

Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 03:49 AM EDT

PDB ID	:	3W1K
Title	:	Crystal structure of the selenocysteine synthase SelA and tRNASec complex
Authors	:	Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on	:	2012-11-15
Resolution	:	7.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 7.50 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RNA backbone	3102	1079 (11.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Q	uality of chain	
1	А	452	44%	54%	•
1	В	452	46%	54%	
1	С	452	48%	51%	•
1	D	452	47%	52%	•
1	Е	452	46%	53%	•
2	F	95	16%	78%	• •



Mol	Chain	Length		Quality of chain		
2	G	95	14%	79%	•	·
2	Н	95	17%	77%	•	·
2	Ι	95	14%	76%	7%	•
2	J	95	14%	78%	5%	•



3W1K

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

Mol	Chain	Residues		I	Atom	s			ZeroOcc	AltConf	Trace
1	Δ	459	Total	С	Ν	Ο	Р	\mathbf{S}	0	0	0
1	Л	402	3575	2278	620	665	1	11	0	0	0
1	В	459	Total	С	Ν	Ο	Р	\mathbf{S}	0	0	0
1	D	402	3575	2278	620	665	1	11	0	0	0
1	С	459	Total	С	Ν	0	Р	\mathbf{S}	0	0	0
1	U	402	3575	2278	620	665	1	11	0	0	0
1	Л	459	Total	С	Ν	Ο	Р	S	0	0	0
1	D	402	3575	2278	620	665	1	11	0	0	0
1	F	459	Total	С	Ν	Ο	Р	S	0	0	0
		402	3575	2278	620	665	5 1 11 0		0	0	

• Molecule 1 is a protein called L-seryl-tRNA(Sec) selenium transferase.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	19	ALA	LYS	engineered mutation	UNP 067140
А	21	ALA	LYS	engineered mutation	UNP 067140
А	46	ALA	LYS	engineered mutation	UNP 067140
А	48	ALA	LYS	engineered mutation	UNP 067140
В	19	ALA	LYS	engineered mutation	UNP 067140
В	21	ALA	LYS	engineered mutation	UNP 067140
В	46	ALA	LYS	engineered mutation	UNP 067140
В	48	ALA	LYS	engineered mutation	UNP 067140
С	19	ALA	LYS	engineered mutation	UNP 067140
С	21	ALA	LYS	engineered mutation	UNP 067140
С	46	ALA	LYS	engineered mutation	UNP 067140
С	48	ALA	LYS	engineered mutation	UNP 067140
D	19	ALA	LYS	engineered mutation	UNP 067140
D	21	ALA	LYS	engineered mutation	UNP 067140
D	46	ALA	LYS	engineered mutation	UNP 067140
D	48	ALA	LYS	engineered mutation	UNP 067140
Е	19	ALA	LYS	engineered mutation	UNP 067140
Е	21	ALA	LYS	engineered mutation	UNP 067140
E	46	ALA	LYS	engineered mutation	UNP 067140



Chain	Residue	Modelled	Actual	Comment	Reference			
Ε	48	ALA	LYS	engineered mutation	UNP 067140			

• Molecule 2 is a RNA chain called selenocysteine tRNA.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
9	F	02	Total	С	Ν	Ο	Р	0	0	0
	Г	92	1957	873	342	650	92	0	0	0
9	С	02	Total	С	Ν	0	Р	0	0	0
	G	92	1957	873	342	650	92	0	0	0
9	ц	02	Total	С	Ν	0	Р	0	0	0
	11	92	1957	873	342	650	92	0	0	0
0	т	02	Total	С	Ν	0	Р	0	0	0
	1	92	1957	873	342	650	92	0	0	0
0	т	02	Total	С	Ν	0	Р	0	0	0
	J	92	1957	873	342	650	92		U	U



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. 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. 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: L-seryl-tRNA(Sec) selenium transferase

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L319 L319 K229 L324 C323 L230 L325 C323 L231 L326 K329 L233 L330 K329 L234 L331 L332 L242 L3335 K335 L244 L331 K335 L244 L332 K335 L244 L333 L252 L244 L334 L252 L244 L335 L254 L254 L344 L255 L244 L344 L255 L244 L344 L256 L254 L344 L256 L254 L344 L256 L254 L344 L256 L274 L355 L274 L266 K356 K356 L274 L355 L274 L266 L356 L366 L266 L356 L366 L266 L356 L366 L266 L356 L366 L266 L366 L366

13392 13392 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 13395 1402 13407 1413 1413 1413 1413 1413 1413 1413 1413 1413 1425 1428 1426 1428 1428 1428 1429 1428 1421 1428 1428 1428 1428 1428 1428 1428 1428 1428 1428 1428 1428 1438 1439 1438 1448 1448 1448 1448 1448 1448 1445 1445 <t

 \bullet Molecule 1: L-seryl-tRNA (Sec) selenium transferase

> D20 F26 F26 F26 D27 C27 C27 C27 C27 D27 L27

Cha	ain	ı C): '								48	%																5	1%								•			
M1 K2 S3	L4	L5 R6	07 18	6d	010 111	S12	K13 114	V 14 V 15	E16	117	r 10 A19	K20	A21	125	Y26	V27 V00	V 20 K 29	A30	A31	K32 E33	V34	A35 526	E30 K37	Y38	K39 K40	E41	142 143	E44	R.47	A48	D49 1 EO		E55 D56	V57	E58 DE0	09X	161	L64	P67	N68
169 K70 B71	V72	173 N74	A75 776	176 G77	V78 V70		T82 Mo2	CON	R86	A87	189 L89	890 8		600	197	298 700	ה ק ת	N102		PTO/	E113	D116	OTTW	1120	H121 H122	1123	E124 K125	Y126	1 1 30	T131	E1 27		N141 N142	A143	G144	L150	K157	E158	V159 1160	1161
S162 R163 C164	E165	L166 V167	E168 1160	1169 G170	G171 C172	F173	R174 1176	P176	D177	1178 M170	K180	K181	S182	R187	E188	V189	1191 T191	T192	N193	K194	V197			A203	A209	L210	L211 M212	K213	K016	S217	N218 5210	Y220	M221	F224	V225 E226	E227	V228	V234	H238	K239
Y240 G241 T242	P243	T244 Y245	Y246	D24/	L252 1 253		K257	E265	P266		C271	1272	S273	G275	1276	D277	V279	S280		G283 D284	K285	L286 17007		1294	1295 V296	G297	1.301	1302	TROF	K306	K307 N208	P309	I310	R312	A313	R315	I316 D317		1320 L321	S322
G323 L324 F375	M326	T327 L328	K329	L330 Y331	F332 F332	K334	R335 V226	E337	D338	1339	V341	1342	R343 M244	n3 45 L345	T346	0347 D346	D340	A351	L352	R353 Q354	K355	A356 V267	R358	L359	E360 K361	L362	L363 K364	D365	1366 P367	G368	L369 V370	1371	5372 V373		P380	S384	L385 P386	E387	T392	-
V395 A396 T307	R398	H399 D400	R401	L402 S403	S404	E406	L407	0400	R412	1.12	r41/ 1418	V419	C420	1422 1422	R423	E424	0426	L427	L428	r429 D430	M431	R432	V434	F435	D438	L439	140	K443	1 450	S451	1452									
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I73	V78	V79 180	90 Q	K86 A87	P88	890 890		194 N95	F96	197	A101		L107	<u>Y109</u>	-	R116	H122	I123	E124	X125 Y126		E129 1 120	T131		F13/ V138	V139	N140 N141	N142	A143 G144		L150	1160	1161 9160	R163	G164 E165	L166	V167 E168	1169	G171 G171	S172
F173 R174 T175	P176	D177 1178	M179	K180 K181	S182	E188	V189	T191	T192	N193	T195	K196	V197	D199	Y200	E201	1204	N205		1208	L211	M212 V213	CTZU	K216	N216 N218	F219	Y220 M221		F224 V725	E226	E227 V778	K229	L230	L233	V234	H238	K239 Y240	G241	1242 P243	T244
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(1323) (1324) (1324) (1324) (1331) (1333) (1333) (1333) (1333) (1333) (1334) (1334) (1334) (1334) (1334) (1335) (1335) (1336)

 \bullet Molecule 1: L-seryl-tRNA (Sec) selenium transferase



Chain H:	17%	77%	•••
01 01 02 05 05 05 05 05 05 05 05 05 05 05 05 05	C C C C C C C C C C C C C C C C C C C	U34 C35 C35 C35 C35 C35 C35 C35 C35 C42 C42 C42 C42 C42 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	04/G 0471 4471 6477 6477 6477 6477 6470 6470 6470
A47P 648 649 653 054 055 055 055 055 055	U60 U60 663 664 864 866 065 065 065 065 070 068 073 070 071 050 073 072 0 072 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		
• Molecule 2:	selenocysteine tRNA		
Chain I: 14	4%	76% 7	%•
61 62 62 65 65 86 86 87 09	A10 614 614 616 618 618 618 620 723 723 723 723 723 723 723 723 723 723	U33 U34 U34 C35 A36 A37 A37 A37 A37 C42 C42 C42 C42 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	0474 0474 0471 0471 6471 6477 6477 6478 6478
G470 A477 G48 G49 G53 U55 U55 C55 G57 G57	A58 1059 1059 1059 1057 1057 1059 1059 1059 1059 1059 1059 1059 1059		
• Molecule 2:	selenocysteine tRNA		
Chain J: 1	4%	78%	5% •
G G G G G G G G G G G G G G G G G G G	A 10 611 611 612 613 613 614 016 016 016 021 022 022 022 027 027 027 027 027 027 027	C32 U33 C35 C35 C35 C35 C35 C35 A37 A37 A37 A37 A37 C35 C40 C41 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	447E 047F 047F 047H 647J 647Z 647K 647K 647M
A47N 6470 6470 648 648 648 648 652 653 053 054 054	C C C C C C C C C C C C C C C C C C C		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	148.55Å 355.97 Å 165.50 Å	Deperitor
a, b, c, α , β , γ	90.00° 115.41° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	49.94 - 7.50	Depositor
Resolution (A)	49.94 - 7.49	EDS
% Data completeness	98.2 (49.94-7.50)	Depositor
(in resolution range)	98.0(49.94-7.49)	EDS
R _{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.28 (at 7.37 \text{\AA})$	Xtriage
Refinement program	CNS 1.3	Depositor
D D	0.194 , 0.240	Depositor
Λ, Λ_{free}	0.198 , 0.253	DCC
R_{free} test set	475 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	391.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.41,562.8	EDS
L-test for twinning ²	$< L > = 0.38, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	27660	wwPDB-VP
Average B, all atoms $(Å^2)$	525.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mol Chain		Bond lengths		Bond angles	
	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.41	0/3597	0.65	0/4831
1	В	0.39	0/3597	0.65	0/4831
1	С	0.39	0/3597	0.64	0/4831
1	D	0.41	0/3597	0.65	0/4831
1	Е	0.40	0/3597	0.64	0/4831
2	F	0.49	1/2185~(0.0%)	0.75	0/3401
2	G	0.44	1/2185~(0.0%)	0.73	0/3401
2	Н	0.42	1/2185~(0.0%)	0.73	0/3401
2	Ι	0.43	1/2185~(0.0%)	0.72	0/3401
2	J	0.43	1/2185~(0.0%)	0.72	2/3401~(0.1%)
All	All	0.42	5/28910~(0.0%)	0.68	2/41160~(0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	F	1	G	OP3-P	-7.24	1.52	1.61
2	Ι	1	G	OP3-P	-7.05	1.52	1.61
2	J	1	G	OP3-P	-7.05	1.52	1.61
2	Н	1	G	OP3-P	-6.86	1.52	1.61
2	G	1	G	OP3-P	-6.77	1.53	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	47(P)	А	OP2-P-O3'	6.24	118.93	105.20
2	J	27	С	OP2-P-O3'	5.73	117.81	105.20

There are no chirality outliers.

There are no planarity outliers.



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	А	3575	0	3758	296	0
1	В	3575	0	3758	290	0
1	С	3575	0	3758	284	0
1	D	3575	0	3758	300	0
1	Ε	3575	0	3758	256	0
2	F	1957	0	989	102	0
2	G	1957	0	989	124	0
2	Н	1957	0	989	105	0
2	Ι	1957	0	989	112	0
2	J	1957	0	989	91	0
All	All	27660	0	23735	1788	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 35.

All (1788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:157:LYS:HE2	1:C:209:ALA:HB2	1.27	1.14
1:B:1:MET:HG3	1:B:4:LEU:HD12	1.31	1.12
1:C:102:ASN:HB3	1:D:71:ARG:HH22	1.15	1.08
1:A:10:GLN:H	1:A:13:LYS:HD2	1.13	1.08
2:J:32:C:H2'	2:J:33:U:C6	1.93	1.02
1:B:10:GLN:H	1:B:13:LYS:HD2	1.20	1.02
1:C:353:ARG:HE	1:C:357:LYS:HD2	1.24	1.01
1:C:67:PRO:HD3	1:D:329:LYS:HE3	1.42	0.99
1:A:60:LYS:O	1:A:64:LEU:HG	1.63	0.98
1:B:374:ILE:HD11	1:B:428:LEU:HD21	1.42	0.97
1:D:221:MET:HG2	1:E:221:MET:HG2	1.47	0.97
2:G:47(H):U:H2'	2:G:47(I):A:O4'	1.65	0.97
1:D:4:LEU:O	1:D:42:ILE:HD13	1.65	0.95
1:B:423:ARG:HD2	1:B:428:LEU:HD12	1.49	0.95
1:B:373:VAL:HG22	1:B:395:VAL:HG22	1.49	0.94
1:A:157:LYS:HE2	1:A:209:ALA:HB2	1.50	0.94
1:A:442:ILE:O	1:A:446:LEU:HG	1.66	0.94



	1 · · · · · · · · · · · · · · · · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:11:ILE:HD12	2:F:18:G:OP1	1.68	0.93
1:E:5:LEU:HD11	1:E:39:ARG:HA	1.47	0.93
1:A:181:LYS:HG3	1:B:309:PRO:HG2	1.49	0.93
1:C:163:ARG:HD2	1:C:190:GLY:O	1.67	0.93
2:F:36:A:H2'	2:F:37:A:O4'	1.67	0.93
1:C:10:GLN:H	1:C:13:LYS:HD2	1.31	0.92
1:C:83:ASN:HB3	1:D:109:TYR:HD2	1.36	0.91
1:C:399:HIS:HE1	1:C:401:ARG:HD3	1.35	0.91
1:B:10:GLN:HB3	1:B:13:LYS:HG3	1.51	0.91
1:E:187:ARG:HE	1:E:203:ALA:HB1	1.34	0.91
1:C:332:PHE:CZ	1:D:29:LYS:HD2	2.06	0.91
1:D:150:LEU:HD13	1:D:179:MET:HG3	1.52	0.91
2:J:7:G:H22	2:J:66:A:H2	1.18	0.90
1:A:97:ILE:HD11	1:A:323:GLY:HA3	1.52	0.90
1:E:254:ILE:HD11	1:E:259:PHE:CE2	2.08	0.89
2:I:33:U:H5'	2:I:34:U:OP2	1.70	0.89
1:B:366:ILE:HB	1:B:369:LEU:HD12	1.55	0.89
2:F:47(H):U:H2'	2:F:47(I):A:O4'	1.74	0.88
2:I:7:G:H22	2:I:66:A:H2	1.19	0.88
1:A:171:GLY:HA3	1:B:116:ARG:NH2	1.86	0.88
1:A:68:ASN:HD22	1:B:122:HIS:HA	1.37	0.88
2:G:29:A:H2'	2:G:30:G:O4'	1.74	0.87
2:F:7:G:H22	2:F:66:A:H2	1.23	0.87
2:G:7:G:H22	2:G:66:A:H2	1.20	0.87
1:B:221:MET:HG2	1:C:221:MET:HG2	1.56	0.86
1:D:29:LYS:HD3	1:D:64:LEU:HD13	1.55	0.86
1:B:358:ARG:HH21	1:B:439:LEU:HD12	1.39	0.86
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.39	0.86
1:B:231:GLU:HG3	1:B:274:LEU:HD11	1.58	0.85
1:E:330:LEU:HD23	1:E:335:ARG:HD3	1.58	0.85
2:G:65:C:H2'	2:G:66:A:C8	2.11	0.85
1:C:73:ILE:HB	1:C:418:ILE:HG12	1.57	0.85
1:B:10:GLN:HG2	1:B:12:SER:H	1.42	0.85
1:B:176:PRO:HG3	1:C:191:THR:HG22	1.59	0.84
1:A:136:SER:HB3	1:A:296:VAL:HG12	1.60	0.84
2:I:47(A):C:H2'	2:I:47(B):G:H8	1.40	0.84
1:E:1:MET:CG	1:E:4:LEU:HD12	2.07	0.84
1:C:29:LYS:HD2	1:D:332:PHE:CZ	2.11	0.84
1:E:252:LEU:HD21	1:E:256:LEU:HG	1.58	0.84
1:B:298:LYS:HB2	1:B:301:LEU:HD12	1.60	0.83
2:I:25:U:O2'	2:I:26:C:H5'	1.79	0.83



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:167:VAL:HG12	1:D:219:PHE:HE2	1.41	0.83
1:A:90:SER:HB3	1:A:338:ASP:O	1.77	0.83
2:F:47(G):U:H6	2:F:47(G):U:O5'	1.62	0.83
1:E:443:LYS:O	1:E:447:GLN:HG2	1.79	0.83
2:F:32:C:H2'	2:F:33:U:O4'	1.80	0.82
1:C:5:LEU:HD11	1:C:39:ARG:HA	1.60	0.82
2:I:47(H):U:H2'	2:I:47(I):A:O4'	1.80	0.82
1:B:263:VAL:HG11	1:B:388:LEU:HD13	1.62	0.82
2:H:7:G:H22	2:H:66:A:H2	1.24	0.81
1:A:10:GLN:HB2	1:A:13:LYS:HE3	1.61	0.81
1:A:29:LYS:HD2	1:B:332:PHE:CZ	2.16	0.81
1:B:97:ILE:HD11	1:B:323:GLY:HA3	1.61	0.81
1:D:362:LEU:HB3	1:D:443:LYS:HD2	1.62	0.81
2:G:25:U:H2'	2:G:26:C:H6	1.46	0.81
1:B:411:LEU:HD22	1:B:418:ILE:HD12	1.61	0.80
1:C:126:TYR:CB	1:C:328:LEU:HD13	2.12	0.80
1:A:171:GLY:HA3	1:B:116:ARG:HH22	1.44	0.80
2:G:25:U:H2'	2:G:26:C:C6	2.17	0.80
1:E:187:ARG:NE	1:E:203:ALA:HB1	1.97	0.80
2:J:47(L):C:H2'	2:J:47(M):G:C8	2.17	0.80
2:G:27:C:H2'	2:G:28:U:O4'	1.80	0.80
1:A:5:LEU:HD11	1:A:39:ARG:HG2	1.63	0.79
1:A:28:VAL:O	1:A:32:ARG:HG3	1.80	0.79
1:A:12:SER:O	1:A:16:GLU:HG3	1.82	0.79
1:B:60:LYS:O	1:B:64:LEU:HG	1.83	0.79
1:D:5:LEU:HD12	1:D:8:ILE:HD12	1.62	0.79
1:C:102:ASN:HB3	1:D:71:ARG:NH2	1.96	0.79
1:D:176:PRO:HG3	1:E:191:THR:HG22	1.64	0.79
2:J:47(L):C:H2'	2:J:47(M):G:H8	1.48	0.79
1:B:10:GLN:H	1:B:13:LYS:CD	1.95	0.79
1:A:366:ILE:HB	1:A:369:LEU:CD1	2.12	0.79
2:J:38:A:O2'	2:J:39:U:H5'	1.82	0.79
1:B:217:SER:O	1:B:386:PRO:HD3	1.83	0.79
2:H:67(A):A:H2'	2:H:68:C:C6	2.18	0.79
1:A:10:GLN:N	1:A:13:LYS:HD2	1.96	0.78
1:C:97:ILE:HD11	1:C:323:GLY:HA3	1.65	0.78
1:E:366:ILE:HB	1:E:369:LEU:HD12	1.66	0.78
1:C:234:VAL:CG2	1:C:276:ILE:HD13	2.14	0.78
1:D:344:MET:O	1:D:432:ARG:HD2	1.81	0.78
1:C:11:ILE:HB	2:I:16:U:H4'	1.65	0.78
1:B:197:VAL:HG22	1:B:228:VAL:HG13	1.64	0.78



