Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:20 PM EDT

PDB ID	:	1FJG
Title	:	STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL SUBUNIT IN COMPLEX WITH THE ANTIBIOTICS STREPTOMYCIN, SPECTINOMYCIN, AND PAROMOMYCIN
Authors	:	Carter, A.P.; Clemons Jr., W.M.; Brodersen, D.E.; Wimberly, B.T.; Morgan-Warren, R.J.; Ramakrishnan, V.
Deposited on	:	2000-08-08
Resolution	:	3.00 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 (i)) were used in the production of this report:

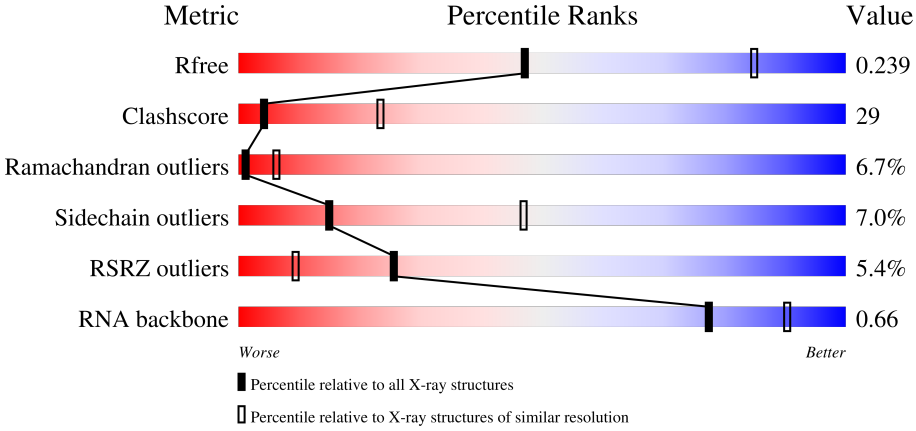
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	6%; 36%, 49%, 12%, • •
2	X	6	33%; 83%, 17%
3	B	256	%; 28%, 56%, 8%, 7%
4	C	239	23%, 53%, 9%, •, 14%

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Mol	Chain	Length	Quality of chain
5	D	209	7% 46% 46% 7%
6	E	162	.% 40% 48% • • 7%
7	F	101	5% 37% 60% •
8	G	156	2% 39% 54% 6% •
9	H	138	.% 50% 46% •
10	I	128	12% 42% 47% 9% ••
11	J	105	9% 24% 54% 13% • 7%
12	K	129	8% 36% 48% 6% • 8%
13	L	135	.% 36% 50% • • 7%
14	M	126	14% 30% 52% 16% ••
15	N	61	5% 25% 62% 11% •
16	O	89	2% 62% 33% • •
17	P	88	.% 44% 44% 6% 6%
18	Q	105	10% 48% 40% 10% ••
19	R	88	5% 18% 53% 11% 17%
20	S	93	17% 27% 55% 9% 10%
21	T	106	3% 40% 45% 8% • 7%
22	V	26	8% 27% 62% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1550	-	-	-	X
24	MG	A	1557	-	-	-	X
24	MG	A	1573	-	-	-	X
24	MG	A	1583	-	-	-	X
24	MG	A	1586	-	-	-	X
24	MG	A	1615	-	-	-	X
24	MG	A	1619	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	210	-	-	-	X
24	MG	A	211	-	-	-	X
24	MG	A	212	-	-	-	X

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 51995 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.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1507	32391	14418	6002	10465	1506	22	0	0

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	6	117	54	13	45	5	0	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	237	1923	1226	344	348	5	0	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	206	1612	1016	314	281	1	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	208	1703	1066	339	291	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLN	ASN	CONFLICT	UNP P80373
D	201	ASN	GLN	CONFLICT	UNP P80373

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	150	1146	724	217	201	4	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	F	101	843	531	155	154	3	0	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	155	1257	781	252	218	6	0	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	138	1116	705	215	193	3	0	0	0

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	127	1011	639	198	174	0	0	0

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	98	792	498	156	137	1	0	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	119	885	549	168	165	3	0	0	0

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	125	975	614	196	164	1	0	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	125	997	617	207	171	2	0	0	0

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	60	492	312	104	72	4	0	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	O	88	734	459	147	126	2	0	0	0

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	83	700	443	139	117	1	0	0	0

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	104	857	547	161	147	2	0	0	0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	R	73	597	380	118	99	0	0	0

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	84	674	430	126	116	2	0	0	0

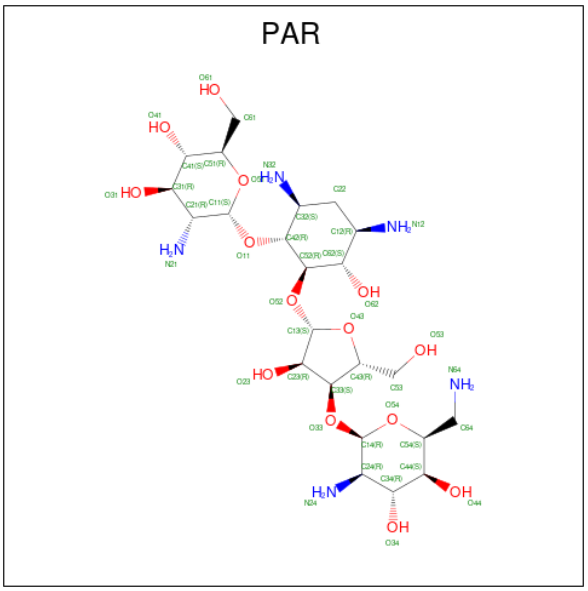
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	T	99	762	469	162	129	2	0	0	0

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	V	24	208	128	50	30	0	0	0

- Molecule 23 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	A	1	42	23	5	14	0	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
24	A	94	94	94	0	0

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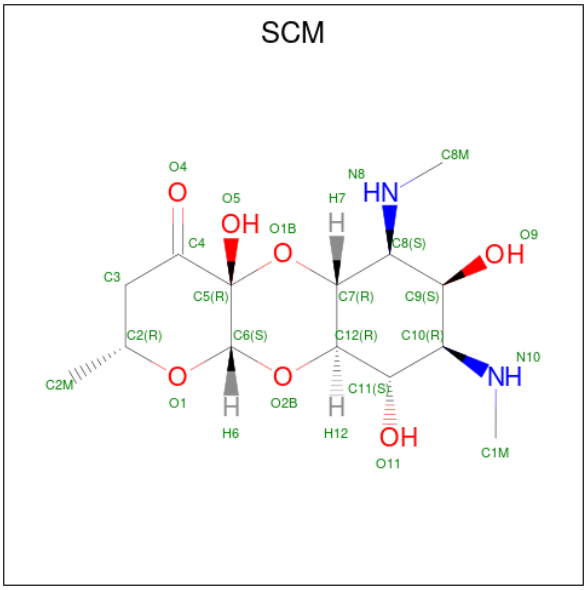
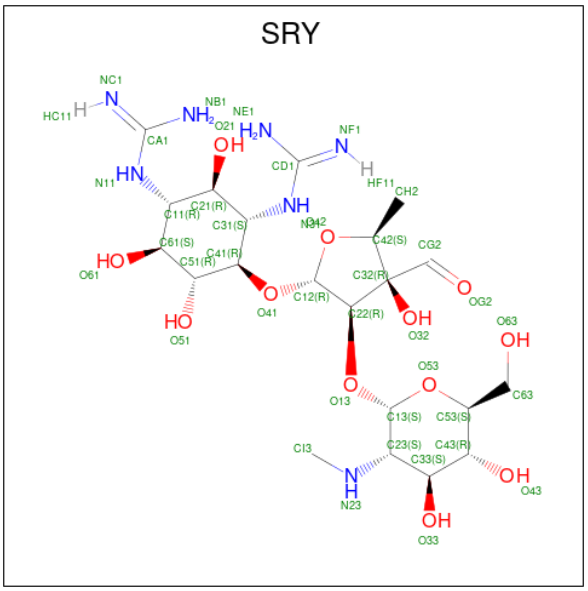
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Mg 1 1	0	0
24	H	1	Total Mg 1 1	0	0

- Molecule 25 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C N O 23 14 2 7	0	0

- Molecule 26 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
26	A	1	40	21	7	12	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

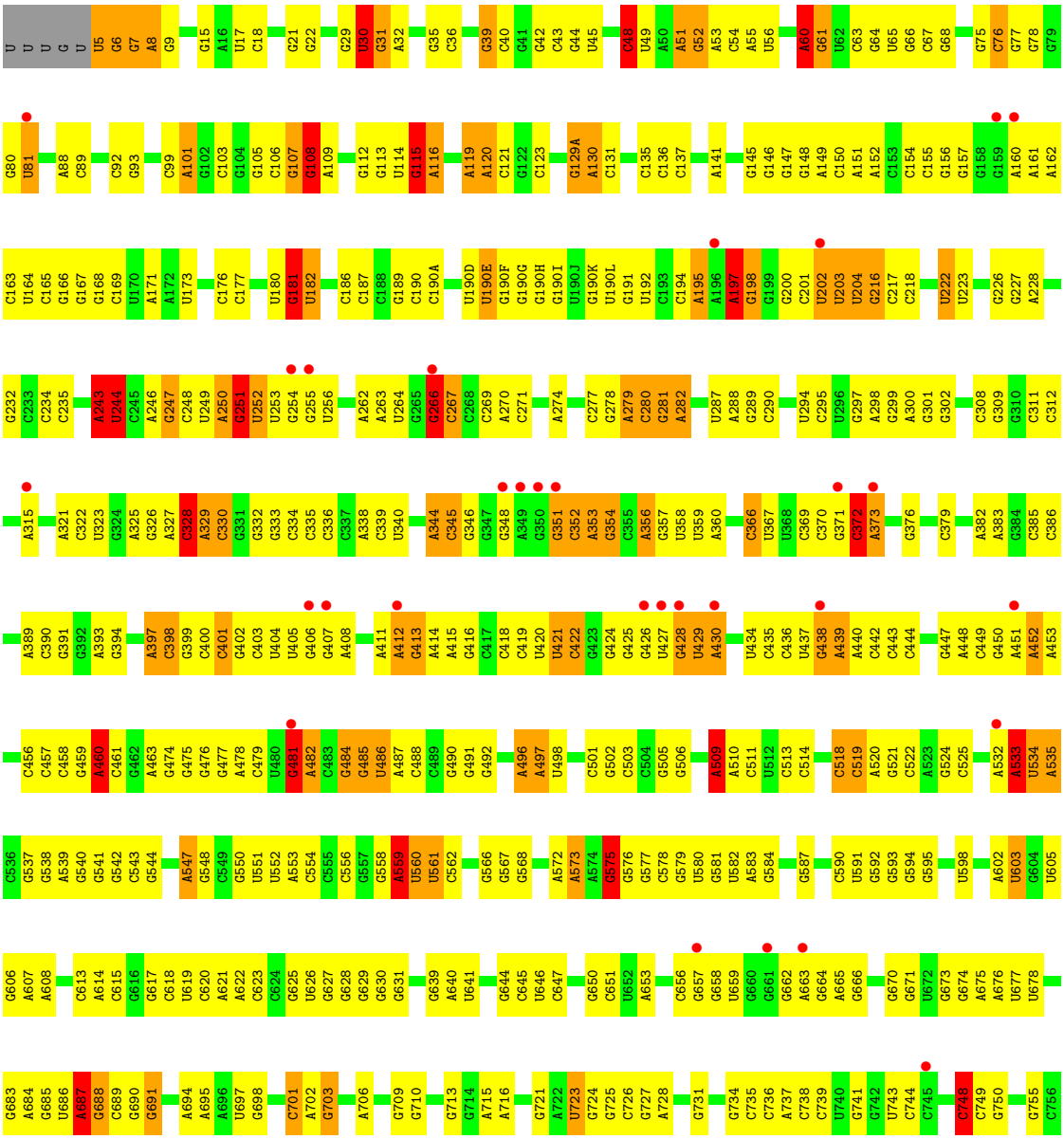
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
27	D	1	1	1	0	0
			Total	Zn		
27	N	1	1	1	0	0

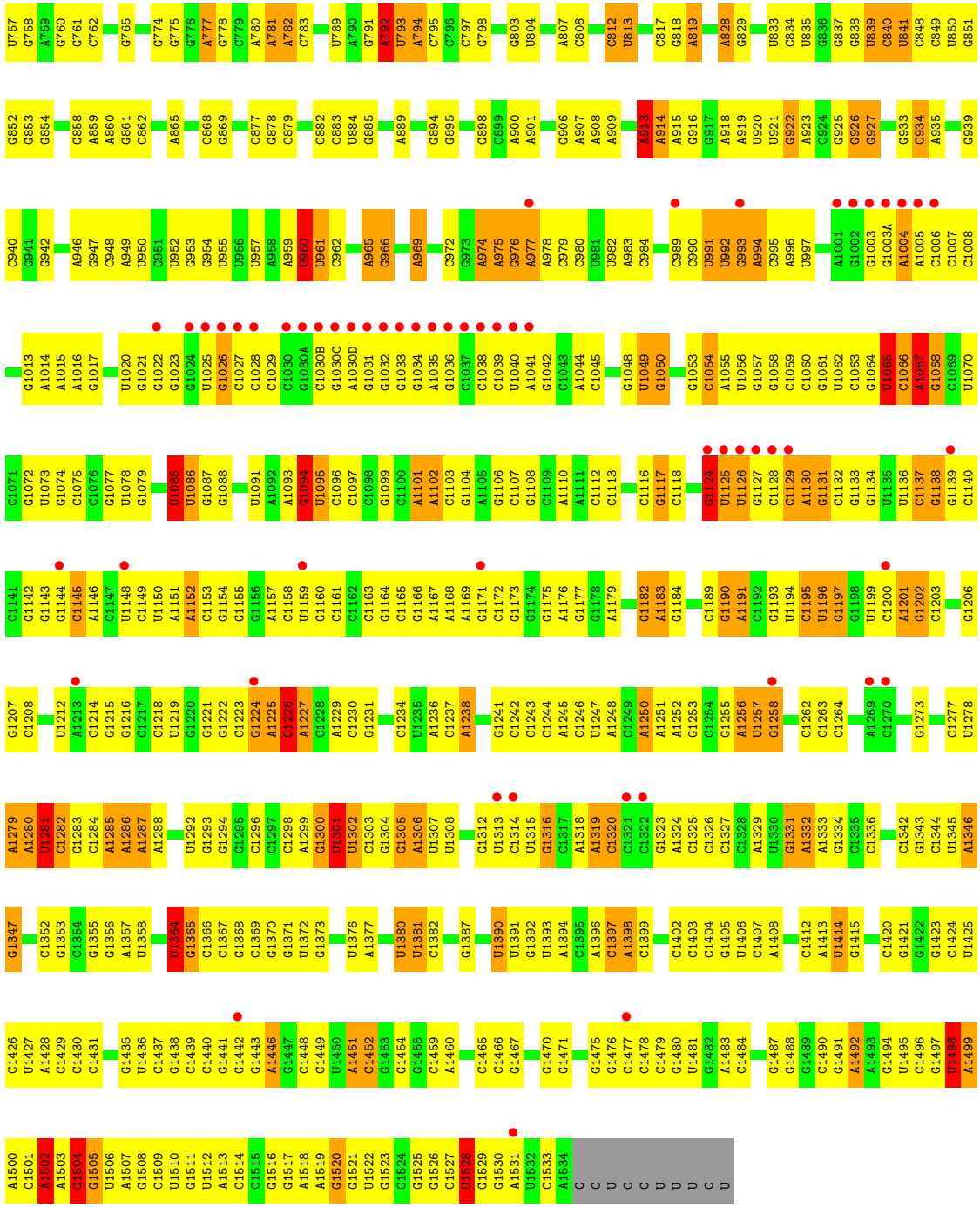
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 16S RIBOSOMAL RNA

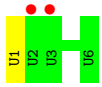
Chain A:





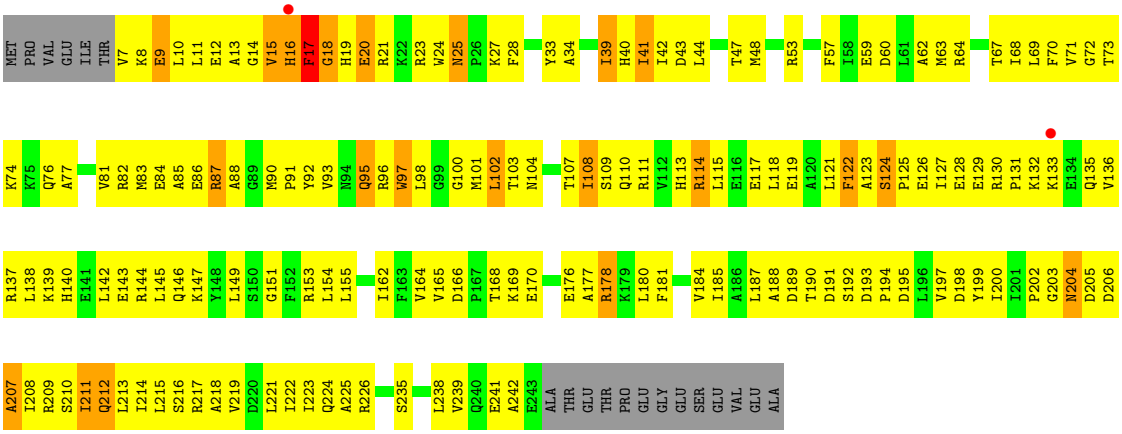
• Molecule 2: FRAGMENT OF MESSENGER RNA

Chain X:



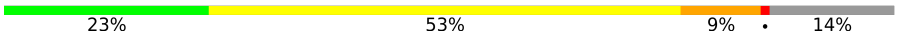
• Molecule 3: 30S RIBOSOMAL PROTEIN S2

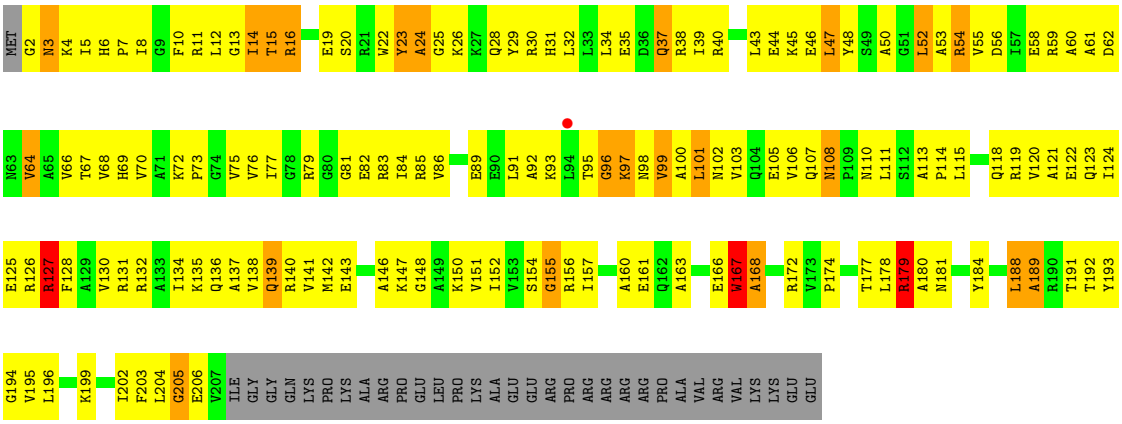
Chain B:



- Molecule 4: 30S RIBOSOMAL PROTEIN S3

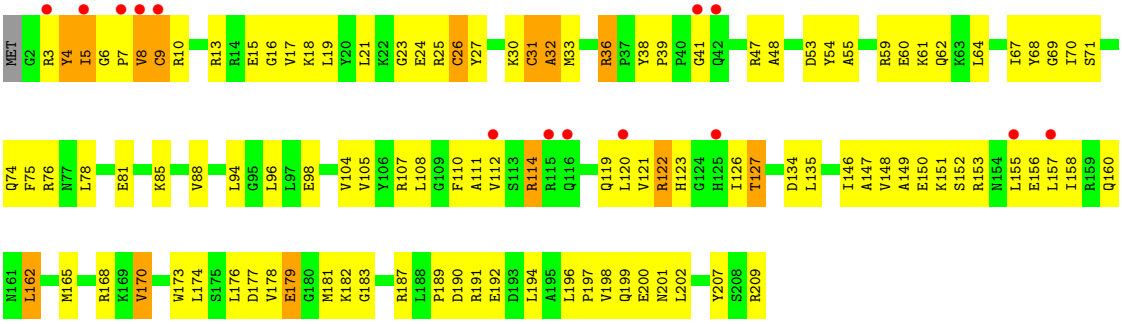
Chain C:





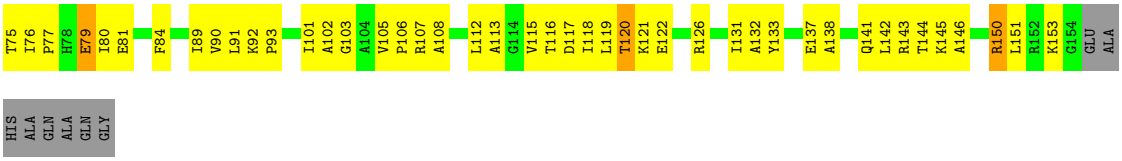
- Molecule 5: 30S RIBOSOMAL PROTEIN S4

Chain D:



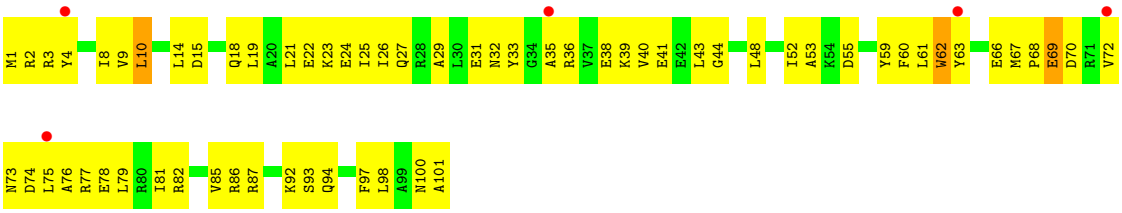
- Molecule 6: 30S RIBOSOMAL PROTEIN S5

Chain E:



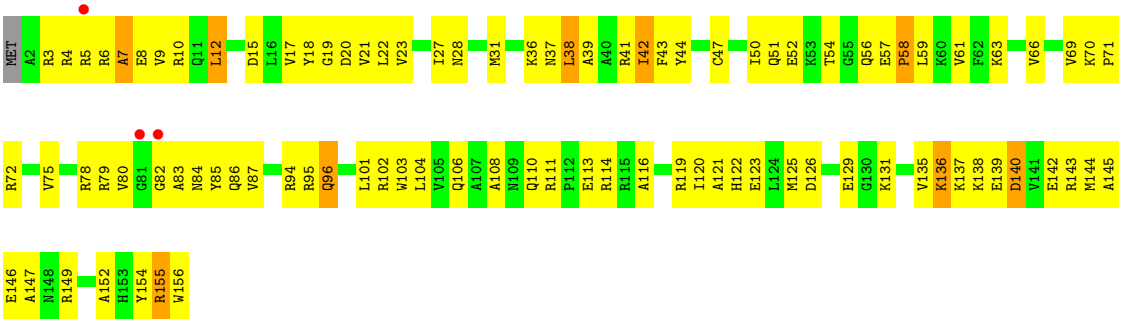
• Molecule 7: 30S RIBOSOMAL PROTEIN S6

Chain F:



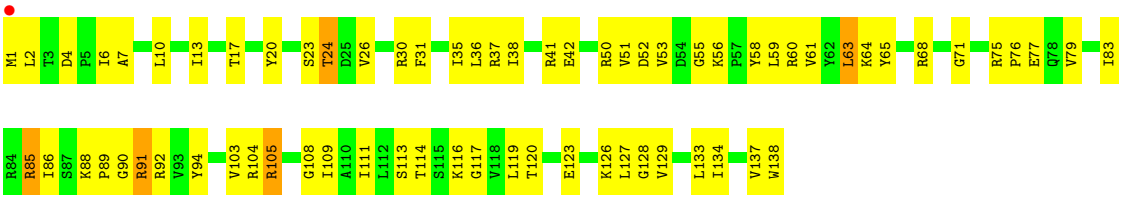
• Molecule 8: 30S RIBOSOMAL PROTEIN S7

Chain G:



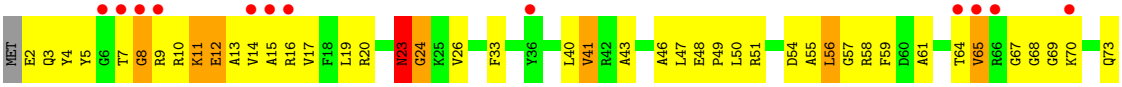
• Molecule 9: 30S RIBOSOMAL PROTEIN S8

Chain H:



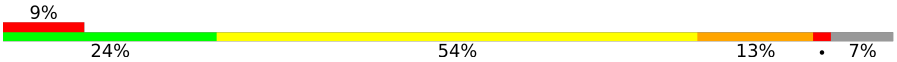
• Molecule 10: 30S RIBOSOMAL PROTEIN S9

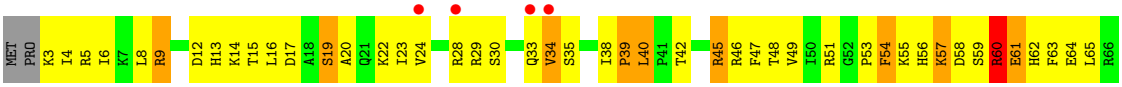
Chain I:

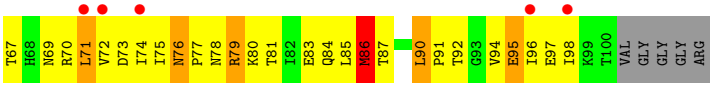


• Molecule 11: 30S RIBOSOMAL PROTEIN S10

Chain J:

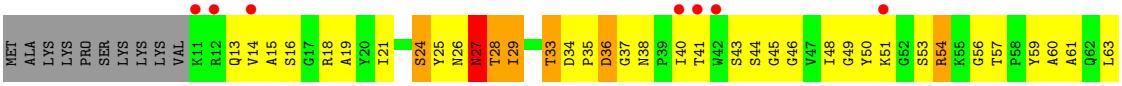


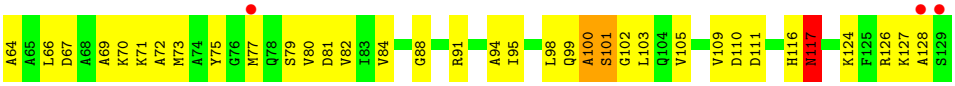




• Molecule 12: 30S RIBOSOMAL PROTEIN S11

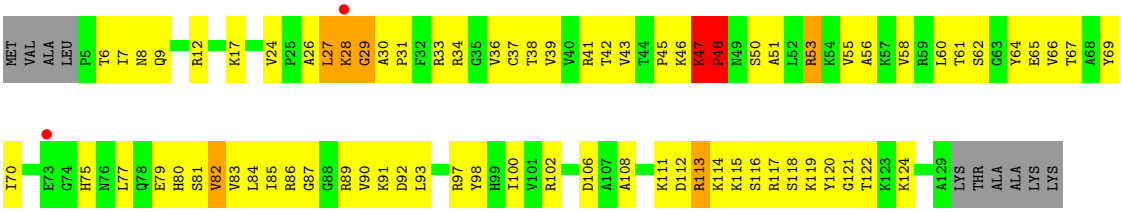
Chain K:





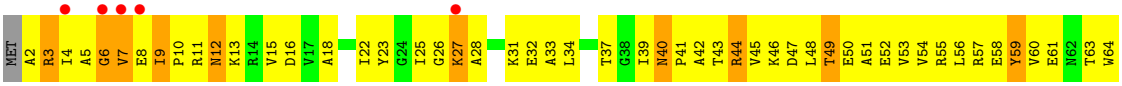
• Molecule 13: 30S RIBOSOMAL PROTEIN S12

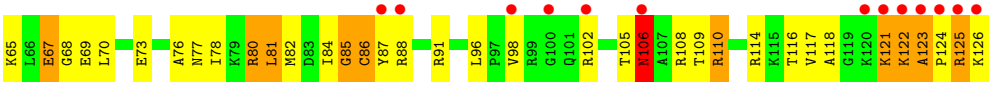
Chain L:



• Molecule 14: 30S RIBOSOMAL PROTEIN S13

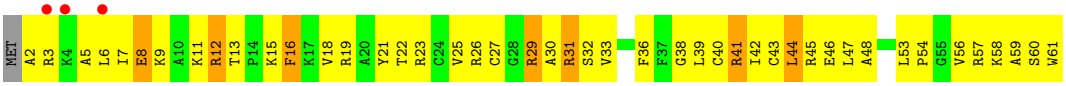
Chain M:





• Molecule 15: 30S RIBOSOMAL PROTEIN S14

Chain N:

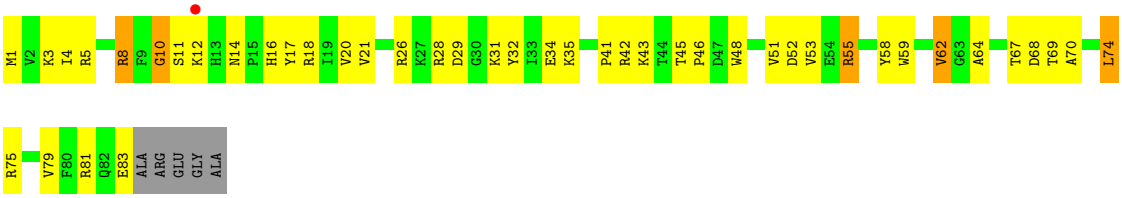


• Molecule 16: 30S RIBOSOMAL PROTEIN S15

Chain O:

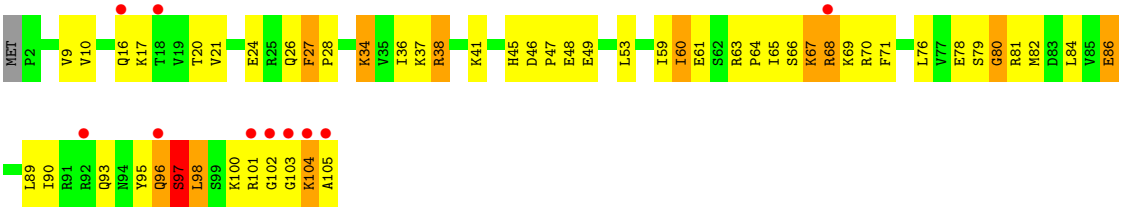
• Molecule 17: 30S RIBOSOMAL PROTEIN S16

Chain P:



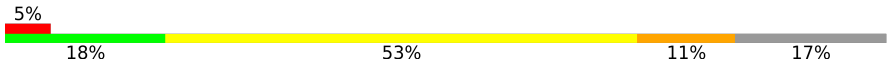
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

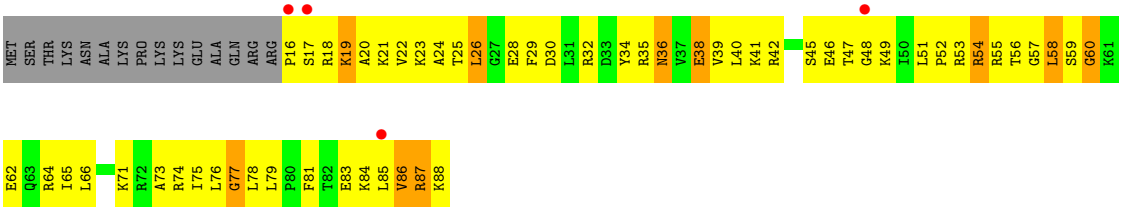
Chain Q:



• Molecule 19: 30S RIBOSOMAL PROTEIN S18

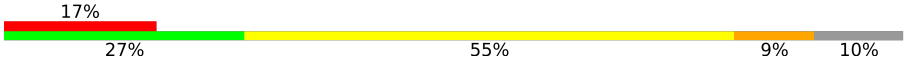
Chain R:

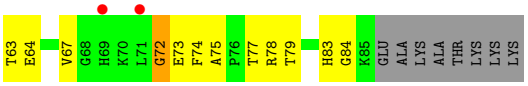




• Molecule 20: 30S RIBOSOMAL PROTEIN S19

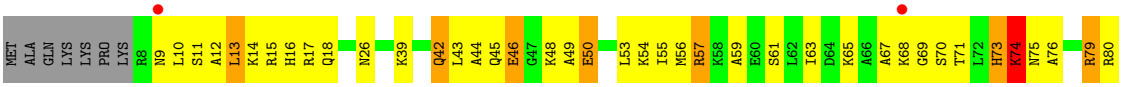
Chain S:

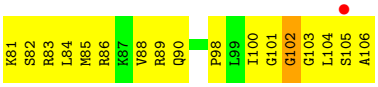




• Molecule 21: 30S RIBOSOMAL PROTEIN S20

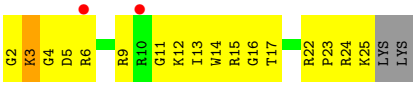
Chain T:





• Molecule 22: 30S RIBOSOMAL PROTEIN THX

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.00Å 402.00Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.35 – 3.00 97.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (95.35-3.00) 91.0 (97.50-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.255 0.207 , 0.239	Depositor DCC
R_{free} test set	13237 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	51995	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PAR, MG, ZN, SCM, SRY

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	A	0.48	0/36259	0.74	39/56593 (0.1%)
2	X	1.41	1/128 (0.8%)	1.72	5/196 (2.6%)
3	B	0.34	0/1958	0.65	0/2640
4	C	0.37	0/1636	0.66	0/2205
5	D	0.38	0/1733	0.63	0/2318
6	E	0.46	0/1162	0.71	0/1564
7	F	0.32	0/856	0.60	0/1154
8	G	0.34	0/1276	0.60	0/1709
9	H	0.44	0/1136	0.71	0/1527
10	I	0.36	0/1029	0.64	0/1378
11	J	0.35	0/805	0.66	1/1082 (0.1%)
12	K	0.36	0/900	0.65	0/1213
13	L	0.41	0/991	0.79	1/1327 (0.1%)
14	M	0.32	0/1008	0.65	0/1347
15	N	0.39	0/501	0.69	0/664
16	O	0.36	0/745	0.62	1/992 (0.1%)
17	P	0.43	0/716	0.73	0/963
18	Q	0.45	0/870	0.77	1/1159 (0.1%)
19	R	0.37	0/603	0.64	0/799
20	S	0.31	0/689	0.72	2/926 (0.2%)
21	T	0.38	0/764	0.71	0/1006
22	V	0.42	0/212	0.65	0/277
All	All	0.45	1/55977 (0.0%)	0.73	50/83039 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	39

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	U	C4-O4	13.50	1.34	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1	U	N3-C4-C5	12.17	121.90	114.60
2	X	1	U	C2-N3-C4	-11.66	120.00	127.00
1	A	1498	U	C2'-C3'-O3'	9.77	130.99	109.50
2	X	1	U	C5-C4-O4	-9.60	120.14	125.90
1	A	559	A	C2'-C3'-O3'	9.52	130.44	109.50
1	A	243	A	C2'-C3'-O3'	9.24	129.82	109.50
1	A	115	G	C2'-C3'-O3'	9.10	129.53	109.50
1	A	1528	U	C2'-C3'-O3'	8.80	128.86	109.50
1	A	366	C	C2'-C3'-O3'	8.67	128.58	109.50
1	A	792	A	C2'-C3'-O3'	8.56	128.32	109.50
1	A	575	G	C2'-C3'-O3'	8.54	128.28	109.50
1	A	181	G	C2'-C3'-O3'	8.50	128.20	109.50
1	A	1364	U	C2'-C3'-O3'	7.49	125.97	109.50
1	A	60	A	C2'-C3'-O3'	7.32	125.59	109.50
1	A	48	C	C2'-C3'-O3'	7.30	125.57	109.50
1	A	1195	C	N1-C1'-C2'	7.28	123.46	114.00
2	X	1	U	N1-C2-N3	7.21	119.23	114.90
1	A	509	A	C2'-C3'-O3'	7.20	125.34	109.50
1	A	372	C	C2'-C3'-O3'	6.93	124.80	113.70
1	A	30	U	C2'-C3'-O3'	6.64	124.32	113.70
1	A	266	G	C2'-C3'-O3'	6.47	124.06	113.70
1	A	460	A	N9-C1'-C2'	6.42	122.35	114.00
1	A	266	G	N9-C1'-C2'	6.38	122.29	114.00
1	A	960	U	C2'-C3'-O3'	6.30	123.78	113.70
20	S	72	GLY	N-CA-C	-6.30	97.36	113.10
1	A	1380	U	C2'-C3'-O3'	6.28	123.75	113.70
1	A	5	U	N1-C1'-C2'	6.19	122.05	114.00
1	A	328	C	C2'-C3'-O3'	6.12	123.50	113.70
1	A	197	A	C2'-C3'-O3'	6.02	123.33	113.70
1	A	1067	A	C2'-C3'-O3'	5.97	123.25	113.70
1	A	1504	G	C2'-C3'-O3'	5.95	123.22	113.70
11	J	60	ARG	N-CA-C	5.88	126.88	111.00
1	A	1124	G	N9-C1'-C2'	5.67	121.37	114.00
1	A	533	A	N9-C1'-C2'	5.61	121.30	114.00
1	A	63	C	C5'-C4'-C3'	-5.50	107.20	116.00
20	S	54	GLY	N-CA-C	-5.41	99.59	113.10
16	O	45	VAL	N-CA-C	-5.38	96.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	G	O4'-C1'-N9	5.32	112.46	108.20
18	Q	67	LYS	N-CA-C	-5.30	96.67	111.00
1	A	1065	U	C1'-O4'-C4'	-5.27	105.68	109.90
1	A	913	A	OP2-P-O3'	5.23	116.71	105.20
1	A	115	G	C4'-C3'-C2'	5.19	107.79	102.60
1	A	1528	U	C4'-C3'-O3'	5.18	123.35	113.00
1	A	687	A	C2'-C3'-O3'	5.17	121.98	113.70
1	A	618	C	C5'-C4'-C3'	5.12	124.20	116.00
2	X	1	U	N1-C2-O2	-5.09	119.23	122.80
1	A	107	G	N9-C1'-C2'	-5.08	106.41	112.00
13	L	26	ALA	N-CA-C	-5.07	97.30	111.00
1	A	244	U	C5'-C4'-C3'	-5.03	107.94	116.00
1	A	1502	A	N9-C1'-C2'	5.01	120.51	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	559	A	C3'
1	A	1498	U	C3'
1	A	1528	U	C3'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	G	Sidechain
1	A	1048	G	Sidechain
1	A	1077	G	Sidechain
1	A	1079	G	Sidechain
1	A	108	G	Sidechain
1	A	1085	U	Sidechain
1	A	1094	G	Sidechain
1	A	1226	C	Sidechain
1	A	1281	U	Sidechain
1	A	1301	U	Sidechain
1	A	1316	G	Sidechain
1	A	1390	U	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	197	A	Sidechain
1	A	222	U	Sidechain
1	A	251	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	266	G	Sidechain
1	A	274	A	Sidechain
1	A	290	C	Sidechain
1	A	297	G	Sidechain
1	A	356	A	Sidechain
1	A	401	C	Sidechain
1	A	481	G	Sidechain
1	A	535	A	Sidechain
1	A	561	U	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	603	U	Sidechain
1	A	641	U	Sidechain
1	A	691	G	Sidechain
1	A	727	G	Sidechain
1	A	748	C	Sidechain
1	A	76	C	Sidechain
1	A	868	C	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	942	G	Sidechain

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	A	32391	0	16348	1037	0
2	X	117	0	63	0	0
3	B	1923	0	1968	208	0
4	C	1612	0	1677	188	0
5	D	1703	0	1763	128	0
6	E	1146	0	1207	104	0
7	F	843	0	857	74	0
8	G	1257	0	1296	108	0
9	H	1116	0	1177	75	0
10	I	1011	0	1043	104	0
11	J	792	0	835	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	885	0	904	68	0
13	L	975	0	1062	90	0
14	M	997	0	1072	113	0
15	N	492	0	529	67	0
16	O	734	0	771	34	0
17	P	700	0	720	45	0
18	Q	857	0	930	88	0
19	R	597	0	668	83	0
20	S	674	0	699	72	0
21	T	762	0	859	73	0
22	V	208	0	221	22	0
23	A	42	0	45	4	0
24	A	94	0	0	0	0
24	D	1	0	0	0	0
24	H	1	0	0	0	0
25	A	23	0	24	2	0
26	A	40	0	37	5	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	51995	0	36775	2610	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 29.

