Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:33 AM GMT

PDB ID	:	2R7X
Title	:	Crystal Structure of Rotavirus SA11 VP1/RNA (UGUGACC)/GTP complex
Authors	:	Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on	:	2007-09-10
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

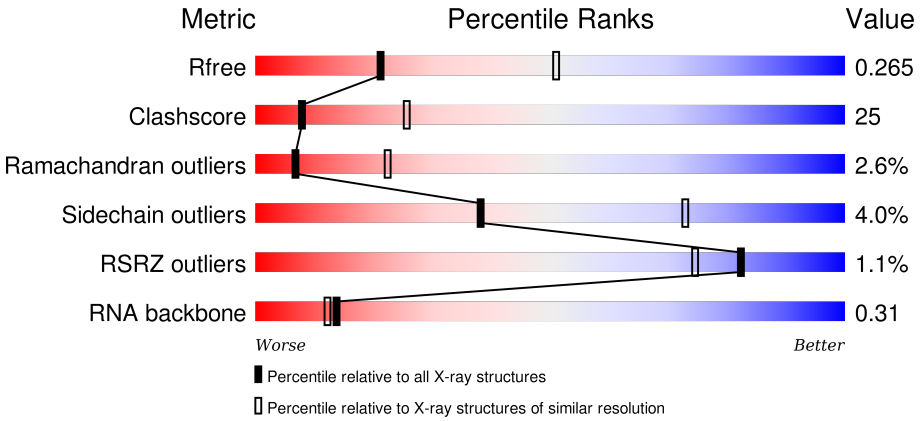
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	X	7	29% 71%
1	Y	7	29% 71%
2	A	1095	% 53% 41%
2	B	1095	% 52% 42%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GTP	A	1111	-	-	-	X
3	GTP	B	1111	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

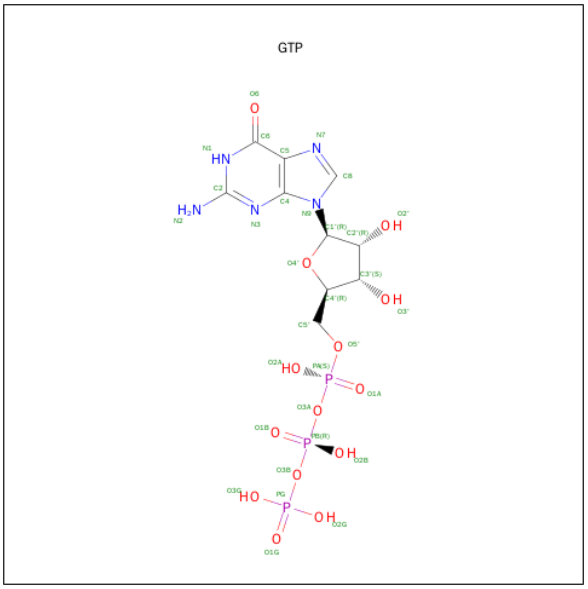
- Molecule 1 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	7	Total	C	N	O	P	0	0	0
			145	66	25	48	6			
1	Y	7	Total	C	N	O	P	0	0	0
			145	66	25	48	6			

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1073	Total	C	N	O	S	0	0	0
			8695	5576	1447	1634	38			
2	B	1073	Total	C	N	O	S	0	0	0
			8695	5576	1447	1634	38			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3')

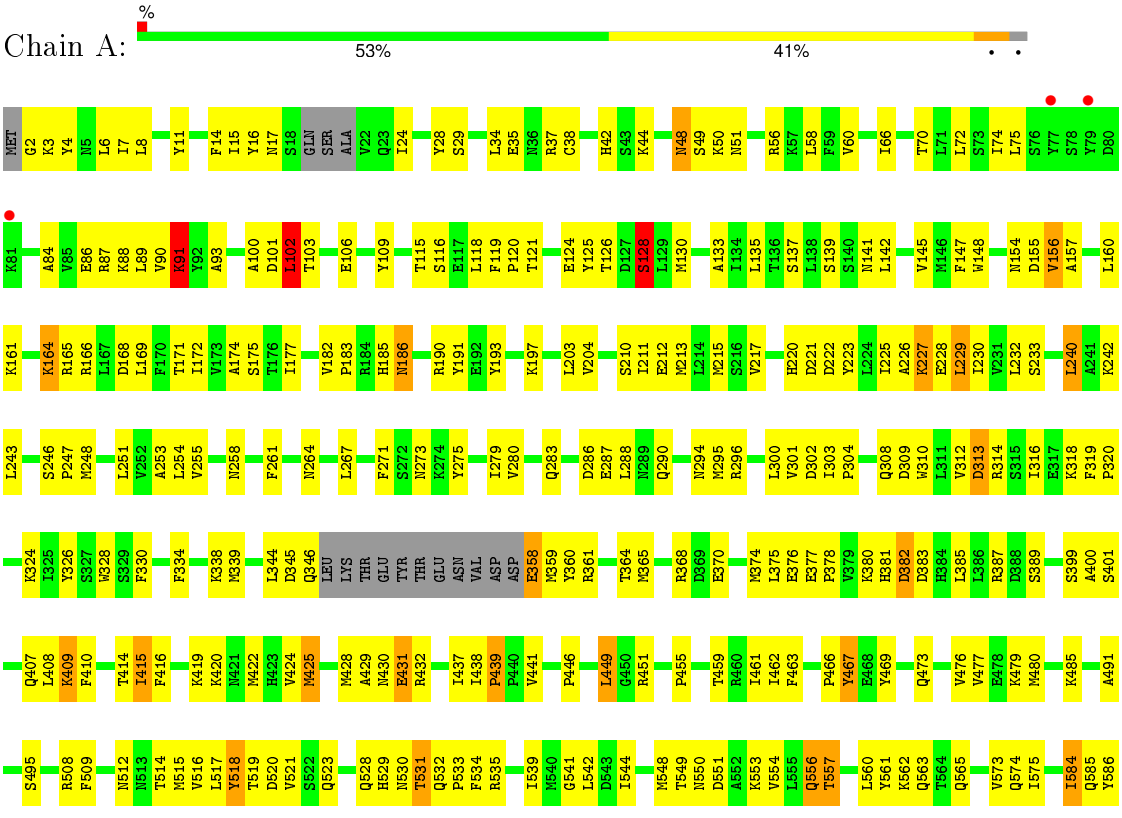
Chain X:

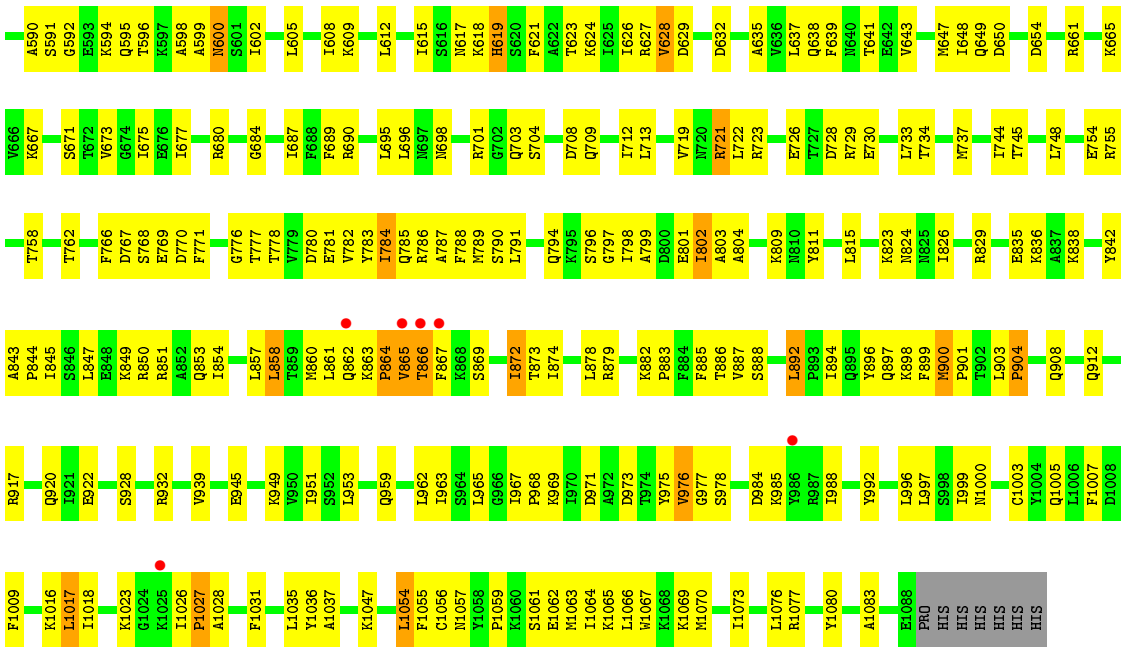
- Molecule 1: RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3')

Chain Y:

- Molecule 2: RNA-dependent RNA polymerase

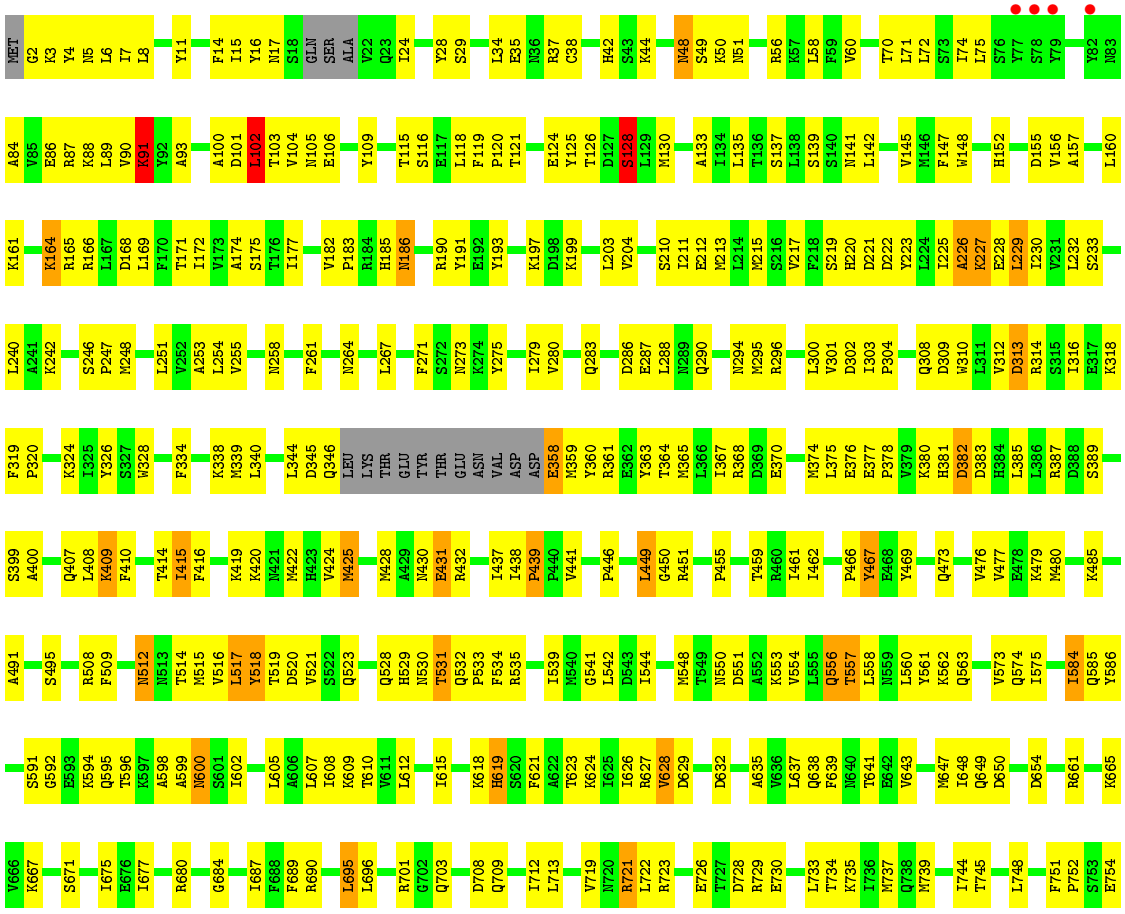
Chain A:

