43
20:LL:494:ARG:HE	20:LL:498:LEU:HD11	1.83	0.43
21:LM:249:LYS:HE3	21:LM:249:LYS:HB3	1.87	0.43
21:LM:336:LEU:HD22	21:LM:373:ILE:HD13	2.00	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
22:LN:67:LEU:HD23	22:LN:81:PRO:HG3	1.99	0.43
22:LN:313:LYS:HD2	22:LN:313:LYS:HA	1.78	0.43
23:LO:261:ALA:HB1	23:LO:279:PHE:HB3	2.00	0.43
24:LP:279:LYS:HA	24:LP:279:LYS:HD2	1.86	0.43
25:LQ:937:ARG:HD2	25:LQ:937:ARG:HA	1.78	0.43
26:LS:512:ASP:N	26:LS:512:ASP:OD1	2.51	0.43
27:LT:931:GLY:N	57:LR:801:GLU:OE2	2.51	0.43
37:SH:290:GLY:HA3	37:SH:293:GLN:HG3	2.00	0.43
38:SI:992:GLU:OE1	53:8:564:G:O2'	2.32	0.43
51:NH:675:GLU:HA	51:NH:702:LYS:HA	1.99	0.43
57:LR:513:LYS:HE2	57:LR:513:LYS:HB3	1.83	0.43
4:L0:189:U:H3	4:L0:209:G:H22	1.66	0.43
4:L0:331:U:H3	23:LO:656:ARG:HH12	1.64	0.43
21:LM:218:ILE:HD12	21:LM:263:VAL:HB	2.00	0.43
21:LM:276:LEU:HD23	21:LM:276:LEU:HA	1.90	0.43
23:LO:516:SER:HB3	23:LO:536:LYS:HD3	1.99	0.43
34:SD:242:ALA:HB3	34:SD:269:ILE:HA	1.99	0.43
37:SH:156:ARG:HD2	37:SH:198:THR:HG21	2.00	0.43
38:SI:179:SER:OG	38:SI:182:THR:OG1	2.35	0.43
42:SN:41:ASN:OD1	42:SN:41:ASN:N	2.51	0.43
49:SZ:380:TYR:HA	53:8:1220:C:H4'	1.99	0.43
53:8:52:U:H2'	53:8:53:G:C8	2.52	0.43
53:8:154:G:N3	63:L6:56:ASN:ND2	2.67	0.43
53:8:262:U:H2'	53:8:263:C:H4'	2.00	0.43
53:8:406:U:H2'	53:8:407:A:C8	2.53	0.43
53:8:1655:A:H2	53:8:1745:G:H22	1.66	0.43
57:LR:548:LEU:N	57:LR:560:TRP:O	2.49	0.43
57:LR:655:GLU:HA	57:LR:658:LYS:HB2	2.00	0.43
4:L0:82:A:N7	17:LH:256:THR:OG1	2.46	0.43
4:L0:114:G:H2'	4:L0:115:G:H8	1.82	0.43
4:L0:529:A:H2'	4:L0:530:A:C8	2.53	0.43
7:L4:57:ASN:N	7:L4:60:GLU:OE2	2.51	0.43
8:L5:185:ARG:NH2	53:8:1472:C:OP1	2.50	0.43
9:L7:35:LYS:HA	9:L7:38:LEU:HB2	1.98	0.43
12:LC:14:LYS:NZ	53:8:1610:G:N7	2.66	0.43
22:LN:130:THR:HG23	22:LN:132:LEU:H	1.81	0.43
27:LT:30:ILE:HG13	27:LT:380:LEU:HD23	1.99	0.43
28:LU:85:THR:HG21	28:LU:372:VAL:HG21	2.01	0.43
28:LU:114:THR:OG1	28:LU:139:CYS:SG	2.66	0.43
34:SC:253:ILE:HD13	34:SC:253:ILE:HA	1.89	0.43
53:8:164:A:H2'	53:8:165:G:C8	2.54	0.43



A + 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
57:LR:433:HIS:HE1	57:LR:437:VAL:HB	1.83	0.43
62:LX:9:ARG:HH21	62:LX:199:LEU:HD21	1.83	0.43
62:LX:748:ARG:HD3	62:LX:748:ARG:HA	1.80	0.43
65:5:332:ASP:OD1	65:5:332:ASP:N	2.46	0.43
65:5:418:LEU:HD13	65:5:441:SER:HB2	2.01	0.43
5:L2:1:G:H2'	5:L2:2:U:C6	2.53	0.43
11:L9:26:ALA:HA	40:SL:55:TYR:HE2	1.83	0.43
13:LD:59:PRO:HA	13:LD:64:VAL:HG23	2.00	0.43
17:LH:212:CYS:SG	17:LH:224:SER:OG	2.74	0.43
22:LN:249:ARG:NH2	22:LN:309:GLN:OE1	2.51	0.43
22:LN:635:GLY:HA3	22:LN:649:TRP:CE2	2.53	0.43
23:LO:147:GLN:HB3	23:LO:166:LYS:HB2	2.00	0.43
25:LQ:668:ASP:OD1	25:LQ:668:ASP:N	2.52	0.43
35:SF:21:LEU:HA	35:SF:24:VAL:HG22	1.99	0.43
36:SG:457:GLU:OE2	36:SG:461:LYS:NZ	2.51	0.43
37:SH:17:PHE:N	38:SI:609:GLU:OE2	2.52	0.43
38:SI:751:TYR:HB2	45:SR:77:ILE:HG22	2.00	0.43
48:SY:229:SER:HB2	48:SY:245:LYS:HB2	1.99	0.43
53:8:1049:U:H2'	53:8:1050:G:C8	2.53	0.43
53:8:1274:C:H2'	53:8:1275:A:C8	2.53	0.43
57:LR:554:ASP:OD1	57:LR:554:ASP:N	2.49	0.43
62:LX:73:ARG:HH22	62:LX:99:SER:HA	1.83	0.43
62:LX:587:GLN:O	62:LX:636:VAL:N	2.48	0.43
66:6:98:ARG:HH22	66:6:101:GLN:HG2	1.83	0.43
66:6:339:SER:O	66:6:345:LYS:NZ	2.51	0.43
2:SA:171:ASP:N	2:SA:171:ASP:OD1	2.49	0.43
7:L4:112:HIS:CD2	7:L4:239:PRO:HG3	2.53	0.43
10:L8:184:LEU:HG	10:L8:189:LEU:HG	1.99	0.43
11:L9:82:ARG:NH1	66:6:323:GLU:OE1	2.49	0.43
15:LF:45:ALA:HA	15:LF:50:ALA:HB3	1.99	0.43
18:LJ:117:LEU:HD23	18:LJ:118:LEU:HB2	2.00	0.43
20:LL:518:ASN:OD1	20:LL:518:ASN:N	2.50	0.43
21:LM:166:ASN:HD21	59:SB:409:THR:HG22	1.83	0.43
21:LM:304:GLN:HA	21:LM:346:LYS:HD2	2.01	0.43
25:LQ:392:THR:HG23	25:LQ:409:ALA:HB1	2.01	0.43
25:LQ:539:VAL:HG22	25:LQ:546:LEU:HD12	2.00	0.43
30:LW:109:LYS:HD3	30:LW:396:THR:HB	2.00	0.43
30:LW:312:VAL:HG21	30:LW:353:PRO:HG2	2.00	0.43
42:SN:180:LEU:HA	42:SN:183:ILE:HG22	2.01	0.43
4:L0:133:U:H2'	4:L0:134:A:H8	1.84	0.43
7:L4:148:ARG:HH12	53:8:125:U:H5'	1.83	0.43



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
14:LE:12:ASN:OD1	14:LE:12:ASN:N	2.51	0.43
17:LH:363:ASN:ND2	17:LH:390:PRO:O	2.50	0.43
19:LK:439:LYS:HA	19:LK:439:LYS:HD2	1.83	0.43
20:LL:104:SER:O	20:LL:104:SER:OG	2.33	0.43
21:LM:201:LYS:HE2	21:LM:201:LYS:HB3	1.85	0.43
22:LN:382:VAL:HG11	22:LN:755:ILE:HD13	2.00	0.43
28:LU:174:ARG:HD2	28:LU:209:LEU:HD21	2.00	0.43
40:SL:16:THR:OG1	40:SL:17:LEU:N	2.49	0.43
53:8:109:G:O3'	66:6:227:ARG:NH2	2.51	0.43
53:8:878:G:H2'	53:8:879:G:C8	2.53	0.43
62:LX:92:ASP:HB3	62:LX:95:GLU:H	1.83	0.43
62:LX:139:ILE:HG13	62:LX:486:LEU:HD13	2.00	0.43
1:NA:315:GLU:HG2	38:SI:1038:ILE:HG21	2.01	0.43
4:L0:423:C:H2'	4:L0:424:G:H8	1.83	0.43
5:L2:8:U:H2'	5:L2:9:A:C8	2.54	0.43
7:L4:193:GLY:H	7:L4:194:THR:HG23	1.84	0.43
17:LH:43:ASN:N	17:LH:43:ASN:OD1	2.52	0.43
20:LL:80:MET:SD	20:LL:86:TRP:NE1	2.91	0.43
20:LL:302:ASN:HD21	20:LL:314:PHE:HB3	1.84	0.43
25:LQ:175:ASP:HA	25:LQ:191:LEU:HB2	1.99	0.43
25:LQ:189:TRP:HA	25:LQ:196:CYS:HA	2.01	0.43
26:LS:444:ILE:HG22	26:LS:445:ARG:HG2	2.01	0.43
27:LT:432:THR:OG1	27:LT:443:TRP:NE1	2.37	0.43
29:LV:104:PHE:HE1	29:LV:114:SER:HB2	1.84	0.43
33:NK:44:LEU:HA	33:NK:79:SER:HA	2.01	0.43
34:SC:242:ALA:HB3	34:SC:269:ILE:HA	1.99	0.43
36:SG:476:THR:HG22	36:SG:491:SER:HA	2.00	0.43
37:SH:292:ASN:OD1	37:SH:292:ASN:N	2.51	0.43
38:SI:108:VAL:HA	38:SI:114:ARG:HB3	2.00	0.43
38:SI:373:ILE:HB	62:LX:6:ILE:HD11	2.01	0.43
41:SM:60:GLN:OE1	58:NE:207:ARG:NH2	2.51	0.43
41:SM:190:ILE:HB	41:SM:223:THR:HA	2.01	0.43
42:SN:231:GLN:N	42:SN:231:GLN:OE1	2.51	0.43
47:ST:444:ASN:OD1	47:ST:444:ASN:N	2.52	0.43
53:8:590:C:H2'	53:8:591:A:C8	2.54	0.43
57:LR:314:ILE:HD13	57:LR:329:VAL:HA	2.00	0.43
57:LR:437:VAL:HA	57:LR:458:SER:HA	2.01	0.43
57:LR:733:ASP:OD1	57:LR:733:ASP:N	2.43	0.43
58:NE:248:LYS:HE2	58:NE:248:LYS:HB2	1.93	0.43
1:NA:341:LEU:HD22	6:L3:116:LEU:HD11	2.00	0.43
1:NA:354:VAL:HG21	41:SM:168:HIS:HB2	2.01	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:NA:362:THR:HG22	41:SM:234:ARG:HH12	1.84	0.43
4:L0:486:U:H4'	4:L0:487:A:H5"	2.01	0.43
7:L4:202:ASP:OD1	7:L4:202:ASP:N	2.52	0.43
12:LC:39:VAL:HG12	12:LC:41:PRO:HD2	2.00	0.43
12:LC:98:ASP:HA	27:LT:490:GLN:HG3	2.00	0.43
15:LF:20:ARG:HG2	15:LF:76:TYR:HE2	1.84	0.43
18:LJ:226:ILE:HG23	18:LJ:239:LEU:HD11	1.99	0.43
18:LJ:494:GLU:HG3	20:LL:540:LEU:HD13	2.01	0.43
21:LM:382:LEU:HD23	21:LM:382:LEU:HA	1.90	0.43
23:LO:192:ASP:HB2	23:LO:212:ASP:HB3	2.00	0.43
25:LQ:449:THR:OG1	25:LQ:451:ASN:O	2.37	0.43
29:LV:171:ARG:HG2	65:5:468:VAL:HA	2.00	0.43
36:SG:495:SER:HB2	36:SG:513:GLU:HG3	2.00	0.43
37:SH:70:THR:HG23	37:SH:72:THR:H	1.84	0.43
39:SK:169:ASP:OD1	39:SK:169:ASP:N	2.51	0.43
57:LR:77:THR:HG21	57:LR:117:LEU:HG	2.00	0.43
58:NE:247:VAL:HA	58:NE:250:ILE:HB	2.01	0.43
62:LX:392:ILE:O	62:LX:546:TYR:OH	2.34	0.43
5:L2:17:G:H2'	5:L2:18:G:H8	1.84	0.43
5:L2:47:G:O2'	40:SL:15:ARG:NH2	2.52	0.43
22:LN:744:VAL:HG13	22:LN:752:LEU:HD11	2.00	0.43
23:LO:211:LYS:HE3	23:LO:262:LYS:HD3	1.99	0.43
38:SI:1021:LEU:HA	38:SI:1026:LYS:HG2	2.01	0.43
40:SL:78:LYS:HE3	40:SL:177:GLY:H	1.83	0.43
41:SM:107:ILE:HD13	41:SM:107:ILE:HA	1.90	0.43
53:8:1499:G:H1	53:8:1508:U:H3	1.66	0.43
53:8:1694:A:H2'	53:8:1695:G:C5	2.54	0.43
62:LY:506:GLY:HA3	65:5:489:GLN:HB2	2.01	0.43
63:L6:1:MET:HG2	63:L6:24:ILE:HD13	2.00	0.43
65:5:497:LEU:HB3	65:5:500:GLN:HB3	1.99	0.43
2:SA:194:ARG:HD2	59:SB:169:LEU:HD12	2.01	0.43
4:L0:397:A:H2'	4:L0:398:A:C8	2.54	0.43
12:LC:8:GLN:HE21	12:LC:10:PHE:HE1	1.67	0.43
23:LO:3:SER:HB2	23:LO:612:LEU:HD13	2.01	0.43
23:LO:559:ILE:HG23	23:LO:598:ASN:HD22	1.83	0.43
25:LQ:7:ARG:HH21	25:LQ:71:ALA:HA	1.84	0.43
30:LW:109:LYS:HB2	30:LW:109:LYS:HE2	1.79	0.43
35:SF:17:THR:HG23	35:SF:81:VAL:HG12	2.01	0.43
47:ST:577:VAL:HG23	47:ST:585:PRO:HG3	2.00	0.43
53:8:868:G:H21	64:NF:90:TYR:H	1.66	0.43
62:LX:529:VAL:O	62:LX:533:PHE:N	2.44	0.43