All (2610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:A:H4'	1:A:244:U:H5'	1.30	1.13
5:D:23:GLY:HA3	5:D:112:VAL:HG12	1.31	1.12
11:J:51:ARG:HB2	11:J:59:SER:HB3	1.27	1.11
12:K:54:ARG:HB3	12:K:54:ARG:HH11	1.13	1.09
1:A:761:G:C2	18:Q:105:ALA:HA	1.88	1.08
4:C:191:THR:HG22	4:C:193:TYR:H	1.14	1.08
3:B:77:ALA:HB2	3:B:211:ILE:HD13	1.18	1.06
18:Q:97:SER:HB2	18:Q:103:GLY:HA2	1.26	1.06
4:C:157:ILE:HD13	4:C:166:GLU:HG2	1.35	1.06
14:M:10:PRO:HB2	14:M:18:ALA:HB1	1.35	1.06
20:S:33:THR:HG22	20:S:35:SER:H	1.20	1.05
5:D:156:GLU:HG2	5:D:160:GLN:HE21	1.19	1.04
13:L:60:LEU:HD11	13:L:85:ILE:HD12	1.39	1.03
1:A:761:G:H1'	18:Q:104:LYS:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:40:ILE:HD13	20:S:62:ILE:HD13	1.38	1.01
3:B:84:GLU:HB3	3:B:219:VAL:HG21	1.41	1.00
13:L:27:LEU:O	13:L:29:GLY:N	1.94	0.99
21:T:74:LYS:HG2	21:T:75:ASN:H	1.26	0.99
1:A:1305:G:O2'	1:A:1306:A:H8	1.44	0.98
1:A:761:G:H4'	18:Q:103:GLY:N	1.77	0.98
1:A:1250:A:H4'	10:I:68:GLY:H	1.29	0.97
20:S:55:LYS:HG2	20:S:56:GLN:HE21	1.28	0.97
4:C:3:ASN:HD22	4:C:3:ASN:N	1.58	0.97
11:J:49:VAL:HG13	15:N:41:ARG:HB2	1.44	0.97
3:B:91:PRO:HG3	3:B:154:LEU:HB2	1.41	0.97
1:A:1256:A:H4'	1:A:1257:U:H5'	1.46	0.95
13:L:47:LYS:HB3	13:L:48:PRO:HD3	1.44	0.95
1:A:187:C:N3	21:T:105:SER:HB3	1.82	0.94
1:A:1044:A:H2'	1:A:1045:C:H5'	1.48	0.94
1:A:1443:G:H5"	1:A:1446:A:C5'	1.96	0.94
19:R:55:ARG:HH11	19:R:55:ARG:HA	1.29	0.94
13:L:38:THR:HG22	13:L:39:VAL:HG23	1.50	0.94
1:A:1117:G:H4'	10:I:104:ARG:NH1	1.81	0.93
1:A:1443:G:H5"	1:A:1446:A:H5'	1.50	0.93
3:B:102:LEU:HD21	3:B:162:ILE:HD11	1.48	0.93
1:A:839:U:H5'	1:A:840:C:C5	2.02	0.93
12:K:54:ARG:O	12:K:57:THR:HG22	1.69	0.93
6:E:12:LEU:HD13	6:E:31:LEU:HB2	1.49	0.93
1:A:975:A:H5'	1:A:975:A:H8	1.30	0.92
12:K:54:ARG:HB3	12:K:54:ARG:NH1	1.83	0.92
22:V:6:ARG:HD3	22:V:15:ARG:NH2	1.83	0.92
1:A:1226:C:H1'	20:S:83:HIS:NE2	1.84	0.92
3:B:130:ARG:HB3	3:B:131:PRO:HD2	1.53	0.91
18:Q:67:LYS:HA	18:Q:70:ARG:HH12	1.35	0.91
1:A:1101:A:H4'	1:A:1102:A:O5'	1.68	0.91
1:A:1279:A:H5"	1:A:1280:A:OP1	1.72	0.90
1:A:351:G:H4'	1:A:352:C:OP1	1.68	0.90
1:A:839:U:H5'	1:A:840:C:H5	1.35	0.90
1:A:1250:A:H4'	10:I:68:GLY:N	1.86	0.90
5:D:23:GLY:HA3	5:D:112:VAL:CG1	2.02	0.89
18:Q:97:SER:CB	18:Q:103:GLY:HA2	2.02	0.89
3:B:178:ARG:HH11	3:B:178:ARG:HG3	1.34	0.89
12:K:18:ARG:HB2	12:K:33:THR:HG22	1.54	0.89
4:C:47:LEU:HD21	4:C:68:VAL:HG11	1.54	0.89
18:Q:21:VAL:HG21	18:Q:59:ILE:HD11	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:86:VAL:HG12	19:R:87:ARG:H	1.35	0.89
1:A:371:G:O2'	1:A:372:C:H5'	1.71	0.89
1:A:975:A:H5'	1:A:975:A:C8	2.07	0.89
20:S:43:GLU:H	20:S:43:GLU:CD	1.74	0.89
18:Q:104:LYS:HE3	18:Q:104:LYS:HA	1.53	0.88
7:F:36:ARG:HH12	7:F:38:GLU:HG2	1.34	0.88
4:C:157:ILE:CD1	4:C:166:GLU:HG2	2.02	0.88
1:A:664:G:H22	1:A:741:G:H1	1.19	0.88
16:O:87:ILE:HG22	16:O:88:ARG:H	1.36	0.88
19:R:55:ARG:HA	19:R:55:ARG:NH1	1.89	0.88
3:B:15:VAL:HG13	3:B:209:ARG:HG3	1.54	0.88
6:E:80:ILE:HD11	6:E:91:LEU:HD12	1.56	0.88
20:S:15:LEU:HA	20:S:18:LYS:HB3	1.56	0.88
3:B:197:VAL:HB	3:B:200:ILE:HG12	1.57	0.87
10:I:93:ARG:HD3	10:I:97:LYS:HZ2	1.40	0.87
1:A:371:G:C2'	1:A:372:C:H5'	2.05	0.87
1:A:761:G:N3	18:Q:105:ALA:HA	1.88	0.86
1:A:1086:U:H3	1:A:1099:G:H22	1.23	0.86
7:F:94:GLN:HE21	19:R:32:ARG:HD3	1.38	0.86
19:R:53:ARG:HH11	19:R:59:SER:HA	1.40	0.86
1:A:992:U:H4'	1:A:993:G:O5'	1.76	0.86
5:D:151:LYS:H	5:D:151:LYS:HD2	1.40	0.86
11:J:19:SER:HB2	11:J:91:PRO:HG2	1.58	0.86
5:D:153:ARG:HG2	5:D:181:MET:SD	2.16	0.85
1:A:235:C:H5'	18:Q:70:ARG:HG2	1.57	0.85
1:A:1195:C:H3'	1:A:1196:U:H5"	1.58	0.85
12:K:40:ILE:HG22	12:K:41:THR:HG23	1.57	0.85
4:C:34:LEU:HG	15:N:25:VAL:HG11	1.57	0.85
1:A:438:G:H4'	1:A:439:A:OP1	1.77	0.85
1:A:1305:G:HO2'	1:A:1306:A:H8	0.88	0.85
3:B:18:GLY:HA2	3:B:41:ILE:HA	1.58	0.85
1:A:1502:A:H2	1:A:1505:G:H1	1.22	0.85
1:A:1364:U:O2'	1:A:1365:G:H5"	1.76	0.84
1:A:447:G:H2'	1:A:485:G:N2	1.93	0.84
1:A:112:G:H21	1:A:354:G:H5'	1.43	0.84
14:M:4:ILE:HD13	14:M:56:LEU:HD22	1.58	0.84
1:A:1223:C:P	20:S:78:ARG:HH12	2.00	0.83
8:G:113:GLU:HG2	8:G:119:ARG:HG2	1.58	0.83
1:A:1226:C:H4'	1:A:1227:A:OP1	1.79	0.83
1:A:1305:G:H5'	22:V:4:GLY:HA3	1.59	0.83
3:B:57:PHE:O	3:B:60:ASP:HB3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:81:LEU:HD23	14:M:82:MET:N	1.94	0.83
19:R:47:THR:HA	19:R:83:GLU:HB2	1.60	0.83
1:A:1278:U:H5"	1:A:1279:A:H5'	1.61	0.82
18:Q:104:LYS:HG3	18:Q:105:ALA:H	1.44	0.82
11:J:3:LYS:HG2	11:J:75:ILE:HG23	1.60	0.82
14:M:22:ILE:HD12	14:M:25:ILE:HD12	1.59	0.82
20:S:72:GLY:C	20:S:74:PHE:H	1.82	0.82
11:J:39:PRO:HA	11:J:70:ARG:HH11	1.43	0.82
1:A:1307:U:H5'	14:M:109:THR:HG21	1.62	0.82
1:A:1502:A:H2	1:A:1505:G:N1	1.77	0.81
10:I:118:LYS:O	10:I:119:ALA:HB3	1.80	0.81
21:T:67:ALA:HA	21:T:73:HIS:H	1.43	0.81
1:A:173:U:H5'	1:A:197:A:O4'	1.80	0.81
1:A:838:G:H2'	1:A:839:U:H5"	1.61	0.81
1:A:1152:A:H5"	11:J:13:HIS:CD2	2.16	0.81
12:K:48:ILE:HG22	12:K:49:GLY:H	1.46	0.81
5:D:150:GLU:H	5:D:150:GLU:CD	1.83	0.81
12:K:19:ALA:HB2	12:K:80:VAL:HG11	1.61	0.81
3:B:128:GLU:HA	3:B:135:GLN:HE22	1.43	0.80
13:L:47:LYS:CB	13:L:48:PRO:HD3	2.11	0.80
16:O:78:TYR:CZ	16:O:82:ILE:HD11	2.15	0.80
1:A:1054:C:O2'	1:A:1055:A:H5"	1.81	0.80
1:A:1131:G:H1	1:A:1143:G:H21	1.28	0.80
7:F:86:ARG:O	7:F:87:ARG:HG2	1.81	0.80
13:L:46:LYS:HD2	13:L:47:LYS:HD2	1.63	0.80
21:T:74:LYS:HG2	21:T:75:ASN:N	1.96	0.80
6:E:12:LEU:CD1	6:E:31:LEU:HB2	2.11	0.80
11:J:49:VAL:O	11:J:60:ARG:O	1.99	0.80
6:E:41:VAL:HG22	6:E:113:ALA:HA	1.62	0.80
3:B:18:GLY:CA	3:B:41:ILE:HA	2.11	0.80
1:A:243:A:C4'	1:A:244:U:H5'	2.10	0.80
21:T:73:HIS:O	21:T:74:LYS:HD3	1.82	0.80
3:B:97:TRP:HZ3	3:B:176:GLU:OE2	1.65	0.80
21:T:10:LEU:HD11	21:T:12:ALA:HB3	1.64	0.79
21:T:10:LEU:HD13	21:T:12:ALA:H	1.48	0.79
18:Q:59:ILE:CG2	18:Q:71:PHE:HB3	2.13	0.79
14:M:8:GLU:HG3	14:M:22:ILE:HG23	1.65	0.79
1:A:502:G:H4'	1:A:550:G:H4'	1.63	0.79
4:C:126:ARG:O	4:C:127:ARG:HB2	1.83	0.79
1:A:130:A:OP2	1:A:190(E):U:H2'	1.83	0.79
7:F:100:ASN:HD22	19:R:23:LYS:HG2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:41:ARG:HG2	13:L:42:THR:H	1.48	0.79
1:A:243:A:H4'	1:A:244:U:C5'	2.12	0.78
16:O:26:GLU:OE1	16:O:77:ARG:HD2	1.83	0.78
1:A:80:G:H3'	1:A:81:U:H5"	1.64	0.78
1:A:112:G:N2	1:A:354:G:H5'	1.97	0.78
3:B:15:VAL:CG1	3:B:209:ARG:HG3	2.13	0.78
4:C:35:GLU:HG3	4:C:95:THR:HG21	1.65	0.78
8:G:78:ARG:NH1	8:G:154:TYR:HB3	1.98	0.78
1:A:1094:G:H5"	1:A:1095:U:H5	1.48	0.78
1:A:1044:A:C2'	1:A:1045:C:H5'	2.13	0.78
1:A:1231:G:O3'	10:I:126:SER:HB3	1.83	0.78
19:R:76:LEU:O	19:R:78:LEU:HG	1.82	0.78
1:A:382:A:H2'	1:A:383:A:C8	2.18	0.78
1:A:974:A:OP1	15:N:31:ARG:HG2	1.84	0.78
11:J:30:SER:OG	11:J:81:THR:HA	1.83	0.77
15:N:26:ARG:NH1	15:N:47:LEU:HG	1.98	0.77
20:S:40:ILE:HG21	20:S:62:ILE:HD11	1.67	0.77
1:A:818:G:C3'	1:A:819:A:H5"	2.15	0.77
1:A:1064:G:H4'	1:A:1065:U:H5"	1.66	0.77
3:B:7:VAL:HG11	3:B:221:LEU:HD23	1.66	0.77
4:C:110:ASN:ND2	4:C:140:ARG:HB3	1.99	0.77
5:D:199:GLN:HE21	5:D:201:ASN:H	1.30	0.77
13:L:83:VAL:HG22	13:L:84:LEU:N	2.00	0.76
12:K:48:ILE:HD11	12:K:64:ALA:N	2.00	0.76
15:N:27:CYS:SG	15:N:29:ARG:HB2	2.26	0.76
1:A:1021:G:H2'	1:A:1022:G:O4'	1.85	0.76
5:D:31:CYS:O	5:D:33:MET:N	2.19	0.76
8:G:59:LEU:O	8:G:63:LYS:HG2	1.84	0.76
4:C:174:PRO:HB2	4:C:177:THR:HG22	1.66	0.76
1:A:1142:G:H2'	1:A:1143:G:O4'	1.85	0.76
12:K:57:THR:HG23	12:K:60:ALA:H	1.51	0.76
1:A:173:U:H5"	1:A:197:A:H5'	1.68	0.76
1:A:1137:C:H4'	1:A:1138:G:C2	2.20	0.76
8:G:54:THR:HG22	8:G:56:GLN:H	1.51	0.76
12:K:13:GLN:HA	12:K:75:TYR:O	1.86	0.76
1:A:1016:A:H2'	1:A:1017:G:O4'	1.86	0.76
5:D:162:LEU:HD22	5:D:178:VAL:HG13	1.68	0.75
22:V:6:ARG:HD3	22:V:15:ARG:HH22	1.50	0.75
1:A:1366:C:H2'	1:A:1367:C:H6	1.51	0.75
3:B:166:ASP:OD2	3:B:169:LYS:HB2	1.86	0.75
1:A:579:G:H5'	1:A:728:A:H1'	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:U:O2	1:A:839:U:H2'	1.87	0.75
1:A:761:G:H4'	18:Q:103:GLY:H	1.51	0.75
5:D:162:LEU:HD13	5:D:181:MET:HG2	1.68	0.75
8:G:5:ARG:H	8:G:5:ARG:HD2	1.51	0.75
3:B:12:GLU:HG2	3:B:213:LEU:HD11	1.68	0.75
3:B:114:ARG:NH1	3:B:118:LEU:HD21	2.01	0.75
7:F:2:ARG:NE	7:F:69:GLU:HG2	2.02	0.75
1:A:761:G:C1'	18:Q:104:LYS:O	2.34	0.75
1:A:1117:G:H4'	10:I:104:ARG:HH11	1.50	0.75
14:M:13:LYS:HA	14:M:44:ARG:HH12	1.50	0.75
1:A:250:A:H4'	1:A:251:G:O5'	1.87	0.75
4:C:47:LEU:HD11	4:C:76:VAL:HG22	1.68	0.75
4:C:179:ARG:HD3	4:C:206:GLU:HG2	1.69	0.75
6:E:15:ARG:O	6:E:27:ARG:O	2.05	0.75
6:E:10:MET:SD	6:E:13:ILE:HG23	2.26	0.74
4:C:131:ARG:HG2	4:C:135:LYS:HE3	1.69	0.74
5:D:3:ARG:HD2	5:D:69:GLY:O	1.86	0.74
9:H:113:SER:HB2	9:H:134:ILE:HD11	1.67	0.74
6:E:51:VAL:HB	6:E:52:PRO:HD3	1.69	0.74
10:I:97:LYS:CG	10:I:102:LEU:HD12	2.16	0.74
13:L:45:PRO:HG3	13:L:53:ARG:HD3	1.70	0.74
20:S:5:LEU:O	20:S:6:LYS:HB2	1.86	0.74
1:A:1256:A:C4'	1:A:1257:U:H5'	2.18	0.74
3:B:84:GLU:OE1	3:B:216:SER:HA	1.87	0.74
1:A:474:G:H2'	1:A:475:G:H8	1.50	0.74
1:A:382:A:H2'	1:A:383:A:H8	1.53	0.74
5:D:156:GLU:HG2	5:D:160:GLN:NE2	1.98	0.74
12:K:77:MET:HE3	12:K:80:VAL:HG22	1.68	0.74
1:A:677:U:H3	1:A:713:G:H22	1.35	0.74
1:A:1278:U:H5"	1:A:1279:A:C5'	2.18	0.74
3:B:208:ILE:HD12	3:B:242:ALA:CB	2.18	0.74
7:F:94:GLN:NE2	19:R:32:ARG:HD3	2.02	0.74
13:L:75:HIS:HD2	13:L:77:LEU:H	1.36	0.74
4:C:3:ASN:N	4:C:3:ASN:ND2	2.31	0.74
10:I:127:LYS:HB2	14:M:126:LYS:NZ	2.02	0.73
4:C:6:HIS:CD2	4:C:8:ILE:HB	2.22	0.73
7:F:43:LEU:HD22	7:F:43:LEU:H	1.53	0.73
15:N:9:LYS:HE3	15:N:21:TYR:O	1.87	0.73
1:A:1443:G:H5"	1:A:1446:A:H5"	1.69	0.73
1:A:80:G:C3'	1:A:81:U:H5"	2.18	0.73
1:A:1116:C:H2'	1:A:1117:G:H5"	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:45:HIS:NE2	18:Q:47:PRO:HG3	2.02	0.73
14:M:5:ALA:HB3	14:M:8:GLU:HG3	1.71	0.73
1:A:187:C:C2	21:T:105:SER:HB3	2.22	0.73
3:B:142:LEU:HB3	3:B:146:GLN:HE21	1.53	0.73
5:D:170:VAL:HG13	5:D:174:LEU:HB2	1.70	0.73
7:F:61:LEU:O	7:F:62:TRP:HB2	1.88	0.73
1:A:328:C:O2	1:A:328:C:H2'	1.87	0.73
1:A:761:G:H1'	18:Q:104:LYS:C	2.10	0.73
5:D:98:GLU:HG2	5:D:189:PRO:HG3	1.71	0.73
13:L:24:VAL:O	13:L:24:VAL:HG12	1.88	0.73
5:D:108:LEU:HD13	5:D:183:GLY:HA3	1.69	0.72
1:A:975:A:H4'	1:A:976:G:O5'	1.87	0.72
5:D:26:CYS:HA	5:D:31:CYS:HB2	1.70	0.72
14:M:40:ASN:HD22	14:M:41:PRO:HD2	1.54	0.72
19:R:36:ASN:O	19:R:39:VAL:HG12	1.89	0.72
10:I:11:LYS:O	10:I:11:LYS:HG2	1.90	0.72
19:R:53:ARG:NH1	19:R:59:SER:HA	2.03	0.72
1:A:447:G:H2'	1:A:485:G:H22	1.50	0.72
1:A:1216:G:H5"	15:N:5:ALA:CB	2.20	0.72
1:A:1356:G:H2'	1:A:1357:A:C8	2.24	0.72
11:J:39:PRO:O	11:J:40:LEU:HB2	1.88	0.72
4:C:5:ILE:O	4:C:5:ILE:HD12	1.90	0.72
4:C:13:GLY:HA3	15:N:57:ARG:NH2	2.05	0.72
5:D:23:GLY:CA	5:D:112:VAL:HG12	2.17	0.72
6:E:31:LEU:HD22	6:E:43:LEU:HD21	1.72	0.72
16:O:87:ILE:HG22	16:O:88:ARG:N	2.02	0.72
7:F:101:ALA:HA	19:R:28:GLU:HB3	1.70	0.72
19:R:36:ASN:ND2	19:R:38:GLU:HG2	2.03	0.72
4:C:77:ILE:HG22	4:C:81:GLY:HA2	1.71	0.72
1:A:1075:C:H5'	3:B:103:THR:HG21	1.71	0.71
10:I:69:GLY:O	10:I:73:GLN:HG3	1.90	0.71
14:M:13:LYS:HA	14:M:44:ARG:NH1	2.04	0.71
1:A:1236:A:H4'	1:A:1304:G:H4'	1.69	0.71
1:A:657:G:H4'	16:O:28:GLN:HG2	1.72	0.71
1:A:1285:A:H4'	1:A:1286:A:O5'	1.90	0.71
5:D:151:LYS:HD2	5:D:151:LYS:N	2.06	0.71
8:G:69:VAL:HG21	8:G:104:LEU:HD21	1.73	0.71
13:L:70:ILE:HD13	13:L:77:LEU:HD12	1.70	0.71
1:A:581:G:O2'	18:Q:105:ALA:CB	2.38	0.71
1:A:818:G:H3'	1:A:819:A:H5"	1.71	0.71
8:G:50:ILE:O	8:G:54:THR:HB	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:90:LEU:HB2	11:J:91:PRO:HD3	1.72	0.71
13:L:70:ILE:HG12	13:L:100:ILE:HD12	1.72	0.71
18:Q:67:LYS:CA	18:Q:70:ARG:HH12	2.02	0.71
3:B:73:THR:HG23	3:B:95:GLN:O	1.90	0.71
9:H:120:THR:OG1	9:H:123:GLU:HG3	1.91	0.71
1:A:1281:U:H4'	1:A:1282:C:OP2	1.91	0.71
4:C:58:GLU:HB3	11:J:92:THR:HG21	1.72	0.71
14:M:3:ARG:HA	14:M:8:GLU:O	1.90	0.71
3:B:142:LEU:HB3	3:B:146:GLN:NE2	2.05	0.71
4:C:101:LEU:HD22	4:C:102:ASN:H	1.55	0.70
11:J:49:VAL:HG11	15:N:41:ARG:O	1.91	0.70
1:A:1015:A:H2'	1:A:1016:A:C8	2.25	0.70
6:E:80:ILE:HD11	6:E:91:LEU:HB2	1.72	0.70
14:M:40:ASN:HD22	14:M:41:PRO:CD	2.04	0.70
15:N:11:LYS:C	15:N:13:THR:H	1.94	0.70
1:A:1365:G:H5'	1:A:1365:G:H8	1.54	0.70
4:C:52:LEU:N	4:C:52:LEU:HD23	2.07	0.70
1:A:518:C:O2'	13:L:50:SER:HB3	1.92	0.70
6:E:144:THR:HG22	6:E:146:ALA:H	1.55	0.70
16:O:4:THR:OG1	16:O:7:GLU:HG3	1.91	0.70
1:A:452:A:HO2'	1:A:453:A:H8	1.35	0.70
1:A:1031:G:H2'	1:A:1032:G:H8	1.57	0.70
1:A:1144:G:N2	1:A:1146:A:H62	1.90	0.70
1:A:1315:U:H5	20:S:6:LYS:HZ1	1.38	0.70
11:J:80:LYS:HD3	11:J:83:GLU:HB3	1.73	0.70
1:A:1132:C:H2'	1:A:1133:G:H8	1.56	0.70
3:B:59:GLU:CG	3:B:221:LEU:HD11	2.22	0.70
4:C:23:TYR:O	4:C:24:ALA:O	2.10	0.70
1:A:353:A:H5'	1:A:353:A:H8	1.56	0.70
11:J:78:ASN:O	11:J:80:LYS:N	2.25	0.70
1:A:434:U:H2'	1:A:435:C:C6	2.26	0.70
1:A:1329:A:P	14:M:28:ALA:HB3	2.32	0.70
14:M:34:LEU:HD13	14:M:41:PRO:HA	1.74	0.70
20:S:41:VAL:HG23	20:S:43:GLU:HG2	1.74	0.70
1:A:522:C:H41	13:L:53:ARG:HH22	1.38	0.70
3:B:12:GLU:OE1	3:B:12:GLU:HA	1.91	0.70
3:B:16:HIS:NE2	3:B:214:ILE:HG12	2.05	0.70
1:A:35:G:H2'	1:A:36:C:C6	2.27	0.69
1:A:393:A:O2'	1:A:394:G:H5'	1.90	0.69
1:A:1281:U:H5'	1:A:1282:C:H5	1.57	0.69
1:A:1391:U:H2'	1:A:1392:G:C8	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:81:LEU:HD23	14:M:82:MET:H	1.56	0.69
8:G:86:GLN:HA	8:G:86:GLN:HE21	1.56	0.69
18:Q:59:ILE:HG22	18:Q:71:PHE:CD1	2.27	0.69
22:V:5:ASP:O	22:V:11:GLY:HA3	1.92	0.69
1:A:1035:A:H2'	1:A:1036:G:H8	1.56	0.69
1:A:1053:G:H4'	1:A:1054:C:H5'	1.74	0.69
1:A:1072:G:H2'	1:A:1073:U:C6	2.27	0.69
8:G:121:ALA:O	8:G:125:MET:HG3	1.92	0.69
21:T:89:ARG:HH22	21:T:106:ALA:HA	1.57	0.69
3:B:208:ILE:HD12	3:B:242:ALA:HB1	1.75	0.69
8:G:78:ARG:HB2	8:G:156:TRP:CZ3	2.27	0.69
1:A:1128:C:H1'	1:A:1146:A:H61	1.57	0.69
1:A:135:C:O2	17:P:1:MET:HB2	1.91	0.69
3:B:59:GLU:HG2	3:B:221:LEU:HD11	1.74	0.69
3:B:224:GLN:HG2	3:B:225:ALA:N	2.07	0.69
4:C:30:ARG:HG2	4:C:30:ARG:HH11	1.57	0.69
4:C:53:ALA:O	4:C:54:ARG:HB2	1.92	0.69
1:A:1112:C:O2	4:C:179:ARG:HB3	1.93	0.69
3:B:178:ARG:HG3	3:B:178:ARG:NH1	2.02	0.69
8:G:122:HIS:HA	8:G:125:MET:HE2	1.75	0.69
10:I:8:GLY:HA2	10:I:79:LEU:HD13	1.73	0.69
16:O:16:ALA:HB1	16:O:21:ASP:HB3	1.73	0.69
1:A:190(F):G:H4'	1:A:190(G):G:OP2	1.92	0.68
1:A:838:G:C2'	1:A:839:U:H5"	2.22	0.68
1:A:1163:C:H2'	1:A:1164:G:H8	1.58	0.68
6:E:80:ILE:CD1	6:E:91:LEU:HB2	2.22	0.68
4:C:15:THR:O	4:C:16:ARG:HB2	1.93	0.68
10:I:93:ARG:HD3	10:I:97:LYS:NZ	2.08	0.68
14:M:50:GLU:O	14:M:54:VAL:HG23	1.94	0.68
5:D:25:ARG:C	5:D:27:TYR:H	1.95	0.68
1:A:840:C:H5'	1:A:848:C:O2	1.93	0.68
1:A:1053:G:HO2'	1:A:1199:U:H5	1.42	0.68
1:A:1366:C:H2'	1:A:1367:C:C6	2.29	0.68
3:B:9:GLU:HB2	3:B:217:ARG:HH12	1.57	0.68
3:B:25:ASN:HD22	3:B:27:LYS:H	1.41	0.68
5:D:191:ARG:O	5:D:191:ARG:HD2	1.94	0.68
1:A:1066:C:O2'	1:A:1067:A:H5'	1.93	0.68
1:A:429:U:H2'	5:D:25:ARG:HH12	1.58	0.68
1:A:1116:C:C2'	1:A:1117:G:H5"	2.22	0.68
14:M:54:VAL:O	14:M:58:GLU:HG2	1.94	0.68
1:A:701:C:H5'	1:A:703:G:O4'	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:38:ARG:HH11	4:C:38:ARG:HG3	1.58	0.68
4:C:174:PRO:O	4:C:177:THR:HG22	1.94	0.68
8:G:110:GLN:HA	8:G:110:GLN:NE2	2.09	0.68
12:K:80:VAL:HG21	12:K:103:LEU:HD13	1.76	0.68
8:G:12:LEU:H	8:G:12:LEU:HD12	1.59	0.68
3:B:69:LEU:HD12	3:B:155:LEU:HD11	1.76	0.68
11:J:61:GLU:OE1	15:N:45:ARG:NH1	2.25	0.68
13:L:81:SER:O	13:L:82:VAL:HB	1.94	0.68
17:P:34:GLU:OE2	17:P:55:ARG:HD3	1.93	0.68
1:A:1193:G:O2'	1:A:1194:U:H5'	1.94	0.67
3:B:121:LEU:HD21	3:B:130:ARG:NH2	2.08	0.67
18:Q:24:GLU:OE2	18:Q:37:LYS:HD3	1.95	0.67
20:S:16:LEU:O	20:S:19:VAL:HG12	1.94	0.67
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.95	0.67
4:C:150:LYS:HE2	4:C:152:ILE:HD11	1.75	0.67
1:A:1201:A:H4'	1:A:1202:G:O5'	1.94	0.67
1:A:1225:A:H5'	1:A:1226:C:OP2	1.95	0.67
5:D:61:LYS:HD2	5:D:207:TYR:OH	1.93	0.67
3:B:72:GLY:HA3	3:B:81:VAL:HG21	1.76	0.67
4:C:188:LEU:HD13	4:C:195:VAL:HG13	1.76	0.67
15:N:23:ARG:HA	15:N:29:ARG:O	1.93	0.67
1:A:429:U:H2'	5:D:25:ARG:NH1	2.09	0.67
20:S:40:ILE:HG21	20:S:62:ILE:CD1	2.24	0.67
1:A:794:A:H2'	1:A:795:C:C6	2.29	0.67
1:A:979:C:H2'	1:A:980:C:H5'	1.74	0.67
1:A:1044:A:H2'	1:A:1045:C:C5'	2.23	0.67
3:B:17:PHE:HD1	3:B:18:GLY:N	1.91	0.67
20:S:72:GLY:O	20:S:74:PHE:N	2.28	0.67
6:E:118:ILE:HG22	6:E:119:LEU:N	2.10	0.67
7:F:14:LEU:HA	7:F:18:GLN:NE2	2.10	0.67
14:M:59:TYR:O	14:M:63:THR:HG22	1.94	0.67
21:T:10:LEU:CD1	21:T:12:ALA:HB3	2.24	0.67
1:A:760:G:C6	18:Q:104:LYS:O	2.46	0.67
1:A:538:G:P	13:L:115:LYS:HG3	2.34	0.67
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.25	0.67
1:A:1004:A:H5"	1:A:1025:U:C4	2.30	0.67
4:C:47:LEU:CD2	4:C:68:VAL:HG11	2.24	0.67
4:C:134:ILE:O	4:C:138:VAL:HG23	1.95	0.67
8:G:38:LEU:HD12	8:G:38:LEU:O	1.95	0.67
1:A:17:U:H2'	1:A:18:C:C6	2.30	0.66
1:A:80:G:H2'	1:A:81:U:H5"	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:A:N7	4:C:161:GLU:HB2	2.10	0.66
1:A:1128:C:O2'	1:A:1130:A:N7	2.27	0.66
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.66
4:C:48:TYR:HA	4:C:52:LEU:HD22	1.76	0.66
4:C:191:THR:HB	4:C:194:GLY:O	1.95	0.66
1:A:972:C:O5'	11:J:57:LYS:HD2	1.96	0.66
4:C:10:PHE:CZ	4:C:178:LEU:HD13	2.30	0.66
8:G:23:VAL:O	8:G:27:ILE:HG13	1.94	0.66
20:S:13:ASP:HA	20:S:16:LEU:HB3	1.77	0.66
21:T:70:SER:HA	21:T:73:HIS:CD2	2.31	0.66
26:A:1634:SRY:H61	13:L:47:LYS:HD3	1.78	0.66
7:F:4:TYR:CZ	7:F:72:VAL:HG21	2.31	0.66
9:H:119:LEU:HB3	9:H:123:GLU:HB2	1.78	0.66
13:L:47:LYS:HB3	13:L:48:PRO:CD	2.19	0.66
3:B:204:ASN:C	3:B:204:ASN:HD22	1.99	0.66
4:C:52:LEU:HD23	4:C:52:LEU:H	1.61	0.66
1:A:1130:A:H3'	1:A:1130:A:OP2	1.95	0.66
1:A:1182:G:H4'	1:A:1183:A:O5'	1.94	0.66
1:A:1392:G:H21	1:A:1502:A:H8	1.41	0.66
8:G:72:ARG:HG2	8:G:142:GLU:OE1	1.96	0.66
1:A:1125:U:H3	11:J:5:ARG:NH2	1.93	0.66
6:E:116:THR:HG23	6:E:117:ASP:OD2	1.96	0.66
9:H:64:LYS:HG3	9:H:79:VAL:HG21	1.77	0.66
21:T:46:GLU:HG2	21:T:48:LYS:NZ	2.11	0.66
1:A:269:C:H2'	1:A:270:A:C8	2.30	0.66
13:L:83:VAL:HG22	13:L:84:LEU:H	1.59	0.66
19:R:47:THR:HG23	19:R:83:GLU:H	1.59	0.66
21:T:50:GLU:HB3	21:T:54:LYS:HE3	1.76	0.66
3:B:76:GLN:NE2	3:B:207:ALA:H	1.93	0.66
5:D:13:ARG:HD2	5:D:38:TYR:O	1.95	0.66
11:J:59:SER:O	11:J:60:ARG:HB2	1.94	0.66
20:S:51:VAL:HG23	20:S:75:ALA:HB2	1.77	0.66
3:B:7:VAL:O	3:B:8:LYS:HB2	1.94	0.66
1:A:255:G:H1'	18:Q:16:GLN:NE2	2.10	0.66
6:E:8:GLU:HG2	6:E:34:VAL:HG22	1.76	0.66
11:J:6:ILE:HG12	11:J:98:ILE:HG12	1.78	0.66
1:A:646:U:H2'	1:A:647:C:C6	2.30	0.65
1:A:109:A:H2'	1:A:326:G:N2	2.11	0.65
1:A:1163:C:H2'	1:A:1164:G:C8	2.31	0.65
3:B:121:LEU:HD21	3:B:130:ARG:HH22	1.61	0.65
5:D:114:ARG:HH11	5:D:114:ARG:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:28:LYS:HD2	13:L:33:ARG:HH12	1.60	0.65
13:L:47:LYS:HA	13:L:47:LYS:HE3	1.78	0.65
15:N:44:LEU:HD12	15:N:44:LEU:O	1.96	0.65
21:T:76:ALA:O	21:T:80:ARG:HG2	1.96	0.65
1:A:581:G:O2'	18:Q:105:ALA:HB1	1.96	0.65
18:Q:104:LYS:HE3	18:Q:104:LYS:CA	2.25	0.65
1:A:270:A:H2'	1:A:271:C:C6	2.32	0.65
14:M:15:VAL:HG23	14:M:43:THR:O	1.97	0.65
19:R:51:LEU:HB3	19:R:55:ARG:HB2	1.77	0.65
1:A:761:G:C4'	18:Q:103:GLY:H	2.09	0.65
4:C:177:THR:HG23	4:C:180:ALA:HB2	1.78	0.65
5:D:25:ARG:HH21	5:D:30:LYS:HD3	1.60	0.65
1:A:353:A:H5'	1:A:353:A:C8	2.31	0.65
1:A:1495:U:H2'	1:A:1496:C:H6	1.62	0.65
4:C:7:PRO:HG2	4:C:184:TYR:HB2	1.79	0.65
7:F:23:LYS:O	7:F:27:GLN:HG2	1.96	0.65
3:B:12:GLU:HG2	3:B:213:LEU:CD1	2.26	0.65
18:Q:97:SER:OG	18:Q:98:LEU:N	2.29	0.65
3:B:10:LEU:HB3	3:B:48:MET:SD	2.36	0.65
13:L:47:LYS:CB	13:L:48:PRO:CD	2.74	0.65
1:A:424:G:O2'	1:A:425:G:H5'	1.97	0.65
3:B:143:GLU:O	3:B:147:LYS:HG3	1.96	0.65
10:I:97:LYS:HG3	10:I:102:LEU:HD12	1.78	0.65
1:A:1352:C:H2'	1:A:1353:G:C8	2.32	0.65
12:K:48:ILE:HG22	12:K:49:GLY:N	2.12	0.65
14:M:52:GLU:HG2	14:M:55:ARG:HH21	1.60	0.65
1:A:969:A:H61	14:M:126:LYS:HB2	1.62	0.64
3:B:178:ARG:NH2	9:H:68:ARG:HH22	1.94	0.64
11:J:35:SER:HB2	11:J:73:ASP:HB3	1.79	0.64
11:J:69:ASN:O	11:J:70:ARG:HD3	1.97	0.64
3:B:204:ASN:ND2	3:B:206:ASP:H	1.95	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.62	0.64
6:E:76:ILE:HG23	6:E:77:PRO:HD2	1.77	0.64
6:E:80:ILE:CD1	6:E:91:LEU:HD12	2.27	0.64
10:I:97:LYS:N	10:I:98:PRO:HD2	2.12	0.64
11:J:9:ARG:HB3	11:J:9:ARG:NH1	2.11	0.64
12:K:48:ILE:HD13	12:K:63:LEU:HB2	1.79	0.64
1:A:141:A:H1'	1:A:182:U:O2	1.96	0.64
1:A:1038:C:H2'	1:A:1039:C:C6	2.33	0.64
1:A:1218:C:H2'	1:A:1219:U:C6	2.32	0.64
1:A:1296:C:H4'	1:A:1302:U:C5	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:GLN:HA	3:B:113:HIS:HD2	1.62	0.64
10:I:97:LYS:HG2	10:I:102:LEU:HD12	1.78	0.64
20:S:72:GLY:C	20:S:74:PHE:N	2.50	0.64
1:A:254:G:OP1	18:Q:67:LYS:O	2.15	0.64
1:A:1347:G:N2	1:A:1373:G:H2'	2.12	0.64
1:A:1441:G:H4'	1:A:1442:G:C5	2.32	0.64
4:C:52:LEU:H	4:C:52:LEU:CD2	2.10	0.64
7:F:44:GLY:HA2	7:F:59:TYR:CE1	2.33	0.64
8:G:72:ARG:HH22	8:G:138:LYS:NZ	1.95	0.64
10:I:4:TYR:CE2	10:I:88:TYR:HA	2.33	0.64
19:R:86:VAL:HG12	19:R:87:ARG:N	2.11	0.64
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.32	0.64
1:A:551:U:H2'	1:A:552:U:C6	2.32	0.64
1:A:1425:U:H2'	1:A:1426:C:C6	2.33	0.64
9:H:60:ARG:HH11	9:H:60:ARG:HG3	1.62	0.64
1:A:357:G:O2'	1:A:358:U:H5'	1.98	0.64
1:A:1064:G:H4'	1:A:1065:U:C5'	2.27	0.64
1:A:1236:A:H2'	1:A:1237:C:C6	2.33	0.64
1:A:1396:A:H4'	1:A:1397:C:H5"	1.80	0.64
4:C:101:LEU:CD2	4:C:102:ASN:H	2.11	0.64
21:T:73:HIS:C	21:T:74:LYS:HD3	2.16	0.64
3:B:77:ALA:HB2	3:B:211:ILE:CD1	2.11	0.64
1:A:1221:G:O3'	20:S:77:THR:HG21	1.98	0.64
21:T:57:ARG:HH21	21:T:102:GLY:HA3	1.63	0.64
1:A:1443:G:C5'	1:A:1446:A:H5'	2.25	0.63
4:C:191:THR:HG21	4:C:193:TYR:CZ	2.33	0.63
10:I:70:LYS:O	10:I:74:ILE:HG13	1.97	0.63
13:L:75:HIS:CD2	13:L:77:LEU:H	2.15	0.63
21:T:56:MET:HE3	21:T:88:VAL:HG11	1.78	0.63
22:V:12:LYS:HB3	22:V:22:ARG:HD2	1.79	0.63
1:A:156:G:O2'	1:A:157:G:H5'	1.98	0.63
1:A:923:A:OP1	6:E:21:ALA:HB2	1.98	0.63
1:A:1030(C):G:H2'	1:A:1030(D):A:H8	1.61	0.63
6:E:76:ILE:HD13	6:E:142:LEU:HD11	1.81	0.63
10:I:8:GLY:HA2	10:I:79:LEU:HB3	1.79	0.63
1:A:918:A:H2'	1:A:919:A:C8	2.33	0.63
1:A:1319:A:H5'	1:A:1320:C:OP1	1.98	0.63
4:C:5:ILE:HD13	4:C:10:PHE:HB2	1.81	0.63
14:M:37:THR:HG22	14:M:39:ILE:HD11	1.79	0.63
19:R:45:SER:C	19:R:47:THR:H	2.02	0.63
1:A:405:U:H3'	1:A:406:G:H5'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:G:O2'	1:A:854:G:H5'	1.99	0.63
1:A:1132:C:H2'	1:A:1133:G:C8	2.32	0.63
1:A:1497:G:C2'	1:A:1498:U:H5'	2.29	0.63
5:D:64:LEU:HD23	5:D:198:VAL:HG21	1.80	0.63
10:I:118:LYS:O	10:I:119:ALA:CB	2.46	0.63
1:A:80:G:H3'	1:A:81:U:C5'	2.28	0.63
1:A:1127:G:H1	1:A:1145:C:H42	1.46	0.63
1:A:164:U:H2'	1:A:165:C:H6	1.60	0.63
1:A:418:C:H2'	1:A:419:C:H6	1.64	0.63
1:A:1238:A:H5'	1:A:1336:C:H41	1.62	0.63
1:A:1495:U:H2'	1:A:1496:C:C6	2.33	0.63
9:H:38:ILE:N	9:H:38:ILE:HD12	2.14	0.63
1:A:959:A:H3'	1:A:960:U:H5"	1.81	0.63
3:B:25:ASN:HD22	3:B:25:ASN:C	2.00	0.63
4:C:139:GLN:O	4:C:143:GLU:N	2.26	0.63
6:E:115:VAL:CG1	6:E:118:ILE:HG13	2.29	0.63
14:M:77:ASN:O	14:M:81:LEU:HD22	1.98	0.63
16:O:17:ARG:HG3	16:O:17:ARG:HH11	1.64	0.63
1:A:812:C:O2'	1:A:813:U:P	2.56	0.63
1:A:939:G:H5"	8:G:102:ARG:NH2	2.13	0.63
1:A:1306:A:N6	1:A:1331:G:H1'	2.14	0.63
1:A:1499:A:O2'	1:A:1500:A:H5'	1.99	0.63
1:A:1149:C:H2'	1:A:1150:U:C6	2.34	0.62
5:D:61:LYS:NZ	5:D:62:GLN:NE2	2.47	0.62
1:A:1128:C:H4'	10:I:16:ARG:HH12	1.64	0.62
1:A:1257:U:H4'	1:A:1258:G:O5'	1.98	0.62
3:B:27:LYS:HD3	3:B:195:ASP:OD2	1.99	0.62
7:F:82:ARG:HA	7:F:82:ARG:HE	1.64	0.62
8:G:58:PRO:HG2	8:G:59:LEU:H	1.64	0.62
1:A:397:A:H5'	1:A:398:C:OP1	1.99	0.62
1:A:840:C:H5"	1:A:841:U:OP1	1.99	0.62
1:A:865:A:H5'	1:A:1078:U:O4	1.99	0.62
1:A:1263:C:H2'	1:A:1264:C:C6	2.35	0.62
10:I:98:PRO:HG2	10:I:99:LEU:HD22	1.82	0.62
11:J:12:ASP:O	11:J:15:THR:HG22	1.99	0.62
6:E:115:VAL:HG11	6:E:118:ILE:CD1	2.29	0.62
7:F:2:ARG:CZ	7:F:69:GLU:HG2	2.29	0.62
11:J:15:THR:HG23	11:J:94:VAL:HG22	1.79	0.62
1:A:80:G:C2'	1:A:81:U:H5"	2.28	0.62
1:A:190(L):U:N3	21:T:105:SER:OG	2.31	0.62
1:A:993:G:H4'	1:A:994:A:OP2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:10:LEU:HD11	7:F:59:TYR:HD2	1.65	0.62
13:L:86:ARG:HH11	13:L:86:ARG:HG3	1.63	0.62
1:A:1241:G:H2'	1:A:1242:C:C6	2.34	0.62
12:K:33:THR:HG1	12:K:38:ASN:C	2.01	0.62
14:M:23:TYR:HB3	14:M:67:GLU:HA	1.82	0.62
17:P:81:ARG:HG3	17:P:83:GLU:HG2	1.82	0.62
1:A:664:G:OP1	19:R:64:ARG:HD2	2.00	0.62
15:N:9:LYS:HD3	15:N:9:LYS:C	2.20	0.62
21:T:59:ALA:O	21:T:63:ILE:HG13	1.99	0.62
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.62
7:F:43:LEU:HD22	7:F:43:LEU:N	2.14	0.62
1:A:190(L):U:H3	21:T:105:SER:HG	1.46	0.62
7:F:15:ASP:H	7:F:18:GLN:NE2	1.97	0.62
18:Q:9:VAL:HG21	18:Q:84:LEU:HD13	1.80	0.62
21:T:73:HIS:HB3	21:T:74:LYS:HD2	1.82	0.62
1:A:1158:C:H5"	3:B:133:LYS:HE3	1.81	0.61
1:A:1479:C:H2'	1:A:1480:G:H8	1.65	0.61
5:D:8:VAL:HG12	5:D:21:LEU:CD1	2.30	0.61
14:M:81:LEU:O	14:M:86:CYS:HB3	2.00	0.61
15:N:22:THR:O	15:N:23:ARG:HB2	2.00	0.61
1:A:1049:U:C5	15:N:2:ALA:N	2.69	0.61
1:A:1392:G:N2	1:A:1502:A:H8	1.98	0.61
5:D:17:VAL:HG12	5:D:18:LYS:N	2.15	0.61
7:F:36:ARG:NH1	7:F:38:GLU:HG2	2.11	0.61
19:R:25:THR:O	19:R:26:LEU:HB2	2.00	0.61
1:A:948:C:OP1	14:M:109:THR:HG22	1.99	0.61
3:B:17:PHE:CD1	3:B:18:GLY:N	2.68	0.61
5:D:151:LYS:H	5:D:151:LYS:CD	2.12	0.61
10:I:46:ALA:HB2	10:I:74:ILE:HG23	1.82	0.61
8:G:22:LEU:HD21	8:G:66:VAL:HG21	1.82	0.61
14:M:59:TYR:C	14:M:63:THR:HG22	2.20	0.61
1:A:1223:C:OP1	1:A:1224:G:H3'	2.00	0.61
5:D:170:VAL:CG1	5:D:174:LEU:HB2	2.31	0.61
5:D:176:LEU:HD12	5:D:182:LYS:O	1.99	0.61
8:G:106:GLN:O	8:G:110:GLN:HG2	2.00	0.61
13:L:60:LEU:HD21	13:L:66:VAL:HG22	1.82	0.61
21:T:26:ASN:HB3	21:T:71:THR:HG23	1.83	0.61
1:A:266:G:O3'	18:Q:67:LYS:HB2	2.01	0.61
4:C:52:LEU:HD21	4:C:118:GLN:HE22	1.66	0.61
11:J:80:LYS:HA	11:J:83:GLU:CB	2.31	0.61
13:L:113:ARG:HB2	13:L:122:THR:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:U:OP1	19:R:64:ARG:NH2	2.33	0.61
1:A:1305:G:N2	1:A:1331:G:O2'	2.33	0.61
26:A:1634:SRY:H631	26:A:1634:SRY:HN31	1.66	0.61
6:E:120:THR:HG23	6:E:121:LYS:N	2.15	0.61
6:E:150:ARG:HG3	6:E:150:ARG:HH11	1.64	0.61
1:A:474:G:H2'	1:A:475:G:C8	2.35	0.61
1:A:915:A:H2'	1:A:916:G:H5'	1.82	0.61
3:B:97:TRP:CZ3	3:B:176:GLU:OE2	2.50	0.61
4:C:3:ASN:O	4:C:4:LYS:HB2	2.01	0.61
4:C:195:VAL:HG12	4:C:196:LEU:N	2.15	0.61
1:A:1133:G:H2'	1:A:1134:G:H8	1.64	0.61
1:A:1256:A:H2	1:A:1258:G:C2	2.18	0.61
1:A:1303:C:H2'	1:A:1304:G:H5'	1.83	0.61
1:A:1428:A:H2'	1:A:1429:C:C6	2.36	0.61
1:A:1475:G:H2'	1:A:1476:G:H8	1.66	0.61
4:C:180:ALA:HB1	4:C:203:PHE:CE1	2.36	0.61
13:L:24:VAL:HG13	13:L:98:TYR:CE2	2.35	0.61
5:D:30:LYS:O	5:D:32:ALA:N	2.34	0.61
5:D:156:GLU:CG	5:D:160:GLN:HE21	2.05	0.61
9:H:91:ARG:HG2	13:L:7:ILE:HG21	1.81	0.61
18:Q:26:GLN:O	18:Q:27:PHE:HB3	2.01	0.61
1:A:818:G:H3'	1:A:819:A:C5'	2.31	0.60
1:A:1203:C:OP1	15:N:2:ALA:N	2.34	0.60
1:A:1230:C:H1'	14:M:126:LYS:HA	1.83	0.60
3:B:111:ARG:HB3	3:B:149:LEU:HD11	1.84	0.60
3:B:219:VAL:HG12	3:B:223:ILE:HD13	1.82	0.60
6:E:11:ILE:HB	6:E:31:LEU:HB3	1.81	0.60
1:A:309:G:H1'	1:A:608:A:C2	2.37	0.60
1:A:559:A:OP1	6:E:126:ARG:NH2	2.33	0.60
18:Q:95:TYR:O	18:Q:97:SER:N	2.35	0.60
19:R:21:LYS:HD2	19:R:21:LYS:N	2.14	0.60
20:S:15:LEU:HD22	20:S:49:ILE:HD13	1.83	0.60
3:B:204:ASN:HB3	3:B:210:SER:OG	2.02	0.60
4:C:180:ALA:O	4:C:181:ASN:HB3	2.00	0.60
1:A:189:G:H2'	1:A:190:C:C6	2.36	0.60
1:A:617:G:H5'	17:P:45:THR:HG22	1.84	0.60
1:A:765:G:H1	1:A:812:C:H2'	1.66	0.60
1:A:1106:G:H5"	4:C:172:ARG:HG2	1.82	0.60
1:A:1343:G:H2'	1:A:1344:C:C6	2.36	0.60
4:C:157:ILE:HD13	4:C:166:GLU:CG	2.20	0.60
8:G:78:ARG:HB2	8:G:156:TRP:CH2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:G:OP1	18:Q:68:ARG:HB3	2.01	0.60
3:B:73:THR:HB	3:B:170:GLU:OE2	2.01	0.60
8:G:78:ARG:HH11	8:G:154:TYR:HB3	1.66	0.60
9:H:6:ILE:HD12	9:H:35:ILE:CD1	2.32	0.60
13:L:89:ARG:HA	13:L:97:ARG:HA	1.82	0.60
18:Q:97:SER:CB	18:Q:103:GLY:CA	2.77	0.60
1:A:31:G:N1	1:A:48:C:H5"	2.16	0.60
1:A:190(K):G:H2'	1:A:190(L):U:H6	1.66	0.60
1:A:613:C:O2'	1:A:614:A:H5'	2.02	0.60
1:A:1369:C:H2'	1:A:1370:G:C8	2.36	0.60
3:B:91:PRO:HG3	3:B:154:LEU:CB	2.23	0.60
8:G:86:GLN:HA	8:G:86:GLN:NE2	2.16	0.60
1:A:538:G:OP2	13:L:115:LYS:HG3	2.01	0.60
1:A:1116:C:H2'	1:A:1117:G:C5'	2.32	0.60
1:A:1420:C:H2'	1:A:1421:G:H8	1.66	0.60
6:E:45:PHE:CE2	6:E:47:LYS:HE3	2.37	0.60
10:I:50:LEU:HD23	10:I:85:LEU:HD11	1.82	0.60
13:L:33:ARG:HE	13:L:62:SER:HB3	1.65	0.60
1:A:913:A:H4'	1:A:914:A:O5'	2.01	0.60
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.36	0.60
1:A:1286:A:H4'	22:V:25:LYS:HE3	1.84	0.60
3:B:71:VAL:HG12	3:B:170:GLU:HG2	1.84	0.60
5:D:148:VAL:HG11	5:D:158:ILE:HG21	1.84	0.60
8:G:145:ALA:C	8:G:147:ALA:H	2.05	0.60
10:I:127:LYS:HB2	14:M:126:LYS:HZ1	1.63	0.60
11:J:80:LYS:HA	11:J:83:GLU:HB3	1.83	0.60
14:M:26:GLY:O	14:M:28:ALA:N	2.34	0.60
14:M:44:ARG:HB2	14:M:47:ASP:OD2	2.02	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.37	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.37	0.60
4:C:121:ALA:O	4:C:125:GLU:HG3	2.01	0.60
6:E:13:ILE:HA	6:E:29:GLY:O	2.02	0.60
9:H:91:ARG:HG3	13:L:7:ILE:HG13	1.84	0.60
9:H:103:VAL:HG21	9:H:109:ILE:O	2.01	0.60
14:M:6:GLY:O	14:M:7:VAL:HG22	2.02	0.60
1:A:513:C:O2'	1:A:514:C:H5'	2.02	0.60
1:A:673:G:H2'	1:A:674:G:C8	2.36	0.60
1:A:913:A:O2'	1:A:914:A:P	2.60	0.60
3:B:110:GLN:HA	3:B:113:HIS:CD2	2.37	0.60
6:E:75:THR:HG23	6:E:76:ILE:N	2.17	0.60
6:E:115:VAL:HG11	6:E:118:ILE:HG13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:34:VAL:HG22	11:J:74:ILE:HG12	1.84	0.60
14:M:5:ALA:HB3	14:M:8:GLU:CG	2.32	0.60
1:A:123:C:OP1	1:A:312:C:H5'	2.02	0.59
1:A:1033:G:H2'	1:A:1034:G:H8	1.66	0.59
5:D:119:GLN:HG2	5:D:123:HIS:CD2	2.37	0.59
10:I:3:GLN:HG3	10:I:20:ARG:HG2	1.84	0.59
11:J:3:LYS:N	11:J:77:PRO:HD3	2.17	0.59
12:K:54:ARG:HH11	12:K:54:ARG:CB	2.03	0.59
15:N:25:VAL:HG23	15:N:38:GLY:O	2.02	0.59
20:S:51:VAL:CG2	20:S:75:ALA:HB2	2.31	0.59
1:A:412:A:H4'	1:A:413:G:H8	1.66	0.59
1:A:1035:A:H2'	1:A:1036:G:C8	2.36	0.59
1:A:1145:C:O2'	1:A:1146:A:H8	1.84	0.59
1:A:1365:G:H5'	1:A:1365:G:C8	2.37	0.59
4:C:96:GLY:O	4:C:98:ASN:N	2.33	0.59
4:C:174:PRO:HB2	4:C:177:THR:CG2	2.31	0.59
6:E:102:ALA:HB1	6:E:120:THR:HG21	1.83	0.59
10:I:26:VAL:HB	10:I:33:PHE:HB2	1.83	0.59
15:N:9:LYS:HD3	15:N:9:LYS:O	2.01	0.59
20:S:36:ARG:HH12	20:S:75:ALA:HB3	1.67	0.59
1:A:168:G:O2'	1:A:169:C:H5'	2.02	0.59
11:J:8:LEU:HD22	11:J:96:ILE:HG12	1.84	0.59
11:J:45:ARG:HH11	11:J:45:ARG:HG3	1.66	0.59
12:K:48:ILE:HD11	12:K:64:ALA:CA	2.32	0.59
14:M:49:THR:HG22	14:M:52:GLU:H	1.68	0.59
1:A:1117:G:H5'	1:A:1117:G:H8	1.67	0.59
1:A:1368:G:O2'	1:A:1369:C:H5'	2.02	0.59
6:E:92:LYS:HB3	6:E:119:LEU:HB2	1.85	0.59
1:A:1498:U:H4'	1:A:1519:A:C2	2.37	0.59
4:C:134:ILE:HG22	4:C:168:ALA:HB3	1.85	0.59
8:G:23:VAL:HG12	8:G:27:ILE:HD11	1.84	0.59
13:L:119:LYS:O	13:L:120:TYR:HB2	2.02	0.59
1:A:575:G:OP1	1:A:575:G:H4'	2.02	0.59
1:A:954:G:H21	1:A:1227:A:H62	1.51	0.59
3:B:103:THR:HB	3:B:176:GLU:OE1	2.03	0.59
1:A:8:A:C6	5:D:209:ARG:HB2	2.37	0.59
1:A:31:G:H1	1:A:48:C:H5"	1.67	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.37	0.59
1:A:582:U:C6	18:Q:105:ALA:OXT	2.55	0.59
1:A:1196:U:OP1	1:A:1197:G:H5'	2.02	0.59
1:A:1405:G:OP2	23:A:1545:PAR:O34	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:122:GLU:HG2	6:E:131:ILE:HD12	1.84	0.59
7:F:19:LEU:C	7:F:19:LEU:HD23	2.23	0.59
12:K:67:ASP:OD1	12:K:71:LYS:HE3	2.02	0.59
13:L:83:VAL:CG2	13:L:84:LEU:N	2.66	0.59
1:A:484:G:H4'	1:A:485:G:O5'	2.02	0.59
1:A:518:C:H5"	1:A:519:C:C6	2.38	0.59
1:A:551:U:H2'	1:A:552:U:H6	1.67	0.59
1:A:1381:U:O2'	1:A:1382:C:H5'	2.03	0.59
3:B:212:GLN:HG3	3:B:239:VAL:CG2	2.32	0.59
4:C:35:GLU:CG	4:C:95:THR:HG21	2.33	0.59
5:D:3:ARG:CZ	5:D:71:SER:H	2.16	0.59
1:A:1527:C:O2'	1:A:1528:U:H5'	2.03	0.59
3:B:74:LYS:HD3	3:B:76:GLN:HB2	1.85	0.59
5:D:8:VAL:HG12	5:D:21:LEU:HD13	1.85	0.59
9:H:4:ASP:OD2	9:H:7:ALA:HB2	2.02	0.59
11:J:30:SER:CB	11:J:84:GLN:HE21	2.16	0.59
12:K:48:ILE:HD13	12:K:63:LEU:CB	2.32	0.59
13:L:83:VAL:HG21	13:L:100:ILE:CG2	2.32	0.59
20:S:53:ASN:HD22	20:S:53:ASN:N	2.01	0.59
21:T:39:LYS:CD	21:T:55:ILE:HD13	2.33	0.59
1:A:1151:A:HO2'	1:A:1152:A:H8	1.49	0.58
1:A:1257:U:O2'	1:A:1258:G:OP2	2.21	0.58
11:J:4:ILE:CG2	11:J:98:ILE:HG23	2.33	0.58
13:L:83:VAL:CG2	13:L:84:LEU:H	2.16	0.58
13:L:111:LYS:O	13:L:112:ASP:HB2	2.01	0.58
17:P:28:ARG:HG3	17:P:29:ASP:OD2	2.02	0.58
1:A:946:A:H2'	1:A:947:G:C8	2.38	0.58
4:C:14:ILE:HG22	4:C:15:THR:H	1.68	0.58
19:R:46:GLU:H	19:R:46:GLU:CD	2.05	0.58
20:S:20:LEU:HA	20:S:23:ASN:HD22	1.66	0.58
21:T:79:ARG:HH11	21:T:79:ARG:HG3	1.68	0.58
1:A:1230:C:O2'	14:M:126:LYS:HG2	2.03	0.58
4:C:13:GLY:HA3	15:N:57:ARG:CZ	2.33	0.58
4:C:30:ARG:HG2	4:C:30:ARG:NH1	2.18	0.58
4:C:147:LYS:HE2	4:C:205:GLY:HA2	1.86	0.58
14:M:37:THR:HG22	14:M:39:ILE:CD1	2.34	0.58
20:S:9:VAL:CG1	20:S:39:THR:HG21	2.33	0.58
1:A:620:C:N1	5:D:135:LEU:HD13	2.18	0.58
5:D:173:TRP:CD2	5:D:189:PRO:HB3	2.38	0.58
6:E:93:PRO:HG2	9:H:105:ARG:HH21	1.67	0.58
13:L:45:PRO:HD3	13:L:51:ALA:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:G:H4'	1:A:429:U:O5'	2.03	0.58
1:A:1250:A:H5"	10:I:67:GLY:C	2.24	0.58
3:B:132:LYS:O	3:B:136:VAL:HG23	2.04	0.58
4:C:14:ILE:O	4:C:16:ARG:N	2.36	0.58
4:C:119:ARG:HH12	4:C:126:ARG:NH2	2.00	0.58
4:C:191:THR:HG21	4:C:193:TYR:CE1	2.39	0.58
5:D:4:TYR:O	5:D:5:ILE:HB	2.02	0.58
12:K:126:ARG:O	12:K:127:LYS:HB2	2.03	0.58
17:P:26:ARG:HE	17:P:31:LYS:HB3	1.69	0.58
20:S:45:VAL:HA	20:S:62:ILE:HG13	1.85	0.58
1:A:421:U:H4'	1:A:422:C:OP2	2.02	0.58
1:A:1040:U:H2'	1:A:1041:A:C8	2.38	0.58
11:J:5:ARG:HG3	11:J:73:ASP:OD1	2.04	0.58
11:J:28:ARG:HH12	11:J:33:GLN:HB3	1.67	0.58
1:A:407:G:H2'	1:A:408:A:H8	1.69	0.58
1:A:443:C:O2'	1:A:444:C:H5'	2.03	0.58
4:C:3:ASN:HD22	4:C:3:ASN:H	1.43	0.58
1:A:438:G:C4'	1:A:439:A:OP1	2.50	0.58
1:A:533:A:H2'	1:A:535:A:OP2	2.03	0.58
1:A:1108:G:H4'	1:A:1191:A:O4'	2.03	0.58
1:A:1325:C:O3'	22:V:17:THR:HG21	2.04	0.58
3:B:126:GLU:HA	3:B:129:GLU:OE2	2.03	0.58
4:C:147:LYS:HE2	4:C:205:GLY:CA	2.34	0.58
7:F:101:ALA:HA	19:R:28:GLU:CB	2.34	0.58
1:A:1033:G:H2'	1:A:1034:G:C8	2.39	0.58
1:A:1136:U:H5"	1:A:1137:C:OP2	2.04	0.58
1:A:1195:C:C3'	1:A:1196:U:H5"	2.32	0.58
1:A:1238:A:H5'	1:A:1336:C:N4	2.19	0.58
4:C:34:LEU:HD23	4:C:34:LEU:O	2.04	0.58
7:F:10:LEU:HD12	7:F:59:TYR:HB3	1.86	0.58
10:I:48:GLU:N	10:I:49:PRO:HD2	2.19	0.58
14:M:39:ILE:HD12	14:M:52:GLU:HB3	1.85	0.58
18:Q:10:VAL:O	18:Q:53:LEU:HD12	2.04	0.58
18:Q:66:SER:O	18:Q:70:ARG:NH1	2.36	0.58
19:R:71:LYS:O	19:R:74:ARG:HB2	2.04	0.58
1:A:107:G:H2'	1:A:108:G:H5'	1.84	0.57
1:A:476:G:O2'	1:A:477:G:H5'	2.03	0.57
8:G:114:ARG:HG2	8:G:114:ARG:HH11	1.69	0.57
9:H:116:LYS:HZ3	9:H:127:LEU:HD12	1.67	0.57
19:R:21:LYS:HB3	19:R:57:GLY:HA3	1.85	0.57
20:S:15:LEU:O	20:S:19:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:52:TYR:HA	20:S:56:GLN:O	2.04	0.57
1:A:112:G:H21	1:A:354:G:C5'	2.14	0.57
1:A:411:A:C4	1:A:413:G:H1'	2.39	0.57
1:A:620:C:H2'	1:A:621:A:O4'	2.03	0.57
1:A:1025:U:H2'	1:A:1026:G:C8	2.38	0.57
4:C:91:LEU:HD23	4:C:91:LEU:C	2.24	0.57
10:I:9:ARG:HG3	10:I:14:VAL:HG13	1.85	0.57
21:T:11:SER:C	21:T:13:LEU:H	2.07	0.57
1:A:99:C:H2'	1:A:101:A:C8	2.39	0.57
1:A:1014:A:H2'	1:A:1015:A:C8	2.38	0.57
3:B:39:ILE:HG22	3:B:41:ILE:H	1.68	0.57
4:C:123:GLN:HE22	4:C:140:ARG:HH22	1.52	0.57
8:G:110:GLN:HA	8:G:110:GLN:HE21	1.68	0.57
1:A:15:G:H21	6:E:18:ARG:HA	1.70	0.57
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.85	0.57
3:B:218:ALA:O	3:B:222:ILE:HG13	2.04	0.57
4:C:126:ARG:HD2	4:C:128:PHE:CE1	2.39	0.57
11:J:30:SER:HB3	11:J:84:GLN:HE21	1.69	0.57
1:A:1392:G:O2'	1:A:1502:A:H5"	2.03	0.57
4:C:177:THR:HG23	4:C:177:THR:O	2.04	0.57
6:E:12:LEU:HD22	6:E:12:LEU:C	2.24	0.57
6:E:102:ALA:HB2	6:E:120:THR:HB	1.86	0.57
9:H:10:LEU:HD23	9:H:83:ILE:HD11	1.87	0.57
10:I:8:GLY:CA	10:I:79:LEU:HB3	2.34	0.57
1:A:761:G:C4	18:Q:105:ALA:O	2.58	0.57
1:A:812:C:O2'	1:A:813:U:OP2	2.23	0.57
1:A:1497:G:H2'	1:A:1498:U:H5'	1.86	0.57
6:E:79:GLU:CD	6:E:79:GLU:H	2.08	0.57
10:I:7:THR:O	10:I:15:ALA:O	2.22	0.57
16:O:17:ARG:HD3	16:O:26:GLU:OE2	2.04	0.57
21:T:10:LEU:HD13	21:T:12:ALA:N	2.16	0.57
1:A:1241:G:H2'	1:A:1242:C:H6	1.69	0.57
4:C:107:GLN:O	4:C:108:ASN:HB3	2.04	0.57
17:P:43:LYS:HG3	17:P:48:TRP:CD2	2.39	0.57
1:A:113:G:H1'	1:A:354:G:H5'	1.85	0.57
1:A:149:A:H2'	1:A:150:C:C6	2.40	0.57
1:A:301:G:O2'	1:A:302:G:H5'	2.04	0.57
1:A:614:A:H2'	1:A:615:C:C6	2.39	0.57
1:A:982:U:H5"	15:N:6:LEU:HD11	1.86	0.57
1:A:1251:A:H2'	1:A:1252:A:C8	2.40	0.57
4:C:195:VAL:O	4:C:196:LEU:HD22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:72:ARG:HH22	8:G:138:LYS:HZ1	1.52	0.57
18:Q:59:ILE:HG22	18:Q:71:PHE:HB3	1.86	0.57
1:A:52:G:O2'	1:A:53:A:H5'	2.04	0.57
1:A:269:C:H2'	1:A:270:A:H8	1.67	0.57
1:A:581:G:H1'	18:Q:105:ALA:HB1	1.87	0.57
1:A:737:A:H1'	7:F:73:ASN:ND2	2.20	0.57
1:A:1086:U:H3	1:A:1099:G:N2	1.98	0.57
11:J:6:ILE:O	11:J:71:LEU:O	2.23	0.57
1:A:321:A:O2'	1:A:322:C:H5'	2.05	0.57
10:I:56:LEU:C	10:I:58:ARG:H	2.07	0.57
20:S:20:LEU:HA	20:S:23:ASN:ND2	2.19	0.57
1:A:107:G:C2'	1:A:108:G:H5'	2.34	0.56
1:A:191:G:C4	21:T:105:SER:HB2	2.39	0.56
3:B:188:ALA:O	3:B:202:PRO:HA	2.05	0.56
4:C:6:HIS:HD2	4:C:8:ILE:H	1.53	0.56
11:J:3:LYS:HA	11:J:75:ILE:HA	1.85	0.56
14:M:117:VAL:HG12	14:M:118:ALA:N	2.19	0.56
15:N:3:ARG:CZ	15:N:6:LEU:HG	2.35	0.56
1:A:435:C:H2'	1:A:436:C:H6	1.69	0.56
1:A:953:G:H1'	14:M:125:ARG:HA	1.87	0.56
1:A:1237:C:H2'	1:A:1336:C:C5	2.39	0.56
1:A:1250:A:H5"	10:I:68:GLY:N	2.20	0.56
3:B:102:LEU:HD21	3:B:162:ILE:CD1	2.31	0.56
6:E:81:GLU:HG2	6:E:90:VAL:HG13	1.87	0.56
6:E:105:VAL:HB	6:E:106:PRO:HD3	1.86	0.56
13:L:53:ARG:N	13:L:53:ARG:HD2	2.19	0.56
17:P:45:THR:HB	17:P:46:PRO:HD2	1.85	0.56
20:S:5:LEU:O	20:S:6:LYS:CB	2.51	0.56
1:A:448:A:OP2	1:A:485:G:N2	2.35	0.56
1:A:519:C:H2'	1:A:520:A:C8	2.41	0.56
1:A:760:G:O6	18:Q:105:ALA:C	2.44	0.56
1:A:1216:G:H5"	15:N:5:ALA:HB2	1.87	0.56
5:D:8:VAL:C	5:D:10:ARG:H	2.07	0.56
6:E:74:GLY:HA3	6:E:116:THR:HG22	1.87	0.56
13:L:24:VAL:HG13	13:L:98:TYR:HE2	1.70	0.56
