



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:31 AM UTC

PDB ID : 6IFO / pdb_00006ifo
Title : Crystal structure of AcrIIA2-SpyCas9-sgRNA ternary complex
Authors : Liu, L.; Wang, Y.
Deposited on : 2018-09-20
Resolution : 3.31 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

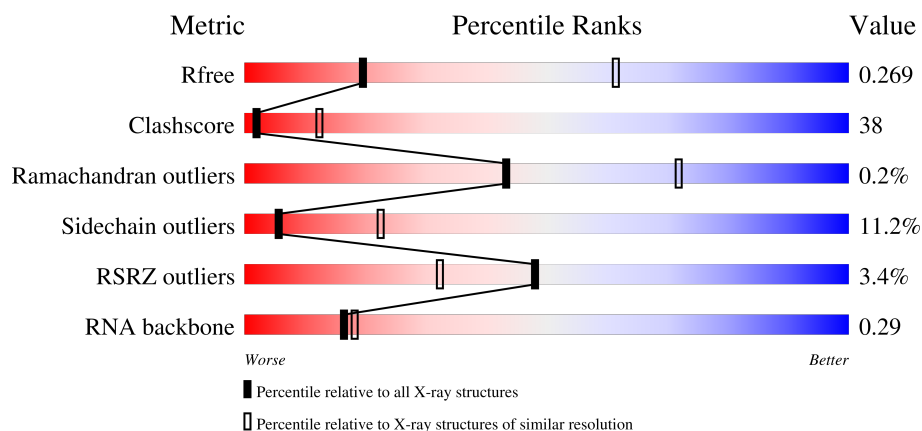
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)
RNA backbone	3983	1067 (3.64-3.00)

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 $\leq 5\%$. 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	1369	3% 63% 30% 6%
1	B	1369	3% 61% 32% 7%
2	C	99	% 37% 28% 19% 11%
2	D	99	% 25% 40% 20% 5% 9%

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Mol	Chain	Length	Quality of chain
3	E	123	7% 26% 43% 23% • 7%
3	F	123	9% 18% 51% 24% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27432 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1360	Total	C	N	O	S	0	0	0
			10904	6939	1886	2055	24			
1	B	1360	Total	C	N	O	S	0	0	0
			10900	6937	1886	2053	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q99ZW2
B	0	SER	-	expression tag	UNP Q99ZW2

- Molecule 2 is a RNA chain called RNA (99-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	88	Total	C	N	O	P	0	0	0
			1881	841	338	614	88			
2	D	90	Total	C	N	O	P	0	0	0
			1927	861	348	628	90			

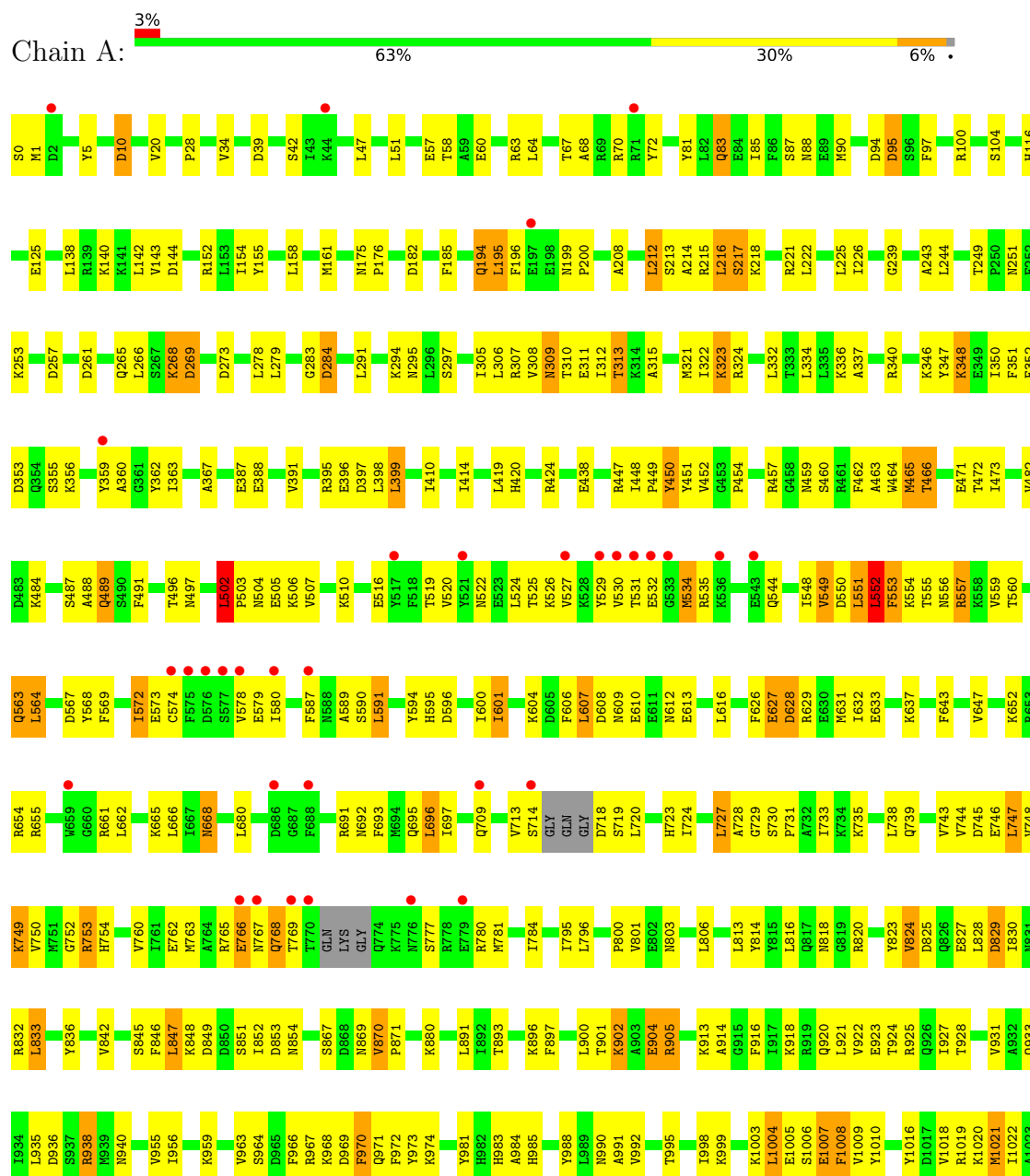
- Molecule 3 is a protein called AcrIIA2.

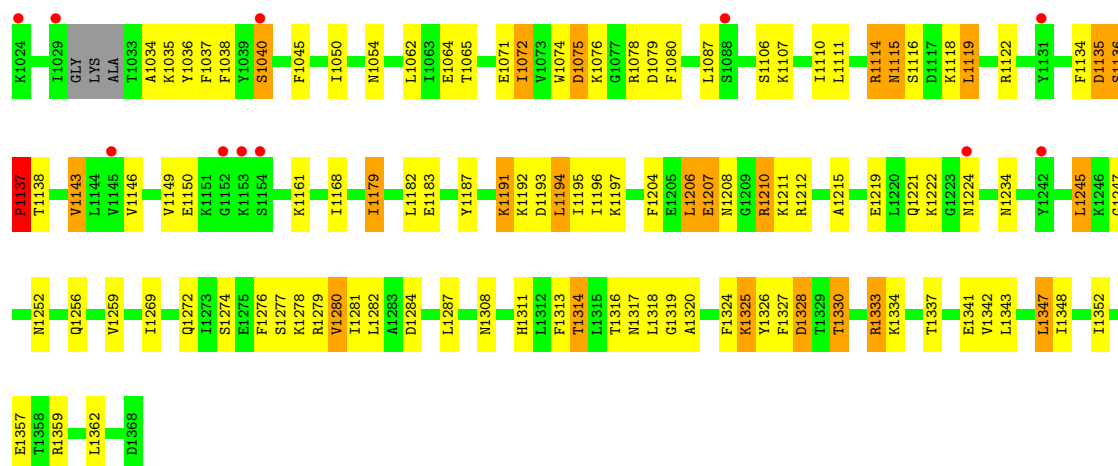
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	118	Total	C	N	O	S	0	0	0
			920	575	136	205	4			
3	E	115	Total	C	N	O	S	0	0	0
			900	565	136	195	4			

3 Residue-property plots

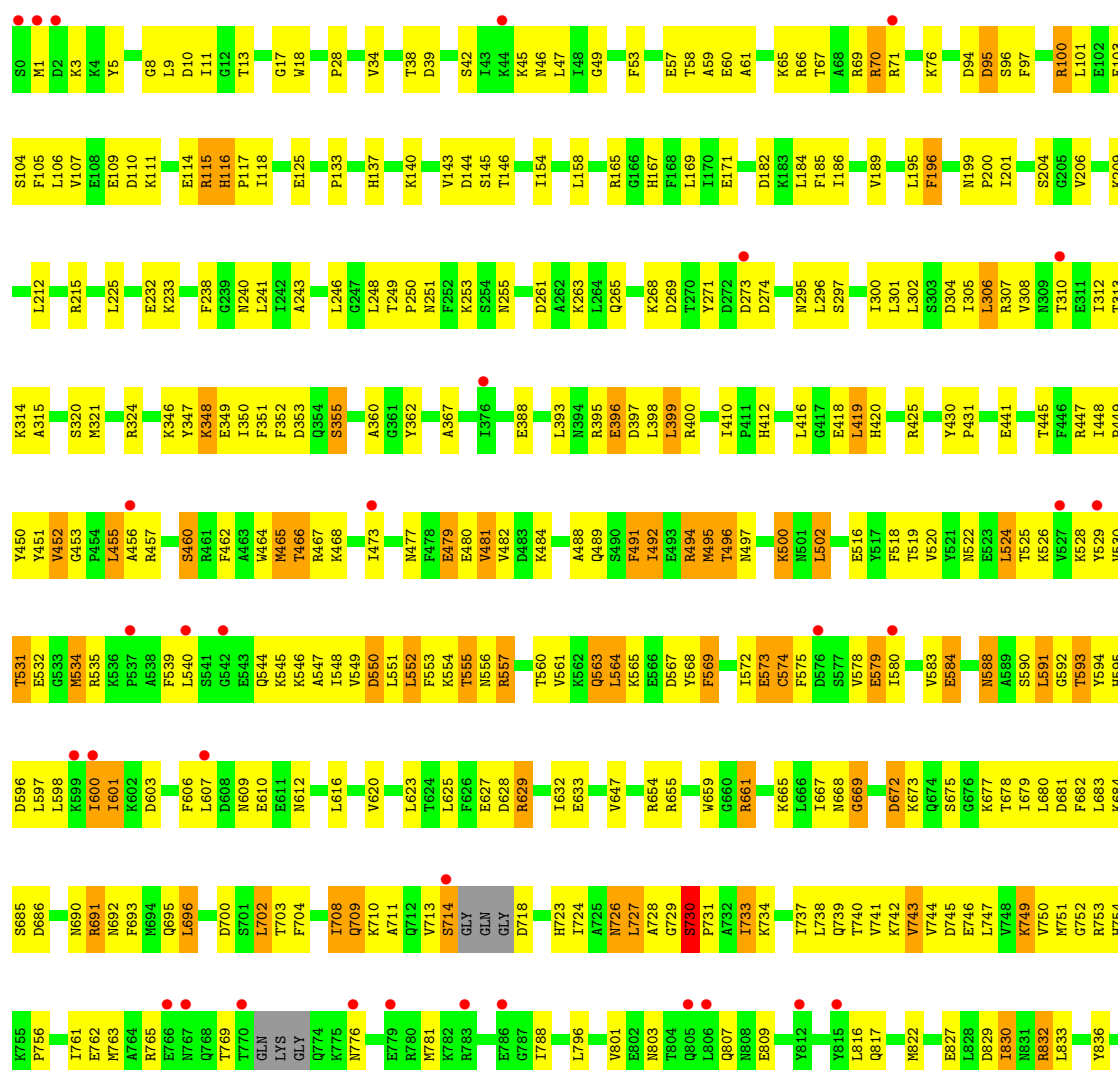
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

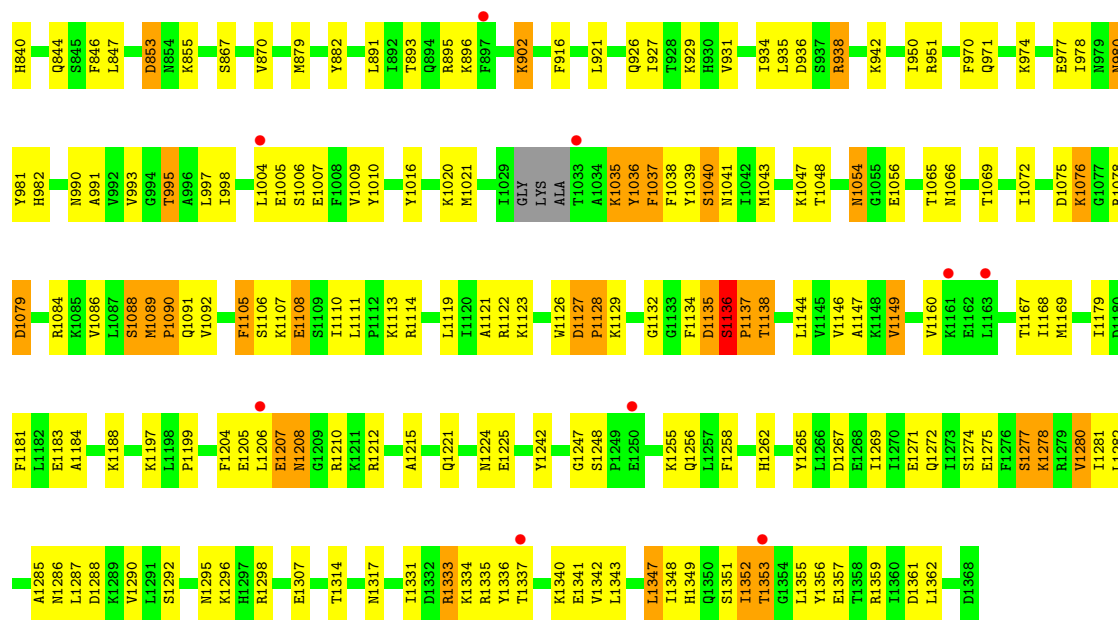
- Molecule 1: CRISPR-associated endonuclease Cas9/Csn1





• Molecule 1: CRISPR-associated endonuclease Cas9/Csn1

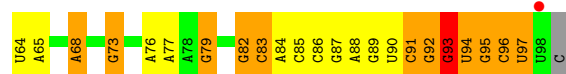
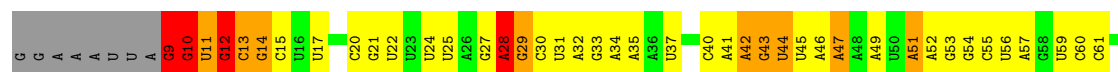
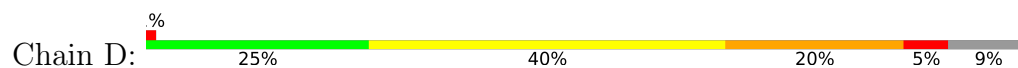




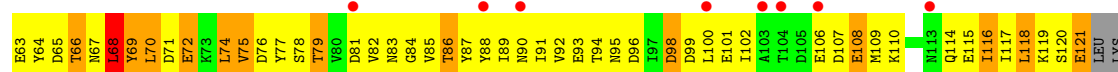
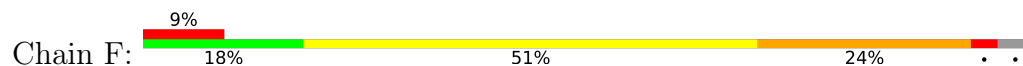
• Molecule 2: RNA (99-MER)



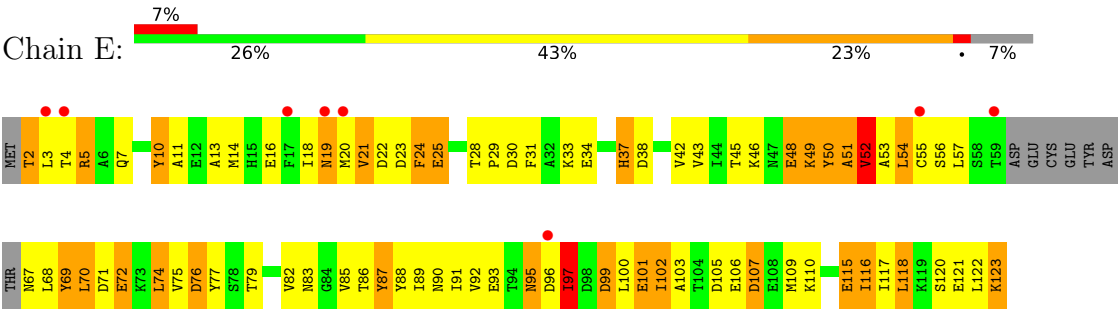
• Molecule 2: RNA (99-MER)



• Molecule 3: AcrIIA2



● Molecule 3: AcrIIA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.16Å 214.57Å 131.97Å 90.00° 102.89° 90.00°	Depositor
Resolution (Å)	49.51 – 3.31 49.51 – 3.31	Depositor EDS
% Data completeness (in resolution range)	66.1 (49.51-3.31) 66.1 (49.51-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.269	Depositor DCC
R_{free} test set	4234 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27432	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.73	6/11097 (0.1%)	0.96	24/14959 (0.2%)
1	B	0.79	12/11093 (0.1%)	1.02	35/14954 (0.2%)
2	C	0.52	0/2105	0.94	8/3279 (0.2%)
2	D	0.53	0/2157	0.94	9/3361 (0.3%)
3	E	0.66	0/911	1.10	5/1237 (0.4%)
3	F	0.83	0/932	1.25	9/1269 (0.7%)
All	All	0.73	18/28295 (0.1%)	1.00	90/39059 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	ASN	C-N	6.19	1.40	1.33
1	B	1136	SER	C-N	6.11	1.40	1.33
1	B	502	LEU	C-N	6.11	1.41	1.33
1	A	448	ILE	C-N	6.03	1.40	1.33
1	A	870	VAL	C-N	5.97	1.40	1.33
1	A	502	LEU	C-N	5.91	1.40	1.33
1	A	199	ASN	C-N	5.87	1.40	1.33
1	B	448	ILE	C-N	5.74	1.40	1.33
1	B	453	GLY	C-N	5.56	1.40	1.33
1	A	200	PRO	N-CD	5.52	1.55	1.47
1	B	1089	MET	C-N	5.49	1.40	1.34
1	B	200	PRO	N-CD	5.38	1.55	1.47
1	B	730	SER	C-N	5.25	1.40	1.33
1	B	1137	PRO	N-CD	5.22	1.55	1.47
1	B	1128	PRO	N-CD	5.18	1.55	1.47
1	A	871	PRO	N-CD	5.10	1.54	1.47
1	B	1090	PRO	N-CD	5.04	1.54	1.47
1	B	117	PRO	N-CD	5.03	1.54	1.47

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	GLY	N-CA-C	10.41	125.09	112.49
3	E	97	ILE	N-CA-C	9.17	119.97	110.62
3	F	24	PHE	N-CA-C	8.99	120.69	111.07
3	F	43	VAL	N-CA-C	8.56	121.45	109.29
1	B	1036	TYR	N-CA-C	8.02	120.03	111.28
1	A	462	PHE	N-CA-C	8.01	120.09	111.36
1	B	1108	GLU	N-CA-C	7.84	119.91	111.36
3	F	42	VAL	CB-CA-C	-7.54	98.93	111.29
1	B	1136	SER	CA-C-N	-7.47	112.99	120.31
1	B	1136	SER	C-N-CA	-7.47	112.99	120.31
2	C	42	A	C2'-C3'-O3'	7.25	124.57	113.70
1	B	199	ASN	CA-C-N	-7.20	113.26	120.31
1	B	199	ASN	C-N-CA	-7.20	113.26	120.31
2	D	10	G	C3'-C2'-O2'	-7.17	99.95	110.70
3	F	49	LYS	CA-C-N	-7.04	113.36	122.79
3	F	49	LYS	C-N-CA	-7.04	113.36	122.79
1	A	502	LEU	CA-C-N	-6.99	113.50	120.21
1	A	502	LEU	C-N-CA	-6.99	113.50	120.21
1	B	600	ILE	N-CA-C	6.96	117.08	110.53
1	A	199	ASN	CA-C-N	-6.86	113.24	120.03
1	A	199	ASN	C-N-CA	-6.86	113.24	120.03
2	D	93	G	C4'-C3'-O3'	-6.85	102.73	113.00
1	A	870	VAL	CA-C-N	-6.75	113.34	120.03
1	A	870	VAL	C-N-CA	-6.75	113.34	120.03
1	A	448	ILE	CA-C-N	-6.63	113.46	120.03
1	A	448	ILE	C-N-CA	-6.63	113.46	120.03
1	B	502	LEU	CA-C-N	-6.62	113.47	120.03
1	B	502	LEU	C-N-CA	-6.62	113.47	120.03
1	B	1079	ASP	N-CA-C	6.61	118.56	111.36
2	C	28	A	C2'-C3'-O3'	6.53	119.30	109.50
1	B	448	ILE	CA-C-N	-6.49	113.60	120.03
1	B	448	ILE	C-N-CA	-6.49	113.60	120.03
2	C	94	U	C3'-C2'-O2'	6.38	120.28	110.70
1	B	453	GLY	CA-C-N	-6.31	113.26	119.76
1	B	453	GLY	C-N-CA	-6.31	113.26	119.76
1	A	535	ARG	CB-CA-C	-6.27	109.36	116.63
1	B	452	VAL	N-CA-C	6.20	116.94	110.62
1	A	1245	LEU	N-CA-C	6.19	118.11	111.36
1	B	726	ASN	N-CA-C	6.14	117.97	111.28
1	B	462	PHE	N-CA-C	6.09	117.92	111.28
1	A	552	LEU	N-CA-C	6.07	117.69	111.14
1	A	312	ILE	N-CA-C	-6.05	104.61	110.72
3	F	43	VAL	CB-CA-C	-5.85	103.75	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	769	THR	N-CA-C	5.79	118.70	111.24
1	B	1135	ASP	N-CA-C	5.76	117.55	111.28
2	D	30	C	C3'-C2'-O2'	5.73	119.30	110.70
1	B	481	VAL	N-CA-C	5.71	116.48	110.72
1	A	1280	VAL	N-CA-C	5.69	116.12	111.62
3	F	75	VAL	N-CA-C	5.67	115.74	108.82
2	D	47	A	C4'-C3'-O3'	-5.67	104.50	113.00
2	C	92	G	C4'-C3'-O3'	-5.62	104.56	113.00
1	A	1320	ALA	CA-C-N	5.61	125.54	119.76
1	A	1320	ALA	C-N-CA	5.61	125.54	119.76
1	A	1279	ARG	N-CA-C	5.57	117.43	111.36
1	A	549	VAL	N-CA-C	-5.54	104.97	110.62
1	B	708	ILE	N-CA-C	5.50	116.22	110.62
2	D	53	G	C3'-C2'-O2'	5.49	118.94	110.70
1	A	553	PHE	N-CA-C	5.49	117.34	111.36
1	B	535	ARG	N-CA-C	5.42	117.26	111.36
1	B	3	LYS	N-CA-C	-5.38	106.58	112.72
1	B	730	SER	CA-C-N	-5.37	113.37	119.28
1	B	730	SER	C-N-CA	-5.37	113.37	119.28
1	A	1079	ASP	N-CA-C	5.36	117.20	111.36
1	A	1314	THR	N-CA-C	-5.35	105.56	111.71
1	B	169	LEU	N-CA-C	5.33	118.88	112.38
3	E	51	ALA	N-CA-C	5.33	118.16	110.28
1	B	743	VAL	CB-CA-C	-5.32	105.16	111.97
2	C	21	G	C4'-C3'-O3'	-5.32	105.02	113.00
1	A	1135	ASP	N-CA-C	5.31	119.74	112.68
2	C	92	G	C2'-C3'-O3'	5.26	121.60	113.70
1	B	206	VAL	N-CA-C	5.25	117.20	109.63
3	E	24	PHE	N-CA-C	5.25	117.01	111.28
1	A	194	GLN	N-CA-C	-5.25	105.56	111.28
3	E	76	ASP	N-CA-C	5.23	117.62	110.24
1	B	1127	ASP	CA-C-N	-5.21	113.26	119.05
1	B	1127	ASP	C-N-CA	-5.21	113.26	119.05
2	C	27	G	C1'-C2'-O2'	5.21	116.22	108.40
3	F	10	TYR	N-CA-C	-5.21	105.60	111.28
2	D	9	G	C2'-C3'-O3'	5.17	121.45	113.70
1	B	584	GLU	N-CA-C	-5.16	99.80	110.80
3	F	20	MET	N-CA-C	-5.16	105.66	111.28
1	B	116	HIS	CA-C-N	-5.15	113.40	119.84
1	B	116	HIS	C-N-CA	-5.15	113.40	119.84
2	D	28	A	C4'-C3'-O3'	5.15	117.13	109.40
1	A	1137	PRO	CA-N-CD	-5.15	104.79	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	87	TYR	N-CA-C	-5.13	100.05	108.41
2	C	19	G	C2'-C3'-O3'	-5.10	106.05	113.70
1	B	978	ILE	CB-CA-C	-5.07	105.48	111.97
2	D	79	G	C4'-C3'-O3'	-5.02	105.47	113.00
2	D	12	G	C2'-C3'-O3'	-5.00	106.20	113.70

There are no chirality outliers.

There are no planarity outliers.

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	10904	0	10832	644	0
1	B	10900	0	10835	791	0
2	C	1881	0	945	76	0
2	D	1927	0	966	168	0
3	E	900	0	831	191	0
3	F	920	0	824	293	0
All	All	27432	0	25233	2012	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 38.