	1 · · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:I:55:U:H2'	2:I:57:G:OP2	1.84	0.78
2:J:47(H):U:H2'	2:J:47(I):A:O4'	1.84	0.78
1:B:405:GLN:HE22	1:B:422:ILE:HG21	1.49	0.78
1:C:126:TYR:HB2	1:C:328:LEU:HD13	1.64	0.78
1:C:253:LEU:HD23	1:C:331:TYR:CD1	2.19	0.78
1:D:10:GLN:HG2	1:D:12:SER:H	1.49	0.78
1:E:1:MET:C	1:E:3:SER:H	1.86	0.78
1:E:343:ARG:O	1:E:347:GLN:HG3	1.83	0.77
1:D:39:ARG:O	1:D:43:ILE:HG13	1.85	0.77
1:A:332:PHE:CZ	1:B:29:LYS:HD2	2.20	0.77
1:D:42:ILE:HD11	1:D:50:LEU:HD21	1.66	0.77
1:A:366:ILE:HB	1:A:369:LEU:HD12	1.64	0.77
1:C:126:TYR:CE2	1:C:325:GLU:HG3	2.20	0.77
1:B:37:LYS:O	1:B:41:GLU:HG3	1.85	0.76
2:I:47(A):C:H2'	2:I:47(B):G:C8	2.18	0.76
1:C:397:ILE:HD11	1:C:427:LEU:HD23	1.67	0.76
1:A:399:HIS:HE1	1:A:401:ARG:HD3	1.50	0.76
1:A:163:ARG:HD2	1:A:190:GLY:O	1.85	0.76
1:B:90:SER:HB3	1:B:338:ASP:O	1.84	0.76
1:E:5:LEU:CD1	1:E:39:ARG:HA	2.16	0.76
1:D:10:GLN:HB2	2:H:19:G:H3'	1.66	0.76
1:B:5:LEU:HD11	1:B:39:ARG:HA	1.68	0.76
1:A:217:SER:O	1:A:386:PRO:HD3	1.86	0.76
2:G:65:C:H2'	2:G:66:A:H8	1.52	0.75
1:C:130:LEU:HD13	1:C:253:LEU:HD21	1.69	0.75
2:F:65:C:H2'	2:F:66:A:C8	2.20	0.75
2:H:15:C:H2'	2:H:16:U:C6	2.20	0.75
1:D:1:MET:HG3	1:D:2:LYS:N	2.00	0.75
1:D:399:HIS:CE1	1:D:450:LEU:HD22	2.21	0.75
1:E:37:LYS:O	1:E:41:GLU:HG3	1.87	0.75
1:E:163:ARG:HD2	1:E:190:GLY:O	1.87	0.75
2:F:37:A:H2'	2:F:38:A:O4'	1.87	0.75
1:A:216:LYS:HG2	1:A:219:PHE:CZ	2.22	0.74
1:A:60:LYS:HD2	1:A:64:LEU:HD21	1.67	0.74
1:E:363:LEU:CD2	1:E:446:LEU:HD12	2.16	0.74
1:C:181:LYS:HG3	1:D:309:PRO:HG2	1.68	0.74
1:E:72:VAL:HG22	1:E:417:PRO:HG2	1.69	0.74
2:I:8:A:N6	2:I:21:U:O4	2.20	0.74
1:C:29:LYS:HD3	1:C:64:LEU:HD13	1.69	0.74
1:A:145:ALA:O	1:A:149:VAL:HG23	1.88	0.74
1:B:399:HIS:CE1	1:B:450:LEU:HD22	2.22	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:301:LEU:O	1:C:305:ILE:HG13	1.87	0.74
1:D:366:ILE:HB	1:D:369:LEU:HD12	1.69	0.74
2:F:47:U:H2'	2:F:47(A):C:C6	2.22	0.74
2:J:65:C:H2'	2:J:66:A:C8	2.23	0.74
1:A:28:VAL:HG12	1:A:32:ARG:NE	2.03	0.73
1:A:61:ILE:O	1:A:65:MET:HG3	1.88	0.73
1:B:169:ILE:O	1:B:173:PHE:HB3	1.88	0.73
1:E:73:ILE:HB	1:E:418:ILE:HG12	1.69	0.73
1:B:12:SER:O	1:B:16:GLU:HG3	1.88	0.73
1:E:363:LEU:HD21	1:E:446:LEU:HD12	1.69	0.73
2:H:46:C:C2'	2:H:47:U:H5'	2.18	0.73
2:G:58:A:H1'	2:G:60:U:OP2	1.88	0.73
1:A:147:PHE:HB2	1:A:178:ILE:HD11	1.69	0.73
2:G:28:U:O2'	2:G:29:A:H5'	1.88	0.73
1:C:39:ARG:HH22	2:I:18:G:H2'	1.54	0.73
1:A:68:ASN:ND2	1:B:122:HIS:HA	2.02	0.73
1:B:10:GLN:HB3	1:B:13:LYS:HE3	1.70	0.72
2:F:58:A:H1'	2:F:60:U:OP2	1.89	0.72
1:B:150:LEU:HD13	1:B:179:MET:HG3	1.70	0.72
1:D:5:LEU:HD11	1:D:39:ARG:HG3	1.70	0.72
1:B:39:ARG:O	1:B:43:ILE:HG13	1.88	0.72
2:J:55:U:H2'	2:J:57:G:OP2	1.89	0.72
1:C:359:LEU:HB2	1:C:439:LEU:HD22	1.70	0.72
2:F:47(A):C:H2'	2:F:47(B):G:H8	1.53	0.72
1:B:25:ILE:HG13	1:B:26:TYR:N	2.04	0.72
1:E:280:SER:HA	1:E:294:ILE:O	1.90	0.72
2:J:47(I):A:H2'	2:J:47(J):A:O4'	1.89	0.72
1:B:10:GLN:HB2	2:F:19:G:H3'	1.71	0.72
1:B:163:ARG:NH1	1:C:188:GLU:OE1	2.22	0.72
2:I:15:C:H2'	2:I:16:U:C6	2.24	0.72
1:B:224:PHE:CD1	1:C:218:ASN:HB2	2.25	0.72
2:F:47(A):C:H2'	2:F:47(B):G:C8	2.25	0.72
1:B:10:GLN:N	1:B:13:LYS:HD2	2.00	0.71
2:I:47:U:H2'	2:I:47(A):C:C6	2.26	0.71
1:B:336:TYR:O	1:B:339:ILE:HG12	1.90	0.71
1:E:30:ALA:O	1:E:34:VAL:HG23	1.91	0.71
2:H:37:A:H2'	2:H:38:A:O4'	1.91	0.71
2:G:47(J):A:O2'	2:G:47(K):G:H5'	1.91	0.71
1:D:169:ILE:HG22	1:D:218:ASN:OD1	1.91	0.71
2:G:63:C:H2'	2:G:64:A:C8	2.25	0.71
1:A:330:LEU:HD23	1:A:335:ARG:HD3	1.72	0.71



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:35:C:H2'	2:F:36:A:C8	2.26	0.71
2:F:63:C:H2'	2:F:64:A:C8	2.25	0.71
1:A:11:ILE:O	1:A:15:VAL:HG23	1.90	0.71
1:B:159:VAL:HG22	1:B:210:LEU:HB3	1.70	0.71
1:E:1:MET:SD	1:E:4:LEU:HD12	2.30	0.71
1:D:280:SER:HA	1:D:294:ILE:O	1.90	0.71
2:I:9:U:H4'	2:I:45:U:C2	2.26	0.71
1:A:407:LEU:CD2	1:A:427:LEU:HD22	2.21	0.70
1:B:28:VAL:HG12	1:B:32:ARG:NE	2.04	0.70
2:H:46:C:H2'	2:H:47:U:O4'	1.91	0.70
2:I:47(G):U:H2'	2:I:47(H):U:O4'	1.90	0.70
1:B:77:GLY:HA2	1:B:433:THR:HG23	1.73	0.70
1:E:90:SER:HB3	1:E:338:ASP:O	1.90	0.70
2:J:37:A:H2'	2:J:38:A:O4'	1.92	0.70
1:B:1:MET:HG3	1:B:4:LEU:CD1	2.18	0.70
1:B:163:ARG:HD2	1:B:190:GLY:O	1.92	0.70
1:C:12:SER:O	1:C:16:GLU:HG3	1.91	0.70
1:D:407:LEU:CD2	1:D:427:LEU:HD22	2.21	0.70
1:A:138:VAL:HG13	1:A:293:GLY:O	1.91	0.70
1:B:280:SER:HA	1:B:294:ILE:O	1.92	0.70
1:B:285:LLP:OP4	1:B:285:LLP:H4'1	1.91	0.70
1:E:330:LEU:CD2	1:E:335:ARG:HD3	2.22	0.70
2:F:47(O):G:H2'	2:F:47(P):A:C8	2.27	0.70
1:A:301:LEU:O	1:A:305:ILE:HG13	1.91	0.70
1:D:5:LEU:CD1	1:D:8:ILE:HD12	2.22	0.70
1:E:77:GLY:HA3	1:E:430:ASP:CG	2.12	0.70
1:E:211:LEU:HG	1:E:242:ILE:CG2	2.21	0.70
1:E:1:MET:HG3	1:E:4:LEU:HD12	1.72	0.70
1:D:408:SER:O	1:D:412:ARG:HG3	1.91	0.69
1:E:217:SER:O	1:E:386:PRO:HD3	1.93	0.69
2:G:47:U:H2'	2:G:47(A):C:C6	2.27	0.69
2:H:47:U:H2'	2:H:47(A):C:C6	2.27	0.69
1:B:290:PRO:HB2	1:B:320:THR:HG22	1.75	0.69
1:C:10:GLN:HG3	2:I:19:G:O5'	1.91	0.69
1:C:280:SER:HA	1:C:294:ILE:O	1.93	0.69
1:E:230:LEU:HD23	1:E:233:LEU:HD12	1.74	0.69
1:E:435:PHE:HB3	1:E:437:GLU:OE1	1.93	0.69
1:B:1:MET:CG	1:B:4:LEU:HD12	2.18	0.69
1:A:280:SER:HA	1:A:294:ILE:O	1.93	0.69
2:J:47(A):C:H2'	2:J:47(B):G:H8	1.57	0.69
2:I:37:A:H2'	2:I:38:A:O4'	1.91	0.69



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:374:ILE:HD11	1:B:428:LEU:CD2	2.21	0.69
1:C:28:VAL:O	1:C:32:ARG:HG3	1.91	0.69
1:E:11:ILE:HG21	1:E:28:VAL:HG13	1.73	0.69
2:F:55:U:H2'	2:F:57:G:OP2	1.93	0.69
2:J:47:U:H2'	2:J:47(A):C:C6	2.28	0.69
1:A:253:LEU:HD23	1:A:331:TYR:CD1	2.28	0.69
1:D:200:TYR:CE2	1:D:228:VAL:HG21	2.28	0.69
2:G:37:A:H2'	2:G:38:A:O4'	1.93	0.69
1:E:10:GLN:HG2	1:E:12:SER:H	1.57	0.68
2:I:6:A:H2'	2:I:7:G:C8	2.29	0.68
1:B:187:ARG:HE	1:B:203:ALA:HB1	1.58	0.68
2:F:47(I):A:H2'	2:F:47(J):A:O4'	1.93	0.68
1:A:399:HIS:CE1	1:A:401:ARG:HD3	2.28	0.68
1:C:402:LEU:HD22	1:C:406:GLU:HG2	1.76	0.68
1:E:141:ASN:OD1	1:E:143:ALA:HB3	1.93	0.68
1:B:407:LEU:HD23	1:B:427:LEU:HD22	1.76	0.68
1:D:8:ILE:HD11	1:D:38:TYR:HB3	1.74	0.68
1:E:405:GLN:HE22	1:E:422:ILE:HG21	1.56	0.68
2:F:38:A:C2'	2:F:39:U:H5'	2.23	0.68
1:D:298:LYS:HB2	1:D:301:LEU:HD12	1.75	0.68
2:H:47(H):U:H2'	2:H:47(I):A:O4'	1.93	0.68
2:I:28:U:O2'	2:I:29:A:H5'	1.94	0.68
1:A:345:LEU:CD2	1:A:380:PRO:HB3	2.24	0.68
1:E:358:ARG:HH21	1:E:439:LEU:HD12	1.58	0.68
1:B:390:LEU:HB2	1:B:432:ARG:NH2	2.09	0.68
1:C:366:ILE:HG23	1:C:367:PRO:HD2	1.75	0.68
2:G:25:U:O2'	2:G:26:C:H5'	1.94	0.68
2:H:47(A):C:H2'	2:H:47(B):G:H8	1.59	0.68
1:A:320:THR:HG22	1:B:319:LEU:HD12	1.76	0.68
1:E:234:VAL:HG22	1:E:276:ILE:HD13	1.74	0.68
1:D:126:TYR:O	1:D:130:LEU:HG	1.94	0.67
2:F:65:C:H2'	2:F:66:A:H8	1.56	0.67
2:J:47(A):C:H2'	2:J:47(B):G:C8	2.29	0.67
1:E:162:SER:HB2	1:E:200:TYR:OH	1.94	0.67
1:E:197:VAL:HG22	1:E:228:VAL:HG13	1.77	0.67
2:I:47(L):C:H2'	2:I:47(M):G:C8	2.29	0.67
1:C:42:ILE:HD11	1:C:50:LEU:HD21	1.76	0.67
1:E:159:VAL:HG22	1:E:210:LEU:HB3	1.75	0.67
1:A:2:LYS:O	1:A:6:ARG:HG3	1.94	0.67
1:A:10:GLN:H	1:A:13:LYS:CD	2.00	0.67
2:J:47(O):G:H2'	2:J:47(P):A:C8	2.29	0.67



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:194:LYS:HG2	1:B:226:GLU:HB2	1.76	0.67
1:B:390:LEU:CB	1:B:432:ARG:HH22	2.08	0.67
1:C:39:ARG:O	1:C:43:ILE:HG13	1.94	0.67
1:E:420:CYS:SG	1:E:427:LEU:HD11	2.35	0.67
1:E:8:ILE:HD11	1:E:38:TYR:HB3	1.75	0.67
1:A:85:GLY:HA2	1:B:107:LEU:HD23	1.76	0.67
1:A:123:ILE:CD1	1:A:325:GLU:HB2	2.23	0.67
1:B:256:LEU:HD23	1:B:263:VAL:CG2	2.24	0.67
1:C:302:ILE:HD13	1:C:305:ILE:HD12	1.76	0.67
1:D:2:LYS:HE2	1:D:6:ARG:NH2	2.10	0.67
1:E:8:ILE:CD1	1:E:38:TYR:HB3	2.24	0.67
1:B:28:VAL:HG12	1:B:32:ARG:HE	1.59	0.67
1:E:407:LEU:HD23	1:E:427:LEU:HD22	1.77	0.67
1:E:423:ARG:HD2	1:E:428:LEU:CD1	2.25	0.67
2:I:47(O):G:H2'	2:I:47(P):A:C8	2.30	0.67
1:A:392:THR:HG21	1:A:430:ASP:OD2	1.95	0.66
1:A:10:GLN:HB2	1:A:13:LYS:CE	2.25	0.66
1:C:187:ARG:HE	1:C:203:ALA:HB1	1.59	0.66
1:A:39:ARG:O	1:A:43:ILE:HG13	1.95	0.66
1:B:145:ALA:O	1:B:149:VAL:HG23	1.95	0.66
1:C:5:LEU:HD12	1:C:42:ILE:HD12	1.76	0.66
1:D:97:ILE:HD11	1:D:323:GLY:HA3	1.76	0.66
2:H:36:A:O2'	2:H:37:A:H5'	1.95	0.66
2:I:38:A:C2'	2:I:39:U:H5'	2.25	0.66
2:J:58:A:H1'	2:J:60:U:OP2	1.95	0.66
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.77	0.66
1:A:165:GLU:OE1	1:A:213:LYS:HG3	1.96	0.66
1:A:343:ARG:O	1:A:347:GLN:HG3	1.95	0.66
1:C:399:HIS:CD2	1:C:450:LEU:HD13	2.30	0.66
1:C:90:SER:HB3	1:C:338:ASP:O	1.95	0.66
1:C:167:VAL:HG12	1:C:219:PHE:HE2	1.61	0.66
1:D:340:PRO:O	1:D:344:MET:HG3	1.95	0.66
2:I:63:C:H2'	2:I:64:A:C8	2.31	0.66
1:A:30:ALA:O	1:A:34:VAL:HG23	1.95	0.66
1:B:390:LEU:HB2	1:B:432:ARG:HH22	1.58	0.66
2:G:30:G:O2'	2:G:31:A:H5'	1.95	0.66
2:H:58:A:H1'	2:H:60:U:OP2	1.95	0.66
1:A:361:LYS:HA	1:A:364:LYS:HE3	1.77	0.66
1:D:242:ILE:HG23	1:D:243:PRO:HD2	1.77	0.66
1:E:12:SER:O	1:E:16:GLU:HG3	1.96	0.66
2:J:27:C:H2'	2:J:28:U:O4'	1.95	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:263:VAL:HG12	1:A:265:GLU:H	1.59	0.65
1:B:412:ARG:HD2	1:B:419:VAL:HG22	1.78	0.65
2:G:63:C:H2'	2:G:64:A:H8	1.61	0.65
1:A:169:ILE:HG13	1:A:173:PHE:HD2	1.60	0.65
1:C:11:ILE:HG21	1:C:28:VAL:HG13	1.78	0.65
1:C:37:LYS:O	1:C:41:GLU:HG3	1.96	0.65
1:D:217:SER:O	1:D:386:PRO:HD3	1.96	0.65
2:G:47(O):G:H2'	2:G:47(P):A:C8	2.30	0.65
1:A:68:ASN:HD22	1:B:122:HIS:CA	2.07	0.65
1:A:302:ILE:CG2	1:A:306:LYS:HE3	2.27	0.65
1:D:302:ILE:CG2	1:D:306:LYS:HE3	2.26	0.65
1:E:130:LEU:HD13	1:E:253:LEU:HD21	1.79	0.65
1:E:211:LEU:HG	1:E:242:ILE:HG22	1.78	0.65
2:J:24:C:O2'	2:J:25:U:H5'	1.96	0.65
1:A:401:ARG:NH1	1:A:450:LEU:O	2.28	0.65
1:C:72:VAL:HG13	1:C:417:PRO:HG2	1.79	0.65
1:E:39:ARG:O	1:E:43:ILE:HG13	1.97	0.65
2:J:63:C:H2'	2:J:64:A:C8	2.32	0.65
1:D:39:ARG:HG2	2:H:56:C:N4	2.10	0.65
1:A:68:ASN:ND2	1:B:122:HIS:CD2	2.64	0.65
2:F:28:U:O2'	2:F:29:A:H5'	1.96	0.65
2:G:31:A:N7	2:G:32:C:C4	2.64	0.65
1:A:309:PRO:HG2	1:B:181:LYS:HG3	1.78	0.65
1:E:371:ILE:HG12	1:E:397:ILE:HG22	1.77	0.65
1:A:123:ILE:HG23	1:A:328:LEU:HD12	1.77	0.65
2:F:67(A):A:H2'	2:F:68:C:C6	2.32	0.65
2:F:69:U:H2'	2:F:70:C:C6	2.32	0.65
2:H:47(O):G:H2'	2:H:47(P):A:C8	2.32	0.65
1:A:83:ASN:HB3	1:B:109:TYR:HD2	1.62	0.65
1:B:32:ARG:HH22	2:F:18:G:P	2.19	0.65
1:A:13:LYS:HA	1:A:16:GLU:OE1	1.97	0.64
2:G:36:A:H2'	2:G:37:A:C8	2.31	0.64
1:D:250:SER:HB2	1:D:286:LEU:CD1	2.27	0.64
2:J:25:U:O2'	2:J:26:C:H5'	1.96	0.64
1:B:352:LEU:HD13	1:B:392:THR:HA	1.78	0.64
1:B:423:ARG:HD2	1:B:428:LEU:CD1	2.26	0.64
1:C:333:GLU:HA	1:D:25:ILE:HD12	1.80	0.64
1:D:218:ASN:ND2	1:E:224:PHE:HB2	2.13	0.64
2:I:47(L):C:H2'	2:I:47(M):G:H8	1.60	0.64
1:D:11:ILE:HG22	2:H:16:U:H4'	1.78	0.64
1:A:271:CYS:O	1:A:276:ILE:HG12	1.98	0.64



