



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:00 am GMT

PDB ID : 4V4J
Title : Interactions and Dynamics of the Shine-Dalgarno Helix in the 70S Ribosome.
Authors : Korostelev, A.; Trakhanov, S.; Asahara, H.; Laurberg, M.; Noller, H.F.
Deposited on : 2007-07-18
Resolution : 3.83 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

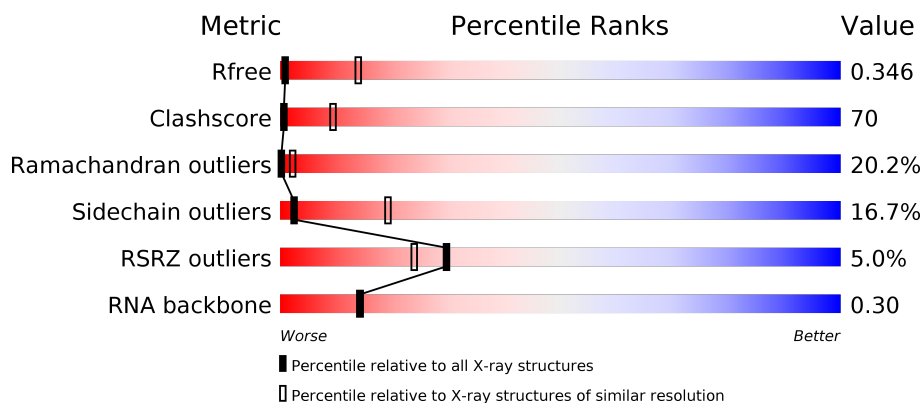
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.83 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.



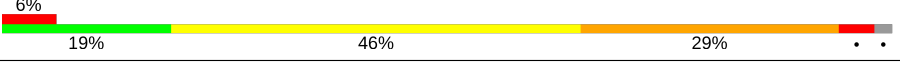

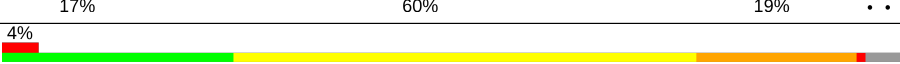
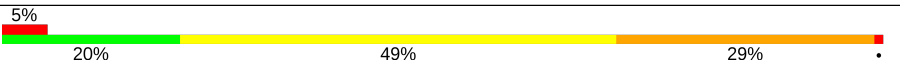
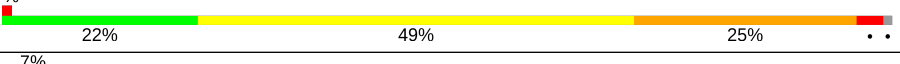

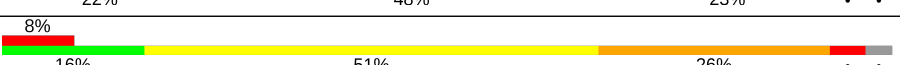
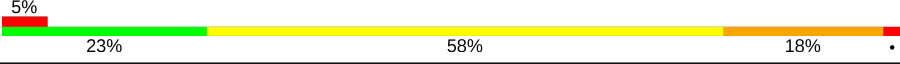
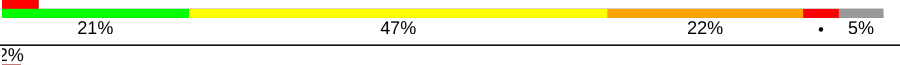
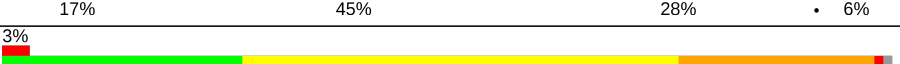
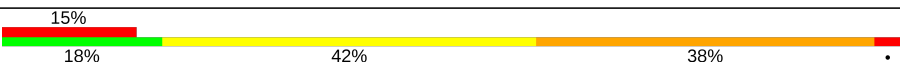
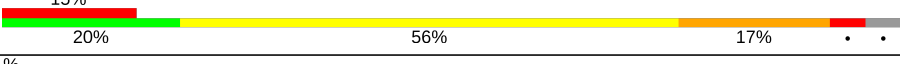

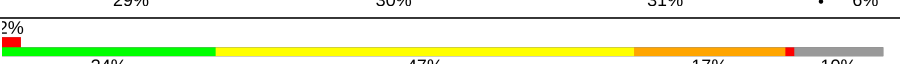

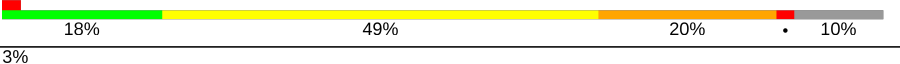
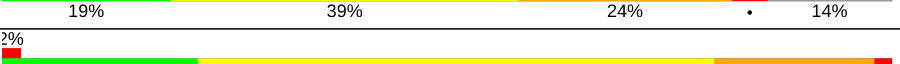
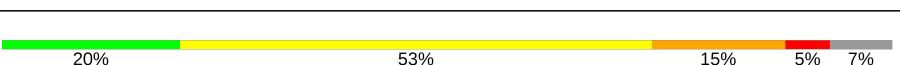
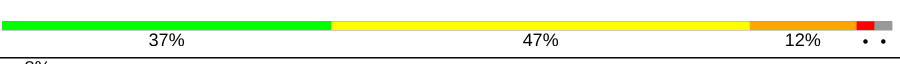




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1000 (4.12-3.56)
Clashscore	112137	1045 (4.10-3.58)
Ramachandran outliers	110173	1008 (4.10-3.58)
Sidechain outliers	110143	1001 (4.10-3.58)
RSRZ outliers	101464	1014 (4.12-3.56)
RNA backbone	2435	1017 (4.76-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	w	2889	<div> <div>4%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
2	x	120	<div> <div>61%</div> <div>38%</div> <div>.</div> </div>
3	A	229	<div> <div>3%</div> <div>15%</div> <div>28%</div> <div>10%</div> <div>.</div> <div>45%</div> </div>
4	B	276	<div> <div>7%</div> <div>16%</div> <div>55%</div> <div>26%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	206	
6	D	205	
7	E	182	
8	F	180	
9	G	148	
10	H	140	
11	I	122	
12	J	150	
13	K	141	
14	L	118	
15	M	112	
16	N	146	
17	O	118	
18	P	101	
19	Q	113	
20	R	96	
21	S	110	
22	T	206	
23	U	85	
24	V	98	
25	W	72	
26	X	60	
27	Y	60	
28	Z	49	
29	a	65	

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Mol	Chain	Length	Quality of chain
30	b	37	
31	y	1522	
32	z	77	
33	2	76	
34	3	18	
35	c	256	
36	d	239	
37	e	209	
38	f	162	
39	g	101	
40	h	156	
41	i	138	
42	j	128	
43	k	105	
44	l	129	
45	m	132	
46	n	126	
47	o	61	
48	p	89	
49	q	88	
50	r	105	
51	s	88	
52	t	93	
53	u	106	
54	v	27	

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 147125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	2889	Total	C	N	O	P	0	0	0
			62213	27690	11624	20011	2888			

- Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	x	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	127	Total	C	N	O	S	0	0	0
			996	627	184	184	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	201	Total	C	N	O	S	0	0	0
			1541	974	295	267	5			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	194	Total	C	N	O	S	0	0	0
			1517	969	283	263	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	180	Total	C	N	O	S	0	0	0
			1468	938	267	259	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	173	Total	C	N	O	S	0	0	0
			1319	839	245	234	1			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	148	Total	C	N	O	S	0	0	0
			1156	737	204	214	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1103	712	206	182	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	24	VAL	MET	CONFLICT	UNP Q72IN1

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	137	Total	C	N	O	S	0	0	0
			1089	698	207	177	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	106	Total	C	N	O	S	0	0	0
			846	534	168	144				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	109	Total	C	N	O	S	0	0	0
			868	547	170	150	1			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	92	Total	C	N	O			
			725	471	131	123	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	103	Total	C	N	O	S		
			793	510	151	126	6	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	185	Total	C	N	O	S		
			1475	941	262	269	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	76	Total	C	N	O	S		
			605	376	126	102	1	0	0

- Molecule 24 is a protein called LSU ribosomal protein L28P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	V	88	Total	C	N	O			
			694	435	141	118		0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	W	62	Total	C	N	O	S		
			520	325	102	91	2	0	0

- Molecule 26 is a protein called LSU ribosomal protein L30P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	X	60	Total	C	N	O	S		
			477	303	91	82	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	56	Total	C	N	O	S	0	0	0
			436	275	84	72	5			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	a	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	b	35	Total	C	N	O	S	0	0	0
			294	181	66	44	3			

- Molecule 31 is a RNA chain called 16S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1514	Total	C	N	O	P	0	0	0
			32546	14494	6022	10517	1513			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	466	G	C	CONFLICT	GB 155076

- Molecule 32 is a RNA chain called P-site tRNA^fMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2	76	Total	C	N	O	P	0	0	0
			1621	725	293	528	75			

- Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	3	18	Total	C	N	O	P	0	0	0
			390	176	80	117	17			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	c	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	d	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	e	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	f	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	g	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	h	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	i	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	j	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	k	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	l	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	m	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	n	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	o	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	p	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	q	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	r	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	s	81	Total	C	N	O	0	0	0
			668	423	135	110			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	t	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	u	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

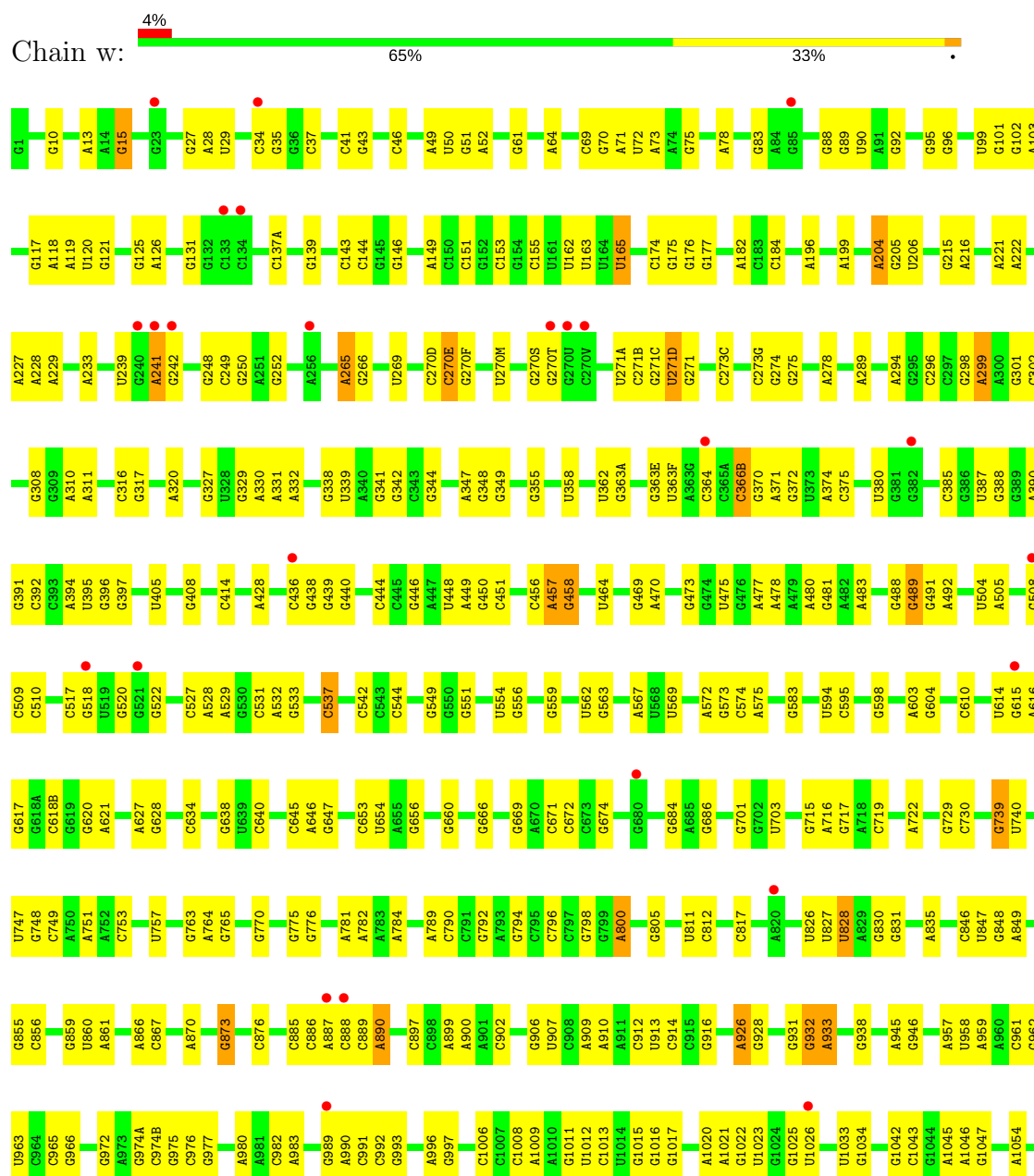
- Molecule 54 is a protein called 30S ribosomal protein Thx.

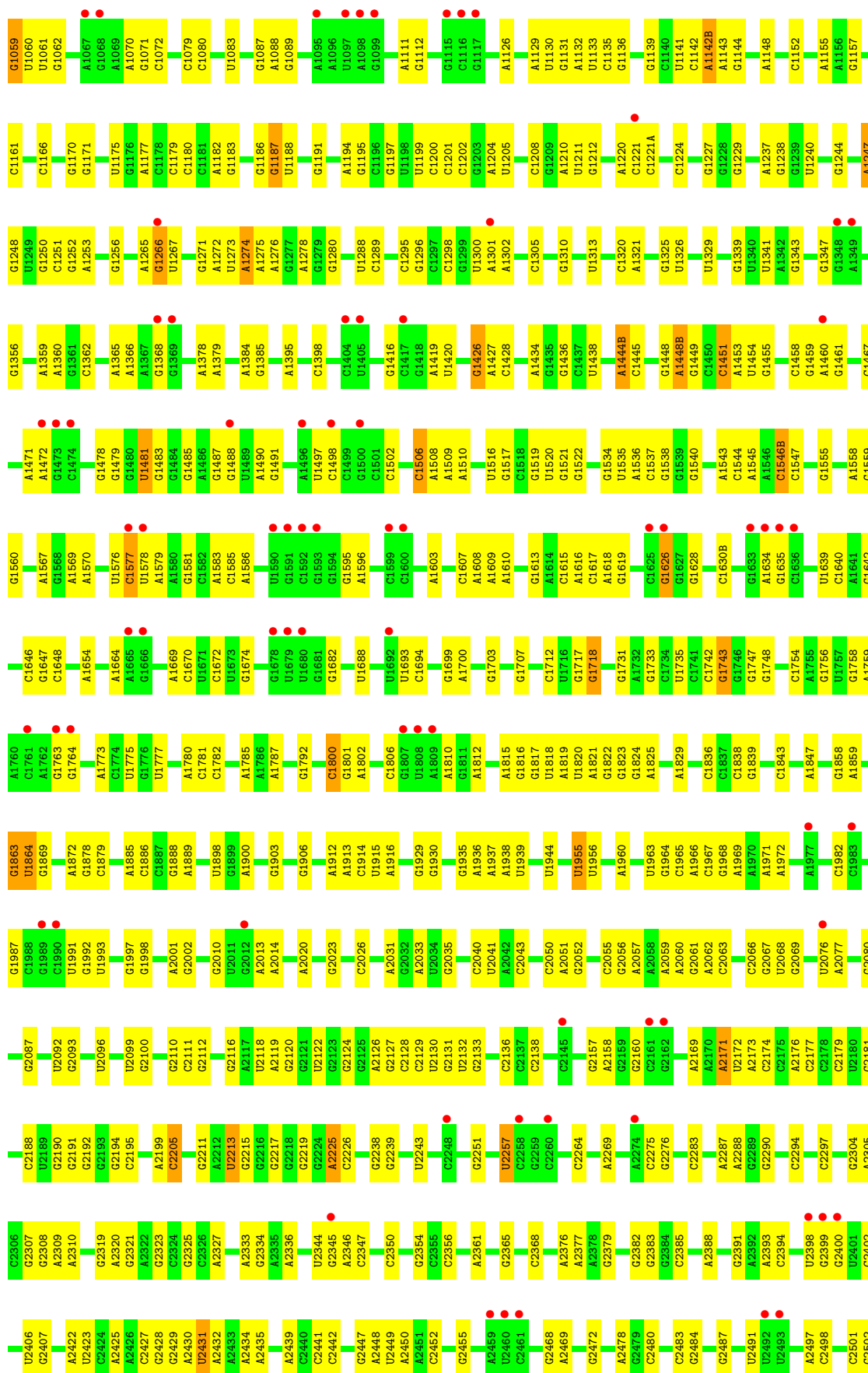
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	v	24	Total	C	N	O	0	0	0
			208	128	50	30			

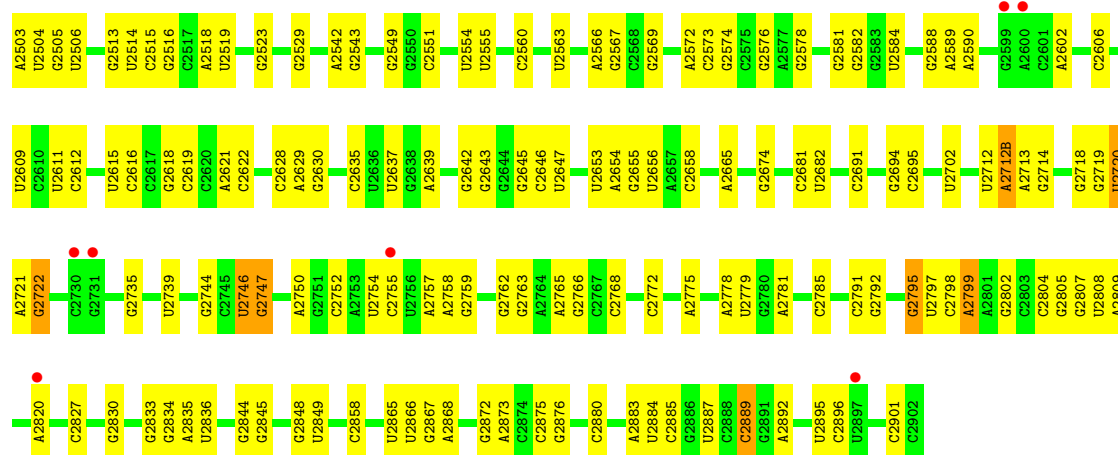
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

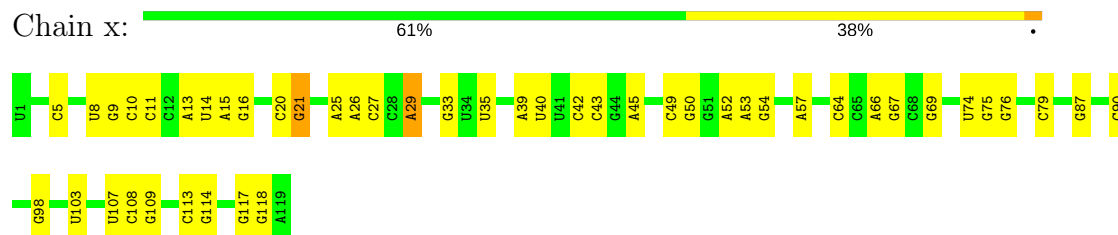
• Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



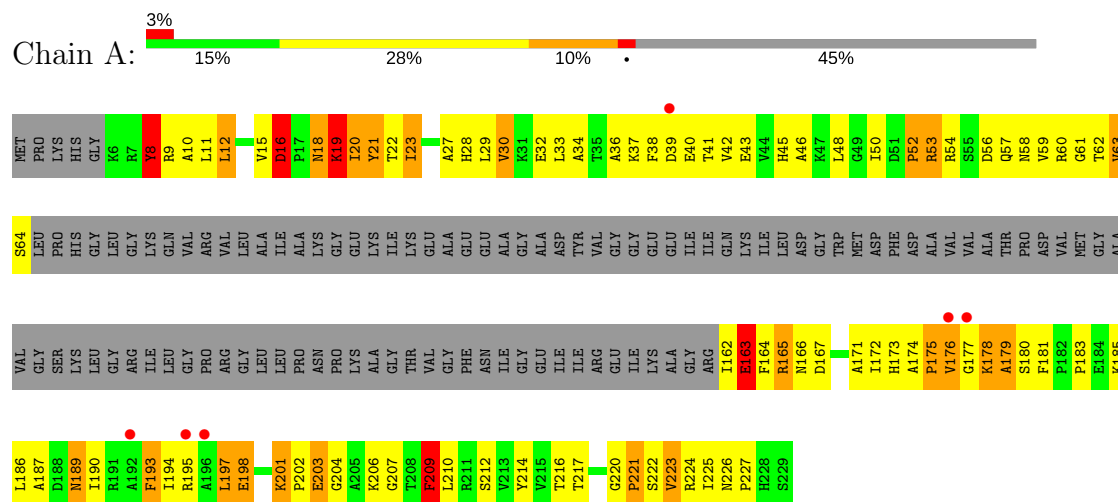




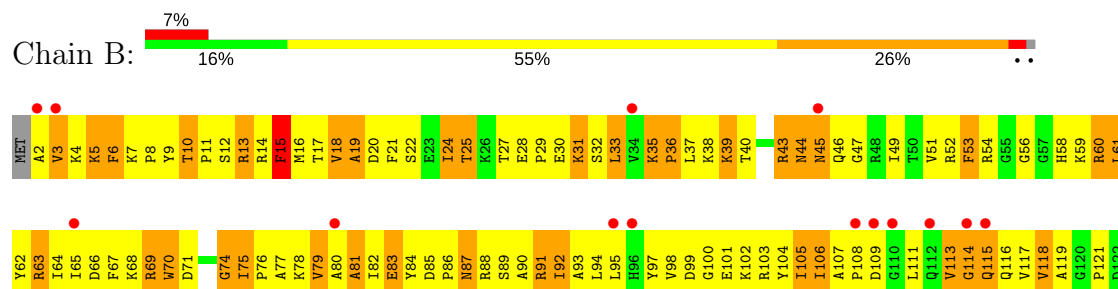
• Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA

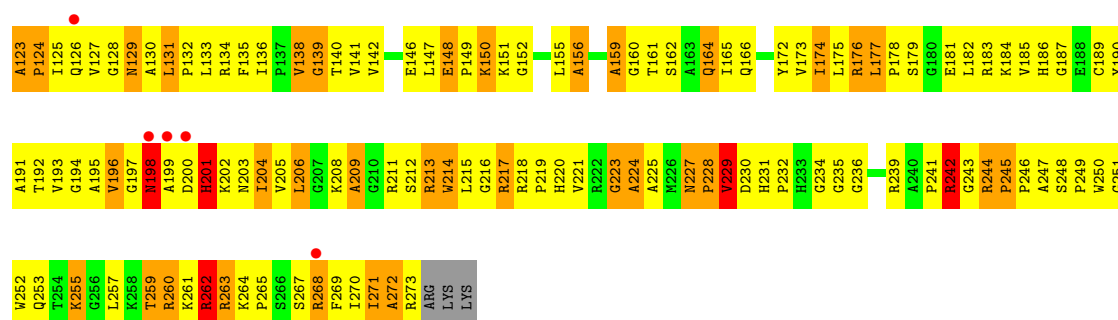


• Molecule 3: 50S ribosomal protein L1

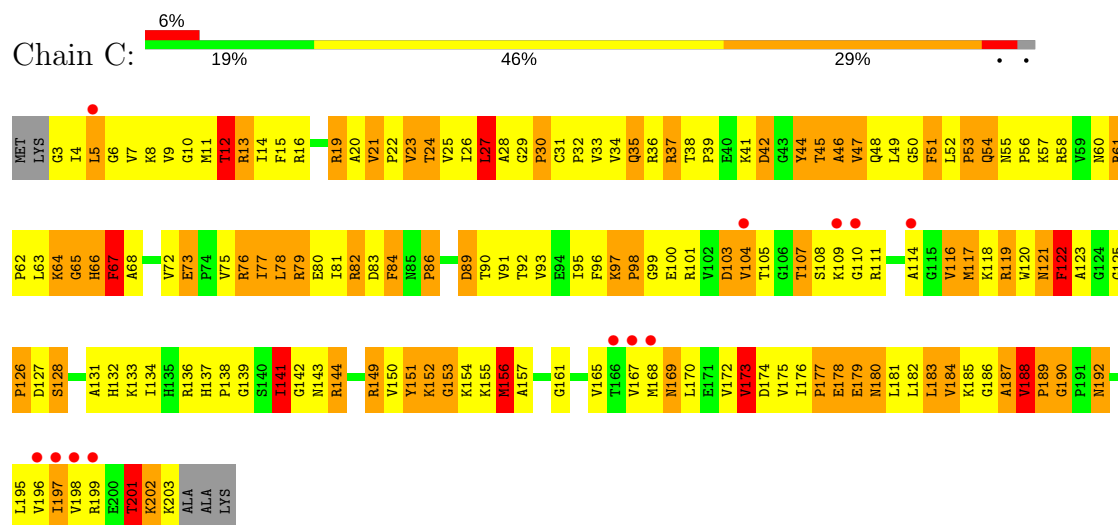


• Molecule 4: 50S ribosomal protein L2

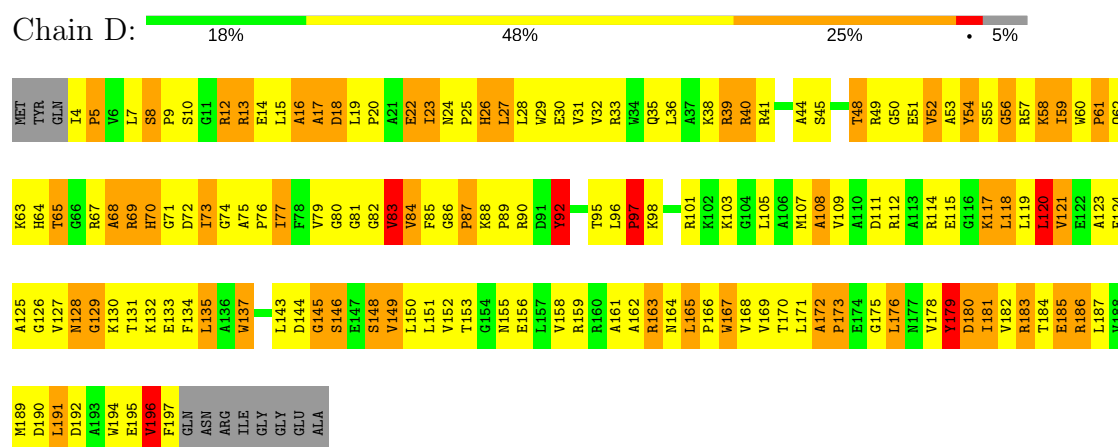




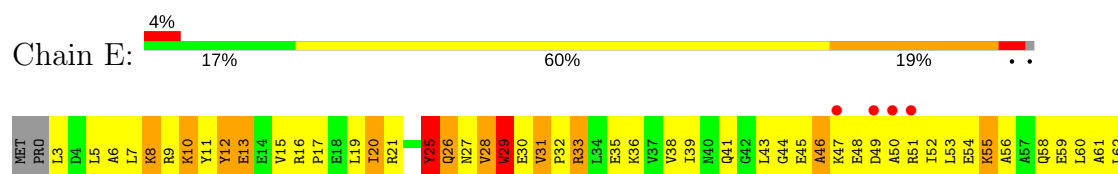
• Molecule 5: 50S ribosomal protein L3

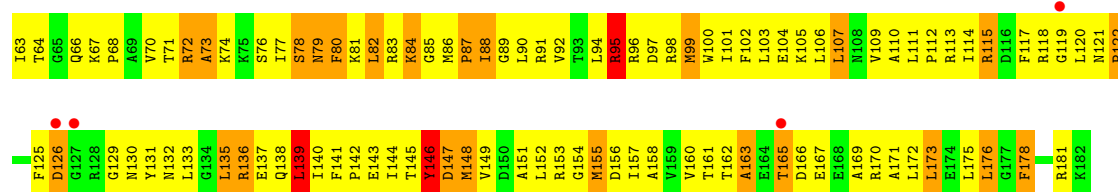


• Molecule 6: 50S ribosomal protein L4

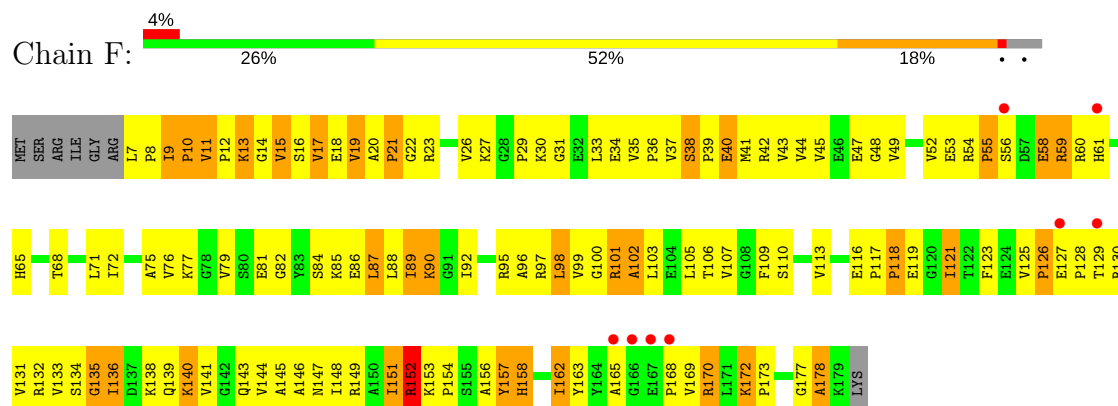


• Molecule 7: 50S ribosomal protein L5

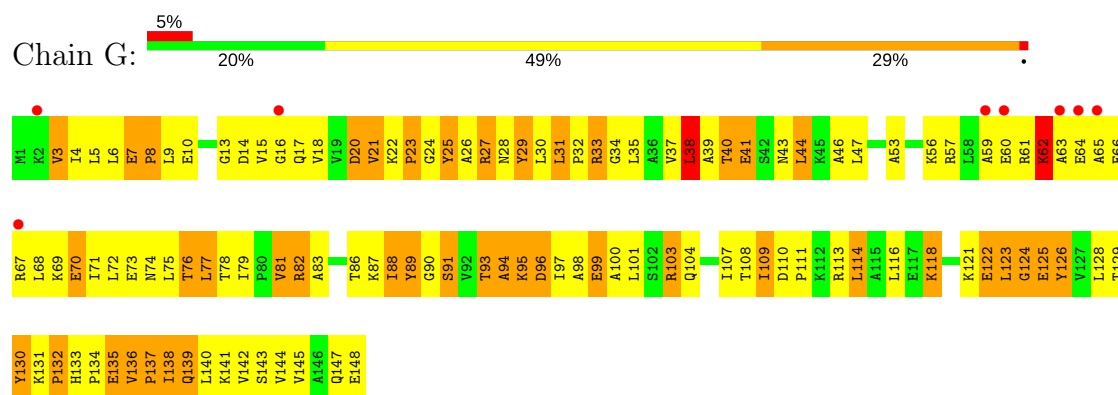




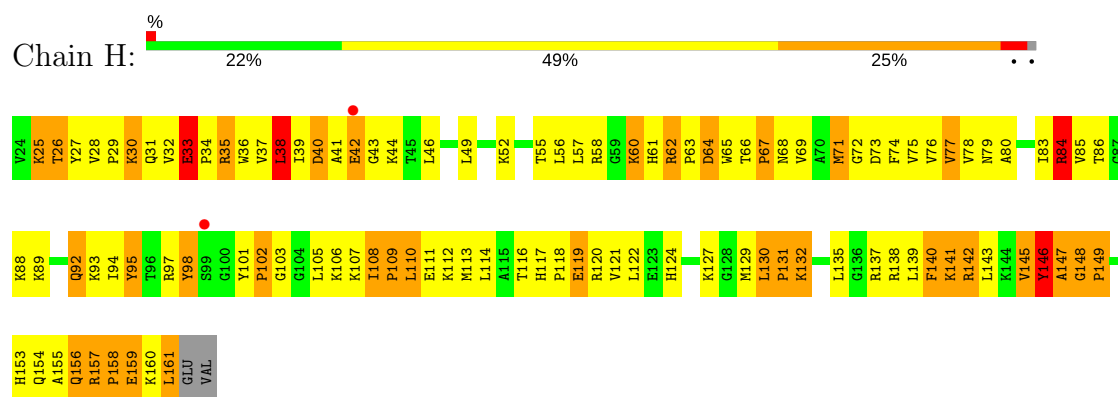
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L9

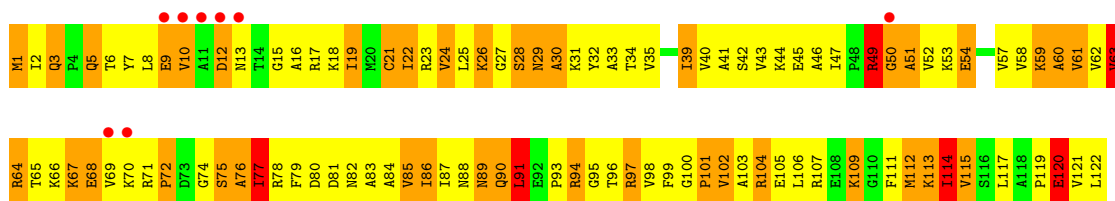


• Molecule 10: 50S ribosomal protein L13

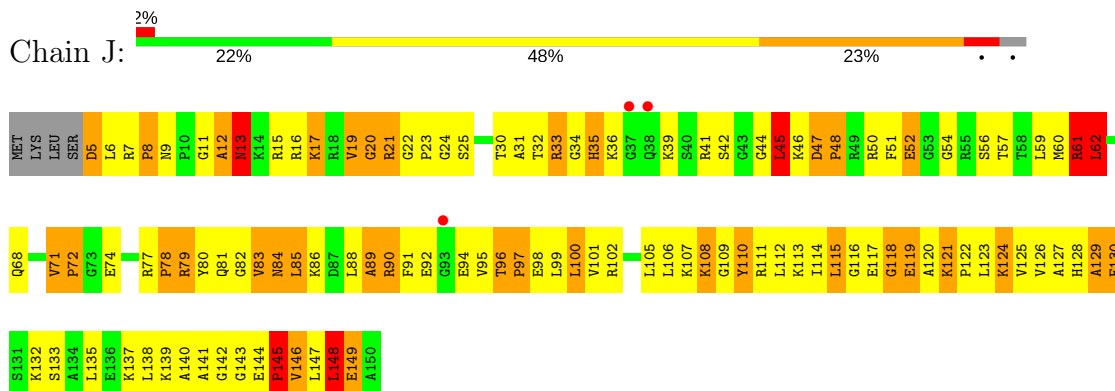


• Molecule 11: 50S ribosomal protein L14

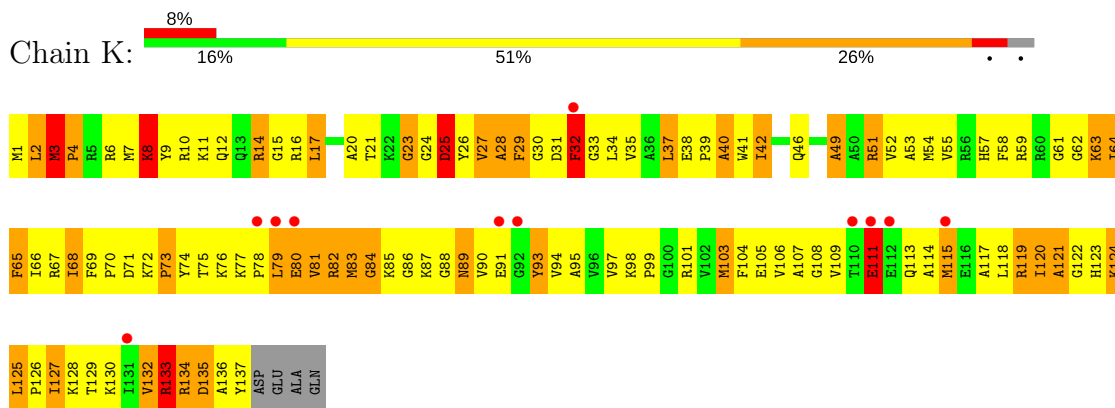




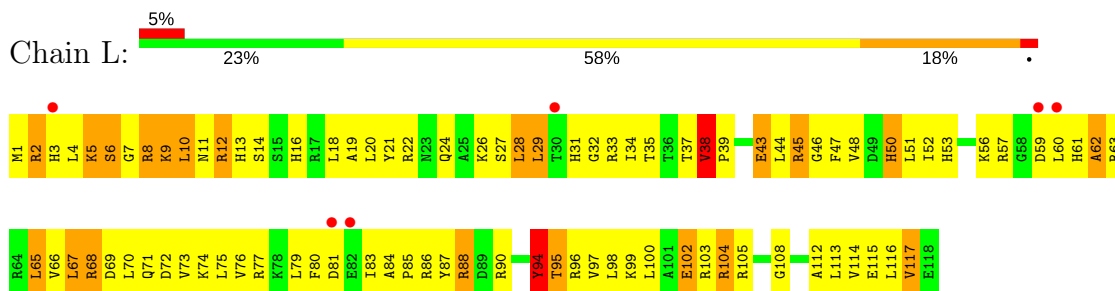
• Molecule 12: 50S ribosomal protein L15



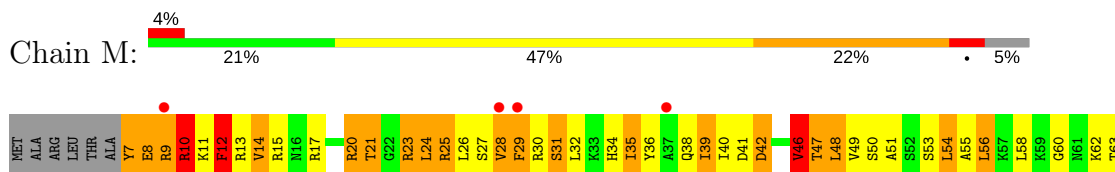
• Molecule 13: 50S ribosomal protein L16

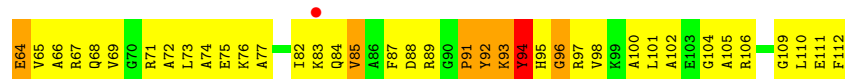


• Molecule 14: 50S ribosomal protein L17

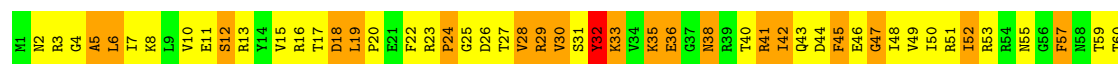
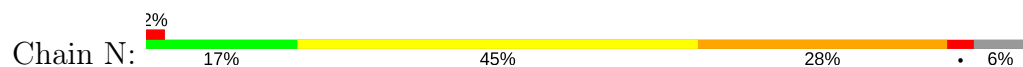


• Molecule 15: 50S ribosomal protein L18

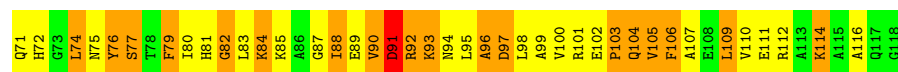
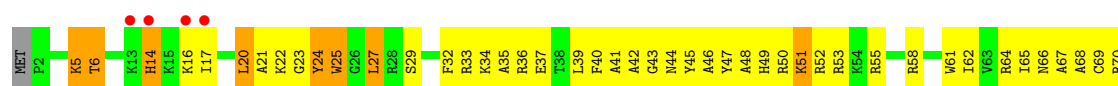




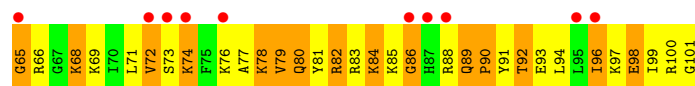
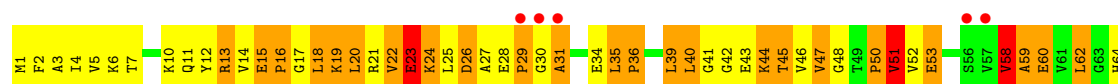
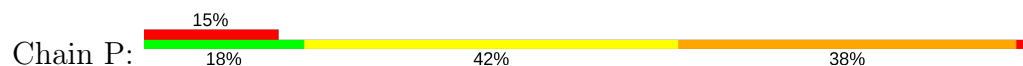
• Molecule 16: 50S ribosomal protein L19



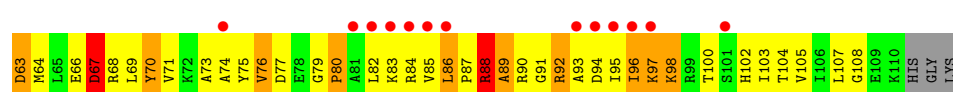
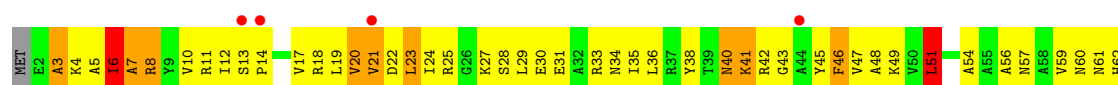
• Molecule 17: 50S ribosomal protein L20



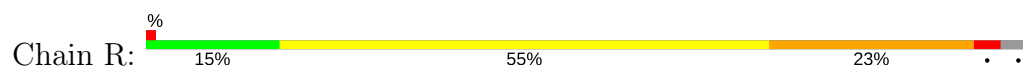
• Molecule 18: 50S ribosomal protein L21

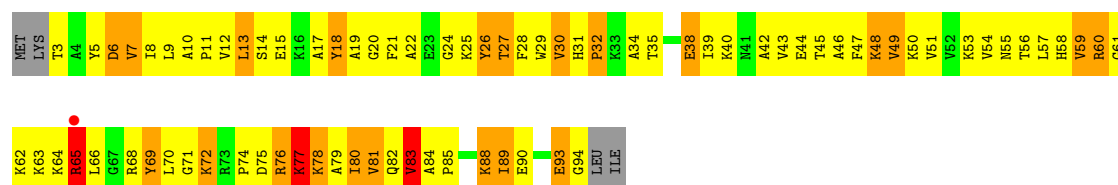


• Molecule 19: 50S ribosomal protein L22

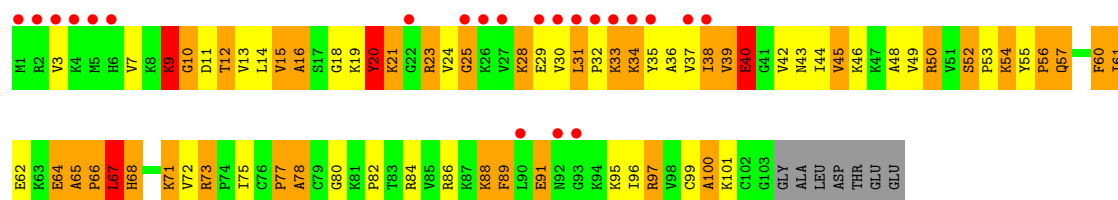
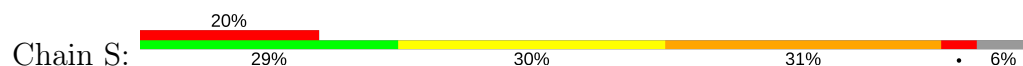


• Molecule 20: 50S ribosomal protein L23

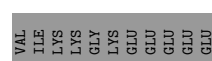
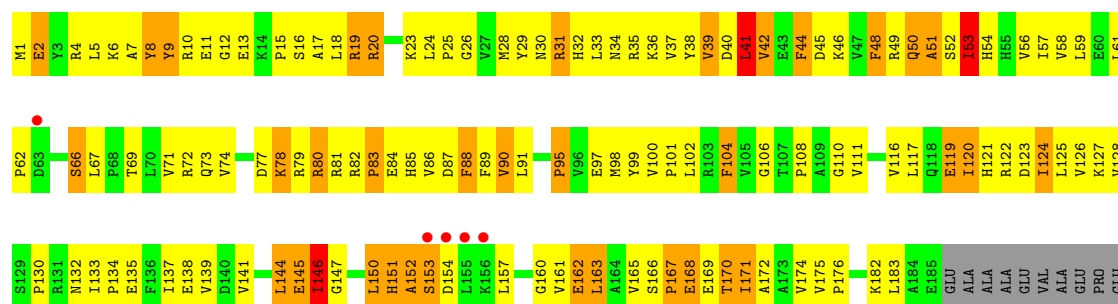




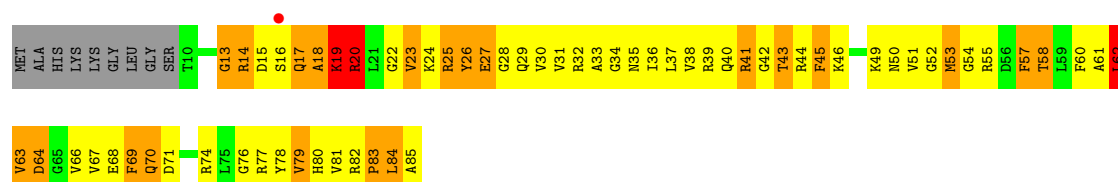
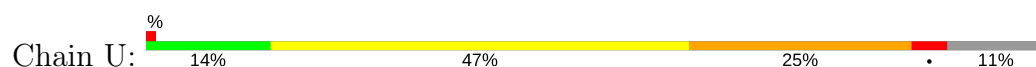
- Molecule 21: 50S ribosomal protein L24



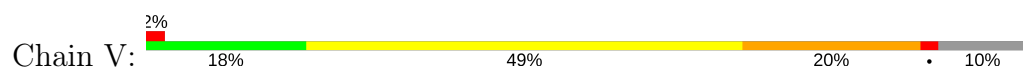
- Molecule 22: 50S ribosomal protein L25

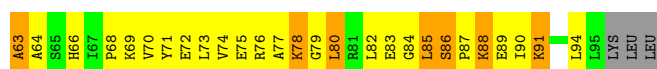


- Molecule 23: 50S ribosomal protein L27

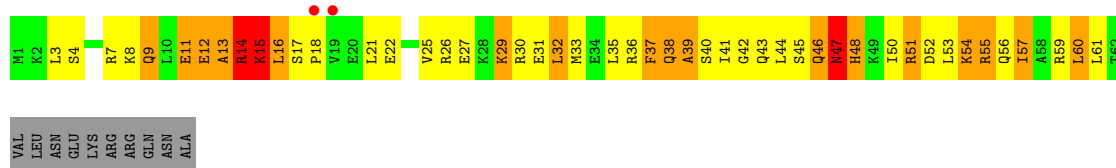
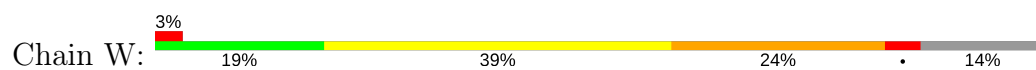


- Molecule 24: LSU ribosomal protein L28P

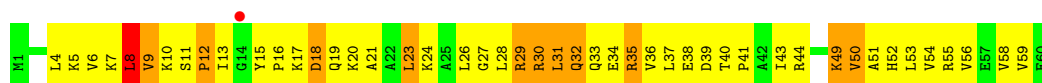




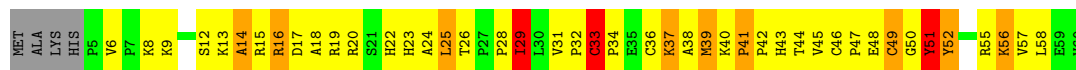
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: LSU ribosomal protein L30P



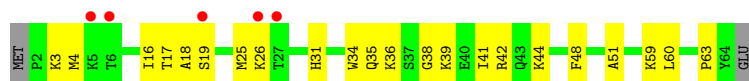
- Molecule 27: 50S ribosomal protein L32



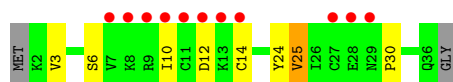
- Molecule 28: 50S ribosomal protein L34



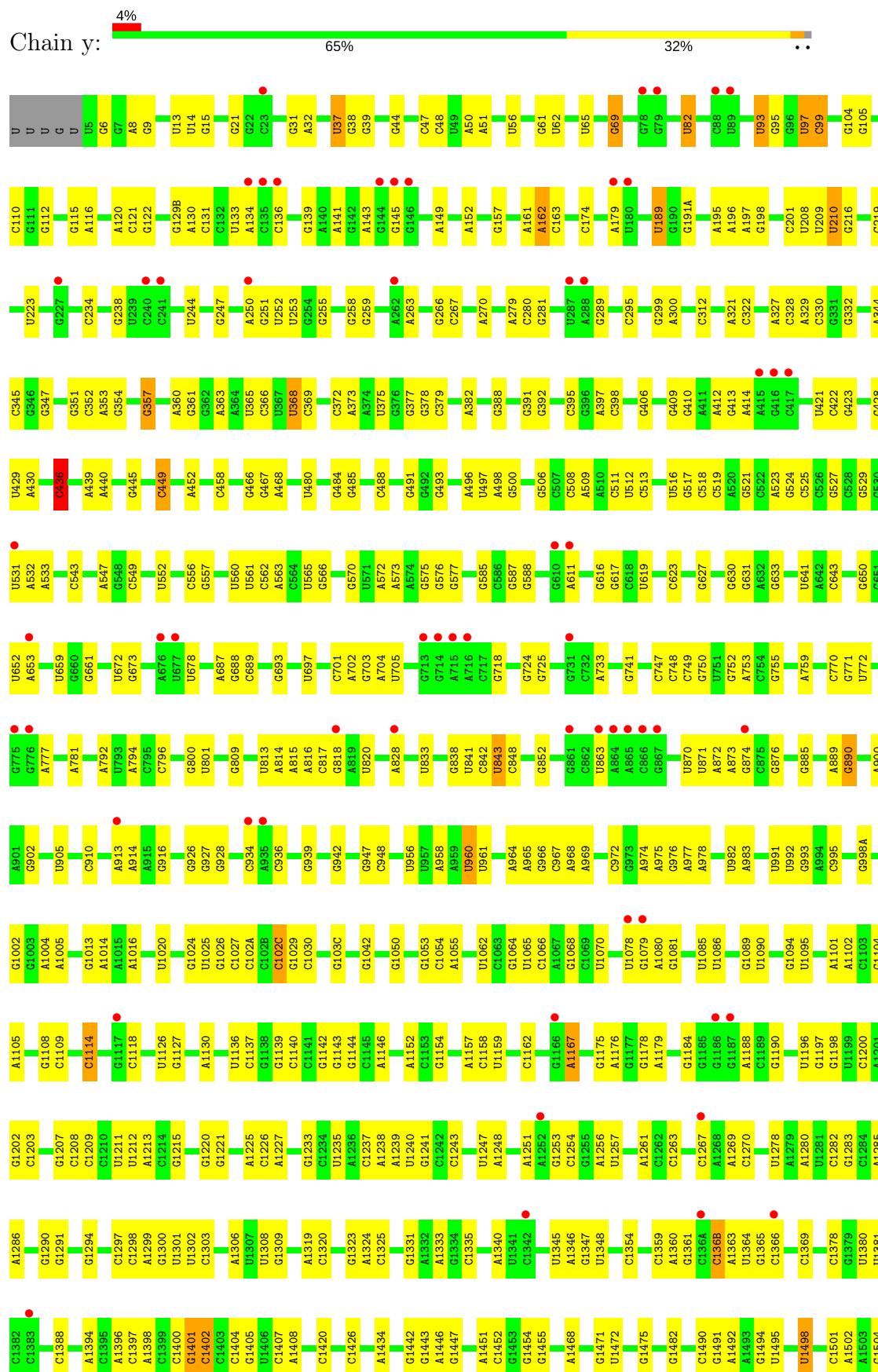
- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36

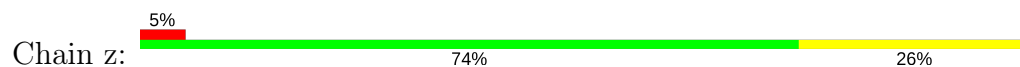


- Molecule 31: 16S RNA

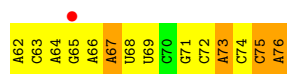
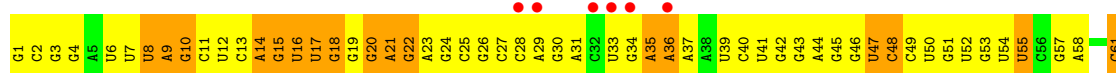
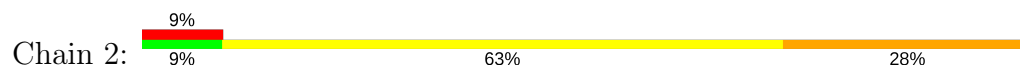




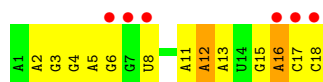
• Molecule 32: P-site tRNA^fMET



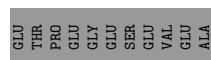
• Molecule 33: E-site tRNA



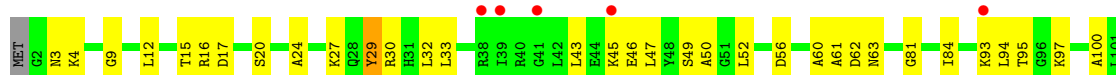
• Molecule 34: MRNA



• Molecule 35: 30S ribosomal protein S2

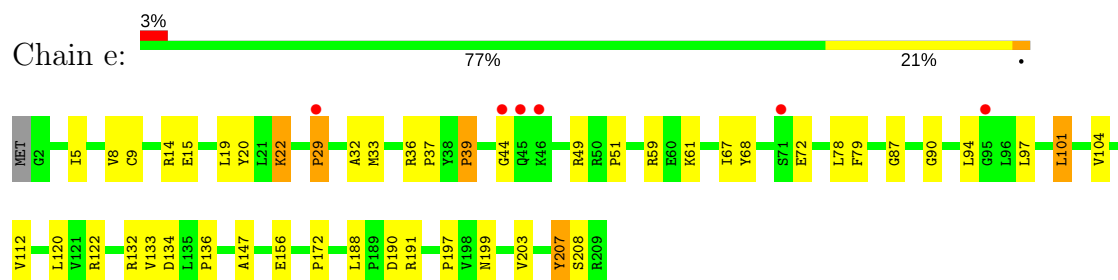


• Molecule 36: 30S ribosomal protein S3

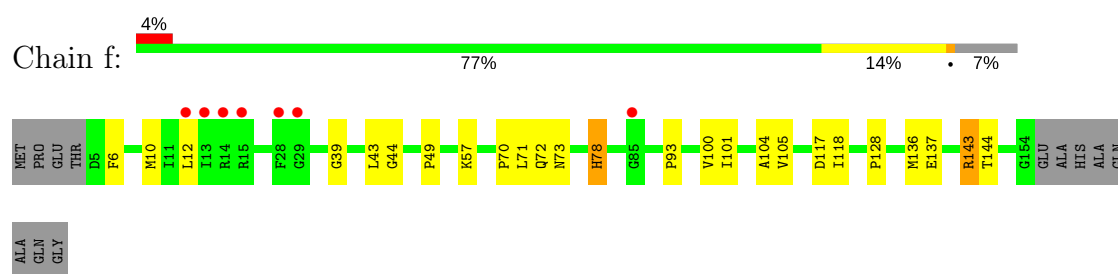


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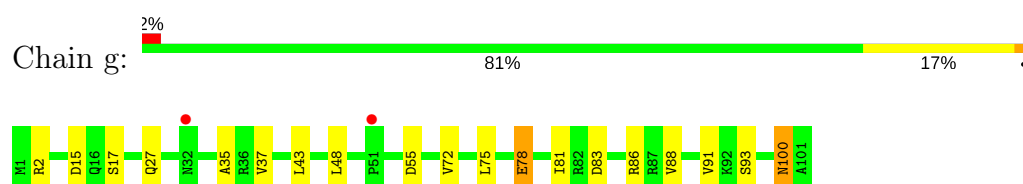
• Molecule 37: 30S ribosomal protein S4



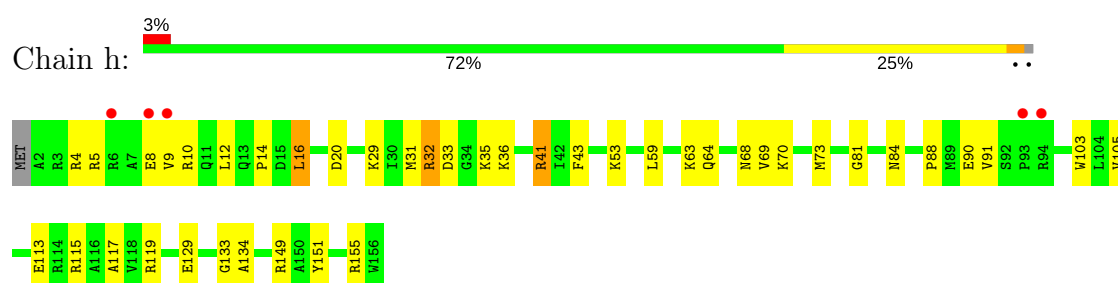
• Molecule 38: 30S ribosomal protein S5



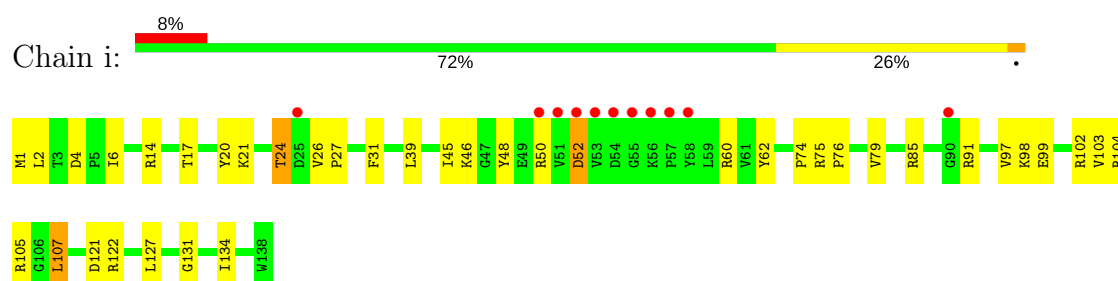
• Molecule 39: 30S ribosomal protein S6



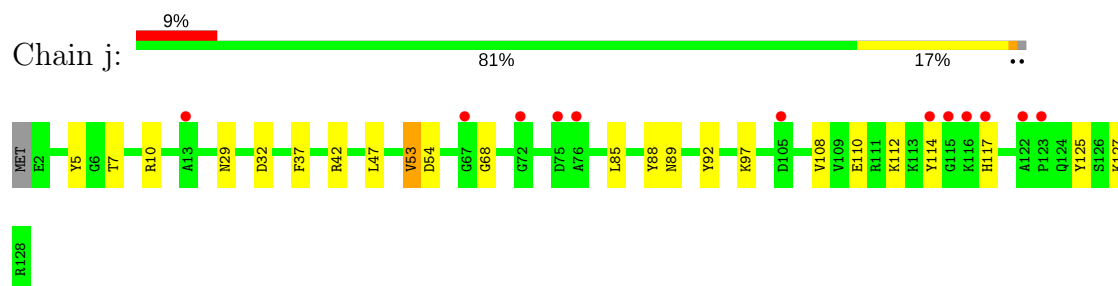
• Molecule 40: 30S ribosomal protein S7



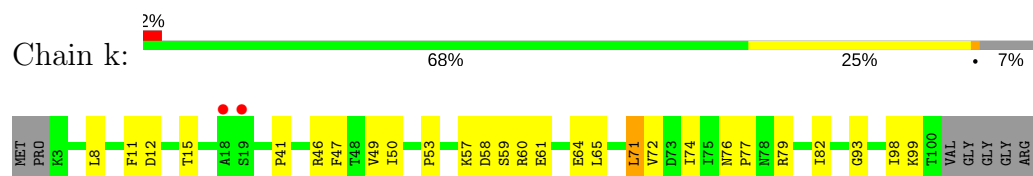
• Molecule 41: 30S ribosomal protein S8



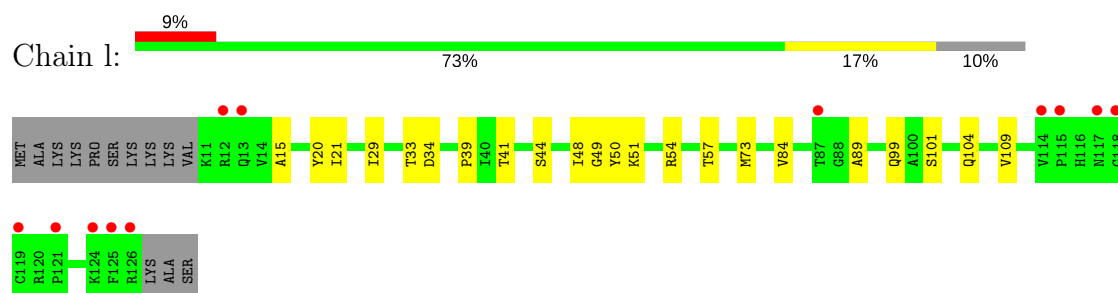
- Molecule 42: 30S ribosomal protein S9



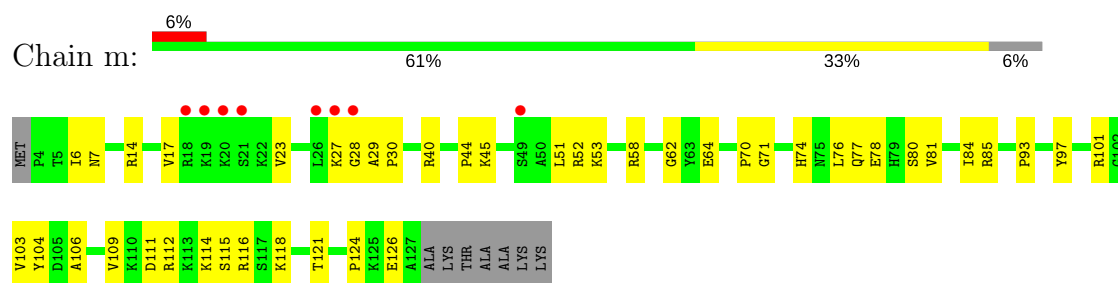
- Molecule 43: 30S ribosomal protein S10



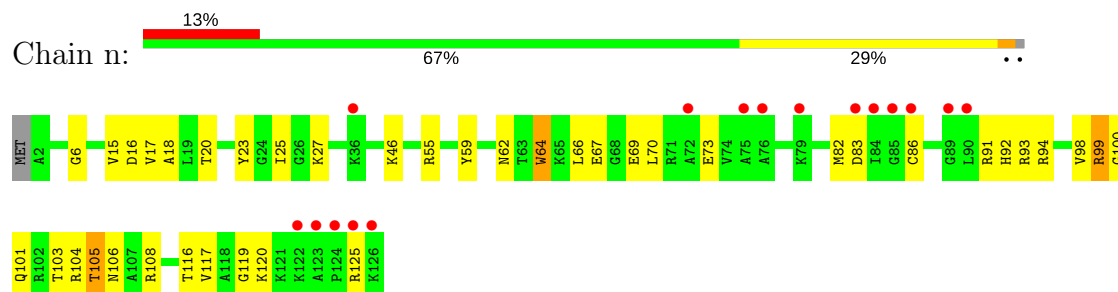
- Molecule 44: 30S ribosomal protein S11



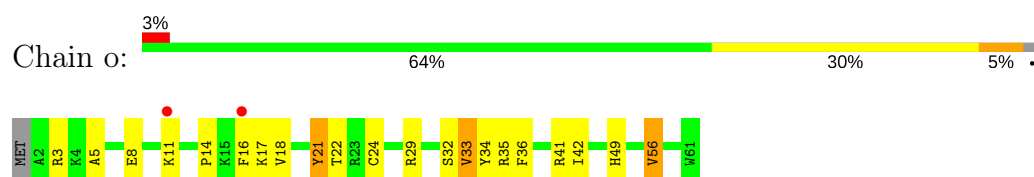
- Molecule 45: 30S ribosomal protein S12



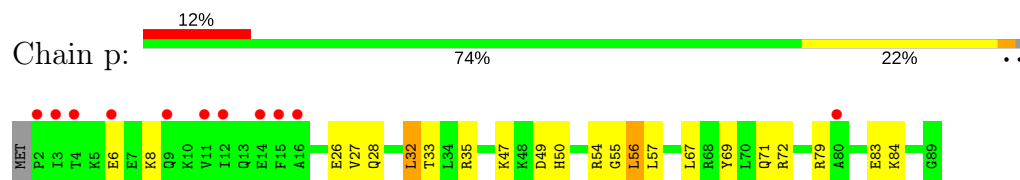
- Molecule 46: 30S ribosomal protein S13



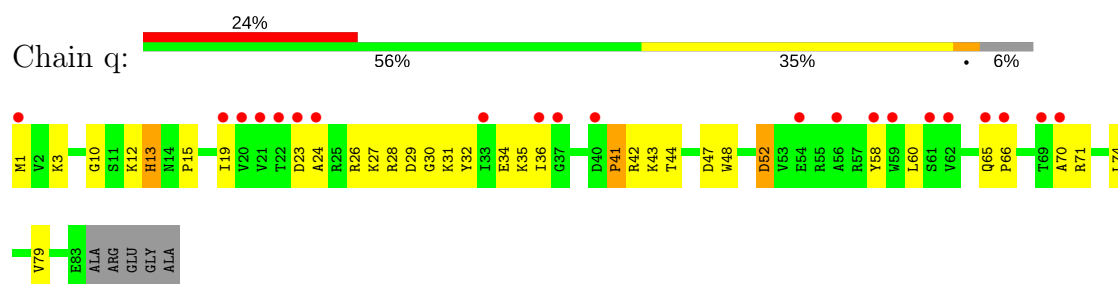
- Molecule 47: 30S ribosomal protein S14 type Z



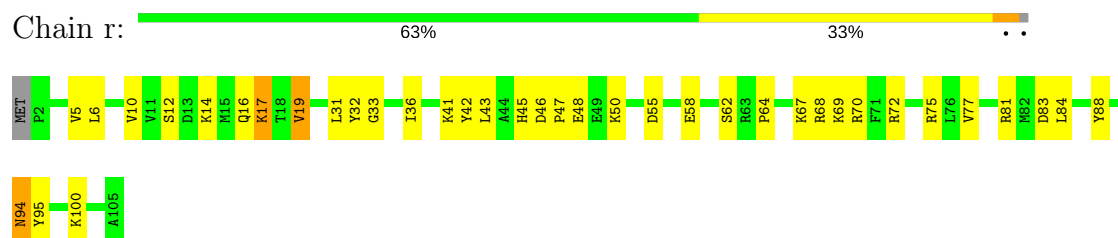
- Molecule 48: 30S ribosomal protein S15



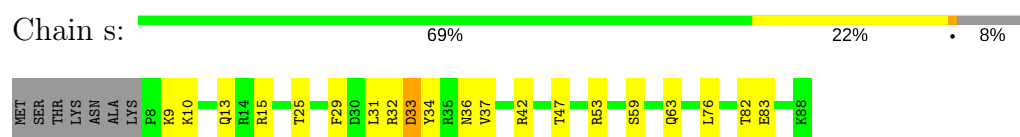
- Molecule 49: 30S ribosomal protein S16



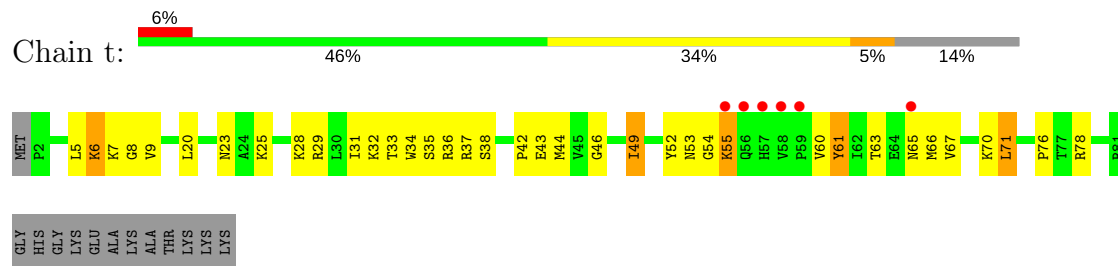
- Molecule 50: 30S ribosomal protein S17



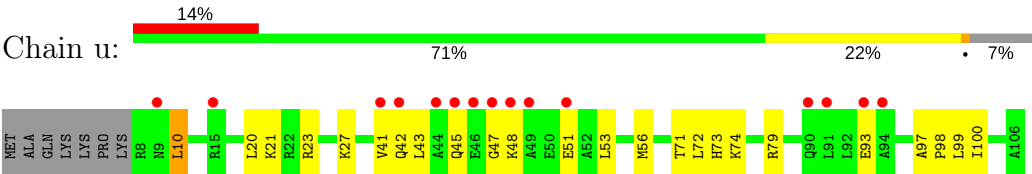
- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



