



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:42 PM 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 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/ValidationPDFNotes.html>

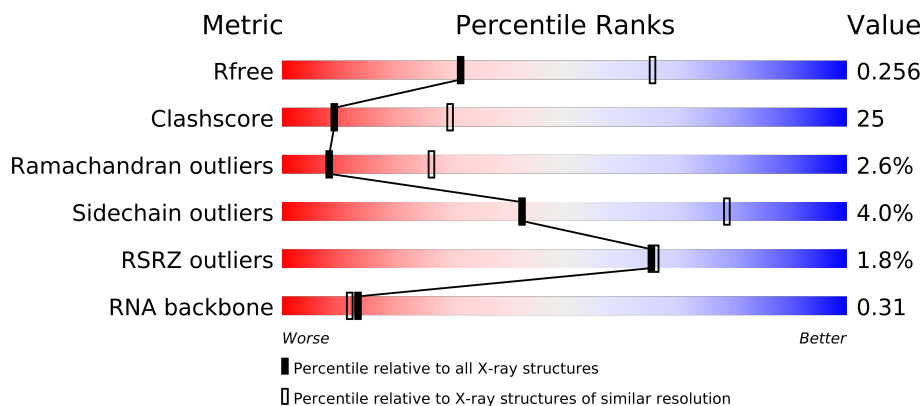
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	X	7	
1	Y	7	
2	A	1095	
2	B	1095	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition i

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

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.

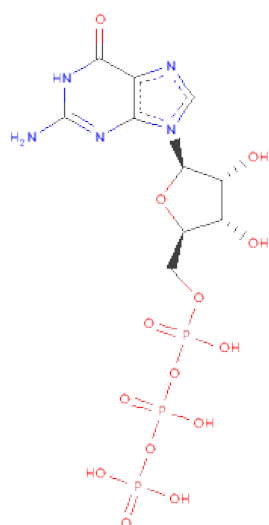
- Molecule 1 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3').

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			

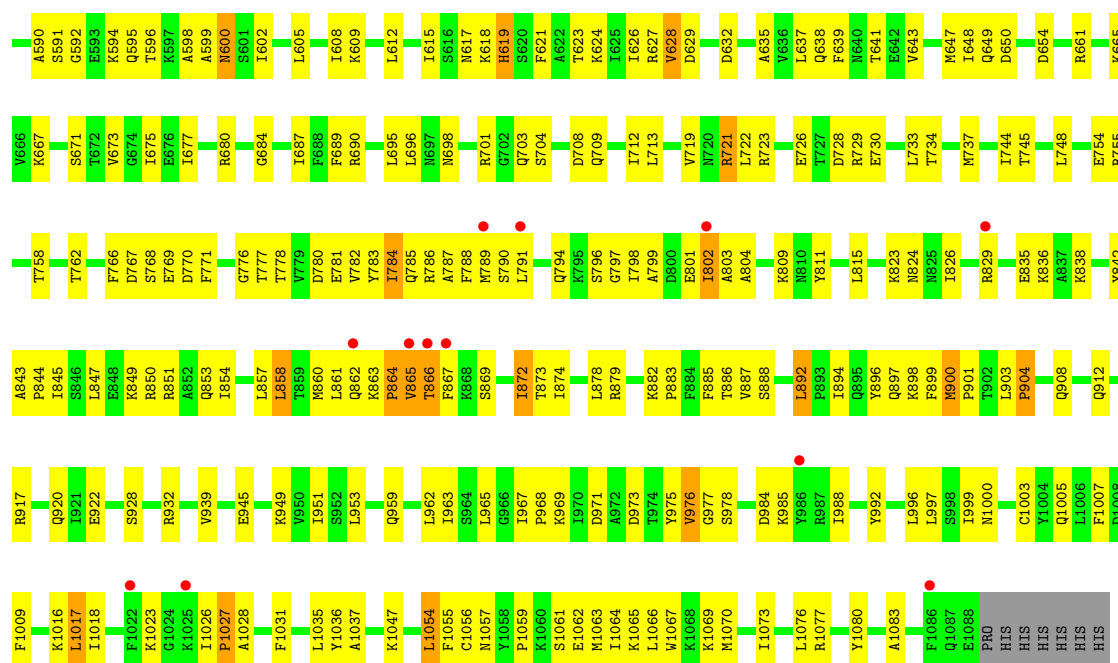
- Molecule 2 is a protein called RNA-dependent RNA polymerase.