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:408:SER:OG	1:D:422:ILE:HD11	1.98	0.64
1:E:152:THR:HG21	1:E:305:ILE:HA	1.79	0.64
2:G:24:C:O2'	2:G:25:U:H5'	1.97	0.64
2:G:29:A:C2'	2:G:30:G:O4'	2.46	0.64
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.62	0.64
1:D:302:ILE:HG22	1:D:306:LYS:HE3	1.80	0.64
1:D:359:LEU:HB2	1:D:439:LEU:HD22	1.79	0.64
1:B:359:LEU:HB2	1:B:439:LEU:HD22	1.79	0.64
1:A:373:VAL:HG22	1:A:395:VAL:HG22	1.80	0.64
1:D:353:ARG:HB2	1:D:393:TYR:CE2	2.31	0.64
2:J:65:C:H2'	2:J:66:A:H8	1.62	0.64
2:F:6:A:H2'	2:F:7:G:C8	2.33	0.64
1:D:218:ASN:HD22	1:E:224:PHE:HB2	1.63	0.64
1:D:250:SER:HB2	1:D:286:LEU:HD12	1.79	0.64
1:E:86:ARG:NH1	1:E:285:LLP:HE2	2.12	0.64
1:B:10:GLN:NE2	2:F:19:G:OP1	2.31	0.63
1:C:11:ILE:O	1:C:15:VAL:HG23	1.97	0.63
1:D:161:ILE:HG21	1:D:166:LEU:HD21	1.79	0.63
1:A:309:PRO:CG	1:B:181:LYS:HG3	2.28	0.63
1:C:211:LEU:HG	1:C:242:ILE:HG21	1.80	0.63
1:D:3:SER:O	1:D:7:GLN:HG2	1.98	0.63
2:I:10:A:H4'	2:I:45:U:O4'	1.98	0.63
1:C:339:ILE:HD11	1:C:342:ILE:HG13	1.80	0.63
1:A:28:VAL:HG12	1:A:32:ARG:HE	1.63	0.63
1:C:5:LEU:CD1	1:C:42:ILE:HD12	2.28	0.63
1:D:259:PHE:HB3	1:D:346:THR:HG21	1.80	0.63
2:I:10:A:C5'	2:I:45:U:O4'	2.47	0.63
1:A:270:ASP:O	1:A:274:LEU:HG	1.98	0.63
1:C:317:ASP:HA	1:D:291:GLN:OE1	1.98	0.63
1:C:431:MET:CE	1:C:434:VAL:HG21	2.28	0.63
1:B:12:SER:OG	2:F:16:U:H1'	1.99	0.63
2:H:21:U:H2'	2:H:22:G:C8	2.34	0.63
2:H:63:C:H2'	2:H:64:A:C8	2.34	0.63
2:I:35:C:H2'	2:I:36:A:O4'	1.98	0.63
1:A:161:ILE:HG23	1:A:166:LEU:HD21	1.80	0.63
1:B:25:ILE:HG13	1:B:26:TYR:H	1.60	0.63
1:E:4:LEU:O	1:E:42:ILE:HD13	1.99	0.63
2:G:47(E):A:H2	2:G:47(I):A:N7	1.96	0.63
2:I:30:G:O2'	2:I:31:A:H5'	1.98	0.63
1:E:423:ARG:HD2	1:E:428:LEU:HD12	1.81	0.63
2:F:24:C:O2'	2:F:25:U:H5'	1.99	0.63



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:32:ARG:HH11	1:B:32:ARG:HG2	1.63	0.62
1:B:32:ARG:NH1	2:F:18:G:OP1	2.32	0.62
1:B:128:ASN:HD21	1:B:135:SER:HA	1.64	0.62
1:D:224:PHE:HD1	1:E:218:ASN:HB2	1.62	0.62
2:H:47(A):C:H2'	2:H:47(B):G:C8	2.34	0.62
1:B:178:ILE:HG23	1:B:179:MET:N	2.14	0.62
1:A:302:ILE:HG22	1:A:306:LYS:HE3	1.81	0.62
1:C:25:ILE:HG13	1:C:26:TYR:N	2.14	0.62
2:H:32:C:H2'	2:H:33:U:C6	2.34	0.62
1:E:396:ALA:HB2	1:E:428:LEU:HD23	1.82	0.62
2:F:63:C:H2'	2:F:64:A:H8	1.62	0.62
1:D:5:LEU:HD21	1:D:39:ARG:HG2	1.82	0.62
2:G:67(A):A:H2'	2:G:68:C:C6	2.34	0.62
1:A:37:LYS:O	1:A:41:GLU:HG3	1.99	0.62
1:B:33:GLU:OE1	1:B:60:LYS:HD2	2.00	0.62
2:G:47(H):U:O2'	2:G:47(I):A:H5'	1.99	0.62
2:G:32:C:H2'	2:G:33:U:C6	2.34	0.62
1:A:11:ILE:HD12	2:G:18:G:OP1	2.00	0.62
1:A:25:ILE:HG13	1:A:26:TYR:N	2.14	0.62
1:B:123:ILE:HD11	1:B:325:GLU:HB2	1.81	0.62
2:I:47(E):A:H2'	2:I:47(F):U:O4'	2.00	0.62
2:I:58:A:H1'	2:I:60:U:OP2	2.00	0.62
1:B:187:ARG:NE	1:B:203:ALA:HB1	2.14	0.62
1:C:57:VAL:O	1:C:61:ILE:HG13	2.00	0.62
1:C:312:ARG:HG2	1:D:173:PHE:HB2	1.82	0.62
1:D:1:MET:CG	1:D:2:LYS:N	2.62	0.62
1:A:425:ASP:CG	1:A:425:ASP:O	2.37	0.61
1:C:32:ARG:HG2	1:C:32:ARG:HH11	1.64	0.61
2:F:69:U:H2'	2:F:70:C:H6	1.64	0.61
1:A:69:ILE:HG12	1:B:122:HIS:ND1	2.14	0.61
1:C:67:PRO:HB2	1:D:96:PHE:CZ	2.34	0.61
1:C:187:ARG:NE	1:C:203:ALA:HB1	2.15	0.61
1:C:362:LEU:O	1:C:443:LYS:HG3	2.00	0.61
2:F:47(G):U:O5'	2:F:47(G):U:C6	2.51	0.61
1:C:348:ASP:HB2	1:C:351:ALA:HB2	1.82	0.61
1:B:61:ILE:O	1:B:65:MET:HG3	1.99	0.61
1:C:30:ALA:O	1:C:34:VAL:HG23	2.01	0.61
1:C:99:GLU:O	1:D:71:ARG:NH2	2.33	0.61
1:D:79:VAL:HG21	1:D:345:LEU:HG	1.81	0.61
1:E:33:GLU:OE1	1:E:60:LYS:HD2	2.01	0.61
1:C:150:LEU:HD13	1:C:179:MET:HG3	1.83	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:405:GLN:HG3	2:G:1:G:O4'	2.01	0.61
1:E:363:LEU:HB2	1:E:371:ILE:CD1	2.31	0.61
1:A:445:THR:O	1:A:449:LEU:HG	2.01	0.61
1:B:123:ILE:CD1	1:B:325:GLU:HB2	2.31	0.61
2:G:54:U:H2'	2:G:55:U:O4'	2.01	0.61
2:H:6:A:H2'	2:H:7:G:C8	2.36	0.61
2:I:67(A):A:H2'	2:I:68:C:C6	2.36	0.61
2:J:30:G:O2'	2:J:31:A:H5'	2.01	0.61
1:C:355:LYS:HG3	1:C:439:LEU:HD11	1.83	0.61
2:G:29:A:O2'	2:G:30:G:H5'	2.01	0.61
2:G:69:U:H2'	2:G:70:C:C6	2.35	0.61
1:B:405:GLN:NE2	1:B:422:ILE:HG21	2.15	0.61
1:C:102:ASN:CB	1:D:71:ARG:HH22	2.04	0.60
1:D:125:LYS:O	1:D:129:GLU:HG3	2.00	0.60
1:D:347:GLN:NE2	1:D:352:LEU:HD21	2.16	0.60
1:B:452:ILE:HG23	1:B:452:ILE:OXT	2.00	0.60
1:C:75:ALA:HB3	1:C:420:CYS:HB3	1.83	0.60
1:D:347:GLN:HE21	1:D:352:LEU:HD21	1.66	0.60
1:E:10:GLN:OE1	1:E:13:LYS:HE3	2.01	0.60
1:E:11:ILE:O	1:E:15:VAL:HG23	2.01	0.60
2:G:71:C:H2'	2:G:72:C:C6	2.36	0.60
1:A:251:GLY:HA2	1:A:268:PHE:HE2	1.66	0.60
1:E:158:GLU:OE2	1:E:187:ARG:HD2	2.00	0.60
2:H:69:U:H2'	2:H:70:C:C6	2.36	0.60
1:A:130:LEU:HD13	1:A:253:LEU:HD21	1.83	0.60
2:F:30:G:O2'	2:F:31:A:H5'	2.01	0.60
2:H:53:G:O2'	2:H:54:U:H5'	2.00	0.60
2:G:47(A):C:H2'	2:G:47(B):G:H8	1.66	0.60
2:I:71:C:H2'	2:I:72:C:C6	2.36	0.60
1:A:420:CYS:SG	1:A:427:LEU:HD21	2.41	0.60
1:E:88:PRO:HG2	1:E:340:PRO:CB	2.31	0.60
1:B:10:GLN:HG2	1:B:12:SER:N	2.15	0.60
1:B:57:VAL:O	1:B:61:ILE:HG13	2.01	0.60
1:C:344:MET:O	1:C:432:ARG:HD2	2.01	0.60
1:D:163:ARG:HH11	1:E:166:LEU:CD1	2.14	0.60
1:D:216:LYS:HG2	1:D:219:PHE:CZ	2.37	0.60
1:A:399:HIS:HE1	1:A:401:ARG:CD	2.14	0.60
1:B:28:VAL:O	1:B:32:ARG:HG3	2.02	0.60
1:D:123:ILE:CD1	1:D:325:GLU:HB2	2.32	0.60
1:E:57:VAL:O	1:E:61:ILE:HG13	2.01	0.60
2:I:69:U:H2'	2:I:70:C:C6	2.36	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:6:A:H2'	2:J:7:G:C8	2.37	0.60
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.16	0.60
1:B:11:ILE:O	1:B:15:VAL:HG23	2.02	0.60
1:B:178:ILE:CG2	1:B:179:MET:N	2.65	0.60
1:C:285:LLP:OP1	1:D:312:ARG:NH1	2.33	0.60
1:D:200:TYR:CD2	1:D:228:VAL:HG21	2.36	0.60
2:G:15:C:H2'	2:G:16:U:C6	2.37	0.60
1:A:363:LEU:O	1:A:371:ILE:HD11	2.02	0.60
1:C:14:VAL:HG13	1:C:18:PHE:HE2	1.66	0.60
1:C:423:ARG:HD2	1:C:428:LEU:CD1	2.32	0.60
2:G:6:A:H2'	2:G:7:G:C8	2.37	0.60
1:A:10:GLN:HB3	1:A:13:LYS:HG3	1.84	0.59
1:C:11:ILE:CB	2:I:16:U:H4'	2.32	0.59
2:F:71:C:H2'	2:F:72:C:C6	2.36	0.59
1:D:336:TYR:O	1:D:339:ILE:HG12	2.02	0.59
1:E:107:LEU:HD11	1:E:321:LEU:HD23	1.84	0.59
2:J:69:U:H2'	2:J:70:C:C6	2.36	0.59
1:B:10:GLN:CB	1:B:13:LYS:HE3	2.31	0.59
1:C:399:HIS:CE1	1:C:401:ARG:HD3	2.27	0.59
1:A:397:ILE:HD11	1:A:427:LEU:HD23	1.84	0.59
1:D:32:ARG:O	1:D:36:GLU:HG2	2.02	0.59
1:E:107:LEU:O	1:E:122:HIS:HE1	1.85	0.59
2:I:10:A:C2	2:I:26:C:O2	2.54	0.59
2:J:38:A:HO2'	2:J:39:U:H5'	1.67	0.59
1:B:32:ARG:HG2	1:B:32:ARG:NH1	2.18	0.59
1:C:93:VAL:HA	1:C:326:MET:HG2	1.84	0.59
1:C:187:ARG:HD3	1:C:203:ALA:HB1	1.84	0.59
1:A:10:GLN:HG3	2:G:19:G:P	2.43	0.59
2:I:38:A:O2'	2:I:39:U:H5'	2.02	0.59
2:J:71:C:H2'	2:J:72:C:C6	2.37	0.59
1:A:150:LEU:HD13	1:A:179:MET:HG3	1.84	0.59
1:D:2:LYS:HG2	1:D:2:LYS:O	2.03	0.59
1:D:208:THR:HG22	1:D:242:ILE:HD13	1.85	0.59
1:E:187:ARG:CD	1:E:203:ALA:HB1	2.32	0.59
1:C:10:GLN:HG3	2:I:19:G:P	2.43	0.59
1:C:366:ILE:HB	1:C:369:LEU:CD1	2.33	0.59
1:D:373:VAL:HG22	1:D:395:VAL:HG22	1.85	0.59
2:I:63:C:H2'	2:I:64:A:H8	1.67	0.59
1:A:193:ASN:O	1:A:225:VAL:HG13	2.03	0.59
1:B:12:SER:HG	2:F:16:U:H1'	1.68	0.59
1:C:285:LLP:P	1:D:312:ARG:HH22	2.26	0.59



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:2:LYS:O	1:E:6:ARG:HG3	2.02	0.59
1:B:30:ALA:O	1:B:34:VAL:HG23	2.02	0.58
2:G:4:A:H2'	2:G:5:G:C8	2.38	0.58
2:H:67(A):A:H2'	2:H:68:C:H6	1.68	0.58
1:A:153:LEU:HD11	1:A:301:LEU:HD22	1.85	0.58
1:B:242:ILE:HG23	1:B:243:PRO:HD2	1.85	0.58
1:C:13:LYS:HA	1:C:16:GLU:OE1	2.03	0.58
1:C:32:ARG:HG2	1:C:32:ARG:NH1	2.18	0.58
1:C:83:ASN:HB3	1:D:109:TYR:CD2	2.27	0.58
1:C:373:VAL:HG22	1:C:395:VAL:HG22	1.84	0.58
1:D:66:LYS:NZ	1:D:415:GLU:OE2	2.36	0.58
1:D:420:CYS:SG	1:D:427:LEU:HD11	2.43	0.58
2:G:39:U:H2'	2:G:40:C:O4'	2.04	0.58
1:B:1:MET:C	1:B:3:SER:H	2.06	0.58
2:F:67:U:H2'	2:F:67(A):A:H8	1.68	0.58
2:H:24:C:O2'	2:H:25:U:H5'	2.03	0.58
1:A:409:ARG:NH1	1:A:413:LEU:CD1	2.67	0.58
1:E:169:ILE:O	1:E:173:PHE:HB3	2.04	0.58
1:E:396:ALA:HB1	1:E:426:GLN:CD	2.24	0.58
2:I:10:A:C4'	2:I:45:U:O4'	2.51	0.58
1:A:126:TYR:CB	1:A:328:LEU:HD13	2.34	0.58
1:A:181:LYS:HG3	1:B:309:PRO:CG	2.29	0.58
1:B:256:LEU:HD23	1:B:263:VAL:HG21	1.83	0.58
1:D:10:GLN:HG2	1:D:12:SER:N	2.16	0.58
2:H:35:C:N4	2:H:36:A:N6	2.50	0.58
2:H:69:U:H2'	2:H:70:C:H6	1.68	0.58
2:J:53:G:H2'	2:J:54:U:H6	1.68	0.58
1:C:55:GLU:O	1:C:59:ARG:HG3	2.03	0.58
1:C:332:PHE:HZ	1:D:29:LYS:HD2	1.61	0.58
1:C:344:MET:O	1:C:432:ARG:CD	2.52	0.58
1:E:7:GLN:HB2	1:E:50:LEU:CD1	2.33	0.58
1:E:399:HIS:CE1	1:E:450:LEU:HD22	2.38	0.58
2:F:4:A:H2'	2:F:5:G:H8	1.69	0.58
2:H:71:C:H2'	2:H:72:C:C6	2.39	0.58
1:B:358:ARG:NH2	1:B:439:LEU:HD12	2.16	0.58
1:C:272:ILE:HD11	1:C:296:VAL:HG23	1.86	0.58
2:H:21:U:H2'	2:H:22:G:H8	1.67	0.58
2:I:59:U:O2'	2:I:60:U:H5'	2.03	0.58
2:J:69:U:H2'	2:J:70:C:H6	1.69	0.58
1:B:298:LYS:O	1:B:302:ILE:HG12	2.03	0.58
1:D:33:GLU:OE1	1:D:60:LYS:HD2	2.03	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:38:A:O2'	2:F:39:U:H5'	2.03	0.58
1:C:69:ILE:HD11	1:D:321:LEU:HG	1.85	0.58
1:D:344:MET:O	1:D:432:ARG:CD	2.52	0.58
2:J:54:U:H2'	2:J:55:U:O4'	2.04	0.58
1:B:32:ARG:O	1:B:36:GLU:HG2	2.04	0.58
1:C:363:LEU:HD22	1:C:366:ILE:HD12	1.86	0.58
1:D:37:LYS:O	1:D:41:GLU:HG3	2.04	0.58
2:J:18:G:O2'	2:J:57:G:N2	2.35	0.58
2:J:53:G:O2'	2:J:54:U:H5'	2.03	0.57
2:J:63:C:H2'	2:J:64:A:H8	1.69	0.57
1:A:409:ARG:HH12	1:A:413:LEU:CD1	2.17	0.57
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.70	0.57
1:C:10:GLN:HB3	1:C:13:LYS:HG3	1.85	0.57
1:D:224:PHE:CD1	1:E:218:ASN:HB2	2.38	0.57
1:E:353:ARG:HB2	1:E:393:TYR:CE2	2.39	0.57
2:G:4:A:H2'	2:G:5:G:H8	1.69	0.57
2:H:7:G:C2	2:H:49:G:C8	2.92	0.57
2:J:28:U:O2'	2:J:29:A:H5'	2.04	0.57
1:A:85:GLY:HA2	1:B:107:LEU:CD2	2.35	0.57
1:A:435:PHE:HB2	1:A:438:ASP:OD2	2.04	0.57
1:B:24:GLU:O	1:B:28:VAL:HG23	2.04	0.57
1:C:49:ASP:OD1	1:C:50:LEU:N	2.37	0.57
1:E:120:ILE:HG21	1:E:137:PHE:CD1	2.39	0.57
2:F:6:A:O2'	2:F:7:G:H5'	2.04	0.57
2:G:26:C:H2'	2:G:27:C:O4'	2.04	0.57
2:G:53:G:H2'	2:G:54:U:H6	1.68	0.57
2:J:53:G:H2'	2:J:54:U:C6	2.39	0.57
1:B:3:SER:O	1:B:7:GLN:HG2	2.04	0.57
1:B:10:GLN:HB2	2:F:19:G:C3'	2.34	0.57
2:F:54:U:H2'	2:F:55:U:O4'	2.04	0.57
2:H:30:G:O2'	2:H:31:A:H5'	2.05	0.57
2:H:53:G:H2'	2:H:54:U:H6	1.70	0.57
1:C:157:LYS:HE2	1:C:209:ALA:CB	2.19	0.57
1:C:423:ARG:HD2	1:C:428:LEU:HD12	1.86	0.57
1:D:399:HIS:CE1	1:D:401:ARG:HB2	2.40	0.57
2:F:71:C:H2'	2:F:72:C:H6	1.70	0.57
1:B:224:PHE:HD1	1:C:218:ASN:HB2	1.69	0.57
2:F:4:A:H2'	2:F:5:G:C8	2.39	0.57
2:G:25:U:C2	2:G:26:C:C5	2.93	0.57
2:H:48:G:H4'	2:H:49:G:H5"	1.86	0.57
1:A:251:GLY:HA2	1:A:268:PHE:CE2	2.40	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:359:LEU:HB2	1:A:439:LEU:HD22	1.87	0.57
1:C:386:PRO:HG2	1:C:387:GLU:H	1.70	0.57
1:D:407:LEU:HD23	1:D:427:LEU:HD22	1.86	0.57
2:F:35:C:O2'	2:F:36:A:H5'	2.03	0.57
2:H:15:C:H2'	2:H:16:U:H6	1.70	0.57
1:B:175:ILE:N	1:B:176:PRO:HD2	2.19	0.57
1:C:339:ILE:CD1	1:C:342:ILE:HG13	2.34	0.57
1:C:421:ARG:HH11	1:C:421:ARG:HG2	1.68	0.57
1:E:169:ILE:HG22	1:E:218:ASN:OD1	2.05	0.57
1:E:408:SER:O	1:E:412:ARG:HG3	2.04	0.57
1:B:137:PHE:CE1	1:B:306:LYS:HG2	2.40	0.57
1:C:187:ARG:CD	1:C:203:ALA:HB1	2.33	0.57
1:D:234:VAL:HG11	1:D:275:GLY:HA3	1.87	0.57
1:E:25:ILE:HG13	1:E:26:TYR:N	2.19	0.57
2:F:53:G:H2'	2:F:54:U:H6	1.69	0.57
2:I:47(I):A:H2'	2:I:47(J):A:O4'	2.05	0.57
1:A:161:ILE:CG2	1:A:166:LEU:HD21	2.35	0.57
1:B:10:GLN:HB3	1:B:13:LYS:CG	2.30	0.57
2:G:26:C:O2'	2:G:27:C:H5'	2.04	0.57
2:H:4:A:H2'	2:H:5:G:H8	1.70	0.57
2:I:54:U:H2'	2:I:55:U:O4'	2.03	0.57
1:A:137:PHE:CD1	1:A:306:LYS:HG2	2.40	0.56
1:A:169:ILE:O	1:A:173:PHE:HB3	2.05	0.56
1:A:360:GLU:O	1:A:364:LYS:HG3	2.05	0.56
1:C:11:ILE:HD12	2:I:18:G:OP1	2.05	0.56
1:D:87:ALA:CB	1:D:341:VAL:HG21	2.35	0.56
1:E:299:LYS:O	1:E:303:GLU:HG2	2.05	0.56
2:F:53:G:O2'	2:F:54:U:H5'	2.05	0.56
2:G:43:G:H5'	2:G:43:G:H8	1.70	0.56
1:A:194:LYS:HG2	1:A:226:GLU:HB2	1.87	0.56
1:B:216:LYS:HG2	1:B:219:PHE:CZ	2.40	0.56
1:B:443:LYS:O	1:B:447:GLN:HG2	2.05	0.56
2:G:69:U:H2'	2:G:70:C:H6	1.69	0.56
2:I:38:A:H2'	2:I:39:U:O4'	2.04	0.56
2:J:14:G:O2'	2:J:15:C:H5'	2.05	0.56
1:C:6:ARG:NH1	2:I:20:U:O4	2.38	0.56
1:C:14:VAL:HG13	1:C:18:PHE:CE2	2.40	0.56
1:C:69:ILE:CD1	1:D:321:LEU:HG	2.36	0.56
1:C:141:ASN:OD1	1:C:143:ALA:HB3	2.05	0.56
1:D:360:GLU:HG3	1:D:371:ILE:HG21	1.87	0.56
1:E:1:MET:HG3	1:E:4:LEU:CD1	2.35	0.56