• Molecule 54: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	507.21Å 507.21Å 692.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.83 78.70 – 3.70	Depositor EDS
% Data completeness (in resolution range)	81.7 (30.00-3.83) 68.4 (78.70-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.327 , 0.351 0.328 , 0.346	Depositor DCC
R_{free} test set	10090 reflections (2.99%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , -110.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.22$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.267 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.260 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	147125	wwPDB-VP
Average B, all atoms (Å ²)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.08% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MG, 5MC, M2G, 7MG, PSU

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	w	1.00	42/69679 (0.1%)	1.03	92/108779 (0.1%)
2	x	0.65	1/2878 (0.0%)	0.90	1/4490 (0.0%)
3	A	0.53	0/1015	0.63	0/1369
4	B	0.53	0/2165	0.70	0/2919
5	C	0.56	0/1574	0.69	0/2125
6	D	0.58	0/1551	0.69	0/2101
7	E	0.58	0/1492	0.72	1/2006 (0.0%)
8	F	0.56	0/1345	0.70	0/1819
9	G	0.51	0/1171	0.70	0/1583
10	H	0.54	0/1130	0.71	1/1525 (0.1%)
11	I	0.57	0/942	0.74	1/1268 (0.1%)
12	J	0.57	0/1131	0.76	1/1504 (0.1%)
13	K	0.58	0/1110	0.74	1/1483 (0.1%)
14	L	0.49	0/982	0.69	0/1312
15	M	0.51	0/856	0.63	0/1138
16	N	0.56	0/1157	0.72	0/1544
17	O	0.53	0/982	0.64	0/1306
18	P	0.58	0/790	0.69	0/1057
19	Q	0.51	0/878	0.74	1/1179 (0.1%)
20	R	0.60	0/739	0.75	0/993
21	S	0.61	0/806	0.70	0/1074
22	T	0.54	0/1507	0.66	0/2045
23	U	0.56	0/613	0.75	0/816
24	V	0.64	0/701	0.71	0/932
25	W	0.53	0/522	0.75	0/690
26	X	0.51	0/482	0.66	0/646
27	Y	0.53	0/449	0.69	0/606
28	Z	0.52	0/426	0.65	0/561
29	a	0.56	0/515	0.70	0/679
30	b	0.60	0/297	0.63	0/392
31	y	0.72	23/36178 (0.1%)	0.93	44/56463 (0.1%)
32	z	0.62	0/1831	0.88	0/2853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.65	0/1791	0.85	0/2791
34	3	0.63	0/439	0.90	0/684
35	c	0.56	0/1935	0.67	0/2609
36	d	0.51	0/1636	0.68	0/2205
37	e	0.55	0/1733	0.68	1/2318 (0.0%)
38	f	0.60	0/1162	0.68	0/1564
39	g	0.55	0/856	0.70	0/1154
40	h	0.54	0/1276	0.63	0/1709
41	i	0.51	0/1136	0.68	0/1527
42	j	0.58	0/1029	0.66	0/1378
43	k	0.59	0/807	0.66	0/1085
44	l	0.58	0/879	0.64	0/1187
45	m	0.55	0/986	0.75	0/1320
46	n	0.54	0/1008	0.68	0/1347
47	o	0.52	0/501	0.67	0/664
48	p	0.50	0/745	0.64	0/992
49	q	0.57	0/716	0.70	0/963
50	r	0.55	0/870	0.71	0/1159
51	s	0.60	0/675	0.67	0/894
52	t	0.59	0/661	0.68	1/890 (0.1%)
53	u	0.46	0/764	0.65	0/1006
54	v	0.58	0/212	0.60	0/277
All	All	0.81	66/159711 (0.0%)	0.92	145/238980 (0.1%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	41	C	O3'-P	43.37	2.13	1.61
1	w	1506	C	O3'-P	40.09	2.09	1.61
1	w	489	G	O3'-P	39.72	2.08	1.61
1	w	1448(B)	A	O3'-P	38.61	2.07	1.61
1	w	436	C	O3'-P	36.62	2.05	1.61
1	w	554	U	O3'-P	36.54	2.04	1.61
1	w	1743	G	O3'-P	36.44	2.04	1.61
1	w	1712	C	O3'-P	36.33	2.04	1.61
1	w	2213	U	O3'-P	35.61	2.03	1.61
1	w	366(B)	C	O3'-P	35.53	2.03	1.61
1	w	2712(B)	A	O3'-P	35.29	2.03	1.61
1	w	890	A	O3'-P	34.85	2.02	1.61
1	w	926	A	O3'-P	34.47	2.02	1.61
1	w	155	C	O3'-P	34.19	2.02	1.61
1	w	1583	A	O3'-P	33.94	2.01	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	99	U	O3'-P	33.39	2.01	1.61
1	w	1718	G	O3'-P	33.29	2.01	1.61
1	w	1481	U	O3'-P	31.86	1.99	1.61
1	w	1451	C	O3'-P	31.83	1.99	1.61
1	w	1735	U	O3'-P	31.62	1.99	1.61
1	w	537	C	O3'-P	31.45	1.98	1.61
1	w	1864	U	O3'-P	30.27	1.97	1.61
1	w	1171	G	O3'-P	30.16	1.97	1.61
1	w	1546(B)	C	O3'-P	29.62	1.96	1.61
1	w	1630(B)	C	O3'-P	29.10	1.96	1.61
1	w	1872	A	O3'-P	28.59	1.95	1.61
1	w	1142(B)	A	O3'-P	28.49	1.95	1.61
1	w	2219	G	O3'-P	28.38	1.95	1.61
1	w	1221(A)	C	O3'-P	27.85	1.94	1.61
1	w	165	U	O3'-P	27.37	1.94	1.61
1	w	1444(B)	A	O3'-P	26.83	1.93	1.61
1	w	1133	U	O3'-P	25.03	1.91	1.61
31	y	201	C	O3'-P	23.92	1.89	1.61
1	w	2199	A	O3'-P	21.55	1.87	1.61
31	y	97	U	O3'-P	18.57	1.83	1.61
1	w	2799	A	O3'-P	17.20	1.81	1.61
1	w	2746	U	O5'-C5'	16.23	1.70	1.44
1	w	2795	G	O3'-P	15.55	1.79	1.61
31	y	99	C	O3'-P	15.40	1.79	1.61
31	y	103(C)	G	O3'-P	15.38	1.79	1.61
31	y	1455	G	O3'-P	14.53	1.78	1.61
31	y	843	U	O3'-P	13.63	1.77	1.61
31	y	136(B)	C	O3'-P	13.10	1.76	1.61
31	y	458	C	O3'-P	13.00	1.76	1.61
31	y	1498	U	C4-O4	12.92	1.33	1.23
31	y	102(C)	C	O3'-P	12.51	1.76	1.61
1	w	2746	U	O3'-P	11.80	1.75	1.61
31	y	838	G	O3'-P	11.41	1.74	1.61
1	w	2889	C	O3'-P	11.28	1.74	1.61
31	y	93	U	O3'-P	9.74	1.72	1.61
31	y	1167	A	O3'-P	8.96	1.72	1.61
1	w	2747	G	P-O5'	8.92	1.68	1.59
31	y	1402	C	P-O5'	8.88	1.68	1.59
1	w	2746	U	P-O5'	8.37	1.68	1.59
1	w	2722	G	O5'-C5'	7.90	1.57	1.44
31	y	1402	C	O5'-C5'	7.66	1.56	1.44
31	y	99	C	P-O5'	7.37	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	1402	C	C4-N4	7.28	1.40	1.33
31	y	69	G	O3'-P	7.14	1.69	1.61
1	w	2720	U	O5'-C5'	6.96	1.55	1.44
2	x	29	A	P-O5'	5.49	1.65	1.59
31	y	97	U	O5'-C5'	5.49	1.53	1.44
31	y	449	C	O5'-C5'	5.45	1.53	1.44
31	y	162	A	O5'-C5'	5.27	1.52	1.44
31	y	1114	C	O5'-C5'	5.08	1.52	1.44
31	y	37	U	O5'-C5'	5.02	1.52	1.44

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2712(B)	A	P-O3'-C3'	-23.05	92.04	119.70
1	w	489	G	P-O3'-C3'	-18.72	97.23	119.70
31	y	97	U	P-O3'-C3'	-16.92	99.40	119.70
1	w	41	C	P-O3'-C3'	-15.29	101.35	119.70
1	w	1712	C	P-O3'-C3'	-15.07	101.61	119.70
31	y	99	C	P-O3'-C3'	-15.02	101.68	119.70
1	w	155	C	P-O3'-C3'	-13.31	103.73	119.70
1	w	537	C	P-O3'-C3'	-12.70	104.46	119.70
1	w	1718	G	P-O3'-C3'	-12.30	104.94	119.70
1	w	2746	U	P-O5'-C5'	-11.99	101.71	120.90
31	y	136(B)	C	P-O3'-C3'	-11.73	105.63	119.70
1	w	436	C	P-O3'-C3'	-11.65	105.72	119.70
1	w	99	U	P-O3'-C3'	-11.53	105.86	119.70
1	w	2393	A	N9-C1'-C2'	-11.49	99.07	114.00
31	y	201	C	P-O3'-C3'	-10.95	106.56	119.70
31	y	93	U	P-O3'-C3'	-10.73	106.83	119.70
1	w	1735	U	P-O3'-C3'	-10.67	106.90	119.70
1	w	1506	C	P-O3'-C3'	-10.31	107.32	119.70
1	w	1133	U	P-O3'-C3'	-10.18	107.49	119.70
31	y	838	G	P-O3'-C3'	-10.06	107.63	119.70
1	w	890	A	P-O3'-C3'	-9.59	108.19	119.70
1	w	1221(A)	C	P-O3'-C3'	-9.46	108.35	119.70
31	y	1402	C	P-O5'-C5'	-9.20	106.18	120.90
1	w	1743	G	P-O3'-C3'	-9.02	108.88	119.70
1	w	2799	A	O3'-P-O5'	9.00	121.11	104.00
1	w	1448(B)	A	P-O3'-C3'	-8.98	108.92	119.70
31	y	1455	G	OP1-P-O3'	8.80	124.56	105.20
31	y	103(C)	G	P-O3'-C3'	-8.77	109.18	119.70
1	w	2805	G	OP2-P-O3'	8.38	123.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	926	A	P-O3'-C3'	-8.35	109.69	119.70
1	w	1577	C	N1-C1'-C2'	-8.29	102.88	112.00
1	w	2795	G	P-O3'-C3'	-8.10	109.97	119.70
1	w	1955	U	N1-C1'-C2'	8.07	124.49	114.00
1	w	1822	G	N9-C1'-C2'	-8.05	103.15	112.00
31	y	99	C	OP2-P-O3'	8.05	122.90	105.20
1	w	2795	G	OP2-P-O3'	7.77	122.29	105.20
1	w	2257	U	N1-C1'-C2'	-7.67	103.57	112.00
1	w	2431	U	N1-C1'-C2'	-7.47	103.78	112.00
1	w	2805	G	OP1-P-O3'	-7.41	88.90	105.20
1	w	1863	G	N9-C1'-C2'	-7.38	103.88	112.00
31	y	1401	G	C3'-C2'-C1'	-7.37	95.60	101.50
1	w	1872	A	P-O3'-C3'	-7.29	110.95	119.70
31	y	82	U	P-O3'-C3'	7.22	128.37	119.70
1	w	366(B)	C	P-O3'-C3'	-7.15	111.12	119.70
1	w	458	G	C1'-O4'-C4'	-7.11	104.21	109.90
1	w	1955	U	O4'-C1'-N1	6.93	113.75	108.20
1	w	1187	G	N9-C1'-C2'	6.92	123.00	114.00
31	y	99	C	O3'-P-O5'	-6.86	90.96	104.00
1	w	1059	G	O4'-C1'-N9	6.86	113.69	108.20
1	w	362	U	C3'-C2'-C1'	-6.85	96.02	101.50
31	y	1401	G	P-O3'-C3'	-6.84	111.49	119.70
1	w	1444(B)	A	P-O3'-C3'	-6.80	111.54	119.70
1	w	1451	C	O3'-P-O5'	-6.77	91.14	104.00
31	y	210	U	P-O3'-C3'	6.69	127.73	119.70
1	w	873	G	N9-C1'-C2'	-6.64	104.70	112.00
1	w	2213	U	P-O3'-C3'	-6.62	111.75	119.70
2	x	21	G	N9-C1'-C2'	-6.58	104.76	112.00
19	Q	51	LEU	CA-CB-CG	6.58	130.43	115.30
1	w	800	A	O4'-C1'-N9	6.53	113.43	108.20
1	w	1171	G	P-O3'-C3'	-6.50	111.90	119.70
31	y	890	G	N9-C1'-C2'	-6.39	104.97	112.00
1	w	1274	A	N9-C1'-C2'	-6.39	104.98	112.00
1	w	1822	G	O4'-C1'-N9	6.38	113.30	108.20
31	y	1498	U	N1-C1'-C2'	6.35	122.26	114.00
31	y	189	U	N1-C1'-C2'	-6.35	105.02	112.00
31	y	93	U	OP2-P-O3'	6.22	118.88	105.20
1	w	1516	U	N1-C1'-C2'	-6.11	105.28	112.00
1	w	458	G	O4'-C1'-N9	6.09	113.07	108.20
31	y	1517	G	C3'-C2'-C1'	-6.07	96.64	101.50
1	w	265	A	N9-C1'-C2'	5.97	121.77	114.00
31	y	99	C	P-O5'-C5'	-5.95	111.39	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	136(B)	C	OP2-P-O3'	5.94	118.28	105.20
31	y	843	U	OP1-P-O3'	5.88	118.13	105.20
1	w	828	U	N1-C1'-C2'	5.87	121.63	114.00
1	w	2885	C	C3'-C2'-C1'	-5.84	96.83	101.50
1	w	1577	C	O4'-C1'-N1	5.80	112.84	108.20
31	y	102(C)	C	OP2-P-O3'	5.78	117.92	105.20
1	w	1221(A)	C	OP2-P-O3'	5.78	117.91	105.20
31	y	102(C)	C	O3'-P-O5'	-5.77	93.04	104.00
1	w	362	U	N1-C1'-C2'	-5.77	105.66	112.00
1	w	2746	U	P-O3'-C3'	-5.74	112.81	119.70
31	y	210	U	OP1-P-O3'	-5.74	92.57	105.20
1	w	227	A	P-O3'-C3'	5.74	126.58	119.70
31	y	1498	U	C5-C4-O4	-5.73	122.46	125.90
1	w	1800	C	O4'-C1'-N1	5.73	112.78	108.20
1	w	1615	C	O4'-C1'-N1	5.69	112.75	108.20
31	y	1105	A	N9-C1'-C2'	-5.65	105.78	112.00
31	y	587	G	O4'-C1'-N9	5.63	112.71	108.20
1	w	241	A	O4'-C1'-N9	5.63	112.70	108.20
1	w	271(D)	U	O4'-C1'-N1	5.62	112.70	108.20
52	t	71	LEU	CA-CB-CG	5.62	128.23	115.30
1	w	15	G	N9-C1'-C2'	-5.61	105.83	112.00
31	y	1455	G	O3'-P-O5'	-5.59	93.38	104.00
1	w	70	G	N9-C1'-C2'	5.57	121.24	114.00
1	w	2393	A	O4'-C1'-N9	5.56	112.65	108.20
1	w	1288	U	P-O3'-C3'	5.55	126.36	119.70
31	y	436	C	N1-C1'-C2'	-5.53	105.92	112.00
1	w	2468	G	N9-C1'-C2'	-5.53	105.92	112.00
1	w	913	U	P-O3'-C3'	5.51	126.32	119.70
31	y	1254	C	N1-C1'-C2'	-5.51	105.94	112.00
1	w	99	U	OP1-P-O3'	5.48	117.25	105.20
1	w	2225	A	P-O3'-C3'	5.48	126.27	119.70
1	w	2171	A	N9-C1'-C2'	5.47	121.12	114.00
31	y	69	G	O3'-P-O5'	-5.46	93.63	104.00
1	w	932	G	N9-C1'-C2'	5.46	121.09	114.00
1	w	1626	G	O4'-C1'-N9	5.43	112.54	108.20
12	J	148	LEU	CA-CB-CG	5.42	127.77	115.30
1	w	1898	U	N1-C1'-C2'	5.41	121.03	114.00
1	w	2497	A	P-O3'-C3'	5.36	126.14	119.70
1	w	2171	A	P-O3'-C3'	5.36	126.13	119.70
31	y	210	U	OP2-P-O3'	5.35	116.97	105.20
31	y	468	A	O3'-P-O5'	5.34	114.14	104.00
7	E	139	LEU	CA-CB-CG	5.33	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	91	LEU	CA-CB-CG	5.32	127.54	115.30
1	w	933	A	O4'-C1'-N9	5.30	112.44	108.20
31	y	250	A	N9-C1'-C2'	-5.30	106.17	112.00
31	y	1521	G	N9-C1'-C2'	-5.28	106.19	112.00
1	w	448	U	C1'-O4'-C4'	-5.28	105.67	109.90
13	K	37	LEU	CA-CB-CG	5.28	127.45	115.30
1	w	270(E)	C	N1-C1'-C2'	5.28	120.86	114.00
1	w	2002	G	O4'-C1'-N9	5.28	112.42	108.20
31	y	1220	G	N9-C1'-C2'	-5.27	106.20	112.00
1	w	2205	C	N1-C1'-C2'	-5.27	106.20	112.00
1	w	739	G	P-O3'-C3'	5.26	126.02	119.70
31	y	1401	G	N9-C1'-C2'	-5.24	106.24	112.00
1	w	1775	U	C3'-C2'-C1'	-5.24	97.31	101.50
31	y	960	U	N1-C1'-C2'	5.24	120.81	114.00
31	y	1498	U	N1-C2-N3	5.21	118.03	114.90
31	y	659	U	C3'-C2'-C1'	-5.21	97.34	101.50
31	y	1498	U	C2-N3-C4	-5.20	123.88	127.00
1	w	1247	A	C1'-O4'-C4'	-5.19	105.75	109.90
1	w	299	A	O4'-C1'-N9	5.18	112.34	108.20
1	w	1266	G	P-O3'-C3'	5.18	125.91	119.70
10	H	38	LEU	CA-CB-CG	5.17	127.20	115.30
37	e	19	LEU	CA-CB-CG	5.15	127.14	115.30
1	w	520	G	C3'-C2'-C1'	-5.15	97.38	101.50
1	w	1426	G	N9-C1'-C2'	5.13	120.68	114.00
1	w	554	U	P-O3'-C3'	-5.13	113.54	119.70
1	w	1812	A	C4'-C3'-C2'	-5.10	97.50	102.60
1	w	204	A	C3'-C2'-C1'	5.09	105.57	101.50
1	w	1356	G	O4'-C1'-N9	5.09	112.27	108.20
31	y	1402	C	C3'-C2'-C1'	5.06	105.55	101.50
1	w	1534	G	C3'-C2'-C1'	-5.04	97.47	101.50
1	w	457	A	N9-C1'-C2'	5.02	120.53	114.00
1	w	2848	G	O4'-C1'-N9	5.01	112.20	108.20

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	w	62213	0	31375	0	0
2	x	2573	0	1306	0	0
3	A	996	0	1013	124	0
4	B	2115	0	2195	368	0
5	C	1541	0	1599	276	0
6	D	1517	0	1565	225	0
7	E	1468	0	1529	224	0
8	F	1319	0	1399	148	0
9	G	1156	0	1239	188	6
10	H	1103	0	1177	181	0
11	I	932	0	994	188	0
12	J	1114	0	1187	155	0
13	K	1089	0	1156	198	0
14	L	968	0	1033	140	0
15	M	846	0	902	143	0
16	N	1143	0	1211	186	0
17	O	964	0	1022	150	0
18	P	779	0	852	155	0
19	Q	868	0	929	121	0
20	R	725	0	778	106	0
21	S	793	0	890	76	0
22	T	1475	0	1504	190	0
23	U	605	0	628	123	0
24	V	694	0	764	128	0
25	W	520	0	575	72	0
26	X	477	0	529	74	0
27	Y	436	0	460	62	0
28	Z	418	0	467	31	0
29	a	507	0	576	0	0
30	b	294	0	323	0	0
31	y	32546	0	16450	0	6
32	z	1639	0	837	0	0
33	2	1621	0	821	150	0
34	3	390	0	198	12	0
35	c	1900	0	1951	0	0
36	d	1612	0	1677	0	0
37	e	1703	0	1767	0	0
38	f	1146	0	1207	0	0
39	g	843	0	857	0	0
40	h	1257	0	1296	0	0
41	i	1116	0	1177	0	0
42	j	1011	0	1043	0	0
43	k	794	0	840	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l	864	0	881	0	0
45	m	970	0	1057	0	0
46	n	997	0	1072	0	0
47	o	492	0	533	0	0
48	p	734	0	771	0	0
49	q	700	0	720	0	0
50	r	857	0	930	0	0
51	s	668	0	748	0	0
52	t	647	0	673	0	0
53	u	762	0	859	0	0
54	v	208	0	221	0	0
All	All	147125	0	99763	4100	6

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 70.

