Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:10 AM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

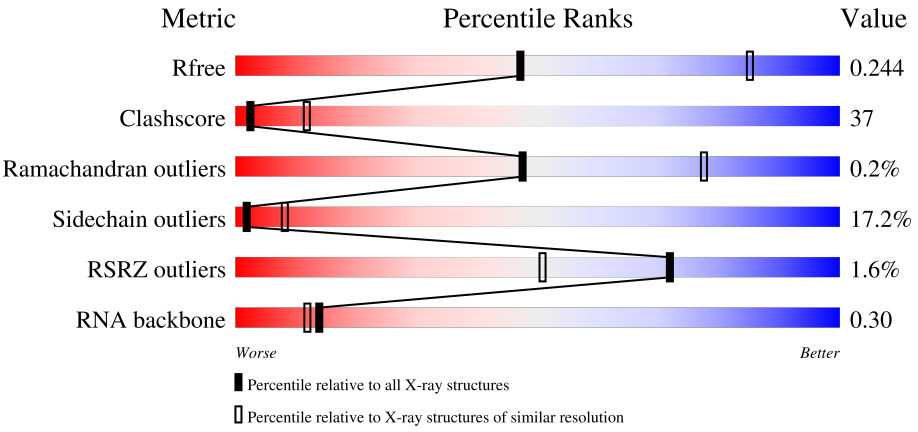
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)
RNA backbone	3102	1063 (3.36-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1160	46% 42% 9%
1	B	1160	44% 42% 9%
2	C	59	20% 37% 37%
2	E	59	25% 42% 29%

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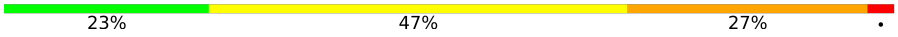
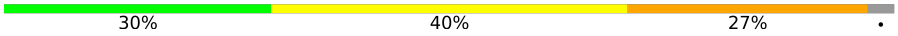
Mol	Chain	Length	Quality of chain
3	D	30	
3	F	30	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21838 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Uncharacterized protein.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 4 is water.

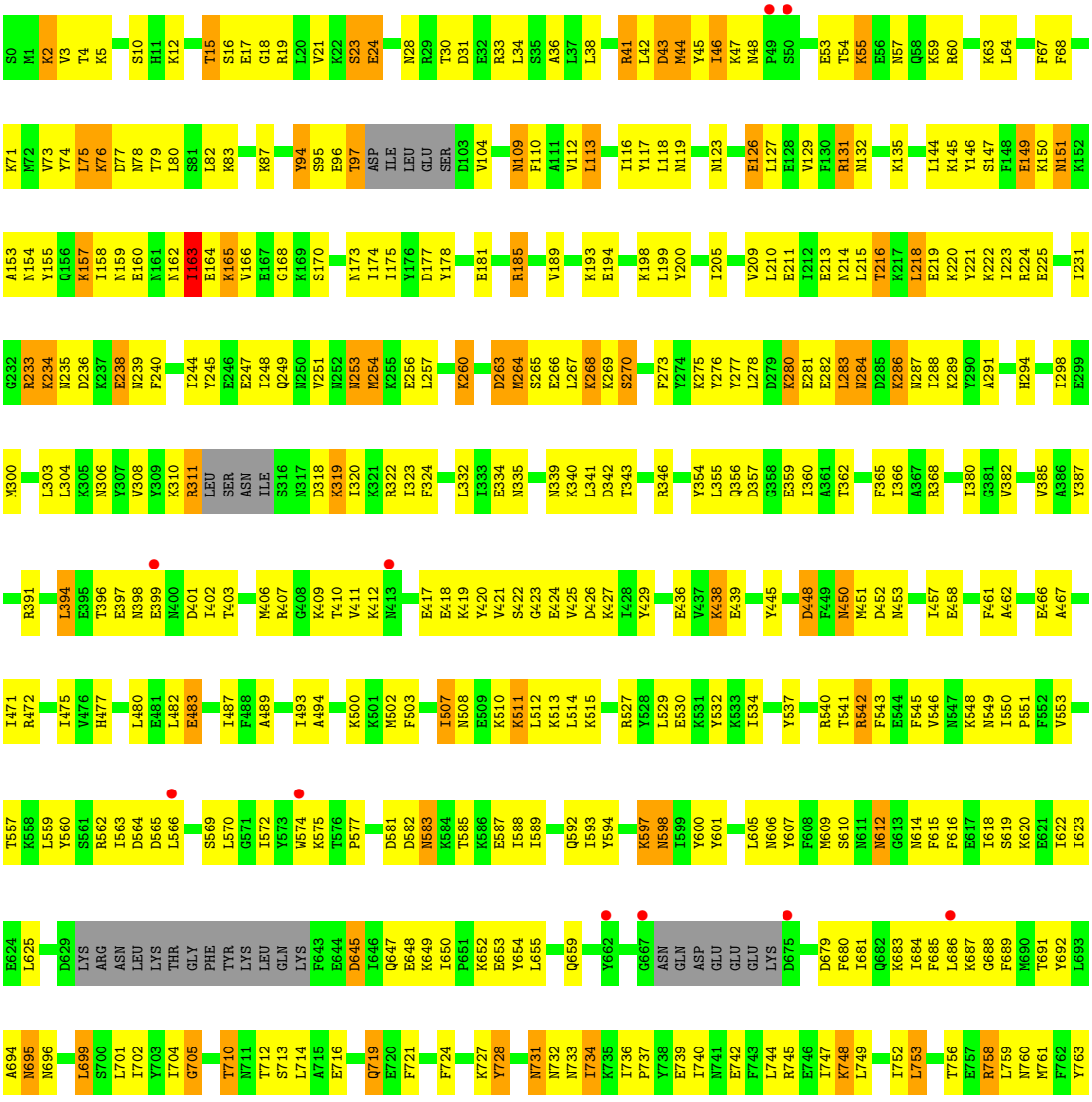
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	2	Total O 2 2	0	0

