Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:10 AM EDT

PDB ID	:	5XWP
Title	:	Crystal structure of LbuCas13a-crRNA-target RNA ternary complex
Authors	:	Liu, L.; Li, X.; Li, Z.; Wang, Y.
Deposited on	:	2017-06-30
Resolution	:	3.09 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:

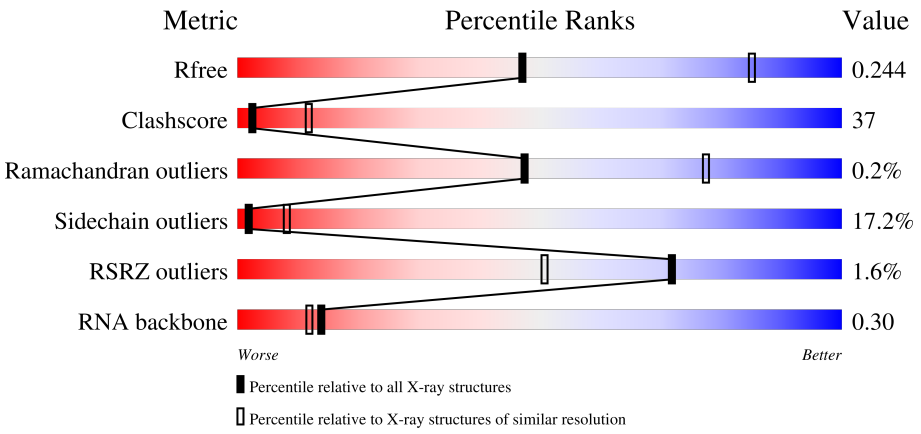
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)
RNA backbone	3102	1063 (3.36-2.80)

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	1160	.% 46% 42% 9% •
1	B	1160	2% 44% 42% 9% •
2	C	59	20% 37% 37% • •
2	E	59	25% 42% 29% • •

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Mol	Chain	Length	Quality of chain
3	D	30	23% 47% 27% •
3	F	30	30% 40% 27% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21838 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 protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1125	9160	5877	1539	1720	3	21	0	0	0
1	B	1114	8940	5718	1508	1690	3	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP C7NBY4
A	1048	ALA	ARG	engineered mutation	UNP C7NBY4
A	1053	ALA	HIS	engineered mutation	UNP C7NBY4
B	0	SER	-	expression tag	UNP C7NBY4
B	1048	ALA	ARG	engineered mutation	UNP C7NBY4
B	1053	ALA	HIS	engineered mutation	UNP C7NBY4

- Molecule 2 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	58	1229	553	224	394	58	0	0	0
2	E	58	1229	553	224	394	58	0	0	0

- Molecule 3 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	30	644	288	116	210	30	0	0	0
3	F	29	624	279	113	203	29	0	0	0

- Molecule 4 is water.

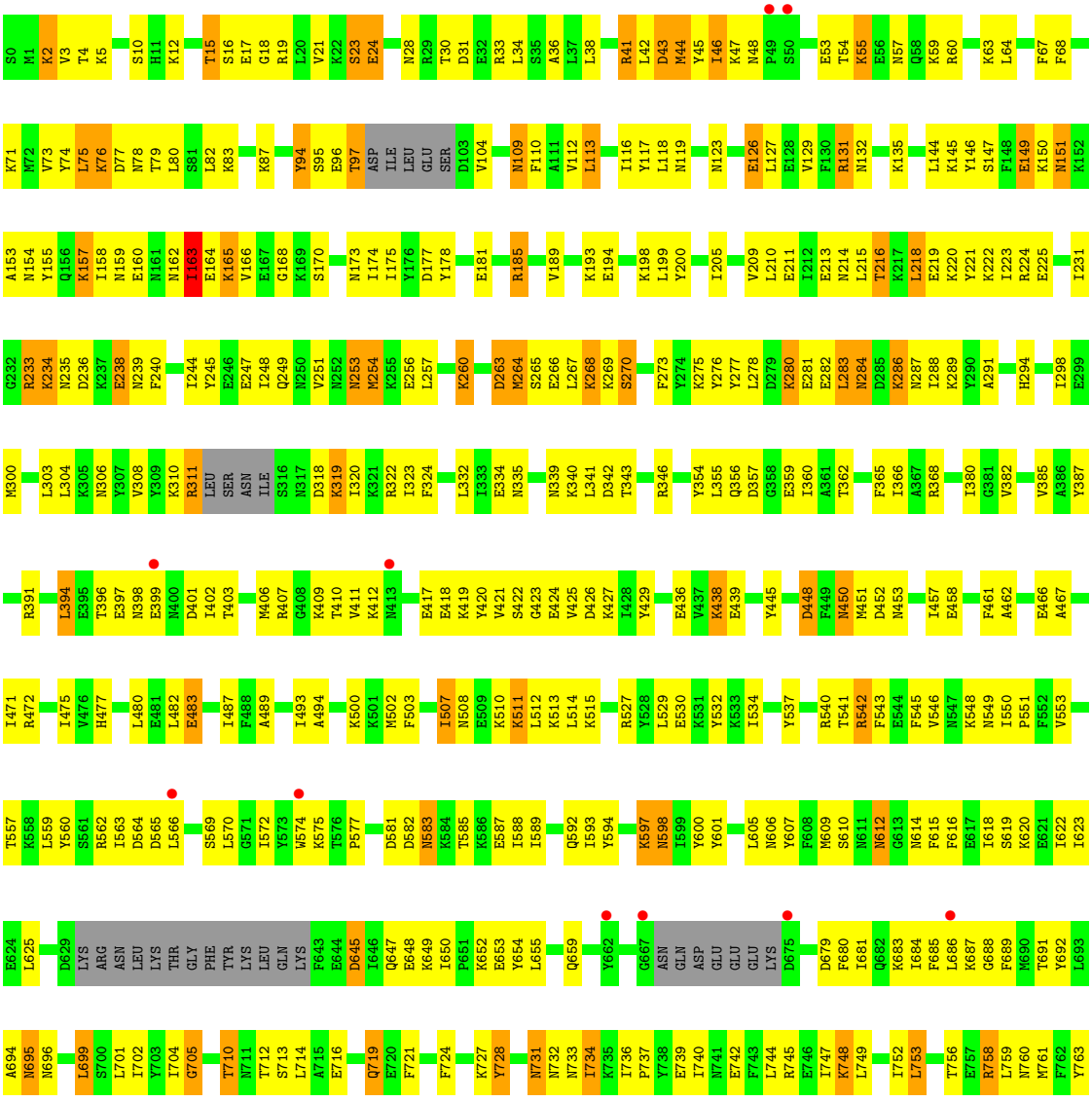
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	10	10	10	0	0
			Total	O		
4	B	2	2	2	0	0

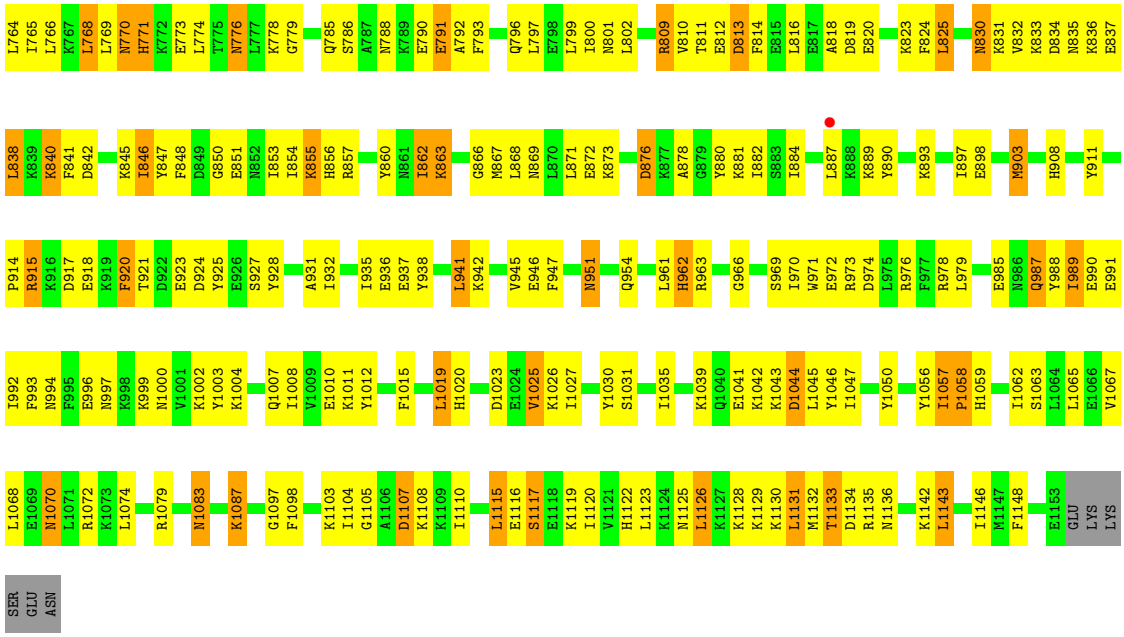
3 Residue-property plots (i)

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: Uncharacterized protein

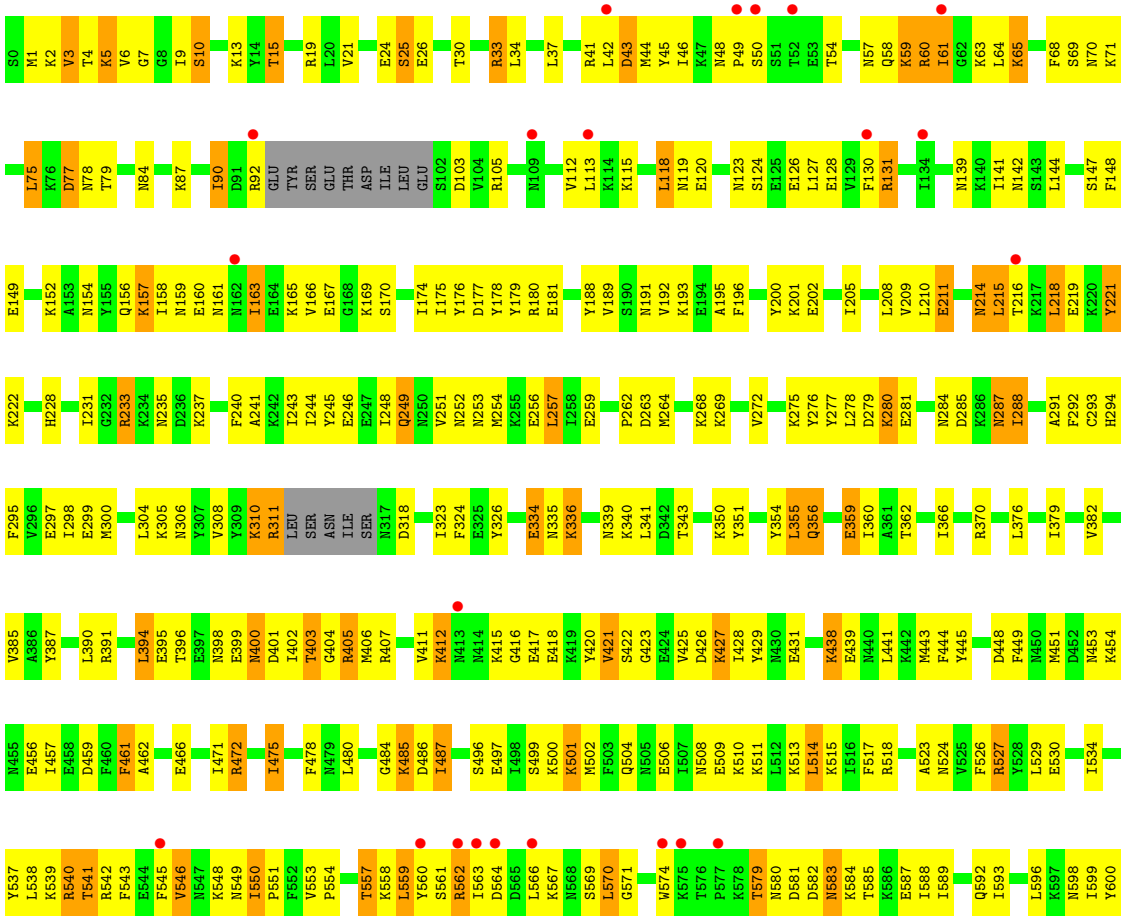
Chain A:





• Molecule 1: Uncharacterized protein

Chain B:



Y601 G602 E603 F604 L605 N606 Y607 F608 M609 S610 N611 N614 F615 F616 E617 I618 S619 K620 E621 I622 I623 E624 L625 N626 D629 K630 R631 N632 LEU LYS THR GLY PHE TYR LYS LEU GLN LYS PHE GLU ASP ILE GLN GLU LYS ILE P651 K652 L655 A656 Q659 N665 A666 GLY ASN

GLN ASP GLU GLU GLU LYS D675 T676 Y677 I678 D679 F680 I681 Q682 K683 I684 F685 L686 K687 G688 F689 M690 T691 Y692 L693 A694 N695 N696 G697 R698 L699 S700 L701 I702 Y703 I704 G705 S706 D707 T710 N711 T712 S713 L714 Q719 E720 F721 D722 L725 K726 K727 Y728 E729 Q730 N731 N732 N733

I734 K735 I736 P737 Y738 E739 I740 N741 L744 R745 E746 I747 K748 I752 L753 K754 Y755 T756 E757 R758 L759 N760 M761 F762 Y763 L764 K767 L768 L769 N770 H771 K772 E773 L774 K778 E782 K783 Y784 A787 D795 Q796 L799 I800 N801 L802 L803 N804 N808 R809 V810

F814 E815 L816 G822 K823 F824 L825 D826 F827 K831 V832 K833 D834 L838 K839 K840 F841 D842 T843 N844 K845 I846 Y847 F848 D849 I853 I854 K855 H856 R857 Y860 N861 I862 G866 M867 L868 N869 L870 L871 E872 A878 G879 Y880 K881 I882 E885 E886 L887 K888 K889 Y890 S891

N892 K893 K894 I897 E898 H901 K902 M903 Q904 E905 N906 L907 H908 R909 K910 Y911 A912 E913 P914 R915 K916 F920 T921 D922 E923 D924 Y925 E926 S927 Y928 K929 Q930 A931 I932 E933 N934 I935 E936 E937 Y938 L941 K942 N943 K944 V945 E946 F947 N948 E949 R959 H962 R963 G966

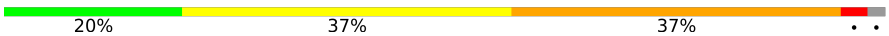
I970 R973 R976 F977 R978 L979 E982 F983 P984 E985 N986 Q987 Y988 I989 E990 E991 I992 F993 N994 F995 E996 N997 K998 K999 N1000 V1001 K1004 G1005 G1006 Q1007 I1008 V1009 E1010 K1011 Y1012 I1013 K1014 F1015 Y1016 L1019 H1020 E1024 K1029 Y1030 S1031 I1035 Q1040 E1041 K1042 K1043

D1044 L1045 Y1046 I1047 A1048 P1058 S1063 L1064 L1065 L1068 R1072 R1079 K1087 S1088 V1099 A1100 T1101 F1102 K1103 I1104 I1110 Q1113 T1114 L1115 E1116 S1117 E1118 K1119 I1120 L1123 K1124 N1125 L1126 K1129 D1134 R1135 N1136 E1139 L1140 C1141 K1142 L1143 V1144 K1145 I1146 E1149

Y1150 K1151 M1152 E1153 GLU LYS LYS SER GLU ASN

- Molecule 2: RNA (59-MER)

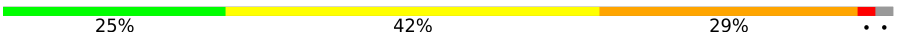
Chain C:



G G1 A2 C3 C4 A5 C6 C7 C8 C9 A10 A11 A12 A13 A14 U15 G16 A17 A18 G19 G20 G21 G22 A23 C24 U25 A26 A27 A28 A29 C30 A31 C32 A33 A34 A35 U36 C37 U38 A39 U46 A47 A48 U54 C55 U56 U57 C58

- Molecule 2: RNA (59-MER)

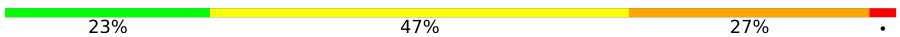
Chain E:



G G1 A2 C3 C4 A5 C6 C7 A10 A11 A12 A13 A14 U15 G16 A17 A18 G19 G20 G21 G22 A23 C24 U25 A26 A27 A28 A29 C30 A31 C32 A33 A34 A35 U36 C37 U38 A39 U40 U46 A47 A48 U54 C55 U56 U57 C58

- Molecule 3: RNA (30-MER)

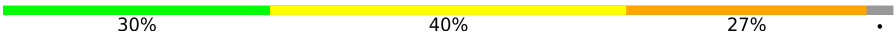
Chain D:

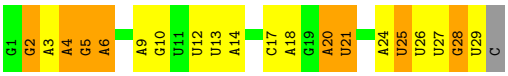


G1 G2 A3 A4 G5 A6 A7 G8 A9 G10 U11 U12 U13 A14 G19 A20 U21 A22 G23 A24 U25 U26 U27 G28 U29 C30

- Molecule 3: RNA (30-MER)

Chain F:


30%
40%
27%


G1
G2
A3
A4
G5
A6
A9
G10
U11
U12
U13
A14
C17
A18
G19
A20
U21
A24
U25
U26
U27
G28
U29
C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.58Å 132.87Å 139.96Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	48.18 – 3.09 48.18 – 3.09	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.18-3.09) 91.3 (48.18-3.09)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.18 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.218 , 0.244 0.220 , 0.244	Depositor DCC
R_{free} test set	2881 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , -23.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21838	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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)

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	0.70	0/9290	0.79	10/12431 (0.1%)
1	B	0.67	0/9063	0.83	15/12146 (0.1%)
2	C	0.86	4/1375 (0.3%)	0.81	1/2137 (0.0%)
2	E	0.79	1/1375 (0.1%)	0.78	0/2137
3	D	0.72	3/721 (0.4%)	0.76	1/1122 (0.1%)
3	F	0.75	2/699 (0.3%)	0.75	1/1088 (0.1%)
All	All	0.71	10/22523 (0.0%)	0.81	28/31061 (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	0	2
1	B	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	A	O3'-P	-9.91	1.49	1.61
2	C	2	A	O3'-P	-9.17	1.50	1.61
2	C	1	G	O3'-P	-6.05	1.53	1.61
3	F	12	U	O3'-P	-5.86	1.54	1.61
3	D	2	G	C4'-O4'	5.58	1.52	1.45
2	C	28	A	O3'-P	-5.50	1.54	1.61
3	D	21	U	O3'-P	-5.39	1.54	1.61
3	F	2	G	C4'-O4'	-5.17	1.38	1.45
2	C	39	A	O3'-P	-5.11	1.55	1.61
3	D	8	G	O3'-P	-5.04	1.55	1.61

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	403	THR	N-CA-C	-14.91	70.75	111.00
1	B	570	LEU	N-CA-C	12.38	144.44	111.00
1	B	678	ILE	CB-CA-C	-8.31	94.97	111.60
1	B	570	LEU	CB-CA-C	-8.22	94.59	110.20
1	B	65	LYS	CB-CA-C	-7.21	95.99	110.40
3	F	2	G	C5'-C4'-O4'	-7.01	100.68	109.10
1	B	404	GLY	C-N-CA	-6.69	104.98	121.70
1	A	601	TYR	CB-CA-C	6.18	122.75	110.40
1	B	855	LYS	CB-CA-C	-5.98	98.45	110.40
1	B	571	GLY	N-CA-C	-5.91	98.33	113.10
1	B	848	PHE	CB-CA-C	-5.88	98.64	110.40
1	A	542	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	494	ALA	C-N-CD	5.88	140.74	128.40
1	B	913	ARG	C-N-CD	5.83	140.64	128.40
3	D	2	G	C1'-O4'-C4'	-5.80	105.26	109.90
1	A	540	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	728	TYR	CB-CA-C	-5.50	99.39	110.40
2	C	1	G	C4'-C3'-O3'	-5.38	98.09	109.40
1	A	163	ILE	N-CA-C	5.37	125.50	111.00
1	B	922	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	629	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	1044	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	1044	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	565	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	77	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	564	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	263	ASP	N-CA-C	-5.15	97.09	111.00
1	B	963	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	VAL	Peptide
1	A	705	GLY	Peptide
1	B	421	VAL	Peptide
1	B	695	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9160	0	9025	680	0
1	B	8940	0	8665	681	0
2	C	1229	0	627	87	0
2	E	1229	0	627	95	0
3	D	644	0	321	40	0
3	F	624	0	310	36	0
4	A	10	0	0	0	0
4	B	2	0	0	0	0
All	All	21838	0	19575	1546	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 37.