All (4100) 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)
11:I:97:ARG:HE	11:I:97:ARG:HA	1.04	1.15
4:B:65:ILE:HD12	4:B:105:ILE:HG13	1.18	1.15
15:M:17:ARG:HE	15:M:89:ARG:HD2	1.06	1.14
14:L:96:ARG:HG3	14:L:117:VAL:HG23	1.31	1.11
22:T:10:ARG:HG2	22:T:37:VAL:HA	1.33	1.11
13:K:133:ARG:HG2	13:K:134:ARG:H	1.14	1.11
26:X:5:LYS:HA	26:X:36:VAL:HG12	1.23	1.11
15:M:28:VAL:HG12	15:M:29:PHE:H	1.10	1.10
6:D:150:LEU:HD12	6:D:169:VAL:HB	1.30	1.10
27:Y:38:ALA:HB2	27:Y:49:CYS:HB3	1.28	1.10
3:A:30:VAL:HA	3:A:33:LEU:HB2	1.34	1.09
18:P:15:GLU:HB3	18:P:16:PRO:HD3	1.29	1.09
4:B:124:PRO:HG2	4:B:129:ASN:HD21	0.94	1.09
5:C:93:VAL:HG12	5:C:182:LEU:HB2	1.18	1.09
17:O:51:LYS:HE3	17:O:55:ARG:HE	1.09	1.09
19:Q:11:ARG:HA	19:Q:100:THR:HG22	1.34	1.09
33:2:67:A:O2'	33:2:68:U:H5'	1.52	1.08
6:D:149:VAL:HB	6:D:186:ARG:HB2	1.09	1.08
24:V:48:LYS:HG2	24:V:63:ALA:HA	1.30	1.08
11:I:114:ILE:H	11:I:114:ILE:HD13	1.13	1.07
25:W:26:ARG:HD3	25:W:29:LYS:HD2	1.35	1.07
13:K:61:GLY:HA2	22:T:183:LEU:HG	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:96:ILE:HG22	18:P:97:LYS:H	1.13	1.07
33:2:35:A:H2'	33:2:36:A:C8	1.89	1.06
15:M:30:ARG:HD2	15:M:31:SER:H	1.18	1.06
22:T:6:LYS:HD3	22:T:6:LYS:H	4.64	1.06
4:B:35:LYS:HD3	4:B:64:ILE:HG22	1.37	1.06
13:K:32:PHE:HB2	13:K:106:VAL:HB	1.38	1.06
18:P:66:ARG:HD2	18:P:68:LYS:HG3	1.36	1.06
5:C:185:LYS:HG3	5:C:186:GLY:H	1.12	1.05
20:R:12:VAL:HG22	20:R:13:LEU:H	1.21	1.05
12:J:50:ARG:HG2	12:J:50:ARG:HH21	1.18	1.05
12:J:71:VAL:HG13	12:J:72:PRO:HD3	1.31	1.05
20:R:10:ALA:O	20:R:29:TRP:HB2	1.56	1.04
4:B:107:ALA:O	4:B:197:GLY:HA2	1.57	1.04
9:G:132:PRO:HD3	9:G:138:ILE:HG22	1.39	1.04
23:U:68:GLU:HB3	23:U:80:HIS:H	1.21	1.04
21:S:52:SER:HB3	21:S:53:PRO:HD2	1.38	1.04
4:B:126:GLN:HG2	4:B:129:ASN:HD22	1.23	1.04
17:O:90:VAL:HG13	17:O:91:ASP:H	1.19	1.04
6:D:48:THR:O	6:D:52:VAL:HB	1.59	1.03
33:2:34:G:H2'	33:2:35:A:H5''	1.40	1.03
14:L:2:ARG:HG3	14:L:3:HIS:H	1.20	1.03
4:B:69:ARG:HH22	4:B:76:PRO:HG3	1.20	1.02
3:A:59:VAL:O	3:A:165:ARG:HA	1.60	1.02
24:V:91:LYS:HA	24:V:94:LEU:HD22	1.41	1.02
5:C:108:SER:HA	5:C:189:PRO:HG3	1.39	1.02
21:S:88:LYS:HG3	21:S:89:PHE:H	1.21	1.01
11:I:24:VAL:HG22	11:I:25:LEU:H	1.24	1.01
23:U:40:GLN:HG2	23:U:41:ARG:H	1.17	1.01
23:U:66:VAL:O	23:U:81:VAL:HA	1.61	1.01
15:M:39:ILE:HD11	15:M:49:VAL:HG13	1.43	1.00
24:V:40:ARG:HG2	24:V:41:ARG:H	1.25	1.00
3:A:190:ILE:O	3:A:194:ILE:HG12	1.61	1.00
6:D:150:LEU:HD23	6:D:181:ILE:HG12	1.41	1.00
11:I:85:VAL:HG12	11:I:86:ILE:H	1.25	1.00
17:O:98:LEU:HD11	17:O:105:VAL:HB	1.42	1.00
5:C:170:LEU:HD23	5:C:185:LYS:HB3	1.44	1.00
9:G:3:VAL:HB	9:G:21:VAL:HG21	1.38	1.00
26:X:8:LEU:HG	26:X:9:VAL:H	1.22	1.00
15:M:53:SER:OG	15:M:69:VAL:HG21	1.62	0.99
16:N:135:VAL:HG13	16:N:136:GLN:H	1.26	0.99
33:2:48:C:H5''	33:2:48:C:H6	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:77:ILE:HB	16:N:74:ARG:HD2	1.44	0.99
11:I:68:GLU:HB2	11:I:76:ALA:HB1	1.41	0.99
24:V:66:HIS:HB3	24:V:69:LYS:HG2	1.39	0.99
7:E:7:LEU:HB3	7:E:100:TRP:HE1	1.26	0.99
8:F:149:ARG:HA	8:F:153:LYS:HG3	1.44	0.99
14:L:63:ARG:HH22	14:L:76:VAL:HG12	1.27	0.99
4:B:131:LEU:HD21	4:B:135:PHE:HB2	1.45	0.98
10:H:36:TRP:HB2	10:H:156:GLN:HB3	1.44	0.98
16:N:112:ARG:HA	16:N:115:ARG:HH21	1.22	0.98
20:R:13:LEU:HD22	20:R:29:TRP:HZ2	1.28	0.98
33:2:6:U:H2'	33:2:7:U:H5''	1.44	0.98
23:U:37:LEU:HD12	23:U:38:VAL:H	1.29	0.98
15:M:13:ARG:HG3	15:M:91:PRO:HA	1.42	0.98
26:X:35:ARG:HA	26:X:35:ARG:HE	1.28	0.97
5:C:28:ALA:CB	5:C:93:VAL:HG13	1.95	0.97
3:A:60:ARG:HA	3:A:164:PHE:O	1.65	0.97
6:D:8:SER:HB2	6:D:9:PRO:HD3	1.47	0.97
12:J:113:LYS:HA	12:J:129:ALA:O	1.64	0.97
22:T:80:ARG:HD2	22:T:82:ARG:HD3	1.46	0.97
7:E:144:ILE:HG23	7:E:147:ASP:HB2	1.46	0.97
24:V:54:ALA:HA	24:V:58:ILE:HG13	1.46	0.97
23:U:51:VAL:HG23	23:U:81:VAL:HG23	1.45	0.97
4:B:124:PRO:HG2	4:B:129:ASN:ND2	1.79	0.96
33:2:74:C:H2'	33:2:75:C:C1'	1.95	0.96
15:M:17:ARG:NE	15:M:89:ARG:HD2	1.78	0.96
10:H:60:LYS:NZ	17:O:67:ALA:HB2	1.80	0.96
23:U:36:ILE:HG12	23:U:39:ARG:NH2	1.79	0.96
4:B:43:ARG:H	4:B:43:ARG:HD3	1.30	0.96
9:G:4:ILE:HA	9:G:17:GLN:O	1.64	0.96
21:S:67:LEU:HD13	21:S:68:HIS:H	1.30	0.96
26:X:20:LYS:O	26:X:23:LEU:HG	1.62	0.96
20:R:65:ARG:NE	20:R:65:ARG:HA	1.81	0.96
20:R:12:VAL:CG2	20:R:13:LEU:H	1.79	0.96
9:G:7:GLU:H	9:G:8:PRO:HD3	1.30	0.95
22:T:150:LEU:HG	22:T:171:ILE:HD11	1.48	0.95
11:I:97:ARG:HA	11:I:97:ARG:NE	1.80	0.95
18:P:96:ILE:HG22	18:P:97:LYS:N	1.80	0.95
13:K:37:LEU:HG	13:K:128:LYS:H	1.31	0.95
19:Q:21:VAL:HG11	19:Q:76:VAL:HG11	1.48	0.95
18:P:7:THR:HG21	18:P:22:VAL:HG23	1.49	0.95
3:A:167:ASP:H	3:A:171:ALA:HA	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:5:LEU:O	22:T:59:LEU:HA	1.67	0.94
24:V:10:LYS:O	24:V:12:PRO:HD2	1.66	0.94
28:Z:2:LYS:H	28:Z:2:LYS:HD3	1.32	0.94
4:B:211:ARG:HA	4:B:214:TRP:CE3	2.03	0.94
13:K:16:ARG:HG3	13:K:17:LEU:H	1.32	0.94
22:T:7:ALA:HB2	22:T:59:LEU:HB3	1.49	0.94
9:G:27:ARG:H	9:G:27:ARG:HD3	1.32	0.94
17:O:84:LYS:HA	17:O:89:GLU:HG2	1.50	0.94
10:H:63:PRO:HA	17:O:64:ARG:NH2	1.82	0.94
4:B:81:ALA:HB3	4:B:94:LEU:HB3	1.49	0.94
5:C:174:ASP:H	5:C:183:LEU:HD11	1.33	0.94
6:D:33:ARG:HH12	12:J:12:ALA:H	1.06	0.93
6:D:149:VAL:CB	6:D:186:ARG:HB2	1.98	0.93
19:Q:88:ARG:HD2	19:Q:94:ASP:H	1.30	0.93
13:K:46:GLN:HE22	13:K:126:PRO:HD3	1.33	0.93
16:N:30:VAL:HG21	16:N:84:GLN:HG3	1.49	0.93
22:T:110:GLY:HA3	22:T:146:ILE:HG23	1.51	0.93
10:H:79:ASN:O	10:H:83:ILE:HD11	1.66	0.93
22:T:84:GLU:HG3	22:T:85:HIS:H	1.33	0.93
33:2:74:C:H2'	33:2:75:C:O4'	1.67	0.93
14:L:68:ARG:HB3	14:L:68:ARG:HH11	1.34	0.93
19:Q:77:ASP:H	19:Q:103:ILE:HG22	1.34	0.93
14:L:48:VAL:O	14:L:52:ILE:HG12	1.69	0.93
3:A:197:LEU:HG	3:A:198:GLU:HG3	1.51	0.93
7:E:139:LEU:HB2	7:E:146:TYR:H	1.33	0.92
12:J:92:GLU:OE2	12:J:123:LEU:HB3	1.69	0.92
14:L:76:VAL:HA	14:L:79:LEU:HG	1.51	0.92
7:E:141:PHE:HD2	7:E:144:ILE:H	1.05	0.92
33:2:34:G:C2'	33:2:35:A:H5''	1.99	0.92
12:J:101:VAL:HA	12:J:105:LEU:O	1.70	0.92
10:H:107:LYS:HG3	10:H:108:ILE:H	1.32	0.92
4:B:142:VAL:HG23	4:B:193:VAL:HA	1.52	0.92
6:D:117:LYS:NZ	6:D:117:LYS:HA	1.85	0.92
16:N:17:THR:HG23	16:N:18:ASP:H	1.35	0.92
11:I:75:SER:HA	16:N:75:ILE:O	1.70	0.92
19:Q:11:ARG:HB3	19:Q:98:LYS:HE2	1.49	0.92
4:B:126:GLN:HG2	4:B:129:ASN:ND2	1.85	0.92
12:J:42:SER:HB2	12:J:45:LEU:HA	1.51	0.92
15:M:66:ALA:HB1	15:M:101:LEU:HG	1.49	0.92
17:O:37:GLU:HA	17:O:40:PHE:CD1	2.05	0.92
20:R:12:VAL:HG22	20:R:13:LEU:N	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:3:GLN:OE1	11:I:5:GLN:HB3	1.71	0.91
33:2:49:C:H2'	33:2:50:U:H6	1.33	0.91
3:A:164:PHE:HB2	3:A:172:ILE:HG21	1.51	0.91
9:G:129:THR:HA	9:G:139:GLN:HA	1.51	0.91
18:P:7:THR:HG21	18:P:22:VAL:CG2	2.00	0.91
4:B:82:ILE:HG21	4:B:91:ARG:HH21	1.35	0.91
7:E:68:PRO:HB3	7:E:92:VAL:HB	1.51	0.91
5:C:28:ALA:HB2	5:C:93:VAL:HG13	1.52	0.91
4:B:123:ALA:HB1	4:B:124:PRO:HD2	1.50	0.91
11:I:1:MET:H2	11:I:67:LYS:HG2	1.35	0.91
11:I:71:ARG:HH22	16:N:74:ARG:HH22	1.18	0.91
4:B:164:GLN:HE22	4:B:166:GLN:HG3	1.35	0.90
4:B:44:ASN:HA	4:B:49:ILE:HA	1.53	0.90
7:E:7:LEU:HB3	7:E:100:TRP:NE1	1.86	0.90
4:B:259:THR:HG22	4:B:260:ARG:N	1.86	0.90
4:B:65:ILE:HG22	4:B:104:TYR:HD1	1.34	0.90
33:2:49:C:H2'	33:2:50:U:C6	2.05	0.90
33:2:9:A:N6	33:2:23:A:N7	2.18	0.90
22:T:97:GLU:CD	22:T:125:LEU:HG	1.91	0.90
16:N:24:PRO:HA	16:N:49:VAL:HG11	1.52	0.90
24:V:88:LYS:HG3	24:V:89:GLU:H	1.36	0.90
23:U:83:PRO:O	23:U:84:LEU:HB2	1.69	0.90
4:B:131:LEU:HD23	4:B:132:PRO:HD2	1.53	0.90
11:I:101:PRO:O	11:I:102:VAL:HG13	1.72	0.90
7:E:46:ALA:HB1	7:E:53:LEU:HD11	1.51	0.90
13:K:34:LEU:HD11	13:K:118:LEU:HG	1.54	0.90
14:L:87:TYR:OH	14:L:116:LEU:HB3	1.71	0.90
13:K:98:LYS:HB2	13:K:101:ARG:HB2	1.52	0.90
8:F:38:SER:HB2	8:F:39:PRO:HD2	1.50	0.89
20:R:8:ILE:HA	20:R:30:VAL:HG23	1.53	0.89
4:B:133:LEU:HD13	4:B:136:ILE:HD12	1.54	0.89
5:C:93:VAL:HB	5:C:182:LEU:HD13	1.53	0.89
13:K:133:ARG:CG	13:K:134:ARG:H	1.82	0.89
18:P:13:ARG:H	18:P:13:ARG:HH11	1.15	0.89
6:D:149:VAL:HB	6:D:186:ARG:CB	2.02	0.89
19:Q:85:VAL:HG13	19:Q:95:ILE:HG22	1.54	0.89
6:D:4:ILE:HB	6:D:5:PRO:HD3	1.53	0.89
13:K:37:LEU:HD11	13:K:128:LYS:HB2	1.54	0.89
11:I:65:THR:HA	11:I:82:ASN:ND2	1.87	0.89
8:F:20:ALA:HB1	8:F:21:PRO:HD2	1.54	0.89
3:A:223:VAL:HG12	3:A:224:ARG:H	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:47:VAL:HG12	5:C:48:GLN:H	1.36	0.89
3:A:201:LYS:HB2	3:A:202:PRO:HD2	1.55	0.89
5:C:119:ARG:HG3	5:C:157:ALA:HA	1.53	0.89
16:N:106:SER:HA	16:N:110:ILE:HD13	1.53	0.89
33:2:16:U:H2'	33:2:17:U:H5'	1.53	0.88
5:C:104:VAL:HG22	5:C:198:VAL:HA	1.54	0.88
5:C:66:HIS:O	5:C:67:PHE:HB2	1.71	0.88
23:U:62:LEU:HD23	23:U:63:VAL:HG23	1.55	0.88
16:N:33:LYS:HD3	16:N:41:ARG:HB3	1.52	0.88
14:L:33:ARG:HA	14:L:114:VAL:O	1.74	0.88
26:X:7:LYS:HG3	26:X:55:ARG:HB3	1.55	0.88
6:D:59:ILE:HD11	6:D:71:GLY:HA2	1.54	0.88
11:I:85:VAL:HG12	11:I:86:ILE:N	1.85	0.88
13:K:114:ALA:O	13:K:118:LEU:HD13	1.73	0.88
13:K:34:LEU:HB3	13:K:129:THR:OG1	1.73	0.88
19:Q:23:LEU:HD13	27:Y:25:LEU:HG	1.54	0.88
11:I:17:ARG:HH21	11:I:47:ILE:HB	1.37	0.88
4:B:174:ILE:HG22	4:B:175:LEU:H	1.37	0.87
7:E:74:LYS:HE3	7:E:88:ILE:HD11	1.55	0.87
14:L:24:GLN:O	14:L:28:LEU:HG	1.73	0.87
26:X:23:LEU:HA	26:X:26:LEU:HD12	1.54	0.87
13:K:125:LEU:HB3	13:K:126:PRO:HD2	1.54	0.87
33:2:36:A:H2'	33:2:37:A:H5'	1.57	0.87
9:G:3:VAL:H	9:G:21:VAL:CG2	1.87	0.87
11:I:64:ARG:O	11:I:82:ASN:HA	1.73	0.87
5:C:188:VAL:HG22	5:C:189:PRO:HD2	1.56	0.87
6:D:48:THR:HG23	6:D:49:ARG:H	1.40	0.87
13:K:39:PRO:HB3	13:K:99:PRO:HG3	1.55	0.87
5:C:11:MET:HB2	5:C:23:VAL:O	1.74	0.87
8:F:17:VAL:HG22	8:F:45:VAL:HB	1.57	0.87
22:T:80:ARG:HH11	22:T:82:ARG:HB2	1.37	0.87
4:B:19:ALA:HB1	4:B:24:ILE:HD11	1.56	0.87
4:B:39:LYS:HG3	4:B:40:THR:H	1.40	0.87
11:I:97:ARG:HE	11:I:97:ARG:CA	1.86	0.86
7:E:46:ALA:HB2	7:E:87:PRO:HG3	1.56	0.86
4:B:221:VAL:HG23	4:B:223:GLY:H	1.41	0.86
22:T:53:ILE:HA	22:T:98:MET:SD	2.15	0.86
14:L:34:ILE:HG22	14:L:35:THR:H	1.38	0.86
15:M:28:VAL:HG12	15:M:29:PHE:N	1.90	0.86
17:O:51:LYS:HE3	17:O:55:ARG:NE	1.89	0.86
7:E:172:LEU:HA	7:E:175:LEU:HB2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:63:C:H2'	33:2:64:A:H8	1.41	0.86
9:G:109:ILE:O	9:G:111:PRO:HD3	1.75	0.86
14:L:9:LYS:HG3	14:L:10:LEU:H	1.41	0.86
10:H:57:LEU:CD1	10:H:139:LEU:HB3	2.05	0.86
5:C:174:ASP:N	5:C:183:LEU:HD11	1.90	0.86
5:C:28:ALA:HB2	5:C:93:VAL:CG1	2.05	0.86
6:D:27:LEU:HD13	6:D:27:LEU:H	1.41	0.86
23:U:28:GLY:HA3	23:U:67:VAL:O	1.74	0.86
33:2:18:G:N1	33:2:57:G:N1	2.24	0.86
7:E:175:LEU:HB3	7:E:176:LEU:HD23	1.56	0.85
22:T:69:THR:HG21	22:T:88:PHE:CE1	2.11	0.85
15:M:67:ARG:HA	15:M:100:ALA:O	1.74	0.85
6:D:181:ILE:HA	6:D:184:THR:OG1	1.77	0.85
11:I:61:VAL:HG13	11:I:85:VAL:H	1.38	0.85
5:C:185:LYS:HG3	5:C:186:GLY:N	1.91	0.85
21:S:19:LYS:O	21:S:20:TYR:HB2	1.75	0.85
7:E:5:LEU:HD13	7:E:9:ARG:HD3	1.59	0.85
15:M:30:ARG:HD2	15:M:31:SER:N	1.92	0.85
23:U:45:PHE:HA	23:U:77:ARG:O	1.77	0.85
7:E:6:ALA:HB3	7:E:100:TRP:CZ2	2.12	0.85
11:I:19:ILE:HG22	11:I:43:VAL:HA	1.57	0.85
23:U:36:ILE:HA	23:U:60:PHE:HB2	1.56	0.85
9:G:63:ALA:HA	9:G:66:GLU:HB2	1.59	0.85
9:G:3:VAL:HG12	9:G:21:VAL:HG11	1.57	0.85
9:G:98:ALA:HA	9:G:111:PRO:HG2	1.57	0.85
14:L:57:ARG:HG3	14:L:61:HIS:HB3	1.59	0.85
24:V:90:ILE:HB	24:V:91:LYS:HZ2	1.40	0.85
25:W:13:ALA:HB3	25:W:15:LYS:HE3	1.58	0.85
3:A:53:ARG:HG3	33:2:54:U:O2'	1.75	0.84
4:B:133:LEU:HG	4:B:173:VAL:HG11	1.59	0.84
10:H:36:TRP:CB	10:H:156:GLN:HB3	2.06	0.84
17:O:49:HIS:HA	17:O:52:ARG:HB2	1.58	0.84
15:M:63:THR:OG1	15:M:100:ALA:HB2	1.77	0.84
18:P:15:GLU:HB3	18:P:16:PRO:CD	2.07	0.84
8:F:118:PRO:HD2	8:F:121:ILE:HG21	1.59	0.84
10:H:117:HIS:O	10:H:121:VAL:HG23	1.77	0.84
22:T:150:LEU:HD12	22:T:151:HIS:N	1.91	0.84
4:B:3:VAL:HA	4:B:17:THR:HG23	1.60	0.84
15:M:28:VAL:CG1	15:M:29:PHE:H	1.91	0.84
12:J:50:ARG:HG2	12:J:50:ARG:NH2	1.92	0.84
16:N:100:TYR:HA	16:N:103:ARG:HH12	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:111:ARG:H	16:N:111:ARG:HD2	1.42	0.84
22:T:53:ILE:HD13	22:T:53:ILE:H	1.42	0.84
13:K:3:MET:H	13:K:4:PRO:CD	1.90	0.84
5:C:64:LYS:O	5:C:66:HIS:N	2.10	0.84
14:L:84:ALA:O	14:L:88:ARG:HB2	1.78	0.84
20:R:42:ALA:O	20:R:46:ALA:HB2	1.76	0.84
22:T:24:LEU:HD11	22:T:41:LEU:HA	1.60	0.84
33:2:18:G:C6	33:2:57:G:N1	2.45	0.83
4:B:35:LYS:HE3	4:B:64:ILE:H	1.41	0.83
7:E:46:ALA:HA	7:E:53:LEU:HD21	1.60	0.83
18:P:89:GLN:OE1	18:P:91:TYR:HB2	1.78	0.83
22:T:6:LYS:CD	22:T:6:LYS:H	3.99	0.83
12:J:85:LEU:HD23	12:J:120:ALA:H	1.42	0.83
20:R:13:LEU:HD22	20:R:29:TRP:CZ2	2.12	0.83
20:R:30:VAL:HG22	20:R:31:HIS:H	1.41	0.83
6:D:180:ASP:O	6:D:184:THR:HG23	1.78	0.83
11:I:19:ILE:CG2	11:I:43:VAL:HA	2.07	0.83
11:I:22:ILE:HG13	11:I:23:ARG:H	1.41	0.83
18:P:14:VAL:HG21	18:P:98:GLU:HG2	1.60	0.83
3:A:63:VAL:HG22	3:A:64:SER:H	1.41	0.83
12:J:85:LEU:HD21	12:J:119:GLU:H	1.43	0.83
4:B:211:ARG:HA	4:B:214:TRP:HE3	1.37	0.83
16:N:100:TYR:O	16:N:102:ILE:N	2.12	0.83
7:E:125:PHE:HB2	7:E:166:ASP:CG	1.97	0.83
16:N:47:GLY:HA2	16:N:64:ARG:O	1.78	0.83
21:S:23:ARG:HD3	21:S:38:ILE:HG21	1.59	0.83
4:B:259:THR:HG22	4:B:260:ARG:H	1.40	0.83
7:E:47:LYS:HB2	7:E:72:ARG:HH12	1.43	0.83
13:K:32:PHE:CB	13:K:106:VAL:HB	2.07	0.83
13:K:8:LYS:HB3	13:K:12:GLN:HE21	1.44	0.83
9:G:38:LEU:HD13	9:G:40:THR:HG22	1.61	0.83
10:H:62:ARG:HE	10:H:63:PRO:HD2	1.44	0.83
15:M:110:LEU:HG	15:M:111:GLU:H	1.43	0.83
19:Q:10:VAL:HG12	19:Q:11:ARG:H	1.43	0.82
15:M:17:ARG:HE	15:M:89:ARG:CD	1.90	0.82
26:X:35:ARG:HG3	26:X:37:LEU:HD21	1.61	0.82
19:Q:27:LYS:O	19:Q:71:VAL:HB	1.78	0.82
22:T:108:PRO:HB3	22:T:144:LEU:HB3	1.59	0.82
4:B:126:GLN:O	4:B:193:VAL:HG22	1.78	0.82
16:N:51:ARG:HG2	16:N:52:ILE:N	1.94	0.82
21:S:31:LEU:HD23	21:S:31:LEU:H	2.55	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:12:U:H3	33:2:23:A:H61	1.26	0.82
17:O:92:ARG:HB2	18:P:11:GLN:OE1	1.79	0.82
11:I:17:ARG:HG2	11:I:46:ALA:HA	1.61	0.82
22:T:97:GLU:HB2	22:T:126:VAL:O	1.77	0.82
12:J:79:ARG:HB3	12:J:109:GLY:HA2	1.62	0.82
22:T:151:HIS:HB3	22:T:168:GLU:HA	1.61	0.82
11:I:68:GLU:HA	11:I:77:ILE:O	1.78	0.82
11:I:15:GLY:O	11:I:46:ALA:HB1	1.78	0.82
13:K:30:GLY:HA3	13:K:65:PHE:CZ	2.15	0.82
12:J:113:LYS:H	12:J:113:LYS:HD2	4.94	0.81
6:D:169:VAL:HG13	6:D:170:THR:H	1.45	0.81
7:E:136:ARG:HA	7:E:155:MET:SD	2.20	0.81
17:O:92:ARG:HB3	17:O:95:LEU:HG	1.60	0.81
23:U:67:VAL:HG13	23:U:79:VAL:HG12	1.61	0.81
27:Y:33:CYS:HB3	27:Y:49:CYS:SG	2.20	0.81
8:F:41:MET:HG3	8:F:54:ARG:HA	1.61	0.81
12:J:88:LEU:O	12:J:88:LEU:HG	1.80	0.81
5:C:185:LYS:CG	5:C:186:GLY:H	1.93	0.81
7:E:170:ARG:HB2	7:E:173:LEU:HD23	1.60	0.81
11:I:6:THR:HG22	11:I:7:TYR:H	1.45	0.81
3:A:8:TYR:HB2	3:A:11:LEU:HB2	1.61	0.81
20:R:12:VAL:HG13	20:R:17:ALA:HB2	1.60	0.81
18:P:10:LYS:HZ1	18:P:22:VAL:HA	1.45	0.81
4:B:106:ILE:HG22	4:B:197:GLY:H	1.44	0.81
4:B:172:TYR:HD1	4:B:186:HIS:HA	1.43	0.81
25:W:3:LEU:HD11	25:W:8:LYS:HD3	1.62	0.81
26:X:5:LYS:HA	26:X:36:VAL:CG1	2.08	0.81
25:W:47:ASN:HA	25:W:50:ILE:O	1.81	0.81
9:G:94:ALA:HB2	9:G:116:LEU:HD21	1.63	0.81
11:I:88:ASN:H	11:I:93:PRO:HA	1.45	0.81
4:B:247:ALA:HA	4:B:253:GLN:HA	1.61	0.80
4:B:93:ALA:HB2	4:B:107:ALA:HB2	1.64	0.80
15:M:26:LEU:HD22	15:M:39:ILE:CG2	2.12	0.80
24:V:11:ARG:HB2	24:V:12:PRO:CD	2.10	0.80
3:A:29:LEU:O	3:A:33:LEU:HG	1.81	0.80
22:T:4:ARG:HA	22:T:58:VAL:HB	1.62	0.80
23:U:40:GLN:CG	23:U:41:ARG:H	1.93	0.80
4:B:133:LEU:CD2	4:B:189:CYS:HB2	2.12	0.80
5:C:154:LYS:HD2	5:C:155:LYS:H	1.44	0.80
5:C:93:VAL:CG1	5:C:182:LEU:HB2	2.09	0.80
21:S:15:VAL:HG13	21:S:16:ALA:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:6:LYS:HD3	22:T:6:LYS:N	4.93	0.80
12:J:71:VAL:CG1	12:J:72:PRO:HD3	2.12	0.80
13:K:51:ARG:NH1	13:K:51:ARG:HB2	1.97	0.80
18:P:15:GLU:CB	18:P:16:PRO:HD3	2.11	0.80
4:B:69:ARG:NH2	4:B:76:PRO:HG3	1.95	0.80
16:N:29:ARG:O	16:N:85:LYS:HE2	1.82	0.80
13:K:24:GLY:H	13:K:98:LYS:HB3	1.46	0.80
24:V:12:PRO:O	24:V:13:ILE:HD12	1.81	0.80
24:V:50:ARG:NE	24:V:61:ARG:HB2	1.97	0.80
6:D:27:LEU:CD1	6:D:27:LEU:H	1.94	0.80
3:A:27:ALA:HB2	3:A:186:LEU:HD11	1.64	0.80
7:E:68:PRO:HB2	7:E:91:ARG:O	1.81	0.80
18:P:66:ARG:HD2	18:P:68:LYS:CG	2.12	0.80
16:N:31:SER:H	16:N:42:ILE:HB	1.47	0.80
5:C:97:LYS:HB2	5:C:98:PRO:HD2	1.64	0.80
10:H:113:MET:HA	10:H:116:THR:HG22	1.61	0.80
12:J:146:VAL:HG13	12:J:147:LEU:H	1.47	0.80
9:G:23:PRO:HB2	9:G:27:ARG:NE	1.96	0.79
10:H:60:LYS:HZ2	17:O:67:ALA:HB2	1.44	0.79
18:P:34:GLU:HB2	18:P:64:HIS:CE1	2.17	0.79
6:D:18:ASP:O	6:D:22:GLU:HG2	1.82	0.79
10:H:114:LEU:HA	10:H:121:VAL:HG13	1.64	0.79
10:H:41:ALA:O	10:H:83:ILE:HD12	1.83	0.79
11:I:87:ILE:HD13	11:I:93:PRO:HB3	1.63	0.79
33:2:54:U:H3	33:2:58:A:H62	1.27	0.79
13:K:114:ALA:C	13:K:118:LEU:HD13	2.03	0.79
10:H:114:LEU:HA	10:H:121:VAL:CG1	2.12	0.79
17:O:27:LEU:HD12	17:O:34:LYS:HG3	1.65	0.79
23:U:15:ASP:O	23:U:20:ARG:HD2	1.83	0.79
11:I:34:THR:HG22	11:I:35:VAL:H	1.46	0.79
15:M:25:ARG:HE	15:M:89:ARG:NH1	1.80	0.79
8:F:123:PHE:HB2	8:F:131:VAL:HG13	1.65	0.79
21:S:49:VAL:HG12	21:S:50:ARG:H	1.45	0.79
5:C:105:THR:HB	5:C:197:ILE:HD11	1.64	0.78
13:K:46:GLN:HE22	13:K:126:PRO:CD	1.96	0.78
26:X:8:LEU:CG	26:X:9:VAL:H	1.96	0.78
4:B:83:GLU:HB2	4:B:92:ILE:HD11	1.64	0.78
8:F:145:ALA:O	8:F:149:ARG:HB2	1.82	0.78
15:M:25:ARG:HH21	15:M:89:ARG:NH2	1.80	0.78
16:N:99:LEU:HG	16:N:102:ILE:HG12	1.65	0.78
6:D:151:LEU:H	6:D:169:VAL:CG1	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:169:VAL:HG13	6:D:170:THR:N	1.99	0.78
10:H:44:LYS:O	10:H:83:ILE:HG22	1.82	0.78
16:N:84:GLN:O	16:N:86:ILE:HG13	1.83	0.78
19:Q:88:ARG:HD2	19:Q:94:ASP:N	1.98	0.78
11:I:79:PHE:HE2	11:I:102:VAL:HG11	1.48	0.78
10:H:63:PRO:HA	17:O:64:ARG:HH22	1.42	0.78
23:U:68:GLU:HB3	23:U:80:HIS:N	1.98	0.78
4:B:91:ARG:HD3	4:B:198:ASN:HB2	1.65	0.78
13:K:132:VAL:HG13	13:K:133:ARG:N	1.98	0.78
4:B:108:PRO:HG2	4:B:111:LEU:HB2	1.66	0.78
18:P:65:GLY:H	18:P:96:ILE:HG13	1.49	0.78
20:R:81:VAL:HG22	20:R:82:GLN:H	1.47	0.78
4:B:60:ARG:CZ	4:B:60:ARG:HA	2.14	0.78
6:D:117:LYS:HZ2	6:D:117:LYS:HA	1.45	0.78
6:D:179:TYR:HD2	6:D:179:TYR:H	1.32	0.78
8:F:151:ILE:C	8:F:152:ARG:HD2	2.03	0.78
9:G:9:LEU:HD23	9:G:10:GLU:H	1.48	0.78
11:I:71:ARG:NH2	16:N:74:ARG:HH22	1.82	0.78
12:J:88:LEU:HD22	12:J:100:LEU:HG	1.63	0.78
7:E:79:ASN:CG	7:E:80:PHE:H	1.86	0.78
33:2:9:A:H62	33:2:23:A:H62	1.32	0.77
9:G:87:LYS:HB3	9:G:121:LYS:HD3	1.65	0.77
11:I:65:THR:O	11:I:79:PHE:HB2	1.84	0.77
5:C:77:ILE:HG22	5:C:78:LEU:H	1.49	0.77
6:D:96:LEU:HB3	6:D:97:PRO:CD	2.15	0.77
14:L:79:LEU:HA	14:L:83:ILE:CG1	2.14	0.77
17:O:99:ALA:HA	17:O:106:PHE:CE1	2.19	0.77
20:R:5:TYR:HE2	25:W:26:ARG:HG2	1.50	0.77
25:W:55:ARG:N	25:W:55:ARG:HH11	1.81	0.77
15:M:66:ALA:HB3	15:M:100:ALA:HB3	1.67	0.77
17:O:40:PHE:HB3	18:P:78:LYS:HD3	1.64	0.77
26:X:35:ARG:HA	26:X:35:ARG:NE	1.99	0.77
4:B:78:LYS:HE3	4:B:114:GLY:HA2	1.66	0.77
10:H:148:GLY:HA3	10:H:149:PRO:O	1.83	0.77
12:J:107:LYS:HG3	12:J:108:LYS:H	1.49	0.77
26:X:8:LEU:O	26:X:9:VAL:HG22	1.85	0.77
17:O:98:LEU:HD21	17:O:105:VAL:HG21	1.66	0.77
4:B:126:GLN:CG	4:B:129:ASN:HD22	1.96	0.77
5:C:28:ALA:HB3	5:C:180:ASN:C	2.04	0.77
13:K:133:ARG:HG2	13:K:134:ARG:N	1.97	0.77
16:N:29:ARG:HG3	16:N:30:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:40:GLN:HG2	23:U:41:ARG:N	1.98	0.77
9:G:107:ILE:HG12	9:G:109:ILE:HG12	1.67	0.77
9:G:81:VAL:HG23	9:G:82:ARG:H	1.48	0.77
10:H:46:LEU:HD21	10:H:83:ILE:HB	1.66	0.77
20:R:12:VAL:CG1	20:R:17:ALA:HB2	2.14	0.77
4:B:108:PRO:HG3	4:B:127:VAL:HG13	1.64	0.77
14:L:97:VAL:O	14:L:98:LEU:HG	1.84	0.77
25:W:8:LYS:HA	25:W:11:GLU:CB	2.14	0.77
4:B:259:THR:O	4:B:260:ARG:HG2	1.83	0.77
6:D:111:ASP:HA	6:D:114:ARG:HG2	1.66	0.77
6:D:172:ALA:HB3	6:D:173:PRO:CD	2.14	0.77
6:D:26:HIS:HA	12:J:13:ASN:HB3	1.67	0.77
6:D:15:LEU:HD22	6:D:19:LEU:HD22	1.66	0.77
10:H:57:LEU:HD11	10:H:139:LEU:HB3	1.66	0.77
11:I:21:CYS:SG	11:I:22:ILE:N	2.57	0.77
4:B:138:VAL:HG13	4:B:139:GLY:H	1.47	0.77
5:C:93:VAL:HA	5:C:182:LEU:HD22	1.66	0.77
7:E:70:VAL:HG12	7:E:90:LEU:HD21	1.66	0.77
10:H:55:THR:O	10:H:60:LYS:HB3	1.85	0.77
14:L:68:ARG:NH1	14:L:68:ARG:HB3	2.00	0.77
11:I:79:PHE:HD2	16:N:70:VAL:HG11	1.51	0.77
24:V:26:ARG:H	24:V:26:ARG:HD3	1.49	0.77
4:B:69:ARG:NH2	4:B:119:ALA:HB2	1.99	0.76
9:G:77:LEU:HD12	9:G:142:VAL:HG13	1.65	0.76
18:P:47:VAL:HG13	18:P:48:GLY:N	2.00	0.76
21:S:88:LYS:HG3	21:S:89:PHE:N	2.00	0.76
4:B:77:ALA:O	4:B:117:VAL:HG23	1.84	0.76
7:E:139:LEU:CB	7:E:146:TYR:H	1.97	0.76
7:E:35:GLU:OE2	7:E:160:VAL:HG12	1.85	0.76
8:F:118:PRO:HG2	8:F:121:ILE:HB	1.67	0.76
9:G:23:PRO:HB2	9:G:27:ARG:HE	1.50	0.76
17:O:48:ALA:O	17:O:52:ARG:HG2	1.85	0.76
15:M:25:ARG:HH21	15:M:89:ARG:HH22	1.31	0.76
23:U:26:TYR:CD2	23:U:29:GLN:HB2	2.20	0.76
4:B:79:VAL:HA	4:B:95:LEU:CB	2.15	0.76
13:K:51:ARG:CZ	13:K:51:ARG:HB2	2.14	0.76
4:B:6:PHE:HE1	4:B:18:VAL:HB	1.51	0.76
5:C:7:VAL:H	5:C:27:LEU:HD22	1.49	0.76
11:I:77:ILE:HD12	11:I:79:PHE:CE1	2.20	0.76
21:S:88:LYS:CG	21:S:89:PHE:H	1.97	0.76
8:F:134:SER:HA	8:F:138:LYS:NZ	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:23:LEU:HG	19:Q:24:ILE:N	1.99	0.76
4:B:123:ALA:HB1	4:B:124:PRO:CD	2.16	0.76
10:H:118:PRO:O	10:H:121:VAL:HB	1.85	0.76
22:T:110:GLY:CA	22:T:146:ILE:HD12	2.16	0.76
13:K:34:LEU:HD21	13:K:118:LEU:HD23	1.67	0.76
21:S:31:LEU:CD2	21:S:31:LEU:H	2.67	0.76
33:2:74:C:H2'	33:2:75:C:H1'	1.67	0.75
4:B:164:GLN:NE2	4:B:166:GLN:HG3	2.01	0.75
5:C:122:PHE:CE2	5:C:138:PRO:HB3	2.22	0.75
8:F:146:ALA:HA	8:F:149:ARG:HB3	1.68	0.75
10:H:40:ASP:HB2	10:H:77:VAL:HG13	1.67	0.75
20:R:27:THR:HA	20:R:78:LYS:HB3	1.67	0.75
9:G:59:ALA:O	9:G:63:ALA:HB3	1.86	0.75
17:O:103:PRO:O	17:O:105:VAL:N	2.19	0.75
33:2:41:U:H2'	33:2:42:G:H8	1.52	0.75
3:A:58:ASN:HA	3:A:166:ASN:OD1	1.86	0.75
11:I:34:THR:HG22	11:I:35:VAL:N	2.01	0.75
12:J:100:LEU:O	12:J:101:VAL:HG22	1.86	0.75
9:G:88:ILE:HG23	9:G:89:TYR:H	1.52	0.75
16:N:26:ASP:OD2	16:N:91:ARG:HB3	1.86	0.75
20:R:12:VAL:HG13	20:R:17:ALA:CB	2.15	0.75
6:D:137:TRP:HA	6:D:137:TRP:CE3	2.22	0.75
8:F:153:LYS:HB2	8:F:154:PRO:HD3	1.68	0.75
9:G:3:VAL:CB	9:G:21:VAL:HG21	2.17	0.75
12:J:6:LEU:C	12:J:8:PRO:HD3	2.06	0.75
14:L:72:ASP:O	14:L:76:VAL:HG23	1.85	0.75
33:2:68:U:H2'	33:2:69:U:C6	2.21	0.75
4:B:35:LYS:HB2	4:B:36:PRO:HA	1.68	0.75
13:K:136:ALA:O	13:K:137:TYR:HB2	1.85	0.75
13:K:72:LYS:C	13:K:72:LYS:HD3	2.07	0.75
15:M:30:ARG:CD	15:M:31:SER:H	1.99	0.75
22:T:166:SER:OG	22:T:169:GLU:HB2	1.87	0.75
25:W:29:LYS:HD3	25:W:30:ARG:N	2.01	0.75
3:A:21:TYR:N	3:A:21:TYR:CD2	2.55	0.75
12:J:79:ARG:NH1	12:J:108:LYS:HB2	2.02	0.75
19:Q:38:TYR:CD2	27:Y:41:PRO:HG3	2.22	0.75
4:B:108:PRO:HD2	4:B:111:LEU:CD2	2.17	0.75
6:D:165:LEU:HG	6:D:169:VAL:O	1.87	0.75
7:E:120:LEU:HD22	7:E:121:ASN:H	1.52	0.75
22:T:15:PRO:O	22:T:19:ARG:HD2	1.86	0.75
12:J:148:LEU:HD22	12:J:149:GLU:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:7:LYS:HA	26:X:34:GLU:HA	1.67	0.75
4:B:65:ILE:CG2	4:B:105:ILE:HA	2.15	0.75
7:E:43:LEU:HG	7:E:153:ARG:NE	2.02	0.75
24:V:90:ILE:HB	24:V:91:LYS:NZ	2.02	0.75
24:V:17:SER:HB2	24:V:44:PRO:O	1.86	0.75
3:A:217:THR:OG1	3:A:220:GLY:N	2.20	0.74
7:E:3:LEU:HB2	7:E:100:TRP:CH2	2.22	0.74
11:I:64:ARG:HD3	11:I:102:VAL:HG21	1.69	0.74
13:K:23:GLY:HA3	13:K:98:LYS:HA	1.67	0.74
16:N:51:ARG:HG2	16:N:52:ILE:H	1.52	0.74
19:Q:33:ARG:HG3	19:Q:34:ASN:N	2.00	0.74
34:3:15:G:O2'	34:3:16:A:H5''	1.87	0.74
7:E:61:ALA:O	7:E:64:THR:HG22	1.87	0.74
8:F:105:LEU:O	8:F:113:VAL:HB	1.87	0.74
11:I:16:ALA:HA	11:I:46:ALA:HB1	1.69	0.74
13:K:64:ILE:HG12	13:K:106:VAL:HA	1.70	0.74
9:G:22:LYS:HB2	9:G:23:PRO:HD2	1.69	0.74
16:N:26:ASP:HA	16:N:48:ILE:HG23	1.69	0.74
33:2:48:C:C6	33:2:48:C:H5''	2.16	0.74
4:B:182:LEU:HB3	4:B:271:ILE:HG22	1.68	0.74
11:I:77:ILE:HG13	16:N:72:VAL:HG13	1.68	0.74
6:D:121:VAL:HA	6:D:189:MET:O	1.87	0.74
14:L:53:HIS:O	14:L:56:LYS:HG2	1.88	0.74
24:V:85:LEU:HB2	24:V:87:PRO:HD2	1.68	0.74
12:J:148:LEU:CD2	12:J:149:GLU:H	2.00	0.74
5:C:108:SER:HA	5:C:189:PRO:CG	2.18	0.74
8:F:38:SER:HB2	8:F:39:PRO:CD	2.17	0.74
9:G:7:GLU:N	9:G:8:PRO:HD3	2.03	0.74
11:I:109:LYS:HE3	11:I:109:LYS:HA	1.68	0.74
20:R:20:GLY:HA2	20:R:24:GLY:O	1.87	0.74
22:T:171:ILE:HD13	22:T:171:ILE:H	1.51	0.74
22:T:42:VAL:HG12	22:T:46:LYS:HD2	1.68	0.74
14:L:9:LYS:O	14:L:10:LEU:HB2	1.85	0.74
22:T:128:VAL:HG23	22:T:160:GLY:O	1.86	0.74
26:X:8:LEU:HG	26:X:9:VAL:N	2.01	0.74
4:B:118:VAL:HG22	4:B:119:ALA:H	1.53	0.74
7:E:111:LEU:O	7:E:114:ILE:HB	1.88	0.74
11:I:16:ALA:HA	11:I:46:ALA:CB	2.16	0.74
33:2:29:A:O2'	33:2:30:G:H5'	1.87	0.74
3:A:185:LYS:O	3:A:189:ASN:HB2	1.88	0.74
4:B:108:PRO:HD2	4:B:111:LEU:HD23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:SER:H	25:W:7:ARG:HG3	1.53	0.74
3:A:63:VAL:HG22	3:A:64:SER:N	2.03	0.73
5:C:110:GLY:HA2	5:C:161:GLY:HA3	1.71	0.73
7:E:71:THR:O	7:E:88:ILE:HB	1.87	0.73
22:T:88:PHE:C	22:T:88:PHE:CD2	2.61	0.73
22:T:97:GLU:OE1	22:T:125:LEU:HG	1.86	0.73
23:U:31:VAL:O	23:U:64:ASP:HA	1.87	0.73
11:I:114:ILE:H	11:I:114:ILE:CD1	1.90	0.73
6:D:155:ASN:O	6:D:158:VAL:HG12	1.88	0.73
9:G:122:GLU:HG2	9:G:123:LEU:N	2.01	0.73
34:3:8:U:H3'	34:3:8:U:H6	1.52	0.73
15:M:41:ASP:HB3	15:M:46:VAL:HG23	1.69	0.73
18:P:43:GLU:CD	18:P:44:LYS:H	1.92	0.73
7:E:114:ILE:HG12	7:E:115:ARG:H	1.52	0.73
9:G:27:ARG:H	9:G:27:ARG:CD	2.00	0.73
14:L:39:PRO:O	14:L:43:GLU:HG2	1.88	0.73
19:Q:88:ARG:CD	19:Q:94:ASP:H	2.00	0.73
5:C:38:THR:HG22	5:C:39:PRO:HD2	1.71	0.73
9:G:124:GLY:O	9:G:143:SER:HA	1.88	0.73
23:U:32:ARG:HA	23:U:64:ASP:OD1	1.89	0.73
25:W:8:LYS:HA	25:W:11:GLU:HB2	1.69	0.73
27:Y:16:ARG:HG3	27:Y:17:ASP:H	1.54	0.73
6:D:119:LEU:O	6:D:121:VAL:N	2.22	0.73
16:N:93:ARG:H	16:N:116:ALA:HA	1.53	0.73
16:N:50:ILE:HD11	16:N:64:ARG:HB2	1.70	0.73
21:S:39:VAL:HG12	21:S:40:GLU:H	1.53	0.73
24:V:90:ILE:O	24:V:94:LEU:HD13	1.87	0.73
6:D:8:SER:HB2	6:D:9:PRO:CD	2.17	0.73
12:J:7:ARG:N	12:J:8:PRO:HD3	2.03	0.73
24:V:14:VAL:O	24:V:46:LEU:HD11	1.89	0.73
5:C:28:ALA:HB1	5:C:93:VAL:HG13	1.70	0.73
18:P:34:GLU:HB2	18:P:64:HIS:NE2	2.02	0.73
33:2:51:G:H2'	33:2:52:U:C6	2.24	0.73
3:A:41:THR:O	3:A:217:THR:HB	1.88	0.73
4:B:131:LEU:HD23	4:B:132:PRO:CD	2.18	0.73
4:B:65:ILE:HG21	4:B:105:ILE:HA	1.70	0.73
4:B:79:VAL:HA	4:B:95:LEU:HB3	1.71	0.73
6:D:96:LEU:HB3	6:D:97:PRO:HD2	1.69	0.73
13:K:37:LEU:HG	13:K:128:LYS:N	2.04	0.73
14:L:29:LEU:HD21	14:L:75:LEU:HD13	1.70	0.73
21:S:9:LYS:HG3	21:S:10:GLY:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:31:LYS:HE3	4:B:32:SER:O	1.89	0.73
13:K:72:LYS:O	13:K:94:VAL:HG22	1.89	0.73
17:O:90:VAL:HG13	17:O:91:ASP:N	2.00	0.73
18:P:24:LYS:HG2	18:P:25:LEU:N	2.04	0.73
18:P:66:ARG:HE	18:P:94:LEU:HD21	1.52	0.73
3:A:46:ALA:HA	3:A:212:SER:O	1.89	0.73
4:B:97:TYR:HB2	4:B:102:LYS:HA	1.71	0.73
5:C:47:VAL:HG12	5:C:48:GLN:N	2.04	0.73
7:E:103:LEU:O	7:E:107:LEU:HG	1.89	0.73
18:P:78:LYS:HB2	18:P:83:ARG:NH1	2.02	0.73
23:U:28:GLY:CA	23:U:67:VAL:O	2.37	0.73
25:W:47:ASN:HB2	25:W:51:ARG:NH2	2.04	0.73
6:D:150:LEU:CD1	6:D:169:VAL:HB	2.16	0.72
11:I:10:VAL:HG11	11:I:17:ARG:HA	1.71	0.72
21:S:52:SER:HB3	21:S:53:PRO:CD	2.19	0.72
12:J:96:THR:HG23	12:J:99:LEU:HB2	1.70	0.72
33:2:63:C:H2'	33:2:64:A:C8	2.24	0.72
12:J:85:LEU:HD21	12:J:119:GLU:N	2.05	0.72
15:M:8:GLU:HG2	15:M:11:LYS:HE3	1.70	0.72
3:A:21:TYR:H	3:A:21:TYR:HD2	1.34	0.72
4:B:81:ALA:HB3	4:B:94:LEU:CB	2.18	0.72
8:F:22:GLY:O	8:F:37:VAL:HG22	1.88	0.72
14:L:83:ILE:O	14:L:87:TYR:HD1	1.72	0.72
20:R:32:PRO:HG3	20:R:72:LYS:HE2	1.69	0.72
27:Y:33:CYS:CB	27:Y:38:ALA:HB3	2.20	0.72
11:I:77:ILE:HD12	11:I:79:PHE:CD1	2.25	0.72
14:L:66:VAL:HA	14:L:68:ARG:HH12	1.53	0.72
14:L:76:VAL:HA	14:L:79:LEU:CG	2.18	0.72
15:M:49:VAL:HG22	15:M:50:SER:H	1.53	0.72
21:S:65:ALA:HB3	21:S:66:PRO:HD3	1.71	0.72
28:Z:21:ARG:C	28:Z:23:ARG:H	1.91	0.72
3:A:34:ALA:HB2	3:A:179:ALA:HB1	1.72	0.72
3:A:61:GLY:O	3:A:163:GLU:HA	1.90	0.72
4:B:20:ASP:O	4:B:24:ILE:HB	1.89	0.72
5:C:22:PRO:O	5:C:23:VAL:HG13	1.88	0.72
18:P:24:LYS:HB2	18:P:94:LEU:HG	1.71	0.72
23:U:15:ASP:HB3	23:U:20:ARG:HH11	1.54	0.72
24:V:87:PRO:HB2	24:V:91:LYS:HD2	1.70	0.72
5:C:131:ALA:O	5:C:133:LYS:HG2	1.90	0.72
13:K:72:LYS:HZ2	13:K:73:PRO:HB2	1.54	0.72
16:N:72:VAL:CG1	16:N:74:ARG:HG2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:96:THR:HG23	12:J:99:LEU:CB	2.19	0.72
6:D:59:ILE:HD11	6:D:71:GLY:CA	2.20	0.72
7:E:104:GLU:HA	7:E:107:LEU:HD12	1.70	0.72
16:N:30:VAL:HA	16:N:42:ILE:HB	1.71	0.72
19:Q:4:LYS:HD2	19:Q:62:HIS:HE1	1.55	0.72
24:V:83:GLU:O	24:V:88:LYS:HE2	1.89	0.72
33:2:13:C:H2'	33:2:14:A:O4'	1.89	0.72
5:C:37:ARG:HA	5:C:42:ASP:CG	2.11	0.72
11:I:17:ARG:NH2	11:I:47:ILE:HB	2.03	0.72
20:R:68:ARG:O	20:R:69:TYR:HB2	1.90	0.72
14:L:2:ARG:HG3	14:L:3:HIS:N	2.01	0.72
21:S:50:ARG:HG3	21:S:54:LYS:NZ	2.05	0.72
26:X:8:LEU:CD2	26:X:33:GLN:H	2.03	0.72
4:B:106:ILE:HG22	4:B:197:GLY:N	2.05	0.71
5:C:77:ILE:HG22	5:C:78:LEU:N	2.04	0.71
6:D:69:ARG:HH21	6:D:69:ARG:HG3	1.53	0.71
7:E:144:ILE:HG23	7:E:147:ASP:CB	2.18	0.71
8:F:134:SER:HA	8:F:138:LYS:HZ1	1.54	0.71
10:H:29:PRO:HB3	10:H:64:ASP:HB3	1.72	0.71
13:K:64:ILE:HD11	13:K:106:VAL:HG22	1.71	0.71
15:M:25:ARG:NE	15:M:89:ARG:NH1	2.37	0.71
25:W:47:ASN:HB2	25:W:51:ARG:CZ	2.20	0.71
6:D:129:GLY:O	6:D:161:ALA:HA	1.90	0.71
7:E:115:ARG:O	7:E:118:ARG:HG2	9.95	0.71
10:H:135:LEU:HD12	10:H:135:LEU:H	1.53	0.71
24:V:9:GLY:HA3	24:V:61:ARG:CZ	2.20	0.71
3:A:21:TYR:O	3:A:225:ILE:HA	1.91	0.71
17:O:44:ASN:O	17:O:48:ALA:HB2	1.90	0.71
4:B:80:ALA:HB3	4:B:94:LEU:O	1.91	0.71
33:2:16:U:C2'	33:2:17:U:H5'	2.19	0.71
8:F:40:GLU:CD	8:F:55:PRO:HB3	2.10	0.71
19:Q:80:PRO:HD2	19:Q:102:HIS:NE2	2.05	0.71
7:E:43:LEU:HG	7:E:153:ARG:HE	1.54	0.71
11:I:1:MET:H2	11:I:67:LYS:CG	2.03	0.71
13:K:37:LEU:HB2	13:K:127:ILE:HB	1.72	0.71
23:U:28:GLY:H	23:U:69:PHE:HB2	1.55	0.71
26:X:8:LEU:HD21	26:X:33:GLN:H	1.55	0.71
21:S:67:LEU:CD1	21:S:68:HIS:H	2.03	0.71
6:D:181:ILE:HD11	6:D:185:GLU:O	1.90	0.71
17:O:27:LEU:CD1	17:O:34:LYS:HG3	2.21	0.71
25:W:55:ARG:H	25:W:55:ARG:HH11	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:122:PRO:HB2	7:E:173:LEU:HD22	1.70	0.71
10:H:119:GLU:HG3	10:H:145:VAL:HG23	1.70	0.71
15:M:17:ARG:HG2	15:M:89:ARG:HA	1.72	0.71
27:Y:31:VAL:HG22	27:Y:40:LYS:O	1.90	0.71
7:E:129:GLY:HA3	7:E:161:THR:O	1.91	0.71
17:O:84:LYS:HE2	17:O:84:LYS:H	1.54	0.71
19:Q:76:VAL:HA	19:Q:103:ILE:HG22	1.70	0.71
20:R:8:ILE:HG13	20:R:42:ALA:HB1	1.71	0.71
28:Z:14:LYS:O	28:Z:20:ALA:HB1	1.90	0.71
4:B:132:PRO:O	4:B:136:ILE:HG13	1.91	0.71
10:H:39:ILE:HG13	10:H:40:ASP:H	1.55	0.71
26:X:4:LEU:HD13	26:X:58:VAL:HG22	1.71	0.71
33:2:6:U:C2'	33:2:7:U:H5''	2.21	0.71
9:G:38:LEU:HD12	9:G:38:LEU:N	2.06	0.71
11:I:77:ILE:HG12	16:N:74:ARG:H	1.54	0.71
33:2:19:G:H5''	33:2:20:G:OP1	1.89	0.71
22:T:110:GLY:HA3	22:T:146:ILE:HD12	1.72	0.71
22:T:151:HIS:CB	22:T:168:GLU:HA	2.20	0.71
24:V:69:LYS:HG3	24:V:70:VAL:N	2.04	0.71
18:P:18:LEU:O	18:P:19:LYS:HB2	1.90	0.70
3:A:48:LEU:HB2	3:A:209:PHE:O	1.90	0.70
4:B:15:PHE:O	4:B:16:MET:HG3	1.91	0.70
7:E:126:ASP:CB	7:E:130:ASN:HB2	2.20	0.70
16:N:90:GLN:HB3	16:N:120:ARG:NH1	2.06	0.70
10:H:49:LEU:HA	10:H:52:LYS:HE2	1.73	0.70
5:C:173:VAL:H	5:C:183:LEU:HD11	1.54	0.70
6:D:150:LEU:O	6:D:187:LEU:HA	1.90	0.70
10:H:62:ARG:NE	10:H:63:PRO:HD2	2.06	0.70
22:T:130:PRO:HA	22:T:133:ILE:CG1	2.21	0.70
16:N:64:ARG:HD3	16:N:102:ILE:HD11	1.72	0.70
7:E:46:ALA:HA	7:E:53:LEU:CD2	2.20	0.70
9:G:133:HIS:NE2	9:G:136:VAL:HG23	2.06	0.70
14:L:66:VAL:CA	14:L:68:ARG:HH12	2.04	0.70
6:D:128:ASN:HA	6:D:134:PHE:CZ	2.26	0.70
22:T:110:GLY:HA3	22:T:146:ILE:CG2	2.21	0.70
3:A:27:ALA:CB	3:A:186:LEU:HD11	2.21	0.70
6:D:120:LEU:HD21	6:D:123:ALA:HB2	1.73	0.70
17:O:33:ARG:O	17:O:36:ARG:HB3	1.90	0.70
23:U:49:LYS:O	23:U:81:VAL:HB	1.91	0.70
23:U:67:VAL:HG13	23:U:79:VAL:CG1	2.21	0.70
33:2:61:C:O2'	33:2:62:A:H5'	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:41:LYS:HG3	5:C:42:ASP:OD2	1.90	0.70
8:F:153:LYS:HD2	8:F:162:ILE:O	1.90	0.70
17:O:51:LYS:HD3	17:O:51:LYS:O	1.92	0.70
3:A:197:LEU:HG	3:A:198:GLU:N	2.07	0.70
4:B:43:ARG:N	4:B:43:ARG:HD3	2.05	0.70
11:I:64:ARG:HB3	11:I:102:VAL:HG21	1.73	0.70
12:J:46:LYS:HB3	12:J:51:PHE:CZ	2.26	0.70
15:M:11:LYS:O	15:M:14:VAL:HG12	1.91	0.70
17:O:40:PHE:CB	18:P:78:LYS:HD3	2.21	0.70
25:W:7:ARG:C	25:W:8:LYS:HD2	2.11	0.70
24:V:9:GLY:HA3	24:V:61:ARG:NH2	2.06	0.70
11:I:13:ASN:H	11:I:97:ARG:HB2	1.55	0.70
22:T:19:ARG:HH21	22:T:25:PRO:HB2	1.56	0.70
14:L:9:LYS:CG	14:L:10:LEU:H	2.00	0.70
4:B:133:LEU:H	4:B:133:LEU:HD22	1.57	0.70
4:B:255:LYS:HD3	4:B:255:LYS:O	1.91	0.70
4:B:52:ARG:NH2	4:B:220:HIS:HA	2.07	0.70
8:F:102:ALA:HB2	8:F:117:PRO:HD3	1.74	0.70
28:Z:19:ARG:HG2	28:Z:23:ARG:NH2	2.07	0.70
4:B:111:LEU:CD1	4:B:115:GLN:HB3	2.22	0.70
5:C:176:ILE:HB	5:C:181:LEU:O	1.92	0.70
6:D:137:TRP:HA	6:D:137:TRP:HE3	1.55	0.70
9:G:6:LEU:HD13	9:G:35:LEU:HD22	1.73	0.70
11:I:68:GLU:HA	11:I:77:ILE:C	2.11	0.70
22:T:99:TYR:HA	22:T:124:ILE:O	1.92	0.70
20:R:31:HIS:CG	20:R:32:PRO:HD2	2.27	0.69
24:V:24:ALA:HB1	24:V:36:GLY:HA2	1.74	0.69
3:A:30:VAL:HA	3:A:33:LEU:CB	2.20	0.69
4:B:63:ARG:HH11	4:B:63:ARG:HG3	1.57	0.69
5:C:25:VAL:HG13	5:C:183:LEU:HA	1.72	0.69
11:I:64:ARG:HE	11:I:83:ALA:HB2	1.57	0.69
15:M:28:VAL:H	15:M:89:ARG:HB2	1.57	0.69
15:M:67:ARG:N	15:M:100:ALA:HB1	2.08	0.69
23:U:36:ILE:HA	23:U:60:PHE:CB	2.20	0.69
10:H:66:THR:O	10:H:68:ASN:N	2.25	0.69
11:I:6:THR:HG22	11:I:7:TYR:N	2.06	0.69
11:I:7:TYR:C	11:I:8:LEU:HD22	2.12	0.69
12:J:85:LEU:HD11	12:J:118:GLY:N	2.07	0.69
4:B:108:PRO:HA	4:B:195:ALA:O	1.91	0.69
5:C:116:VAL:HG22	5:C:117:MET:H	1.57	0.69
6:D:152:VAL:HG23	6:D:171:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:99:GLU:HB3	9:G:103:ARG:NH1	2.08	0.69
4:B:10:THR:OG1	4:B:11:PRO:HD2	1.93	0.69
7:E:35:GLU:HB2	7:E:161:THR:HA	1.73	0.69
13:K:10:ARG:H	13:K:12:GLN:HE22	1.40	0.69
22:T:130:PRO:HA	22:T:133:ILE:HG12	1.72	0.69
22:T:150:LEU:HD11	22:T:154:ASP:OD2	1.91	0.69
22:T:30:ASN:HD21	22:T:32:HIS:HB2	1.56	0.69
22:T:99:TYR:CD1	22:T:125:LEU:HD13	2.27	0.69
26:X:27:GLY:HA2	26:X:29:ARG:HH12	1.57	0.69
4:B:19:ALA:HB1	4:B:24:ILE:CD1	2.22	0.69
6:D:145:GLY:O	6:D:146:SER:HB2	1.93	0.69
6:D:179:TYR:O	6:D:182:VAL:HG22	1.92	0.69
14:L:53:HIS:HA	14:L:56:LYS:HD3	1.75	0.69
3:A:56:ASP:OD2	3:A:57:GLN:HG3	1.91	0.69
9:G:7:GLU:H	9:G:8:PRO:CD	2.05	0.69
10:H:78:VAL:HG23	10:H:79:ASN:OD1	1.92	0.69
13:K:24:GLY:O	13:K:25:ASP:HB3	1.93	0.69
19:Q:11:ARG:HB3	19:Q:98:LYS:CE	2.21	0.69
24:V:48:LYS:HA	24:V:63:ALA:O	1.92	0.69
23:U:29:GLN:HG2	23:U:30:VAL:N	2.07	0.69
4:B:56:GLY:HA2	4:B:213:ARG:O	1.92	0.69
7:E:169:ALA:O	7:E:172:LEU:HG	1.93	0.69
10:H:78:VAL:HG12	10:H:146:TYR:OH	1.93	0.69
18:P:47:VAL:HG13	18:P:48:GLY:H	1.56	0.69
13:K:3:MET:H	13:K:4:PRO:HD2	1.58	0.69
18:P:17:GLY:HA2	18:P:98:GLU:OE2	1.93	0.69
27:Y:29:ILE:H	27:Y:29:ILE:HD13	1.58	0.69
24:V:26:ARG:CD	24:V:26:ARG:H	2.06	0.69
26:X:7:LYS:CA	26:X:34:GLU:HA	2.22	0.69
3:A:21:TYR:HD2	3:A:21:TYR:N	1.88	0.69
3:A:224:ARG:C	3:A:225:ILE:HD12	2.12	0.69
5:C:75:VAL:C	5:C:77:ILE:H	1.94	0.69
10:H:102:PRO:HG2	10:H:103:GLY:H	1.58	0.69
10:H:62:ARG:HE	10:H:63:PRO:CD	2.05	0.69
12:J:17:LYS:HB3	12:J:19:VAL:HG23	1.74	0.69
13:K:125:LEU:HB3	13:K:126:PRO:CD	2.23	0.69
15:M:25:ARG:NH2	15:M:89:ARG:HH22	1.89	0.69
20:R:82:GLN:HG3	20:R:83:VAL:HG22	1.73	0.69
13:K:40:ALA:O	13:K:97:VAL:HB	1.93	0.69
3:A:225:ILE:CG2	3:A:226:ASN:N	2.56	0.69
6:D:32:VAL:O	6:D:36:LEU:HG	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:28:PHE:N	20:R:77:LYS:O	2.19	0.69
24:V:85:LEU:HD12	24:V:85:LEU:H	1.56	0.69
5:C:122:PHE:HE2	5:C:138:PRO:HB3	1.57	0.68
6:D:146:SER:H	6:D:167:TRP:HE1	1.41	0.68
9:G:62:LYS:O	9:G:66:GLU:HG3	1.93	0.68
24:V:19:GLN:HG2	24:V:20:ARG:H	1.57	0.68
4:B:121:PRO:HA	4:B:131:LEU:HG	1.76	0.68
4:B:52:ARG:HH22	4:B:220:HIS:HA	1.57	0.68
5:C:93:VAL:HG11	5:C:181:LEU:O	1.92	0.68
7:E:105:LYS:O	7:E:109:VAL:HB	1.93	0.68
17:O:106:PHE:O	17:O:110:VAL:HG23	1.92	0.68
3:A:41:THR:HG22	3:A:42:VAL:H	1.58	0.68
10:H:79:ASN:O	10:H:83:ILE:CD1	2.38	0.68
12:J:82:GLY:HA2	12:J:113:LYS:O	1.94	0.68
13:K:65:PHE:CE1	13:K:105:GLU:HB2	2.28	0.68
16:N:26:ASP:HA	16:N:48:ILE:HD12	1.75	0.68
10:H:60:LYS:HZ1	17:O:67:ALA:HB2	1.57	0.68
18:P:47:VAL:HG22	18:P:48:GLY:H	1.57	0.68
33:2:43:G:H2'	33:2:44:A:H8	1.59	0.68
4:B:2:ALA:HB2	4:B:20:ASP:OD2	1.94	0.68
7:E:141:PHE:HD2	7:E:144:ILE:N	1.88	0.68
8:F:75:ALA:O	8:F:79:VAL:HG13	1.93	0.68
9:G:122:GLU:HG2	9:G:123:LEU:H	1.57	0.68
22:T:161:VAL:HG12	22:T:162:GLU:N	2.08	0.68
4:B:17:THR:HB	4:B:205:VAL:H	1.58	0.68
4:B:212:SER:OG	4:B:217:ARG:NE	2.27	0.68
5:C:11:MET:O	5:C:12:THR:HG23	1.94	0.68
10:H:98:TYR:O	10:H:105:LEU:HB2	1.94	0.68
11:I:10:VAL:HG22	11:I:17:ARG:O	1.94	0.68
6:D:33:ARG:NH1	12:J:12:ALA:H	1.88	0.68
13:K:65:PHE:CD1	13:K:105:GLU:HB2	2.27	0.68
13:K:133:ARG:CG	13:K:134:ARG:N	2.56	0.68
22:T:73:GLN:O	22:T:87:ASP:HB2	1.93	0.68
6:D:14:GLU:HG2	6:D:16:ALA:H	1.59	0.68
6:D:150:LEU:HA	6:D:169:VAL:HG12	1.74	0.68
9:G:60:GLU:O	9:G:64:GLU:HB2	1.94	0.68
10:H:120:ARG:HG2	10:H:124:HIS:CE1	2.28	0.68
8:F:126:PRO:CG	8:F:130:ARG:HB2	2.24	0.68
13:K:24:GLY:N	13:K:98:LYS:HB3	2.09	0.68
14:L:84:ALA:HB3	14:L:85:PRO:HD3	1.76	0.68
15:M:25:ARG:NE	15:M:89:ARG:HH12	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:65:ILE:HG22	4:B:104:TYR:CD1	2.22	0.68
16:N:26:ASP:HB3	16:N:91:ARG:HG2	1.76	0.68
33:2:1:G:O2'	33:2:2:C:H5'	1.93	0.68
5:C:37:ARG:HA	5:C:42:ASP:OD2	1.94	0.68
9:G:122:GLU:CG	9:G:123:LEU:H	2.06	0.68
18:P:4:ILE:HB	18:P:39:LEU:HD21	1.76	0.68
18:P:43:GLU:O	18:P:44:LYS:HB2	1.93	0.68
13:K:63:LYS:HE3	22:T:116:VAL:CG1	2.23	0.68
13:K:15:GLY:HA2	13:K:72:LYS:HE2	1.76	0.68
27:Y:33:CYS:HB2	27:Y:38:ALA:HB3	1.76	0.68
34:3:4:G:H2'	34:3:5:A:C8	2.28	0.68
4:B:10:THR:HG23	4:B:12:SER:H	1.58	0.68
6:D:54:TYR:H	6:D:54:TYR:HD2	1.42	0.68
7:E:107:LEU:O	7:E:111:LEU:HB3	1.94	0.68
4:B:183:ARG:HD3	4:B:184:LYS:N	2.09	0.67
7:E:172:LEU:HA	7:E:175:LEU:CB	2.24	0.67
28:Z:1:MET:HE2	28:Z:1:MET:O	1.94	0.67
5:C:11:MET:CB	5:C:24:THR:HA	2.25	0.67
6:D:172:ALA:HB3	6:D:173:PRO:HD3	1.76	0.67
14:L:102:GLU:HG2	14:L:103:ARG:N	2.09	0.67
17:O:21:ALA:HB2	17:O:39:LEU:HD21	1.76	0.67
23:U:29:GLN:CG	23:U:30:VAL:H	2.07	0.67
9:G:4:ILE:CG1	9:G:18:VAL:HG22	2.24	0.67
11:I:66:LYS:HA	11:I:79:PHE:O	1.95	0.67
13:K:67:ARG:O	13:K:68:ILE:HG23	1.94	0.67
14:L:79:LEU:HA	14:L:83:ILE:HG13	1.75	0.67
15:M:40:ILE:HG22	15:M:41:ASP:N	2.07	0.67
16:N:64:ARG:NH2	16:N:103:ARG:O	2.27	0.67
17:O:74:LEU:HD21	17:O:79:PHE:HB3	1.76	0.67
18:P:4:ILE:HG13	18:P:13:ARG:HB3	1.75	0.67
19:Q:88:ARG:HG3	19:Q:94:ASP:CG	2.15	0.67
33:2:41:U:H2'	33:2:42:G:C8	2.29	0.67
4:B:160:GLY:HA2	4:B:196:VAL:HB	1.77	0.67
4:B:247:ALA:HB2	4:B:253:GLN:HG2	1.77	0.67
4:B:69:ARG:HH22	4:B:76:PRO:CG	2.03	0.67
5:C:34:VAL:HG13	5:C:67:PHE:CE1	2.29	0.67
9:G:7:GLU:HG3	9:G:35:LEU:HD11	1.75	0.67
11:I:9:GLU:HA	11:I:18:LYS:HD2	1.76	0.67
13:K:75:THR:O	13:K:88:GLY:HA3	1.94	0.67
19:Q:56:ALA:O	19:Q:60:ASN:HB2	1.94	0.67
23:U:39:ARG:HA	23:U:58:THR:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:50:ARG:CZ	24:V:61:ARG:HB2	2.24	0.67
10:H:146:TYR:HD2	10:H:146:TYR:N	1.91	0.67
10:H:57:LEU:O	10:H:72:GLY:HA2	1.95	0.67
12:J:98:GLU:O	12:J:102:ARG:HB3	1.94	0.67
13:K:39:PRO:HB3	13:K:99:PRO:CG	2.23	0.67
15:M:13:ARG:HG3	15:M:91:PRO:CA	2.20	0.67
19:Q:77:ASP:N	19:Q:103:ILE:HG22	2.08	0.67
24:V:40:ARG:HG2	24:V:41:ARG:N	2.04	0.67
3:A:29:LEU:HG	3:A:33:LEU:HG	1.76	0.67
6:D:25:PRO:HA	6:D:28:LEU:HD12	1.77	0.67
7:E:99:MET:O	7:E:103:LEU:HG	1.94	0.67
7:E:73:ALA:H	7:E:87:PRO:HA	1.59	0.67
9:G:81:VAL:O	9:G:148:GLU:HG3	1.94	0.67
11:I:61:VAL:CG1	11:I:85:VAL:HB	2.24	0.67
16:N:24:PRO:CA	16:N:49:VAL:HG11	2.25	0.67
19:Q:66:GLU:O	19:Q:67:ASP:HB2	1.95	0.67
4:B:78:LYS:HE3	4:B:114:GLY:CA	2.25	0.67
13:K:132:VAL:HG22	13:K:133:ARG:H	1.59	0.67
24:V:26:ARG:CB	24:V:34:THR:HG23	2.25	0.67
10:H:29:PRO:CB	10:H:64:ASP:HB3	2.24	0.67
4:B:69:ARG:CZ	4:B:119:ALA:HB2	2.24	0.67
4:B:25:THR:O	4:B:25:THR:HG23	1.95	0.67
9:G:3:VAL:H	9:G:21:VAL:HG21	1.59	0.67
10:H:135:LEU:O	10:H:139:LEU:HG	1.94	0.67
26:X:40:THR:OG1	26:X:43:ILE:HD13	1.95	0.67
4:B:248:SER:HB3	4:B:249:PRO:HD2	1.75	0.67
5:C:117:MET:HA	5:C:122:PHE:N	2.09	0.67
6:D:178:VAL:O	6:D:181:ILE:HG22	1.95	0.67
9:G:81:VAL:HG22	9:G:145:VAL:O	1.95	0.67
12:J:78:PRO:HB3	12:J:110:TYR:HB2	1.75	0.67
18:P:65:GLY:N	18:P:96:ILE:HG13	2.09	0.67
4:B:69:ARG:CG	4:B:190:TYR:HE2	2.08	0.67
5:C:117:MET:HB3	5:C:136:ARG:NH2	2.09	0.67
6:D:181:ILE:O	6:D:181:ILE:HD13	1.95	0.67
8:F:76:VAL:HA	8:F:79:VAL:HG22	1.75	0.67
9:G:93:THR:OG1	9:G:94:ALA:N	2.26	0.67
15:M:62:LYS:HG3	15:M:63:THR:HG22	1.77	0.67
16:N:135:VAL:HG13	16:N:136:GLN:N	2.07	0.67
23:U:28:GLY:HA2	23:U:67:VAL:HB	1.77	0.67
23:U:41:ARG:HG2	23:U:42:GLY:H	1.60	0.67
26:X:15:TYR:HB3	26:X:16:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:27:THR:O	16:N:28:VAL:HG23	1.94	0.67
6:D:112:ARG:NH1	6:D:184:THR:O	2.28	0.66
6:D:150:LEU:HB2	6:D:187:LEU:CD2	2.26	0.66
12:J:85:LEU:HD11	12:J:118:GLY:CA	2.25	0.66
11:I:69:VAL:HG12	11:I:77:ILE:HG22	1.77	0.66
14:L:22:ARG:HH22	14:L:71:GLN:HE21	1.40	0.66
19:Q:7:ALA:HB3	19:Q:103:ILE:O	1.95	0.66
21:S:23:ARG:HG3	21:S:24:VAL:N	2.10	0.66
9:G:95:LYS:HG3	9:G:96:ASP:H	1.60	0.66
4:B:200:ASP:C	4:B:202:LYS:H	1.98	0.66
6:D:162:ALA:HB1	6:D:170:THR:OG1	1.96	0.66
6:D:121:VAL:HG13	6:D:191:LEU:H	1.58	0.66
7:E:73:ALA:N	7:E:87:PRO:HA	2.10	0.66
8:F:34:GLU:HG2	8:F:35:VAL:N	2.09	0.66
9:G:7:GLU:N	9:G:8:PRO:CD	2.58	0.66
16:N:31:SER:HB3	16:N:42:ILE:C	2.16	0.66
18:P:34:GLU:HB2	18:P:64:HIS:HE2	1.60	0.66
22:T:120:ILE:HB	22:T:171:ILE:O	1.94	0.66
24:V:12:PRO:CG	24:V:63:ALA:HB2	2.26	0.66
23:U:74:ARG:O	23:U:74:ARG:HD2	1.94	0.66
5:C:173:VAL:H	5:C:183:LEU:CD1	2.08	0.66
9:G:109:ILE:C	9:G:111:PRO:HD3	2.16	0.66
16:N:112:ARG:HA	16:N:115:ARG:NH2	2.05	0.66
33:2:69:U:H6	33:2:69:U:O5'	1.77	0.66
4:B:242:ARG:HB2	4:B:242:ARG:HH11	1.60	0.66
4:B:242:ARG:HB2	4:B:242:ARG:NH1	2.11	0.66
6:D:176:LEU:O	6:D:179:TYR:CE2	2.49	0.66
11:I:66:LYS:O	11:I:78:ARG:HG3	1.94	0.66
13:K:58:PHE:HZ	13:K:117:ALA:HB1	1.60	0.66
26:X:28:LEU:HD12	26:X:33:GLN:HB3	1.78	0.66
33:2:20:G:H22	33:2:22:G:H1'	1.60	0.66
5:C:117:MET:HA	5:C:122:PHE:H	1.61	0.66
5:C:36:ARG:NH1	5:C:86:PRO:HD2	2.10	0.66
7:E:103:LEU:HD12	7:E:104:GLU:N	2.10	0.66
18:P:15:GLU:CB	18:P:16:PRO:CD	2.73	0.66
22:T:80:ARG:NH1	22:T:82:ARG:HB2	2.10	0.66
23:U:29:GLN:HG2	23:U:30:VAL:H	1.59	0.66
26:X:8:LEU:HA	26:X:54:VAL:HG12	1.76	0.66
33:2:7:U:O2'	33:2:49:C:H5'	1.95	0.66
3:A:54:ARG:NE	3:A:54:ARG:HA	2.10	0.66
4:B:117:VAL:HG22	4:B:127:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:89:ILE:HD11	8:F:129:THR:OG1	1.96	0.66
9:G:5:LEU:HD23	9:G:9:LEU:HD12	1.77	0.66
16:N:32:TYR:HB3	16:N:82:LEU:HA	1.78	0.66
23:U:52:GLY:HA2	23:U:62:LEU:HD13	1.78	0.66
24:V:24:ALA:HA	24:V:37:ILE:HG22	1.78	0.66
5:C:101:ARG:HD3	5:C:169:ASN:HB3	1.78	0.66
5:C:37:ARG:HB3	5:C:42:ASP:CB	2.26	0.66
11:I:1:MET:C	11:I:2:ILE:HD12	2.16	0.66
13:K:35:VAL:O	13:K:129:THR:HA	1.96	0.66
14:L:53:HIS:HB3	14:L:94:TYR:OH	1.94	0.66
15:M:20:ARG:HG3	15:M:21:THR:H	1.60	0.66
22:T:100:VAL:O	22:T:123:ASP:HB3	1.95	0.66
4:B:126:GLN:H	4:B:129:ASN:HD22	1.44	0.66
4:B:174:ILE:HG22	4:B:175:LEU:N	2.09	0.66
4:B:4:LYS:HB2	4:B:18:VAL:HG12	1.76	0.66
7:E:161:THR:HG22	7:E:163:ALA:H	1.58	0.66
10:H:39:ILE:HG13	10:H:40:ASP:N	2.11	0.66
7:E:115:ARG:O	7:E:118:ARG:CG	10.13	0.66
13:K:24:GLY:C	13:K:98:LYS:HD3	2.16	0.66
7:E:120:LEU:HD13	7:E:121:ASN:N	2.11	0.65
8:F:153:LYS:HZ2	8:F:163:TYR:HD1	1.42	0.65
5:C:4:ILE:HG13	5:C:6:GLY:H	1.59	0.65
15:M:12:PHE:CD1	15:M:12:PHE:N	2.63	0.65
4:B:63:ARG:HH11	4:B:63:ARG:CG	2.08	0.65
9:G:3:VAL:H	9:G:21:VAL:HG22	1.60	0.65
16:N:6:LEU:O	16:N:10:VAL:HG23	1.96	0.65
17:O:55:ARG:HG2	17:O:55:ARG:HH11	1.60	0.65
20:R:12:VAL:HB	20:R:27:THR:HB	1.78	0.65
27:Y:38:ALA:HB2	27:Y:49:CYS:CB	2.16	0.65
3:A:193:PHE:CD2	3:A:193:PHE:C	2.70	0.65
3:A:201:LYS:HE3	3:A:203:GLU:HG2	1.78	0.65
7:E:79:ASN:CG	7:E:80:PHE:N	2.50	0.65
22:T:102:LEU:H	22:T:123:ASP:HA	1.59	0.65
26:X:17:LYS:HE2	26:X:21:ALA:HB2	1.77	0.65
28:Z:30:VAL:O	28:Z:33:ARG:HB3	1.96	0.65
6:D:52:VAL:O	6:D:52:VAL:HG13	1.97	0.65
7:E:39:ILE:HG13	7:E:157:ILE:HG23	1.79	0.65
13:K:106:VAL:HG21	13:K:118:LEU:HD11	1.78	0.65
3:A:62:THR:HG22	3:A:63:VAL:H	1.61	0.65
4:B:106:ILE:HG22	4:B:197:GLY:HA3	1.79	0.65
9:G:35:LEU:O	9:G:35:LEU:HD13	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:39:ILE:HD13	11:I:39:ILE:H	1.60	0.65
13:K:78:PRO:HG2	13:K:87:LYS:HG2	1.78	0.65
4:B:218:ARG:HG2	4:B:219:PRO:HD2	1.78	0.65
8:F:170:ARG:HH22	8:F:172:LYS:HE3	1.60	0.65
11:I:71:ARG:HG2	11:I:72:PRO:HD2	1.78	0.65
12:J:85:LEU:HD11	12:J:117:GLU:C	2.17	0.65
16:N:3:ARG:O	16:N:7:ILE:HG12	1.96	0.65
22:T:25:PRO:HA	22:T:38:TYR:CB	2.27	0.65
24:V:12:PRO:HG3	24:V:63:ALA:N	2.10	0.65
16:N:50:ILE:HD12	16:N:62:THR:OG1	1.96	0.65
34:3:8:U:H3'	34:3:8:U:C6	2.30	0.65
3:A:167:ASP:N	3:A:171:ALA:HA	2.08	0.65
4:B:172:TYR:CD1	4:B:186:HIS:HA	2.30	0.65
5:C:169:ASN:C	5:C:170:LEU:HD12	2.16	0.65
11:I:61:VAL:HG11	11:I:85:VAL:HB	1.79	0.65
12:J:114:ILE:HG12	12:J:130:PHE:HA	1.78	0.65
15:M:66:ALA:HB1	15:M:101:LEU:CG	2.27	0.65
10:H:78:VAL:HB	10:H:149:PRO:HA	1.79	0.65
20:R:6:ASP:HA	25:W:26:ARG:HH22	1.62	0.65
8:F:26:VAL:HB	8:F:33:LEU:HB2	1.78	0.65
11:I:43:VAL:HG11	11:I:53:LYS:HA	1.77	0.65
16:N:101:PHE:C	16:N:103:ARG:H	2.01	0.65
16:N:45:PHE:HE2	16:N:64:ARG:HA	1.62	0.65
17:O:92:ARG:HG2	17:O:94:ASN:HD22	1.62	0.65
4:B:58:HIS:O	4:B:60:ARG:N	2.30	0.65
17:O:92:ARG:HG2	17:O:94:ASN:ND2	2.12	0.65
19:Q:12:ILE:HG22	19:Q:13:SER:H	1.60	0.65
26:X:8:LEU:O	26:X:54:VAL:HA	1.96	0.65
33:2:74:C:C2'	33:2:75:C:O4'	2.42	0.64
4:B:126:GLN:H	4:B:129:ASN:ND2	1.94	0.64
5:C:175:VAL:HA	5:C:182:LEU:HD12	1.79	0.64
6:D:75:ALA:N	6:D:76:PRO:HD3	2.10	0.64
8:F:98:LEU:HB3	8:F:123:PHE:CZ	2.32	0.64
18:P:73:SER:HB2	18:P:89:GLN:H	1.62	0.64
33:2:14:A:C2	33:2:22:G:C2	2.85	0.64
22:T:17:ALA:O	22:T:20:ARG:HG3	1.97	0.64
33:2:14:A:N6	33:2:21:A:C2	2.65	0.64
9:G:28:ASN:O	9:G:29:TYR:HB2	1.97	0.64
9:G:38:LEU:HD12	9:G:38:LEU:H	1.61	0.64
13:K:80:GLU:O	13:K:81:VAL:HG13	1.97	0.64
15:M:39:ILE:HD13	15:M:39:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:45:TYR:HA	17:O:48:ALA:HB3	1.79	0.64
19:Q:25:ARG:HH21	19:Q:74:ALA:HB3	1.61	0.64
12:J:147:LEU:HD13	12:J:148:LEU:HD13	1.78	0.64
3:A:225:ILE:HG22	3:A:226:ASN:N	2.13	0.64
4:B:35:LYS:HB2	4:B:36:PRO:CA	2.26	0.64
6:D:166:PRO:O	6:D:167:TRP:HB2	1.96	0.64
8:F:76:VAL:O	8:F:79:VAL:HG22	1.97	0.64
10:H:108:ILE:HG21	10:H:112:LYS:HD2	1.78	0.64
10:H:65:TRP:HB3	17:O:64:ARG:NE	2.12	0.64
11:I:71:ARG:CG	11:I:72:PRO:HD2	2.26	0.64
13:K:106:VAL:HG11	13:K:114:ALA:HB1	1.78	0.64
14:L:9:LYS:HG3	14:L:10:LEU:N	2.10	0.64
16:N:11:GLU:C	16:N:13:ARG:H	1.98	0.64
17:O:92:ARG:HD2	18:P:11:GLN:HB2	1.78	0.64
18:P:10:LYS:NZ	18:P:22:VAL:HA	2.11	0.64
26:X:30:ARG:HD2	26:X:33:GLN:HB2	1.80	0.64
28:Z:21:ARG:O	28:Z:23:ARG:N	2.31	0.64
18:P:34:GLU:N	18:P:64:HIS:CE1	2.66	0.64
5:C:103:ASP:HB2	5:C:199:ARG:HD3	1.78	0.64
5:C:184:VAL:HG12	5:C:185:LYS:H	1.61	0.64
10:H:40:ASP:HA	10:H:44:LYS:HG3	1.80	0.64
12:J:137:LYS:HB2	12:J:138:LEU:HD12	1.80	0.64
16:N:50:ILE:CD1	16:N:64:ARG:HB2	2.27	0.64
33:2:48:C:H4'	33:2:49:C:H5''	1.80	0.64
4:B:76:PRO:HA	4:B:97:TYR:CE1	2.32	0.64
5:C:12:THR:HG21	16:N:57:PHE:HB3	1.80	0.64
5:C:170:LEU:HB3	5:C:185:LYS:HB3	1.79	0.64
11:I:77:ILE:CB	16:N:74:ARG:HD2	2.24	0.64
4:B:133:LEU:HB2	4:B:187:GLY:O	1.97	0.64
5:C:14:ILE:O	5:C:20:ALA:HA	1.98	0.64
5:C:170:LEU:CD2	5:C:185:LYS:HB3	2.24	0.64
7:E:110:ALA:HB1	7:E:140:ILE:HG13	1.80	0.64
13:K:63:LYS:HE3	22:T:116:VAL:HG13	1.78	0.64
5:C:55:ASN:OD1	5:C:75:VAL:HG23	1.97	0.64
6:D:109:VAL:HA	6:D:112:ARG:HG2	1.79	0.64
14:L:56:LYS:HD2	14:L:87:TYR:O	1.98	0.64
15:M:67:ARG:H	15:M:100:ALA:HB1	1.60	0.64
16:N:70:VAL:HG12	16:N:71:GLY:N	2.12	0.64
22:T:28:MET:HG2	22:T:37:VAL:HG22	1.79	0.64
24:V:51:VAL:O	24:V:52:ARG:HB2	1.98	0.64
17:O:95:LEU:C	17:O:97:ASP:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:37:VAL:CG1	10:H:38:LEU:N	2.60	0.64
9:G:81:VAL:HG11	9:G:144:VAL:HG13	1.80	0.64
11:I:85:VAL:CG1	11:I:86:ILE:H	1.93	0.64
15:M:12:PHE:HD1	15:M:12:PHE:N	1.96	0.64
24:V:88:LYS:HG3	24:V:89:GLU:N	2.12	0.64
4:B:228:PRO:O	4:B:230:ASP:N	2.31	0.64
10:H:36:TRP:O	10:H:37:VAL:HG23	1.98	0.64
11:I:17:ARG:HE	11:I:47:ILE:H	1.44	0.64
17:O:100:VAL:HG23	17:O:101:ARG:HD2	1.80	0.64
18:P:78:LYS:HB2	18:P:83:ARG:HH11	1.60	0.64
22:T:8:TYR:CD1	22:T:39:VAL:HG13	2.33	0.64
23:U:15:ASP:HB3	23:U:20:ARG:HG3	1.80	0.64
4:B:184:LYS:HG2	4:B:185:VAL:H	1.63	0.64
4:B:69:ARG:HG3	4:B:190:TYR:HE2	1.62	0.64
6:D:151:LEU:H	6:D:169:VAL:HG11	1.62	0.64
13:K:14:ARG:N	13:K:14:ARG:HD2	2.13	0.64
16:N:86:ILE:HG22	16:N:87:ASP:N	2.13	0.64
18:P:94:LEU:HB3	18:P:96:ILE:HD13	1.79	0.64
21:S:67:LEU:HD13	21:S:68:HIS:N	2.09	0.64
22:T:39:VAL:HG12	22:T:40:ASP:H	1.63	0.64
24:V:26:ARG:HB3	24:V:34:THR:HG23	1.80	0.63
4:B:248:SER:HB3	4:B:249:PRO:CD	2.27	0.63
4:B:45:ASN:CG	4:B:46:GLN:H	2.01	0.63
5:C:28:ALA:N	5:C:181:LEU:HA	2.11	0.63
5:C:175:VAL:HA	5:C:182:LEU:CD1	2.28	0.63
5:C:27:LEU:CD2	5:C:29:GLY:H	2.10	0.63
9:G:27:ARG:N	9:G:27:ARG:HD3	2.09	0.63
10:H:95:TYR:CD1	10:H:108:ILE:O	2.51	0.63
10:H:146:TYR:CD2	10:H:146:TYR:N	2.63	0.63
11:I:93:PRO:HG3	11:I:114:ILE:CG2	2.27	0.63
12:J:148:LEU:H	12:J:148:LEU:HD13	1.62	0.63
13:K:25:ASP:HB3	13:K:101:ARG:HD2	1.80	0.63
24:V:87:PRO:HA	24:V:91:LYS:NZ	2.13	0.63
26:X:49:LYS:HA	26:X:49:LYS:NZ	2.14	0.63
26:X:31:LEU:O	26:X:32:GLN:HB2	1.98	0.63
3:A:225:ILE:CG2	3:A:226:ASN:H	2.11	0.63
4:B:208:LYS:NZ	4:B:209:ALA:HB3	2.14	0.63
8:F:84:SER:OG	8:F:138:LYS:HE3	1.98	0.63
22:T:24:LEU:CD1	22:T:41:LEU:HA	2.28	0.63
22:T:88:PHE:C	22:T:88:PHE:HD2	2.00	0.63
23:U:66:VAL:O	23:U:81:VAL:CA	2.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:109:ASP:HB2	4:B:199:ALA:HB2	1.79	0.63
6:D:19:LEU:HA	6:D:22:GLU:HG3	1.79	0.63
7:E:70:VAL:HG12	7:E:90:LEU:CD2	2.27	0.63
14:L:44:LEU:HD23	14:L:47:PHE:CZ	2.33	0.63
22:T:141:VAL:CG2	22:T:144:LEU:HB2	2.29	0.63
17:O:106:PHE:HA	17:O:109:LEU:CG	2.29	0.63
33:2:68:U:H2'	33:2:69:U:H6	1.61	0.63
4:B:20:ASP:C	4:B:24:ILE:HB	2.18	0.63
10:H:65:TRP:CH2	10:H:67:PRO:HA	2.34	0.63
19:Q:88:ARG:NH1	19:Q:93:ALA:HA	2.14	0.63
25:W:29:LYS:HB2	25:W:29:LYS:HZ3	1.64	0.63
18:P:96:ILE:CG2	18:P:97:LYS:N	2.53	0.63
22:T:80:ARG:HD2	22:T:82:ARG:CD	2.26	0.63
19:Q:24:ILE:HD12	19:Q:25:ARG:N	2.13	0.63
23:U:42:GLY:O	23:U:43:THR:OG1	2.15	0.63
4:B:91:ARG:HD3	4:B:198:ASN:CB	2.28	0.63
9:G:124:GLY:HA2	9:G:144:VAL:H	1.64	0.63
10:H:108:ILE:CG2	10:H:112:LYS:HD2	2.27	0.63
10:H:95:TYR:HB2	10:H:107:LYS:O	1.98	0.63
20:R:51:VAL:HB	20:R:79:ALA:HB1	1.80	0.63
26:X:35:ARG:HG3	26:X:37:LEU:CD2	2.27	0.63
17:O:90:VAL:CG1	17:O:91:ASP:H	2.02	0.63
27:Y:38:ALA:HB1	27:Y:40:LYS:CG	2.29	0.63
3:A:223:VAL:HG12	3:A:224:ARG:N	2.11	0.63
4:B:102:LYS:O	4:B:103:ARG:HG2	1.98	0.63
5:C:172:VAL:HG12	5:C:173:VAL:H	1.62	0.63
7:E:146:TYR:CG	7:E:147:ASP:N	2.67	0.63
11:I:111:PHE:O	11:I:114:ILE:HG12	1.98	0.63
15:M:8:GLU:H	15:M:10:ARG:NH1	1.95	0.63
15:M:13:ARG:CG	15:M:91:PRO:HA	2.21	0.63
17:O:79:PHE:C	17:O:79:PHE:CD2	2.72	0.63
23:U:50:ASN:O	23:U:62:LEU:HB3	1.98	0.63
4:B:92:ILE:HA	4:B:105:ILE:O	1.98	0.63
6:D:150:LEU:HD23	6:D:181:ILE:CG1	2.24	0.63
9:G:56:LYS:HG3	9:G:57:ARG:HD2	1.80	0.63
27:Y:16:ARG:HG3	27:Y:17:ASP:N	2.14	0.63
33:2:18:G:C2	33:2:57:G:C2	2.87	0.63
4:B:183:ARG:HA	4:B:269:PHE:O	1.99	0.63
4:B:75:ILE:HG22	4:B:75:ILE:O	1.98	0.63
6:D:175:GLY:O	6:D:176:LEU:HB2	1.98	0.63
10:H:40:ASP:OD1	10:H:41:ALA:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:61:VAL:O	11:I:84:ALA:HA	1.99	0.63
13:K:72:LYS:HD3	13:K:73:PRO:N	2.13	0.63
15:M:26:LEU:HB2	15:M:87:PHE:HA	1.81	0.63
16:N:19:LEU:HD22	16:N:83:ILE:O	1.98	0.63
16:N:61:PHE:CD1	16:N:61:PHE:N	2.67	0.63
16:N:70:VAL:HG12	16:N:71:GLY:H	1.64	0.63
4:B:133:LEU:HG	4:B:173:VAL:CG1	2.27	0.62
5:C:11:MET:HE3	5:C:23:VAL:H	1.64	0.62
5:C:7:VAL:HG22	5:C:27:LEU:HD22	1.81	0.62
6:D:45:SER:O	6:D:87:PRO:HG2	1.99	0.62
7:E:136:ARG:O	7:E:137:GLU:HG2	1.98	0.62
7:E:35:GLU:HB2	7:E:161:THR:CA	2.28	0.62
8:F:140:LYS:HD2	8:F:141:VAL:HG23	1.81	0.62
10:H:27:TYR:OH	17:O:64:ARG:HD3	2.00	0.62
23:U:52:GLY:CA	23:U:62:LEU:HB2	2.29	0.62
7:E:28:VAL:HG13	7:E:33:ARG:HE	1.64	0.62
8:F:11:VAL:O	8:F:11:VAL:HG12	2.00	0.62
9:G:122:GLU:CG	9:G:123:LEU:N	2.61	0.62
13:K:58:PHE:CD1	13:K:62:GLY:HA3	2.34	0.62
24:V:85:LEU:C	24:V:87:PRO:HD2	2.19	0.62
26:X:9:VAL:HG12	26:X:32:GLN:HA	1.80	0.62
3:A:48:LEU:HB3	3:A:210:LEU:HD23	1.81	0.62
4:B:106:ILE:HG22	4:B:197:GLY:CA	2.29	0.62
6:D:112:ARG:O	6:D:117:LYS:HE2	2.00	0.62
22:T:132:ASN:O	22:T:134:PRO:HD3	2.00	0.62
22:T:77:ASP:H	22:T:83:PRO:HA	1.64	0.62
23:U:37:LEU:CD1	23:U:38:VAL:H	2.07	0.62
3:A:23:ILE:HG12	3:A:225:ILE:HG21	1.80	0.62
7:E:73:ALA:H	7:E:87:PRO:CA	2.13	0.62
9:G:132:PRO:HD2	9:G:137:PRO:HA	1.81	0.62
19:Q:48:ALA:O	19:Q:51:LEU:HD13	1.98	0.62
33:2:14:A:H3'	33:2:15:G:C8	2.34	0.62
5:C:77:ILE:CG2	5:C:78:LEU:H	2.12	0.62
6:D:44:ALA:HB1	6:D:87:PRO:HB2	1.82	0.62
7:E:144:ILE:HG22	7:E:144:ILE:O	1.99	0.62
10:H:77:VAL:HB	10:H:145:VAL:CG1	2.29	0.62
12:J:138:LEU:HA	12:J:142:GLY:N	2.14	0.62
22:T:90:VAL:O	22:T:91:LEU:HD23	1.99	0.62
28:Z:13:ALA:HA	28:Z:17:GLY:HA3	1.82	0.62
14:L:86:ARG:HG3	14:L:87:TYR:CD1	2.35	0.62
4:B:124:PRO:CG	4:B:129:ASN:HD21	1.90	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:169:VAL:O	6:D:170:THR:HB	2.00	0.62
21:S:45:VAL:HA	21:S:57:GLN:HG2	1.81	0.62
33:2:66:A:N6	33:2:67:A:H62	1.96	0.62
9:G:130:TYR:HB3	9:G:138:ILE:O	1.99	0.62
20:R:47:PHE:O	20:R:48:LYS:HB2	1.99	0.62
34:3:15:G:O3'	34:3:16:A:H4'	2.00	0.62
4:B:74:GLY:HA2	4:B:119:ALA:HB3	1.80	0.62
14:L:76:VAL:O	14:L:79:LEU:HB2	2.00	0.62
24:V:11:ARG:HB2	24:V:12:PRO:HD2	1.81	0.62
7:E:114:ILE:HG12	7:E:115:ARG:N	2.15	0.62
8:F:170:ARG:HH22	8:F:172:LYS:CE	2.12	0.62
9:G:4:ILE:O	9:G:37:VAL:HB	2.00	0.62
18:P:73:SER:O	18:P:74:LYS:HB2	2.00	0.62
20:R:60:ARG:HB2	20:R:74:PRO:HG3	1.80	0.62
7:E:7:LEU:HB3	7:E:100:TRP:CD1	2.35	0.62
8:F:12:PRO:C	8:F:14:GLY:H	2.02	0.62
13:K:133:ARG:HG3	22:T:81:ARG:NH2	2.14	0.62
6:D:117:LYS:HZ2	6:D:186:ARG:HA	1.65	0.62
12:J:114:ILE:HD11	12:J:130:PHE:HB3	1.81	0.62
13:K:58:PHE:HZ	13:K:117:ALA:CB	2.13	0.62
15:M:28:VAL:HG21	15:M:87:PHE:CZ	2.34	0.62
19:Q:69:LEU:HA	19:Q:108:GLY:O	2.00	0.62
26:X:27:GLY:HA2	26:X:29:ARG:NH1	2.13	0.62
33:2:34:G:H2'	33:2:35:A:C5'	2.22	0.61
4:B:97:TYR:CB	4:B:102:LYS:HA	2.29	0.61
4:B:247:ALA:CA	4:B:253:GLN:HA	2.30	0.61
6:D:192:ASP:O	6:D:195:GLU:HG2	2.00	0.61
16:N:92:GLY:HA2	16:N:114:LEU:HB3	1.80	0.61
9:G:122:GLU:HG3	9:G:123:LEU:HD22	1.81	0.61
10:H:79:ASN:CA	10:H:147:ALA:HA	2.30	0.61
14:L:75:LEU:O	14:L:79:LEU:HG	2.00	0.61
18:P:50:PRO:HG2	18:P:51:VAL:H	1.65	0.61
22:T:146:ILE:H	22:T:146:ILE:HD13	1.65	0.61
20:R:82:GLN:O	20:R:83:VAL:HG13	2.00	0.61
22:T:161:VAL:HG12	22:T:162:GLU:H	1.64	0.61
4:B:208:LYS:HD3	4:B:209:ALA:N	2.15	0.61
4:B:24:ILE:HG12	4:B:82:ILE:O	2.00	0.61
5:C:173:VAL:N	5:C:183:LEU:HD11	2.15	0.61
6:D:127:VAL:O	6:D:129:GLY:N	2.33	0.61
11:I:93:PRO:C	11:I:95:GLY:H	2.04	0.61
7:E:78:SER:O	7:E:79:ASN:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:41:GLU:O	9:G:44:LEU:HB3	1.99	0.61
14:L:29:LEU:HG	14:L:75:LEU:HD22	1.82	0.61
20:R:88:LYS:O	20:R:89:ILE:HB	2.00	0.61
22:T:150:LEU:HB3	22:T:172:ALA:HB3	1.81	0.61
19:Q:76:VAL:HA	19:Q:103:ILE:CG2	2.31	0.61
33:2:36:A:C2'	33:2:37:A:H5'	2.29	0.61
9:G:33:ARG:HD3	9:G:34:GLY:N	2.14	0.61
6:D:183:ARG:HG2	12:J:7:ARG:HB3	1.81	0.61
13:K:109:VAL:O	13:K:114:ALA:HB2	2.00	0.61
16:N:91:ARG:HA	16:N:116:ALA:HB2	1.82	0.61
21:S:15:VAL:HG13	21:S:16:ALA:N	2.14	0.61
21:S:50:ARG:HG3	21:S:54:LYS:HZ2	1.65	0.61
23:U:29:GLN:CG	23:U:30:VAL:N	2.63	0.61
22:T:124:ILE:HD12	22:T:125:LEU:H	1.64	0.61
5:C:154:LYS:HZ2	5:C:155:LYS:HD2	1.65	0.61
6:D:163:ARG:HG3	6:D:164:ASN:H	1.66	0.61
19:Q:21:VAL:CG1	19:Q:76:VAL:HG11	2.28	0.61
10:H:38:LEU:HD22	10:H:76:VAL:HB	1.82	0.61
4:B:33:LEU:C	4:B:35:LYS:H	2.03	0.61
12:J:85:LEU:HD21	12:J:118:GLY:HA3	1.81	0.61
11:I:77:ILE:HG12	16:N:74:ARG:N	2.15	0.61
4:B:161:THR:O	4:B:196:VAL:HG23	2.01	0.61
4:B:75:ILE:HG23	4:B:98:VAL:HB	1.82	0.61
5:C:24:THR:HB	5:C:186:GLY:HA2	1.81	0.61
9:G:124:GLY:C	9:G:144:VAL:H	2.04	0.61
13:K:52:VAL:HG23	13:K:53:ALA:N	2.16	0.61
19:Q:23:LEU:HD21	19:Q:24:ILE:HG23	1.83	0.61
27:Y:44:THR:HG22	27:Y:45:VAL:N	2.15	0.61
4:B:221:VAL:HG23	4:B:223:GLY:N	2.14	0.61
5:C:65:GLY:HA3	5:C:73:GLU:OE1	2.00	0.61
6:D:33:ARG:HH12	12:J:12:ALA:N	1.88	0.61
15:M:95:HIS:O	15:M:98:VAL:N	2.31	0.61
16:N:106:SER:HA	16:N:110:ILE:CD1	2.29	0.61
16:N:26:ASP:HB2	16:N:88:ILE:HD12	1.81	0.61
22:T:69:THR:HG21	22:T:88:PHE:HE1	1.65	0.61
19:Q:30:GLU:HA	19:Q:33:ARG:HG2	1.82	0.61
11:I:64:ARG:HD3	11:I:102:VAL:CG2	2.31	0.61
16:N:47:GLY:CA	16:N:64:ARG:O	2.49	0.61
20:R:12:VAL:CG1	20:R:17:ALA:CB	2.78	0.61
24:V:27:GLU:HA	33:2:74:C:H4'	1.81	0.61
33:2:51:G:H2'	33:2:52:U:H6	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:THR:HG22	3:A:63:VAL:N	2.16	0.61
4:B:133:LEU:HA	4:B:136:ILE:HB	1.81	0.61
5:C:30:PRO:HB3	5:C:90:THR:HG21	1.83	0.61
7:E:101:ILE:O	7:E:104:GLU:HG2	2.00	0.61
13:K:126:PRO:O	13:K:127:ILE:HG23	2.01	0.61
14:L:97:VAL:HA	14:L:113:LEU:O	2.00	0.61
15:M:49:VAL:HG22	15:M:50:SER:N	2.15	0.61
20:R:14:SER:O	20:R:17:ALA:HB3	2.00	0.61
22:T:146:ILE:N	22:T:146:ILE:HD13	2.15	0.61
26:X:8:LEU:HD21	26:X:30:ARG:O	2.00	0.61
5:C:201:THR:HG22	5:C:202:LYS:H	1.65	0.60
9:G:138:ILE:O	9:G:138:ILE:HG23	2.01	0.60
18:P:42:GLY:O	18:P:47:VAL:HG11	2.01	0.60
23:U:52:GLY:HA3	23:U:62:LEU:HB2	1.83	0.60
24:V:86:SER:N	24:V:87:PRO:HD2	2.16	0.60
5:C:103:ASP:O	5:C:104:VAL:HB	2.01	0.60
11:I:114:ILE:N	11:I:114:ILE:HD13	1.99	0.60
13:K:15:GLY:CA	13:K:72:LYS:HE2	2.31	0.60
11:I:109:LYS:HA	11:I:109:LYS:CE	2.30	0.60
12:J:146:VAL:HG13	12:J:147:LEU:N	2.15	0.60
4:B:212:SER:CB	4:B:217:ARG:HG2	2.31	0.60
4:B:3:VAL:HA	4:B:17:THR:CG2	2.30	0.60
4:B:20:ASP:HB2	4:B:91:ARG:NH1	2.17	0.60
4:B:75:ILE:CG2	4:B:98:VAL:HB	2.31	0.60
5:C:56:PRO:HB2	5:C:58:ARG:HH11	1.65	0.60
7:E:68:PRO:CB	7:E:92:VAL:HB	2.28	0.60
8:F:103:LEU:HG	8:F:123:PHE:CE2	2.37	0.60
9:G:131:LYS:HZ3	9:G:134:PRO:HA	1.67	0.60
16:N:31:SER:H	16:N:42:ILE:CB	2.15	0.60
16:N:26:ASP:H	16:N:91:ARG:H	1.50	0.60
17:O:41:ALA:C	17:O:43:GLY:H	2.04	0.60
17:O:69:CYS:HB2	17:O:74:LEU:HD13	1.82	0.60
27:Y:13:LYS:O	27:Y:16:ARG:HG3	2.01	0.60
27:Y:19:ARG:HG3	27:Y:20:ARG:HG3	1.83	0.60
17:O:98:LEU:HD11	17:O:105:VAL:CB	2.25	0.60
23:U:37:LEU:HD12	23:U:38:VAL:N	2.11	0.60
5:C:107:THR:O	5:C:189:PRO:HG2	2.00	0.60
17:O:66:ASN:HD21	17:O:70:ARG:NH2	1.98	0.60
3:A:186:LEU:HD12	3:A:187:ALA:N	2.16	0.60
5:C:13:ARG:HB3	5:C:22:PRO:HA	1.83	0.60
6:D:171:LEU:HD23	6:D:172:ALA:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:9:LEU:HD23	9:G:10:GLU:N	2.15	0.60
13:K:58:PHE:CZ	13:K:117:ALA:HB1	2.37	0.60
13:K:37:LEU:CG	13:K:128:LYS:H	2.10	0.60
14:L:86:ARG:HG3	14:L:87:TYR:CE1	2.37	0.60
18:P:47:VAL:HG22	18:P:48:GLY:N	2.16	0.60
22:T:90:VAL:HG22	22:T:91:LEU:H	1.64	0.60
11:I:6:THR:CG2	11:I:7:TYR:H	2.12	0.60
3:A:15:VAL:O	3:A:16:ASP:O	2.20	0.60
4:B:24:ILE:HG23	4:B:25:THR:HG22	1.82	0.60
4:B:261:LYS:HE2	4:B:261:LYS:HA	1.83	0.60
9:G:43:ASN:HA	9:G:46:ALA:HB3	1.84	0.60
11:I:7:TYR:O	11:I:8:LEU:HD13	2.02	0.60
14:L:38:VAL:HB	14:L:39:PRO:HD3	1.84	0.60
18:P:21:ARG:O	18:P:22:VAL:HB	2.01	0.60
18:P:5:VAL:HG22	18:P:6:LYS:N	2.16	0.60
22:T:84:GLU:HG3	22:T:85:HIS:N	2.12	0.60
15:M:110:LEU:HD21	15:M:112:PHE:CZ	2.37	0.60
4:B:133:LEU:HD21	4:B:189:CYS:HB2	1.81	0.60
6:D:69:ARG:NH2	6:D:69:ARG:HG3	2.17	0.60
10:H:79:ASN:HA	10:H:147:ALA:HA	1.82	0.60
18:P:39:LEU:CD1	18:P:40:LEU:H	2.14	0.60
19:Q:23:LEU:CD1	27:Y:25:LEU:HG	2.28	0.60
22:T:30:ASN:ND2	22:T:32:HIS:HB2	2.17	0.60
7:E:28:VAL:CG1	7:E:33:ARG:HH11	2.14	0.60
11:I:29:ASN:HD22	11:I:29:ASN:C	2.05	0.60
11:I:34:THR:CG2	11:I:35:VAL:H	2.14	0.60
12:J:90:ARG:HG2	12:J:91:PHE:HD1	1.66	0.60
8:F:96:ALA:HB3	8:F:128:PRO:O	2.02	0.60
9:G:88:ILE:HG23	9:G:89:TYR:N	2.17	0.60
14:L:79:LEU:O	14:L:83:ILE:HB	2.00	0.60
16:N:91:ARG:HA	16:N:116:ALA:CB	2.32	0.60
22:T:141:VAL:HG22	22:T:144:LEU:HB2	1.83	0.60
33:2:67:A:C2'	33:2:68:U:H5'	2.31	0.60
24:V:27:GLU:HA	33:2:74:C:C5'	2.32	0.60
3:A:217:THR:HG1	3:A:220:GLY:H	1.48	0.60
7:E:120:LEU:HD12	7:E:178:PHE:HB3	1.84	0.60
8:F:100:GLY:O	8:F:101:ARG:HB3	2.02	0.60
10:H:88:LYS:HE3	10:H:92:GLN:HG3	1.82	0.60
12:J:71:VAL:HG13	12:J:72:PRO:CD	2.20	0.60
14:L:66:VAL:C	14:L:68:ARG:HH12	2.03	0.60
11:I:77:ILE:CG1	16:N:72:VAL:HG13	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:13:LYS:HA	27:Y:16:ARG:HG2	1.84	0.60
23:U:35:ASN:H	23:U:61:ALA:HB3	1.67	0.59
4:B:38:LYS:HG3	4:B:38:LYS:O	2.02	0.59
4:B:79:VAL:HB	4:B:111:LEU:HG	1.83	0.59
5:C:66:HIS:O	5:C:67:PHE:CB	2.49	0.59
7:E:139:LEU:HB2	7:E:146:TYR:N	2.10	0.59
7:E:78:SER:O	7:E:79:ASN:CB	2.50	0.59
7:E:96:ARG:HD3	7:E:97:ASP:N	2.17	0.59
13:K:8:LYS:CB	13:K:12:GLN:HE21	2.15	0.59
16:N:28:VAL:O	16:N:29:ARG:HB2	2.02	0.59
17:O:111:GLU:HA	17:O:114:LYS:HD3	1.83	0.59
19:Q:87:PRO:O	19:Q:88:ARG:HB3	2.01	0.59
20:R:83:VAL:HG23	20:R:85:PRO:HD2	1.83	0.59
27:Y:33:CYS:HB3	27:Y:38:ALA:HB3	1.83	0.59
27:Y:38:ALA:CB	27:Y:49:CYS:HB3	2.18	0.59
4:B:8:PRO:CG	4:B:15:PHE:H	2.15	0.59
6:D:149:VAL:C	6:D:150:LEU:HD22	2.23	0.59
11:I:24:VAL:HG22	11:I:25:LEU:N	2.04	0.59
33:2:8:U:H2'	33:2:9:A:H5''	1.85	0.59
8:F:153:LYS:HD2	8:F:163:TYR:HA	1.84	0.59
14:L:65:LEU:O	14:L:68:ARG:NH1	2.36	0.59
24:V:91:LYS:O	24:V:94:LEU:HB2	2.02	0.59
33:2:14:A:H62	33:2:21:A:H2	1.49	0.59
33:2:66:A:N6	33:2:67:A:N6	2.50	0.59
9:G:81:VAL:C	9:G:148:GLU:HG3	2.23	0.59
15:M:62:LYS:O	15:M:65:VAL:HG22	2.01	0.59
33:2:20:G:N2	33:2:22:G:H1'	2.17	0.59
4:B:200:ASP:O	4:B:202:LYS:N	2.34	0.59
4:B:33:LEU:HD23	4:B:33:LEU:O	2.03	0.59
6:D:27:LEU:N	6:D:27:LEU:HD13	2.16	0.59
7:E:141:PHE:CD2	7:E:144:ILE:HB	2.37	0.59
14:L:79:LEU:HD23	14:L:83:ILE:HG13	1.82	0.59
15:M:26:LEU:HD22	15:M:39:ILE:HG21	1.83	0.59
16:N:107:ASP:O	16:N:111:ARG:HD3	2.02	0.59
17:O:105:VAL:HG22	18:P:43:GLU:CD	2.23	0.59
20:R:42:ALA:O	20:R:46:ALA:CB	2.49	0.59
9:G:98:ALA:CA	9:G:111:PRO:HG2	2.28	0.59
14:L:63:ARG:HA	14:L:66:VAL:HG22	1.84	0.59
15:M:84:GLN:HE21	15:M:112:PHE:HE2	1.49	0.59
15:M:82:ILE:CG2	15:M:85:VAL:HB	2.33	0.59
4:B:196:VAL:HG12	4:B:197:GLY:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:65:ILE:HB	4:B:104:TYR:O	2.03	0.59
5:C:154:LYS:NZ	5:C:155:LYS:HD2	2.17	0.59
6:D:15:LEU:HD22	6:D:19:LEU:CD2	2.32	0.59
7:E:15:VAL:HG12	7:E:15:VAL:O	2.03	0.59
7:E:70:VAL:HA	7:E:90:LEU:HG	1.83	0.59
22:T:151:HIS:HB3	22:T:168:GLU:CA	2.32	0.59
27:Y:8:LYS:O	27:Y:9:LYS:HB2	2.01	0.59
19:Q:11:ARG:HD2	19:Q:98:LYS:NZ	2.18	0.59
24:V:11:ARG:HB2	24:V:12:PRO:HD3	1.84	0.59
27:Y:31:VAL:O	27:Y:39:MET:HA	2.03	0.59
4:B:118:VAL:HG22	4:B:119:ALA:N	2.17	0.59
4:B:140:THR:HG23	4:B:165:ILE:HD13	1.83	0.59
4:B:60:ARG:NH2	4:B:86:PRO:HB2	2.17	0.59
8:F:12:PRO:HD2	8:F:15:VAL:HG21	1.84	0.59
9:G:4:ILE:HG12	9:G:18:VAL:HG22	1.83	0.59
19:Q:17:VAL:HG21	19:Q:103:ILE:HD13	1.84	0.59
22:T:25:PRO:HA	22:T:38:TYR:HB3	1.84	0.59
23:U:41:ARG:HG2	23:U:41:ARG:HH11	1.68	0.59
17:O:66:ASN:HA	17:O:69:CYS:SG	2.43	0.59
5:C:51:PHE:N	5:C:76:ARG:HB3	2.17	0.59
7:E:30:GLU:HG3	7:E:30:GLU:O	2.03	0.59
7:E:3:LEU:HB2	7:E:100:TRP:HH2	1.65	0.59
8:F:125:VAL:HB	8:F:128:PRO:CB	2.33	0.59
10:H:27:TYR:CE1	17:O:64:ARG:HD3	2.38	0.59
10:H:65:TRP:HB3	17:O:64:ARG:CD	2.32	0.59
13:K:120:ILE:O	13:K:124:LYS:HB3	2.03	0.59
14:L:1:MET:HG3	14:L:5:LYS:HA	1.84	0.59
15:M:73:LEU:HA	15:M:76:LYS:HE3	1.85	0.59
18:P:66:ARG:NE	18:P:94:LEU:HD21	2.18	0.59
4:B:105:ILE:HG23	4:B:106:ILE:H	1.67	0.59
4:B:4:LYS:HD3	4:B:19:ALA:O	2.03	0.59
8:F:11:VAL:HA	8:F:15:VAL:HG22	1.84	0.59
11:I:106:LEU:HB2	11:I:115:VAL:HG22	1.85	0.59
12:J:133:SER:O	12:J:137:LYS:HG2	2.03	0.59
14:L:18:LEU:O	14:L:21:TYR:HB2	2.03	0.59
21:S:23:ARG:HG3	21:S:24:VAL:H	1.66	0.59
3:A:48:LEU:HD23	3:A:48:LEU:H	1.68	0.59
5:C:116:VAL:HG21	5:C:122:PHE:CD1	2.37	0.59
5:C:90:THR:HG22	5:C:91:VAL:H	1.67	0.59
12:J:79:ARG:HG2	12:J:108:LYS:O	2.03	0.59
13:K:133:ARG:HE	13:K:134:ARG:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:83:LEU:HD23	17:O:84:LYS:HZ3	1.67	0.59
28:Z:19:ARG:O	28:Z:22:MET:HB3	2.03	0.59
33:2:49:C:H1'	33:2:66:A:C2	2.38	0.59
4:B:24:ILE:O	4:B:25:THR:C	2.41	0.59
28:Z:2:LYS:CD	28:Z:2:LYS:H	2.09	0.59
22:T:117:LEU:H	22:T:117:LEU:HD23	1.68	0.58
4:B:10:THR:HG22	4:B:13:ARG:HB2	1.85	0.58
5:C:105:THR:O	5:C:197:ILE:HD13	2.01	0.58
9:G:81:VAL:O	9:G:82:ARG:HB2	2.03	0.58
27:Y:46:CYS:O	27:Y:57:VAL:HG21	2.02	0.58
4:B:166:GLN:HE21	4:B:176:ARG:HB2	1.69	0.58
7:E:96:ARG:O	7:E:99:MET:HG3	2.02	0.58
10:H:38:LEU:HD13	10:H:39:ILE:N	2.19	0.58
14:L:66:VAL:HB	14:L:70:LEU:HD12	1.83	0.58
16:N:27:THR:HG22	16:N:87:ASP:HB3	1.85	0.58
33:2:18:G:N1	33:2:57:G:C6	2.71	0.58
9:G:44:LEU:O	9:G:47:LEU:HG	2.03	0.58
12:J:61:ARG:N	12:J:61:ARG:HE	2.01	0.58
12:J:85:LEU:HD22	12:J:85:LEU:C	2.23	0.58
19:Q:17:VAL:O	19:Q:20:VAL:N	2.36	0.58
33:2:43:G:H2'	33:2:44:A:C8	2.37	0.58
10:H:37:VAL:HG13	10:H:38:LEU:H	1.68	0.58
12:J:24:GLY:HA2	12:J:30:THR:HG23	1.85	0.58
6:D:172:ALA:CB	6:D:173:PRO:CD	2.80	0.58
7:E:73:ALA:H	7:E:87:PRO:CB	2.15	0.58
15:M:106:ARG:NH1	15:M:111:GLU:HA	2.18	0.58
18:P:40:LEU:HB2	18:P:50:PRO:HB3	1.84	0.58
18:P:66:ARG:CD	18:P:68:LYS:HG3	2.25	0.58
33:2:65:G:C2'	33:2:66:A:H5'	2.33	0.58
4:B:148:GLU:O	4:B:151:LYS:HB2	2.03	0.58
6:D:67:ARG:O	6:D:68:ALA:HB2	2.03	0.58
8:F:12:PRO:O	8:F:14:GLY:N	2.34	0.58
9:G:64:GLU:HG3	9:G:67:ARG:NH2	2.18	0.58
10:H:132:LYS:N	10:H:132:LYS:HE3	2.18	0.58
12:J:97:PRO:CD	12:J:126:VAL:HB	2.32	0.58
15:M:25:ARG:HH12	15:M:41:ASP:C	2.07	0.58
16:N:45:PHE:HE2	16:N:64:ARG:CA	2.16	0.58
19:Q:28:SER:HB3	19:Q:29:LEU:HD23	1.85	0.58
20:R:30:VAL:H	20:R:76:ARG:HG3	1.68	0.58
24:V:66:HIS:HB3	24:V:69:LYS:CG	2.25	0.58
23:U:28:GLY:HA2	23:U:67:VAL:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:141:PHE:HB3	7:E:144:ILE:HB	1.84	0.58
16:N:45:PHE:HD2	16:N:63:VAL:HG23	1.68	0.58
4:B:184:LYS:HZ2	4:B:269:PHE:HE2	1.51	0.58
4:B:81:ALA:O	4:B:93:ALA:HA	2.03	0.58
4:B:6:PHE:HB3	4:B:8:PRO:HD3	1.84	0.58
4:B:82:ILE:HG22	4:B:91:ARG:HE	1.68	0.58
14:L:116:LEU:O	14:L:117:VAL:HG12	2.02	0.58
16:N:112:ARG:CA	16:N:115:ARG:HH21	2.08	0.58
25:W:41:ILE:HD13	25:W:44:LEU:HD13	1.86	0.58
26:X:21:ALA:HA	26:X:24:LYS:NZ	2.17	0.58
28:Z:19:ARG:HG2	28:Z:23:ARG:HH21	1.67	0.58
11:I:15:GLY:H	11:I:17:ARG:HH22	1.51	0.58
12:J:97:PRO:HG3	12:J:126:VAL:O	2.02	0.58
33:2:14:A:C6	33:2:22:G:C6	2.91	0.58
33:2:26:G:O2'	33:2:27:C:H5'	2.02	0.58
4:B:76:PRO:HG2	4:B:117:VAL:HG12	1.83	0.58
4:B:56:GLY:HA3	4:B:215:LEU:C	2.23	0.58
9:G:109:ILE:HG22	9:G:111:PRO:HG3	1.85	0.58
20:R:32:PRO:CG	20:R:72:LYS:HE2	2.33	0.58
22:T:4:ARG:C	22:T:5:LEU:HD22	2.23	0.58
33:2:35:A:H2'	33:2:36:A:N9	2.17	0.58
5:C:44:TYR:HE2	5:C:46:ALA:HB3	1.69	0.58
5:C:98:PRO:HG3	5:C:174:ASP:HA	1.86	0.58
11:I:26:LYS:HB3	11:I:30:ALA:HB2	1.86	0.58
23:U:37:LEU:HD12	23:U:38:VAL:HG23	1.85	0.58
24:V:51:VAL:HG12	24:V:52:ARG:N	2.19	0.58
27:Y:58:LEU:H	27:Y:58:LEU:HD12	1.69	0.58
14:L:20:LEU:O	14:L:24:GLN:HG2	2.01	0.58
8:F:135:GLY:N	8:F:138:LYS:HZ2	2.02	0.58
8:F:14:GLY:C	8:F:16:SER:H	2.06	0.58
12:J:79:ARG:HH12	12:J:108:LYS:HB2	1.67	0.58
17:O:105:VAL:HG13	18:P:43:GLU:OE2	2.03	0.58
3:A:166:ASN:HA	3:A:171:ALA:CB	2.34	0.58
5:C:44:TYR:CE2	5:C:46:ALA:HB3	2.38	0.58
7:E:135:LEU:HA	7:E:136:ARG:HH11	1.67	0.58
18:P:1:MET:HG3	18:P:43:GLU:O	2.04	0.58
18:P:73:SER:OG	18:P:89:GLN:HB3	2.04	0.58
4:B:130:ALA:HA	4:B:191:ALA:O	2.03	0.58
4:B:212:SER:HB2	4:B:217:ARG:HG2	1.85	0.58
4:B:3:VAL:HG23	4:B:200:ASP:C	2.24	0.58
6:D:153:THR:OG1	6:D:158:VAL:HG11	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:4:ILE:HB	6:D:5:PRO:CD	2.32	0.58
21:S:25:GLY:HA2	21:S:37:VAL:HB	1.85	0.58
23:U:19:LYS:HZ3	23:U:19:LYS:HB2	1.67	0.58
20:R:9:LEU:O	25:W:30:ARG:HB2	2.04	0.58
28:Z:10:ARG:HH11	28:Z:14:LYS:HE3	1.69	0.58
4:B:141:VAL:HG12	4:B:162:SER:OG	2.04	0.58
5:C:25:VAL:CG1	5:C:182:LEU:O	2.51	0.58
6:D:105:LEU:O	6:D:109:VAL:HG22	2.04	0.58
6:D:128:ASN:HA	6:D:134:PHE:HZ	1.69	0.58
8:F:23:ARG:HG2	8:F:36:PRO:HA	1.86	0.58
10:H:113:MET:O	10:H:121:VAL:HG22	2.04	0.58
12:J:41:ARG:HE	12:J:42:SER:H	1.51	0.58
13:K:134:ARG:NH2	13:K:137:TYR:HA	2.19	0.58
15:M:28:VAL:HG21	15:M:87:PHE:CE1	2.39	0.58
16:N:101:PHE:C	16:N:103:ARG:N	2.57	0.58
17:O:106:PHE:HA	17:O:109:LEU:HG	1.86	0.58
33:2:34:G:C3'	33:2:35:A:H5''	2.34	0.57
33:2:26:G:H1	33:2:44:A:H61	1.52	0.57
5:C:37:ARG:HB3	5:C:42:ASP:HB2	1.86	0.57
5:C:84:PHE:HD1	5:C:86:PRO:HD3	1.68	0.57
7:E:43:LEU:HD22	7:E:45:GLU:HG2	1.85	0.57
9:G:4:ILE:HG13	9:G:18:VAL:HG22	1.85	0.57
10:H:93:LYS:HB3	10:H:110:LEU:HD21	1.86	0.57
12:J:25:SER:H	12:J:31:ALA:HB2	1.68	0.57
13:K:114:ALA:O	13:K:117:ALA:HB3	2.04	0.57
13:K:119:ARG:O	13:K:120:ILE:C	2.42	0.57
13:K:16:ARG:HG3	13:K:17:LEU:N	2.11	0.57
16:N:86:ILE:HG22	16:N:87:ASP:H	1.67	0.57
33:2:45:G:H2'	33:2:46:G:H5''	1.86	0.57
26:X:5:LYS:O	26:X:56:VAL:HA	2.04	0.57
19:Q:19:LEU:C	27:Y:25:LEU:HD23	2.24	0.57
33:2:35:A:C6	33:2:36:A:N6	2.73	0.57
33:2:8:U:O2	33:2:21:A:H2	1.86	0.57
4:B:270:ILE:O	4:B:271:ILE:HD12	2.04	0.57
7:E:62:LEU:HD12	7:E:63:ILE:N	2.19	0.57
8:F:144:VAL:HG22	8:F:148:ILE:HD13	1.86	0.57
9:G:124:GLY:CA	9:G:144:VAL:H	2.17	0.57
15:M:27:SER:HB3	15:M:89:ARG:NH1	2.19	0.57
18:P:69:LYS:HD3	18:P:71:LEU:HD21	1.87	0.57
23:U:16:SER:O	23:U:17:GLN:HB2	2.05	0.57
24:V:51:VAL:HG12	24:V:52:ARG:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:25:VAL:O	25:W:29:LYS:HG3	2.05	0.57
3:A:198:GLU:HB2	3:A:201:LYS:HG2	1.86	0.57
4:B:35:LYS:HD2	4:B:62:TYR:O	2.05	0.57
8:F:153:LYS:HA	8:F:162:ILE:O	2.04	0.57
23:U:50:ASN:HB2	23:U:81:VAL:CB	2.33	0.57
5:C:187:ALA:O	5:C:188:VAL:HB	2.04	0.57
5:C:33:VAL:HG13	5:C:47:VAL:HG11	1.85	0.57
7:E:77:ILE:HG23	7:E:78:SER:N	2.20	0.57
9:G:38:LEU:HD13	9:G:40:THR:CG2	2.31	0.57
10:H:27:TYR:CE2	17:O:100:VAL:HG13	2.39	0.57
10:H:78:VAL:HA	10:H:146:TYR:CE2	2.39	0.57
12:J:138:LEU:HG	12:J:142:GLY:HA3	1.85	0.57
12:J:45:LEU:HD23	12:J:46:LYS:H	1.69	0.57
12:J:78:PRO:CB	12:J:110:TYR:HB2	2.34	0.57
18:P:10:LYS:HZ1	18:P:22:VAL:HG23	1.69	0.57
19:Q:86:LEU:HD13	19:Q:87:PRO:HD2	1.86	0.57
21:S:45:VAL:HG12	21:S:57:GLN:HG2	1.85	0.57
21:S:82:PRO:HB3	21:S:97:ARG:NH1	2.18	0.57
24:V:15:ALA:HB2	24:V:48:LYS:NZ	2.20	0.57
33:2:9:A:N7	33:2:12:U:O4	2.36	0.57
3:A:198:GLU:CB	3:A:201:LYS:HG2	2.34	0.57
3:A:225:ILE:HG23	3:A:226:ASN:H	1.68	0.57
5:C:174:ASP:O	5:C:182:LEU:HD12	2.04	0.57
7:E:7:LEU:CB	7:E:100:TRP:HE1	2.10	0.57
7:E:96:ARG:HD3	7:E:97:ASP:H	1.69	0.57
8:F:13:LYS:HE2	8:F:29:PRO:HA	1.85	0.57
9:G:21:VAL:HG23	9:G:22:LYS:N	2.19	0.57
10:H:161:LEU:HD12	10:H:161:LEU:H	1.70	0.57
11:I:111:PHE:HB3	11:I:114:ILE:HG12	1.87	0.57
12:J:84:ASN:OD1	12:J:85:LEU:HD13	2.04	0.57
13:K:16:ARG:CG	13:K:17:LEU:H	2.12	0.57
14:L:34:ILE:HG22	14:L:35:THR:N	2.16	0.57
15:M:40:ILE:HG22	15:M:41:ASP:H	1.68	0.57
17:O:91:ASP:O	17:O:92:ARG:O	2.23	0.57
18:P:77:ALA:O	18:P:78:LYS:HB3	2.04	0.57
20:R:13:LEU:H	20:R:13:LEU:HD23	1.68	0.57
21:S:28:LYS:HA	21:S:35:TYR:HB3	1.86	0.57
22:T:146:ILE:HB	22:T:176:PRO:HD3	1.87	0.57
23:U:50:ASN:HB2	23:U:81:VAL:HB	1.87	0.57
4:B:69:ARG:CG	4:B:190:TYR:CE2	2.87	0.57
4:B:28:GLU:N	4:B:29:PRO:HD2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:97:TYR:HB2	4:B:102:LYS:CA	2.32	0.57
5:C:36:ARG:HG2	5:C:36:ARG:HH11	1.70	0.57
15:M:26:LEU:HD22	15:M:39:ILE:HG22	1.86	0.57
17:O:95:LEU:HD11	18:P:11:GLN:HB3	1.86	0.57
22:T:10:ARG:HG3	22:T:11:GLU:N	2.18	0.57
25:W:3:LEU:CD1	25:W:8:LYS:HD3	2.33	0.57
4:B:131:LEU:O	4:B:136:ILE:HD11	2.04	0.57
4:B:4:LYS:CB	4:B:18:VAL:HG12	2.34	0.57
4:B:45:ASN:CG	4:B:46:GLN:N	2.57	0.57
4:B:35:LYS:CE	4:B:64:ILE:H	2.17	0.57
8:F:26:VAL:HG12	8:F:27:LYS:N	2.19	0.57
13:K:33:GLY:HA3	13:K:132:VAL:HB	1.87	0.57
16:N:30:VAL:HG21	16:N:84:GLN:CG	2.28	0.57
17:O:109:LEU:HA	17:O:112:ARG:HG3	1.87	0.57
24:V:58:ILE:HG12	24:V:82:LEU:HD11	1.87	0.57
4:B:65:ILE:CB	4:B:105:ILE:HA	2.34	0.57
5:C:28:ALA:HB3	5:C:181:LEU:N	2.20	0.57
10:H:135:LEU:HD12	10:H:135:LEU:N	2.20	0.57
10:H:37:VAL:HG13	10:H:38:LEU:N	2.19	0.57
16:N:121:ILE:O	16:N:121:ILE:HD13	2.04	0.57
25:W:21:LEU:HD23	25:W:21:LEU:C	2.25	0.57
4:B:111:LEU:HD12	4:B:115:GLN:HB3	1.85	0.57
4:B:94:LEU:HA	4:B:103:ARG:O	2.04	0.57
5:C:173:VAL:HG23	5:C:183:LEU:HD22	1.87	0.57
5:C:51:PHE:C	5:C:76:ARG:HB2	2.25	0.57
8:F:153:LYS:CB	8:F:154:PRO:HD3	2.35	0.57
11:I:104:ARG:HD2	11:I:104:ARG:H	1.69	0.57
16:N:87:ASP:OD1	16:N:87:ASP:N	2.37	0.57
19:Q:20:VAL:HA	19:Q:23:LEU:CD2	2.35	0.57
28:Z:12:ARG:O	28:Z:17:GLY:N	2.38	0.57
33:2:67:A:HO2'	33:2:68:U:H5'	1.68	0.57
9:G:63:ALA:CA	9:G:66:GLU:HB2	2.32	0.57
13:K:58:PHE:CZ	13:K:117:ALA:CB	2.87	0.57
14:L:5:LYS:HG2	14:L:6:SER:H	1.69	0.57
14:L:5:LYS:HG2	14:L:6:SER:N	2.20	0.57
16:N:11:GLU:O	16:N:13:ARG:N	2.37	0.57
17:O:99:ALA:HA	17:O:106:PHE:HE1	1.69	0.57
18:P:4:ILE:CG1	18:P:13:ARG:HB3	2.35	0.57
21:S:60:PHE:O	21:S:61:ILE:HG13	2.04	0.57
23:U:20:ARG:CG	23:U:20:ARG:HH11	2.18	0.57
4:B:80:ALA:N	4:B:95:LEU:HA	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:83:GLU:CB	4:B:92:ILE:HD11	2.35	0.56
5:C:103:ASP:HA	5:C:168:MET:HA	1.87	0.56
5:C:24:THR:HB	5:C:186:GLY:CA	2.35	0.56
10:H:89:LYS:C	10:H:110:LEU:HG	2.25	0.56
11:I:22:ILE:HG13	11:I:23:ARG:N	2.16	0.56
14:L:63:ARG:HD3	14:L:67:LEU:CD2	2.35	0.56
16:N:50:ILE:HG13	16:N:63:VAL:C	2.25	0.56
17:O:93:LYS:HD2	17:O:93:LYS:N	2.20	0.56
17:O:94:ASN:OD1	17:O:95:LEU:HD23	2.05	0.56
22:T:44:PHE:CG	22:T:45:ASP:N	2.73	0.56
28:Z:10:ARG:O	28:Z:14:LYS:HD3	2.05	0.56
24:V:33:LYS:HG2	24:V:34:THR:H	1.70	0.56
33:2:73:A:N1	33:2:74:C:N4	2.54	0.56
4:B:60:ARG:CZ	4:B:86:PRO:HB2	2.34	0.56
6:D:171:LEU:HD21	6:D:173:PRO:O	2.05	0.56
9:G:103:ARG:HD2	9:G:104:GLN:N	2.19	0.56
10:H:119:GLU:HG3	10:H:145:VAL:CG2	2.35	0.56
13:K:109:VAL:HG23	13:K:114:ALA:HB2	1.86	0.56
19:Q:4:LYS:HD2	19:Q:62:HIS:CE1	2.37	0.56
24:V:15:ALA:HB2	24:V:48:LYS:HZ2	1.70	0.56
6:D:134:PHE:HD1	6:D:134:PHE:N	2.03	0.56
6:D:150:LEU:HB2	6:D:187:LEU:HD23	1.87	0.56
7:E:12:TYR:O	7:E:13:GLU:HB2	2.03	0.56
7:E:131:TYR:O	7:E:158:ALA:HB1	2.05	0.56
7:E:11:TYR:HA	7:E:15:VAL:HB	1.86	0.56
10:H:89:LYS:O	10:H:110:LEU:HG	2.04	0.56
12:J:85:LEU:HD11	12:J:118:GLY:HA3	1.87	0.56
13:K:106:VAL:HG11	13:K:118:LEU:HD11	1.86	0.56
15:M:34:HIS:HB3	15:M:36:TYR:CE1	2.40	0.56
16:N:99:LEU:CG	16:N:102:ILE:HG12	2.33	0.56
16:N:46:GLU:CD	16:N:65:LYS:HG2	2.26	0.56
17:O:41:ALA:C	17:O:43:GLY:N	2.59	0.56
19:Q:57:ASN:HD22	19:Q:61:ASN:ND2	2.02	0.56
22:T:53:ILE:H	22:T:53:ILE:CD1	2.16	0.56
24:V:91:LYS:HE3	24:V:91:LYS:N	2.19	0.56
25:W:45:SER:O	25:W:46:GLN:HB2	2.04	0.56
25:W:46:GLN:C	25:W:48:HIS:H	2.09	0.56
26:X:7:LYS:HB3	26:X:34:GLU:HB3	1.88	0.56
34:3:17:C:C4	34:3:18:C:N4	2.73	0.56
3:A:166:ASN:HA	3:A:171:ALA:HA	1.87	0.56
5:C:30:PRO:HG3	5:C:92:THR:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:178:VAL:O	6:D:182:VAL:HG13	2.05	0.56
7:E:139:LEU:CB	7:E:146:TYR:N	2.68	0.56
8:F:126:PRO:HG2	8:F:130:ARG:HB2	1.87	0.56
9:G:4:ILE:C	9:G:37:VAL:HB	2.25	0.56
15:M:73:LEU:O	15:M:76:LYS:HB2	2.05	0.56
18:P:72:VAL:HG13	18:P:88:ARG:HD3	1.86	0.56
33:2:44:A:N6	33:2:45:G:N2	2.53	0.56
6:D:24:ASN:O	6:D:28:LEU:HG	2.04	0.56
9:G:16:GLY:O	9:G:18:VAL:HG23	2.06	0.56
11:I:27:GLY:O	11:I:28:SER:CB	2.53	0.56
11:I:60:ALA:HA	11:I:86:ILE:HA	1.87	0.56
12:J:83:VAL:CG1	12:J:114:ILE:HA	2.35	0.56
14:L:38:VAL:CB	14:L:39:PRO:HD3	2.36	0.56
16:N:24:PRO:HB3	16:N:49:VAL:HG21	1.87	0.56
22:T:45:ASP:O	22:T:49:ARG:HG3	2.06	0.56
4:B:91:ARG:HD3	4:B:198:ASN:OD1	2.06	0.56
5:C:90:THR:HG22	5:C:91:VAL:N	2.21	0.56
6:D:134:PHE:CD1	6:D:134:PHE:N	2.73	0.56
6:D:165:LEU:H	6:D:165:LEU:HD13	1.71	0.56
7:E:20:ILE:HG22	7:E:21:ARG:N	2.20	0.56
7:E:81:LYS:O	7:E:82:LEU:CB	2.53	0.56
7:E:46:ALA:CB	7:E:87:PRO:HG3	2.33	0.56
10:H:108:ILE:HD13	10:H:112:LYS:HE3	1.88	0.56
16:N:93:ARG:N	16:N:116:ALA:HA	2.20	0.56
17:O:90:VAL:C	17:O:92:ARG:H	2.09	0.56
18:P:24:LYS:CG	18:P:25:LEU:N	2.68	0.56
19:Q:20:VAL:HA	19:Q:23:LEU:HD22	1.88	0.56
22:T:106:GLY:O	22:T:108:PRO:HD3	2.06	0.56
22:T:150:LEU:CG	22:T:171:ILE:HD11	2.30	0.56
5:C:178:GLU:HG3	5:C:179:GLU:N	2.20	0.56
33:2:8:U:O2	33:2:21:A:C2	2.59	0.56
33:2:8:U:C2'	33:2:9:A:H5''	2.36	0.56
8:F:157:TYR:HA	8:F:172:LYS:H	1.71	0.56
4:B:63:ARG:HG2	4:B:86:PRO:HD2	1.88	0.56
4:B:82:ILE:HG23	4:B:107:ALA:HB3	1.87	0.56
5:C:34:VAL:HB	5:C:48:GLN:HB3	1.86	0.56
7:E:66:GLN:HE22	7:E:94:LEU:HD21	1.69	0.56
8:F:11:VAL:N	8:F:12:PRO:CD	2.69	0.56
9:G:88:ILE:HG12	9:G:89:TYR:N	2.20	0.56
11:I:79:PHE:CE2	11:I:102:VAL:HG11	2.36	0.56
16:N:115:ARG:O	16:N:116:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:11:GLU:C	16:N:57:PHE:HZ	2.09	0.56
16:N:61:PHE:HD1	16:N:61:PHE:N	2.03	0.56
20:R:89:ILE:O	20:R:89:ILE:HG22	2.05	0.56
5:C:116:VAL:HG23	5:C:120:TRP:HD1	1.71	0.56
6:D:56:GLY:O	6:D:57:ARG:HB2	2.05	0.56
7:E:148:MET:N	7:E:148:MET:SD	2.79	0.56
9:G:130:TYR:HD2	9:G:131:LYS:N	2.04	0.56
12:J:35:HIS:CG	12:J:36:LYS:H	2.23	0.56
13:K:86:GLY:C	13:K:87:LYS:HD2	2.25	0.56
18:P:34:GLU:N	18:P:64:HIS:HE1	2.02	0.56
18:P:66:ARG:HE	18:P:94:LEU:CD2	2.18	0.56
19:Q:24:ILE:HG21	19:Q:36:LEU:HD11	1.88	0.56
21:S:45:VAL:HG12	21:S:57:GLN:HE21	1.71	0.56
22:T:141:VAL:HG21	22:T:144:LEU:HD23	1.87	0.56
24:V:50:ARG:HG2	24:V:61:ARG:HA	1.87	0.56
3:A:197:LEU:CG	3:A:198:GLU:HG3	2.32	0.56
4:B:65:ILE:HB	4:B:105:ILE:HA	1.86	0.56
4:B:95:LEU:HD23	4:B:95:LEU:H	1.71	0.56
5:C:134:ILE:HG22	5:C:137:HIS:HB2	1.87	0.56
5:C:51:PHE:HB3	5:C:76:ARG:NE	2.21	0.56
7:E:145:THR:O	7:E:146:TYR:HB3	2.05	0.56
10:H:46:LEU:HD22	10:H:122:LEU:HG	1.87	0.56
10:H:29:PRO:HG3	10:H:69:VAL:HG11	1.88	0.56
12:J:61:ARG:HD2	12:J:62:LEU:N	2.21	0.56
13:K:78:PRO:O	13:K:79:LEU:CB	2.54	0.56
19:Q:20:VAL:HG11	19:Q:47:VAL:HG11	1.87	0.56
22:T:33:LEU:HD12	22:T:34:ASN:H	1.71	0.56
27:Y:12:SER:C	27:Y:14:ALA:H	2.09	0.56
27:Y:56:LYS:HD2	27:Y:57:VAL:H	1.71	0.56
33:2:16:U:C3'	33:2:17:U:H5'	2.36	0.56
34:3:18:C:H6	34:3:18:C:O5'	1.89	0.56
3:A:193:PHE:HD2	3:A:193:PHE:O	1.88	0.56
4:B:130:ALA:HB1	4:B:190:TYR:CZ	2.41	0.56
7:E:73:ALA:H	7:E:87:PRO:HB3	1.69	0.56
9:G:114:LEU:HB3	9:G:130:TYR:CD1	2.41	0.56
17:O:62:ILE:O	17:O:65:ILE:HB	2.05	0.56
24:V:15:ALA:HA	24:V:46:LEU:HG	1.88	0.56
24:V:57:GLU:O	24:V:82:LEU:HD11	2.06	0.56
4:B:78:LYS:HB2	4:B:114:GLY:HA2	1.87	0.56
12:J:88:LEU:CD2	12:J:100:LEU:HG	2.34	0.56
12:J:112:LEU:H	12:J:128:HIS:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:58:LEU:HD23	15:M:60:GLY:H	1.71	0.56
15:M:93:LYS:O	15:M:94:TYR:C	2.44	0.56
5:C:192:ASN:OD1	16:N:4:GLY:HA2	2.06	0.56
5:C:47:VAL:CG1	5:C:48:GLN:H	2.12	0.56
11:I:69:VAL:CG1	11:I:77:ILE:HG22	2.35	0.56
12:J:19:VAL:O	12:J:19:VAL:HG12	2.06	0.56
18:P:34:GLU:H	18:P:64:HIS:HE1	1.53	0.56
22:T:9:TYR:CD2	22:T:37:VAL:HG11	2.41	0.56
22:T:5:LEU:CD2	22:T:57:ILE:HD11	2.36	0.56
5:C:180:ASN:O	5:C:181:LEU:HD13	2.06	0.55
6:D:117:LYS:HZ3	6:D:117:LYS:HA	1.71	0.55
7:E:66:GLN:NE2	7:E:94:LEU:HD21	2.21	0.55
10:H:77:VAL:HB	10:H:145:VAL:HG13	1.88	0.55
17:O:42:ALA:O	17:O:46:ALA:CB	2.54	0.55
20:R:8:ILE:CG1	20:R:42:ALA:HB1	2.35	0.55
26:X:10:LYS:HB2	26:X:53:LEU:HA	1.88	0.55
28:Z:46:VAL:HG12	28:Z:47:ARG:N	2.21	0.55
15:M:93:LYS:N	15:M:93:LYS:HD2	2.21	0.55
19:Q:12:ILE:HG22	19:Q:13:SER:N	2.20	0.55
25:W:7:ARG:O	25:W:8:LYS:HD2	2.06	0.55
7:E:25:TYR:H	7:E:25:TYR:HD1	1.49	0.55
8:F:14:GLY:C	8:F:16:SER:N	2.58	0.55
8:F:149:ARG:O	8:F:153:LYS:HB2	2.06	0.55
10:H:119:GLU:CG	10:H:145:VAL:HG23	2.37	0.55
10:H:73:ASP:O	10:H:75:VAL:HG23	2.06	0.55
13:K:106:VAL:HG12	13:K:107:ALA:N	2.21	0.55
13:K:8:LYS:NZ	13:K:8:LYS:N	2.55	0.55
14:L:5:LYS:CG	14:L:6:SER:H	2.18	0.55
14:L:99:LYS:HB3	27:Y:43:HIS:HD2	1.71	0.55
15:M:27:SER:CB	15:M:89:ARG:HG3	2.36	0.55
33:2:63:C:O2'	33:2:64:A:H5'	2.06	0.55
4:B:264:LYS:HD3	4:B:265:PRO:HD2	1.89	0.55
5:C:182:LEU:HG	5:C:183:LEU:H	1.72	0.55
5:C:38:THR:CG2	5:C:39:PRO:HD2	2.36	0.55
6:D:16:ALA:O	6:D:18:ASP:N	2.40	0.55
7:E:82:LEU:HD22	7:E:83:ARG:H	1.72	0.55
10:H:88:LYS:HE3	10:H:92:GLN:CG	2.35	0.55
13:K:106:VAL:HG21	13:K:118:LEU:CG	2.36	0.55
15:M:74:ALA:HB3	15:M:109:GLY:HA3	1.88	0.55
15:M:82:ILE:HG21	15:M:85:VAL:HB	1.87	0.55
22:T:137:ILE:HG12	22:T:138:GLU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:34:GLY:HA2	23:U:60:PHE:CD2	2.42	0.55
5:C:9:VAL:HG11	5:C:27:LEU:HB2	1.88	0.55
18:P:100:ARG:HD2	18:P:101:GLY:N	2.22	0.55
33:2:7:U:C2'	33:2:49:C:H5'	2.35	0.55
7:E:46:ALA:CA	7:E:53:LEU:HD21	2.35	0.55
12:J:85:LEU:H	12:J:85:LEU:CD1	2.18	0.55
19:Q:17:VAL:HG21	19:Q:103:ILE:CD1	2.37	0.55
5:C:176:ILE:HD13	5:C:182:LEU:HA	1.89	0.55
6:D:112:ARG:HB3	6:D:117:LYS:HD2	1.89	0.55
7:E:165:THR:C	7:E:167:GLU:H	2.09	0.55
10:H:114:LEU:HA	10:H:121:VAL:HG11	1.87	0.55
11:I:22:ILE:HG12	11:I:40:VAL:O	2.06	0.55
11:I:64:ARG:HB3	11:I:102:VAL:CG2	2.36	0.55
12:J:83:VAL:HG22	12:J:84:ASN:N	2.21	0.55
13:K:75:THR:HG23	13:K:77:LYS:NZ	2.21	0.55
14:L:38:VAL:HG23	14:L:39:PRO:HD3	1.88	0.55
16:N:91:ARG:HG3	16:N:92:GLY:N	2.22	0.55
19:Q:23:LEU:CD2	19:Q:24:ILE:HG23	2.37	0.55
26:X:40:THR:HB	26:X:41:PRO:HD2	1.88	0.55
20:R:5:TYR:O	20:R:7:VAL:N	2.39	0.55
34:3:8:U:C3'	34:3:8:U:C6	2.89	0.55
4:B:79:VAL:HB	4:B:111:LEU:CD1	2.37	0.55
4:B:91:ARG:HD3	4:B:198:ASN:CG	2.26	0.55
5:C:11:MET:HB3	5:C:24:THR:HA	1.88	0.55
8:F:125:VAL:HG12	8:F:131:VAL:HG23	1.88	0.55
8:F:41:MET:SD	8:F:55:PRO:HD3	2.47	0.55
8:F:87:LEU:O	8:F:130:ARG:HA	2.06	0.55
8:F:8:PRO:HB3	8:F:49:VAL:HA	1.88	0.55
11:I:107:ARG:HB2	11:I:115:VAL:HG11	1.88	0.55
13:K:132:VAL:HG22	13:K:133:ARG:CZ	2.37	0.55
18:P:34:GLU:H	18:P:64:HIS:CE1	2.23	0.55
25:W:37:PHE:O	25:W:38:GLN:C	2.45	0.55
4:B:105:ILE:HG12	4:B:106:ILE:N	2.22	0.55
4:B:211:ARG:HA	4:B:214:TRP:CZ3	2.42	0.55
4:B:82:ILE:HG21	4:B:91:ARG:NH2	2.15	0.55
5:C:47:VAL:HG23	5:C:84:PHE:HB3	1.89	0.55
7:E:144:ILE:HA	7:E:147:ASP:OD2	2.07	0.55
7:E:173:LEU:HA	7:E:178:PHE:HD2	1.71	0.55
7:E:28:VAL:O	7:E:30:GLU:N	2.40	0.55
11:I:10:VAL:HG13	11:I:17:ARG:C	2.27	0.55
11:I:77:ILE:C	11:I:77:ILE:HD13	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:79:PHE:HE2	11:I:102:VAL:CG1	2.18	0.55
20:R:81:VAL:HG22	20:R:82:GLN:N	2.20	0.55
22:T:119:GLU:O	22:T:121:HIS:N	2.40	0.55
23:U:36:ILE:HG12	23:U:39:ARG:HH21	1.67	0.55
3:A:54:ARG:HE	3:A:54:ARG:HA	1.69	0.55
5:C:156:MET:HE1	5:C:157:ALA:H	1.71	0.55
6:D:62:GLN:O	6:D:63:LYS:C	2.45	0.55
6:D:7:LEU:H	6:D:7:LEU:HD12	1.71	0.55
9:G:109:ILE:CG2	9:G:110:ASP:N	2.69	0.55
10:H:32:VAL:HG21	10:H:71:MET:CE	2.37	0.55
16:N:112:ARG:NH2	16:N:113:LYS:HE3	2.22	0.55
22:T:174:VAL:O	22:T:175:VAL:HG23	2.05	0.55
33:2:28:C:O5'	33:2:28:C:H6	1.90	0.55
6:D:179:TYR:CD2	6:D:179:TYR:N	2.62	0.55
6:D:196:VAL:O	6:D:196:VAL:HG13	2.06	0.55
8:F:149:ARG:CA	8:F:153:LYS:HG3	2.29	0.55
14:L:53:HIS:HB2	14:L:56:LYS:HE2	1.88	0.55
16:N:30:VAL:HG12	16:N:42:ILE:HG21	1.89	0.55
16:N:45:PHE:CE2	16:N:64:ARG:HA	2.41	0.55
22:T:78:LYS:H	22:T:78:LYS:HD2	1.72	0.55
26:X:21:ALA:HA	26:X:24:LYS:HZ2	1.72	0.55
4:B:27:THR:C	4:B:29:PRO:HD2	2.27	0.55
6:D:149:VAL:HG22	6:D:168:VAL:CG1	2.37	0.55
6:D:112:ARG:NH1	6:D:185:GLU:OE2	2.37	0.55
7:E:31:VAL:HG22	7:E:32:PRO:CD	2.37	0.55
9:G:6:LEU:HD22	9:G:7:GLU:HG2	1.89	0.55
10:H:37:VAL:HG22	10:H:158:PRO:O	2.07	0.55
13:K:42:ILE:O	13:K:94:VAL:HA	2.06	0.55
15:M:106:ARG:HD3	15:M:111:GLU:HA	1.88	0.55
15:M:24:LEU:H	15:M:85:VAL:HG23	1.73	0.55
17:O:109:LEU:O	17:O:112:ARG:HB2	2.07	0.55
18:P:43:GLU:CG	18:P:44:LYS:N	2.70	0.55
22:T:77:ASP:HB3	22:T:82:ARG:O	2.07	0.55
23:U:50:ASN:HB3	23:U:64:ASP:O	2.06	0.55
33:2:47:U:O4	33:2:50:U:H5''	2.07	0.54
10:H:65:TRP:CZ3	10:H:71:MET:SD	3.00	0.54
13:K:51:ARG:O	13:K:54:MET:HB3	2.08	0.54
24:V:12:PRO:HG3	24:V:63:ALA:HB2	1.88	0.54
33:2:17:U:H6	33:2:17:U:O5'	1.90	0.54
3:A:53:ARG:HA	3:A:53:ARG:HE	1.73	0.54
3:A:54:ARG:HB3	3:A:56:ASP:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:VAL:HG12	4:B:118:VAL:H	1.71	0.54
5:C:174:ASP:H	5:C:183:LEU:CD1	2.15	0.54
8:F:156:ALA:O	8:F:158:HIS:N	2.40	0.54
15:M:38:GLN:HA	15:M:50:SER:HB3	1.89	0.54
18:P:3:ALA:HA	18:P:41:GLY:O	2.07	0.54
19:Q:20:VAL:O	19:Q:20:VAL:HG12	2.07	0.54
18:P:24:LYS:HG2	18:P:25:LEU:H	1.70	0.54
24:V:31:GLY:O	24:V:32:LYS:HB2	2.07	0.54
4:B:79:VAL:HB	4:B:111:LEU:CG	2.37	0.54
5:C:52:LEU:HB3	5:C:76:ARG:N	2.22	0.54
9:G:98:ALA:CB	9:G:111:PRO:HG2	2.38	0.54
15:M:7:TYR:O	15:M:8:GLU:HB2	2.06	0.54
17:O:76:TYR:CG	17:O:77:SER:N	2.74	0.54
21:S:61:ILE:CG2	21:S:62:GLU:N	2.70	0.54
24:V:10:LYS:HD2	24:V:15:ALA:H	1.73	0.54
33:2:34:G:OP1	33:2:34:G:H8	1.90	0.54
33:2:55:PSU:O2'	33:2:57:G:N7	2.36	0.54
6:D:24:ASN:HB3	6:D:27:LEU:HD11	1.90	0.54
8:F:126:PRO:HG3	8:F:130:ARG:HB2	1.88	0.54
10:H:140:PHE:CE2	10:H:141:LYS:HD3	2.42	0.54
11:I:15:GLY:HA2	11:I:47:ILE:O	2.07	0.54
16:N:78:LEU:O	16:N:81:PRO:HD2	2.07	0.54
20:R:63:LYS:HD3	20:R:64:LYS:N	2.22	0.54
25:W:4:SER:N	25:W:7:ARG:HG3	2.23	0.54
5:C:31:CYS:HB2	5:C:91:VAL:CG2	2.37	0.54
24:V:58:ILE:HG12	24:V:82:LEU:CD1	2.37	0.54
4:B:129:ASN:O	4:B:192:THR:HA	2.08	0.54
5:C:84:PHE:CD1	5:C:86:PRO:HD3	2.43	0.54
7:E:79:ASN:ND2	7:E:86:MET:SD	2.81	0.54
9:G:124:GLY:O	9:G:144:VAL:N	2.41	0.54
12:J:35:HIS:N	12:J:36:LYS:HZ3	2.05	0.54
23:U:26:TYR:CE2	23:U:29:GLN:HB2	2.42	0.54
26:X:6:VAL:HB	26:X:35:ARG:O	2.08	0.54
27:Y:16:ARG:HB2	27:Y:20:ARG:HH12	1.71	0.54
3:A:9:ARG:C	3:A:9:ARG:HD3	2.27	0.54
5:C:109:LYS:HG3	5:C:189:PRO:HB2	1.89	0.54
5:C:170:LEU:HD23	5:C:185:LYS:CB	2.27	0.54
5:C:172:VAL:HG12	5:C:173:VAL:N	2.22	0.54
5:C:50:GLY:O	5:C:51:PHE:HB2	2.06	0.54
6:D:5:PRO:HD2	6:D:9:PRO:HG2	1.88	0.54
7:E:120:LEU:CD1	7:E:178:PHE:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:44:LYS:HB2	10:H:83:ILE:CG2	2.37	0.54
13:K:46:GLN:NE2	13:K:126:PRO:HD3	2.13	0.54
15:M:39:ILE:O	15:M:48:LEU:HB2	2.08	0.54
16:N:17:THR:HG23	16:N:18:ASP:N	2.16	0.54
22:T:59:LEU:HB2	22:T:67:LEU:HB3	1.87	0.54
23:U:34:GLY:HA2	23:U:60:PHE:CE2	2.43	0.54
25:W:3:LEU:HD23	25:W:4:SER:N	2.23	0.54
19:Q:40:ASN:O	19:Q:41:LYS:HB2	2.08	0.54
28:Z:21:ARG:C	28:Z:23:ARG:N	2.61	0.54
3:A:34:ALA:HB2	3:A:179:ALA:CB	2.37	0.54
4:B:224:ALA:HA	4:B:231:HIS:HD2	1.73	0.54
5:C:27:LEU:HG	5:C:28:ALA:N	2.22	0.54
8:F:152:ARG:HB3	8:F:153:LYS:HD2	7.09	0.54
9:G:122:GLU:CG	9:G:123:LEU:HD22	2.38	0.54
9:G:7:GLU:CG	9:G:35:LEU:HD11	2.37	0.54
11:I:68:GLU:HB2	11:I:76:ALA:CB	2.27	0.54
12:J:96:THR:C	12:J:98:GLU:H	2.11	0.54
14:L:22:ARG:HH12	14:L:71:GLN:NE2	2.06	0.54
15:M:110:LEU:CG	15:M:111:GLU:H	2.19	0.54
19:Q:5:ALA:HB2	19:Q:54:ALA:HB2	1.90	0.54
20:R:54:VAL:HG22	20:R:55:ASN:N	2.23	0.54
22:T:23:LYS:O	22:T:25:PRO:HD3	2.06	0.54
25:W:38:GLN:O	25:W:40:SER:N	2.40	0.54
25:W:57:ILE:O	25:W:57:ILE:HG13	2.08	0.54
4:B:183:ARG:HD3	4:B:184:LYS:O	2.08	0.54
5:C:5:LEU:HD12	5:C:5:LEU:N	2.23	0.54
5:C:61:ARG:HD2	5:C:62:PRO:HD3	1.89	0.54
5:C:93:VAL:HG12	5:C:182:LEU:CB	2.13	0.54
6:D:150:LEU:O	6:D:187:LEU:HD23	2.08	0.54
9:G:63:ALA:HA	9:G:66:GLU:CB	2.33	0.54
11:I:121:VAL:O	11:I:122:LEU:HG	2.08	0.54
12:J:7:ARG:HG3	12:J:7:ARG:O	2.08	0.54
13:K:29:PHE:CE1	22:T:120:ILE:O	2.61	0.54
15:M:87:PHE:HB2	15:M:112:PHE:HE1	1.73	0.54
16:N:25:GLY:C	16:N:48:ILE:HG23	2.28	0.54
19:Q:80:PRO:HD2	19:Q:102:HIS:CD2	2.43	0.54
23:U:71:ASP:HA	23:U:78:TYR:H	1.73	0.54
19:Q:82:LEU:O	19:Q:97:LYS:HA	2.08	0.54
24:V:88:LYS:CG	24:V:89:GLU:H	2.16	0.54
5:C:44:TYR:HE2	5:C:46:ALA:CB	2.21	0.54
17:O:95:LEU:HD13	18:P:4:ILE:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:5:LEU:HB2	9:G:13:GLY:HA2	1.90	0.54
12:J:95:VAL:O	12:J:125:VAL:HG23	2.08	0.54
14:L:68:ARG:HG2	14:L:69:ASP:N	2.22	0.54
20:R:80:ILE:O	20:R:81:VAL:HB	2.07	0.54
21:S:73:ARG:HD3	21:S:78:ALA:HB2	1.89	0.54
22:T:9:TYR:HB2	22:T:62:PRO:HG2	1.90	0.54
25:W:31:GLU:O	25:W:32:LEU:O	2.26	0.54
25:W:29:LYS:O	25:W:32:LEU:HB2	2.07	0.54
27:Y:41:PRO:HB2	27:Y:42:PRO:HD2	1.89	0.54
4:B:111:LEU:HD12	4:B:115:GLN:CB	2.38	0.53
4:B:193:VAL:HG23	4:B:194:GLY:N	2.23	0.53
5:C:61:ARG:N	5:C:62:PRO:HD2	2.23	0.53
8:F:125:VAL:HG12	8:F:131:VAL:CG2	2.38	0.53
9:G:4:ILE:C	9:G:5:LEU:HD22	2.27	0.53
12:J:34:GLY:O	12:J:35:HIS:HB3	2.08	0.53
13:K:106:VAL:HG21	13:K:118:LEU:CD1	2.38	0.53
13:K:78:PRO:HD3	13:K:87:LYS:HB3	1.89	0.53
22:T:150:LEU:O	22:T:171:ILE:HD13	2.08	0.53
27:Y:8:LYS:O	27:Y:9:LYS:HE2	2.08	0.53
13:K:34:LEU:HA	13:K:130:LYS:O	2.08	0.53
13:K:33:GLY:CA	13:K:132:VAL:HB	2.38	0.53
4:B:69:ARG:NH2	4:B:118:VAL:O	2.42	0.53
9:G:131:LYS:HZ3	9:G:134:PRO:CA	2.22	0.53
10:H:42:GLU:HA	10:H:83:ILE:CD1	2.38	0.53
10:H:74:PHE:HA	10:H:142:ARG:HB2	1.90	0.53
13:K:32:PHE:C	13:K:132:VAL:HG11	2.28	0.53
13:K:73:PRO:HB3	13:K:89:ASN:O	2.08	0.53
16:N:99:LEU:CD1	16:N:102:ILE:HG12	2.38	0.53
22:T:150:LEU:HG	22:T:171:ILE:CD1	2.31	0.53
24:V:48:LYS:HG2	24:V:63:ALA:CA	2.22	0.53
16:N:26:ASP:HB3	16:N:91:ARG:CG	2.38	0.53
26:X:7:LYS:HA	26:X:33:GLN:O	2.08	0.53
4:B:155:LEU:O	4:B:156:ALA:HB3	2.08	0.53
4:B:6:PHE:C	4:B:8:PRO:HD3	2.28	0.53
6:D:149:VAL:HG22	6:D:168:VAL:HG12	1.90	0.53
11:I:43:VAL:HB	11:I:54:GLU:N	2.24	0.53
12:J:127:ALA:N	12:J:145:PRO:HG3	2.24	0.53
14:L:76:VAL:HA	14:L:79:LEU:CD1	2.38	0.53
16:N:66:VAL:HA	16:N:71:GLY:HA2	1.90	0.53
17:O:98:LEU:HD22	17:O:101:ARG:O	2.08	0.53
20:R:43:VAL:HA	20:R:46:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:23:ARG:HD3	21:S:38:ILE:CG2	2.36	0.53
25:W:36:ARG:C	25:W:38:GLN:H	2.10	0.53
26:X:49:LYS:HA	26:X:49:LYS:HZ2	1.72	0.53
33:2:2:C:H6	33:2:2:C:O5'	1.90	0.53
33:2:64:A:H2'	33:2:65:G:C8	2.43	0.53
19:Q:3:ALA:HB1	19:Q:107:LEU:HB2	1.89	0.53
17:O:74:LEU:HD22	17:O:75:ASN:N	2.23	0.53
6:D:48:THR:HG23	6:D:85:PHE:CZ	2.44	0.53
7:E:89:GLY:C	7:E:90:LEU:HD12	2.29	0.53
9:G:77:LEU:HD11	9:G:79:ILE:HB	1.89	0.53
10:H:80:ALA:HB3	10:H:146:TYR:H	1.73	0.53
11:I:10:VAL:CG2	11:I:17:ARG:O	2.57	0.53