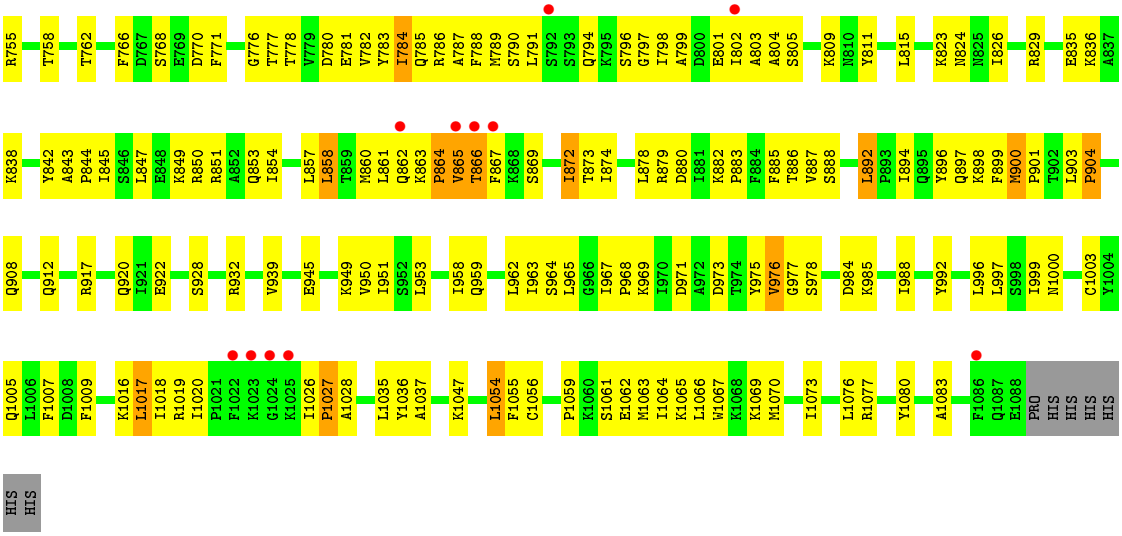




• Molecule 2: RNA-dependent RNA polymerase

Chain B:




R755 T758 T762 F766 D767 S768 E769 D770 F771 G776 T777 T778 V779 D780 E781 V782 Y783 I784 Q785 R786 A787 F788 M789 S790 L791 S792 S793 Q794 K795 S796 G797 I798 A799 D800 E801 I802 A803 A804 S805 K809 N810 Y811 L815 K823 N824 N825 I826 R829 E835 K836 A837
K838 Y842 A843 P844 I845 S846 L847 E848 K849 R850 R851 A852 Q853 I854 L857 L858 T859 M860 L861 Q862 K863 P864 V865 T866 F867 K868 S869 I872 T873 I874 L878 R879 D880 I881 K882 P883 F884 F885 T886 V887 S888 L892 P893 I894 Q895 Y896 Q897 K898 F899 M900 P901 T902 L903 P904
Q908 Q912 R917 Q920 I921 E922 S928 R932 V939 E945 K949 V950 I951 S952 L953 I958 Q959 L962 I963 S964 L965 G966 I967 P968 K969 I970 D971 A972 D973 T974 Y975 V976 G977 S978 D984 K985 I988 Y992 L996 L997 S998 I999 N1000 C1003 Y1004
Q1005 L1006 F1007 D1008 F1009 K1016 L1017 I1018 R1019 I1020 P1021 F1022 K1023 G1024 K1025 I1026 P1027 A1028 L1035 Y1036 A1037 K1047 L1054 F1055 C1056 P1059 K1060 S1061 E1062 M1063 I1064 K1065 L1066 W1067 K1068 K1069 M1070 I1073 L1076 R1077 Y1080 A1083 F1086 Q1087 E1088 PRO HIS HIS HIS HIS
HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.00Å 143.77Å 112.83Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 35.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.1 (30.00-2.80) 80.7 (35.94-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.277 0.224 , 0.265	Depositor DCC
R_{free} test set	4650 reflections (10.20%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 17.5	EDS
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 57725 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	X	0.52	0/161	0.97	0/249
1	Y	0.46	0/161	0.96	0/249
2	A	0.41	0/8866	0.63	0/11985
2	B	0.40	0/8866	0.62	0/11985
All	All	0.41	0/18054	0.63	0/24468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	X	145	0	77	16	0
1	Y	145	0	77	16	0
2	A	8695	0	8782	433	0
2	B	8695	0	8782	436	0
3	A	32	0	12	2	0
3	B	32	0	12	2	0
All	All	17744	0	17742	884	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 25.