All (1546) 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:566:LEU:HD12	1:A:686:LEU:CD1	1.58	1.30
1:A:406:MSE:CE	1:A:461:PHE:HB3	1.62	1.30
1:B:920:PHE:O	1:B:921:THR:CG2	1.82	1.24
1:A:265:SER:HB3	1:A:268:LYS:HG2	1.24	1.19
1:B:846:ILE:HD11	1:B:887:LEU:HD21	1.21	1.15
1:B:920:PHE:O	1:B:921:THR:HG23	0.96	1.13
1:B:846:ILE:CD1	1:B:887:LEU:HD21	1.78	1.13
1:B:251:VAL:CG1	1:B:256:GLU:HB2	1.78	1.13
1:A:74:TYR:CE1	1:A:83:LYS:HE3	1.84	1.12
1:B:251:VAL:HG11	1:B:256:GLU:HB2	1.28	1.11
1:B:376:LEU:O	1:B:475:ILE:HG21	1.49	1.11
1:B:502:MSE:HE3	1:B:763:TYR:HE2	1.14	1.09
1:A:566:LEU:HD12	1:A:686:LEU:HD13	1.29	1.08
2:E:28:A:OP2	1:B:1088:SER:HB3	1.54	1.07
1:A:240:PHE:O	1:A:244:ILE:HG13	1.53	1.07
1:A:727:LYS:C	1:A:734:ILE:HD11	1.75	1.06
1:A:511:LYS:HG2	1:A:728:TYR:OH	1.55	1.06
1:B:688:GLY:O	1:B:691:THR:HG22	1.56	1.06
1:A:915:ARG:H	1:A:915:ARG:HD2	1.19	1.06
1:A:607:TYR:O	1:A:610:SER:HB3	1.55	1.05
2:E:40:U:H5"	1:B:546:VAL:HG22	1.31	1.05
1:A:503:PHE:O	1:A:507:ILE:HG22	1.54	1.05
1:A:727:LYS:O	1:A:734:ILE:HD11	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:ILE:HG23	1:A:973:ARG:NH1	1.71	1.05
1:A:406:MSE:HE2	1:A:461:PHE:HB3	1.39	1.04
1:A:406:MSE:HE3	1:A:461:PHE:HB3	1.39	1.03
1:A:862:ILE:HG13	1:A:951:ASN:HD21	1.20	1.03
1:B:299:GLU:OE2	1:B:340:LYS:HE2	1.56	1.03
1:A:566:LEU:CD1	1:A:686:LEU:CD1	2.35	1.03
1:B:574:TRP:CZ3	1:B:702:ILE:HG23	1.93	1.03
1:B:901:HIS:O	1:B:905:GLU:HG3	1.59	1.03
1:A:1039:LYS:HE3	1:A:1046:TYR:CE2	1.92	1.03
1:A:566:LEU:CD1	1:A:686:LEU:HD13	1.89	1.02
2:E:33:A:H5'	2:E:33:A:H8	1.25	1.02
1:A:932:ILE:HD11	1:A:1131:LEU:HD11	1.39	1.02
1:B:264:MSE:CE	1:B:269:LYS:HG3	1.91	1.01
1:B:157:LYS:HE2	1:B:355:LEU:O	1.60	1.01
1:A:160:GLU:CB	1:A:163:ILE:HG22	1.90	1.00
1:A:694:ALA:HA	1:A:699:LEU:HD12	1.42	1.00
1:B:584:LYS:O	1:B:588:ILE:HG13	1.62	0.99
1:A:265:SER:HB3	1:A:268:LYS:CG	1.92	0.99
2:C:32:C:H42	3:D:28:G:H1	1.07	0.98
1:B:615:PHE:CE2	1:B:651:PRO:N	2.30	0.98
3:D:5:G:H5"	3:D:5:G:H8	1.28	0.98
1:B:251:VAL:HG11	1:B:256:GLU:CB	1.93	0.98
1:B:761:MSE:HE1	1:B:764:LEU:HD12	1.46	0.97
1:A:160:GLU:OE1	1:A:162:ASN:HB3	1.64	0.97
1:B:60:ARG:HH12	1:B:103:ASP:H	1.05	0.97
2:E:31:A:H2'	2:E:32:C:H5"	1.45	0.97
1:B:678:ILE:HA	1:B:681:ILE:HG22	1.43	0.97
1:A:163:ILE:HG13	1:A:165:LYS:HD2	1.47	0.97
1:A:936:GLU:OE1	1:A:1133:THR:HG22	1.64	0.96
1:A:687:LYS:O	1:A:691:THR:HG23	1.65	0.96
2:C:17:A:H5"	2:C:17:A:N3	1.81	0.96
1:A:450:ASN:O	1:A:457:ILE:HD11	1.66	0.95
1:B:502:MSE:HE3	1:B:763:TYR:CE2	2.01	0.95
1:B:608:PHE:HD2	1:B:609:MSE:HE2	1.32	0.95
1:B:305:LYS:O	1:B:310:LYS:HB2	1.64	0.95
1:A:862:ILE:HG13	1:A:951:ASN:ND2	1.82	0.95
1:A:970:ILE:HG22	1:A:974:ASP:OD2	1.63	0.95
3:F:3:A:H2'	3:F:4:A:C5'	1.96	0.94
1:A:200:TYR:HB3	1:A:205:ILE:HD11	1.49	0.94
1:A:719:GLN:H	1:A:719:GLN:HE21	0.94	0.94
1:B:77:ASP:O	1:B:79:THR:HG23	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:CG1	1:A:419:LYS:HG2	1.98	0.94
1:B:244:ILE:O	1:B:248:ILE:HG13	1.66	0.94
1:A:422:SER:HB2	1:A:427:LYS:HE2	1.50	0.93
2:E:21:G:H2'	2:E:22:G:H5'	1.48	0.93
2:E:31:A:O2'	2:E:32:C:OP1	1.84	0.93
1:B:284:ASN:H	1:B:287:ASN:HD21	0.98	0.93
1:B:846:ILE:CD1	1:B:887:LEU:CD2	2.46	0.93
1:A:74:TYR:CZ	1:A:83:LYS:HE3	2.05	0.92
1:B:678:ILE:O	1:B:682:GLN:HB2	1.68	0.92
2:C:32:C:N4	3:D:28:G:H1	1.67	0.92
1:A:932:ILE:HD11	1:A:1131:LEU:CD1	2.00	0.92
1:A:438:LYS:HB2	1:A:451:MSE:HE3	1.51	0.91
2:C:21:G:H2'	2:C:22:G:H5'	1.50	0.91
1:B:690:MSE:SE	1:B:693:LEU:HD23	2.21	0.91
3:F:3:A:H2'	3:F:4:A:H5'	1.52	0.91
1:A:80:LEU:CB	1:A:127:LEU:HB3	2.01	0.91
1:A:411:VAL:HG13	1:A:419:LYS:HG2	1.53	0.91
1:A:15:THR:HG22	1:A:360:ILE:HD13	1.53	0.91
1:A:60:ARG:HD3	1:A:97:THR:HG22	1.54	0.90
1:B:615:PHE:CZ	1:B:651:PRO:N	2.40	0.89
1:A:915:ARG:HG3	1:A:915:ARG:HH11	1.34	0.89
1:B:241:ALA:O	1:B:244:ILE:HG22	1.72	0.89
1:B:678:ILE:HA	1:B:681:ILE:CG2	2.01	0.89
1:A:42:LEU:HD12	1:A:71:LYS:HB2	1.54	0.89
1:A:507:ILE:HD11	1:A:752:ILE:HG23	1.55	0.88
1:A:991:GLU:HG2	1:A:1000:ASN:HB3	1.54	0.88
1:A:75:LEU:HD21	1:A:79:THR:N	1.87	0.88
1:B:550:ILE:HG23	1:B:551:PRO:HD2	1.55	0.88
1:A:231:ILE:HD12	1:A:267:LEU:HD22	1.53	0.88
1:A:406:MSE:CE	1:A:461:PHE:CB	2.52	0.88
1:B:211:GLU:OE2	1:B:222:LYS:HE2	1.72	0.87
1:A:566:LEU:HD12	1:A:686:LEU:HD12	1.53	0.87
1:B:761:MSE:HA	1:B:761:MSE:HE3	1.56	0.87
1:A:265:SER:N	1:A:268:LYS:HD2	1.89	0.87
1:A:112:VAL:HG13	1:A:126:GLU:OE1	1.75	0.86
2:E:40:U:H5"	1:B:546:VAL:CG2	2.05	0.86
1:B:502:MSE:CE	1:B:763:TYR:HE2	1.89	0.86
1:B:254:MSE:HE2	1:B:264:MSE:HE1	1.57	0.86
1:B:310:LYS:HA	1:B:310:LYS:CE	2.04	0.86
1:A:247:GLU:OE1	1:A:260:LYS:HD3	1.76	0.86
1:A:932:ILE:CD1	1:A:1131:LEU:HD11	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MSE:HE1	1:B:269:LYS:HG3	1.57	0.86
1:A:701:LEU:O	1:A:704:ILE:HG13	1.76	0.85
3:F:27:U:C2'	3:F:28:G:H5'	2.06	0.85
1:A:719:GLN:H	1:A:719:GLN:NE2	1.72	0.85
1:A:1030:TYR:O	1:A:1035:ILE:HD11	1.77	0.85
1:B:615:PHE:CE2	1:B:651:PRO:CD	2.60	0.85
3:F:4:A:C2'	3:F:5:G:O5'	2.24	0.84
1:A:15:THR:HG21	1:A:360:ILE:HD12	1.60	0.84
1:A:1039:LYS:HE3	1:A:1046:TYR:HE2	1.41	0.84
1:B:57:ASN:O	1:B:61:ILE:HG13	1.77	0.84
1:B:1019:LEU:HD23	1:B:1020:HIS:CE1	2.12	0.84
1:A:15:THR:HG22	1:A:360:ILE:CD1	2.07	0.84
1:A:185:ARG:O	1:A:189:VAL:HG23	1.78	0.83
1:B:518:ARG:HG3	1:B:725:LEU:HD13	1.58	0.83
1:B:401:ASP:OD1	1:B:403:THR:HG23	1.79	0.83
1:B:574:TRP:CZ3	1:B:702:ILE:CG2	2.61	0.83
1:A:15:THR:CG2	1:A:360:ILE:HD12	2.08	0.83
1:A:737:PRO:HG2	1:A:740:ILE:CG1	2.08	0.83
1:B:254:MSE:CE	1:B:264:MSE:HE1	2.09	0.83
1:B:251:VAL:CG1	1:B:256:GLU:CB	2.52	0.83
1:B:920:PHE:C	1:B:921:THR:HG23	1.98	0.83
2:E:17:A:H5"	2:E:17:A:N3	1.93	0.83
1:A:719:GLN:HE21	1:A:719:GLN:N	1.75	0.83
1:B:60:ARG:NH1	1:B:103:ASP:H	1.75	0.83
1:B:845:LYS:HB3	1:B:848:PHE:O	1.78	0.83
1:A:756:THR:HB	1:A:759:LEU:HB2	1.58	0.82
1:A:513:LYS:HE2	1:A:744:LEU:O	1.79	0.82
1:A:240:PHE:CE2	1:A:263:ASP:O	2.32	0.82
1:A:251:VAL:HB	1:A:256:GLU:HB3	1.60	0.82
1:A:46:ILE:HG23	1:A:104:VAL:O	1.78	0.82
1:A:841:PHE:HE1	1:A:887:LEU:HD11	1.44	0.82
1:A:816:LEU:HD13	1:A:863:LYS:HG2	1.59	0.82
1:A:75:LEU:CD2	1:A:79:THR:H	1.92	0.82
1:A:163:ILE:HG13	1:A:165:LYS:CD	2.10	0.82
1:A:655:LEU:HD13	1:A:681:ILE:HD11	1.61	0.81
1:A:737:PRO:HG2	1:A:740:ILE:HG13	1.61	0.81
1:A:846:ILE:O	1:A:854:ILE:HD12	1.79	0.81
1:B:737:PRO:HB2	1:B:740:ILE:HD11	1.59	0.81
1:B:154:ASN:OD1	1:B:170:SER:HB3	1.79	0.81
2:C:7:C:C2'	2:C:8:C:H5'	2.10	0.81
1:A:265:SER:CB	1:A:268:LYS:HG2	2.07	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:CB	1:A:127:LEU:CB	2.58	0.81
1:B:737:PRO:CG	1:B:740:ILE:HD11	2.11	0.80
1:B:160:GLU:O	1:B:163:ILE:HG13	1.80	0.80
1:A:694:ALA:CA	1:A:699:LEU:HD12	2.11	0.80
1:B:60:ARG:HH12	1:B:103:ASP:N	1.79	0.80
1:B:609:MSE:HE3	1:B:685:PHE:HE1	1.46	0.80
1:B:737:PRO:CB	1:B:740:ILE:HD11	2.11	0.80
1:B:846:ILE:HD13	1:B:887:LEU:CD2	2.10	0.80
1:A:550:ILE:HG22	1:A:551:PRO:HD2	1.64	0.80
1:A:566:LEU:CD1	1:A:686:LEU:HD12	2.09	0.80
2:E:21:G:C2'	2:E:22:G:H5'	2.10	0.80
1:B:398:ASN:HD22	1:B:400:ASN:H	1.30	0.79
1:A:320:ILE:HG23	1:A:324:PHE:HD2	1.47	0.79
1:A:438:LYS:CD	1:A:451:MSE:CE	2.59	0.79
1:A:240:PHE:CG	1:A:268:LYS:NZ	2.50	0.79
1:A:699:LEU:CD2	1:A:702:ILE:HD11	2.11	0.79
1:A:882:ILE:CD1	1:A:947:PHE:HE1	1.95	0.79
2:C:7:C:H2'	2:C:8:C:H5'	1.64	0.79
2:C:10:A:C8	2:C:10:A:H5"	2.16	0.79
1:B:453:ASN:HB3	1:B:456:GLU:HB2	1.63	0.79
1:B:617:GLU:HA	1:B:620:LYS:CB	2.11	0.79
3:D:5:G:H5"	3:D:5:G:C8	2.15	0.79
1:B:925:TYR:HD2	1:B:1126:LEU:HD21	1.47	0.79
1:A:75:LEU:HD23	1:A:79:THR:O	1.83	0.79
1:A:131:ARG:HB2	1:A:131:ARG:HH11	1.47	0.79
1:B:756:THR:CG2	1:B:758:ARG:HG3	2.13	0.79
1:A:75:LEU:CD2	1:A:79:THR:N	2.45	0.79
1:A:283:LEU:HD13	1:A:288:ILE:HD12	1.65	0.79
1:B:178:TYR:CD2	1:B:288:ILE:CD1	2.65	0.79
1:B:219:GLU:O	1:B:222:LYS:HG2	1.83	0.79
1:B:560:TYR:HA	1:B:563:ILE:CD1	2.13	0.79
3:F:4:A:H2'	3:F:5:G:O5'	1.81	0.79
1:B:735:LYS:H	1:B:735:LYS:HD3	1.47	0.79
2:C:58:C:H6	2:C:58:C:H5"	1.48	0.78
2:E:31:A:H2'	2:E:32:C:H6	1.49	0.78
1:B:412:LYS:HB2	1:B:417:GLU:O	1.83	0.78
1:A:549:ASN:HB2	2:C:38:U:O2'	1.84	0.78
2:E:1:G:H8	2:E:1:G:H3'	1.49	0.78
1:B:925:TYR:CD2	1:B:1126:LEU:CD2	2.67	0.78
1:A:15:THR:CG2	1:A:360:ILE:CD1	2.61	0.78
1:B:351:TYR:HB3	1:B:355:LEU:HD22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:O	1:B:396:THR:HG23	1.83	0.78
1:B:376:LEU:HD21	1:B:484:GLY:HA2	1.64	0.78
1:A:283:LEU:CD1	1:A:288:ILE:HD12	2.14	0.77
1:B:530:GLU:OE2	1:B:710:THR:HG21	1.83	0.77
1:B:566:LEU:O	1:B:569:SER:HB2	1.84	0.77
1:A:109:ASN:O	1:A:113:LEU:HD12	1.84	0.77
1:A:198:LYS:HD3	1:A:266:GLU:HG2	1.66	0.77
1:A:970:ILE:HG23	1:A:973:ARG:HH12	1.44	0.77
1:A:160:GLU:HB3	1:A:163:ILE:HG22	1.64	0.77
1:A:502:MSE:HE2	1:A:763:TYR:HE2	1.50	0.77
1:A:607:TYR:O	1:A:610:SER:CB	2.33	0.77
2:C:2:A:H2'	2:C:3:C:H5'	1.67	0.77
2:E:33:A:H5'	2:E:33:A:C8	2.15	0.77
1:A:46:ILE:CG2	1:A:104:VAL:O	2.34	0.76
1:A:175:ILE:HD11	1:A:278:LEU:HD11	1.66	0.76
1:A:320:ILE:HG23	1:A:324:PHE:CD2	2.20	0.76
2:C:21:G:C2'	2:C:22:G:H5'	2.15	0.76
1:B:1:MSE:HE3	1:B:37:LEU:HD22	1.67	0.76
1:B:75:LEU:HD23	1:B:75:LEU:O	1.85	0.76
1:B:415:LYS:N	1:B:416:GLY:HA2	1.98	0.76
3:D:2:G:C2	1:B:998:LYS:HG3	2.21	0.76
1:B:118:LEU:HD13	1:B:120:GLU:OE2	1.85	0.76
1:B:846:ILE:HD11	1:B:887:LEU:CD2	2.06	0.76
1:B:754:LYS:H	1:B:754:LYS:HD2	1.49	0.76
2:C:56:U:O2'	2:C:57:U:H5'	1.85	0.76
1:B:581:ASP:HB3	1:B:584:LYS:CB	2.15	0.76
1:A:362:THR:O	1:A:366:ILE:HG13	1.86	0.76
1:B:517:PHE:CZ	1:B:740:ILE:HG22	2.21	0.76
1:B:205:ILE:O	1:B:209:VAL:HG23	1.86	0.76
1:A:962:HIS:CD2	2:C:28:A:H61	2.04	0.75
1:A:991:GLU:HG2	1:A:1000:ASN:CB	2.16	0.75
1:B:614:ASN:CB	1:B:618:ILE:CD1	2.64	0.75
1:B:761:MSE:CE	1:B:764:LEU:HD12	2.15	0.75
1:B:1041:GLU:HB2	1:B:1043:LYS:HG3	1.68	0.75
1:A:731:ASN:HD22	1:A:731:ASN:C	1.89	0.75
1:A:221:TYR:O	1:A:225:GLU:HB2	1.86	0.75
1:A:294:HIS:CE1	1:A:298:ILE:HD11	2.22	0.75
1:A:1107:ASP:O	1:A:1108:LYS:HG2	1.87	0.75
1:A:265:SER:H	1:A:268:LYS:HD2	1.51	0.75
1:B:306:ASN:O	1:B:311:ARG:HB3	1.86	0.75
1:A:560:TYR:O	1:A:563:ILE:HG13	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:LYS:HZ3	1:A:937:GLU:CD	1.90	0.75
1:B:574:TRP:CZ2	1:B:592:GLN:OE1	2.39	0.75
2:E:32:C:H42	3:F:28:G:H1	1.31	0.75
1:B:618:ILE:CD1	1:B:691:THR:HG21	2.16	0.75
3:F:3:A:H2'	3:F:4:A:H5"	1.68	0.75
1:A:5:LYS:HD2	2:C:31:A:C8	2.22	0.74
1:B:157:LYS:HG2	1:B:166:VAL:HG22	1.66	0.74
1:A:112:VAL:O	1:A:116:ILE:HG13	1.85	0.74
1:A:438:LYS:CB	1:A:451:MSE:HE3	2.17	0.74
2:C:56:U:C2	3:D:5:G:N2	2.55	0.74
1:A:131:ARG:HB2	1:A:131:ARG:NH1	2.03	0.74
1:A:648:GLU:O	1:A:649:LYS:HG3	1.86	0.74
1:A:936:GLU:OE1	1:A:1133:THR:CG2	2.35	0.74
1:B:339:ASN:O	1:B:343:THR:HG23	1.86	0.74
1:B:989:ILE:HD12	1:B:1015:PHE:CE2	2.22	0.74
1:B:562:ARG:CZ	1:B:682:GLN:NE2	2.50	0.74
1:A:655:LEU:HD13	1:A:681:ILE:CD1	2.17	0.74
1:B:846:ILE:HG13	1:B:847:TYR:H	1.52	0.74
1:B:997:ASN:HD22	1:B:997:ASN:H	1.34	0.74
1:B:609:MSE:CE	1:B:685:PHE:CE1	2.71	0.74
1:B:756:THR:HG22	1:B:758:ARG:HG3	1.68	0.74
1:A:320:ILE:CG2	1:A:324:PHE:HD2	2.02	0.73
1:B:278:LEU:HD12	1:B:278:LEU:O	1.88	0.73
1:B:618:ILE:HD13	1:B:691:THR:HG21	1.70	0.73
1:B:608:PHE:CD2	1:B:609:MSE:HE2	2.22	0.73
1:A:160:GLU:CG	1:A:163:ILE:HG22	2.18	0.73
1:A:618:ILE:CD1	1:A:688:GLY:HA2	2.18	0.73
1:A:841:PHE:CE1	1:A:887:LEU:HD11	2.24	0.73
2:E:28:A:OP2	1:B:1088:SER:CB	2.36	0.73
1:B:771:HIS:HB3	1:B:808:ASN:HD22	1.54	0.73
3:F:27:U:H2'	3:F:28:G:H5'	1.69	0.73
1:A:406:MSE:O	1:A:425:VAL:HG12	1.88	0.73
1:A:339:ASN:O	1:A:343:THR:HG23	1.89	0.73
1:A:970:ILE:HG23	1:A:973:ARG:HH11	1.53	0.73
1:A:1007:GLN:HB2	1:A:1010:GLU:OE2	1.88	0.72
1:A:1120:ILE:HD11	1:A:1135:ARG:HG2	1.71	0.72
1:B:517:PHE:CE1	1:B:526:PHE:CE2	2.77	0.72
1:B:816:LEU:HB3	1:B:853:ILE:HD11	1.72	0.72
1:B:970:ILE:HG23	1:B:973:ARG:HH21	1.54	0.72
1:A:131:ARG:HG3	1:A:132:ASN:N	2.04	0.72
2:E:31:A:C2'	2:E:32:C:H5"	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:OG	1:A:24:GLU:N	2.20	0.72
1:B:609:MSE:CE	1:B:685:PHE:HE1	2.02	0.72
1:A:224:ARG:HD2	2:C:18:A:C8	2.24	0.72
1:A:75:LEU:HD21	1:A:78:ASN:CA	2.20	0.72
1:A:76:LYS:HA	1:A:76:LYS:CE	2.18	0.72
1:A:593:ILE:O	1:A:597:LYS:HB2	1.88	0.72
1:B:989:ILE:HD12	1:B:1015:PHE:HE2	1.55	0.72
1:A:549:ASN:CB	2:C:38:U:O2'	2.38	0.72
1:B:259:GLU:O	1:B:262:PRO:HD3	1.90	0.72
1:B:157:LYS:CE	1:B:355:LEU:O	2.37	0.72
1:A:438:LYS:HD3	1:A:451:MSE:CE	2.20	0.71
1:B:341:LEU:O	1:B:341:LEU:HD12	1.89	0.71
1:A:1031:SER:C	1:A:1035:ILE:HD12	2.10	0.71
1:B:906:ASN:O	1:B:909:ARG:HB3	1.91	0.71
1:B:925:TYR:HD2	1:B:1126:LEU:CD2	2.03	0.71
1:B:559:LEU:HD23	1:B:560:TYR:N	2.05	0.71
1:B:167:GLU:HB2	1:B:177:ASP:OD2	1.89	0.71
1:A:240:PHE:HE2	1:A:263:ASP:O	1.72	0.71
1:B:412:LYS:HA	1:B:418:GLU:HA	1.73	0.71
1:B:517:PHE:CZ	1:B:526:PHE:HE2	2.08	0.71
1:B:690:MSE:HA	1:B:693:LEU:HB3	1.73	0.71
2:E:1:G:H3'	2:E:1:G:C8	2.25	0.71
1:A:33:ARG:O	1:A:36:ALA:HB3	1.91	0.71
1:B:54:THR:HG23	1:B:57:ASN:HD22	1.54	0.71
1:A:283:LEU:CD1	1:A:288:ILE:CD1	2.68	0.70
1:A:1065:LEU:HD22	1:A:1110:ILE:HG22	1.73	0.70
2:E:28:A:H2	1:B:966:GLY:HA3	1.56	0.70
2:C:24:C:H6	2:C:24:C:H5'	1.56	0.70
1:B:550:ILE:HG22	1:B:553:VAL:HG12	1.73	0.70
1:A:42:LEU:HD21	1:A:73:VAL:CG2	2.21	0.70
1:A:234:LYS:O	1:A:238:GLU:HB2	1.92	0.70
2:E:56:U:O2'	2:E:57:U:H5'	1.91	0.70
1:A:254:MSE:HE3	1:A:277:TYR:HD2	1.56	0.70
1:A:1063:SER:O	1:A:1067:VAL:HG23	1.92	0.70
1:B:678:ILE:O	1:B:682:GLN:CB	2.40	0.70
1:B:719:GLN:H	1:B:719:GLN:NE2	1.89	0.70
1:B:987:GLN:HG3	1:B:988:TYR:CE1	2.26	0.70
1:A:254:MSE:HG3	1:A:273:PHE:HD1	1.57	0.70
1:A:1019:LEU:O	1:A:1019:LEU:HD22	1.92	0.70
1:B:570:LEU:CB	1:B:687:LYS:HD2	2.21	0.70
1:B:614:ASN:CB	1:B:618:ILE:HD12	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:G:C5'	2:E:2:A:H5'	2.22	0.70
1:B:376:LEU:O	1:B:475:ILE:CG2	2.35	0.70
2:E:32:C:H2'	2:E:33:A:H5"	1.73	0.70
2:C:10:A:H5"	2:C:10:A:H8	1.57	0.69
1:B:362:THR:O	1:B:366:ILE:HG13	1.91	0.69
1:B:611:ASN:O	1:B:611:ASN:ND2	2.21	0.69
1:B:690:MSE:HA	1:B:693:LEU:CB	2.22	0.69
1:A:823:LYS:HD3	1:A:872:GLU:OE1	1.92	0.69
1:A:1031:SER:O	1:A:1035:ILE:HD12	1.91	0.69
1:B:438:LYS:HA	1:B:451:MSE:HE3	1.74	0.69
1:A:503:PHE:O	1:A:507:ILE:CG2	2.38	0.69
1:B:862:ILE:HG23	1:B:868:LEU:HD21	1.73	0.69
1:B:705:GLY:HA2	1:B:711:ASN:HD22	1.57	0.69
1:B:559:LEU:HD23	1:B:559:LEU:C	2.12	0.69
1:A:219:GLU:O	1:A:222:LYS:HB2	1.93	0.69
2:E:7:C:H5"	1:B:340:LYS:HG2	1.73	0.69
1:A:764:LEU:O	1:A:768:LEU:HD22	1.93	0.69
1:B:54:THR:O	1:B:58:GLN:CB	2.41	0.69
1:A:1083:ASN:H	1:A:1083:ASN:HD22	1.39	0.69
1:A:200:TYR:HB3	1:A:205:ILE:CD1	2.22	0.69
1:A:240:PHE:CD1	1:A:268:LYS:NZ	2.58	0.69
1:A:502:MSE:HE2	1:A:763:TYR:CE2	2.28	0.69
2:E:31:A:HO2'	2:E:32:C:P	2.12	0.68
1:B:560:TYR:HA	1:B:563:ILE:HD11	1.74	0.68
1:A:67:PHE:CE2	1:A:117:TYR:HA	2.28	0.68
1:A:897:ILE:HD13	1:A:938:TYR:CZ	2.28	0.68
1:B:823:LYS:HB3	1:B:872:GLU:HG3	1.74	0.68
1:A:790:GLU:HG3	1:A:792:ALA:H	1.59	0.68
1:A:911:TYR:HB2	1:A:920:PHE:CE1	2.28	0.68
1:B:405:ARG:H	1:B:405:ARG:HD2	1.59	0.68
1:A:695:ASN:C	1:A:695:ASN:HD22	1.97	0.68
1:A:1030:TYR:C	1:A:1035:ILE:HD11	2.14	0.68
1:A:727:LYS:C	1:A:734:ILE:CD1	2.58	0.68
1:A:882:ILE:HD12	1:A:947:PHE:HE1	1.59	0.68
2:C:10:A:H5'	2:C:11:A:OP2	1.94	0.68
1:B:21:VAL:HG13	1:B:25:SER:O	1.93	0.68
1:B:1065:LEU:HD22	1:B:1110:ILE:HG22	1.74	0.68
1:A:96:GLU:O	1:A:97:THR:HG23	1.93	0.68
1:A:322:ARG:NH1	2:C:1:G:H2'	2.09	0.68
1:B:592:GLN:HG2	1:B:596:LEU:HD12	1.75	0.68
1:A:354:TYR:CB	1:A:365:PHE:HZ	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ILE:HG22	1:B:475:ILE:HD11	1.75	0.68
1:B:825:LEU:CD1	1:B:841:PHE:CZ	2.77	0.68
1:B:989:ILE:CD1	1:B:1015:PHE:CE2	2.76	0.68
1:B:1004:LYS:O	1:B:1004:LYS:HG2	1.94	0.68
1:A:254:MSE:CE	1:A:277:TYR:CD2	2.77	0.67
1:B:65:LYS:HA	1:B:68:PHE:CB	2.24	0.67
1:A:42:LEU:HD21	1:A:73:VAL:HG23	1.74	0.67
1:A:585:THR:O	1:A:589:ILE:HG13	1.93	0.67
1:B:735:LYS:HD3	1:B:735:LYS:N	2.08	0.67
1:B:215:LEU:HB3	1:B:219:GLU:HB3	1.75	0.67
1:B:880:TYR:O	1:B:881:LYS:HD2	1.94	0.67
1:B:15:THR:HG23	1:B:360:ILE:CD1	2.25	0.67
1:B:299:GLU:OE2	1:B:340:LYS:CE	2.38	0.67
1:A:75:LEU:HD21	1:A:78:ASN:C	2.14	0.67
3:D:8:G:O2'	3:D:9:A:H5'	1.94	0.67
1:B:1029:LYS:HB2	1:B:1029:LYS:NZ	2.08	0.67
1:A:728:TYR:HA	1:A:734:ILE:CD1	2.25	0.67
1:B:574:TRP:HZ2	1:B:592:GLN:OE1	1.77	0.67
3:D:28:G:H2'	3:D:29:U:H5'	1.76	0.67
1:B:264:MSE:HE3	1:B:269:LYS:HG3	1.77	0.67
1:A:42:LEU:HD12	1:A:71:LYS:CB	2.24	0.66
1:A:254:MSE:HE2	1:A:277:TYR:CD2	2.31	0.66
1:A:254:MSE:HG3	1:A:273:PHE:CD1	2.31	0.66
1:B:929:LYS:O	1:B:933:GLU:HG3	1.94	0.66
1:B:959:ARG:HA	1:B:962:HIS:CE1	2.31	0.66
1:A:824:PHE:C	1:A:825:LEU:HD23	2.16	0.66
1:A:882:ILE:CD1	1:A:947:PHE:CE1	2.78	0.66
1:B:1068:LEU:O	1:B:1072:ARG:HG3	1.95	0.66
1:B:34:LEU:HD22	1:B:141:ILE:HG23	1.78	0.66
1:B:677:TYR:O	1:B:681:ILE:HG22	1.95	0.66
1:B:825:LEU:HD11	1:B:841:PHE:CE2	2.30	0.66
1:B:678:ILE:CA	1:B:681:ILE:HG22	2.23	0.66
1:A:438:LYS:HD2	1:A:451:MSE:CE	2.24	0.66
1:A:1007:GLN:OE1	1:A:1007:GLN:HA	1.96	0.66