23:U:41:ARG:HA	23:U:57:PHE:CG	2.43	0.53
24:V:9:GLY:HA3	24:V:61:ARG:NH1	2.24	0.53
19:Q:38:TYR:HD2	27:Y:41:PRO:HG3	1.70	0.53
22:T:77:ASP:HB2	22:T:84:GLU:HB3	1.89	0.53
25:W:22:GLU:O	25:W:25:VAL:HG22	2.08	0.53
7:E:17:PRO:HB3	7:E:20:ILE:HD12	1.90	0.53
7:E:56:ALA:O	7:E:60:LEU:HG	2.08	0.53
8:F:152:ARG:N	8:F:152:ARG:HD2	2.22	0.53
10:H:157:ARG:N	10:H:158:PRO:CD	2.71	0.53
13:K:32:PHE:HZ	13:K:111:GLU:HB3	1.72	0.53
14:L:38:VAL:CG2	14:L:39:PRO:HD3	2.39	0.53
17:O:98:LEU:HD12	17:O:106:PHE:CG	2.42	0.53
18:P:34:GLU:O	18:P:62:LEU:HD23	2.09	0.53
23:U:40:GLN:CG	23:U:41:ARG:N	2.67	0.53
23:U:37:LEU:HG	23:U:60:PHE:HA	1.91	0.53
22:T:128:VAL:HG13	22:T:133:ILE:HD13	1.90	0.53
33:2:14:A:H2'	33:2:15:G:H5'	1.91	0.53
3:A:216:THR:HA	3:A:221:PRO:O	2.09	0.53
5:C:127:ASP:O	5:C:128:SER:CB	2.56	0.53
5:C:93:VAL:O	5:C:96:PHE:O	2.26	0.53
6:D:52:VAL:O	6:D:52:VAL:CG1	2.56	0.53
7:E:12:TYR:N	7:E:12:TYR:CD2	2.76	0.53
12:J:46:LYS:HB3	12:J:51:PHE:CE2	2.44	0.53
19:Q:21:VAL:CG2	19:Q:22:ASP:N	2.71	0.53
13:K:61:GLY:CA	22:T:183:LEU:HG	2.23	0.53
25:W:59:ARG:O	25:W:61:LEU:N	2.37	0.53
16:N:107:ASP:O	16:N:111:ARG:CD	2.56	0.53
19:Q:66:GLU:O	19:Q:67:ASP:CB	2.57	0.53
4:B:117:VAL:HG12	4:B:118:VAL:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:112:ARG:CB	6:D:117:LYS:HD2	2.39	0.53
6:D:51:GLU:O	6:D:52:VAL:HG12	2.08	0.53
8:F:55:PRO:HG3	8:F:61:HIS:CE1	2.43	0.53
21:S:32:PRO:O	21:S:33:LYS:HB2	2.09	0.53
22:T:150:LEU:C	22:T:150:LEU:HD12	2.28	0.53
22:T:59:LEU:HD23	22:T:67:LEU:HD12	1.90	0.53
22:T:41:LEU:HD13	22:T:42:VAL:HG23	1.90	0.53
4:B:198:ASN:HB3	4:B:201:HIS:CE1	2.43	0.53
7:E:47:LYS:HB2	7:E:72:ARG:NH1	2.18	0.53
9:G:82:ARG:HG2	9:G:83:ALA:H	1.72	0.53
28:Z:24:THR:H	28:Z:28:ARG:CD	2.21	0.53
27:Y:16:ARG:HB2	27:Y:20:ARG:NH1	2.24	0.53
4:B:79:VAL:CB	4:B:111:LEU:HG	2.39	0.53
4:B:177:LEU:C	4:B:179:SER:H	2.12	0.53
5:C:177:PRO:O	5:C:180:ASN:N	2.39	0.53
7:E:83:ARG:O	7:E:85:GLY:N	2.42	0.53
8:F:144:VAL:C	8:F:146:ALA:H	2.11	0.53
8:F:41:MET:SD	8:F:55:PRO:CD	2.97	0.53
13:K:115:MET:O	13:K:118:LEU:HB2	2.09	0.53
19:Q:19:LEU:C	19:Q:21:VAL:H	2.12	0.53
24:V:27:GLU:HB2	24:V:33:LYS:O	2.08	0.53
33:2:75:C:H5'	33:2:76:A:OP1	2.09	0.53
13:K:35:VAL:C	13:K:103:MET:SD	2.88	0.53
4:B:69:ARG:HG2	4:B:190:TYR:CE2	2.43	0.53
4:B:8:PRO:HG2	4:B:15:PHE:H	1.74	0.53
11:I:101:PRO:CB	11:I:120:GLU:HB3	2.39	0.53
16:N:42:ILE:HG13	16:N:43:GLN:N	2.24	0.53
23:U:18:ALA:O	23:U:19:LYS:HB2	2.09	0.53
7:E:6:ALA:HB3	7:E:100:TRP:HZ2	1.69	0.53
9:G:61:ARG:C	9:G:63:ALA:H	2.11	0.53
14:L:63:ARG:HA	14:L:66:VAL:CG2	2.39	0.53
4:B:212:SER:C	4:B:217:ARG:HG2	2.29	0.52
5:C:28:ALA:H	5:C:181:LEU:HA	1.73	0.52
5:C:60:ASN:HB2	5:C:62:PRO:HD2	1.90	0.52
6:D:150:LEU:HB2	6:D:187:LEU:HD21	1.91	0.52
6:D:77:ILE:HG13	6:D:81:GLY:HA2	9.72	0.52
13:K:30:GLY:HA3	13:K:65:PHE:CE1	2.44	0.52
19:Q:8:ARG:HH11	19:Q:8:ARG:HG2	1.74	0.52
23:U:51:VAL:HG21	23:U:79:VAL:HB	1.90	0.52
22:T:71:VAL:HG13	22:T:87:ASP:O	2.09	0.52
23:U:16:SER:HA	23:U:20:ARG:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:ARG:C	3:A:197:LEU:H	2.12	0.52
3:A:59:VAL:HG22	3:A:166:ASN:HB3	1.90	0.52
4:B:79:VAL:HB	4:B:111:LEU:HD11	1.91	0.52
11:I:27:GLY:O	11:I:28:SER:HB3	2.09	0.52
11:I:16:ALA:HA	11:I:46:ALA:HB2	1.89	0.52
12:J:61:ARG:HE	12:J:61:ARG:H	1.57	0.52
12:J:83:VAL:CG2	12:J:84:ASN:N	2.72	0.52
14:L:11:ASN:O	14:L:12:ARG:HB2	2.09	0.52
23:U:51:VAL:HG11	23:U:79:VAL:HG23	1.90	0.52
33:2:73:A:C6	33:2:74:C:N4	2.77	0.52
15:M:20:ARG:HG3	15:M:21:THR:N	2.25	0.52
17:O:92:ARG:NE	18:P:11:GLN:OE1	2.42	0.52
17:O:95:LEU:C	17:O:97:ASP:N	2.62	0.52
23:U:44:ARG:H	23:U:57:PHE:HZ	1.56	0.52
23:U:16:SER:O	23:U:17:GLN:CB	2.56	0.52
21:S:37:VAL:O	21:S:39:VAL:N	2.36	0.52
22:T:138:GLU:HG2	22:T:139:VAL:N	2.24	0.52
10:H:66:THR:O	10:H:69:VAL:HG12	2.09	0.52
13:K:37:LEU:HB2	13:K:127:ILE:CB	2.38	0.52
16:N:18:ASP:O	16:N:19:LEU:C	2.48	0.52
22:T:106:GLY:C	22:T:108:PRO:HD3	2.29	0.52
27:Y:48:GLU:C	27:Y:50:GLY:H	2.13	0.52
20:R:12:VAL:CG2	20:R:13:LEU:N	2.47	0.52
5:C:173:VAL:N	5:C:183:LEU:CD1	2.72	0.52
7:E:3:LEU:HB2	7:E:100:TRP:CZ3	2.43	0.52
18:P:24:LYS:HB3	18:P:92:THR:OG1	2.10	0.52
23:U:28:GLY:H	23:U:69:PHE:HD2	1.57	0.52
10:H:140:PHE:CG	10:H:141:LYS:N	2.78	0.52
16:N:31:SER:HB3	16:N:42:ILE:O	2.10	0.52
25:W:14:ARG:HB3	25:W:54:LYS:HE2	1.91	0.52
25:W:26:ARG:HA	25:W:29:LYS:HG3	1.92	0.52
34:3:17:C:H2'	34:3:18:C:C6	2.44	0.52
6:D:196:VAL:O	6:D:196:VAL:CG1	2.56	0.52
16:N:42:ILE:HG13	16:N:43:GLN:H	1.72	0.52
4:B:88:ARG:HD2	4:B:90:ALA:HB2	1.91	0.52
5:C:25:VAL:HG13	5:C:183:LEU:CA	2.39	0.52
10:H:157:ARG:N	10:H:158:PRO:HD3	2.25	0.52
10:H:26:THR:O	10:H:27:TYR:HB3	2.09	0.52
11:I:74:GLY:O	11:I:75:SER:HB2	2.10	0.52
12:J:95:VAL:HA	12:J:100:LEU:HD21	1.91	0.52
13:K:3:MET:N	13:K:4:PRO:CD	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:42:ILE:CG2	13:K:95:ALA:HB3	2.39	0.52
17:O:14:HIS:O	17:O:17:ILE:HB	2.09	0.52
17:O:103:PRO:C	17:O:105:VAL:N	2.60	0.52
23:U:23:VAL:HG13	23:U:38:VAL:HG22	1.91	0.52
23:U:66:VAL:N	23:U:81:VAL:HG13	2.24	0.52
3:A:11:LEU:HD12	3:A:11:LEU:H	1.75	0.52
3:A:62:THR:CG2	3:A:63:VAL:H	2.23	0.52
4:B:221:VAL:C	4:B:223:GLY:H	2.12	0.52
4:B:7:LYS:N	4:B:8:PRO:HD3	2.24	0.52
7:E:103:LEU:HA	7:E:106:LEU:HD23	1.92	0.52
7:E:122:PRO:HA	7:E:131:TYR:OH	2.10	0.52
8:F:125:VAL:HB	8:F:128:PRO:HB2	1.91	0.52
8:F:44:VAL:HG22	8:F:45:VAL:N	2.24	0.52
11:I:64:ARG:HH12	11:I:100:GLY:HA3	1.75	0.52
12:J:47:ASP:HB2	12:J:48:PRO:HA	1.92	0.52
13:K:16:ARG:NH1	13:K:17:LEU:HD21	2.25	0.52
16:N:23:ARG:HH21	16:N:94:ALA:HB2	1.74	0.52
10:H:65:TRP:HD1	17:O:64:ARG:HE	1.54	0.52
19:Q:57:ASN:HA	19:Q:60:ASN:HB3	1.92	0.52
19:Q:6:ILE:N	19:Q:6:ILE:HD13	2.23	0.52
19:Q:18:ARG:NH1	19:Q:76:VAL:HG23	2.25	0.52
21:S:28:LYS:N	21:S:28:LYS:HD3	2.23	0.52
27:Y:36:CYS:O	27:Y:37:LYS:HB2	2.08	0.52
33:2:33:U:H3	33:2:36:A:P	2.32	0.52
9:G:63:ALA:HA	9:G:66:GLU:HG3	1.92	0.52
33:2:13:C:H2'	33:2:14:A:C1'	2.39	0.52
5:C:61:ARG:H	5:C:62:PRO:HD2	1.75	0.52
5:C:75:VAL:C	5:C:77:ILE:N	2.63	0.52
11:I:13:ASN:N	11:I:97:ARG:HB2	2.24	0.52
13:K:23:GLY:HA3	13:K:98:LYS:CA	2.39	0.52
5:C:111:ARG:HG3	14:L:3:HIS:HD2	1.73	0.52
15:M:40:ILE:CG2	15:M:41:ASP:N	2.71	0.52
20:R:77:LYS:HE3	20:R:77:LYS:HA	1.92	0.52
23:U:24:LYS:HG3	23:U:25:ARG:HG2	1.91	0.52
27:Y:12:SER:OG	27:Y:15:ARG:NH2	2.42	0.52
27:Y:41:PRO:HG2	27:Y:44:THR:OG1	2.09	0.52
8:F:135:GLY:H	8:F:138:LYS:HZ2	1.57	0.52
9:G:68:LEU:O	9:G:72:LEU:HG	2.10	0.52
10:H:106:LYS:HG3	10:H:107:LYS:H	1.75	0.52
11:I:16:ALA:C	11:I:17:ARG:HD3	2.30	0.52
24:V:21:ARG:HG3	24:V:22:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:223:GLY:C	4:B:225:ALA:H	2.12	0.52
14:L:29:LEU:CD2	14:L:75:LEU:HD22	2.40	0.52
16:N:26:ASP:CA	16:N:48:ILE:HD12	2.40	0.52
16:N:45:PHE:CD2	16:N:63:VAL:HG23	2.45	0.52
16:N:51:ARG:HB3	16:N:62:THR:CG2	2.39	0.52
18:P:18:LEU:H	18:P:98:GLU:CD	2.13	0.52
20:R:53:LYS:O	20:R:79:ALA:HA	2.10	0.52
8:F:177:GLY:O	8:F:178:ALA:HB3	2.10	0.52
3:A:54:ARG:HH12	33:2:53:G:H1'	1.75	0.52
3:A:176:VAL:HG13	3:A:177:GLY:H	1.75	0.52
9:G:82:ARG:HG2	9:G:83:ALA:N	2.24	0.52
10:H:40:ASP:OD1	10:H:79:ASN:O	2.28	0.52
11:I:24:VAL:CG2	11:I:25:LEU:H	2.07	0.52
11:I:85:VAL:CG1	11:I:86:ILE:N	2.56	0.52
12:J:144:GLU:HB3	12:J:145:PRO:HD2	1.92	0.52
12:J:7:ARG:N	12:J:8:PRO:CD	2.72	0.52
14:L:63:ARG:CD	14:L:67:LEU:HD21	2.39	0.52
16:N:95:ARG:O	16:N:96:ARG:HB3	2.10	0.52
27:Y:12:SER:C	27:Y:14:ALA:N	2.62	0.52
9:G:53:ALA:O	9:G:57:ARG:HD3	2.10	0.52
19:Q:23:LEU:HD13	27:Y:25:LEU:CG	2.34	0.52
33:2:34:G:C3'	33:2:35:A:C5'	2.88	0.52
14:L:94:TYR:HB3	14:L:117:VAL:HG11	1.91	0.52
4:B:181:GLU:HG3	4:B:272:ALA:O	2.10	0.52
4:B:19:ALA:HA	4:B:201:HIS:HD2	1.74	0.52
4:B:267:SER:O	4:B:268:ARG:HB2	2.10	0.52
5:C:116:VAL:C	5:C:118:LYS:H	2.13	0.52
6:D:151:LEU:N	6:D:151:LEU:HD23	2.25	0.52
8:F:59:ARG:HG2	8:F:60:ARG:N	2.24	0.52
11:I:41:ALA:O	11:I:57:VAL:HA	2.10	0.52
12:J:138:LEU:HD23	12:J:143:GLY:N	2.25	0.52
15:M:26:LEU:HD21	15:M:85:VAL:HG11	1.92	0.52
10:H:64:ASP:OD2	17:O:100:VAL:HG12	2.10	0.52
18:P:72:VAL:HG12	18:P:73:SER:N	2.25	0.52
19:Q:18:ARG:HH11	19:Q:76:VAL:HG23	1.74	0.52
13:K:42:ILE:HG22	13:K:95:ALA:O	2.10	0.52
33:2:7:U:H2'	33:2:49:C:H5'	1.91	0.51
4:B:79:VAL:HG12	4:B:113:VAL:O	2.10	0.51
5:C:103:ASP:O	5:C:104:VAL:CB	2.58	0.51
6:D:163:ARG:HG3	6:D:164:ASN:N	2.24	0.51
6:D:163:ARG:NH2	6:D:164:ASN:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:29:TRP:HB3	6:D:33:ARG:HH11	1.75	0.51
7:E:109:VAL:O	7:E:112:PRO:HD2	2.09	0.51
12:J:84:ASN:HD21	12:J:86:LYS:HB2	1.75	0.51
14:L:28:LEU:HB3	14:L:34:ILE:HG12	1.91	0.51
14:L:2:ARG:CG	14:L:3:HIS:H	2.04	0.51
17:O:68:ALA:O	17:O:72:HIS:HB2	2.11	0.51
18:P:4:ILE:HG22	18:P:5:VAL:N	2.25	0.51
20:R:74:PRO:HB2	20:R:76:ARG:HE	1.74	0.51
13:K:135:ASP:HA	22:T:48:PHE:CE1	2.45	0.51
22:T:81:ARG:O	22:T:83:PRO:HD3	2.10	0.51
22:T:99:TYR:CG	22:T:125:LEU:HD13	2.45	0.51
25:W:15:LYS:O	25:W:17:SER:N	2.40	0.51
28:Z:13:ALA:O	28:Z:20:ALA:HB3	2.11	0.51
4:B:147:LEU:O	4:B:148:GLU:C	2.48	0.51
4:B:78:LYS:HA	4:B:115:GLN:O	2.10	0.51
6:D:29:TRP:HB3	6:D:33:ARG:NH1	2.24	0.51
9:G:109:ILE:HG23	9:G:110:ASP:N	2.24	0.51
10:H:56:LEU:CD1	10:H:61:HIS:HB3	2.40	0.51
13:K:119:ARG:N	13:K:119:ARG:HD2	2.25	0.51
13:K:72:LYS:HZ2	13:K:73:PRO:CB	2.22	0.51
15:M:35:ILE:CD1	15:M:66:ALA:HA	2.40	0.51
15:M:51:ALA:HB3	15:M:73:LEU:HD11	1.92	0.51
16:N:17:THR:O	16:N:19:LEU:N	2.43	0.51
16:N:31:SER:OG	16:N:32:TYR:N	2.43	0.51
16:N:3:ARG:O	16:N:4:GLY:C	2.48	0.51
17:O:5:LYS:HD2	17:O:5:LYS:O	2.10	0.51
21:S:20:TYR:O	21:S:21:LYS:HB2	2.10	0.51
22:T:72:ARG:O	22:T:73:GLN:HG3	2.11	0.51
5:C:122:PHE:HE2	5:C:138:PRO:CB	2.21	0.51
7:E:149:VAL:C	7:E:151:ALA:H	2.12	0.51
8:F:40:GLU:OE1	8:F:55:PRO:HB3	2.09	0.51
9:G:27:ARG:HH21	9:G:27:ARG:HB2	1.76	0.51
25:W:54:LYS:C	25:W:55:ARG:HD2	2.31	0.51
3:A:197:LEU:HG	3:A:198:GLU:H	1.75	0.51
7:E:120:LEU:CD2	7:E:121:ASN:H	2.22	0.51
7:E:135:LEU:HD13	7:E:155:MET:HG2	1.92	0.51
7:E:31:VAL:HG22	7:E:32:PRO:HD2	1.91	0.51
14:L:12:ARG:HG3	14:L:12:ARG:HH11	1.75	0.51
14:L:1:MET:O	14:L:2:ARG:C	2.48	0.51
15:M:54:LEU:O	15:M:56:LEU:O	2.28	0.51
16:N:28:VAL:HG22	16:N:44:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:42:ALA:O	17:O:46:ALA:HB2	2.11	0.51
19:Q:82:LEU:HD13	19:Q:83:LYS:N	2.25	0.51
22:T:150:LEU:HD12	22:T:151:HIS:C	2.30	0.51
22:T:30:ASN:HA	22:T:89:PHE:CE1	2.45	0.51
26:X:49:LYS:HG3	26:X:50:VAL:N	2.26	0.51
14:L:13:HIS:HB3	14:L:16:HIS:CD2	2.45	0.51
14:L:83:ILE:O	14:L:87:TYR:CD1	2.57	0.51
3:A:167:ASP:H	3:A:171:ALA:CA	2.14	0.51
4:B:3:VAL:HG13	4:B:17:THR:OG1	2.11	0.51
7:E:111:LEU:O	7:E:112:PRO:C	2.48	0.51
8:F:87:LEU:HD23	8:F:133:VAL:HG13	1.93	0.51
9:G:27:ARG:HH22	9:G:28:ASN:ND2	2.09	0.51
12:J:35:HIS:CG	12:J:36:LYS:N	2.79	0.51
13:K:78:PRO:O	13:K:79:LEU:HB2	2.11	0.51
18:P:36:PRO:O	18:P:59:ALA:HB1	2.09	0.51
21:S:53:PRO:O	21:S:54:LYS:CB	2.59	0.51
23:U:22:GLY:O	23:U:24:LYS:N	2.44	0.51
17:O:83:LEU:HD23	17:O:84:LYS:NZ	2.26	0.51
4:B:208:LYS:HZ3	4:B:209:ALA:HB3	1.76	0.51
4:B:224:ALA:HA	4:B:231:HIS:CD2	2.46	0.51
5:C:7:VAL:O	5:C:9:VAL:HG13	2.11	0.51
6:D:12:ARG:O	6:D:13:ARG:HB3	2.11	0.51
6:D:172:ALA:CB	6:D:173:PRO:HD3	2.39	0.51
7:E:107:LEU:O	7:E:111:LEU:CB	2.59	0.51
9:G:77:LEU:HD22	9:G:78:THR:N	2.25	0.51
9:G:5:LEU:CD2	9:G:9:LEU:HD12	2.40	0.51
12:J:88:LEU:O	12:J:88:LEU:CG	2.57	0.51
13:K:134:ARG:HD3	13:K:135:ASP:N	2.26	0.51
14:L:90:ARG:HB2	14:L:94:TYR:CE2	2.45	0.51
15:M:67:ARG:HA	15:M:104:GLY:HA3	1.92	0.51
15:M:68:GLN:O	15:M:71:ARG:HG2	2.10	0.51
22:T:44:PHE:CD2	22:T:45:ASP:N	2.79	0.51
25:W:51:ARG:HH11	25:W:51:ARG:HG3	1.74	0.51
26:X:34:GLU:O	26:X:36:VAL:HG13	2.11	0.51
27:Y:44:THR:HG22	27:Y:45:VAL:H	1.75	0.51
14:L:102:GLU:CG	14:L:103:ARG:N	2.74	0.51
25:W:8:LYS:HA	25:W:11:GLU:HB3	1.92	0.51
5:C:79:ARG:O	5:C:80:GLU:HG3	2.11	0.51
6:D:58:LYS:O	6:D:59:ILE:HG23	2.11	0.51
8:F:86:GLU:HA	8:F:132:ARG:HA	1.92	0.51
8:F:11:VAL:HA	8:F:15:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:55:PRO:HG2	8:F:61:HIS:CG	2.46	0.51
12:J:46:LYS:HB3	12:J:51:PHE:HZ	1.75	0.51
12:J:83:VAL:HG13	12:J:114:ILE:HA	1.93	0.51
17:O:21:ALA:HB2	17:O:39:LEU:CD2	2.41	0.51
22:T:39:VAL:HG12	22:T:40:ASP:N	2.25	0.51
24:V:21:ARG:HG3	24:V:22:GLY:H	1.75	0.51
21:S:49:VAL:O	21:S:54:LYS:O	2.29	0.51
3:A:214:TYR:CD2	3:A:222:SER:HB2	2.46	0.51
5:C:184:VAL:O	5:C:184:VAL:HG23	4.60	0.51
6:D:32:VAL:HG23	6:D:33:ARG:N	2.25	0.51
9:G:24:GLY:O	9:G:27:ARG:NH2	2.44	0.51
10:H:35:ARG:HD2	10:H:73:ASP:OD2	2.11	0.51
10:H:41:ALA:C	10:H:43:GLY:H	2.13	0.51
11:I:111:PHE:HB3	11:I:114:ILE:CG1	2.39	0.51
12:J:132:LYS:O	12:J:135:LEU:HB3	2.11	0.51
13:K:37:LEU:CD1	13:K:128:LYS:HB2	2.36	0.51
5:C:176:ILE:HG21	5:C:181:LEU:HD23	1.92	0.51
5:C:8:LYS:HG2	5:C:190:GLY:O	2.10	0.51
7:E:79:ASN:ND2	7:E:81:LYS:H	2.08	0.51
8:F:127:GLU:N	8:F:128:PRO:HA	2.25	0.51
8:F:77:LYS:O	8:F:77:LYS:HD3	2.11	0.51
9:G:77:LEU:CD2	9:G:100:ALA:HB1	2.40	0.51
9:G:131:LYS:NZ	9:G:134:PRO:HA	2.26	0.51
12:J:97:PRO:HG2	12:J:126:VAL:HB	1.93	0.51
19:Q:85:VAL:CG1	19:Q:95:ILE:HG22	2.35	0.51
20:R:57:LEU:HD21	20:R:59:VAL:HG22	1.91	0.51
19:Q:38:TYR:O	27:Y:28:PRO:HG3	2.10	0.51
33:2:69:U:O5'	33:2:69:U:C6	2.63	0.51
13:K:89:ASN:ND2	13:K:90:VAL:H	2.09	0.51
15:M:40:ILE:CG2	15:M:41:ASP:H	2.24	0.51
4:B:93:ALA:O	4:B:104:TYR:HA	2.11	0.51
4:B:140:THR:CG2	4:B:165:ILE:HD13	2.41	0.51
4:B:259:THR:CG2	4:B:260:ARG:N	2.60	0.51
5:C:37:ARG:HB2	5:C:45:THR:N	2.26	0.51
12:J:50:ARG:NH2	12:J:57:THR:OG1	2.44	0.51
12:J:96:THR:O	12:J:98:GLU:N	2.44	0.51
16:N:50:ILE:HG13	16:N:63:VAL:CA	2.41	0.51
17:O:14:HIS:HA	17:O:17:ILE:HD13	1.93	0.51
20:R:65:ARG:CZ	20:R:65:ARG:HA	2.38	0.51
24:V:21:ARG:O	24:V:39:LYS:HG3	2.11	0.51
25:W:37:PHE:O	25:W:39:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:15:LEU:HD23	6:D:114:ARG:HH12	1.76	0.50
6:D:166:PRO:O	6:D:167:TRP:CB	2.57	0.50
6:D:176:LEU:CD2	6:D:178:VAL:HG22	2.41	0.50
6:D:48:THR:HG23	6:D:49:ARG:N	2.20	0.50
7:E:115:ARG:HA	7:E:115:ARG:HH11	1.76	0.50
7:E:59:GLU:OE2	7:E:151:ALA:HB1	2.11	0.50
9:G:69:LYS:O	9:G:69:LYS:HD3	2.11	0.50
14:L:51:LEU:HD12	14:L:52:ILE:N	2.27	0.50
15:M:35:ILE:O	15:M:35:ILE:HG23	2.10	0.50
15:M:62:LYS:HA	15:M:97:ARG:NH1	2.27	0.50
18:P:78:LYS:O	18:P:78:LYS:HG3	2.10	0.50
22:T:19:ARG:HE	22:T:25:PRO:HG2	1.76	0.50
23:U:62:LEU:HD23	23:U:63:VAL:CG2	2.36	0.50
23:U:81:VAL:O	23:U:83:PRO:HD3	2.11	0.50
24:V:70:VAL:HG23	24:V:71:TYR:H	1.74	0.50
17:O:16:LYS:O	17:O:20:LEU:HD23	2.11	0.50
33:2:68:U:O2'	33:2:69:U:H5'	2.12	0.50
4:B:133:LEU:HD23	4:B:189:CYS:HB2	1.93	0.50
7:E:12:TYR:HD2	7:E:12:TYR:H	1.58	0.50
9:G:130:TYR:HB3	9:G:138:ILE:HG23	1.93	0.50
9:G:23:PRO:HB2	9:G:27:ARG:CZ	2.41	0.50
16:N:35:LYS:HE2	16:N:40:THR:OG1	2.11	0.50
17:O:50:ARG:HH21	17:O:50:ARG:HG2	1.76	0.50
17:O:92:ARG:O	17:O:94:ASN:N	2.44	0.50
19:Q:88:ARG:HH11	19:Q:93:ALA:HA	1.74	0.50
22:T:8:TYR:HD1	22:T:39:VAL:HG13	1.75	0.50
24:V:88:LYS:CG	24:V:89:GLU:OE2	2.59	0.50
25:W:50:ILE:O	25:W:51:ARG:CB	2.58	0.50
18:P:58:VAL:O	18:P:59:ALA:HB2	2.11	0.50
7:E:81:LYS:O	7:E:82:LEU:HB2	2.11	0.50
11:I:77:ILE:HG23	11:I:79:PHE:CE1	2.46	0.50
12:J:13:ASN:O	12:J:13:ASN:ND2	2.44	0.50
13:K:81:VAL:HG21	13:K:82:ARG:NH1	2.27	0.50
16:N:32:TYR:O	16:N:33:LYS:O	2.29	0.50
16:N:83:ILE:HG13	16:N:84:GLN:H	1.76	0.50
18:P:60:GLU:OE1	18:P:62:LEU:HD22	2.11	0.50
20:R:27:THR:HA	20:R:78:LYS:CB	2.38	0.50
22:T:28:MET:SD	22:T:35:ARG:HB2	2.52	0.50
23:U:28:GLY:N	23:U:69:PHE:HB2	2.23	0.50
18:P:64:HIS:HA	18:P:96:ILE:HG23	1.94	0.50
25:W:53:LEU:HD23	25:W:54:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:88:ARG:HH11	4:B:88:ARG:HG2	1.77	0.50
6:D:128:ASN:HA	6:D:134:PHE:CE1	2.46	0.50
6:D:132:LYS:HA	6:D:135:LEU:HB3	1.93	0.50
8:F:7:LEU:HB2	8:F:8:PRO:HD3	1.94	0.50
10:H:39:ILE:CG1	10:H:40:ASP:H	2.24	0.50
12:J:50:ARG:NH2	12:J:50:ARG:CG	2.65	0.50
13:K:133:ARG:HG3	22:T:81:ARG:HH21	1.76	0.50
14:L:11:ASN:O	14:L:12:ARG:CB	2.60	0.50
19:Q:45:TYR:CG	19:Q:45:TYR:O	2.63	0.50
25:W:54:LYS:N	25:W:55:ARG:HD2	2.25	0.50
27:Y:41:PRO:HB2	27:Y:42:PRO:CD	2.41	0.50
3:A:223:VAL:CG1	3:A:224:ARG:H	2.09	0.50
4:B:126:GLN:O	4:B:193:VAL:CG2	2.57	0.50
5:C:81:ILE:O	5:C:83:ASP:N	2.44	0.50
12:J:41:ARG:NH1	12:J:45:LEU:HG	2.27	0.50
13:K:119:ARG:O	13:K:121:ALA:N	2.45	0.50
14:L:22:ARG:HH22	14:L:71:GLN:NE2	2.09	0.50
5:C:109:LYS:HZ3	14:L:4:LEU:HD11	1.76	0.50
27:Y:29:ILE:HG12	27:Y:42:PRO:HD3	1.93	0.50
15:M:49:VAL:CG2	15:M:50:SER:H	2.23	0.50
24:V:87:PRO:HA	24:V:91:LYS:HZ2	1.77	0.50
6:D:129:GLY:HA2	6:D:161:ALA:HB2	1.93	0.50
6:D:130:LYS:HD3	6:D:131:THR:H	1.77	0.50
10:H:25:LYS:O	10:H:27:TYR:N	2.44	0.50
16:N:50:ILE:CG1	16:N:64:ARG:HB2	2.42	0.50
18:P:40:LEU:HD13	18:P:41:GLY:N	2.25	0.50
18:P:23:GLU:HB3	18:P:91:TYR:OH	2.11	0.50
19:Q:88:ARG:O	19:Q:89:ALA:O	2.30	0.50
22:T:28:MET:O	22:T:29:TYR:HB3	2.11	0.50
26:X:10:LYS:HB2	26:X:53:LEU:CA	2.42	0.50
26:X:7:LYS:HB3	26:X:34:GLU:CB	2.42	0.50
14:L:27:SER:C	14:L:29:LEU:H	2.14	0.50
13:K:66:ILE:HG22	13:K:104:PHE:CD1	2.46	0.50
33:2:51:G:H2'	33:2:52:U:O4'	2.11	0.50
13:K:26:TYR:CD2	13:K:27:VAL:HG22	2.46	0.50
33:2:31:A:H61	33:2:39:U:H3	1.60	0.50
14:L:62:ALA:HB1	14:L:80:PHE:CE1	2.47	0.50
15:M:40:ILE:HG12	15:M:47:THR:HA	1.93	0.50
16:N:42:ILE:O	16:N:43:GLN:HB2	2.11	0.50
17:O:61:TRP:HB3	17:O:93:LYS:O	2.12	0.50
23:U:35:ASN:N	23:U:61:ALA:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:5:TYR:CE2	25:W:26:ARG:HG2	2.38	0.50
4:B:90:ALA:O	4:B:92:ILE:N	2.45	0.50
5:C:149:ARG:HH12	5:C:152:LYS:HD2	1.75	0.50
10:H:97:ARG:HH12	10:H:127:LYS:HB3	1.75	0.50
10:H:77:VAL:HB	10:H:145:VAL:HG12	1.93	0.50
10:H:36:TRP:CE3	10:H:155:ALA:O	2.64	0.50
10:H:57:LEU:C	10:H:57:LEU:HD13	2.32	0.50
11:I:93:PRO:C	11:I:95:GLY:N	2.65	0.50
14:L:79:LEU:C	14:L:83:ILE:HB	2.31	0.50
18:P:43:GLU:CG	18:P:44:LYS:H	2.25	0.50
19:Q:11:ARG:O	19:Q:98:LYS:HE2	2.12	0.50
23:U:41:ARG:HG2	23:U:42:GLY:N	2.27	0.50
4:B:100:GLY:O	4:B:101:GLU:HG3	2.12	0.50
5:C:120:TRP:O	5:C:121:ASN:CB	2.59	0.50
7:E:120:LEU:HD13	7:E:121:ASN:C	2.32	0.50
7:E:43:LEU:HG	7:E:153:ARG:CZ	2.42	0.50
9:G:24:GLY:H	9:G:27:ARG:NH1	2.10	0.50
10:H:146:TYR:CG	10:H:147:ALA:N	2.80	0.50
10:H:25:LYS:HD2	10:H:25:LYS:H	1.77	0.50
12:J:96:THR:HG23	12:J:99:LEU:HB3	1.92	0.50
16:N:67:SER:O	16:N:69:GLY:N	2.45	0.50
16:N:78:LEU:HD23	16:N:79:HIS:HB2	1.94	0.50
18:P:13:ARG:HH11	18:P:13:ARG:N	1.96	0.50
23:U:52:GLY:HA2	23:U:62:LEU:CD1	2.40	0.50
24:V:91:LYS:CA	24:V:91:LYS:HE3	2.41	0.50
14:L:76:VAL:HG13	14:L:79:LEU:HD12	1.93	0.50
26:X:17:LYS:O	26:X:18:ASP:C	2.50	0.50
18:P:79:VAL:HG12	18:P:80:GLN:N	2.27	0.49
6:D:120:LEU:CD2	6:D:123:ALA:HB2	2.41	0.49
9:G:38:LEU:H	9:G:38:LEU:CD1	2.21	0.49
9:G:5:LEU:HB2	9:G:13:GLY:CA	2.42	0.49
9:G:81:VAL:CG1	9:G:144:VAL:HG13	2.42	0.49
10:H:79:ASN:N	10:H:147:ALA:HA	2.27	0.49
10:H:29:PRO:CA	10:H:64:ASP:HB3	2.41	0.49
12:J:5:ASP:C	12:J:6:LEU:HD12	2.32	0.49
14:L:79:LEU:CD2	14:L:83:ILE:HG13	2.42	0.49
16:N:30:VAL:O	16:N:85:LYS:HG2	2.12	0.49
16:N:47:GLY:O	16:N:63:VAL:HB	2.11	0.49
16:N:64:ARG:HG2	16:N:65:LYS:N	2.26	0.49
18:P:13:ARG:H	18:P:13:ARG:NH1	1.97	0.49
20:R:88:LYS:O	20:R:89:ILE:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:101:PRO:HA	22:T:123:ASP:OD1	2.12	0.49
22:T:120:ILE:HG21	22:T:170:THR:O	2.11	0.49
25:W:13:ALA:O	25:W:14:ARG:HG2	2.12	0.49
26:X:11:SER:O	26:X:53:LEU:HD13	2.12	0.49
26:X:49:LYS:C	26:X:51:ALA:H	2.15	0.49
22:T:167:PRO:C	22:T:169:GLU:H	2.15	0.49
33:2:72:C:N4	33:2:73:A:N6	2.59	0.49
4:B:174:ILE:O	4:B:175:LEU:HB2	2.12	0.49
4:B:228:PRO:C	4:B:229:VAL:HG23	2.32	0.49
5:C:114:ALA:O	5:C:157:ALA:HB1	2.12	0.49
5:C:154:LYS:HG3	5:C:155:LYS:O	2.11	0.49
5:C:33:VAL:HG13	5:C:47:VAL:CG1	2.40	0.49
6:D:72:ASP:C	6:D:74:GLY:H	2.15	0.49
6:D:44:ALA:CB	6:D:87:PRO:HB2	2.41	0.49
8:F:163:TYR:OH	8:F:169:VAL:HG11	2.12	0.49
8:F:72:ILE:O	8:F:75:ALA:HB3	2.12	0.49
10:H:145:VAL:C	10:H:146:TYR:HD2	2.15	0.49
12:J:85:LEU:CD2	12:J:119:GLU:H	2.19	0.49
13:K:8:LYS:N	13:K:8:LYS:HZ2	2.10	0.49
14:L:28:LEU:HA	14:L:34:ILE:HD11	1.93	0.49
16:N:123:LYS:O	16:N:123:LYS:HD2	2.12	0.49
17:O:106:PHE:O	17:O:109:LEU:HG	2.12	0.49
24:V:55:GLY:H	24:V:58:ILE:HD11	1.77	0.49
26:X:36:VAL:O	26:X:37:LEU:HD13	2.12	0.49
27:Y:13:LYS:O	27:Y:16:ARG:CG	2.60	0.49
16:N:45:PHE:CE1	16:N:72:VAL:HB	2.47	0.49
16:N:50:ILE:HG13	16:N:64:ARG:N	2.28	0.49
18:P:24:LYS:HG2	18:P:25:LEU:O	2.12	0.49
33:2:65:G:C2	33:2:66:A:C8	3.00	0.49
8:F:87:LEU:CD2	8:F:133:VAL:HG13	2.42	0.49
20:R:63:LYS:CD	20:R:64:LYS:H	2.25	0.49
3:A:45:HIS:ND1	3:A:173:HIS:HB3	2.26	0.49
4:B:105:ILE:HG12	4:B:106:ILE:H	1.78	0.49
8:F:14:GLY:O	8:F:16:SER:N	2.45	0.49
8:F:39:PRO:O	8:F:41:MET:N	2.38	0.49
11:I:39:ILE:HD13	11:I:39:ILE:N	2.26	0.49
12:J:57:THR:HG23	12:J:57:THR:O	2.11	0.49
16:N:26:ASP:CA	16:N:48:ILE:HG23	2.40	0.49
18:P:34:GLU:C	18:P:35:LEU:HD23	2.32	0.49
21:S:25:GLY:HA3	21:S:28:LYS:HE3	1.94	0.49
21:S:50:ARG:HG3	21:S:54:LYS:HZ3	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:40:GLU:CB	21:S:62:GLU:HG2	2.41	0.49
25:W:18:PRO:O	25:W:22:GLU:HB2	2.12	0.49
28:Z:15:THR:O	28:Z:16:HIS:ND1	2.46	0.49
13:K:55:VAL:O	13:K:58:PHE:N	2.44	0.49
3:A:193:PHE:HD2	3:A:193:PHE:C	2.15	0.49
5:C:117:MET:CA	5:C:122:PHE:H	2.24	0.49
6:D:95:THR:C	6:D:96:LEU:HD22	2.32	0.49
11:I:61:VAL:CG1	11:I:85:VAL:H	2.18	0.49
12:J:85:LEU:H	12:J:85:LEU:HD13	1.76	0.49
18:P:90:PRO:O	18:P:91:TYR:HB3	2.12	0.49
19:Q:24:ILE:CG2	19:Q:36:LEU:HD11	2.42	0.49
22:T:26:GLY:HA2	22:T:85:HIS:CD2	2.47	0.49
4:B:228:PRO:O	4:B:229:VAL:HG23	2.12	0.49
5:C:93:VAL:CB	5:C:182:LEU:HD13	2.32	0.49
5:C:50:GLY:O	5:C:76:ARG:HD2	2.12	0.49
7:E:139:LEU:HA	7:E:144:ILE:O	2.13	0.49
7:E:96:ARG:CG	7:E:97:ASP:H	2.25	0.49
9:G:130:TYR:CD2	9:G:131:LYS:N	2.80	0.49
11:I:50:GLY:O	11:I:51:ALA:HB2	2.13	0.49
15:M:27:SER:HB2	15:M:89:ARG:HG3	1.95	0.49
17:O:106:PHE:HA	17:O:109:LEU:HD21	1.95	0.49
21:S:61:ILE:HG23	21:S:62:GLU:N	2.28	0.49
22:T:99:TYR:CE1	22:T:125:LEU:HD22	2.48	0.49
7:E:99:MET:SD	7:E:100:TRP:N	2.85	0.49
9:G:15:VAL:CG1	9:G:17:GLN:HG2	2.42	0.49
10:H:108:ILE:CG2	10:H:113:MET:HB2	2.43	0.49
28:Z:11:LYS:HE3	28:Z:15:THR:OG1	2.13	0.49
33:2:49:C:O5'	33:2:49:C:H6	1.95	0.49
3:A:214:TYR:HD2	3:A:222:SER:HB2	1.78	0.49
4:B:138:VAL:HG13	4:B:139:GLY:N	2.22	0.49
4:B:166:GLN:NE2	4:B:176:ARG:HB2	2.27	0.49
7:E:96:ARG:CD	7:E:97:ASP:H	2.25	0.49
15:M:58:LEU:HD23	15:M:60:GLY:N	2.26	0.49
16:N:106:SER:CA	16:N:110:ILE:HD13	2.34	0.49
10:H:60:LYS:O	17:O:64:ARG:NH1	2.45	0.49
18:P:23:GLU:CD	18:P:24:LYS:H	2.16	0.49
21:S:13:VAL:HA	21:S:23:ARG:O	2.11	0.49
23:U:39:ARG:HD3	23:U:58:THR:HG21	1.95	0.49
7:E:152:LEU:O	7:E:153:ARG:HB2	2.12	0.49
21:S:37:VAL:HG23	21:S:37:VAL:O	2.12	0.49
27:Y:39:MET:N	27:Y:39:MET:SD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:156:GLU:HA	6:D:159:ARG:HG3	1.93	0.49
6:D:48:THR:N	6:D:52:VAL:HG21	2.27	0.49
10:H:57:LEU:HD12	10:H:139:LEU:HB3	1.88	0.49
13:K:28:ALA:HB1	13:K:105:GLU:OE2	2.12	0.49
16:N:84:GLN:OE1	16:N:86:ILE:HD11	2.12	0.49
21:S:28:LYS:HA	21:S:35:TYR:CB	2.42	0.49
22:T:51:ALA:HA	22:T:54:HIS:HB2	1.94	0.49
23:U:50:ASN:HD22	23:U:81:VAL:CG1	2.25	0.49
33:2:24:G:H2'	33:2:25:C:O4'	2.13	0.49
4:B:39:LYS:HG3	4:B:40:THR:N	2.18	0.49
4:B:2:ALA:O	4:B:3:VAL:C	2.50	0.49
4:B:76:PRO:CG	4:B:117:VAL:HG12	2.41	0.49
9:G:43:ASN:O	9:G:47:LEU:HD23	2.12	0.49
9:G:90:GLY:O	9:G:91:SER:CB	2.61	0.49
13:K:136:ALA:O	13:K:137:TYR:CB	2.59	0.49
5:C:111:ARG:HG3	14:L:3:HIS:CD2	2.46	0.49
16:N:53:ARG:O	16:N:59:THR:OG1	2.24	0.49
17:O:35:ALA:O	17:O:39:LEU:HG	2.13	0.49
19:Q:7:ALA:HB2	19:Q:20:VAL:HG22	11.06	0.49
24:V:89:GLU:HG2	24:V:90:ILE:H	1.78	0.49
33:2:49:C:C2	33:2:66:A:C2	3.01	0.49
4:B:89:SER:O	4:B:159:ALA:HA	2.13	0.49
4:B:3:VAL:HG23	4:B:200:ASP:HB3	1.95	0.49
6:D:121:VAL:HG13	6:D:191:LEU:N	2.27	0.49
7:E:16:ARG:HB3	7:E:17:PRO:CD	2.42	0.49
10:H:102:PRO:CG	10:H:103:GLY:H	2.24	0.49
12:J:24:GLY:HA3	12:J:31:ALA:HB2	1.95	0.49
17:O:47:TYR:O	17:O:51:LYS:HB2	2.13	0.49
17:O:66:ASN:O	17:O:70:ARG:HG3	2.12	0.49
18:P:7:THR:HG21	18:P:22:VAL:HG22	1.89	0.49
19:Q:5:ALA:HB3	19:Q:105:VAL:HB	1.95	0.49
22:T:124:ILE:HG13	22:T:125:LEU:N	2.28	0.49
23:U:28:GLY:O	23:U:66:VAL:HB	2.12	0.49
23:U:51:VAL:HG21	23:U:79:VAL:CG2	2.43	0.49
33:2:53:G:N3	33:2:62:A:C2	2.81	0.49
4:B:117:VAL:HG13	4:B:128:GLY:C	2.33	0.49
4:B:43:ARG:O	4:B:51:VAL:HG22	2.13	0.49
6:D:179:TYR:HD2	6:D:179:TYR:N	2.05	0.49
6:D:19:LEU:N	6:D:20:PRO:HD2	2.28	0.49
14:L:84:ALA:O	14:L:87:TYR:C	2.51	0.49
16:N:50:ILE:O	16:N:97:ALA:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:63:LYS:HB2	20:R:70:LEU:HB3	1.95	0.49
26:X:52:HIS:NE2	26:X:53:LEU:HD22	2.28	0.49
24:V:18:ILE:N	24:V:18:ILE:HD12	2.27	0.49
4:B:146:GLU:OE2	4:B:150:LYS:HA	2.12	0.49
4:B:146:GLU:HA	4:B:152:GLY:O	2.13	0.49
9:G:81:VAL:O	9:G:82:ARG:CB	2.61	0.49
22:T:110:GLY:HA2	22:T:146:ILE:HD12	1.92	0.49
3:A:201:LYS:NZ	3:A:203:GLU:HA	2.28	0.48
4:B:20:ASP:O	4:B:22:SER:N	2.46	0.48
8:F:34:GLU:HG2	8:F:35:VAL:H	1.78	0.48
11:I:91:LEU:HB2	11:I:111:PHE:HE1	1.78	0.48
11:I:88:ASN:N	11:I:93:PRO:HA	2.23	0.48
16:N:131:ALA:O	16:N:132:LYS:HG3	2.13	0.48
11:I:77:ILE:HD13	11:I:78:ARG:C	2.33	0.48
16:N:26:ASP:O	16:N:26:ASP:OD1	2.31	0.48
17:O:32:PHE:O	17:O:36:ARG:HB2	2.13	0.48
18:P:62:LEU:N	18:P:62:LEU:CD2	2.75	0.48
33:2:36:A:N6	33:2:37:A:C5	2.82	0.48
6:D:112:ARG:O	6:D:117:LYS:HG2	2.13	0.48
6:D:146:SER:N	6:D:167:TRP:CZ2	2.81	0.48
6:D:29:TRP:O	6:D:32:VAL:HG22	2.12	0.48
7:E:11:TYR:HD2	7:E:12:TYR:CD2	2.31	0.48
7:E:167:GLU:O	7:E:170:ARG:HG2	2.13	0.48
7:E:35:GLU:O	7:E:36:LYS:HG3	2.13	0.48
7:E:48:GLU:HG2	7:E:84:LYS:HB3	1.95	0.48
7:E:55:LYS:HD3	7:E:56:ALA:N	2.28	0.48
8:F:147:ASN:O	8:F:151:ILE:HG13	2.13	0.48
8:F:153:LYS:NZ	8:F:163:TYR:HD1	2.11	0.48
9:G:121:LYS:O	9:G:122:GLU:O	2.31	0.48
9:G:5:LEU:HB3	9:G:8:PRO:HD2	1.94	0.48
18:P:77:ALA:O	18:P:78:LYS:CB	2.61	0.48
21:S:34:LYS:HA	21:S:64:GLU:O	2.13	0.48
22:T:80:ARG:HG3	22:T:82:ARG:H	1.78	0.48
24:V:58:ILE:CG2	24:V:86:SER:HB2	2.42	0.48
18:P:51:VAL:HG12	18:P:52:VAL:H	1.78	0.48
7:E:125:PHE:HB3	7:E:131:TYR:CE1	2.48	0.48
11:I:10:VAL:HG13	11:I:17:ARG:O	2.13	0.48
24:V:87:PRO:CB	24:V:91:LYS:HD2	2.42	0.48
26:X:23:LEU:HA	26:X:26:LEU:HB2	1.95	0.48
20:R:40:LYS:O	20:R:44:GLU:HB3	2.13	0.48
24:V:18:ILE:HA	24:V:44:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:25:C:O5'	33:2:25:C:H6	1.95	0.48
4:B:17:THR:HB	4:B:205:VAL:N	2.27	0.48
5:C:141:ILE:HD13	5:C:141:ILE:N	2.28	0.48
5:C:25:VAL:HG13	5:C:182:LEU:O	2.13	0.48
6:D:145:GLY:HA2	6:D:167:TRP:CE2	2.48	0.48
6:D:183:ARG:HG2	12:J:7:ARG:CB	2.43	0.48
7:E:109:VAL:HG11	7:E:142:PRO:HB3	1.95	0.48
8:F:127:GLU:HB2	8:F:129:THR:H	1.78	0.48
8:F:10:PRO:HB2	8:F:12:PRO:HD3	1.96	0.48
8:F:18:GLU:O	8:F:19:VAL:HB	2.13	0.48
16:N:38:ASN:H	16:N:38:ASN:HD22	1.59	0.48
18:P:4:ILE:HG23	18:P:12:TYR:O	2.13	0.48
18:P:94:LEU:HD13	18:P:96:ILE:HD13	1.95	0.48
23:U:19:LYS:O	23:U:20:ARG:HB2	2.13	0.48
4:B:75:ILE:H	4:B:76:PRO:HD3	1.78	0.48
5:C:117:MET:HB3	5:C:136:ARG:HH22	1.76	0.48
5:C:154:LYS:HD2	5:C:155:LYS:N	2.19	0.48
5:C:192:ASN:OD1	16:N:4:GLY:CA	2.60	0.48
7:E:59:GLU:OE2	7:E:151:ALA:CB	2.62	0.48
11:I:104:ARG:HD3	11:I:104:ARG:N	3.14	0.48
12:J:89:ALA:O	12:J:121:LYS:HD2	2.12	0.48
15:M:28:VAL:O	15:M:29:PHE:HB2	2.12	0.48
15:M:85:VAL:O	15:M:85:VAL:HG22	2.13	0.48
24:V:87:PRO:HA	24:V:91:LYS:HZ3	1.78	0.48
33:2:53:G:C6	33:2:54:U:C4	3.01	0.48
24:V:51:VAL:CG1	24:V:52:ARG:H	2.25	0.48
4:B:196:VAL:CG1	4:B:197:GLY:N	2.76	0.48
5:C:108:SER:HB3	5:C:165:VAL:CG2	2.43	0.48
5:C:155:LYS:O	5:C:156:MET:HB2	2.12	0.48
5:C:32:PRO:HD3	5:C:51:PHE:HD2	1.78	0.48
7:E:156:ASP:C	7:E:157:ILE:HD12	2.34	0.48
7:E:94:LEU:HA	7:E:95:ARG:NH1	2.28	0.48
10:H:106:LYS:HG3	10:H:107:LYS:N	2.29	0.48
12:J:139:LYS:O	12:J:140:ALA:HB3	2.13	0.48
16:N:124:ASP:N	16:N:124:ASP:OD1	2.46	0.48
21:S:99:CYS:O	21:S:100:ALA:HB2	2.13	0.48
21:S:12:THR:O	21:S:13:VAL:HG23	2.14	0.48
22:T:163:LEU:HD12	22:T:163:LEU:H	1.78	0.48
4:B:118:VAL:O	4:B:129:ASN:HA	2.13	0.48
4:B:227:ASN:O	4:B:228:PRO:O	2.32	0.48
24:V:11:ARG:CB	24:V:12:PRO:CD	2.83	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:79:VAL:HG13	6:D:79:VAL:O	2.13	0.48
7:E:11:TYR:HD2	7:E:12:TYR:CG	2.32	0.48
9:G:65:ALA:HB1	9:G:133:HIS:HD1	1.78	0.48
10:H:107:LYS:HG3	10:H:108:ILE:N	2.14	0.48
10:H:113:MET:HA	10:H:116:THR:CG2	2.38	0.48
16:N:11:GLU:C	16:N:13:ARG:N	2.66	0.48
17:O:95:LEU:O	17:O:97:ASP:N	2.47	0.48
18:P:18:LEU:O	18:P:19:LYS:CB	2.61	0.48
28:Z:43:THR:HG23	28:Z:43:THR:O	2.14	0.48
19:Q:28:SER:C	19:Q:71:VAL:HG23	2.34	0.48
20:R:30:VAL:HG13	20:R:31:HIS:N	2.29	0.48
11:I:16:ALA:O	11:I:17:ARG:HD3	2.14	0.48
33:2:73:A:C2	33:2:74:C:C4	3.01	0.48
8:F:9:ILE:HD12	8:F:10:PRO:HD2	1.95	0.48
10:H:101:TYR:N	10:H:102:PRO:CD	2.77	0.48
13:K:98:LYS:HB2	13:K:101:ARG:HD3	1.95	0.48
14:L:21:TYR:HA	14:L:24:GLN:HG3	1.96	0.48
16:N:112:ARG:HH21	16:N:113:LYS:HE3	1.77	0.48
16:N:16:ARG:O	16:N:79:HIS:CE1	2.66	0.48
18:P:30:GLY:O	18:P:31:ALA:HB2	2.14	0.48
18:P:14:VAL:HB	18:P:98:GLU:OE1	2.14	0.48
23:U:27:GLU:HA	23:U:69:PHE:CD2	2.48	0.48
23:U:68:GLU:O	23:U:79:VAL:HA	2.12	0.48
26:X:7:LYS:HB3	26:X:34:GLU:CA	2.43	0.48
19:Q:23:LEU:CB	27:Y:25:LEU:HG	2.43	0.48
26:X:49:LYS:HE3	26:X:52:HIS:CE1	2.49	0.48
17:O:91:ASP:O	17:O:95:LEU:HB2	2.13	0.48
3:A:197:LEU:CG	3:A:198:GLU:N	2.77	0.48
5:C:150:VAL:O	5:C:151:TYR:C	2.52	0.48
5:C:48:GLN:HG2	5:C:78:LEU:HB2	1.95	0.48
12:J:20:GLY:O	12:J:21:ARG:HG2	2.14	0.48
12:J:44:GLY:O	12:J:45:LEU:O	2.31	0.48
13:K:52:VAL:CG2	13:K:53:ALA:N	2.76	0.48
17:O:55:ARG:HG2	17:O:55:ARG:NH1	2.25	0.48
24:V:85:LEU:O	24:V:86:SER:HB2	2.13	0.48
26:X:4:LEU:HD11	26:X:56:VAL:HB	1.95	0.48
24:V:76:ARG:NH2	24:V:94:LEU:HG	2.28	0.48
33:2:49:C:C1'	33:2:66:A:C2	2.96	0.48
4:B:88:ARG:HG3	4:B:89:SER:N	2.28	0.48
8:F:89:ILE:HD12	8:F:89:ILE:H	1.79	0.48
9:G:77:LEU:HD23	9:G:100:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:42:GLU:HA	10:H:83:ILE:HD13	1.96	0.48
10:H:41:ALA:H	10:H:44:LYS:HG3	1.79	0.48
11:I:24:VAL:HA	11:I:39:ILE:HG22	1.95	0.48
11:I:64:ARG:HE	11:I:83:ALA:CB	2.25	0.48
12:J:126:VAL:HA	12:J:145:PRO:HB3	1.95	0.48
12:J:39:LYS:HZ2	12:J:39:LYS:HB3	1.79	0.48
15:M:63:THR:HG23	15:M:64:GLU:N	2.29	0.48
18:P:22:VAL:O	18:P:23:GLU:HG3	2.13	0.48
18:P:43:GLU:HG3	18:P:44:LYS:N	2.29	0.48
20:R:5:TYR:OH	25:W:30:ARG:NH2	2.46	0.48
21:S:39:VAL:HG12	21:S:40:GLU:N	2.24	0.48
23:U:24:LYS:HG2	23:U:37:LEU:O	2.13	0.48
34:3:11:A:H2'	34:3:12:A:C2	2.48	0.48
3:A:162:ILE:HG13	3:A:162:ILE:O	2.13	0.48
3:A:176:VAL:HG13	3:A:177:GLY:N	2.29	0.48
3:A:41:THR:HA	3:A:178:LYS:HD2	1.95	0.48
4:B:108:PRO:HD2	4:B:111:LEU:HD22	1.91	0.48
5:C:81:ILE:O	5:C:82:ARG:C	2.52	0.48
9:G:125:GLU:O	9:G:126:TYR:CB	2.62	0.48
11:I:77:ILE:HG23	11:I:79:PHE:HE1	1.79	0.48
12:J:56:SER:O	12:J:59:LEU:HB3	2.13	0.48
14:L:62:ALA:HB1	14:L:80:PHE:CZ	2.49	0.48
14:L:62:ALA:O	14:L:66:VAL:HG13	2.14	0.48
26:X:12:PRO:HG2	26:X:13:ILE:H	1.79	0.48
24:V:58:ILE:HG21	24:V:86:SER:HB2	1.95	0.48
27:Y:16:ARG:CG	27:Y:17:ASP:N	2.76	0.48
22:T:18:LEU:HD13	22:T:38:TYR:CD2	2.49	0.47
4:B:69:ARG:HH12	4:B:76:PRO:HD3	1.78	0.47
5:C:151:TYR:HD1	5:C:151:TYR:H	1.62	0.47
6:D:45:SER:O	6:D:87:PRO:CG	2.62	0.47
7:E:55:LYS:O	7:E:58:GLN:HB3	2.14	0.47
10:H:145:VAL:C	10:H:146:TYR:CD2	2.88	0.47
10:H:29:PRO:HB3	10:H:64:ASP:C	2.35	0.47
11:I:32:TYR:O	11:I:33:ALA:HB2	2.13	0.47
12:J:148:LEU:H	12:J:148:LEU:CD1	2.26	0.47
13:K:28:ALA:HB1	13:K:105:GLU:CD	2.34	0.47
15:M:39:ILE:HD11	15:M:49:VAL:CG1	2.29	0.47
16:N:42:ILE:CG1	16:N:43:GLN:H	2.25	0.47
16:N:99:LEU:HG	16:N:102:ILE:CG1	2.40	0.47
20:R:29:TRP:CG	20:R:76:ARG:HG2	2.49	0.47
3:A:209:PHE:CD1	3:A:210:LEU:HG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:75:ILE:HG21	4:B:99:ASP:HB3	1.95	0.47
5:C:47:VAL:O	5:C:80:GLU:HG2	2.13	0.47
5:C:8:LYS:O	5:C:192:ASN:HA	2.13	0.47
6:D:112:ARG:N	6:D:112:ARG:HD2	2.29	0.47
6:D:117:LYS:HE3	6:D:185:GLU:HG3	1.96	0.47
8:F:100:GLY:O	8:F:101:ARG:CB	2.62	0.47
8:F:125:VAL:HB	8:F:128:PRO:CA	2.44	0.47
9:G:69:LYS:O	9:G:70:GLU:HB2	2.14	0.47
15:M:62:LYS:HG3	15:M:63:THR:N	2.29	0.47
15:M:8:GLU:O	15:M:9:ARG:HB2	2.14	0.47
17:O:27:LEU:C	17:O:29:SER:H	2.18	0.47
22:T:4:ARG:O	22:T:5:LEU:HD22	2.13	0.47
33:2:28:C:C2'	33:2:29:A:H5'	2.44	0.47
6:D:44:ALA:HB1	6:D:87:PRO:CB	2.43	0.47
7:E:132:ASN:C	7:E:133:LEU:HD22	2.34	0.47
9:G:94:ALA:O	9:G:97:ILE:HG12	2.13	0.47
18:P:73:SER:HB2	18:P:89:GLN:N	2.27	0.47
19:Q:59:VAL:HG12	19:Q:59:VAL:O	2.14	0.47
26:X:7:LYS:HB3	26:X:34:GLU:HA	1.95	0.47
27:Y:46:CYS:HB3	27:Y:47:PRO:HD2	1.96	0.47
6:D:163:ARG:HH22	6:D:164:ASN:HB3	1.79	0.47
3:A:29:LEU:C	3:A:33:LEU:HG	2.34	0.47
4:B:103:ARG:HA	4:B:103:ARG:NE	2.29	0.47
4:B:147:LEU:HG	4:B:148:GLU:H	1.78	0.47
4:B:6:PHE:CD1	4:B:16:MET:O	2.67	0.47
5:C:53:PRO:O	5:C:55:ASN:OD1	2.33	0.47
6:D:28:LEU:O	6:D:32:VAL:HG22	2.14	0.47
6:D:32:VAL:HG23	6:D:33:ARG:H	1.79	0.47
6:D:39:ARG:HG3	6:D:40:ARG:H	1.79	0.47
8:F:8:PRO:CB	8:F:49:VAL:HA	2.44	0.47
8:F:90:LYS:HD3	8:F:90:LYS:N	2.29	0.47
12:J:135:LEU:O	12:J:139:LYS:HB2	2.15	0.47
13:K:107:ALA:O	13:K:109:VAL:N	2.47	0.47
13:K:115:MET:HA	13:K:118:LEU:HD22	1.97	0.47
16:N:12:SER:HA	16:N:15:VAL:HG22	1.97	0.47
17:O:51:LYS:NZ	17:O:55:ARG:HH21	2.12	0.47
17:O:66:ASN:ND2	17:O:70:ARG:NH2	2.61	0.47
21:S:19:LYS:O	21:S:20:TYR:CB	2.57	0.47
28:Z:13:ALA:O	28:Z:20:ALA:CB	2.63	0.47
17:O:74:LEU:HD22	17:O:75:ASN:O	2.14	0.47
22:T:145:GLU:O	22:T:147:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:161:VAL:CG1	22:T:162:GLU:N	2.77	0.47
25:W:53:LEU:O	25:W:54:LYS:HB3	2.14	0.47
4:B:111:LEU:HD13	4:B:115:GLN:HB3	1.95	0.47
5:C:151:TYR:C	5:C:153:GLY:H	2.17	0.47
10:H:157:ARG:O	10:H:159:GLU:N	2.47	0.47
10:H:58:ARG:HD2	10:H:65:TRP:CZ2	2.50	0.47
22:T:24:LEU:CG	22:T:41:LEU:HA	2.44	0.47
24:V:26:ARG:N	24:V:26:ARG:HD3	2.23	0.47
27:Y:38:ALA:HB1	27:Y:40:LYS:HG3	1.95	0.47
27:Y:51:TYR:O	27:Y:52:TYR:HB3	2.13	0.47
25:W:52:ASP:HA	25:W:55:ARG:NH2	2.30	0.47
4:B:255:LYS:NZ	4:B:255:LYS:HB2	2.29	0.47
4:B:63:ARG:CB	4:B:85:ASP:HB2	2.44	0.47
6:D:109:VAL:CA	6:D:112:ARG:HG2	2.45	0.47
6:D:149:VAL:HG23	6:D:150:LEU:N	2.29	0.47
9:G:128:LEU:HD23	9:G:140:LEU:O	2.14	0.47
11:I:70:LYS:H	11:I:76:ALA:CB	2.27	0.47
12:J:107:LYS:CG	12:J:108:LYS:H	2.21	0.47
14:L:99:LYS:HG2	14:L:100:LEU:N	2.29	0.47
18:P:92:THR:OG1	18:P:93:GLU:N	2.46	0.47
21:S:31:LEU:CD2	21:S:31:LEU:N	3.27	0.47
22:T:66:SER:O	22:T:67:LEU:HB2	2.15	0.47
23:U:31:VAL:HB	23:U:61:ALA:CB	2.44	0.47
4:B:35:LYS:HE3	4:B:64:ILE:N	2.22	0.47
22:T:33:LEU:HD12	22:T:34:ASN:N	2.28	0.47
33:2:9:A:H62	33:2:23:A:N6	2.08	0.47
4:B:177:LEU:O	4:B:179:SER:N	2.47	0.47
9:G:73:GLU:C	9:G:75:LEU:H	2.18	0.47
11:I:43:VAL:HB	11:I:53:LYS:C	2.35	0.47
11:I:74:GLY:O	11:I:75:SER:CB	2.62	0.47
13:K:64:ILE:HG23	13:K:65:PHE:N	2.29	0.47
15:M:104:GLY:C	15:M:106:ARG:H	2.18	0.47
15:M:95:HIS:O	15:M:96:GLY:C	2.53	0.47
20:R:12:VAL:HG23	20:R:13:LEU:HD23	1.96	0.47
22:T:99:TYR:CE2	22:T:125:LEU:HB2	2.49	0.47
24:V:21:ARG:CG	24:V:22:GLY:N	2.77	0.47
28:Z:43:THR:O	28:Z:44:PRO:C	2.53	0.47
3:A:37:LYS:HG3	3:A:38:PHE:H	1.80	0.47
4:B:77:ALA:O	4:B:117:VAL:CG2	2.60	0.47
5:C:79:ARG:C	5:C:80:GLU:HG3	2.35	0.47
6:D:108:ALA:O	6:D:112:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:108:ALA:C	6:D:112:ARG:HG2	2.35	0.47
7:E:71:THR:HB	7:E:88:ILE:HD12	1.96	0.47
15:M:106:ARG:HD2	15:M:110:LEU:O	2.14	0.47
22:T:9:TYR:CE2	22:T:61:LEU:HD11	2.50	0.47
24:V:66:HIS:CG	24:V:69:LYS:HE3	2.49	0.47
24:V:88:LYS:HG3	24:V:89:GLU:OE2	2.15	0.47
33:2:36:A:OP2	33:2:36:A:H8	1.97	0.47
22:T:135:GLU:OE2	22:T:135:GLU:N	2.47	0.47
22:T:58:VAL:C	22:T:59:LEU:HD22	2.35	0.47
26:X:30:ARG:HD3	26:X:30:ARG:O	2.14	0.47
14:L:63:ARG:HD3	14:L:67:LEU:HD21	1.96	0.47
17:O:93:LYS:CD	17:O:93:LYS:H	2.28	0.47
19:Q:62:HIS:N	19:Q:62:HIS:CD2	2.83	0.47
33:2:29:A:HO2'	33:2:30:G:H5'	1.76	0.47
4:B:119:ALA:HB1	4:B:190:TYR:OH	2.14	0.47
6:D:15:LEU:HD23	6:D:114:ARG:NH1	2.30	0.47
7:E:8:LYS:O	7:E:12:TYR:HD2	1.98	0.47
8:F:156:ALA:C	8:F:158:HIS:H	2.18	0.47
8:F:153:LYS:CD	8:F:163:TYR:HA	2.44	0.47
8:F:20:ALA:HB3	8:F:23:ARG:O	2.15	0.47
10:H:94:ILE:HG13	10:H:95:TYR:N	2.30	0.47
10:H:95:TYR:N	10:H:95:TYR:CD1	2.83	0.47
11:I:104:ARG:HH11	11:I:104:ARG:CG	2.27	0.47
11:I:112:MET:O	11:I:113:LYS:C	2.53	0.47
12:J:46:LYS:CB	12:J:51:PHE:HZ	2.28	0.47
16:N:115:ARG:O	16:N:116:ALA:CB	2.63	0.47
18:P:30:GLY:CA	18:P:65:GLY:HA2	2.44	0.47
19:Q:104:THR:HG22	19:Q:105:VAL:N	2.30	0.47
22:T:150:LEU:CD1	22:T:154:ASP:CG	2.83	0.47
25:W:59:ARG:HG2	25:W:59:ARG:O	2.15	0.47
12:J:84:ASN:HA	12:J:116:GLY:HA3	1.97	0.47
16:N:29:ARG:HG2	16:N:86:ILE:HB	1.95	0.47
18:P:22:VAL:C	18:P:23:GLU:HG3	2.34	0.47
4:B:247:ALA:CB	4:B:253:GLN:HA	2.44	0.47
4:B:60:ARG:NH2	4:B:86:PRO:CB	2.77	0.47
5:C:156:MET:CE	5:C:157:ALA:H	2.28	0.47
5:C:37:ARG:O	5:C:45:THR:HA	2.15	0.47
6:D:117:LYS:O	6:D:118:LEU:HB2	2.14	0.47
7:E:67:LYS:O	7:E:67:LYS:HG3	2.15	0.47
8:F:151:ILE:O	8:F:152:ARG:HB2	2.15	0.47
10:H:101:TYR:N	10:H:102:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:49:LEU:O	10:H:52:LYS:HB2	2.14	0.47
11:I:117:LEU:O	11:I:119:PRO:HD3	2.15	0.47
11:I:85:VAL:O	11:I:86:ILE:HG13	2.14	0.47
12:J:126:VAL:HA	12:J:145:PRO:CB	2.45	0.47
13:K:83:MET:HG2	13:K:84:GLY:N	2.30	0.47
17:O:44:ASN:O	17:O:48:ALA:CB	2.61	0.47
19:Q:11:ARG:HD2	19:Q:98:LYS:HZ3	1.79	0.47
20:R:12:VAL:HG13	20:R:17:ALA:HB1	1.96	0.47
13:K:55:VAL:HG11	22:T:182:LYS:O	2.15	0.47
23:U:62:LEU:CD2	23:U:63:VAL:HG23	2.38	0.47
24:V:89:GLU:HG2	24:V:90:ILE:HG13	1.97	0.47
23:U:50:ASN:HB2	23:U:81:VAL:HG11	1.97	0.47
14:L:29:LEU:CG	14:L:75:LEU:HD22	2.44	0.47
18:P:22:VAL:HG22	18:P:22:VAL:O	2.15	0.47
33:2:65:G:O2'	33:2:66:A:H5'	2.15	0.47
4:B:62:TYR:CE2	4:B:64:ILE:HD12	2.50	0.47
5:C:51:PHE:HB3	5:C:76:ARG:CZ	2.45	0.47
6:D:186:ARG:O	6:D:187:LEU:HG	2.15	0.47
6:D:48:THR:H	6:D:52:VAL:HG21	1.79	0.47
9:G:122:GLU:OE1	9:G:126:TYR:HB2	2.15	0.47
19:Q:14:PRO:O	19:Q:17:VAL:HG22	2.15	0.47
4:B:83:GLU:HB2	4:B:92:ILE:CD1	2.41	0.47
14:L:103:ARG:O	14:L:104:ARG:O	2.33	0.47
6:D:73:ILE:C	6:D:75:ALA:N	2.69	0.46
7:E:141:PHE:CE2	7:E:143:GLU:HB3	2.50	0.46
11:I:93:PRO:HG3	11:I:114:ILE:HG23	1.97	0.46
17:O:89:GLU:O	17:O:90:VAL:HB	2.15	0.46
23:U:15:ASP:H	23:U:20:ARG:NH1	2.13	0.46
33:2:26:G:C2'	33:2:27:C:H5'	2.45	0.46
15:M:77:ALA:HB1	15:M:82:ILE:O	2.16	0.46
4:B:70:TRP:N	4:B:70:TRP:CE3	2.83	0.46
5:C:134:ILE:HG22	5:C:137:HIS:CD2	2.50	0.46
5:C:154:LYS:CD	5:C:155:LYS:N	2.79	0.46
6:D:22:GLU:O	6:D:107:MET:SD	2.73	0.46
10:H:131:PRO:O	10:H:132:LYS:HB3	2.15	0.46
10:H:68:ASN:HD22	10:H:68:ASN:HA	3.33	0.46
14:L:32:GLY:O	14:L:115:GLU:HA	2.16	0.46
18:P:64:HIS:HA	18:P:96:ILE:CG2	2.45	0.46
20:R:21:PHE:HD2	20:R:26:TYR:HE1	1.63	0.46
22:T:29:TYR:OH	22:T:73:GLN:NE2	2.46	0.46
22:T:71:VAL:HG11	22:T:74:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:89:GLU:HG2	24:V:90:ILE:N	2.31	0.46
33:2:18:G:C4	33:2:57:G:N2	2.83	0.46
16:N:23:ARG:HD3	16:N:120:ARG:HD3	1.97	0.46
21:S:49:VAL:HG12	21:S:50:ARG:N	2.24	0.46
26:X:10:LYS:HB3	26:X:11:SER:H	1.49	0.46
22:T:13:GLU:O	22:T:15:PRO:HD3	2.15	0.46
3:A:54:ARG:NH2	33:2:53:G:N3	2.58	0.46
33:2:65:G:H2'	33:2:66:A:H5'	1.97	0.46
4:B:91:ARG:CB	4:B:198:ASN:HB2	2.45	0.46
4:B:53:PHE:HA	4:B:218:ARG:CB	2.44	0.46
7:E:126:ASP:HB3	7:E:130:ASN:HB2	1.97	0.46
9:G:38:LEU:HB2	9:G:39:ALA:H	1.46	0.46
11:I:101:PRO:CG	11:I:120:GLU:HB3	2.45	0.46
11:I:77:ILE:HD13	11:I:78:ARG:N	2.30	0.46
23:U:66:VAL:O	23:U:81:VAL:HG13	2.16	0.46
16:N:31:SER:N	16:N:42:ILE:HB	2.24	0.46
26:X:52:HIS:CD2	26:X:53:LEU:HD22	2.51	0.46
33:2:28:C:O2'	33:2:29:A:H5'	2.15	0.46
33:2:14:A:C2'	33:2:15:G:H5'	2.46	0.46
5:C:16:ARG:O	5:C:19:ARG:CG	2.63	0.46
5:C:77:ILE:HG21	5:C:79:ARG:NH2	2.31	0.46
6:D:172:ALA:HB3	6:D:173:PRO:HD2	1.94	0.46
12:J:59:LEU:O	12:J:61:ARG:NE	2.49	0.46
17:O:43:GLY:O	17:O:47:TYR:HB3	2.16	0.46
18:P:29:PRO:HA	18:P:66:ARG:HB3	1.97	0.46
18:P:82:ARG:HG2	18:P:82:ARG:HH11	1.80	0.46
18:P:96:ILE:O	18:P:97:LYS:HE2	2.16	0.46
20:R:81:VAL:HG13	20:R:82:GLN:N	2.31	0.46
21:S:42:VAL:HB	21:S:61:ILE:HG22	1.97	0.46
24:V:13:ILE:HD13	24:V:66:HIS:CE1	2.50	0.46
33:2:36:A:H2'	33:2:37:A:C5'	2.36	0.46
5:C:105:THR:HB	5:C:197:ILE:CD1	2.42	0.46
5:C:78:LEU:H	5:C:78:LEU:HD23	1.79	0.46
6:D:152:VAL:CG2	6:D:171:LEU:HD22	2.43	0.46
10:H:132:LYS:H	10:H:132:LYS:HE3	1.81	0.46
10:H:29:PRO:HA	10:H:64:ASP:HB3	1.96	0.46
10:H:63:PRO:O	10:H:65:TRP:N	2.49	0.46
10:H:69:VAL:O	10:H:69:VAL:HG13	2.15	0.46
11:I:71:ARG:HG2	11:I:72:PRO:CD	2.44	0.46
11:I:81:ASP:C	11:I:82:ASN:OD1	2.54	0.46
12:J:24:GLY:CA	12:J:31:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:1:MET:O	13:K:2:LEU:HB2	2.16	0.46
13:K:23:GLY:HA2	13:K:98:LYS:HG2	1.98	0.46
14:L:26:LYS:O	14:L:29:LEU:HB3	2.16	0.46
16:N:65:LYS:HD2	16:N:66:VAL:N	2.30	0.46
20:R:29:TRP:HA	20:R:76:ARG:CG	2.45	0.46
20:R:93:GLU:HG3	20:R:94:GLY:N	2.31	0.46
22:T:8:TYR:N	22:T:8:TYR:CD1	2.82	0.46
24:V:73:LEU:O	24:V:75:GLU:N	2.48	0.46
11:I:62:VAL:HG12	11:I:63:VAL:N	2.30	0.46
27:Y:13:LYS:CA	27:Y:16:ARG:HG2	2.45	0.46
7:E:113:ARG:O	7:E:140:ILE:HD11	2.15	0.46
7:E:139:LEU:C	7:E:141:PHE:H	2.19	0.46
9:G:77:LEU:HD12	9:G:142:VAL:CG1	2.40	0.46
9:G:88:ILE:HG12	9:G:89:TYR:H	1.80	0.46
3:A:166:ASN:HA	3:A:171:ALA:CA	2.46	0.46
4:B:200:ASP:C	4:B:202:LYS:N	2.67	0.46
4:B:68:LYS:O	4:B:69:ARG:HB2	2.15	0.46
4:B:70:TRP:N	4:B:70:TRP:HE3	2.14	0.46
6:D:159:ARG:C	6:D:161:ALA:H	2.19	0.46
10:H:118:PRO:HA	10:H:121:VAL:CG2	2.46	0.46
12:J:97:PRO:CG	12:J:126:VAL:HB	2.45	0.46
13:K:3:MET:O	13:K:4:PRO:O	2.34	0.46
13:K:7:MET:HA	13:K:8:LYS:NZ	2.31	0.46
16:N:50:ILE:HG12	16:N:64:ARG:HB2	1.98	0.46
17:O:51:LYS:HZ2	17:O:55:ARG:NH2	2.13	0.46
18:P:3:ALA:C	18:P:4:ILE:HD12	2.36	0.46
18:P:4:ILE:CG2	18:P:5:VAL:N	2.78	0.46
19:Q:33:ARG:HG3	19:Q:34:ASN:H	1.78	0.46
20:R:59:VAL:H	20:R:74:PRO:HG2	1.81	0.46
22:T:7:ALA:CB	22:T:59:LEU:HB3	2.32	0.46
24:V:50:ARG:HD3	24:V:60:PHE:O	2.16	0.46
17:O:93:LYS:HD2	17:O:93:LYS:H	1.81	0.46
9:G:4:ILE:HG22	9:G:37:VAL:HG21	1.98	0.46
13:K:39:PRO:CB	13:K:99:PRO:HG3	2.35	0.46
14:L:44:LEU:O	14:L:48:VAL:HG23	2.15	0.46
19:Q:21:VAL:HG11	19:Q:76:VAL:CG1	2.32	0.46
34:3:2:A:H8	34:3:2:A:O5'	1.99	0.46
3:A:165:ARG:O	3:A:171:ALA:HB1	2.16	0.46
3:A:40:GLU:OE2	3:A:220:GLY:N	2.49	0.46
4:B:165:ILE:CG2	4:B:166:GLN:N	2.79	0.46
4:B:248:SER:HB2	4:B:252:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:259:THR:C	4:B:260:ARG:HG2	2.35	0.46
5:C:25:VAL:HG12	5:C:26:ILE:N	2.30	0.46
6:D:120:LEU:HD11	6:D:123:ALA:HB3	1.97	0.46
6:D:163:ARG:CG	6:D:164:ASN:H	2.28	0.46
7:E:120:LEU:C	7:E:120:LEU:HD22	2.93	0.46
8:F:102:ALA:HB2	8:F:117:PRO:CD	2.44	0.46
8:F:143:GLN:O	8:F:146:ALA:HB3	2.15	0.46
8:F:96:ALA:O	8:F:97:ARG:HB2	2.15	0.46
10:H:130:LEU:HB3	10:H:131:PRO:HD2	1.98	0.46
15:M:35:ILE:HD12	15:M:66:ALA:HA	1.97	0.46
22:T:73:GLN:HB2	22:T:87:ASP:CB	2.45	0.46
13:K:35:VAL:HG22	13:K:130:LYS:HB2	1.98	0.46
6:D:4:ILE:HD13	6:D:12:ARG:HE	1.81	0.46
22:T:104:PHE:HD1	22:T:104:PHE:O	1.99	0.46
22:T:73:GLN:HB2	22:T:87:ASP:HB2	1.97	0.46
4:B:3:VAL:O	4:B:5:LYS:HD2	2.16	0.46
24:V:27:GLU:HA	33:2:74:C:H5'	1.97	0.46
5:C:24:THR:HG23	5:C:25:VAL:N	2.30	0.46
9:G:130:TYR:O	9:G:138:ILE:N	2.48	0.46
11:I:111:PHE:O	11:I:115:VAL:HG23	2.16	0.46
11:I:23:ARG:HG2	11:I:24:VAL:N	2.30	0.46
13:K:23:GLY:CA	13:K:98:LYS:HG2	2.46	0.46
15:M:110:LEU:HG	15:M:111:GLU:N	2.22	0.46
16:N:79:HIS:HB3	16:N:80:SER:H	1.37	0.46
24:V:12:PRO:HG2	24:V:13:ILE:H	1.80	0.46
33:2:44:A:N6	33:2:45:G:C2	2.83	0.46
3:A:63:VAL:HG13	3:A:64:SER:N	2.30	0.46
4:B:133:LEU:HD13	4:B:136:ILE:CD1	2.36	0.46
4:B:211:ARG:CA	4:B:214:TRP:HE3	2.20	0.46
4:B:60:ARG:NH1	4:B:60:ARG:HA	2.31	0.46
6:D:178:VAL:HA	6:D:181:ILE:HG22	1.98	0.46
9:G:25:TYR:CG	9:G:30:LEU:HD12	2.51	0.46
13:K:37:LEU:HB2	13:K:127:ILE:CG2	2.45	0.46
14:L:97:VAL:HG13	14:L:112:ALA:HB1	1.97	0.46
15:M:83:LYS:O	15:M:110:LEU:HD12	2.16	0.46
19:Q:86:LEU:O	19:Q:88:ARG:HD3	2.16	0.46
20:R:54:VAL:HG22	20:R:55:ASN:H	1.81	0.46
23:U:50:ASN:HD22	23:U:81:VAL:HG12	1.80	0.46
26:X:20:LYS:HA	26:X:23:LEU:HD21	1.96	0.46
28:Z:37:LYS:HZ1	28:Z:39:ARG:NH2	2.14	0.46
11:I:70:LYS:HG3	11:I:71:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:47:PHE:HA	14:L:50:HIS:HB2	1.98	0.46
17:O:36:ARG:HG2	17:O:40:PHE:CZ	2.51	0.46
18:P:40:LEU:HD13	18:P:41:GLY:H	1.81	0.46
18:P:39:LEU:HD12	18:P:40:LEU:H	1.81	0.46
18:P:66:ARG:HH11	18:P:66:ARG:HG2	1.81	0.46
4:B:259:THR:C	4:B:261:LYS:H	2.19	0.46
5:C:23:VAL:HG12	5:C:185:LYS:HD3	1.98	0.46
5:C:3:GLY:HA3	5:C:95:ILE:HD13	1.98	0.46
6:D:131:THR:OG1	6:D:163:ARG:HD3	2.16	0.46
6:D:55:SER:O	6:D:57:ARG:N	2.48	0.46
7:E:172:LEU:HD12	7:E:172:LEU:C	2.36	0.46
8:F:58:GLU:HG2	8:F:61:HIS:CD2	2.51	0.46
9:G:3:VAL:HG12	9:G:21:VAL:CG1	2.38	0.46
18:P:71:LEU:O	18:P:90:PRO:O	2.33	0.46
22:T:72:ARG:C	22:T:73:GLN:HG3	2.35	0.46
23:U:15:ASP:HB3	23:U:20:ARG:NH1	2.29	0.46
3:A:15:VAL:O	3:A:21:TYR:OH	2.34	0.45
4:B:91:ARG:HH11	4:B:198:ASN:CG	2.20	0.45
6:D:156:GLU:HA	6:D:159:ARG:CG	2.44	0.45
6:D:190:ASP:O	6:D:194:TRP:HB2	2.16	0.45
7:E:26:GLN:HG3	7:E:27:ASN:OD1	2.16	0.45
9:G:129:THR:HG23	9:G:139:GLN:HG3	1.98	0.45
11:I:49:ARG:HD3	11:I:49:ARG:H	1.81	0.45
15:M:63:THR:HG23	15:M:64:GLU:H	1.81	0.45
16:N:29:ARG:HB3	16:N:86:ILE:H	1.80	0.45
16:N:26:ASP:OD1	16:N:90:GLN:N	2.49	0.45
18:P:45:THR:HG22	18:P:46:VAL:HG23	1.99	0.45
20:R:5:TYR:O	20:R:7:VAL:HG12	2.16	0.45
22:T:2:GLU:HA	22:T:56:VAL:HG23	1.98	0.45
25:W:41:ILE:C	25:W:43:GLN:H	2.20	0.45
10:H:95:TYR:N	10:H:95:TYR:HD1	2.15	0.45
11:I:34:THR:CG2	11:I:35:VAL:N	2.70	0.45
11:I:89:ASN:O	11:I:90:GLN:C	2.54	0.45
13:K:106:VAL:HG12	13:K:107:ALA:H	1.80	0.45
5:C:109:LYS:HZ1	14:L:4:LEU:HD21	1.81	0.45
5:C:154:LYS:CD	5:C:155:LYS:H	2.21	0.45
6:D:182:VAL:CG2	6:D:183:ARG:N	2.79	0.45
6:D:64:HIS:O	6:D:65:THR:HG22	2.15	0.45
6:D:98:LYS:HA	6:D:101:ARG:HB3	1.98	0.45
8:F:76:VAL:HA	8:F:79:VAL:CG2	2.45	0.45
9:G:124:GLY:HA2	9:G:144:VAL:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:66:VAL:HG23	14:L:67:LEU:HD22	1.98	0.45
15:M:20:ARG:HB2	15:M:88:ASP:OD1	2.16	0.45
16:N:85:LYS:HZ3	16:N:85:LYS:C	2.19	0.45
17:O:99:ALA:HA	17:O:106:PHE:CZ	2.50	0.45
23:U:29:GLN:HG2	23:U:30:VAL:HG12	1.97	0.45
26:X:31:LEU:O	26:X:32:GLN:CB	2.61	0.45
3:A:172:ILE:HD13	3:A:174:ALA:HB2	1.99	0.45
4:B:3:VAL:HG22	4:B:201:HIS:HA	1.99	0.45
5:C:99:GLY:H	5:C:172:VAL:C	2.19	0.45
6:D:165:LEU:N	6:D:165:LEU:HD13	2.30	0.45
7:E:11:TYR:HA	7:E:15:VAL:CG2	2.46	0.45
7:E:125:PHE:HB2	7:E:166:ASP:OD1	2.16	0.45
7:E:16:ARG:HB3	7:E:17:PRO:HD3	1.98	0.45
8:F:121:ILE:O	8:F:121:ILE:HG12	2.17	0.45
8:F:26:VAL:CG1	8:F:27:LYS:N	2.80	0.45
11:I:114:ILE:N	11:I:114:ILE:CD1	2.69	0.45
13:K:121:ALA:O	13:K:125:LEU:HD12	2.16	0.45
13:K:26:TYR:O	13:K:67:ARG:NH1	2.49	0.45
18:P:39:LEU:HD13	18:P:40:LEU:H	1.79	0.45
26:X:49:LYS:O	26:X:51:ALA:N	2.48	0.45
4:B:146:GLU:OE1	4:B:189:CYS:HA	2.16	0.45
5:C:118:LYS:HD2	5:C:118:LYS:HA	1.77	0.45
7:E:120:LEU:HD12	7:E:178:PHE:CB	2.46	0.45
8:F:38:SER:CB	8:F:39:PRO:CD	2.88	0.45
11:I:91:LEU:O	11:I:91:LEU:HD22	2.16	0.45
16:N:86:ILE:CG2	16:N:87:ASP:H	2.30	0.45
17:O:103:PRO:C	17:O:105:VAL:H	2.18	0.45
19:Q:5:ALA:O	19:Q:6:ILE:HG23	2.17	0.45
27:Y:50:GLY:O	27:Y:51:TYR:HB2	2.16	0.45
33:2:67:A:H2'	33:2:68:U:H6	1.82	0.45
33:2:66:A:C6	33:2:67:A:N6	2.84	0.45
4:B:186:HIS:HB3	4:B:189:CYS:SG	2.56	0.45
4:B:35:LYS:CB	4:B:36:PRO:CA	2.95	0.45
4:B:63:ARG:NH1	4:B:63:ARG:CG	2.72	0.45
8:F:88:LEU:HD12	8:F:130:ARG:HD2	1.99	0.45
8:F:43:VAL:HB	8:F:53:GLU:H	1.82	0.45
9:G:113:ARG:HB2	9:G:130:TYR:CE2	2.52	0.45
14:L:38:VAL:HG23	14:L:39:PRO:CD	2.47	0.45
15:M:26:LEU:HD21	15:M:85:VAL:CG1	2.46	0.45
23:U:13:GLY:O	23:U:14:ARG:HB2	2.16	0.45
23:U:17:GLN:O	23:U:18:ALA:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:19:GLN:H	24:V:44:PRO:HD3	1.82	0.45
24:V:39:LYS:O	24:V:40:ARG:HB2	2.17	0.45
14:L:80:PHE:O	14:L:84:ALA:HB3	2.17	0.45
16:N:25:GLY:O	16:N:48:ILE:HG23	2.17	0.45
18:P:10:LYS:HZ1	18:P:22:VAL:CA	2.24	0.45
6:D:125:ALA:HA	6:D:137:TRP:CD1	2.52	0.45
7:E:141:PHE:CB	7:E:144:ILE:HB	2.47	0.45
8:F:88:LEU:HB2	8:F:130:ARG:HG2	1.98	0.45
10:H:29:PRO:HB3	10:H:64:ASP:CB	2.44	0.45
11:I:101:PRO:HB3	11:I:119:PRO:O	2.15	0.45
11:I:15:GLY:H	11:I:17:ARG:NH2	2.13	0.45
12:J:122:PRO:HG2	12:J:141:ALA:O	2.17	0.45
13:K:24:GLY:O	13:K:25:ASP:CB	2.62	0.45
18:P:3:ALA:O	18:P:13:ARG:HA	2.16	0.45
20:R:27:THR:HG22	20:R:77:LYS:O	2.17	0.45
21:S:67:LEU:CG	21:S:68:HIS:H	2.29	0.45
24:V:12:PRO:HG3	24:V:63:ALA:CB	2.47	0.45
13:K:124:LYS:HG3	13:K:125:LEU:N	2.32	0.45
3:A:52:PRO:CG	3:A:167:ASP:HA	2.46	0.45
4:B:155:LEU:O	4:B:156:ALA:CB	2.65	0.45
4:B:203:ASN:O	4:B:205:VAL:N	2.50	0.45
4:B:5:LYS:O	4:B:6:PHE:O	2.33	0.45
4:B:36:PRO:HG2	4:B:61:LEU:HG	1.98	0.45
5:C:100:GLU:O	5:C:172:VAL:HG23	2.16	0.45
5:C:48:GLN:HA	5:C:79:ARG:O	2.17	0.45
5:C:92:THR:HB	5:C:93:VAL:H	1.60	0.45
7:E:171:ALA:O	7:E:175:LEU:HB2	2.16	0.45
7:E:28:VAL:HG12	7:E:29:TRP:N	2.31	0.45
7:E:49:ASP:O	7:E:50:ALA:HB3	2.17	0.45
7:E:55:LYS:HD3	7:E:56:ALA:H	1.81	0.45
9:G:130:TYR:C	9:G:130:TYR:CD2	2.90	0.45
9:G:29:TYR:O	9:G:32:PRO:HD2	2.16	0.45
10:H:58:ARG:HA	10:H:139:LEU:HD13	1.98	0.45
12:J:88:LEU:O	12:J:90:ARG:N	2.49	0.45
13:K:72:LYS:HG2	13:K:73:PRO:HD2	1.97	0.45
14:L:87:TYR:HH	14:L:116:LEU:HB3	1.76	0.45
15:M:68:GLN:HA	15:M:71:ARG:HG2	1.99	0.45
17:O:88:ILE:C	17:O:89:GLU:HG3	2.37	0.45
17:O:96:ALA:C	17:O:98:LEU:N	2.70	0.45
20:R:81:VAL:CG2	20:R:82:GLN:H	2.19	0.45
21:S:72:VAL:HG13	21:S:72:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:150:LEU:HD13	22:T:154:ASP:CG	2.37	0.45
23:U:51:VAL:HG21	23:U:79:VAL:HG23	1.99	0.45
24:V:24:ALA:HB2	24:V:39:LYS:HZ2	1.82	0.45
24:V:12:PRO:HG2	24:V:63:ALA:HB2	1.99	0.45
24:V:86:SER:N	24:V:87:PRO:CD	2.79	0.45
25:W:16:LEU:C	25:W:16:LEU:HD23	2.36	0.45
25:W:45:SER:O	25:W:46:GLN:CB	2.65	0.45
13:K:74:TYR:C	13:K:88:GLY:O	2.55	0.45
33:2:7:U:N3	33:2:67:A:N6	2.65	0.45
28:Z:37:LYS:HZ1	28:Z:39:ARG:CZ	2.29	0.45
4:B:206:LEU:H	4:B:206:LEU:HD22	1.82	0.45
4:B:20:ASP:HB3	4:B:24:ILE:HG13	1.98	0.45
4:B:181:GLU:HA	4:B:273:ARG:HA	1.98	0.45
6:D:117:LYS:NZ	6:D:186:ARG:HA	2.31	0.45
9:G:33:ARG:HG3	9:G:34:GLY:H	1.82	0.45
10:H:27:TYR:CZ	17:O:64:ARG:HD3	2.51	0.45
13:K:109:VAL:HG11	13:K:113:GLN:OE1	2.16	0.45
14:L:1:MET:HB2	14:L:4:LEU:O	2.17	0.45
14:L:22:ARG:HH12	14:L:71:GLN:CD	2.19	0.45
14:L:5:LYS:CG	14:L:6:SER:N	2.80	0.45
14:L:94:TYR:HB2	14:L:95:THR:H	1.64	0.45
15:M:74:ALA:O	15:M:77:ALA:HB3	2.17	0.45
11:I:79:PHE:CD2	16:N:70:VAL:HG11	2.40	0.45
16:N:89:VAL:HG12	16:N:121:ILE:HG13	1.99	0.45
17:O:81:HIS:O	17:O:82:GLY:C	2.54	0.45
19:Q:12:ILE:CG2	19:Q:13:SER:H	2.27	0.45
19:Q:27:LYS:HB3	19:Q:27:LYS:NZ	5.20	0.45
19:Q:85:VAL:HG12	19:Q:86:LEU:N	2.32	0.45
22:T:124:ILE:CG1	22:T:125:LEU:N	2.80	0.45
23:U:15:ASP:CB	23:U:20:ARG:HG3	2.46	0.45
23:U:30:VAL:O	23:U:31:VAL:HG13	2.16	0.45
24:V:20:ARG:HA	24:V:41:ARG:HA	1.97	0.45
26:X:10:LYS:HB2	26:X:53:LEU:HB2	1.98	0.45
26:X:8:LEU:HD23	26:X:33:GLN:H	1.81	0.45
23:U:70:GLN:HB3	23:U:71:ASP:H	1.63	0.45
5:C:55:ASN:HD21	5:C:75:VAL:CG2	2.30	0.45
7:E:157:ILE:HG22	7:E:158:ALA:N	2.32	0.45
7:E:32:PRO:HA	7:E:162:THR:OG1	2.17	0.45
8:F:85:LYS:O	8:F:132:ARG:HG3	2.17	0.45
11:I:98:VAL:HG22	11:I:99:PHE:N	2.32	0.45
14:L:27:SER:O	14:L:29:LEU:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:63:ARG:NH2	14:L:76:VAL:HG12	2.11	0.45
15:M:68:GLN:HA	15:M:71:ARG:HD3	1.99	0.45
21:S:65:ALA:CB	21:S:66:PRO:HD3	2.46	0.45
25:W:51:ARG:C	25:W:53:LEU:H	2.20	0.45
19:Q:21:VAL:HG22	19:Q:22:ASP:N	2.31	0.45
21:S:77:PRO:O	21:S:78:ALA:HB2	2.17	0.45
26:X:23:LEU:HA	26:X:26:LEU:CD1	2.38	0.45
33:2:10:G:H2'	33:2:11:C:C6	2.52	0.45
33:2:72:C:C4	33:2:73:A:N6	2.84	0.45
4:B:147:LEU:HG	4:B:148:GLU:N	2.32	0.45
4:B:140:THR:HG22	4:B:165:ILE:HB	1.99	0.45
5:C:16:ARG:HB2	5:C:19:ARG:HG3	1.99	0.45
9:G:31:LEU:HD21	9:G:38:LEU:HD23	1.98	0.45
11:I:66:LYS:H	11:I:82:ASN:HD21	1.64	0.45
13:K:8:LYS:NZ	13:K:8:LYS:H	2.15	0.45
17:O:103:PRO:O	17:O:106:PHE:CD2	2.70	0.45
18:P:89:GLN:HE21	18:P:89:GLN:HB3	1.65	0.45
19:Q:89:ALA:O	19:Q:91:GLY:N	2.49	0.45
20:R:84:ALA:N	20:R:85:PRO:CD	2.80	0.45
23:U:23:VAL:HA	23:U:38:VAL:HA	1.98	0.45
5:C:93:VAL:CA	5:C:182:LEU:HD22	2.43	0.45
11:I:91:LEU:HB2	11:I:111:PHE:CE1	2.52	0.45
18:P:43:GLU:O	18:P:44:LYS:CB	2.62	0.45
4:B:262:ARG:O	4:B:264:LYS:N	2.40	0.44
4:B:69:ARG:NH1	4:B:76:PRO:HD3	2.32	0.44
6:D:130:LYS:HB3	6:D:133:GLU:HB2	1.99	0.44
6:D:67:ARG:O	6:D:68:ALA:CB	2.64	0.44
8:F:12:PRO:O	8:F:15:VAL:HG13	2.17	0.44
8:F:177:GLY:O	8:F:178:ALA:CB	2.65	0.44
9:G:114:LEU:C	9:G:114:LEU:HD12	2.38	0.44
9:G:130:TYR:C	9:G:130:TYR:HD2	2.21	0.44
10:H:160:LYS:HA	10:H:160:LYS:HD3	1.68	0.44
13:K:134:ARG:HH12	13:K:137:TYR:HE2	1.63	0.44
13:K:49:ALA:O	13:K:52:VAL:HG22	2.17	0.44
14:L:66:VAL:O	14:L:68:ARG:NH1	2.50	0.44
15:M:23:ARG:HB2	15:M:85:VAL:O	2.17	0.44
17:O:98:LEU:HD12	17:O:106:PHE:CD1	2.52	0.44
18:P:40:LEU:HB2	18:P:50:PRO:CB	2.45	0.44
22:T:78:LYS:N	22:T:78:LYS:HD2	2.31	0.44
24:V:71:TYR:O	24:V:72:GLU:C	2.55	0.44
20:R:48:LYS:O	20:R:50:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:21:A:N6	33:2:46:G:O2'	2.50	0.44
20:R:32:PRO:HG3	20:R:72:LYS:CE	2.44	0.44
21:S:48:ALA:HA	21:S:56:PRO:HA	1.98	0.44
25:W:41:ILE:CD1	25:W:44:LEU:HD13	2.46	0.44
14:L:73:VAL:O	14:L:77:ARG:HG3	2.16	0.44
4:B:28:GLU:N	4:B:29:PRO:CD	2.80	0.44
5:C:44:TYR:CE2	5:C:46:ALA:CB	2.99	0.44
6:D:18:ASP:O	6:D:22:GLU:CG	2.61	0.44
7:E:120:LEU:HG	7:E:178:PHE:HB3	1.99	0.44
7:E:139:LEU:C	7:E:141:PHE:N	2.70	0.44
8:F:136:ILE:O	8:F:138:LYS:HE2	2.17	0.44
9:G:128:LEU:O	9:G:139:GLN:HB3	2.18	0.44
10:H:146:TYR:O	10:H:147:ALA:HB2	2.16	0.44
11:I:104:ARG:CD	11:I:104:ARG:H	2.29	0.44
11:I:50:GLY:O	11:I:51:ALA:CB	2.65	0.44
15:M:26:LEU:HG	15:M:85:VAL:HG13	2.00	0.44
17:O:37:GLU:O	17:O:40:PHE:HB2	2.17	0.44
25:W:54:LYS:O	25:W:55:ARG:HG2	2.18	0.44
26:X:9:VAL:HG23	26:X:9:VAL:O	2.17	0.44
9:G:77:LEU:HB3	9:G:142:VAL:HG13	1.99	0.44
11:I:113:LYS:O	11:I:117:LEU:HG	2.17	0.44
3:A:198:GLU:O	3:A:198:GLU:OE2	2.35	0.44
3:A:201:LYS:HB2	3:A:202:PRO:CD	2.36	0.44
4:B:53:PHE:HA	4:B:218:ARG:HB3	1.99	0.44
5:C:176:ILE:N	5:C:176:ILE:HD12	2.33	0.44
6:D:117:LYS:O	6:D:118:LEU:CB	2.65	0.44
6:D:23:ILE:O	6:D:23:ILE:HG13	2.17	0.44
6:D:29:TRP:O	6:D:33:ARG:HG3	2.18	0.44
6:D:86:GLY:N	6:D:87:PRO:HD2	2.32	0.44
7:E:51:ARG:HA	7:E:54:GLU:HG3	1.99	0.44
8:F:7:LEU:HB2	8:F:8:PRO:CD	2.47	0.44
11:I:29:ASN:HD22	11:I:30:ALA:N	2.15	0.44
13:K:134:ARG:HH22	13:K:137:TYR:HA	1.81	0.44
15:M:25:ARG:NH1	15:M:41:ASP:C	2.69	0.44
17:O:106:PHE:HA	17:O:109:LEU:CD2	2.46	0.44
18:P:62:LEU:N	18:P:62:LEU:HD23	2.32	0.44
18:P:5:VAL:CG2	18:P:6:LYS:N	2.79	0.44
20:R:26:TYR:CD1	20:R:26:TYR:N	2.85	0.44
20:R:59:VAL:O	20:R:74:PRO:HD2	2.17	0.44
24:V:41:ARG:O	24:V:42:GLN:HB3	2.17	0.44
11:I:69:VAL:H	11:I:77:ILE:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:97:VAL:O	13:K:97:VAL:HG12	2.16	0.44
10:H:27:TYR:HE1	17:O:64:ARG:CD	2.30	0.44
21:S:42:VAL:HG12	21:S:43:ASN:N	2.31	0.44
33:2:2:C:O5'	33:2:2:C:C6	2.70	0.44
20:R:44:GLU:HG2	20:R:44:GLU:O	2.17	0.44
33:2:18:G:C2	33:2:57:G:N1	2.85	0.44
3:A:29:LEU:HG	3:A:33:LEU:CG	2.44	0.44
5:C:154:LYS:CG	5:C:155:LYS:N	2.81	0.44
5:C:55:ASN:HD21	5:C:75:VAL:HG23	1.83	0.44
9:G:29:TYR:C	9:G:32:PRO:HD2	2.38	0.44
13:K:106:VAL:CG2	13:K:118:LEU:HD11	2.46	0.44
13:K:32:PHE:HB2	13:K:106:VAL:CB	2.27	0.44
13:K:34:LEU:HD21	13:K:118:LEU:CD2	2.43	0.44
15:M:17:ARG:HB3	15:M:89:ARG:HD3	2.00	0.44
16:N:28:VAL:O	16:N:29:ARG:CB	2.66	0.44
18:P:16:PRO:O	18:P:98:GLU:OE2	2.36	0.44
27:Y:46:CYS:O	27:Y:50:GLY:HA2	2.17	0.44
33:2:33:U:O5'	33:2:33:U:H6	2.01	0.44
7:E:72:ARG:HD2	7:E:73:ALA:N	2.33	0.44
7:E:74:LYS:HE3	7:E:88:ILE:CD1	2.38	0.44
13:K:51:ARG:HA	13:K:54:MET:SD	2.56	0.44
15:M:64:GLU:H	15:M:64:GLU:CD	3.85	0.44
15:M:94:TYR:OH	15:M:102:ALA:HB1	2.17	0.44
16:N:19:LEU:HD12	16:N:79:HIS:HA	1.99	0.44
17:O:98:LEU:HD21	18:P:43:GLU:HG2	1.99	0.44
18:P:39:LEU:HD12	18:P:39:LEU:H	1.83	0.44
24:V:13:ILE:HB	24:V:66:HIS:HE1	1.82	0.44
27:Y:44:THR:CG2	27:Y:45:VAL:N	2.79	0.44
20:R:43:VAL:HG13	20:R:44:GLU:N	2.33	0.44
22:T:120:ILE:HB	22:T:171:ILE:C	2.38	0.44
17:O:64:ARG:O	17:O:67:ALA:HB3	2.17	0.44
10:H:25:LYS:HG3	18:P:13:ARG:NH2	2.33	0.44
20:R:40:LYS:O	20:R:45:THR:HG23	2.18	0.44
3:A:172:ILE:HG12	3:A:173:HIS:N	2.33	0.44
4:B:80:ALA:H	4:B:95:LEU:HA	1.81	0.44
5:C:169:ASN:O	5:C:170:LEU:HD12	2.17	0.44
5:C:98:PRO:HG3	5:C:174:ASP:CA	2.46	0.44
6:D:16:ALA:O	6:D:17:ALA:C	2.55	0.44
7:E:17:PRO:HA	7:E:20:ILE:HG13	1.99	0.44
9:G:97:ILE:O	9:G:101:LEU:HD23	2.18	0.44
14:L:62:ALA:O	14:L:66:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:100:TYR:CA	16:N:103:ARG:HH12	2.23	0.44
17:O:42:ALA:O	17:O:46:ALA:HB3	2.18	0.44
22:T:124:ILE:CD1	22:T:125:LEU:H	2.28	0.44
22:T:19:ARG:H	22:T:19:ARG:HD2	1.81	0.44
14:L:79:LEU:HA	14:L:83:ILE:HB	1.99	0.44
16:N:30:VAL:HA	16:N:42:ILE:CB	2.45	0.44
4:B:142:VAL:HG23	4:B:193:VAL:CA	2.35	0.44
4:B:58:HIS:CD2	4:B:58:HIS:C	2.91	0.44
5:C:7:VAL:HG22	5:C:27:LEU:HD13	2.00	0.44
7:E:154:GLY:C	7:E:155:MET:SD	2.96	0.44
7:E:41:GLN:O	7:E:89:GLY:HA3	2.18	0.44
7:E:48:GLU:OE1	7:E:52:ILE:HG13	2.18	0.44
7:E:86:MET:N	7:E:87:PRO:CD	2.81	0.44
8:F:118:PRO:CD	8:F:121:ILE:HD12	2.48	0.44
8:F:123:PHE:HA	8:F:132:ARG:O	2.18	0.44
8:F:126:PRO:HD3	8:F:130:ARG:O	2.18	0.44
8:F:89:ILE:HG12	8:F:129:THR:HB	1.99	0.44
9:G:123:LEU:O	9:G:144:VAL:O	2.36	0.44
10:H:113:MET:O	10:H:121:VAL:CG2	2.66	0.44
10:H:113:MET:SD	10:H:116:THR:O	2.75	0.44
11:I:10:VAL:HB	11:I:99:PHE:CE2	2.52	0.44
12:J:35:HIS:N	12:J:36:LYS:NZ	2.66	0.44
12:J:61:ARG:O	12:J:62:LEU:HB3	2.17	0.44
13:K:17:LEU:N	13:K:17:LEU:HD13	2.33	0.44
13:K:8:LYS:HZ3	13:K:70:PRO:CG	2.30	0.44
17:O:79:PHE:CE2	17:O:80:ILE:HD13	2.53	0.44
19:Q:18:ARG:O	19:Q:21:VAL:HG13	2.18	0.44
19:Q:45:TYR:O	19:Q:46:PHE:CG	2.71	0.44
22:T:161:VAL:CG1	22:T:162:GLU:H	2.30	0.44
24:V:33:LYS:CG	24:V:34:THR:H	2.29	0.44
26:X:7:LYS:CB	26:X:34:GLU:HA	2.47	0.44
4:B:92:ILE:HD12	4:B:92:ILE:C	2.37	0.44
5:C:63:LEU:O	5:C:65:GLY:N	2.50	0.44
3:A:20:ILE:HG22	3:A:20:ILE:O	2.17	0.44
5:C:11:MET:HB2	5:C:24:THR:HA	1.97	0.44
5:C:47:VAL:CG2	5:C:84:PHE:HB3	2.48	0.44
5:C:47:VAL:CG2	5:C:84:PHE:O	2.65	0.44
7:E:101:ILE:HG23	7:E:102:PHE:N	2.33	0.44
7:E:109:VAL:C	7:E:112:PRO:HD2	2.39	0.44
7:E:165:THR:C	7:E:167:GLU:N	2.71	0.44
7:E:38:VAL:O	7:E:157:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:17:VAL:HG22	8:F:45:VAL:CB	2.38	0.44
8:F:58:GLU:O	8:F:59:ARG:C	2.56	0.44
9:G:98:ALA:HA	9:G:111:PRO:CG	2.40	0.44
11:I:10:VAL:CG1	11:I:17:ARG:HA	2.46	0.44
13:K:37:LEU:O	13:K:127:ILE:HG21	2.18	0.44
13:K:34:LEU:HB3	13:K:129:THR:HG1	1.77	0.44
16:N:79:HIS:C	16:N:81:PRO:HD2	2.37	0.44
17:O:17:ILE:HA	17:O:39:LEU:HD11	1.98	0.44
19:Q:92:ARG:HB3	19:Q:93:ALA:H	1.51	0.44
22:T:58:VAL:O	22:T:59:LEU:HD13	2.17	0.44
23:U:46:LYS:NZ	23:U:76:GLY:HA2	2.33	0.44
4:B:117:VAL:HG13	4:B:128:GLY:HA3	1.99	0.44
26:X:38:GLU:HG2	26:X:39:ASP:N	2.33	0.44
10:H:39:ILE:CG1	10:H:40:ASP:N	2.80	0.44
19:Q:82:LEU:CD1	19:Q:84:ARG:HG3	2.47	0.44
20:R:63:LYS:CD	20:R:64:LYS:N	2.81	0.44
23:U:41:ARG:HA	23:U:57:PHE:CD2	2.53	0.44
4:B:177:LEU:CD1	4:B:181:GLU:HB3	2.47	0.44
4:B:97:TYR:HB2	4:B:102:LYS:C	2.38	0.44
5:C:57:LYS:O	5:C:58:ARG:HG3	2.17	0.44
6:D:59:ILE:HB	6:D:60:TRP:H	1.44	0.44
7:E:46:ALA:CB	7:E:53:LEU:HD11	2.36	0.44
7:E:82:LEU:HD22	7:E:83:ARG:N	2.33	0.44
8:F:8:PRO:O	8:F:9:ILE:HB	2.17	0.44
9:G:116:LEU:O	9:G:116:LEU:HD12	2.18	0.44
12:J:111:ARG:O	12:J:111:ARG:HG3	4.61	0.44
14:L:63:ARG:HD2	14:L:67:LEU:HD21	2.00	0.44
15:M:106:ARG:HH11	15:M:111:GLU:HA	1.83	0.44
17:O:74:LEU:H	17:O:74:LEU:HD12	1.83	0.44
22:T:88:PHE:O	22:T:88:PHE:HD2	2.01	0.44
17:O:88:ILE:HG22	18:P:51:VAL:O	2.18	0.43
18:P:36:PRO:HD2	18:P:60:GLU:CD	2.39	0.43
20:R:28:PHE:O	20:R:29:TRP:HD1	2.00	0.43
20:R:35:THR:O	20:R:35:THR:HG22	2.18	0.43
26:X:40:THR:O	26:X:44:ARG:HD3	2.18	0.43
3:A:190:ILE:HA	3:A:193:PHE:HB3	1.99	0.43
3:A:39:ASP:O	3:A:40:GLU:HB3	2.17	0.43
4:B:177:LEU:HD12	4:B:181:GLU:HB3	1.99	0.43
4:B:214:TRP:C	4:B:215:LEU:HD12	2.38	0.43
5:C:50:GLY:C	5:C:76:ARG:HB3	2.38	0.43
5:C:61:ARG:HG3	5:C:61:ARG:H	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:121:VAL:HG13	6:D:191:LEU:HA	1.99	0.43
7:E:25:TYR:CD1	7:E:25:TYR:N	2.79	0.43
10:H:93:LYS:HB3	10:H:110:LEU:CD2	2.47	0.43
11:I:59:LYS:NZ	11:I:88:ASN:HA	2.33	0.43
12:J:114:ILE:O	12:J:115:LEU:HB3	2.17	0.43
12:J:35:HIS:H	12:J:36:LYS:NZ	2.16	0.43
13:K:106:VAL:HG21	13:K:118:LEU:HG	1.99	0.43
13:K:3:MET:H	13:K:4:PRO:HD3	1.76	0.43
14:L:86:ARG:NH2	14:L:116:LEU:HD13	2.33	0.43
15:M:94:TYR:OH	15:M:102:ALA:CB	2.66	0.43
15:M:91:PRO:HG2	15:M:92:TYR:CE2	2.53	0.43
10:H:29:PRO:O	10:H:30:LYS:O	2.36	0.43
10:H:32:VAL:HG21	10:H:71:MET:HE1	2.00	0.43
14:L:10:LEU:HA	14:L:10:LEU:HD23	1.89	0.43
3:A:175:PRO:HB2	3:A:176:VAL:H	1.59	0.43
5:C:180:ASN:C	5:C:181:LEU:HD22	2.37	0.43
5:C:53:PRO:O	5:C:54:GLN:C	2.56	0.43
5:C:72:VAL:O	5:C:73:GLU:O	2.35	0.43
7:E:111:LEU:HB3	7:E:112:PRO:HD3	1.99	0.43
7:E:120:LEU:HD22	7:E:121:ASN:N	2.28	0.43
8:F:89:ILE:O	8:F:89:ILE:HD12	2.18	0.43
9:G:44:LEU:HD13	9:G:44:LEU:C	2.39	0.43
9:G:64:GLU:O	9:G:67:ARG:HG2	2.17	0.43
10:H:32:VAL:HG11	10:H:71:MET:CB	2.48	0.43
10:H:80:ALA:HB3	10:H:146:TYR:O	2.18	0.43
10:H:43:GLY:C	10:H:84:ARG:HB2	2.39	0.43
12:J:97:PRO:HD2	12:J:126:VAL:HB	1.98	0.43
18:P:13:ARG:N	18:P:13:ARG:HD3	2.34	0.43
19:Q:95:ILE:O	19:Q:96:ILE:HG23	2.17	0.43
20:R:15:GLU:OE2	20:R:18:TYR:HB2	2.18	0.43
20:R:8:ILE:HA	20:R:30:VAL:CG2	2.37	0.43
21:S:39:VAL:O	21:S:62:GLU:HG2	2.18	0.43
23:U:51:VAL:HG21	23:U:79:VAL:CB	2.48	0.43
23:U:20:ARG:CG	23:U:20:ARG:NH1	2.81	0.43
23:U:66:VAL:HG22	23:U:82:ARG:HB2	2.00	0.43
5:C:176:ILE:HB	5:C:181:LEU:C	2.39	0.43
5:C:47:VAL:CG1	5:C:48:GLN:N	2.74	0.43
17:O:79:PHE:C	17:O:79:PHE:HD2	2.20	0.43
33:2:16:U:C3'	33:2:17:U:C5'	2.97	0.43
7:E:126:ASP:CG	7:E:130:ASN:HB2	2.38	0.43
7:E:28:VAL:C	7:E:30:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:141:VAL:O	8:F:141:VAL:HG12	2.18	0.43
9:G:118:LYS:O	9:G:118:LYS:HG2	2.18	0.43
9:G:47:LEU:HD12	9:G:47:LEU:C	2.38	0.43
10:H:80:ALA:HB3	10:H:146:TYR:N	2.34	0.43
11:I:77:ILE:HG23	11:I:77:ILE:O	2.18	0.43
21:S:84:ARG:HD3	21:S:91:GLU:HG2	2.01	0.43
23:U:53:MET:SD	23:U:54:GLY:N	2.85	0.43
24:V:83:GLU:HG2	24:V:88:LYS:NZ	2.32	0.43
25:W:35:LEU:HA	25:W:37:PHE:CE2	2.54	0.43
25:W:46:GLN:C	25:W:48:HIS:N	2.71	0.43
17:O:51:LYS:C	17:O:51:LYS:HD3	2.38	0.43
3:A:28:HIS:HA	3:A:183:PRO:HG3	2.01	0.43
3:A:62:THR:CG2	3:A:63:VAL:N	2.81	0.43
6:D:169:VAL:CG1	6:D:170:THR:H	2.22	0.43
6:D:173:PRO:HA	6:D:194:TRP:HZ2	1.84	0.43
7:E:176:LEU:N	7:E:176:LEU:HD23	2.34	0.43
9:G:14:ASP:N	9:G:14:ASP:OD2	2.49	0.43
10:H:112:LYS:HD3	10:H:116:THR:HG21	2.00	0.43
10:H:57:LEU:HD21	10:H:142:ARG:HG3	2.00	0.43
14:L:79:LEU:HA	14:L:83:ILE:CB	2.49	0.43
15:M:24:LEU:HD22	15:M:24:LEU:N	2.33	0.43
15:M:34:HIS:CD2	15:M:36:TYR:OH	2.71	0.43
15:M:7:TYR:O	15:M:8:GLU:CB	2.66	0.43
16:N:45:PHE:O	16:N:46:GLU:C	2.56	0.43
19:Q:18:ARG:HG2	19:Q:38:TYR:HA	20.05	0.43
20:R:83:VAL:HG23	20:R:85:PRO:CD	2.47	0.43
26:X:28:LEU:CD1	26:X:33:GLN:HB3	2.45	0.43
26:X:7:LYS:O	26:X:55:ARG:N	2.50	0.43
21:S:23:ARG:HH11	21:S:38:ILE:HG21	1.83	0.43
22:T:58:VAL:HG13	22:T:66:SER:HB3	2.00	0.43
24:V:24:ALA:CB	24:V:36:GLY:HA2	2.46	0.43
3:A:23:ILE:HG13	3:A:23:ILE:H	1.70	0.43
4:B:38:LYS:CG	4:B:38:LYS:O	2.66	0.43
5:C:126:PRO:HB2	5:C:127:ASP:H	1.68	0.43
6:D:101:ARG:O	6:D:105:LEU:HG	2.18	0.43
6:D:148:SER:O	6:D:184:THR:HB	2.18	0.43
6:D:83:VAL:HB	6:D:84:VAL:H	1.56	0.43
8:F:17:VAL:CG2	8:F:45:VAL:H	2.31	0.43
9:G:132:PRO:HD3	9:G:138:ILE:CG2	2.28	0.43
12:J:100:LEU:N	12:J:100:LEU:HD22	2.33	0.43
13:K:37:LEU:HG	13:K:128:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:78:PRO:CG	13:K:87:LYS:HG2	2.47	0.43
16:N:64:ARG:HD3	16:N:102:ILE:CD1	2.46	0.43
17:O:21:ALA:HB1	17:O:24:TYR:CE1	2.54	0.43
19:Q:29:LEU:H	19:Q:29:LEU:HD23	1.83	0.43
23:U:84:LEU:O	23:U:85:ALA:HB2	2.18	0.43
20:R:89:ILE:O	20:R:89:ILE:CG2	2.66	0.43
9:G:76:THR:HA	9:G:141:LYS:O	2.18	0.43
11:I:19:ILE:HB	11:I:42:SER:O	2.19	0.43
14:L:76:VAL:CA	14:L:79:LEU:HG	2.34	0.43
20:R:20:GLY:O	20:R:21:PHE:C	2.57	0.43
23:U:45:PHE:C	23:U:46:LYS:HD2	2.38	0.43
33:2:20:G:N2	33:2:22:G:C1'	2.81	0.43
33:2:36:A:C6	33:2:37:A:C4	3.07	0.43
4:B:250:TRP:O	4:B:250:TRP:CD1	2.72	0.43
5:C:151:TYR:O	5:C:153:GLY:N	2.49	0.43
5:C:75:VAL:O	5:C:77:ILE:N	2.51	0.43
8:F:152:ARG:O	8:F:153:LYS:C	2.56	0.43
8:F:55:PRO:HB2	8:F:56:SER:H	1.61	0.43
12:J:9:ASN:O	12:J:11:GLY:N	2.51	0.43
21:S:36:ALA:HA	21:S:62:GLU:HB2	2.01	0.43
22:T:78:LYS:HG2	22:T:79:ARG:N	2.33	0.43
23:U:63:VAL:O	23:U:64:ASP:OD1	2.37	0.43
24:V:27:GLU:HA	33:2:74:C:C4'	2.47	0.43
24:V:15:ALA:HA	24:V:46:LEU:CG	2.48	0.43
25:W:29:LYS:HD3	25:W:29:LYS:C	2.38	0.43
33:2:53:G:C5	33:2:54:U:C5	3.06	0.43
33:2:54:U:C2'	33:2:55:PSU:O5'	2.66	0.43
33:2:7:U:C5'	33:2:7:U:H6	2.32	0.43
5:C:4:ILE:HD11	5:C:27:LEU:O	2.19	0.43
5:C:4:ILE:HG13	5:C:6:GLY:N	2.31	0.43
6:D:148:SER:HB3	6:D:184:THR:HB	2.00	0.43
7:E:148:MET:O	7:E:151:ALA:HB3	2.19	0.43
7:E:161:THR:HG22	7:E:163:ALA:N	2.31	0.43
8:F:105:LEU:HD11	8:F:107:VAL:HG23	2.01	0.43
8:F:95:ARG:HG3	8:F:95:ARG:HH21	1.84	0.43
10:H:137:ARG:O	10:H:138:ARG:C	2.57	0.43
14:L:50:HIS:HA	14:L:53:HIS:HE1	1.84	0.43
23:U:67:VAL:CG1	23:U:79:VAL:HG12	2.40	0.43
25:W:37:PHE:CG	25:W:37:PHE:O	2.71	0.43
17:O:65:ILE:HD11	17:O:96:ALA:HB3	2.00	0.43
23:U:13:GLY:O	23:U:14:ARG:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:VAL:O	4:B:118:VAL:HB	2.19	0.43
4:B:182:LEU:HD22	4:B:271:ILE:HB	2.01	0.43
4:B:8:PRO:HB2	4:B:14:ARG:HA	2.01	0.43
5:C:127:ASP:O	5:C:128:SER:HB3	2.18	0.43
5:C:132:HIS:HB3	5:C:133:LYS:H	1.57	0.43
5:C:97:LYS:HD3	5:C:97:LYS:N	2.34	0.43
6:D:182:VAL:O	12:J:6:LEU:HA	2.19	0.43
7:E:149:VAL:C	7:E:151:ALA:N	2.72	0.43
8:F:12:PRO:C	8:F:14:GLY:N	2.70	0.43
9:G:27:ARG:NH2	9:G:27:ARG:HB2	2.34	0.43
9:G:67:ARG:O	9:G:71:ILE:HG22	2.19	0.43
9:G:88:ILE:HG12	9:G:89:TYR:CD1	2.54	0.43
17:O:97:ASP:C	17:O:99:ALA:N	2.70	0.43
18:P:4:ILE:O	18:P:39:LEU:HG	2.17	0.43
21:S:40:GLU:HB2	21:S:62:GLU:OE2	2.18	0.43
22:T:108:PRO:HD2	22:T:111:VAL:HG21	2.00	0.43
23:U:74:ARG:C	23:U:74:ARG:HD2	2.39	0.43
24:V:62:VAL:HG11	24:V:70:VAL:HG12	2.01	0.43
19:Q:23:LEU:CG	27:Y:25:LEU:HG	2.49	0.43
13:K:37:LEU:CB	13:K:127:ILE:HB	2.47	0.43
14:L:68:ARG:CZ	14:L:69:ASP:H	2.32	0.43
22:T:130:PRO:CA	22:T:133:ILE:HG12	2.43	0.43
22:T:2:GLU:HA	22:T:56:VAL:CG2	2.49	0.43
10:H:63:PRO:HA	17:O:64:ARG:CZ	2.48	0.43
3:A:37:LYS:HZ2	3:A:38:PHE:HD2	1.64	0.43
4:B:259:THR:O	4:B:261:LYS:N	2.52	0.43
5:C:167:VAL:HG22	5:C:170:LEU:HD11	2.00	0.43
7:E:28:VAL:C	7:E:30:GLU:N	2.71	0.43
9:G:6:LEU:O	9:G:14:ASP:N	2.51	0.43
11:I:70:LYS:H	11:I:76:ALA:HA	1.83	0.43
13:K:72:LYS:HD3	13:K:73:PRO:O	2.18	0.43
15:M:62:LYS:HG3	15:M:63:THR:H	1.83	0.43
16:N:4:GLY:O	16:N:7:ILE:HB	2.19	0.43
17:O:105:VAL:HB	17:O:106:PHE:H	1.62	0.43
18:P:35:LEU:HA	18:P:62:LEU:HD21	1.99	0.43
19:Q:75:TYR:O	19:Q:103:ILE:HB	2.19	0.43
20:R:65:ARG:O	20:R:66:LEU:HB2	2.19	0.43
21:S:23:ARG:CG	21:S:24:VAL:N	2.79	0.43
10:H:34:PRO:HB3	10:H:72:GLY:O	2.18	0.43
11:I:88:ASN:O	11:I:89:ASN:C	2.56	0.43
16:N:90:GLN:HB3	16:N:120:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:TYR:O	3:A:12:LEU:HD13	2.19	0.43
4:B:182:LEU:O	4:B:271:ILE:N	2.51	0.43
7:E:120:LEU:HD13	7:E:121:ASN:H	1.79	0.43
7:E:125:PHE:HB2	7:E:166:ASP:CB	2.48	0.43
7:E:139:LEU:HD13	7:E:139:LEU:H	1.83	0.43
7:E:46:ALA:HA	7:E:53:LEU:CG	2.48	0.43
7:E:95:ARG:HA	7:E:99:MET:HG2	2.01	0.43
12:J:121:LYS:O	12:J:121:LYS:HD3	2.19	0.43
12:J:95:VAL:HG23	12:J:125:VAL:HA	2.00	0.43
15:M:26:LEU:CB	15:M:39:ILE:HG22	2.49	0.43
18:P:91:TYR:CG	18:P:92:THR:N	2.87	0.43
19:Q:3:ALA:CB	19:Q:107:LEU:HB2	2.48	0.43
22:T:102:LEU:HB2	22:T:123:ASP:O	2.17	0.43
23:U:51:VAL:HG11	23:U:79:VAL:CG2	2.48	0.43
33:2:36:A:C5	33:2:37:A:C8	3.07	0.43
11:I:107:ARG:N	11:I:115:VAL:HG21	2.34	0.43
15:M:30:ARG:HB3	15:M:92:TYR:CE1	2.53	0.43
16:N:95:ARG:O	16:N:96:ARG:CB	2.67	0.43
11:I:86:ILE:O	11:I:93:PRO:CB	2.66	0.43
13:K:52:VAL:HG23	13:K:53:ALA:H	1.84	0.42
15:M:74:ALA:HB3	15:M:109:GLY:CA	2.49	0.42
19:Q:88:ARG:HD2	19:Q:93:ALA:CA	2.49	0.42
17:O:92:ARG:C	17:O:94:ASN:H	2.22	0.42
24:V:85:LEU:HD12	24:V:85:LEU:N	2.30	0.42
33:2:45:G:C2'	33:2:46:G:H5''	2.48	0.42
4:B:65:ILE:CD1	4:B:105:ILE:HG13	2.13	0.42
4:B:63:ARG:HB3	4:B:85:ASP:HB2	2.01	0.42
5:C:28:ALA:O	5:C:30:PRO:HD3	2.19	0.42
6:D:53:ALA:O	6:D:54:TYR:C	2.57	0.42
9:G:113:ARG:O	9:G:131:LYS:O	2.36	0.42
9:G:147:GLN:O	9:G:148:GLU:HB2	2.18	0.42
9:G:24:GLY:H	9:G:27:ARG:CZ	2.32	0.42
9:G:88:ILE:HG23	9:G:90:GLY:H	1.84	0.42
11:I:2:ILE:HB	11:I:33:ALA:O	2.19	0.42
13:K:3:MET:SD	13:K:3:MET:O	2.77	0.42
15:M:24:LEU:O	15:M:25:ARG:C	2.57	0.42
17:O:96:ALA:C	17:O:98:LEU:H	2.22	0.42
21:S:31:LEU:CB	21:S:32:PRO:CD	2.97	0.42
26:X:10:LYS:O	26:X:12:PRO:HD3	2.19	0.42
18:P:24:LYS:C	18:P:25:LEU:HD12	2.39	0.42
20:R:38:GLU:H	20:R:38:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:141:VAL:HG21	22:T:144:LEU:HB2	1.99	0.42
22:T:151:HIS:O	22:T:152:ALA:C	2.57	0.42
24:V:64:ALA:C	24:V:66:HIS:H	2.22	0.42
18:P:86:GLY:C	18:P:88:ARG:H	4.51	0.42
27:Y:22:HIS:O	27:Y:23:HIS:C	2.57	0.42
4:B:76:PRO:HD2	4:B:118:VAL:HA	2.01	0.42
4:B:25:THR:O	4:B:25:THR:CG2	2.63	0.42
4:B:76:PRO:HA	4:B:97:TYR:CD1	2.54	0.42
5:C:142:GLY:O	5:C:144:ARG:N	2.51	0.42
5:C:186:GLY:O	5:C:187:ALA:HB2	2.19	0.42
7:E:39:ILE:HG13	7:E:157:ILE:CG2	2.45	0.42
11:I:100:GLY:HA2	11:I:101:PRO:HD3	1.87	0.42
12:J:128:HIS:HA	12:J:147:LEU:HA	2.01	0.42
6:D:30:GLU:OE1	12:J:12:ALA:HB1	2.19	0.42
13:K:14:ARG:H	13:K:14:ARG:HD2	1.82	0.42
14:L:28:LEU:HB3	14:L:34:ILE:CG1	2.49	0.42
15:M:27:SER:OG	15:M:40:ILE:HG13	2.19	0.42
15:M:91:PRO:HG2	15:M:92:TYR:CD2	2.55	0.42
18:P:47:VAL:CG1	18:P:48:GLY:H	2.22	0.42
24:V:69:LYS:HG3	24:V:70:VAL:H	1.81	0.42
25:W:26:ARG:HA	25:W:29:LYS:CG	2.49	0.42
16:N:31:SER:OG	16:N:32:TYR:HD1	2.02	0.42
10:H:46:LEU:CD2	10:H:83:ILE:HB	2.42	0.42
13:K:73:PRO:HD3	13:K:93:TYR:CZ	2.55	0.42
14:L:44:LEU:HA	14:L:47:PHE:HE2	1.83	0.42
14:L:48:VAL:HG12	14:L:52:ILE:HD11	2.01	0.42
3:A:45:HIS:CD2	3:A:216:THR:HG22	2.53	0.42
5:C:92:THR:O	5:C:95:ILE:HG22	2.18	0.42
5:C:98:PRO:HG3	5:C:174:ASP:N	2.33	0.42
8:F:156:ALA:C	8:F:158:HIS:N	2.72	0.42
10:H:114:LEU:O	10:H:121:VAL:HG11	2.19	0.42
10:H:27:TYR:O	10:H:28:VAL:C	2.57	0.42
12:J:85:LEU:N	12:J:85:LEU:HD13	2.35	0.42
16:N:35:LYS:O	16:N:36:GLU:C	2.57	0.42
16:N:77:PRO:HB2	16:N:78:LEU:H	1.56	0.42
17:O:51:LYS:NZ	17:O:55:ARG:NH2	2.66	0.42
21:S:55:TYR:HB2	21:S:56:PRO:HD2	2.00	0.42
22:T:137:ILE:HG12	22:T:138:GLU:N	2.34	0.42
24:V:87:PRO:HB2	24:V:91:LYS:CD	2.43	0.42
13:K:32:PHE:HA	13:K:132:VAL:HG11	2.00	0.42
15:M:104:GLY:O	15:M:106:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:83:VAL:CG2	12:J:84:ASN:H	2.32	0.42
24:V:78:LYS:HD3	24:V:80:LEU:HD12	2.01	0.42
24:V:10:LYS:O	24:V:48:LYS:HE2	2.20	0.42
24:V:53:VAL:CG1	24:V:54:ALA:N	2.83	0.42
4:B:118:VAL:CG2	4:B:119:ALA:H	2.27	0.42
6:D:68:ALA:O	6:D:70:HIS:N	2.52	0.42
9:G:137:PRO:HB2	9:G:138:ILE:H	1.62	0.42
10:H:78:VAL:O	10:H:79:ASN:C	2.56	0.42
11:I:106:LEU:HD12	11:I:106:LEU:H	1.85	0.42
12:J:12:ALA:HB3	12:J:16:ARG:HG3	2.00	0.42
12:J:32:THR:O	12:J:33:ARG:CG	2.68	0.42
21:S:60:PHE:O	21:S:61:ILE:CG1	2.67	0.42
22:T:146:ILE:CD1	22:T:146:ILE:H	2.31	0.42
24:V:48:LYS:O	24:V:49:VAL:HG23	2.19	0.42
28:Z:11:LYS:O	28:Z:12:ARG:C	2.57	0.42
12:J:15:ARG:HG2	12:J:15:ARG:H	1.64	0.42
14:L:44:LEU:O	14:L:45:ARG:C	2.57	0.42
15:M:25:ARG:NH1	15:M:42:ASP:HB3	2.34	0.42
19:Q:11:ARG:HD2	19:Q:98:LYS:HZ1	1.84	0.42
20:R:13:LEU:CD2	20:R:13:LEU:N	2.83	0.42
21:S:13:VAL:HG12	21:S:14:LEU:O	2.19	0.42
24:V:77:ALA:O	24:V:78:LYS:HB3	2.18	0.42
33:2:22:G:O2'	33:2:23:A:H5'	2.20	0.42
4:B:221:VAL:C	4:B:223:GLY:N	2.72	0.42
4:B:250:TRP:O	4:B:250:TRP:HD1	2.03	0.42
5:C:170:LEU:HB3	5:C:185:LYS:CB	2.48	0.42
5:C:188:VAL:CG2	5:C:189:PRO:HD2	2.38	0.42
5:C:36:ARG:HG2	5:C:36:ARG:NH1	2.33	0.42
7:E:173:LEU:HA	7:E:178:PHE:CD2	2.53	0.42
7:E:96:ARG:O	7:E:99:MET:HE3	2.20	0.42
11:I:101:PRO:HB2	11:I:120:GLU:HB3	2.01	0.42
16:N:86:ILE:CG2	16:N:87:ASP:N	2.79	0.42
20:R:65:ARG:HE	20:R:65:ARG:HA	1.74	0.42
3:A:48:LEU:HG	3:A:50:ILE:HG12	2.01	0.42
4:B:147:LEU:CG	4:B:148:GLU:H	2.33	0.42
5:C:183:LEU:O	5:C:183:LEU:HD12	2.20	0.42
5:C:185:LYS:CG	5:C:186:GLY:N	2.62	0.42
5:C:37:ARG:HG2	5:C:46:ALA:O	2.20	0.42
6:D:124:PHE:CE1	6:D:126:GLY:O	2.71	0.42
10:H:113:MET:CA	10:H:116:THR:HG22	2.41	0.42
10:H:34:PRO:HA	10:H:35:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:52:GLU:O	12:J:54:GLY:N	2.51	0.42
13:K:130:LYS:HA	13:K:130:LYS:HD3	1.85	0.42
14:L:99:LYS:HE2	27:Y:42:PRO:HB2	2.01	0.42
15:M:77:ALA:O	15:M:82:ILE:N	2.51	0.42
17:O:87:GLY:O	17:O:89:GLU:HG3	2.20	0.42
17:O:94:ASN:CG	17:O:95:LEU:N	2.72	0.42
18:P:40:LEU:C	18:P:40:LEU:HD22	2.40	0.42
20:R:47:PHE:O	20:R:48:LYS:CB	2.67	0.42
20:R:57:LEU:CD2	20:R:59:VAL:HG22	2.49	0.42
20:R:77:LYS:O	20:R:78:LYS:HB3	2.18	0.42
21:S:9:LYS:O	21:S:11:ASP:N	2.53	0.42
22:T:108:PRO:O	22:T:111:VAL:N	2.53	0.42
27:Y:31:VAL:HB	27:Y:32:PRO:CD	2.50	0.42
3:A:9:ARG:HD3	3:A:10:ALA:N	2.35	0.42
4:B:184:LYS:HE3	4:B:269:PHE:HD2	1.84	0.42
4:B:63:ARG:H	4:B:87:ASN:HD21	1.66	0.42
5:C:175:VAL:C	5:C:176:ILE:HD12	2.40	0.42
5:C:37:ARG:HG2	5:C:37:ARG:H	1.54	0.42
7:E:87:PRO:HB2	7:E:88:ILE:H	1.68	0.42
8:F:157:TYR:O	8:F:158:HIS:HB2	2.19	0.42
10:H:28:VAL:HA	10:H:29:PRO:HD2	1.76	0.42
12:J:144:GLU:HB3	12:J:145:PRO:CD	2.49	0.42
12:J:7:ARG:O	12:J:7:ARG:CG	2.67	0.42
13:K:98:LYS:HB2	13:K:101:ARG:CB	2.37	0.42
15:M:13:ARG:O	15:M:17:ARG:HG3	2.19	0.42
17:O:98:LEU:CD1	17:O:105:VAL:HB	2.30	0.42
18:P:10:LYS:NZ	18:P:22:VAL:HG23	2.31	0.42
18:P:89:GLN:O	18:P:90:PRO:C	2.58	0.42
24:V:76:ARG:CZ	24:V:94:LEU:HD11	2.50	0.42
24:V:88:LYS:HG2	24:V:89:GLU:OE2	2.19	0.42
4:B:115:GLN:NE2	4:B:127:VAL:HG21	2.35	0.42
8:F:121:ILE:O	8:F:121:ILE:HG23	2.20	0.42
17:O:105:VAL:HG21	18:P:43:GLU:HG2	2.02	0.42
4:B:12:SER:O	4:B:13:ARG:HD2	2.20	0.42
10:H:101:TYR:CD1	10:H:101:TYR:N	2.87	0.42
10:H:65:TRP:CZ2	10:H:67:PRO:HG3	2.55	0.42
13:K:132:VAL:O	13:K:133:ARG:HB3	2.20	0.42
18:P:52:VAL:O	18:P:53:GLU:HB2	2.19	0.42
19:Q:29:LEU:HD22	19:Q:69:LEU:O	2.20	0.42
22:T:151:HIS:HB2	22:T:168:GLU:HA	2.00	0.42
23:U:41:ARG:NH1	23:U:42:GLY:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:50:ASN:HB2	23:U:81:VAL:CG1	2.48	0.42
19:Q:88:ARG:CZ	19:Q:92:ARG:O	2.68	0.42
20:R:12:VAL:CG2	20:R:13:LEU:HD23	2.50	0.42
20:R:63:LYS:HD3	20:R:64:LYS:HG2	2.02	0.42
33:2:47:U:C4	33:2:50:U:H5"	2.54	0.42
4:B:79:VAL:HG12	4:B:113:VAL:HA	2.01	0.42
4:B:164:GLN:HE22	4:B:166:GLN:CG	2.19	0.42
4:B:17:THR:CG2	4:B:204:ILE:HA	2.49	0.42
4:B:2:ALA:O	4:B:4:LYS:HD2	2.20	0.42
4:B:69:ARG:HH12	4:B:76:PRO:CG	2.33	0.42
4:B:75:ILE:N	4:B:76:PRO:CD	2.83	0.42
7:E:103:LEU:HD12	7:E:104:GLU:H	1.84	0.42
9:G:81:VAL:HG11	9:G:144:VAL:CG1	2.48	0.42
9:G:94:ALA:HA	9:G:97:ILE:HG12	2.02	0.42
10:H:33:GLU:HA	10:H:34:PRO:HD3	1.75	0.42
6:D:26:HIS:CA	12:J:13:ASN:HB3	2.45	0.42
16:N:70:VAL:CG1	16:N:71:GLY:N	2.82	0.42
16:N:85:LYS:HZ3	16:N:85:LYS:HB3	1.83	0.42
17:O:104:GLN:O	17:O:107:ALA:HB3	2.19	0.42
17:O:64:ARG:HB3	17:O:64:ARG:HH21	1.85	0.42
23:U:17:GLN:O	23:U:18:ALA:HB3	2.20	0.42
25:W:29:LYS:HB2	25:W:29:LYS:NZ	2.32	0.42
25:W:41:ILE:O	25:W:43:GLN:N	2.53	0.42
18:P:58:VAL:HB	18:P:59:ALA:H	1.71	0.42
19:Q:70:TYR:HD2	19:Q:70:TYR:O	2.03	0.42
23:U:51:VAL:HG23	23:U:81:VAL:CG2	2.34	0.42
24:V:12:PRO:HG3	24:V:63:ALA:H	1.84	0.42
26:X:16:PRO:O	26:X:19:GLN:HB2	2.19	0.42
4:B:92:ILE:HD12	4:B:93:ALA:N	2.34	0.42
5:C:116:VAL:HG13	5:C:122:PHE:HB2	2.00	0.42
5:C:30:PRO:HG3	5:C:92:THR:HG22	2.02	0.42
7:E:17:PRO:HA	7:E:20:ILE:CG1	2.50	0.42
8:F:116:GLU:O	8:F:118:PRO:HD3	2.19	0.42
9:G:147:GLN:HA	9:G:147:GLN:HE21	1.85	0.42
10:H:112:LYS:NZ	10:H:116:THR:HG21	2.35	0.42
13:K:63:LYS:HE3	22:T:116:VAL:HG11	1.98	0.42
14:L:29:LEU:HD11	14:L:75:LEU:HB2	2.02	0.42
15:M:89:ARG:HH11	15:M:89:ARG:HG2	1.85	0.42
20:R:17:ALA:C	20:R:19:ALA:H	2.24	0.42
27:Y:58:LEU:N	27:Y:58:LEU:HD12	2.35	0.42
3:A:166:ASN:O	3:A:167:ASP:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:48:LEU:CB	3:A:209:PHE:O	2.65	0.41
6:D:39:ARG:O	6:D:40:ARG:C	2.58	0.41
7:E:8:LYS:C	7:E:10:LYS:H	2.23	0.41
7:E:161:THR:CG2	7:E:163:ALA:H	2.31	0.41
11:I:10:VAL:HG12	11:I:12:ASP:O	2.19	0.41
11:I:62:VAL:C	11:I:63:VAL:HG22	2.40	0.41
11:I:70:LYS:HG3	11:I:71:ARG:H	1.85	0.41
11:I:79:PHE:HD2	16:N:70:VAL:CG1	2.27	0.41
11:I:8:LEU:HD22	11:I:8:LEU:N	2.34	0.41
15:M:63:THR:HG1	15:M:100:ALA:HB2	1.84	0.41
18:P:84:LYS:HE3	18:P:84:LYS:HB3	2.57	0.41
24:V:31:GLY:O	24:V:32:LYS:CB	2.68	0.41
7:E:103:LEU:HA	7:E:106:LEU:CD2	2.50	0.41
33:2:16:U:H3'	33:2:17:U:C5'	2.50	0.41
4:B:69:ARG:HH12	4:B:76:PRO:CD	2.33	0.41
5:C:116:VAL:C	5:C:118:LYS:N	2.72	0.41
10:H:108:ILE:HG23	10:H:112:LYS:HD2	2.00	0.41
13:K:132:VAL:HG13	13:K:133:ARG:H	1.79	0.41
15:M:26:LEU:HB3	15:M:39:ILE:HG22	2.02	0.41
17:O:33:ARG:HG3	17:O:34:LYS:N	2.36	0.41
19:Q:29:LEU:HD11	19:Q:67:ASP:H	1.85	0.41
19:Q:86:LEU:HA	19:Q:87:PRO:HD3	1.88	0.41
20:R:57:LEU:HD23	20:R:58:HIS:N	2.36	0.41
22:T:127:LYS:HB3	22:T:162:GLU:HG3	2.00	0.41
23:U:49:LYS:H	23:U:49:LYS:HD2	1.86	0.41
33:2:54:U:H2'	33:2:55:PSU:O5'	2.19	0.41
4:B:113:VAL:O	4:B:115:GLN:N	2.51	0.41
4:B:117:VAL:HG13	4:B:128:GLY:CA	2.50	0.41
4:B:132:PRO:C	4:B:136:ILE:HG13	2.41	0.41
5:C:122:PHE:HB3	5:C:123:ALA:H	1.52	0.41
5:C:173:VAL:HG23	5:C:183:LEU:HD13	2.01	0.41
5:C:89:ASP:O	5:C:90:THR:OG1	2.31	0.41
6:D:31:VAL:O	6:D:32:VAL:C	2.59	0.41
7:E:47:LYS:HD2	7:E:72:ARG:HH22	1.85	0.41
8:F:105:LEU:CD1	8:F:107:VAL:HG23	2.50	0.41
13:K:75:THR:HG23	13:K:77:LYS:HZ1	1.83	0.41
15:M:106:ARG:O	15:M:106:ARG:HD2	2.19	0.41
16:N:60:THR:OG1	16:N:75:ILE:HG23	2.20	0.41
11:I:77:ILE:HD11	16:N:72:VAL:HA	2.02	0.41
17:O:5:LYS:O	17:O:6:THR:C	2.59	0.41
17:O:80:ILE:O	17:O:81:HIS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:92:ARG:HH12	18:P:10:LYS:N	2.18	0.41
21:S:9:LYS:HG3	21:S:10:GLY:N	2.30	0.41
22:T:108:PRO:CB	22:T:144:LEU:HB3	2.40	0.41
22:T:150:LEU:HD13	22:T:154:ASP:OD1	2.20	0.41
23:U:54:GLY:O	23:U:57:PHE:O	2.37	0.41
26:X:59:VAL:O	26:X:59:VAL:HG23	2.21	0.41
10:H:38:LEU:HB3	10:H:159:GLU:HB2	2.02	0.41
13:K:119:ARG:C	13:K:123:HIS:HB2	2.41	0.41
14:L:18:LEU:HA	14:L:21:TYR:HB2	2.01	0.41
23:U:36:ILE:HG13	23:U:60:PHE:HB3	2.01	0.41
33:2:1:G:H2'	33:2:2:C:H6	1.85	0.41
3:A:194:ILE:O	3:A:197:LEU:HD23	2.21	0.41
3:A:42:VAL:HG22	3:A:217:THR:HG22	2.02	0.41
4:B:248:SER:HB2	4:B:252:TRP:NE1	2.34	0.41
5:C:35:GLN:HB2	5:C:48:GLN:HB2	2.02	0.41
6:D:61:PRO:O	6:D:65:THR:HB	2.20	0.41
6:D:73:ILE:HG12	6:D:73:ILE:O	2.21	0.41
7:E:46:ALA:C	7:E:48:GLU:H	2.24	0.41
7:E:98:ARG:O	7:E:101:ILE:HG22	2.20	0.41
8:F:105:LEU:HD13	8:F:106:THR:N	2.36	0.41
9:G:93:THR:O	9:G:94:ALA:C	2.59	0.41
16:N:107:ASP:N	16:N:111:ARG:HH11	2.18	0.41
18:P:76:LYS:HE2	18:P:85:LYS:HB3	2.02	0.41
19:Q:22:ASP:HA	19:Q:25:ARG:HD2	2.02	0.41
25:W:36:ARG:C	25:W:38:GLN:N	2.73	0.41
12:J:118:GLY:O	12:J:119:GLU:HB3	2.21	0.41
21:S:32:PRO:O	21:S:33:LYS:CB	2.68	0.41
3:A:183:PRO:HA	3:A:186:LEU:HG	2.03	0.41
3:A:226:ASN:HA	3:A:227:PRO:HD2	1.95	0.41
4:B:92:ILE:HA	4:B:106:ILE:HA	2.02	0.41
4:B:140:THR:O	4:B:164:GLN:HA	2.21	0.41
4:B:174:ILE:CG2	4:B:175:LEU:H	2.20	0.41
4:B:228:PRO:HD3	4:B:236:GLY:HA2	2.03	0.41
5:C:119:ARG:HB3	5:C:120:TRP:CD1	2.56	0.41
5:C:172:VAL:O	5:C:173:VAL:HG13	2.21	0.41
5:C:173:VAL:HG23	5:C:183:LEU:CD2	2.49	0.41
5:C:20:ALA:O	5:C:21:VAL:HG13	2.20	0.41
8:F:101:ARG:HD2	8:F:121:ILE:HG23	2.02	0.41
9:G:132:PRO:HG2	9:G:133:HIS:ND1	2.36	0.41
10:H:41:ALA:H	10:H:44:LYS:CG	2.33	0.41
11:I:5:GLN:NE2	11:I:5:GLN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:18:LEU:C	14:L:18:LEU:HD23	2.41	0.41
16:N:105:LEU:O	16:N:110:ILE:HD13	2.21	0.41
19:Q:79:GLY:HA3	19:Q:102:HIS:CD2	2.55	0.41
19:Q:7:ALA:HB3	19:Q:103:ILE:HG13	2.02	0.41
19:Q:7:ALA:HB2	19:Q:20:VAL:CG2	10.40	0.41
19:Q:63:ASP:O	19:Q:64:MET:HG2	2.20	0.41
20:R:12:VAL:HG11	20:R:17:ALA:HB2	1.99	0.41
20:R:27:THR:O	20:R:28:PHE:HD2	2.03	0.41
21:S:97:ARG:HD2	21:S:97:ARG:C	2.41	0.41
22:T:67:LEU:HD11	22:T:88:PHE:CZ	2.55	0.41
23:U:28:GLY:HA2	23:U:67:VAL:O	2.19	0.41
24:V:84:GLY:C	24:V:86:SER:N	2.73	0.41
28:Z:46:VAL:HG12	28:Z:47:ARG:H	1.84	0.41
3:A:63:VAL:HG13	3:A:64:SER:H	1.86	0.41
6:D:98:LYS:HD3	6:D:101:ARG:HH21	1.84	0.41
13:K:32:PHE:CA	13:K:132:VAL:HG11	2.51	0.41
6:D:109:VAL:HA	6:D:112:ARG:CG	2.49	0.41
13:K:24:GLY:O	13:K:98:LYS:HD3	2.19	0.41
19:Q:10:VAL:HG12	19:Q:11:ARG:N	2.23	0.41
9:G:99:GLU:HB3	9:G:103:ARG:HH12	1.83	0.41
10:H:95:TYR:CE1	10:H:109:PRO:HA	2.55	0.41
27:Y:15:ARG:HA	27:Y:18:ALA:HB3	2.01	0.41
13:K:134:ARG:HD3	13:K:134:ARG:C	2.40	0.41
27:Y:9:LYS:HD3	27:Y:9:LYS:HA	1.91	0.41
28:Z:23:ARG:HG2	28:Z:23:ARG:HH11	1.85	0.41
24:V:39:LYS:HA	24:V:39:LYS:HD2	1.82	0.41
13:K:72:LYS:NZ	13:K:73:PRO:HB2	2.30	0.41
33:2:49:C:C6	33:2:49:C:O5'	2.73	0.41
3:A:179:ALA:O	3:A:181:PHE:N	2.53	0.41
3:A:45:HIS:CD2	3:A:216:THR:CG2	3.03	0.41
3:A:41:THR:HG22	3:A:42:VAL:N	2.29	0.41
4:B:4:LYS:HZ1	4:B:22:SER:H	1.68	0.41
9:G:109:ILE:HG23	9:G:110:ASP:H	1.85	0.41
9:G:63:ALA:HA	9:G:66:GLU:CG	2.50	0.41
12:J:25:SER:N	12:J:31:ALA:HB2	2.34	0.41
13:K:132:VAL:HG22	13:K:133:ARG:N	2.32	0.41
13:K:52:VAL:CG2	13:K:53:ALA:H	2.32	0.41
15:M:67:ARG:CA	15:M:100:ALA:O	2.57	0.41
20:R:75:ASP:C	20:R:76:ARG:HD3	2.41	0.41
20:R:7:VAL:HG13	20:R:8:ILE:N	2.36	0.41
22:T:36:LYS:O	22:T:37:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:50:ASN:CB	23:U:81:VAL:HG11	2.50	0.41
21:S:37:VAL:HG22	21:S:62:GLU:OE1	2.20	0.41
16:N:135:VAL:CG1	16:N:136:GLN:H	2.09	0.41
22:T:167:PRO:O	22:T:169:GLU:N	2.49	0.41
3:A:193:PHE:CD2	3:A:193:PHE:O	2.72	0.41
4:B:25:THR:H	4:B:82:ILE:C	2.24	0.41
5:C:77:ILE:HB	5:C:79:ARG:NE	2.36	0.41
8:F:89:ILE:CG1	8:F:129:THR:HB	2.51	0.41
8:F:20:ALA:O	8:F:22:GLY:N	2.54	0.41
9:G:24:GLY:O	9:G:25:TYR:C	2.58	0.41
12:J:123:LEU:O	12:J:124:LYS:C	2.59	0.41
13:K:7:MET:HA	13:K:8:LYS:HZ2	1.86	0.41
15:M:68:GLN:O	15:M:72:ALA:N	2.54	0.41
16:N:100:TYR:CD1	16:N:100:TYR:N	2.88	0.41
18:P:28:GLU:O	18:P:29:PRO:O	2.37	0.41
24:V:18:ILE:HD12	24:V:18:ILE:H	1.86	0.41
24:V:79:GLY:O	24:V:80:LEU:HG	2.21	0.41
25:W:7:ARG:HG2	25:W:7:ARG:H	1.71	0.41
19:Q:19:LEU:O	27:Y:25:LEU:HD23	2.20	0.41
17:O:32:PHE:CG	17:O:33:ARG:N	2.88	0.41
17:O:92:ARG:C	17:O:94:ASN:N	2.74	0.41
33:2:43:G:O2'	33:2:44:A:H5'	2.20	0.41
11:I:87:ILE:HA	11:I:93:PRO:HA	2.03	0.41
27:Y:44:THR:CG2	27:Y:45:VAL:H	2.33	0.41
24:V:78:LYS:C	24:V:78:LYS:HD2	2.41	0.41
4:B:133:LEU:N	4:B:133:LEU:HD22	2.32	0.41
5:C:75:VAL:HG12	5:C:75:VAL:O	2.21	0.41
6:D:178:VAL:CA	6:D:181:ILE:HG22	2.51	0.41
7:E:82:LEU:HD13	7:E:83:ARG:C	2.41	0.41
9:G:3:VAL:N	9:G:21:VAL:HG21	2.31	0.41
9:G:90:GLY:O	9:G:91:SER:OG	2.32	0.41
11:I:77:ILE:CD1	11:I:79:PHE:CD1	3.01	0.41
12:J:122:PRO:O	12:J:123:LEU:HB2	2.21	0.41
15:M:106:ARG:CD	15:M:111:GLU:HA	2.51	0.41
16:N:5:ALA:O	16:N:8:LYS:N	2.54	0.41
16:N:95:ARG:HG3	16:N:96:ARG:NH1	2.36	0.41
18:P:21:ARG:O	18:P:22:VAL:CB	2.69	0.41
19:Q:29:LEU:N	19:Q:29:LEU:HD23	2.36	0.41
20:R:21:PHE:CD2	20:R:26:TYR:HE1	2.39	0.41
20:R:39:ILE:HD13	20:R:43:VAL:HG12	2.02	0.41
22:T:11:GLU:O	22:T:13:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:151:HIS:O	22:T:153:SER:N	2.53	0.41
22:T:26:GLY:HA3	22:T:86:VAL:CG2	2.50	0.41
24:V:55:GLY:N	24:V:58:ILE:HD11	2.35	0.41
4:B:242:ARG:HB3	4:B:243:GLY:H	1.55	0.41
4:B:44:ASN:HA	4:B:49:ILE:CA	2.36	0.41
4:B:30:GLU:HB3	4:B:63:ARG:HH22	1.85	0.41
4:B:75:ILE:H	4:B:76:PRO:CD	2.32	0.41
5:C:77:ILE:HG21	5:C:79:ARG:HH21	1.86	0.41
6:D:132:LYS:HA	6:D:135:LEU:CB	2.51	0.41
7:E:125:PHE:HB3	7:E:131:TYR:HE1	1.84	0.41
7:E:43:LEU:HB3	7:E:44:GLY:H	1.77	0.41
7:E:72:ARG:HD2	7:E:87:PRO:HB3	2.03	0.41
8:F:76:VAL:CA	8:F:79:VAL:HG22	2.46	0.41
10:H:62:ARG:HA	10:H:63:PRO:HD2	1.96	0.41
13:K:72:LYS:O	13:K:73:PRO:O	2.38	0.41
13:K:7:MET:HB2	13:K:93:TYR:CD2	2.56	0.41
14:L:19:ALA:HB3	14:L:81:ASP:O	28.73	0.41
15:M:54:LEU:O	15:M:55:ALA:C	2.59	0.41
11:I:12:ASP:OD1	11:I:86:ILE:HD12	2.20	0.41
18:P:23:GLU:O	18:P:24:LYS:CB	2.68	0.41
21:S:71:LYS:NZ	21:S:73:ARG:HE	2.18	0.41
14:L:102:GLU:O	14:L:103:ARG:C	2.59	0.41
15:M:24:LEU:HB2	15:M:85:VAL:CG2	2.51	0.41
16:N:17:THR:O	16:N:18:ASP:C	2.59	0.41
16:N:88:ILE:HB	16:N:89:VAL:H	1.50	0.41
25:W:60:LEU:O	25:W:60:LEU:HD13	2.21	0.41
20:R:61:GLY:HA2	20:R:71:GLY:O	2.21	0.41
22:T:99:TYR:CD2	22:T:124:ILE:C	2.94	0.41
28:Z:19:ARG:CG	28:Z:23:ARG:HH21	2.32	0.41
13:K:114:ALA:O	13:K:115:MET:C	2.58	0.41
3:A:53:ARG:CG	33:2:54:U:O2'	2.57	0.41
3:A:195:ARG:C	3:A:197:LEU:N	2.73	0.41
5:C:176:ILE:CG2	5:C:181:LEU:HD23	2.51	0.41
5:C:173:VAL:CA	5:C:183:LEU:HD11	2.51	0.41
5:C:105:THR:O	5:C:196:VAL:HG22	2.21	0.41
6:D:162:ALA:O	6:D:163:ARG:C	2.60	0.41
6:D:165:LEU:HD12	6:D:170:THR:HB	2.03	0.41
7:E:151:ALA:O	7:E:152:LEU:HB3	2.20	0.41
7:E:5:LEU:CD1	7:E:9:ARG:HD3	2.39	0.41
8:F:127:GLU:H	8:F:128:PRO:HA	1.85	0.41
10:H:62:ARG:CZ	10:H:63:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:137:LYS:CB	12:J:138:LEU:HD12	2.49	0.41
14:L:7:GLY:O	14:L:8:ARG:HB2	2.20	0.41
18:P:50:PRO:C	18:P:51:VAL:HG23	2.42	0.41
19:Q:29:LEU:HD11	19:Q:67:ASP:N	2.36	0.41
22:T:31:ARG:HG3	22:T:32:HIS:CE1	2.56	0.41
33:2:11:C:C4	33:2:12:U:C5	3.08	0.41
13:K:53:ALA:O	13:K:57:HIS:HB2	2.21	0.41
19:Q:40:ASN:O	19:Q:41:LYS:CB	2.67	0.41
3:A:198:GLU:HA	3:A:201:LYS:HB3	2.03	0.40
4:B:134:ARG:HA	4:B:134:ARG:HD2	1.93	0.40
4:B:244:ARG:HA	4:B:245:PRO:HA	1.89	0.40
5:C:27:LEU:HG	5:C:28:ALA:H	1.83	0.40
5:C:34:VAL:HG13	5:C:67:PHE:HE1	1.81	0.40
5:C:84:PHE:C	5:C:84:PHE:CD1	2.95	0.40
6:D:130:LYS:HD3	6:D:131:THR:N	2.35	0.40
6:D:149:VAL:O	6:D:150:LEU:HD13	2.20	0.40
6:D:196:VAL:HG22	6:D:197:PHE:CD1	2.55	0.40
6:D:92:TYR:CD1	6:D:92:TYR:N	2.89	0.40
9:G:124:GLY:HA2	9:G:144:VAL:O	2.21	0.40
11:I:43:VAL:HG12	11:I:44:LYS:N	2.36	0.40
11:I:47:ILE:HG22	11:I:49:ARG:HG2	2.04	0.40
11:I:88:ASN:HB2	11:I:94:ARG:HB2	2.03	0.40
12:J:137:LYS:C	12:J:138:LEU:HD12	2.42	0.40
13:K:33:GLY:N	13:K:132:VAL:HG11	2.37	0.40
13:K:42:ILE:C	13:K:42:ILE:HD13	2.42	0.40
13:K:72:LYS:HA	13:K:73:PRO:HD3	1.98	0.40
14:L:21:TYR:O	14:L:24:GLN:HB2	2.21	0.40
22:T:125:LEU:HA	22:T:125:LEU:HD12	1.84	0.40
22:T:58:VAL:HG12	22:T:59:LEU:N	2.36	0.40
28:Z:22:MET:HG2	28:Z:22:MET:O	2.22	0.40
22:T:9:TYR:HD2	22:T:9:TYR:HA	1.77	0.40
26:X:8:LEU:HD11	26:X:31:LEU:HA	2.03	0.40
16:N:44:ASP:OD2	16:N:85:LYS:HD2	2.22	0.40
25:W:50:ILE:O	25:W:51:ARG:HB2	2.20	0.40
4:B:2:ALA:HA	4:B:200:ASP:HB2	2.02	0.40
5:C:183:LEU:CD1	5:C:183:LEU:C	2.89	0.40
5:C:61:ARG:HG3	5:C:62:PRO:CD	2.52	0.40
6:D:129:GLY:HA2	6:D:161:ALA:CB	2.51	0.40
6:D:35:GLN:HE21	6:D:39:ARG:HH22	1.69	0.40
7:E:99:MET:HE3	7:E:100:TRP:HB2	2.02	0.40
7:E:135:LEU:C	7:E:136:ARG:HE	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:95:ARG:HH11	7:E:95:ARG:N	2.19	0.40
8:F:11:VAL:N	8:F:12:PRO:HD3	2.36	0.40
9:G:88:ILE:CG2	9:G:89:TYR:H	2.21	0.40
13:K:119:ARG:O	13:K:122:GLY:N	2.54	0.40
17:O:90:VAL:C	17:O:92:ARG:N	2.74	0.40
18:P:36:PRO:HD2	18:P:60:GLU:OE1	2.21	0.40
34:3:4:G:H2'	34:3:5:A:H8	1.84	0.40
5:C:151:TYR:HB2	5:C:154:LYS:CB	2.52	0.40
12:J:21:ARG:HB3	12:J:22:GLY:H	1.52	0.40
22:T:151:HIS:HB3	22:T:168:GLU:C	2.42	0.40
33:2:3:G:H2'	33:2:4:G:H5'	2.04	0.40
5:C:4:ILE:C	5:C:5:LEU:HD12	2.42	0.40
5:C:5:LEU:CD1	5:C:5:LEU:N	2.83	0.40
8:F:60:ARG:HA	8:F:60:ARG:HD3	1.95	0.40
9:G:24:GLY:N	9:G:27:ARG:CZ	2.84	0.40
9:G:62:LYS:HD2	9:G:135:GLU:HB3	2.02	0.40
11:I:101:PRO:HB2	11:I:120:GLU:C	2.42	0.40
11:I:26:LYS:CB	11:I:30:ALA:HB2	2.49	0.40
12:J:85:LEU:HD22	12:J:86:LYS:N	2.37	0.40
12:J:88:LEU:CD1	12:J:90:ARG:HH21	2.34	0.40
12:J:91:PHE:CD2	12:J:92:GLU:N	2.90	0.40
13:K:106:VAL:CG1	13:K:118:LEU:HD11	2.51	0.40
15:M:38:GLN:HA	15:M:50:SER:CB	2.49	0.40
16:N:15:VAL:O	16:N:19:LEU:HD23	9.62	0.40
23:U:37:LEU:CD1	23:U:38:VAL:HG23	2.50	0.40
28:Z:5:TRP:HA	28:Z:5:TRP:CE3	2.57	0.40
15:M:38:GLN:HB2	15:M:38:GLN:HE21	1.61	0.40
15:M:17:ARG:CZ	15:M:89:ARG:HD2	2.47	0.40
25:W:12:GLU:O	25:W:14:ARG:N	2.54	0.40
16:N:97:ALA:HB3	16:N:98:LYS:NZ	2.37	0.40
25:W:14:ARG:CB	25:W:54:LYS:HE2	2.50	0.40
14:L:66:VAL:C	14:L:68:ARG:H	2.22	0.40
3:A:8:TYR:N	3:A:8:TYR:CD1	2.89	0.40
5:C:176:ILE:HD13	5:C:182:LEU:CA	2.50	0.40
5:C:4:ILE:HG22	5:C:91:VAL:C	2.41	0.40
6:D:148:SER:HB3	6:D:184:THR:HG22	2.03	0.40
6:D:194:TRP:C	6:D:196:VAL:N	2.75	0.40
10:H:127:LYS:HA	10:H:130:LEU:HD11	2.03	0.40
13:K:71:ASP:N	13:K:94:VAL:O	2.55	0.40
17:O:103:PRO:O	17:O:104:GLN:C	2.60	0.40
22:T:17:ALA:HA	22:T:20:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:29:LYS:C	25:W:29:LYS:HZ2	2.24	0.40
25:W:55:ARG:HB2	25:W:56:GLN:OE1	2.21	0.40
19:Q:70:TYR:C	19:Q:70:TYR:CD2	2.94	0.40
33:2:71:G:C6	33:2:72:C:C4	3.09	0.40
3:A:18:ASN:HB3	3:A:19:LYS:H	1.74	0.40
4:B:92:ILE:HG22	4:B:105:ILE:O	2.22	0.40
4:B:151:LYS:HD2	4:B:151:LYS:HA	1.94	0.40
5:C:189:PRO:HB2	5:C:190:GLY:H	1.63	0.40
5:C:52:LEU:HB3	5:C:76:ARG:H	1.85	0.40
5:C:55:ASN:ND2	5:C:75:VAL:HG23	2.37	0.40
8:F:34:GLU:CG	8:F:35:VAL:N	2.81	0.40
9:G:65:ALA:CB	9:G:133:HIS:HD1	2.35	0.40
12:J:12:ALA:O	12:J:13:ASN:C	2.60	0.40
14:L:3:HIS:O	14:L:4:LEU:HG	2.22	0.40
4:B:24:ILE:CG2	4:B:25:THR:HG22	2.51	0.40
15:M:25:ARG:NH2	15:M:89:ARG:NH2	2.55	0.40
16:N:33:LYS:HG3	16:N:42:ILE:O	2.22	0.40
21:S:49:VAL:CG1	21:S:50:ARG:H	2.26	0.40
19:Q:57:ASN:HD22	19:Q:61:ASN:HD22	1.69	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:10:GLU:O	31:y:436:C:OP1[4_555]	1.78	0.42
9:G:89:TYR:O	31:y:357:G:O2'[4_555]	2.00	0.20
9:G:90:GLY:O	31:y:368:U:OP2[4_555]	2.11	0.09
9:G:90:GLY:O	31:y:368:U:OP1[4_555]	2.14	0.06
9:G:91:SER:O	31:y:368:U:OP1[4_555]	2.17	0.03
9:G:91:SER:OG	31:y:368:U:OP1[4_555]	2.19	0.01