All (884) 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)
2:A:865:VAL:HG13	2:A:866:THR:H	1.14	1.08
2:B:865:VAL:HG13	2:B:866:THR:H	1.14	1.08
2:B:520:ASP:HB3	2:B:667:LYS:HG2	1.45	0.98
2:A:520:ASP:HB3	2:A:667:LYS:HG2	1.46	0.97
2:B:186:ASN:ND2	2:B:190:ARG:H	1.65	0.95
2:A:186:ASN:ND2	2:A:190:ARG:H	1.67	0.93
1:X:1105:A:H5'	2:A:400:ALA:HB1	1.50	0.92
2:B:556:GLN:HA	2:B:556:GLN:HE21	1.36	0.90
2:A:556:GLN:HE21	2:A:556:GLN:HA	1.37	0.89
1:Y:1105:A:H5'	2:B:400:ALA:HB1	1.56	0.87
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.74	0.86
2:B:177:ILE:HD13	2:B:203:LEU:HD11	1.56	0.86
2:B:283:GLN:OE1	2:B:649:GLN:HG3	1.75	0.85
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.57	0.84
2:A:689:PHE:HB3	2:A:723:ARG:NH1	1.92	0.84
2:B:420:LYS:O	2:B:424:VAL:HG23	1.79	0.82
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.15	0.81
2:B:689:PHE:HB3	2:B:723:ARG:NH1	1.94	0.81
2:B:161:LYS:O	2:B:165:ARG:HG3	1.82	0.80
2:A:161:LYS:O	2:A:165:ARG:HG3	1.83	0.79
2:A:286:ASP:O	2:A:290:GLN:HG3	1.82	0.79
2:B:461:ILE:HD11	2:B:586:TYR:CZ	2.17	0.79
2:A:865:VAL:HG13	2:A:866:THR:N	1.95	0.79
2:B:865:VAL:HG13	2:B:866:THR:N	1.96	0.79
2:A:8:LEU:HD23	2:A:74:ILE:HD12	1.64	0.79
2:A:420:LYS:O	2:A:424:VAL:HG23	1.83	0.78
2:B:887:VAL:HG22	2:B:1054:LEU:HD11	1.64	0.78
2:B:286:ASP:O	2:B:290:GLN:HG3	1.84	0.78
2:B:120:PRO:HD2	2:B:124:GLU:OE2	1.83	0.77
2:A:120:PRO:HD2	2:A:124:GLU:OE2	1.83	0.77
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.65	0.77
2:A:477:VAL:HA	2:A:480:MET:CE	2.15	0.76
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.67	0.76
2:B:186:ASN:HD21	2:B:190:ARG:H	1.33	0.76
2:B:316:ILE:HD13	2:B:684:GLY:HA3	1.68	0.76
2:B:135:LEU:HD13	2:B:709:GLN:HE22	1.51	0.76
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.67	0.75
2:B:428:MET:HE1	2:B:811:TYR:HD1	1.52	0.75
2:B:8:LEU:HD23	2:B:74:ILE:HD12	1.68	0.75
2:A:598:ALA:O	2:A:602:ILE:HG13	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:VAL:HA	2:B:480:MET:CE	2.17	0.75
2:B:744:ILE:HG22	2:B:745:THR:HG23	1.69	0.74
2:B:254:LEU:HD23	2:B:280:VAL:HG21	1.67	0.74
2:B:312:VAL:HG23	2:B:313:ASP:OD2	1.86	0.74
2:A:87:ARG:O	2:A:90:VAL:HG22	1.88	0.73
2:B:165:ARG:HE	2:B:220:HIS:HA	1.53	0.73
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.70	0.73
2:A:190:ARG:HG2	2:A:701:ARG:NH2	2.04	0.73
2:B:190:ARG:HG2	2:B:701:ARG:NH2	2.04	0.72
2:A:135:LEU:HD13	2:A:709:GLN:HE22	1.55	0.72
2:A:316:ILE:HD13	2:A:684:GLY:HA3	1.71	0.72
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.55	0.72
2:A:66:ILE:CG2	2:B:894:ILE:HD11	2.19	0.72
2:A:312:VAL:HG23	2:A:313:ASP:OD2	1.88	0.72
2:A:165:ARG:HE	2:A:220:HIS:HA	1.54	0.72
2:A:186:ASN:HD21	2:A:190:ARG:H	1.37	0.72
2:B:87:ARG:O	2:B:90:VAL:HG22	1.90	0.72
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.25	0.72
2:A:959:GLN:HE21	2:A:976:VAL:HG11	1.54	0.71
2:B:892:LEU:HD22	2:B:1017:LEU:HD11	1.71	0.71
2:B:509:PHE:CD2	2:B:624:LYS:HB3	2.25	0.71
2:A:886:THR:HG22	2:B:512:ASN:ND2	2.06	0.71
2:B:598:ALA:O	2:B:602:ILE:HG13	1.92	0.70
2:B:428:MET:CE	2:B:811:TYR:HD1	2.05	0.70
2:B:959:GLN:HE21	2:B:976:VAL:HG11	1.55	0.70
1:X:1105:A:H5'	2:A:400:ALA:CB	2.21	0.70
2:B:44:LYS:HB3	2:B:58:LEU:HD21	1.74	0.70
2:A:324:LYS:O	2:A:328:TRP:HD1	1.75	0.69
2:B:473:GLN:HG2	2:B:561:TYR:CE1	2.26	0.69
2:B:50:LYS:HG2	2:B:50:LYS:O	1.91	0.69
2:A:968:PRO:HG2	2:A:971:ASP:OD2	1.92	0.69
2:A:44:LYS:HB3	2:A:58:LEU:HD21	1.75	0.68
2:A:66:ILE:HG21	2:B:894:ILE:HD11	1.75	0.68
2:B:419:LYS:HB2	2:B:422:MET:HG3	1.74	0.68
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.28	0.68
2:A:102:LEU:H	2:A:102:LEU:HD22	1.59	0.68
2:B:865:VAL:CG1	2:B:866:THR:H	1.97	0.68
1:Y:1105:A:H5'	2:B:400:ALA:CB	2.23	0.68
2:B:789:MET:HE1	2:B:873:THR:HG21	1.74	0.68
2:B:324:LYS:O	2:B:328:TRP:HD1	1.77	0.67
2:B:102:LEU:H	2:B:102:LEU:HD22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:865:VAL:CG1	2:A:866:THR:H	1.97	0.67
2:A:951:ILE:HG12	2:A:985:LYS:HA	1.76	0.67
2:B:295:MET:O	2:B:300:LEU:HB2	1.94	0.67
2:A:428:MET:CE	2:A:811:TYR:HD1	2.08	0.67
2:A:532:GLN:HB2	2:A:533:PRO:HD3	1.77	0.67
2:A:155:ASP:O	2:A:160:LEU:HD13	1.95	0.67
2:A:975:TYR:O	2:A:977:GLY:N	2.28	0.67
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.76	0.67
2:A:409:LYS:HG3	2:A:414:THR:HG22	1.77	0.67
2:A:370:GLU:HG2	2:A:602:ILE:HG23	1.77	0.66
2:B:975:TYR:O	2:B:977:GLY:N	2.29	0.66
2:B:141:ASN:O	2:B:145:VAL:HG23	1.95	0.66
2:A:477:VAL:HA	2:A:480:MET:HE3	1.77	0.66
2:A:50:LYS:O	2:A:50:LYS:HG2	1.94	0.66
2:B:968:PRO:HG2	2:B:971:ASP:OD2	1.96	0.66
2:B:778:THR:O	2:B:782:VAL:HG23	1.95	0.66
2:A:963:ILE:HD11	2:A:969:LYS:HG2	1.78	0.66
2:A:309:ASP:O	2:A:312:VAL:HG22	1.96	0.66
2:B:951:ILE:HG12	2:B:985:LYS:HA	1.77	0.65
2:B:744:ILE:HB	2:B:748:LEU:HD22	1.77	0.65
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.31	0.65
2:B:409:LYS:HG3	2:B:414:THR:HG22	1.79	0.65
2:B:370:GLU:HG2	2:B:602:ILE:HG23	1.78	0.65
2:A:514:THR:HG22	2:A:638:GLN:HG3	1.77	0.65
2:A:361:ARG:O	2:A:365:MET:HG2	1.97	0.65
2:A:377:GLU:HB2	2:A:378:PRO:HD3	1.78	0.65
2:A:477:VAL:HG21	2:A:594:LYS:HG3	1.78	0.65
2:A:473:GLN:OE1	2:A:595:GLN:HG2	1.95	0.65
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.79	0.65
2:B:477:VAL:HG21	2:B:594:LYS:HG3	1.77	0.65
2:B:462:ILE:HG23	2:B:591:SER:O	1.97	0.65
2:B:477:VAL:HA	2:B:480:MET:HE3	1.78	0.65
2:A:296:ARG:HH22	2:A:308:GLN:HE22	1.43	0.65
2:B:532:GLN:HB2	2:B:533:PRO:HD3	1.79	0.65
2:B:963:ILE:HD11	2:B:969:LYS:HG2	1.78	0.65
2:B:155:ASP:O	2:B:160:LEU:HD13	1.97	0.65
2:B:687:ILE:HG23	2:B:900:MET:HG3	1.80	0.64
2:B:361:ARG:O	2:B:365:MET:HG2	1.97	0.64
2:A:135:LEU:HD22	2:A:709:GLN:HE21	1.63	0.64
2:B:898:LYS:HD3	2:B:908:GLN:HG2	1.79	0.64
2:B:296:ARG:HH22	2:B:308:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:477:VAL:HA	2:A:480:MET:HE2	1.79	0.64
2:A:898:LYS:HD3	2:A:908:GLN:HG2	1.79	0.64
2:A:744:ILE:HB	2:A:748:LEU:HD22	1.79	0.64
2:B:473:GLN:OE1	2:B:595:GLN:HG2	1.97	0.64
1:Y:1106:C:H5'	1:Y:1107:C:OP2	1.98	0.64
2:B:253:ALA:HB1	2:B:671:SER:HB2	1.78	0.64
2:A:319:PHE:N	2:A:320:PRO:CD	2.61	0.64
2:B:539:ILE:HG23	2:B:562:LYS:HG3	1.80	0.63
2:A:789:MET:HE1	2:A:873:THR:HG21	1.79	0.63
2:B:309:ASP:O	2:B:312:VAL:HG22	1.97	0.63
2:A:539:ILE:HG23	2:A:562:LYS:HG3	1.80	0.63
2:A:126:THR:OG1	2:A:128:SER:HB3	1.98	0.63
2:B:377:GLU:HB2	2:B:378:PRO:HD3	1.80	0.63
2:A:141:ASN:O	2:A:145:VAL:HG23	1.98	0.63
2:B:319:PHE:N	2:B:320:PRO:CD	2.62	0.63
2:B:191:TYR:CE2	2:B:204:VAL:HG11	2.33	0.63
2:A:90:VAL:HG23	2:A:91:LYS:H	1.64	0.63
2:A:528:GLN:O	2:A:531:THR:HG22	1.98	0.63
2:B:528:GLN:O	2:B:531:THR:HG22	1.98	0.63
2:B:126:THR:OG1	2:B:128:SER:HB3	1.98	0.63
2:A:462:ILE:HG23	2:A:591:SER:O	1.99	0.63
2:B:1059:PRO:O	2:B:1063:MET:HG3	1.98	0.63
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.80	0.63
2:B:687:ILE:CG2	2:B:900:MET:HG3	2.29	0.63
2:A:3:LYS:O	2:A:7:ILE:HG12	1.99	0.63
2:B:90:VAL:HG23	2:B:91:LYS:H	1.64	0.62
2:A:6:LEU:HD22	2:A:6:LEU:N	2.14	0.62
2:B:477:VAL:HA	2:B:480:MET:HE2	1.81	0.62
2:B:253:ALA:CB	2:B:671:SER:HB2	2.29	0.62
2:A:623:THR:CG2	2:A:626:ILE:HG13	2.29	0.62
2:B:514:THR:HG22	2:B:638:GLN:HG3	1.81	0.62
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.99	0.62
2:B:84:ALA:O	2:B:88:LYS:HG3	1.98	0.62
2:B:962:LEU:O	2:B:967:ILE:HB	2.00	0.62
2:A:137:SER:HB2	2:A:185:HIS:CD2	2.35	0.62
1:X:1106:C:H5'	1:X:1107:C:OP2	2.00	0.62
2:B:279:ILE:HG22	2:B:648:ILE:HD12	1.82	0.62
2:A:253:ALA:CB	2:A:671:SER:HB2	2.30	0.62
2:B:618:LYS:HD2	2:B:654:ASP:OD2	2.00	0.62
2:B:734:THR:HA	2:B:737:MET:HE3	1.82	0.61
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:687:ILE:CG2	2:A:900:MET:HG3	2.30	0.61
2:A:242:LYS:O	2:A:246:SER:HB2	2.00	0.61
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.82	0.61
2:A:295:MET:O	2:A:300:LEU:HB2	2.00	0.61
2:A:618:LYS:HD2	2:A:654:ASP:OD2	2.01	0.61
2:B:3:LYS:O	2:B:7:ILE:HG12	2.01	0.61
2:B:777:THR:HG21	2:B:882:LYS:HE3	1.82	0.61
2:A:623:THR:HG21	2:A:626:ILE:HG13	1.82	0.61
2:A:449:LEU:HD22	2:A:573:VAL:HG13	1.83	0.61
2:B:6:LEU:HD22	2:B:6:LEU:N	2.16	0.61
2:B:115:THR:HB	2:B:197:LYS:HA	1.80	0.61
2:A:84:ALA:O	2:A:88:LYS:HG3	2.00	0.61
2:A:784:ILE:HD12	2:A:788:PHE:CE2	2.35	0.61
2:B:784:ILE:HD12	2:B:788:PHE:CE2	2.35	0.61
2:B:623:THR:CG2	2:B:626:ILE:HG13	2.31	0.61
2:B:86:GLU:OE2	2:B:182:VAL:HB	2.00	0.61
2:A:708:ASP:O	2:A:712:ILE:HG13	2.01	0.61
2:B:169:LEU:HD21	2:B:227:LYS:HB2	1.83	0.60
2:B:520:ASP:HB2	2:B:667:LYS:HE2	1.83	0.60
2:A:962:LEU:O	2:A:967:ILE:HB	2.02	0.60
2:B:11:TYR:HA	2:B:147:PHE:CE1	2.36	0.60
2:B:261:PHE:CD2	2:B:899:PHE:HB3	2.36	0.60
2:A:627:ARG:HG2	2:A:627:ARG:HH11	1.66	0.60
2:B:556:GLN:HA	2:B:556:GLN:NE2	2.12	0.60
2:B:887:VAL:HG22	2:B:1054:LEU:CD1	2.31	0.60
1:Y:1105:A:C5'	2:B:400:ALA:HB1	2.32	0.60
2:B:885:PHE:CE1	2:B:1056:CYS:HB2	2.37	0.60
2:A:796:SER:HB2	2:A:849:LYS:HE3	1.84	0.60
1:Y:1101:U:O4	2:B:415:ILE:HG13	2.02	0.59
2:A:778:THR:O	2:A:782:VAL:HG23	2.01	0.59
2:B:137:SER:HB2	2:B:185:HIS:CD2	2.38	0.59
2:B:485:LYS:HE2	2:B:495:SER:HA	1.84	0.59
2:A:446:PRO:HB2	2:A:574:GLN:HG3	1.83	0.59
2:B:449:LEU:CD1	2:B:573:VAL:HG22	2.32	0.59
2:B:449:LEU:HD22	2:B:573:VAL:HG13	1.85	0.59
2:A:56:ARG:O	2:A:60:VAL:HG23	2.02	0.59
2:B:312:VAL:HG23	2:B:313:ASP:H	1.68	0.59
2:B:449:LEU:HD11	2:B:573:VAL:HG22	1.84	0.59
2:B:242:LYS:O	2:B:246:SER:HB2	2.03	0.59
2:A:86:GLU:OE2	2:A:182:VAL:HB	2.02	0.59
2:B:708:ASP:O	2:B:712:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:556:GLN:NE2	2:A:556:GLN:HA	2.14	0.59
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.83	0.58
2:A:11:TYR:HA	2:A:147:PHE:CE1	2.38	0.58
2:B:623:THR:HG21	2:B:626:ILE:HG13	1.84	0.58
2:A:115:THR:HB	2:A:197:LYS:HA	1.83	0.58
2:A:449:LEU:CD1	2:A:573:VAL:HG22	2.33	0.58
2:B:446:PRO:HB2	2:B:574:GLN:HG3	1.83	0.58
2:B:56:ARG:O	2:B:60:VAL:HG23	2.03	0.58
2:A:133:ALA:HB1	2:A:701:ARG:HG3	1.85	0.58
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.39	0.58
2:B:591:SER:HB2	2:B:596:THR:HG21	1.86	0.58
2:B:794:GLN:HG2	2:B:853:GLN:OE1	2.03	0.58