1:A:547:A:H4'	1:A:548:G:O5'	2.04	0.56
4:C:148:GLY:HA3	4:C:172:ARG:O	2.06	0.56
11:J:75:ILE:O	11:J:76:ASN:HB2	2.06	0.56
14:M:40:ASN:HD22	14:M:40:ASN:C	2.08	0.56
1:A:216:G:H2'	1:A:217:C:C6	2.40	0.56
1:A:412:A:H4'	1:A:413:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:C:O2'	1:A:1491:G:H5'	2.06	0.56
13:L:115:LYS:O	13:L:117:ARG:HG3	2.06	0.56
14:M:37:THR:HG23	14:M:55:ARG:HB3	1.86	0.56
1:A:222:U:H2'	1:A:223:U:C6	2.41	0.56
6:E:15:ARG:HD3	6:E:26:PHE:HB3	1.87	0.56
20:S:63:THR:HG22	20:S:64:GLU:N	2.21	0.56
1:A:490:G:H2'	1:A:491:G:H8	1.69	0.56
1:A:1229:A:OP2	14:M:114:ARG:HD3	2.06	0.56
1:A:1305:G:H22	1:A:1331:G:H2'	1.68	0.56
6:E:47:LYS:N	6:E:47:LYS:HD2	2.20	0.56
18:Q:24:GLU:CD	18:Q:37:LYS:HD3	2.26	0.56
1:A:1521:G:H2'	1:A:1522:U:C6	2.41	0.56
3:B:215:LEU:O	3:B:219:VAL:HG23	2.06	0.56
6:E:120:THR:CG2	6:E:121:LYS:N	2.69	0.56
9:H:65:TYR:HA	9:H:79:VAL:HG23	1.88	0.56
14:M:11:ARG:HG2	14:M:12:ASN:N	2.21	0.56
3:B:108:ILE:O	3:B:108:ILE:HG22	2.05	0.56
5:D:60:GLU:OE1	5:D:60:GLU:HA	2.04	0.56
9:H:83:ILE:HG23	9:H:83:ILE:O	2.06	0.56
12:K:27:ASN:C	12:K:27:ASN:HD22	2.08	0.56
14:M:88:ARG:HA	14:M:98:VAL:HG13	1.87	0.56
15:N:41:ARG:HG2	15:N:41:ARG:HH11	1.71	0.56
19:R:73:ALA:HB3	19:R:79:LEU:HD12	1.87	0.56
20:S:5:LEU:O	20:S:6:LYS:HE3	2.06	0.56
3:B:17:PHE:HB3	3:B:44:LEU:HD11	1.88	0.56
6:E:81:GLU:HG2	6:E:90:VAL:HG22	1.87	0.56
10:I:127:LYS:HB2	14:M:126:LYS:HZ3	1.71	0.56
11:J:8:LEU:CD2	11:J:96:ILE:HG12	2.36	0.56
21:T:82:SER:O	21:T:86:ARG:HB2	2.06	0.56
1:A:76:C:O2'	1:A:77:G:H5'	2.06	0.55
1:A:1305:G:C5'	22:V:4:GLY:HA3	2.34	0.55
19:R:19:LYS:H	19:R:19:LYS:HD3	1.70	0.55
1:A:344:A:H5"	1:A:345:C:H5	1.70	0.55
1:A:352:C:H4'	1:A:354:G:OP1	2.05	0.55
1:A:1157:A:H4'	1:A:1158:C:O5'	2.06	0.55
1:A:1168:A:H2'	1:A:1169:A:C8	2.41	0.55
3:B:25:ASN:ND2	3:B:27:LYS:H	2.03	0.55
5:D:199:GLN:HE21	5:D:201:ASN:N	2.00	0.55
8:G:143:ARG:O	8:G:147:ALA:HB2	2.06	0.55
12:K:82:VAL:HG23	12:K:105:VAL:HG13	1.89	0.55
15:N:60:SER:O	15:N:61:TRP:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:8:ARG:HB2	17:P:28:ARG:NH1	2.21	0.55
1:A:706:A:H1'	12:K:29:ILE:HD11	1.88	0.55
1:A:1499:A:H1'	1:A:1520:G:H5'	1.87	0.55
7:F:14:LEU:HA	7:F:18:GLN:HE21	1.69	0.55
13:L:43:VAL:HG12	13:L:93:LEU:HD22	1.89	0.55
1:A:566:G:H4'	1:A:567:G:OP1	2.06	0.55
1:A:1364:U:O2'	1:A:1365:G:C5'	2.53	0.55
4:C:191:THR:HG22	4:C:193:TYR:N	2.00	0.55
5:D:30:LYS:O	5:D:31:CYS:C	2.44	0.55
7:F:1:MET:HB3	7:F:67:MET:O	2.06	0.55
7:F:43:LEU:H	7:F:43:LEU:CD2	2.19	0.55
8:G:85:TYR:O	8:G:87:VAL:HG23	2.06	0.55
11:J:30:SER:HB3	11:J:80:LYS:HG3	1.87	0.55
11:J:60:ARG:O	11:J:61:GLU:O	2.23	0.55
19:R:47:THR:HG22	19:R:48:GLY:N	2.22	0.55
21:T:39:LYS:HG2	21:T:55:ILE:HD13	1.88	0.55
3:B:28:PHE:CZ	3:B:189:ASP:HA	2.42	0.55
4:C:28:GLN:HA	4:C:31:HIS:HD2	1.71	0.55
4:C:43:LEU:O	4:C:47:LEU:HB3	2.07	0.55
4:C:126:ARG:O	4:C:127:ARG:CB	2.54	0.55
4:C:134:ILE:CG2	4:C:168:ALA:HB3	2.36	0.55
4:C:142:MET:HA	4:C:142:MET:HE3	1.87	0.55
8:G:66:VAL:HG12	8:G:70:LYS:HE3	1.88	0.55
11:J:39:PRO:HA	11:J:70:ARG:NH1	2.18	0.55
12:K:33:THR:HG23	12:K:34:ASP:O	2.07	0.55
1:A:1263:C:H2'	1:A:1264:C:H6	1.70	0.55
3:B:139:LYS:O	3:B:143:GLU:HG3	2.07	0.55
8:G:22:LEU:HD11	8:G:101:LEU:HD21	1.89	0.55
19:R:16:PRO:HG2	19:R:18:ARG:HB3	1.88	0.55
1:A:176:C:H2'	1:A:177:C:H6	1.71	0.55
1:A:1497:G:O2'	1:A:1498:U:H5'	2.07	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.55
3:B:114:ARG:HH12	3:B:118:LEU:HD21	1.67	0.55
3:B:168:THR:OG1	3:B:192:SER:HB3	2.06	0.55
5:D:25:ARG:O	5:D:27:TYR:N	2.39	0.55
13:L:28:LYS:O	13:L:29:GLY:C	2.44	0.55
19:R:39:VAL:HG13	19:R:40:LEU:N	2.21	0.55
1:A:358:U:H2'	1:A:359:U:H6	1.72	0.55
1:A:737:A:H1'	7:F:73:ASN:HD21	1.71	0.55
5:D:199:GLN:NE2	5:D:201:ASN:H	2.02	0.55
9:H:20:TYR:CE1	9:H:76:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:16:ASP:HB3	14:M:41:PRO:HB3	1.88	0.55
1:A:202:U:H4'	1:A:203:U:OP1	2.07	0.55
3:B:20:GLU:HB2	3:B:190:THR:HB	1.88	0.55
4:C:52:LEU:N	4:C:52:LEU:CD2	2.70	0.55
4:C:108:ASN:ND2	4:C:111:LEU:HG	2.22	0.55
17:P:4:ILE:HA	17:P:20:VAL:O	2.07	0.55
18:Q:69:LYS:O	18:Q:70:ARG:HD2	2.06	0.55
1:A:376:G:OP2	17:P:67:THR:HG21	2.07	0.55
1:A:939:G:H5"	8:G:102:ARG:HH22	1.71	0.55
10:I:24:GLY:HA2	10:I:59:PHE:O	2.07	0.55
14:M:8:GLU:C	14:M:9:ILE:HG13	2.27	0.55
16:O:81:LEU:HD22	16:O:85:LEU:CD1	2.36	0.55
17:P:58:TYR:O	17:P:62:VAL:HG23	2.06	0.55
1:A:975:A:H4'	1:A:976:G:C5'	2.36	0.54
1:A:1531:A:O5'	1:A:1531:A:H8	1.90	0.54
4:C:6:HIS:CD2	4:C:8:ILE:H	2.25	0.54
8:G:154:TYR:O	8:G:156:TRP:N	2.40	0.54
20:S:33:THR:HG22	20:S:34:TRP:N	2.22	0.54
1:A:427:U:OP1	5:D:13:ARG:NH2	2.37	0.54
1:A:620:C:C2	5:D:135:LEU:HD13	2.41	0.54
1:A:914:A:OP1	26:A:1634:SRY:H13	2.06	0.54
1:A:1190:G:OP1	4:C:4:LYS:HA	2.07	0.54
5:D:148:VAL:CG1	5:D:158:ILE:HD13	2.37	0.54
1:A:501:C:H2'	1:A:502:G:H8	1.72	0.54
1:A:1091:U:O2	1:A:1093:A:C8	2.61	0.54
1:A:1113:C:H1'	4:C:178:LEU:HD21	1.89	0.54
4:C:85:ARG:HD2	4:C:85:ARG:O	2.07	0.54
9:H:10:LEU:HD12	9:H:85:ARG:HG3	1.90	0.54
11:J:16:LEU:HD23	11:J:94:VAL:HG13	1.89	0.54
19:R:46:GLU:CD	19:R:46:GLU:N	2.60	0.54
1:A:335:C:H2'	1:A:336:C:C6	2.41	0.54
1:A:959:A:H2'	1:A:960:U:O4'	2.06	0.54
1:A:1154:G:H2'	1:A:1155:G:H8	1.71	0.54
5:D:122:ARG:NH2	5:D:134:ASP:OD2	2.40	0.54
5:D:152:SER:HB3	5:D:155:LEU:HD12	1.88	0.54
7:F:35:ALA:HA	7:F:67:MET:HB3	1.88	0.54
8:G:70:LYS:HB3	8:G:96:GLN:HG2	1.88	0.54
15:N:11:LYS:C	15:N:13:THR:N	2.61	0.54
19:R:36:ASN:HD21	19:R:38:GLU:HG2	1.71	0.54
1:A:913:A:H1'	1:A:914:A:O4'	2.07	0.54
1:A:1131:G:H2'	1:A:1132:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:N2	1:A:1331:G:C2'	2.71	0.54
1:A:1423:G:O2'	1:A:1424:C:H5'	2.07	0.54
1:A:1487:G:O2'	1:A:1488:G:H5'	2.06	0.54
8:G:20:ASP:OD2	8:G:63:LYS:NZ	2.41	0.54
19:R:59:SER:O	19:R:60:GLY:C	2.45	0.54
1:A:939:G:H2'	1:A:940:C:C6	2.43	0.54
1:A:1501:C:OP2	1:A:1504:G:H2'	2.08	0.54
26:A:1634:SRY:C61	13:L:47:LYS:HD3	2.38	0.54
3:B:128:GLU:HA	3:B:135:GLN:NE2	2.19	0.54
4:C:29:TYR:OH	15:N:54:PRO:O	2.22	0.54
6:E:27:ARG:HG2	6:E:28:PHE:N	2.23	0.54
10:I:5:TYR:HA	10:I:17:VAL:O	2.07	0.54
15:N:42:ILE:O	15:N:46:GLU:HG3	2.07	0.54
20:S:43:GLU:CD	20:S:43:GLU:N	2.53	0.54
1:A:781:A:H2'	1:A:782:A:H5'	1.89	0.54
5:D:191:ARG:HH12	5:D:196:LEU:H	1.56	0.54
7:F:1:MET:HE3	7:F:66:GLU:HG2	1.90	0.54
9:H:10:LEU:CD2	9:H:83:ILE:HD11	2.38	0.54
9:H:24:THR:HG23	9:H:61:VAL:HB	1.88	0.54
16:O:87:ILE:CG2	16:O:88:ARG:H	2.13	0.54
18:Q:97:SER:HB2	18:Q:103:GLY:CA	2.17	0.54
1:A:192:U:O4'	21:T:103:GLY:HA2	2.08	0.54
1:A:246:A:N6	1:A:281:G:H1'	2.23	0.54
1:A:735:C:O2'	1:A:736:C:H5'	2.07	0.54
1:A:1438:G:H2'	1:A:1439:C:C6	2.43	0.54
1:A:1498:U:H4'	1:A:1519:A:H2	1.73	0.54
4:C:64:VAL:HB	4:C:99:VAL:CG2	2.37	0.54
5:D:162:LEU:CD2	5:D:178:VAL:HG13	2.36	0.54
1:A:247:G:OP2	18:Q:100:LYS:HG2	2.08	0.54
1:A:542:G:OP1	5:D:10:ARG:NH2	2.40	0.54
1:A:628:G:O2'	1:A:629:G:H5'	2.08	0.54
1:A:761:G:H4'	18:Q:102:GLY:C	2.29	0.54
3:B:130:ARG:CB	3:B:131:PRO:HD2	2.33	0.54
11:J:42:THR:HG23	11:J:67:THR:O	2.08	0.54
19:R:39:VAL:CG1	19:R:40:LEU:N	2.70	0.54
1:A:166:G:O2'	1:A:167:G:H5'	2.07	0.54
1:A:192:U:H4'	21:T:103:GLY:H	1.73	0.54
1:A:579:G:H2'	1:A:580:U:C6	2.43	0.54
1:A:1149:C:H2'	1:A:1150:U:H6	1.73	0.54
3:B:76:GLN:HE21	3:B:206:ASP:HB3	1.73	0.54
3:B:208:ILE:HD12	3:B:242:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:10:PHE:CE2	4:C:178:LEU:HD13	2.43	0.54
18:Q:97:SER:OG	18:Q:103:GLY:CA	2.56	0.54
1:A:1041:A:H2'	1:A:1042:G:C8	2.42	0.53
5:D:13:ARG:HA	5:D:33:MET:SD	2.48	0.53
4:C:191:THR:CG2	4:C:192:THR:N	2.70	0.53
7:F:26:ILE:HG21	7:F:63:TYR:CE2	2.43	0.53
8:G:42:ILE:HG22	8:G:120:ILE:HD12	1.90	0.53
11:J:38:ILE:O	11:J:70:ARG:HA	2.09	0.53
19:R:19:LYS:HD3	19:R:19:LYS:N	2.22	0.53
1:A:399:G:H2'	1:A:400:C:C6	2.43	0.53
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.43	0.53
26:A:1634:SRY:O51	13:L:47:LYS:HG2	2.09	0.53
3:B:12:GLU:HG3	3:B:12:GLU:O	2.08	0.53
3:B:131:PRO:O	3:B:135:GLN:HG3	2.09	0.53
7:F:53:ALA:C	7:F:55:ASP:H	2.11	0.53
10:I:112:LYS:HD3	10:I:112:LYS:C	2.29	0.53
1:A:861:G:O2'	1:A:862:C:H5'	2.09	0.53
1:A:1060:C:C5	4:C:2:GLY:CA	2.92	0.53
1:A:1064:G:C4'	1:A:1065:U:C5'	2.86	0.53
7:F:74:ASP:HA	7:F:77:ARG:CD	2.38	0.53
11:J:28:ARG:NH1	11:J:33:GLN:HB3	2.23	0.53
1:A:335:C:H2'	1:A:336:C:H6	1.73	0.53
1:A:1281:U:H5'	1:A:1282:C:C5	2.41	0.53
1:A:1426:C:O2'	1:A:1427:U:H5'	2.09	0.53
4:C:64:VAL:CG2	4:C:99:VAL:HB	2.38	0.53
15:N:11:LYS:O	15:N:13:THR:N	2.42	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.09	0.53
6:E:118:ILE:CG2	6:E:119:LEU:N	2.72	0.53
8:G:71:PRO:HD3	8:G:103:TRP:CZ3	2.42	0.53
8:G:80:VAL:HG21	8:G:154:TYR:CE1	2.42	0.53
9:H:61:VAL:O	9:H:63:LEU:HD13	2.09	0.53
21:T:44:ALA:HB2	21:T:88:VAL:HG13	1.91	0.53
22:V:24:ARG:O	22:V:25:LYS:HB2	2.08	0.53
1:A:287:U:O2'	1:A:288:A:H5'	2.08	0.53
1:A:685:G:O2'	1:A:686:U:H5'	2.08	0.53
1:A:1112:C:N3	4:C:178:LEU:N	2.57	0.53
1:A:1315:U:H5	20:S:6:LYS:NZ	2.05	0.53
3:B:59:GLU:HG3	3:B:221:LEU:HD11	1.89	0.53
3:B:67:THR:HA	3:B:90:MET:HE1	1.91	0.53
3:B:82:ARG:O	3:B:86:GLU:HG3	2.09	0.53
6:E:19:MET:SD	6:E:24:ARG:NH1	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:19:LEU:HD23	10:I:61:ALA:HB2	1.91	0.53
18:Q:104:LYS:CG	18:Q:105:ALA:H	2.19	0.53
1:A:119:A:H4'	1:A:120:A:O5'	2.09	0.53
1:A:358:U:H2'	1:A:359:U:C6	2.43	0.53
1:A:598:U:H4'	9:H:94:TYR:CD1	2.44	0.53
1:A:724:G:O2'	1:A:725:G:H5'	2.09	0.53
1:A:761:G:C4'	18:Q:103:GLY:N	2.60	0.53
3:B:128:GLU:CA	3:B:135:GLN:HE22	2.16	0.53
4:C:91:LEU:HD21	4:C:99:VAL:CG1	2.38	0.53
6:E:107:ARG:HG2	6:E:108:ALA:N	2.23	0.53
1:A:401:C:O2'	1:A:402:G:H5'	2.09	0.53
1:A:894:G:O2'	1:A:895:G:H5'	2.08	0.53
1:A:974:A:OP1	1:A:974:A:H8	1.92	0.53
1:A:1316:G:O2'	15:N:18:VAL:HG11	2.08	0.53
5:D:105:VAL:HG13	5:D:110:PHE:HB2	1.91	0.53
15:N:8:GLU:HG2	15:N:9:LYS:N	2.24	0.53
1:A:1038:C:H2'	1:A:1039:C:C5	2.43	0.53
1:A:1167:A:H2'	1:A:1168:A:C8	2.44	0.53
1:A:1237:C:H2'	1:A:1336:C:H5	1.74	0.53
7:F:82:ARG:HA	7:F:82:ARG:NE	2.23	0.53
15:N:39:LEU:HD13	15:N:47:LEU:HD12	1.91	0.53
1:A:1127:G:H1	1:A:1145:C:N4	2.06	0.52
1:A:1152:A:H5"	11:J:13:HIS:HD2	1.67	0.52
1:A:1247:U:O2'	1:A:1248:A:H5'	2.09	0.52
3:B:130:ARG:HB3	3:B:131:PRO:CD	2.34	0.52
6:E:151:LEU:HD11	9:H:77:GLU:OE2	2.08	0.52
7:F:69:GLU:OE1	7:F:69:GLU:N	2.41	0.52
22:V:24:ARG:HG3	22:V:24:ARG:HH11	1.73	0.52
1:A:106:C:O2	1:A:379:C:H4'	2.09	0.52
1:A:791:G:H2'	1:A:792:A:C5'	2.39	0.52
1:A:1102:A:H2'	1:A:1103:C:C6	2.44	0.52
1:A:1148:U:H2'	1:A:1149:C:O4'	2.09	0.52
1:A:1459:C:O2'	1:A:1460:A:H5'	2.09	0.52
17:P:81:ARG:CG	17:P:83:GLU:HG2	2.40	0.52
1:A:105:G:H2'	1:A:106:C:C6	2.44	0.52
1:A:518:C:HO2'	13:L:50:SER:HB3	1.73	0.52
1:A:1394:A:C6	1:A:1501:C:H4'	2.44	0.52
3:B:93:VAL:HG11	3:B:97:TRP:CD1	2.44	0.52
5:D:64:LEU:HD12	5:D:75:PHE:CZ	2.45	0.52
9:H:113:SER:HB2	9:H:134:ILE:CD1	2.37	0.52
14:M:44:ARG:HG3	14:M:44:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:67:THR:HG22	17:P:68:ASP:N	2.24	0.52
22:V:12:LYS:HG2	22:V:22:ARG:HB3	1.91	0.52
1:A:187:C:O2	21:T:105:SER:HB3	2.08	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.52
1:A:513:C:H2'	1:A:514:C:H6	1.74	0.52
1:A:828:A:H2'	1:A:829:G:O4'	2.08	0.52
1:A:877:C:O2'	1:A:878:G:H5'	2.08	0.52
1:A:1250:A:H5"	10:I:67:GLY:CA	2.39	0.52
3:B:108:ILE:O	3:B:108:ILE:CG2	2.57	0.52
4:C:64:VAL:HG23	4:C:99:VAL:HB	1.92	0.52
5:D:8:VAL:O	5:D:10:ARG:N	2.42	0.52
13:L:28:LYS:HD2	13:L:33:ARG:NH1	2.24	0.52
14:M:49:THR:HB	14:M:52:GLU:HG3	1.91	0.52
14:M:121:LYS:O	14:M:123:ALA:N	2.42	0.52
16:O:25:THR:HG21	16:O:70:LEU:HB2	1.92	0.52
1:A:463:A:H2'	1:A:474:G:O4'	2.09	0.52
1:A:537:G:OP1	13:L:113:ARG:NH2	2.42	0.52
1:A:592:G:H2'	1:A:593:G:H8	1.74	0.52
4:C:48:TYR:HD1	4:C:52:LEU:HD21	1.75	0.52
8:G:59:LEU:HD11	8:G:63:LYS:HE2	1.91	0.52
8:G:108:ALA:O	8:G:119:ARG:HD2	2.10	0.52
22:V:17:THR:O	22:V:22:ARG:HD3	2.10	0.52
1:A:204:U:H4'	1:A:216:G:O5'	2.09	0.52
1:A:254:G:O2'	1:A:255:G:H5'	2.09	0.52
1:A:255:G:H2'	1:A:256:U:C6	2.45	0.52
3:B:10:LEU:HD13	3:B:48:MET:SD	2.49	0.52
7:F:67:MET:HB2	7:F:68:PRO:CD	2.40	0.52
8:G:95:ARG:HG3	8:G:95:ARG:HH11	1.73	0.52
10:I:19:LEU:CD1	10:I:85:LEU:HD12	2.40	0.52
12:K:84:VAL:HG21	12:K:95:ILE:HD11	1.92	0.52
13:L:83:VAL:HG21	13:L:100:ILE:HG23	1.91	0.52
15:N:26:ARG:HH11	15:N:47:LEU:HG	1.69	0.52
19:R:39:VAL:O	19:R:42:ARG:HB2	2.09	0.52
1:A:1195:C:H3'	1:A:1196:U:C5'	2.34	0.52
5:D:36:ARG:HB3	5:D:38:TYR:CZ	2.45	0.52
8:G:136:LYS:HD2	8:G:136:LYS:C	2.29	0.52
9:H:56:LYS:HD2	9:H:56:LYS:N	2.25	0.52
14:M:40:ASN:C	14:M:40:ASN:ND2	2.63	0.52
17:P:10:GLY:HA3	17:P:14:ASN:O	2.09	0.52
20:S:42:PRO:O	20:S:45:VAL:HB	2.10	0.52
1:A:277:C:O2'	1:A:278:G:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:H5"	4:C:155:GLY:H	1.74	0.52
4:C:22:TRP:CH2	4:C:32:LEU:HB2	2.45	0.52
6:E:115:VAL:HG11	6:E:118:ILE:CG1	2.40	0.52
9:H:108:GLY:HA3	9:H:138:TRP:HB3	1.92	0.52
16:O:81:LEU:HD22	16:O:85:LEU:HD12	1.91	0.52
1:A:485:G:O2'	1:A:486:U:P	2.68	0.52
1:A:1420:C:H2'	1:A:1421:G:C8	2.45	0.52
3:B:124:SER:O	3:B:127:ILE:HG22	2.10	0.52
4:C:141:VAL:HG11	4:C:202:ILE:HG12	1.92	0.52
5:D:61:LYS:NZ	5:D:62:GLN:HE22	2.08	0.52
5:D:78:LEU:HD22	5:D:96:LEU:HB3	1.92	0.52
14:M:27:LYS:HD2	14:M:31:LYS:HE3	1.92	0.52
19:R:48:GLY:O	19:R:74:ARG:NH2	2.40	0.52
1:A:129(A):G:N3	1:A:190(E):U:H5'	2.24	0.52
1:A:136:C:H2'	1:A:137:C:H6	1.74	0.52
1:A:750:G:H1'	16:O:22:THR:OG1	2.10	0.52
1:A:1250:A:H2'	1:A:1251:A:C8	2.44	0.52
1:A:1279:A:O2'	1:A:1282:C:N4	2.43	0.52
3:B:15:VAL:CG1	3:B:210:SER:HA	2.40	0.52
3:B:221:LEU:O	3:B:221:LEU:HD13	2.10	0.52
6:E:31:LEU:HD22	6:E:43:LEU:CD2	2.38	0.52
8:G:18:TYR:HB3	8:G:59:LEU:HD22	1.93	0.52
12:K:72:ALA:O	12:K:77:MET:HB2	2.10	0.52
14:M:40:ASN:HD22	14:M:41:PRO:N	2.08	0.52
1:A:619:U:N3	5:D:134:ASP:OD1	2.39	0.51
1:A:1182:G:O2'	1:A:1183:A:OP2	2.26	0.51
3:B:178:ARG:NH1	3:B:178:ARG:CG	2.71	0.51
6:E:20:GLN:OE1	6:E:25:ARG:HD2	2.10	0.51
21:T:69:GLY:O	21:T:73:HIS:CE1	2.63	0.51
1:A:452:A:O2'	1:A:453:A:H8	1.92	0.51
1:A:858:G:O6	1:A:869:G:H3'	2.11	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.44	0.51
1:A:1202:G:O2'	1:A:1203:C:H5'	2.11	0.51
1:A:1244:C:O2'	1:A:1245:A:H5'	2.10	0.51
1:A:1405:G:P	23:A:1545:PAR:O34	2.68	0.51
3:B:93:VAL:HG11	3:B:97:TRP:HD1	1.75	0.51
4:C:132:ARG:HH11	4:C:132:ARG:HG3	1.76	0.51
4:C:156:ARG:HB3	4:C:160:ALA:O	2.11	0.51
9:H:111:ILE:O	9:H:134:ILE:HB	2.10	0.51
19:R:38:GLU:H	19:R:38:GLU:CD	2.12	0.51
1:A:77:G:O2'	1:A:78:G:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:U:H4'	1:A:1050:G:OP2	2.11	0.51
3:B:17:PHE:CD1	3:B:17:PHE:C	2.84	0.51
3:B:126:GLU:HG2	3:B:129:GLU:OE2	2.10	0.51
5:D:189:PRO:HB2	5:D:194:LEU:CD2	2.41	0.51
5:D:189:PRO:HB2	5:D:194:LEU:HD21	1.92	0.51
9:H:51:VAL:HG21	9:H:60:ARG:HG2	1.93	0.51
10:I:4:TYR:CZ	10:I:88:TYR:HD1	2.27	0.51
11:J:56:HIS:O	11:J:58:ASP:N	2.43	0.51
13:L:38:THR:HG22	13:L:39:VAL:CG2	2.33	0.51
1:A:130:A:C8	18:Q:63:ARG:HG3	2.46	0.51
1:A:407:G:H2'	1:A:408:A:C8	2.43	0.51
1:A:457:C:H2'	1:A:458:C:H6	1.75	0.51
1:A:509:A:H5'	5:D:54:TYR:HD2	1.75	0.51
1:A:738:C:H2'	1:A:739:C:H6	1.74	0.51
1:A:1068:G:OP2	1:A:1068:G:H8	1.93	0.51
4:C:34:LEU:HG	15:N:25:VAL:CG1	2.36	0.51
4:C:45:LYS:C	4:C:47:LEU:H	2.13	0.51
8:G:152:ALA:C	8:G:154:TYR:H	2.12	0.51
10:I:116:LYS:HE2	10:I:122:ALA:HB2	1.92	0.51
16:O:70:LEU:HD12	16:O:78:TYR:HA	1.91	0.51
21:T:39:LYS:CG	21:T:55:ILE:HD13	2.41	0.51
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.46	0.51
1:A:1021:G:C2	1:A:1022:G:H1'	2.45	0.51
1:A:1131:G:H1	1:A:1143:G:N2	2.02	0.51
3:B:178:ARG:NH1	9:H:71:GLY:O	2.44	0.51
11:J:8:LEU:HD12	11:J:20:ALA:HB2	1.91	0.51
11:J:16:LEU:CD2	11:J:94:VAL:HG13	2.41	0.51
12:K:46:GLY:O	12:K:48:ILE:O	2.28	0.51
14:M:52:GLU:HG2	14:M:55:ARG:NH2	2.25	0.51
19:R:42:ARG:HG3	19:R:42:ARG:NH1	2.25	0.51
20:S:72:GLY:O	20:S:74:PHE:HD1	1.94	0.51
21:T:39:LYS:HD3	21:T:55:ILE:HD13	1.93	0.51
1:A:390:C:O3'	17:P:28:ARG:NH2	2.43	0.51
1:A:797:C:OP1	12:K:124:LYS:HE2	2.10	0.51
8:G:18:TYR:CD2	8:G:59:LEU:HB2	2.46	0.51
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.10	0.51
1:A:267:C:OP2	18:Q:67:LYS:HD2	2.11	0.51
1:A:1060:C:C5	4:C:2:GLY:HA3	2.46	0.51
1:A:1245:A:H2'	1:A:1246:C:C6	2.46	0.51
3:B:212:GLN:HG3	3:B:239:VAL:HG21	1.92	0.51
9:H:126:LYS:C	9:H:128:GLY:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:9:ARG:CB	11:J:9:ARG:HH11	2.24	0.51
15:N:57:ARG:HG2	15:N:58:LYS:N	2.25	0.51
20:S:53:ASN:N	20:S:53:ASN:ND2	2.59	0.51
21:T:14:LYS:HG2	21:T:18:GLN:NE2	2.26	0.51
1:A:1117:G:H4'	10:I:104:ARG:HH12	1.69	0.51
3:B:68:ILE:HB	3:B:90:MET:HE3	1.92	0.51
5:D:25:ARG:C	5:D:27:TYR:N	2.64	0.51
7:F:53:ALA:O	7:F:55:ASP:N	2.43	0.51
14:M:122:LYS:O	14:M:123:ALA:HB2	2.11	0.51
1:A:130:A:OP2	1:A:190(E):U:C2'	2.57	0.51
1:A:164:U:H2'	1:A:165:C:C6	2.45	0.51
1:A:376:G:P	17:P:67:THR:HG21	2.51	0.51
1:A:449:C:O2	17:P:42:ARG:HD2	2.11	0.51
1:A:991:U:O2'	1:A:992:U:H5'	2.10	0.51
1:A:1056:U:H5'	4:C:163:ALA:HB2	1.93	0.51
1:A:1405:G:O2'	1:A:1406:U:H5'	2.11	0.51
5:D:61:LYS:HZ1	5:D:62:GLN:HE22	1.59	0.51
17:P:20:VAL:HG11	17:P:32:TYR:HB3	1.93	0.51
20:S:55:LYS:HG2	20:S:56:GLN:NE2	2.11	0.51
1:A:558:G:H2'	1:A:559:A:H2	1.76	0.51
1:A:979:C:O2	15:N:19:ARG:HG2	2.10	0.51
1:A:1366:C:HO2'	1:A:1367:C:H5'	1.76	0.51
10:I:121:ARG:NH1	10:I:122:ALA:O	2.44	0.51
13:L:115:LYS:O	13:L:117:ARG:N	2.42	0.51
17:P:21:VAL:HG21	17:P:59:TRP:CD1	2.45	0.51
19:R:47:THR:C	19:R:49:LYS:H	2.14	0.51
21:T:43:LEU:CD1	21:T:55:ILE:HD12	2.41	0.51
21:T:53:LEU:O	21:T:56:MET:HB3	2.10	0.51
1:A:443:C:H2'	1:A:444:C:H6	1.74	0.50
1:A:501:C:O2'	1:A:502:G:H5'	2.11	0.50
1:A:639:G:O2'	1:A:640:A:H5'	2.10	0.50
1:A:644:G:O2'	1:A:645:C:H5'	2.11	0.50
1:A:953:G:H1'	14:M:125:ARG:CA	2.41	0.50
1:A:1479:C:H2'	1:A:1480:G:C8	2.45	0.50
4:C:113:ALA:HB3	4:C:114:PRO:HD3	1.93	0.50
8:G:23:VAL:HG13	8:G:43:PHE:CE2	2.46	0.50
9:H:51:VAL:HG21	9:H:60:ARG:CG	2.41	0.50
14:M:40:ASN:ND2	14:M:41:PRO:HD2	2.24	0.50
18:Q:104:LYS:O	18:Q:105:ALA:O	2.29	0.50
19:R:36:ASN:HD22	19:R:36:ASN:C	2.13	0.50
21:T:43:LEU:HD12	21:T:55:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:9:ARG:HH12	22:V:23:PRO:HD2	1.76	0.50
1:A:60:A:H4'	1:A:61:G:O5'	2.11	0.50
3:B:34:ALA:O	3:B:40:HIS:O	2.30	0.50
4:C:24:ALA:CB	11:J:9:ARG:HD2	2.41	0.50
5:D:38:TYR:HB2	5:D:39:PRO:HD2	1.93	0.50
5:D:70:ILE:HD11	5:D:74:GLN:HB3	1.93	0.50
20:S:30:LEU:O	20:S:31:ILE:HD13	2.11	0.50
1:A:532:A:N6	4:C:160:ALA:HA	2.26	0.50
1:A:791:G:H2'	1:A:792:A:H5'	1.92	0.50
1:A:818:G:C2'	1:A:819:A:H5"	2.40	0.50
3:B:219:VAL:O	3:B:223:ILE:HD13	2.10	0.50
4:C:131:ARG:CG	4:C:135:LYS:HE3	2.38	0.50
12:K:27:ASN:O	12:K:28:THR:CB	2.59	0.50
1:A:478:A:O2'	1:A:479:C:H5'	2.11	0.50
1:A:833:U:H2'	1:A:834:C:C6	2.47	0.50
1:A:1508:G:H2'	1:A:1509:C:C6	2.47	0.50
3:B:16:HIS:NE2	3:B:214:ILE:CG1	2.73	0.50
8:G:69:VAL:HG21	8:G:104:LEU:CD2	2.41	0.50
9:H:38:ILE:HD12	9:H:38:ILE:H	1.76	0.50
11:J:49:VAL:CG1	15:N:41:ARG:HB2	2.30	0.50
13:L:119:LYS:O	13:L:120:TYR:CB	2.59	0.50
14:M:108:ARG:NE	14:M:108:ARG:HA	2.27	0.50
1:A:328:C:O2	1:A:328:C:C2'	2.57	0.50
4:C:179:ARG:HD2	4:C:179:ARG:C	2.32	0.50
5:D:150:GLU:CD	5:D:150:GLU:N	2.61	0.50
12:K:25:TYR:CE2	12:K:88:GLY:HA2	2.46	0.50
12:K:27:ASN:O	12:K:28:THR:HB	2.11	0.50
20:S:7:LYS:HG3	20:S:7:LYS:O	2.10	0.50
1:A:524:G:H2'	1:A:525:C:C6	2.47	0.50
1:A:1133:G:H2'	1:A:1134:G:C8	2.46	0.50
3:B:84:GLU:HB3	3:B:219:VAL:CG2	2.29	0.50
3:B:187:LEU:HD11	3:B:204:ASN:O	2.12	0.50
8:G:80:VAL:HG21	8:G:154:TYR:CD1	2.46	0.50
14:M:77:ASN:O	14:M:80:ARG:HB3	2.12	0.50
17:P:20:VAL:CG1	17:P:21:VAL:N	2.74	0.50
1:A:748:C:O2'	1:A:749:C:C6	2.62	0.50
1:A:782:A:H2'	1:A:783:C:O4'	2.12	0.50
1:A:1039:C:H2'	1:A:1040:U:H6	1.76	0.50
1:A:1160:G:O2'	1:A:1161:C:H5'	2.12	0.50
4:C:110:ASN:HD22	4:C:140:ARG:HB3	1.76	0.50
4:C:113:ALA:N	4:C:202:ILE:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:104:VAL:HG11	5:D:146:ILE:CD1	2.42	0.50
6:E:16:THR:HG23	6:E:27:ARG:O	2.12	0.50
10:I:10:ARG:O	10:I:11:LYS:C	2.49	0.50
11:J:20:ALA:O	11:J:24:VAL:HG23	2.11	0.50
15:N:27:CYS:HB3	15:N:43:CYS:SG	2.52	0.50
18:Q:104:LYS:HG3	18:Q:105:ALA:N	2.22	0.50
22:V:23:PRO:C	22:V:25:LYS:H	2.15	0.50
1:A:334:C:H2'	1:A:335:C:C6	2.47	0.50
1:A:953:G:C1'	14:M:125:ARG:HA	2.41	0.50
1:A:1137:C:H4'	1:A:1138:G:N1	2.27	0.50
1:A:1372:U:O2'	1:A:1373:G:H5'	2.12	0.50
3:B:111:ARG:NE	3:B:111:ARG:HA	2.27	0.50
3:B:204:ASN:HD22	3:B:205:ASP:N	2.08	0.50
8:G:80:VAL:C	8:G:82:GLY:H	2.12	0.50
9:H:123:GLU:O	9:H:127:LEU:HD23	2.12	0.50
13:L:55:VAL:HG12	13:L:56:ALA:H	1.76	0.50
1:A:263:A:P	21:T:79:ARG:HH12	2.35	0.50
1:A:915:A:C2'	1:A:916:G:H5'	2.42	0.50
1:A:990:C:H2'	1:A:991:U:O4'	2.12	0.50
4:C:52:LEU:CD2	4:C:118:GLN:HE22	2.24	0.50
6:E:76:ILE:O	6:E:93:PRO:HB3	2.12	0.50
9:H:6:ILE:HD11	9:H:31:PHE:CD2	2.47	0.50
11:J:39:PRO:O	11:J:69:ASN:O	2.30	0.50
11:J:53:PRO:O	11:J:54:PHE:O	2.29	0.50
12:K:14:VAL:HG12	12:K:16:SER:O	2.12	0.50
14:M:98:VAL:O	14:M:98:VAL:HG12	2.12	0.50
16:O:67:LEU:HD11	16:O:87:ILE:HD13	1.94	0.50
1:A:116:A:O5'	1:A:116:A:H8	1.93	0.49
1:A:513:C:H2'	1:A:514:C:C6	2.47	0.49
1:A:818:G:C3'	1:A:819:A:C5'	2.87	0.49
1:A:974:A:OP2	15:N:41:ARG:NH1	2.45	0.49
1:A:1346:A:H4'	1:A:1347:G:O5'	2.11	0.49
4:C:115:LEU:HD23	4:C:118:GLN:OE1	2.11	0.49
5:D:61:LYS:HE3	5:D:62:GLN:HE21	1.77	0.49
5:D:165:MET:SD	5:D:168:ARG:HD2	2.51	0.49
8:G:111:ARG:HB3	8:G:113:GLU:OE2	2.11	0.49
12:K:14:VAL:HG21	12:K:40:ILE:HD11	1.93	0.49
13:L:86:ARG:HG3	13:L:86:ARG:NH1	2.28	0.49
15:N:57:ARG:HG2	15:N:58:LYS:H	1.76	0.49
18:Q:101:ARG:HH11	18:Q:101:ARG:HG3	1.75	0.49
1:A:115:G:H1'	1:A:116:A:N7	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:C:O2'	1:A:370:C:H5'	2.11	0.49
1:A:559:A:P	6:E:126:ARG:HH22	2.35	0.49
3:B:107:THR:C	3:B:109:SER:H	2.15	0.49
3:B:165:VAL:O	3:B:187:LEU:O	2.29	0.49
4:C:134:ILE:HG23	4:C:151:VAL:HB	1.94	0.49
7:F:3:ARG:HB3	7:F:93:SER:OG	2.11	0.49
8:G:57:GLU:O	8:G:61:VAL:HG23	2.11	0.49
17:P:75:ARG:HH11	17:P:75:ARG:HG3	1.77	0.49
19:R:42:ARG:HG3	19:R:42:ARG:HH11	1.76	0.49
1:A:88:A:H2'	1:A:89:C:O4'	2.11	0.49
1:A:148:G:O2'	1:A:149:A:H5'	2.12	0.49
1:A:162:A:N3	1:A:348:G:H4'	2.27	0.49
1:A:502:G:OP1	13:L:118:SER:CB	2.61	0.49
1:A:594:G:C2'	1:A:595:G:H5'	2.42	0.49
1:A:1305:G:H22	1:A:1331:G:C2'	2.25	0.49
3:B:63:MET:HG3	3:B:64:ARG:N	2.27	0.49
5:D:199:GLN:HG3	5:D:202:LEU:HG	1.95	0.49
8:G:83:ALA:HB3	8:G:85:TYR:CE2	2.48	0.49
18:Q:27:PHE:HB2	18:Q:28:PRO:HD2	1.93	0.49
1:A:155:C:H2'	1:A:156:G:H8	1.76	0.49
1:A:164:U:O2'	1:A:165:C:H5'	2.13	0.49
1:A:448:A:H2'	1:A:449:C:C6	2.48	0.49
1:A:1074:G:O2'	3:B:103:THR:HG22	2.12	0.49
1:A:1175:G:O2'	1:A:1176:A:H5'	2.12	0.49
4:C:154:SER:OG	4:C:155:GLY:N	2.45	0.49
6:E:102:ALA:CB	6:E:120:THR:HG21	2.42	0.49
9:H:13:ILE:O	9:H:17:THR:HG23	2.13	0.49
10:I:95:LYS:C	10:I:98:PRO:HD2	2.32	0.49
12:K:77:MET:CE	12:K:80:VAL:HG22	2.39	0.49
17:P:52:ASP:O	17:P:52:ASP:OD2	2.30	0.49
1:A:1053:G:C4'	1:A:1054:C:H5'	2.42	0.49
1:A:1230:C:H2'	1:A:1231:G:H8	1.78	0.49
1:A:1305:G:H5'	22:V:4:GLY:CA	2.37	0.49
1:A:1313:U:OP2	20:S:6:LYS:HA	2.12	0.49
4:C:177:THR:CG2	4:C:180:ALA:HB2	2.43	0.49
6:E:11:ILE:HG12	6:E:33:VAL:HG23	1.94	0.49
8:G:15:ASP:OD1	8:G:17:VAL:N	2.45	0.49
10:I:120:ARG:O	10:I:121:ARG:C	2.49	0.49
14:M:110:ARG:HG2	14:M:110:ARG:HH11	1.77	0.49
1:A:112:G:H4'	1:A:389:A:H5"	1.94	0.49
1:A:155:C:H2'	1:A:156:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:G:O2'	1:A:282:A:OP2	2.26	0.49
1:A:1231:G:H5"	10:I:126:SER:HB2	1.93	0.49
1:A:1292:U:O2'	1:A:1293:G:H5'	2.13	0.49
3:B:111:ARG:HD3	3:B:145:LEU:HD21	1.94	0.49
4:C:26:LYS:HE2	11:J:45:ARG:HH12	1.77	0.49
4:C:38:ARG:HG3	4:C:38:ARG:NH1	2.23	0.49
4:C:131:ARG:HG2	4:C:135:LYS:CE	2.40	0.49
6:E:15:ARG:O	6:E:15:ARG:HD2	2.12	0.49
6:E:103:GLY:O	6:E:106:PRO:HD2	2.12	0.49
7:F:101:ALA:HB2	19:R:28:GLU:HB2	1.94	0.49
8:G:135:VAL:O	8:G:139:GLU:HG3	2.12	0.49
10:I:98:PRO:HG2	10:I:99:LEU:CD2	2.42	0.49
11:J:47:PHE:HB2	11:J:63:PHE:HB2	1.94	0.49
21:T:79:ARG:HD3	21:T:83:ARG:CZ	2.42	0.49
1:A:189:G:H2'	1:A:190:C:H6	1.77	0.49
1:A:373:A:H1'	1:A:481:G:H1'	1.93	0.49
1:A:1189:C:OP1	11:J:51:ARG:NH2	2.40	0.49
3:B:17:PHE:HD1	3:B:17:PHE:C	2.16	0.49
6:E:60:TYR:O	6:E:64:ARG:HG2	2.13	0.49
1:A:662:G:H2'	1:A:663:A:C8	2.47	0.49
3:B:100:GLY:O	3:B:104:ASN:N	2.40	0.49
1:A:992:U:O2'	1:A:993:G:OP2	2.31	0.49
1:A:1128:C:H5'	10:I:16:ARG:HH22	1.77	0.49
1:A:1470:G:O2'	1:A:1471:G:H5'	2.13	0.49
3:B:23:ARG:HG3	3:B:23:ARG:O	2.11	0.49
4:C:167:TRP:O	4:C:168:ALA:HB3	2.11	0.49
5:D:191:ARG:HG2	5:D:200:GLU:OE2	2.13	0.49
12:K:27:ASN:HA	12:K:56:GLY:HA2	1.94	0.49
16:O:45:VAL:HG12	16:O:46:HIS:ND1	2.28	0.49
20:S:50:ALA:HA	20:S:58:VAL:O	2.13	0.49
1:A:541:G:O2'	1:A:542:G:H5'	2.13	0.49
1:A:1030(B):C:H2'	1:A:1030(C):G:O4'	2.12	0.49
5:D:199:GLN:CG	5:D:202:LEU:HG	2.42	0.49
6:E:11:ILE:CG1	6:E:33:VAL:HG23	2.43	0.49
10:I:19:LEU:HD11	10:I:85:LEU:HD12	1.95	0.49
1:A:532:A:H2'	1:A:533:A:H5'	1.96	0.48
1:A:646:U:H2'	1:A:647:C:H6	1.73	0.48
1:A:760:G:N7	18:Q:105:ALA:O	2.46	0.48
1:A:839:U:O2	1:A:839:U:C2'	2.58	0.48
1:A:952:U:H2'	1:A:953:G:H8	1.77	0.48
1:A:1118:C:H1'	1:A:1179:A:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:C:H5"	3:B:133:LYS:CE	2.43	0.48
1:A:1202:G:C2'	1:A:1203:C:H5'	2.43	0.48
1:A:1305:G:O2'	1:A:1306:A:P	2.71	0.48
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.48
4:C:70:VAL:C	4:C:106:VAL:HG23	2.34	0.48
9:H:7:ALA:HA	9:H:85:ARG:HG3	1.95	0.48
16:O:45:VAL:O	16:O:46:HIS:HB2	2.12	0.48
1:A:29:G:O2'	1:A:30:U:H5'	2.13	0.48
1:A:163:C:O2'	1:A:164:U:H5'	2.12	0.48
1:A:192:U:C4'	21:T:103:GLY:H	2.26	0.48
1:A:450:G:N7	1:A:481:G:C6	2.81	0.48
1:A:1126:U:OP2	1:A:1281:U:O2	2.30	0.48
1:A:1256:A:C3'	1:A:1257:U:H5'	2.43	0.48
1:A:1326:C:OP1	22:V:12:LYS:NZ	2.40	0.48
1:A:1407:C:O2'	1:A:1408:A:H5'	2.14	0.48
3:B:88:ALA:C	3:B:90:MET:H	2.16	0.48
11:J:35:SER:CB	11:J:73:ASP:HB3	2.43	0.48
16:O:17:ARG:HG3	16:O:17:ARG:NH1	2.28	0.48
19:R:74:ARG:CD	19:R:81:PHE:HA	2.43	0.48
21:T:73:HIS:C	21:T:74:LYS:CD	2.81	0.48
1:A:840:C:H4'	1:A:841:U:O5'	2.13	0.48
1:A:1095:U:H2'	1:A:1096:C:C6	2.48	0.48
5:D:17:VAL:HG11	5:D:197:PRO:CB	2.43	0.48
5:D:114:ARG:HG3	5:D:114:ARG:NH1	2.27	0.48
6:E:11:ILE:HD11	6:E:108:ALA:HB3	1.96	0.48
16:O:70:LEU:HD12	16:O:78:TYR:CA	2.43	0.48
18:Q:59:ILE:HG22	18:Q:71:PHE:HD1	1.75	0.48
1:A:7:G:O2'	6:E:120:THR:O	2.31	0.48
1:A:505:G:H2'	1:A:506:G:C8	2.48	0.48
5:D:157:LEU:HD23	5:D:157:LEU:C	2.34	0.48
13:L:36:VAL:HG22	13:L:82:VAL:HG22	1.94	0.48
18:Q:89:LEU:O	18:Q:93:GLN:HG3	2.14	0.48
1:A:200:G:H2'	1:A:201:C:O4'	2.13	0.48
1:A:397:A:H5'	1:A:398:C:P	2.54	0.48
1:A:533:A:O2'	1:A:534:U:OP1	2.28	0.48
1:A:757:U:H2'	1:A:758:G:O4'	2.13	0.48
1:A:1056:U:H5'	4:C:163:ALA:CB	2.44	0.48
1:A:1301:U:O2'	1:A:1302:U:P	2.71	0.48
3:B:42:ILE:HD12	3:B:203:GLY:HA2	1.96	0.48
3:B:90:MET:HA	3:B:91:PRO:HD3	1.73	0.48
4:C:79:ARG:C	4:C:81:GLY:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:91:LEU:HD21	4:C:99:VAL:HG11	1.95	0.48
6:E:36:ASP:O	6:E:37:ARG:HB2	2.13	0.48
7:F:60:PHE:CZ	19:R:78:LEU:HD21	2.48	0.48
8:G:38:LEU:HD11	8:G:42:ILE:HD11	1.94	0.48
9:H:55:GLY:C	9:H:56:LYS:HD2	2.32	0.48
18:Q:45:HIS:CG	18:Q:65:ILE:HD13	2.49	0.48
18:Q:69:LYS:C	18:Q:70:ARG:HD2	2.33	0.48
19:R:88:LYS:OXT	19:R:88:LYS:HG2	2.13	0.48
1:A:252:U:H2'	1:A:253:U:C6	2.48	0.48
1:A:922:G:H2'	1:A:923:A:C8	2.48	0.48
1:A:975:A:O2'	15:N:32:SER:HB2	2.14	0.48
1:A:1216:G:H5"	15:N:5:ALA:HB1	1.94	0.48
1:A:1292:U:OP2	8:G:41:ARG:NH2	2.46	0.48
4:C:67:THR:O	4:C:69:HIS:HD2	1.96	0.48
6:E:35:GLY:HA3	6:E:112:LEU:HB3	1.94	0.48
18:Q:27:PHE:CE1	18:Q:36:ILE:HD11	2.49	0.48
1:A:145:G:O2'	1:A:146:G:H5'	2.14	0.48
1:A:160:A:H2'	1:A:161:A:O4'	2.14	0.48
1:A:321:A:H2'	1:A:322:C:H6	1.78	0.48
1:A:501:C:H2'	1:A:502:G:C8	2.48	0.48
1:A:920:U:H2'	1:A:921:U:C6	2.48	0.48
1:A:1041:A:H2'	1:A:1042:G:H8	1.78	0.48
1:A:1225:A:H2'	1:A:1225:A:N3	2.29	0.48
1:A:1366:C:O2'	1:A:1367:C:H5'	2.12	0.48
1:A:1402:C:O2	1:A:1500:A:N1	2.47	0.48
4:C:19:GLU:O	4:C:40:ARG:NH2	2.47	0.48
4:C:35:GLU:CD	4:C:59:ARG:HH22	2.17	0.48
7:F:97:PHE:HB2	19:R:32:ARG:HH21	1.78	0.48
9:H:103:VAL:HG12	9:H:108:GLY:HA3	1.96	0.48
10:I:99:LEU:HD22	10:I:99:LEU:N	2.29	0.48
11:J:46:ARG:HG2	11:J:46:ARG:HH11	1.79	0.48
18:Q:17:LYS:HA	18:Q:46:ASP:O	2.13	0.48
1:A:485:G:C2'	1:A:486:U:OP2	2.61	0.48
1:A:965:A:O2'	1:A:966:G:OP2	2.32	0.48
3:B:60:ASP:O	3:B:64:ARG:HB2	2.13	0.48
4:C:155:GLY:HA3	4:C:196:LEU:HD13	1.96	0.48
8:G:31:MET:HA	8:G:39:ALA:HB2	1.96	0.48
10:I:9:ARG:CG	10:I:14:VAL:HG13	2.43	0.48
11:J:51:ARG:H	11:J:59:SER:HB2	1.79	0.48
13:L:102:ARG:NH2	13:L:108:ALA:O	2.42	0.48
1:A:270:A:H2'	1:A:271:C:H6	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:U:O2'	1:A:359:U:H5'	2.13	0.48
1:A:738:C:H2'	1:A:739:C:C6	2.48	0.48
1:A:1257:U:H5"	1:A:1258:G:H5'	1.95	0.48
7:F:15:ASP:H	7:F:18:GLN:HE21	1.62	0.48
8:G:51:GLN:HG2	8:G:51:GLN:O	2.13	0.48
8:G:79:ARG:HG3	8:G:84:ASN:OD1	2.14	0.48
16:O:41:GLU:OE2	16:O:41:GLU:HA	2.12	0.48
21:T:57:ARG:NH2	21:T:102:GLY:HA3	2.28	0.48
22:V:24:ARG:HG3	22:V:24:ARG:NH1	2.29	0.48
1:A:627:G:O2'	1:A:628:G:H5'	2.13	0.48
1:A:1004:A:N7	1:A:1036:G:O6	2.47	0.48
1:A:1039:C:H2'	1:A:1040:U:C6	2.49	0.48
1:A:1125:U:H3	11:J:5:ARG:HH21	1.61	0.48
1:A:1355:G:O2'	1:A:1356:G:H5'	2.14	0.48
1:A:1367:C:H4'	11:J:48:THR:HG21	1.96	0.48
3:B:85:ALA:O	3:B:88:ALA:O	2.32	0.48
3:B:180:LEU:O	3:B:181:PHE:HB2	2.13	0.48
4:C:6:HIS:HD2	4:C:8:ILE:HB	1.74	0.48
4:C:25:GLY:O	4:C:29:TYR:HB2	2.13	0.48
5:D:98:GLU:OE1	5:D:194:LEU:HD11	2.13	0.48
7:F:78:GLU:HA	7:F:81:ILE:CD1	2.44	0.48
11:J:9:ARG:HB3	11:J:9:ARG:HH11	1.79	0.48
11:J:22:LYS:HZ2	11:J:90:LEU:HB2	1.78	0.48
14:M:65:LYS:HG3	14:M:69:GLU:OE2	2.14	0.48
19:R:45:SER:C	19:R:47:THR:N	2.68	0.48
19:R:52:PRO:HD2	19:R:55:ARG:CG	2.44	0.48
21:T:57:ARG:HH11	21:T:57:ARG:CG	2.27	0.48
21:T:74:LYS:CG	21:T:75:ASN:N	2.61	0.48
1:A:255:G:H1'	18:Q:16:GLN:HE22	1.78	0.47
1:A:613:C:H2'	1:A:614:A:C8	2.49	0.47
1:A:687:A:H4'	1:A:688:G:O5'	2.14	0.47
1:A:1279:A:O2'	1:A:1281:U:OP2	2.31	0.47
1:A:1314:C:O2'	1:A:1315:U:H5'	2.14	0.47
6:E:137:GLU:O	6:E:141:GLN:HG3	2.14	0.47
7:F:97:PHE:N	19:R:30:ASP:OD1	2.46	0.47
11:J:51:ARG:HB2	11:J:59:SER:CB	2.20	0.47
11:J:75:ILE:O	11:J:76:ASN:CB	2.61	0.47
14:M:78:ILE:O	14:M:82:MET:HB2	2.14	0.47
20:S:17:GLU:O	20:S:21:GLU:HG3	2.14	0.47
1:A:715:A:H2'	1:A:716:A:C8	2.49	0.47
1:A:748:C:O2'	1:A:749:C:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:U:H4'	20:S:79:THR:O	2.15	0.47
1:A:1128:C:H1'	1:A:1146:A:N6	2.26	0.47
1:A:1405:G:O4'	1:A:1519:A:H4'	2.13	0.47
5:D:3:ARG:CZ	5:D:70:ILE:HA	2.44	0.47
13:L:53:ARG:HD2	13:L:53:ARG:H	1.79	0.47
16:O:34:LEU:C	16:O:34:LEU:HD23	2.33	0.47
1:A:54:C:H2'	1:A:352:C:H41	1.79	0.47
1:A:75:G:H2'	1:A:76:C:H6	1.79	0.47
1:A:322:C:O2'	1:A:323:U:H5'	2.14	0.47
1:A:883:C:O2'	1:A:884:U:H5'	2.14	0.47
1:A:1014:A:C2	1:A:1219:U:H1'	2.49	0.47
1:A:1138:G:H3'	1:A:1138:G:N3	2.28	0.47
1:A:1250:A:H5'	10:I:68:GLY:O	2.14	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.47
1:A:1522:U:O2'	1:A:1523:G:H5'	2.14	0.47
3:B:10:LEU:HD22	3:B:48:MET:SD	2.54	0.47
3:B:39:ILE:HG22	3:B:41:ILE:N	2.27	0.47
3:B:95:GLN:HG3	3:B:147:LYS:O	2.13	0.47
3:B:123:ALA:O	3:B:124:SER:CB	2.63	0.47
9:H:23:SER:OG	9:H:24:THR:N	2.47	0.47
10:I:47:LEU:C	10:I:49:PRO:HD2	2.34	0.47
11:J:4:ILE:HG21	11:J:98:ILE:HG23	1.95	0.47
11:J:62:HIS:HB3	15:N:59:ALA:HB3	1.95	0.47
18:Q:48:GLU:O	18:Q:49:GLU:C	2.52	0.47
1:A:666:G:H5'	1:A:726:C:H1'	1.97	0.47
1:A:882:C:O2'	1:A:883:C:H5'	2.14	0.47
1:A:1508:G:O2'	1:A:1509:C:H5'	2.14	0.47
3:B:47:THR:HG23	3:B:202:PRO:O	2.15	0.47
3:B:114:ARG:HH11	3:B:118:LEU:HD11	1.79	0.47
3:B:122:PHE:C	3:B:124:SER:H	2.18	0.47
5:D:64:LEU:HD12	5:D:75:PHE:HZ	1.78	0.47
7:F:9:VAL:HG22	7:F:60:PHE:CD2	2.50	0.47
8:G:15:ASP:O	8:G:19:GLY:HA2	2.14	0.47
11:J:71:LEU:O	11:J:73:ASP:N	2.47	0.47
15:N:26:ARG:NH1	15:N:47:LEU:CG	2.74	0.47
1:A:965:A:H4'	1:A:966:G:O5'	2.15	0.47
1:A:1125:U:O4	11:J:5:ARG:NE	2.46	0.47
1:A:1151:A:O2'	1:A:1152:A:H8	1.97	0.47
1:A:1222:G:H5'	20:S:77:THR:HG21	1.96	0.47
1:A:1223:C:P	20:S:78:ARG:NH1	2.78	0.47
1:A:1305:G:N2	1:A:1331:G:HO2'	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:84:PHE:CE2	6:E:133:TYR:HD1	2.33	0.47
7:F:9:VAL:HB	7:F:87:ARG:HB2	1.96	0.47
10:I:111:ARG:HG3	10:I:111:ARG:NH1	2.29	0.47
13:L:37:CYS:O	13:L:79:GLU:O	2.32	0.47
13:L:81:SER:O	13:L:106:ASP:HB2	2.14	0.47
14:M:125:ARG:HD2	14:M:125:ARG:C	2.35	0.47
20:S:10:PHE:HE2	20:S:12:ASP:OD1	1.98	0.47
1:A:248:C:O2'	1:A:249:U:H5'	2.14	0.47
1:A:338:A:H2'	1:A:339:C:C6	2.49	0.47
1:A:1110:A:H8	1:A:1110:A:O5'	1.97	0.47
1:A:1124:G:H5'	11:J:35:SER:O	2.14	0.47
1:A:1424:C:O2'	1:A:1425:U:H5'	2.15	0.47
3:B:149:LEU:O	3:B:153:ARG:HB2	2.15	0.47
7:F:75:LEU:C	7:F:75:LEU:HD13	2.35	0.47
8:G:44:TYR:HE1	10:I:41:VAL:HG11	1.79	0.47
10:I:97:LYS:O	10:I:100:GLY:N	2.46	0.47
12:K:110:ASP:OD2	19:R:88:LYS:NZ	2.48	0.47
22:V:2:GLY:O	22:V:4:GLY:N	2.48	0.47
1:A:51:A:H4'	1:A:52:G:C5'	2.44	0.47
1:A:344:A:C5'	1:A:345:C:H5	2.28	0.47
1:A:393:A:C2'	1:A:394:G:H5'	2.45	0.47
1:A:630:G:O2'	1:A:631:G:H5'	2.14	0.47
1:A:959:A:H2	1:A:1221:G:N3	2.11	0.47
1:A:979:C:C2'	1:A:980:C:H5'	2.45	0.47
1:A:1201:A:O2'	1:A:1202:G:OP2	2.32	0.47
3:B:9:GLU:CD	3:B:217:ARG:HH22	2.18	0.47
9:H:90:GLY:O	18:Q:34:LYS:HE2	2.15	0.47
10:I:56:LEU:C	10:I:58:ARG:N	2.67	0.47
11:J:60:ARG:HD2	11:J:60:ARG:N	2.24	0.47
12:K:73:MET:CE	12:K:102:GLY:HA3	2.44	0.47
13:L:8:ASN:O	13:L:12:ARG:HG3	2.15	0.47
14:M:5:ALA:O	14:M:6:GLY:C	2.53	0.47
14:M:11:ARG:O	14:M:13:LYS:HG3	2.14	0.47
15:N:33:VAL:HA	15:N:40:CYS:HA	1.96	0.47
19:R:21:LYS:HD2	19:R:21:LYS:H	1.79	0.47
19:R:65:ILE:O	19:R:66:LEU:C	2.52	0.47
20:S:28:LYS:HD3	20:S:31:ILE:CD1	2.44	0.47
20:S:41:VAL:HB	20:S:43:GLU:OE2	2.13	0.47
1:A:147:G:O2'	1:A:148:G:H5'	2.14	0.47
1:A:217:C:O2'	1:A:218:C:H5'	2.15	0.47
1:A:839:U:C5'	1:A:840:C:H5	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
1:A:1057:G:H2'	1:A:1058:G:O4'	2.15	0.47
3:B:19:HIS:HD2	3:B:205:ASP:OD1	1.97	0.47
3:B:82:ARG:O	3:B:83:MET:C	2.53	0.47
4:C:26:LYS:HD3	11:J:45:ARG:HH22	1.80	0.47
9:H:60:ARG:HG3	9:H:60:ARG:NH1	2.30	0.47
13:L:6:THR:OG1	13:L:9:GLN:HG3	2.14	0.47
14:M:11:ARG:HG2	14:M:12:ASN:H	1.80	0.47
17:P:3:LYS:O	17:P:21:VAL:HA	2.14	0.47
19:R:18:ARG:HG3	19:R:18:ARG:O	2.15	0.47
19:R:21:LYS:H	19:R:21:LYS:CD	2.28	0.47
1:A:113:G:H1'	1:A:354:G:C5'	2.44	0.47
1:A:543:C:O2'	1:A:544:G:H5'	2.15	0.47
1:A:743:U:H2'	1:A:744:C:C6	2.50	0.47
1:A:792:A:H4'	1:A:793:U:H5"	1.97	0.47
1:A:1059:C:O2'	1:A:1060:C:H5'	2.15	0.47
3:B:238:LEU:HD23	3:B:241:GLU:OE1	2.15	0.47
4:C:137:ALA:HA	4:C:140:ARG:HD2	1.97	0.47
8:G:72:ARG:NH2	8:G:138:LYS:NZ	2.63	0.47
10:I:8:GLY:HA2	10:I:79:LEU:CD1	2.41	0.47
20:S:24:ALA:HB3	20:S:25:LYS:HD2	1.97	0.47
1:A:949:A:N7	14:M:106:ASN:ND2	2.63	0.47
1:A:1074:G:O3'	3:B:103:THR:CG2	2.63	0.47
1:A:1169:A:H2'	1:A:1171:G:O4'	2.14	0.47
1:A:1439:C:H2'	1:A:1440:C:H6	1.80	0.47
1:A:1504:G:OP1	1:A:1507:A:H4'	2.15	0.47
3:B:12:GLU:C	3:B:14:GLY:N	2.67	0.47
5:D:47:ARG:HG2	5:D:48:ALA:N	2.30	0.47
8:G:28:ASN:OD1	8:G:36:LYS:NZ	2.48	0.47
17:P:4:ILE:HG13	17:P:64:ALA:HB1	1.97	0.47
1:A:42:G:H2'	1:A:43:C:C6	2.50	0.46
1:A:226:G:O2'	1:A:227:G:H5'	2.14	0.46
1:A:1387:G:H5"	25:A:1633:SCM:H8M3	1.98	0.46
3:B:8:LYS:O	3:B:9:GLU:HG3	2.15	0.46
3:B:76:GLN:HE21	3:B:207:ALA:H	1.61	0.46
3:B:122:PHE:O	3:B:125:PRO:HD2	2.15	0.46
6:E:5:ASP:CG	6:E:6:PHE:H	2.16	0.46
6:E:28:PHE:O	6:E:47:LYS:HA	2.15	0.46
6:E:74:GLY:CA	6:E:116:THR:HG22	2.45	0.46
9:H:4:ASP:CG	9:H:85:ARG:HH11	2.18	0.46
12:K:33:THR:HG23	12:K:34:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:9:ARG:O	22:V:13:ILE:HG13	2.15	0.46
1:A:359:U:H2'	1:A:360:A:C8	2.51	0.46
1:A:425:G:O2'	1:A:426:G:H5'	2.15	0.46
1:A:1329:A:OP1	14:M:26:GLY:O	2.33	0.46
4:C:188:LEU:O	4:C:189:ALA:HB2	2.15	0.46
5:D:19:LEU:HD22	5:D:67:ILE:CG1	2.46	0.46
8:G:37:ASN:HD21	10:I:40:LEU:HA	1.80	0.46
9:H:63:LEU:N	9:H:63:LEU:CD1	2.77	0.46
9:H:75:ARG:HA	9:H:76:PRO:HD3	1.78	0.46
10:I:16:ARG:HB2	10:I:64:THR:HB	1.96	0.46
10:I:125:TYR:CD1	10:I:128:ARG:HB2	2.50	0.46
14:M:13:LYS:CA	14:M:44:ARG:NH1	2.77	0.46
15:N:7:ILE:O	15:N:7:ILE:HG22	2.14	0.46
19:R:59:SER:OG	19:R:62:GLU:HG3	2.15	0.46
1:A:401:C:H2'	1:A:402:G:H8	1.80	0.46
1:A:437:U:O2'	5:D:123:HIS:CD2	2.68	0.46
1:A:792:A:H1'	1:A:794:A:N7	2.31	0.46
1:A:1397:C:O2'	1:A:1398:A:P	2.73	0.46
4:C:43:LEU:HD12	4:C:55:VAL:HG11	1.97	0.46
7:F:39:LYS:HE3	7:F:62:TRP:CZ3	2.50	0.46
8:G:71:PRO:HD3	8:G:103:TRP:HZ3	1.81	0.46
11:J:23:ILE:HD12	11:J:23:ILE:H	1.79	0.46
12:K:33:THR:OG1	12:K:38:ASN:C	2.54	0.46
14:M:5:ALA:H	14:M:8:GLU:HB2	1.80	0.46
15:N:57:ARG:CG	15:N:58:LYS:H	2.28	0.46
19:R:19:LYS:H	19:R:19:LYS:CD	2.27	0.46
20:S:15:LEU:CA	20:S:18:LYS:HB3	2.35	0.46
1:A:371:G:H2'	1:A:372:C:H5'	1.93	0.46
1:A:448:A:H2'	1:A:449:C:H6	1.80	0.46
1:A:953:G:H2'	1:A:954:G:O4'	2.15	0.46
1:A:1250:A:C4'	10:I:68:GLY:H	2.15	0.46
3:B:204:ASN:HD22	3:B:206:ASP:H	1.63	0.46
4:C:119:ARG:O	4:C:122:GLU:HB2	2.15	0.46
5:D:3:ARG:NH1	5:D:70:ILE:HA	2.31	0.46
5:D:94:LEU:CD1	5:D:191:ARG:HD3	2.46	0.46
8:G:113:GLU:HG2	8:G:119:ARG:CG	2.37	0.46
12:K:27:ASN:C	12:K:27:ASN:ND2	2.69	0.46
13:L:34:ARG:O	13:L:61:THR:HG23	2.14	0.46
1:A:67:C:H2'	1:A:68:G:C8	2.51	0.46
1:A:281:G:HO2'	1:A:282:A:P	2.38	0.46
1:A:329:A:H4'	1:A:330:C:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:C:H2'	1:A:340:U:H6	1.81	0.46
1:A:502:G:H1'	1:A:550:G:H5'	1.98	0.46
1:A:900:A:H2'	1:A:901:A:C8	2.50	0.46
1:A:1031:G:H2'	1:A:1032:G:C8	2.44	0.46
1:A:1085:U:O3'	1:A:1086:U:H6	1.99	0.46
1:A:1207:G:H2'	1:A:1208:C:H6	1.81	0.46
1:A:1439:C:H2'	1:A:1440:C:C6	2.51	0.46
10:I:78:LYS:HD3	10:I:101:PHE:CD2	2.50	0.46
11:J:12:ASP:OD1	11:J:14:LYS:N	2.49	0.46
11:J:34:VAL:HG12	11:J:35:SER:N	2.30	0.46
13:L:27:LEU:HD13	13:L:64:TYR:HE1	1.80	0.46
14:M:33:ALA:HA	14:M:59:TYR:CE2	2.51	0.46
14:M:65:LYS:HE3	14:M:69:GLU:OE2	2.15	0.46
14:M:123:ALA:O	14:M:125:ARG:N	2.48	0.46
18:Q:76:LEU:C	18:Q:76:LEU:HD23	2.35	0.46
1:A:21:G:H2'	1:A:22:G:C8	2.50	0.46
1:A:107:G:N7	21:T:15:ARG:NH2	2.56	0.46