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	
3	A	123/229 (54%)	72 (58%)	31 (25%)	20 (16%)	0	4
4	B	270/276 (98%)	134 (50%)	64 (24%)	72 (27%)	0	1
5	C	199/206 (97%)	99 (50%)	47 (24%)	53 (27%)	0	1
6	D	192/205 (94%)	91 (47%)	45 (23%)	56 (29%)	0	0
7	E	178/182 (98%)	97 (54%)	55 (31%)	26 (15%)	0	5
8	F	171/180 (95%)	90 (53%)	40 (23%)	41 (24%)	0	1
9	G	146/148 (99%)	83 (57%)	35 (24%)	28 (19%)	0	2
10	H	136/140 (97%)	62 (46%)	45 (33%)	29 (21%)	0	2
11	I	120/122 (98%)	62 (52%)	24 (20%)	34 (28%)	0	0
12	J	144/150 (96%)	63 (44%)	46 (32%)	35 (24%)	0	1
13	K	135/141 (96%)	56 (42%)	41 (30%)	38 (28%)	0	0
14	L	116/118 (98%)	64 (55%)	30 (26%)	22 (19%)	0	3
15	M	104/112 (93%)	58 (56%)	22 (21%)	24 (23%)	0	1
16	N	135/146 (92%)	56 (42%)	40 (30%)	39 (29%)	0	0
17	O	115/118 (98%)	66 (57%)	28 (24%)	21 (18%)	0	3
18	P	99/101 (98%)	39 (39%)	28 (28%)	32 (32%)	0	0
19	Q	107/113 (95%)	64 (60%)	23 (22%)	20 (19%)	0	3
20	R	90/96 (94%)	29 (32%)	36 (40%)	25 (28%)	0	0
21	S	101/110 (92%)	28 (28%)	31 (31%)	42 (42%)	0	0
22	T	183/206 (89%)	115 (63%)	45 (25%)	23 (13%)	0	7
23	U	74/85 (87%)	31 (42%)	21 (28%)	22 (30%)	0	0
24	V	86/98 (88%)	41 (48%)	29 (34%)	16 (19%)	0	3
25	W	60/72 (83%)	33 (55%)	11 (18%)	16 (27%)	0	1
26	X	58/60 (97%)	31 (53%)	20 (34%)	7 (12%)	0	8
27	Y	54/60 (90%)	27 (50%)	16 (30%)	11 (20%)	0	2
28	Z	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	0	10
29	a	61/65 (94%)	28 (46%)	20 (33%)	13 (21%)	0	2
30	b	33/37 (89%)	16 (48%)	10 (30%)	7 (21%)	0	2
35	c	232/256 (91%)	142 (61%)	59 (25%)	31 (13%)	0	6
36	d	204/239 (85%)	102 (50%)	60 (29%)	42 (21%)	0	2
37	e	206/209 (99%)	120 (58%)	60 (29%)	26 (13%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	f	148/162 (91%)	102 (69%)	32 (22%)	14 (10%)	1	14
39	g	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	17
40	h	153/156 (98%)	96 (63%)	30 (20%)	27 (18%)	0	3
41	i	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	5
42	j	125/128 (98%)	81 (65%)	29 (23%)	15 (12%)	0	8
43	k	96/105 (91%)	55 (57%)	25 (26%)	16 (17%)	0	4
44	l	114/129 (88%)	74 (65%)	28 (25%)	12 (10%)	0	11
45	m	122/132 (92%)	67 (55%)	35 (29%)	20 (16%)	0	4
46	n	123/126 (98%)	70 (57%)	35 (28%)	18 (15%)	0	5
47	o	58/61 (95%)	30 (52%)	16 (28%)	12 (21%)	0	2
48	p	86/89 (97%)	51 (59%)	24 (28%)	11 (13%)	0	7
49	q	81/88 (92%)	34 (42%)	25 (31%)	22 (27%)	0	0
50	r	102/105 (97%)	54 (53%)	24 (24%)	24 (24%)	0	1
51	s	79/88 (90%)	45 (57%)	21 (27%)	13 (16%)	0	4
52	t	78/93 (84%)	30 (38%)	26 (33%)	22 (28%)	0	0
53	u	97/106 (92%)	47 (48%)	35 (36%)	15 (16%)	0	4
54	v	22/27 (82%)	8 (36%)	6 (27%)	8 (36%)	0	0
All	All	5697/6163 (92%)	3030 (53%)	1515 (27%)	1152 (20%)	0	2