All (2012) 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:B:569:PHE:HE1	1:B:578:VAL:CG1	1.05	1.61
1:B:531:THR:HG21	1:B:575:PHE:CE2	1.09	1.58
1:A:970:PHE:CD1	1:A:1080:PHE:CE1	1.94	1.52
1:B:569:PHE:CE1	1:B:578:VAL:HG11	1.02	1.52
1:B:569:PHE:CD1	1:B:578:VAL:HG21	1.41	1.50
3:E:31:PHE:CD1	3:E:91:ILE:HD11	1.43	1.50
1:A:564:LEU:CD2	1:A:580:ILE:CD1	1.91	1.48
1:B:531:THR:CG2	1:B:575:PHE:CE2	1.93	1.46
3:F:50:TYR:HE1	3:F:88:TYR:CD1	1.33	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:GLU:HG2	1:B:990:ASN:ND2	1.30	1.44
3:E:31:PHE:CD1	3:E:91:ILE:CD1	1.99	1.43
1:B:569:PHE:HD1	1:B:578:VAL:CG2	1.28	1.43
1:A:568:TYR:HE2	1:A:569:PHE:CE1	1.35	1.43
2:D:12:G:H8	2:D:13:C:C5	1.36	1.43
3:F:50:TYR:CE1	3:F:88:TYR:CD1	2.06	1.42
1:B:1347:LEU:HD12	1:B:1348:ILE:N	1.34	1.41
3:F:52:VAL:CG1	3:F:110:LYS:HG2	1.51	1.41
1:A:970:PHE:CE1	1:A:1080:PHE:CZ	2.09	1.40
1:A:560:THR:CG2	1:A:563:GLN:OE1	1.66	1.39
3:F:66:THR:CB	3:F:69:TYR:CE2	2.06	1.39
3:E:31:PHE:CE1	3:E:91:ILE:HD11	1.59	1.37
1:B:569:PHE:CE1	1:B:578:VAL:CG1	1.86	1.36
1:B:531:THR:HG21	1:B:575:PHE:CD2	1.59	1.36
1:B:596:ASP:O	1:B:600:ILE:CD1	1.72	1.35
3:F:81:ASP:OD1	3:F:86:THR:CG2	1.76	1.34
1:B:1106:SER:HB2	1:B:1136:SER:O	1.25	1.32
1:B:1206:LEU:CD1	1:B:1210:ARG:HE	1.43	1.31
1:A:568:TYR:CE2	1:A:569:PHE:CE1	2.20	1.30
3:F:52:VAL:HG11	3:F:110:LYS:CG	1.60	1.29
1:A:569:PHE:CD2	1:A:578:VAL:HG11	1.68	1.28
3:F:70:LEU:HD11	3:F:106:GLU:OE1	1.12	1.28
3:E:10:TYR:CE1	3:E:14:MET:HG2	1.65	1.28
1:B:531:THR:CG2	1:B:575:PHE:HE2	1.39	1.27
1:B:547:ALA:O	1:B:551:LEU:HD12	1.12	1.27
1:A:718:ASP:N	1:A:723:HIS:HE2	1.31	1.27
3:E:48:GLU:HG3	3:E:86:THR:OG1	1.32	1.27
1:A:564:LEU:HD23	1:A:580:ILE:CD1	1.59	1.26
3:E:57:LEU:CB	3:E:68:LEU:HD23	1.63	1.26
1:B:709:GLN:OE1	1:B:929:LYS:NZ	1.67	1.26
1:A:970:PHE:HD1	1:A:1080:PHE:CE1	1.38	1.26
1:B:304:ASP:O	1:B:307:ARG:NH2	1.68	1.26
1:B:846:PHE:O	1:B:1040:SER:HB3	1.12	1.25
3:F:4:THR:CB	3:F:7:GLN:HB2	1.63	1.25
1:A:564:LEU:HD21	1:A:580:ILE:CD1	1.56	1.25
1:A:568:TYR:CE2	1:A:569:PHE:CD1	2.26	1.24
3:F:71:ASP:O	3:F:95:ASN:CB	1.85	1.24
1:B:561:VAL:HG22	1:B:583:VAL:CG1	1.66	1.23
3:F:23:ASP:O	3:F:25:GLU:OE2	1.57	1.23
3:E:31:PHE:CE1	3:E:91:ILE:CD1	2.17	1.22
1:A:728:ALA:HB1	2:C:11:U:OP1	1.38	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:CD2	1:A:569:PHE:HD1	1.58	1.21
1:A:1313:PHE:O	1:A:1317:ASN:ND2	1.71	1.21
2:D:12:G:C8	2:D:13:C:C5	2.27	1.21
1:B:1206:LEU:HD13	1:B:1210:ARG:NE	1.56	1.21
1:B:597:LEU:O	1:B:601:ILE:CG2	1.87	1.20
1:B:1206:LEU:HD13	1:B:1210:ARG:HE	1.06	1.20
1:B:71:ARG:NE	2:D:17:U:C5	2.10	1.20
1:A:970:PHE:CE1	1:A:1080:PHE:HZ	1.53	1.20
3:F:50:TYR:OH	3:F:88:TYR:CZ	1.94	1.19
1:B:477:ASN:O	1:B:481:VAL:HG23	1.41	1.18
3:F:52:VAL:CG1	3:F:110:LYS:CG	2.19	1.17
3:F:79:THR:HG23	3:F:88:TYR:CE1	1.80	1.17
1:A:970:PHE:CD1	1:A:1080:PHE:HE1	1.42	1.16
3:E:48:GLU:OE1	3:E:85:VAL:HG13	1.39	1.16
3:F:50:TYR:CE1	3:F:88:TYR:CE1	2.34	1.16
1:A:568:TYR:CD2	1:A:569:PHE:CD1	2.34	1.15
1:B:561:VAL:CG2	1:B:583:VAL:CG1	2.25	1.15
1:A:564:LEU:CD2	1:A:580:ILE:HD13	1.65	1.15
1:A:1191:LYS:HB2	1:A:1194:LEU:HG	1.26	1.15
1:B:1206:LEU:CD1	1:B:1210:ARG:NE	2.08	1.14
3:F:81:ASP:OD1	3:F:86:THR:HG23	1.39	1.14
1:B:1336:TYR:HA	3:F:59:THR:CG2	1.78	1.14
1:A:970:PHE:HE1	1:A:1080:PHE:CZ	1.57	1.13
1:A:548:ILE:HG23	1:A:552:LEU:CD2	1.79	1.13
1:A:557:ARG:O	1:A:590:SER:OG	1.65	1.12
1:B:1242:TYR:HE2	1:B:1256:GLN:CD	1.57	1.12
2:D:10:G:HO2'	2:D:11:U:C5'	1.62	1.12
1:B:547:ALA:C	1:B:551:LEU:HD12	1.74	1.12
3:E:48:GLU:CG	3:E:86:THR:OG1	1.98	1.12
1:B:488:ALA:O	1:B:492:ILE:HG13	1.50	1.12
1:A:963:VAL:HG21	1:A:990:ASN:OD1	1.48	1.11
1:B:71:ARG:NH2	2:D:17:U:O4	1.84	1.11
1:A:564:LEU:HD23	1:A:580:ILE:HD12	1.22	1.11
1:A:728:ALA:O	1:A:927:ILE:HD13	1.51	1.10
3:F:14:MET:HE2	3:F:28:THR:HB	1.33	1.10
1:A:83:GLN:NE2	1:A:155:TYR:OH	1.85	1.10
1:A:194:GLN:OE1	1:A:557:ARG:NH1	1.83	1.10
1:A:1191:LYS:HD3	1:A:1194:LEU:HD11	1.33	1.10
1:A:1247:GLY:O	1:A:1252:ASN:OD1	1.69	1.10
1:B:545:LYS:O	1:B:548:ILE:HG22	1.51	1.10
1:B:596:ASP:O	1:B:600:ILE:HD12	0.94	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:LEU:HA	3:F:110:LYS:HD3	1.21	1.10
1:B:569:PHE:CD1	1:B:578:VAL:HG11	1.85	1.10
3:F:39:SER:O	3:F:93:GLU:HA	1.52	1.10
3:E:70:LEU:CD1	3:E:103:ALA:HB2	1.80	1.10
1:B:560:THR:HG22	1:B:563:GLN:OE1	1.52	1.09
1:B:561:VAL:CG2	1:B:583:VAL:HG11	1.83	1.09
1:B:746:GLU:OE1	1:B:1351:SER:OG	1.69	1.09
1:A:548:ILE:HG23	1:A:552:LEU:HD23	1.30	1.09
1:A:1021:MET:HG2	1:A:1036:TYR:CD1	1.86	1.09
1:B:460:SER:OG	2:D:61:C:P	2.10	1.09
1:B:547:ALA:O	1:B:551:LEU:CD1	1.99	1.09
3:E:51:ALA:HB3	3:E:90:ASN:CB	1.81	1.09
3:E:57:LEU:CB	3:E:68:LEU:CD2	2.29	1.09
1:B:1106:SER:CB	1:B:1136:SER:O	2.00	1.08
3:E:4:THR:HB	3:E:7:GLN:HB2	1.30	1.08
1:A:569:PHE:CE2	1:A:578:VAL:HG11	1.89	1.08
1:A:1021:MET:HG2	1:A:1036:TYR:HD1	1.12	1.08
1:A:530:VAL:CA	1:A:534:MET:HG2	1.82	1.07
1:B:597:LEU:O	1:B:601:ILE:HG22	0.91	1.07
3:F:14:MET:HE1	3:F:89:ILE:HD11	1.36	1.07
1:B:94:ASP:OD2	1:B:100:ARG:NH2	1.88	1.07
3:F:55:CYS:HB3	3:F:69:TYR:O	1.53	1.07
3:F:70:LEU:HD11	3:F:106:GLU:CD	1.80	1.07
1:B:195:LEU:C	1:B:196:PHE:HD2	1.61	1.07
1:B:1054:ASN:ND2	1:B:1056:GLU:OE1	1.88	1.07
3:E:70:LEU:HD11	3:E:103:ALA:HB2	1.36	1.07
1:A:1064:GLU:HG2	1:A:1076:LYS:NZ	1.68	1.06
1:B:846:PHE:HB3	1:B:1040:SER:HB2	1.37	1.06
3:E:48:GLU:HG3	3:E:86:THR:HG1	0.94	1.06
3:F:81:ASP:OD1	3:F:86:THR:HG22	1.48	1.06
3:F:93:GLU:HG3	3:F:94:THR:H	1.17	1.06
1:A:1179:ILE:HD11	1:A:1192:LYS:HE3	1.13	1.06
1:A:1247:GLY:HA3	1:A:1252:ASN:HD21	1.17	1.06
1:A:472:THR:HG23	2:C:59:U:OP2	1.55	1.06
1:B:1206:LEU:HD13	1:B:1210:ARG:CZ	1.85	1.06
1:B:601:ILE:HG21	1:B:607:LEU:HD21	1.08	1.05
1:B:977:GLU:N	1:B:977:GLU:OE1	1.88	1.05
2:D:10:G:O2'	2:D:11:U:O5'	1.73	1.05
1:A:1075:ASP:OD2	1:A:1078:ARG:N	1.88	1.05
1:A:1146:VAL:CG2	1:A:1194:LEU:HD12	1.86	1.05
3:F:4:THR:HB	3:F:7:GLN:HB2	1.10	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:ALA:CB	3:E:90:ASN:CB	2.35	1.05
1:A:901:THR:C	1:A:905:ARG:HH21	1.63	1.05
3:F:70:LEU:CD1	3:F:106:GLU:OE1	2.05	1.05
1:A:273:ASP:OD2	3:E:3:LEU:HD11	1.57	1.05
1:A:727:LEU:HD23	1:A:727:LEU:H	1.19	1.04
3:E:31:PHE:CD1	3:E:91:ILE:HD12	1.84	1.04
1:B:846:PHE:O	1:B:1040:SER:CB	2.05	1.04
1:A:346:LYS:O	1:A:350:ILE:HG13	1.55	1.04
1:B:71:ARG:CZ	2:D:17:U:O4	2.06	1.04
1:B:520:VAL:CG1	1:B:553:PHE:CE1	2.40	1.04
1:A:1106:SER:HB2	1:A:1136:SER:O	1.57	1.03
1:B:1336:TYR:HA	3:F:59:THR:HG21	1.36	1.03
1:A:451:TYR:O	1:A:464:TRP:CZ2	2.11	1.03
1:B:520:VAL:HG13	1:B:553:PHE:CE1	1.93	1.03
1:B:665:LYS:O	1:B:669:GLY:N	1.90	1.03
3:F:4:THR:HB	3:F:7:GLN:CB	1.87	1.03
3:F:54:LEU:HA	3:F:110:LYS:CD	1.87	1.03
1:A:1204:PHE:CE1	1:A:1347:LEU:HD12	1.93	1.03
3:F:64:TYR:O	3:F:66:THR:N	1.91	1.03
3:E:71:ASP:O	3:E:95:ASN:HB2	1.57	1.03
1:B:1075:ASP:N	1:B:1079:ASP:OD2	1.92	1.03
1:A:530:VAL:HA	1:A:534:MET:HG2	1.05	1.03
1:B:94:ASP:CG	1:B:100:ARG:HH22	1.66	1.03
1:B:1205:GLU:OE2	1:B:1359:ARG:NH2	1.92	1.02
1:B:1206:LEU:HD11	1:B:1212:ARG:HG2	1.41	1.02
1:B:1206:LEU:HD13	1:B:1210:ARG:NH2	1.75	1.01
3:F:52:VAL:HG11	3:F:110:LYS:HG2	1.11	1.01
3:E:54:LEU:HD11	3:E:110:LYS:CB	1.90	1.01
3:E:116:ILE:H	3:E:116:ILE:HD12	1.21	1.01
1:A:970:PHE:CD1	1:A:1080:PHE:CZ	2.40	1.01
1:A:451:TYR:O	1:A:464:TRP:HZ2	1.44	1.01
1:B:573:GLU:HG3	1:B:575:PHE:CD1	1.95	1.01
3:E:52:VAL:HG21	3:E:92:VAL:CG2	1.89	1.00
1:A:901:THR:C	1:A:905:ARG:NH2	2.19	1.00
1:B:1347:LEU:CD1	1:B:1348:ILE:H	1.75	1.00
3:F:18:ILE:HG23	3:F:24:PHE:HE1	1.26	1.00
1:B:569:PHE:CD1	1:B:578:VAL:CB	2.43	0.99
1:A:560:THR:HG22	1:A:563:GLN:CD	1.87	0.99
1:B:531:THR:H	1:B:534:MET:CG	1.75	0.99
1:B:1147:ALA:O	1:B:1160:VAL:CG2	2.11	0.99
2:D:10:G:O2'	2:D:11:U:C5'	2.07	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:GLU:CG	1:B:990:ASN:ND2	2.24	0.99
1:B:926:GLN:HG3	2:D:9:G:C3'	1.93	0.99
3:F:31:PHE:HE1	3:F:76:ASP:CB	1.76	0.99
3:F:50:TYR:OH	3:F:88:TYR:CE1	2.11	0.99
3:E:52:VAL:HG21	3:E:92:VAL:HG21	1.44	0.99
1:A:1179:ILE:HD11	1:A:1192:LYS:CE	1.92	0.99
1:B:46:ASN:ND2	1:B:1089:MET:HE2	1.77	0.99
1:A:530:VAL:HA	1:A:534:MET:CG	1.93	0.98
1:A:568:TYR:CE2	1:A:569:PHE:HE1	1.71	0.98
1:A:1064:GLU:CG	1:A:1076:LYS:NZ	2.25	0.98
1:A:1146:VAL:HG21	1:A:1194:LEU:HD12	1.43	0.98
1:B:569:PHE:CD1	1:B:578:VAL:CG2	2.17	0.98
3:F:45:THR:HG21	3:F:49:LYS:CB	1.94	0.98
3:F:52:VAL:HG12	3:F:110:LYS:HG2	1.42	0.98
3:E:2:THR:O	3:E:3:LEU:HG	1.63	0.98
1:B:561:VAL:HG22	1:B:583:VAL:HG11	0.98	0.98
1:B:926:GLN:CG	2:D:9:G:H5''	1.93	0.98
1:B:500:LYS:HD2	2:D:12:G:H1	1.28	0.97
1:B:665:LYS:HG3	1:B:669:GLY:HA3	1.44	0.97
1:B:71:ARG:CD	2:D:17:U:C5	2.47	0.97
1:B:171:GLU:HG2	1:B:629:ARG:NH1	1.80	0.97
3:F:66:THR:CB	3:F:69:TYR:HE2	1.69	0.97
1:B:1334:LYS:HZ3	3:F:57:LEU:HD13	1.29	0.97
3:F:50:TYR:CE1	3:F:88:TYR:CG	2.52	0.97
1:B:531:THR:N	1:B:534:MET:HG3	1.80	0.97
1:B:569:PHE:HA	1:B:573:GLU:HB2	1.45	0.96
1:B:71:ARG:NE	2:D:17:U:C4	2.32	0.96
1:B:1105:PHE:CE1	2:D:51:A:C6	2.52	0.96
3:E:70:LEU:CD2	3:E:101:GLU:HB3	1.96	0.96
1:B:1084:ARG:O	1:B:1088:SER:OG	1.84	0.96
1:B:1147:ALA:O	1:B:1160:VAL:HG22	1.65	0.96
1:A:273:ASP:OD2	3:E:3:LEU:CD1	2.13	0.95
1:A:564:LEU:HD21	1:A:580:ILE:HD13	0.97	0.95
1:A:970:PHE:CE1	1:A:1080:PHE:CE1	2.47	0.95
1:A:144:ASP:OD2	1:A:313:THR:HG22	1.65	0.95
3:F:14:MET:HE2	3:F:28:THR:CB	1.96	0.95
1:A:1179:ILE:CD1	1:A:1192:LYS:HE3	1.96	0.95
1:B:1277:SER:HA	1:B:1281:ILE:HG12	1.48	0.95
1:B:601:ILE:CG2	1:B:607:LEU:HD21	1.97	0.95
1:B:1335:ARG:O	3:F:59:THR:HG23	1.66	0.95
2:D:9:G:O2'	2:D:10:G:OP1	1.85	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:66:THR:CB	3:F:69:TYR:CZ	2.49	0.95
3:F:50:TYR:CZ	3:F:88:TYR:CE1	2.53	0.94
3:E:42:VAL:HB	3:E:121:GLU:OE2	1.67	0.94
1:B:1347:LEU:CD1	1:B:1348:ILE:N	2.28	0.94
1:A:718:ASP:N	1:A:723:HIS:NE2	2.14	0.94
1:A:999:LYS:HD3	1:A:1071:GLU:OE1	1.67	0.94
1:A:1064:GLU:HG2	1:A:1076:LYS:HZ2	1.19	0.94
3:E:5:ARG:NH2	3:E:122:LEU:O	1.99	0.94
1:B:1105:PHE:CE1	2:D:51:A:N6	2.35	0.94
2:D:11:U:O2'	2:D:12:G:OP2	1.85	0.94
3:F:42:VAL:HG23	3:F:121:GLU:CD	1.92	0.94
1:A:97:PHE:CD2	1:A:152:ARG:HG2	2.03	0.94
1:B:530:VAL:HA	1:B:534:MET:SD	2.07	0.94
1:B:547:ALA:HB1	1:B:551:LEU:CD1	1.97	0.94
1:B:980:ASN:ND2	1:B:1225:GLU:OE1	2.00	0.94
3:F:54:LEU:CA	3:F:110:LYS:HD3	1.97	0.94
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.33	0.93
1:B:846:PHE:CB	1:B:1040:SER:HB2	1.97	0.93
1:B:926:GLN:HG3	2:D:9:G:H3'	1.47	0.93
1:A:395:ARG:HD2	1:A:397:ASP:HB2	1.50	0.93
1:A:745:ASP:OD2	1:A:938:ARG:NH1	2.00	0.93
1:B:71:ARG:CZ	2:D:17:U:C4	2.51	0.93
1:B:991:ALA:O	1:B:995:THR:OG1	1.85	0.93
3:F:4:THR:OG1	3:F:7:GLN:CG	2.16	0.93
1:A:1191:LYS:HB2	1:A:1194:LEU:CG	1.98	0.93
1:B:1210:ARG:HA	1:B:1280:VAL:HG12	1.51	0.93
1:B:531:THR:CG2	1:B:575:PHE:CD2	2.36	0.93
1:B:569:PHE:CD1	1:B:578:VAL:CG1	2.49	0.93
1:B:1242:TYR:CE2	1:B:1256:GLN:CD	2.45	0.93
1:B:1108:GLU:O	1:B:1134:PHE:HE2	1.52	0.93
3:F:50:TYR:HE1	3:F:88:TYR:CE1	1.77	0.93
1:B:569:PHE:CE1	1:B:578:VAL:CB	2.51	0.93
3:F:43:VAL:CG2	3:F:44:ILE:N	2.32	0.92
3:E:75:VAL:HG12	3:E:76:ASP:H	1.34	0.92
1:A:569:PHE:HD2	1:A:578:VAL:HG11	1.22	0.92
1:B:71:ARG:HD3	2:D:17:U:C5	2.05	0.92
3:F:15:HIS:CE1	3:F:19:ASN:OD1	2.22	0.92
1:A:564:LEU:CD2	1:A:580:ILE:HD11	1.97	0.92
1:B:488:ALA:O	1:B:492:ILE:CG1	2.18	0.92
3:F:14:MET:CE	3:F:28:THR:HB	1.98	0.92
3:E:31:PHE:HD1	3:E:91:ILE:CD1	1.60	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:115:GLU:OE1	3:E:115:GLU:N	2.03	0.92
1:B:477:ASN:CG	1:B:481:VAL:HG21	1.94	0.92
3:E:10:TYR:HE1	3:E:14:MET:HG2	1.05	0.92
1:A:560:THR:HG22	1:A:563:GLN:OE1	0.75	0.92
3:F:22:ASP:HB3	3:F:82:VAL:CG1	2.00	0.92
1:B:460:SER:OG	2:D:61:C:OP1	1.85	0.92
1:B:71:ARG:HD3	2:D:17:U:C6	2.04	0.91
3:F:20:MET:SD	3:F:117:ILE:HD11	2.10	0.91
1:A:746:GLU:O	1:A:750:VAL:HG23	1.70	0.91
1:B:926:GLN:HG3	2:D:9:G:H5''	1.48	0.91
1:B:1242:TYR:CE2	1:B:1256:GLN:NE2	2.37	0.91
1:A:1146:VAL:HG21	1:A:1194:LEU:CD1	1.98	0.91
1:A:1204:PHE:CE2	1:A:1342:VAL:HG11	2.06	0.91
3:F:39:SER:HB2	3:F:91:ILE:CG2	2.01	0.91
3:E:70:LEU:HD23	3:E:101:GLU:HB3	1.51	0.91
1:A:215:ARG:C	1:A:216:LEU:HD12	1.95	0.91
1:A:828:LEU:HD22	1:A:836:TYR:CE2	2.06	0.91
1:B:398:LEU:HD21	1:B:399:LEU:HG	1.53	0.91
1:B:520:VAL:HG11	1:B:553:PHE:CD1	2.04	0.91
1:B:749:LYS:HE2	1:B:753:ARG:HH12	1.33	0.91
1:B:1242:TYR:HE2	1:B:1256:GLN:NE2	1.69	0.91
1:B:846:PHE:C	1:B:1040:SER:HB3	1.94	0.91
3:F:4:THR:CB	3:F:7:GLN:CB	2.45	0.91
3:F:22:ASP:HB3	3:F:82:VAL:HG11	1.53	0.91
1:B:395:ARG:HD2	1:B:397:ASP:HB2	1.50	0.91
1:B:601:ILE:HG21	1:B:607:LEU:CD2	1.99	0.91
1:B:829:ASP:HB3	1:B:832:ARG:HG3	1.52	0.91
3:E:31:PHE:HD1	3:E:91:ILE:HD11	1.12	0.91
3:E:49:LYS:CE	3:E:49:LYS:HA	1.98	0.91
3:F:45:THR:HG21	3:F:49:LYS:O	1.70	0.90
3:F:18:ILE:HG23	3:F:24:PHE:CE1	2.06	0.90
1:B:665:LYS:O	1:B:669:GLY:CA	2.19	0.90
1:A:465:MET:HE3	1:A:482:VAL:HG22	1.52	0.90
1:A:693:PHE:CZ	1:A:697:ILE:HD11	2.06	0.90
1:A:144:ASP:CG	1:A:313:THR:HG22	1.97	0.90
1:A:846:PHE:O	1:A:1040:SER:CB	2.19	0.90
1:B:916:PHE:HD1	1:B:1040:SER:HG	1.00	0.90
1:A:1191:LYS:CD	1:A:1194:LEU:HD11	2.02	0.90
1:B:520:VAL:HG13	1:B:553:PHE:HE1	1.33	0.90
1:B:531:THR:HG22	1:B:575:PHE:HE2	1.34	0.90
1:A:1107:LYS:HE2	3:E:93:GLU:OE2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:LEU:HD22	3:E:75:VAL:O	1.71	0.89
1:A:548:ILE:CG2	1:A:552:LEU:HD23	2.01	0.89
3:F:43:VAL:HG23	3:F:44:ILE:N	1.84	0.89
3:E:10:TYR:C	3:E:10:TYR:HD1	1.80	0.89
3:E:10:TYR:C	3:E:10:TYR:CD1	2.45	0.89
1:B:460:SER:OG	2:D:61:C:C5'	2.20	0.89
3:F:17:PHE:HE2	3:F:44:ILE:HG21	1.36	0.89
3:F:69:TYR:HA	3:F:102:ILE:HG12	1.52	0.89
2:D:10:G:O2'	2:D:11:U:H5'	1.70	0.89
1:A:796:LEU:HD22	1:A:801:VAL:HG12	1.54	0.89
1:B:398:LEU:HD23	1:B:399:LEU:HB2	1.54	0.89
1:A:766:GLU:HA	1:A:768:GLN:HE22	1.37	0.89
1:A:1311:HIS:O	1:A:1314:THR:HG23	1.72	0.89
1:A:1313:PHE:C	1:A:1317:ASN:ND2	2.31	0.89
1:B:749:LYS:HE2	1:B:753:ARG:NH1	1.87	0.89
1:B:554:LYS:HG2	1:B:594:TYR:CE2	2.08	0.88
1:B:520:VAL:HG11	1:B:553:PHE:CE1	2.09	0.88
3:F:23:ASP:C	3:F:25:GLU:OE2	2.16	0.88
1:B:96:SER:OG	1:B:100:ARG:NH1	2.06	0.88
1:B:460:SER:HG	2:D:61:C:P	1.91	0.88
1:B:603:ASP:OD1	1:B:606:PHE:N	2.05	0.88
1:B:673:LYS:N	1:B:703:THR:OG1	2.07	0.88
3:E:69:TYR:HB3	3:E:101:GLU:O	1.74	0.88
1:A:465:MET:CE	1:A:482:VAL:HG22	2.04	0.88
1:B:46:ASN:ND2	1:B:1089:MET:CE	2.36	0.88
1:B:1206:LEU:HD12	1:B:1210:ARG:NE	1.88	0.88
1:B:1334:LYS:HG2	3:F:57:LEU:HD22	1.56	0.88
3:E:14:MET:HE2	3:E:28:THR:HB	1.56	0.88
1:B:1286:ASN:ND2	1:B:1334:LYS:HG3	1.89	0.88
3:F:50:TYR:CZ	3:F:88:TYR:CZ	2.61	0.88
1:A:568:TYR:HE2	1:A:569:PHE:HE1	0.91	0.88
1:A:692:ASN:O	1:A:696:LEU:HD12	1.74	0.88
3:F:4:THR:OG1	3:F:7:GLN:HG3	1.74	0.88
1:A:144:ASP:OD1	1:A:313:THR:CG2	2.21	0.88
1:B:100:ARG:HH11	1:B:100:ARG:HG3	1.37	0.88
1:B:672:ASP:OD2	1:B:675:SER:N	2.05	0.87
1:B:1206:LEU:HD13	1:B:1210:ARG:HH21	1.35	0.87
3:E:31:PHE:CE1	3:E:91:ILE:CG1	2.57	0.87
1:A:1136:SER:OG	3:E:96:ASP:OD2	1.91	0.87
3:F:15:HIS:HE1	3:F:19:ASN:OD1	1.56	0.87
1:A:1211:LYS:HG3	1:A:1224:ASN:HD21	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1242:TYR:CE2	1:B:1256:GLN:CG	2.57	0.87
1:B:494:ARG:HG2	1:B:494:ARG:HH11	1.38	0.87
1:B:539:PHE:HB3	1:B:690:ASN:ND2	1.90	0.87
1:B:1105:PHE:HE1	2:D:51:A:N6	1.71	0.87
3:F:93:GLU:HG3	3:F:94:THR:N	1.88	0.87
1:B:1334:LYS:NZ	3:F:57:LEU:HD13	1.89	0.86
1:B:451:TYR:O	1:B:464:TRP:CZ2	2.29	0.86
1:B:1336:TYR:HA	3:F:59:THR:HG23	1.56	0.86
3:F:45:THR:CG2	3:F:49:LYS:CB	2.53	0.86
2:D:12:G:H8	2:D:13:C:H5	1.11	0.86
1:B:528:LYS:O	1:B:580:ILE:HG23	1.74	0.86
3:F:42:VAL:CG2	3:F:121:GLU:CD	2.49	0.86
1:A:901:THR:O	1:A:905:ARG:NH2	2.07	0.86
3:E:48:GLU:OE1	3:E:85:VAL:CG1	2.21	0.86
1:B:195:LEU:O	1:B:196:PHE:HD2	1.57	0.86
1:B:762:GLU:HG2	1:B:990:ASN:HD22	1.36	0.86
1:B:1242:TYR:CE2	1:B:1256:GLN:HG2	2.11	0.86
1:A:569:PHE:CD2	1:A:578:VAL:CG1	2.58	0.86
3:E:2:THR:C	3:E:3:LEU:HG	2.00	0.86
1:B:661:ARG:HB2	2:D:10:G:N2	1.90	0.86
1:B:554:LYS:HG2	1:B:594:TYR:HE2	1.40	0.85
3:F:57:LEU:HB2	3:F:68:LEU:HD12	1.59	0.85
1:A:569:PHE:HD2	1:A:578:VAL:CG1	1.90	0.85
1:B:460:SER:OG	2:D:61:C:H5'	1.75	0.85
1:B:672:ASP:HB2	1:B:702:LEU:HD23	1.58	0.85
1:B:1206:LEU:HD12	1:B:1210:ARG:HE	1.42	0.85
1:A:846:PHE:HE1	1:A:913:LYS:HE3	1.42	0.85
1:B:1113:LYS:HB2	1:B:1129:LYS:O	1.75	0.85
1:B:195:LEU:O	1:B:196:PHE:CD2	2.30	0.85
1:B:560:THR:HG22	1:B:563:GLN:CD	2.02	0.85
1:A:10:ASP:OD2	1:A:983:HIS:O	1.95	0.85
1:B:762:GLU:CG	1:B:990:ASN:HD21	1.85	0.84
1:B:1210:ARG:HG3	1:B:1280:VAL:HA	1.57	0.84
2:D:85:C:C4	2:D:86:C:N4	2.45	0.84
3:E:2:THR:O	3:E:3:LEU:CG	2.24	0.84
1:A:496:THR:HG21	1:A:506:LYS:HG2	1.60	0.84
1:B:564:LEU:HD11	1:B:580:ILE:HD12	1.58	0.84
1:B:1086:VAL:O	1:B:1089:MET:HG2	1.76	0.84
3:F:47:ASN:O	3:F:49:LYS:N	2.10	0.84
1:A:531:THR:N	1:A:534:MET:SD	2.50	0.84
1:B:1108:GLU:OE2	3:F:37:HIS:CG	2.30	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:THR:N	1:B:534:MET:SD	2.49	0.84
1:B:597:LEU:C	1:B:601:ILE:HG22	2.00	0.84
3:E:19:ASN:O	3:E:21:VAL:HG23	1.77	0.84
3:F:31:PHE:HE1	3:F:76:ASP:HB2	1.40	0.84
1:B:569:PHE:HA	1:B:573:GLU:CB	2.08	0.84
1:B:665:LYS:C	1:B:669:GLY:H	1.86	0.84
3:E:72:GLU:HG2	3:E:92:VAL:HG11	1.59	0.84
1:B:195:LEU:C	1:B:196:PHE:CD2	2.53	0.84
3:F:69:TYR:HB3	3:F:101:GLU:O	1.78	0.84
3:E:67:ASN:O	3:E:69:TYR:CE1	2.30	0.84
1:A:1204:PHE:CD2	1:A:1342:VAL:CG1	2.61	0.83
1:B:1258:PHE:O	1:B:1262:HIS:ND1	2.11	0.83
1:A:1114:ARG:CZ	1:A:1114:ARG:HB3	2.08	0.83
1:B:531:THR:O	1:B:534:MET:HG3	1.78	0.83
1:A:849:ASP:OD1	1:A:851:SER:OG	1.96	0.83
1:B:829:ASP:CB	1:B:832:ARG:HG3	2.09	0.83
1:A:1337:THR:HG22	3:E:97:ILE:HD11	1.58	0.83
1:B:1210:ARG:HG3	1:B:1280:VAL:HG12	1.60	0.83
1:A:728:ALA:O	1:A:927:ILE:CD1	2.26	0.83
1:B:573:GLU:HG3	1:B:575:PHE:CE1	2.14	0.83
3:F:31:PHE:CE1	3:F:76:ASP:HB2	2.14	0.83
1:A:554:LYS:NZ	1:A:608:ASP:OD2	2.11	0.83
1:B:561:VAL:CG2	1:B:583:VAL:HG13	2.08	0.83
1:B:1206:LEU:HD11	1:B:1212:ARG:CG	2.08	0.83
1:A:568:TYR:HD2	1:A:569:PHE:CD1	1.96	0.82
1:B:672:ASP:HA	1:B:703:THR:HB	1.61	0.82
2:D:87:G:H3'	2:D:87:G:N3	1.93	0.82
3:F:19:ASN:O	3:F:21:VAL:HG23	1.78	0.82
3:F:67:ASN:C	3:F:68:LEU:HD13	2.04	0.82
3:F:45:THR:HG21	3:F:49:LYS:C	2.04	0.82
3:F:45:THR:CG2	3:F:49:LYS:O	2.27	0.82
1:A:1308:ASN:HB3	1:A:1326:TYR:CD1	2.14	0.82
3:F:17:PHE:CE2	3:F:44:ILE:HG21	2.15	0.82
1:A:846:PHE:O	1:A:1040:SER:HB3	1.79	0.82
1:B:583:VAL:HG13	1:B:584:GLU:O	1.79	0.82
3:F:14:MET:HE1	3:F:89:ILE:CD1	2.07	0.82
3:F:74:LEU:HD22	3:F:75:VAL:O	1.78	0.82
3:E:51:ALA:HB1	3:E:52:VAL:HG22	1.60	0.82
1:A:829:ASP:CG	1:A:832:ARG:HG3	2.05	0.82
1:A:1204:PHE:CD2	1:A:1342:VAL:HG11	2.15	0.82
1:B:547:ALA:HB1	1:B:551:LEU:HD11	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLU:HG2	1:A:990:ASN:ND2	1.94	0.81
1:A:846:PHE:HE1	1:A:913:LYS:CE	1.93	0.81
1:B:569:PHE:HE1	1:B:578:VAL:HG12	1.38	0.81
3:E:31:PHE:HE1	3:E:91:ILE:HD11	1.43	0.81
3:E:54:LEU:CD1	3:E:110:LYS:CB	2.58	0.81
3:E:18:ILE:HD11	3:E:24:PHE:HZ	1.45	0.81
1:A:897:PHE:O	1:A:901:THR:HG23	1.79	0.81
1:A:1064:GLU:CG	1:A:1076:LYS:HZ1	1.92	0.81
1:A:1333:ARG:HH11	1:A:1333:ARG:HG3	1.45	0.81
1:B:465:MET:HE1	1:B:473:ILE:CD1	2.11	0.81
1:B:556:ASN:OD1	1:B:563:GLN:NE2	2.13	0.81
1:A:531:THR:HB	1:A:534:MET:SD	2.21	0.81
1:B:10:ASP:OD1	1:B:762:GLU:OE1	1.99	0.81
1:B:557:ARG:O	1:B:590:SER:OG	1.98	0.81
1:A:1333:ARG:HG3	1:A:1333:ARG:NH1	1.96	0.80
1:B:457:ARG:NH2	2:D:57:A:OP1	2.13	0.80
1:B:488:ALA:O	1:B:492:ILE:CD1	2.30	0.80
1:B:829:ASP:CG	1:B:832:ARG:HG3	2.06	0.80
1:B:554:LYS:O	1:B:595:HIS:HE1	1.63	0.80
1:B:564:LEU:HD11	1:B:580:ILE:CD1	2.11	0.80
1:A:555:THR:C	1:A:556:ASN:HD22	1.90	0.80
1:A:520:VAL:HG11	1:A:553:PHE:CD1	2.16	0.80
1:A:853:ASP:OD2	1:A:893:THR:HG21	1.82	0.80
1:B:665:LYS:O	1:B:669:GLY:HA3	1.82	0.80
1:B:926:GLN:CG	2:D:9:G:H3'	2.11	0.80
3:F:52:VAL:CG1	3:F:110:LYS:HG3	2.11	0.80
1:A:559:VAL:HG13	1:A:563:GLN:HG3	1.61	0.79
1:A:1204:PHE:CG	1:A:1342:VAL:HG13	2.16	0.79
1:B:46:ASN:CG	1:B:1089:MET:CE	2.55	0.79
1:B:1206:LEU:HB2	1:B:1210:ARG:HB3	1.62	0.79
1:B:796:LEU:HD22	1:B:801:VAL:HG12	1.63	0.79
1:B:1036:TYR:HB2	1:B:1037:PHE:CE1	2.18	0.79
3:E:10:TYR:HE1	3:E:14:MET:CG	1.91	0.79
1:B:549:VAL:HA	1:B:553:PHE:HB2	1.65	0.79
1:B:749:LYS:CE	1:B:753:ARG:HH12	1.95	0.79
3:E:51:ALA:HB2	3:E:90:ASN:CB	2.13	0.79
1:A:1204:PHE:CG	1:A:1342:VAL:CG1	2.66	0.78
3:F:55:CYS:SG	3:F:110:LYS:HE3	2.23	0.78
1:B:553:PHE:HB3	1:B:591:LEU:HD11	1.65	0.78
1:B:677:LYS:NZ	1:B:685:SER:O	2.16	0.78
1:B:1267:ASP:OD1	1:B:1298:ARG:NH2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:MET:HE1	1:A:473:ILE:CD1	2.13	0.78
1:A:728:ALA:CB	2:C:11:U:OP1	2.28	0.78
1:A:1146:VAL:HG23	1:A:1194:LEU:HD12	1.65	0.78
1:A:140:LYS:NZ	1:A:144:ASP:OD1	2.16	0.78
1:B:730:SER:O	1:B:733:ILE:HG22	1.84	0.78
1:B:1340:LYS:NZ	1:B:1343:LEU:HD12	1.99	0.78
1:A:936:ASP:HB2	1:A:955:VAL:HG11	1.66	0.78
3:E:70:LEU:HD11	3:E:103:ALA:CB	2.12	0.78
1:B:395:ARG:HD2	1:B:397:ASP:CB	2.14	0.78
1:B:71:ARG:HE	2:D:17:U:H5	1.32	0.77
1:A:963:VAL:CG2	1:A:990:ASN:OD1	2.31	0.77
1:B:500:LYS:HD2	2:D:12:G:N1	1.98	0.77
3:E:31:PHE:CE1	3:E:91:ILE:HG13	2.18	0.77
1:B:762:GLU:HG2	1:B:990:ASN:HD21	0.96	0.77
1:B:1147:ALA:O	1:B:1160:VAL:HG23	1.83	0.77
1:B:1105:PHE:CD2	1:B:1169:MET:HG3	2.19	0.77
3:F:4:THR:OG1	3:F:7:GLN:CB	2.32	0.77
3:F:43:VAL:HG23	3:F:44:ILE:H	1.46	0.77
1:A:268:LYS:NZ	3:E:28:THR:O	2.15	0.77
1:A:520:VAL:CG1	1:A:553:PHE:CE1	2.67	0.77
1:A:1247:GLY:CA	1:A:1252:ASN:HD21	1.96	0.77
1:B:201:ILE:HD11	1:B:232:GLU:CD	2.08	0.77
1:B:531:THR:N	1:B:534:MET:CG	2.42	0.77
1:B:561:VAL:HG21	1:B:583:VAL:CG1	2.14	0.77
1:B:846:PHE:CA	1:B:1040:SER:HB2	2.14	0.77
3:F:29:PRO:HG2	3:F:78:SER:OG	1.85	0.77
1:A:1247:GLY:HA3	1:A:1252:ASN:ND2	1.98	0.76
1:B:46:ASN:CG	1:B:1089:MET:HE2	2.11	0.76
2:D:20:C:H6	2:D:20:C:H5''	1.48	0.76
2:D:93:G:C3'	2:D:94:U:H5'	2.16	0.76
3:F:42:VAL:O	3:F:42:VAL:HG12	1.83	0.76
1:B:307:ARG:NH1	1:B:397:ASP:OD2	2.18	0.76
1:B:830:ILE:O	1:B:833:LEU:HG	1.84	0.76
1:B:1206:LEU:HD22	1:B:1341:GLU:OE2	1.85	0.76
1:B:677:LYS:HD3	1:B:682:PHE:CE1	2.21	0.76
1:A:829:ASP:OD1	1:A:832:ARG:N	2.17	0.76
1:A:563:GLN:O	1:A:567:ASP:N	2.18	0.76
1:B:569:PHE:O	1:B:574:CYS:N	2.18	0.76
2:D:13:C:O2	2:D:14:G:C2	2.38	0.76
3:E:31:PHE:HE1	3:E:91:ILE:CG1	1.99	0.76