	le us pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:200:TYR:CE2	1:E:228:VAL:HG21	2.41	0.56
1:E:336:TYR:O	1:E:339:ILE:HG12	2.04	0.56
2:G:53:G:H2'	2:G:54:U:C6	2.40	0.56
2:H:36:A:H2'	2:H:37:A:O4'	2.05	0.56
2:J:4:A:H2'	2:J:5:G:H8	1.70	0.56
1:C:169:ILE:O	1:C:173:PHE:HB3	2.05	0.56
2:H:41:U:O2'	2:H:42:A:H5'	2.05	0.56
2:H:47(E):A:H2'	2:H:47(F):U:H5'	1.88	0.56
1:B:15:VAL:HA	1:B:27:VAL:HG11	1.88	0.56
1:B:187:ARG:CD	1:B:203:ALA:HB1	2.36	0.56
1:C:194:LYS:NZ	1:C:224:PHE:HB3	2.21	0.56
1:C:211:LEU:HG	1:C:242:ILE:CG2	2.34	0.56
1:D:107:LEU:HD11	1:D:321:LEU:HD23	1.88	0.56
1:E:1:MET:C	1:E:3:SER:N	2.57	0.56
1:E:18:PHE:HB3	1:E:21:ALA:HB3	1.87	0.56
2:I:10:A:H5'	2:I:45:U:O4'	2.06	0.56
2:J:35:C:H2'	2:J:36:A:O4'	2.06	0.56
1:D:22:TYR:CG	1:D:61:ILE:HG21	2.41	0.56
1:E:401:ARG:NH1	1:E:450:LEU:O	2.39	0.56
2:G:47(K):G:O2'	2:G:47(L):C:H5'	2.06	0.56
2:H:32:C:C4	2:H:33:U:C4	2.93	0.56
2:H:47(E):A:C2'	2:H:47(F):U:H5'	2.35	0.56
2:I:15:C:H2'	2:I:16:U:H6	1.70	0.56
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.88	0.56
1:D:194:LYS:HB2	1:E:168:GLU:OE1	2.06	0.56
2:H:4:A:H2'	2:H:5:G:C8	2.40	0.56
1:D:5:LEU:HD21	2:H:56:C:N4	2.21	0.56
1:D:194:LYS:HG2	1:D:226:GLU:HB2	1.87	0.56
1:E:88:PRO:HG2	1:E:340:PRO:HB2	1.88	0.56
1:E:161:ILE:HG13	1:E:212:MET:O	2.05	0.56
1:E:269:ARG:HH11	1:E:269:ARG:HG3	1.71	0.56
2:G:53:G:O2'	2:G:54:U:H5'	2.05	0.56
1:B:40:LYS:O	1:B:44:GLU:HG3	2.06	0.56
1:C:26:TYR:OH	1:D:333:GLU:CG	2.54	0.56
1:C:285:LLP:OP3	1:D:312:ARG:NH2	2.26	0.56
1:D:30:ALA:O	1:D:34:VAL:HG23	2.06	0.56
2:I:53:G:O2'	2:I:54:U:H5'	2.06	0.56
1:C:39:ARG:HH22	2:I:18:G:C2'	2.17	0.56
2:J:4:A:H2'	2:J:5:G:C8	2.41	0.56
1:A:57:VAL:O	1:A:61:ILE:HG13	2.05	0.55
1:B:402:LEU:HD12	1:B:450:LEU:CD2	2.36	0.55



	io ao pagoni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:230:LEU:O	1:D:234:VAL:HG23	2.06	0.55
1:E:213:LYS:HE3	1:E:246:TYR:HE1	1.71	0.55
2:F:27:C:H2'	2:F:28:U:O4'	2.06	0.55
2:I:39:U:H2'	2:I:40:C:O4'	2.05	0.55
2:I:69:U:H2'	2:I:70:C:H6	1.69	0.55
1:A:366:ILE:HG23	1:A:367:PRO:HD2	1.89	0.55
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.88	0.55
1:D:201:GLU:OE2	1:D:239:LYS:NZ	2.37	0.55
1:E:399:HIS:CE1	1:E:401:ARG:HD3	2.41	0.55
2:F:67:U:H2'	2:F:67(A):A:C8	2.42	0.55
1:D:27:VAL:HG22	1:D:61:ILE:HD13	1.88	0.55
1:D:123:ILE:HD11	1:D:325:GLU:HB2	1.89	0.55
1:D:163:ARG:HG2	1:D:188:GLU:HB2	1.87	0.55
1:D:220:TYR:CD2	1:D:387:GLU:HG2	2.41	0.55
1:E:87:ALA:CB	1:E:341:VAL:HG21	2.37	0.55
1:A:39:ARG:NH2	2:G:18:G:O2'	2.40	0.55
1:C:107:LEU:O	1:C:122:HIS:HE1	1.90	0.55
1:C:420:CYS:SG	1:C:427:LEU:HD11	2.47	0.55
1:E:169:ILE:HD11	1:E:285:LLP:H5'1	1.87	0.55
2:I:4:A:H2'	2:I:5:G:C8	2.42	0.55
2:I:53:G:H2'	2:I:54:U:H6	1.72	0.55
1:A:123:ILE:HD11	1:A:325:GLU:HB2	1.87	0.55
1:A:234:VAL:HG12	1:A:238:HIS:CD2	2.41	0.55
1:C:216:LYS:HG2	1:C:219:PHE:CZ	2.42	0.55
1:C:242:ILE:HG23	1:C:243:PRO:HD2	1.88	0.55
2:F:59:U:O2'	2:F:60:U:H5'	2.07	0.55
2:G:47(A):C:H2'	2:G:47(B):G:C8	2.42	0.55
2:G:59:U:O2'	2:G:60:U:H5'	2.06	0.55
1:B:399:HIS:CD2	1:B:450:LEU:HD13	2.41	0.55
1:A:194:LYS:HG2	1:A:226:GLU:CB	2.36	0.55
1:D:326:MET:O	1:D:330:LEU:HG	2.06	0.55
1:A:157:LYS:CE	1:A:209:ALA:HB2	2.32	0.55
1:A:169:ILE:HG13	1:A:173:PHE:CD2	2.41	0.55
1:C:39:ARG:NH2	2:I:18:G:O2'	2.39	0.55
1:C:363:LEU:HD21	1:C:443:LYS:HA	1.88	0.55
1:D:150:LEU:HB3	1:D:182:SER:OG	2.07	0.55
2:H:47(L):C:H2'	2:H:47(M):G:C8	2.41	0.55
2:J:43:G:H5'	2:J:43:G:H8	1.72	0.55
1:A:348:ASP:O	1:A:351:ALA:HB3	2.06	0.55
1:C:26:TYR:OH	1:D:333:GLU:HG2	2.07	0.55
1:C:270:ASP:O	1:C:274:LEU:HG	2.06	0.55



	io ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:285:LLP:H4'1	1:C:285:LLP:OP4	2.05	0.55
1:D:10:GLN:HB2	2:H:19:G:C3'	2.37	0.55
2:G:41:U:O2'	2:G:42:A:H5'	2.07	0.55
2:H:28:U:O2'	2:H:29:A:H5'	2.06	0.55
2:H:63:C:H2'	2:H:64:A:H8	1.71	0.55
2:J:47(G):U:H2'	2:J:47(H):U:O4'	2.07	0.55
1:B:10:GLN:CB	1:B:13:LYS:HG3	2.33	0.55
1:D:163:ARG:HD2	1:D:190:GLY:O	2.07	0.55
1:E:80:ILE:O	1:E:80:ILE:HG22	2.07	0.55
1:B:208:THR:HG22	1:B:242:ILE:HD13	1.90	0.54
1:C:313:ALA:HB1	1:D:144:GLY:CA	2.37	0.54
1:E:74:ASN:HB2	1:E:84:LEU:HD13	1.89	0.54
1:E:278:LEU:HD23	1:E:297:GLY:HA3	1.89	0.54
1:E:430:ASP:OD1	1:E:432:ARG:HB3	2.06	0.54
2:F:47(K):G:O2'	2:F:47(L):C:H5'	2.07	0.54
2:J:3:G:H2'	2:J:4:A:O4'	2.08	0.54
1:A:436:HIS:CD2	1:A:439:LEU:HD12	2.42	0.54
1:C:435:PHE:HB2	1:C:438:ASP:OD2	2.07	0.54
2:F:38:A:H2'	2:F:39:U:H5'	1.90	0.54
1:A:239:LYS:HD3	1:A:240:TYR:CE2	2.42	0.54
1:C:171:GLY:HA3	1:D:116:ARG:NH2	2.22	0.54
1:D:402:LEU:HD12	1:D:450:LEU:CD2	2.38	0.54
2:H:47(F):U:O2'	2:H:47(G):U:H5"	2.08	0.54
2:J:26:C:O2'	2:J:27:C:H5'	2.08	0.54
2:J:39:U:H2'	2:J:40:C:O4'	2.07	0.54
1:A:265:GLU:HB2	1:A:385:LEU:HD21	1.90	0.54
1:B:169:ILE:HG22	1:B:218:ASN:OD1	2.08	0.54
1:C:317:ASP:HB3	1:D:291:GLN:HB3	1.90	0.54
1:D:392:THR:HG21	1:D:430:ASP:OD2	2.07	0.54
2:I:3:G:H2'	2:I:4:A:O4'	2.08	0.54
2:I:4:A:H2'	2:I:5:G:H8	1.72	0.54
1:A:396:ALA:HB2	1:A:428:LEU:CD2	2.37	0.54
1:D:57:VAL:O	1:D:61:ILE:HG13	2.07	0.54
1:C:278:LEU:HD23	1:C:297:GLY:HA3	1.89	0.54
1:C:302:ILE:CG2	1:C:306:LYS:HE3	2.38	0.54
1:D:405:GLN:HE22	1:D:422:ILE:HG21	1.72	0.54
1:D:438:ASP:O	1:D:442:ILE:HG13	2.08	0.54
2:I:47(K):G:O2'	2:I:47(L):C:H5'	2.07	0.54
1:A:40:LYS:O	1:A:44:GLU:HG3	2.08	0.54
1:A:388:LEU:HD21	1:A:390:LEU:HD11	1.90	0.54
1:C:10:GLN:N	1:C:13:LYS:HD2	2.13	0.54



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:283:GLY:O	1:C:287:LEU:HB3	2.08	0.54
1:C:420:CYS:HB2	1:C:428:LEU:O	2.06	0.54
2:I:71:C:H2'	2:I:72:C:H6	1.72	0.54
1:A:100:ILE:HD12	1:B:69:ILE:HG22	1.90	0.54
1:C:234:VAL:HG22	1:C:276:ILE:HD13	1.88	0.54
1:C:421:ARG:HG2	1:C:421:ARG:NH1	2.22	0.54
1:D:14:VAL:CG1	1:D:18:PHE:HE2	2.21	0.54
1:D:86:ARG:HD2	1:D:284:ASP:OD2	2.08	0.54
1:E:347:GLN:NE2	1:E:352:LEU:HD21	2.22	0.54
2:J:71:C:H2'	2:J:72:C:H6	1.73	0.54
1:A:25:ILE:HG13	1:A:26:TYR:H	1.71	0.54
1:A:96:PHE:O	1:A:100:ILE:HG12	2.08	0.54
1:C:407:LEU:CD2	1:C:427:LEU:HD22	2.38	0.54
1:D:139:VAL:HB	1:D:314:LEU:HB3	1.89	0.54
2:H:53:G:H2'	2:H:54:U:C6	2.43	0.54
1:A:263:VAL:HG12	1:A:264:ASP:N	2.22	0.54
1:C:28:VAL:HG11	2:I:16:U:OP1	2.08	0.54
1:D:176:PRO:HG3	1:E:191:THR:CG2	2.36	0.54
1:D:256:LEU:HD23	1:D:263:VAL:CG2	2.37	0.54
1:D:423:ARG:HD2	1:D:428:LEU:CD1	2.38	0.54
1:E:28:VAL:HG12	1:E:32:ARG:HE	1.71	0.54
1:E:220:TYR:HD2	1:E:386:PRO:HB2	1.74	0.53
2:G:55:U:H2'	2:G:57:G:OP2	2.08	0.53
2:G:64:A:H2'	2:G:65:C:C6	2.43	0.53
1:A:171:GLY:CA	1:B:116:ARG:NH2	2.67	0.53
1:D:191:THR:HG22	1:E:176:PRO:HG3	1.90	0.53
2:F:53:G:H2'	2:F:54:U:C6	2.42	0.53
2:G:5(A):U:C2'	2:G:6:A:H5'	2.38	0.53
2:H:59:U:O2'	2:H:60:U:H5'	2.08	0.53
2:I:39:U:H2'	2:I:40:C:C6	2.43	0.53
1:A:102:ASN:HB3	1:B:71:ARG:HH12	1.72	0.53
1:C:194:LYS:HG2	1:C:226:GLU:HB2	1.90	0.53
1:D:239:LYS:HD3	1:D:240:TYR:CE2	2.43	0.53
1:E:136:SER:HB3	1:E:296:VAL:HG12	1.89	0.53
2:G:71:C:H2'	2:G:72:C:H6	1.72	0.53
1:A:420:CYS:SG	1:A:427:LEU:HD11	2.49	0.53
1:D:348:ASP:HB2	1:D:351:ALA:HB2	1.90	0.53
1:E:32:ARG:O	1:E:36:GLU:HG2	2.08	0.53
2:G:10:A:C6	2:G:44:G:N1	2.76	0.53
1:A:340:PRO:HA	1:A:343:ARG:NH1	2.23	0.53
1:B:351:ALA:O	1:B:354:GLN:HB3	2.09	0.53



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:399:HIS:CE1	1:B:401:ARG:HB2	2.44	0.53
1:C:10:GLN:OE1	2:I:20:U:OP1	2.26	0.53
1:C:179:MET:O	1:C:182:SER:HB3	2.09	0.53
1:C:343:ARG:O	1:C:347:GLN:HG3	2.09	0.53
1:D:47:ARG:HD3	1:D:49:ASP:O	2.08	0.53
1:D:179:MET:HA	1:D:182:SER:HB3	1.90	0.53
1:E:178:ILE:HG23	1:E:179:MET:N	2.23	0.53
2:G:35:C:N4	2:G:36:A:N6	2.56	0.53
2:J:47(K):G:O2'	2:J:47(L):C:H5'	2.07	0.53
1:A:10:GLN:CB	1:A:13:LYS:HE3	2.35	0.53
1:C:159:VAL:HG13	1:C:210:LEU:HB3	1.90	0.53
1:D:7:GLN:HB2	1:D:50:LEU:CD1	2.39	0.53
1:D:39:ARG:NE	2:H:19:G:O6	2.42	0.53
1:D:107:LEU:O	1:D:122:HIS:HE1	1.92	0.53
1:D:197:VAL:HG22	1:D:228:VAL:HG13	1.91	0.53
1:E:79:VAL:HG12	1:E:341:VAL:HG13	1.91	0.53
1:B:10:GLN:HG3	2:F:19:G:P	2.48	0.53
1:C:29:LYS:CD	1:D:332:PHE:CZ	2.89	0.53
1:E:161:ILE:HG21	1:E:166:LEU:HD21	1.90	0.53
1:E:200:TYR:CD2	1:E:228:VAL:HG21	2.44	0.53
1:E:234:VAL:HG12	1:E:238:HIS:CD2	2.44	0.53
2:J:46:C:C4	2:J:47:U:C4	2.97	0.53
1:B:187:ARG:HD3	1:B:203:ALA:HB1	1.91	0.53
1:D:270:ASP:O	1:D:274:LEU:HG	2.08	0.53
1:E:79:VAL:HG13	1:E:344:MET:SD	2.48	0.53
2:F:39:U:H2'	2:F:40:C:O4'	2.08	0.53
2:J:15:C:H2'	2:J:16:U:C6	2.43	0.53
1:A:97:ILE:HD11	1:A:323:GLY:CA	2.34	0.53
1:B:194:LYS:HD3	1:C:168:GLU:OE2	2.09	0.53
2:H:3:G:H2'	2:H:4:A:O4'	2.09	0.53
1:A:231:GLU:O	1:A:235:LYS:HG3	2.09	0.52
1:A:347:GLN:NE2	1:A:352:LEU:HD21	2.24	0.52
1:B:179:MET:O	1:B:182:SER:HB3	2.09	0.52
1:A:11:ILE:HG21	1:A:28:VAL:HG13	1.90	0.52
1:A:334:LYS:HD2	1:A:336:TYR:OH	2.09	0.52
1:B:142:ASN:HB3	1:B:285:LLP:OP4	2.08	0.52
1:B:263:VAL:CG1	1:B:388:LEU:HD13	2.35	0.52
1:D:363:LEU:HB2	1:D:371:ILE:HD13	1.90	0.52
2:I:18:G:O2'	2:I:57:G:N2	2.38	0.52
1:A:161:ILE:HG13	1:A:212:MET:O	2.09	0.52
1:A:399:HIS:CE1	1:A:401:ARG:HB2	2.44	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:162:SER:HB2	1:B:200:TYR:OH	2.08	0.52
1:B:425:ASP:O	1:B:425:ASP:CG	2.48	0.52
1:C:11:ILE:CG2	2:I:16:U:H4'	2.39	0.52
1:C:86:ARG:NH1	1:C:285:LLP:HE2	2.24	0.52
1:D:396:ALA:HB1	1:D:426:GLN:CD	2.30	0.52
1:C:131:THR:HG21	1:C:296:VAL:HG11	1.92	0.52
1:C:165:GLU:OE2	1:C:213:LYS:NZ	2.38	0.52
1:D:77:GLY:HA3	1:D:430:ASP:CG	2.30	0.52
2:G:10:A:C6	2:G:44:G:C6	2.97	0.52
2:G:39:U:H2'	2:G:40:C:C6	2.45	0.52
2:I:31:A:H2'	2:I:32:C:O4'	2.09	0.52
2:I:41:U:O2'	2:I:42:A:H5'	2.08	0.52
1:B:200:TYR:CE2	1:B:228:VAL:HG21	2.44	0.52
1:B:210:LEU:HD12	1:B:243:PRO:HG2	1.92	0.52
1:C:25:ILE:HG13	1:C:26:TYR:H	1.72	0.52
1:C:407:LEU:HD23	1:C:427:LEU:HD22	1.90	0.52
1:E:211:LEU:HG	1:E:242:ILE:HG21	1.91	0.52
2:G:3:G:H2'	2:G:4:A:O4'	2.10	0.52
2:I:53:G:H2'	2:I:54:U:C6	2.44	0.52
1:D:165:GLU:OE1	1:D:213:LYS:HG3	2.10	0.52
2:H:71:C:H2'	2:H:72:C:H6	1.74	0.52
1:B:234:VAL:CG2	1:B:276:ILE:HD13	2.39	0.52
1:C:212:MET:HE3	1:C:245:TYR:HE1	1.75	0.52
1:D:169:ILE:HD12	1:D:169:ILE:O	2.09	0.52
1:E:194:LYS:HG2	1:E:226:GLU:HB2	1.91	0.52
2:J:5(A):U:C2'	2:J:6:A:H5'	2.39	0.52
1:A:370:LYS:HB2	1:A:398:ARG:O	2.10	0.52
1:B:252:LEU:HD12	1:B:253:LEU:N	2.25	0.52
1:C:28:VAL:HG12	1:C:32:ARG:NE	2.25	0.52
1:E:208:THR:HG22	1:E:242:ILE:HD13	1.92	0.52
1:B:169:ILE:O	1:B:169:ILE:HG13	2.08	0.52
1:C:47:ARG:HD3	1:C:49:ASP:O	2.09	0.52
1:D:35:ALA:HB1	1:D:39:ARG:NH2	2.25	0.52
1:D:254:ILE:HD13	1:D:336:TYR:HE1	1.74	0.52
1:E:25:ILE:HG13	1:E:26:TYR:H	1.73	0.52
2:G:47(E):A:C2	2:G:47(I):A:N7	2.77	0.52
2:H:6:A:O2'	2:H:7:G:H5'	2.10	0.52
1:A:427:LEU:HD23	1:A:429:PHE:HE1	1.75	0.51
1:B:230:LEU:HB3	1:B:274:LEU:CD2	2.39	0.51
1:E:147:PHE:HB2	1:E:178:ILE:HD11	1.92	0.51
1:B:38:TYR:O	1:B:42:ILE:HG13	2.10	0.51