1:A:401:C:H1'	1:A:622:A:H1'	1.98	0.46
1:A:487:A:H2'	1:A:488:C:O4'	2.16	0.46
1:A:780:A:O2'	1:A:781:A:H5"	2.16	0.46
1:A:925:G:C2	1:A:927:G:C8	3.04	0.46
1:A:1298:C:OP2	8:G:114:ARG:NH2	2.48	0.46
7:F:22:GLU:OE1	7:F:22:GLU:HA	2.15	0.46
8:G:129:GLU:CB	8:G:131:LYS:HE2	2.46	0.46
8:G:136:LYS:HD2	8:G:136:LYS:O	2.16	0.46
9:H:53:VAL:HB	9:H:58:TYR:CD1	2.51	0.46
11:J:15:THR:HG23	11:J:94:VAL:CG2	2.44	0.46
14:M:32:GLU:OE1	14:M:64:TRP:HZ2	1.97	0.46
14:M:117:VAL:CG1	14:M:118:ALA:N	2.78	0.46
16:O:64:ARG:HH11	16:O:64:ARG:HG3	1.78	0.46
21:T:46:GLU:HG2	21:T:48:LYS:HZ3	1.78	0.46
1:A:109:A:C6	1:A:327:A:C6	3.04	0.46
1:A:521:G:O2'	1:A:522:C:H5'	2.16	0.46
1:A:1325:C:O2'	1:A:1326:C:H5'	2.15	0.46
3:B:189:ASP:HB3	3:B:203:GLY:O	2.16	0.46
5:D:17:VAL:HG12	5:D:18:LYS:H	1.80	0.46
5:D:98:GLU:CG	5:D:189:PRO:HG3	2.45	0.46
6:E:80:ILE:HD12	6:E:91:LEU:HB2	1.97	0.46
10:I:11:LYS:O	10:I:11:LYS:CG	2.62	0.46
14:M:8:GLU:CD	14:M:22:ILE:HA	2.36	0.46
18:Q:79:SER:O	18:Q:80:GLY:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:A:N3	12:K:117:ASN:O	2.49	0.46
1:A:797:C:O2'	1:A:798:G:H5'	2.15	0.46
3:B:119:GLU:OE2	3:B:153:ARG:NH2	2.48	0.46
4:C:91:LEU:CD2	4:C:99:VAL:HG13	2.46	0.46
7:F:82:ARG:HB2	7:F:85:VAL:HB	1.98	0.46
8:G:15:ASP:OD2	8:G:23:VAL:HG11	2.15	0.46
14:M:59:TYR:CD2	14:M:63:THR:HG21	2.50	0.46
17:P:59:TRP:HB3	17:P:64:ALA:HB2	1.97	0.46
1:A:837:G:H2'	1:A:838:G:C8	2.51	0.46
1:A:933:G:OP2	8:G:3:ARG:HB2	2.16	0.46
1:A:1053:G:O2'	1:A:1199:U:H5	1.98	0.46
1:A:1366:C:O2'	11:J:60:ARG:NH2	2.49	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.81	0.46
1:A:1448:C:H2'	1:A:1449:C:C6	2.51	0.46
3:B:15:VAL:HG11	3:B:210:SER:HA	1.97	0.46
4:C:105:GLU:HG2	4:C:106:VAL:N	2.31	0.46
8:G:41:ARG:O	8:G:42:ILE:C	2.54	0.46
8:G:129:GLU:HB3	8:G:131:LYS:HE2	1.96	0.46
20:S:12:ASP:HB3	20:S:14:HIS:CD2	2.51	0.46
21:T:57:ARG:HG2	21:T:57:ARG:NH1	2.30	0.46
1:A:190(L):U:H3	21:T:105:SER:CB	2.29	0.46
1:A:302:G:N3	1:A:556:C:H4'	2.31	0.46
1:A:321:A:H2'	1:A:322:C:C6	2.50	0.46
1:A:451:A:OP1	1:A:481:G:N2	2.49	0.46
1:A:491:G:O2'	1:A:492:G:H5'	2.16	0.46
1:A:613:C:H2'	1:A:614:A:H8	1.81	0.46
1:A:677:U:O2	1:A:777:A:O2'	2.32	0.46
1:A:996:A:N1	1:A:1045:C:O2'	2.48	0.46
1:A:1028:C:H2'	1:A:1029:C:C6	2.51	0.46
1:A:1060:C:C5	4:C:2:GLY:HA2	2.50	0.46
1:A:1231:G:H4'	10:I:126:SER:CB	2.45	0.46
1:A:1300:G:O2'	1:A:1301:U:H6	1.99	0.46
1:A:1364:U:HO2'	1:A:1365:G:H5"	1.80	0.46
1:A:1430:C:H2'	1:A:1431:C:H6	1.81	0.46
3:B:19:HIS:CD2	3:B:205:ASP:OD1	2.69	0.46
3:B:204:ASN:ND2	3:B:206:ASP:N	2.64	0.46
4:C:23:TYR:CG	11:J:95:GLU:HB2	2.51	0.46
6:E:93:PRO:HG2	9:H:105:ARG:NH2	2.31	0.46
13:L:81:SER:O	13:L:106:ASP:OD1	2.34	0.46
1:A:1061:G:O2'	1:A:1062:U:H5'	2.16	0.45
1:A:1229:A:H2'	1:A:1230:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:G:H5"	10:I:126:SER:CB	2.46	0.45
4:C:204:LEU:O	4:C:205:GLY:C	2.54	0.45
5:D:190:ASP:O	5:D:194:LEU:HD23	2.16	0.45
7:F:74:ASP:HA	7:F:77:ARG:HD2	1.99	0.45
11:J:69:ASN:O	11:J:70:ARG:CD	2.63	0.45
17:P:51:VAL:O	17:P:51:VAL:CG1	2.64	0.45
19:R:18:ARG:HA	19:R:21:LYS:NZ	2.31	0.45
20:S:25:LYS:HD2	20:S:25:LYS:N	2.31	0.45
22:V:14:TRP:C	22:V:16:GLY:H	2.19	0.45
1:A:281:G:O2'	1:A:282:A:C8	2.70	0.45
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.45
1:A:1256:A:O2'	1:A:1257:U:P	2.75	0.45
1:A:1316:G:H4'	15:N:18:VAL:CG1	2.46	0.45
1:A:1483:A:H2'	1:A:1484:C:O4'	2.16	0.45
4:C:7:PRO:HG2	4:C:184:TYR:CB	2.45	0.45
5:D:16:GLY:O	5:D:33:MET:HE2	2.16	0.45
5:D:17:VAL:HG11	5:D:197:PRO:HG3	1.97	0.45
6:E:19:MET:CE	6:E:24:ARG:HH12	2.29	0.45
6:E:80:ILE:HD11	6:E:91:LEU:CD1	2.36	0.45
8:G:9:VAL:CG1	8:G:94:ARG:NH1	2.80	0.45
10:I:55:ALA:O	10:I:57:GLY:N	2.49	0.45
18:Q:45:HIS:CD2	18:Q:47:PRO:HG3	2.52	0.45
18:Q:86:GLU:HA	18:Q:86:GLU:OE1	2.16	0.45
1:A:858:G:O2'	1:A:859:A:H5'	2.17	0.45
1:A:1097:C:P	3:B:144:ARG:HH22	2.39	0.45
4:C:77:ILE:CG2	4:C:81:GLY:HA2	2.43	0.45
6:E:80:ILE:HD12	6:E:80:ILE:O	2.15	0.45
8:G:6:ARG:O	8:G:7:ALA:O	2.34	0.45
8:G:79:ARG:CG	8:G:84:ASN:OD1	2.65	0.45
9:H:116:LYS:HZ2	9:H:127:LEU:HB3	1.81	0.45
10:I:4:TYR:O	10:I:19:LEU:N	2.50	0.45
12:K:91:ARG:NH2	19:R:88:LYS:NZ	2.65	0.45
13:L:87:GLY:HA2	13:L:98:TYR:HA	1.99	0.45
16:O:29:VAL:HG12	16:O:85:LEU:HD11	1.97	0.45
16:O:42:HIS:O	16:O:45:VAL:O	2.33	0.45
19:R:34:TYR:CD1	19:R:35:ARG:HG3	2.51	0.45
1:A:55:A:O2'	1:A:56:U:H5'	2.17	0.45
1:A:602:A:O2'	1:A:603:U:H5'	2.17	0.45
1:A:989:C:O2	1:A:1216:G:N2	2.41	0.45
3:B:70:PHE:O	3:B:92:TYR:HA	2.17	0.45
4:C:130:VAL:O	4:C:134:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:154:SER:O	4:C:155:GLY:O	2.33	0.45
7:F:26:ILE:HG21	7:F:63:TYR:HE2	1.79	0.45
14:M:110:ARG:HH11	14:M:110:ARG:CG	2.29	0.45
1:A:186:C:O3'	21:T:82:SER:HB3	2.16	0.45
1:A:670:G:H2'	1:A:671:G:O4'	2.17	0.45
1:A:838:G:H2'	1:A:839:U:C5'	2.41	0.45
1:A:976:G:C8	1:A:1358:U:C2	3.05	0.45
1:A:1465:C:O2'	1:A:1466:C:H5'	2.17	0.45
4:C:167:TRP:HB3	4:C:168:ALA:H	1.44	0.45
5:D:7:PRO:HG2	5:D:10:ARG:HD2	1.98	0.45
7:F:10:LEU:CD1	7:F:59:TYR:HD2	2.28	0.45
8:G:59:LEU:CD1	8:G:63:LYS:HE2	2.46	0.45
8:G:145:ALA:C	8:G:147:ALA:N	2.70	0.45
15:N:26:ARG:HH11	15:N:47:LEU:CG	2.29	0.45
17:P:18:ARG:HD3	17:P:35:LYS:HD2	1.99	0.45
17:P:20:VAL:HG13	17:P:21:VAL:N	2.32	0.45
20:S:63:THR:HG22	20:S:64:GLU:H	1.79	0.45
1:A:228:A:H4'	17:P:62:VAL:HG11	1.98	0.45
1:A:734:G:H21	19:R:75:ILE:HD11	1.82	0.45
1:A:1201:A:HO2'	1:A:1202:G:P	2.40	0.45
1:A:1226:C:H5'	14:M:96:LEU:CD1	2.47	0.45
3:B:142:LEU:CB	3:B:146:GLN:HE21	2.25	0.45
4:C:29:TYR:OH	15:N:54:PRO:HG2	2.17	0.45
6:E:107:ARG:O	6:E:108:ALA:C	2.54	0.45
8:G:38:LEU:O	8:G:42:ILE:HG13	2.16	0.45
21:T:26:ASN:CB	21:T:71:THR:HG23	2.46	0.45
1:A:281:G:O2'	1:A:282:A:P	2.74	0.45
1:A:996:A:H2'	1:A:997:U:C6	2.52	0.45
1:A:1014:A:H4'	20:S:14:HIS:CE1	2.51	0.45
1:A:1491:G:C5	23:A:1545:PAR:H21	2.52	0.45
4:C:12:LEU:HD23	4:C:16:ARG:O	2.17	0.45
5:D:173:TRP:HB2	5:D:187:ARG:O	2.17	0.45
6:E:150:ARG:HG3	6:E:150:ARG:NH1	2.31	0.45
7:F:48:LEU:HD13	7:F:52:ILE:HG13	1.97	0.45
7:F:52:ILE:O	7:F:53:ALA:HB3	2.16	0.45
7:F:97:PHE:HB2	19:R:32:ARG:NH2	2.32	0.45
15:N:32:SER:OG	15:N:41:ARG:HG2	2.17	0.45
1:A:1283:G:O2'	1:A:1284:C:H5'	2.16	0.45
6:E:79:GLU:OE1	9:H:105:ARG:HD3	2.17	0.45
8:G:95:ARG:HG3	8:G:95:ARG:NH1	2.32	0.45
11:J:80:LYS:HA	11:J:83:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:34:ASP:C	12:K:36:ASP:H	2.20	0.45
14:M:116:THR:HG22	14:M:117:VAL:N	2.31	0.45
1:A:154:C:H2'	1:A:155:C:C6	2.52	0.45
1:A:198:G:OP2	1:A:198:G:H8	1.99	0.45
1:A:502:G:H2'	1:A:503:C:O4'	2.17	0.45
1:A:961:U:O2'	1:A:962:C:H5'	2.16	0.45
1:A:1006:C:H2'	1:A:1007:C:H6	1.82	0.45
1:A:1394:A:C5	1:A:1501:C:H4'	2.52	0.45
3:B:169:LYS:HD2	3:B:170:GLU:OE2	2.17	0.45
4:C:5:ILE:HD13	4:C:10:PHE:CB	2.45	0.45
4:C:142:MET:HA	4:C:142:MET:CE	2.46	0.45
12:K:33:THR:HG21	12:K:37:GLY:HA2	1.97	0.45
17:P:74:LEU:O	17:P:79:VAL:HG23	2.17	0.45
18:Q:96:GLN:O	18:Q:97:SER:HB3	2.15	0.45
22:V:3:LYS:HB3	22:V:14:TRP:CD1	2.51	0.45
1:A:190:C:H2'	1:A:190(A):C:H6	1.82	0.45
1:A:420:U:H2'	1:A:422:C:C5	2.51	0.45
1:A:889:A:N1	1:A:907:A:H5"	2.32	0.45
1:A:1152:A:H2'	1:A:1153:C:C6	2.51	0.45
1:A:1402:C:H2'	1:A:1403:C:O4'	2.17	0.45
10:I:3:GLN:HG3	10:I:20:ARG:CG	2.46	0.45
10:I:93:ARG:O	10:I:95:LYS:N	2.50	0.45
14:M:67:GLU:HB3	14:M:68:GLY:H	1.49	0.45
16:O:26:GLU:HG3	16:O:81:LEU:HG	1.98	0.45
17:P:67:THR:HG22	17:P:69:THR:H	1.82	0.45
18:Q:82:MET:O	18:Q:86:GLU:HB2	2.17	0.45
20:S:20:LEU:HD12	20:S:21:GLU:N	2.32	0.45
20:S:44:MET:O	20:S:47:HIS:HB2	2.17	0.45
1:A:308:C:H2'	1:A:309:G:H8	1.81	0.44
1:A:321:A:H62	1:A:328:C:H1'	1.82	0.44
1:A:656:C:O2'	16:O:28:GLN:OE1	2.34	0.44
1:A:663:A:O2'	1:A:664:G:H5'	2.17	0.44
1:A:1128:C:H5'	10:I:16:ARG:NH2	2.32	0.44
1:A:1250:A:C5'	10:I:68:GLY:N	2.80	0.44
7:F:31:GLU:O	7:F:33:TYR:N	2.51	0.44
9:H:1:MET:HG2	9:H:2:LEU:N	2.32	0.44
12:K:66:LEU:O	12:K:70:LYS:HG3	2.18	0.44
15:N:15:LYS:HB3	15:N:16:PHE:CE1	2.53	0.44
19:R:25:THR:O	19:R:25:THR:HG22	2.17	0.44
1:A:129(A):G:N3	1:A:190(E):U:C5'	2.80	0.44
1:A:154:C:H2'	1:A:155:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:C:H2'	1:A:335:C:H6	1.81	0.44
1:A:657:G:C4'	16:O:28:GLN:HG2	2.45	0.44
1:A:678:U:H4'	1:A:778:G:OP1	2.17	0.44
1:A:1027:C:H2'	1:A:1028:C:C6	2.52	0.44
1:A:1299:A:C8	1:A:1301:U:H1'	2.52	0.44
1:A:1318:A:O2'	20:S:37:ARG:HD2	2.17	0.44
3:B:74:LYS:CD	3:B:76:GLN:HB2	2.46	0.44
4:C:82:GLU:O	4:C:86:VAL:HG23	2.17	0.44
4:C:136:GLN:O	4:C:139:GLN:HB2	2.17	0.44
11:J:45:ARG:HG3	11:J:45:ARG:NH1	2.32	0.44
11:J:48:THR:HG23	11:J:62:HIS:CD2	2.52	0.44
12:K:25:TYR:CD2	12:K:88:GLY:HA2	2.51	0.44
12:K:34:ASP:O	12:K:36:ASP:N	2.51	0.44
13:L:27:LEU:C	13:L:29:GLY:N	2.67	0.44
20:S:15:LEU:HD12	20:S:16:LEU:N	2.32	0.44
21:T:39:LYS:HE3	21:T:55:ILE:HD11	1.99	0.44
21:T:56:MET:CE	21:T:88:VAL:HB	2.47	0.44
1:A:160:A:O2'	1:A:344:A:N6	2.50	0.44
1:A:202:U:H5"	1:A:203:U:OP2	2.17	0.44
1:A:1376:U:H2'	1:A:1377:A:C8	2.53	0.44
1:A:1491:G:O6	23:A:1545:PAR:H531	2.18	0.44
4:C:97:LYS:O	4:C:98:ASN:HB3	2.17	0.44
14:M:26:GLY:O	14:M:27:LYS:C	2.56	0.44
14:M:96:LEU:O	14:M:110:ARG:NH1	2.50	0.44
14:M:102:ARG:HD2	14:M:105:THR:OG1	2.17	0.44
1:A:42:G:H2'	1:A:43:C:H6	1.83	0.44
1:A:1347:G:H22	1:A:1373:G:H2'	1.81	0.44
1:A:1448:C:H2'	1:A:1449:C:H6	1.82	0.44
3:B:189:ASP:OD1	3:B:205:ASP:HB3	2.18	0.44
5:D:3:ARG:NH2	5:D:71:SER:H	2.14	0.44
5:D:8:VAL:HG12	5:D:21:LEU:HD12	1.99	0.44
14:M:11:ARG:CG	14:M:12:ASN:N	2.80	0.44
14:M:84:ILE:O	14:M:86:CYS:N	2.50	0.44
18:Q:104:LYS:HA	18:Q:104:LYS:CE	2.29	0.44
19:R:21:LYS:N	19:R:21:LYS:CD	2.80	0.44
21:T:46:GLU:HB3	21:T:48:LYS:HG3	1.99	0.44
1:A:92:C:O2'	1:A:93:G:H5'	2.17	0.44
1:A:1070:U:H4'	6:E:25:ARG:HH21	1.83	0.44
1:A:1127:G:N2	1:A:1145:C:N3	2.65	0.44
1:A:1371:G:O3'	10:I:69:GLY:HA3	2.17	0.44
1:A:1502:A:C2	1:A:1505:G:N1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:68:ILE:N	3:B:90:MET:HE3	2.32	0.44
4:C:195:VAL:CG1	4:C:196:LEU:N	2.80	0.44
8:G:31:MET:HB2	8:G:39:ALA:CB	2.48	0.44
11:J:9:ARG:NH1	11:J:9:ARG:CB	2.80	0.44
12:K:111:ASP:OD1	19:R:84:LYS:HE2	2.16	0.44
18:Q:45:HIS:HB2	18:Q:65:ILE:CD1	2.47	0.44
19:R:24:ALA:O	19:R:26:LEU:N	2.49	0.44
21:T:67:ALA:HA	21:T:73:HIS:N	2.22	0.44
1:A:232:G:H1'	1:A:262:A:N1	2.33	0.44
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.44
1:A:954:G:H2'	1:A:955:U:C6	2.53	0.44
1:A:1039:C:O2'	1:A:1040:U:H5'	2.17	0.44
3:B:25:ASN:C	3:B:25:ASN:ND2	2.71	0.44
3:B:114:ARG:NH1	3:B:118:LEU:HD11	2.32	0.44
3:B:129:GLU:H	3:B:135:GLN:NE2	2.15	0.44
4:C:139:GLN:O	4:C:140:ARG:C	2.56	0.44
8:G:44:TYR:O	8:G:47:CYS:HB2	2.18	0.44
9:H:117:GLY:O	9:H:119:LEU:HG	2.18	0.44
10:I:118:LYS:HB3	10:I:118:LYS:HE2	1.70	0.44
19:R:87:ARG:O	19:R:88:LYS:HB3	2.18	0.44
20:S:13:ASP:OD2	20:S:13:ASP:N	2.49	0.44
1:A:187:C:N3	21:T:105:SER:CB	2.69	0.44
1:A:370:C:O2'	1:A:371:G:H5'	2.18	0.44
1:A:440:A:H3'	1:A:442:C:C6	2.53	0.44
1:A:650:G:O2'	1:A:651:C:H5'	2.17	0.44
1:A:1064:G:C4'	1:A:1065:U:H5"	2.41	0.44
1:A:1393:U:O4'	1:A:1502:A:H5'	2.18	0.44
1:A:1478:C:O2'	1:A:1479:C:H5'	2.18	0.44
1:A:1496:C:H2'	1:A:1497:G:O4'	2.18	0.44
1:A:1511:G:H2'	1:A:1512:U:O4'	2.17	0.44
3:B:162:ILE:HD12	3:B:177:ALA:HB2	1.99	0.44
3:B:204:ASN:C	3:B:204:ASN:ND2	2.67	0.44
5:D:17:VAL:CG1	5:D:18:LYS:N	2.80	0.44
8:G:15:ASP:HB3	8:G:20:ASP:H	1.83	0.44
8:G:137:LYS:O	8:G:138:LYS:C	2.56	0.44
12:K:16:SER:HA	12:K:79:SER:O	2.16	0.44
12:K:50:TYR:CD1	12:K:60:ALA:HB2	2.52	0.44
13:L:83:VAL:CG2	13:L:100:ILE:HG23	2.48	0.44
22:V:2:GLY:C	22:V:4:GLY:N	2.68	0.44
1:A:186:C:H2'	1:A:187:C:C6	2.53	0.44
1:A:723:U:O2	1:A:723:U:H2'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:H2'	1:A:978:A:H5"	1.99	0.44
1:A:1312:G:O2'	1:A:1313:U:H5'	2.18	0.44
1:A:1342:C:O2'	1:A:1343:G:H5'	2.18	0.44
1:A:1372:U:C2'	1:A:1373:G:H5'	2.48	0.44
1:A:1533:C:O2	1:A:1533:C:H2'	2.17	0.44
4:C:6:HIS:HD2	4:C:8:ILE:N	2.16	0.44
6:E:12:LEU:CD1	6:E:31:LEU:HD12	2.47	0.44
6:E:13:ILE:HG22	6:E:30:ALA:CB	2.48	0.44
6:E:143:ARG:NH1	9:H:77:GLU:CD	2.71	0.44
8:G:23:VAL:HG12	8:G:27:ILE:CD1	2.48	0.44
10:I:48:GLU:OE1	10:I:48:GLU:HA	2.18	0.44
11:J:19:SER:O	11:J:22:LYS:N	2.50	0.44
11:J:86:MET:N	11:J:86:MET:SD	2.89	0.44
17:P:20:VAL:HG11	17:P:32:TYR:CB	2.48	0.44
1:A:533:A:O2'	1:A:534:U:P	2.76	0.44
1:A:960:U:O2'	1:A:1223:C:H4'	2.18	0.44
1:A:1190:G:O2'	1:A:1191:A:P	2.76	0.44
1:A:1492:A:OP1	13:L:47:LYS:N	2.51	0.44
3:B:59:GLU:HG2	3:B:221:LEU:CD1	2.44	0.44
6:E:33:VAL:HG12	6:E:112:LEU:HD12	1.98	0.44
10:I:23:ASN:HD22	10:I:23:ASN:C	2.20	0.44
11:J:60:ARG:HD2	11:J:60:ARG:HA	1.78	0.44
13:L:70:ILE:CD1	13:L:77:LEU:HD12	2.44	0.44
15:N:21:TYR:HE2	15:N:23:ARG:NE	2.16	0.44
21:T:79:ARG:HH11	21:T:79:ARG:CG	2.31	0.44
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.43
1:A:180:U:H2'	1:A:181:G:H5'	2.00	0.43
1:A:428:G:O2'	1:A:429:U:P	2.76	0.43
1:A:1057:G:H5"	4:C:154:SER:OG	2.17	0.43
1:A:1243:C:H2'	1:A:1244:C:C6	2.53	0.43
1:A:1508:G:H2'	1:A:1509:C:H6	1.83	0.43
3:B:53:ARG:NH1	3:B:199:TYR:CD2	2.86	0.43
3:B:82:ARG:HG2	3:B:86:GLU:CD	2.38	0.43
3:B:126:GLU:HA	3:B:129:GLU:CD	2.38	0.43
4:C:191:THR:HG21	4:C:193:TYR:CE2	2.53	0.43
6:E:15:ARG:O	6:E:16:THR:O	2.36	0.43
14:M:80:ARG:HG2	14:M:81:LEU:N	2.32	0.43
17:P:20:VAL:HG13	17:P:32:TYR:HB2	2.00	0.43
1:A:280:C:O2	18:Q:38:ARG:HG3	2.17	0.43
1:A:851:G:H2'	1:A:852:G:H8	1.83	0.43
1:A:1234:C:H5'	1:A:1365:G:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:A:H2'	1:A:1334:G:O4'	2.18	0.43
1:A:1437:C:H2'	1:A:1438:G:H8	1.83	0.43
3:B:12:GLU:OE1	3:B:12:GLU:CA	2.63	0.43
4:C:83:ARG:C	4:C:85:ARG:N	2.72	0.43
4:C:128:PHE:N	4:C:128:PHE:CD1	2.86	0.43
5:D:3:ARG:NE	5:D:71:SER:H	2.15	0.43
9:H:60:ARG:CG	9:H:60:ARG:NH1	2.81	0.43
9:H:126:LYS:C	9:H:128:GLY:N	2.72	0.43
12:K:100:ALA:O	12:K:101:SER:O	2.35	0.43
13:L:55:VAL:HG12	13:L:56:ALA:N	2.33	0.43
14:M:45:VAL:O	14:M:48:LEU:HB2	2.18	0.43
18:Q:67:LYS:O	18:Q:68:ARG:CB	2.67	0.43
19:R:52:PRO:HD2	19:R:55:ARG:HG3	2.01	0.43
20:S:8:GLY:O	20:S:9:VAL:C	2.56	0.43
1:A:475:G:H2'	1:A:476:G:H8	1.83	0.43
1:A:484:G:O2'	1:A:485:G:OP2	2.32	0.43
1:A:1207:G:H2'	1:A:1208:C:C6	2.53	0.43
3:B:178:ARG:NH2	9:H:68:ARG:NH2	2.64	0.43
4:C:188:LEU:HD13	4:C:189:ALA:H	1.83	0.43
5:D:107:ARG:HB3	5:D:174:LEU:HD11	2.00	0.43
7:F:48:LEU:HD13	7:F:52:ILE:CG1	2.48	0.43
8:G:12:LEU:H	8:G:12:LEU:CD1	2.21	0.43
9:H:23:SER:O	9:H:24:THR:HB	2.18	0.43
10:I:93:ARG:CG	10:I:97:LYS:HE3	2.49	0.43
11:J:61:GLU:OE1	15:N:45:ARG:HD2	2.18	0.43
12:K:14:VAL:O	12:K:15:ALA:HB3	2.18	0.43
17:P:43:LYS:HG3	17:P:48:TRP:CE2	2.53	0.43
20:S:5:LEU:O	20:S:6:LYS:CE	2.66	0.43
1:A:103:C:P	21:T:17:ARG:HH11	2.41	0.43
1:A:496:A:H4'	1:A:497:A:OP1	2.18	0.43
1:A:502:G:C1'	1:A:550:G:H5'	2.48	0.43
1:A:738:C:P	7:F:92:LYS:HE3	2.58	0.43
1:A:1390:U:H2'	1:A:1391:U:C6	2.53	0.43
1:A:1451:A:O2'	1:A:1452:C:OP1	2.34	0.43
5:D:120:LEU:HD23	5:D:120:LEU:HA	1.87	0.43
10:I:97:LYS:N	10:I:98:PRO:CD	2.80	0.43
12:K:24:SER:C	12:K:26:ASN:H	2.21	0.43
21:T:46:GLU:HG2	21:T:48:LYS:HZ2	1.80	0.43
1:A:39:G:O2'	1:A:40:C:H5'	2.18	0.43
1:A:80:G:C3'	1:A:81:U:C5'	2.93	0.43
1:A:481:G:C2'	1:A:482:A:N7	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:G:O2'	1:A:594:G:H5'	2.18	0.43
1:A:683:G:H2'	1:A:684:A:C8	2.54	0.43
4:C:37:GLN:O	4:C:38:ARG:C	2.56	0.43
4:C:188:LEU:HD13	4:C:195:VAL:CG1	2.45	0.43
5:D:199:GLN:NE2	5:D:201:ASN:HB2	2.34	0.43
6:E:43:LEU:HD11	6:E:132:ALA:HB1	2.00	0.43
7:F:40:VAL:HG22	7:F:41:GLU:N	2.34	0.43
13:L:46:LYS:HD2	13:L:47:LYS:CD	2.41	0.43
14:M:44:ARG:NH1	14:M:44:ARG:HG3	2.32	0.43
14:M:44:ARG:HB3	14:M:46:LYS:HG3	2.00	0.43
15:N:44:LEU:O	15:N:48:ALA:HB2	2.18	0.43
1:A:160:A:H1'	1:A:344:A:C5	2.53	0.43
1:A:234:C:H2'	1:A:235:C:H6	1.84	0.43
1:A:262:A:C6	1:A:263:A:C6	3.06	0.43
1:A:1102:A:H2'	1:A:1103:C:H6	1.84	0.43
1:A:1152:A:C6	1:A:1153:C:C4	3.06	0.43
1:A:1404:C:H2'	1:A:1405:G:C8	2.54	0.43
1:A:1521:G:H2'	1:A:1522:U:H6	1.82	0.43
7:F:25:ILE:HD12	7:F:82:ARG:HD2	2.01	0.43
10:I:111:ARG:HD2	10:I:113:LYS:HD2	2.01	0.43
13:L:41:ARG:CG	13:L:42:THR:H	2.21	0.43
14:M:49:THR:HG22	14:M:51:ALA:N	2.34	0.43
14:M:116:THR:CG2	14:M:117:VAL:N	2.82	0.43
1:A:294:U:H2'	1:A:295:C:C6	2.54	0.43
1:A:338:A:H2	1:A:351:G:H22	1.65	0.43
1:A:404:U:H2'	1:A:405:U:C6	2.54	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.18	0.43
1:A:622:A:H3'	1:A:623:C:H6	1.84	0.43
1:A:761:G:O2'	18:Q:103:GLY:O	2.33	0.43
1:A:865:A:H5'	1:A:1078:U:C4	2.54	0.43
1:A:1498:U:C4'	1:A:1519:A:H2	2.32	0.43
3:B:113:HIS:O	3:B:117:GLU:HG3	2.18	0.43
4:C:89:GLU:O	4:C:93:LYS:HG2	2.19	0.43
5:D:148:VAL:HG13	5:D:158:ILE:HD13	2.00	0.43
7:F:27:GLN:HA	7:F:27:GLN:NE2	2.34	0.43
9:H:51:VAL:HG12	9:H:52:ASP:N	2.34	0.43
11:J:85:LEU:O	11:J:87:THR:N	2.51	0.43
14:M:2:ALA:O	14:M:10:PRO:HD2	2.18	0.43
14:M:5:ALA:HB3	14:M:8:GLU:CB	2.49	0.43
14:M:49:THR:O	14:M:52:GLU:N	2.52	0.43
1:A:35:G:H2'	1:A:36:C:H6	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:G:O2'	1:A:168:G:H5'	2.18	0.43
1:A:428:G:HO2'	1:A:429:U:P	2.42	0.43
1:A:429:U:H1'	1:A:430:A:H5"	1.99	0.43
1:A:1026:G:H2'	1:A:1027:C:H5'	2.00	0.43
1:A:1129:C:O2'	1:A:1130:A:P	2.77	0.43
1:A:1516:G:H2'	1:A:1518:A:OP2	2.19	0.43
4:C:44:GLU:HA	4:C:52:LEU:HD12	2.01	0.43
5:D:111:ALA:HB2	5:D:120:LEU:HD12	2.00	0.43
7:F:100:ASN:ND2	19:R:23:LYS:HG2	2.24	0.43
11:J:16:LEU:O	11:J:17:ASP:C	2.56	0.43
11:J:45:ARG:NH1	15:N:36:PHE:CE2	2.87	0.43
17:P:11:SER:O	17:P:12:LYS:C	2.56	0.43
1:A:848:C:O2'	1:A:849:C:H5'	2.18	0.43
1:A:1229:A:H2'	1:A:1230:C:C6	2.54	0.43
5:D:13:ARG:HB3	5:D:38:TYR:O	2.18	0.43
5:D:76:ARG:HG2	5:D:76:ARG:HH11	1.84	0.43
5:D:105:VAL:HG21	5:D:126:ILE:HG13	2.00	0.43
7:F:8:ILE:HD11	7:F:79:LEU:HD13	2.01	0.43
7:F:31:GLU:C	7:F:33:TYR:H	2.22	0.43
8:G:12:LEU:HD12	8:G:12:LEU:N	2.29	0.43
8:G:116:ALA:HA	8:G:119:ARG:NH2	2.33	0.43
10:I:23:ASN:C	10:I:23:ASN:ND2	2.71	0.43
13:L:43:VAL:CG1	13:L:93:LEU:HD22	2.49	0.43
17:P:52:ASP:OD2	17:P:52:ASP:C	2.57	0.43
20:S:9:VAL:O	20:S:9:VAL:HG12	2.17	0.43
1:A:645:C:H2'	1:A:646:U:C6	2.54	0.43
1:A:738:C:OP1	7:F:92:LYS:HE3	2.19	0.43
1:A:807:A:H2'	1:A:808:C:C6	2.54	0.43
1:A:1085:U:O3'	1:A:1086:U:C6	2.71	0.43
1:A:1104:G:P	3:B:111:ARG:HD2	2.58	0.43
1:A:1226:C:H5'	14:M:96:LEU:HD13	2.00	0.43
1:A:1288:A:O4'	1:A:1353:G:H4'	2.19	0.43
3:B:88:ALA:HB2	3:B:219:VAL:HG13	2.00	0.43
3:B:126:GLU:HG2	3:B:129:GLU:CD	2.39	0.43
5:D:149:ALA:HB3	5:D:152:SER:CB	2.49	0.43
9:H:86:ILE:O	9:H:88:LYS:HG3	2.19	0.43
9:H:89:PRO:C	9:H:91:ARG:H	2.22	0.43
12:K:21:ILE:HD13	12:K:94:ALA:CB	2.49	0.43
15:N:44:LEU:HD12	15:N:44:LEU:C	2.39	0.43
17:P:43:LYS:HD2	17:P:43:LYS:N	2.33	0.43
1:A:190:C:H2'	1:A:190(A):C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:C:O2'	1:A:1061:G:H5'	2.18	0.42
1:A:1149:C:P	10:I:9:ARG:NH1	2.92	0.42
1:A:1262:C:H42	1:A:1273:G:H1	1.67	0.42
1:A:1438:G:H2'	1:A:1439:C:H6	1.83	0.42
3:B:13:ALA:C	3:B:15:VAL:H	2.23	0.42
3:B:16:HIS:HE1	3:B:213:LEU:HB3	1.83	0.42
4:C:26:LYS:HE2	11:J:45:ARG:NH1	2.33	0.42
5:D:119:GLN:CG	5:D:123:HIS:CD2	3.02	0.42
5:D:149:ALA:HB3	5:D:152:SER:HB2	2.01	0.42
10:I:9:ARG:HA	10:I:13:ALA:O	2.19	0.42
11:J:28:ARG:NH1	11:J:28:ARG:HG2	2.34	0.42
12:K:69:ALA:O	12:K:72:ALA:HB3	2.19	0.42
15:N:41:ARG:HG2	15:N:41:ARG:NH1	2.33	0.42
19:R:75:ILE:C	19:R:77:GLY:H	2.22	0.42
21:T:98:PRO:O	21:T:100:ILE:HG13	2.19	0.42
1:A:129(A):G:O2'	1:A:130:A:OP2	2.38	0.42
1:A:345:C:H4'	1:A:346:G:O5'	2.19	0.42
1:A:583:A:H2'	1:A:584:G:O4'	2.19	0.42
1:A:594:G:O2'	1:A:595:G:H5'	2.18	0.42
1:A:1315:U:H2'	1:A:1316:G:O4'	2.19	0.42
3:B:34:ALA:O	3:B:41:ILE:HB	2.19	0.42
5:D:24:GLU:O	5:D:27:TYR:HB2	2.19	0.42
9:H:114:THR:HG21	9:H:129:VAL:HG23	2.01	0.42
11:J:45:ARG:HB2	11:J:65:LEU:HB3	2.01	0.42
11:J:96:ILE:HG22	11:J:97:GLU:N	2.33	0.42
14:M:5:ALA:HB3	14:M:8:GLU:HB2	2.00	0.42
21:T:14:LYS:HE2	21:T:18:GLN:HE22	1.84	0.42
1:A:194:C:H2'	1:A:195:A:H5"	2.00	0.42
1:A:411:A:OP2	5:D:25:ARG:NH2	2.52	0.42
1:A:582:U:H1'	1:A:760:G:O6	2.19	0.42
1:A:1190:G:O2'	1:A:1191:A:OP2	2.36	0.42
1:A:1202:G:H1'	15:N:29:ARG:HD2	2.02	0.42
1:A:1221:G:OP1	20:S:36:ARG:HD3	2.19	0.42
1:A:1316:G:N2	1:A:1318:A:H3'	2.34	0.42
3:B:223:ILE:HG22	3:B:224:GLN:N	2.34	0.42
4:C:13:GLY:CA	15:N:57:ARG:CZ	2.96	0.42
4:C:29:TYR:CZ	15:N:54:PRO:HG2	2.55	0.42
4:C:73:PRO:HD3	4:C:105:GLU:HG3	2.02	0.42
5:D:55:ALA:O	5:D:59:ARG:HG2	2.19	0.42
5:D:104:VAL:HG11	5:D:146:ILE:HD12	2.01	0.42
6:E:51:VAL:CB	6:E:52:PRO:HD3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:53:VAL:HB	9:H:58:TYR:CE1	2.54	0.42
10:I:93:ARG:HG2	10:I:97:LYS:HE3	2.01	0.42
11:J:8:LEU:HD23	11:J:96:ILE:HG23	2.01	0.42
1:A:440:A:H3'	1:A:442:C:H6	1.85	0.42
1:A:694:A:H5'	12:K:53:SER:HB2	2.00	0.42
1:A:706:A:C1'	12:K:29:ILE:HD11	2.49	0.42
1:A:1172:C:O2'	1:A:1173:G:H5'	2.19	0.42
1:A:1331:G:HO2'	1:A:1332:A:P	2.42	0.42
3:B:83:MET:O	3:B:86:GLU:HB2	2.20	0.42
3:B:144:ARG:O	3:B:147:LYS:N	2.50	0.42
4:C:62:ASP:HA	4:C:97:LYS:CD	2.49	0.42
4:C:91:LEU:HD23	4:C:92:ALA:N	2.34	0.42
4:C:134:ILE:HG22	4:C:168:ALA:CB	2.49	0.42
9:H:138:TRP:HE3	9:H:138:TRP:OXT	2.02	0.42
11:J:29:ARG:HB2	11:J:84:GLN:HE22	1.85	0.42
12:K:59:TYR:C	12:K:61:ALA:N	2.72	0.42
12:K:80:VAL:HG12	12:K:81:ASP:N	2.34	0.42
1:A:325:A:OP2	21:T:70:SER:HB2	2.20	0.42
1:A:333:G:H4'	21:T:16:HIS:CD2	2.55	0.42
1:A:590:C:O2'	1:A:591:U:H5'	2.19	0.42
1:A:908:A:H2'	1:A:909:A:C8	2.54	0.42
1:A:1049:U:H5	15:N:2:ALA:N	2.14	0.42
1:A:1296:C:H4'	1:A:1302:U:C4	2.54	0.42
1:A:1301:U:HO2'	1:A:1302:U:P	2.41	0.42
1:A:1509:C:O2'	1:A:1510:U:H5'	2.19	0.42
3:B:10:LEU:O	3:B:11:LEU:C	2.57	0.42
3:B:123:ALA:O	3:B:124:SER:HB3	2.20	0.42
3:B:235:SER:O	3:B:238:LEU:HB2	2.18	0.42
4:C:52:LEU:HG	4:C:52:LEU:O	2.19	0.42
7:F:101:ALA:CB	19:R:28:GLU:HB2	2.49	0.42
14:M:11:ARG:HA	14:M:45:VAL:HB	2.01	0.42
14:M:85:GLY:O	14:M:86:CYS:C	2.58	0.42
19:R:40:LEU:O	19:R:41:LYS:C	2.58	0.42
19:R:58:LEU:HB3	19:R:59:SER:H	1.67	0.42
20:S:12:ASP:HB2	20:S:35:SER:OG	2.20	0.42
1:A:302:G:H5"	13:L:17:LYS:HE2	2.01	0.42
1:A:413:G:H2'	1:A:428:G:N2	2.34	0.42
1:A:553:A:H2'	1:A:554:C:C6	2.54	0.42
1:A:605:U:O2'	1:A:606:G:H5'	2.20	0.42
1:A:1279:A:C5'	1:A:1280:A:OP1	2.57	0.42
8:G:38:LEU:HD12	8:G:38:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:48:GLU:N	10:I:49:PRO:CD	2.82	0.42
10:I:65:VAL:O	10:I:65:VAL:CG1	2.67	0.42
13:L:28:LYS:O	13:L:30:ALA:N	2.53	0.42
16:O:25:THR:HG21	16:O:70:LEU:HD23	2.02	0.42
19:R:87:ARG:HB3	19:R:88:LYS:H	1.64	0.42
20:S:62:ILE:HD12	20:S:63:THR:N	2.35	0.42
1:A:75:G:H2'	1:A:76:C:C6	2.54	0.42
1:A:190(E):U:O2'	18:Q:63:ARG:NH2	2.53	0.42
1:A:244:U:O4	1:A:906:G:H1'	2.20	0.42
1:A:452:A:OP1	17:P:43:LYS:NZ	2.51	0.42
1:A:675:A:H1'	12:K:116:HIS:CD2	2.55	0.42
1:A:959:A:C2	1:A:1222:G:O4'	2.72	0.42
1:A:1107:C:C4	1:A:1108:G:C8	3.07	0.42
3:B:87:ARG:HB2	3:B:219:VAL:HG11	2.01	0.42
5:D:17:VAL:HG11	5:D:197:PRO:CG	2.50	0.42
8:G:101:LEU:HD23	8:G:101:LEU:N	2.35	0.42
8:G:108:ALA:HA	8:G:111:ARG:HD2	2.01	0.42
10:I:4:TYR:CE1	10:I:88:TYR:HD1	2.37	0.42
10:I:40:LEU:O	10:I:41:VAL:C	2.58	0.42
12:K:109:VAL:HG13	19:R:85:LEU:O	2.20	0.42
14:M:87:TYR:CZ	14:M:91:ARG:HD3	2.55	0.42
20:S:28:LYS:HB3	20:S:31:ILE:HD11	2.02	0.42
1:A:67:C:O2'	1:A:171:A:H1'	2.19	0.42
1:A:248:C:C2'	1:A:249:U:H5'	2.50	0.42
1:A:266:G:O2'	1:A:267:C:P	2.78	0.42
1:A:373:A:C1'	1:A:481:G:O2'	2.68	0.42
1:A:737:A:H2'	1:A:738:C:C6	2.55	0.42
1:A:792:A:C4	1:A:794:A:C5	3.08	0.42
1:A:1202:G:C2	15:N:42:ILE:HG21	2.55	0.42
1:A:1277:C:HO2'	1:A:1278:U:H5'	1.85	0.42
1:A:1342:C:O2'	10:I:124:GLN:HB2	2.20	0.42
6:E:43:LEU:HD23	6:E:43:LEU:HA	1.82	0.42
6:E:80:ILE:HG22	9:H:104:ARG:HH12	1.83	0.42
8:G:41:ARG:O	8:G:43:PHE:N	2.53	0.42
12:K:43:SER:O	12:K:44:SER:HB3	2.19	0.42
13:L:27:LEU:HD13	13:L:64:TYR:CE1	2.54	0.42
1:A:114:U:H2'	1:A:115:G:C8	2.55	0.42
1:A:774:G:O2'	1:A:775:G:H5'	2.20	0.42
1:A:983:A:HO2'	1:A:1049:U:HO2'	1.67	0.42
1:A:1152:A:H2'	1:A:1153:C:H6	1.85	0.42
1:A:1306:A:O2'	14:M:109:THR:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:C:H2'	1:A:1327:C:C6	2.55	0.42
1:A:1480:G:O2'	1:A:1481:U:H5'	2.19	0.42
3:B:33:TYR:O	3:B:34:ALA:HB2	2.19	0.42
3:B:60:ASP:HA	3:B:64:ARG:NH2	2.35	0.42
8:G:85:TYR:HD1	8:G:154:TYR:HE1	1.66	0.42
9:H:38:ILE:N	9:H:38:ILE:CD1	2.82	0.42
21:T:68:LYS:HD2	21:T:68:LYS:HA	1.79	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.42
1:A:1293:G:O2'	1:A:1294:G:H5'	2.20	0.42
1:A:1346:A:C4	8:G:10:ARG:NH2	2.88	0.42
3:B:178:ARG:HH21	9:H:68:ARG:HH22	1.62	0.42
3:B:184:VAL:N	3:B:198:ASP:OD2	2.52	0.42
5:D:81:GLU:O	5:D:85:LYS:HG3	2.18	0.42
10:I:65:VAL:O	10:I:65:VAL:HG12	2.20	0.42
11:J:78:ASN:H	11:J:81:THR:CB	2.32	0.42
11:J:78:ASN:H	11:J:81:THR:HB	1.84	0.42
14:M:11:ARG:CG	14:M:12:ASN:H	2.33	0.42
19:R:26:LEU:HB2	19:R:42:ARG:HH12	1.85	0.42
21:T:81:LYS:O	21:T:85:MET:HG3	2.20	0.42
1:A:60:A:N1	1:A:107:G:O2'	2.45	0.41
1:A:792:A:H4'	1:A:793:U:C5'	2.50	0.41
1:A:1064:G:H4'	1:A:1065:U:OP1	2.20	0.41
1:A:1072:G:C5	1:A:1073:U:C4	3.08	0.41
1:A:1230:C:O2'	1:A:1231:G:H5'	2.20	0.41
1:A:1476:G:O2'	1:A:1477:C:H5'	2.20	0.41
3:B:107:THR:C	3:B:109:SER:N	2.72	0.41
11:J:28:ARG:HG2	11:J:28:ARG:HH11	1.85	0.41
12:K:98:LEU:O	12:K:99:GLN:C	2.58	0.41
16:O:85:LEU:HD13	16:O:87:ILE:HD11	2.02	0.41
18:Q:67:LYS:O	18:Q:68:ARG:HB3	2.20	0.41
1:A:264:U:H4'	18:Q:63:ARG:HD3	2.01	0.41
1:A:481:G:H2'	1:A:482:A:N7	2.35	0.41
1:A:533:A:C2'	1:A:535:A:OP2	2.67	0.41
1:A:686:U:O4	1:A:703:G:H1'	2.20	0.41
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.41
3:B:53:ARG:NH1	3:B:199:TYR:HD2	2.17	0.41
3:B:209:ARG:HH11	3:B:209:ARG:HG2	1.85	0.41
4:C:72:LYS:O	4:C:75:VAL:HG23	2.20	0.41
12:K:19:ALA:HB2	12:K:80:VAL:CG1	2.41	0.41
13:L:30:ALA:HA	13:L:31:PRO:HD3	1.84	0.41
1:A:279:A:H4'	1:A:280:C:OP2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:G:H2'	1:A:1088:G:C8	2.55	0.41
1:A:1154:G:H2'	1:A:1155:G:C8	2.54	0.41
1:A:1347:G:N7	10:I:10:ARG:NH2	2.68	0.41
25:A:1633:SCM:H32	6:E:21:ALA:O	2.20	0.41
3:B:154:LEU:O	3:B:155:LEU:C	2.59	0.41
4:C:91:LEU:HD21	4:C:99:VAL:HG13	2.01	0.41
6:E:19:MET:HE2	6:E:24:ARG:HH12	1.85	0.41
6:E:31:LEU:HD23	6:E:31:LEU:HA	1.80	0.41
8:G:111:ARG:HE	8:G:123:GLU:HB2	1.86	0.41
10:I:5:TYR:HE2	10:I:16:ARG:HB3	1.85	0.41
10:I:10:ARG:O	10:I:12:GLU:N	2.53	0.41
11:J:51:ARG:CB	11:J:59:SER:HB3	2.21	0.41
12:K:27:ASN:HD21	12:K:45:GLY:H	1.68	0.41
14:M:9:ILE:HD12	14:M:9:ILE:N	2.36	0.41
15:N:57:ARG:CG	15:N:58:LYS:N	2.81	0.41
17:P:17:TYR:HE1	17:P:41:PRO:HG2	1.85	0.41
19:R:22:VAL:HG23	19:R:55:ARG:O	2.19	0.41
20:S:40:ILE:HG22	20:S:67:VAL:HA	2.01	0.41
1:A:397:A:H3'	1:A:397:A:N3	2.34	0.41
1:A:411:A:C6	1:A:429:U:C4	3.08	0.41
1:A:691:G:O2'	1:A:797:C:H4'	2.20	0.41
1:A:761:G:H5"	18:Q:102:GLY:HA3	2.03	0.41
1:A:803:G:H2'	1:A:804:U:C6	2.56	0.41
1:A:975:A:O5'	1:A:976:G:H5'	2.20	0.41
1:A:1007:C:O2'	1:A:1008:C:H5'	2.20	0.41
1:A:1063:C:H3'	1:A:1064:G:H2'	2.02	0.41
1:A:1255:G:O2'	1:A:1258:G:H1'	2.21	0.41
1:A:1442:G:C5	1:A:1446:A:C6	3.09	0.41
3:B:13:ALA:O	3:B:15:VAL:N	2.53	0.41
3:B:88:ALA:HB1	3:B:90:MET:HG2	2.02	0.41
4:C:83:ARG:O	4:C:86:VAL:N	2.54	0.41
4:C:113:ALA:N	4:C:114:PRO:CD	2.83	0.41
4:C:120:VAL:O	4:C:124:ILE:HG13	2.20	0.41
5:D:108:LEU:HA	5:D:108:LEU:HD23	1.83	0.41
6:E:45:PHE:CD2	6:E:47:LYS:HE3	2.55	0.41
6:E:63:ARG:HE	6:E:63:ARG:HB2	1.58	0.41
7:F:25:ILE:HD12	7:F:82:ARG:HH11	1.85	0.41
9:H:42:GLU:HG3	9:H:109:ILE:HD13	2.02	0.41
10:I:12:GLU:HG2	10:I:12:GLU:O	2.20	0.41
11:J:45:ARG:O	11:J:64:GLU:HA	2.20	0.41
13:L:112:ASP:O	13:L:114:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:63:ARG:HG2	18:Q:64:PRO:HD2	2.02	0.41
18:Q:78:GLU:O	18:Q:78:GLU:HG3	2.20	0.41
1:A:22:G:H4'	1:A:885:G:C8	2.56	0.41
1:A:542:G:H5'	5:D:41:GLY:HA3	2.02	0.41
1:A:761:G:C5	18:Q:105:ALA:O	2.73	0.41
1:A:1190:G:C2'	1:A:1191:A:OP2	2.69	0.41
3:B:20:GLU:OE2	3:B:205:ASP:OD1	2.39	0.41
5:D:127:THR:HG23	5:D:147:ALA:O	2.20	0.41
5:D:177:ASP:OD1	5:D:179:GLU:HB2	2.21	0.41
6:E:24:ARG:HG2	6:E:24:ARG:HH11	1.85	0.41
7:F:26:ILE:O	7:F:29:ALA:HB3	2.21	0.41
8:G:69:VAL:HG12	8:G:69:VAL:O	2.20	0.41
9:H:36:LEU:HD12	9:H:59:LEU:HD13	2.02	0.41
9:H:104:ARG:CZ	9:H:138:TRP:CZ3	3.03	0.41
11:J:83:GLU:HA	11:J:83:GLU:OE1	2.20	0.41
12:K:91:ARG:CZ	19:R:88:LYS:HZ1	2.33	0.41
13:L:90:VAL:O	13:L:92:ASP:N	2.52	0.41
17:P:34:GLU:OE1	17:P:55:ARG:NH1	2.53	0.41
18:Q:9:VAL:CG2	18:Q:84:LEU:HD13	2.48	0.41
18:Q:68:ARG:N	18:Q:70:ARG:NH1	2.69	0.41
21:T:42:GLN:O	21:T:45:GLN:HB3	2.20	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.84	0.41
1:A:255:G:H2'	1:A:256:U:H6	1.86	0.41
1:A:385:C:H2'	1:A:386:C:C6	2.56	0.41
1:A:485:G:O2'	1:A:486:U:OP2	2.39	0.41
1:A:625:G:H4'	17:P:16:HIS:CD2	2.55	0.41
1:A:1072:G:H2'	1:A:1073:U:H6	1.79	0.41
3:B:27:LYS:O	3:B:194:PRO:HG3	2.20	0.41
4:C:174:PRO:CB	4:C:177:THR:HG22	2.45	0.41
5:D:68:TYR:N	5:D:68:TYR:CD1	2.88	0.41
10:I:111:ARG:HD3	10:I:112:LYS:N	2.36	0.41
13:L:69:TYR:HB2	13:L:90:VAL:HG21	2.02	0.41
19:R:29:PHE:CD2	19:R:29:PHE:N	2.88	0.41
19:R:53:ARG:HA	19:R:56:THR:OG1	2.20	0.41
1:A:315:A:O4'	1:A:353:A:C2	2.73	0.41
1:A:403:C:O2'	1:A:404:U:H5'	2.20	0.41
1:A:411:A:N9	1:A:413:G:H1'	2.36	0.41
1:A:456:C:O2'	1:A:457:C:H5'	2.21	0.41
1:A:481:G:O2'	1:A:482:A:N7	2.43	0.41
1:A:622:A:C8	1:A:623:C:C6	3.08	0.41
1:A:644:G:C5	1:A:645:C:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:A:H8	1:A:923:A:O5'	2.04	0.41
1:A:975:A:H4'	1:A:976:G:H5'	2.01	0.41
1:A:1129:C:O5'	1:A:1130:A:H5'	2.21	0.41
3:B:115:LEU:HD23	3:B:115:LEU:C	2.41	0.41
4:C:139:GLN:CA	4:C:139:GLN:HE21	2.31	0.41
7:F:39:LYS:HE3	7:F:62:TRP:HZ3	1.84	0.41
8:G:52:GLU:C	8:G:54:THR:H	2.23	0.41
8:G:113:GLU:CD	8:G:113:GLU:H	2.21	0.41
8:G:116:ALA:HA	8:G:119:ARG:CZ	2.51	0.41
18:Q:90:ILE:HA	18:Q:93:GLN:OE1	2.20	0.41
21:T:75:ASN:N	21:T:75:ASN:OD1	2.53	0.41
1:A:228:A:C4'	17:P:62:VAL:HG11	2.51	0.41
1:A:502:G:OP1	13:L:118:SER:HB3	2.20	0.41
1:A:525:C:OP1	13:L:89:ARG:HD3	2.20	0.41
1:A:538:G:H2'	1:A:539:A:C8	2.56	0.41
1:A:789:U:H2'	1:A:791:G:OP2	2.20	0.41
1:A:949:A:OP2	14:M:106:ASN:HB2	2.20	0.41
1:A:972:C:H4'	11:J:57:LYS:CG	2.51	0.41
1:A:1064:G:O4'	1:A:1065:U:H5'	2.21	0.41
1:A:1466:C:H2'	1:A:1467:G:O4'	2.21	0.41
3:B:137:ARG:O	3:B:140:HIS:HB2	2.21	0.41
3:B:224:GLN:HG2	3:B:225:ALA:H	1.85	0.41
4:C:7:PRO:CG	4:C:184:TYR:HB2	2.50	0.41
5:D:148:VAL:HG11	5:D:158:ILE:HD13	2.03	0.41
6:E:11:ILE:HG22	6:E:12:LEU:HD12	2.02	0.41
11:J:71:LEU:HA	11:J:71:LEU:HD23	1.86	0.41
14:M:57:ARG:CG	14:M:61:GLU:OE2	2.68	0.41
14:M:73:GLU:O	14:M:76:ALA:N	2.53	0.41
17:P:21:VAL:HG21	17:P:59:TRP:CG	2.55	0.41
18:Q:20:THR:HG21	18:Q:41:LYS:HD2	2.03	0.41
18:Q:60:ILE:HD13	18:Q:61:GLU:N	2.36	0.41
1:A:66:G:H4'	1:A:173:U:C5	2.56	0.41
1:A:119:A:C4'	1:A:120:A:O5'	2.69	0.41
1:A:204:U:H5'	1:A:216:G:OP1	2.21	0.41
1:A:578:C:H2'	1:A:579:G:O4'	2.21	0.41
1:A:849:C:O2'	1:A:850:U:H5'	2.20	0.41
1:A:926:G:H3'	1:A:1505:G:H21	1.85	0.41
1:A:934:C:C4	1:A:1345:U:C5	3.09	0.41
1:A:960:U:O2	1:A:960:U:H2'	2.20	0.41
1:A:1021:G:O2'	1:A:1022:G:H5'	2.21	0.41
1:A:1149:C:P	10:I:9:ARG:HH11	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:C:C2'	1:A:1166:G:H5'	2.50	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.55	0.41
3:B:151:GLY:C	3:B:153:ARG:H	2.23	0.41
4:C:20:SER:O	15:N:54:PRO:HB3	2.21	0.41
4:C:101:LEU:O	4:C:102:ASN:CG	2.59	0.41
4:C:139:GLN:CA	4:C:139:GLN:NE2	2.84	0.41
5:D:149:ALA:O	5:D:150:GLU:C	2.57	0.41
6:E:43:LEU:HD22	6:E:44:GLY:N	2.36	0.41
6:E:50:GLU:HB2	6:E:53:LEU:HD12	2.03	0.41
8:G:21:VAL:HG23	8:G:22:LEU:N	2.36	0.41
8:G:83:ALA:HB3	8:G:85:TYR:HE2	1.83	0.41
8:G:136:LYS:O	8:G:140:ASP:HB2	2.20	0.41
8:G:140:ASP:OD1	8:G:143:ARG:NH2	2.54	0.41
9:H:7:ALA:HB2	9:H:85:ARG:HD2	2.02	0.41
9:H:83:ILE:HG13	9:H:137:VAL:HG22	2.02	0.41
13:L:75:HIS:HD2	13:L:77:LEU:N	2.11	0.41
13:L:79:GLU:OE1	13:L:80:HIS:CE1	2.74	0.41
13:L:90:VAL:O	13:L:90:VAL:HG12	2.21	0.41
14:M:4:ILE:HG23	14:M:57:ARG:HA	2.03	0.41
15:N:21:TYR:CE2	15:N:23:ARG:HG2	2.55	0.41
16:O:34:LEU:C	16:O:34:LEU:CD2	2.89	0.41
17:P:5:ARG:HA	17:P:70:ALA:HB2	2.03	0.41
19:R:17:SER:HB2	19:R:54:ARG:HB3	2.03	0.41
21:T:70:SER:HA	21:T:73:HIS:NE2	2.35	0.41
21:T:86:ARG:O	21:T:90:GLN:HG3	2.20	0.41
1:A:44:G:H2'	1:A:45:U:O4'	2.21	0.41
1:A:539:A:H2'	1:A:540:G:C8	2.56	0.41
1:A:607:A:O2'	1:A:608:A:H5'	2.21	0.41
1:A:761:G:H2'	1:A:762:C:H6	1.85	0.41
1:A:1058:G:OP1	4:C:199:LYS:HE3	2.21	0.41
3:B:209:ARG:HG2	3:B:209:ARG:NH1	2.36	0.41
4:C:12:LEU:HD23	4:C:12:LEU:HA	1.87	0.41
5:D:6:GLY:O	5:D:7:PRO:C	2.59	0.41
5:D:61:LYS:HZ2	5:D:62:GLN:NE2	2.16	0.41
5:D:121:VAL:O	5:D:134:ASP:HA	2.21	0.41
6:E:11:ILE:CD1	6:E:108:ALA:HB3	2.50	0.41
6:E:80:ILE:HD13	6:E:138:ALA:HB1	2.03	0.41
6:E:144:THR:HG22	6:E:145:LYS:N	2.36	0.41
9:H:86:ILE:HD12	9:H:133:LEU:HD22	2.03	0.41
10:I:48:GLU:OE1	10:I:51:ARG:HD2	2.21	0.41
18:Q:84:LEU:HD23	18:Q:84:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:36:ASN:HD22	19:R:38:GLU:HG2	1.84	0.41
20:S:8:GLY:O	20:S:10:PHE:N	2.54	0.41
1:A:459:G:H3'	1:A:460:A:H5"	2.03	0.40
1:A:736:C:H2'	1:A:737:A:C8	2.56	0.40
1:A:949:A:H2'	1:A:950:U:O4'	2.21	0.40
1:A:972:C:P	11:J:57:LYS:HD2	2.61	0.40
1:A:990:C:H2'	1:A:991:U:C1'	2.51	0.40
1:A:1005:A:C5	1:A:1025:U:H1'	2.56	0.40
3:B:88:ALA:O	3:B:90:MET:N	2.51	0.40
3:B:121:LEU:HD23	3:B:138:LEU:HD13	2.02	0.40
3:B:215:LEU:HD23	3:B:215:LEU:HA	1.87	0.40
6:E:13:ILE:O	6:E:13:ILE:HG13	2.20	0.40
6:E:101:ILE:O	6:E:120:THR:HB	2.21	0.40
7:F:2:ARG:CD	7:F:69:GLU:HG2	2.49	0.40
8:G:51:GLN:O	8:G:51:GLN:CG	2.69	0.40
9:H:30:ARG:NH1	9:H:50:ARG:HH22	2.19	0.40
10:I:26:VAL:CG1	10:I:33:PHE:HB2	2.51	0.40
13:L:41:ARG:HG2	13:L:42:THR:N	2.26	0.40
16:O:29:VAL:HG12	16:O:85:LEU:CD1	2.52	0.40
16:O:87:ILE:C	16:O:89:GLY:N	2.75	0.40
1:A:123:C:OP1	1:A:311:C:O2'	2.37	0.40
1:A:300:A:H8	1:A:300:A:O5'	2.05	0.40
1:A:477:G:H2'	1:A:478:A:H8	1.85	0.40
1:A:1055:A:C6	1:A:1206:G:C5	3.10	0.40
1:A:1064:G:C4'	1:A:1065:U:H5'	2.51	0.40
1:A:1148:U:O3'	10:I:14:VAL:HG11	2.22	0.40
3:B:7:VAL:HG12	3:B:8:LYS:N	2.36	0.40
3:B:102:LEU:HB3	3:B:180:LEU:HD12	2.03	0.40
7:F:33:TYR:HB2	7:F:75:LEU:HD23	2.03	0.40
9:H:37:ARG:HD2	9:H:41:ARG:NH2	2.35	0.40
9:H:61:VAL:HG12	9:H:63:LEU:HD12	2.03	0.40
11:J:51:ARG:H	11:J:59:SER:CB	2.33	0.40
14:M:37:THR:HG23	14:M:55:ARG:CB	2.50	0.40
14:M:53:VAL:HG12	14:M:53:VAL:O	2.21	0.40
14:M:88:ARG:HD2	20:S:3:ARG:HH21	1.87	0.40
16:O:36:ILE:N	16:O:59:MET:HE1	2.35	0.40
19:R:17:SER:HA	19:R:19:LYS:HE2	2.02	0.40
20:S:33:THR:HG22	20:S:34:TRP:H	1.86	0.40
1:A:356:A:O2'	1:A:357:G:H5'	2.21	0.40
1:A:404:U:H2'	1:A:405:U:H6	1.86	0.40
1:A:533:A:O2'	1:A:535:A:OP2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:C2'	1:A:645:C:H5'	2.51	0.40
1:A:658:G:H2'	1:A:659:U:C6	2.56	0.40
1:A:676:A:H2'	1:A:677:U:H6	1.86	0.40
1:A:921:U:O2	6:E:19:MET:HB2	2.21	0.40
1:A:991:U:O2	1:A:993:G:H8	2.05	0.40
1:A:1005:A:C2'	1:A:1006:C:H5'	2.51	0.40
1:A:1028:C:O2'	1:A:1029:C:H5'	2.20	0.40
1:A:1054:C:HO2'	1:A:1055:A:H5"	1.80	0.40
1:A:1065:U:H4'	1:A:1066:C:O5'	2.21	0.40
1:A:1231:G:C4'	10:I:126:SER:HB3	2.51	0.40
3:B:68:ILE:H	3:B:90:MET:HE3	1.86	0.40
3:B:98:LEU:O	3:B:101:MET:HG3	2.21	0.40
3:B:189:ASP:OD2	3:B:205:ASP:OD1	2.39	0.40
3:B:193:ASP:HA	3:B:194:PRO:HD2	1.96	0.40
3:B:213:LEU:CD2	3:B:213:LEU:C	2.90	0.40
4:C:58:GLU:O	4:C:59:ARG:HG3	2.21	0.40
4:C:77:ILE:HA	4:C:84:ILE:HB	2.03	0.40
6:E:20:GLN:O	6:E:22:GLY:N	2.55	0.40
9:H:31:PHE:HZ	9:H:134:ILE:CD1	2.33	0.40
13:L:7:ILE:HD13	13:L:7:ILE:HA	1.86	0.40
15:N:53:LEU:HB3	15:N:56:VAL:HG21	2.03	0.40
1:A:415:A:H2'	1:A:416:G:C8	2.57	0.40
1:A:625:G:O2'	1:A:626:U:H5'	2.21	0.40
1:A:954:G:H2'	1:A:955:U:H6	1.87	0.40
1:A:1087:G:H2'	1:A:1088:G:H8	1.85	0.40
1:A:1300:G:C2'	1:A:1301:U:OP2	2.69	0.40
1:A:1331:G:O2'	1:A:1332:A:P	2.79	0.40
1:A:1391:U:H2'	1:A:1392:G:H8	1.80	0.40
1:A:1478:C:H2'	1:A:1479:C:H6	1.86	0.40
1:A:1525:G:O2'	1:A:1526:G:H5'	2.21	0.40
7:F:21:LEU:O	7:F:24:GLU:HB3	2.21	0.40
7:F:74:ASP:HA	7:F:77:ARG:HG3	2.02	0.40
7:F:76:ALA:O	7:F:77:ARG:C	2.60	0.40
8:G:155:ARG:O	8:G:156:TRP:CB	2.69	0.40
10:I:111:ARG:HH11	10:I:111:ARG:CG	2.35	0.40
12:K:41:THR:HG21	12:K:71:LYS:HB3	2.03	0.40
13:L:58:VAL:O	13:L:65:GLU:HA	2.21	0.40
21:T:57:ARG:HH11	21:T:57:ARG:HG2	1.86	0.40
1:A:6:G:H4'	1:A:298:A:H4'	2.03	0.40
1:A:6:G:C4	6:E:119:LEU:HD11	2.57	0.40
1:A:389:A:C6	1:A:390:C:H1'	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:U:H5'	1:A:566:G:N2	2.36	0.40
1:A:697:U:H2'	1:A:698:G:H5'	2.02	0.40
1:A:709:G:H2'	1:A:710:G:H8	1.87	0.40
1:A:983:A:H5'	1:A:984:C:OP2	2.22	0.40
1:A:993:G:HO2'	1:A:994:A:P	2.45	0.40
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.40
1:A:1346:A:C5	8:G:10:ARG:NH2	2.89	0.40
3:B:185:ILE:HA	3:B:199:TYR:O	2.22	0.40
3:B:213:LEU:C	3:B:213:LEU:HD23	2.42	0.40
10:I:58:ARG:NH2	10:I:88:TYR:OH	2.54	0.40
11:J:90:LEU:CB	11:J:91:PRO:HD3	2.47	0.40
12:K:21:ILE:HD13	12:K:94:ALA:HB3	2.02	0.40
21:T:61:SER:O	21:T:65:LYS:HG3	2.22	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	Percentiles
3	B	235/256 (92%)	172 (73%)	43 (18%)	20 (8%)	1 4
4	C	204/239 (85%)	135 (66%)	43 (21%)	26 (13%)	0 1
5	D	206/209 (99%)	173 (84%)	25 (12%)	8 (4%)	3 17
6	E	148/162 (91%)	130 (88%)	16 (11%)	2 (1%)	11 43
7	F	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	3 17
8	G	153/156 (98%)	123 (80%)	25 (16%)	5 (3%)	4 21
9	H	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22 60
10	I	125/128 (98%)	96 (77%)	18 (14%)	11 (9%)	1 3
11	J	96/105 (91%)	64 (67%)	18 (19%)	14 (15%)	0 1
12	K	117/129 (91%)	91 (78%)	19 (16%)	7 (6%)	1 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	123/135 (91%)	95 (77%)	19 (15%)	9 (7%)	1	5
14	M	123/126 (98%)	92 (75%)	14 (11%)	17 (14%)	0	1
15	N	58/61 (95%)	44 (76%)	11 (19%)	3 (5%)	2	12
16	O	86/89 (97%)	69 (80%)	12 (14%)	5 (6%)	1	10
17	P	81/88 (92%)	72 (89%)	8 (10%)	1 (1%)	13	48
18	Q	102/105 (97%)	86 (84%)	11 (11%)	5 (5%)	2	13
19	R	71/88 (81%)	49 (69%)	16 (22%)	6 (8%)	1	4
20	S	82/93 (88%)	60 (73%)	16 (20%)	6 (7%)	1	5
21	T	97/106 (92%)	77 (79%)	12 (12%)	8 (8%)	1	4
22	V	22/26 (85%)	17 (77%)	4 (18%)	1 (4%)	2	14
All	All	2364/2540 (93%)	1851 (78%)	354 (15%)	159 (7%)	1	6