3:E:48:GLU:O	3:E:49:LYS:HE3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TYR:CD2	1:A:569:PHE:CE2	2.73	0.76
1:A:1333:ARG:H	1:A:1333:ARG:HD2	1.50	0.76
3:F:54:LEU:HD23	3:F:55:CYS:N	2.01	0.76
1:A:100:ARG:HG3	1:A:100:ARG:NH1	1.98	0.75
1:A:745:ASP:CG	1:A:938:ARG:HH12	1.94	0.75
3:F:51:ALA:HB2	3:F:90:ASN:OD1	1.85	0.75
1:A:544:GLN:O	1:A:548:ILE:HG13	1.84	0.75
3:F:20:MET:HE2	3:F:117:ILE:CG1	2.16	0.75
1:B:301:LEU:O	1:B:305:ILE:HG13	1.86	0.75
1:B:315:ALA:HB1	1:B:418:GLU:OE2	1.86	0.75
1:B:1065:THR:HG22	1:B:1072:ILE:HA	1.68	0.75
1:A:1337:THR:CG2	3:E:97:ILE:HD11	2.15	0.75
3:E:14:MET:HE2	3:E:28:THR:CB	2.16	0.75
2:C:16:U:C4	2:C:17:U:C4	2.75	0.75
1:B:1122:ARG:O	1:B:1123:LYS:HG2	1.87	0.75
1:B:672:ASP:HA	1:B:703:THR:CB	2.16	0.75
1:A:449:PRO:HD2	1:A:452:VAL:HB	1.69	0.75
3:E:48:GLU:CD	3:E:85:VAL:HG13	2.11	0.74
3:E:102:ILE:HD12	3:E:102:ILE:N	2.02	0.74
1:A:1337:THR:HG22	3:E:97:ILE:CD1	2.16	0.74
1:B:451:TYR:O	1:B:464:TRP:HZ2	1.70	0.74
1:B:449:PRO:HD2	1:B:452:VAL:CG2	2.16	0.74
1:B:561:VAL:HG21	1:B:583:VAL:HG13	1.68	0.74
1:B:628:ASP:O	1:B:632:ILE:HG13	1.86	0.74
1:A:1122:ARG:HG2	1:A:1134:PHE:CE1	2.22	0.74
1:B:416:LEU:HD12	1:B:416:LEU:O	1.86	0.74
1:A:216:LEU:HD12	1:A:216:LEU:N	2.03	0.74
1:B:465:MET:HE1	1:B:473:ILE:HD11	1.70	0.74
1:B:606:PHE:O	1:B:612:ASN:ND2	2.18	0.74
1:B:727:LEU:N	1:B:727:LEU:HD23	2.02	0.74
1:B:1020:LYS:O	1:B:1035:LYS:HD2	1.87	0.74
1:A:591:LEU:HD23	1:A:591:LEU:N	2.03	0.74
3:F:24:PHE:HD1	3:F:24:PHE:H	1.33	0.74
1:A:90:MET:SD	1:A:97:PHE:HD2	2.11	0.74
1:A:829:ASP:OD1	1:A:832:ARG:HG3	1.87	0.74
1:A:999:LYS:CD	1:A:1071:GLU:OE1	2.36	0.74
1:B:1274:SER:O	1:B:1278:LYS:HG3	1.88	0.74
1:A:692:ASN:C	1:A:696:LEU:HD12	2.12	0.73
1:B:661:ARG:HB2	2:D:10:G:C2	2.23	0.73
1:B:1210:ARG:CG	1:B:1280:VAL:HG12	2.18	0.73
1:A:1072:ILE:N	1:A:1072:ILE:HD12	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:LEU:HD12	1:B:1210:ARG:HB3	1.71	0.73
1:B:398:LEU:CD2	1:B:399:LEU:HG	2.18	0.73
3:F:53:ALA:O	3:F:72:GLU:OE1	2.06	0.73
3:E:4:THR:HB	3:E:7:GLN:CB	2.15	0.73
1:A:520:VAL:HG11	1:A:553:PHE:CE1	2.23	0.73
1:A:766:GLU:HA	1:A:768:GLN:NE2	2.03	0.73
3:F:13:ALA:HB2	3:F:119:LYS:HD3	1.69	0.73
3:F:47:ASN:C	3:F:49:LYS:H	1.96	0.73
1:A:457:ARG:NH2	2:C:57:A:H5''	2.03	0.73
1:A:1333:ARG:HH11	1:A:1333:ARG:CG	2.02	0.73
1:B:846:PHE:CA	1:B:1040:SER:CB	2.67	0.73
3:F:10:TYR:OH	3:F:29:PRO:O	2.06	0.73
3:E:49:LYS:HA	3:E:49:LYS:HE2	1.69	0.73
1:A:144:ASP:OD1	1:A:313:THR:HG22	1.87	0.73
1:A:195:LEU:C	1:A:196:PHE:HD2	1.97	0.73
1:A:999:LYS:HG2	1:A:1071:GLU:OE1	1.89	0.73
1:A:1194:LEU:N	1:A:1194:LEU:HD23	2.04	0.73
3:F:50:TYR:CD1	3:F:77:TYR:CE1	2.77	0.73
1:B:710:LYS:O	1:B:713:VAL:HG23	1.89	0.73
3:F:4:THR:CB	3:F:7:GLN:HG3	2.18	0.73
1:B:70:ARG:NH1	2:D:15:C:OP1	2.22	0.72
1:A:1211:LYS:HG3	1:A:1224:ASN:ND2	2.04	0.72
2:C:87:G:C8	2:C:92:G:C2	2.77	0.72
1:A:557:ARG:NH2	1:A:596:ASP:N	2.37	0.72
1:A:1191:LYS:CB	1:A:1194:LEU:HG	2.14	0.72
3:F:118:LEU:HD23	3:F:118:LEU:C	2.15	0.72
1:A:488:ALA:O	1:A:491:PHE:HB3	1.90	0.72
1:B:398:LEU:HD23	1:B:398:LEU:C	2.15	0.72
1:B:728:ALA:CB	2:D:10:G:O5'	2.38	0.72
1:A:526:LYS:HE3	1:A:692:ASN:HB3	1.72	0.72
2:D:85:C:N3	2:D:86:C:N4	2.37	0.72
1:A:1191:LYS:HB2	1:A:1194:LEU:CD1	2.20	0.72
1:A:1333:ARG:H	1:A:1333:ARG:CD	2.03	0.72
1:B:665:LYS:CG	1:B:669:GLY:HA3	2.16	0.72
1:B:419:LEU:C	1:B:419:LEU:HD13	2.15	0.72
1:B:661:ARG:HB2	2:D:10:G:H22	1.53	0.72
1:B:1286:ASN:HD21	1:B:1334:LYS:HG3	1.53	0.72
3:E:2:THR:O	3:E:3:LEU:CD2	2.38	0.72
3:F:50:TYR:OH	3:F:88:TYR:OH	2.06	0.72
1:A:97:PHE:CE2	1:A:152:ARG:HG2	2.25	0.71
1:A:901:THR:OG1	1:A:905:ARG:NH2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:LYS:NZ	1:A:905:ARG:NH1	2.38	0.71
1:B:1336:TYR:CD2	3:F:59:THR:HG21	2.25	0.71
1:A:846:PHE:O	1:A:1040:SER:HB2	1.88	0.71
1:B:1333:ARG:NH1	3:F:71:ASP:OD2	2.23	0.71
3:F:31:PHE:CE1	3:F:76:ASP:CB	2.66	0.71
1:B:96:SER:C	1:B:100:ARG:NH1	2.48	0.71
1:B:867:SER:O	1:B:1054:ASN:OD1	2.09	0.71
1:B:544:GLN:HG2	1:B:568:TYR:OH	1.91	0.71
1:B:1108:GLU:OE2	3:F:37:HIS:ND1	2.24	0.71
2:D:11:U:O3'	2:D:12:G:O4'	2.08	0.71
2:C:97:U:H6	2:C:97:U:H5'	1.55	0.71
1:B:564:LEU:C	1:B:564:LEU:HD12	2.15	0.71
1:B:1285:ALA:HB3	1:B:1334:LYS:CE	2.21	0.71
1:B:926:GLN:HG3	2:D:9:G:C5'	2.19	0.71
2:D:11:U:H5'	2:D:12:G:C2	2.25	0.71
3:E:45:THR:HG21	3:E:51:ALA:HA	1.72	0.71
1:B:547:ALA:CA	1:B:551:LEU:HD12	2.21	0.71
1:A:1064:GLU:HG3	1:A:1076:LYS:HZ1	1.56	0.71
3:E:116:ILE:HD12	3:E:116:ILE:N	2.03	0.71
1:B:526:LYS:HE3	1:B:692:ASN:HB3	1.71	0.71
1:A:64:LEU:HD21	3:E:2:THR:OG1	1.91	0.70
1:A:465:MET:HE1	1:A:473:ILE:HD11	1.72	0.70
1:A:727:LEU:HD23	1:A:727:LEU:N	2.01	0.70
1:B:573:GLU:OE1	1:B:573:GLU:HA	1.89	0.70
2:D:13:C:O2	2:D:14:G:N1	2.24	0.70
3:E:10:TYR:CE1	3:E:14:MET:CG	2.60	0.70
1:A:81:TYR:O	1:A:85:ILE:HG13	1.91	0.70
2:D:9:G:H2'	2:D:9:G:N3	2.07	0.70
3:F:5:ARG:CZ	3:F:5:ARG:HB3	2.21	0.70
1:A:520:VAL:HG21	1:A:591:LEU:CD2	2.22	0.70
3:F:43:VAL:C	3:F:44:ILE:HD13	2.16	0.70
3:F:108:GLU:HA	3:F:108:GLU:OE2	1.91	0.70
1:B:100:ARG:NH1	1:B:100:ARG:HG3	1.97	0.70
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.25	0.70
1:A:564:LEU:CD2	1:A:580:ILE:HD12	1.87	0.70
1:A:1065:THR:HG22	1:A:1072:ILE:HA	1.73	0.70
3:F:57:LEU:HD23	3:F:57:LEU:C	2.16	0.70
2:D:46:A:C2	2:D:47:A:C5	2.80	0.70
3:F:79:THR:HG23	3:F:88:TYR:HE1	1.54	0.70
1:B:451:TYR:HA	1:B:491:PHE:CD1	2.27	0.70
3:F:52:VAL:HG12	3:F:110:LYS:CG	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HE2	1:A:351:PHE:CD1	2.26	0.69
1:A:1247:GLY:C	1:A:1252:ASN:OD1	2.35	0.69
2:D:11:U:H4'	2:D:12:G:C4	2.26	0.69
3:E:18:ILE:HD11	3:E:24:PHE:CZ	2.27	0.69
1:A:846:PHE:CE1	1:A:913:LYS:CE	2.75	0.69
3:F:4:THR:OG1	3:F:7:GLN:HB2	1.90	0.69
1:A:967:ARG:NH1	1:A:974:LYS:HB2	2.06	0.69
1:A:784:ILE:HD12	1:A:806:LEU:HD21	1.75	0.69
1:A:1003:LYS:HB3	1:A:1016:TYR:HD1	1.58	0.69
1:A:1206:LEU:HD11	1:A:1341:GLU:OE2	1.92	0.69
2:C:84:A:N1	2:C:94:U:O4	2.26	0.69
1:B:46:ASN:OD1	1:B:1089:MET:HE1	1.92	0.69
3:F:52:VAL:HG11	3:F:110:LYS:CB	2.23	0.69
1:A:601:ILE:HD11	1:A:643:PHE:CE1	2.28	0.69
1:A:762:GLU:HG2	1:A:990:ASN:HD21	1.54	0.69
2:C:84:A:C2	2:C:85:C:C4	2.81	0.69
1:B:673:LYS:H	1:B:703:THR:HG1	1.41	0.69
1:B:708:ILE:O	1:B:711:ALA:HB3	1.93	0.69
1:B:1274:SER:O	1:B:1278:LYS:CG	2.41	0.69
3:F:54:LEU:HA	3:F:110:LYS:CE	2.23	0.69
3:F:67:ASN:O	3:F:68:LEU:HD22	1.92	0.69
1:B:747:LEU:CD2	1:B:1353:THR:CG2	2.71	0.69
1:B:1207:GLU:OE1	1:B:1210:ARG:NH1	2.26	0.69
1:A:1204:PHE:HE1	1:A:1347:LEU:HD12	1.58	0.68
1:B:477:ASN:CG	1:B:481:VAL:CG2	2.65	0.68
3:E:75:VAL:HG12	3:E:76:ASP:N	2.05	0.68
1:A:921:LEU:HD11	1:A:1004:LEU:HD23	1.75	0.68
1:B:846:PHE:HB3	1:B:1040:SER:CB	2.20	0.68
1:A:20:VAL:CG2	1:A:747:LEU:CD2	2.71	0.68
3:F:35:VAL:HG13	3:F:75:VAL:HG11	1.75	0.68
1:B:460:SER:OG	2:D:60:C:O3'	2.10	0.68
1:B:733:ILE:HD11	1:B:763:MET:CE	2.24	0.68
1:A:964:SER:O	1:A:968:LYS:HG2	1.93	0.68
1:B:737:ILE:O	1:B:741:VAL:HG23	1.93	0.68
1:B:1285:ALA:HB3	1:B:1334:LYS:NZ	2.08	0.68
3:F:22:ASP:N	3:F:22:ASP:OD1	2.26	0.68
1:A:1106:SER:CB	1:A:1136:SER:O	2.40	0.68
1:B:398:LEU:HD23	1:B:399:LEU:CB	2.23	0.68
3:F:98:ASP:OD1	3:F:98:ASP:N	2.25	0.68
3:F:100:LEU:O	3:F:101:GLU:HG3	1.93	0.68
1:A:465:MET:HE3	1:A:482:VAL:CG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TYR:HB3	1:A:1021:MET:HE1	1.76	0.68
1:B:201:ILE:HD12	1:B:232:GLU:HG3	1.74	0.68
1:A:520:VAL:HG13	1:A:553:PHE:CE1	2.28	0.68
3:F:31:PHE:CE1	3:F:76:ASP:C	2.71	0.68
3:F:118:LEU:HD23	3:F:118:LEU:O	1.94	0.68
1:A:1247:GLY:O	1:A:1252:ASN:CG	2.37	0.68
1:B:870:VAL:HG21	1:B:902:LYS:HB3	1.76	0.68
1:B:1204:PHE:CD2	1:B:1342:VAL:HG11	2.28	0.68
1:B:1343:LEU:O	1:B:1362:LEU:HB3	1.94	0.68
3:F:31:PHE:CE1	3:F:76:ASP:O	2.47	0.68
3:E:99:ASP:O	3:E:100:LEU:HG	1.94	0.68
1:A:847:LEU:HD21	1:A:849:ASP:HB2	1.75	0.68
1:B:547:ALA:C	1:B:551:LEU:CD1	2.61	0.68
3:F:52:VAL:HG11	3:F:110:LYS:CA	2.23	0.68
1:A:83:GLN:NE2	1:A:155:TYR:CZ	2.62	0.67
1:B:495:MET:CE	2:D:14:G:C1'	2.72	0.67
1:B:531:THR:CB	1:B:575:PHE:CD2	2.77	0.67
1:B:1333:ARG:CZ	3:F:71:ASP:OD2	2.42	0.67
2:C:16:U:C5	2:C:17:U:C4	2.83	0.67
3:F:7:GLN:HG2	3:F:36:LEU:HD12	1.76	0.67
1:A:560:THR:CG2	1:A:563:GLN:CD	2.56	0.67
1:B:661:ARG:HD2	2:D:10:G:C6	2.29	0.67
1:A:158:LEU:HD22	1:A:419:LEU:HD22	1.76	0.67
1:A:1334:LYS:HE2	3:E:57:LEU:O	1.94	0.67
1:A:309:ASN:OD1	1:A:309:ASN:N	2.27	0.67
1:A:529:TYR:HD2	1:A:569:PHE:CE2	2.12	0.67
1:A:1308:ASN:HB3	1:A:1326:TYR:CE1	2.30	0.67
1:B:1204:PHE:CD2	1:B:1342:VAL:CG1	2.78	0.67
1:B:1287:LEU:O	1:B:1290:VAL:HG22	1.94	0.67
3:E:42:VAL:O	3:E:42:VAL:HG13	1.92	0.67
1:B:497:ASN:OD1	2:D:14:G:N2	2.26	0.66
1:B:1351:SER:HB2	1:B:1356:TYR:HB2	1.76	0.66
1:A:525:THR:HG23	1:A:526:LYS:HD3	1.76	0.66
1:A:531:THR:HG22	1:A:532:GLU:N	2.09	0.66
1:A:548:ILE:CG2	1:A:552:LEU:CD2	2.64	0.66
1:B:557:ARG:HH22	1:B:596:ASP:N	1.94	0.66
1:B:1204:PHE:CG	1:B:1342:VAL:HG13	2.31	0.66
2:D:12:G:C8	2:D:13:C:C4	2.83	0.66
3:F:92:VAL:HG12	3:F:93:GLU:O	1.96	0.66
1:A:777:SER:OG	1:A:803:ASN:O	2.14	0.66
1:B:201:ILE:CD1	1:B:232:GLU:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:GLU:CG	3:F:94:THR:N	2.54	0.66
3:E:48:GLU:CG	3:E:86:THR:HG1	1.84	0.66
2:C:34:A:H5'	2:C:34:A:H8	1.60	0.66
1:B:253:LYS:HB2	1:B:261:ASP:HA	1.78	0.66
1:A:765:ARG:HE	1:A:925:ARG:NH1	1.93	0.66
3:E:16:GLU:OE1	3:E:117:ILE:HD13	1.94	0.66
1:A:353:ASP:OD2	1:A:356:LYS:HD3	1.95	0.66
1:A:846:PHE:CE1	1:A:913:LYS:HE2	2.31	0.66
2:D:46:A:H2'	2:D:47:A:C8	2.30	0.66
1:A:531:THR:O	1:A:534:MET:HB2	1.96	0.66
3:F:51:ALA:HB2	3:F:90:ASN:CG	2.20	0.66
1:A:1206:LEU:CD1	1:A:1341:GLU:OE2	2.44	0.66
2:D:11:U:H4'	2:D:12:G:N3	2.11	0.66
3:F:77:TYR:HB2	3:F:89:ILE:O	1.96	0.66
1:B:455:LEU:N	1:B:455:LEU:HD23	2.10	0.65
3:F:63:GLU:HG3	3:F:64:TYR:N	2.10	0.65
1:A:1072:ILE:HD12	1:A:1072:ILE:H	1.60	0.65
1:A:1107:LYS:CE	3:E:93:GLU:OE2	2.42	0.65
1:A:1313:PHE:C	1:A:1317:ASN:HD21	2.03	0.65
1:B:569:PHE:HD1	1:B:578:VAL:HG21	0.51	0.65
1:A:269:ASP:OD2	1:A:269:ASP:N	2.23	0.65
1:A:451:TYR:O	1:A:464:TRP:CE2	2.48	0.65
1:B:516:GLU:OE2	1:B:592:GLY:N	2.29	0.65
3:F:4:THR:CB	3:F:7:GLN:CG	2.72	0.65
1:A:194:GLN:CD	1:A:557:ARG:NH1	2.55	0.65
1:A:348:LYS:O	1:A:352:PHE:HB2	1.97	0.65
1:B:96:SER:C	1:B:100:ARG:HH12	2.03	0.65
1:B:739:GLN:O	1:B:743:VAL:HG23	1.96	0.65
1:A:1045:PHE:O	1:A:1076:LYS:HE3	1.96	0.65
1:B:447:ARG:HG3	2:D:17:U:H5'	1.79	0.65
1:B:522:ASN:OD1	1:B:693:PHE:HB3	1.97	0.65
1:B:555:THR:C	1:B:556:ASN:HD22	2.04	0.65
3:F:31:PHE:HE1	3:F:76:ASP:HB3	1.59	0.65
1:B:547:ALA:CB	1:B:551:LEU:CD1	2.73	0.65
1:B:980:ASN:ND2	1:B:1225:GLU:CD	2.54	0.65
1:A:1003:LYS:HB3	1:A:1016:TYR:CD1	2.31	0.65
1:B:1111:LEU:CD1	1:B:1135:ASP:HB2	2.26	0.65
3:F:51:ALA:HB2	3:F:90:ASN:CB	2.26	0.65
3:E:18:ILE:CD1	3:E:24:PHE:CZ	2.80	0.65
1:A:5:TYR:OH	1:A:754:HIS:O	2.14	0.65
1:B:496:THR:HG23	1:B:659:TRP:CH2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:G:N3	2:D:87:G:C3'	2.60	0.65
1:B:867:SER:C	1:B:1054:ASN:OD1	2.40	0.65
1:A:594:TYR:CE1	1:A:607:LEU:HB3	2.32	0.64
1:A:1122:ARG:HG2	1:A:1134:PHE:HE1	1.61	0.64
1:B:560:THR:HG22	1:B:563:GLN:CG	2.26	0.64
1:B:1286:ASN:ND2	1:B:1334:LYS:HE2	2.12	0.64
1:B:1204:PHE:CE2	1:B:1342:VAL:HG11	2.31	0.64
3:E:77:TYR:CD2	3:E:88:TYR:CD1	2.86	0.64
1:B:1210:ARG:HA	1:B:1280:VAL:CG1	2.24	0.64
3:F:93:GLU:CG	3:F:94:THR:H	2.01	0.64
1:A:999:LYS:CG	1:A:1071:GLU:OE1	2.45	0.64
1:A:1138:THR:HB	1:A:1168:ILE:HD12	1.80	0.64
1:B:560:THR:HG22	1:B:563:GLN:HG2	1.78	0.64
1:B:746:GLU:CD	1:B:1351:SER:HG	1.99	0.64
1:B:1333:ARG:NH2	3:F:72:GLU:OE2	2.31	0.64
1:A:718:ASP:CA	1:A:723:HIS:HE2	2.09	0.64
2:C:84:A:H2	2:C:85:C:C2	2.16	0.64
1:B:158:LEU:HD22	1:B:419:LEU:CD2	2.27	0.64
1:B:494:ARG:HG2	1:B:494:ARG:NH1	2.10	0.64
1:B:449:PRO:HD2	1:B:452:VAL:HG21	1.78	0.64
1:B:629:ARG:HH11	1:B:629:ARG:CG	2.11	0.64
1:B:1108:GLU:O	1:B:1134:PHE:CE2	2.43	0.64
1:B:1340:LYS:HZ2	1:B:1343:LEU:HD12	1.60	0.64
1:A:1204:PHE:CE2	1:A:1342:VAL:CG1	2.81	0.64
1:B:557:ARG:NH2	1:B:596:ASP:N	2.45	0.64
1:B:840:HIS:HE1	1:B:855:LYS:HE3	1.62	0.64
2:D:13:C:O2	2:D:14:G:C6	2.51	0.64
1:B:525:THR:HG23	1:B:526:LYS:HD3	1.79	0.64
1:B:1210:ARG:NH1	1:B:1282:LEU:HD11	2.12	0.64
3:E:52:VAL:CG2	3:E:92:VAL:CG2	2.72	0.64
3:E:70:LEU:HD23	3:E:101:GLU:CB	2.25	0.64
3:E:72:GLU:CG	3:E:92:VAL:HG11	2.27	0.64
1:A:175:ASN:HB2	1:A:176:PRO:HD2	1.80	0.64
1:A:763:MET:SD	1:A:928:THR:HG22	2.38	0.64
2:C:11:U:O2'	2:C:12:G:OP2	2.14	0.64
1:B:306:LEU:HA	1:B:320:SER:OG	1.98	0.63
1:B:544:GLN:O	1:B:548:ILE:HB	1.98	0.63
1:B:552:LEU:HD11	1:B:564:LEU:HA	1.79	0.63
1:B:1334:LYS:HZ3	3:F:57:LEU:CD1	2.10	0.63
1:B:1334:LYS:CG	3:F:57:LEU:HD22	2.26	0.63
3:F:35:VAL:O	3:F:39:SER:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:THR:HG22	3:F:86:THR:HG21	1.79	0.63
1:A:529:TYR:CD2	1:A:569:PHE:HE2	2.16	0.63
1:A:564:LEU:HD23	1:A:580:ILE:HD11	1.61	0.63
1:B:1108:GLU:OE2	3:F:37:HIS:CE1	2.52	0.63
1:B:1242:TYR:CD2	1:B:1256:GLN:NE2	2.66	0.63
1:B:1334:LYS:HA	3:F:57:LEU:O	1.98	0.63
1:A:560:THR:HG23	1:A:563:GLN:HG2	1.79	0.63
1:A:1210:ARG:HE	1:A:1212:ARG:NH2	1.96	0.63
1:B:420:HIS:ND1	1:B:441:GLU:OE1	2.30	0.63
1:A:273:ASP:OD2	3:E:3:LEU:HD13	1.97	0.63
2:C:12:G:H2'	2:C:13:C:C6	2.32	0.63
1:B:489:GLN:CD	1:B:492:ILE:HD13	2.24	0.63
3:E:30:ASP:OD1	3:E:30:ASP:O	2.17	0.63
1:A:628:ASP:OD2	1:A:631:MET:N	2.18	0.63
1:B:263:LYS:NZ	3:F:25:GLU:HA	2.13	0.63
1:B:477:ASN:C	1:B:481:VAL:HG23	2.23	0.63
1:B:1206:LEU:HB3	1:B:1210:ARG:NH2	2.13	0.63
1:B:926:GLN:HG3	2:D:9:G:O3'	1.99	0.63
2:D:10:G:C2'	2:D:11:U:O5'	2.47	0.63
1:A:398:LEU:HG	1:A:399:LEU:HG	1.80	0.63
1:B:980:ASN:HD22	1:B:1225:GLU:CD	2.06	0.63
1:A:560:THR:O	1:A:563:GLN:HG2	1.99	0.63
1:B:548:ILE:O	1:B:552:LEU:HB2	1.98	0.63
1:B:840:HIS:CE1	1:B:855:LYS:HE3	2.34	0.63
2:D:44:U:O2'	2:D:45:U:H5'	1.97	0.63
1:B:495:MET:CE	2:D:14:G:C2'	2.77	0.62
1:B:452:VAL:O	1:B:465:MET:HB2	1.98	0.62
1:B:539:PHE:HB3	1:B:690:ASN:HD21	1.64	0.62
1:B:560:THR:CG2	1:B:563:GLN:OE1	2.37	0.62
3:F:10:TYR:O	3:F:14:MET:N	2.31	0.62
1:B:1333:ARG:HH21	3:F:54:LEU:HD22	1.63	0.62
1:A:519:THR:HG23	1:A:589:ALA:HB1	1.80	0.62
1:A:1247:GLY:C	1:A:1252:ASN:CG	2.68	0.62
1:B:346:LYS:O	1:B:350:ILE:HG13	1.98	0.62
1:B:545:LYS:O	1:B:549:VAL:HG13	1.99	0.62
1:B:846:PHE:HA	1:B:1040:SER:CB	2.29	0.62
1:B:847:LEU:HD13	1:B:916:PHE:HB3	1.80	0.62
1:A:395:ARG:O	1:A:395:ARG:HG2	1.99	0.62
1:B:718:ASP:OD2	1:B:718:ASP:N	2.32	0.62
1:B:746:GLU:HG2	1:B:1353:THR:CG2	2.29	0.62
1:A:362:TYR:HA	1:A:367:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:PRO:O	1:A:504:ASN:HB2	1.99	0.62
1:A:820:ARG:NH2	1:A:825:ASP:OD1	2.32	0.62
3:F:45:THR:HG21	3:F:49:LYS:CA	2.29	0.62
1:A:395:ARG:HD2	1:A:397:ASP:CB	2.29	0.62
1:A:465:MET:HG2	1:A:466:THR:N	2.15	0.62
1:B:853:ASP:OD2	1:B:893:THR:HG21	2.00	0.62
1:B:998:ILE:HD11	1:B:1005:GLU:HG3	1.82	0.62
1:B:1206:LEU:CD1	1:B:1210:ARG:NH2	2.60	0.62
1:B:105:PHE:CE1	2:D:24:U:H1'	2.34	0.62
1:B:728:ALA:HB1	2:D:10:G:O5'	1.99	0.62
1:B:1347:LEU:HD12	1:B:1347:LEU:C	2.15	0.62
1:A:348:LYS:O	1:A:348:LYS:HD3	1.98	0.62
2:C:18:G:O2'	2:C:19:G:H5'	1.98	0.62
3:E:2:THR:O	3:E:3:LEU:HD23	1.99	0.62
3:E:48:GLU:HG2	3:E:86:THR:OG1	1.97	0.62
1:A:559:VAL:CG1	1:A:563:GLN:HG3	2.30	0.62
1:B:313:THR:HG22	1:B:315:ALA:H	1.63	0.62
1:B:921:LEU:HD11	1:B:1004:LEU:HD23	1.80	0.62
1:B:1210:ARG:HG3	1:B:1280:VAL:CG1	2.30	0.62
2:C:12:G:C2'	2:C:13:C:H5'	2.30	0.61
1:B:1048:THR:HG22	1:B:1076:LYS:HD3	1.81	0.61
1:B:1347:LEU:HD12	1:B:1348:ILE:H	0.80	0.61
1:A:780:ARG:HB3	1:A:806:LEU:HD23	1.82	0.61
1:B:846:PHE:HA	1:B:1040:SER:N	2.15	0.61
1:A:727:LEU:H	1:A:727:LEU:CD2	1.98	0.61
1:B:269:ASP:OD2	1:B:269:ASP:N	2.31	0.61
1:A:718:ASP:O	1:A:723:HIS:CE1	2.53	0.61
1:A:1114:ARG:HH21	1:A:1114:ARG:CG	2.14	0.61
1:B:531:THR:OG1	1:B:532:GLU:N	2.29	0.61
1:B:665:LYS:HG3	1:B:669:GLY:CA	2.25	0.61
1:A:1021:MET:CG	1:A:1036:TYR:CD1	2.75	0.61
1:A:1314:THR:HA	1:A:1317:ASN:ND2	2.16	0.61
3:F:15:HIS:HA	3:F:18:ILE:HG13	1.82	0.61
1:A:348:LYS:HD3	1:A:348:LYS:C	2.25	0.61
1:B:395:ARG:O	1:B:395:ARG:HG2	2.00	0.61
1:B:675:SER:OG	1:B:677:LYS:HB2	2.00	0.61
3:E:19:ASN:C	3:E:21:VAL:HG23	2.25	0.61
2:D:93:G:H3'	2:D:94:U:H5'	1.82	0.61
3:F:39:SER:CB	3:F:91:ILE:CG2	2.76	0.61
1:A:569:PHE:HD2	1:A:578:VAL:CB	2.12	0.61
2:C:84:A:C2	2:C:85:C:C2	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:LYS:HZ3	1:B:1343:LEU:CD1	2.14	0.61
3:F:75:VAL:HG12	3:F:76:ASP:N	2.15	0.61
1:A:353:ASP:O	1:A:360:ALA:HB3	2.01	0.61
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.12	0.61
1:B:1114:ARG:HD3	1:B:1119:LEU:HD11	1.83	0.61
1:A:745:ASP:CG	1:A:938:ARG:NH1	2.56	0.61
1:A:1210:ARG:HD2	1:A:1280:VAL:O	2.01	0.61
1:A:1219:GLU:OE1	3:E:97:ILE:HD12	2.01	0.61
1:B:563:GLN:O	1:B:567:ASP:N	2.33	0.61
1:A:1022:ILE:O	1:A:1035:LYS:HE3	2.01	0.60
1:A:502:LEU:C	1:A:502:LEU:HD12	2.25	0.60
1:A:505:GLU:OE1	1:A:505:GLU:HA	1.99	0.60
1:B:495:MET:HE2	2:D:14:G:H1'	1.82	0.60
1:A:728:ALA:HB1	2:C:11:U:P	2.41	0.60
1:B:560:THR:CG2	1:B:563:GLN:HG2	2.31	0.60
1:B:95:ASP:N	1:B:95:ASP:OD1	2.31	0.60
3:E:116:ILE:H	3:E:116:ILE:CD1	1.99	0.60
1:A:284:ASP:OD1	1:A:510:LYS:NZ	2.33	0.60
1:A:1114:ARG:HH21	1:A:1114:ARG:HG2	1.65	0.60
1:B:201:ILE:CD1	1:B:232:GLU:CG	2.79	0.60
1:B:353:ASP:OD1	1:B:355:SER:OG	2.18	0.60
1:A:569:PHE:HB3	1:A:578:VAL:HG21	1.82	0.60
2:D:10:G:O2'	2:D:11:U:P	2.60	0.60
1:B:273:ASP:OD2	3:F:3:LEU:HG	2.01	0.60
1:A:268:LYS:CE	3:E:28:THR:O	2.48	0.60
1:A:359:TYR:HE1	1:A:363:ILE:HG13	1.66	0.60
1:A:399:LEU:N	1:A:399:LEU:HD23	2.17	0.60
1:A:556:ASN:O	1:A:595:HIS:NE2	2.35	0.60
1:B:249:THR:HG22	1:B:265:GLN:HB2	1.84	0.60
1:B:746:GLU:HG2	1:B:1353:THR:HG21	1.82	0.60
3:F:24:PHE:O	3:F:25:GLU:HB2	2.01	0.60
3:E:10:TYR:CD1	3:E:10:TYR:O	2.53	0.60
1:B:468:LYS:HD2	1:B:480:GLU:O	2.01	0.60
1:B:729:GLY:O	1:B:734:LYS:NZ	2.29	0.60
3:F:50:TYR:CD1	3:F:77:TYR:CD1	2.90	0.60
3:F:75:VAL:HG12	3:F:76:ASP:H	1.65	0.60
1:A:828:LEU:HB3	1:A:836:TYR:HE2	1.67	0.59
1:A:1064:GLU:CG	1:A:1076:LYS:HZ2	2.00	0.59
2:C:34:A:H5''	2:C:34:A:C8	2.37	0.59
1:B:477:ASN:HB2	1:B:481:VAL:CG2	2.32	0.59
2:D:45:U:H2'	2:D:46:A:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:HH21	1:A:596:ASP:N	1.98	0.59
1:B:492:ILE:HG23	1:B:625:LEU:HD13	1.84	0.59
1:A:557:ARG:O	1:A:590:SER:CB	2.49	0.59
1:A:781:MET:HE2	1:A:803:ASN:HB3	1.83	0.59
1:B:451:TYR:O	1:B:464:TRP:CE2	2.55	0.59
1:B:479:GLU:HG2	1:B:484:LYS:NZ	2.18	0.59
1:B:548:ILE:CG2	1:B:549:VAL:N	2.66	0.59
1:B:568:TYR:HD2	1:B:569:PHE:CE2	2.21	0.59
3:F:53:ALA:HB3	3:F:70:LEU:HD21	1.84	0.59
1:B:531:THR:O	1:B:534:MET:CG	2.50	0.59
1:A:83:GLN:O	1:A:87:SER:HB3	2.03	0.59
3:F:20:MET:CE	3:F:117:ILE:HD11	2.32	0.59
3:E:75:VAL:CG1	3:E:76:ASP:H	2.13	0.59
2:D:87:G:C8	2:D:92:G:N1	2.70	0.59
2:D:93:G:C5'	2:D:93:G:N3	2.65	0.59
3:F:85:VAL:HG12	3:F:86:THR:N	2.16	0.59
1:A:693:PHE:CE2	1:A:697:ILE:CD1	2.86	0.59
2:C:92:G:C2'	2:C:93:G:OP1	2.51	0.59
1:B:745:ASP:CG	1:B:938:ARG:HH12	2.11	0.59
1:B:1047:LYS:O	1:B:1076:LYS:NZ	2.30	0.59
3:F:51:ALA:N	3:F:90:ASN:OD1	2.36	0.59
1:A:1256:GLN:O	1:A:1259:VAL:HG22	2.02	0.59
1:B:1146:VAL:HG23	1:B:1146:VAL:O	2.02	0.59
1:B:1215:ALA:HB2	1:B:1221:GLN:HG3	1.85	0.59
1:B:1343:LEU:O	1:B:1362:LEU:CB	2.51	0.59
3:F:22:ASP:OD2	3:F:82:VAL:HG21	2.03	0.59
3:E:49:LYS:NZ	3:E:50:TYR:HE1	2.00	0.59
1:A:569:PHE:HE2	1:A:578:VAL:HG11	1.65	0.59
1:A:1019:ARG:HA	1:A:1022:ILE:HD12	1.84	0.59
1:A:973:TYR:HB2	1:A:1234:ASN:OD1	2.03	0.58
1:B:310:THR:HG22	1:B:310:THR:O	2.02	0.58
1:A:1146:VAL:HG23	1:A:1146:VAL:O	2.01	0.58
1:B:531:THR:HB	1:B:575:PHE:HD2	1.68	0.58
1:B:846:PHE:C	1:B:1040:SER:CB	2.65	0.58
1:B:1036:TYR:CB	1:B:1037:PHE:CE1	2.85	0.58
1:A:842:VAL:H	1:A:854:ASN:HD21	1.49	0.58
1:B:846:PHE:HA	1:B:1040:SER:H	1.68	0.58
2:D:88:A:C8	2:D:92:G:O6	2.56	0.58
3:E:49:LYS:CE	3:E:50:TYR:CE1	2.86	0.58
3:E:74:LEU:HD23	3:E:91:ILE:O	2.02	0.58
1:A:1114:ARG:HB3	1:A:1114:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:G:C2'	2:C:19:G:H5'	2.33	0.58
2:C:34:A:C8	2:C:34:A:C5'	2.86	0.58
1:B:1210:ARG:CA	1:B:1280:VAL:HG12	2.30	0.58
1:B:1281:ILE:O	1:B:1336:TYR:OH	2.18	0.58
1:A:496:THR:HG21	1:A:506:LYS:CG	2.31	0.58
1:B:569:PHE:HD2	1:B:569:PHE:N	2.02	0.58
1:B:1206:LEU:CD1	1:B:1210:ARG:HH21	2.12	0.58
3:E:18:ILE:HG12	3:E:24:PHE:CE1	2.38	0.58
1:B:714:SER:HB2	1:B:726:ASN:HD21	1.68	0.58
3:E:43:VAL:HG11	3:E:52:VAL:CG2	2.33	0.58
1:A:668:ASN:OD1	1:A:680:LEU:HB3	2.03	0.58
1:A:902:LYS:N	1:A:905:ARG:NH2	2.52	0.58
3:E:18:ILE:HG12	3:E:24:PHE:HE1	1.68	0.58
1:A:612:ASN:O	1:A:616:LEU:HG	2.04	0.58
1:B:522:ASN:OD1	1:B:693:PHE:CB	2.52	0.57
3:F:51:ALA:CB	3:F:90:ASN:OD1	2.52	0.57
1:B:1107:LYS:HB3	3:F:38:ASP:OD1	2.04	0.57
3:F:39:SER:CB	3:F:91:ILE:HG21	2.34	0.57
3:F:42:VAL:HG23	3:F:121:GLU:OE2	2.04	0.57
1:B:557:ARG:NH2	1:B:596:ASP:H	2.02	0.57
1:B:1340:LYS:HZ3	1:B:1343:LEU:HD12	1.69	0.57
2:D:93:G:C2'	2:D:94:U:H5'	2.34	0.57
1:B:495:MET:CE	2:D:14:G:H1'	2.34	0.57
1:B:1336:TYR:CD2	3:F:59:THR:CG2	2.88	0.57
1:A:489:GLN:O	1:A:489:GLN:NE2	2.38	0.57
1:B:714:SER:HB2	1:B:726:ASN:ND2	2.19	0.57
1:B:1111:LEU:HD11	1:B:1135:ASP:HB2	1.85	0.57
1:A:294:LYS:O	1:A:297:SER:HB3	2.05	0.57
1:A:724:ILE:HA	1:A:727:LEU:HD21	1.84	0.57
1:B:49:GLY:HA2	1:B:1092:VAL:HG13	1.85	0.57
1:B:746:GLU:CD	1:B:1351:SER:OG	2.45	0.57
1:B:1337:THR:OG1	3:F:58:SER:HB3	2.05	0.57
3:E:37:HIS:O	3:E:122:LEU:HD21	2.05	0.57
1:A:355:SER:OG	1:A:356:LYS:HD2	2.05	0.57
1:B:489:GLN:NE2	1:B:492:ILE:HD13	2.19	0.57
1:B:723:HIS:O	1:B:727:LEU:HD21	2.05	0.57
1:B:846:PHE:HA	1:B:1040:SER:HB2	1.86	0.57
1:A:529:TYR:HD2	1:A:569:PHE:HE2	1.49	0.57
1:B:673:LYS:H	1:B:703:THR:CB	2.18	0.57
1:B:1210:ARG:HG3	1:B:1280:VAL:CA	2.30	0.57
2:D:45:U:C2	2:D:46:A:C8	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:GLU:CA	1:A:768:GLN:HE22	2.13	0.57
1:B:1037:PHE:N	1:B:1037:PHE:CD1	2.73	0.57
3:F:24:PHE:HB3	3:F:82:VAL:HA	1.85	0.57
1:A:249:THR:HG22	1:A:265:GLN:HB2	1.87	0.57
1:A:520:VAL:HG13	1:A:553:PHE:HE1	1.69	0.57
1:A:1247:GLY:CA	1:A:1252:ASN:ND2	2.64	0.57
2:C:12:G:H2'	2:C:13:C:H6	1.70	0.57
1:B:182:ASP:OD1	1:B:182:ASP:N	2.36	0.57
1:B:1206:LEU:N	1:B:1210:ARG:O	2.38	0.57
3:F:5:ARG:CG	3:F:5:ARG:HH11	2.17	0.57
3:E:43:VAL:HG11	3:E:52:VAL:HG21	1.86	0.57
1:B:212:LEU:HD13	1:B:300:ILE:HD11	1.88	0.56
1:B:240:ASN:HD22	1:B:255:ASN:HD21	1.51	0.56