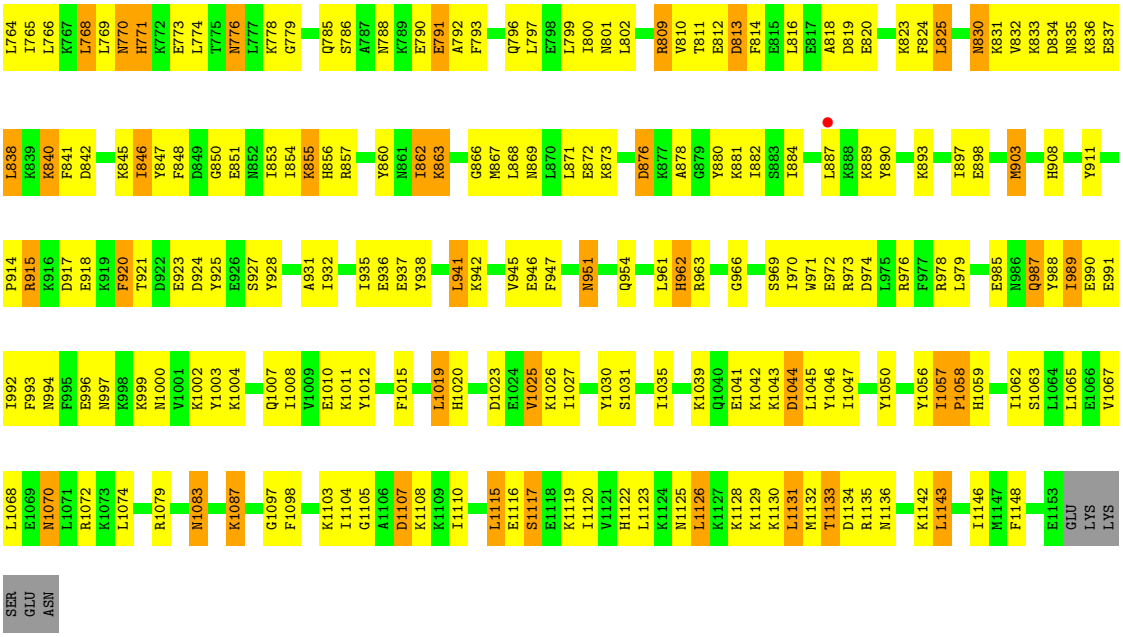
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncharacterized protein