Atom-1	Atom-2	Interatomic	Clash
	1100m -	distance (Å)	overlap (Å)
4:L0:295:A:OP2	27:LT:385:GLN:NE2	2.45	0.42
6:L3:63:GLN:HA	6:L3:66:LEU:HB2	2.01	0.42
17:LH:437:THR:HG21	17:LH:706:HIS:HB3	2.00	0.42
17:LH:451:PHE:HB2	17:LH:458:GLN:HB3	2.01	0.42
18:LJ:34:GLN:HE21	18:LJ:329:ILE:HD12	1.83	0.42
21:LM:103:LEU:HD23	21:LM:103:LEU:HA	1.92	0.42
23:LO:477:SER:N	23:LO:491:ALA:O	2.41	0.42
23:LO:746:ASN:OD1	23:LO:777:ARG:NE	2.49	0.42
25:LQ:270:SER:OG	25:LQ:286:ILE:O	2.34	0.42
25:LQ:287:ARG:NH1	25:LQ:323:SER:O	2.51	0.42
25:LQ:673:VAL:HG22	25:LQ:683:ILE:HG12	2.00	0.42
26:LS:429:TYR:CD1	26:LS:448:LYS:HE2	2.54	0.42
26:LS:431:GLU:HB3	26:LS:446:ARG:HH21	1.83	0.42
27:LT:100:ILE:HD13	27:LT:149:TYR:HB2	2.01	0.42
31:LZ:75:GLU:HG3	31:LZ:94:ILE:HG12	2.00	0.42
33:NK:166:VAL:HA	33:NK:171:VAL:HA	2.01	0.42
34:SD:121:LYS:HG2	34:SD:143:VAL:HG11	2.01	0.42
35:SF:73:ASP:OD1	35:SF:73:ASP:N	2.52	0.42
36:SG:363:ASP:N	36:SG:363:ASP:OD1	2.43	0.42
36:SG:501:ILE:HG22	36:SG:508:PHE:HB3	2.01	0.42
47:ST:444:ASN:O	47:ST:447:SER:OG	2.37	0.42
53:8:22:A:O2'	53:8:23:G:O4'	2.37	0.42
55:LI:69:ILE:HA	55:LI:79:ASN:HA	2.01	0.42
57:LR:175:TRP:HA	57:LR:182:CYS:HA	2.01	0.42
57:LR:403:ILE:HD12	57:LR:415:TRP:HB2	2.00	0.42
57:LR:589:GLN:HA	57:LR:603:ASP:HA	2.01	0.42
58:NE:230:LYS:HD3	58:NE:230:LYS:HA	1.79	0.42
62:LX:21:LYS:HB3	62:LX:477:ALA:HB2	2.01	0.42
2:SA:146:ASP:N	2:SA:146:ASP:OD1	2.48	0.42
5:L2:30:A:C5	28:LU:57:PRO:HG2	2.55	0.42
9:L7:85:PHE:HB3	9:L7:88:ARG:HB2	2.00	0.42
17:LH:868:ASN:OD1	17:LH:868:ASN:N	2.49	0.42
22:LN:262:ILE:HD11	22:LN:283:VAL:HG11	2.00	0.42
22:LN:580:LYS:HG3	22:LN:596:MET:HB2	2.00	0.42
23:LO:336:SER:HA	27:LT:745:LYS:HA	2.00	0.42
24:LP:286:ILE:HD13	24:LP:286:ILE:HA	1.93	0.42
28:LU:143:LYS:HE2	28:LU:143:LYS:HB2	1.84	0.42
34:SC:272:LYS:HA	34:SC:313:HIS:HD2	1.84	0.42
37:SH:143:LYS:HD2	37:SH:143:LYS:HA	1.82	0.42
44:SQ:79:LYS:HA	44:SQ:79:LYS:HD2	1.80	0.42
47:ST:102:ARG:O	47:ST:106:LYS:NZ	2.41	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
47:ST:607:THR:OG1	47:ST:608:LYS:N	2.53	0.42
53:8:487:G:H2'	53:8:488:G:C8	2.54	0.42
53:8:939:A:H61	53:8:975:C:H1'	1.84	0.42
53:8:1130:G:H3'	53:8:1131:A:H4'	2.00	0.42
54:SU:130:GLU:HG2	54:SU:134:PHE:HB2	2.01	0.42
55:LI:563:LEU:HD13	55:LI:598:GLU:HG3	2.02	0.42
57:LR:24:THR:HG21	57:LR:68:LYS:HD3	2.01	0.42
57:LR:294:LEU:HB2	57:LR:303:PHE:HB2	2.01	0.42
62:LX:86:ARG:HH21	62:LX:91:MET:HA	1.84	0.42
62:LX:653:ALA:HA	62:LX:656:LEU:HB2	2.00	0.42
2:SA:393:SER:N	35:SF:62:GLU:OE2	2.52	0.42
3:NB:509:ARG:NE	53:8:1504:G:OP1	2.52	0.42
4:L0:409:C:H5"	38:SI:1089:GLN:HE21	1.85	0.42
13:LD:84:ILE:HG12	13:LD:111:VAL:HB	2.01	0.42
17:LH:449:LEU:N	17:LH:460:PHE:O	2.52	0.42
26:LS:229:PRO:HA	26:LS:230:PRO:HD3	1.91	0.42
26:LS:571:SER:OG	26:LS:575:GLY:N	2.52	0.42
28:LU:230:ASN:HB2	28:LU:274:ALA:HB2	2.01	0.42
29:LV:6:THR:HG22	29:LV:12:SER:HA	2.00	0.42
29:LV:101:ASN:HA	29:LV:118:GLN:HG3	2.00	0.42
44:SQ:119:ARG:HG2	44:SQ:174:LEU:HD22	2.01	0.42
57:LR:228:LYS:HD2	57:LR:228:LYS:HA	1.78	0.42
1:NA:480:GLN:HG3	1:NA:482:LEU:H	1.83	0.42
4:L0:210:U:H2'	4:L0:211:G:C8	2.54	0.42
11:L9:120:LYS:HB2	11:L9:120:LYS:HE3	1.80	0.42
22:LN:116:SER:OG	22:LN:117:ILE:N	2.53	0.42
23:LO:522:SER:HB3	23:LO:583:ILE:HG22	2.02	0.42
27:LT:428:GLU:OE2	27:LT:452:ARG:NH1	2.52	0.42
29:LV:101:ASN:OD1	29:LV:118:GLN:NE2	2.51	0.42
38:SI:284:PRO:HD3	38:SI:779:ARG:HH22	1.84	0.42
38:SI:371:VAL:HG13	62:LX:6:ILE:HD12	2.01	0.42
41:SM:268:ASN:HD22	41:SM:271:ALA:HB2	1.83	0.42
44:SQ:75:LYS:NZ	44:SQ:76:LYS:O	2.51	0.42
44:SQ:130:LEU:HA	44:SQ:187:PHE:HZ	1.84	0.42
47:ST:419:LYS:HE3	47:ST:419:LYS:HB2	1.75	0.42
62:LX:69:HIS:CE1	62:LX:71:LYS:HB2	2.53	0.42
14:LE:117:ARG:O	14:LE:120:HIS:ND1	2.51	0.42
21:LM:175:THR:OG1	21:LM:176:ALA:N	2.52	0.42
22:LN:111:SER:HA	22:LN:524:LYS:HA	2.01	0.42
22:LN:325:ASN:OD1	22:LN:325:ASN:N	2.50	0.42
23:LO:99:CYS:HA	23:LO:115:SER:HA	2.01	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
23:LO:335:GLU:O	25:LQ:924:TYR:OH	2.37	0.42
23:LO:478:CYS:SG	23:LO:479:LEU:N	2.93	0.42
24:LP:169:GLN:HE22	46:SS:338:LEU:HD22	1.83	0.42
27:LT:482:GLY:HA2	27:LT:505:VAL:HG23	2.01	0.42
27:LT:930:MET:HA	27:LT:933:ALA:HB3	2.02	0.42
29:LV:59:SER:OG	29:LV:74:THR:OG1	2.28	0.42
37:SH:53:LEU:HD22	37:SH:65:ILE:HD13	2.02	0.42
48:SY:223:GLU:HA	48:SY:226:LYS:HE3	2.02	0.42
59:SB:201:ASP:HB3	59:SB:204:ALA:HB3	2.02	0.42
62:LX:202:ASP:OD2	62:LX:206:ASN:ND2	2.53	0.42
65:5:290:ARG:NH1	66:6:101:GLN:HE21	2.17	0.42
11:L9:25:ASP:HA	11:L9:28:LEU:HB3	2.00	0.42
11:L9:80:LEU:HA	11:L9:83:VAL:HG22	2.00	0.42
22:LN:207:ASP:HB3	22:LN:209:ARG:HE	1.84	0.42
22:LN:481:ILE:HB	22:LN:485:LYS:HB3	2.00	0.42
24:LP:115:ASN:ND2	44:SQ:70:ASP:OD1	2.53	0.42
26:LS:234:ASP:OD2	26:LS:234:ASP:N	2.41	0.42
27:LT:579:ARG:NE	27:LT:614:LEU:O	2.52	0.42
34:SD:177:SER:OG	34:SD:202:ARG:NH1	2.53	0.42
38:SI:853:ARG:HH21	38:SI:1020:SER:HB3	1.85	0.42
39:SJ:136:ARG:NH2	53:8:1196:A:N3	2.58	0.42
39:SK:51:GLU:OE2	39:SK:51:GLU:N	2.52	0.42
53:8:1049:U:H2'	53:8:1050:G:H8	1.84	0.42
62:LX:516:PHE:HD1	62:LX:711:LYS:HA	1.85	0.42
2:SA:218:LYS:HA	2:SA:218:LYS:HD2	1.65	0.42
2:SA:224:LYS:HB3	2:SA:268:MET:HE3	2.01	0.42
9:L7:8:ILE:HD12	9:L7:8:ILE:HG23	1.85	0.42
10:L8:26:LYS:HE3	10:L8:26:LYS:HB3	1.82	0.42
11:L9:68:LYS:HB2	11:L9:68:LYS:HE2	1.84	0.42
20:LL:85:ILE:HB	20:LL:99:PHE:HB2	2.01	0.42
22:LN:422:LEU:HD13	22:LN:444:ARG:HH22	1.83	0.42
23:LO:397:LYS:HZ2	23:LO:442:GLY:H	1.67	0.42
25:LQ:332:ILE:HG12	25:LQ:379:PRO:HG3	2.01	0.42
25:LQ:931:SER:O	25:LQ:936:LYS:NZ	2.45	0.42
26:LS:496:ARG:HA	26:LS:496:ARG:HD2	1.86	0.42
36:SG:310:ASN:N	36:SG:310:ASN:OD1	2.52	0.42
36:SG:481:ILE:H	36:SG:481:ILE:HD12	1.84	0.42
39:SK:148:LEU:HD11	53:8:1575:G:H21	1.84	0.42
41:SM:285:ASN:OD1	41:SM:285:ASN:N	2.48	0.42
44:SQ:177:LEU:HD12	44:SQ:177:LEU:HA	1.93	0.42
53:8:126:A:N6	53:8:290:G:H1	2.17	0.42



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
53:8:399:A:H1'	53:8:401:A:H5'	2.02	0.42
57:LR:453:PHE:HB2	57:LR:465:LYS:HD2	2.01	0.42
62:LX:69:HIS:HE1	62:LX:71:LYS:HB2	1.84	0.42
14:LE:55:ASP:OD2	14:LE:57:ARG:NH1	2.53	0.42
17:LH:308:ASP:OD1	17:LH:308:ASP:N	2.46	0.42
17:LH:603:ASN:O	55:LI:592:ARG:NH2	2.52	0.42
23:LO:172:ILE:HD11	23:LO:206:ILE:HG12	2.01	0.42
23:LO:431:ILE:HG21	23:LO:452:ASN:HB2	2.02	0.42
24:LP:388:UNK:O	24:LP:392:UNK:N	2.53	0.42
25:LQ:626:GLN:NE2	25:LQ:668:ASP:O	2.44	0.42
34:SC:165:ALA:HB3	34:SC:168:LYS:HB2	2.01	0.42
36:SG:442:ILE:HD12	36:SG:470:LEU:HD22	2.01	0.42
38:SI:943:LYS:NZ	53:8:1595:U:O2	2.40	0.42
38:SI:966:ILE:HD11	38:SI:1001:VAL:HB	2.01	0.42
38:SI:1153:ASP:HA	38:SI:1156:LYS:HE3	2.00	0.42
42:SN:35:ASP:OD1	42:SN:35:ASP:N	2.43	0.42
53:8:199:G:N3	53:8:201:G:N2	2.68	0.42
53:8:362:G:H2'	53:8:363:G:C8	2.55	0.42
56:ND:181:LEU:HD23	56:ND:181:LEU:HA	1.89	0.42
57:LR:63:GLU:O	57:LR:81:GLN:N	2.53	0.42
59:SB:157:ASP:HA	59:SB:279:ARG:HH21	1.85	0.42
62:LX:185:ASN:OD1	62:LX:185:ASN:N	2.53	0.42
2:SA:389:ILE:HG22	35:SF:62:GLU:HB3	2.02	0.42
18:LJ:499:LYS:HB3	18:LJ:503:ARG:HH12	1.84	0.42
22:LN:645:ARG:HD3	22:LN:656:ARG:HH22	1.84	0.42
23:LO:69:LEU:HD23	23:LO:69:LEU:HA	1.92	0.42
23:LO:317:LEU:HD12	23:LO:332:TRP:HB3	2.02	0.42
25:LQ:279:LYS:HE2	25:LQ:279:LYS:HB2	1.91	0.42
27:LT:90:VAL:HG13	27:LT:101:TYR:HB2	2.01	0.42
27:LT:316:ASP:OD1	27:LT:316:ASP:N	2.51	0.42
38:SI:150:MET:HA	38:SI:153:MET:HB3	2.00	0.42
39:SJ:52:THR:HG21	39:SJ:146:HIS:CE1	2.55	0.42
39:SK:72:ASP:OD2	39:SK:73:HIS:ND1	2.41	0.42
41:SM:109:LEU:HD12	41:SM:109:LEU:HA	1.90	0.42
53:8:322:G:C8	65:5:460:LYS:HE3	2.54	0.42
55:LI:562:PRO:HB2	55:LI:565:GLU:HB2	2.01	0.42
57:LR:16:TYR:OH	57:LR:21:ALA:O	2.31	0.42
57:LR:43:ILE:HG22	57:LR:52:ILE:HA	2.02	0.42
4:L0:415:U:H2'	4:L0:416:A:H8	1.85	0.42
15:LF:20:ARG:HG2	15:LF:76:TYR:CE2	2.55	0.42
17:LH:378:ASP:O	26:LS:344:ARG:NH1	2.53	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
18:LJ:492:ARG:HH21	18:LJ:495:ILE:HD12	1.85	0.42
22:LN:631:GLU:HG2	22:LN:651:ALA:HB3	2.02	0.42
25:LQ:590:THR:HG1	25:LQ:600:TRP:HE1	1.66	0.42
28:LU:174:ARG:NH2	28:LU:206:VAL:O	2.49	0.42
28:LU:448:ARG:HE	53:8:1050:G:H21	1.68	0.42
30:LW:254:GLY:HA2	30:LW:277:VAL:HG23	2.02	0.42
35:SE:111:LYS:HA	35:SE:111:LYS:HD2	1.78	0.42
36:SG:257:ASP:HB2	36:SG:259:LYS:HE2	2.02	0.42
37:SH:231:ARG:HA	37:SH:231:ARG:HD3	1.90	0.42
42:SN:44:LYS:HD2	42:SN:236:LYS:HB2	2.00	0.42
44:SQ:117:VAL:HG23	44:SQ:149:ILE:HD11	2.01	0.42
53:8:243:G:H2'	53:8:244:A:H8	1.84	0.42
53:8:591:A:H2'	53:8:592:A:C8	2.55	0.42
53:8:1659:A:H2'	53:8:1660:A:C8	2.54	0.42
53:8:1661:U:H2'	53:8:1662:G:H8	1.85	0.42
54:SU:227:LYS:HA	54:SU:227:LYS:HD2	1.75	0.42
58:NE:199:ASP:N	58:NE:199:ASP:OD1	2.48	0.42
62:LX:18:VAL:HG11	62:LX:44:MET:HB2	2.00	0.42
62:LX:906:SER:OG	62:LX:907:ASN:N	2.53	0.42
66:6:249:ILE:O	66:6:253:SER:OG	2.31	0.42
4:L0:264:C:H2'	4:L0:265:A:C8	2.55	0.41
5:L2:18:G:H2'	5:L2:19:A:H8	1.85	0.41
9:L7:49:ILE:HG12	9:L7:172:VAL:HG12	2.01	0.41
17:LH:60:ARG:HB2	20:LL:341:ALA:HB1	2.02	0.41
18:LJ:109:ASP:OD1	18:LJ:109:ASP:N	2.51	0.41
19:LK:447:ASN:O	55:LI:671:ARG:NH2	2.51	0.41
20:LL:110:ILE:HD11	20:LL:117:LEU:HD21	2.02	0.41
20:LL:212:LEU:HB2	20:LL:226:LEU:HB2	2.02	0.41
23:LO:30:LEU:HD22	23:LO:39:VAL:HG22	2.02	0.41
25:LQ:553:ASN:HD22	25:LQ:573:LYS:H	1.66	0.41
25:LQ:659:GLU:O	25:LQ:677:HIS:N	2.49	0.41
28:LU:75:LYS:H	28:LU:75:LYS:HG2	1.70	0.41
29:LV:144:LEU:HB2	29:LV:155:VAL:HG22	2.02	0.41
36:SG:430:LYS:H	66:6:254:ASP:HB2	1.85	0.41
36:SG:523:LYS:HD2	36:SG:523:LYS:HA	1.85	0.41
38:SI:137:LEU:HD22	38:SI:232:PHE:HE1	1.84	0.41
38:SI:257:LEU:HA	38:SI:260:THR:HG22	2.01	0.41
41:SM:287:LYS:NZ	53:8:562:G:OP1	2.39	0.41
42:SN:227:SER:OG	42:SN:228:LYS:N	2.52	0.41
47:ST:753:LYS:HA	47:ST:753:LYS:HD2	1.79	0.41
53:8:329:G:H2'	53:8:330:G:C8	2.55	0.41