1:B:569:PHE:N	1:B:569:PHE:CD2	2.73	0.56
3:F:69:TYR:HA	3:F:102:ILE:CG1	2.32	0.56
1:A:116:HIS:HB3	1:A:125:GLU:HG3	1.86	0.56
1:A:606:PHE:CD1	1:A:612:ASN:ND2	2.73	0.56
1:B:158:LEU:HD22	1:B:419:LEU:HD22	1.87	0.56
1:B:353:ASP:O	1:B:360:ALA:HB3	2.05	0.56
1:B:629:ARG:NH1	1:B:629:ARG:HG3	2.20	0.56
1:B:747:LEU:HD21	1:B:1353:THR:CG2	2.34	0.56
1:B:1207:GLU:O	1:B:1208:ASN:HB2	2.06	0.56
2:D:11:U:C4'	2:D:12:G:C4	2.88	0.56
3:E:72:GLU:CG	3:E:92:VAL:CG1	2.83	0.56
1:A:552:LEU:HD13	1:A:552:LEU:N	2.20	0.56
1:B:529:TYR:HB3	1:B:580:ILE:HG12	1.87	0.56
1:B:661:ARG:HB2	2:D:10:G:N1	2.20	0.56
1:B:1206:LEU:CD1	1:B:1210:ARG:CZ	2.64	0.56
2:D:82:G:C6	2:D:83:C:C4	2.94	0.56
3:E:49:LYS:NZ	3:E:50:TYR:CE1	2.73	0.56
1:A:1280:VAL:HG23	1:A:1281:ILE:N	2.19	0.56
1:B:140:LYS:NZ	1:B:144:ASP:OD1	2.37	0.56
1:B:747:LEU:CD2	1:B:1353:THR:HG21	2.35	0.56
1:A:914:ALA:HB1	1:A:1018:VAL:HB	1.86	0.56
1:A:459:ASN:OD1	2:C:56:U:O2	2.22	0.56
1:A:718:ASP:C	1:A:723:HIS:NE2	2.64	0.56
1:A:1337:THR:CB	3:E:97:ILE:HD11	2.36	0.56
1:B:479:GLU:HG2	1:B:484:LYS:HZ3	1.71	0.56
1:B:547:ALA:O	1:B:551:LEU:N	2.35	0.56
1:B:588:ASN:N	1:B:588:ASN:OD1	2.39	0.56
1:A:531:THR:CB	1:A:534:MET:SD	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:PHE:CZ	1:A:697:ILE:CD1	2.86	0.56
1:B:171:GLU:HG2	1:B:629:ARG:HH12	1.64	0.56
1:B:776:ASN:HD21	1:B:807:GLN:HE22	1.53	0.56
1:A:606:PHE:CE1	1:A:612:ASN:ND2	2.73	0.56
1:B:420:HIS:CE1	1:B:441:GLU:OE1	2.59	0.56
1:B:477:ASN:CB	1:B:481:VAL:CG2	2.84	0.56
1:A:897:PHE:HA	1:A:900:LEU:HD12	1.87	0.56
1:B:321:MET:HE1	1:B:324:ARG:CZ	2.36	0.56
3:E:52:VAL:O	3:E:53:ALA:HB3	2.06	0.56
1:A:58:THR:HG22	1:A:731:PRO:HG2	1.87	0.56
1:A:970:PHE:O	1:A:971:GLN:HB2	2.05	0.56
1:B:59:ALA:HB3	2:D:13:C:OP2	2.06	0.56
1:B:569:PHE:HB3	1:B:575:PHE:HB2	1.88	0.56
1:B:727:LEU:HD21	1:B:934:ILE:HD11	1.88	0.56
1:B:733:ILE:HD11	1:B:763:MET:HE3	1.88	0.56
3:F:20:MET:O	3:F:21:VAL:HB	2.06	0.56
3:F:52:VAL:HG11	3:F:110:LYS:HA	1.88	0.56
3:F:68:LEU:HD13	3:F:68:LEU:N	2.21	0.56
3:E:46:LYS:CB	3:E:87:TYR:CZ	2.89	0.56
1:A:306:LEU:HD11	1:A:414:ILE:HD13	1.87	0.55
1:A:970:PHE:CD2	1:A:970:PHE:N	2.73	0.55
2:C:92:G:O6	2:C:93:G:C6	2.59	0.55
1:A:144:ASP:OD1	1:A:313:THR:HG21	2.04	0.55
1:B:492:ILE:CG2	1:B:625:LEU:HD13	2.35	0.55
1:B:563:GLN:O	1:B:567:ASP:HB2	2.06	0.55
1:B:629:ARG:HH11	1:B:629:ARG:HG3	1.72	0.55
1:B:1105:PHE:CE1	2:D:51:A:C5	2.94	0.55
3:E:106:GLU:O	3:E:109:MET:N	2.39	0.55
1:B:455:LEU:HD13	1:B:473:ILE:HG21	1.88	0.55
1:B:496:THR:CG2	1:B:659:TRP:CH2	2.89	0.55
3:E:50:TYR:CD1	3:E:50:TYR:N	2.73	0.55
1:B:143:VAL:HG11	1:B:315:ALA:HB2	1.87	0.55
1:A:520:VAL:HG21	1:A:591:LEU:HD23	1.88	0.55
1:B:548:ILE:HG23	1:B:549:VAL:N	2.21	0.55
1:B:1108:GLU:OE2	3:F:37:HIS:CD2	2.59	0.55
3:E:5:ARG:CZ	3:E:122:LEU:O	2.55	0.55
1:A:20:VAL:CG2	1:A:747:LEU:HD22	2.35	0.55
1:A:693:PHE:CE2	1:A:697:ILE:HD12	2.42	0.55
2:C:84:A:C2	2:C:85:C:N3	2.73	0.55
3:F:53:ALA:CB	3:F:70:LEU:HD21	2.37	0.55
1:A:813:LEU:HD21	1:A:852:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:TYR:CE1	1:B:756:PRO:HB3	2.42	0.55
1:B:57:GLU:O	2:D:64:U:O2'	2.19	0.55
1:B:629:ARG:HH11	1:B:629:ARG:HB2	1.71	0.55
1:B:672:ASP:CB	1:B:702:LEU:HD23	2.34	0.55
1:A:194:GLN:CD	1:A:557:ARG:HH11	2.15	0.55
1:B:398:LEU:CD2	1:B:399:LEU:HB2	2.33	0.55
1:B:479:GLU:CG	1:B:484:LYS:NZ	2.69	0.55
1:B:1210:ARG:CZ	1:B:1282:LEU:HD11	2.37	0.55
3:F:69:TYR:CD2	3:F:69:TYR:N	2.73	0.55
3:E:107:ASP:OD1	3:E:107:ASP:N	2.40	0.55
1:A:1357:GLU:OE1	1:A:1359:ARG:NH1	2.34	0.55
1:A:531:THR:CA	1:A:534:MET:SD	2.95	0.55
1:B:1179:ILE:O	1:B:1183:GLU:HG3	2.07	0.55
3:E:10:TYR:O	3:E:13:ALA:HB3	2.07	0.55
1:A:913:LYS:NZ	1:A:1038:PHE:CE1	2.75	0.54
1:B:606:PHE:C	1:B:606:PHE:CD2	2.85	0.54
2:D:85:C:N4	2:D:86:C:N4	2.55	0.54
3:E:77:TYR:HD2	3:E:88:TYR:CD1	2.24	0.54
1:A:140:LYS:NZ	1:A:313:THR:HG21	2.22	0.54
1:A:449:PRO:HD2	1:A:452:VAL:CB	2.36	0.54
1:B:238:PHE:HA	1:B:241:LEU:HD12	1.89	0.54
3:F:94:THR:HG23	3:F:94:THR:O	2.06	0.54
3:E:48:GLU:HA	3:E:86:THR:OG1	2.07	0.54
1:A:269:ASP:OD2	3:E:30:ASP:OD2	2.23	0.54
1:A:966:PHE:C	1:A:966:PHE:CD2	2.85	0.54
1:A:1161:LYS:O	1:A:1343:LEU:HD13	2.07	0.54
1:A:1204:PHE:CE1	1:A:1347:LEU:CD1	2.81	0.54
1:B:46:ASN:HD21	1:B:1089:MET:CE	2.17	0.54
1:B:1147:ALA:HB1	1:B:1188:LYS:O	2.07	0.54
3:F:47:ASN:C	3:F:49:LYS:N	2.54	0.54
3:E:20:MET:HA	3:E:20:MET:HE3	1.90	0.54
1:A:825:ASP:OD2	1:B:314:LYS:NZ	2.41	0.54
1:A:1204:PHE:CD1	1:A:1342:VAL:CG1	2.90	0.54
2:C:12:G:C5	2:C:13:C:C4	2.96	0.54
2:C:75:A:H2'	2:C:76:A:N3	2.23	0.54
1:B:416:LEU:HD22	1:B:445:THR:CG2	2.37	0.54
1:B:569:PHE:CD1	1:B:578:VAL:HB	2.38	0.54
1:B:1353:THR:HB	1:B:1355:LEU:HG	1.89	0.54
3:E:70:LEU:HD13	3:E:70:LEU:N	2.22	0.54
1:A:472:THR:HG23	2:C:59:U:P	2.47	0.54
1:A:1003:LYS:HG2	1:A:1016:TYR:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:ILE:HD11	1:B:763:MET:HE1	1.88	0.54
2:D:87:G:O2'	2:D:88:A:H5'	2.07	0.54
3:E:5:ARG:HH12	3:E:122:LEU:HD23	1.73	0.54
2:C:97:U:H6	2:C:97:U:C5'	2.19	0.54
3:F:10:TYR:C	3:F:10:TYR:CD1	2.85	0.54
1:B:491:PHE:CD2	1:B:491:PHE:C	2.86	0.54
1:B:547:ALA:CA	1:B:551:LEU:CD1	2.85	0.54
1:B:601:ILE:HD12	1:B:601:ILE:O	2.07	0.54
1:B:661:ARG:CB	2:D:10:G:C2	2.90	0.54
1:B:1105:PHE:N	1:B:1105:PHE:CD1	2.73	0.54
3:F:39:SER:HB2	3:F:91:ILE:HG22	1.86	0.54
1:A:1122:ARG:NH2	2:C:49:A:N3	2.56	0.54
1:B:45:LYS:HA	1:B:1091:GLN:HE22	1.73	0.54
1:B:196:PHE:HD2	1:B:196:PHE:N	2.02	0.54
3:F:81:ASP:CG	3:F:86:THR:HG23	2.27	0.54
1:A:336:LYS:HE2	1:A:351:PHE:CE1	2.42	0.54
1:B:395:ARG:CD	1:B:397:ASP:HB2	2.32	0.54
3:F:22:ASP:HB3	3:F:82:VAL:HG13	1.84	0.54
1:B:116:HIS:HB3	1:B:125:GLU:HG3	1.90	0.54
1:B:557:ARG:NH2	1:B:595:HIS:HB2	2.23	0.54
2:D:87:G:N3	2:D:87:G:H5''	2.22	0.53
3:F:17:PHE:CD1	3:F:17:PHE:C	2.85	0.53
3:F:20:MET:HE2	3:F:117:ILE:HG13	1.89	0.53
3:F:79:THR:HG22	3:F:86:THR:CG2	2.37	0.53
3:E:89:ILE:O	3:E:89:ILE:HG22	2.07	0.53
1:A:569:PHE:CD2	1:A:578:VAL:HG21	2.43	0.53
1:A:1219:GLU:OE1	3:E:97:ILE:CD1	2.56	0.53
1:B:347:TYR:C	1:B:347:TYR:CD2	2.86	0.53
1:B:480:GLU:OE1	1:B:480:GLU:HA	2.07	0.53
2:D:85:C:N3	2:D:86:C:C4	2.77	0.53
3:E:69:TYR:CD1	3:E:69:TYR:N	2.76	0.53
3:E:77:TYR:CD2	3:E:88:TYR:HD1	2.26	0.53
1:B:1107:LYS:HB3	3:F:38:ASP:CG	2.32	0.53
1:B:1122:ARG:NH2	2:D:49:A:N3	2.57	0.53
3:F:20:MET:CE	3:F:116:ILE:HG22	2.38	0.53
3:E:70:LEU:HD22	3:E:101:GLU:C	2.34	0.53
1:A:347:TYR:C	1:A:347:TYR:CD2	2.86	0.53
1:A:560:THR:H	1:A:563:GLN:CD	2.16	0.53
1:A:1146:VAL:HG21	1:A:1194:LEU:HD13	1.89	0.53
1:B:569:PHE:CE1	1:B:578:VAL:HB	2.42	0.53
1:B:728:ALA:HB3	2:D:10:G:O5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:SER:CA	1:B:1136:SER:O	2.56	0.53
2:D:93:G:H2'	2:D:94:U:H5'	1.90	0.53
3:E:54:LEU:CG	3:E:110:LYS:CB	2.86	0.53
1:A:336:LYS:HG2	1:A:351:PHE:CE1	2.43	0.53
1:A:1308:ASN:CB	1:A:1326:TYR:CE1	2.92	0.53
1:B:465:MET:HE2	1:B:482:VAL:HG13	1.91	0.53
1:B:677:LYS:CD	1:B:682:PHE:CE1	2.89	0.53
1:A:969:ASP:HB3	1:A:970:PHE:CD2	2.44	0.53
1:A:1075:ASP:CG	1:A:1078:ARG:HB3	2.32	0.53
1:B:186:ILE:O	1:B:189:VAL:HG22	2.09	0.53
3:F:5:ARG:HH11	3:F:5:ARG:HG3	1.72	0.53
3:F:72:GLU:HG2	3:F:92:VAL:HG11	1.89	0.53
1:A:460:SER:OG	1:A:463:ALA:HB3	2.08	0.53
1:A:559:VAL:O	1:A:587:PHE:HD1	1.92	0.53
1:A:744:VAL:O	1:A:748:VAL:HG23	2.08	0.53
1:A:269:ASP:OD1	3:E:30:ASP:OD2	2.27	0.53
1:A:902:LYS:HZ1	1:A:905:ARG:NH1	2.05	0.53
1:A:1191:LYS:CB	1:A:1194:LEU:CD1	2.86	0.53
1:B:212:LEU:HD22	1:B:246:LEU:HD21	1.89	0.53
1:B:627:GLU:HG2	1:B:655:ARG:NE	2.24	0.53
3:F:5:ARG:CZ	3:F:5:ARG:CB	2.86	0.53
3:F:57:LEU:HD12	3:F:68:LEU:CD1	2.38	0.53
3:F:69:TYR:CA	3:F:102:ILE:HG12	2.33	0.53
3:F:77:TYR:HB3	3:F:90:ASN:HD22	1.73	0.53
3:E:49:LYS:HA	3:E:49:LYS:HE3	1.86	0.53
1:A:305:ILE:HD13	1:A:410:ILE:HD11	1.90	0.53
1:A:520:VAL:HG21	1:A:591:LEU:HD21	1.90	0.53
1:A:936:ASP:OD2	1:A:940:ASN:ND2	2.42	0.53
1:B:522:ASN:O	1:B:525:THR:HG22	2.09	0.53
1:A:359:TYR:HE1	1:A:363:ILE:CG1	2.22	0.53
1:B:349:GLU:O	1:B:353:ASP:HB2	2.09	0.53
1:B:761:ILE:HD11	1:B:935:LEU:HD12	1.91	0.53
1:B:1333:ARG:NH2	3:F:54:LEU:HD22	2.23	0.53
1:B:1336:TYR:CA	3:F:59:THR:HG21	2.25	0.53
3:E:99:ASP:O	3:E:100:LEU:CG	2.57	0.53
1:A:970:PHE:N	1:A:970:PHE:HD2	2.06	0.52
1:B:531:THR:CB	1:B:575:PHE:HD2	2.19	0.52
1:B:683:LEU:HD21	1:B:696:LEU:HD22	1.91	0.52
3:F:43:VAL:O	3:F:44:ILE:HD13	2.09	0.52
3:E:46:LYS:CB	3:E:116:ILE:HD11	2.38	0.52
1:A:719:SER:O	1:A:723:HIS:CG	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:U:C5	2:C:17:U:C5	2.97	0.52
1:B:1105:PHE:N	1:B:1105:PHE:HD1	2.06	0.52
3:E:16:GLU:O	3:E:19:ASN:HB3	2.09	0.52
1:A:729:GLY:N	2:C:11:U:OP1	2.41	0.52
1:A:847:LEU:HB2	1:A:916:PHE:HB3	1.91	0.52
1:A:902:LYS:HA	1:A:905:ARG:NH2	2.25	0.52
1:B:661:ARG:CB	2:D:10:G:N2	2.67	0.52
1:B:1048:THR:CG2	1:B:1076:LYS:HD3	2.39	0.52
3:F:10:TYR:O	3:F:14:MET:HB2	2.09	0.52
1:A:291:LEU:O	1:A:295:ASN:ND2	2.42	0.52
1:A:555:THR:O	1:A:555:THR:HG22	2.09	0.52
2:C:11:U:C2	2:C:12:G:C8	2.98	0.52
1:B:144:ASP:O	1:B:425:ARG:NH2	2.41	0.52
1:B:531:THR:HG22	1:B:575:PHE:CE2	2.15	0.52
1:B:1262:HIS:O	1:B:1265:TYR:HB2	2.10	0.52
3:F:5:ARG:CB	3:F:5:ARG:NH1	2.73	0.52
3:F:69:TYR:CB	3:F:101:GLU:O	2.55	0.52
1:A:140:LYS:HZ3	1:A:313:THR:HG21	1.73	0.52
1:A:420:HIS:CE1	1:A:424:ARG:HD2	2.45	0.52
1:B:184:LEU:HD11	1:B:295:ASN:HB3	1.91	0.52
1:B:1127:ASP:OD2	1:B:1129:LYS:N	2.43	0.52
2:C:35:A:OP2	2:C:35:A:H8	1.92	0.52
1:B:546:LYS:O	1:B:550:ASP:HB2	2.09	0.52
3:F:14:MET:HE2	3:F:28:THR:OG1	2.10	0.52
1:A:836:TYR:N	1:A:836:TYR:CD1	2.73	0.52
1:B:686:ASP:OD2	1:B:691:ARG:HB2	2.09	0.52
1:B:691:ARG:HB3	1:B:696:LEU:CD1	2.40	0.52
1:B:1277:SER:HA	1:B:1281:ILE:CG1	2.29	0.52
2:D:9:G:N3	2:D:9:G:C2'	2.72	0.52
3:F:37:HIS:CD2	3:F:37:HIS:C	2.88	0.52
3:E:82:VAL:CG1	3:E:83:ASN:N	2.73	0.52
1:A:28:PRO:HG2	1:A:47:LEU:HD12	1.92	0.52
1:A:626:PHE:O	1:A:632:ILE:HD11	2.10	0.52
1:A:569:PHE:CE2	1:A:578:VAL:CG1	2.80	0.52
1:A:693:PHE:CE2	1:A:697:ILE:HD11	2.45	0.52
1:A:1114:ARG:NH2	1:A:1114:ARG:CB	2.73	0.52
1:B:238:PHE:O	1:B:241:LEU:HB2	2.09	0.52
1:B:1114:ARG:O	1:B:1129:LYS:HA	2.09	0.52
1:B:1137:PRO:HB2	1:B:1167:THR:CG2	2.38	0.52
1:B:268:LYS:HE2	3:F:28:THR:O	2.11	0.51
1:B:306:LEU:HD12	1:B:306:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:LYS:NZ	1:B:1343:LEU:CD1	2.69	0.51
3:E:82:VAL:HG12	3:E:83:ASN:N	2.25	0.51
1:A:144:ASP:CG	1:A:313:THR:CG2	2.70	0.51
1:A:279:LEU:O	1:A:283:GLY:N	2.43	0.51
1:A:548:ILE:HG23	1:A:552:LEU:HD22	1.87	0.51
1:B:1336:TYR:HD2	3:F:59:THR:HG21	1.72	0.51
1:A:988:TYR:O	1:A:992:VAL:HG23	2.10	0.51
1:B:59:ALA:CB	2:D:13:C:OP2	2.59	0.51
1:B:552:LEU:CD1	1:B:564:LEU:HA	2.40	0.51
2:D:84:A:C2	2:D:95:G:C6	2.99	0.51
3:F:15:HIS:O	3:F:16:GLU:C	2.52	0.51
3:F:53:ALA:O	3:F:54:LEU:HB3	2.11	0.51
3:E:14:MET:HE3	3:E:28:THR:HG21	1.92	0.51
3:E:18:ILE:CD1	3:E:24:PHE:CE1	2.93	0.51
1:A:1149:VAL:HG12	1:A:1187:TYR:HA	1.91	0.51
2:C:84:A:H2	2:C:85:C:N3	2.08	0.51
1:B:315:ALA:CB	1:B:418:GLU:OE2	2.56	0.51
1:B:530:VAL:CA	1:B:534:MET:SD	2.90	0.51
1:B:833:LEU:HA	1:B:836:TYR:CD2	2.45	0.51
1:B:893:THR:HG23	1:B:896:LYS:H	1.75	0.51
3:F:42:VAL:CG2	3:F:121:GLU:OE1	2.58	0.51
3:F:54:LEU:HG	3:F:55:CYS:H	1.75	0.51
3:E:48:GLU:CG	3:E:85:VAL:HG13	2.40	0.51
1:A:573:GLU:O	1:A:574:CYS:SG	2.66	0.51
1:A:1324:PHE:C	1:A:1324:PHE:CD2	2.88	0.51
1:B:451:TYR:O	1:B:464:TRP:NE1	2.43	0.51
1:B:495:MET:HE1	2:D:14:G:H2'	1.93	0.51
1:B:682:PHE:CE2	1:B:702:LEU:HD21	2.45	0.51
1:B:816:LEU:HA	1:B:891:LEU:HD22	1.92	0.51
3:F:84:GLY:C	3:F:85:VAL:HG23	2.36	0.51
3:E:34:GLU:O	3:E:38:ASP:OD1	2.28	0.51
1:A:924:THR:HG23	1:A:959:LYS:NZ	2.26	0.51
1:A:1314:THR:CA	1:A:1317:ASN:ND2	2.73	0.51
1:B:980:ASN:ND2	1:B:980:ASN:H	2.08	0.51
1:B:1335:ARG:C	3:F:59:THR:HG23	2.36	0.51
3:E:42:VAL:O	3:E:42:VAL:CG1	2.58	0.51
1:A:1115:ASN:ND2	1:A:1115:ASN:H	2.08	0.51
1:B:28:PRO:HG2	1:B:47:LEU:HD12	1.92	0.51
1:B:492:ILE:H	1:B:492:ILE:HD12	1.75	0.51
3:F:50:TYR:CD1	3:F:88:TYR:CG	2.97	0.51
1:A:215:ARG:N	1:A:216:LEU:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:C	1:A:489:GLN:HE21	2.17	0.51
1:A:531:THR:CG2	1:A:532:GLU:N	2.73	0.51
1:A:752:GLY:C	1:A:753:ARG:HG3	2.36	0.51
1:A:1111:LEU:CD1	1:A:1135:ASP:HB2	2.41	0.51
1:A:1328:ASP:OD2	1:A:1328:ASP:N	2.31	0.51
1:B:1036:TYR:HB2	1:B:1037:PHE:CD1	2.45	0.51
1:A:1018:VAL:O	1:A:1021:MET:HB2	2.11	0.51
1:B:829:ASP:O	1:B:833:LEU:HD23	2.11	0.51
1:B:1007:GLU:OE2	1:B:1007:GLU:HA	2.11	0.51
1:B:1041:ASN:OD1	1:B:1043:MET:N	2.42	0.51
2:D:54:G:C6	2:D:55:C:N4	2.79	0.51
1:B:215:ARG:CZ	1:B:395:ARG:HH12	2.24	0.51
1:B:492:ILE:O	1:B:496:THR:OG1	2.28	0.51
1:B:693:PHE:C	1:B:693:PHE:CD1	2.89	0.51
1:B:1128:PRO:HA	1:B:1132:GLY:O	2.11	0.51
3:F:24:PHE:CD1	3:F:24:PHE:N	2.73	0.51
3:F:43:VAL:HG22	3:F:44:ILE:N	2.19	0.51
1:A:496:THR:HG21	1:A:506:LYS:HB3	1.93	0.50
1:A:1204:PHE:CE1	1:A:1342:VAL:HG12	2.47	0.50
1:B:723:HIS:O	1:B:727:LEU:CD2	2.59	0.50
2:D:44:U:HO2'	2:D:45:U:H5'	1.76	0.50
3:F:54:LEU:CG	3:F:55:CYS:H	2.25	0.50
3:E:103:ALA:HB1	3:E:106:GLU:OE1	2.11	0.50
1:A:454:PRO:HB2	1:A:463:ALA:HB2	1.93	0.50
1:A:497:ASN:O	1:A:507:VAL:HG22	2.11	0.50
1:A:531:THR:N	1:A:534:MET:HG2	2.25	0.50
1:A:1204:PHE:CD1	1:A:1342:VAL:HG12	2.46	0.50
1:A:1325:LYS:HB3	1:A:1330:THR:HG23	1.92	0.50
2:C:84:A:C6	2:C:94:U:O4	2.64	0.50
1:B:569:PHE:CA	1:B:573:GLU:CB	2.86	0.50
1:B:942:LYS:HB2	1:B:950:ILE:HD12	1.93	0.50
1:B:1285:ALA:HB3	1:B:1334:LYS:HZ1	1.73	0.50
3:F:39:SER:HB2	3:F:91:ILE:HG21	1.88	0.50
3:E:67:ASN:O	3:E:69:TYR:HE1	1.89	0.50
1:A:154:ILE:O	1:A:158:LEU:HG	2.11	0.50
1:B:1224:ASN:CG	1:B:1280:VAL:HG11	2.36	0.50
2:D:11:U:C4'	2:D:12:G:N3	2.73	0.50
3:F:45:THR:CB	3:F:49:LYS:O	2.59	0.50
3:F:48:GLU:HA	3:F:88:TYR:CE2	2.46	0.50
1:A:505:GLU:OE2	1:A:665:LYS:HD3	2.12	0.50
1:A:531:THR:H	1:A:534:MET:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:PHE:HD2	1:A:578:VAL:HG21	1.76	0.50
1:A:1111:LEU:HD11	1:A:1135:ASP:HB2	1.93	0.50
1:B:520:VAL:CG1	1:B:553:PHE:HE1	1.95	0.50
3:F:54:LEU:H	3:F:110:LYS:HZ2	1.59	0.50
3:E:48:GLU:OE1	3:E:85:VAL:HG22	2.11	0.50
1:A:451:TYR:O	1:A:464:TRP:NE1	2.44	0.50
2:D:11:U:H5'	2:D:12:G:N2	2.26	0.50
3:F:15:HIS:C	3:F:15:HIS:HD1	2.20	0.50
3:E:10:TYR:HD1	3:E:11:ALA:N	2.08	0.50
1:A:195:LEU:C	1:A:196:PHE:CD2	2.85	0.50
1:A:454:PRO:HD3	2:C:15:C:O3'	2.12	0.50
1:A:627:GLU:HA	1:A:655:ARG:HD2	1.93	0.50
1:A:922:VAL:O	1:A:959:LYS:HE2	2.11	0.50
2:C:65:A:O5'	2:C:65:A:H8	1.94	0.50
1:B:998:ILE:HD11	1:B:1005:GLU:CG	2.41	0.50
2:D:46:A:C2	2:D:47:A:C4	3.00	0.50
2:D:88:A:N9	2:D:92:G:O6	2.45	0.50
3:F:100:LEU:O	3:F:101:GLU:CG	2.60	0.50
3:E:54:LEU:HD11	3:E:110:LYS:CA	2.41	0.50
3:E:106:GLU:O	3:E:107:ASP:C	2.54	0.50
1:A:97:PHE:CD1	1:A:97:PHE:C	2.86	0.50
1:A:244:LEU:O	1:A:266:LEU:HD12	2.11	0.50
1:A:531:THR:HG22	1:A:532:GLU:H	1.74	0.50
1:A:766:GLU:CA	1:A:768:GLN:NE2	2.73	0.50
1:A:902:LYS:HZ3	1:A:905:ARG:NH1	2.08	0.50
2:C:75:A:C6	2:C:76:A:C6	3.00	0.50
1:B:11:ILE:HB	1:B:763:MET:HG2	1.94	0.50
3:E:24:PHE:O	3:E:25:GLU:HB2	2.12	0.50
3:E:45:THR:HG22	3:E:115:GLU:HB3	1.94	0.50
1:A:347:TYR:C	1:A:347:TYR:HD2	2.19	0.50
1:A:933:GLN:HB2	1:A:1010:TYR:CE1	2.47	0.50
1:B:495:MET:HE2	2:D:14:G:C1'	2.41	0.50
1:B:678:THR:O	1:B:681:ASP:HB2	2.12	0.50
2:D:12:G:C8	2:D:13:C:H5	1.96	0.50
3:F:77:TYR:CB	3:F:90:ASN:HD22	2.25	0.50
1:A:1272:GLN:NE2	2:C:89:G:O6	2.36	0.50
1:B:165:ARG:O	1:B:412:HIS:HA	2.12	0.50
1:B:781:MET:HE2	1:B:803:ASN:HB3	1.92	0.50
1:B:822:MET:O	1:B:879:MET:HE2	2.12	0.50
3:F:69:TYR:H	3:F:69:TYR:HD2	1.58	0.50
1:A:182:ASP:OD1	1:A:182:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD13	1:A:359:TYR:HE2	1.76	0.49
1:A:609:ASN:O	1:A:610:GLU:HB2	2.12	0.49
1:A:816:LEU:HA	1:A:891:LEU:HD22	1.94	0.49
1:A:1074:TRP:HE1	1:A:1080:PHE:HE2	1.57	0.49
1:B:58:THR:HG21	2:D:12:G:H5'	1.94	0.49
1:B:830:ILE:C	1:B:833:LEU:HG	2.37	0.49
1:B:1048:THR:HG22	1:B:1076:LYS:CD	2.42	0.49
3:F:77:TYR:CB	3:F:89:ILE:O	2.58	0.49
1:A:269:ASP:CG	3:E:30:ASP:OD2	2.55	0.49
1:A:555:THR:O	1:A:556:ASN:ND2	2.45	0.49
1:A:749:LYS:HE3	1:A:753:ARG:NH2	2.28	0.49
1:B:465:MET:CE	1:B:473:ILE:HD13	2.41	0.49
1:B:495:MET:HE1	2:D:14:G:C2'	2.42	0.49
1:B:1271:GLU:O	1:B:1275:GLU:HG2	2.12	0.49
2:D:31:U:O4	2:D:32:A:N6	2.45	0.49
3:F:114:GLN:O	3:F:114:GLN:HG3	2.12	0.49
1:A:214:ALA:C	1:A:216:LEU:HD12	2.37	0.49
1:A:1274:SER:O	1:A:1278:LYS:HG3	2.12	0.49
1:B:104:SER:O	1:B:111:LYS:NZ	2.46	0.49
3:F:54:LEU:CD2	3:F:55:CYS:H	2.25	0.49
3:E:5:ARG:HH12	3:E:122:LEU:CD2	2.25	0.49
1:A:347:TYR:HD2	1:A:347:TYR:O	1.94	0.49
1:A:767:ASN:N	1:A:768:GLN:NE2	2.60	0.49
1:A:823:TYR:C	1:A:824:VAL:CG2	2.85	0.49
1:B:49:GLY:HA2	1:B:1092:VAL:CG1	2.42	0.49
1:B:58:THR:HG22	1:B:731:PRO:HD2	1.94	0.49
3:F:63:GLU:C	3:F:65:ASP:H	2.19	0.49
3:E:101:GLU:C	3:E:102:ILE:HD12	2.36	0.49
1:A:214:ALA:HB1	1:A:216:LEU:HD11	1.94	0.49
1:A:970:PHE:HE1	1:A:1080:PHE:HZ	1.00	0.49
1:B:46:ASN:CG	1:B:1089:MET:HE1	2.27	0.49
1:B:196:PHE:CD2	1:B:196:PHE:N	2.73	0.49
1:B:201:ILE:CD1	1:B:232:GLU:CD	2.82	0.49
1:B:465:MET:CE	1:B:473:ILE:CD1	2.87	0.49
1:B:600:ILE:O	1:B:647:VAL:HG23	2.12	0.49
3:E:5:ARG:C	3:E:5:ARG:CD	2.85	0.49
1:A:524:LEU:O	1:A:527:VAL:HG12	2.12	0.49
1:B:253:LYS:HD2	1:B:261:ASP:HB3	1.95	0.49
1:B:665:LYS:CA	1:B:669:GLY:HA3	2.42	0.49
1:B:749:LYS:CE	1:B:753:ARG:NH1	2.64	0.49
2:D:28:A:O3'	2:D:29:G:H4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:A:C2	2:D:95:G:O6	2.65	0.49
3:E:51:ALA:C	3:E:52:VAL:CG2	2.85	0.49
1:A:600:ILE:HG22	1:A:647:VAL:HG23	1.94	0.49
1:A:1207:GLU:O	1:A:1208:ASN:HB2	2.12	0.49
1:B:593:THR:HG21	1:B:620:VAL:HG21	1.94	0.49
3:F:20:MET:HE2	3:F:117:ILE:HD11	1.93	0.49
3:F:85:VAL:CG1	3:F:86:THR:N	2.75	0.49
1:A:336:LYS:CG	1:A:351:PHE:CE1	2.96	0.49
1:A:359:TYR:CE1	1:A:363:ILE:CG1	2.96	0.49
1:B:464:TRP:NE1	1:B:491:PHE:HB2	2.28	0.49
1:B:529:TYR:CB	1:B:580:ILE:HG12	2.43	0.49
3:F:72:GLU:HB3	3:F:92:VAL:CG1	2.42	0.49
1:A:560:THR:HG23	1:A:563:GLN:H	1.77	0.49
1:A:1045:PHE:O	1:A:1076:LYS:CE	2.60	0.49
1:B:1169:MET:HG2	2:D:52:A:C2	2.47	0.49
1:B:1247:GLY:O	1:B:1248:SER:C	2.53	0.49
1:A:214:ALA:C	1:A:216:LEU:CD1	2.86	0.49
1:A:348:LYS:C	1:A:348:LYS:CD	2.85	0.49
1:A:1204:PHE:CD2	1:A:1342:VAL:HG13	2.37	0.49
1:B:269:ASP:OD2	3:F:30:ASP:OD2	2.30	0.49
1:B:496:THR:CG2	1:B:659:TRP:CZ3	2.96	0.49
2:D:11:U:HO2'	2:D:12:G:P	2.26	0.49
1:A:922:VAL:O	1:A:959:LYS:CE	2.61	0.48
1:A:1122:ARG:O	2:C:52:A:H5''	2.13	0.48
1:B:154:ILE:O	1:B:158:LEU:HG	2.13	0.48
1:B:629:ARG:HH11	1:B:629:ARG:CB	2.26	0.48
1:B:926:GLN:HG3	2:D:9:G:C4'	2.42	0.48
3:F:35:VAL:CG1	3:F:75:VAL:HG11	2.41	0.48
1:A:278:LEU:O	1:A:278:LEU:HD12	2.12	0.48
1:A:449:PRO:HD2	1:A:452:VAL:CG2	2.44	0.48
1:B:201:ILE:HD11	1:B:232:GLU:OE2	2.11	0.48
1:B:980:ASN:HD22	1:B:980:ASN:H	1.60	0.48
3:E:29:PRO:HD2	3:E:89:ILE:CD1	2.43	0.48
1:A:752:GLY:C	1:A:753:ARG:CG	2.85	0.48
1:B:557:ARG:CZ	1:B:595:HIS:HB2	2.43	0.48
1:B:1336:TYR:CA	3:F:59:THR:HG23	2.37	0.48
1:B:1349:HIS:HB3	2:D:68:A:N3	2.27	0.48
1:A:1191:LYS:CG	1:A:1194:LEU:HD11	2.43	0.48
1:B:45:LYS:CA	1:B:1091:GLN:HE22	2.25	0.48
1:B:419:LEU:HD13	1:B:419:LEU:O	2.13	0.48
1:B:449:PRO:CD	1:B:452:VAL:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ILE:O	1:B:931:VAL:HG23	2.14	0.48
1:B:1206:LEU:HD12	1:B:1210:ARG:CB	2.40	0.48
1:B:1295:ASN:O	1:B:1298:ARG:HG3	2.13	0.48
3:F:4:THR:OG1	3:F:7:GLN:CD	2.56	0.48
3:F:20:MET:HE2	3:F:117:ILE:CD1	2.43	0.48
3:F:20:MET:HE3	3:F:116:ILE:HG22	1.94	0.48
1:A:557:ARG:HA	1:A:595:HIS:CD2	2.48	0.48
2:D:92:G:OP1	2:D:92:G:H4'	2.13	0.48
3:E:51:ALA:CB	3:E:52:VAL:HG22	2.37	0.48
1:A:457:ARG:NH2	2:C:57:A:OP1	2.47	0.48
1:A:823:TYR:O	1:A:824:VAL:HG22	2.13	0.48
1:A:1206:LEU:CD2	1:A:1206:LEU:N	2.77	0.48
1:A:1247:GLY:C	1:A:1252:ASN:ND2	2.72	0.48
1:B:464:TRP:CE2	1:B:491:PHE:HB2	2.49	0.48
1:B:549:VAL:HG23	1:B:550:ASP:N	2.28	0.48
1:B:1204:PHE:CG	1:B:1342:VAL:CG1	2.96	0.48
3:E:70:LEU:HD13	3:E:103:ALA:HB2	1.86	0.48
1:B:240:ASN:ND2	1:B:255:ASN:HD21	2.11	0.48
1:B:1242:TYR:OH	1:B:1256:GLN:HB3	2.14	0.48
2:D:29:G:C2	2:D:41:A:N3	2.81	0.48
2:D:93:G:C3'	2:D:94:U:C5'	2.91	0.48
3:F:31:PHE:CZ	3:F:76:ASP:O	2.67	0.48
3:F:52:VAL:HG21	3:F:110:LYS:HA	1.96	0.48
3:F:53:ALA:O	3:F:72:GLU:HB2	2.13	0.48
1:A:95:ASP:OD1	1:A:95:ASP:N	2.46	0.48
1:A:560:THR:HG23	1:A:563:GLN:CG	2.43	0.48
1:A:1146:VAL:CG2	1:A:1194:LEU:CD1	2.68	0.48
1:B:830:ILE:HA	1:B:833:LEU:HG	1.95	0.48
1:B:1009:VAL:HG12	1:B:1010:TYR:N	2.28	0.48
1:B:1274:SER:O	1:B:1278:LYS:HG2	2.11	0.48
2:D:13:C:O2'	2:D:14:G:O4'	2.32	0.48
3:F:52:VAL:HG11	3:F:110:LYS:HG3	1.68	0.48
1:A:1114:ARG:CG	1:A:1114:ARG:NH2	2.73	0.48
1:A:1325:LYS:CB	1:A:1325:LYS:NZ	2.76	0.48
1:B:97:PHE:HA	1:B:100:ARG:CZ	2.44	0.48
1:B:321:MET:HE2	1:B:321:MET:HA	1.96	0.48
1:B:552:LEU:HA	1:B:555:THR:OG1	2.14	0.48
3:F:17:PHE:CD2	3:F:44:ILE:HG13	2.49	0.48
1:A:143:VAL:HG11	1:A:315:ALA:HB2	1.96	0.48
1:A:450:TYR:CD1	2:C:16:U:H1'	2.47	0.48
1:A:1191:LYS:CG	1:A:1194:LEU:CD1	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:C:H2'	2:C:84:A:H8	1.78	0.48
1:B:554:LYS:O	1:B:595:HIS:CE1	2.53	0.48
1:B:746:GLU:O	1:B:750:VAL:HG23	2.14	0.48
1:B:1137:PRO:HB2	1:B:1167:THR:HG21	1.96	0.48
2:D:95:G:H2'	2:D:96:C:C5'	2.44	0.48
1:B:796:LEU:HD22	1:B:801:VAL:CG1	2.40	0.47
1:A:814:TYR:CZ	1:A:830:ILE:HB	2.49	0.47
1:B:449:PRO:HD2	1:B:452:VAL:CB	2.45	0.47
1:B:672:ASP:HA	1:B:703:THR:OG1	2.14	0.47
1:B:974:LYS:HD2	1:B:982:HIS:HB2	1.96	0.47
1:B:1105:PHE:CE2	1:B:1169:MET:HG3	2.48	0.47
3:F:99:ASP:O	3:F:100:LEU:HD23	2.14	0.47
1:A:195:LEU:O	1:A:196:PHE:HD2	1.96	0.47
1:A:449:PRO:HG2	1:A:452:VAL:HG21	1.95	0.47
1:A:557:ARG:NH2	1:A:596:ASP:CG	2.72	0.47
1:A:720:LEU:O	1:A:723:HIS:HB2	2.14	0.47
1:B:449:PRO:HD2	1:B:452:VAL:HB	1.96	0.47
1:B:494:ARG:NH1	1:B:494:ARG:CG	2.73	0.47
1:B:547:ALA:CB	1:B:551:LEU:HD11	2.37	0.47
1:B:1107:LYS:HD2	1:B:1136:SER:HB2	1.95	0.47
1:B:1204:PHE:CD2	1:B:1342:VAL:HG13	2.49	0.47
3:F:29:PRO:CG	3:F:78:SER:OG	2.60	0.47
3:F:66:THR:CB	3:F:69:TYR:OH	2.62	0.47
3:F:70:LEU:N	3:F:101:GLU:O	2.44	0.47
1:A:195:LEU:HB3	1:A:196:PHE:CD2	2.49	0.47
1:A:795:ILE:HD12	1:A:818:ASN:C	2.39	0.47
1:B:516:GLU:HA	1:B:519:THR:HG22	1.96	0.47
1:B:569:PHE:CA	1:B:573:GLU:HB3	2.44	0.47
1:B:788:ILE:HG21	1:B:796:LEU:HG	1.95	0.47
1:B:817:GLN:O	1:B:882:TYR:OH	2.31	0.47
2:D:93:G:N3	2:D:93:G:O5'	2.47	0.47