	A la C	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:91:LYS:HE2	1:B:95:ASN:HD21	1.75	0.51
1:B:142:ASN:HD22	1:B:285:LLP:C5	2.23	0.51
1:B:218:ASN:ND2	1:C:224:PHE:HB2	2.25	0.51
1:B:224:PHE:HB2	1:C:218:ASN:ND2	2.25	0.51
1:B:360:GLU:HG3	1:B:371:ILE:CG2	2.41	0.51
1:C:29:LYS:HD2	1:D:332:PHE:CE2	2.45	0.51
1:A:15:VAL:HA	1:A:27:VAL:HG11	1.91	0.51
1:B:5:LEU:HD12	1:B:8:ILE:CD1	2.41	0.51
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.92	0.51
1:E:234:VAL:HG11	1:E:275:GLY:HA3	1.92	0.51
2:F:39:U:H2'	2:F:40:C:C6	2.45	0.51
2:F:47(E):A:O2'	2:F:47(I):A:N6	2.41	0.51
2:G:6:A:O2'	2:G:7:G:H5'	2.11	0.51
2:G:27:C:O2'	2:G:28:U:H5'	2.10	0.51
1:A:278:LEU:HD11	1:A:305:ILE:HD11	1.93	0.51
1:C:2:LYS:O	1:C:6:ARG:HG3	2.09	0.51
1:D:227:GLU:HG2	1:D:228:VAL:N	2.26	0.51
2:F:43:G:H5'	2:F:43:G:H8	1.75	0.51
2:F:47:U:H2'	2:F:47(A):C:H6	1.72	0.51
2:F:67(A):A:H2'	2:F:68:C:H6	1.76	0.51
2:G:47(G):U:H2'	2:G:47(H):U:O4'	2.11	0.51
2:H:39:U:H2'	2:H:40:C:O4'	2.10	0.51
2:I:6:A:O2'	2:I:7:G:H5'	2.09	0.51
1:A:33:GLU:CD	1:A:60:LYS:HE3	2.30	0.51
1:D:208:THR:CG2	1:D:242:ILE:HD13	2.39	0.51
1:E:363:LEU:HD22	1:E:446:LEU:HD12	1.91	0.51
2:J:6:A:O2'	2:J:7:G:H5'	2.10	0.51
1:B:147:PHE:C	1:B:147:PHE:CD2	2.83	0.51
1:B:396:ALA:HB2	1:B:428:LEU:HD23	1.93	0.51
2:F:64:A:H2'	2:F:65:C:C6	2.46	0.51
2:J:59:U:O2'	2:J:60:U:H5'	2.10	0.51
1:C:361:LYS:HA	1:C:364:LYS:HE3	1.93	0.51
2:F:3:G:H2'	2:F:4:A:O4'	2.10	0.51
2:F:47(G):U:H2'	2:F:47(H):U:O4'	2.11	0.51
2:H:7:G:O2'	2:H:8:A:H5'	2.11	0.51
2:H:54:U:H2'	2:H:55:U:O4'	2.09	0.51
2:I:14:G:O2'	2:I:15:C:H5'	2.10	0.51
2:I:43:G:H5'	2:I:43:G:H8	1.75	0.51
2:J:41:U:O2'	2:J:42:A:H5'	2.11	0.51
2:J:64:A:H2'	2:J:65:C:C6	2.45	0.51
1:B:14:VAL:O	1:B:18:PHE:HD2	1.93	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:H:14:G:O2'	2:H:15:C:H5'	2.11	0.51
2:J:52:G:O2'	2:J:53:G:H5'	2.11	0.51
2:I:64:A:H2'	2:I:65:C:C6	2.46	0.51
2:I:67:U:H2'	2:I:67(A):A:H8	1.76	0.51
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.76	0.51
1:B:5:LEU:CD1	1:B:42:ILE:HD12	2.41	0.51
1:B:10:GLN:NE2	1:B:12:SER:OG	2.44	0.51
1:B:11:ILE:HG22	2:F:16:U:H4'	1.93	0.51
1:B:404:SER:OG	1:B:425:ASP:HA	2.11	0.51
1:C:392:THR:HG21	1:C:430:ASP:OD2	2.10	0.51
1:E:1:MET:O	1:E:3:SER:N	2.44	0.51
1:E:242:ILE:HG23	1:E:243:PRO:HD2	1.93	0.51
1:E:261:ILE:HG22	1:E:263:VAL:HG13	1.92	0.51
1:E:285:LLP:O3	1:E:285:LLP:NZ	2.44	0.51
2:F:36:A:O2'	2:F:37:A:H5'	2.11	0.51
1:A:3:SER:O	1:A:7:GLN:HG2	2.10	0.50
1:A:87:ALA:CB	1:A:341:VAL:HG21	2.41	0.50
1:A:179:MET:O	1:A:182:SER:HB3	2.11	0.50
2:G:31:A:N7	2:G:32:C:C5	2.80	0.50
1:B:5:LEU:HD12	1:B:8:ILE:HD12	1.93	0.50
1:B:337:GLU:OE1	1:B:337:GLU:N	2.43	0.50
1:C:252:LEU:HD13	1:C:286:LEU:HB3	1.94	0.50
2:G:25:U:N3	2:G:26:C:C4	2.80	0.50
2:H:47(K):G:O2'	2:H:47(L):C:H5'	2.11	0.50
2:H:47(L):C:H2'	2:H:47(M):G:H8	1.75	0.50
2:H:64:A:H2'	2:H:65:C:C6	2.45	0.50
1:A:126:TYR:HB2	1:A:328:LEU:HD13	1.92	0.50
1:A:153:LEU:CD1	1:A:301:LEU:HD22	2.42	0.50
1:C:173:PHE:HB2	1:D:312:ARG:HG2	1.93	0.50
1:D:25:ILE:HG13	1:D:26:TYR:N	2.27	0.50
2:J:32:C:H2'	2:J:33:U:C5	2.41	0.50
1:C:4:LEU:O	1:C:42:ILE:HD13	2.12	0.50
1:C:12:SER:OG	2:I:16:U:H1'	2.11	0.50
1:C:79:VAL:HG21	1:C:345:LEU:CD2	2.42	0.50
1:D:452:ILE:OXT	1:D:452:ILE:HG23	2.12	0.50
1:E:363:LEU:CB	1:E:371:ILE:CD1	2.89	0.50
2:H:45:U:H2'	2:H:46:C:O4'	2.12	0.50
1:A:34:VAL:HG12	1:A:53:PHE:CE1	2.46	0.50
1:A:357:LYS:O	1:A:361:LYS:HG3	2.11	0.50
1:B:230:LEU:HB3	1:B:274:LEU:HD21	1.94	0.50
1:C:68:ASN:ND2	1:D:122:HIS:CD2	2.79	0.50



	A de la constantina d	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:157:LYS:CE	1:C:209:ALA:HB2	2.20	0.50
1:C:358:ARG:NH2	1:C:439:LEU:HD12	2.27	0.50
1:D:278:LEU:HD23	1:D:297:GLY:HA3	1.94	0.50
1:D:369:LEU:HD21	1:D:450:LEU:CD1	2.42	0.50
2:G:5(A):U:H2'	2:G:6:A:H5'	1.93	0.50
1:A:396:ALA:HB2	1:A:428:LEU:HD21	1.94	0.50
1:C:168:GLU:O	1:C:168:GLU:HG2	2.12	0.50
1:D:299:LYS:O	1:D:303:GLU:HG2	2.11	0.50
1:A:72:VAL:HG22	1:A:417:PRO:HG2	1.94	0.50
1:B:123:ILE:O	1:B:125:LYS:N	2.44	0.50
1:D:6:ARG:NH1	2:H:20:U:O4	2.45	0.50
1:D:18:PHE:HB3	1:D:21:ALA:HB3	1.92	0.50
1:E:34:VAL:HG21	1:E:57:VAL:HA	1.94	0.50
2:H:46:C:H2'	2:H:47:U:H5'	1.93	0.50
1:A:161:ILE:HG22	1:A:186:LEU:HD11	1.93	0.50
1:B:55:GLU:O	1:B:59:ARG:HG3	2.11	0.50
1:C:161:ILE:CG2	1:C:166:LEU:HD21	2.41	0.50
1:D:90:SER:HB3	1:D:338:ASP:O	2.12	0.50
1:E:34:VAL:O	1:E:38:TYR:HD1	1.95	0.50
2:H:25:U:O2'	2:H:26:C:H5'	2.11	0.50
2:H:46:C:O2'	2:H:47:U:H5'	2.12	0.50
2:I:24:C:O2'	2:I:25:U:H5'	2.11	0.50
2:I:26:C:H2'	2:I:27:C:O4'	2.11	0.50
1:B:22:TYR:CG	1:B:61:ILE:HG21	2.46	0.50
1:B:186:LEU:HD12	1:B:187:ARG:N	2.27	0.50
1:C:161:ILE:HD13	1:C:166:LEU:CD2	2.42	0.50
1:E:7:GLN:HB2	1:E:50:LEU:HD11	1.92	0.50
1:E:97:ILE:HD11	1:E:323:GLY:HA3	1.94	0.50
1:B:396:ALA:HB2	1:B:428:LEU:CD2	2.41	0.49
1:D:396:ALA:HB1	1:D:426:GLN:HG2	1.94	0.49
1:E:79:VAL:CG1	1:E:341:VAL:HG13	2.41	0.49
1:E:396:ALA:HB2	1:E:428:LEU:CD2	2.41	0.49
1:E:435:PHE:HB2	1:E:438:ASP:OD2	2.12	0.49
2:G:9:U:C4	2:G:48:G:C8	2.99	0.49
2:J:47(N):A:C6	2:J:47(O):G:C6	3.00	0.49
1:A:340:PRO:O	1:A:344:MET:HG3	2.12	0.49
1:B:174:ARG:C	1:B:176:PRO:HD2	2.33	0.49
1:D:72:VAL:HG22	1:D:417:PRO:HG2	1.94	0.49
1:D:363:LEU:HB2	1:D:371:ILE:CD1	2.42	0.49
2:I:47:U:H2'	2:I:47(A):C:H6	1.76	0.49
1:D:163:ARG:HG3	1:D:189:VAL:O	2.13	0.49



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:200:TYR:HE2	1:D:228:VAL:HG21	1.75	0.49
1:E:28:VAL:HG12	1:E:32:ARG:NE	2.28	0.49
2:H:43:G:H5'	2:H:43:G:H8	1.77	0.49
1:A:409:ARG:NH1	1:A:413:LEU:HD11	2.27	0.49
1:B:18:PHE:HB3	1:B:21:ALA:HB3	1.93	0.49
2:F:5(A):U:C2'	2:F:6:A:H5'	2.42	0.49
2:I:25:U:C2'	2:I:26:C:H5'	2.42	0.49
2:I:47(I):A:C2'	2:I:47(J):A:H5'	2.43	0.49
1:C:194:LYS:HG2	1:C:226:GLU:N	2.27	0.49
2:H:39:U:H2'	2:H:40:C:C6	2.47	0.49
2:H:47(F):U:C2'	2:H:47(G):U:H5"	2.42	0.49
2:H:67:U:H2'	2:H:67(A):A:H8	1.77	0.49
2:J:31:A:H2'	2:J:32:C:O4'	2.13	0.49
1:A:8:ILE:CD1	1:A:38:TYR:HB3	2.42	0.49
1:C:312:ARG:HD2	1:C:315:ARG:NH1	2.28	0.49
1:E:77:GLY:HA3	1:E:430:ASP:CB	2.42	0.49
1:E:347:GLN:NE2	1:E:352:LEU:CD2	2.75	0.49
2:F:47(L):C:H2'	2:F:47(M):G:C8	2.48	0.49
1:A:313:ALA:HB1	1:B:144:GLY:CA	2.43	0.49
1:C:1:MET:HG3	1:C:4:LEU:HD12	1.94	0.49
1:C:123:ILE:HG23	1:C:328:LEU:HD12	1.95	0.49
1:C:257:LYS:HD2	2:H:5:G:H4'	1.94	0.49
1:D:358:ARG:HH21	1:D:439:LEU:HD12	1.76	0.49
1:D:360:GLU:HG3	1:D:371:ILE:CG2	2.42	0.49
1:E:399:HIS:HE1	1:E:401:ARG:HD3	1.77	0.49
2:J:5(A):U:H2'	2:J:6:A:H5'	1.95	0.49
2:J:47(E):A:H2	2:J:47(I):A:N7	2.11	0.49
1:A:200:TYR:CD2	1:A:233:LEU:HD21	2.48	0.49
1:A:250:SER:HB2	1:A:286:LEU:HD12	1.94	0.49
1:C:172:SER:OG	1:D:312:ARG:HB2	2.13	0.49
1:C:330:LEU:HD22	1:C:335:ARG:HD3	1.95	0.49
1:D:163:ARG:NH1	1:E:188:GLU:OE1	2.46	0.49
1:D:178:ILE:CG2	1:D:179:MET:N	2.76	0.49
1:E:366:ILE:HG23	1:E:367:PRO:HD2	1.95	0.49
2:G:47(G):U:O5'	2:G:47(G):U:H6	1.95	0.49
1:A:5:LEU:HD12	1:A:8:ILE:HD12	1.94	0.49
1:B:408:SER:O	1:B:412:ARG:HG3	2.12	0.49
1:D:161:ILE:HD13	1:D:166:LEU:HD23	1.94	0.49
2:G:67:U:H2'	2:G:67(A):A:H8	1.78	0.49
2:I:26:C:O2'	2:I:27:C:H5'	2.13	0.49
2:I:46:C:C4	2:I:47:U:C4	3.00	0.49



	A de la constantina d	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:145:ALA:HB1	1:B:295:ILE:HD11	1.95	0.49
1:D:196:LYS:N	1:D:199:ASP:OD2	2.46	0.49
1:B:324:LEU:HD12	1:B:324:LEU:O	2.12	0.48
1:C:266:PRO:HB2	1:C:271:CYS:SG	2.53	0.48
1:D:123:ILE:O	1:D:125:LYS:N	2.46	0.48
1:E:363:LEU:HD22	1:E:366:ILE:HD12	1.95	0.48
1:E:370:LYS:HG3	1:E:398:ARG:O	2.13	0.48
1:E:421:ARG:HG2	1:E:421:ARG:NH1	2.27	0.48
2:F:28:U:H2'	2:F:29:A:C8	2.48	0.48
2:G:14:G:O2'	2:G:15:C:H5'	2.13	0.48
2:G:49:G:C8	2:G:49:G:O5'	2.66	0.48
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.78	0.48
1:A:197:VAL:HG22	1:A:228:VAL:HG13	1.95	0.48
1:A:344:MET:O	1:A:432:ARG:CD	2.60	0.48
1:A:377:LYS:HE2	1:A:389:GLU:OE2	2.14	0.48
1:B:229:LYS:HB2	1:B:232:ASP:OD2	2.13	0.48
1:B:231:GLU:O	1:B:235:LYS:HG3	2.12	0.48
1:B:335:ARG:NH1	1:B:338:ASP:OD2	2.45	0.48
1:B:339:ILE:HG13	1:B:342:ILE:HB	1.95	0.48
1:C:89:LEU:HD12	1:D:101:ALA:HB1	1.95	0.48
1:D:11:ILE:O	1:D:15:VAL:HG23	2.13	0.48
1:D:439:LEU:HD23	1:D:442:ILE:HD12	1.96	0.48
1:E:406:GLU:OE1	1:E:406:GLU:HA	2.11	0.48
2:G:46:C:O2'	2:G:47:U:H5'	2.13	0.48
1:A:163:ARG:HG2	1:A:188:GLU:HB2	1.94	0.48
1:C:194:LYS:HZ1	1:C:224:PHE:HB3	1.78	0.48
1:C:408:SER:O	1:C:412:ARG:HG3	2.13	0.48
1:E:72:VAL:HG22	1:E:417:PRO:CG	2.42	0.48
1:E:353:ARG:HB2	1:E:393:TYR:CD2	2.47	0.48
2:I:35:C:O2'	2:I:36:A:H5'	2.14	0.48
1:A:286:LEU:HG	1:A:384:SER:HB2	1.95	0.48
1:A:442:ILE:O	1:A:446:LEU:CG	2.53	0.48
1:B:211:LEU:HG	1:B:242:ILE:HG21	1.94	0.48
1:B:219:PHE:CD2	1:C:193:ASN:HB3	2.48	0.48
1:C:370:LYS:HB2	1:C:398:ARG:O	2.14	0.48
1:D:254:ILE:HD12	1:D:259:PHE:CE2	2.49	0.48
1:E:96:PHE:O	1:E:100:ILE:HG12	2.13	0.48
2:G:34:U:O5'	2:G:34:U:H6	1.96	0.48
2:H:5(A):U:C2'	2:H:6:A:H5'	2.42	0.48
2:H:47(E):A:H2'	2:H:47(F):U:O4'	2.13	0.48
2:I:47(E):A:C2'	2:I:47(F):U:H5'	2.43	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:I:67:U:H2'	2:I:67(A):A:C8	2.49	0.48
1:A:250:SER:O	1:A:286:LEU:HB2	2.13	0.48
1:A:268:PHE:H	1:A:268:PHE:HD2	1.62	0.48
1:D:11:ILE:HG21	1:D:28:VAL:HG13	1.95	0.48
1:E:163:ARG:CD	1:E:190:GLY:O	2.61	0.48
1:E:204:ILE:HG22	1:E:205:ASN:N	2.28	0.48
1:A:126:TYR:HB3	1:A:328:LEU:HD13	1.95	0.48
1:A:442:ILE:CG2	1:A:446:LEU:HD11	2.43	0.48
1:B:400:ASP:OD1	1:B:401:ARG:N	2.47	0.48
1:B:411:LEU:CD2	1:B:418:ILE:HD12	2.37	0.48
1:C:169:ILE:HG13	1:C:173:PHE:HD2	1.77	0.48
1:C:212:MET:CE	1:C:245:TYR:HE1	2.26	0.48
1:D:5:LEU:CD1	1:D:39:ARG:HA	2.44	0.48
1:D:163:ARG:NH1	1:E:166:LEU:HD13	2.28	0.48
1:E:421:ARG:HG2	1:E:421:ARG:HH11	1.77	0.48
2:F:14:G:O2'	2:F:15:C:H5'	2.14	0.48
2:I:45:U:H2'	2:I:46:C:O4'	2.13	0.48
2:I:48:G:H4'	2:I:49:G:H5"	1.96	0.48
2:J:3:G:O2'	2:J:4:A:H5'	2.13	0.48
1:B:254:ILE:CD1	1:B:259:PHE:HE2	2.27	0.48
1:C:5:LEU:HD13	1:C:42:ILE:HB	1.95	0.48
1:C:123:ILE:HD13	1:C:325:GLU:HB2	1.96	0.48
1:C:197:VAL:CG2	1:C:228:VAL:HG13	2.43	0.48
1:D:39:ARG:HG2	2:H:56:C:H42	1.78	0.48
2:G:10:A:H4'	2:G:45:U:O4'	2.14	0.48
2:I:10:A:C2	2:I:26:C:C2	3.00	0.48
1:A:210:LEU:HD12	1:A:243:PRO:HG2	1.96	0.48
1:A:231:GLU:H	1:A:231:GLU:CD	2.16	0.48
1:A:366:ILE:HB	1:A:369:LEU:HD11	1.92	0.48
1:A:432:ARG:O	1:A:432:ARG:HG3	2.12	0.48
1:B:165:GLU:OE1	1:B:213:LYS:HG3	2.13	0.48
1:C:40:LYS:O	1:C:44:GLU:HG3	2.14	0.48
1:C:200:TYR:CE2	1:C:228:VAL:HG21	2.48	0.48
2:F:9:U:H5	2:F:48:G:H5'	1.78	0.48
1:A:108:GLU:HB2	1:B:83:ASN:HA	1.96	0.48
1:A:165:GLU:OE2	1:A:213:LYS:NZ	2.47	0.48
1:C:68:ASN:HD22	1:D:122:HIS:CB	2.26	0.48
1:C:363:LEU:O	1:C:371:ILE:HD11	2.13	0.48
1:D:10:GLN:CG	1:D:12:SER:H	2.22	0.48
1:D:131:THR:O	1:D:269:ARG:HA	2.13	0.48
1:D:176:PRO:CG	1:E:191:THR:HG22	2.39	0.48