A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
53:8:523:G:N2	53:8:529:A:H62	2.17	0.41
53:8:1690:G:H2'	53:8:1691:A:H8	1.84	0.41
62:LX:197:ASN:OD1	62:LX:197:ASN:N	2.52	0.41
65:5:297:TRP:HE1	66:6:59:SER:HG	1.68	0.41
3:NB:560:ASN:ND2	53:8:477:A:OP1	2.53	0.41
8:L5:133:VAL:HG22	8:L5:198:LEU:HD13	2.01	0.41
12:LC:94:GLN:HE22	31:LZ:182:PHE:HB3	1.84	0.41
14:LE:39:GLN:O	14:LE:43:LYS:N	2.46	0.41
17:LH:491:GLN:H	17:LH:491:GLN:HG2	1.65	0.41
17:LH:698:VAL:HA	17:LH:701:VAL:HG22	2.01	0.41
19:LK:506:LEU:HB3	55:LI:655:LEU:HD21	2.02	0.41
20:LL:150:LYS:HD2	20:LL:150:LYS:HA	1.89	0.41
22:LN:741:LEU:HA	22:LN:756:GLU:HA	2.02	0.41
27:LT:169:SER:HG	27:LT:171:GLN:HE21	1.66	0.41
27:LT:932:VAL:HG22	57:LR:808:TYR:HB2	2.02	0.41
28:LU:195:ALA:HB2	28:LU:203:LEU:HD12	2.01	0.41
30:LW:46:LEU:HD13	46:SS:859:ARG:HH12	1.84	0.41
30:LW:123:THR:OG1	30:LW:140:ARG:NH2	2.53	0.41
37:SH:125:HIS:NE2	37:SH:263:ASP:OD1	2.45	0.41
38:SI:140:LEU:HD11	38:SI:152:THR:HB	2.01	0.41
38:SI:1135:ARG:HH11	53:8:494:U:H3'	1.85	0.41
40:SL:18:ASN:HD22	40:SL:21:LYS:HD2	1.84	0.41
40:SL:67:ILE:HG23	40:SL:71:PHE:HD2	1.85	0.41
41:SM:288:ASP:OD1	41:SM:288:ASP:N	2.51	0.41
53:8:972:G:H2'	53:8:973:A:H8	1.85	0.41
53:8:1672:G:H2'	53:8:1673:G:C8	2.55	0.41
54:SU:341:LEU:HD23	54:SU:341:LEU:HA	1.93	0.41
55:LI:68:PRO:O	55:LI:80:ALA:N	2.50	0.41
62:LX:916:ILE:HA	62:LX:919:LYS:HD2	2.02	0.41
65:5:458:ALA:HB2	65:5:463:LYS:HE3	2.02	0.41
1:NA:345:LEU:HD11	38:SI:961:PHE:HZ	1.85	0.41
5:L2:63:C:H2'	5:L2:64:A:H8	1.85	0.41
7:L4:62:LYS:NZ	53:8:454:U:OP2	2.44	0.41
7:L4:178:GLY:O	7:L4:231:GLN:NE2	2.49	0.41
8:L5:79:ASN:OD1	53:8:1583:A:O2'	2.36	0.41
9:L7:123:ASP:HA	9:L7:126:LEU:HG	2.02	0.41
9:L7:163:ASP:HA	9:L7:166:LEU:HD23	2.02	0.41
10:L8:195:ARG:NH2	13:LD:10:GLU:O	2.54	0.41
12:LC:13:LYS:HD2	12:LC:13:LYS:HA	1.89	0.41
17:LH:168:LEU:HD23	17:LH:168:LEU:HA	1.94	0.41
22:LN:71:ARG:HB2	22:LN:75:ASN:HB2	2.02	0.41



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
23:LO:538:GLN:HG3	23:LO:554:ASP:HA	2.01	0.41
25:LQ:656:HIS:CE1	25:LQ:660:VAL:HG22	2.55	0.41
27:LT:293:GLU:OE1	27:LT:293:GLU:N	2.52	0.41
28:LU:2:LYS:HZ2	30:LW:77:GLU:HG3	1.84	0.41
28:LU:48:THR:HA	28:LU:51:GLU:HG2	2.02	0.41
29:LV:158:SER:H	29:LV:183:VAL:HG12	1.86	0.41
34:SC:272:LYS:HG2	34:SC:275:CYS:H	1.85	0.41
39:SJ:97:LEU:HD23	39:SJ:97:LEU:HA	1.94	0.41
39:SJ:115:GLN:HB3	39:SJ:121:LEU:HD13	2.02	0.41
39:SJ:229:ASN:OD1	39:SJ:229:ASN:N	2.53	0.41
51:NH:1098:PHE:H	51:NH:1184:GLY:HA3	1.84	0.41
53:8:1208:A:N6	53:8:1454:G:C6	2.88	0.41
57:LR:548:LEU:O	57:LR:560:TRP:N	2.44	0.41
63:L6:102:VAL:HG23	63:L6:106:LEU:HG	2.02	0.41
4:L0:145:A:H2'	4:L0:146:G:C8	2.54	0.41
12:LC:26:LYS:H	12:LC:26:LYS:HG2	1.73	0.41
17:LH:730:ASP:HB3	17:LH:734:VAL:HG22	2.02	0.41
17:LH:847:ASP:N	17:LH:847:ASP:OD1	2.53	0.41
21:LM:160:LEU:HD23	59:SB:412:VAL:HG11	2.02	0.41
22:LN:474:SER:OG	22:LN:475:THR:N	2.52	0.41
23:LO:11:LEU:HD11	23:LO:372:TRP:HB3	2.03	0.41
25:LQ:220:THR:HB	25:LQ:259:ILE:HD11	2.02	0.41
27:LT:417:LEU:HG	27:LT:432:THR:HG22	2.01	0.41
29:LV:80:GLN:HB3	29:LV:82:HIS:CD2	2.56	0.41
31:LZ:135:HIS:HB3	31:LZ:166:ILE:HG21	2.02	0.41
34:SD:244:VAL:HG11	34:SD:252:ILE:HG21	2.02	0.41
35:SF:24:VAL:HG12	35:SF:102:ILE:HD11	2.03	0.41
36:SG:410:ASP:OD1	36:SG:410:ASP:N	2.53	0.41
37:SH:133:ILE:HG23	37:SH:137:LEU:HD12	2.03	0.41
53:8:202:A:O2'	53:8:203:U:O4'	2.38	0.41
63:L6:3:LEU:HD12	63:L6:111:LEU:HD11	2.01	0.41
2:SA:6:TYR:HE1	2:SA:19:LYS:HD2	1.86	0.41
2:SA:302:ASN:OD1	2:SA:401:GLY:N	2.53	0.41
4:L0:89:C:H5"	4:L0:90:G:H5'	2.02	0.41
4:L0:192:G:H2'	4:L0:193:G:C8	2.56	0.41
9:L7:45:SER:OG	9:L7:47:ARG:NH1	2.53	0.41
9:L7:165:LYS:HE2	9:L7:169:PHE:HZ	1.85	0.41
13:LD:90:TYR:O	13:LD:92:HIS:ND1	2.54	0.41
17:LH:648:LYS:HE2	17:LH:648:LYS:HB2	1.88	0.41
18:LJ:262:GLU:HG3	18:LJ:270:SER:HB3	2.02	0.41
21:LM:316:PRO:HD2	21:LM:319:ILE:HD12	2.03	0.41



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
22:LN:143:VAL:HB	56:ND:198:ILE:HD13	2.02	0.41
23:LO:641:LEU:HD12	23:LO:641:LEU:HA	1.93	0.41
23:LO:728:GLU:HA	23:LO:731:ARG:HD2	2.01	0.41
25:LQ:142:ASP:OD1	25:LQ:142:ASP:N	2.39	0.41
25:LQ:676:SER:OG	25:LQ:678:ASP:OD1	2.27	0.41
26:LS:251:ILE:HG12	26:LS:584:GLY:HA2	2.03	0.41
28:LU:233:ASP:HB3	28:LU:249:LEU:HB2	2.01	0.41
28:LU:267:ILE:HG22	28:LU:279:THR:HG22	2.03	0.41
29:LV:80:GLN:HB3	29:LV:82:HIS:HD2	1.85	0.41
30:LW:203:TYR:HE2	30:LW:433:LEU:HA	1.85	0.41
34:SC:291:GLN:HE21	40:SL:128:LEU:HB2	1.85	0.41
38:SI:98:LEU:HB2	38:SI:101:ILE:HD11	2.02	0.41
38:SI:841:THR:HG22	38:SI:860:TYR:H	1.84	0.41
39:SJ:46:ALA:HA	39:SJ:115:GLN:HG2	2.01	0.41
40:SL:185:LEU:HD23	40:SL:186:PRO:HD2	2.02	0.41
46:SS:837:LYS:HD3	46:SS:837:LYS:HA	1.89	0.41
53:8:415:C:OP1	62:LX:70:ARG:NH1	2.52	0.41
53:8:1131:A:O2'	53:8:1136:U:O4	2.34	0.41
54:SU:130:GLU:HB3	54:SU:144:PRO:HG3	2.02	0.41
54:SU:136:SER:O	54:SU:136:SER:OG	2.36	0.41
55:LI:608:GLN:HA	55:LI:611:ILE:HG12	2.03	0.41
62:LX:15:ARG:HH21	62:LX:47:ALA:HB2	1.84	0.41
1:NA:437:ILE:HD11	31:LZ:61:LEU:HG	2.03	0.41
4:L0:68:U:O4	17:LH:422:LYS:NZ	2.53	0.41
7:L4:69:HIS:HD2	15:LF:17:LEU:HB2	1.85	0.41
9:L7:81:LEU:HD23	9:L7:81:LEU:HA	1.87	0.41
17:LH:96:ILE:HG12	17:LH:108:THR:HG21	2.02	0.41
22:LN:497:ILE:HD11	22:LN:555:LEU:HD13	2.02	0.41
26:LS:154:LYS:HB3	26:LS:154:LYS:HE2	1.83	0.41
26:LS:247:SER:OG	26:LS:248:HIS:N	2.54	0.41
27:LT:474:PHE:HE1	27:LT:495:ARG:HG3	1.86	0.41
38:SI:54:LEU:HD23	45:SR:50:LYS:HB2	2.03	0.41
38:SI:568:ARG:HA	38:SI:568:ARG:HD3	1.80	0.41
38:SI:1123:LYS:HE2	38:SI:1123:LYS:HB2	1.91	0.41
39:SJ:152:SER:O	39:SJ:155:SER:OG	2.28	0.41
44:SQ:60:LYS:H	44:SQ:60:LYS:HG2	1.70	0.41
45:SR:58:GLY:HA3	45:SR:69:ARG:HA	2.02	0.41
47:ST:267:UNK:O	47:ST:271:UNK:N	2.53	0.41
53:8:140:A:N9	63:L6:184:LEU:N	2.69	0.41
53:8:144:U:H2'	53:8:145:A:H4'	2.02	0.41
53:8:890:C:H2'	53:8:891:A:C8	2.55	0.41



Atom-1	Atom-2	Interatomic	\mathbf{Clash}_{\circ}
		distance (Å)	overlap (Å)
55:LI:170:LYS:HA	55:LI:177:SER:HA	2.03	0.41
55:LI:248:LEU:HA	55:LI:264:SER:HA	2.02	0.41
59:SB:153:LYS:HE3	59:SB:378:GLU:HB2	2.02	0.41
1:NA:357:ILE:HD13	41:SM:234:ARG:HH21	1.86	0.41
2:SA:180:LEU:HD13	59:SB:183:ARG:HG2	2.03	0.41
2:SA:388:ARG:HB3	35:SF:63:ILE:HA	2.02	0.41
4:L0:411:A:H2'	4:L0:412:A:C8	2.56	0.41
4:L0:489:G:H22	24:LP:125:SER:H	1.69	0.41
10:L8:32:GLN:HE22	10:L8:34:ALA:HB2	1.84	0.41
17:LH:31:ASN:OD1	17:LH:31:ASN:N	2.53	0.41
20:LL:20:VAL:HG12	20:LL:29:VAL:HG22	2.03	0.41
22:LN:287:THR:HG21	22:LN:337:CYS:HA	2.03	0.41
23:LO:557:LYS:HD3	23:LO:557:LYS:HA	1.88	0.41
26:LS:150:TYR:HE1	30:LW:80:LEU:HA	1.86	0.41
26:LS:529:ILE:HD12	26:LS:591:LEU:HD13	2.02	0.41
27:LT:184:THR:OG1	27:LT:187:ASN:OD1	2.32	0.41
28:LU:255:THR:OG1	28:LU:256:GLN:N	2.53	0.41
28:LU:401:LYS:HE3	28:LU:401:LYS:HB2	1.79	0.41
29:LV:81:ILE:HD12	29:LV:81:ILE:HA	1.96	0.41
30:LW:148:LEU:HD23	30:LW:148:LEU:HA	1.96	0.41
30:LW:182:THR:HG22	40:SL:15:ARG:HG2	2.02	0.41
30:LW:204:LEU:HD12	30:LW:204:LEU:HA	1.93	0.41
30:LW:384:VAL:HA	30:LW:385:PRO:HD3	1.92	0.41
38:SI:776:GLN:HA	38:SI:780:ILE:HG22	2.01	0.41
46:SS:277:ARG:HA	46:SS:280:GLN:HG2	2.03	0.41
48:SY:125:LEU:HD12	48:SY:125:LEU:HA	1.93	0.41
53:8:999:U:N3	53:8:1002:G:OP1	2.42	0.41
54:SU:383:LEU:O	54:SU:387:THR:OG1	2.28	0.41
62:LY:744:PRO:HA	62:LY:762:MET:HA	2.03	0.41
62:LX:132:PRO:HA	62:LX:135:LEU:HD12	2.02	0.41
65:5:406:TYR:O	66:6:82:ARG:NH2	2.54	0.41
65:5:470:ASP:OD1	65:5:471:PRO:HD3	2.20	0.41
2:SA:324:ASN:HA	2:SA:327:LYS:HB2	2.03	0.41
4:L0:289:U:H2'	4:L0:290:G:C8	2.56	0.41
4:L0:409:C:H2'	4:L0:410:A:C8	2.56	0.41
10:L8:32:GLN:H	10:L8:32:GLN:HG3	1.70	0.41
13:LD:32:LYS:HE2	13:LD:32:LYS:HB2	1.82	0.41
17:LH:690:ASN:ND2	17:LH:750:LEU:O	2.54	0.41
18:LJ:507:MET:HE2	18:LJ:507:MET:HB3	1.96	0.41
22:LN:105:SER:O	22:LN:105:SER:OG	2.34	0.41
24:LP:410:UNK:O	24:LP:414:UNK:N	2.54	0.41