2:B:798:ILE:O	2:B:802:ILE:HG22	2.04	0.58
2:B:133:ALA:HB1	2:B:701:ARG:HG3	1.85	0.58
2:A:476:VAL:O	2:A:480:MET:HG3	2.02	0.58
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.86	0.58
2:A:449:LEU:HD11	2:A:573:VAL:HG22	1.86	0.58
2:A:383:ASP:O	2:A:387:ARG:HG3	2.04	0.58
1:X:1101:U:O4	2:A:415:ILE:HG13	2.04	0.57
2:B:530:ASN:O	2:B:533:PRO:HD2	2.04	0.57
2:A:887:VAL:HG22	2:A:1054:LEU:CD1	2.33	0.57
2:A:959:GLN:NE2	2:A:976:VAL:HG11	2.19	0.57
2:A:514:THR:CG2	2:A:638:GLN:HG3	2.34	0.57
2:B:627:ARG:HG2	2:B:627:ARG:HH11	1.69	0.57
2:B:882:LYS:HB3	2:B:883:PRO:HD3	1.85	0.57
2:B:135:LEU:HD22	2:B:709:GLN:HE21	1.69	0.57
2:B:14:PHE:CE2	2:B:147:PHE:HB2	2.40	0.57
2:A:621:PHE:CE1	2:A:637:LEU:HD13	2.40	0.57
2:B:796:SER:HB2	2:B:849:LYS:HE3	1.87	0.57
2:A:407:GLN:HE22	2:A:416:PHE:HB3	1.70	0.57
2:A:296:ARG:HH22	2:A:308:GLN:NE2	2.02	0.57
2:A:520:ASP:HB2	2:A:667:LYS:HE2	1.86	0.57
2:A:530:ASN:O	2:A:533:PRO:HD2	2.05	0.57
2:B:860:MET:HE1	2:B:864:PRO:HA	1.86	0.57
2:B:605:LEU:HD11	2:B:609:LYS:HE3	1.86	0.57
2:A:485:LYS:HE2	2:A:495:SER:HA	1.86	0.57
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.40	0.57
2:A:605:LEU:HD11	2:A:609:LYS:HE3	1.86	0.57
1:X:1105:A:C5'	2:A:400:ALA:HB1	2.28	0.57
2:B:959:GLN:NE2	2:B:976:VAL:HG11	2.20	0.57
2:B:862:GLN:O	2:B:863:LYS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:156:VAL:HG23	2:A:157:ALA:N	2.20	0.57
2:A:798:ILE:O	2:A:802:ILE:HG22	2.05	0.57
2:B:383:ASP:O	2:B:387:ARG:HG3	2.05	0.57
2:A:407:GLN:NE2	2:A:416:PHE:HB3	2.20	0.56
2:B:928:SER:O	2:B:932:ARG:HG3	2.04	0.56
2:B:894:ILE:O	2:B:894:ILE:HG13	2.05	0.56
2:B:514:THR:CG2	2:B:638:GLN:HG3	2.35	0.56
2:B:621:PHE:CE1	2:B:637:LEU:HD13	2.41	0.56
2:A:997:LEU:HD12	2:A:1035:LEU:HD21	1.87	0.56
2:A:169:LEU:HD21	2:A:227:LYS:HB2	1.87	0.56
2:A:794:GLN:HG2	2:A:853:GLN:OE1	2.05	0.56
2:A:928:SER:O	2:A:932:ARG:HG3	2.04	0.56
2:B:35:GLU:O	2:B:38:CYS:HB2	2.05	0.56
2:B:892:LEU:CD2	2:B:1017:LEU:HD11	2.36	0.56
2:A:945:GLU:HG2	2:A:992:TYR:CE1	2.39	0.56
2:A:161:LYS:O	2:A:165:ARG:NH1	2.38	0.56
2:B:476:VAL:O	2:B:480:MET:HG3	2.05	0.56
2:B:312:VAL:HG23	2:B:313:ASP:N	2.21	0.56
2:A:312:VAL:HG23	2:A:313:ASP:H	1.71	0.56
2:A:573:VAL:CG1	2:A:575:ILE:HG13	2.36	0.56
2:B:466:PRO:HD2	2:B:469:TYR:CD2	2.41	0.56
2:A:1028:ALA:HB1	2:A:1070:MET:HE3	1.88	0.56
2:B:28:TYR:HD2	2:B:72:LEU:HB2	1.70	0.56
2:B:799:ALA:HB2	2:B:845:ILE:HD13	1.88	0.56
2:A:1016:LYS:O	2:A:1018:ILE:N	2.39	0.56
2:A:154:ASN:ND2	2:B:1019:ARG:HA	2.21	0.56
2:B:148:TRP:CZ3	2:B:166:ARG:HD2	2.41	0.55
2:A:35:GLU:O	2:A:38:CYS:HB2	2.06	0.55
2:A:591:SER:HB2	2:A:596:THR:HG21	1.89	0.55
2:B:518:TYR:HD2	2:B:518:TYR:H	1.52	0.55
2:A:860:MET:HE1	2:A:864:PRO:HA	1.87	0.55
2:A:862:GLN:O	2:A:863:LYS:HB2	2.05	0.55
2:B:161:LYS:O	2:B:165:ARG:NH1	2.38	0.55
2:A:66:ILE:HG22	2:B:894:ILE:HD11	1.88	0.55
2:A:799:ALA:HB2	2:A:845:ILE:HD13	1.88	0.55
2:B:573:VAL:CG1	2:B:575:ILE:HG13	2.36	0.55
3:A:1111:GTP:O1B	3:A:1111:GTP:O3G	2.25	0.55
2:B:477:VAL:HG21	2:B:594:LYS:CG	2.36	0.55
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.70	0.55
2:B:407:GLN:NE2	2:B:416:PHE:HB3	2.22	0.55
2:B:438:ILE:HD12	2:B:563:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:PHE:HD2	2:B:899:PHE:HB3	1.71	0.55
2:B:695:LEU:HG	2:B:713:LEU:CD1	2.36	0.55
2:A:148:TRP:CZ3	2:A:166:ARG:HD2	2.42	0.55
2:B:296:ARG:HH22	2:B:308:GLN:NE2	2.05	0.55
2:B:407:GLN:HE22	2:B:416:PHE:HB3	1.72	0.55
2:A:1062:GLU:HA	2:A:1065:LYS:HD3	1.87	0.55
2:B:15:ILE:HG22	2:B:16:TYR:CD1	2.41	0.55
1:X:1103:U:O2'	1:X:1104:G:O5'	2.25	0.54
2:A:864:PRO:HA	2:A:867:PHE:HE2	1.71	0.54
2:B:945:GLU:HG2	2:B:992:TYR:CE1	2.41	0.54
2:B:1016:LYS:O	2:B:1018:ILE:N	2.39	0.54
2:B:186:ASN:HD21	2:B:190:ARG:N	2.01	0.54
2:A:477:VAL:HG21	2:A:594:LYS:CG	2.37	0.54
2:B:156:VAL:HG23	2:B:157:ALA:N	2.23	0.54
2:B:535:ARG:O	2:B:539:ILE:HG13	2.06	0.54
2:A:15:ILE:HG22	2:A:16:TYR:CD1	2.42	0.54
2:B:864:PRO:HA	2:B:867:PHE:HE2	1.72	0.54
2:B:1000:ASN:C	2:B:1005:GLN:HB3	2.28	0.54
2:B:619:HIS:ND1	2:B:619:HIS:N	2.56	0.54
2:B:165:ARG:HD3	2:B:223:TYR:CB	2.38	0.54
2:B:1062:GLU:HA	2:B:1065:LYS:HD3	1.88	0.54
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.72	0.54
2:B:399:SER:HB3	2:B:838:LYS:HB3	1.89	0.54
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.38	0.54
2:B:748:LEU:C	2:B:748:LEU:HD23	2.27	0.54
2:A:2:GLY:HA2	2:A:754:GLU:OE2	2.08	0.54
2:A:165:ARG:HD3	2:A:223:TYR:HB2	1.90	0.54
2:B:116:SER:HB3	2:B:197:LYS:HG3	1.89	0.54
2:B:2:GLY:HA2	2:B:754:GLU:OE2	2.08	0.54
2:A:703:GLN:CD	2:A:703:GLN:N	2.62	0.54
2:A:166:ARG:HD3	2:A:215:MET:SD	2.48	0.54
2:A:591:SER:HB2	2:A:596:THR:CG2	2.38	0.53
2:B:997:LEU:HD12	2:B:1035:LEU:HD21	1.90	0.53
2:B:826:ILE:O	2:B:829:ARG:HG2	2.08	0.53
2:B:385:LEU:HD23	2:B:479:LYS:HE2	1.89	0.53
2:A:992:TYR:O	2:A:996:LEU:HG	2.08	0.53
2:B:992:TYR:O	2:B:996:LEU:HG	2.08	0.53
2:A:748:LEU:C	2:A:748:LEU:HD23	2.28	0.53
2:A:28:TYR:HD2	2:A:72:LEU:HB2	1.72	0.53
2:B:11:TYR:O	2:B:14:PHE:HB3	2.09	0.53
2:A:523:GLN:HB2	2:A:665:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.90	0.53
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.90	0.53
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.38	0.53
2:A:312:VAL:HG23	2:A:313:ASP:N	2.24	0.53
2:B:523:GLN:HB2	2:B:665:LYS:O	2.08	0.53
2:A:466:PRO:HD2	2:A:469:TYR:CD2	2.44	0.53
2:A:50:LYS:NZ	2:A:50:LYS:HB2	2.23	0.53
2:B:703:GLN:CD	2:B:703:GLN:N	2.62	0.53
2:A:882:LYS:HG3	2:A:1036:TYR:OH	2.09	0.53
2:A:451:ARG:NH2	2:A:459:THR:HG21	2.24	0.53
1:Y:1103:U:O2'	1:Y:1104:G:O5'	2.27	0.53
2:A:886:THR:HG22	2:B:512:ASN:CG	2.29	0.53
2:B:835:GLU:OE1	2:B:838:LYS:HD2	2.09	0.53
2:A:437:ILE:O	2:A:439:PRO:HD3	2.09	0.53
2:B:917:ARG:HD3	2:B:1007:PHE:O	2.09	0.53
2:B:4:TYR:HD1	2:B:733:LEU:HD22	1.73	0.53
2:A:894:ILE:HG13	2:A:894:ILE:O	2.08	0.53
1:Y:1103:U:O2'	1:Y:1104:G:H5"	2.09	0.53
2:A:892:LEU:CD2	2:A:1017:LEU:HD11	2.36	0.53
2:A:879:ARG:HH11	2:A:879:ARG:HG3	1.74	0.53
2:B:632:ASP:OD2	2:B:677:ILE:HB	2.08	0.53
1:Y:1101:U:O2'	1:Y:1102:G:P	2.67	0.53
2:B:166:ARG:HD3	2:B:215:MET:SD	2.49	0.53
2:B:56:ARG:HG2	2:B:56:ARG:HH11	1.74	0.52
2:A:621:PHE:CD1	2:A:637:LEU:HD13	2.43	0.52
2:A:4:TYR:HD1	2:A:733:LEU:HD22	1.73	0.52
2:B:898:LYS:HD3	2:B:908:GLN:CG	2.39	0.52
2:A:535:ARG:O	2:A:539:ILE:HG13	2.08	0.52
2:A:826:ILE:O	2:A:829:ARG:HG2	2.09	0.52
2:B:811:TYR:CZ	2:B:815:LEU:HD11	2.45	0.52
2:B:734:THR:HA	2:B:737:MET:CE	2.39	0.52
2:B:287:GLU:HA	2:B:290:GLN:OE1	2.09	0.52
2:B:50:LYS:HB2	2:B:50:LYS:NZ	2.24	0.52
2:B:667:LYS:HG3	2:B:667:LYS:O	2.08	0.52
1:X:1101:U:O2'	1:X:1102:G:P	2.68	0.52
2:A:8:LEU:HA	2:A:737:MET:SD	2.49	0.52
2:A:1018:ILE:HD12	2:A:1037:ALA:HB1	1.90	0.52
2:A:1000:ASN:C	2:A:1005:GLN:HB3	2.30	0.52
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.90	0.52
2:A:874:ILE:O	2:A:878:LEU:HG	2.10	0.52
1:X:1102:G:H4'	1:X:1103:U:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:HD3	2:B:223:TYR:HB2	1.92	0.52
2:A:186:ASN:HD21	2:A:190:ARG:N	2.04	0.52
2:B:591:SER:HB2	2:B:596:THR:CG2	2.39	0.52
2:A:116:SER:HA	2:A:119:PHE:O	2.09	0.52
2:B:518:TYR:N	2:B:518:TYR:CD2	2.77	0.52
2:A:410:PHE:HE1	2:A:425:MET:HE2	1.74	0.52
2:A:762:THR:HA	2:A:1077:ARG:O	2.10	0.52
2:B:945:GLU:HG2	2:B:992:TYR:HE1	1.74	0.52
2:B:75:LEU:C	2:B:75:LEU:HD23	2.31	0.52
2:B:387:ARG:HA	2:B:553:LYS:HB3	1.92	0.52
2:B:882:LYS:HG3	2:B:1036:TYR:OH	2.10	0.52
2:B:794:GLN:HG2	2:B:853:GLN:CD	2.30	0.52
2:A:835:GLU:OE1	2:A:838:LYS:HD2	2.10	0.52
2:B:516:VAL:HG21	2:B:675:ILE:CG2	2.40	0.52
2:A:917:ARG:HD3	2:A:1007:PHE:O	2.10	0.52
2:B:116:SER:HA	2:B:119:PHE:O	2.09	0.51
2:B:556:GLN:HE21	2:B:556:GLN:CA	2.09	0.51
2:B:168:ASP:OD2	2:B:223:TYR:OH	2.21	0.51
2:A:116:SER:HB3	2:A:197:LYS:HG3	1.91	0.51
2:B:874:ILE:O	2:B:878:LEU:HG	2.10	0.51
2:B:879:ARG:HG3	2:B:879:ARG:HH11	1.75	0.51
2:A:619:HIS:N	2:A:619:HIS:ND1	2.59	0.51
2:A:734:THR:HA	2:A:737:MET:CE	2.41	0.51
2:B:762:THR:HA	2:B:1077:ARG:O	2.10	0.51
2:A:75:LEU:HD23	2:A:75:LEU:C	2.31	0.51
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.25	0.51
2:B:15:ILE:HG22	2:B:16:TYR:CE1	2.44	0.51
2:A:15:ILE:HG22	2:A:16:TYR:CE1	2.44	0.51
2:A:387:ARG:HA	2:A:553:LYS:HB3	1.92	0.51
2:A:794:GLN:HG2	2:A:853:GLN:CD	2.31	0.51
2:A:318:LYS:NZ	2:A:318:LYS:HB2	2.25	0.51
2:A:28:TYR:CE2	2:A:70:THR:HB	2.46	0.51
2:A:168:ASP:OD2	2:A:223:TYR:OH	2.20	0.51
2:B:375:LEU:C	2:B:378:PRO:HD2	2.31	0.51
2:A:56:ARG:HH11	2:A:56:ARG:HG2	1.76	0.51
1:X:1103:U:O2'	1:X:1104:G:H5"	2.11	0.51
2:A:811:TYR:CZ	2:A:815:LEU:HD11	2.46	0.51
2:A:776:GLY:HA3	2:A:785:GLN:NE2	2.26	0.51
2:B:776:GLY:HA3	2:B:785:GLN:NE2	2.26	0.51
2:B:621:PHE:CD1	2:B:637:LEU:HD13	2.45	0.51
2:A:11:TYR:O	2:A:14:PHE:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:ILE:O	2:B:439:PRO:HD3	2.11	0.51
2:A:287:GLU:HA	2:A:290:GLN:OE1	2.11	0.50
2:B:410:PHE:HE1	2:B:425:MET:HE2	1.76	0.50
2:B:1000:ASN:O	2:B:1005:GLN:HB3	2.11	0.50
2:B:318:LYS:HB2	2:B:318:LYS:NZ	2.25	0.50
1:Y:1103:U:O2'	1:Y:1104:G:C5'	2.59	0.50
2:A:514:THR:HG22	2:A:638:GLN:CG	2.41	0.50
2:B:387:ARG:NH1	2:B:553:LYS:HG3	2.27	0.50
2:B:553:LYS:O	2:B:557:THR:HG23	2.11	0.50
2:B:514:THR:HG22	2:B:638:GLN:CB	2.41	0.50
2:B:29:SER:OG	2:B:34:LEU:HD23	2.11	0.50
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.42	0.50
2:A:898:LYS:HD3	2:A:908:GLN:CG	2.41	0.50
2:A:553:LYS:O	2:A:557:THR:HG23	2.11	0.50
2:A:518:TYR:N	2:A:518:TYR:CD2	2.79	0.50
2:B:8:LEU:HD13	2:B:737:MET:HG2	1.93	0.50
2:B:248:MET:HG2	2:B:326:TYR:CD1	2.47	0.50
2:B:28:TYR:CE2	2:B:70:THR:HB	2.47	0.50
2:B:1028:ALA:HB1	2:B:1070:MET:HE3	1.94	0.50
2:A:667:LYS:HG3	2:A:667:LYS:O	2.10	0.50
2:B:680:ARG:HB3	2:B:689:PHE:CE1	2.47	0.50
2:B:370:GLU:O	2:B:374:MET:HG3	2.12	0.50
2:B:44:LYS:HB3	2:B:58:LEU:CD2	2.40	0.50
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.47	0.50
2:A:853:GLN:HE21	2:A:853:GLN:HA	1.77	0.50
1:X:1103:U:O2'	1:X:1104:G:C5'	2.60	0.49
2:B:8:LEU:HA	2:B:737:MET:SD	2.52	0.49
2:B:959:GLN:NE2	2:B:973:ASP:OD1	2.45	0.49
2:B:1018:ILE:HD12	2:B:1037:ALA:HB1	1.93	0.49
1:Y:1101:U:O2'	1:Y:1102:G:OP1	2.29	0.49