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:146:VAL:HG22	1:E:245:TYR:OH	2.13	0.48
1:E:425:ASP:CG	1:E:425:ASP:O	2.51	0.48
2:F:26:C:H2'	2:F:27:C:O4'	2.13	0.48
2:F:37:A:O2'	2:F:38:A:H5'	2.14	0.48
2:G:36:A:O2'	2:G:37:A:H5'	2.14	0.48
2:J:35:C:H2'	2:J:36:A:C8	2.49	0.48
1:A:34:VAL:O	1:A:38:TYR:HD1	1.97	0.47
1:A:87:ALA:HB2	1:A:341:VAL:HG21	1.96	0.47
1:A:242:ILE:HG23	1:A:243:PRO:HD2	1.95	0.47
1:B:150:LEU:HB3	1:B:182:SER:OG	2.14	0.47
1:C:313:ALA:HB1	1:D:144:GLY:HA2	1.95	0.47
1:D:335:ARG:NH1	1:D:338:ASP:OD2	2.47	0.47
1:E:452:ILE:HG23	1:E:452:ILE:OXT	2.14	0.47
2:I:3:G:O2'	2:I:4:A:H5'	2.14	0.47
1:B:5:LEU:CD1	1:B:39:ARG:HA	2.42	0.47
1:B:128:ASN:ND2	1:B:135:SER:HA	2.29	0.47
1:B:285:LLP:O3	1:B:285:LLP:NZ	2.43	0.47
1:B:409:ARG:HH12	1:B:413:LEU:HD11	1.79	0.47
1:D:191:THR:HB	1:E:166:LEU:O	2.14	0.47
2:F:41:U:O2'	2:F:42:A:H5'	2.14	0.47
2:G:31:A:C8	2:G:32:C:C5	3.02	0.47
2:H:5(A):U:H2'	2:H:6:A:H5'	1.96	0.47
2:I:5(A):U:C2'	2:I:6:A:H5'	2.44	0.47
2:I:37:A:O2'	2:I:38:A:H5'	2.14	0.47
1:E:344:MET:O	1:E:432:ARG:CD	2.63	0.47
2:G:27:C:C2'	2:G:28:U:O4'	2.58	0.47
1:A:116:ARG:HD3	1:B:83:ASN:OD1	2.15	0.47
1:B:42:ILE:HD11	1:B:50:LEU:HD21	1.96	0.47
1:C:302:ILE:HA	1:C:305:ILE:HD12	1.94	0.47
1:C:358:ARG:HH21	1:C:439:LEU:HD12	1.79	0.47
1:E:187:ARG:HD3	1:E:203:ALA:HB1	1.95	0.47
1:E:298:LYS:O	1:E:302:ILE:HG12	2.14	0.47
2:F:61:C:H2'	2:F:62:C:C6	2.49	0.47
2:G:10:A:C4	2:G:44:G:C2	3.02	0.47
2:J:67:U:H2'	2:J:67(A):A:H8	1.78	0.47
1:A:33:GLU:OE1	1:A:60:LYS:HD2	2.14	0.47
1:A:138:VAL:HG22	1:A:294:ILE:HA	1.96	0.47
1:C:363:LEU:HB2	1:C:371:ILE:HD13	1.97	0.47
1:D:24:GLU:O	1:D:24:GLU:HG3	2.14	0.47
1:D:228:VAL:CG1	1:D:233:LEU:HG	2.45	0.47
1:D:339:ILE:HG13	1:D:339:ILE:O	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:10:GLN:HG2	1:E:12:SER:N	2.25	0.47
2:I:47(E):A:H2'	2:I:47(F):U:H5'	1.95	0.47
1:B:166:LEU:O	1:C:191:THR:HB	2.15	0.47
1:C:68:ASN:HD22	1:D:122:HIS:HB3	1.80	0.47
1:D:87:ALA:HB2	1:D:341:VAL:HG21	1.97	0.47
1:E:216:LYS:HG2	1:E:219:PHE:CE2	2.49	0.47
2:I:47(I):A:H2'	2:I:47(J):A:H5'	1.96	0.47
2:J:39:U:H2'	2:J:40:C:C6	2.48	0.47
1:A:55:GLU:O	1:A:59:ARG:HG3	2.14	0.47
1:A:178:ILE:HG23	1:A:179:MET:N	2.29	0.47
1:A:406:GLU:OE1	1:A:406:GLU:HA	2.13	0.47
1:A:407:LEU:HD21	1:A:427:LEU:HD22	1.94	0.47
1:B:10:GLN:HB3	1:B:13:LYS:CE	2.43	0.47
1:B:423:ARG:HG2	1:B:423:ARG:NH1	2.30	0.47
1:C:18:PHE:HB3	1:C:21:ALA:HB3	1.96	0.47
1:C:33:GLU:OE1	1:C:60:LYS:HD2	2.14	0.47
1:C:60:LYS:HA	1:C:60:LYS:HD3	1.70	0.47
1:C:366:ILE:CG2	1:C:367:PRO:HD2	2.43	0.47
1:D:131:THR:HG22	1:D:268:PHE:HB3	1.97	0.47
1:D:163:ARG:NH1	1:E:166:LEU:CD1	2.78	0.47
1:E:37:LYS:O	1:E:41:GLU:CG	2.59	0.47
1:E:123:ILE:O	1:E:126:TYR:N	2.41	0.47
1:E:161:ILE:CG2	1:E:166:LEU:HD21	2.45	0.47
1:E:188:GLU:H	1:E:188:GLU:HG2	1.47	0.47
1:E:194:LYS:HE3	1:E:224:PHE:HB3	1.95	0.47
1:E:283:GLY:O	1:E:287:LEU:HB3	2.14	0.47
2:G:31:A:C5	2:G:32:C:C4	3.01	0.47
2:H:26:C:H2'	2:H:27:C:O4'	2.14	0.47
2:I:47(P):A:H2'	2:I:48:G:H5'	1.96	0.47
2:J:8:A:HO2'	2:J:9:U:P	2.37	0.47
2:J:36:A:H2'	2:J:37:A:O4'	2.14	0.47
1:B:402:LEU:HD12	1:B:450:LEU:HD21	1.97	0.47
1:C:181:LYS:HB3	1:D:310:ILE:HD11	1.96	0.47
1:E:8:ILE:HD13	1:E:38:TYR:HB3	1.96	0.47
1:E:139:VAL:HB	1:E:314:LEU:HB3	1.97	0.47
1:E:348:ASP:O	1:E:351:ALA:HB3	2.14	0.47
2:F:47(E):A:H2'	2:F:47(F):U:H5'	1.97	0.47
2:H:65:C:H2'	2:H:66:A:H8	1.79	0.47
1:A:72:VAL:HG22	1:A:417:PRO:CG	2.45	0.47
1:C:309:PRO:HG2	1:D:181:LYS:HG3	1.96	0.47
1:D:161:ILE:CG2	1:D:166:LEU:HD21	2.45	0.47



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:175:ILE:N	1:D:176:PRO:HD2	2.29	0.47
1:D:251:GLY:HA2	1:D:268:PHE:HE2	1.79	0.47
1:D:318:LYS:HB3	1:D:318:LYS:HE2	1.73	0.47
1:E:107:LEU:O	1:E:122:HIS:CE1	2.66	0.47
2:G:37:A:O2'	2:G:38:A:H5'	2.15	0.47
1:B:123:ILE:O	1:B:126:TYR:N	2.43	0.47
1:D:7:GLN:CB	1:D:50:LEU:CD1	2.93	0.47
1:D:335:ARG:O	1:D:338:ASP:HB2	2.15	0.47
2:F:42:A:O2'	2:F:43:G:C8	2.68	0.47
2:G:10:A:N6	2:G:44:G:C6	2.83	0.47
2:G:40:C:H2'	2:G:41:U:C6	2.51	0.47
2:H:43:G:O2'	2:H:44:G:H5'	2.15	0.47
2:I:59:U:C2'	2:I:60:U:H5'	2.45	0.47
1:A:18:PHE:HB3	1:A:21:ALA:HB3	1.97	0.46
1:A:366:ILE:CG2	1:A:367:PRO:HD2	2.45	0.46
1:B:444:LYS:O	1:B:448:GLU:HG3	2.15	0.46
1:C:285:LLP:O3	1:C:285:LLP:NZ	2.46	0.46
1:C:348:ASP:HB2	1:C:351:ALA:CB	2.44	0.46
1:E:255:ASN:HB3	1:E:258:GLU:OE2	2.15	0.46
1:E:429:PHE:HB3	1:E:431:MET:CE	2.46	0.46
2:G:47(F):U:O2'	2:G:47(H):U:OP2	2.21	0.46
1:A:72:VAL:HG13	1:A:417:PRO:HG2	1.97	0.46
1:A:175:ILE:N	1:A:176:PRO:HD2	2.30	0.46
1:A:399:HIS:ND1	1:A:401:ARG:HB2	2.30	0.46
1:B:161:ILE:HG22	1:B:186:LEU:HD11	1.97	0.46
1:D:107:LEU:CD1	1:D:321:LEU:HD23	2.45	0.46
1:E:123:ILE:O	1:E:125:LYS:N	2.48	0.46
1:E:230:LEU:O	1:E:234:VAL:HG23	2.15	0.46
2:G:25:U:C2	2:G:26:C:C6	3.04	0.46
1:A:68:ASN:HD22	1:B:122:HIS:CB	2.27	0.46
1:A:80:ILE:HD12	1:A:285:LLP:HA	1.97	0.46
1:A:345:LEU:CD2	1:A:380:PRO:CB	2.91	0.46
2:I:47(H):U:O2'	2:I:47(I):A:H5'	2.16	0.46
2:J:47:U:H2'	2:J:47(A):C:H6	1.76	0.46
1:A:2:LYS:O	1:A:6:ARG:NE	2.48	0.46
1:B:344:MET:O	1:B:432:ARG:HD2	2.15	0.46
1:C:302:ILE:HG22	1:C:306:LYS:HE3	1.97	0.46
1:D:7:GLN:HB2	1:D:50:LEU:HD13	1.95	0.46
1:D:234:VAL:HG12	1:D:238:HIS:CD2	2.50	0.46
2:I:65:C:H2'	2:I:66:A:C8	2.50	0.46
1:A:369:LEU:HD21	1:A:450:LEU:CD1	2.45	0.46



	i agein	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:11:ILE:HG21	1:B:28:VAL:HG13	1.98	0.46
1:B:130:LEU:O	1:B:269:ARG:NH2	2.49	0.46
1:C:68:ASN:HD21	1:D:122:HIS:HD2	1.63	0.46
1:C:123:ILE:O	1:C:125:LYS:N	2.48	0.46
1:C:169:ILE:HD11	1:C:285:LLP:H5'1	1.98	0.46
1:C:317:ASP:HA	1:D:291:GLN:CD	2.36	0.46
1:D:34:VAL:HG21	1:D:57:VAL:HA	1.97	0.46
1:E:254:ILE:HD11	1:E:259:PHE:CZ	2.50	0.46
1:E:270:ASP:O	1:E:274:LEU:HG	2.15	0.46
2:H:9:U:H4'	2:H:45:U:C2	2.50	0.46
2:J:46:C:C4	2:J:47:U:O4	2.69	0.46
1:C:123:ILE:HG23	1:C:328:LEU:CD1	2.45	0.46
1:D:2:LYS:CE	2:H:56:C:O2'	2.63	0.46
1:D:228:VAL:HG11	1:D:233:LEU:HG	1.98	0.46
1:D:316:ILE:H	1:D:316:ILE:HG12	1.48	0.46
1:D:339:ILE:HG13	1:D:342:ILE:HB	1.97	0.46
1:A:334:LYS:CD	1:A:336:TYR:OH	2.64	0.46
1:B:160:ILE:HD12	1:B:211:LEU:CD2	2.45	0.46
1:C:87:ALA:HB2	1:C:341:VAL:HG21	1.97	0.46
1:C:308:ASN:OD1	1:C:310:ILE:HG13	2.16	0.46
1:C:320:THR:O	1:C:324:LEU:HB2	2.15	0.46
1:D:2:LYS:HE2	1:D:6:ARG:CZ	2.45	0.46
1:E:442:ILE:O	1:E:446:LEU:HG	2.15	0.46
2:F:36:A:C2'	2:F:37:A:H5'	2.46	0.46
2:F:47(J):A:N6	2:F:47(K):G:O6	2.48	0.46
2:G:9:U:O4	2:G:48:G:C8	2.68	0.46
2:G:25:U:O2'	2:G:26:C:C5'	2.64	0.46
1:A:68:ASN:O	1:A:70:LYS:HE3	2.15	0.46
1:A:348:ASP:HB2	1:A:351:ALA:HB2	1.97	0.46
1:A:427:LEU:HD23	1:A:429:PHE:CE1	2.50	0.46
1:A:436:HIS:HD2	1:A:439:LEU:HD12	1.81	0.46
1:B:246:TYR:OH	1:B:266:PRO:HG3	2.16	0.46
1:B:326:MET:O	1:B:330:LEU:HG	2.15	0.46
1:C:67:PRO:HB2	1:D:96:PHE:CE1	2.51	0.46
1:D:60:LYS:HD3	1:D:60:LYS:HA	1.77	0.46
2:G:10:A:C5	2:G:44:G:C2	3.04	0.46
1:B:126:TYR:O	1:B:130:LEU:HG	2.15	0.46
1:C:60:LYS:O	1:C:64:LEU:HG	2.16	0.46
1:D:169:ILE:O	1:D:173:PHE:HB3	2.15	0.46
2:F:26:C:O2'	2:F:27:C:H5'	2.15	0.46
2:H:8:A:O2'	2:H:9:U:P	2.74	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:67:U:H2'	2:H:67(A):A:C8	2.50	0.46
2:I:47(E):A:C2	2:I:47(J):A:C6	3.04	0.46
2:J:59:U:C2'	2:J:60:U:H5'	2.46	0.46
1:A:24:GLU:O	1:A:28:VAL:HG23	2.16	0.46
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.73	0.46
1:A:116:ARG:HH22	1:B:171:GLY:HA3	1.81	0.46
1:A:120:ILE:HD11	1:A:315:ARG:HG3	1.97	0.46
1:A:309:PRO:HG3	1:B:181:LYS:HG3	1.97	0.46
1:A:320:THR:CG2	1:B:319:LEU:HD12	2.45	0.46
1:B:370:LYS:HB2	1:B:398:ARG:O	2.16	0.46
1:E:40:LYS:O	1:E:44:GLU:HG3	2.16	0.46
1:E:109:TYR:OH	1:E:114:GLY:O	2.32	0.46
1:B:14:VAL:CG1	1:B:18:PHE:HE2	2.29	0.45
1:C:234:VAL:HG12	1:C:238:HIS:CD2	2.51	0.45
1:D:167:VAL:HG12	1:D:219:PHE:CE2	2.34	0.45
1:E:73:ILE:HD13	1:E:438:ASP:HB3	1.97	0.45
1:A:68:ASN:ND2	1:B:122:HIS:HD2	2.11	0.45
1:A:181:LYS:HE3	1:B:309:PRO:HD2	1.99	0.45
1:D:347:GLN:NE2	1:D:352:LEU:CD2	2.80	0.45
2:G:40:C:H2'	2:G:41:U:O4'	2.16	0.45
2:G:67:U:H2'	2:G:67(A):A:C8	2.51	0.45
2:I:36:A:H2'	2:I:37:A:O4'	2.16	0.45
1:A:123:ILE:O	1:A:126:TYR:N	2.45	0.45
1:A:375:LYS:NZ	1:A:391:PRO:HB2	2.32	0.45
1:C:14:VAL:O	1:C:18:PHE:HD2	1.98	0.45
1:C:67:PRO:CG	1:D:96:PHE:CE1	2.99	0.45
1:C:431:MET:HE2	1:C:434:VAL:HG21	1.98	0.45
1:D:212:MET:HG2	1:D:213:LYS:N	2.29	0.45
1:E:432:ARG:O	1:E:432:ARG:HG3	2.16	0.45
2:G:31:A:C6	2:G:32:C:N3	2.84	0.45
2:J:65:C:H2'	2:J:66:A:O4'	2.17	0.45
1:A:420:CYS:HB2	1:A:428:LEU:O	2.16	0.45
1:D:123:ILE:HG12	1:D:321:LEU:HD11	1.99	0.45
1:D:285:LLP:H4'1	1:D:285:LLP:OP4	2.16	0.45
1:D:409:ARG:NH1	1:D:413:LEU:HD11	2.30	0.45
2:F:38:A:H2'	2:F:39:U:C5'	2.46	0.45
1:B:92:ASP:CG	1:B:335:ARG:HH12	2.19	0.45
1:C:181:LYS:HG3	1:D:309:PRO:CG	2.44	0.45
1:E:14:VAL:CG1	1:E:18:PHE:HE2	2.29	0.45
1:E:234:VAL:HG12	1:E:238:HIS:HD2	1.80	0.45
2:G:18:G:O2'	2:G:57:G:N2	2.50	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:G:28:U:H2'	2:G:29:A:C8	2.52	0.45
2:H:55:U:H2'	2:H:57:G:OP2	2.17	0.45
1:C:73:ILE:CB	1:C:418:ILE:HG12	2.40	0.45
1:C:107:LEU:O	1:C:122:HIS:CE1	2.68	0.45
1:D:1:MET:CG	1:D:2:LYS:H	2.28	0.45
1:D:169:ILE:HG13	1:D:173:PHE:HD2	1.82	0.45
1:E:15:VAL:HA	1:E:27:VAL:HG11	1.98	0.45
1:E:187:ARG:HE	1:E:203:ALA:CB	2.15	0.45
1:E:360:GLU:O	1:E:364:LYS:HG3	2.16	0.45
1:E:445:THR:O	1:E:449:LEU:HG	2.16	0.45
2:F:8:A:HO2'	2:F:9:U:P	2.39	0.45
2:F:25:U:O2'	2:F:26:C:H5'	2.16	0.45
2:G:47(C):C:O2'	2:G:47(D):U:H5'	2.16	0.45
2:I:25:U:HO2'	2:I:26:C:H5'	1.78	0.45
1:D:33:GLU:CD	1:D:60:LYS:HE3	2.37	0.45
2:G:25:U:C4	2:G:26:C:N4	2.85	0.45
2:H:47(E):A:H2'	2:H:47(F):U:C5'	2.45	0.45
2:I:5(A):U:H2'	2:I:6:A:H5'	1.99	0.45
2:I:21:U:H2'	2:I:22:G:H8	1.81	0.45
2:I:28:U:H2'	2:I:29:A:C8	2.52	0.45
2:I:47(I):A:H2'	2:I:47(J):A:C5'	2.47	0.45
2:J:67:U:H2'	2:J:67(A):A:C8	2.50	0.45
1:A:283:GLY:O	1:A:287:LEU:HB3	2.17	0.45
1:B:34:VAL:HG21	1:B:57:VAL:HA	1.99	0.45
1:B:360:GLU:O	1:B:364:LYS:HG3	2.17	0.45
1:C:70:LYS:O	1:C:72:VAL:HG23	2.17	0.45
1:D:188:GLU:OE1	1:E:163:ARG:NH1	2.38	0.45
1:E:88:PRO:HD2	1:E:341:VAL:HG22	1.98	0.45
2:F:43:G:O2'	2:F:44:G:H5'	2.17	0.45
2:H:42:A:O2'	2:H:43:G:C8	2.64	0.45
1:B:363:LEU:O	1:B:371:ILE:HD11	2.17	0.45
1:E:89:LEU:HB2	1:E:94:ILE:HD11	1.99	0.45
1:E:193:ASN:HB2	1:E:224:PHE:O	2.17	0.45
1:E:344:MET:O	1:E:432:ARG:HD2	2.17	0.45
1:A:34:VAL:HG21	1:A:57:VAL:HA	1.98	0.45
1:A:353:ARG:HB2	1:A:393:TYR:CE2	2.52	0.45
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.58	0.45
1:D:10:GLN:HA	2:H:19:G:H2'	1.98	0.45
1:D:219:PHE:CD2	1:E:193:ASN:HB3	2.52	0.45
2:H:46:C:H2'	2:H:47:U:C5'	2.46	0.45
2:J:28:U:H2'	2:J:29:A:C8	2.52	0.45