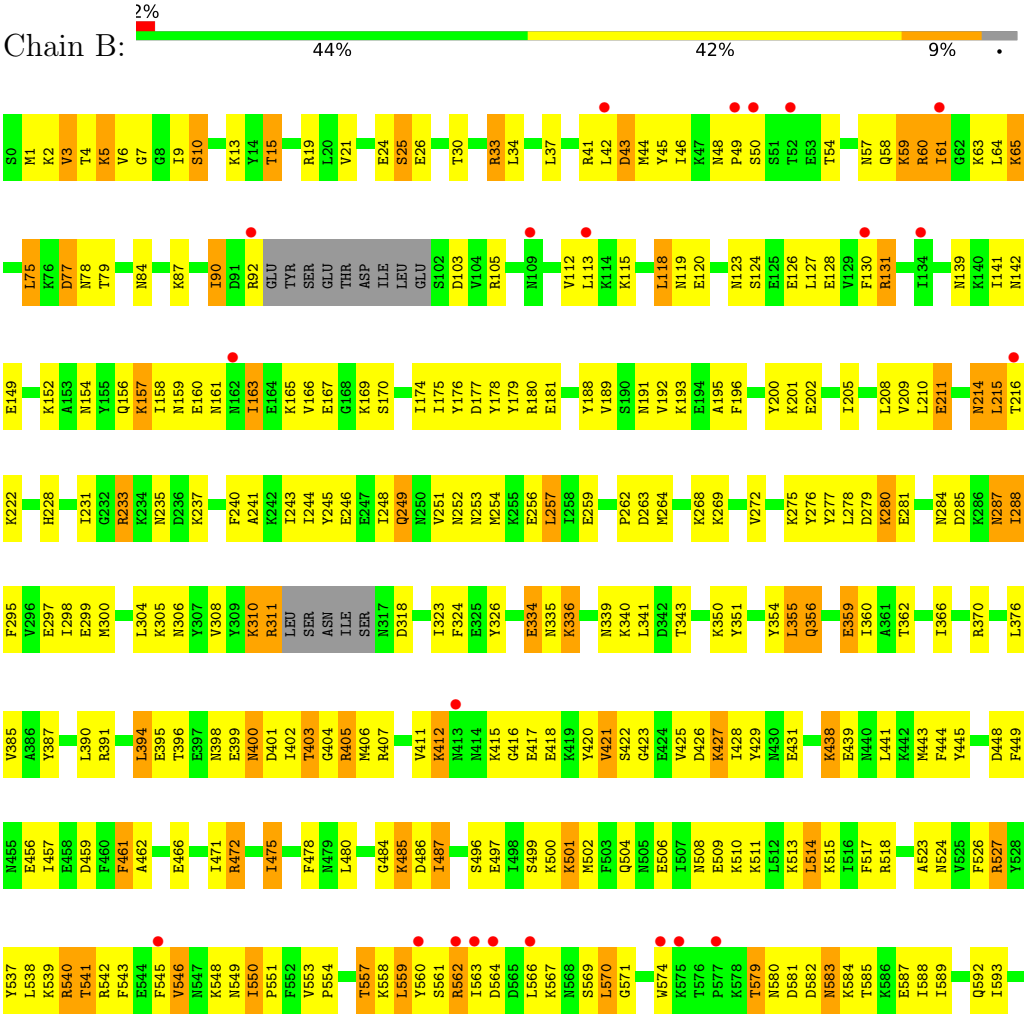
Chain A:

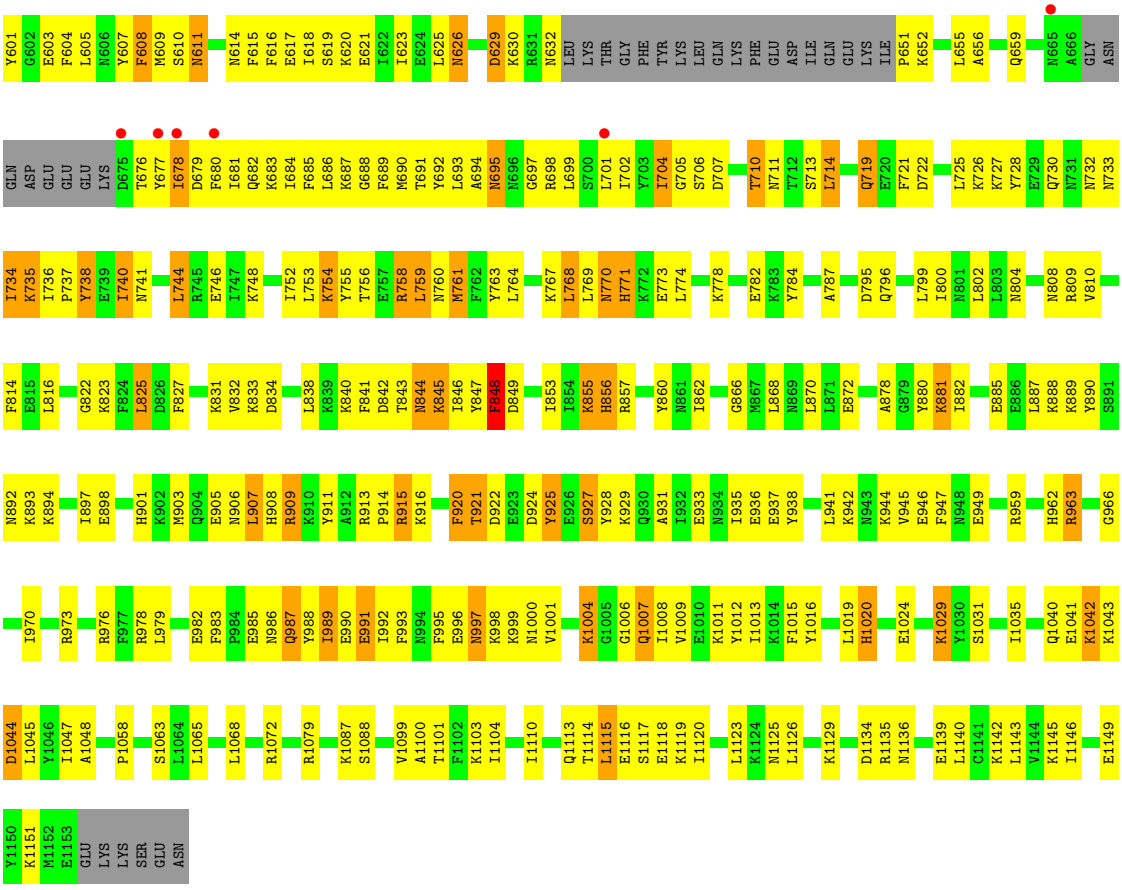




• Molecule 1: Uncharacterized protein

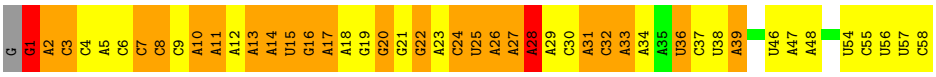
Chain B:





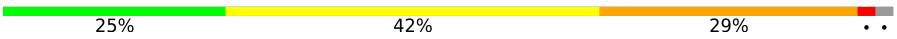
• Molecule 2: RNA (59-MER)

Chain C:



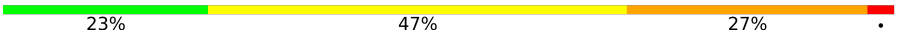
• Molecule 2: RNA (59-MER)

Chain E:



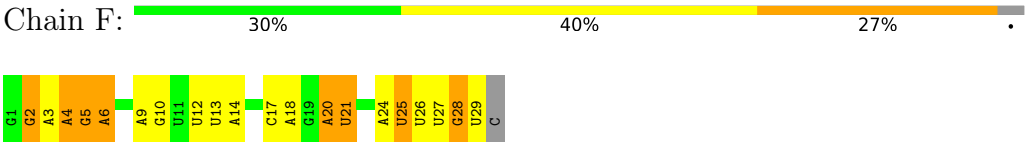
• Molecule 3: RNA (30-MER)

Chain D:



• Molecule 3: RNA (30-MER)

Chain F:


30%
40%
27%
G1
G2
A3
A4
G5
A6
A9
G10
U11
U12
U13
A14
C17
A18
G19
A20
U21
A24
U25
U26
U27
G28
U29
C

4 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	0/9290	0.79	10/12431 (0.1%)
1	B	0.67	0/9063	0.83	15/12146 (0.1%)
2	C	0.86	4/1375 (0.3%)	0.81	1/2137 (0.0%)
2	E	0.79	1/1375 (0.1%)	0.78	0/2137
3	D	0.72	3/721 (0.4%)	0.76	1/1122 (0.1%)
3	F	0.75	2/699 (0.3%)	0.75	1/1088 (0.1%)
All	All	0.71	10/22523 (0.0%)	0.81	28/31061 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (10) bond length outliers are listed below:

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

All (28) bond angle outliers are listed below:

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

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:MSE:HB2	1:A:954:GLN:OE1	2.21	0.40
1:A:872:GLU:O	1:A:876:ASP:HB2	2.22	0.40
1:A:971:TRP:CD1	1:A:1074:LEU:HD21	2.57	0.40
2:C:8:C:H6	2:C:8:C:O5'	2.03	0.40
2:C:18:A:O2'	2:C:19:G:H5'	2.21	0.40
1:B:914:PRO:O	1:B:916:LYS:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1115/1160 (96%)	1079 (97%)	34 (3%)	2 (0%)	47 77
1	B	1104/1160 (95%)	1064 (96%)	38 (3%)	2 (0%)	47 77
All	All	2219/2320 (96%)	2143 (97%)	72 (3%)	4 (0%)	47 77

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

analysed, and the total number of residues.

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA (i)

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

All (68) RNA backbone outliers are listed below:

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

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

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

All (11) RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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

All (39) RSRZ outliers are listed below:

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

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.