2:A:556:GLN:CA	2:A:556:GLN:HE21	2.09	0.49
2:B:899:PHE:O	2:B:901:PRO:HD3	2.11	0.49
2:A:248:MET:HG2	2:A:326:TYR:CD1	2.48	0.49
2:B:93:ALA:HB1	2:B:175:SER:HA	1.94	0.49
2:A:210:SER:OG	2:A:230:ILE:HG23	2.13	0.49
2:B:193:TYR:CZ	2:B:197:LYS:HD2	2.47	0.49
2:A:334:PHE:CE2	2:A:455:PRO:HD3	2.48	0.49
2:A:368:ARG:HG3	2:A:541:GLY:N	2.28	0.49
2:A:90:VAL:HG23	2:A:91:LYS:N	2.27	0.49
2:A:102:LEU:N	2:A:102:LEU:HD22	2.25	0.49
2:B:853:GLN:HE21	2:B:853:GLN:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:VAL:HA	2:B:647:MET:SD	2.52	0.49
2:A:857:LEU:O	2:A:861:LEU:HD13	2.12	0.49
2:A:461:ILE:HD11	2:A:586:TYR:CE1	2.47	0.49
2:B:313:ASP:OD2	2:B:313:ASP:N	2.35	0.49
2:B:90:VAL:HG23	2:B:91:LYS:N	2.27	0.49
2:B:650:ASP:O	2:B:654:ASP:OD1	2.31	0.49
2:B:485:LYS:HE2	2:B:495:SER:CA	2.42	0.49
2:A:29:SER:H	2:A:35:GLU:HG2	1.78	0.49
2:A:93:ALA:HB1	2:A:175:SER:HA	1.95	0.49
2:A:303:ILE:HB	2:A:304:PRO:HD3	1.92	0.49
2:B:102:LEU:HD22	2:B:102:LEU:N	2.25	0.49
2:B:853:GLN:NE2	2:B:853:GLN:HA	2.28	0.49
2:A:853:GLN:NE2	2:A:853:GLN:HA	2.28	0.49
2:B:29:SER:H	2:B:35:GLU:HG2	1.78	0.49
1:Y:1102:G:H4'	1:Y:1103:U:OP2	2.13	0.49
2:B:165:ARG:HE	2:B:220:HIS:CA	2.24	0.49
2:A:313:ASP:O	2:A:314:ARG:HB2	2.13	0.49
2:B:358:GLU:OE2	2:B:359:MET:HG3	2.12	0.49
2:B:857:LEU:O	2:B:861:LEU:HD13	2.12	0.49
2:A:410:PHE:CE1	2:A:425:MET:HE2	2.48	0.49
2:A:251:LEU:HD22	2:A:310:TRP:CZ3	2.48	0.49
2:A:139:SER:O	2:A:142:LEU:HB2	2.13	0.49
2:B:437:ILE:HD12	2:B:437:ILE:N	2.28	0.48
2:B:164:LYS:O	2:B:165:ARG:C	2.51	0.48
2:A:8:LEU:HD13	2:A:737:MET:HG2	1.95	0.48
2:A:8:LEU:CD2	2:A:74:ILE:HD12	2.38	0.48
2:A:370:GLU:O	2:A:374:MET:HG3	2.13	0.48
2:A:100:ALA:O	2:A:102:LEU:HD22	2.13	0.48
2:A:375:LEU:C	2:A:378:PRO:HD2	2.33	0.48
2:A:467:TYR:C	2:A:467:TYR:CD1	2.87	0.48
2:B:212:GLU:HB2	2:B:696:LEU:HD12	1.94	0.48
2:A:165:ARG:NE	2:A:220:HIS:HA	2.23	0.48
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.46	0.48
2:A:514:THR:HG22	2:A:638:GLN:CB	2.43	0.48
2:A:650:ASP:O	2:A:654:ASP:OD1	2.32	0.48
1:X:1101:U:O2'	1:X:1102:G:OP1	2.30	0.48
2:B:165:ARG:NE	2:B:220:HIS:HA	2.24	0.48
2:A:419:LYS:HB2	2:A:422:MET:CG	2.41	0.48
2:B:514:THR:HG22	2:B:638:GLN:CG	2.43	0.48
2:A:109:TYR:HA	2:A:118:LEU:CD2	2.44	0.48
2:A:44:LYS:HB3	2:A:58:LEU:CD2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:LYS:HB2	2:B:422:MET:CG	2.41	0.48
2:B:967:ILE:N	2:B:967:ILE:HD12	2.28	0.48
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.49	0.48
2:A:229:LEU:O	2:A:233:SER:HB3	2.13	0.48
2:B:251:LEU:HD22	2:B:310:TRP:CZ3	2.48	0.48
2:A:364:THR:OG1	2:A:533:PRO:HB3	2.12	0.48
2:B:4:TYR:CD1	2:B:733:LEU:HD22	2.49	0.48
2:B:461:ILE:HD11	2:B:586:TYR:CE1	2.48	0.48
2:A:4:TYR:CD1	2:A:733:LEU:HD22	2.49	0.48
2:A:358:GLU:OE2	2:A:359:MET:HG3	2.13	0.48
2:B:344:LEU:O	2:B:346:GLN:N	2.46	0.48
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.49	0.48
2:B:89:LEU:HD11	2:B:174:ALA:HA	1.95	0.48
2:B:221:ASP:O	2:B:225:ILE:HG13	2.13	0.48
2:A:168:ASP:O	2:A:171:THR:HB	2.13	0.48
2:A:313:ASP:N	2:A:313:ASP:OD2	2.36	0.48
2:A:437:ILE:N	2:A:437:ILE:HD12	2.29	0.48
2:A:1000:ASN:O	2:A:1005:GLN:HB3	2.13	0.48
2:B:786:ARG:HD3	2:B:869:SER:CB	2.43	0.48
2:A:632:ASP:OD2	2:A:677:ILE:HB	2.13	0.48
2:B:842:TYR:CE2	2:B:844:PRO:HB2	2.49	0.48
2:A:887:VAL:HG12	2:A:888:SER:N	2.28	0.48
2:B:145:VAL:CG2	2:B:211:ILE:HG23	2.44	0.48
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.95	0.48
2:B:303:ILE:HB	2:B:304:PRO:HD3	1.94	0.48
2:B:451:ARG:NH2	2:B:459:THR:HG21	2.29	0.48
2:B:364:THR:OG1	2:B:533:PRO:HB3	2.12	0.47
2:B:84:ALA:HB1	2:B:88:LYS:NZ	2.28	0.47
2:A:899:PHE:O	2:A:901:PRO:HD3	2.13	0.47
2:A:872:ILE:HD11	2:A:1069:LYS:HE3	1.95	0.47
2:A:999:ILE:HD11	2:A:1009:PHE:CZ	2.49	0.47
2:A:539:ILE:HA	2:A:542:LEU:HD12	1.95	0.47
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.28	0.47
2:B:467:TYR:C	2:B:467:TYR:CD1	2.88	0.47
2:B:168:ASP:O	2:B:171:THR:HB	2.14	0.47
2:A:165:ARG:HE	2:A:220:HIS:CA	2.25	0.47
2:A:430:ASN:O	2:A:432:ARG:N	2.47	0.47
2:B:193:TYR:CE2	2:B:197:LYS:HD2	2.50	0.47
2:B:301:VAL:C	2:B:304:PRO:HD2	2.34	0.47
2:B:382:ASP:OD1	2:B:551:ASP:HB2	2.14	0.47
2:A:627:ARG:HG2	2:A:627:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:485:LYS:HE2	2:A:495:SER:CA	2.44	0.47
2:A:605:LEU:HD12	2:A:605:LEU:O	2.15	0.47
2:A:344:LEU:O	2:A:346:GLN:N	2.47	0.47
2:A:382:ASP:OD1	2:A:551:ASP:HB2	2.14	0.47
2:B:313:ASP:O	2:B:314:ARG:HB2	2.15	0.47
2:A:518:TYR:H	2:A:518:TYR:HD2	1.60	0.47
2:B:771:PHE:HB3	2:B:1003:CYS:SG	2.55	0.47
2:B:886:THR:OG1	2:B:1055:PHE:HB3	2.14	0.47
2:A:786:ARG:HD3	2:A:869:SER:CB	2.44	0.47
2:B:539:ILE:HA	2:B:542:LEU:HD12	1.96	0.47
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.96	0.47
2:B:368:ARG:HG3	2:B:541:GLY:N	2.30	0.47
2:A:89:LEU:HD11	2:A:174:ALA:HA	1.96	0.47
2:A:48:ASN:N	2:A:48:ASN:HD22	2.13	0.47
2:B:430:ASN:O	2:B:432:ARG:N	2.48	0.47
2:B:56:ARG:HG2	2:B:56:ARG:NH1	2.30	0.47
2:A:387:ARG:NH1	2:A:553:LYS:HG3	2.30	0.47
2:A:34:LEU:O	2:A:37:ARG:HB2	2.15	0.47
2:B:410:PHE:CE1	2:B:425:MET:HE2	2.50	0.47
2:B:229:LEU:O	2:B:233:SER:HB3	2.15	0.46
2:A:967:ILE:N	2:A:967:ILE:HD12	2.30	0.46
2:B:101:ASP:OD1	2:B:103:THR:HB	2.15	0.46
2:B:109:TYR:HA	2:B:118:LEU:CD2	2.45	0.46
2:A:680:ARG:HB3	2:A:689:PHE:CE1	2.50	0.46
2:A:796:SER:HB3	2:A:799:ALA:HB3	1.96	0.46
2:A:1018:ILE:HD12	2:A:1037:ALA:CB	2.46	0.46
2:A:29:SER:OG	2:A:34:LEU:HD23	2.15	0.46
2:B:804:ALA:HA	2:B:809:LYS:HE3	1.95	0.46
2:A:164:LYS:O	2:A:165:ARG:C	2.53	0.46
2:A:886:THR:OG1	2:A:1055:PHE:HB3	2.14	0.46
2:B:789:MET:HE2	2:B:1076:LEU:HD21	1.98	0.46
2:A:1067:TRP:O	2:A:1070:MET:HB2	2.15	0.46
2:A:212:GLU:HB2	2:A:696:LEU:HD12	1.96	0.46
2:A:290:GLN:O	2:A:294:ASN:ND2	2.48	0.46
2:B:887:VAL:HG12	2:B:888:SER:N	2.30	0.46
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.46	0.46
2:B:796:SER:HB3	2:B:799:ALA:HB3	1.96	0.46
2:B:515:MET:HG2	2:B:639:PHE:HE2	1.80	0.46
2:B:1018:ILE:HD12	2:B:1037:ALA:CB	2.46	0.46
2:B:843:ALA:HB3	2:B:844:PRO:HD3	1.97	0.46
2:B:271:PHE:CZ	2:B:273:ASN:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:584:ILE:HD12	2:B:585:GLN:O	2.16	0.46
2:B:389:SER:OG	2:B:557:THR:HG21	2.16	0.46
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.81	0.46
2:A:246:SER:N	2:A:247:PRO:CD	2.78	0.46
2:B:326:TYR:HE2	2:B:690:ARG:HB2	1.81	0.46
2:A:326:TYR:HE2	2:A:690:ARG:HB2	1.81	0.46
2:B:999:ILE:HD11	2:B:1009:PHE:CZ	2.51	0.46
2:A:643:VAL:HA	2:A:647:MET:SD	2.55	0.46
2:B:721:ARG:HD2	2:B:726:GLU:HG3	1.97	0.46
3:B:1111:GTP:O3G	3:B:1111:GTP:O1B	2.34	0.46
2:A:428:MET:C	2:A:430:ASN:H	2.19	0.46
2:A:56:ARG:HG2	2:A:56:ARG:NH1	2.31	0.46
2:B:89:LEU:HD11	2:B:174:ALA:CB	2.46	0.46
2:B:896:TYR:HB2	2:B:912:GLN:HA	1.98	0.46
2:B:48:ASN:N	2:B:48:ASN:HD22	2.14	0.46
2:B:438:ILE:HD11	2:B:560:LEU:HB3	1.96	0.46
2:B:210:SER:OG	2:B:230:ILE:HG23	2.17	0.45
2:A:221:ASP:O	2:A:225:ILE:HG13	2.16	0.45
2:B:428:MET:C	2:B:430:ASN:H	2.20	0.45
2:B:28:TYR:CZ	2:B:784:ILE:HG12	2.50	0.45
2:B:11:TYR:CZ	2:B:15:ILE:HG13	2.52	0.45
2:A:997:LEU:HD12	2:A:1035:LEU:CD2	2.46	0.45
2:A:326:TYR:CE2	2:A:690:ARG:HB2	2.52	0.45
2:A:228:GLU:OE2	2:A:302:ASP:HB2	2.16	0.45
2:B:387:ARG:HB3	2:B:387:ARG:NH1	2.31	0.45
2:B:1067:TRP:O	2:B:1070:MET:HB2	2.15	0.45
2:A:381:HIS:O	2:A:382:ASP:C	2.54	0.45
2:A:89:LEU:HD11	2:A:174:ALA:CB	2.46	0.45
2:B:135:LEU:HD22	2:B:709:GLN:NE2	2.30	0.45
2:A:11:TYR:CZ	2:A:15:ILE:HG13	2.51	0.45
2:A:217:VAL:HG13	2:A:223:TYR:N	2.31	0.45
2:B:797:GLY:O	2:B:801:GLU:HG3	2.17	0.45
2:B:556:GLN:NE2	2:B:556:GLN:CA	2.75	0.45
2:B:596:THR:O	2:B:600:ASN:HB2	2.16	0.45
2:A:217:VAL:HG13	2:A:222:ASP:CB	2.47	0.45
2:B:339:MET:CE	2:B:449:LEU:HB3	2.46	0.45
2:A:438:ILE:HD11	2:A:560:LEU:HB3	1.97	0.45
2:A:984:ASP:O	2:A:988:ILE:HG12	2.17	0.45
2:A:721:ARG:HD2	2:A:726:GLU:HG3	1.98	0.45
2:A:758:THR:HG22	2:A:766:PHE:O	2.16	0.45
2:B:217:VAL:HG13	2:B:222:ASP:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:182:VAL:HA	2:A:183:PRO:HD3	1.80	0.45
2:B:999:ILE:HA	2:B:999:ILE:HD12	1.77	0.45
2:B:872:ILE:HD11	2:B:1069:LYS:HE3	1.98	0.45
2:A:612:LEU:HD23	2:A:615:ILE:HD11	1.98	0.45
2:A:896:TYR:HB2	2:A:912:GLN:HA	1.99	0.45
2:B:334:PHE:CE2	2:B:455:PRO:HD3	2.52	0.45
2:A:1026:ILE:HA	2:A:1027:PRO:HD2	1.59	0.45
2:B:34:LEU:O	2:B:37:ARG:HB2	2.17	0.45
2:A:441:VAL:HG13	2:A:469:TYR:OH	2.17	0.45
1:Y:1101:U:HO2'	1:Y:1102:G:P	2.40	0.45
2:B:217:VAL:HG13	2:B:223:TYR:N	2.31	0.45
2:A:374:MET:CE	2:A:480:MET:HB3	2.47	0.45
2:A:959:GLN:HE21	2:A:973:ASP:HA	1.82	0.45
2:B:326:TYR:CE2	2:B:690:ARG:HB2	2.52	0.45
2:A:797:GLY:O	2:A:801:GLU:HG3	2.17	0.45
2:A:803:ALA:HB1	2:A:836:LYS:HE3	1.99	0.45
2:B:959:GLN:HE21	2:B:973:ASP:HA	1.82	0.45
2:B:963:ILE:CD1	2:B:969:LYS:HG2	2.46	0.45
2:B:605:LEU:HB2	2:B:628:VAL:HG11	1.99	0.45
2:B:1026:ILE:HA	2:B:1027:PRO:HD2	1.58	0.45
2:B:627:ARG:NH1	2:B:627:ARG:HG2	2.31	0.44
2:A:271:PHE:CZ	2:A:273:ASN:HA	2.52	0.44
2:A:584:ILE:HD12	2:A:585:GLN:O	2.17	0.44
2:B:125:TYR:CG	2:B:126:THR:N	2.85	0.44
2:B:246:SER:N	2:B:247:PRO:CD	2.80	0.44
2:B:100:ALA:O	2:B:102:LEU:HD22	2.17	0.44
2:A:999:ILE:HA	2:A:999:ILE:HD12	1.79	0.44
2:B:380:LYS:HE3	2:B:548:MET:CE	2.48	0.44
2:A:963:ILE:CD1	2:A:969:LYS:HG2	2.46	0.44
1:X:1102:G:O2'	1:X:1103:U:P	2.75	0.44
1:X:1105:A:C6	2:A:462:ILE:HD13	2.52	0.44
2:B:428:MET:HE1	2:B:811:TYR:CD1	2.42	0.44
2:A:28:TYR:CZ	2:A:784:ILE:HG12	2.52	0.44
2:B:182:VAL:HA	2:B:183:PRO:HD3	1.80	0.44
2:A:857:LEU:HD23	2:A:857:LEU:C	2.37	0.44
2:A:596:THR:O	2:A:600:ASN:HB2	2.17	0.44
2:A:8:LEU:HD12	2:A:737:MET:SD	2.58	0.44
2:A:255:VAL:HG11	2:A:316:ILE:HD13	2.00	0.44
2:B:784:ILE:HG22	2:B:785:GLN:N	2.33	0.44
2:B:139:SER:O	2:B:142:LEU:HB2	2.18	0.44
1:Y:1105:A:C6	2:B:462:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HD13	2:B:709:GLN:NE2	2.26	0.44
2:A:125:TYR:CG	2:A:126:THR:N	2.86	0.44
2:B:381:HIS:O	2:B:382:ASP:C	2.56	0.44
2:B:450:GLY:O	2:B:462:ILE:N	2.50	0.43
2:B:8:LEU:CD2	2:B:74:ILE:HD12	2.42	0.43
2:B:408:LEU:O	2:B:414:THR:HA	2.17	0.43
2:B:1070:MET:O	2:B:1073:ILE:HG13	2.18	0.43