All (1152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	8	TYR
3	A	16	ASP
3	A	63	VAL
3	A	176	VAL
3	A	179	ALA
3	A	180	SER
3	A	209	PHE
4	B	3	VAL
4	B	6	PHE
4	B	15	PHE
4	B	21	PHE
4	B	36	PRO
4	B	39	LYS
4	B	44	ASN

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Mol	Chain	Res	Type
4	B	59	LYS
4	B	69	ARG
4	B	83	GLU
4	B	91	ARG
4	B	105	ILE
4	B	138	VAL
4	B	149	PRO
4	B	156	ALA
4	B	196	VAL
4	B	206	LEU
4	B	209	ALA
4	B	227	ASN
4	B	228	PRO
4	B	235	GLY
4	B	239	ARG
4	B	259	THR
4	B	262	ARG
4	B	263	ARG
5	C	35	GLN
5	C	51	PHE
5	C	54	GLN
5	C	65	GLY
5	C	67	PHE
5	C	73	GLU
5	C	77	ILE
5	C	82	ARG
5	C	104	VAL
5	C	121	ASN
5	C	122	PHE
5	C	128	SER
5	C	143	ASN
5	C	144	ARG
5	C	149	ARG
5	C	178	GLU
5	C	189	PRO
6	D	17	ALA
6	D	18	ASP
6	D	23	ILE
6	D	38	LYS
6	D	48	THR
6	D	54	TYR
6	D	58	LYS