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
25:LQ:400:SER:HB3	25:LQ:404:LYS:HB3	2.03	0.41
25:LQ:824:MET:HA	25:LQ:825:PRO:HD3	1.94	0.41
27:LT:187:ASN:OD1	27:LT:187:ASN:N	2.51	0.41
28:LU:26:ARG:NH2	46:SS:867:GLN:O	2.54	0.41
28:LU:142:ASP:OD1	28:LU:142:ASP:N	2.48	0.41
28:LU:254:PRO:HG2	46:SS:284:ARG:NE	2.36	0.41
29:LV:126:GLN:HE21	29:LV:130:GLY:HA2	1.86	0.41
31:LZ:57:LEU:HA	31:LZ:57:LEU:HD12	1.85	0.41
36:SG:553:ILE:HD12	36:SG:553:ILE:HA	1.99	0.41
38:SI:838:ILE:HD11	53:8:578:U:C4	2.56	0.41
38:SI:969:VAL:HG12	38:SI:1000:ILE:H	1.85	0.41
52:NI:41:ARG:HA	52:NI:53:LEU:HA	2.02	0.41
53:8:600:U:H2'	53:8:601:A:C8	2.55	0.41
53:8:1110:G:O2'	53:8:1111:G:O4'	2.37	0.41
53:8:1661:U:H2'	53:8:1662:G:C8	2.56	0.41
2:SA:15:TYR:CZ	2:SA:78:LEU:HB2	2.55	0.41
4:L0:114:G:H2'	4:L0:115:G:C8	2.56	0.41
4:L0:223:C:H2'	4:L0:224:G:C8	2.56	0.41
7:L4:36:HIS:CE1	7:L4:85:GLY:HA3	2.56	0.41
7:L4:125:LYS:HB3	7:L4:142:HIS:HD2	1.85	0.41
8:L5:196:GLU:OE2	8:L5:200:ASN:ND2	2.45	0.41
9:L7:56:LYS:HB2	9:L7:88:ARG:HH12	1.86	0.41
9:L7:91:ILE:HG21	9:L7:129:LEU:HD12	2.03	0.41
11:L9:173:ALA:HB2	53:8:511:A:H5'	2.03	0.41
14:LE:19:LYS:HD3	14:LE:19:LYS:HA	1.83	0.41
17:LH:780:GLU:O	17:LH:782:THR:N	2.54	0.41
18:LJ:90:ARG:HG3	18:LJ:92:ASP:H	1.85	0.41
21:LM:284:SER:OG	21:LM:285:ASN:N	2.53	0.41
23:LO:482:SER:OG	23:LO:486:SER:N	2.53	0.41
23:LO:791:HIS:O	23:LO:795:ASN:ND2	2.54	0.41
26:LS:156:ASN:OD1	26:LS:156:ASN:N	2.54	0.41
27:LT:59:GLN:HG2	27:LT:71:VAL:HG12	2.02	0.41
27:LT:173:LEU:HD23	27:LT:173:LEU:HA	1.90	0.41
28:LU:247:TYR:HD1	28:LU:254:PRO:HB3	1.86	0.41
29:LV:102:VAL:HG23	29:LV:117:LEU:HD23	2.03	0.41
35:SE:21:LEU:HA	35:SE:24:VAL:HG22	2.02	0.41
35:SE:37:ALA:HA	35:SE:99:ALA:HB3	2.03	0.41
36:SG:274:ILE:HA	36:SG:275:PRO:HD3	1.89	0.41
36:SG:343:ASP:OD1	36:SG:343:ASP:N	2.47	0.41
36:SG:523:LYS:NZ	36:SG:525:GLN:OE1	2.41	0.41
37:SH:24:ALA:HA	37:SH:27:SER:HB3	2.03	0.41



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
37:SH:134:LYS:HB3	37:SH:134:LYS:HE2	1.90	0.41
37:SH:298:ILE:HD13	37:SH:298:ILE:HA	1.95	0.41
38:SI:780:ILE:HD12	38:SI:780:ILE:HA	1.92	0.41
39:SK:88:ARG:HE	39:SK:88:ARG:HB3	1.64	0.41
39:SK:188:ARG:HG2	39:SK:190:GLN:HB2	2.03	0.41
42:SN:242:ILE:HG12	42:SN:255:TYR:HB3	2.03	0.41
45:SR:104:LEU:HD13	45:SR:104:LEU:HA	1.92	0.41
47:ST:495:ASN:ND2	47:ST:617:HIS:O	2.53	0.41
47:ST:575:PHE:HD1	47:ST:600:LEU:HB2	1.84	0.41
52:NI:40:LYS:O	52:NI:54:PHE:N	2.53	0.41
53:8:9:U:H5"	58:NE:292:LYS:HE2	2.01	0.41
53:8:107:C:H2'	53:8:108:A:H8	1.86	0.41
53:8:116:U:H2'	53:8:117:U:C6	2.56	0.41
53:8:222:A:H5'	53:8:246:G:C2	2.56	0.41
53:8:312:A:H4'	53:8:313:U:H5'	2.03	0.41
53:8:477:A:H2'	53:8:478:A:H8	1.85	0.41
53:8:911:U:H5'	57:LR:534:ARG:HB2	2.02	0.41
53:8:1783:C:H2'	53:8:1784:C:C6	2.56	0.41
55:LI:572:SER:HB3	55:LI:574:ARG:NH1	2.36	0.41
55:LI:604:LYS:HB2	55:LI:604:LYS:HE2	1.86	0.41
57:LR:87:ILE:HG12	57:LR:97:ARG:HB2	2.03	0.41
57:LR:284:PRO:HB2	57:LR:288:LEU:HD23	2.03	0.41
63:L6:201:GLN:O	63:L6:205:ALA:N	2.50	0.41
2:SA:18:PHE:HD1	2:SA:50:LEU:HA	1.86	0.41
2:SA:411:ARG:HA	2:SA:411:ARG:HD3	1.94	0.41
3:NB:559:ARG:HE	53:8:545:A:H8	1.67	0.41
3:NB:604:ARG:NH1	53:8:498:G:O3'	2.50	0.41
4:L0:467:A:N1	4:L0:468:A:N6	2.69	0.41
11:L9:77:ILE:HG23	11:L9:86:LEU:HD23	2.03	0.41
12:LC:39:VAL:O	12:LC:45:ARG:NH2	2.54	0.41
14:LE:40:VAL:O	14:LE:44:HIS:ND1	2.40	0.41
16:LG:21:SER:OG	16:LG:25:VAL:O	2.28	0.41
18:LJ:101:ALA:HA	18:LJ:126:PRO:HB3	2.03	0.41
20:LL:198:THR:HG23	20:LL:200:GLU:H	1.86	0.41
22:LN:112:LEU:HD11	22:LN:525:VAL:HG22	2.02	0.41
22:LN:197:LYS:HA	22:LN:197:LYS:HD3	1.76	0.41
22:LN:393:SER:OG	22:LN:394:TRP:N	2.54	0.41
23:LO:539:ILE:HB	23:LO:553:ILE:HG13	2.02	0.41
26:LS:541:LEU:O	26:LS:542:ARG:NH1	2.42	0.41
28:LU:186:ASP:HB2	28:LU:225:LEU:HG	2.03	0.41
35:SE:106:ASP:OD1	35:SE:106:ASP:N	2.54	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
36:SG:461:LYS:HA	36:SG:461:LYS:HD3	1.92	0.41
38:SI:118:LEU:HD23	38:SI:131:ILE:HD11	2.01	0.41
47:ST:426:THR:HG22	47:ST:462:LEU:HD13	2.02	0.41
57:LR:768:ASN:HB3	57:LR:771:LYS:HE3	2.03	0.41
65:5:486:SER:OG	65:5:488:ASP:OD1	2.29	0.41
3:NB:518:ILE:HD13	3:NB:518:ILE:HA	1.91	0.40
4:L0:409:C:H2'	4:L0:410:A:H8	1.87	0.40
7:L4:75:LYS:HB2	7:L4:77:ARG:HG2	2.02	0.40
9:L7:76:LYS:HA	9:L7:76:LYS:HD2	1.89	0.40
13:LD:74:THR:O	13:LD:87:ARG:N	2.54	0.40
17:LH:75:SER:HA	17:LH:79:LEU:HB2	2.02	0.40
17:LH:600:SER:HB2	17:LH:638:PHE:HB3	2.03	0.40
23:LO:188:ASN:N	23:LO:188:ASN:OD1	2.52	0.40
29:LV:24:SER:H	29:LV:49:LEU:HD21	1.86	0.40
29:LV:177:LYS:HA	29:LV:177:LYS:HD2	1.81	0.40
34:SC:104:ASP:OD1	44:SQ:127:ARG:NH1	2.54	0.40
34:SD:304:LEU:HD23	34:SD:306:LEU:HD12	2.04	0.40
38:SI:129:ILE:HD11	38:SI:853:ARG:HD2	2.03	0.40
39:SJ:174:LYS:HG2	39:SJ:199:ASP:HB3	2.03	0.40
39:SJ:175:CYS:SG	39:SJ:176:ARG:N	2.94	0.40
41:SM:263:LEU:HD12	41:SM:263:LEU:HA	1.91	0.40
42:SN:125:VAL:HG13	42:SN:151:PRO:HA	2.02	0.40
53:8:340:U:H2'	53:8:341:A:H8	1.86	0.40
53:8:922:G:H2'	53:8:923:A:C8	2.56	0.40
53:8:1695:G:C2	53:8:1706:C:C2	3.08	0.40
59:SB:53:ALA:HB3	59:SB:56:ALA:HB3	2.03	0.40
59:SB:210:LEU:HD11	59:SB:260:GLU:HB3	2.03	0.40
59:SB:299:LEU:HD23	59:SB:341:LEU:HD23	2.03	0.40
2:SA:82:LEU:HD23	2:SA:82:LEU:HA	1.81	0.40
4:L0:250:G:H1	4:L0:262:U:H3	1.70	0.40
4:L0:523:U:H5"	28:LU:126:LYS:HA	2.02	0.40
9:L7:166:LEU:HA	9:L7:169:PHE:CD1	2.56	0.40
15:LF:59:GLY:HA3	15:LF:72:PHE:HB3	2.03	0.40
20:LL:516:ILE:HG23	20:LL:519:LEU:HD21	2.04	0.40
23:LO:526:ASP:HA	23:LO:815:TYR:CZ	2.57	0.40
25:LQ:292:UNK:O	25:LQ:296:UNK:N	2.54	0.40
27:LT:847:LEU:O	27:LT:851:SER:OG	2.31	0.40
28:LU:58:PHE:HE1	28:LU:373:ARG:HG2	1.86	0.40
28:LU:92:ILE:HG13	28:LU:106:PHE:HB2	2.02	0.40
28:LU:109:HIS:CG	28:LU:140:SER:HB2	2.55	0.40
28:LU:263:ARG:O	28:LU:281:ASN:ND2	2.54	0.40



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
30:LW:458:THR:HA	46:SS:854:ARG:HD3	2.02	0.40
32:NG:21:ALA:HA	32:NG:26:THR:HA	2.02	0.40
36:SG:225:LYS:HE3	36:SG:225:LYS:HB3	1.92	0.40
37:SH:244:THR:HG23	37:SH:259:GLU:HB3	2.02	0.40
37:SH:307:ASP:OD1	38:SI:765:ASN:ND2	2.46	0.40
43:SO:263:LEU:HA	43:SO:266:VAL:HG22	2.02	0.40
45:SR:130:VAL:HG13	45:SR:135:LEU:HD21	2.02	0.40
46:SS:278:ILE:H	46:SS:278:ILE:HD12	1.86	0.40
53:8:1733:C:H2'	53:8:1734:U:H6	1.87	0.40
57:LR:200:GLU:O	57:LR:256:ARG:NH2	2.54	0.40
62:LX:658:ARG:HD3	62:LX:766:LEU:HD13	2.04	0.40
65:5:416:VAL:O	65:5:420:ASP:N	2.45	0.40
3:NB:591:TYR:OH	3:NB:594:GLU:O	2.32	0.40
4:L0:286:U:H2'	4:L0:287:G:H8	1.86	0.40
4:L0:494:C:H2'	4:L0:495:G:C8	2.56	0.40
5:L2:45:U:O2'	40:SL:23:GLN:OE1	2.28	0.40
5:L2:310:G:H2'	5:L2:311:G:C8	2.55	0.40
9:L7:154:LEU:HD12	9:L7:185:ILE:HG22	2.03	0.40
10:L8:78:ILE:HA	10:L8:104:ILE:HG22	2.02	0.40
17:LH:546:LYS:HE2	17:LH:548:ILE:HD11	2.02	0.40
18:LJ:256:THR:HG21	18:LJ:277:LEU:HD13	2.03	0.40
21:LM:31:ALA:HB1	21:LM:154:ILE:HG23	2.03	0.40
21:LM:83:ARG:HE	21:LM:91:ILE:HD11	1.86	0.40
21:LM:124:ARG:HA	21:LM:124:ARG:HD2	1.87	0.40
23:LO:425:PHE:HB3	23:LO:458:TRP:CD1	2.56	0.40
23:LO:496:THR:HG22	23:LO:513:GLU:HB3	2.03	0.40
23:LO:612:LEU:HD23	23:LO:612:LEU:HA	1.90	0.40
27:LT:814:GLU:OE1	27:LT:822:ARG:NH1	2.55	0.40
27:LT:856:GLU:HB2	43:SO:252:LEU:HD11	2.03	0.40
31:LZ:55:ARG:HG2	31:LZ:98:GLU:HG2	2.03	0.40
34:SD:163:PHE:CG	34:SD:266:GLY:HA3	2.56	0.40
35:SE:68:PRO:HA	35:SE:71:CYS:HB2	2.02	0.40
37:SH:113:LYS:HE3	37:SH:113:LYS:HB3	1.94	0.40
38:SI:180:GLN:HA	38:SI:183:LEU:HB3	2.03	0.40
38:SI:310:THR:HA	38:SI:311:PRO:HD3	1.96	0.40
38:SI:832:HIS:CD2	38:SI:834:TRP:HB2	2.56	0.40
39:SJ:150:ILE:HD12	39:SJ:160:LEU:HD12	2.02	0.40
47:ST:643:LEU:HD23	47:ST:684:ILE:HD13	2.03	0.40
53:8:1210:C:H2'	53:8:1211:A:C8	2.56	0.40
59:SB:226:ILE:HG13	59:SB:227:LEU:HD12	2.03	0.40
62:LX:62:LYS:HA	62:LX:62:LYS:HD3	1.80	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
62:LX:200:VAL:HG22	62:LX:208:LEU:HD12	2.03	0.40
62:LX:881:GLN:H	62:LX:881:GLN:HG2	1.67	0.40
65:5:194:ILE:HD11	65:5:421:LEU:HD11	2.03	0.40
4:L0:192:G:H2'	4:L0:193:G:H8	1.85	0.40
4:L0:305:A:H2'	4:L0:306:G:C8	2.57	0.40
4:L0:480:C:O2	24:LP:46:ARG:NH1	2.54	0.40
7:L4:112:HIS:NE2	7:L4:237:SER:O	2.55	0.40
18:LJ:62:ARG:HE	18:LJ:62:ARG:HB3	1.76	0.40
18:LJ:128:HIS:CE1	18:LJ:172:ARG:HH21	2.40	0.40
21:LM:131:ASN:OD1	21:LM:131:ASN:N	2.48	0.40
21:LM:218:ILE:HG23	21:LM:263:VAL:HG11	2.02	0.40
22:LN:394:TRP:HB3	22:LN:399:VAL:HG13	2.02	0.40
22:LN:639:ASP:OD2	22:LN:647:TRP:NE1	2.52	0.40
25:LQ:589:ILE:HG12	25:LQ:599:ILE:HG12	2.03	0.40
28:LU:326:ASP:OD1	28:LU:326:ASP:N	2.46	0.40
29:LV:195:LEU:HD13	29:LV:207:TRP:HB2	2.04	0.40
29:LV:238:ASN:N	29:LV:238:ASN:OD1	2.55	0.40
35:SE:20:ILE:HD13	35:SE:79:VAL:HG21	2.04	0.40
47:ST:571:ILE:HD13	47:ST:571:ILE:HA	1.89	0.40
47:ST:573:LEU:HD23	47:ST:573:LEU:HA	1.93	0.40
53:8:631:G:O6	53:8:968:U:O4	2.39	0.40
53:8:1512:G:H2'	53:8:1513:G:C8	2.56	0.40
57:LR:299:ASN:O	57:LR:301:GLN:NE2	2.41	0.40
57:LR:536:LEU:HA	57:LR:552:SER:HA	2.04	0.40
4:L0:505:G:H2'	4:L0:506:G:C8	2.56	0.40
20:LL:58:LEU:HD13	20:LL:80:MET:HE1	2.04	0.40
20:LL:469:ILE:HB	20:LL:508:ILE:HD12	2.04	0.40
21:LM:6:ASP:OD1	21:LM:6:ASP:N	2.54	0.40
22:LN:758:ASN:HB2	22:LN:763:HIS:CD2	2.57	0.40
23:LO:162:LEU:HD13	23:LO:197:ALA:HB3	2.04	0.40
23:LO:750:LEU:HD23	23:LO:750:LEU:HA	1.84	0.40
25:LQ:341:ALA:HB1	25:LQ:353:LEU:HD11	2.03	0.40
25:LQ:395:ARG:HA	25:LQ:395:ARG:HD3	1.85	0.40
27:LT:544:ALA:HB3	27:LT:562:LEU:HD22	2.02	0.40
34:SC:178:GLY:HA2	34:SC:181:VAL:HG12	2.02	0.40
34:SD:253:ILE:HD13	34:SD:253:ILE:HA	1.94	0.40
38:SI:241:HIS:HB3	38:SI:851:TRP:HE1	1.86	0.40
38:SI:833:ARG:HH12	45:SR:141:GLU:HG3	1.86	0.40
39:SJ:136:ARG:HD3	53:8:1195:C:C2	2.56	0.40
41:SM:16:LYS:HE2	41:SM:16:LYS:HB2	1.95	0.40
42:SN:223:LEU:HD12	42:SN:235:ILE:HG13	2.03	0.40