2:B:719:VAL:HG12	2:B:723:ARG:HD2	2.00	0.43
2:B:126:THR:HG23	2:B:126:THR:O	2.18	0.43
2:A:949:LYS:O	2:A:953:LEU:HG	2.19	0.43
2:B:228:GLU:OE2	2:B:302:ASP:HB2	2.18	0.43
1:X:1102:G:N1	2:A:190:ARG:HD3	2.33	0.43
2:B:213:MET:O	2:B:217:VAL:HG23	2.19	0.43
2:A:387:ARG:NH1	2:A:387:ARG:HB3	2.33	0.43
2:B:780:ASP:O	2:B:783:TYR:HB3	2.18	0.43
2:B:605:LEU:O	2:B:605:LEU:HD12	2.18	0.43
2:B:992:TYR:CE1	2:B:996:LEU:HD21	2.53	0.43
2:A:556:GLN:NE2	2:A:556:GLN:CA	2.77	0.43
2:B:8:LEU:HD12	2:B:737:MET:SD	2.58	0.43
2:A:1028:ALA:O	2:A:1031:PHE:HB3	2.18	0.43
2:A:334:PHE:CD2	2:A:455:PRO:HD3	2.53	0.43
2:B:612:LEU:HD23	2:B:615:ILE:HD11	2.00	0.43
2:A:783:TYR:CZ	2:A:864:PRO:HB2	2.53	0.43
2:A:264:ASN:O	2:A:267:LEU:N	2.49	0.43
2:B:491:ALA:HB3	2:B:629:ASP:HB2	2.00	0.43
2:A:784:ILE:HG22	2:A:785:GLN:N	2.34	0.43
2:B:863:LYS:HE3	2:B:863:LYS:HB2	1.80	0.43
2:B:101:ASP:C	2:B:101:ASP:OD1	2.56	0.43
2:B:803:ALA:HB1	2:B:836:LYS:HE3	2.01	0.43
2:A:771:PHE:HB3	2:A:1003:CYS:SG	2.59	0.43
1:Y:1102:G:N1	2:B:190:ARG:HD3	2.33	0.43
2:B:301:VAL:O	2:B:304:PRO:HD2	2.18	0.43
2:B:984:ASP:O	2:B:988:ILE:HG12	2.19	0.43
2:A:897:GLN:N	2:A:897:GLN:OE1	2.40	0.43
2:A:186:ASN:N	2:A:186:ASN:HD22	2.16	0.43
1:X:1103:U:O2'	1:X:1104:G:P	2.76	0.43
2:A:608:ILE:HD11	2:A:635:ALA:HB2	2.00	0.43
2:A:101:ASP:OD1	2:A:103:THR:HB	2.19	0.43
2:A:787:ALA:O	2:A:790:SER:HB3	2.19	0.43
2:A:860:MET:C	2:A:862:GLN:H	2.21	0.43
2:A:101:ASP:OD1	2:A:101:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:LEU:O	2:A:243:LEU:HB2	2.19	0.43
2:A:903:LEU:C	2:A:904:PRO:O	2.57	0.43
2:A:380:LYS:HE3	2:A:548:MET:CE	2.49	0.43
2:A:24:ILE:HG22	2:A:24:ILE:O	2.19	0.43
2:A:1066:LEU:O	2:A:1069:LYS:N	2.52	0.42
2:B:360:TYR:OH	2:B:529:HIS:HB3	2.19	0.42
2:B:186:ASN:N	2:B:186:ASN:HD22	2.16	0.42
2:A:408:LEU:O	2:A:414:THR:HA	2.19	0.42
2:B:7:ILE:HG22	2:B:7:ILE:O	2.19	0.42
2:B:860:MET:HA	2:B:860:MET:HE3	2.00	0.42
2:A:519:THR:HG22	2:A:521:VAL:HG13	2.02	0.42
2:B:1061:SER:O	2:B:1064:ILE:HG22	2.19	0.42
2:B:728:ASP:OD1	2:B:730:GLU:HB2	2.19	0.42
2:B:177:ILE:HD13	2:B:203:LEU:CD1	2.38	0.42
2:A:177:ILE:HD13	2:A:203:LEU:CD1	2.38	0.42
2:A:734:THR:HA	2:A:737:MET:HE3	2.01	0.42
2:A:854:ILE:O	2:A:858:LEU:HB2	2.19	0.42
2:B:255:VAL:HG11	2:B:316:ILE:HD13	2.01	0.42
2:B:338:LYS:O	2:B:339:MET:C	2.58	0.42
2:B:860:MET:C	2:B:862:GLN:H	2.21	0.42
2:A:780:ASP:O	2:A:783:TYR:HB3	2.19	0.42
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.54	0.42
2:A:729:ARG:HE	2:A:770:ASP:CG	2.23	0.42
2:B:258:ASN:OD1	2:B:275:TYR:HD1	2.02	0.42
2:B:823:LYS:HG2	2:B:824:ASN:N	2.34	0.42
2:B:164:LYS:O	2:B:166:ARG:N	2.53	0.42
2:A:7:ILE:O	2:A:7:ILE:HG22	2.20	0.42
2:B:783:TYR:CZ	2:B:864:PRO:HB2	2.55	0.42
2:A:544:ILE:O	2:A:548:MET:HG3	2.19	0.42
2:B:5:ASN:CG	2:B:71:LEU:HD23	2.39	0.42
1:Y:1102:G:O2'	1:Y:1103:U:P	2.77	0.42
2:B:375:LEU:O	2:B:378:PRO:HD2	2.19	0.42
2:A:863:LYS:HE3	2:A:863:LYS:HB2	1.81	0.42
2:B:264:ASN:O	2:B:267:LEU:N	2.50	0.42
2:B:517:LEU:C	2:B:517:LEU:CD2	2.88	0.42
2:B:949:LYS:O	2:B:953:LEU:HG	2.20	0.42
2:A:339:MET:CE	2:A:449:LEU:HB3	2.49	0.42
2:B:449:LEU:HA	2:B:449:LEU:HD12	1.77	0.42
2:A:1026:ILE:O	2:A:1026:ILE:HG12	2.20	0.42
2:A:823:LYS:HG2	2:A:824:ASN:N	2.34	0.42
2:A:1047:LYS:HE3	2:A:1047:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:854:ILE:O	2:B:858:LEU:HB2	2.19	0.42
2:B:340:LEU:HD13	2:B:575:ILE:HG21	2.02	0.42
2:B:997:LEU:HD12	2:B:1035:LEU:CD2	2.49	0.42
2:A:301:VAL:C	2:A:304:PRO:HD2	2.39	0.42
2:B:544:ILE:O	2:B:548:MET:HG3	2.20	0.42
2:A:689:PHE:HB3	2:A:723:ARG:HH12	1.75	0.42
2:A:428:MET:HE1	2:A:811:TYR:CD1	2.45	0.42
2:A:338:LYS:O	2:A:339:MET:C	2.58	0.42
2:A:781:GLU:O	2:A:785:GLN:HG3	2.20	0.42
2:B:226:ALA:O	2:B:227:LYS:C	2.58	0.42
2:B:722:LEU:HD21	2:B:771:PHE:CE1	2.54	0.42
2:A:1061:SER:O	2:A:1064:ILE:HG22	2.20	0.42
2:B:729:ARG:HE	2:B:770:ASP:CG	2.23	0.42
2:B:735:LYS:O	2:B:739:MET:HG3	2.19	0.42
1:X:1104:G:H5'	2:A:401:SER:HB2	2.01	0.42
2:B:148:TRP:HB3	2:B:215:MET:HE1	2.02	0.42
2:B:255:VAL:CG1	2:B:316:ILE:HB	2.50	0.42
2:B:409:LYS:HZ3	2:B:409:LYS:HB2	1.85	0.42
2:A:109:TYR:HA	2:A:118:LEU:HD22	2.01	0.42
2:B:584:ILE:HD12	2:B:585:GLN:N	2.35	0.42
2:A:491:ALA:HB3	2:A:629:ASP:HB2	2.01	0.42
2:A:1080:TYR:O	2:A:1083:ALA:HB3	2.19	0.42
2:B:897:GLN:N	2:B:897:GLN:OE1	2.42	0.42
2:A:133:ALA:O	2:A:698:ASN:HB2	2.19	0.42
2:A:719:VAL:HG12	2:A:723:ARG:HD2	2.02	0.42
2:B:171:THR:O	2:B:172:ILE:C	2.58	0.42
2:A:164:LYS:O	2:A:166:ARG:N	2.53	0.42
2:B:374:MET:CE	2:B:480:MET:HB3	2.50	0.42
2:A:1070:MET:O	2:A:1073:ILE:HG13	2.20	0.42
2:A:563:GLN:NE2	2:A:563:GLN:HA	2.34	0.42
2:B:519:THR:HG22	2:B:521:VAL:HG13	2.02	0.42
2:A:847:LEU:O	2:A:851:ARG:HG3	2.19	0.42
2:A:255:VAL:CG1	2:A:316:ILE:HB	2.50	0.41
2:A:847:LEU:HD23	2:A:850:ARG:NH1	2.34	0.41
2:B:758:THR:HG22	2:B:766:PHE:O	2.20	0.41
2:B:534:PHE:CZ	2:B:599:ALA:HB1	2.54	0.41
2:B:903:LEU:C	2:B:904:PRO:O	2.57	0.41
2:A:232:LEU:CD2	2:A:300:LEU:HG	2.50	0.41
2:A:449:LEU:HD12	2:A:449:LEU:HA	1.76	0.41
2:A:992:TYR:CE1	2:A:996:LEU:HD21	2.55	0.41
2:B:49:SER:C	2:B:51:ASN:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:VAL:HG23	2:B:105:ASN:ND2	2.34	0.41
2:A:920:GLN:HA	2:A:920:GLN:OE1	2.20	0.41
2:A:723:ARG:NH2	3:A:1111:GTP:O3B	2.37	0.41
2:A:213:MET:O	2:A:217:VAL:HG23	2.21	0.41
2:A:70:THR:HG21	2:A:755:ARG:HG2	2.02	0.41
2:A:796:SER:OG	2:A:845:ILE:HG23	2.21	0.41
2:B:842:TYR:CZ	2:B:844:PRO:HG2	2.54	0.41
2:B:667:LYS:CG	2:B:667:LYS:O	2.69	0.41
2:B:680:ARG:HB3	2:B:689:PHE:HE1	1.85	0.41
2:A:704:SER:HB2	2:A:708:ASP:CB	2.50	0.41
2:A:360:TYR:OH	2:A:529:HIS:HB3	2.20	0.41
2:A:258:ASN:OD1	2:A:275:TYR:HD1	2.04	0.41
2:B:1080:TYR:O	2:B:1083:ALA:HB3	2.20	0.41
2:B:363:TYR:CZ	2:B:367:ILE:HD11	2.56	0.41
2:B:661:ARG:HD2	2:B:661:ARG:HA	1.82	0.41
2:B:1047:LYS:HE3	2:B:1047:LYS:HB2	1.75	0.41
2:B:920:GLN:HA	2:B:920:GLN:OE1	2.20	0.41
2:A:415:ILE:HG23	2:A:416:PHE:N	2.35	0.41
2:A:789:MET:CE	2:A:1076:LEU:HD21	2.50	0.41
2:A:410:PHE:HE1	2:A:425:MET:CE	2.32	0.41
2:A:516:VAL:HG21	2:A:675:ILE:HG21	2.01	0.41
2:B:608:ILE:HD11	2:B:635:ALA:HB2	2.02	0.41
2:A:477:VAL:HG11	2:A:594:LYS:HG3	2.03	0.41
2:A:429:ALA:C	2:A:430:ASN:OD1	2.59	0.41
2:B:232:LEU:CD2	2:B:300:LEU:HG	2.50	0.41
2:B:880:ASP:O	2:B:883:PRO:HD2	2.20	0.41
2:B:485:LYS:HE2	2:B:495:SER:C	2.40	0.41
2:B:573:VAL:HG12	2:B:575:ILE:HG13	2.02	0.41
2:B:796:SER:OG	2:B:845:ILE:HG23	2.21	0.41
2:B:860:MET:O	2:B:862:GLN:N	2.44	0.41
2:B:612:LEU:CD2	2:B:637:LEU:HD11	2.50	0.41
2:B:857:LEU:C	2:B:857:LEU:HD23	2.40	0.41
2:A:103:THR:HG22	2:A:103:THR:O	2.21	0.41
2:A:767:ASP:O	2:A:769:GLU:N	2.53	0.41
2:A:661:ARG:HD2	2:A:661:ARG:HA	1.83	0.41
2:A:430:ASN:C	2:A:432:ARG:N	2.74	0.41
2:A:967:ILE:HA	2:A:968:PRO:HD2	1.89	0.41
2:A:573:VAL:HG12	2:A:575:ILE:HG13	2.02	0.41
2:B:70:THR:HG21	2:B:755:ARG:HG2	2.02	0.41
2:A:389:SER:OG	2:A:557:THR:HG21	2.20	0.41
2:A:485:LYS:HE2	2:A:495:SER:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:853:GLN:CA	2:A:853:GLN:HE21	2.33	0.41
2:B:441:VAL:HG13	2:B:469:TYR:OH	2.21	0.41
2:B:786:ARG:HD3	2:B:869:SER:OG	2.20	0.41
2:A:584:ILE:HD12	2:A:585:GLN:N	2.36	0.41
2:A:49:SER:C	2:A:51:ASN:H	2.22	0.41
2:B:950:VAL:O	2:B:958:ILE:HG12	2.21	0.41
2:B:213:MET:SD	2:B:229:LEU:HD23	2.61	0.41
2:B:290:GLN:O	2:B:294:ASN:ND2	2.54	0.41
2:A:965:LEU:HB2	2:A:967:ILE:HD13	2.03	0.41
2:B:965:LEU:HB2	2:B:967:ILE:HD13	2.03	0.41
2:B:900:MET:HB3	2:B:903:LEU:CD1	2.50	0.41
2:A:126:THR:HG23	2:A:126:THR:O	2.21	0.41
2:B:449:LEU:HD11	2:B:573:VAL:CG2	2.49	0.41
2:A:722:LEU:HD21	2:A:771:PHE:CE1	2.55	0.41
2:A:1023:LYS:NZ	2:A:1057:ASN:HA	2.36	0.41
2:A:617:ASN:HD22	2:A:617:ASN:N	2.17	0.41
2:A:744:ILE:HD11	2:A:858:LEU:HD21	2.02	0.41
2:A:254:LEU:CD2	2:A:280:VAL:HG21	2.44	0.41
2:B:781:GLU:O	2:B:785:GLN:HG3	2.21	0.41
2:A:605:LEU:HB2	2:A:628:VAL:HG11	2.03	0.41
2:B:516:VAL:HG21	2:B:675:ILE:HG21	2.01	0.41
2:A:330:PHE:CE1	2:A:690:ARG:CZ	3.04	0.41
2:A:212:GLU:CB	2:A:696:LEU:HD12	2.51	0.41
2:A:515:MET:CE	2:A:639:PHE:CE2	3.04	0.41
2:B:1020:ILE:O	2:B:1020:ILE:HG22	2.20	0.41
2:A:288:LEU:HD12	2:A:288:LEU:O	2.20	0.41
2:B:288:LEU:HD12	2:B:288:LEU:O	2.20	0.41
2:A:463:PHE:CZ	2:A:590:ALA:HB3	2.56	0.41
2:B:254:LEU:CD2	2:B:280:VAL:HG21	2.44	0.41
2:A:430:ASN:C	2:A:432:ARG:H	2.23	0.41
2:A:102:LEU:H	2:A:102:LEU:CD2	2.30	0.41
2:A:539:ILE:HD11	2:A:565:GLN:O	2.20	0.41
2:B:183:PRO:HG3	2:B:199:LYS:HD3	2.02	0.41
2:B:103:THR:HG22	2:B:103:THR:O	2.21	0.41
2:B:515:MET:CE	2:B:639:PHE:CE2	3.04	0.41
2:B:723:ARG:NH2	3:B:1111:GTP:O3B	2.49	0.40
2:B:219:SER:O	2:B:222:ASP:HB2	2.21	0.40
2:A:783:TYR:CE2	2:A:864:PRO:HB2	2.56	0.40
2:B:607:LEU:O	2:B:610:THR:HB	2.21	0.40
2:B:24:ILE:HG22	2:B:24:ILE:O	2.21	0.40
2:B:165:ARG:HB3	2:B:223:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:887:VAL:CG1	2:A:888:SER:N	2.84	0.40
2:A:429:ALA:O	2:A:430:ASN:OD1	2.40	0.40
2:B:789:MET:CE	2:B:1076:LEU:HD21	2.51	0.40
2:B:967:ILE:HA	2:B:968:PRO:HD2	1.90	0.40
2:B:152:HIS:CD2	2:B:155:ASP:OD2	2.75	0.40
2:B:212:GLU:CB	2:B:696:LEU:HD12	2.51	0.40
2:B:109:TYR:HA	2:B:118:LEU:HD22	2.03	0.40
2:B:787:ALA:O	2:B:790:SER:HB3	2.22	0.40
2:A:728:ASP:OD1	2:A:730:GLU:HB2	2.21	0.40
2:A:549:THR:HG21	2:A:554:VAL:HG11	2.04	0.40
2:B:751:PHE:HA	2:B:752:PRO:HD3	1.87	0.40
2:A:171:THR:O	2:A:172:ILE:C	2.60	0.40
2:A:165:ARG:HB3	2:A:223:TYR:HB2	2.04	0.40
2:A:324:LYS:O	2:A:328:TRP:CD1	2.64	0.40
2:B:853:GLN:HE21	2:B:853:GLN:CA	2.33	0.40
2:B:847:LEU:O	2:B:851:ARG:HG3	2.21	0.40
1:Y:1103:U:O2'	1:Y:1104:G:P	2.79	0.40
2:B:217:VAL:HG13	2:B:222:ASP:HB3	2.04	0.40
2:A:135:LEU:HD13	2:A:709:GLN:NE2	2.29	0.40
2:A:860:MET:O	2:A:862:GLN:N	2.45	0.40
2:A:703:GLN:CD	2:A:703:GLN:H	2.23	0.40
2:B:1066:LEU:O	2:B:1069:LYS:N	2.54	0.40
2:B:847:LEU:HD23	2:B:850:ARG:NH1	2.35	0.40
2:B:554:VAL:O	2:B:558:LEU:HB2	2.21	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
2	A	1067/1095 (97%)	915 (86%)	124 (12%)	28 (3%)	7 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1067/1095 (97%)	919 (86%)	120 (11%)	28 (3%)	7 22
All	All	2134/2190 (97%)	1834 (86%)	244 (11%)	56 (3%)	7 22