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:123:ILE:HD13	1:A:325:GLU:HB2	1.99	0.44
1:A:322:SER:OG	1:A:323:GLY:N	2.50	0.44
1:C:335:ARG:O	1:C:338:ASP:HB2	2.17	0.44
1:C:358:ARG:O	1:C:362:LEU:HG	2.17	0.44
1:D:5:LEU:HD13	1:D:39:ARG:HA	1.98	0.44
1:D:396:ALA:HB1	1:D:426:GLN:CG	2.47	0.44
1:C:5:LEU:CD1	1:C:39:ARG:HA	2.40	0.44
1:C:77:GLY:CA	1:C:430:ASP:HB3	2.46	0.44
1:C:120:ILE:HG21	1:C:137:PHE:CD1	2.52	0.44
1:E:165:GLU:OE1	1:E:213:LYS:HG3	2.17	0.44
1:E:438:ASP:O	1:E:442:ILE:HG13	2.18	0.44
2:H:28:U:H2'	2:H:29:A:C8	2.53	0.44
2:H:47:U:H2'	2:H:47(A):C:H6	1.78	0.44
1:A:263:VAL:CG2	1:A:388:LEU:HD13	2.48	0.44
1:A:359:LEU:HD11	1:A:363:LEU:HD11	2.00	0.44
1:C:423:ARG:HD2	1:C:428:LEU:HD11	2.00	0.44
1:E:7:GLN:CB	1:E:50:LEU:CD1	2.95	0.44
2:H:26:C:O2'	2:H:27:C:H5'	2.17	0.44
2:H:37:A:O2'	2:H:38:A:H5'	2.17	0.44
2:H:49:G:C8	2:H:49:G:O5'	2.70	0.44
1:B:348:ASP:O	1:B:351:ALA:HB3	2.17	0.44
1:C:5:LEU:HD12	1:C:8:ILE:CD1	2.48	0.44
1:D:11:ILE:HD13	2:H:18:G:OP1	2.16	0.44
1:E:316:ILE:HD11	1:E:321:LEU:HD13	1.99	0.44
1:E:347:GLN:HE21	1:E:352:LEU:CD2	2.31	0.44
2:F:43:G:H2'	2:F:44:G:C8	2.53	0.44
1:A:14:VAL:HG13	1:A:18:PHE:HE2	1.82	0.44
1:A:94:ILE:HD11	1:B:102:ASN:HA	1.99	0.44
1:A:423:ARG:O	1:A:424:GLU:HB3	2.18	0.44
1:B:87:ALA:HB2	1:B:341:VAL:HG21	2.00	0.44
1:C:123:ILE:O	1:C:126:TYR:N	2.43	0.44
1:C:197:VAL:HG22	1:C:228:VAL:HG13	1.98	0.44
1:E:367:PRO:HG3	1:E:451:SER:OG	2.17	0.44
2:J:26:C:H2'	2:J:27:C:O4'	2.17	0.44
1:A:77:GLY:CA	1:A:430:ASP:HB3	2.47	0.44
1:A:317:ASP:HB2	1:B:291:GLN:HB3	2.00	0.44
1:B:141:ASN:HB2	1:B:285:LLP:OP1	2.18	0.44
1:C:77:GLY:HA3	1:C:430:ASP:HB3	1.99	0.44
1:C:161:ILE:HG21	1:C:166:LEU:HD21	1.98	0.44
1:C:423:ARG:HG2	1:C:423:ARG:HH11	1.82	0.44
1:D:286:LEU:HD21	1:D:384:SER:OG	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:400:ASP:OD1	1:D:401:ARG:N	2.51	0.44
1:E:359:LEU:HB2	1:E:439:LEU:HD22	1.98	0.44
2:F:5(A):U:H2'	2:F:6:A:H5'	1.99	0.44
1:A:131:THR:HG21	1:A:296:VAL:HG11	1.99	0.44
1:A:159:VAL:HG13	1:A:210:LEU:HB3	2.00	0.44
1:A:200:TYR:CE2	1:A:233:LEU:HD21	2.53	0.44
1:C:404:SER:OG	1:C:425:ASP:HA	2.18	0.44
1:D:254:ILE:HD13	1:D:336:TYR:CE1	2.53	0.44
1:D:254:ILE:HD12	1:D:259:PHE:HE2	1.82	0.44
1:E:42:ILE:HD11	1:E:50:LEU:HD21	2.00	0.44
1:E:110:ASN:ND2	1:E:113:GLU:OE1	2.51	0.44
2:G:47:U:H2'	2:G:47(A):C:H6	1.77	0.44
1:C:169:ILE:O	1:C:169:ILE:HG13	2.17	0.44
1:C:178:ILE:CG2	1:C:179:MET:N	2.81	0.44
1:D:2:LYS:NZ	2:H:56:C:O2'	2.49	0.44
1:D:14:VAL:HG12	1:D:18:PHE:CE2	2.52	0.44
1:E:17:ILE:HG22	1:E:17:ILE:O	2.18	0.44
1:E:123:ILE:CD1	1:E:321:LEU:HD12	2.48	0.44
1:E:148:LEU:HG	1:E:305:ILE:HG23	1.99	0.44
1:E:213:LYS:HD3	1:E:230:LEU:HD21	2.00	0.44
2:G:29:A:C2'	2:G:30:G:H5'	2.47	0.44
1:A:347:GLN:HE21	1:A:352:LEU:HD21	1.80	0.44
1:A:375:LYS:HB2	1:A:393:TYR:CE1	2.52	0.44
1:B:366:ILE:HG23	1:B:367:PRO:HD2	2.00	0.44
1:B:409:ARG:NH1	1:B:413:LEU:HD11	2.32	0.44
1:E:77:GLY:CA	1:E:430:ASP:HB3	2.48	0.44
1:E:448:GLU:O	1:E:452:ILE:CG2	2.65	0.44
2:I:47(E):A:H2'	2:I:47(F):U:C5'	2.48	0.44
2:I:65:C:H2'	2:I:66:A:H8	1.83	0.44
2:J:47(E):A:C2	2:J:47(I):A:N7	2.85	0.44
2:J:47(N):A:H2'	2:J:47(O):G:C8	2.52	0.44
1:A:363:LEU:HB2	1:A:371:ILE:HD13	2.00	0.43
1:B:37:LYS:O	1:B:41:GLU:CG	2.59	0.43
1:B:157:LYS:HB3	1:B:207:ASN:O	2.17	0.43
1:C:11:ILE:HD12	2:I:18:G:P	2.58	0.43
1:C:167:VAL:HG12	1:C:219:PHE:CE2	2.48	0.43
1:C:175:ILE:N	1:C:176:PRO:HD2	2.33	0.43
1:C:431:MET:HE1	1:C:434:VAL:HG21	2.00	0.43
1:D:17:ILE:O	1:D:17:ILE:HG22	2.18	0.43
1:D:123:ILE:O	1:D:126:TYR:N	2.44	0.43
1:D:194:LYS:CB	1:E:168:GLU:OE1	2.66	0.43



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:443:LYS:HE2	1:E:447:GLN:OE1	2.18	0.43
2:F:2:G:O2'	2:F:3:G:H5'	2.18	0.43
2:F:15:C:H2'	2:F:16:U:C6	2.53	0.43
2:F:56:C:H2'	2:F:57:G:C8	2.53	0.43
2:G:47(J):A:H2'	2:G:47(K):G:O4'	2.18	0.43
1:A:127:LEU:O	1:A:131:THR:HG23	2.18	0.43
1:A:360:GLU:HG3	1:A:371:ILE:HG21	1.99	0.43
1:B:392:THR:HG21	1:B:430:ASP:OD2	2.19	0.43
1:C:98:SER:HA	1:D:94:ILE:CG2	2.48	0.43
1:E:159:VAL:HG13	1:E:210:LEU:HB3	2.00	0.43
1:E:269:ARG:HG3	1:E:269:ARG:NH1	2.32	0.43
2:F:59:U:C2'	2:F:60:U:H5'	2.48	0.43
2:J:46:C:H2'	2:J:47:U:C6	2.53	0.43
1:A:8:ILE:HD11	1:A:38:TYR:HB3	2.00	0.43
1:A:252:LEU:HD12	1:A:253:LEU:N	2.33	0.43
1:A:271:CYS:HA	1:A:274:LEU:HD12	2.00	0.43
1:D:285:LLP:O3	1:D:285:LLP:NZ	2.50	0.43
1:D:367:PRO:HG3	1:D:451:SER:OG	2.18	0.43
2:F:28:U:H2'	2:F:29:A:H8	1.83	0.43
2:G:10:A:C2	2:G:26:C:O2	2.71	0.43
2:G:31:A:H2'	2:G:32:C:O4'	2.18	0.43
2:I:27:C:C4	2:I:28:U:C4	3.06	0.43
1:A:339:ILE:HG13	1:A:342:ILE:HB	2.01	0.43
1:A:344:MET:O	1:A:432:ARG:HD2	2.17	0.43
1:B:312:ARG:HD2	1:B:315:ARG:NH1	2.33	0.43
1:C:107:LEU:HD11	1:C:321:LEU:HD23	2.00	0.43
1:C:265:GLU:OE1	1:C:385:LEU:CD2	2.66	0.43
1:D:259:PHE:HB3	1:D:346:THR:CG2	2.48	0.43
1:D:259:PHE:CB	1:D:346:THR:HG21	2.48	0.43
1:E:348:ASP:HB2	1:E:351:ALA:HB2	2.00	0.43
2:F:45:U:H2'	2:F:46:C:O4'	2.19	0.43
2:G:29:A:H2'	2:G:30:G:C8	2.53	0.43
1:A:104:TYR:CD1	1:A:104:TYR:N	2.86	0.43
1:A:123:ILE:CG2	1:A:328:LEU:HD12	2.48	0.43
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.80	0.43
1:B:120:ILE:HG21	1:B:137:PHE:CD1	2.54	0.43
1:B:200:TYR:HE2	1:B:228:VAL:HG21	1.83	0.43
1:B:254:ILE:HD12	1:B:259:PHE:HE2	1.82	0.43
1:B:287:LEU:C	1:B:287:LEU:HD23	2.39	0.43
1:C:312:ARG:CD	1:C:315:ARG:NH1	2.82	0.43
1:D:86:ARG:CD	1:D:284:ASP:OD2	2.66	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:366:ILE:HB	1:D:369:LEU:CD1	2.44	0.43
1:E:253:LEU:HD23	1:E:331:TYR:CG	2.54	0.43
2:G:28:U:C2'	2:G:29:A:H5'	2.48	0.43
2:G:47(L):C:H2'	2:G:47(M):G:C8	2.53	0.43
2:J:11:G:C2	2:J:12:G:N7	2.86	0.43
2:J:45:U:H2'	2:J:46:C:O4'	2.18	0.43
2:J:47(P):A:H2'	2:J:48:G:H5'	1.99	0.43
1:A:76:THR:OG1	1:A:78:VAL:HG23	2.17	0.43
1:B:25:ILE:CG1	1:B:26:TYR:N	2.80	0.43
1:B:343:ARG:HH21	1:B:343:ARG:HG2	1.84	0.43
1:D:1:MET:HG3	1:D:2:LYS:H	1.81	0.43
1:E:5:LEU:HD13	1:E:42:ILE:HB	2.00	0.43
2:F:8:A:C5	2:F:48:G:N2	2.86	0.43
1:A:271:CYS:O	1:A:274:LEU:HB2	2.19	0.43
1:A:442:ILE:HG23	1:A:446:LEU:HD11	1.99	0.43
1:B:360:GLU:HG3	1:B:371:ILE:HG22	1.99	0.43
1:D:11:ILE:HB	2:H:16:U:O2'	2.19	0.43
1:D:399:HIS:CD2	1:D:450:LEU:HD13	2.54	0.43
1:E:8:ILE:HD13	1:E:38:TYR:CB	2.49	0.43
1:E:28:VAL:O	1:E:32:ARG:HG3	2.17	0.43
1:E:405:GLN:HE22	1:E:422:ILE:CG2	2.29	0.43
2:G:26:C:C4	2:G:27:C:C4	3.06	0.43
2:J:47(E):A:H2'	2:J:47(F):U:H5'	2.00	0.43
1:A:312:ARG:HB2	1:B:172:SER:OG	2.19	0.43
1:B:77:GLY:CA	1:B:433:THR:HG23	2.47	0.43
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.76	0.43
1:D:370:LYS:HB2	1:D:398:ARG:O	2.18	0.43
1:A:313:ALA:HB1	1:B:144:GLY:HA2	2.00	0.43
1:C:336:TYR:O	1:C:339:ILE:HG12	2.18	0.43
1:D:14:VAL:O	1:D:18:PHE:HD2	2.01	0.43
1:D:169:ILE:HG13	1:D:173:PHE:CD2	2.54	0.43
1:E:88:PRO:HD2	1:E:341:VAL:CG2	2.49	0.43
2:G:47(E):A:H2'	2:G:47(F):U:O4'	2.19	0.43
2:J:38:A:C2'	2:J:39:U:H5'	2.49	0.43
1:A:169:ILE:CG1	1:A:173:PHE:HD2	2.30	0.43
1:B:179:MET:HA	1:B:182:SER:HB3	2.01	0.43
1:B:348:ASP:HB2	1:B:351:ALA:HB2	2.00	0.43
1:C:179:MET:HA	1:C:182:SER:HB3	2.00	0.43
1:C:345:LEU:CD2	1:C:380:PRO:HB3	2.49	0.43
1:E:14:VAL:HG21	1:E:53:PHE:HE2	1.84	0.43
1:A:94:ILE:O	1:A:98:SER:HB2	2.19	0.42



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:325:GLU:OE2	1:B:68:ASN:HB2	2.19	0.42
1:A:345:LEU:HD21	1:A:380:PRO:HB3	2.01	0.42
1:B:87:ALA:CB	1:B:341:VAL:HG21	2.48	0.42
1:C:126:TYR:HB3	1:C:328:LEU:HD13	1.96	0.42
1:D:73:ILE:HB	1:D:418:ILE:HG12	2.00	0.42
2:G:15:C:H2'	2:G:16:U:H6	1.81	0.42
2:H:3:G:O2'	2:H:4:A:H5'	2.19	0.42
2:J:2:G:O2'	2:J:3:G:H5'	2.18	0.42
1:A:79:VAL:HG12	1:A:341:VAL:HG13	2.00	0.42
1:B:10:GLN:HB2	2:F:19:G:C2'	2.49	0.42
1:B:230:LEU:HD22	1:B:276:ILE:HD11	2.00	0.42
1:D:11:ILE:CD1	2:H:18:G:OP1	2.67	0.42
1:D:80:ILE:HD12	1:D:285:LLP:HA	2.01	0.42
1:D:212:MET:HG3	1:D:245:TYR:CD1	2.54	0.42
2:G:8:A:O2'	2:G:9:U:P	2.77	0.42
2:G:59:U:C2'	2:G:60:U:H5'	2.49	0.42
1:A:8:ILE:HA	1:A:9:PRO:HD2	1.82	0.42
1:A:169:ILE:CG1	1:A:173:PHE:CD2	3.03	0.42
1:C:386:PRO:HG2	1:C:387:GLU:N	2.32	0.42
1:D:88:PRO:HG2	1:D:340:PRO:CB	2.49	0.42
1:D:193:ASN:O	1:D:225:VAL:HG13	2.19	0.42
1:E:277:ASP:O	1:E:297:GLY:HA3	2.19	0.42
2:H:47(G):U:H2'	2:H:47(H):U:O4'	2.18	0.42
2:I:21:U:H2'	2:I:22:G:C8	2.55	0.42
1:A:114:GLY:HA3	1:B:412:ARG:NH2	2.35	0.42
1:A:123:ILE:O	1:A:125:LYS:N	2.52	0.42
1:A:161:ILE:CG2	1:A:186:LEU:HD11	2.49	0.42
1:B:70:LYS:O	1:B:72:VAL:HG23	2.18	0.42
1:B:168:GLU:OE2	1:C:194:LYS:HD2	2.20	0.42
1:B:350:LYS:H	1:B:350:LYS:HG3	1.51	0.42
1:C:5:LEU:HD21	1:C:39:ARG:HG2	2.00	0.42
1:D:5:LEU:HD21	1:D:39:ARG:CG	2.48	0.42
1:D:14:VAL:HG12	1:D:18:PHE:HE2	1.84	0.42
1:D:218:ASN:HD22	1:E:224:PHE:CB	2.29	0.42
1:D:427:LEU:HD23	1:D:429:PHE:HE1	1.84	0.42
1:E:216:LYS:HG2	1:E:219:PHE:CZ	2.55	0.42
1:E:347:GLN:HE21	1:E:352:LEU:HD21	1.82	0.42
2:G:36:A:H2'	2:G:37:A:H8	1.81	0.42
2:G:45:U:H2'	2:G:46:C:O4'	2.18	0.42
2:J:22:G:H2'	2:J:23:C:H6	1.83	0.42
1:A:5:LEU:HD11	1:A:39:ARG:CG	2.44	0.42



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:114:GLY:CA	1:B:412:ARG:HH21	2.33	0.42
1:A:355:LYS:HG3	1:A:439:LEU:HD11	2.01	0.42
1:C:239:LYS:HD3	1:C:240:TYR:CE2	2.54	0.42
1:C:343:ARG:HG2	1:C:343:ARG:HH21	1.85	0.42
1:C:425:ASP:O	1:C:425:ASP:CG	2.57	0.42
1:D:25:ILE:HG13	1:D:26:TYR:H	1.84	0.42
1:D:137:PHE:CD1	1:D:306:LYS:HG2	2.54	0.42
1:E:250:SER:O	1:E:286:LEU:HB2	2.20	0.42
1:E:358:ARG:NH2	1:E:439:LEU:HD12	2.28	0.42
2:G:27:C:C4	2:G:28:U:C4	3.08	0.42
2:I:38:A:H2'	2:I:39:U:H5'	2.00	0.42
1:A:169:ILE:HD11	1:A:285:LLP:H5'1	2.02	0.42
1:B:49:ASP:OD1	1:B:50:LEU:N	2.53	0.42
1:C:116:ARG:HH22	1:D:171:GLY:HA3	1.84	0.42
1:D:7:GLN:O	1:D:8:ILE:C	2.58	0.42
1:E:167:VAL:HG12	1:E:219:PHE:HE2	1.85	0.42
1:B:287:LEU:HD23	1:B:287:LEU:O	2.20	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.85	0.42
1:B:394:CYS:HB3	1:B:428:LEU:HD22	2.00	0.42
1:D:16:GLU:OE2	2:H:22:G:H5'	2.20	0.42
1:D:160:ILE:HB	1:D:211:LEU:HD23	2.01	0.42
1:E:300:ASN:O	1:E:304:LYS:HG3	2.20	0.42
2:F:3:G:O2'	2:F:4:A:H5'	2.20	0.42
1:B:13:LYS:O	1:B:17:ILE:HG13	2.20	0.42
1:B:167:VAL:HG12	1:B:219:PHE:HE2	1.85	0.42
1:C:68:ASN:HD22	1:D:122:HIS:HA	1.85	0.42
1:C:82:THR:HG22	1:C:86:ARG:HE	1.85	0.42
1:C:144:GLY:CA	1:D:313:ALA:HB1	2.50	0.42
1:D:141:ASN:OD1	1:D:143:ALA:HB3	2.19	0.42
1:E:126:TYR:CE2	1:E:325:GLU:HG3	2.54	0.42
1:A:97:ILE:HG12	1:A:322:SER:OG	2.20	0.42
1:B:5:LEU:HD12	1:B:42:ILE:HD12	2.01	0.42
1:B:77:GLY:HA3	1:B:430:ASP:CG	2.40	0.42
1:B:363:LEU:HD21	1:B:446:LEU:HD12	2.02	0.42
1:C:423:ARG:HG2	1:C:423:ARG:NH1	2.35	0.42
1:C:452:ILE:OXT	1:C:452:ILE:HG23	2.20	0.42
1:D:194:LYS:HD2	1:E:168:GLU:CD	2.39	0.42
2:F:34:U:O2'	2:F:35:C:H5'	2.20	0.42
2:H:46:C:C2'	2:H:47:U:C5'	2.96	0.42
1:A:4:LEU:O	1:A:42:ILE:HD13	2.19	0.42
1:B:33:GLU:CD	1:B:60:LYS:HE3	2.40	0.42