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Mol	Chain	Res	Type
6	D	59	ILE
6	D	68	ALA
6	D	87	PRO
6	D	120	LEU
6	D	128	ASN
6	D	146	SER
6	D	172	ALA
6	D	176	LEU
6	D	196	VAL
7	E	13	GLU
7	E	26	GLN
7	E	29	TRP
7	E	78	SER
7	E	79	ASN
7	E	82	LEU
7	E	84	LYS
7	E	87	PRO
7	E	88	ILE
7	E	95	ARG
7	E	163	ALA
7	E	181	ARG
8	F	10	PRO
8	F	40	GLU
8	F	52	VAL
8	F	55	PRO
8	F	58	GLU
8	F	71	LEU
8	F	99	VAL
8	F	101	ARG
8	F	109	PHE
8	F	157	TYR
8	F	173	PRO
8	F	178	ALA
9	G	8	PRO
9	G	26	ALA
9	G	29	TYR
9	G	38	LEU
9	G	82	ARG
9	G	94	ALA
9	G	122	GLU
9	G	125	GLU
9	G	132	PRO

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Mol	Chain	Res	Type
9	G	138	ILE
10	H	26	THR
10	H	67	PRO
10	H	102	PRO
10	H	108	ILE
10	H	110	LEU
10	H	146	TYR
10	H	147	ALA
10	H	153	HIS
11	I	5	GLN
11	I	51	ALA
11	I	52	VAL
11	I	54	GLU
11	I	60	ALA
11	I	63	VAL
11	I	75	SER
11	I	85	VAL
11	I	90	GLN
11	I	91	LEU
11	I	115	VAL
12	J	12	ALA
12	J	17	LYS
12	J	33	ARG
12	J	35	HIS
12	J	45	LEU
12	J	52	GLU
12	J	71	VAL
12	J	90	ARG
12	J	106	LEU
12	J	119	GLU
12	J	124	LYS
12	J	148	LEU
13	K	3	MET
13	K	4	PRO
13	K	21	THR
13	K	25	ASP
13	K	27	VAL
13	K	31	ASP
13	K	38	GLU
13	K	68	ILE
13	K	73	PRO
13	K	79	LEU

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Mol	Chain	Res	Type
13	K	80	GLU
13	K	81	VAL
13	K	83	MET
13	K	85	LYS
13	K	108	GLY
13	K	120	ILE
13	K	127	ILE
13	K	133	ARG
14	L	2	ARG
14	L	5	LYS
14	L	12	ARG
14	L	37	THR
14	L	45	ARG
14	L	60	LEU
14	L	62	ALA
14	L	95	THR
14	L	102	GLU
14	L	104	ARG
14	L	117	VAL
15	M	8	GLU
15	M	9	ARG
15	M	10	ARG
15	M	12	PHE
15	M	32	LEU
15	M	35	ILE
16	N	12	SER
16	N	18	ASP
16	N	28	VAL
16	N	30	VAL
16	N	33	LYS
16	N	42	ILE
16	N	45	PHE
16	N	74	ARG
16	N	83	ILE
16	N	96	ARG
16	N	101	PHE
16	N	107	ASP
16	N	135	VAL
17	O	6	THR
17	O	22	LYS
17	O	25	TRP
17	O	76	TYR

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Mol	Chain	Res	Type
17	O	90	VAL
17	O	92	ARG
17	O	104	GLN
17	O	105	VAL
18	P	15	GLU
18	P	22	VAL
18	P	26	ASP
18	P	27	ALA
18	P	29	PRO
18	P	31	ALA
18	P	44	LYS
18	P	50	PRO
18	P	51	VAL
18	P	53	GLU
18	P	68	LYS
18	P	72	VAL
18	P	78	LYS
19	Q	40	ASN
19	Q	67	ASP
19	Q	80	PRO
19	Q	89	ALA
19	Q	90	ARG
19	Q	96	ILE
20	R	6	ASP
20	R	11	PRO
20	R	22	ALA
20	R	30	VAL
20	R	32	PRO
20	R	48	LYS
20	R	49	VAL
20	R	60	ARG
20	R	80	ILE
20	R	81	VAL
20	R	83	VAL
20	R	89	ILE
21	S	7	VAL
21	S	16	ALA
21	S	20	TYR
21	S	21	LYS
21	S	31	LEU
21	S	39	VAL
21	S	46	LYS

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Mol	Chain	Res	Type
21	S	54	LYS
21	S	57	GLN
21	S	61	ILE
21	S	77	PRO
21	S	96	ILE
21	S	100	ALA
22	T	41	LEU
22	T	52	SER
22	T	66	SER
22	T	95	PRO
22	T	146	ILE
23	U	14	ARG
23	U	17	GLN
23	U	18	ALA
23	U	45	PHE
23	U	84	LEU
24	V	11	ARG
24	V	21	ARG
24	V	51	VAL
24	V	52	ARG
24	V	80	LEU
24	V	86	SER
25	W	9	GLN
25	W	13	ALA
25	W	32	LEU
25	W	38	GLN
25	W	39	ALA
25	W	46	GLN
25	W	54	LYS
26	X	8	LEU
26	X	12	PRO
26	X	32	GLN
27	Y	29	ILE
27	Y	34	PRO
27	Y	37	LYS
27	Y	51	TYR
27	Y	52	TYR
28	Z	3	ARG
28	Z	18	PHE
28	Z	22	MET
28	Z	44	PRO
29	a	18	ALA

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Mol	Chain	Res	Type
29	a	19	SER
29	a	26	LYS
29	a	41	ILE
30	b	6	SER
35	c	21	ARG
35	c	91	PRO
35	c	130	ARG
35	c	132	LYS
35	c	165	VAL
35	c	191	ASP
35	c	232	PRO
36	d	24	ALA
36	d	30	ARG
36	d	47	LEU
36	d	49	SER
36	d	62	ASP
36	d	111	LEU
36	d	122	GLU
36	d	127	ARG
36	d	131	ARG
36	d	151	VAL
36	d	152	ILE
36	d	161	GLU
36	d	181	ASN
37	e	5	ILE
37	e	22	LYS
37	e	29	PRO
37	e	32	ALA
37	e	67	ILE
37	e	156	GLU
37	e	172	PRO
37	e	197	PRO
37	e	207	TYR
37	e	208	SER
38	f	44	GLY
38	f	70	PRO
38	f	78	HIS
38	f	101	ILE
38	f	104	ALA
38	f	128	PRO
39	g	35	ALA
39	g	100	ASN

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Mol	Chain	Res	Type
40	h	12	LEU
40	h	20	ASP
40	h	31	MET
40	h	32	ARG
40	h	69	VAL
40	h	133	GLY
40	h	134	ALA
40	h	149	ARG
41	i	27	PRO
41	i	46	LYS
41	i	60	ARG
41	i	76	PRO
41	i	79	VAL
41	i	97	VAL
42	j	37	PHE
42	j	47	LEU
42	j	88	TYR
42	j	110	GLU
42	j	112	LYS
42	j	117	HIS
43	k	59	SER
43	k	60	ARG
43	k	99	LYS
44	l	15	ALA
44	l	50	TYR
44	l	57	THR
45	m	74	HIS
45	m	78	GLU
45	m	97	TYR
45	m	104	TYR
45	m	109	VAL
46	n	17	VAL
46	n	18	ALA
46	n	20	THR
46	n	100	GLY
46	n	116	THR
47	o	3	ARG
47	o	17	LYS
47	o	35	ARG
48	p	28	GLN
48	p	47	LYS
48	p	50	HIS

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Mol	Chain	Res	Type
49	q	3	LYS
49	q	24	ALA
49	q	41	PRO
49	q	47	ASP
50	r	12	SER
50	r	45	HIS
50	r	47	PRO
50	r	68	ARG
50	r	70	ARG
50	r	94	ASN
51	s	15	ARG
51	s	33	ASP
51	s	37	VAL
51	s	59	SER
51	s	83	GLU
52	t	37	ARG
52	t	38	SER
52	t	42	PRO
52	t	65	ASN
52	t	70	LYS
52	t	78	ARG
53	u	10	LEU
53	u	42	GLN
53	u	48	LYS
53	u	71	THR
53	u	73	HIS
53	u	93	GLU
54	v	22	ARG
54	v	23	PRO
3	A	163	GLU
3	A	175	PRO
3	A	223	VAL
4	B	19	ALA
4	B	25	THR
4	B	84	TYR
4	B	113	VAL
4	B	114	GLY
4	B	118	VAL
4	B	174	ILE
4	B	198	ASN
4	B	204	ILE
4	B	223	GLY

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Mol	Chain	Res	Type
4	B	232	PRO
4	B	242	ARG
4	B	272	ALA
5	C	10	GLY
5	C	12	THR
5	C	27	LEU
5	C	46	ALA
5	C	49	LEU
5	C	53	PRO
5	C	64	LYS
5	C	103	ASP
5	C	126	PRO
5	C	151	TYR
5	C	169	ASN
5	C	173	VAL
5	C	177	PRO
5	C	187	ALA
5	C	190	GLY
5	C	195	LEU
5	C	201	THR
6	D	13	ARG
6	D	16	ALA
6	D	56	GLY
6	D	65	THR
6	D	69	ARG
6	D	73	ILE
6	D	82	GLY
6	D	92	TYR
6	D	118	LEU
6	D	129	GLY
6	D	145	GLY
6	D	167	TRP
6	D	173	PRO
6	D	186	ARG
6	D	191	LEU
7	E	8	LYS
7	E	20	ILE
7	E	28	VAL
7	E	46	ALA
7	E	126	ASP
8	F	9	ILE
8	F	13	LYS

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Mol	Chain	Res	Type
8	F	17	VAL
8	F	19	VAL
8	F	21	PRO
8	F	48	GLY
8	F	119	GLU
8	F	136	ILE
8	F	168	PRO
9	G	20	ASP
9	G	23	PRO
9	G	40	THR
9	G	70	GLU
9	G	88	ILE
9	G	89	TYR
9	G	135	GLU
9	G	137	PRO
10	H	30	LYS
10	H	64	ASP
10	H	84	ARG
10	H	85	VAL
10	H	111	GLU
10	H	131	PRO
10	H	148	GLY
10	H	154	GLN
10	H	156	GLN
10	H	158	PRO
11	I	26	LYS
11	I	28	SER
11	I	77	ILE
11	I	89	ASN
11	I	112	MET
11	I	114	ILE
12	J	13	ASN
12	J	21	ARG
12	J	47	ASP
12	J	83	VAL
12	J	89	ALA
12	J	94	GLU
12	J	97	PRO
12	J	115	LEU
12	J	118	GLY
13	K	6	ARG
13	K	20	ALA

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Mol	Chain	Res	Type
13	K	28	ALA
13	K	76	LYS
13	K	119	ARG
14	L	10	LEU
14	L	28	LEU
14	L	74	LYS
15	M	20	ARG
15	M	21	THR
15	M	31	SER
15	M	46	VAL
15	M	91	PRO
15	M	92	TYR
15	M	94	TYR
15	M	96	GLY
15	M	105	ALA
16	N	22	PHE
16	N	29	ARG
16	N	47	GLY
16	N	52	ILE
16	N	68	TYR
16	N	77	PRO
16	N	103	ARG
16	N	116	ALA
17	O	96	ALA
17	O	103	PRO
18	P	2	PHE
18	P	16	PRO
18	P	19	LYS
18	P	36	PRO
18	P	45	THR
18	P	47	VAL
18	P	74	LYS
18	P	86	GLY
18	P	96	ILE
18	P	99	ILE
19	Q	3	ALA
19	Q	6	ILE
19	Q	7	ALA
19	Q	20	VAL
19	Q	41	LYS
19	Q	43	GLY
19	Q	63	ASP

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Mol	Chain	Res	Type
19	Q	92	ARG
20	R	18	TYR
20	R	25	LYS
20	R	69	TYR
20	R	72	LYS
20	R	77	LYS
20	R	93	GLU
21	S	38	ILE
21	S	66	PRO
21	S	68	HIS
21	S	88	LYS
21	S	89	PHE
21	S	91	GLU
21	S	95	LYS
22	T	50	GLN
22	T	51	ALA
22	T	120	ILE
22	T	124	ILE
22	T	152	ALA
22	T	165	VAL
22	T	167	PRO
23	U	13	GLY
23	U	43	THR
23	U	55	ARG
23	U	58	THR
23	U	62	LEU
23	U	63	VAL
23	U	83	PRO
24	V	14	VAL
24	V	18	ILE
24	V	56	GLN
24	V	74	VAL
25	W	42	GLY
25	W	47	ASN
25	W	51	ARG
26	X	50	VAL
27	Y	14	ALA
27	Y	24	ALA
29	a	35	GLN
29	a	39	LYS
29	a	51	ALA
29	a	63	PRO

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Mol	Chain	Res	Type
35	c	9	GLU
35	c	13	ALA
35	c	32	ILE
35	c	74	LYS
35	c	95	GLN
35	c	97	TRP
35	c	131	PRO
35	c	160	ASP
35	c	181	PHE
35	c	229	VAL
36	d	12	LEU
36	d	15	THR
36	d	20	SER
36	d	29	TYR
36	d	45	LYS
36	d	50	ALA
36	d	60	ALA
36	d	63	ASN
36	d	100	ALA
36	d	108	ASN
36	d	109	PRO
36	d	156	ARG
36	d	191	THR
37	e	20	TYR
37	e	39	PRO
37	e	87	GLY
37	e	112	VAL
37	e	190	ASP
38	f	39	GLY
38	f	49	PRO
40	h	8	GLU
40	h	10	ARG
40	h	14	PRO
40	h	16	LEU
40	h	115	ARG
41	i	102	ARG
41	i	131	GLY
42	j	32	ASP
42	j	42	ARG
42	j	68	GLY
43	k	50	ILE
43	k	53	PRO

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Mol	Chain	Res	Type
43	k	58	ASP
43	k	72	VAL
43	k	77	PRO
43	k	93	GLY
44	l	49	GLY
44	l	101	SER
44	l	109	VAL
45	m	7	ASN
45	m	28	GLY
45	m	30	PRO
45	m	62	GLY
45	m	71	GLY
45	m	93	PRO
45	m	106	ALA
45	m	116	ARG
45	m	118	LYS
45	m	124	PRO
46	n	6	GLY
46	n	55	ARG
46	n	64	TRP
46	n	83	ASP
46	n	101	GLN
46	n	106	ASN
47	o	21	TYR
47	o	22	THR
47	o	32	SER
47	o	34	TYR
48	p	27	VAL
48	p	49	ASP
49	q	10	GLY
49	q	12	LYS
49	q	15	PRO
49	q	31	LYS
49	q	36	ILE
49	q	52	ASP
50	r	10	VAL
50	r	17	LYS
50	r	31	LEU
50	r	32	TYR
50	r	33	GLY
50	r	48	GLU
50	r	62	SER

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Mol	Chain	Res	Type
50	r	67	LYS
50	r	75	ARG
51	s	10	LYS
51	s	36	ASN
51	s	47	THR
52	t	7	LYS
52	t	52	TYR
52	t	61	TYR
53	u	41	VAL
53	u	45	GLN
53	u	47	GLY
53	u	74	LYS
53	u	98	PRO
53	u	99	LEU
54	v	15	ARG
54	v	17	THR
3	A	18	ASN
3	A	36	ALA
3	A	206	LYS
3	A	221	PRO
4	B	54	ARG
4	B	75	ILE
4	B	81	ALA
4	B	129	ASN
4	B	139	GLY
4	B	148	GLU
4	B	178	PRO
4	B	201	HIS
4	B	234	GLY
4	B	241	PRO
4	B	260	ARG
5	C	13	ARG
5	C	68	ALA
5	C	76	ARG
5	C	86	PRO
5	C	98	PRO
5	C	152	LYS
5	C	156	MET
6	D	5	PRO
6	D	8	SER
6	D	10	SER
6	D	26	HIS

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Mol	Chain	Res	Type
6	D	40	ARG
6	D	41	ARG
6	D	61	PRO
6	D	90	ARG
6	D	108	ALA
6	D	148	SER
7	E	73	ALA
7	E	117	PHE
7	E	147	ASP
8	F	47	GLU
8	F	59	ARG
8	F	102	ALA
8	F	118	PRO
8	F	135	GLY
8	F	158	HIS
8	F	165	ALA
9	G	7	GLU
9	G	25	TYR
9	G	81	VAL
9	G	86	THR
9	G	91	SER
9	G	95	LYS
9	G	126	TYR
10	H	31	GLN
11	I	30	ALA
11	I	61	VAL
11	I	64	ARG
12	J	72	PRO
12	J	145	PRO
13	K	84	GLY
13	K	91	GLU
13	K	115	MET
14	L	6	SER
14	L	50	HIS
14	L	67	LEU
14	L	94	TYR
14	L	108	GLY
15	M	25	ARG
15	M	28	VAL
15	M	29	PHE
15	M	47	THR
15	M	64	GLU

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Mol	Chain	Res	Type
16	N	2	ASN
16	N	5	ALA
16	N	36	GLU
16	N	93	ARG
16	N	112	ARG
17	O	23	GLY
17	O	24	TYR
17	O	93	LYS
17	O	102	GLU
17	O	116	ALA
18	P	20	LEU
18	P	24	LYS
18	P	59	ALA
18	P	79	VAL
19	Q	42	ARG
19	Q	73	ALA
19	Q	88	ARG
20	R	34	ALA
20	R	59	VAL
20	R	65	ARG
20	R	78	LYS
21	S	9	LYS
21	S	10	GLY
21	S	25	GLY
21	S	29	GLU
21	S	33	LYS
21	S	60	PHE
21	S	65	ALA
21	S	67	LEU
21	S	78	ALA
21	S	101	LYS
22	T	83	PRO
22	T	90	VAL
22	T	122	ARG
23	U	19	LYS
23	U	25	ARG
23	U	70	GLN
24	V	32	LYS
24	V	63	ALA
25	W	14	ARG
25	W	60	LEU
26	X	31	LEU

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Mol	Chain	Res	Type
29	a	31	HIS
29	a	42	ARG
30	b	12	ASP
35	c	54	THR
35	c	60	ASP
35	c	100	GLY
35	c	149	LEU
36	d	43	LEU
36	d	123	GLN
36	d	163	ALA
36	d	178	LEU
37	e	44	GLY
37	e	49	ARG
37	e	147	ALA
38	f	71	LEU
38	f	117	ASP
39	g	81	ILE
39	g	93	SER
40	h	41	ARG
40	h	63	LYS
40	h	73	MET
40	h	90	GLU
40	h	117	ALA
40	h	129	GLU
41	i	20	TYR
41	i	74	PRO
41	i	91	ARG
41	i	107	LEU
41	i	121	ASP
42	j	29	ASN
43	k	12	ASP
43	k	15	THR
44	l	44	SER
44	l	89	ALA
45	m	44	PRO
45	m	103	VAL
46	n	27	LYS
46	n	46	LYS
46	n	67	GLU
47	o	5	ALA
47	o	14	PRO
47	o	18	VAL

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Mol	Chain	Res	Type
48	p	32	LEU
48	p	33	THR
48	p	55	GLY
48	p	56	LEU
48	p	72	ARG
48	p	79	ARG
49	q	13	HIS
49	q	26	ARG
49	q	29	ASP
49	q	30	GLY
49	q	34	GLU
49	q	65	GLN
50	r	83	ASP
51	s	25	THR
51	s	53	ARG
51	s	76	LEU
51	s	82	THR
52	t	5	LEU
52	t	6	LYS
52	t	9	VAL
52	t	28	LYS
52	t	35	SER
52	t	46	GLY
54	v	3	LYS
3	A	19	LYS
3	A	23	ILE
3	A	203	GLU
3	A	207	GLY
4	B	5	LYS
4	B	9	TYR
4	B	35	LYS
4	B	123	ALA
4	B	124	PRO
4	B	159	ALA
4	B	224	ALA
5	C	45	THR
5	C	125	GLY
5	C	153	GLY
5	C	202	LYS
6	D	39	ARG
6	D	70	HIS
6	D	88	LYS

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Mol	Chain	Res	Type
6	D	103	LYS
6	D	179	TYR
6	D	185	GLU
7	E	25	TYR
7	E	76	SER
7	E	122	PRO
8	F	30	LYS
8	F	81	GLU
8	F	126	PRO
8	F	152	ARG
9	G	62	LYS
9	G	74	ASN
10	H	33	GLU
10	H	40	ASP
10	H	42	GLU
10	H	141	LYS
11	I	31	LYS
11	I	49	ARG
11	I	50	GLY
11	I	120	GLU
12	J	23	PRO
12	J	48	PRO
12	J	79	ARG
12	J	108	LYS
12	J	146	VAL
13	K	8	LYS
13	K	23	GLY
13	K	32	PHE
13	K	40	ALA
13	K	125	LEU
13	K	135	ASP
14	L	8	ARG
14	L	46	GLY
15	M	23	ARG
16	N	24	PRO
16	N	32	TYR
16	N	41	ARG
16	N	55	ASN
16	N	131	ALA
16	N	133	GLU
17	O	53	ARG
17	O	77	SER

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Mol	Chain	Res	Type
17	O	91	ASP
19	Q	46	PHE
20	R	7	VAL
20	R	90	GLU
21	S	12	THR
21	S	15	VAL
21	S	18	GLY
21	S	40	GLU
22	T	2	GLU
22	T	39	VAL
22	T	153	SER
23	U	27	GLU
23	U	41	ARG
24	V	62	VAL
24	V	88	LYS
25	W	15	LYS
26	X	9	VAL
35	c	56	ARG
35	c	182	ILE
35	c	209	ARG
35	c	237	ALA
36	d	17	ASP
36	d	129	ALA
36	d	168	ALA
36	d	175	LEU
37	e	101	LEU
38	f	73	ASN
40	h	33	ASP
40	h	36	LYS
40	h	53	LYS
40	h	70	LYS
41	i	52	ASP
42	j	7	THR
42	j	10	ARG
42	j	97	LYS
43	k	71	LEU
44	l	54	ARG
45	m	29	ALA
46	n	105	THR
46	n	117	VAL
47	o	33	VAL
49	q	23	ASP

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Mol	Chain	Res	Type
49	q	28	ARG
49	q	42	ARG
49	q	70	ALA
50	r	50	LYS
50	r	77	VAL
51	s	9	LYS
52	t	20	LEU
52	t	55	LYS
52	t	67	VAL
53	u	43	LEU
54	v	20	LYS
4	B	45	ASN
4	B	47	GLY
4	B	53	PHE
4	B	87	ASN
4	B	116	GLN
4	B	268	ARG
5	C	180	ASN
6	D	12	ARG
6	D	50	GLY
6	D	52	VAL
6	D	83	VAL
6	D	97	PRO
6	D	163	ARG
7	E	107	LEU
7	E	146	TYR
8	F	15	VAL
8	F	38	SER
8	F	170	ARG
10	H	119	GLU
10	H	130	LEU
11	I	24	VAL
11	I	94	ARG
11	I	103	ALA
12	J	61	ARG
12	J	78	PRO
12	J	129	ALA
13	K	2	LEU
13	K	49	ALA
13	K	63	LYS
13	K	121	ALA
13	K	132	VAL

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Mol	Chain	Res	Type
15	M	48	LEU
15	M	56	LEU
16	N	95	ARG
16	N	128	GLU
18	P	23	GLU
18	P	58	VAL
18	P	84	LYS
18	P	90	PRO
19	Q	98	LYS
21	S	3	VAL
21	S	34	LYS
21	S	56	PRO
21	S	86	ARG
22	T	16	SER
22	T	53	ILE
22	T	168	GLU
23	U	20	ARG
23	U	23	VAL
23	U	33	ALA
24	V	68	PRO
25	W	11	GLU
25	W	16	LEU
26	X	18	ASP
29	a	59	LYS
30	b	14	CYS
35	c	19	HIS
35	c	98	LEU
35	c	178	ARG
36	d	9	GLY
36	d	115	LEU
36	d	172	ARG
36	d	204	LEU
37	e	9	CYS
37	e	132	ARG
38	f	143	ARG
39	g	48	LEU
39	g	78	GLU
39	g	88	VAL
40	h	9	VAL
40	h	88	PRO
41	i	24	THR
42	j	54	ASP

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Mol	Chain	Res	Type
43	k	76	ASN
43	k	98	ILE
44	l	39	PRO
45	m	70	PRO
46	n	99	ARG
46	n	119	GLY
49	q	66	PRO
50	r	95	TYR
52	t	8	GLY
54	v	18	TYR
54	v	19	GLY
4	B	251	GLY
5	C	30	PRO
5	C	188	VAL
6	D	89	PRO
8	F	11	VAL
8	F	42	ARG
8	F	82	GLY
8	F	151	ILE
10	H	109	PRO
11	I	22	ILE
11	I	76	ALA
11	I	113	LYS
12	J	8	PRO
13	K	111	GLU
14	L	38	VAL
16	N	20	PRO
16	N	90	GLN
17	O	20	LEU
17	O	88	ILE
19	Q	35	ILE
20	R	88	LYS
21	S	30	VAL
21	S	52	SER
22	T	12	GLY
23	U	57	PHE
25	W	57	ILE
27	Y	55	ARG
29	a	4	MET
29	a	38	GLY
30	b	10	ILE
30	b	30	PRO

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Mol	Chain	Res	Type
35	c	23	ARG
35	c	127	ILE
36	d	61	ALA
36	d	81	GLY
36	d	174	PRO
37	e	51	PRO
40	h	81	GLY
41	i	134	ILE
42	j	53	VAL
45	m	80	SER
50	r	16	GLN
50	r	64	PRO
52	t	76	PRO
3	A	204	GLY
4	B	74	GLY
4	B	125	ILE
6	D	80	GLY
16	N	19	LEU
18	P	65	GLY
27	Y	41	PRO
28	Z	7	PRO
30	b	25	VAL
36	d	116	VAL
37	e	90	GLY
38	f	100	VAL
41	i	6	ILE
43	k	74	ILE
52	t	49	ILE
5	C	139	GLY
7	E	119	GLY
8	F	31	GLY
10	H	77	VAL
10	H	157	ARG
11	I	72	PRO
21	S	45	VAL
21	S	80	GLY
27	Y	33	CYS
38	f	93	PRO
40	h	91	VAL
47	o	56	VAL
49	q	19	ILE
4	B	229	VAL

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Mol	Chain	Res	Type
4	B	246	PRO
5	C	184	VAL
6	D	121	VAL
8	F	121	ILE
9	G	124	GLY
11	I	19	ILE
11	I	101	PRO
12	J	20	GLY
16	N	88	ILE
17	O	82	GLY
22	T	42	VAL
24	V	12	PRO
37	e	37	PRO
37	e	136	PRO
44	l	48	ILE
50	r	46	ASP
52	t	54	GLY
53	u	100	ILE
4	B	92	ILE
4	B	106	ILE
4	B	216	GLY
4	B	244	ARG
5	C	47	VAL
5	C	141	ILE
10	H	149	PRO
11	I	86	ILE
12	J	19	VAL
15	M	85	VAL
16	N	66	VAL
30	b	3	VAL
35	c	164	VAL
37	e	133	VAL
41	i	26	VAL
43	k	41	PRO
50	r	5	VAL
50	r	19	VAL
53	u	97	ALA
3	A	52	PRO
5	C	116	VAL
12	J	62	LEU
23	U	79	VAL
27	Y	6	VAL

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Mol	Chain	Res	Type
39	g	72	VAL
41	i	4	ASP
44	l	21	ILE
4	B	245	PRO

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	
3	A	106/181 (59%)	86 (81%)	20 (19%)	2	13
4	B	214/218 (98%)	179 (84%)	35 (16%)	2	20
5	C	163/166 (98%)	130 (80%)	33 (20%)	1	11
6	D	154/162 (95%)	133 (86%)	21 (14%)	4	28
7	E	154/156 (99%)	130 (84%)	24 (16%)	3	22
8	F	142/148 (96%)	129 (91%)	13 (9%)	11	44
9	G	124/124 (100%)	100 (81%)	24 (19%)	1	12
10	H	117/119 (98%)	96 (82%)	21 (18%)	2	15
11	I	100/100 (100%)	74 (74%)	26 (26%)	0	5
12	J	112/116 (97%)	91 (81%)	21 (19%)	2	13
13	K	108/111 (97%)	84 (78%)	24 (22%)	1	9
14	L	101/101 (100%)	89 (88%)	12 (12%)	6	32
15	M	84/88 (96%)	71 (84%)	13 (16%)	3	22
16	N	121/128 (94%)	101 (84%)	20 (16%)	2	19
17	O	93/94 (99%)	77 (83%)	16 (17%)	2	17
18	P	82/82 (100%)	64 (78%)	18 (22%)	1	9
19	Q	89/92 (97%)	75 (84%)	14 (16%)	3	22
20	R	74/78 (95%)	62 (84%)	12 (16%)	3	20
21	S	86/91 (94%)	73 (85%)	13 (15%)	3	23
22	T	163/179 (91%)	136 (83%)	27 (17%)	2	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	61/67 (91%)	54 (88%)	7 (12%)	6	34
24	V	73/83 (88%)	61 (84%)	12 (16%)	2	20
25	W	58/67 (87%)	47 (81%)	11 (19%)	2	13
26	X	52/52 (100%)	46 (88%)	6 (12%)	6	34
27	Y	49/52 (94%)	40 (82%)	9 (18%)	2	14
28	Z	41/42 (98%)	34 (83%)	7 (17%)	2	18
29	a	53/55 (96%)	44 (83%)	9 (17%)	2	18
30	b	33/34 (97%)	31 (94%)	2 (6%)	22	60
35	c	202/220 (92%)	169 (84%)	33 (16%)	3	20
36	d	160/188 (85%)	130 (81%)	30 (19%)	2	13
37	e	180/181 (99%)	154 (86%)	26 (14%)	4	26
38	f	115/123 (94%)	102 (89%)	13 (11%)	7	35
39	g	90/90 (100%)	77 (86%)	13 (14%)	4	26
40	h	126/127 (99%)	108 (86%)	18 (14%)	4	26
41	i	119/119 (100%)	96 (81%)	23 (19%)	1	13
42	j	98/99 (99%)	89 (91%)	9 (9%)	11	44
43	k	88/92 (96%)	76 (86%)	12 (14%)	4	28
44	l	88/99 (89%)	78 (89%)	10 (11%)	7	34
45	m	104/109 (95%)	80 (77%)	24 (23%)	1	8
46	n	100/101 (99%)	75 (75%)	25 (25%)	1	6
47	o	49/50 (98%)	37 (76%)	12 (24%)	1	6
48	p	79/80 (99%)	66 (84%)	13 (16%)	2	19
49	q	72/74 (97%)	57 (79%)	15 (21%)	1	10
50	r	96/97 (99%)	79 (82%)	17 (18%)	2	16
51	s	71/77 (92%)	63 (89%)	8 (11%)	7	35
52	t	71/80 (89%)	52 (73%)	19 (27%)	0	4
53	u	76/82 (93%)	66 (87%)	10 (13%)	5	28
54	v	19/22 (86%)	16 (84%)	3 (16%)	3	22
All	All	4810/5096 (94%)	4007 (83%)	803 (17%)	2	19

All (803) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	TYR
3	A	12	LEU
3	A	16	ASP
3	A	19	LYS
3	A	20	ILE
3	A	21	TYR
3	A	22	THR
3	A	30	VAL
3	A	32	GLU
3	A	43	GLU
3	A	53	ARG
3	A	163	GLU
3	A	165	ARG
3	A	178	LYS
3	A	189	ASN
3	A	193	PHE
3	A	197	LEU
3	A	198	GLU
3	A	201	LYS
3	A	209	PHE
4	B	10	THR
4	B	13	ARG
4	B	15	PHE
4	B	18	VAL
4	B	24	ILE
4	B	31	LYS
4	B	33	LEU
4	B	37	LEU
4	B	43	ARG
4	B	60	ARG
4	B	61	LEU
4	B	63	ARG
4	B	66	ASP
4	B	67	PHE
4	B	70	TRP
4	B	71	ASP
4	B	79	VAL
4	B	115	GLN
4	B	131	LEU
4	B	150	LYS
4	B	164	GLN
4	B	176	ARG
4	B	177	LEU

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Mol	Chain	Res	Type
4	B	198	ASN
4	B	201	HIS
4	B	213	ARG
4	B	214	TRP
4	B	217	ARG
4	B	229	VAL
4	B	242	ARG
4	B	255	LYS
4	B	257	LEU
4	B	262	ARG
4	B	263	ARG
4	B	271	ILE
5	C	5	LEU
5	C	12	THR
5	C	15	PHE
5	C	19	ARG
5	C	21	VAL
5	C	23	VAL
5	C	24	THR
5	C	27	LEU
5	C	37	ARG
5	C	42	ASP
5	C	44	TYR
5	C	61	ARG
5	C	66	HIS
5	C	67	PHE
5	C	78	LEU
5	C	79	ARG
5	C	84	PHE
5	C	89	ASP
5	C	97	LYS
5	C	107	THR
5	C	117	MET
5	C	119	ARG
5	C	122	PHE
5	C	141	ILE
5	C	156	MET
5	C	173	VAL
5	C	179	GLU
5	C	183	LEU
5	C	188	VAL
5	C	192	ASN

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Mol	Chain	Res	Type
5	C	197	ILE
5	C	201	THR
5	C	203	LYS
6	D	22	GLU
6	D	27	LEU
6	D	77	ILE
6	D	83	VAL
6	D	84	VAL
6	D	92	TYR
6	D	97	PRO
6	D	115	GLU
6	D	117	LYS
6	D	120	LEU
6	D	135	LEU
6	D	137	TRP
6	D	143	LEU
6	D	144	ASP
6	D	149	VAL
6	D	165	LEU
6	D	179	TYR
6	D	180	ASP
6	D	181	ILE
6	D	183	ARG
6	D	196	VAL
7	E	10	LYS
7	E	12	TYR
7	E	19	LEU
7	E	25	TYR
7	E	29	TRP
7	E	31	VAL
7	E	33	ARG
7	E	55	LYS
7	E	72	ARG
7	E	80	PHE
7	E	95	ARG
7	E	99	MET
7	E	115	ARG
7	E	135	LEU
7	E	136	ARG
7	E	138	GLN
7	E	139	LEU
7	E	146	TYR

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Mol	Chain	Res	Type
7	E	148	MET
7	E	155	MET
7	E	165	THR
7	E	173	LEU
7	E	176	LEU
7	E	178	PHE
8	F	65	HIS
8	F	68	THR
8	F	87	LEU
8	F	89	ILE
8	F	90	LYS
8	F	92	ILE
8	F	98	LEU
8	F	110	SER
8	F	139	GLN
8	F	140	LYS
8	F	152	ARG
8	F	162	ILE
8	F	172	LYS
9	G	3	VAL
9	G	20	ASP
9	G	21	VAL
9	G	27	ARG
9	G	31	LEU
9	G	33	ARG
9	G	38	LEU
9	G	41	GLU
9	G	44	LEU
9	G	62	LYS
9	G	76	THR
9	G	77	LEU
9	G	93	THR
9	G	96	ASP
9	G	99	GLU
9	G	103	ARG
9	G	108	THR
9	G	109	ILE
9	G	114	LEU
9	G	118	LYS
9	G	123	LEU
9	G	130	TYR
9	G	136	VAL

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Mol	Chain	Res	Type
9	G	139	GLN
10	H	25	LYS
10	H	33	GLU
10	H	35	ARG
10	H	38	LEU
10	H	60	LYS
10	H	62	ARG
10	H	71	MET
10	H	84	ARG
10	H	86	THR
10	H	92	GLN
10	H	95	TYR
10	H	98	TYR
10	H	129	MET
10	H	132	LYS
10	H	140	PHE
10	H	142	ARG
10	H	143	LEU
10	H	145	VAL
10	H	146	TYR
10	H	159	GLU
10	H	161	LEU
11	I	1	MET
11	I	3	GLN
11	I	9	GLU
11	I	10	VAL
11	I	12	ASP
11	I	21	CYS
11	I	29	ASN
11	I	39	ILE
11	I	45	GLU
11	I	49	ARG
11	I	58	VAL
11	I	59	LYS
11	I	63	VAL
11	I	67	LYS
11	I	68	GLU
11	I	77	ILE
11	I	80	ASP
11	I	91	LEU
11	I	96	THR
11	I	97	ARG

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Mol	Chain	Res	Type
11	I	102	VAL
11	I	104	ARG
11	I	105	GLU
11	I	109	LYS
11	I	114	ILE
11	I	120	GLU
12	J	5	ASP
12	J	13	ASN
12	J	45	LEU
12	J	60	MET
12	J	61	ARG
12	J	62	LEU
12	J	68	GLN
12	J	74	GLU
12	J	77	ARG
12	J	80	TYR
12	J	81	GLN
12	J	84	ASN
12	J	85	LEU
12	J	96	THR
12	J	100	LEU
12	J	110	TYR
12	J	121	LYS
12	J	130	PHE
12	J	145	PRO
12	J	148	LEU
12	J	149	GLU
13	K	3	MET
13	K	8	LYS
13	K	9	TYR
13	K	11	LYS
13	K	14	ARG
13	K	17	LEU
13	K	25	ASP
13	K	29	PHE
13	K	32	PHE
13	K	41	TRP
13	K	42	ILE
13	K	51	ARG
13	K	59	ARG
13	K	64	ILE
13	K	65	PHE

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Mol	Chain	Res	Type
13	K	69	PHE
13	K	82	ARG
13	K	89	ASN
13	K	93	TYR
13	K	103	MET
13	K	111	GLU
13	K	124	LYS
13	K	133	ARG
13	K	134	ARG
14	L	9	LYS
14	L	14	SER
14	L	29	LEU
14	L	31	HIS
14	L	38	VAL
14	L	43	GLU
14	L	59	ASP
14	L	65	LEU
14	L	68	ARG
14	L	88	ARG
14	L	94	TYR
14	L	105	ARG
15	M	7	TYR
15	M	10	ARG
15	M	12	PHE
15	M	14	VAL
15	M	15	ARG
15	M	24	LEU
15	M	39	ILE
15	M	42	ASP
15	M	46	VAL
15	M	54	LEU
15	M	75	GLU
15	M	93	LYS
15	M	94	TYR
16	N	6	LEU
16	N	32	TYR
16	N	35	LYS
16	N	38	ASN
16	N	57	PHE
16	N	61	PHE
16	N	62	THR
16	N	85	LYS

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Mol	Chain	Res	Type
16	N	87	ASP
16	N	88	ILE
16	N	98	LYS
16	N	103	ARG
16	N	107	ASP
16	N	111	ARG
16	N	112	ARG
16	N	113	LYS
16	N	118	ARG
16	N	121	ILE
16	N	123	LYS
16	N	124	ASP
17	O	5	LYS
17	O	14	HIS
17	O	25	TRP
17	O	27	LEU
17	O	51	LYS
17	O	58	ARG
17	O	71	GLN
17	O	74	LEU
17	O	79	PHE
17	O	84	LYS
17	O	85	LYS
17	O	91	ASP
17	O	97	ASP
17	O	106	PHE
17	O	109	LEU
17	O	114	LYS
18	P	13	ARG
18	P	18	LEU
18	P	20	LEU
18	P	23	GLU
18	P	26	ASP
18	P	35	LEU
18	P	39	LEU
18	P	40	LEU
18	P	51	VAL
18	P	58	VAL
18	P	60	GLU
18	P	62	LEU
18	P	80	GLN
18	P	81	TYR

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Mol	Chain	Res	Type
18	P	82	ARG
18	P	89	GLN
18	P	92	THR
18	P	98	GLU
19	Q	6	ILE
19	Q	8	ARG
19	Q	21	VAL
19	Q	23	LEU
19	Q	31	GLU
19	Q	49	LYS
19	Q	51	LEU
19	Q	67	ASP
19	Q	68	ARG
19	Q	70	TYR
19	Q	76	VAL
19	Q	86	LEU
19	Q	88	ARG
19	Q	97	LYS
20	R	3	THR
20	R	13	LEU
20	R	26	TYR
20	R	27	THR
20	R	38	GLU
20	R	49	VAL
20	R	56	THR
20	R	62	LYS
20	R	65	ARG
20	R	76	ARG
20	R	77	LYS
20	R	83	VAL
21	S	9	LYS
21	S	20	TYR
21	S	23	ARG
21	S	28	LYS
21	S	40	GLU
21	S	44	ILE
21	S	50	ARG
21	S	64	GLU
21	S	67	LEU
21	S	71	LYS
21	S	73	ARG
21	S	75	ILE

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Mol	Chain	Res	Type
21	S	97	ARG
22	T	1	MET
22	T	8	TYR
22	T	9	TYR
22	T	19	ARG
22	T	20	ARG
22	T	31	ARG
22	T	41	LEU
22	T	44	PHE
22	T	48	PHE
22	T	50	GLN
22	T	53	ILE
22	T	78	LYS
22	T	80	ARG
22	T	88	PHE
22	T	95	PRO
22	T	104	PHE
22	T	119	GLU
22	T	144	LEU
22	T	145	GLU
22	T	146	ILE
22	T	150	LEU
22	T	151	HIS
22	T	157	LEU
22	T	162	GLU
22	T	163	LEU
22	T	170	THR
22	T	171	ILE
23	U	19	LYS
23	U	20	ARG
23	U	26	TYR
23	U	53	MET
23	U	62	LEU
23	U	64	ASP
23	U	69	PHE
24	V	13	ILE
24	V	18	ILE
24	V	26	ARG
24	V	41	ARG
24	V	43	TYR
24	V	46	LEU
24	V	58	ILE

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Mol	Chain	Res	Type
24	V	60	PHE
24	V	62	VAL
24	V	78	LYS
24	V	85	LEU
24	V	91	LYS
25	W	9	GLN
25	W	12	GLU
25	W	14	ARG
25	W	15	LYS
25	W	27	GLU
25	W	29	LYS
25	W	33	MET
25	W	37	PHE
25	W	47	ASN
25	W	48	HIS
25	W	55	ARG
26	X	8	LEU
26	X	23	LEU
26	X	29	ARG
26	X	30	ARG
26	X	35	ARG
26	X	49	LYS
27	Y	16	ARG
27	Y	25	LEU
27	Y	26	THR
27	Y	29	ILE
27	Y	33	CYS
27	Y	39	MET
27	Y	49	CYS
27	Y	51	TYR
27	Y	56	LYS
28	Z	1	MET
28	Z	2	LYS
28	Z	5	TRP
28	Z	15	THR
28	Z	29	LYS
28	Z	39	ARG
28	Z	44	PRO
29	a	3	LYS
29	a	16	ILE
29	a	17	THR
29	a	25	MET

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Mol	Chain	Res	Type
29	a	34	TRP
29	a	36	LYS
29	a	44	LYS
29	a	48	PHE
29	a	60	LEU
30	b	24	TYR
30	b	25	VAL
35	c	8	LYS
35	c	10	LEU
35	c	17	PHE
35	c	19	HIS
35	c	23	ARG
35	c	42	ILE
35	c	47	THR
35	c	48	MET
35	c	51	LEU
35	c	60	ASP
35	c	67	THR
35	c	71	VAL
35	c	92	TYR
35	c	101	MET
35	c	102	LEU
35	c	118	LEU
35	c	132	LYS
35	c	133	LYS
35	c	136	VAL
35	c	137	ARG
35	c	143	GLU
35	c	146	GLN
35	c	149	LEU
35	c	155	LEU
35	c	156	LYS
35	c	164	VAL
35	c	169	LYS
35	c	172	ILE
35	c	200	ILE
35	c	204	ASN
35	c	209	ARG
35	c	220	ASP
35	c	221	LEU
36	d	3	ASN
36	d	4	LYS

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Mol	Chain	Res	Type
36	d	16	ARG
36	d	27	LYS
36	d	29	TYR
36	d	32	LEU
36	d	33	LEU
36	d	46	GLU
36	d	52	LEU
36	d	56	ASP
36	d	84	ILE
36	d	93	LYS
36	d	94	LEU
36	d	95	THR
36	d	97	LYS
36	d	102	ASN
36	d	107	GLN
36	d	111	LEU
36	d	118	GLN
36	d	123	GLN
36	d	126	ARG
36	d	130	VAL
36	d	131	ARG
36	d	135	LYS
36	d	139	GLN
36	d	175	LEU
36	d	178	LEU
36	d	186	PHE
36	d	193	TYR
36	d	195	VAL
37	e	8	VAL
37	e	14	ARG
37	e	15	GLU
37	e	22	LYS
37	e	29	PRO
37	e	33	MET
37	e	36	ARG
37	e	39	PRO
37	e	59	ARG
37	e	61	LYS
37	e	68	TYR
37	e	72	GLU
37	e	78	LEU
37	e	79	PHE

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Mol	Chain	Res	Type
37	e	94	LEU
37	e	97	LEU
37	e	101	LEU
37	e	104	VAL
37	e	120	LEU
37	e	122	ARG
37	e	134	ASP
37	e	188	LEU
37	e	191	ARG
37	e	199	ASN
37	e	203	VAL
37	e	207	TYR
38	f	6	PHE
38	f	10	MET
38	f	12	LEU
38	f	43	LEU
38	f	57	LYS
38	f	72	GLN
38	f	78	HIS
38	f	105	VAL
38	f	118	ILE
38	f	136	MET
38	f	137	GLU
38	f	143	ARG
38	f	144	THR
39	g	2	ARG
39	g	15	ASP
39	g	17	SER
39	g	27	GLN
39	g	37	VAL
39	g	43	LEU
39	g	55	ASP
39	g	75	LEU
39	g	78	GLU
39	g	83	ASP
39	g	86	ARG
39	g	91	VAL
39	g	100	ASN
40	h	4	ARG
40	h	5	ARG
40	h	16	LEU
40	h	29	LYS

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Mol	Chain	Res	Type
40	h	32	ARG
40	h	35	LYS
40	h	41	ARG
40	h	43	PHE
40	h	59	LEU
40	h	64	GLN
40	h	68	ASN
40	h	84	ASN
40	h	103	TRP
40	h	105	VAL
40	h	113	GLU
40	h	119	ARG
40	h	151	TYR
40	h	155	ARG
41	i	1	MET
41	i	2	LEU
41	i	14	ARG
41	i	17	THR
41	i	21	LYS
41	i	24	THR
41	i	31	PHE
41	i	39	LEU
41	i	45	ILE
41	i	48	TYR
41	i	50	ARG
41	i	52	ASP
41	i	62	TYR
41	i	75	ARG
41	i	85	ARG
41	i	98	LYS
41	i	99	GLU
41	i	103	VAL
41	i	104	ARG
41	i	105	ARG
41	i	107	LEU
41	i	122	ARG
41	i	127	LEU
42	j	5	TYR
42	j	53	VAL
42	j	85	LEU
42	j	89	ASN
42	j	92	TYR

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Mol	Chain	Res	Type
42	j	108	VAL
42	j	114	TYR
42	j	125	TYR
42	j	127	LYS
43	k	8	LEU
43	k	11	PHE
43	k	46	ARG
43	k	47	PHE
43	k	49	VAL
43	k	57	LYS
43	k	61	GLU
43	k	64	GLU
43	k	65	LEU
43	k	71	LEU
43	k	79	ARG
43	k	82	ILE
44	l	20	TYR
44	l	29	ILE
44	l	33	THR
44	l	34	ASP
44	l	41	THR
44	l	51	LYS
44	l	73	MET
44	l	84	VAL
44	l	99	GLN
44	l	104	GLN
45	m	6	ILE
45	m	14	ARG
45	m	17	VAL
45	m	23	VAL
45	m	27	LYS
45	m	40	ARG
45	m	45	LYS
45	m	51	LEU
45	m	52	ARG
45	m	53	LYS
45	m	58	ARG
45	m	64	GLU
45	m	76	LEU
45	m	77	GLN
45	m	81	VAL
45	m	84	ILE

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Mol	Chain	Res	Type
45	m	85	ARG
45	m	101	ARG
45	m	111	ASP
45	m	112	ARG
45	m	114	LYS
45	m	115	SER
45	m	121	THR
45	m	126	GLU
46	n	15	VAL
46	n	16	ASP
46	n	23	TYR
46	n	25	ILE
46	n	59	TYR
46	n	62	ASN
46	n	64	TRP
46	n	66	LEU
46	n	69	GLU
46	n	70	LEU
46	n	73	GLU
46	n	82	MET
46	n	86	CYS
46	n	91	ARG
46	n	92	HIS
46	n	93	ARG
46	n	94	ARG
46	n	98	VAL
46	n	99	ARG
46	n	103	THR
46	n	104	ARG
46	n	105	THR
46	n	108	ARG
46	n	120	LYS
46	n	125	ARG
47	o	8	GLU
47	o	11	LYS
47	o	16	PHE
47	o	21	TYR
47	o	24	CYS
47	o	29	ARG
47	o	33	VAL
47	o	36	PHE
47	o	41	ARG

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Mol	Chain	Res	Type
47	o	42	ILE
47	o	49	HIS
47	o	56	VAL
48	p	6	GLU
48	p	8	LYS
48	p	26	GLU
48	p	32	LEU
48	p	35	ARG
48	p	54	ARG
48	p	56	LEU
48	p	57	LEU
48	p	67	LEU
48	p	69	TYR
48	p	71	GLN
48	p	83	GLU
48	p	84	LYS
49	q	1	MET
49	q	13	HIS
49	q	27	LYS
49	q	32	TYR
49	q	35	LYS
49	q	41	PRO
49	q	43	LYS
49	q	44	THR
49	q	48	TRP
49	q	52	ASP
49	q	58	TYR
49	q	60	LEU
49	q	71	ARG
49	q	74	LEU
49	q	79	VAL
50	r	6	LEU
50	r	14	LYS
50	r	17	LYS
50	r	19	VAL
50	r	36	ILE
50	r	41	LYS
50	r	42	TYR
50	r	43	LEU
50	r	55	ASP
50	r	58	GLU
50	r	69	LYS