1:B:214:ASN:N	1:B:214:ASN:HD22	1.93	0.66
1:A:976:ARG:HB3	1:A:993:PHE:CE2	2.29	0.66
1:B:179:TYR:CD2	1:B:188:TYR:HD1	2.12	0.66
1:A:915:ARG:HG3	1:A:915:ARG:NH1	2.04	0.66
1:A:915:ARG:HD2	1:A:915:ARG:N	2.03	0.65
1:B:264:MSE:HE3	1:B:269:LYS:CB	2.26	0.65
2:C:58:C:H6	2:C:58:C:C5'	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:PHE:CZ	1:B:526:PHE:CE2	2.83	0.65
1:B:46:ILE:HG13	1:B:46:ILE:O	1.96	0.65
1:B:726:LYS:O	1:B:730:GLN:HG3	1.96	0.65
1:A:153:ALA:HB1	1:A:360:ILE:HG22	1.79	0.65
1:A:1023:ASP:OD2	1:A:1027:ILE:CB	2.45	0.65
1:B:264:MSE:HE3	1:B:269:LYS:HA	1.78	0.65
1:A:737:PRO:HG2	1:A:740:ILE:HG12	1.78	0.65
2:E:28:A:C2	1:B:966:GLY:HA3	2.31	0.65
1:B:626:ASN:HA	1:B:629:ASP:HB2	1.78	0.65
1:B:701:LEU:O	1:B:704:ILE:CG1	2.44	0.65
1:A:320:ILE:CG2	1:A:324:PHE:CD2	2.79	0.65
1:A:425:VAL:HG21	1:A:458:GLU:HA	1.78	0.65
1:B:310:LYS:HA	1:B:310:LYS:HE3	1.79	0.65
1:B:925:TYR:CE2	1:B:1126:LEU:CD2	2.80	0.65
1:A:2:LYS:NZ	1:A:4:THR:O	2.30	0.65
1:A:987:GLN:H	1:A:987:GLN:CD	1.99	0.65
1:B:579:THR:HB	1:B:585:THR:HG22	1.76	0.65
1:B:9:ILE:HG13	1:B:33:ARG:HG3	1.79	0.65
1:B:882:ILE:HG13	1:B:944:LYS:NZ	2.11	0.65
1:A:862:ILE:CG1	1:A:951:ASN:HD21	2.04	0.64
1:A:882:ILE:HD11	1:A:947:PHE:HE1	1.62	0.64
1:A:354:TYR:HB3	1:A:365:PHE:CZ	2.32	0.64
1:A:694:ALA:CB	1:A:699:LEU:HD12	2.27	0.64
1:A:770:ASN:OD1	1:A:771:HIS:N	2.30	0.64
1:B:252:ASN:OD1	1:B:253:ASN:N	2.30	0.64
1:B:846:ILE:HG13	1:B:847:TYR:N	2.12	0.64
1:B:992:ILE:HG23	1:B:1011:LYS:HB2	1.79	0.64
1:A:41:ARG:O	1:A:44:MSE:HB2	1.97	0.64
1:A:306:ASN:O	1:A:311:ARG:HG3	1.98	0.64
1:A:951:ASN:N	1:A:951:ASN:HD22	1.93	0.64
1:B:543:PHE:CD2	1:B:598:ASN:ND2	2.64	0.64
1:B:979:LEU:HB3	1:B:989:ILE:HG12	1.79	0.64
1:B:1019:LEU:HD23	1:B:1020:HIS:HE1	1.58	0.64
1:B:771:HIS:HB3	1:B:808:ASN:ND2	2.11	0.64
1:B:846:ILE:HD13	1:B:887:LEU:HD21	1.70	0.64
1:B:300:MSE:HE1	1:B:324:PHE:HE1	1.61	0.64
1:B:754:LYS:HD2	1:B:754:LYS:N	2.13	0.64
1:B:214:ASN:N	1:B:214:ASN:ND2	2.45	0.64
1:B:527:ARG:NH2	1:B:719:GLN:OE1	2.31	0.64
1:B:737:PRO:O	1:B:740:ILE:HG12	1.96	0.64
1:B:989:ILE:HD11	1:B:1015:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:HG2	1:A:728:TYR:HH	1.62	0.64
1:A:606:ASN:O	1:A:610:SER:HB2	1.98	0.64
1:B:756:THR:HB	1:B:759:LEU:HB2	1.80	0.63
1:B:1006:GLY:O	1:B:1011:LYS:HE3	1.98	0.63
1:A:406:MSE:HE3	1:A:461:PHE:CB	2.22	0.63
1:A:785:GLN:HE22	1:A:797:LEU:HD12	1.63	0.63
1:A:878:ALA:HB2	1:A:1146:ILE:HG21	1.80	0.63
2:C:58:C:H5"	2:C:58:C:C6	2.31	0.63
3:F:20:A:C2'	3:F:21:U:H5'	2.29	0.63
2:E:54:U:O2'	2:E:55:C:H5'	1.99	0.63
1:B:976:ARG:NH2	1:B:990:GLU:OE2	2.32	0.63
1:A:175:ILE:CD1	1:A:278:LEU:HD11	2.28	0.63
1:B:237:LYS:HD2	1:B:237:LYS:O	1.98	0.63
1:B:429:TYR:CZ	1:B:454:LYS:HG2	2.33	0.63
1:B:462:ALA:O	1:B:466:GLU:HG3	1.99	0.63
1:B:604:PHE:CE1	1:B:608:PHE:HB2	2.34	0.63
2:E:30:C:N4	1:B:787:ALA:HA	2.12	0.63
1:B:163:ILE:HG21	1:B:985:GLU:HG2	1.80	0.63
1:B:356:GLN:HG3	1:B:359:GLU:OE2	1.99	0.63
1:A:233:ARG:NH2	2:C:18:A:OP1	2.32	0.63
1:A:406:MSE:O	1:A:425:VAL:CG1	2.46	0.63
1:A:477:HIS:ND1	1:A:972:GLU:OE2	2.31	0.63
1:A:566:LEU:O	1:A:569:SER:N	2.32	0.63
1:A:600:TYR:O	1:A:605:LEU:HG	1.98	0.63
2:C:56:U:C2'	2:C:57:U:H5'	2.29	0.63
2:E:34:A:O2'	2:E:35:A:H5'	1.98	0.63
1:A:304:LEU:HD23	1:A:308:VAL:HG21	1.81	0.63
1:A:747:ILE:O	1:A:748:LYS:HD2	1.99	0.63
1:B:240:PHE:O	1:B:244:ILE:HB	1.98	0.63
1:B:287:ASN:HD22	1:B:288:ILE:N	1.97	0.63
1:B:616:PHE:CZ	1:B:651:PRO:HD3	2.34	0.63
1:B:719:GLN:H	1:B:719:GLN:HE21	1.47	0.63
1:B:997:ASN:H	1:B:997:ASN:ND2	1.96	0.63
1:B:523:ALA:O	1:B:524:ASN:HB2	1.99	0.62
1:B:609:MSE:HE1	1:B:685:PHE:CZ	2.34	0.62
1:A:247:GLU:OE1	1:A:260:LYS:CD	2.47	0.62
1:A:278:LEU:O	1:A:278:LEU:HD23	1.98	0.62
1:A:921:THR:O	1:A:924:ASP:HB2	1.99	0.62
1:B:60:ARG:O	1:B:64:LEU:HG	1.99	0.62
1:A:216:THR:OG1	1:A:219:GLU:HG3	1.97	0.62
1:A:1083:ASN:H	1:A:1083:ASN:ND2	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:LEU:HD11	1:A:1057:ILE:HD12	1.81	0.62
1:B:170:SER:O	1:B:174:ILE:HG13	2.00	0.62
1:B:189:VAL:CG1	1:B:334:GLU:OE1	2.48	0.62
1:A:477:HIS:HA	1:A:972:GLU:OE2	1.98	0.62
1:A:854:ILE:HG21	1:A:856:HIS:CE1	2.35	0.62
1:A:94:TYR:O	1:A:95:SER:OG	2.12	0.62
1:A:123:ASN:HB3	1:A:126:GLU:HB3	1.82	0.62
1:A:283:LEU:HD13	1:A:288:ILE:CD1	2.29	0.62
3:D:28:G:O2'	3:D:29:U:H5"	1.99	0.62
1:B:609:MSE:HE1	1:B:685:PHE:CE1	2.34	0.62
1:B:761:MSE:HA	1:B:761:MSE:CE	2.28	0.62
1:B:796:GLN:O	1:B:800:ILE:HG13	2.00	0.62
2:E:38:U:O2'	1:B:549:ASN:ND2	2.32	0.62
1:A:60:ARG:CD	1:A:97:THR:HG22	2.30	0.62
1:A:507:ILE:C	1:A:507:ILE:HD12	2.19	0.62
3:F:5:G:H2'	3:F:6:A:H5"	1.82	0.62
1:B:540:ARG:HB3	1:B:540:ARG:HH21	1.64	0.62
1:A:406:MSE:HE1	1:A:461:PHE:CD1	2.35	0.62
1:B:202:GLU:HB2	1:B:326:TYR:CE1	2.35	0.62
1:B:284:ASN:N	1:B:287:ASN:HD21	1.84	0.61
1:B:710:THR:O	1:B:713:SER:HB2	1.99	0.61
1:B:1120:ILE:HD11	1:B:1135:ARG:HG2	1.80	0.61
1:A:776:ASN:N	1:A:776:ASN:HD22	1.98	0.61
1:A:1068:LEU:O	1:A:1072:ARG:HG3	1.99	0.61
2:E:40:U:C5'	1:B:546:VAL:HG22	2.21	0.61
1:B:937:GLU:O	1:B:941:LEU:HD23	2.01	0.61
1:A:265:SER:HB3	1:A:268:LYS:CD	2.31	0.61
1:B:417:GLU:OE1	1:B:417:GLU:HA	2.00	0.61
1:B:691:THR:O	1:B:695:ASN:HB2	2.00	0.61
1:B:6:VAL:HG11	1:B:33:ARG:HH12	1.66	0.61
1:B:562:ARG:CZ	1:B:682:GLN:HE22	2.13	0.61
1:A:354:TYR:HB3	1:A:365:PHE:HZ	1.66	0.61
1:A:422:SER:CB	1:A:427:LYS:HE2	2.29	0.61
1:A:622:ILE:N	1:A:622:ILE:HD12	2.14	0.61
2:C:10:A:H8	2:C:10:A:C5'	2.14	0.61
1:B:3:VAL:HG23	1:B:4:THR:HG23	1.81	0.61
1:B:728:TYR:O	1:B:732:ASN:N	2.33	0.61
1:B:825:LEU:HD11	1:B:841:PHE:CZ	2.35	0.61
1:B:995:PHE:O	1:B:996:GLU:HB3	2.00	0.61
1:A:244:ILE:HD13	1:A:264:MSE:HE2	1.83	0.61
1:A:450:ASN:O	1:A:457:ILE:CD1	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:GLU:HG2	1:B:1000:ASN:HB3	1.82	0.61
1:A:265:SER:CB	1:A:268:LYS:CG	2.73	0.61
1:B:131:ARG:HH11	1:B:131:ARG:CG	2.14	0.60
1:A:74:TYR:CE2	1:A:76:LYS:HB2	2.36	0.60
1:A:356:GLN:HG2	1:A:359:GLU:OE2	2.01	0.60
1:B:15:THR:CG2	1:B:360:ILE:HD12	2.31	0.60
1:B:156:GLN:CB	1:B:169:LYS:HE3	2.31	0.60
1:B:334:GLU:HG3	1:B:335:ASN:N	2.14	0.60
1:B:686:LEU:HD23	1:B:686:LEU:O	2.01	0.60
1:A:123:ASN:HB3	1:A:126:GLU:CB	2.31	0.60
1:A:280:LYS:HG2	1:A:280:LYS:O	2.00	0.60
1:A:819:ASP:OD1	1:A:820:GLU:N	2.34	0.60
1:A:55:LYS:HE3	1:A:59:LYS:HD2	1.83	0.60
1:B:6:VAL:HG11	1:B:33:ARG:NH1	2.16	0.60
1:B:264:MSE:CE	1:B:269:LYS:CG	2.74	0.60
1:B:284:ASN:O	1:B:287:ASN:ND2	2.33	0.60
1:B:604:PHE:HE1	1:B:608:PHE:CD1	2.19	0.60
1:A:618:ILE:CD1	1:A:688:GLY:CA	2.78	0.60
2:E:2:A:C2'	2:E:3:C:H5'	2.31	0.60
1:B:201:LYS:O	1:B:202:GLU:HB3	2.01	0.60
1:B:759:LEU:HD11	1:B:795:ASP:HB3	1.82	0.60
2:C:2:A:H2'	2:C:3:C:C5'	2.31	0.60
2:E:1:G:OP2	1:B:1079:ARG:NH2	2.34	0.60
1:B:131:ARG:HH11	1:B:131:ARG:HG2	1.66	0.60
1:B:560:TYR:HA	1:B:563:ILE:HG13	1.83	0.60
1:B:893:LYS:HZ1	1:B:937:GLU:CD	2.05	0.60
1:A:728:TYR:O	1:A:732:ASN:HA	2.01	0.60
1:B:846:ILE:HD11	1:B:847:TYR:CE2	2.36	0.60
2:E:11:A:N6	1:B:297:GLU:OE1	2.35	0.60
1:B:996:GLU:O	1:B:996:GLU:HG2	2.00	0.60
1:A:398:ASN:ND2	1:A:424:GLU:OE1	2.35	0.60
1:A:882:ILE:HD12	1:A:947:PHE:CE1	2.37	0.60
1:B:228:HIS:CE1	1:B:233:ARG:HE	2.20	0.60
1:B:351:TYR:HB3	1:B:355:LEU:CD2	2.31	0.60
1:B:737:PRO:CD	1:B:740:ILE:HD11	2.31	0.60
1:A:43:ASP:O	1:A:45:TYR:N	2.35	0.60
3:F:3:A:C2'	3:F:4:A:C5'	2.76	0.60
1:A:816:LEU:HB3	1:A:853:ILE:CD1	2.31	0.59
2:C:10:A:C8	2:C:10:A:C5'	2.85	0.59
1:A:566:LEU:HD13	1:A:686:LEU:HD13	1.80	0.59
3:D:1:G:C8	1:B:1007:GLN:NE2	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:G:C8	2:E:1:G:C3'	2.85	0.59
2:E:2:A:H2'	2:E:3:C:H5'	1.84	0.59
1:B:734:ILE:HG22	1:B:735:LYS:NZ	2.18	0.59
1:A:67:PHE:HE2	1:A:117:TYR:HA	1.67	0.59
1:A:343:THR:HG22	1:A:346:ARG:NH2	2.17	0.59
1:A:842:ASP:OD2	1:A:847:TYR:N	2.34	0.59
1:B:215:LEU:CB	1:B:219:GLU:HB3	2.33	0.59
1:A:74:TYR:HE2	1:A:76:LYS:HB2	1.66	0.59
1:A:728:TYR:O	1:A:732:ASN:N	2.36	0.59
1:B:54:THR:O	1:B:58:GLN:N	2.33	0.59
1:A:618:ILE:HD12	1:A:688:GLY:HA2	1.84	0.59
1:A:978:ARG:NH2	1:A:1012:TYR:OH	2.35	0.59
1:B:15:THR:HG23	1:B:360:ILE:HD12	1.85	0.59
1:B:15:THR:CG2	1:B:360:ILE:CD1	2.80	0.59
1:B:202:GLU:O	1:B:202:GLU:HG2	2.02	0.59
1:A:841:PHE:CE1	1:A:887:LEU:CD1	2.86	0.59
3:F:27:U:O2'	3:F:28:G:H5'	2.03	0.59
1:B:33:ARG:O	1:B:37:LEU:HD12	2.03	0.59
1:B:77:ASP:O	1:B:78:ASN:C	2.38	0.59
1:B:508:ASN:HD21	1:B:510:LYS:HB3	1.67	0.59
1:B:514:LEU:HD23	1:B:728:TYR:CZ	2.38	0.59
1:A:154:ASN:CG	1:A:170:SER:OG	2.42	0.59
1:A:247:GLU:OE1	1:A:260:LYS:HE3	2.03	0.59
2:E:1:G:H5'	2:E:2:A:H5'	1.84	0.59
1:B:43:ASP:C	1:B:43:ASP:OD1	2.41	0.59
1:B:680:PHE:O	1:B:684:ILE:HG13	2.03	0.59
1:A:737:PRO:CG	1:A:740:ILE:HG13	2.31	0.59
1:B:978:ARG:NH2	1:B:1012:TYR:OH	2.34	0.59
1:B:986:ASN:OD1	1:B:988:TYR:N	2.35	0.59
1:B:59:LYS:O	1:B:63:LYS:HG3	2.03	0.58
1:B:178:TYR:CD2	1:B:288:ILE:HD13	2.37	0.58
1:B:862:ILE:CG2	1:B:868:LEU:HD21	2.32	0.58
1:A:401:ASP:OD1	1:A:402:ILE:N	2.35	0.58
1:A:785:GLN:HG2	1:A:790:GLU:O	2.03	0.58
1:B:54:THR:CG2	1:B:57:ASN:HD22	2.15	0.58
1:B:394:LEU:O	1:B:396:THR:N	2.35	0.58
1:A:731:ASN:HB3	1:A:734:ILE:HG12	1.86	0.58
2:E:32:C:H5"	2:E:32:C:H6	1.67	0.58
2:E:56:U:C2	3:F:5:G:N2	2.71	0.58
1:B:517:PHE:CE1	1:B:526:PHE:CZ	2.91	0.58
1:A:175:ILE:HD11	1:A:278:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MSE:HE3	1:A:277:TYR:CD2	2.39	0.58
1:B:560:TYR:HA	1:B:563:ILE:CG1	2.34	0.58
1:A:74:TYR:CZ	1:A:83:LYS:CE	2.84	0.58
1:A:80:LEU:CB	1:A:127:LEU:HB2	2.32	0.58
1:A:175:ILE:HD13	1:A:291:ALA:CB	2.33	0.58
1:A:846:ILE:HG13	1:A:847:TYR:N	2.17	0.58
1:A:880:TYR:CD2	1:A:1143:LEU:HD12	2.38	0.58
1:A:966:GLY:HA3	2:C:28:A:H2	1.69	0.58
1:B:617:GLU:O	1:B:621:GLU:N	2.35	0.58
1:A:399:GLU:OE1	1:A:1059:HIS:CD2	2.56	0.58
1:B:235:ASN:HD21	1:B:240:PHE:HE2	1.51	0.58
1:B:311:ARG:C	1:B:311:ARG:HD3	2.23	0.58
1:A:265:SER:O	1:A:268:LYS:HG3	2.04	0.58
1:A:270:SER:OG	1:A:294:HIS:HB2	2.04	0.58
1:B:405:ARG:HD2	1:B:405:ARG:N	2.18	0.58
1:A:5:LYS:CD	2:C:31:A:C8	2.85	0.58
1:A:41:ARG:NH2	3:D:29:U:OP1	2.32	0.58
1:A:614:ASN:OD1	1:A:618:ILE:HB	2.02	0.58
1:A:728:TYR:HA	1:A:734:ILE:HD11	1.86	0.58
2:C:7:C:O2'	2:C:8:C:H5'	2.03	0.58
1:B:45:TYR:CE2	1:B:130:PHE:CE2	2.92	0.58
1:B:517:PHE:CE1	1:B:526:PHE:HE2	2.22	0.58
1:B:526:PHE:CD2	1:B:721:PHE:CD2	2.92	0.58
1:A:278:LEU:HD23	1:A:278:LEU:C	2.25	0.57
1:A:882:ILE:HD11	1:A:947:PHE:CE1	2.39	0.57
2:E:10:A:N6	2:E:17:A:N7	2.52	0.57
1:B:60:ARG:NH1	1:B:103:ASP:N	2.43	0.57
1:B:215:LEU:N	1:B:215:LEU:HD12	2.18	0.57
1:B:689:PHE:O	1:B:693:LEU:N	2.31	0.57
1:B:941:LEU:O	1:B:945:VAL:HG13	2.04	0.57
1:B:453:ASN:ND2	1:B:456:GLU:OE2	2.36	0.57
1:B:737:PRO:HB2	1:B:740:ILE:CD1	2.33	0.57
1:B:178:TYR:CD2	1:B:288:ILE:HD12	2.38	0.57
2:E:31:A:C8	1:B:5:LYS:HG2	2.40	0.57
1:B:925:TYR:CE2	1:B:1126:LEU:HD23	2.39	0.57
3:F:29:U:H2'	3:F:29:U:O2	2.05	0.57
1:B:275:LYS:HD3	1:B:276:TYR:CZ	2.39	0.57
1:B:554:PRO:HD3	1:B:685:PHE:CD2	2.39	0.57
1:A:157:LYS:CG	1:A:166:VAL:HG22	2.35	0.57
1:A:438:LYS:HD3	1:A:451:MSE:HE2	1.86	0.57
1:B:497:GLU:O	1:B:501:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG23	1:A:57:ASN:H	1.68	0.57
1:A:175:ILE:CD1	1:A:291:ALA:HB1	2.35	0.57
2:C:33:A:O2'	2:C:34:A:H5'	2.04	0.57
1:A:399:GLU:OE2	1:A:1059:HIS:NE2	2.38	0.57
1:B:713:SER:HB2	1:B:714:LEU:HD13	1.86	0.57
1:A:175:ILE:CD1	1:A:291:ALA:CB	2.82	0.57
1:A:898:GLU:HG3	2:C:46:U:H5"	1.86	0.57
1:B:920:PHE:CE2	1:B:1126:LEU:HD11	2.39	0.57
1:A:699:LEU:HD23	1:A:702:ILE:HD11	1.86	0.57
1:B:379:ILE:N	1:B:379:ILE:HD12	2.20	0.57
1:B:689:PHE:O	1:B:693:LEU:HB2	2.05	0.57
1:A:43:ASP:O	1:A:44:MSE:C	2.41	0.56
1:B:253:ASN:HA	1:B:277:TYR:CE1	2.39	0.56
1:B:1029:LYS:HB2	1:B:1029:LYS:HZ1	1.70	0.56
1:B:1044:ASP:CG	1:B:1045:LEU:H	2.08	0.56
1:A:438:LYS:CD	1:A:451:MSE:HE3	2.35	0.56
1:A:996:GLU:HG2	1:A:999:LYS:HG3	1.86	0.56
2:E:32:C:N4	3:F:28:G:H1	2.01	0.56
1:B:144:LEU:O	1:B:147:SER:N	2.39	0.56
1:B:264:MSE:HE3	1:B:269:LYS:CG	2.35	0.56
1:A:218:LEU:HD12	1:A:218:LEU:O	2.04	0.56
3:D:8:G:C2'	3:D:9:A:H5'	2.36	0.56
1:B:15:THR:HG23	1:B:360:ILE:HD13	1.88	0.56
1:B:562:ARG:NH2	1:B:682:GLN:HE22	2.03	0.56
1:B:588:ILE:HD13	1:B:705:GLY:HA3	1.88	0.56
1:B:705:GLY:HA2	1:B:711:ASN:ND2	2.20	0.56
1:A:160:GLU:OE1	1:A:162:ASN:CB	2.48	0.56
1:B:991:GLU:HG2	1:B:1000:ASN:CB	2.35	0.56
1:A:809:ARG:HD3	1:A:809:ARG:H	1.71	0.56
1:B:5:LYS:NZ	1:B:10:SER:OG	2.39	0.56
1:B:46:ILE:HG22	1:B:105:ARG:CB	2.36	0.56
1:B:485:LYS:HG2	1:B:486:ASP:OD1	2.06	0.56
1:B:822:GLY:HA3	1:B:832:VAL:O	2.04	0.56
1:A:728:TYR:N	1:A:734:ILE:HD11	2.19	0.56
1:B:893:LYS:NZ	1:B:937:GLU:CD	2.58	0.56
1:A:438:LYS:HD3	1:A:451:MSE:HE3	1.87	0.56
1:A:897:ILE:HG21	1:A:938:TYR:CD2	2.41	0.56
2:E:2:A:O2'	2:E:3:C:H5'	2.06	0.56
1:B:284:ASN:H	1:B:287:ASN:ND2	1.84	0.56
1:A:163:ILE:HG23	1:A:165:LYS:HD3	1.87	0.56
1:A:898:GLU:HG3	2:C:46:U:C5'	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TYR:CB	1:A:365:PHE:CZ	2.88	0.56
1:A:816:LEU:CD1	1:A:863:LYS:HG2	2.35	0.56
2:E:30:C:H42	1:B:787:ALA:HA	1.71	0.56
1:B:3:VAL:CG2	1:B:4:THR:HG23	2.36	0.56
1:B:600:TYR:HA	1:B:604:PHE:HB3	1.88	0.56
1:A:448:ASP:N	1:A:448:ASP:OD1	2.39	0.55
1:B:4:THR:O	1:B:5:LYS:HB2	2.06	0.55
1:B:825:LEU:HD12	1:B:841:PHE:CZ	2.41	0.55
1:A:462:ALA:O	1:A:466:GLU:HG3	2.07	0.55
1:A:583:ASN:C	1:A:583:ASN:HD22	2.10	0.55
1:A:962:HIS:HD2	2:C:28:A:H61	1.51	0.55
1:A:1105:GLY:HA2	2:C:1:G:N2	2.21	0.55
1:B:550:ILE:HG22	1:B:553:VAL:CG1	2.36	0.55
1:B:882:ILE:HD13	1:B:947:PHE:HE1	1.70	0.55
1:A:160:GLU:HB2	1:A:163:ILE:HG22	1.82	0.55
1:B:993:PHE:HD1	1:B:1008:ILE:HD13	1.71	0.55
1:A:550:ILE:HG13	1:A:605:LEU:HD13	1.89	0.55
1:A:966:GLY:O	1:A:969:SER:HB2	2.05	0.55
1:B:1126:LEU:HG	1:B:1126:LEU:O	2.06	0.55
1:B:678:ILE:HD12	1:B:679:ASP:OD1	2.07	0.55
1:A:157:LYS:NZ	1:A:355:LEU:O	2.34	0.55
1:A:615:PHE:O	1:A:619:SER:HB3	2.07	0.55
1:B:264:MSE:HE3	1:B:269:LYS:CA	2.35	0.55
1:A:131:ARG:HH22	1:A:135:LYS:HE3	1.72	0.55
1:A:247:GLU:OE1	1:A:260:LYS:CE	2.53	0.55
1:B:385:VAL:HG21	1:B:773:GLU:HG3	1.89	0.55
1:A:394:LEU:HD23	1:A:461:PHE:CE1	2.42	0.55
1:A:425:VAL:HG11	1:A:458:GLU:HB2	1.88	0.55
1:B:608:PHE:O	1:B:615:PHE:HB2	2.07	0.55
1:B:652:LYS:O	1:B:656:ALA:N	2.36	0.55
1:A:575:LYS:O	1:A:702:ILE:CG2	2.55	0.55
1:B:112:VAL:HG11	1:B:126:GLU:O	2.06	0.55
1:B:294:HIS:O	1:B:298:ILE:HG13	2.07	0.55
1:B:574:TRP:CE3	1:B:702:ILE:CG2	2.89	0.55
1:B:1063:SER:HB3	1:B:1151:LYS:HG3	1.88	0.55
1:A:560:TYR:OH	1:A:592:GLN:NE2	2.40	0.55
1:A:1044:ASP:CG	1:A:1045:LEU:H	2.11	0.55
1:B:34:LEU:HB3	1:B:141:ILE:CG2	2.36	0.55
1:B:124:SER:O	1:B:128:GLU:N	2.40	0.55
1:B:246:GLU:OE1	1:B:249:GLN:HB2	2.07	0.55
1:B:737:PRO:HD2	1:B:740:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HD21	1:A:702:ILE:HD11	1.87	0.54
2:E:13:A:N6	2:E:14:A:N1	2.55	0.54
2:E:20:G:C2'	2:E:21:G:H5'	2.36	0.54
1:A:399:GLU:CD	1:A:1059:HIS:NE2	2.61	0.54
2:E:10:A:C6	2:E:17:A:N7	2.75	0.54
1:B:34:LEU:HB3	1:B:141:ILE:HG21	1.88	0.54
1:A:988:TYR:CD2	1:A:1002:LYS:CE	2.89	0.54
1:B:268:LYS:HD2	1:B:272:VAL:HG23	1.89	0.54
1:B:736:ILE:HG22	1:B:740:ILE:HG13	1.87	0.54
1:B:987:GLN:CG	1:B:988:TYR:CE1	2.91	0.54
1:A:157:LYS:HG2	1:A:166:VAL:HG22	1.90	0.54
1:A:438:LYS:CD	1:A:451:MSE:HE2	2.35	0.54
1:A:915:ARG:H	1:A:915:ARG:CD	1.95	0.54
1:A:385:VAL:HG21	1:A:773:GLU:HG3	1.88	0.54
1:B:405:ARG:O	1:B:405:ARG:HG2	2.06	0.54
1:B:924:ASP:O	1:B:927:SER:N	2.41	0.54
1:A:284:ASN:OD1	1:A:287:ASN:N	2.36	0.54
1:A:429:TYR:CE2	1:A:451:MSE:O	2.60	0.54
1:A:502:MSE:CE	1:A:763:TYR:HE2	2.20	0.54
1:A:511:LYS:CG	1:A:728:TYR:OH	2.45	0.54
1:A:988:TYR:CD2	1:A:1002:LYS:HE2	2.43	0.54
1:A:1030:TYR:C	1:A:1035:ILE:CD1	2.76	0.54
1:B:592:GLN:HG2	1:B:596:LEU:CD1	2.37	0.54
1:B:778:LYS:NZ	1:B:782:GLU:OE2	2.40	0.54
1:B:1041:GLU:CB	1:B:1043:LYS:HG3	2.37	0.54
2:C:2:A:C2'	2:C:3:C:H5'	2.37	0.54
1:B:659:GLN:HA	1:B:677:TYR:CE1	2.43	0.54
1:B:394:LEU:HB2	1:B:396:THR:HG22	1.90	0.54
1:B:925:TYR:HE2	1:B:1126:LEU:HD23	1.73	0.54
1:A:284:ASN:OD1	1:A:286:LYS:N	2.41	0.54
1:B:128:GLU:OE2	1:B:131:ARG:HD2	2.08	0.54
1:B:537:TYR:OH	1:B:598:ASN:HB3	2.08	0.54
1:B:701:LEU:O	1:B:704:ILE:HG13	2.08	0.54
1:B:735:LYS:O	1:B:735:LYS:HE2	2.08	0.54
1:A:265:SER:H	1:A:268:LYS:CD	2.19	0.54
1:A:1039:LYS:CE	1:A:1046:TYR:CE2	2.80	0.54
1:B:421:VAL:HG22	1:B:422:SER:HB2	1.90	0.54
1:B:562:ARG:NH2	1:B:682:GLN:NE2	2.55	0.54
1:A:163:ILE:HG21	1:A:165:LYS:NZ	2.23	0.53
2:E:35:A:H2'	2:E:36:U:O4'	2.08	0.53
1:B:583:ASN:N	1:B:583:ASN:OD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:O	1:A:239:ASN:HB2	2.08	0.53
1:A:823:LYS:HD3	1:A:872:GLU:CD	2.28	0.53
1:B:771:HIS:CB	1:B:808:ASN:HD22	2.18	0.53
1:B:816:LEU:O	1:B:853:ILE:HD13	2.08	0.53
1:A:701:LEU:HD22	1:A:704:ILE:HD11	1.90	0.53
1:A:1042:LYS:HD3	1:A:1042:LYS:N	2.23	0.53
1:B:6:VAL:HG13	1:B:7:GLY:N	2.22	0.53
1:B:253:ASN:HB2	1:B:281:GLU:OE2	2.08	0.53
1:B:390:LEU:O	1:B:394:LEU:HD12	2.09	0.53
1:B:609:MSE:HE3	1:B:685:PHE:CE1	2.32	0.53
1:B:822:GLY:HA3	1:B:832:VAL:HG13	1.89	0.53
1:A:997:ASN:HB3	1:A:1004:LYS:O	2.08	0.53