3:F:54:LEU:HD23	3:F:55:CYS:H	1.75	0.47
1:A:557:ARG:HH21	1:A:596:ASP:H	1.60	0.47
1:A:936:ASP:HB2	1:A:955:VAL:CG1	2.41	0.47
1:A:1143:VAL:HG13	1:A:1195:ILE:CG2	2.44	0.47
1:A:1337:THR:HB	3:E:97:ILE:HD11	1.96	0.47
1:B:268:LYS:NZ	3:F:30:ASP:OD1	2.40	0.47
1:B:324:ARG:HD3	1:B:400:ARG:HB2	1.97	0.47
1:B:546:LYS:O	1:B:550:ASP:OD2	2.32	0.47
3:F:74:LEU:CD2	3:F:75:VAL:N	2.78	0.47
1:A:718:ASP:C	1:A:723:HIS:CE1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:TYR:CE1	1:A:830:ILE:HD12	2.50	0.47
1:B:171:GLU:CG	1:B:629:ARG:NH1	2.65	0.47
1:B:348:LYS:O	1:B:352:PHE:HB2	2.15	0.47
1:B:419:LEU:C	1:B:419:LEU:CD1	2.85	0.47
1:B:495:MET:HE1	2:D:14:G:N9	2.29	0.47
1:B:680:LEU:O	1:B:684:LYS:HG3	2.15	0.47
1:B:704:PHE:O	1:B:708:ILE:HG13	2.14	0.47
1:B:1286:ASN:HD22	1:B:1334:LYS:HE2	1.80	0.47
3:F:64:TYR:C	3:F:66:THR:N	2.62	0.47
1:A:516:GLU:HA	1:A:519:THR:HG22	1.97	0.47
1:A:606:PHE:CZ	1:A:612:ASN:ND2	2.83	0.47
1:A:743:VAL:HG12	1:A:747:LEU:HD12	1.96	0.47
1:A:1277:SER:HB2	1:A:1287:LEU:HD22	1.97	0.47
2:C:12:G:C8	2:C:13:C:C5	3.02	0.47
2:C:12:G:C4	2:C:13:C:C5	3.03	0.47
1:B:45:LYS:NZ	1:B:1357:GLU:OE2	2.37	0.47
1:B:751:MET:HE3	1:B:751:MET:HB3	1.75	0.47
1:B:1197:LYS:HE2	1:B:1199:PRO:HG3	1.97	0.47
1:B:1242:TYR:HD2	1:B:1256:GLN:HE21	1.59	0.47
3:F:74:LEU:HD22	3:F:75:VAL:N	2.30	0.47
1:A:1191:LYS:CD	1:A:1194:LEU:CD1	2.86	0.47
1:B:34:VAL:HG23	1:B:42:SER:HA	1.97	0.47
3:F:5:ARG:CG	3:F:5:ARG:NH1	2.76	0.47
1:B:665:LYS:C	1:B:669:GLY:HA3	2.37	0.47
1:B:477:ASN:OD1	1:B:481:VAL:HG21	2.12	0.47
1:B:531:THR:C	1:B:534:MET:HG3	2.39	0.47
1:B:563:GLN:HA	1:B:567:ASP:OD2	2.15	0.47
1:B:993:VAL:HG12	1:B:997:LEU:HD12	1.97	0.47
1:B:1255:LYS:O	1:B:1258:PHE:HB3	2.15	0.47
2:D:46:A:H2'	2:D:47:A:H8	1.79	0.47
2:D:92:G:H2'	2:D:92:G:N3	2.30	0.47
1:A:308:VAL:HG12	1:A:309:ASN:C	2.40	0.46
1:A:489:GLN:NE2	1:A:489:GLN:CA	2.74	0.46
1:A:1179:ILE:CG1	1:A:1192:LYS:HE3	2.45	0.46
1:B:45:LYS:HA	1:B:1091:GLN:NE2	2.30	0.46
1:B:926:GLN:CD	2:D:9:G:H5''	2.38	0.46
3:E:49:LYS:HZ3	3:E:50:TYR:HE1	1.61	0.46
1:B:271:TYR:HA	1:B:274:ASP:HB2	1.98	0.46
1:B:492:ILE:CG2	1:B:625:LEU:CD1	2.92	0.46
1:B:846:PHE:O	1:B:1040:SER:C	2.58	0.46
1:B:1106:SER:HB2	1:B:1136:SER:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:106:GLU:O	3:F:109:MET:N	2.48	0.46
3:E:70:LEU:HD22	3:E:70:LEU:H	1.80	0.46
3:E:120:SER:OG	3:E:123:LYS:HG2	2.14	0.46
1:A:334:LEU:O	1:A:337:ALA:HB3	2.15	0.46
1:B:182:ASP:O	1:B:185:PHE:HB3	2.16	0.46
1:B:1121:ALA:HB1	1:B:1126:TRP:O	2.15	0.46
3:E:37:HIS:C	3:E:37:HIS:CD2	2.92	0.46
3:E:54:LEU:HG	3:E:110:LYS:CB	2.45	0.46
1:A:765:ARG:HG3	1:A:925:ARG:HH12	1.81	0.46
1:B:45:LYS:CB	1:B:1091:GLN:HE22	2.29	0.46
1:B:598:LEU:HA	1:B:607:LEU:HD11	1.98	0.46
2:D:88:A:N6	2:D:91:C:N4	2.63	0.46
1:A:216:LEU:N	1:A:216:LEU:CD1	2.73	0.46
1:A:387:GLU:O	1:A:391:VAL:HG23	2.15	0.46
1:A:956:ILE:HG12	1:A:1009:VAL:HG22	1.97	0.46
1:B:556:ASN:HD22	1:B:556:ASN:N	2.13	0.46
1:B:713:VAL:HG12	1:B:714:SER:O	2.16	0.46
1:B:916:PHE:HD1	1:B:1040:SER:OG	1.80	0.46
3:F:31:PHE:CZ	3:F:76:ASP:C	2.94	0.46
3:E:49:LYS:HE2	3:E:50:TYR:CD1	2.51	0.46
1:A:359:TYR:CE1	1:A:363:ILE:HG12	2.51	0.46
2:C:34:A:H3'	2:C:35:A:H8	1.80	0.46
1:B:1286:ASN:HD22	1:B:1334:LYS:HG3	1.79	0.46
1:A:531:THR:N	1:A:534:MET:CG	2.78	0.46
1:A:563:GLN:O	1:A:567:ASP:HB3	2.16	0.46
1:B:456:ALA:O	1:B:467:ARG:NH2	2.49	0.46
1:B:551:LEU:O	1:B:555:THR:OG1	2.34	0.46
1:B:1110:ILE:HB	2:D:22:U:O2'	2.15	0.46
1:B:980:ASN:ND2	1:B:980:ASN:N	2.63	0.46
3:E:74:LEU:CD2	3:E:75:VAL:N	2.79	0.46
1:A:336:LYS:HE2	1:A:351:PHE:HD1	1.79	0.46
1:A:549:VAL:HG13	1:A:550:ASP:N	2.31	0.46
1:A:606:PHE:CG	1:A:612:ASN:ND2	2.83	0.46
1:A:1110:ILE:HG23	1:A:1122:ARG:HD2	1.97	0.46
1:B:302:LEU:O	1:B:306:LEU:HD11	2.16	0.46
3:F:31:PHE:HE1	3:F:76:ASP:C	2.19	0.46
3:F:54:LEU:N	3:F:110:LYS:HZ2	2.14	0.46
3:E:23:ASP:O	3:E:25:GLU:OE1	2.34	0.46
1:A:522:ASN:O	1:A:525:THR:HG22	2.16	0.46
1:A:768:GLN:CD	1:A:768:GLN:N	2.73	0.46
1:A:896:LYS:O	1:A:900:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:ILE:O	1:A:1272:GLN:HB2	2.15	0.46
3:F:74:LEU:CD2	3:F:75:VAL:H	2.28	0.46
1:A:549:VAL:HA	1:A:553:PHE:HB2	1.98	0.45
1:A:1020:LYS:O	1:A:1035:LYS:NZ	2.34	0.45
1:B:518:PHE:CD1	1:B:667:ILE:HG23	2.51	0.45
1:B:677:LYS:HD3	1:B:682:PHE:CZ	2.51	0.45
1:B:747:LEU:HD23	1:B:1353:THR:HG21	1.98	0.45
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.13	0.45
1:A:100:ARG:NH1	1:A:100:ARG:CG	2.73	0.45
1:A:226:ILE:HD11	1:A:239:GLY:HA2	1.98	0.45
1:A:1072:ILE:N	1:A:1072:ILE:CD1	2.73	0.45
1:B:38:THR:HG22	1:B:1361:ASP:HB2	1.99	0.45
1:B:479:GLU:CG	1:B:484:LYS:HZ3	2.27	0.45
1:B:677:LYS:HD3	1:B:682:PHE:CD1	2.51	0.45
1:B:743:VAL:HG22	1:B:1352:ILE:CD1	2.47	0.45
3:E:49:LYS:HE2	3:E:50:TYR:CE1	2.50	0.45
1:A:138:LEU:O	1:A:142:LEU:HG	2.16	0.45
1:A:359:TYR:O	1:A:359:TYR:HD1	2.00	0.45
1:A:569:PHE:HD2	1:A:578:VAL:CG2	2.29	0.45
1:B:65:LYS:O	1:B:69:ARG:HG3	2.16	0.45
1:B:118:ILE:N	1:B:125:GLU:OE2	2.40	0.45
1:B:713:VAL:O	1:B:714:SER:HB3	2.17	0.45
3:E:34:GLU:O	3:E:38:ASP:CG	2.58	0.45
3:E:118:LEU:O	3:E:118:LEU:HG	2.15	0.45
1:A:140:LYS:NZ	1:A:313:THR:CG2	2.80	0.45
1:A:594:TYR:OH	1:A:604:LYS:NZ	2.49	0.45
1:A:1179:ILE:H	1:A:1179:ILE:HD12	1.81	0.45
2:C:12:G:H2'	2:C:13:C:H5'	1.99	0.45
1:B:393:LEU:O	1:B:396:GLU:N	2.47	0.45
1:B:539:PHE:HB3	1:B:690:ASN:HD22	1.77	0.45
1:B:561:VAL:O	1:B:565:LYS:CB	2.64	0.45
1:B:1038:PHE:CE2	1:B:1039:TYR:CE1	3.05	0.45
1:A:718:ASP:N	1:A:718:ASP:OD2	2.50	0.45
1:A:768:GLN:CD	1:A:768:GLN:H	2.23	0.45
1:B:609:ASN:O	1:B:612:ASN:HB2	2.16	0.45
2:D:9:G:HO2'	2:D:10:G:P	2.24	0.45
3:F:4:THR:HB	3:F:7:GLN:CG	2.43	0.45
1:A:969:ASP:HB3	1:A:970:PHE:CE2	2.51	0.45
2:C:73:G:H21	2:C:76:A:H2	1.65	0.45
1:B:9:LEU:HA	1:B:17:GLY:O	2.16	0.45
1:B:549:VAL:CG2	1:B:550:ASP:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:PHE:CG	1:B:578:VAL:HG21	2.28	0.45
1:B:926:GLN:HG2	2:D:9:G:H5'	1.94	0.45
2:D:46:A:N1	2:D:47:A:C6	2.85	0.45
2:D:65:A:H8	2:D:65:A:O5'	1.99	0.45
3:F:45:THR:HB	3:F:49:LYS:O	2.17	0.45
3:F:57:LEU:HD12	3:F:68:LEU:HD12	1.97	0.45
1:A:94:ASP:HB3	1:A:97:PHE:HB2	1.99	0.45
1:A:395:ARG:O	1:A:396:GLU:HB2	2.17	0.45
1:A:853:ASP:O	1:A:896:LYS:HD2	2.17	0.45
1:B:1269:ILE:O	1:B:1272:GLN:HB2	2.16	0.45
2:D:42:A:O2'	2:D:43:G:H5'	2.17	0.45
1:A:83:GLN:O	1:A:87:SER:N	2.50	0.45
1:A:253:LYS:HB2	1:A:261:ASP:HA	1.99	0.45
1:A:1010:TYR:C	1:A:1010:TYR:CD2	2.94	0.45
1:B:105:PHE:CE1	2:D:24:U:C1'	2.99	0.45
1:B:416:LEU:HD12	1:B:416:LEU:C	2.41	0.45
2:D:87:G:N3	2:D:87:G:C5'	2.80	0.45
1:A:981:TYR:O	1:A:984:ALA:N	2.50	0.45
1:A:1038:PHE:O	1:A:1038:PHE:CD1	2.70	0.45
1:B:71:ARG:NE	2:D:17:U:H5	1.87	0.45
1:B:1331:ILE:N	1:B:1331:ILE:HD12	2.32	0.45
3:F:31:PHE:CE1	3:F:76:ASP:HB3	2.44	0.45
3:F:50:TYR:HD1	3:F:77:TYR:CD1	2.34	0.45
1:A:531:THR:CG2	1:A:532:GLU:H	2.30	0.45
1:A:654:ARG:HD3	1:A:655:ARG:N	2.32	0.45
1:A:847:LEU:HG	1:A:848:LYS:N	2.31	0.45
1:A:1008:PHE:H	1:A:1008:PHE:HD1	1.64	0.45
1:A:1334:LYS:CE	3:E:57:LEU:O	2.65	0.45
2:C:92:G:C6	2:C:93:G:C5	3.05	0.45
1:B:495:MET:CE	2:D:14:G:N9	2.80	0.45
2:D:9:G:O2'	2:D:10:G:C5	2.70	0.45
2:D:11:U:O2	2:D:12:G:C6	2.70	0.45
3:F:54:LEU:CG	3:F:55:CYS:N	2.80	0.45
1:A:496:THR:HG21	1:A:506:LYS:CB	2.47	0.44
1:A:568:TYR:HA	1:A:572:ILE:HG13	1.99	0.44
1:A:1280:VAL:CG2	1:A:1281:ILE:N	2.79	0.44
2:C:13:C:O2'	2:C:14:G:H5'	2.17	0.44
1:B:738:LEU:O	1:B:738:LEU:HD12	2.17	0.44
3:F:106:GLU:O	3:F:107:ASP:C	2.61	0.44
1:A:310:THR:HG22	1:A:311:GLU:N	2.32	0.44
1:A:766:GLU:C	1:A:768:GLN:NE2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LYS:O	1:A:1343:LEU:CD1	2.65	0.44
1:B:569:PHE:O	1:B:573:GLU:HB3	2.17	0.44
1:B:829:ASP:CG	1:B:832:ARG:CG	2.85	0.44
2:D:82:G:C5	2:D:83:C:C5	3.06	0.44
3:F:4:THR:HB	3:F:7:GLN:H	1.83	0.44
1:A:449:PRO:HG2	1:A:452:VAL:CG2	2.47	0.44
1:A:846:PHE:CE1	1:A:913:LYS:HE3	2.34	0.44
1:B:568:TYR:HD2	1:B:569:PHE:CD2	2.36	0.44
1:B:693:PHE:CD1	1:B:693:PHE:O	2.70	0.44
2:D:9:G:O2'	2:D:10:G:C4	2.70	0.44
3:F:54:LEU:CD2	3:F:55:CYS:N	2.73	0.44
3:F:63:GLU:CG	3:F:64:TYR:N	2.73	0.44
3:F:67:ASN:C	3:F:68:LEU:CD1	2.85	0.44
1:A:551:LEU:O	1:A:555:THR:HB	2.17	0.44
1:B:573:GLU:CG	1:B:575:PHE:CD1	2.85	0.44
1:B:727:LEU:N	1:B:727:LEU:CD2	2.73	0.44
1:B:1086:VAL:O	1:B:1089:MET:CG	2.59	0.44
2:D:82:G:C5	2:D:83:C:C4	3.05	0.44
3:F:48:GLU:HA	3:F:88:TYR:HE2	1.81	0.44
3:F:87:TYR:CE1	3:F:116:ILE:HD12	2.52	0.44
3:E:43:VAL:HG12	3:E:92:VAL:HG23	2.00	0.44
1:A:350:ILE:HB	1:A:351:PHE:HD2	1.81	0.44
1:A:836:TYR:N	1:A:836:TYR:HD1	2.15	0.44
1:A:1179:ILE:O	1:A:1183:GLU:N	2.45	0.44
1:B:661:ARG:HD2	2:D:10:G:O6	2.17	0.44
1:B:936:ASP:OD1	1:B:951:ARG:NH1	2.51	0.44
1:B:981:TYR:HE2	1:B:1090:PRO:O	2.01	0.44
2:D:83:C:O5'	2:D:83:C:H6	2.01	0.44
1:A:568:TYR:CE2	1:A:569:PHE:HD1	1.82	0.44
1:A:870:VAL:HG21	1:A:902:LYS:HB3	1.99	0.44
2:C:21:G:H2'	2:C:22:U:C6	2.52	0.44
1:B:853:ASP:OD1	1:B:895:ARG:NH1	2.50	0.44
1:B:1242:TYR:CD2	1:B:1256:GLN:HG2	2.51	0.44
2:D:32:A:H2'	2:D:33:G:O4'	2.18	0.44
3:F:15:HIS:C	3:F:15:HIS:ND1	2.75	0.44
3:F:82:VAL:HG12	3:F:83:ASN:N	2.33	0.44
1:A:34:VAL:HG23	1:A:42:SER:HA	1.99	0.44
1:B:167:HIS:ND1	1:B:167:HIS:C	2.75	0.44
2:D:94:U:C5	2:D:95:G:N2	2.85	0.44
3:E:16:GLU:O	3:E:19:ASN:CB	2.65	0.44
1:A:215:ARG:HD2	1:A:395:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:CD2	1:A:569:PHE:CE1	2.81	0.44
1:B:215:ARG:NH2	1:B:395:ARG:HH12	2.16	0.44
1:B:1110:ILE:HD13	1:B:1122:ARG:CZ	2.48	0.44
1:B:1149:VAL:HG21	1:B:1160:VAL:HG11	2.00	0.44
3:F:74:LEU:HD23	3:F:75:VAL:H	1.83	0.44
3:E:74:LEU:HD23	3:E:75:VAL:H	1.83	0.44
1:A:1333:ARG:CD	1:A:1333:ARG:N	2.76	0.44
2:C:84:A:C2	2:C:85:C:C5	3.06	0.44
2:C:92:G:H2'	2:C:93:G:OP1	2.18	0.44
1:B:302:LEU:O	1:B:306:LEU:CD1	2.66	0.44
1:B:465:MET:HG2	1:B:466:THR:N	2.31	0.44
1:B:495:MET:HE3	2:D:14:G:C2'	2.48	0.44
3:F:50:TYR:CZ	3:F:88:TYR:CE2	3.05	0.44
1:A:420:HIS:NE2	1:A:424:ARG:HD2	2.32	0.43
1:B:496:THR:HG22	1:B:659:TRP:CZ3	2.52	0.43
1:B:1206:LEU:CD1	1:B:1210:ARG:HB3	2.46	0.43
2:D:88:A:N6	2:D:91:C:C4	2.86	0.43
2:C:84:A:H2'	2:C:85:C:O4'	2.17	0.43
1:B:692:ASN:OD1	1:B:695:GLN:N	2.36	0.43
1:B:727:LEU:HD23	1:B:727:LEU:H	1.81	0.43
1:B:1123:LYS:HE2	2:D:52:A:OP1	2.18	0.43
3:F:66:THR:O	3:F:67:ASN:HB3	2.18	0.43
1:A:214:ALA:CB	1:A:216:LEU:HD11	2.48	0.43
1:A:457:ARG:HH22	2:C:57:A:H5''	1.81	0.43
1:A:554:LYS:HG2	1:A:594:TYR:CE2	2.54	0.43
2:C:27:G:H5'	2:C:28:A:H5''	2.00	0.43
2:C:91:C:H2'	2:C:92:G:H5''	1.99	0.43
3:F:68:LEU:N	3:F:68:LEU:CD1	2.80	0.43
3:F:100:LEU:C	3:F:101:GLU:HG3	2.44	0.43
1:A:140:LYS:HZ3	1:A:313:THR:CG2	2.30	0.43
1:A:284:ASP:CG	1:A:510:LYS:NZ	2.76	0.43
1:A:916:PHE:C	1:A:920:GLN:HE21	2.25	0.43
1:B:305:ILE:HG21	1:B:410:ILE:HD11	2.01	0.43
1:B:488:ALA:O	1:B:492:ILE:HD11	2.07	0.43
1:B:579:GLU:C	1:B:579:GLU:CD	2.85	0.43
1:B:747:LEU:HD23	1:B:747:LEU:N	2.33	0.43
1:B:1066:ASN:HB3	1:B:1069:THR:OG1	2.18	0.43
1:B:1207:GLU:CD	1:B:1210:ARG:HH12	2.26	0.43
3:F:53:ALA:CB	3:F:70:LEU:CD2	2.95	0.43
3:E:43:VAL:O	3:E:90:ASN:O	2.36	0.43
3:E:67:ASN:O	3:E:69:TYR:CD1	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASP:OD2	1:A:356:LYS:CD	2.65	0.43
1:A:563:GLN:HG2	1:A:563:GLN:H	1.59	0.43
1:A:632:ILE:HG22	1:A:652:LYS:HG2	2.00	0.43
1:A:902:LYS:CA	1:A:905:ARG:NH2	2.82	0.43
1:A:20:VAL:HG21	1:A:747:LEU:CD2	2.48	0.43
1:A:321:MET:HE1	1:A:324:ARG:CZ	2.49	0.43
1:A:628:ASP:O	1:A:632:ILE:HG13	2.18	0.43
1:A:735:LYS:O	1:A:739:GLN:HG2	2.18	0.43
1:A:1106:SER:CB	1:A:1137:PRO:HA	2.48	0.43
2:D:93:G:N3	2:D:93:G:H5''	2.34	0.43
3:E:56:SER:HB2	3:E:71:ASP:CG	2.44	0.43
1:A:20:VAL:HG22	1:A:747:LEU:HD22	2.01	0.43
1:A:51:LEU:HD22	1:A:1352:ILE:CG1	2.49	0.43
1:A:760:VAL:HG21	1:A:991:ALA:HA	2.00	0.43
1:A:813:LEU:HD23	1:A:816:LEU:HD12	2.01	0.43
1:A:1308:ASN:ND2	1:A:1327:PHE:CE1	2.87	0.43
2:C:83:C:H2'	2:C:84:A:C8	2.53	0.43
2:C:92:G:H5''	2:C:92:G:H8	1.83	0.43
1:B:563:GLN:HG2	1:B:563:GLN:H	1.54	0.43
1:B:733:ILE:HG23	1:B:734:LYS:N	2.33	0.43
1:B:1075:ASP:HB3	1:B:1079:ASP:OD2	2.19	0.43
1:B:1292:SER:O	1:B:1296:LYS:HG3	2.19	0.43
1:A:208:ALA:O	1:A:212:LEU:HD12	2.18	0.43
1:A:212:LEU:O	1:A:221:ARG:HD2	2.19	0.43
1:A:347:TYR:CD2	1:A:347:TYR:O	2.70	0.43
1:A:693:PHE:CD2	1:A:693:PHE:C	2.97	0.43
1:B:243:ALA:HB1	1:B:248:LEU:HD12	2.00	0.43
1:B:479:GLU:CG	1:B:484:LYS:HZ2	2.32	0.43
1:B:1206:LEU:HD22	1:B:1210:ARG:HH21	1.83	0.43
3:E:69:TYR:CD2	3:E:102:ILE:HG13	2.54	0.43
1:A:222:LEU:HD21	1:A:243:ALA:HB2	2.00	0.43
1:A:1194:LEU:O	1:A:1196:ILE:HG13	2.19	0.43
1:B:107:VAL:O	1:B:110:ASP:N	2.44	0.43
1:B:747:LEU:HD23	1:B:1353:THR:CG2	2.47	0.43
3:F:54:LEU:H	3:F:110:LYS:NZ	2.17	0.43
1:A:253:LYS:HD2	1:A:261:ASP:HB3	2.00	0.43
1:A:308:VAL:CG1	1:A:309:ASN:N	2.81	0.43
1:A:322:ILE:O	1:A:323:LYS:C	2.62	0.43
1:A:1116:SER:OG	1:A:1118:LYS:HG3	2.19	0.43
1:B:540:LEU:HD22	1:B:544:GLN:HB2	2.00	0.43
1:B:846:PHE:HA	1:B:1040:SER:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:THR:HG22	1:B:1168:ILE:HD12	2.01	0.43
1:B:1314:THR:HA	1:B:1317:ASN:ND2	2.34	0.43
3:F:69:TYR:N	3:F:69:TYR:HD2	2.16	0.43
1:A:0:SER:HB2	2:C:85:C:OP1	2.19	0.42
1:A:20:VAL:HG23	1:A:747:LEU:HD21	2.00	0.42
1:A:923:GLU:HA	1:A:959:LYS:HE2	2.01	0.42
1:A:1245:LEU:HD23	1:A:1245:LEU:HA	1.77	0.42
1:A:1325:LYS:CB	1:A:1325:LYS:HZ2	2.32	0.42
1:A:1342:VAL:O	1:A:1362:LEU:HD12	2.19	0.42
1:B:740:THR:O	1:B:744:VAL:HG23	2.18	0.42
1:B:752:GLY:O	1:B:754:HIS:CD2	2.72	0.42
1:B:115:ARG:HE	1:B:115:ARG:HB2	1.64	0.42
1:B:315:ALA:CA	1:B:418:GLU:OE2	2.66	0.42
3:F:57:LEU:C	3:F:57:LEU:CD2	2.85	0.42
1:A:399:LEU:HD23	1:A:399:LEU:H	1.81	0.42
1:A:496:THR:CG2	1:A:506:LYS:HB3	2.49	0.42
1:A:745:ASP:OD1	1:A:938:ARG:NH1	2.52	0.42
2:C:75:A:C2	2:C:76:A:C5	3.07	0.42
1:B:552:LEU:O	1:B:555:THR:OG1	2.30	0.42
2:D:95:G:H2'	2:D:96:C:O5'	2.19	0.42
3:E:18:ILE:CG1	3:E:24:PHE:HE1	2.31	0.42
1:A:332:LEU:HD13	1:A:359:TYR:CE2	2.54	0.42
1:A:359:TYR:CD1	1:A:359:TYR:C	2.97	0.42
1:A:526:LYS:HA	1:A:526:LYS:HD2	1.81	0.42
1:A:1007:GLU:N	1:A:1007:GLU:OE2	2.52	0.42
1:B:678:THR:O	1:B:679:ILE:C	2.63	0.42
2:D:73:G:H21	2:D:76:A:H2	1.65	0.42
3:F:118:LEU:C	3:F:118:LEU:CD2	2.85	0.42
1:A:765:ARG:NE	1:A:925:ARG:NH1	2.65	0.42
1:A:998:ILE:HD11	1:A:1005:GLU:HG2	2.02	0.42
1:B:249:THR:HG22	1:B:265:GLN:CG	2.49	0.42
1:B:970:PHE:O	1:B:971:GLN:HB2	2.20	0.42
1:B:1206:LEU:HD12	1:B:1210:ARG:CG	2.50	0.42
3:E:18:ILE:HD13	3:E:24:PHE:CE1	2.55	0.42
3:E:29:PRO:HD2	3:E:89:ILE:HD13	2.00	0.42
3:E:70:LEU:HD11	3:E:103:ALA:CA	2.49	0.42
1:A:72:TYR:CE1	2:C:50:U:C4	3.08	0.42
1:A:182:ASP:O	1:A:185:PHE:HB3	2.19	0.42
1:A:724:ILE:O	1:A:727:LEU:HD21	2.19	0.42
1:A:914:ALA:CB	1:A:1018:VAL:HB	2.49	0.42
1:A:1208:ASN:HD22	1:A:1208:ASN:HA	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PRO:O	1:B:263:LYS:HA	2.20	0.42
1:B:1334:LYS:NZ	3:F:57:LEU:CD1	2.71	0.42
3:E:20:MET:O	3:E:21:VAL:HB	2.19	0.42
3:E:82:VAL:CG1	3:E:83:ASN:H	2.32	0.42
1:A:97:PHE:CD1	1:A:97:PHE:O	2.73	0.42
2:C:16:U:C4	2:C:17:U:O4	2.71	0.42
2:C:74:A:H2'	2:C:75:A:C8	2.55	0.42
1:B:8:GLY:O	1:B:18:TRP:HA	2.20	0.42
1:B:249:THR:HG22	1:B:265:GLN:CB	2.47	0.42
1:B:606:PHE:HE2	1:B:616:LEU:HD21	1.84	0.42
1:B:980:ASN:ND2	1:B:1225:GLU:OE2	2.50	0.42
1:B:1016:TYR:HB2	1:B:1021:MET:CE	2.50	0.42
2:D:95:G:H2'	2:D:96:C:H5'	2.02	0.42
1:A:158:LEU:HD22	1:A:419:LEU:CD2	2.48	0.42
1:A:161:MET:HE1	1:A:419:LEU:HA	2.02	0.42
1:A:867:SER:C	1:A:1054:ASN:HD22	2.27	0.42
1:A:967:ARG:HB3	1:A:972:PHE:O	2.20	0.42
1:A:1215:ALA:HB2	1:A:1221:GLN:HG3	2.02	0.42
2:C:76:A:C5	2:C:77:A:H1'	2.55	0.42
1:B:265:GLN:OE1	1:B:268:LYS:HG3	2.19	0.42
1:B:1035:LYS:HE2	1:B:1035:LYS:HB3	1.70	0.42
1:B:1181:PHE:O	1:B:1184:ALA:HB3	2.20	0.42
1:B:1210:ARG:NH2	1:B:1341:GLU:OE2	2.52	0.42
1:A:308:VAL:HG12	1:A:309:ASN:N	2.33	0.42
1:A:718:ASP:C	1:A:723:HIS:HE2	2.27	0.42
1:A:995:THR:HA	1:A:998:ILE:HG22	2.02	0.42
1:A:1114:ARG:HH11	1:A:1116:SER:HB2	1.85	0.42
1:B:524:LEU:HD11	1:B:548:ILE:CG2	2.50	0.42
1:B:539:PHE:CB	1:B:690:ASN:ND2	2.72	0.42
2:D:42:A:C8	2:D:42:A:H3'	2.54	0.42
3:E:18:ILE:O	3:E:21:VAL:HG22	2.19	0.42
3:E:102:ILE:N	3:E:102:ILE:CD1	2.73	0.42
1:A:549:VAL:CG1	1:A:550:ASP:N	2.82	0.42
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.90	0.42
1:A:1204:PHE:CZ	1:A:1342:VAL:CG1	3.02	0.42
1:B:251:ASN:HD21	1:B:261:ASP:HB2	1.84	0.42
3:F:87:TYR:HE1	3:F:116:ILE:HD12	1.84	0.42
1:A:420:HIS:O	1:A:424:ARG:HG3	2.20	0.41
1:A:489:GLN:NE2	1:A:489:GLN:C	2.78	0.41
1:A:720:LEU:O	1:A:723:HIS:N	2.53	0.41
1:A:1195:ILE:H	1:A:1195:ILE:HG13	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:A:C6	2:C:77:A:H1'	2.55	0.41
1:B:66:ARG:O	1:B:67:THR:C	2.62	0.41
1:B:460:SER:HA	2:D:61:C:H5'	2.02	0.41
1:B:477:ASN:CB	1:B:481:VAL:HG23	2.50	0.41
3:F:116:ILE:O	3:F:117:ILE:HG12	2.20	0.41
1:A:530:VAL:C	1:A:534:MET:HG2	2.40	0.41
1:A:842:VAL:H	1:A:854:ASN:ND2	2.17	0.41
1:B:39:ASP:OD2	1:B:39:ASP:N	2.53	0.41
2:D:45:U:H2'	2:D:46:A:O5'	2.20	0.41
2:D:82:G:C6	2:D:83:C:N4	2.88	0.41
3:F:79:THR:HG23	3:F:88:TYR:CZ	2.45	0.41
2:C:11:U:O2'	2:C:12:G:P	2.78	0.41
2:C:83:C:H2'	2:C:84:A:O5'	2.20	0.41
1:B:13:THR:O	1:B:53:PHE:HE1	2.03	0.41
1:B:60:GLU:O	1:B:61:ALA:C	2.63	0.41
1:B:564:LEU:HD12	1:B:564:LEU:O	2.20	0.41
1:B:750:VAL:HG21	1:B:1355:LEU:CD1	2.50	0.41
1:B:1336:TYR:CA	3:F:59:THR:CG2	2.73	0.41
3:F:15:HIS:O	3:F:18:ILE:N	2.53	0.41
1:A:830:ILE:O	1:A:833:LEU:HG	2.20	0.41
1:A:1276:PHE:CE2	1:A:1316:THR:HB	2.55	0.41
2:C:94:U:C2'	2:C:95:G:O5'	2.69	0.41
1:B:546:LYS:O	1:B:549:VAL:HG22	2.20	0.41
1:B:1295:ASN:HA	1:B:1298:ARG:CG	2.50	0.41
3:F:22:ASP:CB	3:F:82:VAL:CG2	2.99	0.41
1:A:780:ARG:CB	1:A:806:LEU:HD23	2.49	0.41
1:B:477:ASN:HB2	1:B:481:VAL:HG23	2.02	0.41
3:F:20:MET:HE2	3:F:117:ILE:HG12	1.99	0.41
1:A:662:LEU:HD22	1:A:666:LEU:CD2	2.51	0.41
1:A:985:HIS:CG	1:A:1087:LEU:HD22	2.55	0.41
1:A:1119:LEU:HD22	1:A:1135:ASP:HA	2.02	0.41
1:B:362:TYR:HA	1:B:367:ALA:HB3	2.02	0.41
1:B:398:LEU:CD2	1:B:399:LEU:CG	2.94	0.41
1:A:60:GLU:HB2	1:A:63:ARG:HH12	1.86	0.41
1:B:531:THR:HG22	1:B:534:MET:SD	2.61	0.41
1:B:568:TYR:CD2	1:B:569:PHE:CD2	3.08	0.41
1:B:1169:MET:HG2	2:D:52:A:N3	2.36	0.41
3:F:12:GLU:HB3	3:F:119:LYS:NZ	2.35	0.41
3:F:33:LYS:H	3:F:33:LYS:HG3	1.58	0.41
1:A:724:ILE:HD13	1:A:738:LEU:HB2	2.03	0.41
1:A:1325:LYS:HB3	1:A:1325:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:G:H2'	2:C:20:C:O4'	2.21	0.41
2:C:83:C:C2	2:C:84:A:N7	2.89	0.41
1:B:395:ARG:HD2	1:B:397:ASP:HB3	2.01	0.41
1:B:495:MET:HE2	2:D:14:G:C4	2.56	0.41
1:B:596:ASP:C	1:B:600:ILE:CD1	2.76	0.41
1:B:623:LEU:HD13	1:B:654:ARG:O	2.21	0.41
1:B:926:GLN:CB	2:D:9:G:H3'	2.49	0.41
1:B:1210:ARG:CD	1:B:1282:LEU:HD11	2.51	0.41
3:E:99:ASP:C	3:E:100:LEU:HG	2.44	0.41
1:A:67:THR:O	1:A:68:ALA:C	2.64	0.41
1:A:214:ALA:CB	1:A:216:LEU:CD1	2.99	0.41
1:A:1314:THR:OG1	1:A:1324:PHE:CD1	2.74	0.41
2:C:22:U:H6	2:C:22:U:O5'	2.04	0.41
1:B:106:LEU:O	2:D:25:U:H4'	2.20	0.41
1:B:268:LYS:HG2	3:F:30:ASP:OD2	2.20	0.41
1:B:271:TYR:O	1:B:274:ASP:HB2	2.20	0.41
1:B:351:PHE:C	1:B:360:ALA:HB2	2.46	0.41
1:B:665:LYS:HA	1:B:669:GLY:CA	2.50	0.41
1:B:1138:THR:HG22	1:B:1168:ILE:CD1	2.51	0.41
2:D:13:C:O2	2:D:14:G:C5	2.73	0.41
2:D:20:C:H2'	2:D:21:G:H5'	2.03	0.41
3:F:21:VAL:O	3:F:21:VAL:HG12	2.20	0.41
3:E:22:ASP:O	3:E:23:ASP:C	2.63	0.41
3:E:52:VAL:CG2	3:E:92:VAL:HG22	2.50	0.41
1:A:90:MET:SD	1:A:97:PHE:CD2	3.03	0.41
1:A:217:SER:O	1:A:218:LYS:C	2.63	0.41
1:A:310:THR:CG2	1:A:311:GLU:N	2.84	0.41
1:A:531:THR:O	1:A:534:MET:SD	2.79	0.41
1:A:752:GLY:O	1:A:753:ARG:HG3	2.20	0.41
1:A:966:PHE:HE2	1:A:972:PHE:CE1	2.39	0.41
2:C:16:U:O4	2:C:17:U:O4	2.38	0.41
1:B:573:GLU:O	1:B:574:CYS:SG	2.79	0.41
2:D:94:U:C2'	2:D:95:G:O5'	2.69	0.41
2:D:96:C:H2'	2:D:97:U:C6	2.55	0.41
3:F:17:PHE:HZ	3:F:87:TYR:CD1	2.39	0.41
3:F:72:GLU:HB3	3:F:92:VAL:HG13	2.02	0.41
1:A:20:VAL:HG23	1:A:747:LEU:CD2	2.51	0.40
1:A:268:LYS:HE3	3:E:28:THR:O	2.19	0.40
1:B:133:PRO:HD2	1:B:137:HIS:CG	2.56	0.40
1:B:530:VAL:CB	1:B:579:GLU:OE1	2.69	0.40
1:B:569:PHE:O	1:B:573:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ARG:HG2	1:B:695:GLN:OE1	2.21	0.40
2:D:42:A:O2'	2:D:43:G:P	2.79	0.40
3:F:24:PHE:CB	3:F:82:VAL:HA	2.49	0.40
3:F:75:VAL:CG1	3:F:76:ASP:N	2.84	0.40
3:E:14:MET:CE	3:E:28:THR:HG21	2.51	0.40
3:E:30:ASP:OD1	3:E:30:ASP:C	2.61	0.40
1:B:713:VAL:O	1:B:714:SER:CB	2.67	0.40
2:D:34:A:OP1	2:D:34:A:H8	2.04	0.40
3:F:35:VAL:O	3:F:39:SER:CB	2.69	0.40
3:E:75:VAL:CG1	3:E:76:ASP:N	2.76	0.40
1:A:730:SER:O	1:A:733:ILE:HG22	2.21	0.40
1:A:1034:ALA:O	1:A:1035:LYS:HD3	2.22	0.40
1:B:145:SER:OG	1:B:146:THR:N	2.55	0.40
1:B:606:PHE:CD2	1:B:612:ASN:ND2	2.90	0.40
1:B:661:ARG:CB	2:D:10:G:N1	2.84	0.40
1:B:661:ARG:O	2:D:10:G:N2	2.55	0.40
1:B:718:ASP:N	1:B:723:HIS:HE2	2.19	0.40
1:B:846:PHE:O	1:B:1041:ASN:N	2.54	0.40
2:D:29:G:N2	2:D:41:A:H1'	2.36	0.40
3:E:48:GLU:OE1	3:E:85:VAL:CG2	2.68	0.40
3:E:72:GLU:HG2	3:E:92:VAL:CG1	2.38	0.40
1:A:251:ASN:HD21	1:A:261:ASP:HB2	1.86	0.40
1:A:880:LYS:HE2	1:A:904:GLU:OE1	2.21	0.40
1:A:1222:LYS:HE3	1:A:1319:GLY:O	2.21	0.40
1:B:103:GLU:OE2	1:B:111:LYS:HD3	2.22	0.40
3:F:54:LEU:C	3:F:55:CYS:SG	3.03	0.40
1:A:356:LYS:HD2	1:A:356:LYS:N	2.37	0.40
1:A:563:GLN:O	1:A:567:ASP:CB	2.70	0.40
1:A:692:ASN:OD1	1:A:695:GLN:HB2	2.21	0.40
1:A:927:ILE:O	1:A:931:VAL:HG23	2.22	0.40
1:A:1347:LEU:O	1:A:1348:ILE:HG12	2.22	0.40
2:C:97:U:H5'	2:C:97:U:C6	2.44	0.40
1:B:296:LEU:O	1:B:297:SER:C	2.65	0.40
1:B:430:TYR:HA	1:B:431:PRO:HD2	1.92	0.40
1:B:747:LEU:HD21	1:B:1353:THR:HG22	2.03	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	
1	A	1352/1369 (99%)	1309 (97%)	42 (3%)	1 (0%)	48	76
1	B	1352/1369 (99%)	1314 (97%)	38 (3%)	0	100	100
3	E	111/123 (90%)	99 (89%)	10 (9%)	2 (2%)	6	30
3	F	114/123 (93%)	98 (86%)	12 (10%)	4 (4%)	3	19
All	All	2929/2984 (98%)	2820 (96%)	102 (4%)	7 (0%)	43	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	21	VAL
3	F	66	THR
3	F	51	ALA
3	F	68	LEU
3	E	52	VAL
1	A	1137	PRO
3	E	21	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	
1	A	1169/1228 (95%)	1052 (90%)	117 (10%)	7	27
1	B	1168/1228 (95%)	1061 (91%)	107 (9%)	8	31
3	E	99/114 (87%)	70 (71%)	29 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	100/114 (88%)	70 (70%)	30 (30%)	0 1
All	All	2536/2684 (94%)	2253 (89%)	283 (11%)	6 22