Atom-1	Atom-1 Atom-2		Clash overlap (Å)
47:ST:418:UNK:O	47:ST:420:GLU:N	2.53	0.40
47:ST:644:ASP:HB3	47:ST:684:ILE:HG12	2.04	0.40
53:8:33:U:H2'	53:8:34:G:C2	2.57	0.40
53:8:1670:G:HO2'	53:8:1671:A:H8	1.67	0.40
54:SU:381:LYS:HE3	54:SU:385:ARG:HH21	1.85	0.40
57:LR:192:ALA:O	57:LR:216:ARG:NH1	2.54	0.40
62:LX:185:ASN:HA	62:LX:188:PHE:HB3	2.04	0.40
62:LX:319:LYS:O	62:LX:323:GLU:N	2.53	0.40
62:LX:862:LEU:O	62:LX:866:TYR:N	2.54	0.40
63:L6:183:ARG:O	63:L6:187:LYS:N	2.52	0.40
65:5:247:ILE:HG23	65:5:262:ALA:HB1	2.03	0.40
66:6:242:MET:HG3	66:6:245:MET:HG2	2.04	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	entiles
1	NA	203/245~(83%)	194 (96%)	8 (4%)	1 (0%)	29	67
2	SA	338/413~(82%)	332~(98%)	6 (2%)	0	100	100
3	NB	126/180~(70%)	118 (94%)	7~(6%)	1 (1%)	19	58
6	L3	100/127~(79%)	91 (91%)	9 (9%)	0	100	100
7	L4	226/228~(99%)	202~(89%)	24 (11%)	0	100	100
8	L5	211/213~(99%)	194~(92%)	17 (8%)	0	100	100
9	L7	161/190~(85%)	142 (88%)	19 (12%)	0	100	100
10	L8	166/200~(83%)	156 (94%)	10 (6%)	0	100	100
11	L9	173/175~(99%)	159 (92%)	14 (8%)	0	100	100
12	LC	123/125~(98%)	113 (92%)	10 (8%)	0	100	100



Conti				
Mol	Chain	Analysed	Favoured	Allowed
13	LD	123/156~(79%)	109 (89%)	14 (11%)
14	LE	125/127~(98%)	115 (92%)	10 (8%)
15	LF	88/90~(98%)	74 (84%)	13 (15%)
16	LG	61/63~(97%)	59 (97%)	2(3%)
17	LH	810/896~(90%)	754 (93%)	56 (7%)
18	LJ	489/513~(95%)	461 (94%)	28 (6%)
19	LK	86/123~(70%)	84 (98%)	2 (2%)