3:D:2:G:O2'	3:D:3:A:H5"	2.08	0.53
1:B:651:PRO:O	1:B:655:LEU:HB2	2.07	0.53
1:B:756:THR:HG21	1:B:758:ARG:HG3	1.90	0.53
1:B:816:LEU:HB3	1:B:853:ILE:CD1	2.38	0.53
1:A:251:VAL:HG21	1:A:257:LEU:N	2.24	0.53
1:A:270:SER:OG	1:A:294:HIS:N	2.41	0.53
1:A:406:MSE:HE2	1:A:461:PHE:CB	2.26	0.53
1:B:914:PRO:O	1:B:915:ARG:HB2	2.08	0.53
1:B:1065:LEU:HD22	1:B:1110:ILE:CG2	2.38	0.53
1:A:194:GLU:OE2	1:A:289:LYS:CE	2.56	0.53
1:A:284:ASN:HD21	1:A:286:LYS:HD2	1.73	0.53
1:A:609:MSE:HE1	1:A:685:PHE:CE1	2.44	0.53
1:B:279:ASP:O	1:B:280:LYS:HD2	2.09	0.53
1:A:756:THR:HG22	1:A:758:ARG:H	1.74	0.53
3:D:9:A:O5'	3:D:9:A:H8	1.91	0.53
1:B:920:PHE:HE2	1:B:1126:LEU:HD11	1.73	0.53
1:B:1007:GLN:O	1:B:1011:LYS:HG3	2.09	0.53
1:A:429:TYR:HE2	1:A:451:MSE:O	1.92	0.53
1:A:1065:LEU:HD22	1:A:1110:ILE:CG2	2.39	0.53
1:B:57:ASN:O	1:B:61:ILE:CG1	2.54	0.53
1:B:300:MSE:HE1	1:B:324:PHE:CE1	2.43	0.53
1:B:540:ARG:HB3	1:B:540:ARG:NH2	2.22	0.53
1:A:251:VAL:HB	1:A:256:GLU:CB	2.37	0.53
1:A:1042:LYS:O	1:A:1070:ASN:ND2	2.42	0.53
1:B:842:ASP:OD2	1:B:847:TYR:HB2	2.08	0.53
1:A:1030:TYR:O	1:A:1035:ILE:CD1	2.53	0.53
1:A:1083:ASN:HD22	1:A:1083:ASN:N	2.01	0.53
1:B:604:PHE:CE1	1:B:608:PHE:CD1	2.97	0.53
1:B:911:TYR:CE2	1:B:1123:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:GLU:O	1:A:947:PHE:HB2	2.09	0.52
2:C:12:A:O5'	2:C:12:A:H8	1.91	0.52
1:B:49:PRO:HG2	1:B:50:SER:OG	2.08	0.52
1:A:67:PHE:CD2	1:A:117:TYR:CD2	2.98	0.52
1:A:445:TYR:CD1	1:A:502:MSE:HE1	2.44	0.52
1:A:854:ILE:CG2	1:A:856:HIS:CE1	2.92	0.52
1:A:253:ASN:HB3	1:A:256:GLU:H	1.74	0.52
1:A:731:ASN:C	1:A:731:ASN:ND2	2.60	0.52
1:B:825:LEU:CD1	1:B:841:PHE:CE2	2.93	0.52
1:B:1113:GLN:O	1:B:1114:THR:HG23	2.09	0.52
1:A:710:THR:O	1:A:713:SER:HB3	2.10	0.52
1:A:1122:HIS:HB2	1:A:1131:LEU:HG	1.91	0.52
1:B:214:ASN:HD22	1:B:214:ASN:H	1.57	0.52
1:A:154:ASN:CG	1:A:170:SER:HG	2.13	0.52
1:A:154:ASN:ND2	1:A:170:SER:OG	2.41	0.52
1:A:170:SER:O	1:A:174:ILE:HG13	2.09	0.52
1:A:513:LYS:HE3	1:A:747:ILE:HB	1.92	0.52
1:B:502:MSE:CE	1:B:763:TYR:CE2	2.79	0.52
1:B:560:TYR:O	1:B:563:ILE:HG13	2.10	0.52
1:B:734:ILE:HG22	1:B:735:LYS:HZ3	1.74	0.52
1:A:12:LYS:HG3	1:A:21:VAL:HG21	1.91	0.52
1:A:209:VAL:O	1:A:213:GLU:HB2	2.09	0.52
3:F:6:A:C5'	3:F:6:A:N3	2.73	0.52
1:B:175:ILE:HD12	1:B:295:PHE:CZ	2.44	0.52
1:B:897:ILE:HD12	1:B:938:TYR:CE1	2.45	0.52
1:A:284:ASN:OD1	1:A:286:LYS:HB2	2.10	0.52
1:A:810:VAL:HG22	1:A:860:TYR:CG	2.44	0.52
1:B:394:LEU:HB2	1:B:396:THR:CG2	2.39	0.52
1:A:618:ILE:HD13	1:A:688:GLY:CA	2.39	0.52
1:A:988:TYR:CE2	1:A:1002:LYS:NZ	2.77	0.52
2:E:10:A:N6	2:E:17:A:C8	2.78	0.52
2:E:17:A:H4'	2:E:17:A:OP2	2.08	0.52
1:B:737:PRO:HD2	1:B:740:ILE:HG13	1.91	0.52
1:A:814:PHE:O	1:A:855:LYS:HE2	2.10	0.52
2:E:17:A:N3	2:E:17:A:C5'	2.71	0.52
3:F:4:A:C8	3:F:4:A:H3'	2.45	0.52
1:A:477:HIS:CB	1:A:972:GLU:OE2	2.58	0.52
1:A:809:ARG:HD3	1:A:809:ARG:N	2.25	0.52
1:A:932:ILE:HD11	1:A:1131:LEU:HD12	1.91	0.52
1:B:629:ASP:O	1:B:632:ASN:CG	2.48	0.52
1:A:43:ASP:OD1	1:A:43:ASP:N	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:TYR:O	1:B:894:LYS:HB2	2.10	0.51
1:A:76:LYS:HA	1:A:76:LYS:HE3	1.93	0.51
1:A:575:LYS:O	1:A:702:ILE:HG23	2.10	0.51
1:A:831:LYS:NZ	1:A:876:ASP:OD2	2.32	0.51
1:A:1083:ASN:ND2	1:A:1083:ASN:N	2.58	0.51
2:E:56:U:C2	3:F:5:G:C2	2.98	0.51
1:B:559:LEU:O	1:B:562:ARG:HG3	2.10	0.51
1:B:832:VAL:O	1:B:832:VAL:HG13	2.10	0.51
1:B:987:GLN:HG2	1:B:988:TYR:CD1	2.44	0.51
1:B:1042:LYS:N	1:B:1042:LYS:CD	2.73	0.51
1:A:889:LYS:HD3	1:A:893:LYS:HZ1	1.75	0.51
2:E:2:A:H2'	2:E:3:C:C5'	2.40	0.51
1:B:3:VAL:O	1:B:33:ARG:HD2	2.11	0.51
1:B:382:VAL:HG13	1:B:769:LEU:HD11	1.92	0.51
1:B:862:ILE:O	1:B:866:GLY:HA3	2.10	0.51
1:A:962:HIS:CD2	2:C:28:A:N6	2.76	0.51
1:A:992:ILE:HG23	1:A:1011:LYS:HB2	1.91	0.51
1:A:1104:ILE:HG12	1:A:1110:ILE:HG13	1.93	0.51
1:B:245:TYR:O	1:B:248:ILE:HB	2.10	0.51
1:B:376:LEU:HB3	1:B:475:ILE:HG23	1.91	0.51
1:B:608:PHE:HD2	1:B:609:MSE:CE	2.13	0.51
1:B:616:PHE:O	1:B:620:LYS:CB	2.59	0.51
1:B:737:PRO:HD2	1:B:740:ILE:CD1	2.40	0.51
1:A:747:ILE:O	1:A:748:LYS:CD	2.59	0.51
1:A:811:THR:HG23	1:A:812:GLU:N	2.25	0.51
1:B:412:LYS:O	1:B:412:LYS:HG3	2.09	0.51
1:A:163:ILE:CD1	1:A:985:GLU:OE1	2.59	0.51
1:B:254:MSE:HG3	1:B:254:MSE:O	2.11	0.51
1:B:305:LYS:O	1:B:310:LYS:CB	2.48	0.51
1:B:496:SER:O	1:B:500:LYS:HB2	2.10	0.51
1:B:822:GLY:CA	1:B:832:VAL:HG13	2.40	0.51
1:A:144:LEU:O	1:A:147:SER:N	2.43	0.51
1:A:159:ASN:O	1:A:160:GLU:HB3	2.11	0.51
1:A:581:ASP:OD2	1:A:583:ASN:HB3	2.11	0.51
1:A:1007:GLN:O	1:A:1011:LYS:HG3	2.09	0.51
2:C:32:C:H2'	2:C:32:C:O2	2.10	0.51
1:B:305:LYS:O	1:B:310:LYS:N	2.37	0.51
1:A:467:ALA:HB2	1:A:761:MSE:HE2	1.93	0.51
1:A:756:THR:HG22	1:A:758:ARG:N	2.25	0.51
1:A:1117:SER:OG	1:A:1134:ASP:HB3	2.10	0.51
2:E:46:U:H5"	1:B:898:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:A:O2'	2:E:34:A:H5'	2.11	0.51
3:F:20:A:O2'	3:F:21:U:H5'	2.11	0.51
1:B:6:VAL:CG1	1:B:7:GLY:N	2.73	0.51
1:B:614:ASN:CB	1:B:618:ILE:HG13	2.41	0.51
1:B:737:PRO:HG2	1:B:740:ILE:HD11	1.91	0.51
1:A:477:HIS:HD1	1:A:972:GLU:CD	2.14	0.51
1:A:650:ILE:HG22	1:A:653:GLU:OE1	2.11	0.51
1:A:728:TYR:O	1:A:732:ASN:CA	2.59	0.51
1:A:903:MSE:HE3	1:A:927:SER:HB3	1.93	0.51
1:B:411:VAL:HG22	1:B:412:LYS:N	2.26	0.51
1:B:614:ASN:O	1:B:618:ILE:HG13	2.11	0.51
1:B:888:LYS:O	1:B:892:ASN:ND2	2.42	0.51
1:B:1145:LYS:O	1:B:1149:GLU:HG2	2.11	0.51
1:A:482:LEU:HD12	1:A:483:GLU:H	1.74	0.50
1:A:951:ASN:ND2	1:A:951:ASN:N	2.59	0.50
1:B:844:ASN:C	1:B:845:LYS:HG3	2.32	0.50
1:B:882:ILE:HG13	1:B:944:LYS:HZ3	1.74	0.50
1:A:75:LEU:HD23	1:A:79:THR:C	2.31	0.50
1:A:236:ASP:OD2	1:A:268:LYS:HB3	2.10	0.50
1:A:411:VAL:O	1:A:418:GLU:HA	2.10	0.50
1:A:423:GLY:O	1:A:426:ASP:N	2.37	0.50
1:A:566:LEU:O	1:A:570:LEU:N	2.44	0.50
1:A:154:ASN:O	1:A:168:GLY:HA2	2.12	0.50
1:B:706:SER:OG	1:B:707:ASP:N	2.44	0.50
1:A:406:MSE:O	1:A:425:VAL:HB	2.10	0.50
2:E:6:C:H5"	1:B:1079:ARG:HG2	1.93	0.50
1:B:202:GLU:HB2	1:B:326:TYR:CZ	2.47	0.50
3:D:27:U:H2'	3:D:28:G:O4'	2.12	0.50
1:B:616:PHE:O	1:B:620:LYS:N	2.45	0.50
1:B:903:MSE:SE	1:B:907:LEU:CD2	3.10	0.50
1:A:118:LEU:O	1:A:119:ASN:HB2	2.12	0.50
1:A:254:MSE:HE2	1:A:277:TYR:CE2	2.45	0.50
3:D:3:A:O2'	3:D:4:A:H5'	2.11	0.50
1:B:6:VAL:CG1	1:B:33:ARG:NH1	2.74	0.50
1:B:34:LEU:HA	1:B:37:LEU:HD12	1.93	0.50
1:A:18:GLY:HA3	1:A:151:ASN:O	2.11	0.50
1:A:54:THR:HG22	1:A:57:ASN:HB2	1.93	0.50
1:A:110:PHE:CD1	1:A:110:PHE:C	2.85	0.50
1:A:240:PHE:HB3	1:A:244:ILE:HD11	1.94	0.50
1:A:728:TYR:HA	1:A:734:ILE:HG13	1.94	0.50
1:A:931:ALA:O	1:A:935:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:VAL:O	1:B:428:ILE:HG13	2.12	0.50
1:B:1100:ALA:HB2	1:B:1115:LEU:CD2	2.42	0.50
1:A:123:ASN:O	1:A:126:GLU:N	2.45	0.49
1:A:731:ASN:ND2	1:A:733:ASN:HB2	2.27	0.49
1:B:989:ILE:HD11	1:B:1015:PHE:CE2	2.47	0.49
1:A:163:ILE:HG12	1:A:165:LYS:HE3	1.93	0.49
1:A:1007:GLN:HB2	1:A:1010:GLU:CD	2.32	0.49
1:B:560:TYR:CA	1:B:563:ILE:HG13	2.41	0.49
1:A:126:GLU:OE2	1:A:126:GLU:HA	2.11	0.49
1:A:319:LYS:O	1:A:319:LYS:HG2	2.12	0.49
1:A:365:PHE:CD1	1:A:365:PHE:C	2.85	0.49
1:A:409:LYS:CB	1:A:421:VAL:HG22	2.42	0.49
1:B:179:TYR:HD2	1:B:188:TYR:HD1	1.58	0.49
1:B:1029:LYS:NZ	1:B:1029:LYS:CB	2.73	0.49
1:B:1099:VAL:HG23	1:B:1118:GLU:HG2	1.93	0.49
1:A:160:GLU:HG3	1:A:163:ILE:HG22	1.93	0.49
1:A:583:ASN:ND2	1:A:587:GLU:OE2	2.46	0.49
1:B:189:VAL:HG13	1:B:334:GLU:OE1	2.11	0.49
1:B:607:TYR:CB	1:B:692:TYR:CE1	2.94	0.49
1:B:1104:ILE:HG12	1:B:1110:ILE:HG13	1.95	0.49
1:A:265:SER:HB3	1:A:268:LYS:HE3	1.93	0.49
1:B:698:ARG:CB	1:B:701:LEU:HD11	2.43	0.49
1:A:880:TYR:O	1:A:881:LYS:HD3	2.13	0.49
3:D:29:U:H5'	3:D:29:U:H6	1.78	0.49
2:E:20:G:O2'	2:E:21:G:H5'	2.13	0.49
3:F:3:A:C2'	3:F:4:A:H5"	2.37	0.49
1:B:449:PHE:HB3	1:B:451:MSE:HE2	1.94	0.49
2:C:15:U:H4'	2:C:16:G:H5"	1.95	0.49
2:C:47:A:H2'	2:C:48:A:C8	2.48	0.49
3:F:4:A:H2'	3:F:5:G:O4'	2.13	0.49
1:B:589:ILE:O	1:B:593:ILE:HG13	2.13	0.49
1:A:991:GLU:HG2	1:A:1000:ASN:CG	2.33	0.49
1:A:245:TYR:O	1:A:248:ILE:HB	2.13	0.49
1:A:423:GLY:O	1:A:427:LYS:N	2.45	0.49
1:A:816:LEU:HB3	1:A:853:ILE:HD11	1.95	0.49
1:B:560:TYR:C	1:B:563:ILE:HG13	2.32	0.49
1:B:920:PHE:HE2	1:B:1126:LEU:CD1	2.25	0.49
1:B:1044:ASP:CG	1:B:1045:LEU:N	2.66	0.49
1:A:224:ARG:CD	2:C:18:A:C8	2.95	0.49
1:A:244:ILE:HG23	1:A:264:MSE:HE3	1.95	0.49
1:B:175:ILE:CD1	1:B:291:ALA:HB1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TYR:CD1	1:B:420:TYR:C	2.85	0.49
1:B:925:TYR:CD1	1:B:925:TYR:C	2.85	0.49
1:A:43:ASP:C	1:A:45:TYR:N	2.64	0.48
1:A:382:VAL:HG13	1:A:769:LEU:HD11	1.95	0.48
1:A:976:ARG:CB	1:A:993:PHE:CE2	2.96	0.48
1:A:988:TYR:O	1:A:991:GLU:HB2	2.13	0.48
2:E:30:C:C1'	2:E:31:A:OP2	2.60	0.48
1:B:54:THR:CG2	1:B:57:ASN:ND2	2.75	0.48
1:B:618:ILE:HG21	1:B:688:GLY:HA2	1.93	0.48
1:A:396:THR:OG1	1:A:398:ASN:ND2	2.46	0.48
1:A:727:LYS:HB3	1:A:734:ILE:CD1	2.43	0.48
2:C:2:A:C2'	2:C:3:C:C5'	2.91	0.48
2:E:31:A:H2'	2:E:32:C:C6	2.39	0.48
1:B:924:ASP:O	1:B:925:TYR:C	2.50	0.48
1:A:588:ILE:HD13	1:A:705:GLY:CA	2.43	0.48
1:A:589:ILE:O	1:A:593:ILE:HG13	2.13	0.48
1:A:917:ASP:OD1	1:A:917:ASP:N	2.36	0.48
1:A:988:TYR:CD2	1:A:1002:LYS:NZ	2.81	0.48
3:D:28:G:C2'	3:D:29:U:H5'	2.41	0.48
2:E:12:A:O5'	2:E:12:A:H8	1.96	0.48
1:B:379:ILE:N	1:B:379:ILE:CD1	2.76	0.48
1:B:554:PRO:HD3	1:B:685:PHE:CE2	2.48	0.48
1:B:997:ASN:ND2	1:B:997:ASN:N	2.60	0.48
1:A:550:ILE:CG2	1:A:551:PRO:HD2	2.40	0.48
1:A:862:ILE:O	1:A:866:GLY:N	2.46	0.48
2:E:1:G:H5"	2:E:2:A:H5'	1.95	0.48
2:E:28:A:H61	1:B:962:HIS:CD2	2.32	0.48
1:B:45:TYR:CE2	1:B:130:PHE:HE2	2.31	0.48
1:B:215:LEU:HD12	1:B:215:LEU:H	1.78	0.48
1:B:600:TYR:CD1	1:B:604:PHE:HD2	2.31	0.48
1:A:406:MSE:CE	1:A:461:PHE:CG	2.96	0.48
1:B:714:LEU:CD1	1:B:714:LEU:N	2.76	0.48
1:A:94:TYR:HB3	1:A:117:TYR:CE1	2.48	0.48
1:A:615:PHE:CD1	1:A:615:PHE:C	2.86	0.48
1:A:721:PHE:CE1	1:A:740:ILE:HD13	2.49	0.48
1:A:915:ARG:NH1	1:A:915:ARG:CG	2.73	0.48
2:C:33:A:C2'	2:C:34:A:H5'	2.44	0.48
1:B:118:LEU:O	1:B:119:ASN:HB2	2.14	0.48
1:B:514:LEU:HD23	1:B:728:TYR:CE2	2.49	0.48
1:B:734:ILE:CG2	1:B:735:LYS:NZ	2.77	0.48
1:B:1044:ASP:OD1	1:B:1045:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:CD2	1:A:308:VAL:HG21	2.42	0.48
1:A:549:ASN:HB3	2:C:38:U:O2'	2.12	0.48
2:E:32:C:H5"	2:E:32:C:C6	2.47	0.48
2:E:33:A:H8	2:E:33:A:C5'	2.11	0.48
1:B:387:TYR:CZ	1:B:391:ARG:HD2	2.49	0.48
1:B:629:ASP:O	1:B:632:ASN:CB	2.61	0.48
1:A:654:TYR:CD1	1:A:654:TYR:C	2.87	0.48
1:A:659:GLN:NE2	3:D:25:U:O2'	2.46	0.48
1:A:823:LYS:HB3	1:A:872:GLU:HG3	1.95	0.48
2:E:27:A:H5'	1:B:963:ARG:NH2	2.28	0.48
1:B:487:ILE:H	1:B:487:ILE:HG13	1.55	0.48
1:B:925:TYR:CD2	1:B:1126:LEU:HD21	2.31	0.48
1:A:510:LYS:HD2	1:A:736:ILE:HD11	1.94	0.48
1:A:1083:ASN:CB	2:C:2:A:H4'	2.44	0.48
2:C:31:A:H5"	2:C:32:C:P	2.54	0.48
2:E:14:A:O4'	1:B:139:ASN:ND2	2.47	0.48
2:E:28:A:H2	1:B:966:GLY:CA	2.23	0.48
1:B:45:TYR:OH	1:B:130:PHE:HD2	1.95	0.48
1:B:249:GLN:NE2	1:B:249:GLN:N	2.60	0.48
1:B:551:PRO:HG3	1:B:652:LYS:HG2	1.94	0.48
1:A:112:VAL:HG13	1:A:126:GLU:CD	2.34	0.48
1:A:194:GLU:OE2	1:A:289:LYS:HE3	2.13	0.48
1:A:695:ASN:C	1:A:695:ASN:ND2	2.66	0.48
1:A:893:LYS:NZ	1:A:937:GLU:CD	2.65	0.48
1:B:679:ASP:O	1:B:683:LYS:CB	2.62	0.48
1:A:59:LYS:HG2	1:A:63:LYS:HE3	1.96	0.47
1:A:812:GLU:HG2	1:A:813:ASP:N	2.29	0.47
1:B:310:LYS:HA	1:B:310:LYS:HE2	1.90	0.47
1:B:614:ASN:O	1:B:618:ILE:HB	2.14	0.47
1:B:701:LEU:O	1:B:704:ILE:HG12	2.13	0.47
1:B:1019:LEU:CD2	1:B:1020:HIS:CE1	2.92	0.47
1:A:185:ARG:NH1	1:A:342:ASP:OD1	2.47	0.47
1:B:457:ILE:HD12	1:B:457:ILE:N	2.29	0.47
1:A:340:LYS:HG2	2:C:7:C:H5"	1.96	0.47
1:A:406:MSE:CE	1:A:461:PHE:CD1	2.97	0.47
1:A:993:PHE:HA	1:A:1008:ILE:HD13	1.95	0.47
1:A:1142:LYS:HD2	1:A:1142:LYS:HA	1.72	0.47
2:E:32:C:H2'	2:E:33:A:C5'	2.44	0.47
1:B:157:LYS:HG2	1:B:166:VAL:CG2	2.41	0.47
1:B:701:LEU:N	1:B:701:LEU:HD12	2.28	0.47
1:A:534:ILE:O	1:A:537:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ILE:O	1:A:866:GLY:HA3	2.14	0.47
1:A:979:LEU:HB3	1:A:989:ILE:HG12	1.95	0.47
2:C:33:A:H2'	2:C:34:A:C5'	2.44	0.47
1:B:131:ARG:CG	1:B:131:ARG:NH1	2.73	0.47
1:B:304:LEU:HD23	1:B:308:VAL:HG21	1.95	0.47
1:B:770:ASN:OD1	1:B:771:HIS:N	2.48	0.47
1:A:406:MSE:O	1:A:425:VAL:CB	2.62	0.47
1:A:615:PHE:HA	1:A:618:ILE:HG22	1.97	0.47
1:A:753:LEU:HD23	1:A:799:LEU:HD12	1.97	0.47
1:A:778:LYS:HE2	1:A:801:ASN:OD1	2.14	0.47
1:A:869:ASN:O	1:A:873:LYS:HG3	2.15	0.47
1:B:64:LEU:O	1:B:68:PHE:N	2.44	0.47
1:B:471:ILE:CG2	1:B:475:ILE:HD11	2.44	0.47
1:B:619:SER:O	1:B:623:ILE:N	2.46	0.47
1:B:698:ARG:CB	1:B:701:LEU:CD1	2.93	0.47
1:B:249:GLN:N	1:B:249:GLN:HE21	2.12	0.47
1:A:236:ASP:OD1	1:A:268:LYS:HE3	2.14	0.47
1:A:380:ILE:HG13	1:A:475:ILE:HG21	1.96	0.47
1:A:482:LEU:HD12	1:A:483:GLU:N	2.29	0.47
1:A:597:LYS:NZ	3:D:14:A:OP1	2.35	0.47
1:A:1050:TYR:CE2	1:A:1062:ILE:HG22	2.49	0.47
1:A:1117:SER:OG	1:A:1135:ARG:N	2.47	0.47
2:C:13:A:H3'	2:C:14:A:C5'	2.43	0.47
2:E:10:A:C6	2:E:17:A:C8	3.02	0.47
1:B:43:ASP:O	1:B:44:MSE:C	2.53	0.47
1:B:160:GLU:O	1:B:163:ILE:N	2.42	0.47
1:B:421:VAL:HG22	1:B:422:SER:CB	2.43	0.47
1:B:554:PRO:CD	1:B:685:PHE:CD2	2.98	0.47
1:A:157:LYS:O	1:A:357:ASP:O	2.32	0.47
1:A:515:LYS:HE2	1:A:545:PHE:CE1	2.50	0.47
1:A:622:ILE:HD12	1:A:622:ILE:H	1.80	0.47
1:A:961:LEU:CD1	1:A:1057:ILE:HD12	2.45	0.47
1:A:1039:LYS:CE	1:A:1046:TYR:HE2	2.19	0.47
1:B:1:MSE:CE	1:B:3:VAL:HG12	2.45	0.47
1:B:453:ASN:O	1:B:457:ILE:HD13	2.15	0.47
1:B:822:GLY:HA2	1:B:832:VAL:CG1	2.44	0.47
1:A:266:GLU:OE1	1:A:269:LYS:NZ	2.48	0.47
1:A:303:LEU:HD11	1:A:332:LEU:HD23	1.97	0.47
1:B:563:ILE:HA	1:B:686:LEU:HD11	1.97	0.47
1:A:304:LEU:HD23	1:A:308:VAL:CG2	2.45	0.47
1:A:785:GLN:HE21	1:A:793:PHE:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:ILE:CG2	1:A:973:ARG:HH12	2.23	0.47
2:E:32:C:N4	2:E:33:A:N6	2.63	0.47
3:F:3:A:N6	3:F:4:A:N6	2.63	0.47
1:B:403:THR:HG21	1:B:472:ARG:CZ	2.45	0.47
1:B:686:LEU:HD23	1:B:686:LEU:C	2.35	0.47
1:A:164:GLU:O	1:A:164:GLU:HG2	2.14	0.46
1:A:300:MSE:HE3	1:A:304:LEU:HG	1.95	0.46
1:A:848:PHE:CE2	1:A:850:GLY:HA2	2.50	0.46
2:C:33:A:H2'	2:C:34:A:O5'	2.14	0.46
1:B:65:LYS:O	1:B:69:SER:N	2.48	0.46
1:B:1136:ASN:HB3	1:B:1140:LEU:HD23	1.97	0.46
1:A:577:PRO:HD3	1:A:592:GLN:OE1	2.15	0.46
2:E:56:U:C2'	2:E:57:U:H5'	2.45	0.46
3:F:4:A:O2'	3:F:5:G:O5'	2.32	0.46
3:F:29:U:OP1	1:B:41:ARG:NH1	2.40	0.46
1:B:423:GLY:N	1:B:426:ASP:OD2	2.48	0.46
1:B:600:TYR:HD1	1:B:604:PHE:HD2	1.64	0.46
1:B:1016:TYR:O	1:B:1020:HIS:ND1	2.42	0.46
1:B:615:PHE:CD2	1:B:651:PRO:N	2.80	0.46
1:B:842:ASP:OD2	1:B:847:TYR:N	2.48	0.46
1:B:991:GLU:HG2	1:B:1000:ASN:CG	2.35	0.46
1:A:231:ILE:HD12	1:A:267:LEU:CD2	2.34	0.46
1:A:244:ILE:HG23	1:A:264:MSE:CE	2.45	0.46
1:A:300:MSE:HE1	1:A:324:PHE:HE1	1.81	0.46
1:B:278:LEU:HD12	1:B:278:LEU:C	2.36	0.46
1:B:690:MSE:HA	1:B:693:LEU:HB2	1.94	0.46
1:B:738:TYR:CD1	1:B:738:TYR:C	2.89	0.46
1:A:55:LYS:HE3	1:A:59:LYS:CD	2.45	0.46
1:A:412:LYS:HA	1:A:417:GLU:O	2.16	0.46
1:A:477:HIS:CA	1:A:972:GLU:OE2	2.64	0.46
1:A:618:ILE:CD1	1:A:688:GLY:N	2.78	0.46
1:A:825:LEU:HD23	1:A:825:LEU:N	2.30	0.46
2:C:14:A:HO2'	2:C:15:U:P	2.38	0.46
3:D:23:G:C2'	3:D:24:A:H5'	2.46	0.46
3:F:4:A:C8	3:F:4:A:C3'	2.99	0.46
1:B:118:LEU:HB3	1:B:120:GLU:HG3	1.97	0.46
1:B:755:TYR:CD1	1:B:756:THR:N	2.83	0.46
1:A:731:ASN:HD21	1:A:733:ASN:HB2	1.81	0.46
1:A:1042:LYS:N	1:A:1042:LYS:CD	2.78	0.46
3:D:5:G:C8	3:D:5:G:C5'	2.94	0.46
1:B:115:LYS:O	1:B:119:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:ILE:HG23	1:B:551:PRO:CD	2.37	0.46
1:A:785:GLN:NE2	1:A:797:LEU:HD12	2.29	0.46
1:A:811:THR:HG22	1:A:860:TYR:OH	2.15	0.46
1:A:857:ARG:NH2	3:D:11:U:OP1	2.49	0.46
1:A:1044:ASP:CG	1:A:1045:LEU:N	2.69	0.46
1:A:1047:ILE:HD13	1:A:1070:ASN:ND2	2.31	0.46
2:E:27:A:N6	2:E:30:C:OP1	2.49	0.46
1:B:814:PHE:H	1:B:814:PHE:HD1	1.64	0.46
1:B:880:TYR:O	1:B:881:LYS:CD	2.63	0.46
1:B:908:HIS:HD2	1:B:928:TYR:OH	1.99	0.46
1:B:987:GLN:CG	1:B:988:TYR:CD1	2.99	0.46
1:B:1047:ILE:HG23	1:B:1048:ALA:N	2.30	0.46
2:E:32:C:C2'	2:E:33:A:H5"	2.43	0.46
1:B:1:MSE:CE	1:B:37:LEU:HD22	2.41	0.46
1:B:524:ASN:ND2	1:B:587:GLU:O	2.41	0.46
1:B:996:GLU:OE2	1:B:999:LYS:HD2	2.15	0.46
2:C:13:A:H3'	2:C:14:A:H5"	1.98	0.46
3:D:28:G:C2'	3:D:29:U:C5'	2.93	0.46
2:E:26:A:C2	2:E:27:A:H1'	2.51	0.46
2:E:30:C:H1'	2:E:31:A:OP2	2.16	0.46
1:B:77:ASP:O	1:B:79:THR:N	2.49	0.46
1:B:175:ILE:CD1	1:B:291:ALA:CB	2.94	0.46
1:B:478:PHE:CE2	1:B:480:LEU:HD23	2.51	0.46
1:B:678:ILE:HD12	1:B:679:ASP:N	2.31	0.46
1:A:153:ALA:HB1	1:A:360:ILE:CG2	2.45	0.46
1:A:622:ILE:N	1:A:622:ILE:CD1	2.79	0.46
1:A:1105:GLY:HA2	2:C:1:G:H21	1.80	0.46
3:D:2:G:N7	1:B:1004:LYS:HE3	2.31	0.46
1:B:398:ASN:ND2	1:B:400:ASN:H	2.06	0.46
1:B:406:MSE:O	1:B:425:VAL:HG23	2.16	0.46
1:B:1020:HIS:ND1	1:B:1020:HIS:N	2.64	0.46
1:A:322:ARG:CZ	2:C:1:G:H2'	2.45	0.45
1:A:699:LEU:O	1:A:702:ILE:HG13	2.15	0.45
1:A:1003:TYR:O	1:A:1011:LYS:HD3	2.16	0.45
2:C:6:C:H2'	2:C:7:C:C6	2.50	0.45