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	866	THR
2	A	976	VAL
2	A	978	SER
2	B	866	THR
2	B	976	VAL
2	B	978	SER
2	A	106	GLU
2	A	128	SER
2	A	226	ALA
2	A	345	ASP
2	A	864	PRO
2	A	865	VAL
2	A	1017	LEU
2	B	106	GLU
2	B	128	SER
2	B	345	ASP
2	B	864	PRO
2	B	865	VAL
2	B	1017	LEU
2	A	91	LYS
2	A	431	GLU
2	A	592	GLY
2	A	768	SER
2	B	91	LYS
2	B	226	ALA
2	B	431	GLU
2	B	592	GLY
2	A	240	LEU
2	A	376	GLU
2	A	382	ASP
2	A	425	MET
2	A	439	PRO
2	A	1027	PRO
2	B	227	LYS
2	B	240	LEU
2	B	376	GLU

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Mol	Chain	Res	Type
2	B	382	ASP
2	B	425	MET
2	B	768	SER
2	B	1027	PRO
2	A	42	HIS
2	A	102	LEU
2	A	164	LYS
2	A	227	LYS
2	A	531	THR
2	B	42	HIS
2	B	102	LEU
2	B	164	LYS
2	B	439	PRO
2	B	508	ARG
2	A	508	ARG
2	A	904	PRO
2	B	531	THR
2	B	964	SER
2	B	904	PRO
2	A	673	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	974/996 (98%)	935 (96%)	39 (4%)	38	73
2	B	974/996 (98%)	935 (96%)	39 (4%)	38	73
All	All	1948/1992 (98%)	1870 (96%)	78 (4%)	38	73