13LD123/156 (79%)109 (89%)14 (11%)010010014LE125/127 (98%)115 (92%)10 (8%)01010010015LF88/90 (98%)74 (84%)13 (15%)1 (1%)145116LG61/63 (97%)59 (97%)2 (3%)010010017LH810/896 (90%)754 (93%)56 (7%)010010018LJ489/513 (95%)461 (94%)28 (6%)010010019LK86/123 (70%)84 (98%)2 (2%)010010020LL465/555 (84%)435 (94%)30 (6%)010010021LM654/748 (87%)610 (93%)43 (7%)10(%)477923LO830/855 (97%)777 (94%)53 (6%)010010024LP259/420 (62%)257 (99%)2 (1%)010010025LQ798/939 (85%)739 (93%)58 (7%)1 (0%)518126LS473/594 (80%)448 (95%)25 (5%)010010010027LT844/921 (92%)805 (95%)39 (5%)010010010028LU453/465 (97%)415 (92%)36 (10%)010010030LW436/438 (100%)449 (95%)27 (6%)010010031LZ180/12 (98%)170 (94%)	Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14LE125/127 (98%)115 (92%)10 (8%)010010010015LF88/90 (98%)74 (84%)13 (15%)1 (1%)145116LG61/63 (97%)59 (97%)2 (3%)010010010017LH810/896 (90%)754 (93%)56 (7%)010010010018LJ489/513 (95%)461 (94%)28 (6%)010010010019LK86/123 (70%)84 (98%)2 (2%)010010010020LL465/555 (84%)435 (94%)30 (6%)010010010021LM654/748 (87%)610 (93%)43 (7%)1 (0%)477923LO830/855 (97%)777 (94%)53 (6%)010010010024LP259/420 (62%)257 (99%)2 (1%)010010010025LQ798/939 (85%)739 (93%)58 (7%)1 (0%)5010010026LS473/594 (80%)448 (95%)25 (5%)010010010027LT844/921 (92%)805 (95%)39 (5%)010010028LU453/465 (97%)170 (94%)36 (10%)010010029LV360/362 (99%)324 (90%)36 (10%)010010030LU436/438 (100%)170 (94%)10 (6%)0100<	13	LD	123/156~(79%)	109 (89%)	14 (11%)	0	100	100
15LF $88/90 (98\%)$ $74 (84\%)$ $13 (15\%)$ $1 (1\%)$ 14 51 16LG $61/63 (97\%)$ $59 (97\%)$ $2 (3\%)$ 0 100 100 100 17LH $810/896 (90\%)$ $754 (93\%)$ $56 (7\%)$ 0 100 100 100 18LJ $489/513 (95\%)$ $461 (94\%)$ $28 (6\%)$ 0 100 100 100 19LK $86/123 (70\%)$ $84 (98\%)$ $2 (2\%)$ 0 100 100 100 20LL $465/555 (84\%)$ $435 (94\%)$ $30 (6\%)$ 0 100 100 100 21LM $424/431 (98\%)$ $407 (96\%)$ $17 (4\%)$ 0 100 100 100 22LN $654/748 (87\%)$ $610 (93\%)$ $43 (7\%)$ $1 (0\%)$ 100 100 100 23LO $830/855 (97\%)$ $777 (94\%)$ $53 (6\%)$ 0 100 100 100 24LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 0 100 100 100 25LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 100 100 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 0 100 100 27LT $844/921 (92\%)$ $36 (10\%)$ $36 (10\%)$ 0 100 100 28LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 0 100 100 30LW $436/438 (100\%)$	14	LE	125/127~(98%)	115 (92%)	10 (8%)	0	100	100
16LG $61/63$ 97% 2 2 0 100 100 100 17LH $810/896$ 754 93% 56 7% 0 100 100 18LJ $489/513$ 95% 461 94% 28 6% 0 100 100 19LK $86/123$ 70% 84 98% 2 2% 0 100 100 20LL $465/555$ 84% 435 94% 30 6% 0 100 100 21LM $424/431$ 98% 407 97 3 6% 100 100 100 22LN $654/748$ 87% 610 33 6% 0 100 100 100 23LO $830/855$ 97% 777 94% 53 6% 0 100 100 24LP $259/420$ 62% 257 90% 1 00 100 100 25LQ $798/939$ 85% 39 5% 1 0% 10 100 26LS $473/594$ 805 93 39 5% 1 0% 100 100 27LT $844/921$ 92% 38 30 0 100 100 100 28LU $453/465$ 97% 36 0 100 100 100 29LV $360/362$ 99% 324 96 0 1	15	LF	88/90~(98%)	74 (84%)	13 (15%)	1 (1%)	14	51
17LH $810/896 (90\%)$ $754 (93\%)$ $56 (7\%)$ 010010018LJ $489/513 (95\%)$ $461 (94\%)$ $28 (6\%)$ 010010019LK $86/123 (70\%)$ $84 (98\%)$ $2 (2\%)$ 010010020LL $465/555 (84\%)$ $435 (94\%)$ $30 (6\%)$ 010010021LM $424/431 (98\%)$ $407 (96\%)$ $17 (4\%)$ 010010022LN $654/748 (87\%)$ $610 (93\%)$ $43 (7\%)$ $1 (0\%)$ 47 79 23LO $830/855 (97\%)$ $777 (94\%)$ $53 (6\%)$ 010010024LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 010010025LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 51 84 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 010010027LT $844/921 (92\%)$ $805 (95\%)$ $39 (5\%)$ 010010028LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 010010029LV $360/362 (99\%)$ $324 (90\%)$ $36 (10\%)$ 010010030LW $436/438 (100\%)$ $409 (94\%)$ $27 (6\%)$ 010010031LZ $180/182 (99\%)$ $170 (94\%)$ $10 (6\%)$ 010010033NK $173/175 (99\%)$ $165 (95\%)$ $8 (5\%)$ 0100100	16	LG	61/63~(97%)	59 (97%)	2 (3%)	0	100	100
18LJ489/513 (95%)461 (94%)28 (6%)010010019LK86/123 (70%)84 (98%)2 (2%)010010020LL465/555 (84%)435 (94%)30 (6%)010010021LM424/431 (98%)407 (96%)17 (4%)010010022LN654/748 (87%)610 (93%)43 (7%)1 (0%)477923LO830/855 (97%)777 (94%)53 (6%)010010024LP259/420 (62%)257 (99%)2 (1%)010010025LQ798/939 (85%)739 (93%)58 (7%)1 (0%)518426LS473/594 (80%)448 (95%)25 (5%)010010027LT844/921 (92%)805 (95%)39 (5%)010010028LU453/465 (97%)415 (92%)38 (8%)010010029IV360/362 (99%)324 (90%)36 (10%)010010030LW436/438 (100%)409 (94%)27 (6%)010010031LZ180/182 (99%)170 (94%)12 (11%)010010033NK173/175 (99%)165 (95%)8 (5%)010010034SC238/247 (96%)227 (95%)11 (5%)010010035SF119/121 (98%)107 (99%)12 (10%)0	17	LH	810/896~(90%)	754 (93%)	56 (7%)	0	100	100
19LK $86/123$ (70%) 84 (98%) 2 (2%)010010020LL $465/555$ (84%) 435 (94%) 30 (6%)010010021LM $424/431$ (98%) 407 (96%) 17 (4%)010010022LN $654/748$ (87%) 610 (93%) 43 (7%) 1 (0%) 47 79 23LO $830/855$ (97%) 777 (94%) 53 (6%)010010024LP $259/420$ (62%) 257 (99%) 2 (1%)010010025LQ $798/939$ (85%) 739 (93%) 58 (7%) 1 (0%) 51 84 26LS $473/594$ (80%) 448 (95%) 25 (5%)010010027LT $844/921$ (92%) 805 (95%) 39 (5%)010010028LU $453/465$ (97%) 415 (92%) 38 (8%)010010029LV $360/362$ (99%) 324 (90%) 36 (10%)010010030LW $436/438$ (100%) 409 (94%) 27 (6%)010010031LZ $180/182$ (99%) 170 (94%) 10 (10%)010010033NK $173/175$ (99%) 165 (55%)8010010034SC $238/247$ (96%) 227 (95%) 11 (5%)010010035SF $119/121$ (98%) 107 (90%) 12 (10%)0100100	18	LJ	489/513~(95%)	461 (94%)	28 (6%)	0	100	100
20LL $465/555$ (84%) 435 (94%) 30 (6%) 0 100 100 21LM $424/431$ (98%) 407 (96%) 17 (4%) 0 100 100 22LN $654/748$ (87%) 610 (93%) 43 (7%) 1 (0%) 47 79 23LO $830/855$ (97%) 777 (94%) 53 (6%) 0 100 100 24LP $259/420$ (62%) 257 (99%) 2 (1%) 0 100 100 25LQ $798/939$ (85%) 739 (93%) 58 (7%) 1 (0%) 10 100 26LS $473/594$ (80%) 448 (95%) 25 (5%) 0 100 100 27LT $844/921$ (92%) 805 (95%) 39 (5%) 0 100 100 28LU $453/465$ (97%) 415 (92%) 38 (8%) 0 100 100 29LV $360/362$ (99%) 324 (90%) 36 (10%) 0 100 100 30LW $436/438$ (100%) 409 (94%) 27 (6%) 0 100 100 31LZ $180/182$ (99%) 170 (94%) 10 (6%) 0 100 100 33 NK $173/175$ (99%) 165 (95%) 8 (5%) 0 100 100 34 SD $224/247$ (91%) 207 (92%) 17 (8%) 0 100 100 35 SF $119/121$ (98%) 107 (90%) 12 (10% 1	19	LK	86/123~(70%)	84 (98%)	2 (2%)	0	100	100
21LM $424/431 (98\%)$ $407 (96\%)$ $17 (4\%)$ 0 100 100 22LN $654/748 (87\%)$ $610 (93\%)$ $43 (7\%)$ $1 (0\%)$ 47 79 23LO $830/855 (97\%)$ $777 (94\%)$ $53 (6\%)$ 0 100 100 24LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 0 100 100 25LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 51 84 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 0 100 100 27LT $844/921 (92\%)$ $805 (95\%)$ $39 (5\%)$ 0 100 100 28LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 0 100 100 29LW $360/362 (99\%)$ $324 (90\%)$ $36 (10\%)$ 0 100 100 30LW $436/438 (100\%)$ $409 (94\%)$ $27 (6\%)$ 0 100 100 31LZ $180/182 (99\%)$ $170 (94\%)$ $10 (6\%)$ 0 100 100 33NK $173/175 (99\%)$ $165 (95\%)$ $8 (5\%)$ 0 100 100 34SD $224/247 (91\%)$ $207 (92\%)$ $11 (5\%)$ 0 100 100 35SF $119/121 (98\%)$ $107 (90\%)$ $12 (10\%)$ 0 100 100 36SG $423/464 (91\%)$ $401 (95\%)$ $22 (5\%)$ 0 100 100 37SH $358/$	20	LL	465/555~(84%)	435 (94%)	30 (6%)	0	100	100
22LN $654/748 (87\%)$ $610 (93\%)$ $43 (7\%)$ $1 (0\%)$ 47 77 23LO $830/855 (97\%)$ $777 (94\%)$ $53 (6\%)$ 0 100 100 24LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 0 100 100 25LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 51 84 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 0 100 100 27LT $844/921 (92\%)$ $805 (95\%)$ $39 (5\%)$ 0 100 100 28LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 0 100 100 29LV $360/362 (99\%)$ $324 (90\%)$ $36 (10\%)$ 0 100 100 30LW $436/438 (100\%)$ $409 (94\%)$ $27 (6\%)$ 0 100 100 31LZ $180/182 (99\%)$ $170 (94\%)$ $10 (6\%)$ 0 100 100 33NK $173/175 (99\%)$ $165 (95\%)$ $8 (5\%)$ 0 100 100 34SC $238/247 (96\%)$ $227 (95\%)$ $11 (5\%)$ 0 100 100 35SE $119/121 (98\%)$ $107 (90\%)$ $12 (10\%)$ 0 100 100 36SG $423/464 (91\%)$ $401 (95\%)$ $22 (5\%)$ 0 100 100 37SH $358/360 (99\%)$ $342 (96\%)$ $16 (4\%)$ 0 100 100 38SI $763/$	21	LM	424/431 (98%)	407 (96%)	17 (4%)	0	100	100
23LO $830/855 (97\%)$ $777 (94\%)$ $53 (6\%)$ 010010024LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 010010025LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 51 84 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 010010027LT $844/921 (92\%)$ $805 (95\%)$ $39 (5\%)$ 010010028LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 010010029LV $360/362 (99\%)$ $324 (90\%)$ $36 (10\%)$ 010010030LW $436/438 (100\%)$ $409 (94\%)$ $27 (6\%)$ 010010031LZ $180/182 (99\%)$ $170 (94\%)$ $10 (6\%)$ 010010033NK $173/175 (99\%)$ $165 (95\%)$ $8 (5\%)$ 010010034SC $238/247 (96\%)$ $227 (95\%)$ $11 (5\%)$ 010010035SF $119/121 (98\%)$ $110 (92\%)$ $9 (8\%)$ 010010036SG $423/464 (91\%)$ $401 (95\%)$ $22 (5\%)$ 010010037SH $358/360 (99\%)$ $342 (96\%)$ $16 (4\%)$ 010010038SI $763/1123 (68\%)$ $727 (95\%)$ $36 (5\%)$ 010010039SK $226/236 (96\%)$ $221 (98\%)$ $5 (2\%)$ 0100100 </td <td>22</td> <td>LN</td> <td>654/748~(87%)</td> <td>610 (93%)</td> <td>43 (7%)</td> <td>1 (0%)</td> <td>47</td> <td>79</td>	22	LN	654/748~(87%)	610 (93%)	43 (7%)	1 (0%)	47	79
24LP $259/420 (62\%)$ $257 (99\%)$ $2 (1\%)$ 0 100 100 25LQ $798/939 (85\%)$ $739 (93\%)$ $58 (7\%)$ $1 (0\%)$ 51 84 26LS $473/594 (80\%)$ $448 (95\%)$ $25 (5\%)$ 0 100 100 27LT $844/921 (92\%)$ $805 (95\%)$ $39 (5\%)$ 0 100 100 28LU $453/465 (97\%)$ $415 (92\%)$ $38 (8\%)$ 0 100 100 29LV $360/362 (99\%)$ $324 (90\%)$ $36 (10\%)$ 0 100 100 30LW $436/438 (100\%)$ $409 (94\%)$ $27 (6\%)$ 0 100 100 31LZ $180/182 (99\%)$ $170 (94\%)$ $10 (6\%)$ 0 100 100 33NK $173/175 (99\%)$ $165 (95\%)$ $8 (5\%)$ 0 100 100 34SC $238/247 (96\%)$ $227 (95\%)$ $11 (5\%)$ 0 100 100 35SE $119/121 (98\%)$ $107 (92\%)$ $17 (8\%)$ 0 100 100 36SG $423/464 (91\%)$ $401 (95\%)$ $22 (5\%)$ 0 100 100 37SH $358/360 (99\%)$ $342 (96\%)$ $16 (4\%)$ 0 100 100 38SI $763/1123 (68\%)$ $727 (95\%)$ $36 (5\%)$ 0 100 100 39SK $226/236 (96\%)$ $221 (98\%)$ $5 (2\%)$ 0 100 100	23	LO	830/855~(97%)	777 (94%)	53 (6%)	0	100	100
25LQ $798/939 (85%)$ $739 (93%)$ $58 (7%)$ $1 (0%)$ 51 84 26 LS $473/594 (80%)$ $448 (95%)$ $25 (5%)$ 0 100 100 27 LT $844/921 (92%)$ $805 (95%)$ $39 (5%)$ 0 100 100 28 LU $453/465 (97%)$ $415 (92%)$ $38 (8%)$ 0 100 100 29 LV $360/362 (99%)$ $324 (90%)$ $36 (10%)$ 0 100 100 30 LW $436/438 (100%)$ $409 (94%)$ $27 (6%)$ 0 100 100 31 LZ $180/182 (99%)$ $170 (94%)$ $10 (6%)$ 0 100 100 32 NG $109/111 (98%)$ $97 (89%)$ $12 (11%)$ 0 100 100 33 NK $173/175 (99%)$ $165 (95%)$ $8 (5%)$ 0 100 100 34 SD $224/247 (96%)$ $227 (95%)$ $11 (5%)$ 0 100 100 35 SE $119/121 (98%)$ $110 (92%)$ $9 (8%)$ 0 100 100 36 SG $423/464 (91%)$ $401 (95%)$ $22 (5%)$ 0 100 100 38 SI $763/1123 (68%)$ $727 (95%)$ $36 (5%)$ 0 100 100 39 SJ $212/236 (90%)$ $205 (97%)$ $7 (3%)$ 0 100 100 39 SK $226/36 (96%)$ $221 (98%)$ $5 (2%)$ 0 100 100 <td>24</td> <td>LP</td> <td>259/420~(62%)</td> <td>257 (99%)</td> <td>2 (1%)</td> <td>0</td> <td>100</td> <td>100</td>	24	LP	259/420~(62%)	257 (99%)	2 (1%)	0	100	100
26 LS 473/594 (80%) 448 (95%) 25 (5%) 0 100 100 27 LT 844/921 (92%) 805 (95%) 39 (5%) 0 100 100 28 LU 453/465 (97%) 415 (92%) 38 (8%) 0 100 100 29 LV 360/362 (99%) 324 (90%) 36 (10%) 0 100 100 100 30 LW 436/438 (100%) 409 (94%) 27 (6%) 0 100 100 100 31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 100 35 SF 119/121 (98%) <t< td=""><td>25</td><td>LQ</td><td>798/939~(85%)</td><td>739 (93%)</td><td>58 (7%)</td><td>1 (0%)</td><td>51</td><td>84</td></t<>	25	LQ	798/939~(85%)	739 (93%)	58 (7%)	1 (0%)	51	84
27 LT 844/921 (92%) 805 (95%) 39 (5%) 0 100 100 28 LU 453/465 (97%) 415 (92%) 38 (8%) 0 100 100 29 LV 360/362 (99%) 324 (90%) 36 (10%) 0 100 100 30 LW 436/438 (100%) 409 (94%) 27 (6%) 0 100 100 31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SF 119/121 (98%) 110 (92%) 9 (8%) 0 100 100	26	LS	473/594~(80%)	448 (95%)	25 (5%)	0	100	100
28 LU 453/465 (97%) 415 (92%) 38 (8%) 0 100 100 29 LV 360/362 (99%) 324 (90%) 36 (10%) 0 100 100 100 30 LW 436/438 (100%) 409 (94%) 27 (6%) 0 100 100 100 31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 100 37 SH	27	LT	844/921~(92%)	805 (95%)	39 (5%)	0	100	100
29 LV 360/362 (99%) 324 (90%) 36 (10%) 0 100 100 30 LW 436/438 (100%) 409 (94%) 27 (6%) 0 100 100 100 31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 <	28	LU	453/465~(97%)	415 (92%)	38 (8%)	0	100	100
30 LW 436/438 (100%) 409 (94%) 27 (6%) 0 100 100 31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100	29	LV	360/362~(99%)	324 (90%)	36 (10%)	0	100	100
31 LZ 180/182 (99%) 170 (94%) 10 (6%) 0 100 100 32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100	30	LW	436/438 (100%)	409 (94%)	27 (6%)	0	100	100
32 NG 109/111 (98%) 97 (89%) 12 (11%) 0 100 100 33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SI 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100	31	LZ	180/182~(99%)	170 (94%)	10 (6%)	0	100	100
33 NK 173/175 (99%) 165 (95%) 8 (5%) 0 100 100 34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 35 SF 119/121 (98%) 107 (90%) 12 (10%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 <t< td=""><td>32</td><td>NG</td><td>109/111 (98%)</td><td>97 (89%)</td><td>12 (11%)</td><td>0</td><td>100</td><td>100</td></t<>	32	NG	109/111 (98%)	97 (89%)	12 (11%)	0	100	100
34 SC 238/247 (96%) 227 (95%) 11 (5%) 0 100 100 34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 100 35 SF 119/121 (98%) 107 (90%) 12 (10%) 0 100	33	NK	173/175~(99%)	165 (95%)	8 (5%)	0	100	100
34 SD 224/247 (91%) 207 (92%) 17 (8%) 0 100 100 35 SE 119/121 (98%) 110 (92%) 9 (8%) 0 100 100 35 SF 119/121 (98%) 107 (90%) 12 (10%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	34	SC	238/247~(96%)	227 (95%)	11 (5%)	0	100	100
35SE119/121 (98%)110 (92%)9 (8%)010010035SF119/121 (98%)107 (90%)12 (10%)010010036SG423/464 (91%)401 (95%)22 (5%)010010037SH358/360 (99%)342 (96%)16 (4%)010010038SI763/1123 (68%)727 (95%)36 (5%)010010039SJ212/236 (90%)205 (97%)7 (3%)010010039SK226/236 (96%)221 (98%)5 (2%)010010040SL170/183 (93%)160 (94%)10 (6%)0100100	34	SD	224/247~(91%)	207 (92%)	17 (8%)	0	100	100
35 SF 119/121 (98%) 107 (90%) 12 (10%) 0 100 100 36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	35	SE	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
36 SG 423/464 (91%) 401 (95%) 22 (5%) 0 100 100 37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	35	SF	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
37 SH 358/360 (99%) 342 (96%) 16 (4%) 0 100 100 38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	36	SG	423/464 (91%)	401 (95%)	22 (5%)	0	100	100
38 SI 763/1123 (68%) 727 (95%) 36 (5%) 0 100 100 39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	37	SH	358/360~(99%)	342 (96%)	16 (4%)	0	100	100
39 SJ 212/236 (90%) 205 (97%) 7 (3%) 0 100 100 39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	38	SI	763/1123~(68%)	727 (95%)	36 (5%)	0	100	100
39 SK 226/236 (96%) 221 (98%) 5 (2%) 0 100 100 40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	39	SJ	212/236~(90%)	205 (97%)	7 (3%)	0	100	100
40 SL 170/183 (93%) 160 (94%) 10 (6%) 0 100 100	39	SK	226/236~(96%)	221 (98%)	5 (2%)	0	100	100
	40	SL	170/183~(93%)	160 (94%)	10 (6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
41	SM	278/290~(96%)	260~(94%)	18~(6%)	0	100	100
42	SN	245/247~(99%)	232~(95%)	13~(5%)	0	100	100
43	SO	177/179~(99%)	163 (92%)	14 (8%)	0	100	100
44	SQ	129/167~(77%)	124 (96%)	5 (4%)	0	100	100
45	SR	102/104~(98%)	91~(89%)	10 (10%)	1 (1%)	15	53
46	\mathbf{SS}	142/197~(72%)	132 (93%)	10 (7%)	0	100	100
47	ST	448/806~(56%)	425 (95%)	22~(5%)	1 (0%)	47	79
48	SY	237/248~(96%)	222~(94%)	15~(6%)	0	100	100
49	SZ	259/261~(99%)	237~(92%)	22 (8%)	0	100	100
50	NJ	263/265~(99%)	259~(98%)	4 (2%)	0	100	100
51	NH	1072/1141~(94%)	1025 (96%)	47 (4%)	0	100	100
52	NI	163/187~(87%)	157 (96%)	6 (4%)	0	100	100
54	SU	471/513~(92%)	447 (95%)	24 (5%)	0	100	100
55	LI	423/687~(62%)	376~(89%)	45 (11%)	2(0%)	29	67
56	ND	58/60~(97%)	58 (100%)	0	0	100	100
57	LR	750/811~(92%)	693~(92%)	57 (8%)	0	100	100
58	NE	157/240~(65%)	139 (88%)	18 (12%)	0	100	100
59	SB	431/436~(99%)	401 (93%)	30 (7%)	0	100	100
60	SV	59/92~(64%)	56~(95%)	3~(5%)	0	100	100
61	SP	2189/2418~(90%)	2132 (97%)	57 (3%)	0	100	100
62	LX	802/923~(87%)	745 (93%)	57 (7%)	0	100	100
62	LY	827/923~(90%)	774 (94%)	53~(6%)	0	100	100
63	L6	161/219~(74%)	150 (93%)	11 (7%)	0	100	100
64	NF	122/124~(98%)	112 (92%)	10 (8%)	0	100	100
65	5	292/534~(55%)	269~(92%)	22 (8%)	1 (0%)	41	75
66	6	273/357~(76%)	259~(95%)	14 (5%)	0	100	100
All	All	23449/27027~(87%)	22060 (94%)	1379 (6%)	10 (0%)	100	100

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	NA	454	VAL
3	NB	441	PRO
	<i>a</i>	1	

Continued from previous page...

Mol	Chain	Res	Type
45	SR	90	ASP
65	5	451	LYS
22	LN	666	ASN
47	ST	419	LYS
55	LI	533	PRO
55	LI	258	PRO
15	m LF	32	ARG
25	LQ	787	LYS

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	ntiles
1	NA	187/223~(84%)	183~(98%)	4 (2%)	53	72
2	SA	296/328~(90%)	293~(99%)	3 (1%)	76	86
3	NB	108/139~(78%)	106 (98%)	2 (2%)	57	75
6	L3	96/108~(89%)	95~(99%)	1 (1%)	76	86
7	L4	196/196~(100%)	182 (93%)	14 (7%)	14	42
8	L5	180/180~(100%)	177~(98%)	3(2%)	60	78
9	L7	146/170~(86%)	139~(95%)	7(5%)	25	53
10	L8	138/161~(86%)	132~(96%)	6 (4%)	29	56
11	L9	150/150~(100%)	142 (95%)	8 (5%)	22	51
12	LC	105/105~(100%)	105 (100%)	0	100	100
13	LD	114/137~(83%)	108~(95%)	6 (5%)	22	51
14	LE	108/108~(100%)	105~(97%)	3~(3%)	43	65
15	$_{ m LF}$	76/76~(100%)	71~(93%)	5(7%)	16	45
16	LG	56/56~(100%)	56~(100%)	0	100	100
17	LH	758/813~(93%)	746~(98%)	12 (2%)	62	79
18	LJ	437/454~(96%)	432~(99%)	5 (1%)	73	85
19	LK	$8\overline{3}/83~(100\%)$	$80 \ (96\%)$	3 (4%)	35	61