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ASP
1	A	39	ASP
1	A	57	GLU
1	A	70	ARG
1	A	83	GLN
1	A	88	ASN
1	A	95	ASP
1	A	104	SER
1	A	195	LEU
1	A	212	LEU
1	A	213	SER
1	A	216	LEU
1	A	217	SER
1	A	225	LEU
1	A	257	ASP
1	A	268	LYS
1	A	269	ASP
1	A	284	ASP
1	A	307	ARG
1	A	309	ASN
1	A	313	THR
1	A	323	LYS
1	A	340	ARG
1	A	348	LYS
1	A	388	GLU
1	A	399	LEU
1	A	438	GLU
1	A	447	ARG
1	A	450	TYR
1	A	465	MET
1	A	466	THR
1	A	471	GLU
1	A	484	LYS
1	A	487	SER
1	A	489	GLN

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Mol	Chain	Res	Type
1	A	502	LEU
1	A	534	MET
1	A	551	LEU
1	A	552	LEU
1	A	557	ARG
1	A	563	GLN
1	A	564	LEU
1	A	572	ILE
1	A	579	GLU
1	A	591	LEU
1	A	601	ILE
1	A	607	LEU
1	A	613	GLU
1	A	627	GLU
1	A	628	ASP
1	A	629	ARG
1	A	633	GLU
1	A	637	LYS
1	A	661	ARG
1	A	668	ASN
1	A	691	ARG
1	A	696	LEU
1	A	709	GLN
1	A	713	VAL
1	A	714	SER
1	A	727	LEU
1	A	747	LEU
1	A	749	LYS
1	A	753	ARG
1	A	766	GLU
1	A	768	GLN
1	A	769	THR
1	A	800	PRO
1	A	824	VAL
1	A	827	GLU
1	A	829	ASP
1	A	833	LEU
1	A	845	SER
1	A	847	LEU
1	A	869	ASN
1	A	902	LYS
1	A	904	GLU