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: C₁₀H₁₆N₅O₁₄P₃).

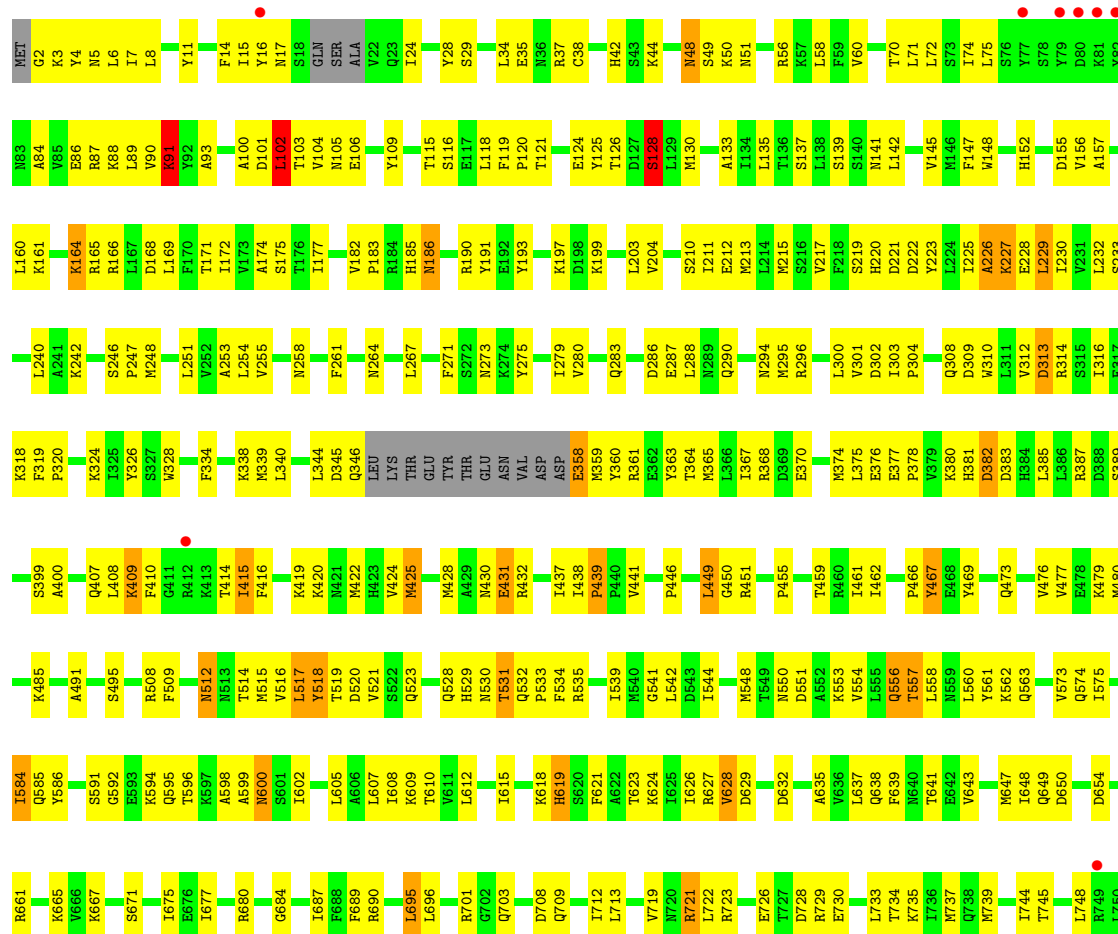


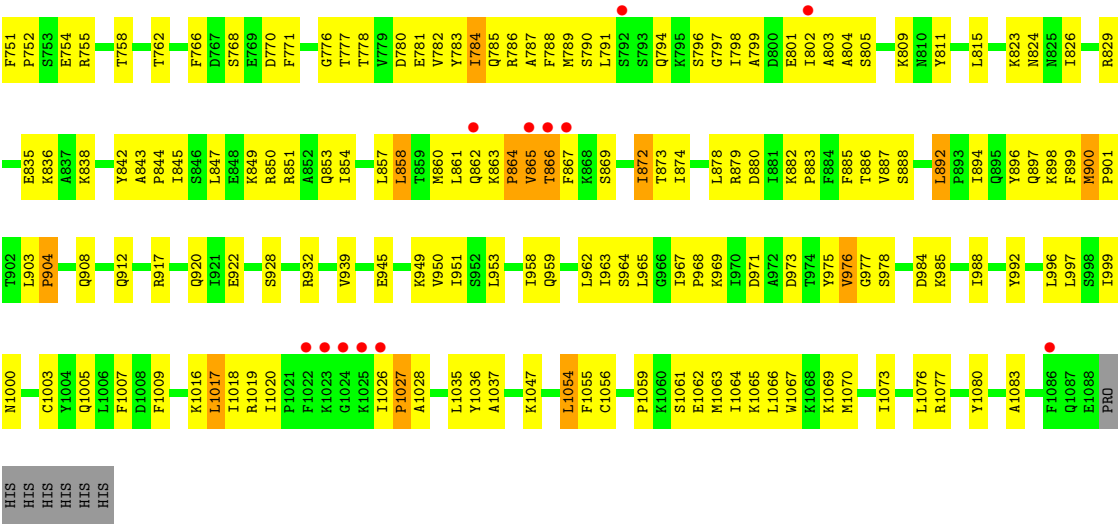
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		



• Molecule 2: RNA-dependent RNA polymerase

Chain B:





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.277 0.223 , 0.256	Depositor DCC
R_{free} test set	3987 reflections (8.75%)	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 , 15.4	EDS
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (884) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:598:ALA:O	2:A:602:ILE:HG13	1.87	0.75
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	Distance(Å)	Clash(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
2:A:477:VAL:HA	2:A:480:MET:HE2	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

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%)	8	26
2	B	1067/1095 (97%)	919 (86%)	120 (11%)	28 (3%)	8	26
All	All	2134/2190 (97%)	1834 (86%)	244 (11%)	56 (3%)	8	26

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	42	79
2	B	974/996 (98%)	935 (96%)	39 (4%)	42	79
All	All	1948/1992 (98%)	1870 (96%)	78 (4%)	42	79

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	34,34,34	2.29	11 (32%)	51,54,54	3.96	16 (31%)
3	GTP	B	1111	-	34,34,34	2.43	11 (32%)	51,54,54	3.97	18 (35%)