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
20	LL	428/497~(86%)	422 (99%)	6 (1%)	67	81
21	LM	391/391~(100%)	390 (100%)	1 (0%)	92	95
22	LN	604/671~(90%)	595~(98%)	9(2%)	65	80
23	LO	730/751~(97%)	717 (98%)	13 (2%)	59	77
24	LP	248/302~(82%)	242 (98%)	6 (2%)	49	69
25	LQ	717/794~(90%)	708 (99%)	9 (1%)	69	82
26	LS	424/529~(80%)	422 (100%)	2 (0%)	88	93
27	LT	745/802~(93%)	741 (100%)	4 (0%)	88	93
28	LU	412/420 (98%)	405 (98%)	7 (2%)	60	78
29	LV	307/326~(94%)	302 (98%)	5 (2%)	62	79
30	LW	373/373~(100%)	371 (100%)	2 (0%)	88	93
31	LZ	171/171~(100%)	169 (99%)	2 (1%)	71	84
34	\mathbf{SC}	202/206~(98%)	200 (99%)	2 (1%)	76	86
34	SD	192/206~(93%)	185 (96%)	7 (4%)	35	61
35	SE	100/100~(100%)	95~(95%)	5 (5%)	24	52
35	SF	100/100~(100%)	97~(97%)	3 (3%)	41	64
36	SG	373/402~(93%)	371 (100%)	2 (0%)	88	93
37	SH	307/307~(100%)	303 (99%)	4 (1%)	69	82
38	SI	684/965~(71%)	666~(97%)	18 (3%)	46	67
39	SJ	195/209~(93%)	190 (97%)	5(3%)	46	67
39	SK	206/209~(99%)	202~(98%)	4 (2%)	57	75
40	SL	156/165~(94%)	146 (94%)	10 (6%)	17	45
41	SM	251/258~(97%)	251 (100%)	0	100	100
42	SN	230/230~(100%)	222 (96%)	8 (4%)	36	61
43	SO	33/156~(21%)	33 (100%)	0	100	100
44	SQ	124/156~(80%)	120 (97%)	4 (3%)	39	62
45	SR	86/86~(100%)	85 (99%)	1 (1%)	71	84
46	SS	135/135~(100%)	130 (96%)	5 (4%)	34	60
47	ST	417/604~(69%)	409 (98%)	8 (2%)	57	75
48	SY	$\overline{226/233}\ (97\%)$	223 (99%)	3 (1%)	69	82
54	SU	$360/\overline{473}\;(76\%)$	354 (98%)	6(2%)	60	78



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	LI	150/634~(24%)	149 (99%)	1 (1%)	84 90
56	ND	57/57~(100%)	54 (95%)	3(5%)	22 51
57	LR	665/713~(93%)	653~(98%)	12 (2%)	59 77
58	NE	119/210~(57%)	116 (98%)	3 (2%)	47 68
59	SB	244/359~(68%)	239~(98%)	5 (2%)	55 73
60	SV	22/87~(25%)	20 (91%)	2(9%)	9 33
62	LX	549/822~(67%)	$531 \ (97\%)$	18 (3%)	38 62
63	L6	139/188~(74%)	131 (94%)	8 (6%)	20 48
65	5	267/482~(55%)	262~(98%)	5 (2%)	57 75
66	6	244/315~(78%)	236 (97%)	8 (3%)	38 62
All	All	15617/18581 (84%)	15309 (98%)	308 (2%)	57 73

All (308) residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	NA	304	GLN
1	NA	455	HIS
1	NA	456	PHE
1	NA	496	TYR
2	SA	193	MET
2	SA	268	MET
2	SA	388	ARG
3	NB	434	PHE
3	NB	495	TYR
6	L3	78	HIS
7	L4	16	HIS
7	L4	24	SER
7	L4	27	TYR
7	L4	47	PHE
7	L4	82	TYR
7	L4	87	MET
7	L4	103	TYR
7	L4	113	ARG
7	L4	138	TYR
7	L4	149	TYR
7	L4	153	ASN
7	L4	205	PHE
7	L4	218	PHE



Mol	Chain	Res	Type
7	L4	226	PHE
8	L5	65	ARG
8	L5	135	ASP
8	L5	209	TYR
9	L7	79	ARG
9	L7	83	LYS
9	L7	86	GLN
9	L7	141	ARG
9	L7	150	GLN
9	L7	163	ASP
9	L7	169	PHE
10	L8	27	PHE
10	L8	58	LEU
10	L8	75	LYS
10	L8	77	ARG
10	L8	113	PHE
10	L8	182	TYR
11	L9	16	LYS
11	L9	63	ASP
11	L9	74	ASN
11	L9	102	GLU
11	L9	103	ASP
11	L9	114	TYR
11	L9	121	SER
11	L9	180	LYS
13	LD	58	CYS
13	LD	67	ARG
13	LD	80	MET
13	LD	88	ARG
13	LD	98	ASN
13	LD	136	ARG
14	LE	41	MET
14	LE	104	LEU
14	LE	111	MET
15	LF	23	PHE
15	LF	40	LEU
15	LF	53	ASP
15	LF	84	LYS
15	LF	89	TYR
17	LH	145	PHE
17	LH	152	ARG
17	LH	267	MET



Mol	Chain	Res	Type
17	LH	336	ARG
17	LH	360	MET
17	LH	432	ARG
17	LH	478	ASN
17	LH	590	HIS
17	LH	605	ASN
17	LH	617	GLN
17	LH	626	PHE
17	LH	875	MET
18	LJ	69	ARG
18	LJ	112	ASN
18	LJ	158	TYR
18	LJ	194	ARG
18	LJ	305	CYS
19	LK	472	ASP
19	LK	481	HIS
19	LK	507	ARG
20	LL	222	THR
20	LL	350	LEU
20	LL	441	LEU
20	LL	450	HIS
20	LL	470	PHE
20	LL	554	PHE
21	LM	382	LEU
22	LN	31	MET
22	LN	113	ARG
22	LN	197	LYS
22	LN	258	SER
22	LN	302	ARG
22	LN	347	LEU
22	LN	369	TYR
22	LN	414	TYR
22	LN	663	PHE
23	LO	193	TYR
23	LO	264	LYS
23	LO	265	CYS
23	LO	293	THR
23	LO	339	LEU
23	LO	353	TYR
23	LO	398	ARG
23	LO	488	LEU
23	LO	505	ARG



Mol	Chain	Res	Type
23	LO	513	GLU
23	LO	680	ARG
23	LO	821	MET
23	LO	826	ARG
24	LP	31	LEU
24	LP	133	TYR
24	LP	174	PHE
24	LP	195	LYS
24	LP	278	MET
24	LP	301	ASN
25	LQ	100	ASP
25	LQ	164	ASP
25	LQ	169	PHE
25	LQ	185	MET
25	LQ	255	ARG
25	LQ	333	ARG
25	LQ	391	ARG
25	LQ	607	CYS
25	LQ	623	PHE
26	LS	176	LYS
26	LS	319	ARG
27	LT	344	ARG
27	LT	510	LEU
27	LT	755	LYS
27	LT	840	PHE
28	LU	89	ASP
28	LU	139	CYS
28	LU	247	TYR
28	LU	268	CYS
28	LU	332	TYR
28	LU	356	TYR
28	LU	407	MET
29	LV	51	GLN
29	LV	85	ASP
29	LV	237	ARG
29	LV	$26\overline{3}$	SER
29	LV	328	MET
30	LW	105	ASP
30	LW	150	LEU
31	LZ	80	ASP
31	LZ	132	GLU
34	\mathbf{SC}	172	TYR



Mol	Chain	Res	Type
34	SC	275	CYS
34	SD	145	ASN
34	SD	148	ARG
34	SD	231	ARG
34	SD	241	PHE
34	SD	259	MET
34	SD	275	CYS
34	SD	303	GLN
35	SE	29	ASN
35	SE	83	SER
35	SE	91	CYS
35	SE	108	SER
35	SE	115	TYR
35	SF	54	MET
35	SF	91	CYS
35	SF	119	ASP
36	SG	114	LYS
36	SG	258	ARG
37	SH	48	TYR
37	SH	69	TYR
37	SH	141	MET
37	SH	301	MET
38	SI	92	ARG
38	SI	100	ASP
38	SI	150	MET
38	SI	177	PHE
38	SI	230	MET
38	SI	308	CYS
38	SI	348	ASP
38	SI	366	MET
38	SI	555	MET
38	SI	772	MET
38	SI	795	LYS
38	SI	833	ARG
38	SI	847	LEU
38	SI	944	ASN
38	SI	960	ARG
38	SI	973	ARG
38	SI	988	ARG
38	SI	997	MET
$\overline{39}$	SJ	70	CYS
39	SJ	76	LEU



Mol	Chain	Res	Type
39	SJ	80	MET
39	SJ	209	MET
39	SJ	242	CYS
39	SK	182	PHE
39	SK	194	GLU
39	SK	241	PHE
39	SK	250	ASN
40	SL	12	LEU
40	SL	55	TYR
40	SL	84	ARG
40	SL	88	ASP
40	SL	100	ASP
40	SL	107	GLU
40	SL	139	ASP
40	SL	150	CYS
40	SL	173	MET
40	SL	178	HIS
42	SN	46	MET
42	SN	73	LEU
42	SN	117	GLN
42	SN	134	LEU
42	SN	139	LEU
42	SN	167	MET
42	SN	175	TYR
42	SN	203	TYR
44	SQ	103	TRP
44	SQ	186	TYR
44	SQ	212	MET
44	SQ	216	ARG
45	SR	131	SER
46	SS	281	ARG
46	SS	314	PRO
46	SS	316	ASN
46	SS	841	LYS
46	SS	878	LEU
47	ST	16	ARG
47	ST	104	MET
47	ST	602	LEU
47	ST	693	LYS
47	ST	713	HIS
47	ST	716	LYS
47	ST	777	TYR



Mol	Chain	Res	Type
47	ST	796	LYS
48	SY	27	PHE
48	SY	63	TYR
48	SY	82	ARG
54	SU	123	TYR
54	SU	174	ASN
54	SU	199	PHE
54	SU	413	MET
54	SU	417	HIS
54	SU	495	MET
55	LI	525	PHE
56	ND	160	ARG
56	ND	195	GLU
56	ND	208	ARG
57	LR	8	LYS
57	LR	50	ARG
57	LR	106	TYR
57	LR	171	MET
57	LR	176	ASP
57	LR	182	CYS
57	LR	217	ASP
57	LR	343	MET
57	LR	464	LYS
57	LR	596	ASP
57	LR	619	ARG
57	LR	626	MET
58	NE	201	GLN
58	NE	255	GLN
58	NE	272	PHE
59	SB	175	LYS
59	SB	178	ASN
59	SB	404	ARG
59	SB	406	LEU
59	SB	407	ARG
60	SV	182	HIS
60	SV	183	ARG
62	LX	32	ARG
62	LX	39	ASN
62	LX	44	MET
62	LX	51	MET
62	LX	91	MET
62	LX	122	CYS



Mol	Chain	Res	Type
62	LX	137	ARG
62	LX	184	PHE
62	LX	185	ASN
62	LX	501	ARG
62	LX	537	MET
62	LX	649	TYR
62	LX	652	ARG
62	LX	785	PHE
62	LX	858	MET
62	LX	896	ASP
62	LX	917	MET
62	LX	920	MET
63	L6	7	TYR
63	L6	27	PHE
63	L6	29	ASP
63	L6	37	ASP
63	L6	92	ARG
63	L6	105	ASP
63	L6	126	ASP
63	L6	208	TYR
65	5	239	PHE
65	5	417	LEU
65	5	445	ARG
65	5	475	TYR
65	5	485	TRP
66	6	49	TYR
66	6	77	MET
66	6	93	MET
66	6	135	TYR
66	6	234	LYS
66	6	271	ARG
66	6	317	MET
66	6	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
8	L5	66	GLN
10	L8	32	GLN
14	LE	15	ASN
17	LH	690	ASN
22	LN	632	ASN



Mol	Chain	Res	Type
23	LO	598	ASN
26	LS	352	GLN
28	LU	133	GLN
28	LU	443	ASN
29	LV	116	HIS
29	LV	126	GLN
35	SF	38	ASN
38	SI	239	ASN
38	SI	1016	ASN
38	SI	1114	GLN
39	SK	190	GLN
42	SN	117	GLN
45	SR	99	ASN
47	ST	738	ASN
55	LI	608	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	LO	483/700~(69%)	164 (33%)	3~(0%)
5	L2	163/333~(48%)	56 (34%)	0
53	8	1169/1807~(64%)	527~(45%)	17 (1%)
All	All	1815/2840~(63%)	747~(41%)	20 (1%)

All (747) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	LO	18	G
4	LO	20	С
4	LO	22	А
4	LO	59	U
4	LO	60	G
4	LO	63	G
4	LO	69	U
4	LO	82	А
4	LO	86	С
4	LO	87	С
4	LO	90	G
4	LO	98	G
4	LO	103	G
4	LO	104	А



Mol	Chain	Res	Type
4	LO	107	G
4	LO	117	G
4	LO	123	С
4	LO	124	А
4	LO	125	G
4	LO	129	U
4	LO	130	G
4	LO	131	С
4	LO	141	А
4	LO	142	U
4	LO	143	А
4	LO	144	С
4	LO	150	G
4	LO	151	U
4	LO	152	U
4	LO	155	А
4	LO	161	А
4	LO	163	G
4	LO	169	А
4	LO	173	G
4	LO	175	А
4	LO	176	U
4	LO	177	U
4	LO	178	G
4	LO	184	U
4	LO	185	А
4	LO	187	А
4	LO	188	А
4	LO	189	U
4	LO	190	U
4	LO	191	U
4	LO	197	G
4	LO	198	A
4	LO	199	А
4	LO	200	A
4	LO	201	U
4	LO	205	С
4	LO	213	G
4	LO	215	U
4	LO	216	U
4	LO	218	U
4	LO	219	U



Mol	Chain	Res	Type
4	LO	220	U
4	LO	227	U
4	LO	233	G
4	LO	234	A
4	LO	235	А
4	LO	236	С
4	LO	238	G
4	LO	239	U
4	LO	240	С
4	LO	243	А
4	LO	252	А
4	LO	253	U
4	LO	254	С
4	LO	255	U
4	LO	256	U
4	LO	259	G
4	LO	261	U
4	LO	262	U
4	LO	267	U
4	LO	268	G
4	LO	279	А
4	LO	280	А
4	LO	281	G
4	LO	284	U
4	LO	304	U
4	LO	305	А
4	LO	309	A
4	LO	310	U
4	LO	311	С
4	LO	312	U
4	LO	313	A
4	LO	314	U
4	LO	315	U
4	LO	316	U
4	LO	322	A
4	LO	323	A
4	LO	324	U
4	LO	325	U
4	LO	326	С
4	LO	331	U
4	LO	332	U
4	LO	337	G



Mol	Chain	Res	Type
4	LO	338	А
4	LO	339	A
4	LO	340	U
4	LO	341	G
4	LO	347	U
4	LO	348	U
4	LO	352	U
4	LO	373	U
4	LO	374	U
4	LO	375	С
4	LO	382	U
4	LO	385	A
4	LO	386	A
4	LO	395	С
4	LO	396	A
4	LO	397	A
4	LO	398	A
4	LO	399	U
4	LO	404	G
4	LO	407	A
4	LO	427	A
4	LO	430	С
4	LO	431	A
4	LO	433	С
4	LO	440	U
4	LO	451	G
4	LO	461	A
4	LO	468	A
4	LO	470	U
4	LO	474	A
4	LO	481	U
4	LO	482	A
4	LO	483	U
4	LO	485	G
4	LO	486	U
4	LO	487	A
4	LO	488	U
4	LO	489	G
4	LO	491	U
4	LO	492	G
4	LO	493	A
4	LO	494	С



Mol	Chain	Res	Type
4	LO	497	А
4	LO	502	G
4	LO	512	А
4	L0	513	G
4	LO	517	А
4	LO	518	А
4	LO	519	А
4	LO	521	G
4	LO	522	С
4	LO	523	U
4	LO	524	U
4	LO	526	U
4	LO	530	А
4	LO	531	С
4	LO	535	G
4	LO	536	A
4	LO	540	U
4	L0	543	С
4	L0	554	G
4	LO	583	U
4	LO	584	U
4	LO	585	С
4	LO	586	А
4	L0	591	U
5	L2	2	U
5	L2	3	С
5	L2	14	А
5	L2	15	U
5	L2	16	А
5	L2	24	U
5	L2	25	U
5	L2	28	A
5	L2	30	A
5	L2	32	G
5	L2	33	A
5	L2	35	U
5	L2	37	G
5	L2	38	U
5	L2	44	U
5	L2	55	A
5	L2	56	A
5	L2	60	А