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Mol	Chain	Res	Type
1	A	905	ARG
1	A	918	LYS
1	A	935	LEU
1	A	938	ARG
1	A	970	PHE
1	A	1004	LEU
1	A	1006	SER
1	A	1007	GLU
1	A	1008	PHE
1	A	1021	MET
1	A	1037	PHE
1	A	1040	SER
1	A	1050	ILE
1	A	1062	LEU
1	A	1072	ILE
1	A	1075	ASP
1	A	1114	ARG
1	A	1115	ASN
1	A	1119	LEU
1	A	1136	SER
1	A	1137	PRO
1	A	1143	VAL
1	A	1150	GLU
1	A	1179	ILE
1	A	1191	LYS
1	A	1193	ASP
1	A	1194	LEU
1	A	1197	LYS
1	A	1206	LEU
1	A	1207	GLU
1	A	1210	ARG
1	A	1282	LEU
1	A	1284	ASP
1	A	1318	LEU
1	A	1325	LYS
1	A	1328	ASP
1	A	1330	THR
1	A	1333	ARG
1	A	1347	LEU
1	B	1	MET
1	B	70	ARG
1	B	76	LYS

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Mol	Chain	Res	Type
1	B	95	ASP
1	B	100	ARG
1	B	101	LEU
1	B	109	GLU
1	B	114	GLU
1	B	115	ARG
1	B	196	PHE
1	B	204	SER
1	B	209	LYS
1	B	225	LEU
1	B	233	LYS
1	B	306	LEU
1	B	308	VAL
1	B	312	ILE
1	B	348	LYS
1	B	355	SER
1	B	388	GLU
1	B	396	GLU
1	B	399	LEU
1	B	419	LEU
1	B	450	TYR
1	B	455	LEU
1	B	460	SER
1	B	465	MET
1	B	466	THR
1	B	479	GLU
1	B	491	PHE
1	B	492	ILE
1	B	494	ARG
1	B	495	MET
1	B	496	THR
1	B	500	LYS
1	B	502	LEU
1	B	524	LEU
1	B	531	THR
1	B	534	MET
1	B	550	ASP
1	B	552	LEU
1	B	555	THR
1	B	557	ARG
1	B	563	GLN
1	B	564	LEU