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASN
2	A	48	ASN
2	A	91	LYS

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Mol	Chain	Res	Type
2	A	102	LEU
2	A	121	THR
2	A	128	SER
2	A	130	MET
2	A	156	VAL
2	A	186	ASN
2	A	229	LEU
2	A	313	ASP
2	A	358	GLU
2	A	409	LYS
2	A	415	ILE
2	A	431	GLU
2	A	449	LEU
2	A	467	TYR
2	A	512	ASN
2	A	517	LEU
2	A	518	TYR
2	A	550	ASN
2	A	556	GLN
2	A	557	THR
2	A	584	ILE
2	A	600	ASN
2	A	619	HIS
2	A	628	VAL
2	A	641	THR
2	A	721	ARG
2	A	784	ILE
2	A	791	LEU
2	A	802	ILE
2	A	858	LEU
2	A	872	ILE
2	A	892	LEU
2	A	900	MET
2	A	922	GLU
2	A	939	VAL
2	A	1054	LEU
2	B	17	ASN
2	B	48	ASN
2	B	91	LYS
2	B	102	LEU
2	B	121	THR
2	B	128	SER

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Mol	Chain	Res	Type
2	B	130	MET
2	B	186	ASN
2	B	229	LEU
2	B	313	ASP
2	B	358	GLU
2	B	409	LYS
2	B	415	ILE
2	B	431	GLU
2	B	449	LEU
2	B	467	TYR
2	B	512	ASN
2	B	517	LEU
2	B	518	TYR
2	B	550	ASN
2	B	556	GLN
2	B	557	THR
2	B	584	ILE
2	B	600	ASN
2	B	619	HIS
2	B	628	VAL
2	B	641	THR
2	B	695	LEU
2	B	721	ARG
2	B	784	ILE
2	B	791	LEU
2	B	805	SER
2	B	858	LEU
2	B	872	ILE
2	B	892	LEU
2	B	900	MET
2	B	922	GLU
2	B	939	VAL
2	B	1054	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	48	ASN
2	A	143	ASN
2	A	152	HIS
2	A	154	ASN

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Mol	Chain	Res	Type
2	A	186	ASN
2	A	289	ASN
2	A	294	ASN
2	A	308	GLN
2	A	407	GLN
2	A	512	ASN
2	A	528	GLN
2	A	556	GLN
2	A	563	GLN
2	A	565	GLN
2	A	574	GLN
2	A	617	ASN
2	A	646	GLN
2	A	649	GLN
2	A	653	ASN
2	A	694	ASN
2	A	709	GLN
2	A	760	ASN
2	A	840	ASN
2	A	853	GLN
2	A	959	GLN
2	B	36	ASN
2	B	48	ASN
2	B	143	ASN
2	B	152	HIS
2	B	186	ASN
2	B	289	ASN
2	B	294	ASN
2	B	308	GLN
2	B	407	GLN
2	B	512	ASN
2	B	528	GLN
2	B	556	GLN
2	B	563	GLN
2	B	565	GLN
2	B	574	GLN
2	B	617	ASN
2	B	638	GLN
2	B	646	GLN
2	B	653	ASN
2	B	694	ASN
2	B	709	GLN

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Mol	Chain	Res	Type
2	B	760	ASN
2	B	840	ASN
2	B	853	GLN
2	B	959	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	7/7 (100%)	4 (57%)	3 (42%)
1	Y	7/7 (100%)	4 (57%)	3 (42%)
All	All	14/14 (100%)	8 (57%)	6 (42%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	1102	G
1	X	1103	U
1	X	1104	G
1	X	1105	A
1	Y	1102	G
1	Y	1103	U
1	Y	1104	G
1	Y	1105	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G
1	X	1103	U
1	Y	1101	U
1	Y	1102	G
1	Y	1103	U

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GTP	A	1111	-	25,34,34	1.74	7 (28%)	34,54,54	4.63	16 (47%)
3	GTP	B	1111	-	25,34,34	1.79	7 (28%)	34,54,54	4.64	16 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	1111	-	-	0/18/38/38	0/3/3/3
3	GTP	B	1111	-	-	0/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1111	GTP	PG-O1G	-4.00	1.38	1.51
3	A	1111	GTP	PG-O1G	-3.70	1.39	1.51
3	B	1111	GTP	C8-N7	-3.41	1.28	1.34
3	B	1111	GTP	O4'-C1'	-3.12	1.37	1.41
3	A	1111	GTP	C8-N7	-3.05	1.28	1.34
3	A	1111	GTP	O4'-C1'	-2.58	1.37	1.41
3	B	1111	GTP	C2'-C3'	2.05	1.59	1.53
3	A	1111	GTP	C2'-C3'	2.12	1.59	1.53
3	A	1111	GTP	C2-N1	2.22	1.39	1.35
3	B	1111	GTP	C2-N1	2.27	1.39	1.35
3	B	1111	GTP	PG-O2G	2.42	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1111	GTP	PG-O2G	2.54	1.63	1.54
3	B	1111	GTP	C6-N1	2.74	1.38	1.33
3	A	1111	GTP	C6-N1	2.94	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1111	GTP	O3G-PG-O1G	-14.08	65.25	110.58
3	A	1111	GTP	O3G-PG-O1G	-14.05	65.36	110.58
3	A	1111	GTP	O2G-PG-O1G	-11.42	73.83	110.58
3	B	1111	GTP	O2G-PG-O1G	-10.99	75.20	110.58
3	A	1111	GTP	PA-O3A-PB	-9.37	106.41	132.73
3	B	1111	GTP	PA-O3A-PB	-8.86	107.86	132.73
3	A	1111	GTP	PB-O3B-PG	-8.50	104.17	132.67
3	B	1111	GTP	PB-O3B-PG	-8.31	104.81	132.67
3	B	1111	GTP	O4'-C4'-C5'	-8.16	80.14	109.32
3	A	1111	GTP	O4'-C4'-C5'	-7.58	82.19	109.32
3	B	1111	GTP	O4'-C4'-C3'	-4.22	96.64	105.15
3	A	1111	GTP	N3-C2-N1	-4.11	121.18	127.44
3	B	1111	GTP	N3-C2-N1	-4.02	121.32	127.44
3	A	1111	GTP	C5-C6-N1	-3.88	118.28	123.59
3	A	1111	GTP	O4'-C4'-C3'	-3.86	97.36	105.15
3	B	1111	GTP	C5-C6-N1	-3.76	118.45	123.59
3	A	1111	GTP	C6-C5-C4	-2.16	118.32	120.90
3	A	1111	GTP	C5'-C4'-C3'	2.11	123.59	115.21
3	B	1111	GTP	C5'-C4'-C3'	2.30	124.36	115.21
3	A	1111	GTP	C2'-C3'-C4'	2.51	107.76	102.61
3	B	1111	GTP	O3A-PA-O5'	2.74	110.20	102.94
3	B	1111	GTP	C2'-C3'-C4'	2.80	108.37	102.61
3	B	1111	GTP	O2G-PG-O3B	2.85	118.00	105.09
3	B	1111	GTP	C4'-O4'-C1'	2.85	112.85	109.72
3	A	1111	GTP	O3A-PA-O5'	2.87	110.55	102.94
3	A	1111	GTP	O2G-PG-O3B	3.09	119.12	105.09
3	B	1111	GTP	C6-N1-C2	3.43	120.70	115.94
3	A	1111	GTP	C6-N1-C2	3.58	120.91	115.94
3	A	1111	GTP	O3G-PG-O2G	5.50	128.31	107.38
3	B	1111	GTP	O3G-PG-O2G	5.64	128.87	107.38
3	A	1111	GTP	C2'-C1'-N9	6.36	124.00	114.29
3	B	1111	GTP	C2'-C1'-N9	6.85	124.76	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1111	GTP	2	0
3	B	1111	GTP	2	0

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	X	7/7 (100%)	0.00	0 100 100	47, 60, 73, 77	0
1	Y	7/7 (100%)	-0.02	0 100 100	47, 59, 72, 77	0
2	A	1073/1095 (97%)	-0.24	9 (0%) 87 81	15, 49, 79, 120	0
2	B	1073/1095 (97%)	-0.19	15 (1%) 78 69	17, 50, 80, 121	0
All	All	2160/2204 (98%)	-0.22	24 (1%) 82 74	15, 50, 79, 121	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	79	TYR	5.0
2	A	865	VAL	4.9
2	B	79	TYR	4.1
2	B	867	PHE	3.9
2	A	866	THR	3.8
2	A	77	TYR	3.7
2	B	792	SER	3.3
2	B	866	THR	3.3
2	B	1024	GLY	3.2
2	B	77	TYR	3.0
2	B	1022	PHE	3.0
2	A	862	GLN	3.0
2	B	862	GLN	2.9
2	B	1023	LYS	2.9
2	B	82	TYR	2.8
2	A	867	PHE	2.6
2	B	1086	PHE	2.5
2	B	1025	LYS	2.3
2	B	865	VAL	2.2
2	B	802	ILE	2.1
2	A	81	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	1025	LYS	2.1
2	A	986	TYR	2.0
2	B	78	SER	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GTP	A	1111	32/32	0.46	0.36	2.74	107,137,145,145	0
3	GTP	B	1111	32/32	0.43	0.41	2.49	112,142,150,150	0

6.5 Other polymers (i)

There are no such residues in this entry.