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	-	-	0/22/38/38	0/1/3/3
3	GTP	B	1111	-	-	0/22/38/38	0/1/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1111	GTP	C2'-C1'	-5.93	1.45	1.53
3	B	1111	GTP	PB-O3B	5.80	1.70	1.59
3	A	1111	GTP	PB-O3B	5.61	1.70	1.59
3	A	1111	GTP	C2'-C1'	-5.40	1.45	1.53
3	B	1111	GTP	PA-O3A	4.74	1.68	1.59
3	B	1111	GTP	PG-O3B	4.24	1.67	1.60
3	A	1111	GTP	PA-O3A	4.24	1.67	1.59
3	A	1111	GTP	PG-O3B	4.22	1.67	1.60
3	B	1111	GTP	PG-O1G	-3.93	1.38	1.51
3	A	1111	GTP	PG-O1G	-3.64	1.39	1.51
3	B	1111	GTP	C2-N2	3.52	1.37	1.32
3	A	1111	GTP	C2-N2	3.34	1.37	1.32
3	B	1111	GTP	C8-N7	-3.31	1.28	1.34
3	B	1111	GTP	PB-O3A	3.25	1.65	1.59
3	A	1111	GTP	C8-N7	-2.97	1.28	1.34
3	B	1111	GTP	O4'-C1'	-2.65	1.37	1.41
3	A	1111	GTP	PB-O3A	2.64	1.64	1.59
3	A	1111	GTP	PG-O2G	2.49	1.63	1.54
3	B	1111	GTP	PG-O2G	2.37	1.63	1.54
3	A	1111	GTP	O4'-C1'	-2.21	1.37	1.41
3	A	1111	GTP	C2'-C3'	2.07	1.59	1.53
3	B	1111	GTP	C2'-C3'	2.01	1.59	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1111	GTP	O3G-PG-O1G	-13.83	65.25	110.44
3	A	1111	GTP	O3G-PG-O1G	-13.79	65.36	110.44
3	A	1111	GTP	O2G-PG-O1G	-11.20	73.83	110.44
3	B	1111	GTP	O2G-PG-O1G	-10.78	75.20	110.44
3	A	1111	GTP	PB-O3B-PG	-9.38	104.17	131.68
3	B	1111	GTP	PB-O3B-PG	-9.16	104.81	131.68
3	A	1111	GTP	PA-O3A-PB	-8.62	106.41	131.68
3	B	1111	GTP	O4'-C4'-C5'	-8.18	80.14	109.36
3	B	1111	GTP	PA-O3A-PB	-8.12	107.86	131.68
3	A	1111	GTP	O3A-PB-O3B	7.99	117.92	101.66
3	A	1111	GTP	O4'-C4'-C5'	-7.61	82.19	109.36
3	B	1111	GTP	O3A-PB-O3B	7.19	116.28	101.66
3	B	1111	GTP	O3G-PG-O2G	5.46	128.87	107.61
3	B	1111	GTP	N3-C4-N9	5.40	134.83	126.91
3	A	1111	GTP	N3-C4-N9	5.33	134.73	126.91
3	A	1111	GTP	O3G-PG-O2G	5.32	128.31	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1111	GTP	C6-C5-N7	-4.91	133.48	134.14
3	B	1111	GTP	C2'-C1'-N9	4.48	124.76	113.27
3	A	1111	GTP	C6-C5-N7	-4.31	133.56	134.14