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE
3	B	21	ARG
3	B	124	SER
4	C	15	THR
4	C	24	ALA
4	C	50	ALA
4	C	54	ARG
4	C	127	ARG
4	C	155	GLY
4	C	179	ARG
4	C	189	ALA
5	D	4	TYR
5	D	31	CYS
5	D	32	ALA
6	E	16	THR
7	F	62	TRP
8	G	4	ARG
8	G	7	ALA
8	G	155	ARG
10	I	126	SER
11	J	34	VAL

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Mol	Chain	Res	Type
11	J	54	PHE
11	J	57	LYS
11	J	61	GLU
11	J	79	ARG
12	K	100	ALA
12	K	101	SER
13	L	28	LYS
13	L	47	LYS
13	L	91	LYS
14	M	27	LYS
14	M	122	LYS
14	M	123	ALA
16	O	85	LEU
18	Q	80	GLY
18	Q	81	ARG
20	S	6	LYS
20	S	9	VAL
3	B	18	GLY
3	B	20	GLU
3	B	95	GLN
3	B	226	ARG
4	C	16	ARG
4	C	23	TYR
4	C	60	ALA
4	C	97	LYS
4	C	100	ALA
4	C	205	GLY
5	D	5	ILE
5	D	26	CYS
5	D	179	GLU
6	E	153	LYS
7	F	98	LEU
8	G	42	ILE
9	H	24	THR
10	I	8	GLY
10	I	94	ALA
11	J	55	LYS
11	J	72	VAL
11	J	86	MET
12	K	27	ASN
12	K	28	THR
12	K	128	ALA