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Mol	Chain	Res	Type
1	B	569	PHE
1	B	572	ILE
1	B	573	GLU
1	B	574	CYS
1	B	579	GLU
1	B	588	ASN
1	B	591	LEU
1	B	593	THR
1	B	601	ILE
1	B	610	GLU
1	B	629	ARG
1	B	633	GLU
1	B	661	ARG
1	B	668	ASN
1	B	672	ASP
1	B	691	ARG
1	B	696	LEU
1	B	700	ASP
1	B	702	LEU
1	B	709	GLN
1	B	714	SER
1	B	724	ILE
1	B	727	LEU
1	B	730	SER
1	B	733	ILE
1	B	742	LYS
1	B	749	LYS
1	B	765	ARG
1	B	809	GLU
1	B	827	GLU
1	B	830	ILE
1	B	832	ARG
1	B	844	GLN
1	B	853	ASP
1	B	902	LYS
1	B	938	ARG
1	B	980	ASN
1	B	995	THR
1	B	1006	SER
1	B	1035	LYS
1	B	1037	PHE
1	B	1040	SER

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Mol	Chain	Res	Type
1	B	1054	ASN
1	B	1076	LYS
1	B	1078	ARG
1	B	1088	SER
1	B	1105	PHE
1	B	1136	SER
1	B	1138	THR
1	B	1144	LEU
1	B	1149	VAL
1	B	1207	GLU
1	B	1208	ASN
1	B	1277	SER
1	B	1278	LYS
1	B	1280	VAL
1	B	1288	ASP
1	B	1307	GLU
1	B	1333	ARG
1	B	1347	LEU
1	B	1352	ILE
1	B	1353	THR
3	F	3	LEU
3	F	4	THR
3	F	5	ARG
3	F	7	GLN
3	F	10	TYR
3	F	18	ILE
3	F	22	ASP
3	F	24	PHE
3	F	26	GLU
3	F	28	THR
3	F	30	ASP
3	F	33	LYS
3	F	37	HIS
3	F	43	VAL
3	F	55	CYS
3	F	68	LEU
3	F	69	TYR
3	F	70	LEU
3	F	72	GLU
3	F	74	LEU
3	F	79	THR
3	F	86	THR

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Mol	Chain	Res	Type
3	F	96	ASP
3	F	98	ASP
3	F	108	GLU
3	F	115	GLU
3	F	116	ILE
3	F	118	LEU
3	F	120	SER
3	F	121	GLU
3	E	2	THR
3	E	5	ARG
3	E	10	TYR
3	E	19	ASN
3	E	25	GLU
3	E	33	LYS
3	E	37	HIS
3	E	48	GLU
3	E	49	LYS
3	E	50	TYR
3	E	52	VAL
3	E	54	LEU
3	E	55	CYS
3	E	69	TYR
3	E	70	LEU
3	E	72	GLU
3	E	74	LEU
3	E	79	THR
3	E	95	ASN
3	E	97	ILE
3	E	99	ASP
3	E	101	GLU
3	E	102	ILE
3	E	105	ASP
3	E	107	ASP
3	E	115	GLU
3	E	116	ILE
3	E	118	LEU
3	E	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	255	ASN
1	A	295	ASN
1	A	354	GLN
1	A	357	ASN
1	A	459	ASN
1	A	489	GLN
1	A	556	ASN
1	A	709	GLN
1	A	768	GLN
1	A	776	ASN
1	A	794	GLN
1	A	803	ASN
1	A	854	ASN
1	A	888	ASN
1	A	926	GLN
1	A	990	ASN
1	A	1101	GLN
1	A	1115	ASN
1	A	1177	ASN
1	A	1208	ASN
1	A	1297	HIS
1	A	1317	ASN
1	B	14	ASN
1	B	99	HIS
1	B	255	ASN
1	B	394	ASN
1	B	489	GLN
1	B	501	ASN
1	B	556	ASN
1	B	563	GLN
1	B	595	HIS
1	B	668	ASN
1	B	754	HIS
1	B	758	ASN
1	B	776	ASN
1	B	840	HIS
1	B	930	HIS
1	B	980	ASN
1	B	985	HIS
1	B	990	ASN
1	B	1177	ASN

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Mol	Chain	Res	Type
1	B	1208	ASN
1	B	1221	GLN
1	B	1286	ASN
1	B	1350	GLN
3	F	15	HIS
3	F	37	HIS
3	E	7	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	87/99 (87%)	30 (34%)	7 (8%)
2	D	90/99 (90%)	31 (34%)	8 (8%)
All	All	177/198 (89%)	61 (34%)	15 (8%)

All (61) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	12	G
2	C	13	C
2	C	16	U
2	C	18	G
2	C	19	G
2	C	28	A
2	C	29	G
2	C	34	A
2	C	35	A
2	C	37	U
2	C	40	C
2	C	43	G
2	C	44	U
2	C	51	A
2	C	56	U
2	C	59	U
2	C	68	A
2	C	74	A
2	C	77	A
2	C	82	G
2	C	87	G
2	C	89	G
2	C	90	U

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Mol	Chain	Res	Type
2	C	91	C
2	C	92	G
2	C	93	G
2	C	94	U
2	C	95	G
2	C	96	C
2	C	97	U
2	D	10	G
2	D	11	U
2	D	12	G
2	D	13	C
2	D	14	G
2	D	27	G
2	D	28	A
2	D	29	G
2	D	35	A
2	D	37	U
2	D	40	C
2	D	43	G
2	D	44	U
2	D	51	A
2	D	56	U
2	D	59	U
2	D	68	A
2	D	73	G
2	D	77	A
2	D	79	G
2	D	82	G
2	D	83	C
2	D	89	G
2	D	90	U
2	D	91	C
2	D	92	G
2	D	93	G
2	D	94	U
2	D	95	G
2	D	96	C
2	D	97	U

All (15) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
2	C	28	A
2	C	33	G
2	C	34	A
2	C	42	A
2	C	92	G
2	C	93	G
2	C	94	U
2	D	9	G
2	D	10	G
2	D	13	C
2	D	28	A
2	D	42	A
2	D	89	G
2	D	92	G
2	D	95	G

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1360/1369 (99%)	0.16	44 (3%)	50	33	32, 64, 102, 160	0
1	B	1360/1369 (99%)	0.16	41 (3%)	52	35	23, 57, 113, 171	0
2	C	88/99 (88%)	-0.09	1 (1%)	78	61	39, 67, 146, 176	0
2	D	90/99 (90%)	-0.11	1 (1%)	78	61	32, 57, 137, 159	0
3	E	115/123 (93%)	0.60	8 (6%)	22	15	52, 83, 109, 120	0
3	F	118/123 (95%)	0.61	11 (9%)	14	11	44, 75, 101, 109	0
All	All	3131/3182 (98%)	0.18	106 (3%)	48	32	23, 63, 110, 176	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	59	THR	5.3
1	B	1337	THR	5.0
1	A	769	THR	4.8
1	A	767	ASN	4.7
1	A	2	ASP	4.5
1	A	574	CYS	4.4
1	A	577	SER	4.4
1	A	714	SER	4.0
3	F	106	GLU	4.0
1	A	1154	SER	3.9
1	B	783	ARG	3.8
1	B	1206	LEU	3.8
1	B	529	TYR	3.7
1	B	527	VAL	3.7
1	A	521	TYR	3.5
3	E	55	CYS	3.5
1	A	576	ASP	3.4
1	A	587	PHE	3.3
1	B	805	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	529	TYR	3.1
2	C	87	G	3.0
1	B	0	SER	3.0
1	B	1004	LEU	3.0
1	A	1242	TYR	3.0
1	A	517	TYR	2.9
1	B	310	THR	2.9
1	B	1163	LEU	2.9
1	B	599	LYS	2.9
3	E	20	MET	2.9
2	D	98	U	2.7
1	A	578	VAL	2.7
3	E	19	ASN	2.7
1	B	770	THR	2.6
1	A	1029	ILE	2.6
1	A	532	GLU	2.6
3	E	4	THR	2.5
3	E	17	PHE	2.5
1	A	580	ILE	2.5
3	F	24	PHE	2.5
1	A	686	ASP	2.5
3	F	104	THR	2.5
3	F	103	ALA	2.4
3	F	81	ASP	2.4
1	B	766	GLU	2.4
1	B	540	LEU	2.4
1	A	543	GLU	2.4
1	A	688	PHE	2.4
1	A	779	GLU	2.4
1	A	1040	SER	2.4
1	A	575	PHE	2.4
1	B	71	ARG	2.4
1	A	1224	ASN	2.3
1	A	359	TYR	2.3
3	F	7	GLN	2.3
1	B	376	ILE	2.3
1	B	456	ALA	2.3
1	B	776	ASN	2.3
1	A	531	THR	2.3
1	B	1	MET	2.3
1	B	812	TYR	2.3
1	B	607	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	90	ASN	2.3
3	F	113	ASN	2.3
1	B	2	ASP	2.3
3	E	96	ASP	2.3
1	B	537	PRO	2.3
1	B	580	ILE	2.3
1	A	536	LYS	2.3
1	B	44	LYS	2.3
1	A	766	GLU	2.2
1	A	1131	TYR	2.2
1	B	576	ASP	2.2
1	A	1152	GLY	2.2
1	B	542	GLY	2.2
1	A	659	TRP	2.2
1	B	1353	THR	2.2
1	A	530	VAL	2.2
1	B	473	ILE	2.2
3	F	55	CYS	2.2
3	F	100	LEU	2.2
1	B	714	SER	2.2
1	A	709	GLN	2.2
1	B	779	GLU	2.2
3	F	88	TYR	2.2
1	B	600	ILE	2.2
1	A	770	THR	2.1
1	A	1088	SER	2.1
1	A	1153	LYS	2.1
1	A	71	ARG	2.1
1	B	1161	LYS	2.1
1	A	197	GLU	2.1
1	A	776	ASN	2.1
1	A	1145	VAL	2.1
1	B	1033	THR	2.1
1	A	44	LYS	2.1
1	A	1024	LYS	2.1
1	B	273	ASP	2.1
1	B	815	TYR	2.1
1	B	1250	GLU	2.1
1	A	527	VAL	2.1
3	E	3	LEU	2.1
1	B	806	LEU	2.0
1	B	767	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	533	GLY	2.0
1	B	897	PHE	2.0
1	B	786	GLU	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 oligosaccharides 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.