Mol	Chain	Res	Type
5	L2	61	G
5	L2	85	G
5	L2	88	U
5	L2	89	С
5	L2	90	С
5	L2	91	С
5	L2	92	А
5	L2	93	U
5	L2	94	А
5	L2	105	С
5	L2	111	G
5	L2	114	А
5	L2	115	G
5	L2	116	А
5	L2	118	А
5	L2	201	С
5	L2	202	G
5	L2	247	U
5	L2	248	G
5	L2	249	G
5	L2	251	G
5	L2	252	С
5	L2	254	А
5	L2	256	G
5	L2	257	А
5	L2	260	U
5	L2	264	С
5	L2	267	А
5	L2	306	G
5	L2	307	G
5	L2	310	G
5	L2	312	U
5	L2	316	А
5	L2	321	С
5	L2	322	А
5	L2	324	U
5	L2	325	С
5	L2	329	С
53	8	-5	G
53	8	-4	A
53	8	-3	U
53	8	-2	А



Mol	Chain	Res	Type
53	8	-1	G
53	8	0	U
53	8	1	U
53	8	8	U
53	8	9	U
53	8	16	G
53	8	18	С
53	8	19	А
53	8	20	G
53	8	21	U
53	8	22	А
53	8	23	G
53	8	26	А
53	8	28	A
53	8	33	U
53	8	34	G
53	8	35	U
53	8	36	С
53	8	37	U
53	8	39	А
53	8	50	С
53	8	51	А
53	8	53	G
53	8	55	А
53	8	99	С
53	8	102	U
53	8	103	А
53	8	104	А
53	8	109	G
53	8	110	U
53	8	111	U
53	8	112	A
53	8	113	U
53	8	114	C
53	8	115	G
53	8	116	U
53	8	119	A
53	8	122	U
53	8	126	A
53	8	127	G
53	8	140	A
53	8	141	U



Mol	Chain	Res	Type
53	8	142	G
53	8	143	G
53	8	144	U
53	8	145	А
53	8	146	U
53	8	147	А
53	8	150	U
53	8	153	G
53	8	159	U
53	8	160	С
53	8	161	U
53	8	162	А
53	8	180	A
53	8	181	A
53	8	185	U
53	8	186	C
53	8	188	А
53	8	190	С
53	8	191	С
53	8	192	U
53	8	194	U
53	8	195	G
53	8	196	G
53	8	197	А
53	8	199	G
53	8	200	А
53	8	201	G
53	8	204	G
53	8	205	U
53	8	207	U
53	8	210	A
53	8	211	U
53	8	212	U
53	8	213	A
53	8	214	G
53	8	223	U
53	8	226	А
53	8	227	U
53	8	228	G
53	8	233	C
53	8	234	G
53	8	235	G



Mol	Chain	Res	Type
53	8	236	А
53	8	237	С
53	8	239	С
53	8	240	U
53	8	241	U
53	8	242	U
53	8	245	U
53	8	246	G
53	8	257	А
53	8	258	С
53	8	261	U
53	8	262	U
53	8	263	С
53	8	264	G
53	8	265	A
53	8	266	A
53	8	267	U
53	8	269	G
53	8	271	А
53	8	273	G
53	8	278	U
53	8	280	U
53	8	281	G
53	8	282	С
53	8	283	U
53	8	284	G
53	8	285	G
53	8	286	С
53	8	287	G
53	8	289	U
53	8	298	С
53	8	300	А
53	8	301	A
53	8	305	С
53	8	306	U
53	8	307	G
53	8	308	С
53	8	312	A
53	8	313	U
53	8	315	A
53	8	316	А
53	8	319	U



Mol	Chain	Res	Type
53	8	320	U
53	8	321	С
53	8	322	G
53	8	323	А
53	8	325	G
53	8	336	G
53	8	337	G
53	8	338	C
53	8	345	U
53	8	346	G
53	8	347	G
53	8	348	U
53	8	351	С
53	8	352	A
53	8	355	G
53	8	359	А
53	8	360	A
53	8	361	С
53	8	362	G
53	8	366	A
53	8	368	U
53	8	369	А
53	8	371	G
53	8	372	G
53	8	373	G
53	8	374	U
53	8	376	С
53	8	377	G
53	8	378	A
53	8	379	U
53	8	382	С
53	8	383	G
53	8	390	G
53	8	396	G
53	8	398	G
53	8	400	A
53	8	401	A
53	8	402	C
53	8	404	G
53	8	407	A
53	8	412	A
53	8	414	С



Mol	Chain	Res	Type
53	8	417	А
53	8	418	G
53	8	420	А
53	8	421	А
53	8	423	G
53	8	431	С
53	8	440	U
53	8	442	С
53	8	444	С
53	8	448	С
53	8	449	С
53	8	452	А
53	8	453	U
53	8	454	U
53	8	455	С
53	8	456	A
53	8	459	G
53	8	460	А
53	8	461	G
53	8	465	G
53	8	466	U
53	8	468	А
53	8	469	С
53	8	470	А
53	8	471	А
53	8	477	А
53	8	480	G
53	8	485	А
53	8	486	G
53	8	487	G
53	8	493	U
53	8	495	С
53	8	496	G
53	8	501	U
53	8	502	U
53	8	504	U
53	8	505	А
53	8	506	А
53	8	507	U
53	8	511	A
53	8	514	G
53	8	515	А



Mol	Chain	Res	Type
53	8	520	А
53	8	527	А
53	8	529	А
53	8	530	С
53	8	532	U
53	8	533	U
53	8	534	А
53	8	535	А
53	8	536	С
53	8	538	А
53	8	539	G
53	8	540	G
53	8	542	А
53	8	543	С
53	8	544	А
53	8	545	А
53	8	546	U
53	8	553	G
53	8	562	G
53	8	563	U
53	8	565	С
53	8	570	А
53	8	572	С
53	8	573	С
53	8	574	G
53	8	576	G
53	8	579	А
53	8	580	А
53	8	581	U
53	8	582	U
53	8	584	С
53	8	585	А
53	8	586	G
53	8	587	С
53	8	594	A
53	8	595	G
53	8	600	U
53	8	603	U
53	8	624	G
53	8	627	C
53	8	629	U
53	8	630	А



Mol	Chain	Res	Type
53	8	632	U
53	8	633	U
53	8	636	A
53	8	637	С
53	8	638	U
53	8	860	U
53	8	861	U
53	8	862	А
53	8	863	А
53	8	864	U
53	8	865	A
53	8	866	G
53	8	870	С
53	8	871	G
53	8	872	G
53	8	877	G
53	8	880	С
53	8	881	А
53	8	882	U
53	8	886	U
53	8	887	А
53	8	892	А
53	8	894	U
53	8	895	G
53	8	896	U
53	8	897	С
53	8	898	А
53	8	899	G
53	8	900	А
53	8	904	G
53	8	905	A
53	8	906	А
53	8	908	U
53	8	911	U
53	8	912	U
53	8	913	G
53	8	914	G
53	8	916	U
53	8	917	U
53	8	918	U
53	8	919	A
53	8	920	U



Mol	Chain	Res	Type
53	8	921	U
53	8	924	А
53	8	925	G
53	8	929	А
53	8	931	С
53	8	932	U
53	8	933	А
53	8	934	С
53	8	935	U
53	8	939	А
53	8	940	А
53	8	942	G
53	8	945	U
53	8	947	U
53	8	948	G
53	8	950	С
53	8	952	А
53	8	955	А
53	8	959	U
53	8	961	U
53	8	962	С
53	8	963	А
53	8	964	U
53	8	965	U
53	8	966	А
53	8	967	А
53	8	969	С
53	8	972	G
53	8	975	С
53	8	976	G
53	8	978	А
53	8	979	А
53	8	980	G
53	8	981	U
53	8	983	A
53	8	984	G
53	8	988	A
53	8	992	А
53	8	993	А
53	8	994	G
53	8	995	A
53	8	996	U


Mol	Chain	Res	Type
53	8	997	G
53	8	998	А
53	8	999	U
53	8	1001	А
53	8	1002	G
53	8	1003	А
53	8	1004	U
53	8	1005	А
53	8	1006	С
53	8	1007	С
53	8	1009	U
53	8	1010	С
53	8	1011	G
53	8	1012	U
53	8	1014	G
53	8	1015	U
53	8	1016	С
53	8	1017	U
53	8	1019	А
53	8	1036	А
53	8	1038	U
53	8	1039	А
53	8	1040	G
53	8	1042	G
53	8	1043	А
53	8	1053	G
53	8	1054	U
53	8	1057	U
53	8	1058	U
53	8	1060	U
53	8	1061	А
53	8	1062	A
53	8	1063	U
53	8	1064	G
53	8	1072	С
53	8	1076	A
53	8	1083	G
53	8	1084	A
53	8	1085	G
53	8	1086	A
53	8	1088	A
53	8	1089	U



Mol	Chain	Res	Type
53	8	1090	С
53	8	1091	А
53	8	1092	А
53	8	1093	А
53	8	1094	G
53	8	1095	U
53	8	1096	С
53	8	1097	U
53	8	1098	U
53	8	1099	U
53	8	1100	G
53	8	1104	U
53	8	1106	U
53	8	1107	G
53	8	1108	G
53	8	1109	G
53	8	1110	G
53	8	1112	G
53	8	1113	А
53	8	1116	А
53	8	1118	G
53	8	1119	G
53	8	1126	G
53	8	1127	G
53	8	1131	А
53	8	1132	А
53	8	1134	С
53	8	1135	U
53	8	1144	U
53	8	1146	G
53	8	1149	G
53	8	1158	C
53	8	1159	C
53	8	1160	A
53	8	1164	G
53	8	$117\overline{4}$	C
53	8	1191	U
53	8	1192	С
53	8	1193	A
53	8	1197	С
53	8	1198	G
53	8	1200	G



Mol	Chain	Res	Type
53	8	1202	А
53	8	1204	А
53	8	1206	U
53	8	1212	G
53	8	1213	G
53	8	1214	U
53	8	1216	С
53	8	1218	G
53	8	1223	А
53	8	1224	А
53	8	1226	А
53	8	1259	U
53	8	1262	U
53	8	1266	U
53	8	1267	G
53	8	1268	G
53	8	1270	G
53	8	1272	U
53	8	1273	G
53	8	1276	U
53	8	1434	U
53	8	1436	А
53	8	1437	U
53	8	1438	G
53	8	1443	U
53	8	1449	U
53	8	1471	А
53	8	1473	U
53	8	1474	G
53	8	1477	G
53	8	1479	А
53	8	1483	А
53	8	1484	G
53	8	1486	G
53	8	1488	G
53	8	1489	U
53	8	1492	А
53	8	1493	А
53	8	1498	G
53	8	1504	G
53	8	1506	G
53	8	1509	С



Mol	Chain	Res	Type
53	8	1531	G
53	8	1533	С
53	8	1534	G
53	8	1573	А
53	8	1574	G
53	8	1575	G
53	8	1576	А
53	8	1583	А
53	8	1584	G
53	8	1590	G
53	8	1595	U
53	8	1596	С
53	8	1597	А
53	8	1600	А
53	8	1602	С
53	8	1614	А
53	8	1618	С
53	8	1628	U
53	8	1629	G
53	8	1630	U
53	8	1632	С
53	8	1639	С
53	8	1640	С
53	8	1645	G
53	8	1652	С
53	8	1653	С
53	8	1657	U
53	8	1658	G
53	8	1666	U
53	8	1670	G
53	8	1678	А
53	8	1680	G
53	8	1681	A
53	8	1682	U
53	8	1683	С
53	8	1684	U
53	8	1693	A
53	8	$1\overline{697}$	G
53	8	1703	С
53	8	1704	U
$\overline{53}$	8	1711	C
53	8	1712	А



Mol	Chain	Res	Type
53	8	1713	G
53	8	1717	G
53	8	1726	G
53	8	1727	G
53	8	1730	А
53	8	1736	G
53	8	1742	U
53	8	1744	А
53	8	1747	G
53	8	1748	G
53	8	1771	U
53	8	1773	С
53	8	1774	G
53	8	1775	U
53	8	1780	G
53	8	1781	А
53	8	1783	С
53	8	1785	U
53	8	1791	А

Continued from previous page...

All (20) RNA pucker outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
4	LO	199	А
4	LO	314	U
4	LO	522	С
53	8	-3	U
53	8	0	U
53	8	22	А
53	8	199	G
53	8	240	U
53	8	283	U
53	8	322	G
53	8	372	G
53	8	876	G
53	8	880	С
53	8	919	А
53	8	997	G
53	8	1057	U
53	8	1094	G
53	8	1573	А
53	8	1638	G



\mathbf{Mol}	Chain	Res	\mathbf{Type}
53	8	1790	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)

There are no ligands in this entry.

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
46	\mathbf{SS}	2
22	LN	2
47	ST	2
24	LP	2
19	LK	2
38	SI	1
17	LH	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SS	408:UNK	С	828:ASN	Ν	85.72
1	SI	417:UNK	С	548:ASN	Ν	63.03
1	LN	730:UNK	С	731:HIS	Ν	39.41
1	ST	316:UNK	С	382:UNK	N	38.49
1	LH	831:UNK	С	846:ASN	Ν	26.10



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LN	716:UNK	С	717:UNK	Ν	21.45
1	LP	416:UNK	С	418:UNK	Ν	15.60
1	ST	252:UNK	С	264:UNK	Ν	14.89
1	LP	369:UNK	С	379:UNK	Ν	11.71
1	LK	426:UNK	С	428:ASP	Ν	11.33
1	SS	363:UNK	С	369:UNK	Ν	10.71
1	LK	402:UNK	С	404:UNK	Ν	4.30

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6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25441. 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: 216



Y Index: 216



Z Index: 216



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: 182

Y Index: 199

Z Index: 219

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 0.007. 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 3693 nm^3 ; this corresponds to an approximate mass of 3336 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 0.251 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25441 and PDB model 7SUK. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.007 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 (0.007).



9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9040	0.3140
5	0.5200	0.1000
6	0.6050	0.1570
8	0.9090	0.2630
LO	0.9890	0.3530
L2	0.9880	0.3600
L3	0.8400	0.3230
L4	0.8350	0.2260
L5	0.9450	0.4070
L6	0.7430	0.1750
L7	0.7720	0.2040
L8	0.8670	0.2410
L9	0.9360	0.3690
LC	0.9570	0.4350
LD	0.8710	0.2350
LE	0.8460	0.2520
m LF	0.9020	0.2620
LG	0.9810	0.4260
LH	0.9480	0.3750
LI	0.9290	0.2260
LJ	0.9540	0.3970
LK	0.9810	0.3210
LL	0.9530	0.3990
LM	0.9460	0.3870
LN	0.9490	0.3700
LO	0.9520	0.4190
LP	0.9710	0.3330
LQ	0.9530	0.3300
LR	0.8190	0.1640
LS	0.9550	0.4190
LT	0.9600	0.4180
LU	0.9370	0.3700
LV	0.8430	0.2340
LW	0.9490	0.4130
LX	0.8470	0.2280



Chain	Atom inclusion	Q-score
LY	0.8620	0.2620
LZ	0.9480	0.4160
NA	0.9010	0.3710
NB	0.9340	0.3810
ND	0.9270	0.3450
NE	0.7280	0.2910
NF	0.4850	0.0300
NG	0.9010	0.2330
NH	0.6270	0.1930
NI	0.3470	0.1710
NJ	0.9320	0.2520
NK	0.9510	0.2180
SA	0.9440	0.3620
SB	0.9440	0.3520
SC	0.9430	0.4130
SD	0.9390	0.3550
SE	0.9240	0.3920
SF	0.9500	0.3550
SG	0.9530	0.3100
SH	0.9470	0.3710
SI	0.9330	0.3620
SJ	0.9480	0.3210
SK	0.9610	0.3840
SL	0.9550	0.4140
SM	0.9260	0.4050
SN	0.9590	0.3740
SO	0.9890	0.3240
SP	0.8630	0.2240
SQ	0.8950	0.3950
SR	0.9210	0.3730
SS	0.9320	0.3350
ST	0.9440	0.3160
SU	0.9440	0.2940
SV	0.9070	0.3540
SY	0.9420	0.3970
SZ	0.9610	0.2440