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Mol	Chain	Res	Type
13	L	27	LEU
14	M	3	ARG
14	M	6	GLY
14	M	12	ASN
14	M	60	VAL
14	M	67	GLU
14	M	80	ARG
14	M	85	GLY
14	M	86	CYS
15	N	12	ARG
17	P	10	GLY
18	Q	96	GLN
18	Q	97	SER
20	S	84	GLY
21	T	9	ASN
21	T	73	HIS
21	T	101	GLY
21	T	104	LEU
3	B	9	GLU
3	B	87	ARG
3	B	122	PHE
3	B	207	ALA
4	C	39	ILE
4	C	96	GLY
4	C	146	ALA
4	C	168	ALA
5	D	9	CYS
7	F	32	ASN
10	I	11	LYS
10	I	23	ASN
10	I	43	ALA
10	I	54	ASP
10	I	56	LEU
11	J	19	SER
11	J	60	ARG
11	J	90	LEU
13	L	116	SER
13	L	121	GLY
14	M	42	ALA
14	M	59	TYR
14	M	106	ASN
14	M	124	PRO

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Mol	Chain	Res	Type
15	N	29	ARG
19	R	26	LEU
19	R	58	LEU
19	R	60	GLY
20	S	47	HIS
20	S	73	GLU
21	T	49	ALA
21	T	50	GLU
3	B	39	ILE
3	B	41	ILE
3	B	62	ALA
3	B	191	ASP
3	B	211	ILE
7	F	70	ASP
11	J	39	PRO
11	J	76	ASN
12	K	35	PRO
16	O	6	GLU
16	O	73	GLU
16	O	86	GLY
21	T	74	LYS
4	C	46	GLU
4	C	47	LEU
4	C	61	ALA
4	C	66	VAL
4	C	108	ASN
4	C	167	TRP
5	D	88	VAL
10	I	12	GLU
11	J	40	LEU
13	L	82	VAL
14	M	121	LYS
19	R	20	ALA
20	S	30	LEU
3	B	212	GLN
10	I	24	GLY
12	K	117	ASN
15	N	30	ALA
18	Q	27	PHE
22	V	3	LYS
13	L	48	PRO
16	O	87	ILE