2:C:31:A:O3'	2:C:32:C:O4'	2.34	0.45
1:B:3:VAL:HG21	1:B:148:PHE:CZ	2.51	0.45
1:B:128:GLU:O	1:B:128:GLU:HG3	2.16	0.45
1:B:920:PHE:O	1:B:921:THR:CB	2.60	0.45
1:B:350:LYS:O	1:B:354:TYR:HD1	1.98	0.45
1:A:648:GLU:C	1:A:649:LYS:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:ILE:HD13	1:A:1070:ASN:HD22	1.81	0.45
2:C:8:C:H2'	2:C:9:C:O5'	2.16	0.45
1:B:33:ARG:HD3	1:B:37:LEU:HD11	1.98	0.45
1:B:800:ILE:O	1:B:804:ASN:HB2	2.16	0.45
1:A:231:ILE:CD1	1:A:267:LEU:HD22	2.36	0.45
1:A:244:ILE:CG2	1:A:264:MSE:CE	2.94	0.45
1:A:976:ARG:HB3	1:A:993:PHE:CZ	2.51	0.45
1:A:1015:PHE:CD1	1:A:1015:PHE:C	2.90	0.45
1:A:1041:GLU:HB3	1:A:1043:LYS:HG3	1.98	0.45
3:F:27:U:H6	3:F:27:U:O5'	1.97	0.45
1:B:210:LEU:HD13	1:B:210:LEU:HA	1.78	0.45
1:B:412:LYS:CB	1:B:417:GLU:O	2.58	0.45
1:B:846:ILE:CD1	1:B:887:LEU:HD22	2.43	0.45
1:A:265:SER:HB3	1:A:268:LYS:CE	2.47	0.45
1:A:812:GLU:HG2	1:A:813:ASP:H	1.81	0.45
2:E:30:C:O2'	2:E:31:A:OP1	2.32	0.45
3:F:9:A:H2'	3:F:10:G:C8	2.52	0.45
1:B:510:LYS:HD2	1:B:736:ILE:HD11	1.97	0.45
1:B:1031:SER:O	1:B:1035:ILE:N	2.44	0.45
1:A:411:VAL:HG22	1:A:412:LYS:N	2.31	0.45
1:A:607:TYR:CE1	1:A:612:ASN:O	2.69	0.45
1:A:618:ILE:HG23	1:A:619:SER:N	2.32	0.45
1:A:1039:LYS:HG2	1:A:1046:TYR:CE2	2.52	0.45
1:A:1120:ILE:O	1:A:1132:MSE:CB	2.64	0.45
3:F:17:C:O2'	3:F:18:A:H5'	2.17	0.45
2:C:31:A:H5"	2:C:32:C:OP2	2.16	0.45
1:B:1:MSE:HE2	1:B:3:VAL:HG12	1.99	0.45
1:B:158:ILE:HG22	1:B:159:ASN:N	2.31	0.45
1:A:411:VAL:HG12	1:A:419:LYS:HG2	1.92	0.45
1:A:925:TYR:CD2	1:A:1128:LYS:HD2	2.52	0.45
1:A:1044:ASP:OD1	1:A:1045:LEU:N	2.50	0.45
1:A:1083:ASN:HB2	2:C:2:A:H4'	1.98	0.45
1:B:235:ASN:ND2	1:B:240:PHE:HE2	2.13	0.45
1:A:145:LYS:NZ	1:A:149:GLU:OE2	2.50	0.45
1:A:235:ASN:OD1	1:A:240:PHE:HE1	1.99	0.45
1:A:489:ALA:O	1:A:758:ARG:HG2	2.17	0.45
1:A:618:ILE:HD11	1:A:688:GLY:N	2.32	0.45
1:A:679:ASP:O	1:A:683:LYS:N	2.39	0.45
1:A:1010:GLU:OE2	1:A:1010:GLU:N	2.46	0.45
2:C:14:A:O2'	2:C:15:U:P	2.75	0.45
2:E:31:A:H2'	2:E:32:C:C5'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:TYR:CD1	1:B:222:LYS:N	2.85	0.45
1:B:604:PHE:CD2	1:B:689:PHE:CD1	3.04	0.45
1:B:728:TYR:CZ	1:B:732:ASN:OD1	2.70	0.45
1:B:882:ILE:HG12	1:B:945:VAL:HA	1.99	0.45
1:B:1110:ILE:N	1:B:1110:ILE:HD12	2.32	0.45
1:A:64:LEU:O	1:A:68:PHE:HD2	1.99	0.45
1:A:75:LEU:HD21	1:A:78:ASN:HA	1.95	0.45
1:A:1135:ARG:NH1	3:D:19:G:O2'	2.50	0.45
3:F:20:A:H2'	3:F:21:U:H5'	1.98	0.45
1:B:678:ILE:O	1:B:682:GLN:N	2.44	0.45
1:B:737:PRO:HD2	1:B:740:ILE:CG1	2.47	0.45
1:A:779:GLY:O	3:D:22:A:H4'	2.17	0.44
1:A:941:LEU:HD12	1:A:945:VAL:HG23	1.99	0.44
1:B:604:PHE:O	1:B:604:PHE:CD1	2.70	0.44
1:B:1142:LYS:HA	1:B:1142:LYS:HD2	1.83	0.44
1:A:158:ILE:O	1:A:164:GLU:HA	2.18	0.44
2:C:8:C:C6	2:C:8:C:C3'	3.00	0.44
3:D:5:G:OP1	1:B:412:LYS:HD2	2.17	0.44
2:E:23:A:C2	2:E:29:A:H2'	2.52	0.44
1:B:444:PHE:O	1:B:767:LYS:HE3	2.17	0.44
1:B:526:PHE:HD2	1:B:721:PHE:CD2	2.34	0.44
1:A:409:LYS:O	1:A:421:VAL:N	2.48	0.44
1:A:588:ILE:HD13	1:A:705:GLY:HA3	2.00	0.44
1:A:680:PHE:O	1:A:684:ILE:HG13	2.17	0.44
2:C:32:C:H5'	2:C:33:A:OP2	2.17	0.44
1:B:878:ALA:HA	1:B:1146:ILE:CD1	2.48	0.44
1:B:1009:VAL:O	1:B:1013:ILE:HG13	2.16	0.44
1:A:1087:LYS:HG2	2:C:3:C:H4'	1.99	0.44
1:A:54:THR:CG2	1:A:57:ASN:HB2	2.46	0.44
1:A:55:LYS:HD2	1:A:55:LYS:C	2.38	0.44
1:A:160:GLU:HG3	1:A:163:ILE:CG2	2.47	0.44
1:A:760:ASN:O	1:A:763:TYR:HB3	2.18	0.44
1:A:936:GLU:OE1	1:A:1133:THR:CB	2.66	0.44
1:B:550:ILE:HB	1:B:553:VAL:HG11	1.99	0.44
1:B:566:LEU:O	1:B:569:SER:CB	2.62	0.44
2:E:11:A:O2'	2:E:12:A:OP2	2.32	0.44
3:F:10:G:H5'	1:B:856:HIS:HA	2.00	0.44
1:B:741:ASN:HA	1:B:744:LEU:HB2	2.00	0.44
1:B:752:ILE:HD12	1:B:752:ILE:HA	1.75	0.44
1:A:163:ILE:CG2	1:A:165:LYS:HD3	2.47	0.44
2:C:26:A:H2'	2:C:27:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:CG2	1:B:412:LYS:N	2.80	0.44
1:B:534:ILE:O	1:B:538:LEU:HG	2.17	0.44
1:B:604:PHE:CD1	1:B:604:PHE:C	2.87	0.44
1:A:240:PHE:CD2	1:A:268:LYS:NZ	2.84	0.44
1:A:251:VAL:HG21	1:A:257:LEU:CA	2.47	0.44
1:A:445:TYR:OH	1:A:768:LEU:CD2	2.66	0.44
1:A:728:TYR:HA	1:A:734:ILE:CG1	2.46	0.44
1:A:1063:SER:OG	1:A:1148:PHE:O	2.35	0.44
2:E:18:A:O2'	2:E:19:G:H5'	2.18	0.44
1:B:165:LYS:HG3	1:B:166:VAL:N	2.32	0.44
1:B:445:TYR:OH	1:B:768:LEU:HD13	2.18	0.44
1:B:614:ASN:CB	1:B:618:ILE:CG1	2.96	0.44
1:B:690:MSE:O	1:B:694:ALA:HB2	2.18	0.44
1:A:961:LEU:CD1	1:A:1057:ILE:CD1	2.95	0.44
1:B:196:PHE:CE1	1:B:200:TYR:HD2	2.36	0.44
1:B:235:ASN:OD1	1:B:240:PHE:CE2	2.71	0.44
1:B:441:LEU:HD12	1:B:451:MSE:HE1	1.99	0.44
1:B:558:LYS:O	1:B:561:SER:HB2	2.18	0.44
1:A:837:GLU:HA	1:A:840:LYS:HD3	1.99	0.43
3:D:21:U:H2'	3:D:22:A:O4'	2.18	0.43
1:B:191:ASN:HB3	1:B:292:PHE:CE2	2.53	0.43
1:B:218:LEU:O	1:B:221:TYR:CD1	2.71	0.43
1:B:427:LYS:O	1:B:431:GLU:HB2	2.18	0.43
1:B:557:THR:OG1	1:B:558:LYS:N	2.51	0.43
1:A:609:MSE:HE1	1:A:685:PHE:HE1	1.82	0.43
1:A:908:HIS:HD2	1:A:928:TYR:OH	2.01	0.43
3:D:29:U:H5'	3:D:29:U:C6	2.53	0.43
1:B:1:MSE:HE2	1:B:1:MSE:HB3	1.67	0.43
1:B:509:GLU:HG2	1:B:513:LYS:HE3	2.00	0.43
1:B:701:LEU:CD1	1:B:701:LEU:H	2.31	0.43
1:A:300:MSE:CE	1:A:324:PHE:HE1	2.31	0.43
2:E:27:A:H5"	2:E:28:A:O5'	2.18	0.43
1:B:42:LEU:HD12	1:B:71:LYS:CB	2.49	0.43
1:B:510:LYS:O	1:B:514:LEU:HB2	2.17	0.43
1:B:524:ASN:ND2	1:B:587:GLU:CA	2.81	0.43
1:A:144:LEU:O	1:A:146:TYR:N	2.52	0.43
1:A:193:LYS:HE3	1:A:334:GLU:OE1	2.19	0.43
1:A:961:LEU:HD11	1:A:1057:ILE:CD1	2.47	0.43
1:A:1025:VAL:O	1:A:1026:LYS:C	2.56	0.43
3:D:6:A:H3'	3:D:7:A:H5"	2.00	0.43
3:D:7:A:H8	3:D:7:A:C5'	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:G:H5"	2:E:2:A:OP1	2.19	0.43
1:B:714:LEU:HD13	1:B:714:LEU:N	2.33	0.43
1:B:870:LEU:HD13	1:B:1058:PRO:O	2.19	0.43
1:A:155:TYR:O	1:A:360:ILE:HA	2.18	0.43
1:A:574:TRP:CZ3	1:A:702:ILE:HG12	2.54	0.43
1:A:689:PHE:O	1:A:692:TYR:HB3	2.19	0.43
1:A:765:ILE:HA	1:A:768:LEU:HD23	1.99	0.43
1:A:785:GLN:HG2	1:A:791:GLU:HA	2.00	0.43
2:C:58:C:C5'	2:C:58:C:C6	2.95	0.43
1:B:509:GLU:CG	1:B:513:LYS:HE3	2.48	0.43
1:B:755:TYR:CD1	1:B:755:TYR:C	2.92	0.43
1:A:94:TYR:HB3	1:A:117:TYR:HE1	1.82	0.43
1:A:160:GLU:OE1	1:A:163:ILE:N	2.39	0.43
1:A:216:THR:OG1	1:A:219:GLU:HB2	2.19	0.43
1:A:220:LYS:HA	1:A:223:ILE:HD12	2.01	0.43
1:A:319:LYS:O	1:A:322:ARG:HB2	2.18	0.43
1:A:594:TYR:CD1	1:A:594:TYR:C	2.92	0.43
2:E:34:A:H2'	2:E:35:A:O5'	2.18	0.43
1:B:976:ARG:HB3	1:B:993:PHE:CE2	2.53	0.43
1:B:993:PHE:CD1	1:B:1008:ILE:HD13	2.52	0.43
1:A:75:LEU:HD21	1:A:78:ASN:N	2.33	0.43
1:A:300:MSE:HE1	1:A:324:PHE:CE1	2.54	0.43
1:A:724:PHE:O	1:A:727:LYS:HB2	2.18	0.43
1:A:728:TYR:N	1:A:734:ILE:CD1	2.80	0.43
2:E:33:A:C8	2:E:33:A:C5'	2.94	0.43
1:B:123:ASN:OD1	1:B:124:SER:N	2.52	0.43
1:B:1117:SER:CB	1:B:1134:ASP:HB3	2.49	0.43
1:A:123:ASN:HB3	1:A:126:GLU:HB2	1.99	0.43
1:A:401:ASP:OD1	1:A:403:THR:OG1	2.36	0.43
1:A:537:TYR:CE1	1:A:541:THR:OG1	2.69	0.43
1:A:764:LEU:O	1:A:768:LEU:CD2	2.64	0.43
1:A:915:ARG:HD3	1:A:918:GLU:CB	2.48	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD23	1.80	0.43
1:A:970:ILE:CG2	1:A:973:ARG:NH1	2.61	0.43
1:B:211:GLU:OE2	1:B:222:LYS:CE	2.57	0.43
1:B:407:ARG:NH1	1:B:459:ASP:OD1	2.46	0.43
1:B:925:TYR:OH	1:B:1129:LYS:O	2.35	0.43
2:E:10:A:C6	2:E:17:A:C5	3.07	0.43
1:A:131:ARG:NH2	1:A:135:LYS:HE3	2.32	0.42
1:A:774:LEU:HD22	1:A:800:ILE:HG23	2.01	0.42
1:A:963:ARG:HH21	2:C:28:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:ASN:HD21	1:A:996:GLU:HB3	1.83	0.42
1:A:1119:LYS:HE3	1:A:1134:ASP:OD1	2.19	0.42
2:C:32:C:N4	3:D:28:G:N1	2.42	0.42
2:C:36:U:C2'	2:C:37:C:H5'	2.49	0.42
1:B:690:MSE:O	1:B:694:ALA:N	2.50	0.42
1:B:704:ILE:C	1:B:706:SER:N	2.72	0.42
1:B:771:HIS:CB	1:B:808:ASN:ND2	2.79	0.42
1:A:30:THR:HG22	1:A:34:LEU:CD1	2.49	0.42
1:A:512:LEU:HB3	1:A:749:LEU:HD11	2.00	0.42
1:A:936:GLU:HG3	1:A:937:GLU:N	2.34	0.42
2:C:8:C:C6	2:C:8:C:H3'	2.54	0.42
2:C:38:U:H2'	2:C:39:A:C8	2.54	0.42
2:E:3:C:H4'	1:B:1087:LYS:HG2	2.00	0.42
3:F:9:A:H2'	3:F:10:G:O5'	2.19	0.42
3:F:25:U:O2'	3:F:26:U:H5'	2.19	0.42
1:B:33:ARG:O	1:B:37:LEU:CD1	2.66	0.42
1:B:188:TYR:O	1:B:192:VAL:HG23	2.19	0.42
1:B:693:LEU:HD12	1:B:693:LEU:HA	1.77	0.42
1:B:774:LEU:HD22	1:B:800:ILE:HG23	2.00	0.42
1:B:1044:ASP:O	1:B:1047:ILE:HG22	2.19	0.42
1:A:471:ILE:CG2	1:A:475:ILE:HD11	2.48	0.42
2:E:2:A:C2'	2:E:3:C:C5'	2.97	0.42
1:B:857:ARG:O	1:B:860:TYR:HB3	2.19	0.42
1:B:890:TYR:OH	1:B:894:LYS:NZ	2.51	0.42
1:B:936:GLU:CG	1:B:937:GLU:N	2.82	0.42
1:A:47:LYS:CG	1:A:48:ASN:N	2.82	0.42
1:A:607:TYR:HE1	1:A:612:ASN:O	2.01	0.42
1:A:655:LEU:HD22	1:A:681:ILE:HD12	2.01	0.42
1:A:655:LEU:CD1	1:A:681:ILE:CD1	2.94	0.42
1:A:728:TYR:O	1:A:728:TYR:CG	2.70	0.42
1:A:1056:TYR:CD1	1:A:1056:TYR:C	2.93	0.42
2:C:56:U:C2	3:D:5:G:C2	3.07	0.42
2:E:32:C:C6	2:E:32:C:C5'	3.03	0.42
2:E:47:A:C2	3:F:14:A:C2	3.08	0.42
1:B:200:TYR:HB3	1:B:205:ILE:HD11	2.02	0.42
1:B:500:LYS:HA	1:B:760:ASN:HD21	1.85	0.42
1:B:1042:LYS:N	1:B:1042:LYS:HD2	2.33	0.42
1:A:728:TYR:CA	1:A:734:ILE:HD11	2.49	0.42
1:B:142:ASN:N	1:B:142:ASN:HD22	2.16	0.42
1:B:211:GLU:OE2	1:B:222:LYS:HG3	2.19	0.42
1:B:280:LYS:HD2	1:B:280:LYS:HA	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:O	1:B:340:LYS:HG3	2.19	0.42
1:B:827:PHE:HZ	1:B:840:LYS:HG2	1.84	0.42
1:B:897:ILE:HD12	1:B:938:TYR:CD1	2.54	0.42
1:B:937:GLU:O	1:B:941:LEU:CD2	2.67	0.42
1:A:17:GLU:OE1	1:A:28:ASN:ND2	2.52	0.42
1:A:30:THR:HG22	1:A:34:LEU:HD12	2.02	0.42
1:A:471:ILE:HG22	1:A:475:ILE:CD1	2.50	0.42
1:A:620:LYS:HA	1:A:623:ILE:HB	2.02	0.42
1:A:1079:ARG:O	1:A:1083:ASN:ND2	2.52	0.42
2:E:47:A:H2'	2:E:48:A:C8	2.55	0.42
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.74	0.42
1:B:176:TYR:O	1:B:179:TYR:N	2.51	0.42
1:B:615:PHE:CE2	1:B:651:PRO:HD3	2.53	0.42
1:B:931:ALA:O	1:B:935:ILE:HG13	2.19	0.42
1:A:385:VAL:HG11	1:A:770:ASN:HB3	2.02	0.42
2:C:7:C:H6	2:C:7:C:O5'	2.01	0.42
2:C:32:C:H2'	2:C:33:A:H5'	2.02	0.42
1:B:257:LEU:HD23	1:B:257:LEU:O	2.19	0.42
1:A:769:LEU:HD23	1:A:769:LEU:HA	1.84	0.42
1:B:189:VAL:O	1:B:193:LYS:HG3	2.19	0.42
1:B:540:ARG:NH2	1:B:541:THR:CG2	2.82	0.42
1:B:618:ILE:HD12	1:B:691:THR:HG21	1.95	0.42
1:B:697:GLY:O	1:B:699:LEU:N	2.50	0.42
1:A:841:PHE:HE1	1:A:887:LEU:CD1	2.17	0.42
1:A:1057:ILE:HA	1:A:1058:PRO:HA	1.77	0.42
2:E:33:A:H2'	2:E:34:A:O5'	2.19	0.42
1:B:178:TYR:OH	1:B:285:ASP:OD1	2.33	0.42
1:B:421:VAL:HG23	1:B:422:SER:OG	2.20	0.42
1:B:769:LEU:HD23	1:B:769:LEU:HA	1.84	0.42
1:A:265:SER:N	1:A:268:LYS:CD	2.72	0.42
1:A:616:PHE:O	1:A:619:SER:OG	2.34	0.42
1:A:742:GLU:OE2	1:A:745:ARG:NH1	2.53	0.42
2:C:15:U:H4'	2:C:16:G:C5'	2.50	0.42
2:E:30:C:C4'	2:E:31:A:OP2	2.68	0.42
1:B:48:ASN:CB	1:B:61:ILE:HG21	2.50	0.42
1:B:734:ILE:CG2	1:B:735:LYS:HZ3	2.32	0.42
1:A:265:SER:H	1:A:268:LYS:HZ2	1.68	0.41
1:A:502:MSE:CE	1:A:763:TYR:CE2	2.98	0.41
1:A:507:ILE:HD12	1:A:507:ILE:O	2.20	0.41
1:A:1097:GLY:O	1:A:1136:ASN:ND2	2.53	0.41
1:B:177:ASP:HA	1:B:180:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HB2	1:B:326:TYR:CD1	2.54	0.41
1:B:231:ILE:HA	1:B:231:ILE:HD12	1.72	0.41
1:B:601:TYR:O	1:B:605:LEU:HD12	2.20	0.41
1:B:686:LEU:C	1:B:686:LEU:CD2	2.88	0.41
1:A:281:GLU:HG3	1:A:282:GLU:N	2.35	0.41
1:A:848:PHE:CE2	1:A:850:GLY:CA	3.03	0.41
1:B:15:THR:HG21	1:B:360:ILE:HD12	2.01	0.41
1:B:991:GLU:OE2	1:B:1001:VAL:N	2.47	0.41
1:A:163:ILE:CG1	1:A:165:LYS:CD	2.92	0.41
1:A:701:LEU:CD2	1:A:704:ILE:HD11	2.49	0.41
2:C:54:U:H3	3:D:6:A:H62	1.67	0.41
2:C:56:U:H3	3:D:4:A:H2	1.67	0.41
2:E:13:A:N6	2:E:14:A:C2	2.88	0.41
2:E:29:A:H62	1:B:784:TYR:HA	1.85	0.41
1:B:625:LEU:O	1:B:629:ASP:N	2.49	0.41
1:B:942:LYS:NZ	1:B:946:GLU:OE1	2.53	0.41
1:A:168:GLY:HA3	1:A:173:ASN:HD22	1.85	0.41
1:A:622:ILE:H	1:A:622:ILE:CD1	2.34	0.41
1:A:921:THR:O	1:A:924:ASP:N	2.53	0.41
1:A:966:GLY:HA3	2:C:28:A:C2	2.51	0.41
1:B:43:ASP:OD1	1:B:44:MSE:N	2.54	0.41
1:B:45:TYR:CE2	1:B:130:PHE:CD2	3.08	0.41
1:B:539:LYS:HG3	1:B:746:GLU:HG2	2.02	0.41
1:B:574:TRP:CH2	1:B:702:ILE:HG23	2.50	0.41
1:A:163:ILE:HG21	1:A:165:LYS:HZ3	1.85	0.41
1:A:753:LEU:HG	1:A:759:LEU:HD21	2.03	0.41
1:A:868:LEU:O	1:A:872:GLU:HB2	2.20	0.41
2:C:20:G:H2'	2:C:21:G:O4'	2.20	0.41
3:D:2:G:O2'	3:D:3:A:P	2.78	0.41
1:B:195:ALA:HB1	1:B:293:CYS:HA	2.01	0.41
1:B:421:VAL:HG13	1:B:421:VAL:O	2.20	0.41
1:B:848:PHE:CD2	1:B:849:ASP:O	2.73	0.41
1:B:949:GLU:HB3	1:B:1140:LEU:HD13	2.03	0.41
1:A:55:LYS:C	1:A:55:LYS:CD	2.89	0.41
1:A:205:ILE:O	1:A:209:VAL:HG23	2.20	0.41
1:A:251:VAL:CG1	1:A:260:LYS:HD2	2.50	0.41
1:A:645:ASP:CG	1:A:647:GLN:HG3	2.41	0.41
1:A:863:LYS:HD2	1:A:863:LYS:HA	1.76	0.41
2:C:25:U:H1'	2:C:26:A:C8	2.55	0.41
1:B:293:CYS:O	1:B:297:GLU:HB2	2.21	0.41
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:982:GLU:HB3	1:B:983:PHE:CE2	2.54	0.41
1:A:452:ASP:O	1:A:453:ASN:CB	2.68	0.41
1:A:607:TYR:HD2	1:A:692:TYR:CD2	2.38	0.41
1:A:759:LEU:HD12	1:A:759:LEU:HA	1.81	0.41
1:A:776:ASN:N	1:A:776:ASN:ND2	2.67	0.41
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.85	0.41
1:B:399:GLU:C	1:B:400:ASN:OD1	2.59	0.41
1:B:441:LEU:HD11	1:B:461:PHE:CE2	2.56	0.41
1:B:524:ASN:ND2	1:B:587:GLU:HA	2.36	0.41
1:B:701:LEU:N	1:B:701:LEU:CD1	2.84	0.41
1:A:334:GLU:HG3	1:A:335:ASN:N	2.36	0.41
1:A:543:PHE:CD1	1:A:598:ASN:OD1	2.74	0.41
1:A:622:ILE:HG12	1:A:684:ILE:HA	2.03	0.41
1:A:766:LEU:HD12	1:A:799:LEU:HD23	2.03	0.41
1:A:911:TYR:CE1	1:A:1126:LEU:HD13	2.56	0.41
1:A:925:TYR:OH	1:A:1129:LYS:O	2.33	0.41
1:B:831:LYS:NZ	1:B:872:GLU:CD	2.74	0.41
1:A:163:ILE:HD11	1:A:985:GLU:OE1	2.21	0.41
1:A:177:ASP:O	1:A:178:TYR:C	2.59	0.41
1:A:420:TYR:CD1	1:A:420:TYR:C	2.94	0.41
1:A:420:TYR:OH	1:A:426:ASP:OD2	2.33	0.41
1:A:445:TYR:OH	1:A:768:LEU:HD22	2.21	0.41
1:A:507:ILE:C	1:A:507:ILE:CD1	2.88	0.41
1:A:508:ASN:OD1	1:A:510:LYS:N	2.53	0.41
1:A:724:PHE:O	1:A:727:LYS:N	2.54	0.41
1:A:763:TYR:HB2	1:A:799:LEU:HD21	2.03	0.41
1:A:971:TRP:CG	1:A:1074:LEU:HD21	2.55	0.41
1:A:991:GLU:OE1	1:A:1002:LYS:O	2.39	0.41
2:C:8:C:C2	2:C:21:G:N2	2.89	0.41
2:C:24:C:H5'	2:C:24:C:C6	2.44	0.41
2:E:35:A:C6	2:E:36:U:C4	3.09	0.41
3:F:9:A:H2'	3:F:10:G:H8	1.85	0.41
1:B:157:LYS:O	1:B:158:ILE:HD13	2.21	0.41
1:B:196:PHE:CD1	1:B:200:TYR:HD2	2.39	0.41
1:B:564:ASP:O	1:B:567:LYS:CB	2.68	0.41
1:B:579:THR:CG2	1:B:580:ASN:N	2.84	0.41
1:B:604:PHE:CD2	1:B:689:PHE:HD1	2.39	0.41
1:B:810:VAL:HA	1:B:860:TYR:CE2	2.55	0.41
1:A:401:ASP:OD2	1:A:403:THR:OG1	2.32	0.41
1:A:513:LYS:CE	1:A:747:ILE:HB	2.50	0.41
1:A:570:LEU:O	1:A:572:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HG12	1:A:622:ILE:CD1	2.51	0.41
1:A:1098:PHE:HB3	1:A:1115:LEU:CD1	2.50	0.41
2:E:4:C:H4'	2:E:5:A:OP2	2.21	0.41
2:E:13:A:C6	2:E:14:A:C6	3.09	0.41
3:F:3:A:C2'	3:F:4:A:H5'	2.36	0.41
3:F:9:A:C2'	3:F:10:G:O5'	2.69	0.41
1:B:251:VAL:HG12	1:B:256:GLU:HB2	1.89	0.41
1:B:412:LYS:HB2	1:B:417:GLU:C	2.39	0.41
1:B:584:LYS:O	1:B:588:ILE:CG1	2.52	0.41
1:B:630:LYS:C	1:B:632:ASN:H	2.24	0.41
1:A:109:ASN:HA	1:A:129:VAL:HG11	2.03	0.40
1:A:890:TYR:CE1	1:A:942:LYS:HG3	2.56	0.40
1:B:249:GLN:HE21	1:B:249:GLN:H	1.68	0.40
1:B:526:PHE:HD2	1:B:721:PHE:HD2	1.69	0.40
1:B:659:GLN:CB	1:B:677:TYR:CZ	3.04	0.40
1:A:283:LEU:CD1	1:A:288:ILE:HD13	2.48	0.40
1:A:423:GLY:C	1:A:426:ASP:H	2.22	0.40
1:A:475:ILE:HD11	1:A:487:ILE:HD11	2.03	0.40
1:A:550:ILE:HB	1:A:553:VAL:CG2	2.51	0.40
1:A:830:ASN:HD22	1:A:830:ASN:HA	1.58	0.40
1:A:1087:LYS:CG	2:C:3:C:H4'	2.51	0.40
3:D:9:A:C8	3:D:9:A:C3'	3.05	0.40
3:D:23:G:H2'	3:D:24:A:H5'	2.04	0.40
1:B:90:ILE:HD12	1:B:90:ILE:H	1.87	0.40
1:B:515:LYS:HE2	1:B:545:PHE:CE1	2.57	0.40
1:B:579:THR:CB	1:B:585:THR:HG22	2.50	0.40
1:B:848:PHE:C	1:B:849:ASP:O	2.59	0.40
1:A:387:TYR:CZ	1:A:391:ARG:HD2	2.57	0.40
1:A:588:ILE:HD13	1:A:705:GLY:HA2	2.03	0.40
1:A:818:ALA:CB	1:A:838:LEU:HD12	2.51	0.40
1:A:862:ILE:HD12	1:A:947:PHE:HB3	2.02	0.40
2:C:33:A:C2	3:D:28:G:C2	3.09	0.40
2:E:27:A:N7	1:B:370:ARG:NH2	2.70	0.40
1:B:123:ASN:O	1:B:127:LEU:N	2.51	0.40
1:B:893:LYS:NZ	1:B:937:GLU:OE2	2.55	0.40
1:B:1119:LYS:HE3	1:B:1134:ASP:OD1	2.22	0.40
1:B:1145:LYS:O	1:B:1145:LYS:HG3	2.20	0.40
1:A:275:LYS:HD3	1:A:276:TYR:CZ	2.56	0.40
1:B:398:ASN:HD22	1:B:400:ASN:N	2.07	0.40
1:B:760:ASN:O	1:B:763:TYR:HB3	2.22	0.40
1:A:530:GLU:HG2	1:A:532:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:MSE:HB2	1:A:954:GLN:OE1	2.21	0.40
1:A:872:GLU:O	1:A:876:ASP:HB2	2.22	0.40
1:A:971:TRP:CD1	1:A:1074:LEU:HD21	2.57	0.40
2:C:8:C:H6	2:C:8:C:O5'	2.03	0.40
2:C:18:A:O2'	2:C:19:G:H5'	2.21	0.40
1:B:914:PRO:O	1:B:916:LYS:N	2.49	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
1	A	1115/1160 (96%)	1079 (97%)	34 (3%)	2 (0%)	47 77
1	B	1104/1160 (95%)	1064 (96%)	38 (3%)	2 (0%)	47 77
All	All	2219/2320 (96%)	2143 (97%)	72 (3%)	4 (0%)	47 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	B	921	THR
1	B	1024	GLU
1	A	914	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	967/1061 (91%)	800 (83%)	167 (17%)	2 8
1	B	925/1061 (87%)	767 (83%)	158 (17%)	2 8
All	All	1892/2122 (89%)	1567 (83%)	325 (17%)	2 8