	io ao pagoni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:363:LEU:CD2	1:B:446:LEU:HD12	2.50	0.42
1:C:6:ARG:HH11	1:C:6:ARG:HG2	1.85	0.42
1:D:77:GLY:CA	1:D:430:ASP:HB3	2.49	0.42
2:G:3:G:O2'	2:G:4:A:H5'	2.19	0.42
2:G:47(E):A:H2'	2:G:47(F):U:H5'	2.01	0.42
2:J:15:C:H2'	2:J:16:U:H6	1.84	0.42
2:J:47(E):A:O2'	2:J:47(I):A:N6	2.53	0.42
1:A:394:CYS:HB2	1:A:428:LEU:HD22	2.01	0.41
1:C:20:LYS:O	1:C:20:LYS:HG2	2.20	0.41
1:D:2:LYS:HE3	2:H:56:C:O2'	2.19	0.41
1:E:392:THR:HG21	1:E:430:ASP:OD2	2.20	0.41
2:H:59:U:C2'	2:H:60:U:H5'	2.50	0.41
1:A:11:ILE:HB	2:G:16:U:H4'	2.02	0.41
1:A:249:GLY:O	1:A:285:LLP:HD3	2.20	0.41
1:A:363:LEU:C	1:A:371:ILE:HD11	2.40	0.41
1:A:368:GLY:O	1:A:399:HIS:HA	2.20	0.41
1:B:444:LYS:HA	1:B:447:GLN:HG2	2.03	0.41
1:C:7:GLN:O	1:C:8:ILE:C	2.58	0.41
1:C:344:MET:O	1:C:432:ARG:HD3	2.19	0.41
1:D:42:ILE:HD11	1:D:50:LEU:CD2	2.44	0.41
1:D:49:ASP:OD1	1:D:50:LEU:N	2.53	0.41
1:E:7:GLN:O	1:E:8:ILE:C	2.56	0.41
2:F:26:C:C4	2:F:27:C:C4	3.07	0.41
2:F:47(E):A:C2'	2:F:47(F):U:H5'	2.49	0.41
2:J:38:A:H2'	2:J:39:U:O4'	2.20	0.41
1:A:268:PHE:CD2	1:A:268:PHE:N	2.88	0.41
1:A:285:LLP:NZ	1:A:285:LLP:O3	2.50	0.41
1:B:249:GLY:O	1:B:285:LLP:HD3	2.19	0.41
1:C:67:PRO:CG	1:D:96:PHE:HE1	2.33	0.41
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.89	0.41
1:C:362:LEU:HB3	1:C:443:LYS:HD2	2.03	0.41
1:D:432:ARG:O	1:D:432:ARG:HG3	2.20	0.41
1:E:189:VAL:HG21	1:E:200:TYR:CD1	2.55	0.41
2:F:9:U:C4	2:F:48:G:C8	3.07	0.41
2:G:7:G:O2'	2:G:8:A:H5'	2.20	0.41
2:G:56:C:H2'	2:G:57:G:C8	2.55	0.41
2:H:32:C:C4	2:H:33:U:O4	2.74	0.41
1:A:114:GLY:CA	1:B:412:ARG:NH2	2.84	0.41
1:A:250:SER:HB2	1:A:286:LEU:CD1	2.50	0.41
1:A:308:ASN:OD1	1:A:308:ASN:C	2.58	0.41
1:B:97:ILE:HD11	1:B:323:GLY:CA	2.41	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:113:GLU:H	1:C:113:GLU:HG3	1.71	0.41
1:D:38:TYR:CE2	1:D:47:ARG:NE	2.88	0.41
1:D:227:GLU:CG	1:D:228:VAL:N	2.83	0.41
1:E:14:VAL:O	1:E:18:PHE:HD2	2.03	0.41
1:E:88:PRO:HG2	1:E:340:PRO:HB3	2.00	0.41
1:E:140:ASN:ND2	1:E:141:ASN:ND2	2.69	0.41
2:F:7:G:O2'	2:F:8:A:H5'	2.19	0.41
1:A:144:GLY:HA2	1:B:313:ALA:HB1	2.03	0.41
1:A:339:ILE:HA	1:A:340:PRO:HD3	1.88	0.41
1:A:388:LEU:HD21	1:A:390:LEU:CD1	2.50	0.41
1:B:175:ILE:N	1:B:176:PRO:CD	2.83	0.41
1:B:247:ASP:C	1:B:247:ASP:OD1	2.59	0.41
1:B:452:ILE:OXT	1:B:452:ILE:CG2	2.68	0.41
1:C:15:VAL:HA	1:C:27:VAL:HG11	2.01	0.41
1:C:355:LYS:CG	1:C:439:LEU:HD11	2.48	0.41
1:D:191:THR:HG22	1:E:176:PRO:CG	2.51	0.41
1:D:298:LYS:O	1:D:302:ILE:HG12	2.19	0.41
1:E:286:LEU:HG	1:E:384:SER:HB2	2.03	0.41
1:E:290:PRO:HB2	1:E:320:THR:HG22	2.03	0.41
1:E:409:ARG:HG3	1:E:412:ARG:NH2	2.34	0.41
2:F:66:A:H2'	2:F:67:U:C6	2.56	0.41
1:A:60:LYS:C	1:A:64:LEU:HG	2.37	0.41
1:A:102:ASN:HB3	1:B:71:ARG:HH22	1.85	0.41
1:A:144:GLY:CA	1:B:313:ALA:HB1	2.50	0.41
1:B:366:ILE:CG2	1:B:367:PRO:HD2	2.51	0.41
1:D:253:LEU:HD23	1:D:331:TYR:CD2	2.55	0.41
1:D:333:GLU:OE1	1:D:335:ARG:HD2	2.21	0.41
2:F:35:C:H2'	2:F:36:A:O4'	2.21	0.41
2:G:43:G:N1	2:G:44:G:C6	2.88	0.41
2:H:46:C:C3'	2:H:47:U:H5'	2.49	0.41
1:A:216:LYS:HG2	1:A:219:PHE:CE2	2.55	0.41
1:A:359:LEU:CD1	1:A:363:LEU:HD11	2.50	0.41
1:A:404:SER:O	1:A:407:LEU:HB3	2.20	0.41
1:A:407:LEU:HD23	1:A:427:LEU:HD22	2.00	0.41
1:B:7:GLN:O	1:B:8:ILE:C	2.58	0.41
1:B:167:VAL:HG12	1:B:219:PHE:CE2	2.55	0.41
1:C:67:PRO:CB	1:D:96:PHE:CE1	3.04	0.41
1:C:178:ILE:HG23	1:C:179:MET:N	2.36	0.41
1:D:277:ASP:O	1:D:278:LEU:HD23	2.20	0.41
1:D:369:LEU:HD21	1:D:450:LEU:HD11	2.03	0.41
1:E:60:LYS:O	1:E:64:LEU:HG	2.20	0.41



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:178:ILE:CG2	1:E:179:MET:N	2.83	0.41
2:G:10:A:N6	2:G:44:G:O6	2.54	0.41
2:I:67(A):A:H2'	2:I:68:C:H6	1.83	0.41
2:J:43:G:H2'	2:J:44:G:C8	2.56	0.41
1:A:77:GLY:HA3	1:A:430:ASP:HB3	2.03	0.41
1:B:160:ILE:HB	1:B:211:LEU:HD23	2.03	0.41
1:B:246:TYR:CE2	1:B:248:ALA:HA	2.56	0.41
1:B:356:ALA:O	1:B:395:VAL:HG21	2.20	0.41
1:B:362:LEU:HD22	1:B:443:LYS:HD2	2.01	0.41
1:C:32:ARG:O	1:C:36:GLU:HG2	2.21	0.41
1:C:79:VAL:HG21	1:C:345:LEU:HG	2.03	0.41
1:D:355:LYS:HG3	1:D:439:LEU:HD11	2.03	0.41
1:E:179:MET:SD	1:E:186:LEU:HB2	2.61	0.41
2:J:32:C:C4	2:J:33:U:O4	2.74	0.41
1:A:12:SER:HG	2:G:16:U:H1'	1.86	0.41
1:A:79:VAL:HG21	1:A:345:LEU:CD2	2.51	0.41
1:A:139:VAL:HB	1:A:314:LEU:HB3	2.02	0.41
1:B:74:ASN:C	1:B:74:ASN:OD1	2.59	0.41
1:B:137:PHE:CD1	1:B:306:LYS:HG2	2.55	0.41
1:B:339:ILE:HG13	1:B:342:ILE:CG1	2.51	0.41
1:B:389:GLU:O	1:B:390:LEU:HD23	2.21	0.41
1:C:72:VAL:HG22	1:C:417:PRO:CG	2.51	0.41
1:D:204:ILE:HG22	1:D:205:ASN:N	2.35	0.41
1:D:256:LEU:HD23	1:D:263:VAL:HG21	2.03	0.41
1:D:265:GLU:HG3	1:D:266:PRO:HD2	2.03	0.41
1:D:399:HIS:ND1	1:D:450:LEU:HD22	2.35	0.41
1:E:90:SER:CB	1:E:338:ASP:O	2.66	0.41
1:E:211:LEU:CD2	1:E:242:ILE:HG21	2.51	0.41
2:H:26:C:C4	2:H:27:C:C4	3.09	0.41
2:I:10:A:C5'	2:I:45:U:C1'	2.99	0.41
2:J:7:G:O2'	2:J:49:G:OP2	2.37	0.41
2:J:47(J):A:H2'	2:J:47(K):G:C8	2.56	0.41
1:A:126:TYR:O	1:A:130:LEU:HG	2.21	0.41
1:A:265:GLU:CD	1:A:266:PRO:HD2	2.40	0.41
1:B:1:MET:C	1:B:3:SER:N	2.74	0.41
1:B:385:LEU:HD13	1:B:388:LEU:HD22	2.03	0.41
1:C:33:GLU:CD	1:C:60:LYS:HE3	2.42	0.41
1:C:432:ARG:O	1:C:432:ARG:HG3	2.20	0.41
1:D:254:ILE:CD1	1:D:336:TYR:CE1	3.04	0.41
1:E:88:PRO:HG3	1:E:344:MET:CE	2.51	0.41
2:I:43:G:H2'	2:I:44:G:C8	2.56	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:29:LYS:HD2	1:B:332:PHE:CE1	2.56	0.40
1:A:84:LEU:HB3	1:B:104:TYR:HB3	2.02	0.40
1:C:438:ASP:O	1:C:442:ILE:HG13	2.20	0.40
1:E:30:ALA:O	1:E:34:VAL:CG2	2.66	0.40
1:E:272:ILE:HD11	1:E:296:VAL:HG23	2.03	0.40
1:E:301:LEU:HD23	1:E:301:LEU:HA	1.75	0.40
1:E:409:ARG:HA	1:E:412:ARG:CZ	2.52	0.40
2:G:47(H):U:H2'	2:G:47(I):A:C4'	2.51	0.40
2:G:66:A:H2'	2:G:67:U:C6	2.56	0.40
2:I:30:G:N2	2:I:40:C:O2	2.44	0.40
1:A:79:VAL:CG1	1:A:341:VAL:HG13	2.51	0.40
1:A:327:THR:O	1:A:331:TYR:HD2	2.05	0.40
1:A:396:ALA:HB2	1:A:428:LEU:HD23	2.03	0.40
1:C:99:GLU:O	1:D:71:ARG:CZ	2.69	0.40
1:D:86:ARG:HB3	1:D:284:ASP:O	2.21	0.40
1:D:163:ARG:HH11	1:E:166:LEU:HD13	1.83	0.40
1:E:15:VAL:HG11	1:E:24:GLU:OE2	2.21	0.40
1:E:231:GLU:CD	1:E:231:GLU:H	2.23	0.40
2:H:65:C:H2'	2:H:66:A:C8	2.56	0.40
2:J:23:C:N4	2:J:24:C:N4	2.69	0.40
1:A:47:ARG:HD3	1:A:49:ASP:O	2.22	0.40
1:A:86:ARG:HD2	1:A:284:ASP:OD2	2.22	0.40
1:A:169:ILE:HG13	1:A:169:ILE:O	2.21	0.40
1:A:263:VAL:CG1	1:A:264:ASP:N	2.85	0.40
1:B:7:GLN:HB2	1:B:50:LEU:CD1	2.51	0.40
1:B:10:GLN:HB2	2:F:19:G:H2'	2.02	0.40
1:B:137:PHE:HD1	1:B:306:LYS:HE2	1.86	0.40
1:C:193:ASN:HB2	1:C:224:PHE:O	2.21	0.40
2:F:38:A:H2'	2:F:39:U:O4'	2.20	0.40
2:I:1:G:H2'	2:I:2:G:C8	2.56	0.40
2:J:47(E):A:C2'	2:J:47(F):U:H5'	2.51	0.40
2:J:56:C:H2'	2:J:57:G:C8	2.56	0.40
1:C:70:LYS:HE2	1:C:70:LYS:HB3	1.88	0.40
1:C:87:ALA:CB	1:C:341:VAL:HG21	2.52	0.40
1:C:247:ASP:OD1	1:C:247:ASP:C	2.60	0.40
1:D:220:TYR:CD1	1:D:220:TYR:C	2.95	0.40
1:D:348:ASP:O	1:D:351:ALA:HB3	2.21	0.40
1:D:363:LEU:O	1:D:371:ILE:HD11	2.22	0.40
1:E:175:ILE:N	1:E:176:PRO:HD2	2.36	0.40
2:G:2:G:H2'	2:G:3:G:C8	2.56	0.40
2:G:29:A:O2'	2:G:30:G:O4'	2.39	0.40



J 1	1 5		
Atom-1	Atom-2	$\begin{array}{l} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
2:I:28:U:H2'	2:I:29:A:H8	1.86	0.40
2:J:35:C:C2'	2:J:36:A:O4'	2.69	0.40
1:A:167:VAL:HG12	1:A:219:PHE:CE2	2.56	0.40
1:A:335:ARG:NE	1:A:338:ASP:OD2	2.54	0.40
1:A:416:PRO:HG3	1:A:441:THR:HG21	2.04	0.40
1:D:416:PRO:CG	1:D:441:THR:HG21	2.51	0.40
1:E:136:SER:CB	1:E:296:VAL:HG12	2.49	0.40
2:H:8:A:HO2'	2:H:9:U:P	2.44	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 X-ray entries followed by that with respect to entries of similar resolution.

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	А	449/452~(99%)	423 (94%)	22 (5%)	4 (1%)	17	57
1	В	449/452~(99%)	419 (93%)	25~(6%)	5 (1%)	14	52
1	С	449/452~(99%)	421 (94%)	24 (5%)	4 (1%)	17	57
1	D	449/452~(99%)	421 (94%)	24 (5%)	4 (1%)	17	57
1	Е	449/452~(99%)	420 (94%)	23 (5%)	6 (1%)	12	48
All	All	2245/2260 (99%)	2104 (94%)	118 (5%)	23 (1%)	15	54

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	PRO
1	Е	9	PRO
1	В	124	GLU
1	С	124	GLU
1	D	124	GLU
1	Е	2	LYS



Mol	Chain	Res	Type
1	Е	124	GLU
1	А	86	ARG
1	А	124	GLU
1	В	19	ALA
1	С	86	ARG
1	D	19	ALA
1	А	19	ALA
1	В	86	ARG
1	С	19	ALA
1	D	86	ARG
1	Е	19	ALA
1	Е	86	ARG
1	A	9	PRO
1	С	9	PRO
1	Е	340	PRO
1	В	9	PRO
1	В	340	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	А	390/390~(100%)	380~(97%)	10 (3%)	46	66
1	В	390/390~(100%)	389~(100%)	1 (0%)	92	95
1	С	390/390~(100%)	385~(99%)	5 (1%)	69	81
1	D	390/390~(100%)	384~(98%)	6 (2%)	65	80
1	Е	390/390~(100%)	389 (100%)	1 (0%)	92	95
All	All	1950/1950~(100%)	1927~(99%)	23 (1%)	71	83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	12	SER
1	А	98	SER



Mol	Chain	Res	Type
1	А	105	SER
1	А	118	SER
1	А	136	SER
1	А	188	GLU
1	А	271	CYS
1	А	287	LEU
1	А	394	CYS
1	A	403	SER
1	В	188	GLU
1	С	3	SER
1	С	188	GLU
1	С	317	ASP
1	С	384	SER
1	С	400	ASP
1	D	24	GLU
1	D	39	ARG
1	D	172	SER
1	D	182	SER
1	D	188	GLU
1	D	316	ILE
1	Е	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	68	ASN
1	А	140	ASN
1	А	347	GLN
1	А	399	HIS
1	А	436	HIS
1	В	10	GLN
1	В	95	ASN
1	В	122	HIS
1	В	142	ASN
1	В	399	HIS
1	В	405	GLN
1	С	10	GLN
1	С	68	ASN
1	С	95	ASN
1	С	122	HIS
1	С	291	GLN
1	С	347	GLN



Mol	Chain	Res	Type
1	С	405	GLN
1	D	122	HIS
1	D	347	GLN
1	D	399	HIS
1	D	436	HIS
1	Е	122	HIS
1	Е	140	ASN
1	Е	238	HIS
1	Е	347	GLN
1	Е	399	HIS
1	Е	405	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	91/95~(95%)	6~(6%)	0
2	G	91/95~(95%)	6~(6%)	0
2	Н	91/95~(95%)	6~(6%)	0
2	Ι	91/95~(95%)	9 (9%)	1 (1%)
2	J	91/95~(95%)	6~(6%)	0
All	All	455/475~(95%)	33~(7%)	1 (0%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	18	G
2	F	20(A)	G
2	F	33	U
2	F	42(A)	С
2	F	43	G
2	F	73	G
2	G	18	G
2	G	20(A)	G
2	G	42(A)	С
2	G	43	G
2	G	47(G)	U
2	G	73	G
2	Н	18	G
2	Н	20(A)	G
2	Н	42(A)	С
2	Н	43	G



Mol	Chain	Res	Type
2	Н	47(G)	U
2	Н	73	G
2	Ι	14	G
2	Ι	18	G
2	Ι	20(A)	G
2	Ι	42(A)	С
2	Ι	43	G
2	Ι	44	G
2	Ι	45	U
2	Ι	47(G)	U
2	Ι	73	G
2	J	18	G
2	J	20(A)	G
2	J	42(A)	С
2	J	43	G
2	J	47(G)	U
2	J	73	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	Ι	44	G

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mal	Mol Type Chain Beg		Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
MOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	А	285	1	23,24,25	1.17	2 (8%)	25,32,34	0.97	1 (4%)
1	LLP	С	285	1	$23,\!24,\!25$	1.14	2 (8%)	25,32,34	0.92	1 (4%)
1	LLP	Е	285	1	23,24,25	1.14	1 (4%)	25,32,34	1.04	1 (4%)
1	LLP	D	285	1	$23,\!24,\!25$	1.14	1 (4%)	25,32,34	0.91	1 (4%)
1	LLP	В	285	1	23,24,25	1.23	2 (8%)	25,32,34	1.04	1 (4%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	А	285	1	-	2/16/17/19	0/1/1/1
1	LLP	С	285	1	-	4/16/17/19	0/1/1/1
1	LLP	Е	285	1	-	2/16/17/19	0/1/1/1
1	LLP	D	285	1	-	3/16/17/19	0/1/1/1
1	LLP	В	285	1	-	6/16/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	285	LLP	C4-C4'	-2.80	1.40	1.46
1	Ε	285	LLP	C4-C4'	-2.58	1.41	1.46
1	А	285	LLP	C4-C4'	-2.47	1.41	1.46
1	С	285	LLP	C4-C4'	-2.24	1.41	1.46
1	А	285	LLP	C2'-C2	2.24	1.53	1.50
1	В	285	LLP	C2'-C2	2.18	1.53	1.50
1	D	285	LLP	C4-C4'	-2.17	1.42	1.46
1	С	285	LLP	C2'-C2	2.13	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Е	285	LLP	OP4-P-OP1	2.80	114.00	106.44
1	В	285	LLP	OP4-P-OP1	2.65	113.59	106.44
1	А	285	LLP	OP4-P-OP1	2.43	113.00	106.44
1	D	285	LLP	OP4-P-OP1	2.33	112.73	106.44
1	С	285	LLP	OP4-P-OP1	2.31	112.69	106.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	285	LLP	O-C-CA-CB
1	В	285	LLP	C4-C5-C5'-OP4
1	В	285	LLP	C6-C5-C5'-OP4
1	В	285	LLP	C-CA-CB-CG
1	В	285	LLP	O-C-CA-CB



Mol	Chain	Res	Type	Atoms
1	С	285	LLP	C4-C5-C5'-OP4
1	С	285	LLP	C6-C5-C5'-OP4
1	С	285	LLP	O-C-CA-CB
1	D	285	LLP	C4-C5-C5'-OP4
1	D	285	LLP	C6-C5-C5'-OP4
1	D	285	LLP	O-C-CA-CB
1	Е	285	LLP	C-CA-CB-CG
1	Ε	285	LLP	O-C-CA-CB
1	В	285	LLP	CE-CD-CG-CB
1	А	285	LLP	C-CA-CB-CG
1	С	285	LLP	C-CA-CB-CG
1	В	285	LLP	CD-CE-NZ-C4'

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There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	285	LLP	4	0
1	С	285	LLP	7	0
1	Ε	285	LLP	3	0
1	D	285	LLP	3	0
1	В	285	LLP	6	0

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)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