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Mol	Chain	Res	Type
19	R	77	GLY
3	B	108	ILE
4	C	103	VAL
8	G	58	PRO
10	I	41	VAL
19	R	86	VAL
21	T	102	GLY
4	C	14	ILE
13	L	29	GLY
14	M	7	VAL

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	Percentiles	
3	B	204/220 (93%)	193 (95%)	11 (5%)	22	57
4	C	160/188 (85%)	147 (92%)	13 (8%)	11	40
5	D	180/181 (99%)	169 (94%)	11 (6%)	18	53
6	E	115/123 (94%)	104 (90%)	11 (10%)	8	32
7	F	90/90 (100%)	88 (98%)	2 (2%)	52	81
8	G	126/127 (99%)	115 (91%)	11 (9%)	10	37
9	H	119/119 (100%)	113 (95%)	6 (5%)	24	60
10	I	98/99 (99%)	91 (93%)	7 (7%)	14	46
11	J	87/92 (95%)	80 (92%)	7 (8%)	12	40
12	K	90/99 (91%)	82 (91%)	8 (9%)	9	35
13	L	104/111 (94%)	98 (94%)	6 (6%)	20	55
14	M	100/101 (99%)	91 (91%)	9 (9%)	9	35
15	N	49/50 (98%)	43 (88%)	6 (12%)	5	21
16	O	79/80 (99%)	76 (96%)	3 (4%)	33	69
17	P	72/74 (97%)	67 (93%)	5 (7%)	15	48
18	Q	96/97 (99%)	88 (92%)	8 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	64/77 (83%)	59 (92%)	5 (8%)	12	42
20	S	73/80 (91%)	69 (94%)	4 (6%)	21	57
21	T	76/82 (93%)	69 (91%)	7 (9%)	9	34
22	V	19/21 (90%)	19 (100%)	0	100	100
All	All	2001/2111 (95%)	1861 (93%)	140 (7%)	15	47

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	17	PHE
3	B	24	TRP
3	B	25	ASN
3	B	43	ASP
3	B	96	ARG
3	B	97	TRP
3	B	102	LEU
3	B	114	ARG
3	B	164	VAL
3	B	178	ARG
3	B	204	ASN
4	C	3	ASN
4	C	11	ARG
4	C	37	GLN
4	C	52	LEU
4	C	56	ASP
4	C	64	VAL
4	C	99	VAL
4	C	101	LEU
4	C	127	ARG
4	C	139	GLN
4	C	167	TRP
4	C	179	ARG
4	C	188	LEU
5	D	8	VAL
5	D	9	CYS
5	D	15	GLU
5	D	36	ARG
5	D	53	ASP
5	D	114	ARG
5	D	122	ARG
5	D	127	THR

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Mol	Chain	Res	Type
5	D	162	LEU
5	D	170	VAL
5	D	192	GLU
6	E	12	LEU
6	E	16	THR
6	E	41	VAL
6	E	43	LEU
6	E	56	GLN
6	E	63	ARG
6	E	73	ASN
6	E	79	GLU
6	E	89	ILE
6	E	120	THR
6	E	150	ARG
7	F	10	LEU
7	F	69	GLU
8	G	8	GLU
8	G	12	LEU
8	G	38	LEU
8	G	75	VAL
8	G	96	GLN
8	G	126	ASP
8	G	136	LYS
8	G	140	ASP
8	G	144	MET
8	G	146	GLU
8	G	149	ARG
9	H	26	VAL
9	H	63	LEU
9	H	85	ARG
9	H	91	ARG
9	H	92	ARG
9	H	105	ARG
10	I	2	GLU
10	I	23	ASN
10	I	65	VAL
10	I	79	LEU
10	I	111	ARG
10	I	113	LYS
10	I	121	ARG
11	J	9	ARG
11	J	45	ARG

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Mol	Chain	Res	Type
11	J	60	ARG
11	J	71	LEU
11	J	79	ARG
11	J	86	MET
11	J	95	GLU
12	K	24	SER
12	K	27	ASN
12	K	29	ILE
12	K	33	THR
12	K	36	ASP
12	K	51	LYS
12	K	54	ARG
12	K	117	ASN
13	L	47	LYS
13	L	48	PRO
13	L	53	ARG
13	L	67	THR
13	L	113	ARG
13	L	124	LYS
14	M	9	ILE
14	M	40	ASN
14	M	44	ARG
14	M	49	THR
14	M	70	LEU
14	M	81	LEU
14	M	106	ASN
14	M	110	ARG
14	M	125	ARG
15	N	8	GLU
15	N	12	ARG
15	N	16	PHE
15	N	31	ARG
15	N	41	ARG
15	N	44	LEU
16	O	57	LEU
16	O	81	LEU
16	O	83	GLU
17	P	8	ARG
17	P	53	VAL
17	P	55	ARG
17	P	62	VAL
17	P	74	LEU

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Mol	Chain	Res	Type
18	Q	34	LYS
18	Q	38	ARG
18	Q	60	ILE
18	Q	68	ARG
18	Q	86	GLU
18	Q	97	SER
18	Q	98	LEU
18	Q	104	LYS
19	R	19	LYS
19	R	36	ASN
19	R	38	GLU
19	R	54	ARG
19	R	87	ARG
20	S	15	LEU
20	S	53	ASN
20	S	61	TYR
20	S	62	ILE
21	T	13	LEU
21	T	42	GLN
21	T	46	GLU
21	T	57	ARG
21	T	74	LYS
21	T	79	ARG
21	T	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	19	HIS
3	B	25	ASN
3	B	45	GLN
3	B	76	GLN
3	B	113	HIS
3	B	135	GLN
3	B	146	GLN
3	B	204	ASN
4	C	3	ASN
4	C	6	HIS
4	C	31	HIS
4	C	69	HIS
4	C	104	GLN
4	C	110	ASN

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Mol	Chain	Res	Type
4	C	123	GLN
4	C	139	GLN
4	C	176	HIS
5	D	42	GLN
5	D	62	GLN
5	D	123	HIS
5	D	160	GLN
5	D	199	GLN
6	E	73	ASN
7	F	16	GLN
7	F	18	GLN
7	F	27	GLN
7	F	32	ASN
7	F	57	GLN
7	F	94	GLN
7	F	100	ASN
8	G	37	ASN
8	G	68	ASN
8	G	86	GLN
8	G	106	GLN
8	G	110	GLN
10	I	23	ASN
10	I	73	GLN
11	J	56	HIS
11	J	62	HIS
11	J	84	GLN
12	K	22	HIS
12	K	27	ASN
12	K	93	GLN
12	K	117	ASN
13	L	49	ASN
13	L	75	HIS
13	L	80	HIS
14	M	12	ASN
14	M	40	ASN
14	M	62	ASN
16	O	13	GLN
16	O	37	ASN
16	O	46	HIS
17	P	76	GLN
18	Q	16	GLN
19	R	36	ASN