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	VAL
1	A	10	SER
1	A	15	THR
1	A	16	SER
1	A	19	ARG
1	A	23	SER
1	A	24	GLU
1	A	31	ASP
1	A	38	LEU
1	A	41	ARG
1	A	43	ASP
1	A	44	MSE
1	A	46	ILE
1	A	53	GLU
1	A	55	LYS
1	A	75	LEU
1	A	76	LYS
1	A	82	LEU
1	A	87	LYS
1	A	94	TYR
1	A	97	THR
1	A	109	ASN
1	A	113	LEU
1	A	126	GLU
1	A	131	ARG
1	A	149	GLU
1	A	150	LYS
1	A	151	ASN
1	A	157	LYS
1	A	163	ILE
1	A	165	LYS
1	A	181	GLU
1	A	185	ARG

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Mol	Chain	Res	Type
1	A	199	LEU
1	A	210	LEU
1	A	211	GLU
1	A	214	ASN
1	A	215	LEU
1	A	216	THR
1	A	218	LEU
1	A	233	ARG
1	A	234	LYS
1	A	238	GLU
1	A	249	GLN
1	A	253	ASN
1	A	254	MSE
1	A	260	LYS
1	A	264	MSE
1	A	268	LYS
1	A	270	SER
1	A	280	LYS
1	A	283	LEU
1	A	284	ASN
1	A	286	LYS
1	A	310	LYS
1	A	311	ARG
1	A	318	ASP
1	A	319	LYS
1	A	323	ILE
1	A	341	LEU
1	A	368	ARG
1	A	394	LEU
1	A	397	GLU
1	A	407	ARG
1	A	410	THR
1	A	436	GLU
1	A	438	LYS
1	A	439	GLU
1	A	448	ASP
1	A	450	ASN
1	A	472	ARG
1	A	480	LEU
1	A	483	GLU
1	A	493	ILE
1	A	500	LYS