3	B	1111	GTP	O4'-C4'-C3'	-4.21	96.64	105.17
3	A	1111	GTP	C2'-C1'-N9	4.18	124.00	113.27
3	A	1111	GTP	C2-N3-C4	4.18	120.96	115.09
3	B	1111	GTP	C2-N3-C4	4.03	120.75	115.09
3	B	1111	GTP	C5-C4-N3	-3.96	120.20	125.94
3	A	1111	GTP	C5-C4-N3	-3.87	120.34	125.94
3	A	1111	GTP	O4'-C4'-C3'	-3.85	97.36	105.17
3	A	1111	GTP	O2G-PG-O3B	2.95	119.12	105.14
3	B	1111	GTP	C2'-C3'-C4'	2.87	108.37	102.65
3	B	1111	GTP	C4'-O4'-C1'	2.86	112.85	109.75
3	B	1111	GTP	O2G-PG-O3B	2.71	118.00	105.14
3	A	1111	GTP	C2'-C3'-C4'	2.56	107.76	102.65
3	B	1111	GTP	O4'-C1'-N9	-2.41	106.19	108.44
3	B	1111	GTP	C5'-C4'-C3'	2.28	124.36	115.21
3	A	1111	GTP	C5'-C4'-C3'	2.09	123.59	115.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	X	7/7 (100%)	0.33	0 100 100	47, 60, 73, 77	0
1	Y	7/7 (100%)	0.26	0 100 100	47, 59, 72, 77	0
2	A	1073/1095 (97%)	-0.19	16 (1%) 70 71	15, 49, 79, 120	0
2	B	1073/1095 (97%)	-0.14	20 (1%) 64 64	17, 50, 80, 121	0
All	All	2160/2204 (98%)	-0.16	36 (1%) 65 68	15, 50, 79, 121	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	865	VAL	5.9
2	A	79	TYR	5.5
2	B	79	TYR	4.6
2	A	866	THR	4.4
2	B	867	PHE	4.3
2	B	866	THR	3.9
2	A	77	TYR	3.8
2	B	1024	GLY	3.7
2	B	792	SER	3.4
2	B	1022	PHE	3.4
2	B	1023	LYS	3.2
2	A	867	PHE	3.2
2	B	77	TYR	3.1
2	B	862	GLN	3.0
2	B	1086	PHE	2.9
2	B	82	TYR	2.9
2	A	862	GLN	2.9
2	B	1025	LYS	2.8
2	B	865	VAL	2.6
2	B	412	ARG	2.6
2	A	1022	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	829	ARG	2.4
2	A	1025	LYS	2.4
2	B	802	ILE	2.4
2	A	986	TYR	2.3
2	A	802	ILE	2.3
2	A	157	ALA	2.2
2	A	81	LYS	2.2
2	B	80	ASP	2.2
2	B	1026	ILE	2.1
2	A	791	LEU	2.1
2	B	749	ARG	2.1
2	B	81	LYS	2.0
2	A	789	MET	2.0
2	A	1086	PHE	2.0
2	B	16	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GTP	B	1111	32/32	0.42	2.63	112,142,150,150	0
3	GTP	A	1111	32/32	0.35	2.48	107,137,145,145	0

6.5 Other polymers ⓘ

There are no such residues in this entry.