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Mol	Chain	Res	Type
20	S	14	HIS
20	S	53	ASN
20	S	56	GLN
21	T	18	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	213 (14%)	88 (5%)
2	X	5/6 (83%)	0	0
All	All	1512/1528 (98%)	213 (14%)	88 (5%)

All (213) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	52	G
1	A	61	G
1	A	64	G
1	A	65	U
1	A	81	U
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	182	U
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A

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Mol	Chain	Res	Type
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
1	A	289	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	482	A
1	A	484	G

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Mol	Chain	Res	Type
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	695	A
1	A	702	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	748	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A

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Mol	Chain	Res	Type
1	A	839	U
1	A	840	C
1	A	841	U
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	1004	A
1	A	1023	G
1	A	1026	G
1	A	1050	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A

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Mol	Chain	Res	Type
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1152	A
1	A	1159	U
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1250	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1306	A
1	A	1319	A
1	A	1320	C
1	A	1332	A
1	A	1347	G

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Mol	Chain	Res	Type
1	A	1364	U
1	A	1365	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1446	A
1	A	1452	C
1	A	1492	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (88) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	30	U
1	A	48	C
1	A	51	A
1	A	60	A
1	A	64	G
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	279	A
1	A	281	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	438	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	518	C
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1085	U
1	A	1094	G
1	A	1101	A
1	A	1129	C

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Mol	Chain	Res	Type
1	A	1139	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1256	A
1	A	1257	U
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1319	A
1	A	1331	G
1	A	1346	A
1	A	1364	U
1	A	1380	U
1	A	1397	C
1	A	1451	A
1	A	1498	U
1	A	1502	A
1	A	1504	G
1	A	1528	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 101 ligands modelled in this entry, 98 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	SCM	A	1633	-	23,25,25	0.97	1 (4%)	26,39,39	1.37	3 (11%)
26	SRY	A	1634	-	40,42,42	1.23	3 (7%)	49,63,63	1.70	9 (18%)
23	PAR	A	1545	-	45,45,45	1.54	9 (20%)	64,67,67	1.18	5 (7%)

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
25	SCM	A	1633	-	-	2/4/57/57	0/3/3/3
26	SRY	A	1634	-	-	6/20/87/87	0/3/3/3
23	PAR	A	1545	-	-	3/18/94/94	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1634	SRY	C31-N31	4.37	1.52	1.45
23	A	1545	PAR	C64-C54	3.93	1.57	1.52
23	A	1545	PAR	O54-C14	3.93	1.51	1.41
26	A	1634	SRY	C11-N11	3.69	1.51	1.45
23	A	1545	PAR	C31-C21	3.12	1.57	1.53
23	A	1545	PAR	C24-N24	2.87	1.51	1.47
23	A	1545	PAR	O51-C11	2.67	1.48	1.41
26	A	1634	SRY	C23-N23	-2.65	1.43	1.47
23	A	1545	PAR	C23-C33	2.39	1.58	1.52
23	A	1545	PAR	O43-C13	2.14	1.45	1.41
25	A	1633	SCM	C10-N10	-2.12	1.43	1.47
23	A	1545	PAR	O54-C54	2.10	1.49	1.44
23	A	1545	PAR	O51-C51	2.02	1.49	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	1634	SRY	C13-O13-C22	-5.96	105.90	116.25
25	A	1633	SCM	C1M-N10-C10	-4.97	107.15	114.38
26	A	1634	SRY	CI3-N23-C23	-4.89	107.26	114.38
26	A	1634	SRY	O41-C12-O42	-4.24	106.84	111.43
23	A	1545	PAR	O33-C14-C24	3.36	114.00	108.22
23	A	1545	PAR	C14-O54-C54	3.22	120.01	113.69
23	A	1545	PAR	O54-C54-C64	3.20	111.97	106.01
26	A	1634	SRY	C13-O53-C53	-3.13	107.54	113.69
26	A	1634	SRY	N31-CD1-NF1	-2.93	115.48	120.59
26	A	1634	SRY	C12-O41-C41	-2.72	111.22	117.96
26	A	1634	SRY	C12-O42-C42	-2.61	104.27	108.38
25	A	1633	SCM	C2M-C2-C3	-2.61	108.13	113.22
23	A	1545	PAR	O23-C23-C33	2.37	117.89	111.17
26	A	1634	SRY	O13-C13-C23	2.26	112.15	108.24
25	A	1633	SCM	C6-O1-C2	-2.19	105.13	112.06
26	A	1634	SRY	NE1-CD1-N31	2.11	124.26	119.55
23	A	1545	PAR	C11-O51-C51	2.00	117.62	113.69

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1633	SCM	C11-C10-N10-C1M
26	A	1634	SRY	NB1-CA1-N11-C11
26	A	1634	SRY	NC1-CA1-N11-C11
26	A	1634	SRY	C13-C23-N23-CI3
26	A	1634	SRY	C43-C53-C63-O63
25	A	1633	SCM	C9-C10-N10-C1M
23	A	1545	PAR	C24-C14-O33-C33
23	A	1545	PAR	C52-C42-O11-C11
26	A	1634	SRY	C33-C23-N23-CI3
26	A	1634	SRY	O53-C53-C63-O63
23	A	1545	PAR	C23-C13-O52-C52

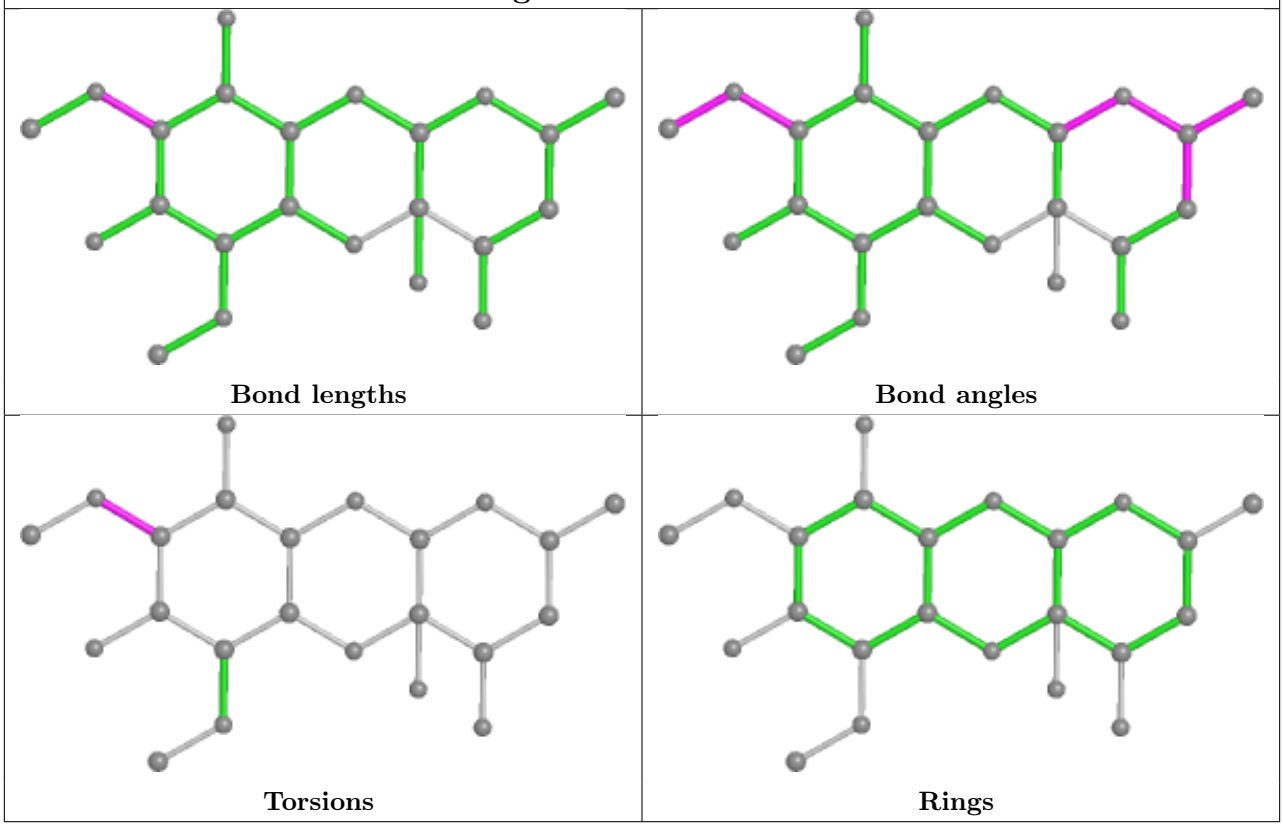
There are no ring outliers.

3 monomers are involved in 11 short contacts:

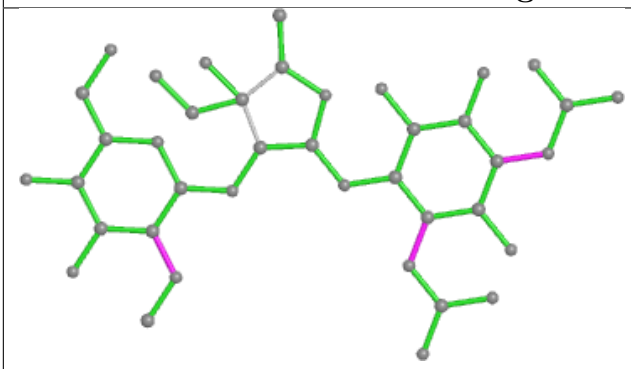
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1633	SCM	2	0
26	A	1634	SRY	5	0
23	A	1545	PAR	4	0

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

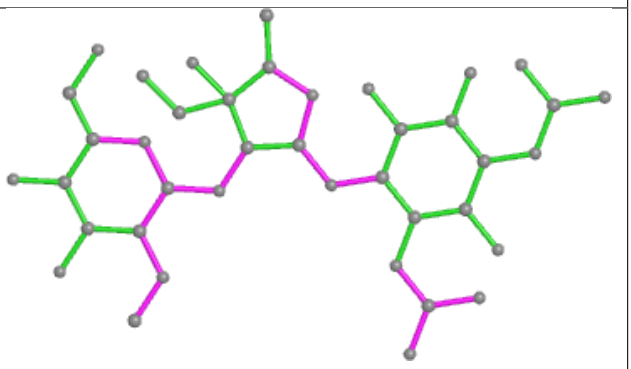
Ligand SCM A 1633



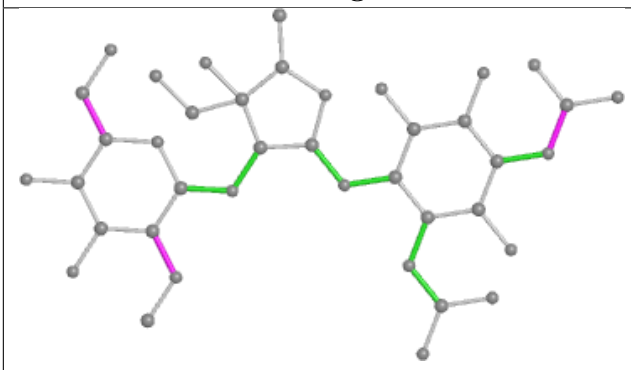
Ligand SRY A 1634



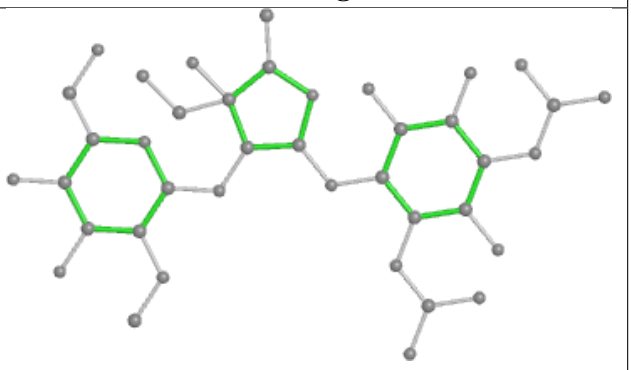
Bond lengths



Bond angles

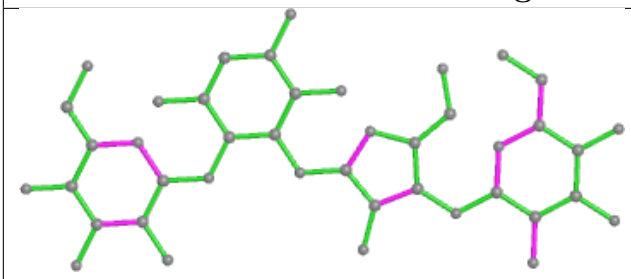


Torsions

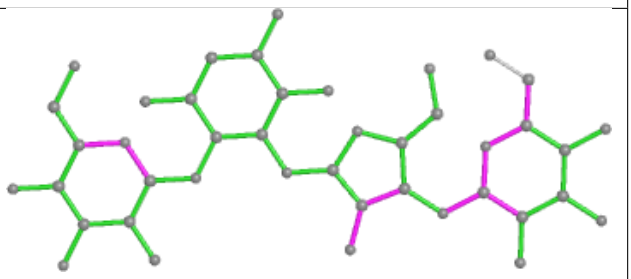


Rings

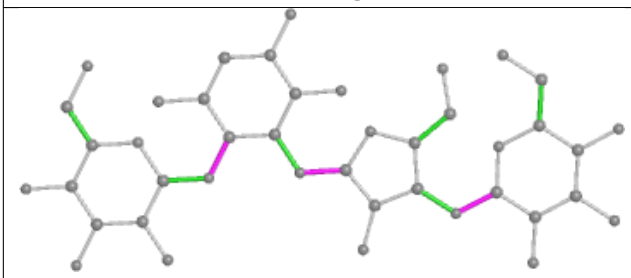
Ligand PAR A 1545



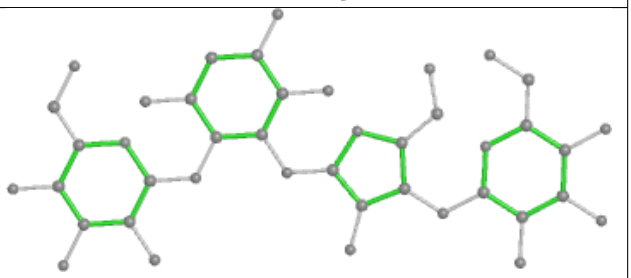
Bond lengths



Bond angles



Torsions



Rings

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1506/1522 (98%)	0.73	86 (5%)	23	8	34, 60, 137, 201	0
2	X	6/6 (100%)	1.38	2 (33%)	0	0	57, 71, 116, 118	0
3	B	237/256 (92%)	0.05	2 (0%)	86	65	35, 83, 162, 185	0
4	C	206/239 (86%)	-0.00	1 (0%)	91	75	32, 79, 136, 190	0
5	D	208/209 (99%)	0.27	14 (6%)	17	5	40, 63, 114, 143	0
6	E	150/162 (92%)	0.14	1 (0%)	87	69	29, 52, 95, 146	0
7	F	101/101 (100%)	0.33	5 (4%)	28	10	49, 89, 138, 165	0
8	G	155/156 (99%)	-0.11	3 (1%)	66	37	40, 72, 141, 177	0
9	H	138/138 (100%)	0.05	1 (0%)	87	69	30, 51, 90, 148	0
10	I	127/128 (99%)	0.58	15 (11%)	4	1	33, 82, 137, 177	0
11	J	98/105 (93%)	0.49	9 (9%)	9	3	42, 109, 179, 201	0
12	K	119/129 (92%)	0.48	10 (8%)	11	3	40, 69, 125, 194	0
13	L	125/135 (92%)	0.21	2 (1%)	72	44	21, 59, 134, 182	0
14	M	125/126 (99%)	0.89	18 (14%)	2	1	47, 83, 146, 185	0
15	N	60/61 (98%)	0.26	3 (5%)	28	10	38, 73, 119, 200	0
16	O	88/89 (98%)	0.13	2 (2%)	60	31	39, 66, 127, 191	0
17	P	83/88 (94%)	0.10	1 (1%)	79	54	37, 53, 90, 159	0
18	Q	104/105 (99%)	0.70	10 (9%)	8	2	26, 58, 143, 201	0
19	R	73/88 (82%)	0.24	4 (5%)	25	9	43, 69, 129, 184	0
20	S	84/93 (90%)	1.22	16 (19%)	1	0	71, 96, 145, 201	0
21	T	99/106 (93%)	0.08	3 (3%)	50	22	39, 64, 119, 166	0
22	V	24/26 (92%)	0.98	2 (8%)	11	3	43, 68, 102, 119	0
All	All	3916/4068 (96%)	0.46	210 (5%)	25	9	21, 66, 142, 201	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	3	ARG	14.3
14	M	123	ALA	13.8
14	M	124	PRO	12.5
18	Q	102	GLY	11.3
1	A	1002	G	11.2
14	M	125	ARG	10.7
18	Q	105	ALA	10.7
18	Q	103	GLY	10.5
18	Q	104	LYS	8.9
1	A	1034	G	7.8
1	A	1003	G	7.5
11	J	33	GLN	7.2
1	A	1038	C	6.4
1	A	1001	A	6.4
1	A	1033	G	6.3
1	A	1006	C	5.8
1	A	1024	G	5.7
1	A	1026	G	5.7
1	A	1129	C	5.7
12	K	128	ALA	5.6
3	B	16	HIS	5.4
14	M	126	LYS	5.4
1	A	1035	A	5.3
12	K	129	SER	5.3
20	S	29	ARG	5.2
1	A	1030(B)	C	5.1
1	A	1004	A	5.1
20	S	2	PRO	4.9
1	A	1039	C	4.9
1	A	1037	C	4.8
1	A	1003(A)	G	4.7
1	A	1124	G	4.7
14	M	122	LYS	4.7
1	A	1032	G	4.5
1	A	532	A	4.4
15	N	6	LEU	4.3
1	A	993	G	4.2
10	I	64	THR	4.2
1	A	1030(D)	A	4.0
1	A	1040	U	4.0
18	Q	101	ARG	4.0
1	A	1027	C	4.0
14	M	7	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
22	V	6	ARG	3.9
1	A	1025	U	3.9
11	J	72	VAL	3.8
1	A	1036	G	3.8
1	A	1005	A	3.8
5	D	7	PRO	3.7
14	M	87	TYR	3.6
14	M	8	GLU	3.6
19	R	48	GLY	3.6
12	K	40	ILE	3.6
1	A	1144	G	3.6
20	S	37	ARG	3.6
1	A	373	A	3.5
14	M	121	LYS	3.5
16	O	22	THR	3.5
9	H	1	MET	3.4
10	I	65	VAL	3.4
1	A	1127	G	3.3
1	A	1126	U	3.3
20	S	34	TRP	3.2
1	A	1031	G	3.2
5	D	157	LEU	3.2
10	I	7	THR	3.2
5	D	112	VAL	3.1
20	S	33	THR	3.1
10	I	66	ARG	3.1
12	K	41	THR	3.1
7	F	63	TYR	3.1
12	K	12	ARG	3.1
21	T	9	ASN	3.1
1	A	1477	C	3.1
8	G	5	ARG	3.1
1	A	1041	A	3.0
1	A	481	G	3.0
3	B	133	LYS	3.0
1	A	1213	A	3.0
20	S	28	LYS	3.0
10	I	70	LYS	3.0
1	A	1139	G	3.0
11	J	98	ILE	3.0
1	A	202	U	2.9
20	S	22	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1224	G	2.9
1	A	1171	G	2.9
10	I	36	TYR	2.9
1	A	1269	A	2.8
10	I	126	SER	2.8
1	A	1270	C	2.8
1	A	1030	C	2.8
1	A	1442	G	2.8
20	S	30	LEU	2.8
19	R	16	PRO	2.8
16	O	23	GLY	2.8
1	A	1314	C	2.8
1	A	254	G	2.7
1	A	81	U	2.7
20	S	4	SER	2.7
1	A	1030(A)	G	2.7
1	A	1128	C	2.7
18	Q	96	GLN	2.7
19	R	17	SER	2.7
1	A	1321	C	2.7
1	A	1030(C)	G	2.6
5	D	116	GLN	2.6
10	I	9	ARG	2.6
15	N	3	ARG	2.6
20	S	31	ILE	2.6
2	X	2	U	2.6
13	L	73	GLU	2.6
14	M	98	VAL	2.6
2	X	3	U	2.6
1	A	1148	U	2.6
1	A	266	G	2.6
12	K	51	LYS	2.6
1	A	657	G	2.5
11	J	74	ILE	2.5
1	A	351	G	2.5
21	T	68	LYS	2.5
1	A	1531	A	2.5
20	S	15	LEU	2.5
1	A	428	G	2.5
1	A	427	U	2.5
10	I	14	VAL	2.5
5	D	41	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
11	J	71	LEU	2.5
18	Q	68	ARG	2.5
19	R	85	LEU	2.4
1	A	426	G	2.4
1	A	349	A	2.4
1	A	350	G	2.4
1	A	407	G	2.4
5	D	5	ILE	2.4
18	Q	16	GLN	2.4
1	A	412	A	2.4
14	M	100	GLY	2.4
1	A	1200	C	2.4
1	A	438	G	2.4
1	A	1022	G	2.4
10	I	16	ARG	2.4
14	M	4	ILE	2.4
10	I	94	ALA	2.3
8	G	82	GLY	2.3
14	M	120	LYS	2.3
20	S	32	LYS	2.3
14	M	6	GLY	2.3
14	M	27	LYS	2.3
5	D	8	VAL	2.3
21	T	105	SER	2.3
22	V	10	ARG	2.3
1	A	255	G	2.3
1	A	663	A	2.3
5	D	42	GLN	2.3
10	I	15	ALA	2.3
1	A	348	G	2.3
10	I	8	GLY	2.3
6	E	21	ALA	2.3
1	A	1322	C	2.3
11	J	28	ARG	2.3
1	A	1028	C	2.2
13	L	28	LYS	2.2
20	S	71	LEU	2.2
11	J	34	VAL	2.2
1	A	160	A	2.2
1	A	745	C	2.2
18	Q	92	ARG	2.2
1	A	1125	U	2.2

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Mol	Chain	Res	Type	RSRZ
17	P	12	LYS	2.2
7	F	75	LEU	2.2
1	A	159	G	2.2
7	F	72	VAL	2.2
11	J	96	ILE	2.2
5	D	120	LEU	2.2
14	M	102	ARG	2.2
5	D	3	ARG	2.2
14	M	88	ARG	2.2
20	S	69	HIS	2.1
1	A	451	A	2.1
12	K	11	LYS	2.1
1	A	1159	U	2.1
5	D	155	LEU	2.1
7	F	4	TYR	2.1
7	F	35	ALA	2.1
1	A	406	G	2.1
4	C	94	LEU	2.1
1	A	977	A	2.1
5	D	115	ARG	2.1
10	I	6	GLY	2.1
18	Q	18	THR	2.1
20	S	6	LYS	2.1
8	G	81	GLY	2.1
1	A	1313	U	2.1
1	A	989	C	2.1
14	M	106	ASN	2.1
1	A	371	G	2.1
1	A	196	A	2.1
1	A	315	A	2.1
12	K	42	TRP	2.0
10	I	119	ALA	2.0
1	A	1258	G	2.0
1	A	430	A	2.0
15	N	4	LYS	2.0
5	D	9	CYS	2.0
1	A	661	G	2.0
5	D	125	HIS	2.0
11	J	24	VAL	2.0
12	K	14	VAL	2.0
12	K	77	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1615	1/1	0.34	0.69	38,38,38,38	1
24	MG	A	1583	1/1	0.41	1.11	38,38,38,38	1
24	MG	A	210	1/1	0.43	0.47	38,38,38,38	1
24	MG	A	1586	1/1	0.50	0.41	38,38,38,38	1
24	MG	A	211	1/1	0.63	0.41	38,38,38,38	1
24	MG	A	1571	1/1	0.71	0.35	38,38,38,38	1
24	MG	A	1550	1/1	0.73	0.40	38,38,38,38	1
24	MG	A	1557	1/1	0.73	0.48	38,38,38,38	1
24	MG	A	1619	1/1	0.74	0.61	38,38,38,38	1
24	MG	A	1573	1/1	0.78	0.78	38,38,38,38	1
24	MG	A	212	1/1	0.78	0.74	38,38,38,38	1
24	MG	A	1620	1/1	0.80	0.15	38,38,38,38	1
24	MG	A	1616	1/1	0.81	1.00	38,38,38,38	1
24	MG	A	1613	1/1	0.81	0.19	38,38,38,38	1
24	MG	A	1582	1/1	0.81	0.20	38,38,38,38	1
24	MG	A	1567	1/1	0.82	0.35	38,38,38,38	0
24	MG	A	1598	1/1	0.83	0.37	38,38,38,38	0
24	MG	A	1600	1/1	0.83	0.23	38,38,38,38	0
24	MG	A	1610	1/1	0.83	0.31	38,38,38,38	1
24	MG	A	1591	1/1	0.83	0.51	38,38,38,38	1
24	MG	A	1621	1/1	0.83	0.26	38,38,38,38	1
24	MG	A	1561	1/1	0.84	0.44	38,38,38,38	1
24	MG	A	1551	1/1	0.85	0.94	38,38,38,38	1
24	MG	A	1580	1/1	0.85	0.31	38,38,38,38	0
24	MG	A	1565	1/1	0.86	0.43	38,38,38,38	1
24	MG	A	1602	1/1	0.86	0.10	38,38,38,38	0
24	MG	A	1601	1/1	0.87	0.26	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1627	1/1	0.87	0.81	38,38,38,38	1
24	MG	D	215	1/1	0.88	0.35	38,38,38,38	0
24	MG	A	1593	1/1	0.89	0.20	38,38,38,38	0
24	MG	A	1611	1/1	0.89	0.19	38,38,38,38	1
24	MG	A	1546	1/1	0.89	0.17	38,38,38,38	1
24	MG	A	1560	1/1	0.89	0.42	38,38,38,38	0
24	MG	A	1552	1/1	0.89	0.35	38,38,38,38	0
24	MG	A	1630	1/1	0.90	0.45	38,38,38,38	1
24	MG	A	1612	1/1	0.90	0.16	38,38,38,38	0
24	MG	A	1595	1/1	0.91	0.29	38,38,38,38	0
24	MG	A	1604	1/1	0.91	0.34	38,38,38,38	0
24	MG	A	1605	1/1	0.91	0.20	38,38,38,38	0
24	MG	A	1563	1/1	0.91	0.48	38,38,38,38	0
24	MG	A	1577	1/1	0.91	0.40	38,38,38,38	0
24	MG	A	1594	1/1	0.91	0.31	38,38,38,38	0
24	MG	A	1564	1/1	0.92	0.09	38,38,38,38	0
23	PAR	A	1545	42/42	0.92	0.24	23,23,23,23	0
24	MG	A	71	1/1	0.92	0.51	38,38,38,38	0
24	MG	A	1596	1/1	0.92	0.34	38,38,38,38	0
24	MG	A	1553	1/1	0.92	0.21	38,38,38,38	1
24	MG	H	213	1/1	0.92	0.61	38,38,38,38	1
24	MG	A	1614	1/1	0.93	0.44	38,38,38,38	1
24	MG	A	1607	1/1	0.93	0.56	38,38,38,38	0
24	MG	A	1629	1/1	0.93	0.44	38,38,38,38	1
24	MG	A	1547	1/1	0.93	0.29	38,38,38,38	0
24	MG	A	214	1/1	0.93	0.20	38,38,38,38	0
24	MG	A	1609	1/1	0.93	0.26	38,38,38,38	0
24	MG	A	1581	1/1	0.94	0.27	38,38,38,38	0
24	MG	A	1587	1/1	0.94	0.40	38,38,38,38	0
24	MG	A	1589	1/1	0.94	0.23	38,38,38,38	0
24	MG	A	1631	1/1	0.94	0.34	38,38,38,38	1
24	MG	A	1549	1/1	0.94	0.34	38,38,38,38	0
24	MG	A	1568	1/1	0.94	0.46	38,38,38,38	0
24	MG	A	1628	1/1	0.95	0.45	38,38,38,38	1
24	MG	A	1618	1/1	0.95	0.14	38,38,38,38	1
24	MG	A	1597	1/1	0.95	0.59	38,38,38,38	1
24	MG	A	1579	1/1	0.95	0.31	38,38,38,38	0
24	MG	A	1584	1/1	0.95	0.11	38,38,38,38	1
24	MG	A	1588	1/1	0.95	0.26	38,38,38,38	0
26	SRY	A	1634	40/40	0.95	0.21	23,23,23,23	0
24	MG	A	1555	1/1	0.96	0.32	38,38,38,38	0
24	MG	A	1592	1/1	0.96	0.60	38,38,38,38	1

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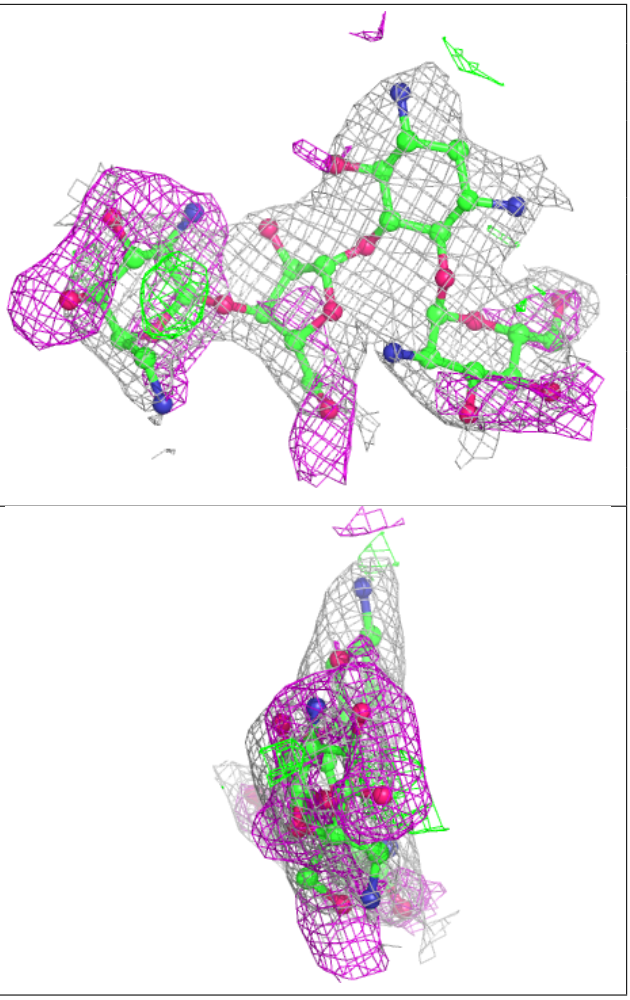
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	1575	1/1	0.96	0.38	38,38,38,38	0
24	MG	A	1576	1/1	0.96	0.07	38,38,38,38	1
24	MG	A	1606	1/1	0.96	0.15	38,38,38,38	0
24	MG	A	1554	1/1	0.96	0.29	38,38,38,38	0
24	MG	A	1569	1/1	0.96	0.39	38,38,38,38	0
24	MG	A	1632	1/1	0.96	0.40	38,38,38,38	1
24	MG	A	1559	1/1	0.96	0.34	38,38,38,38	0
24	MG	A	1572	1/1	0.96	0.43	38,38,38,38	0
25	SCM	A	1633	23/23	0.96	0.21	23,23,23,23	0
24	MG	A	1590	1/1	0.96	0.28	38,38,38,38	1
24	MG	A	1585	1/1	0.97	0.46	38,38,38,38	0
24	MG	A	1617	1/1	0.97	0.15	38,38,38,38	1
24	MG	A	86	1/1	0.97	0.30	38,38,38,38	0
24	MG	A	1599	1/1	0.97	0.33	38,38,38,38	1
24	MG	A	1548	1/1	0.97	0.35	38,38,38,38	0
24	MG	A	1608	1/1	0.97	0.43	38,38,38,38	1
24	MG	A	1624	1/1	0.97	0.53	38,38,38,38	1
24	MG	A	1626	1/1	0.97	0.30	38,38,38,38	1
24	MG	A	1578	1/1	0.97	0.26	38,38,38,38	0
27	ZN	D	300	1/1	0.97	0.31	47,47,47,47	0
24	MG	A	1574	1/1	0.98	0.50	38,38,38,38	0
24	MG	A	1558	1/1	0.98	0.52	38,38,38,38	0
24	MG	A	1625	1/1	0.98	0.34	38,38,38,38	1
24	MG	A	87	1/1	0.98	0.45	38,38,38,38	1
24	MG	A	1556	1/1	0.98	0.23	38,38,38,38	0
24	MG	A	1562	1/1	0.99	0.69	38,38,38,38	0
24	MG	A	1622	1/1	0.99	0.30	38,38,38,38	1
24	MG	A	1566	1/1	0.99	0.64	38,38,38,38	0
24	MG	A	1603	1/1	0.99	0.41	38,38,38,38	0
27	ZN	N	190	1/1	0.99	0.21	47,47,47,47	1
24	MG	A	1623	1/1	1.00	0.37	38,38,38,38	1
24	MG	A	1570	1/1	1.00	0.22	38,38,38,38	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

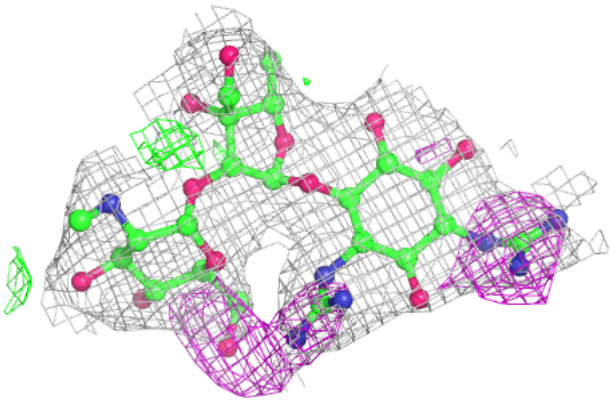
Electron density around PAR A 1545:

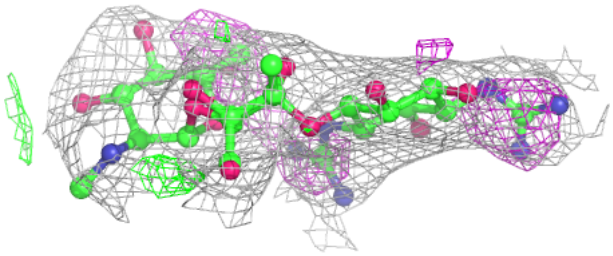
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

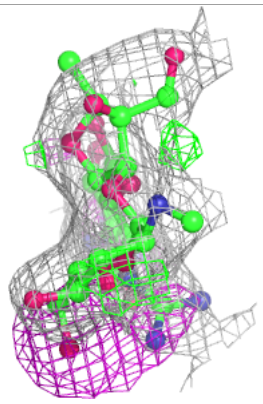


Electron density around SRY A 1634:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

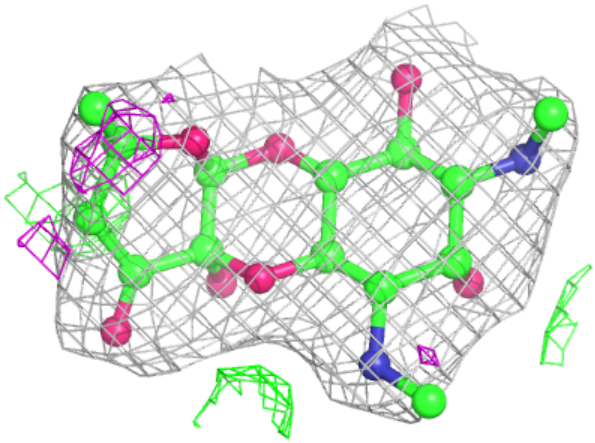


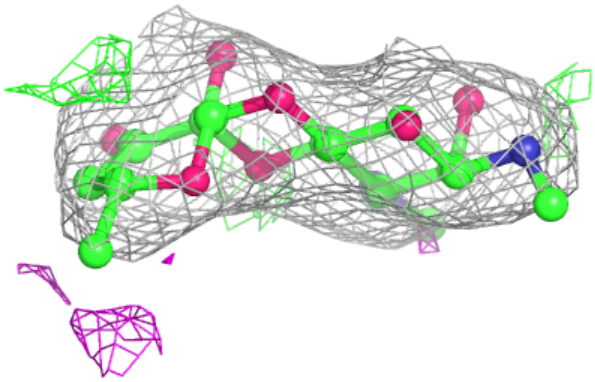


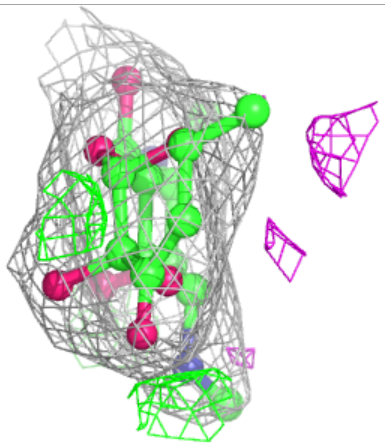


Electron density around SCM A 1633:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.