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Mol	Chain	Res	Type
1	A	507	ILE
1	A	511	LYS
1	A	514	LEU
1	A	527	ARG
1	A	529	LEU
1	A	542	ARG
1	A	546	VAL
1	A	548	LYS
1	A	557	THR
1	A	559	LEU
1	A	562	ARG
1	A	582	ASP
1	A	583	ASN
1	A	597	LYS
1	A	598	ASN
1	A	612	ASN
1	A	625	LEU
1	A	645	ASP
1	A	652	LYS
1	A	695	ASN
1	A	696	ASN
1	A	699	LEU
1	A	710	THR
1	A	712	THR
1	A	714	LEU
1	A	716	GLU
1	A	719	GLN
1	A	731	ASN
1	A	734	ILE
1	A	739	GLU
1	A	748	LYS
1	A	753	LEU
1	A	758	ARG
1	A	768	LEU
1	A	770	ASN
1	A	771	HIS
1	A	776	ASN
1	A	786	SER
1	A	788	ASN
1	A	791	GLU
1	A	796	GLN
1	A	802	LEU

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Mol	Chain	Res	Type
1	A	809	ARG
1	A	813	ASP
1	A	825	LEU
1	A	830	ASN
1	A	832	VAL
1	A	833	LYS
1	A	834	ASP
1	A	835	ASN
1	A	836	LYS
1	A	838	LEU
1	A	840	LYS
1	A	845	LYS
1	A	846	ILE
1	A	851	GLU
1	A	855	LYS
1	A	862	ILE
1	A	863	LYS
1	A	871	LEU
1	A	876	ASP
1	A	884	ILE
1	A	903	MSE
1	A	915	ARG
1	A	920	PHE
1	A	923	GLU
1	A	941	LEU
1	A	951	ASN
1	A	962	HIS
1	A	987	GLN
1	A	989	ILE
1	A	990	GLU
1	A	1019	LEU
1	A	1020	HIS
1	A	1057	ILE
1	A	1058	PRO
1	A	1070	ASN
1	A	1083	ASN
1	A	1087	LYS
1	A	1103	LYS
1	A	1107	ASP
1	A	1115	LEU
1	A	1116	GLU
1	A	1117	SER

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Mol	Chain	Res	Type
1	A	1123	LEU
1	A	1125	ASN
1	A	1126	LEU
1	A	1130	LYS
1	A	1131	LEU
1	A	1133	THR
1	A	1143	LEU
1	B	2	LYS
1	B	3	VAL
1	B	5	LYS
1	B	10	SER
1	B	13	LYS
1	B	15	THR
1	B	19	ARG
1	B	24	GLU
1	B	25	SER
1	B	26	GLU
1	B	30	THR
1	B	33	ARG
1	B	43	ASP
1	B	59	LYS
1	B	60	ARG
1	B	61	ILE
1	B	70	ASN
1	B	75	LEU
1	B	84	ASN
1	B	87	LYS
1	B	90	ILE
1	B	92	ARG
1	B	113	LEU
1	B	118	LEU
1	B	131	ARG
1	B	149	GLU
1	B	152	LYS
1	B	157	LYS
1	B	161	ASN
1	B	163	ILE
1	B	181	GLU
1	B	208	LEU
1	B	211	GLU
1	B	214	ASN
1	B	215	LEU

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Mol	Chain	Res	Type
1	B	216	THR
1	B	218	LEU
1	B	221	TYR
1	B	233	ARG
1	B	243	ILE
1	B	249	GLN
1	B	257	LEU
1	B	263	ASP
1	B	280	LYS
1	B	287	ASN
1	B	288	ILE
1	B	310	LYS
1	B	311	ARG
1	B	318	ASP
1	B	323	ILE
1	B	334	GLU
1	B	336	LYS
1	B	355	LEU
1	B	356	GLN
1	B	359	GLU
1	B	394	LEU
1	B	395	GLU
1	B	400	ASN
1	B	402	ILE
1	B	405	ARG
1	B	412	LYS
1	B	427	LYS
1	B	438	LYS
1	B	439	GLU
1	B	443	MSE
1	B	448	ASP
1	B	461	PHE
1	B	472	ARG
1	B	475	ILE
1	B	485	LYS
1	B	487	ILE
1	B	499	SER
1	B	501	LYS
1	B	504	GLN
1	B	506	GLU
1	B	511	LYS
1	B	514	LEU

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Mol	Chain	Res	Type
1	B	527	ARG
1	B	529	LEU
1	B	540	ARG
1	B	541	THR
1	B	542	ARG
1	B	546	VAL
1	B	548	LYS
1	B	550	ILE
1	B	557	THR
1	B	559	LEU
1	B	562	ARG
1	B	579	THR
1	B	582	ASP
1	B	583	ASN
1	B	599	ILE
1	B	603	GLU
1	B	608	PHE
1	B	610	SER
1	B	611	ASN
1	B	626	ASN
1	B	676	THR
1	B	704	ILE
1	B	710	THR
1	B	714	LEU
1	B	719	GLN
1	B	722	ASP
1	B	727	LYS
1	B	733	ASN
1	B	734	ILE
1	B	735	LYS
1	B	738	TYR
1	B	740	ILE
1	B	744	LEU
1	B	748	LYS
1	B	753	LEU
1	B	754	LYS
1	B	758	ARG
1	B	759	LEU
1	B	761	MSE
1	B	768	LEU
1	B	770	ASN
1	B	771	HIS

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Mol	Chain	Res	Type
1	B	799	LEU
1	B	802	LEU
1	B	809	ARG
1	B	825	LEU
1	B	833	LYS
1	B	834	ASP
1	B	838	LEU
1	B	843	THR
1	B	844	ASN
1	B	845	LYS
1	B	848	PHE
1	B	855	LYS
1	B	856	HIS
1	B	881	LYS
1	B	885	GLU
1	B	889	LYS
1	B	907	LEU
1	B	909	ARG
1	B	915	ARG
1	B	920	PHE
1	B	925	TYR
1	B	927	SER
1	B	987	GLN
1	B	989	ILE
1	B	991	GLU
1	B	997	ASN
1	B	1004	LYS
1	B	1007	GLN
1	B	1020	HIS
1	B	1029	LYS
1	B	1040	GLN
1	B	1042	LYS
1	B	1101	THR
1	B	1103	LYS
1	B	1115	LEU
1	B	1116	GLU
1	B	1125	ASN
1	B	1139	GLU
1	B	1143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	173	ASN
1	A	249	GLN
1	A	271	GLN
1	A	294	HIS
1	A	378	ASN
1	A	583	ASN
1	A	659	GLN
1	A	695	ASN
1	A	719	GLN
1	A	731	ASN
1	A	776	ASN
1	A	785	GLN
1	A	796	GLN
1	A	828	ASN
1	A	830	ASN
1	A	856	HIS
1	A	904	GLN
1	A	908	HIS
1	A	934	ASN
1	A	943	ASN
1	A	951	ASN
1	A	962	HIS
1	A	1070	ASN
1	A	1083	ASN
1	A	1125	ASN
1	A	1136	ASN
1	B	57	ASN
1	B	70	ASN
1	B	84	ASN
1	B	142	ASN
1	B	151	ASN
1	B	214	ASN
1	B	228	HIS
1	B	249	GLN
1	B	271	GLN
1	B	287	ASN
1	B	306	ASN
1	B	398	ASN
1	B	453	ASN
1	B	549	ASN
1	B	626	ASN
1	B	682	GLN

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Mol	Chain	Res	Type
1	B	760	ASN
1	B	807	ASN
1	B	808	ASN
1	B	828	ASN
1	B	861	ASN
1	B	892	ASN
1	B	908	HIS
1	B	943	ASN
1	B	962	HIS
1	B	997	ASN
1	B	1136	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	58/59 (98%)	26 (44%)	5 (8%)
2	E	57/59 (96%)	22 (38%)	4 (7%)
3	D	29/30 (96%)	10 (34%)	0
3	F	28/30 (93%)	10 (35%)	2 (7%)
All	All	172/178 (96%)	68 (39%)	11 (6%)

All (68) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	C
2	C	4	C
2	C	5	A
2	C	7	C
2	C	8	C
2	C	11	A
2	C	13	A
2	C	14	A
2	C	15	U
2	C	16	G
2	C	17	A
2	C	20	G
2	C	22	G
2	C	23	A
2	C	24	C
2	C	25	U
2	C	26	A

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Mol	Chain	Res	Type
2	C	27	A
2	C	28	A
2	C	29	A
2	C	30	C
2	C	31	A
2	C	32	C
2	C	33	A
2	C	36	U
2	C	55	C
3	D	6	A
3	D	7	A
3	D	12	U
3	D	20	A
3	D	21	U
3	D	24	A
3	D	25	U
3	D	28	G
3	D	29	U
3	D	30	C
2	E	2	A
2	E	5	A
2	E	7	C
2	E	14	A
2	E	15	U
2	E	16	G
2	E	17	A
2	E	18	A
2	E	20	G
2	E	22	G
2	E	23	A
2	E	24	C
2	E	25	U
2	E	26	A
2	E	27	A
2	E	28	A
2	E	29	A
2	E	30	C
2	E	31	A
2	E	32	C
2	E	33	A
2	E	36	U
3	F	2	G

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Mol	Chain	Res	Type
3	F	4	A
3	F	5	G
3	F	6	A
3	F	13	U
3	F	20	A
3	F	21	U
3	F	24	A
3	F	25	U
3	F	28	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1	G
2	C	10	A
2	C	14	A
2	C	24	C
2	C	30	C
2	E	24	C
2	E	30	C
2	E	31	A
2	E	32	C
3	F	2	G
3	F	4	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	1104/1160 (95%)	-0.30	11 (0%)	82	66	17, 43, 82, 138	0
1	B	1093/1160 (94%)	-0.17	28 (2%)	56	31	20, 51, 113, 149	0
2	C	58/59 (98%)	-0.49	0	100	100	22, 36, 68, 81	0
2	E	58/59 (98%)	-0.55	0	100	100	29, 43, 82, 92	0
3	D	30/30 (100%)	-0.53	0	100	100	26, 36, 75, 105	0
3	F	29/30 (96%)	-0.63	0	100	100	30, 40, 82, 122	0
All	All	2372/2498 (94%)	-0.26	39 (1%)	72	51	17, 46, 98, 149	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	574	TRP	10.1
1	B	563	ILE	6.8
1	A	49	PRO	6.7
1	B	675	ASP	6.4
1	B	665	ASN	6.0
1	B	575	LYS	5.5
1	A	50	SER	4.6
1	B	680	PHE	4.6
1	B	113	LEU	4.5
1	B	61	ILE	4.1
1	B	130	PHE	3.8
1	B	564	ASP	3.8
1	B	566	LEU	3.6
1	B	49	PRO	3.6
1	A	675	ASP	3.6
1	B	216	THR	3.4
1	B	562	ARG	3.1
1	A	686	LEU	3.0
1	B	42	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	413	ASN	3.0
1	B	162	ASN	2.9
1	B	678	ILE	2.9
1	B	109	ASN	2.7
1	A	667	GLY	2.6
1	B	677	TYR	2.5
1	B	560	TYR	2.4
1	A	566	LEU	2.4
1	B	577	PRO	2.3
1	B	134	ILE	2.3
1	B	413	ASN	2.3
1	A	574	TRP	2.2
1	B	545	PHE	2.2
1	B	52	THR	2.2
1	A	887	LEU	2.1
1	A	399	GLU	2.1
1	B	701	LEU	2.1
1	B	92	ARG	2.0
1	B	50	SER	2.0
1	A	662	TYR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.