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Mol	Chain	Res	Type
50	r	72	ARG
50	r	81	ARG
50	r	84	LEU
50	r	88	TYR
50	r	94	ASN
50	r	100	LYS
51	s	13	GLN
51	s	29	PHE
51	s	31	LEU
51	s	32	ARG
51	s	33	ASP
51	s	34	TYR
51	s	42	ARG
51	s	63	GLN
52	t	6	LYS
52	t	23	ASN
52	t	25	LYS
52	t	29	ARG
52	t	31	ILE
52	t	32	LYS
52	t	33	THR
52	t	34	TRP
52	t	36	ARG
52	t	43	GLU
52	t	44	MET
52	t	49	ILE
52	t	53	ASN
52	t	55	LYS
52	t	60	VAL
52	t	61	TYR
52	t	63	THR
52	t	66	MET
52	t	71	LEU
53	u	10	LEU
53	u	20	LEU
53	u	21	LYS
53	u	23	ARG
53	u	27	LYS
53	u	51	GLU
53	u	53	LEU
53	u	56	MET
53	u	72	LEU

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Mol	Chain	Res	Type
53	u	79	ARG
54	v	6	ARG
54	v	9	ARG
54	v	14	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	ASN
3	A	58	ASN
4	B	46	GLN
4	B	87	ASN
4	B	115	GLN
4	B	129	ASN
4	B	164	GLN
4	B	166	GLN
4	B	198	ASN
4	B	201	HIS
4	B	231	HIS
4	B	253	GLN
5	C	54	GLN
5	C	55	ASN
5	C	66	HIS
5	C	132	HIS
5	C	143	ASN
6	D	35	GLN
6	D	128	ASN
6	D	177	ASN
7	E	40	ASN
7	E	41	GLN
7	E	66	GLN
7	E	79	ASN
7	E	123	ASN
8	F	61	HIS
8	F	65	HIS
8	F	74	ASN
8	F	143	GLN
9	G	28	ASN
9	G	43	ASN
9	G	104	GLN
9	G	147	GLN
10	H	92	GLN

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Mol	Chain	Res	Type
10	H	124	HIS
11	I	3	GLN
11	I	29	ASN
12	J	9	ASN
12	J	38	GLN
12	J	81	GLN
13	K	12	GLN
13	K	45	GLN
13	K	46	GLN
13	K	57	HIS
13	K	123	HIS
14	L	16	HIS
14	L	23	ASN
14	L	71	GLN
15	M	38	GLN
16	N	38	ASN
16	N	90	GLN
17	O	44	ASN
17	O	72	HIS
18	P	64	HIS
18	P	87	HIS
19	Q	57	ASN
20	R	41	ASN
21	S	57	GLN
22	T	34	ASN
22	T	55	HIS
22	T	65	GLN
22	T	73	GLN
22	T	75	ASN
23	U	35	ASN
23	U	40	GLN
23	U	80	HIS
24	V	19	GLN
24	V	45	ASN
25	W	47	ASN
26	X	32	GLN
28	Z	16	HIS
29	a	35	GLN
35	c	25	ASN
35	c	78	GLN
35	c	94	ASN
35	c	135	GLN

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Mol	Chain	Res	Type
35	c	204	ASN
36	d	3	ASN
36	d	6	HIS
36	d	28	GLN
36	d	63	ASN
36	d	102	ASN
36	d	110	ASN
36	d	118	GLN
36	d	136	GLN
36	d	139	GLN
37	e	45	GLN
37	e	74	GLN
37	e	77	ASN
37	e	119	GLN
37	e	129	ASN
37	e	199	ASN
37	e	201	GLN
38	f	20	GLN
38	f	65	ASN
38	f	72	GLN
39	g	18	GLN
39	g	27	GLN
39	g	32	ASN
39	g	94	GLN
40	h	13	GLN
40	h	64	GLN
40	h	68	ASN
40	h	84	ASN
40	h	86	GLN
40	h	97	GLN
40	h	106	GLN
40	h	109	ASN
40	h	110	GLN
40	h	122	HIS
41	i	15	ASN
41	i	70	GLN
42	j	73	GLN
42	j	89	ASN
43	k	56	HIS
43	k	76	ASN
44	l	27	ASN
44	l	38	ASN

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Mol	Chain	Res	Type
45	m	7	ASN
45	m	77	GLN
46	n	40	ASN
46	n	101	GLN
47	o	49	HIS
48	p	13	GLN
48	p	37	ASN
48	p	42	HIS
48	p	62	GLN
49	q	16	HIS
49	q	76	GLN
50	r	26	GLN
51	s	63	GLN
52	t	47	HIS
53	u	26	ASN
53	u	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	983 (34%)	0
2	x	119/120 (99%)	47 (39%)	0
31	y	1511/1522 (99%)	507 (33%)	0
32	z	76/77 (98%)	20 (26%)	0
33	2	75/76 (98%)	22 (29%)	0
34	3	17/18 (94%)	5 (29%)	0
All	All	4686/4702 (99%)	1584 (33%)	0

All (1584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	13	A
1	w	15	G
1	w	27	G
1	w	28	A
1	w	29	U
1	w	34	C
1	w	35	G
1	w	37	C
1	w	43	G

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Mol	Chain	Res	Type
1	w	46	C
1	w	49	A
1	w	50	U
1	w	51	G
1	w	52	A
1	w	61	G
1	w	64	A
1	w	69	C
1	w	71	A
1	w	72	U
1	w	73	A
1	w	75	G
1	w	78	A
1	w	83	G
1	w	88	G
1	w	89	G
1	w	90	U
1	w	92	G
1	w	95	G
1	w	96	G
1	w	101	G
1	w	102	G
1	w	103	A
1	w	117	G
1	w	118	A
1	w	119	A
1	w	120	U
1	w	121	G
1	w	125	G
1	w	126	A
1	w	131	G
1	w	137(A)	C
1	w	139	G
1	w	143	C
1	w	144	C
1	w	146	G
1	w	149	A
1	w	151	C
1	w	153	C
1	w	162	U
1	w	163	U
1	w	165	U

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Mol	Chain	Res	Type
1	w	174	C
1	w	175	G
1	w	176	G
1	w	177	G
1	w	182	A
1	w	184	C
1	w	196	A
1	w	199	A
1	w	204	A
1	w	205	G
1	w	206	U
1	w	215	G
1	w	216	A
1	w	221	A
1	w	222	A
1	w	228	A
1	w	229	A
1	w	233	A
1	w	239	U
1	w	241	A
1	w	242	G
1	w	248	G
1	w	249	C
1	w	250	G
1	w	252	G
1	w	265	A
1	w	266	G
1	w	269	U
1	w	270(D)	C
1	w	270(E)	C
1	w	270(F)	G
1	w	270(M)	U
1	w	270(S)	G
1	w	270(T)	G
1	w	271(A)	U
1	w	271(B)	C
1	w	271(C)	G
1	w	271(D)	U
1	w	271	G
1	w	273(C)	C
1	w	273(G)	C
1	w	274	G

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Mol	Chain	Res	Type
1	w	275	G
1	w	278	A
1	w	289	A
1	w	294	A
1	w	296	C
1	w	298	G
1	w	299	A
1	w	301	G
1	w	302	C
1	w	308	G
1	w	310	A
1	w	311	A
1	w	316	C
1	w	317	G
1	w	320	A
1	w	327	G
1	w	329	G
1	w	330	A
1	w	331	A
1	w	332	A
1	w	338	G
1	w	339	U
1	w	341	G
1	w	342	G
1	w	344	G
1	w	347	A
1	w	348	G
1	w	349	G
1	w	355	G
1	w	358	U
1	w	363(A)	G
1	w	363(E)	G
1	w	363(F)	U
1	w	364	C
1	w	366(B)	C
1	w	370	G
1	w	371	A
1	w	372	G
1	w	374	A
1	w	375	C
1	w	380	U
1	w	385	C

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Mol	Chain	Res	Type
1	w	387	U
1	w	388	G
1	w	390	A
1	w	391	G
1	w	392	C
1	w	394	A
1	w	395	U
1	w	396	G
1	w	397	G
1	w	405	U
1	w	408	G
1	w	414	C
1	w	428	A
1	w	438	G
1	w	439	G
1	w	440	G
1	w	444	C
1	w	446	G
1	w	449	A
1	w	450	G
1	w	451	C
1	w	456	C
1	w	457	A
1	w	458	G
1	w	464	U
1	w	469	G
1	w	470	A
1	w	473	G
1	w	475	U
1	w	477	A
1	w	478	A
1	w	480	A
1	w	481	G
1	w	483	A
1	w	488	G
1	w	489	G
1	w	491	G
1	w	492	A
1	w	504	U
1	w	505	A
1	w	508	G
1	w	509	C

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Mol	Chain	Res	Type
1	w	510	C
1	w	517	C
1	w	518	G
1	w	522	G
1	w	527	C
1	w	528	A
1	w	529	A
1	w	531	C
1	w	532	A
1	w	533	G
1	w	537	C
1	w	542	C
1	w	544	C
1	w	549	G
1	w	551	G
1	w	556	G
1	w	559	G
1	w	562	U
1	w	563	G
1	w	567	A
1	w	569	U
1	w	572	A
1	w	573	G
1	w	574	C
1	w	575	A
1	w	583	G
1	w	594	U
1	w	595	C
1	w	598	G
1	w	603	A
1	w	604	G
1	w	610	C
1	w	614	U
1	w	615	G
1	w	616	A
1	w	617	G
1	w	618(B)	C
1	w	620	G
1	w	621	A
1	w	627	A
1	w	628	G
1	w	634	C

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Mol	Chain	Res	Type
1	w	638	G
1	w	640	C
1	w	645	C
1	w	646	A
1	w	647	G
1	w	653	C
1	w	654	U
1	w	656	G
1	w	660	G
1	w	666	G
1	w	669	G
1	w	671	C
1	w	672	C
1	w	674	G
1	w	684	G
1	w	686	G
1	w	701	G
1	w	703	U
1	w	715	G
1	w	716	A
1	w	717	G
1	w	719	C
1	w	722	A
1	w	729	G
1	w	730	C
1	w	739	G
1	w	740	U
1	w	747	U
1	w	748	G
1	w	749	C
1	w	751	A
1	w	753	C
1	w	757	U
1	w	763	G
1	w	764	A
1	w	765	G
1	w	770	G
1	w	775	G
1	w	776	G
1	w	781	A
1	w	782	A
1	w	784	A

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Mol	Chain	Res	Type
1	w	789	A
1	w	790	C
1	w	792	G
1	w	794	G
1	w	796	C
1	w	798	G
1	w	800	A
1	w	805	G
1	w	811	U
1	w	812	C
1	w	817	C
1	w	826	U
1	w	827	U
1	w	828	U
1	w	830	G
1	w	831	G
1	w	835	A
1	w	846	C
1	w	847	U
1	w	848	G
1	w	849	A
1	w	855	G
1	w	856	C
1	w	859	G
1	w	860	U
1	w	861	A
1	w	866	A
1	w	867	C
1	w	870	A
1	w	873	G
1	w	876	C
1	w	885	C
1	w	886	C
1	w	887	A
1	w	888	C
1	w	889	C
1	w	890	A
1	w	897	C
1	w	899	A
1	w	900	A
1	w	902	C
1	w	906	G

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Mol	Chain	Res	Type
1	w	907	U
1	w	909	A
1	w	910	A
1	w	912	C
1	w	914	C
1	w	916	G
1	w	926	A
1	w	928	G
1	w	931	G
1	w	932	G
1	w	933	A
1	w	938	G
1	w	945	A
1	w	946	G
1	w	957	A
1	w	958	U
1	w	959	A
1	w	961	C
1	w	962	G
1	w	963	U
1	w	965	C
1	w	966	G
1	w	972	G
1	w	974(A)	G
1	w	974(B)	C
1	w	975	G
1	w	976	C
1	w	977	G
1	w	980	A
1	w	982	C
1	w	983	A
1	w	989	G
1	w	990	A
1	w	991	C
1	w	992	C
1	w	993	G
1	w	996	A
1	w	997	G
1	w	1006	C
1	w	1008	C
1	w	1009	A
1	w	1011	G

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Mol	Chain	Res	Type
1	w	1012	U
1	w	1013	C
1	w	1015	G
1	w	1016	G
1	w	1017	G
1	w	1020	A
1	w	1021	A
1	w	1022	G
1	w	1023	U
1	w	1025	G
1	w	1026	U
1	w	1033	U
1	w	1034	G
1	w	1042	G
1	w	1043	C
1	w	1045	A
1	w	1046	A
1	w	1047	G
1	w	1054	A
1	w	1059	G
1	w	1060	U
1	w	1061	U
1	w	1062	G
1	w	1070	A
1	w	1071	G
1	w	1072	C
1	w	1079	C
1	w	1080	C
1	w	1083	U
1	w	1087	G
1	w	1088	A
1	w	1089	G
1	w	1111	A
1	w	1112	G
1	w	1126	A
1	w	1129	A
1	w	1130	U
1	w	1131	G
1	w	1132	A
1	w	1135	C
1	w	1136	G
1	w	1139	G

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Mol	Chain	Res	Type
1	w	1141	U
1	w	1142	C
1	w	1142(B)	A
1	w	1143	A
1	w	1144	G
1	w	1148	A
1	w	1152	C
1	w	1155	A
1	w	1157	G
1	w	1161	C
1	w	1166	C
1	w	1170	G
1	w	1175	U
1	w	1177	A
1	w	1179	C
1	w	1180	C
1	w	1182	A
1	w	1183	G
1	w	1186	G
1	w	1187	G
1	w	1188	U
1	w	1191	G
1	w	1194	A
1	w	1195	G
1	w	1197	G
1	w	1199	U
1	w	1200	C
1	w	1201	C
1	w	1202	C
1	w	1204	A
1	w	1205	U
1	w	1208	C
1	w	1210	A
1	w	1211	U
1	w	1212	G
1	w	1220	A
1	w	1221	C
1	w	1224	C
1	w	1227	G
1	w	1229	G
1	w	1237	A
1	w	1238	G

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Mol	Chain	Res	Type
1	w	1240	U
1	w	1244	G
1	w	1247	A
1	w	1248	G
1	w	1250	G
1	w	1251	C
1	w	1252	G
1	w	1253	A
1	w	1256	G
1	w	1265	A
1	w	1266	G
1	w	1267	U
1	w	1271	G
1	w	1272	A
1	w	1273	U
1	w	1274	A
1	w	1275	A
1	w	1276	A
1	w	1278	A
1	w	1280	G
1	w	1289	C
1	w	1295	C
1	w	1296	G
1	w	1298	C
1	w	1300	U
1	w	1301	A
1	w	1302	A
1	w	1305	C
1	w	1310	G
1	w	1313	U
1	w	1320	C
1	w	1321	A
1	w	1325	G
1	w	1326	U
1	w	1329	U
1	w	1339	G
1	w	1341	U
1	w	1343	G
1	w	1347	G
1	w	1359	A
1	w	1360	A
1	w	1362	C

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Mol	Chain	Res	Type
1	w	1365	A
1	w	1366	A
1	w	1368	G
1	w	1378	A
1	w	1379	A
1	w	1384	A
1	w	1385	G
1	w	1395	A
1	w	1398	C
1	w	1416	G
1	w	1419	A
1	w	1420	U
1	w	1426	G
1	w	1427	A
1	w	1428	C
1	w	1434	A
1	w	1436	G
1	w	1438	U
1	w	1444(B)	A
1	w	1445	C
1	w	1448	G
1	w	1448(B)	A
1	w	1449	G
1	w	1451	C
1	w	1453	A
1	w	1454	U
1	w	1455	G
1	w	1458	C
1	w	1459	G
1	w	1460	A
1	w	1461	G
1	w	1467	C
1	w	1471	A
1	w	1472	A
1	w	1478	G
1	w	1479	G
1	w	1481	U
1	w	1483	G
1	w	1485	G
1	w	1487	G
1	w	1488	G
1	w	1490	A

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Mol	Chain	Res	Type
1	w	1491	G
1	w	1497	U
1	w	1498	C
1	w	1502	C
1	w	1506	C
1	w	1508	A
1	w	1509	A
1	w	1510	A
1	w	1517	G
1	w	1519	G
1	w	1520	U
1	w	1521	G
1	w	1522	G
1	w	1535	U
1	w	1536	A
1	w	1537	C
1	w	1538	G
1	w	1540	G
1	w	1543	A
1	w	1544	C
1	w	1545	A
1	w	1546(B)	C
1	w	1547	C
1	w	1555	G
1	w	1558	A
1	w	1559	G
1	w	1560	G
1	w	1567	A
1	w	1569	A
1	w	1570	A
1	w	1576	U
1	w	1577	C
1	w	1578	U
1	w	1579	A
1	w	1581	G
1	w	1585	C
1	w	1586	A
1	w	1595	G
1	w	1596	A
1	w	1603	A
1	w	1607	C
1	w	1608	A

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Mol	Chain	Res	Type
1	w	1609	A
1	w	1610	A
1	w	1613	G
1	w	1616	A
1	w	1617	C
1	w	1618	A
1	w	1619	G
1	w	1626	G
1	w	1628	G
1	w	1634	A
1	w	1635	G
1	w	1639	U
1	w	1640	C
1	w	1642	G
1	w	1646	C
1	w	1647	G
1	w	1648	C
1	w	1654	A
1	w	1664	A
1	w	1669	A
1	w	1670	C
1	w	1672	C
1	w	1674	G
1	w	1682	G
1	w	1688	U
1	w	1693	U
1	w	1694	C
1	w	1699	G
1	w	1700	A
1	w	1703	G
1	w	1707	G
1	w	1717	G
1	w	1718	G
1	w	1731	G
1	w	1733	G
1	w	1742	C
1	w	1743	G
1	w	1747	G
1	w	1748	G
1	w	1754	C
1	w	1756	G
1	w	1758	G

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Mol	Chain	Res	Type
1	w	1759	A
1	w	1763	G
1	w	1764	G
1	w	1773	A
1	w	1777	U
1	w	1780	A
1	w	1781	C
1	w	1782	C
1	w	1785	A
1	w	1787	A
1	w	1792	G
1	w	1800	C
1	w	1801	G
1	w	1802	A
1	w	1806	C
1	w	1810	A
1	w	1815	A
1	w	1816	G
1	w	1817	G
1	w	1818	U
1	w	1819	A
1	w	1820	U
1	w	1821	A
1	w	1823	G
1	w	1824	G
1	w	1825	A
1	w	1829	A
1	w	1836	C
1	w	1838	C
1	w	1839	G
1	w	1843	C
1	w	1847	A
1	w	1858	G
1	w	1859	A
1	w	1863	G
1	w	1864	U
1	w	1869	G
1	w	1878	G
1	w	1879	C
1	w	1885	A
1	w	1886	C
1	w	1888	G

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Mol	Chain	Res	Type
1	w	1889	A
1	w	1900	A
1	w	1903	G
1	w	1906	G
1	w	1912	A
1	w	1913	A
1	w	1914	C
1	w	1915	U
1	w	1916	A
1	w	1929	G
1	w	1930	G
1	w	1935	G
1	w	1936	A
1	w	1937	A
1	w	1938	A
1	w	1939	U
1	w	1944	U
1	w	1955	U
1	w	1956	U
1	w	1960	A
1	w	1963	U
1	w	1964	G
1	w	1965	C
1	w	1966	A
1	w	1967	C
1	w	1968	G
1	w	1969	A
1	w	1971	A
1	w	1972	A
1	w	1982	C
1	w	1987	G
1	w	1991	U
1	w	1992	G
1	w	1993	U
1	w	1997	G
1	w	1998	G
1	w	2001	A
1	w	2010	G
1	w	2013	A
1	w	2014	A
1	w	2020	A
1	w	2023	G

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Mol	Chain	Res	Type
1	w	2026	C
1	w	2031	A
1	w	2033	A
1	w	2035	G
1	w	2040	C
1	w	2041	U
1	w	2043	C
1	w	2050	C
1	w	2051	A
1	w	2052	G
1	w	2055	C
1	w	2056	G
1	w	2057	A
1	w	2059	A
1	w	2060	A
1	w	2061	G
1	w	2062	A
1	w	2063	C
1	w	2066	C
1	w	2067	G
1	w	2068	U
1	w	2069	G
1	w	2076	U
1	w	2077	A
1	w	2080	G
1	w	2087	G
1	w	2092	U
1	w	2093	G
1	w	2096	U
1	w	2099	U
1	w	2100	G
1	w	2110	G
1	w	2111	C
1	w	2112	G
1	w	2116	G
1	w	2118	U
1	w	2119	A
1	w	2120	G
1	w	2122	U
1	w	2124	G
1	w	2126	A
1	w	2127	G

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Mol	Chain	Res	Type
1	w	2128	C
1	w	2129	C
1	w	2130	U
1	w	2131	G
1	w	2132	U
1	w	2133	G
1	w	2136	C
1	w	2138	C
1	w	2157	G
1	w	2158	A
1	w	2160	G
1	w	2169	A
1	w	2171	A
1	w	2172	U
1	w	2173	A
1	w	2174	C
1	w	2176	A
1	w	2177	C
1	w	2179	C
1	w	2181	G
1	w	2188	C
1	w	2190	G
1	w	2191	G
1	w	2192	G
1	w	2194	G
1	w	2195	C
1	w	2205	C
1	w	2211	G
1	w	2213	U
1	w	2215	G
1	w	2217	G
1	w	2225	A
1	w	2226	C
1	w	2238	G
1	w	2239	G
1	w	2243	U
1	w	2251	G
1	w	2257	U
1	w	2264	C
1	w	2269	A
1	w	2275	C
1	w	2276	G

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Mol	Chain	Res	Type
1	w	2283	C
1	w	2287	A
1	w	2288	A
1	w	2290	G
1	w	2294	C
1	w	2297	C
1	w	2304	G
1	w	2305	A
1	w	2307	G
1	w	2308	G
1	w	2309	A
1	w	2310	A
1	w	2319	G
1	w	2320	A
1	w	2321	G
1	w	2323	G
1	w	2325	G
1	w	2327	A
1	w	2333	A
1	w	2334	G
1	w	2336	A
1	w	2344	U
1	w	2345	G
1	w	2346	A
1	w	2347	C
1	w	2350	C
1	w	2354	G
1	w	2356	C
1	w	2361	A
1	w	2365	G
1	w	2368	C
1	w	2376	A
1	w	2377	A
1	w	2379	G
1	w	2382	G
1	w	2383	G
1	w	2385	C
1	w	2388	A
1	w	2391	G
1	w	2394	C
1	w	2398	U
1	w	2399	G

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Mol	Chain	Res	Type
1	w	2400	G
1	w	2402	C
1	w	2406	U
1	w	2407	G
1	w	2422	A
1	w	2423	U
1	w	2425	A
1	w	2427	C
1	w	2428	G
1	w	2429	G
1	w	2430	A
1	w	2431	U
1	w	2432	A
1	w	2434	A
1	w	2435	A
1	w	2439	A
1	w	2441	C
1	w	2442	C
1	w	2447	G
1	w	2448	A
1	w	2449	U
1	w	2450	A
1	w	2452	C
1	w	2455	G
1	w	2469	A
1	w	2472	G
1	w	2478	A
1	w	2480	C
1	w	2483	C
1	w	2484	G
1	w	2487	G
1	w	2491	U
1	w	2498	C
1	w	2501	C
1	w	2502	G
1	w	2503	A
1	w	2504	U
1	w	2505	G
1	w	2506	U
1	w	2513	G
1	w	2514	U
1	w	2515	C

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Mol	Chain	Res	Type
1	w	2516	G
1	w	2518	A
1	w	2519	U
1	w	2523	G
1	w	2529	G
1	w	2542	A
1	w	2543	G
1	w	2549	G
1	w	2551	C
1	w	2554	U
1	w	2555	U
1	w	2560	C
1	w	2563	U
1	w	2566	A
1	w	2567	G
1	w	2569	G
1	w	2572	A
1	w	2573	C
1	w	2574	G
1	w	2576	G
1	w	2578	G
1	w	2581	G
1	w	2582	G
1	w	2584	U
1	w	2588	G
1	w	2589	A
1	w	2590	A
1	w	2602	A
1	w	2606	C
1	w	2609	U
1	w	2611	U
1	w	2612	C
1	w	2615	U
1	w	2616	C
1	w	2618	G
1	w	2619	C
1	w	2621	A
1	w	2622	C
1	w	2628	C
1	w	2629	A
1	w	2630	G
1	w	2635	C

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Mol	Chain	Res	Type
1	w	2637	U
1	w	2639	A
1	w	2642	G
1	w	2643	G
1	w	2645	G
1	w	2646	C
1	w	2647	U
1	w	2653	U
1	w	2654	A
1	w	2655	G
1	w	2656	U
1	w	2658	C
1	w	2665	A
1	w	2674	G
1	w	2681	C
1	w	2682	U
1	w	2691	C
1	w	2694	G
1	w	2695	C
1	w	2702	U
1	w	2712	U
1	w	2712(B)	A
1	w	2713	A
1	w	2714	G
1	w	2718	G
1	w	2719	G
1	w	2720	U
1	w	2721	A
1	w	2722	G
1	w	2735	G
1	w	2739	U
1	w	2744	G
1	w	2746	U
1	w	2747	G
1	w	2750	A
1	w	2752	C
1	w	2754	U
1	w	2755	C
1	w	2757	A
1	w	2758	A
1	w	2759	G
1	w	2762	G

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Mol	Chain	Res	Type
1	w	2763	G
1	w	2765	A
1	w	2766	G
1	w	2768	C
1	w	2772	C
1	w	2775	A
1	w	2778	A
1	w	2779	U
1	w	2781	A
1	w	2785	C
1	w	2791	C
1	w	2792	G
1	w	2795	G
1	w	2797	U
1	w	2798	C
1	w	2799	A
1	w	2802	G
1	w	2804	C
1	w	2807	G
1	w	2808	U
1	w	2809	A
1	w	2820	A
1	w	2827	C
1	w	2830	G
1	w	2833	G
1	w	2834	G
1	w	2835	A
1	w	2836	U
1	w	2844	G
1	w	2845	G
1	w	2849	U
1	w	2858	C
1	w	2865	U
1	w	2866	U
1	w	2867	G
1	w	2868	A
1	w	2872	G
1	w	2873	A
1	w	2875	C
1	w	2876	G
1	w	2880	C
1	w	2883	A

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Mol	Chain	Res	Type
1	w	2884	U
1	w	2887	U
1	w	2889	C
1	w	2892	A
1	w	2895	U
1	w	2896	C
1	w	2901	C
2	x	5	C
2	x	8	U
2	x	9	G
2	x	10	C
2	x	11	C
2	x	13	A
2	x	14	U
2	x	15	A
2	x	16	G
2	x	20	C
2	x	21	G
2	x	25	A
2	x	26	A
2	x	27	C
2	x	29	A
2	x	33	G
2	x	35	U
2	x	39	A
2	x	40	U
2	x	42	C
2	x	43	C
2	x	45	A
2	x	49	C
2	x	50	G
2	x	52	A
2	x	53	A
2	x	54	G
2	x	57	A
2	x	64	C
2	x	66	A
2	x	67	G
2	x	69	G
2	x	74	U
2	x	75	G
2	x	76	G

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Mol	Chain	Res	Type
2	x	79	C
2	x	87	G
2	x	90	C
2	x	98	G
2	x	103	U
2	x	107	U
2	x	108	C
2	x	109	G
2	x	113	C
2	x	114	G
2	x	117	G
2	x	118	G
31	y	6	G
31	y	8	A
31	y	9	G
31	y	13	U
31	y	14	U
31	y	15	G
31	y	21	G
31	y	31	G
31	y	32	A
31	y	37	U
31	y	38	G
31	y	39	G
31	y	44	G
31	y	47	C
31	y	48	C
31	y	50	A
31	y	51	A
31	y	56	U
31	y	61	G
31	y	62	U
31	y	65	U
31	y	69	G
31	y	82	U
31	y	93	U
31	y	95	G
31	y	97	U
31	y	99	C
31	y	104	G
31	y	105	G
31	y	110	C

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Mol	Chain	Res	Type
31	y	112	G
31	y	115	G
31	y	116	A
31	y	120	A
31	y	121	C
31	y	122	G
31	y	129(B)	G
31	y	130	A
31	y	131	C
31	y	133	U
31	y	134	A
31	y	136	C
31	y	139	G
31	y	141	A
31	y	143	A
31	y	145	G
31	y	149	A
31	y	152	A
31	y	157	G
31	y	161	A
31	y	162	A
31	y	163	C
31	y	174	C
31	y	179	A
31	y	189	U
31	y	191(A)	G
31	y	195	A
31	y	196	A
31	y	197	A
31	y	198	G
31	y	208	U
31	y	209	U
31	y	210	U
31	y	216	G
31	y	219	C
31	y	223	U
31	y	234	C
31	y	238	G
31	y	244	U
31	y	247	G
31	y	251	G
31	y	252	U

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Mol	Chain	Res	Type
31	y	253	U
31	y	255	G
31	y	258	G
31	y	259	G
31	y	263	A
31	y	266	G
31	y	267	C
31	y	270	A
31	y	279	A
31	y	280	C
31	y	281	G
31	y	289	G
31	y	295	C
31	y	299	G
31	y	300	A
31	y	312	C
31	y	321	A
31	y	322	C
31	y	327	A
31	y	328	C
31	y	329	A
31	y	330	C
31	y	332	G
31	y	344	A
31	y	345	C
31	y	347	G
31	y	351	G
31	y	352	C
31	y	353	A
31	y	354	G
31	y	357	G
31	y	360	A
31	y	361	G
31	y	363	A
31	y	365	U
31	y	366	C
31	y	368	U
31	y	369	C
31	y	372	C
31	y	373	A
31	y	375	U
31	y	377	G

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Mol	Chain	Res	Type
31	y	378	G
31	y	379	C
31	y	382	A
31	y	388	G
31	y	391	G
31	y	392	G
31	y	395	C
31	y	397	A
31	y	398	C
31	y	406	G
31	y	409	G
31	y	410	G
31	y	412	A
31	y	413	G
31	y	414	A
31	y	421	U
31	y	422	C
31	y	423	G
31	y	428	G
31	y	429	U
31	y	430	A
31	y	436	C
31	y	439	A
31	y	440	A
31	y	445	G
31	y	449	C
31	y	452	A
31	y	466	G
31	y	467	G
31	y	480	U
31	y	484	G
31	y	485	G
31	y	488	C
31	y	491	G
31	y	493	G
31	y	496	A
31	y	497	U
31	y	498	A
31	y	500	G
31	y	506	G
31	y	508	C
31	y	509	A

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Mol	Chain	Res	Type
31	y	511	C
31	y	512	U
31	y	513	C
31	y	516	PSU
31	y	517	G
31	y	518	C
31	y	519	C
31	y	521	G
31	y	523	A
31	y	524	G
31	y	525	C
31	y	527	7MG
31	y	529	G
31	y	531	U
31	y	532	A
31	y	533	A
31	y	543	C
31	y	547	A
31	y	549	C
31	y	552	U
31	y	556	C
31	y	557	G
31	y	560	U
31	y	561	U
31	y	562	C
31	y	563	A
31	y	565	U
31	y	566	G
31	y	570	G
31	y	572	A
31	y	573	A
31	y	575	G
31	y	576	G
31	y	577	G
31	y	585	G
31	y	588	G
31	y	611	A
31	y	616	G
31	y	617	G
31	y	619	U
31	y	623	C
31	y	627	G

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Mol	Chain	Res	Type
31	y	630	G
31	y	631	G
31	y	633	G
31	y	641	U
31	y	643	C
31	y	650	G
31	y	652	U
31	y	653	A
31	y	661	G
31	y	672	U
31	y	673	G
31	y	678	U
31	y	687	A
31	y	688	G
31	y	689	C
31	y	693	G
31	y	697	U
31	y	701	C
31	y	702	A
31	y	703	G
31	y	704	A
31	y	705	U
31	y	718	G
31	y	724	G
31	y	725	G
31	y	733	A
31	y	741	G
31	y	747	C
31	y	748	C
31	y	749	C
31	y	750	G
31	y	752	G
31	y	753	A
31	y	755	G
31	y	759	A
31	y	770	C
31	y	771	G
31	y	772	U
31	y	777	A
31	y	781	A
31	y	792	A
31	y	794	A

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Mol	Chain	Res	Type
31	y	796	C
31	y	800	G
31	y	801	U
31	y	809	G
31	y	813	U
31	y	814	A
31	y	815	A
31	y	816	A
31	y	817	C
31	y	818	G
31	y	820	U
31	y	828	A
31	y	833	U
31	y	841	U
31	y	842	C
31	y	843	U
31	y	848	C
31	y	852	G
31	y	863	U
31	y	870	U
31	y	871	U
31	y	872	A
31	y	873	A
31	y	874	G
31	y	876	G
31	y	885	G
31	y	889	A
31	y	890	G
31	y	900	A
31	y	902	G
31	y	905	U
31	y	910	C
31	y	913	A
31	y	914	A
31	y	916	G
31	y	926	G
31	y	927	G
31	y	928	G
31	y	934	C
31	y	936	C
31	y	939	G
31	y	942	G

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Mol	Chain	Res	Type
31	y	947	G
31	y	948	C
31	y	956	U
31	y	958	A
31	y	960	U
31	y	961	U
31	y	964	A
31	y	965	A
31	y	966	M2G
31	y	967	5MC
31	y	968	A
31	y	969	A
31	y	972	C
31	y	974	A
31	y	975	A
31	y	976	G
31	y	977	A
31	y	978	A
31	y	982	U
31	y	983	A
31	y	991	U
31	y	992	U
31	y	993	G
31	y	995	C
31	y	998(A)	G
31	y	1002	G
31	y	1004	A
31	y	1005	A
31	y	1013	G
31	y	1014	A
31	y	1016	A
31	y	1020	U
31	y	1024	G
31	y	1025	U
31	y	1026	G
31	y	1027	C
31	y	102(A)	C
31	y	102(C)	C
31	y	1029	G
31	y	1030	C
31	y	1042	G
31	y	1050	G

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Mol	Chain	Res	Type
31	y	1053	G
31	y	1054	C
31	y	1055	A
31	y	1062	U
31	y	1064	G
31	y	1065	U
31	y	1066	C
31	y	1068	G
31	y	1070	U
31	y	1078	U
31	y	1079	G
31	y	1080	A
31	y	1081	G
31	y	1085	U
31	y	1086	U
31	y	1089	G
31	y	1090	U
31	y	1094	G
31	y	1095	U
31	y	1101	A
31	y	1102	A
31	y	1104	G
31	y	1108	G
31	y	1109	C
31	y	1114	C
31	y	1118	C
31	y	1126	U
31	y	1127	G
31	y	1130	A
31	y	1136	U
31	y	1137	C
31	y	1139	G
31	y	1140	C
31	y	1142	G
31	y	1143	G
31	y	1144	G
31	y	1146	A
31	y	1152	A
31	y	1154	G
31	y	1157	A
31	y	1158	C
31	y	1159	U

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Mol	Chain	Res	Type
31	y	1162	C
31	y	1167	A
31	y	1175	G
31	y	1176	A
31	y	1178	G
31	y	1179	A
31	y	1184	G
31	y	1188	A
31	y	1190	G
31	y	1196	U
31	y	1197	G
31	y	1198	G
31	y	1200	C
31	y	1202	G
31	y	1203	C
31	y	1207	2MG
31	y	1208	C
31	y	1209	C
31	y	1211	U
31	y	1212	U
31	y	1213	A
31	y	1215	G
31	y	1221	G
31	y	1225	A
31	y	1226	C
31	y	1227	A
31	y	1233	G
31	y	1235	U
31	y	1237	C
31	y	1238	A
31	y	1239	A
31	y	1240	U
31	y	1241	G
31	y	1243	C
31	y	1247	U
31	y	1248	A
31	y	1251	A
31	y	1253	G
31	y	1256	A
31	y	1257	U
31	y	1261	A
31	y	1263	C

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Mol	Chain	Res	Type
31	y	1267	C
31	y	1269	A
31	y	1270	C
31	y	1278	U
31	y	1280	A
31	y	1282	C
31	y	1283	G
31	y	1285	A
31	y	1286	A
31	y	1290	G
31	y	1291	G
31	y	1294	G
31	y	1297	C
31	y	1298	C
31	y	1299	A
31	y	1300	G
31	y	1301	U
31	y	1302	U
31	y	1303	C
31	y	1306	A
31	y	1308	U
31	y	1309	G
31	y	1319	A
31	y	1320	C
31	y	1323	G
31	y	1324	A
31	y	1325	C
31	y	1331	G
31	y	1333	A
31	y	1335	C
31	y	1340	A
31	y	1345	U
31	y	1346	A
31	y	1347	G
31	y	1348	U
31	y	1354	C
31	y	1359	C
31	y	1360	A
31	y	1361	G
31	y	136(B)	C
31	y	1363	A
31	y	1364	U

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Mol	Chain	Res	Type
31	y	1365	G
31	y	1366	C
31	y	1369	C
31	y	1378	C
31	y	1380	U
31	y	1381	U
31	y	1388	C
31	y	1394	A
31	y	1396	A
31	y	1397	C
31	y	1398	A
31	y	1400	5MC
31	y	1401	G
31	y	1402	C
31	y	1404	5MC
31	y	1405	G
31	y	1407	5MC
31	y	1408	A
31	y	1420	C
31	y	1426	C
31	y	1434	A
31	y	1442	G
31	y	1443	G
31	y	1446	A
31	y	1447	G
31	y	1451	A
31	y	1452	C
31	y	1454	G
31	y	1468	A
31	y	1471	G
31	y	1472	U
31	y	1475	G
31	y	1482	G
31	y	1490	C
31	y	1491	G
31	y	1492	A
31	y	1494	G
31	y	1495	U
31	y	1498	U
31	y	1501	C
31	y	1502	A
31	y	1504	G

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Mol	Chain	Res	Type
31	y	1505	G
31	y	1506	U
31	y	1507	A
31	y	1513	A
31	y	1517	G
31	y	1520	G
31	y	1521	G
31	y	1525	G
31	y	1527	C
31	y	1529	G
31	y	1530	G
31	y	1531	A
31	y	1532	U
31	y	1534	A
31	y	1535	C
32	z	9	G
32	z	16	C
32	z	17	C
32	z	17(A)	U
32	z	18	G
32	z	19	G
32	z	20	U
32	z	21	A
32	z	25	C
32	z	26	G
32	z	30	G
32	z	35	A
32	z	46	A
32	z	48	C
32	z	49	G
32	z	59	A
32	z	65	C
32	z	71	C
32	z	73	A
32	z	76	A
33	2	8	U
33	2	9	A
33	2	10	G
33	2	14	A
33	2	15	G
33	2	16	U
33	2	17	U

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Mol	Chain	Res	Type
33	2	18	G
33	2	20	G
33	2	21	A
33	2	22	G
33	2	35	A
33	2	36	A
33	2	40	C
33	2	47	U
33	2	48	C
33	2	55	PSU
33	2	61	C
33	2	67	A
33	2	73	A
33	2	75	C
33	2	76	A
34	3	3	G
34	3	6	G
34	3	12	A
34	3	13	A
34	3	16	A

There are no RNA pucker outliers to report.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	PSU	2	55	33	16,21,22	1.27	3 (18%)	20,30,33	3.95	8 (40%)
31	2MG	y	1207	31	19,26,27	2.22	5 (26%)	20,38,41	4.03	6 (30%)
31	5MC	y	1400	31	15,22,23	1.12	2 (13%)	17,32,35	0.92	1 (5%)
31	5MC	y	1404	31	15,22,23	1.37	2 (13%)	17,32,35	1.61	1 (5%)
31	5MC	y	1407	31	15,22,23	1.18	2 (13%)	17,32,35	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	MA6	y	1518	31	16,26,27	1.28	0	18,38,41	2.43	6 (33%)
31	MA6	y	1519	31	16,26,27	1.98	3 (18%)	18,38,41	2.28	6 (33%)
31	PSU	y	516	31	16,21,22	1.35	2 (12%)	20,30,33	3.93	6 (30%)
31	7MG	y	527	31	20,26,27	2.55	6 (30%)	22,39,42	2.32	4 (18%)
31	M2G	y	966	31	20,27,28	2.27	4 (20%)	21,40,43	2.84	6 (28%)
31	5MC	y	967	31	15,22,23	1.05	1 (6%)	17,32,35	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PSU	2	55	33	-	0/7/25/26	0/2/2/2
31	2MG	y	1207	31	-	0/5/27/28	0/3/3/3
31	5MC	y	1400	31	-	0/3/25/26	0/2/2/2
31	5MC	y	1404	31	-	0/3/25/26	0/2/2/2
31	5MC	y	1407	31	-	0/3/25/26	0/2/2/2
31	MA6	y	1518	31	-	0/7/29/30	0/3/3/3
31	MA6	y	1519	31	-	0/7/29/30	0/3/3/3
31	PSU	y	516	31	-	0/7/25/26	0/2/2/2
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	M2G	y	966	31	-	0/7/29/30	0/3/3/3
31	5MC	y	967	31	-	0/3/25/26	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	527	7MG	C8-N9	-5.25	1.37	1.45
33	2	55	PSU	C5-C1'	-3.36	1.49	1.52
31	y	527	7MG	C8-N7	-2.58	1.32	1.43
33	2	55	PSU	O5'-C5'	-2.04	1.41	1.44
31	y	1400	5MC	O4'-C1'	2.15	1.44	1.41
33	2	55	PSU	C4-N3	2.21	1.37	1.33
31	y	967	5MC	C4-N4	2.27	1.40	1.34
31	y	966	M2G	C2-N2	2.45	1.38	1.34
31	y	1400	5MC	C4-N4	2.48	1.40	1.34
31	y	1207	2MG	C2-N1	2.51	1.43	1.34
31	y	1407	5MC	C4-N4	2.53	1.40	1.34
31	y	1207	2MG	CM2-N2	2.55	1.49	1.45
31	y	1404	5MC	C4-N4	2.55	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	1407	5MC	O4'-C1'	2.67	1.45	1.41
31	y	516	PSU	C2'-C1'	2.77	1.57	1.53
31	y	516	PSU	C4-N3	2.78	1.38	1.33
31	y	1519	MA6	C9-N6	2.79	1.52	1.45
31	y	1404	5MC	O4'-C1'	2.93	1.45	1.41
31	y	1207	2MG	C6-C5	3.03	1.47	1.41
31	y	527	7MG	C4-N3	3.03	1.38	1.34
31	y	527	7MG	C2-N1	3.75	1.42	1.35
31	y	966	M2G	C6-C5	3.75	1.48	1.41
31	y	1207	2MG	C2-N2	3.79	1.37	1.34
31	y	1519	MA6	C10-N6	3.91	1.55	1.45
31	y	966	M2G	C2-N1	5.13	1.43	1.34
31	y	1519	MA6	O4'-C1'	5.19	1.48	1.41
31	y	527	7MG	C6-C5	5.50	1.47	1.41
31	y	527	7MG	C6-N1	6.04	1.44	1.33
31	y	966	M2G	C6-N1	6.23	1.44	1.33
31	y	1207	2MG	C6-N1	6.72	1.45	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1207	2MG	C4'-O4'-C1'	-13.04	95.89	109.77
31	y	516	PSU	N1-C2-N3	-11.78	119.93	128.40
33	2	55	PSU	N1-C2-N3	-10.91	120.55	128.40
31	y	1207	2MG	C5-C6-N1	-8.45	111.45	123.48
31	y	966	M2G	C5-C6-N1	-8.30	111.67	123.48
31	y	527	7MG	C5-C6-N1	-7.88	111.01	123.37
33	2	55	PSU	C5-C1'-C2'	-7.60	102.45	115.55
33	2	55	PSU	C5-C4-N3	-7.24	119.49	125.43
31	y	516	PSU	C4'-O4'-C1'	-7.21	101.13	109.48
31	y	516	PSU	C5-C4-N3	-6.63	119.99	125.43
31	y	1519	MA6	N3-C2-N1	-6.16	123.50	128.86
31	y	1207	2MG	CM2-N2-C2	-5.78	116.59	123.63
31	y	1518	MA6	N3-C2-N1	-5.51	124.06	128.86
31	y	1404	5MC	C4'-O4'-C1'	-5.41	104.01	109.77
31	y	966	M2G	CM1-N2-C2	-4.56	117.00	121.34
33	2	55	PSU	C5-C6-N1	-3.37	120.03	124.39
31	y	966	M2G	CM2-N2-C2	-2.97	118.52	121.34
31	y	1207	2MG	N3-C2-N1	-2.80	122.00	126.23
31	y	516	PSU	C5-C6-N1	-2.35	121.34	124.39
31	y	527	7MG	C4'-O4'-C1'	-2.29	104.36	109.47
31	y	1518	MA6	O4'-C4'-C3'	2.02	109.19	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	527	7MG	N2-C2-N3	2.03	120.49	117.24
31	y	1400	5MC	O3'-C3'-C4'	2.08	117.16	111.09
31	y	1518	MA6	C1'-N9-C4	2.16	130.36	126.64
31	y	1519	MA6	C10-N6-C9	2.25	123.31	116.03
31	y	1518	MA6	O4'-C4'-C5'	2.56	118.04	109.40
31	y	1519	MA6	C4'-O4'-C1'	2.59	112.53	109.77
31	y	1207	2MG	N2-C2-N3	2.67	119.55	116.95
31	y	966	M2G	O3'-C3'-C2'	2.69	120.44	111.83
31	y	516	PSU	C6-N1-C2	2.70	119.68	115.36
33	2	55	PSU	C6-N1-C2	2.76	119.78	115.36
31	y	1519	MA6	C2'-C3'-C4'	2.82	108.11	102.62
33	2	55	PSU	O4'-C1'-C5	2.83	114.32	109.93
31	y	966	M2G	N3-C2-N2	2.88	120.12	117.15
33	2	55	PSU	C3'-C2'-C1'	3.23	105.65	101.93
31	y	1518	MA6	C2-N1-C6	3.44	120.27	111.82
31	y	1519	MA6	C2-N1-C6	3.50	120.40	111.82
31	y	1519	MA6	N1-C6-N6	4.03	121.28	117.00
31	y	1207	2MG	C6-N1-C2	4.80	123.78	115.18
31	y	527	7MG	C6-N1-C2	5.32	123.72	116.06
33	2	55	PSU	C4-N3-C2	5.76	120.19	115.16
31	y	1518	MA6	N1-C6-N6	6.21	123.59	117.00
31	y	966	M2G	C6-N1-C2	6.48	123.90	116.18
31	y	516	PSU	C4-N3-C2	6.61	120.94	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	55	PSU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	w	32

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	41:C	O3'	43:G	P	2.13
1	w	1506:C	O3'	1508:A	P	2.09
1	w	489:G	O3'	491:G	P	2.08
1	w	1448(B):A	O3'	1449:G	P	2.07
1	w	436:C	O3'	438:G	P	2.05
1	w	554:U	O3'	556:G	P	2.05
1	w	1712:C	O3'	1716:U	P	2.04
1	w	1743:G	O3'	1746:G	P	2.04
1	w	366(B):C	O3'	370:G	P	2.03
1	w	890:A	O3'	892:G	P	2.03
1	w	2213:U	O3'	2215:G	P	2.03
1	w	2712(B):A	O3'	2713:A	P	2.03
1	w	155:C	O3'	161:U	P	2.02
1	w	926:A	O3'	928:G	P	2.02
1	w	99:U	O3'	101:G	P	2.01
1	w	1583:A	O3'	1585:C	P	2.01
1	w	1718:G	O3'	1725:G	P	2.01
1	w	1451:C	O3'	1453:A	P	1.99
1	w	1481:U	O3'	1483:G	P	1.99
1	w	1735:U	O3'	1741:C	P	1.99
1	w	537:C	O3'	539:G	P	1.98
1	w	1171:G	O3'	1173:G	P	1.97
1	w	1864:U	O3'	1869:G	P	1.97
1	w	1546(B):C	O3'	1547:C	P	1.96
1	w	1630(B):C	O3'	1631:A	P	1.96
1	w	1142(B):A	O3'	1143:A	P	1.95
1	w	1872:A	O3'	1878:G	P	1.95
1	w	2219:G	O3'	2224:G	P	1.95
1	w	165:U	O3'	171:G	P	1.94
1	w	1221(A):C	O3'	1222:C	P	1.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	1444(B):A	O3'	1445:C	P	1.93
1	w	1133:U	O3'	1135:C	P	1.91

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	w	2889/2889 (100%)	0.03	107 (3%) 42 34	1, 1, 1, 1	0
2	x	120/120 (100%)	-0.22	0 100 100	1, 1, 1, 1	0
3	A	127/229 (55%)	-0.37	6 (4%) 32 26	1, 1, 1, 1	0
4	B	272/276 (98%)	-0.14	19 (6%) 17 13	1, 1, 1, 1	0
5	C	201/206 (97%)	-0.13	12 (5%) 23 17	1, 1, 1, 1	0
6	D	194/205 (94%)	-0.64	0 100 100	1, 1, 1, 1	0
7	E	180/182 (98%)	-0.30	8 (4%) 35 28	1, 1, 1, 1	0
8	F	173/180 (96%)	-0.46	8 (4%) 33 27	1, 1, 1, 1	0
9	G	148/148 (100%)	-0.21	8 (5%) 26 21	1, 1, 1, 1	0
10	H	138/140 (98%)	-0.43	2 (1%) 75 66	1, 1, 1, 1	0
11	I	122/122 (100%)	-0.17	8 (6%) 19 14	1, 1, 1, 1	0
12	J	146/150 (97%)	-0.51	3 (2%) 64 53	1, 1, 1, 1	0
13	K	137/141 (97%)	-0.08	11 (8%) 13 11	1, 1, 1, 1	0
14	L	118/118 (100%)	-0.24	6 (5%) 29 23	1, 1, 1, 1	0
15	M	106/112 (94%)	-0.16	5 (4%) 32 26	1, 1, 1, 1	0
16	N	137/146 (93%)	-0.24	3 (2%) 62 53	1, 1, 1, 1	0
17	O	117/118 (99%)	-0.40	4 (3%) 46 36	1, 1, 1, 1	0
18	P	101/101 (100%)	0.17	15 (14%) 3 3	1, 1, 1, 1	0
19	Q	109/113 (96%)	0.43	17 (15%) 2 3	1, 1, 1, 1	0
20	R	92/96 (95%)	-0.49	1 (1%) 80 72	1, 1, 1, 1	0
21	S	103/110 (93%)	0.56	22 (21%) 1 1	1, 1, 1, 1	0
22	T	185/206 (89%)	-0.41	5 (2%) 55 44	1, 1, 1, 1	0
23	U	76/85 (89%)	-0.41	1 (1%) 77 68	1, 1, 1, 1	0
24	V	88/98 (89%)	-0.30	2 (2%) 61 51	1, 1, 1, 1	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	62/72 (86%)	-0.12	2 (3%) 48 38	1, 1, 1, 1	0
26	X	60/60 (100%)	-0.14	1 (1%) 70 61	1, 1, 1, 1	0
27	Y	56/60 (93%)	-0.72	0 100 100	1, 1, 1, 1	0
28	Z	48/49 (97%)	-0.69	0 100 100	1, 1, 1, 1	0
29	a	63/65 (96%)	-0.07	5 (7%) 13 11	1, 1, 1, 1	0
30	b	35/37 (94%)	0.97	11 (31%) 0 1	1, 1, 1, 1	0
31	y	1504/1522 (98%)	0.04	62 (4%) 38 30	1, 1, 1, 1	0
32	z	77/77 (100%)	0.23	4 (5%) 28 23	1, 1, 1, 1	0
33	2	75/76 (98%)	0.63	7 (9%) 9 8	1, 1, 1, 1	0
34	3	18/18 (100%)	1.14	6 (33%) 0 1	1, 1, 1, 1	0
35	c	234/256 (91%)	-0.28	10 (4%) 36 28	1, 1, 1, 1	0
36	d	206/239 (86%)	-0.50	7 (3%) 46 36	1, 1, 1, 1	0
37	e	208/209 (99%)	-0.40	6 (2%) 52 42	1, 1, 1, 1	0
38	f	150/162 (92%)	-0.49	7 (4%) 32 26	1, 1, 1, 1	0
39	g	101/101 (100%)	-0.56	2 (1%) 65 56	1, 1, 1, 1	0
40	h	155/156 (99%)	-0.37	5 (3%) 48 38	1, 1, 1, 1	0
41	i	138/138 (100%)	-0.04	11 (7%) 13 11	1, 1, 1, 1	0
42	j	127/128 (99%)	-0.03	12 (9%) 9 8	1, 1, 1, 1	0
43	k	98/105 (93%)	-0.32	2 (2%) 65 56	1, 1, 1, 1	0
44	l	116/129 (89%)	0.07	12 (10%) 7 7	1, 1, 1, 1	0
45	m	124/132 (93%)	-0.25	8 (6%) 20 14	1, 1, 1, 1	0
46	n	125/126 (99%)	0.14	16 (12%) 4 5	1, 1, 1, 1	0
47	o	60/61 (98%)	-0.50	2 (3%) 47 37	1, 1, 1, 1	0
48	p	88/89 (98%)	0.18	11 (12%) 4 5	1, 1, 1, 1	0
49	q	83/88 (94%)	1.02	21 (25%) 1 1	1, 1, 1, 1	0
50	r	104/105 (99%)	-0.59	0 100 100	1, 1, 1, 1	0
51	s	81/88 (92%)	-0.65	0 100 100	1, 1, 1, 1	0
52	t	80/93 (86%)	-0.11	6 (7%) 15 12	1, 1, 1, 1	0
53	u	99/106 (93%)	0.44	15 (15%) 2 3	1, 1, 1, 1	0
54	v	24/27 (88%)	-0.51	0 100 100	1, 1, 1, 1	0
All	All	10478/10865 (96%)	-0.11	524 (5%) 30 24	1, 1, 1, 1	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	3	7	G	9.1
31	y	145	G	8.0
41	i	52	ASP	7.4
1	w	2399	G	7.0
44	l	118	GLY	7.0
1	w	1067	A	6.7
1	w	1591	G	6.6
53	u	46	GLU	6.4
1	w	1473	G	6.4
46	n	124	PRO	6.4
41	i	57	PRO	6.3
31	y	144	G	6.2
1	w	1592	C	6.1
31	y	146	G	6.1
41	i	58	TYR	6.0
31	y	416	G	5.9
49	q	70	ALA	5.9
53	u	45	GLN	5.9
46	n	86	CYS	5.8
31	y	865	A	5.8
5	C	167	VAL	5.8
1	w	1983	C	5.7
21	S	34	LYS	5.7
1	w	2400	G	5.6
52	t	56	GLN	5.6
1	w	1679	U	5.6
1	w	1472	A	5.6
13	K	111	GLU	5.5
44	l	119	CYS	5.5
41	i	53	VAL	5.4
45	m	20	LYS	5.3
46	n	85	GLY	5.2
21	S	30	VAL	5.2
31	y	716	A	5.2
33	2	28	C	5.2
42	j	115	GLY	5.2
48	p	15	PHE	5.1
1	w	1116	C	5.1
38	f	13	ILE	5.1
42	j	123	PRO	5.0
41	i	54	ASP	5.0
18	P	87	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
19	Q	85	VAL	5.0
4	B	109	ASP	5.0
42	j	116	LYS	5.0
22	T	154	ASP	4.9
46	n	126	LYS	4.9
19	Q	97	LYS	4.9
30	b	13	LYS	4.8
19	Q	83	LYS	4.8
46	n	125	ARG	4.8
1	w	518	G	4.8
1	w	2398	U	4.8
52	t	57	HIS	4.7
33	2	34	G	4.7
30	b	29	ASN	4.7
25	W	19	VAL	4.7
48	p	16	ALA	4.7
31	y	23	C	4.7
19	Q	82	LEU	4.7
19	Q	95	ILE	4.7
1	w	1460	A	4.7
8	F	166	GLY	4.6
46	n	123	ALA	4.6
1	w	1635	G	4.6
44	l	115	PRO	4.5
46	n	83	ASP	4.5
21	S	5	MET	4.5
15	M	9	ARG	4.5
1	w	989	G	4.5
21	S	29	GLU	4.5
44	l	125	PHE	4.5
31	y	866	C	4.4
42	j	75	ASP	4.4
1	w	134	C	4.4
37	e	44	GLY	4.4
44	l	117	ASN	4.4
31	y	874	G	4.4
21	S	32	PRO	4.4
18	P	57	VAL	4.3
30	b	28	GLU	4.3
46	n	89	GLY	4.3
19	Q	94	ASP	4.3
45	m	19	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
44	l	126	ARG	4.3
31	y	1079	G	4.2
1	w	1405	U	4.2
45	m	21	SER	4.2
49	q	58	TYR	4.2
41	i	51	VAL	4.2
31	y	135	C	4.2
37	e	46	LYS	4.2
33	2	33	U	4.2
18	P	56	SER	4.2
21	S	1	MET	4.2
1	w	1221	C	4.1
53	u	91	LEU	4.1
48	p	3	ILE	4.1
21	S	31	LEU	4.1
4	B	198	ASN	4.1
1	w	270(T)	G	4.1
31	y	731	G	4.0
5	C	104	VAL	4.0
4	B	199	ALA	4.0
7	E	49	ASP	4.0
17	O	14	HIS	4.0
30	b	8	LYS	4.0
1	w	1590	U	4.0
41	i	55	GLY	4.0
1	w	2493	U	3.9
22	T	155	LEU	3.9
31	y	1383	C	3.9
31	y	227	G	3.9
22	T	156	LYS	3.9
30	b	12	ASP	3.9
1	w	364	C	3.9
9	G	16	GLY	3.9
18	P	86	GLY	3.9
45	m	18	ARG	3.8
34	3	6	G	3.8
49	q	65	GLN	3.8
14	L	59	ASP	3.8
21	S	4	LYS	3.8
1	w	1098	A	3.8
19	Q	93	ALA	3.8
38	f	14	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
43	k	18	ALA	3.7
31	y	1535	C	3.7
18	P	74	LYS	3.7
1	w	1680	U	3.7
19	Q	96	ILE	3.7
31	y	715	A	3.7
11	I	9	GLU	3.7
35	c	65	GLY	3.7
31	y	287	U	3.7
31	y	1078	U	3.7
5	C	5	LEU	3.7
1	w	2461	C	3.7
1	w	2600	A	3.7
41	i	56	LYS	3.6
1	w	1808	U	3.6
35	c	157	ARG	3.6
42	j	117	HIS	3.6
49	q	66	PRO	3.6
49	q	61	SER	3.6
31	y	1267	C	3.6
1	w	1764	G	3.6
1	w	1990	C	3.6
4	B	2	ALA	3.6
33	2	29	A	3.6
53	u	47	GLY	3.6
24	V	26	ARG	3.6
13	K	91	GLU	3.6
30	b	14	CYS	3.5
23	U	16	SER	3.5
1	w	1115	G	3.5
31	y	1117	G	3.5
49	q	21	VAL	3.5
1	w	2820	A	3.5
46	n	84	ILE	3.5
1	w	2492	U	3.5
21	S	92	ASN	3.5
34	3	8	U	3.5
32	z	74	C	3.5
37	e	71	SER	3.5
13	K	110	THR	3.5
49	q	69	THR	3.5
18	P	73	SER	3.5

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Mol	Chain	Res	Type	RSRZ
46	n	79	LYS	3.5
46	n	72	ALA	3.4
13	K	32	PHE	3.4
11	I	69	VAL	3.4
13	K	131	ILE	3.4
49	q	24	ALA	3.4
31	y	611	A	3.4
1	w	2161	C	3.4
49	q	62	VAL	3.4
8	F	127	GLU	3.4
18	P	88	ARG	3.4
30	b	7	VAL	3.3
29	a	19	SER	3.3
31	y	864	A	3.3
9	G	59	ALA	3.3
1	w	133	C	3.3
36	d	38	ARG	3.3
43	k	19	SER	3.3
1	w	2274	A	3.3
31	y	134	A	3.3
31	y	1342	C	3.3
11	I	70	LYS	3.3
42	j	105	ASP	3.3
31	y	677	U	3.3
1	w	1348	G	3.3
46	n	76	ALA	3.2
40	h	8	GLU	3.2
1	w	1600	C	3.2
1	w	1099	G	3.2
9	G	63	ALA	3.2
13	K	112	GLU	3.2
35	c	67	THR	3.2
3	A	39	ASP	3.2
4	B	110	GLY	3.2
1	w	270(V)	C	3.2
13	K	80	GLU	3.2
31	y	417	C	3.2
5	C	109	LYS	3.2
21	S	3	VAL	3.2
42	j	76	ALA	3.2
14	L	60	LEU	3.2
31	y	415	A	3.2

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Mol	Chain	Res	Type	RSRZ
38	f	29	GLY	3.2
1	w	888	C	3.2
1	w	34	C	3.1
48	p	11	VAL	3.1
30	b	10	ILE	3.1
31	y	1536	C	3.1
35	c	37	ASN	3.1
49	q	36	ILE	3.1
9	G	60	GLU	3.1
49	q	19	ILE	3.1
13	K	92	GLY	3.1
44	l	121	PRO	3.1
1	w	241	A	3.1
8	F	165	ALA	3.1
1	w	1626	G	3.1
14	L	81	ASP	3.1
31	y	288	A	3.1
49	q	40	ASP	3.1
49	q	54	GLU	3.1
3	A	192	ALA	3.0
4	B	115	GLN	3.0
9	G	65	ALA	3.0
39	g	51	PRO	3.0
1	w	242	G	3.0
11	I	50	GLY	3.0
1	w	1026	U	3.0
4	B	96	HIS	3.0
42	j	13	ALA	3.0
37	e	95	GLY	3.0
48	p	4	THR	3.0
44	l	87	THR	3.0
21	S	27	VAL	3.0
21	S	26	LYS	3.0
38	f	15	ARG	3.0
48	p	80	ALA	3.0
1	w	270(U)	G	3.0
40	h	9	VAL	3.0
4	B	114	GLY	2.9
52	t	58	VAL	2.9
1	w	1369	G	2.9
38	f	12	LEU	2.9
31	y	179	A	2.9

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Mol	Chain	Res	Type	RSRZ
31	y	1252	A	2.9
13	K	78	PRO	2.9
32	z	17(A)	U	2.9
7	E	126	ASP	2.9
1	w	1761	C	2.9
53	u	51	GLU	2.9
31	y	934	C	2.9
44	l	13	GLN	2.9
49	q	37	GLY	2.9
1	w	2145	C	2.9
1	w	2459	A	2.9
19	Q	21	VAL	2.9
4	B	65	ILE	2.9
31	y	861	G	2.9
5	C	168	MET	2.9
30	b	9	ARG	2.9
11	I	10	VAL	2.9
1	w	1989	G	2.9
31	y	714	G	2.9
33	2	65	G	2.9
12	J	93	GLY	2.8
45	m	49	SER	2.8
1	w	1349	A	2.8
1	w	1404	C	2.8
1	w	1068	G	2.8
49	q	59	TRP	2.8
13	K	79	LEU	2.8
1	w	23	G	2.8
30	b	27	CYS	2.8
31	y	262	A	2.8
34	3	18	C	2.8
8	F	129	THR	2.8
8	F	61	HIS	2.8
1	w	615	G	2.8
4	B	112	GLN	2.8
1	w	1498	C	2.8
29	a	27	THR	2.8
1	w	508	G	2.7
31	y	775	G	2.7
53	u	94	ALA	2.7
3	A	176	VAL	2.7
49	q	33	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
38	f	28	PHE	2.7
37	e	45	GLN	2.7
1	w	1678	G	2.7
25	W	18	PRO	2.7
37	e	29	PRO	2.7
8	F	56	SER	2.7
36	d	93	LYS	2.7
1	w	1625	C	2.7
17	O	17	ILE	2.7
29	a	6	THR	2.7
4	B	268	ARG	2.7
22	T	153	SER	2.7
1	w	1474	C	2.7
42	j	72	GLY	2.7
42	j	114	TYR	2.7
1	w	2258	C	2.7
53	u	41	VAL	2.7
31	y	913	A	2.7
31	y	713	G	2.7
46	n	90	LEU	2.6
9	G	64	GLU	2.6
21	S	6	HIS	2.6
48	p	12	ILE	2.6
41	i	25	ASP	2.6
48	p	6	GLU	2.6
40	h	6	ARG	2.6
5	C	166	THR	2.6
7	E	127	GLY	2.6
19	Q	101	SER	2.6
14	L	3	HIS	2.6
21	S	22	GLY	2.6
42	j	122	ALA	2.6
49	q	56	ALA	2.6
9	G	2	LYS	2.6
33	2	36	A	2.6
21	S	37	VAL	2.6
31	y	250	A	2.6
31	y	653	A	2.6
52	t	59	PRO	2.6
13	K	115	MET	2.5
9	G	67	ARG	2.5
21	S	25	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
31	y	1366	C	2.5
18	P	76	LYS	2.5
1	w	2460	U	2.5
1	w	1301	A	2.5
4	B	200	ASP	2.5
26	X	14	GLY	2.5
1	w	1977	A	2.5
3	A	177	GLY	2.5
7	E	119	GLY	2.5
11	I	11	ALA	2.5
48	p	2	PRO	2.5
31	y	828	A	2.5
21	S	2	ARG	2.5
1	w	2599	G	2.5
45	m	27	LYS	2.5
1	w	1578	U	2.5
31	y	863	U	2.5
39	g	32	ASN	2.5
1	w	2248	C	2.5
35	c	66	GLY	2.5
1	w	2162	G	2.5
31	y	818	G	2.5
47	o	16	PHE	2.5
46	n	75	ALA	2.5
19	Q	84	ARG	2.5
1	w	85	G	2.5
1	w	680	G	2.5
35	c	231	GLU	2.5
18	P	95	LEU	2.5
45	m	28	GLY	2.5
1	w	2260	C	2.5
8	F	168	PRO	2.5
49	q	22	THR	2.5
17	O	16	LYS	2.5
21	S	38	ILE	2.5
1	w	2012	G	2.4
4	B	126	GLN	2.4
36	d	189	ALA	2.4
1	w	1266	G	2.4
53	u	44	ALA	2.4
1	w	2730	C	2.4
3	A	195	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
18	P	30	GLY	2.4
5	C	198	VAL	2.4
29	a	26	LYS	2.4
1	w	1807	G	2.4
41	i	50	ARG	2.4
1	w	1117	G	2.4
14	L	82	GLU	2.4
19	Q	13	SER	2.4
53	u	93	GLU	2.4
1	w	436	C	2.4
18	P	29	PRO	2.4
1	w	1097	U	2.4
36	d	192	THR	2.4
21	S	35	TYR	2.4
40	h	94	ARG	2.4
52	t	65	ASN	2.4
3	A	196	ALA	2.4
44	l	114	VAL	2.4
1	w	1496	A	2.4
32	z	17	C	2.4
16	N	66	VAL	2.3
35	c	158	LEU	2.3
47	o	11	LYS	2.3
44	l	12	ARG	2.3
4	B	3	VAL	2.3
5	C	110	GLY	2.3
21	S	90	LEU	2.3
31	y	241	C	2.3
18	P	96	ILE	2.3
42	j	67	GLY	2.3
31	y	935	A	2.3
1	w	1577	C	2.3
49	q	20	VAL	2.3
1	w	1809	A	2.3
1	w	2345	G	2.3
1	w	1417	C	2.3
17	O	13	LYS	2.3
1	w	382	G	2.3
34	3	16	A	2.3
33	2	32	C	2.3
18	P	72	VAL	2.3
1	w	1634	A	2.3

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Mol	Chain	Res	Type	RSRZ
1	w	1636	C	2.3
19	Q	74	ALA	2.3
34	3	17	C	2.3
1	w	2076	U	2.3
48	p	9	GLN	2.3
53	u	90	GLN	2.3
1	w	256	A	2.3
32	z	62	C	2.3
1	w	1593	G	2.3
7	E	50	ALA	2.3
12	J	38	GLN	2.3
21	S	33	LYS	2.3
30	b	11	CYS	2.3
1	w	240	G	2.3
1	w	1692	U	2.3
22	T	63	ASP	2.3
48	p	14	GLU	2.3
53	u	42	GLN	2.3
16	N	67	SER	2.3
20	R	65	ARG	2.3
1	w	1488	G	2.2
31	y	867	G	2.2
36	d	45	LYS	2.2
35	c	131	PRO	2.2
40	h	93	PRO	2.2
31	y	180	U	2.2
7	E	165	THR	2.2
10	H	42	GLU	2.2
19	Q	81	ALA	2.2
1	w	887	A	2.2
31	y	136	C	2.2
52	t	55	LYS	2.2
4	B	34	VAL	2.2
31	y	610	G	2.2
31	y	1187	G	2.2
5	C	197	ILE	2.2
31	y	78	G	2.2
36	d	41	GLY	2.2
1	w	1599	C	2.2
31	y	89	U	2.2
53	u	15	ARG	2.2
38	f	85	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
11	I	12	ASP	2.2
1	w	1368	G	2.2
1	w	2897	U	2.2
14	L	30	THR	2.1
31	y	676	A	2.1
31	y	79	G	2.1
31	y	1186	G	2.1
31	y	531	U	2.1
1	w	1665	A	2.1
10	H	99	SER	2.1
18	P	65	GLY	2.1
21	S	93	GLY	2.1
4	B	80	ALA	2.1
44	l	124	LYS	2.1
8	F	167	GLU	2.1
35	c	129	GLU	2.1
15	M	29	PHE	2.1
1	w	521	G	2.1
7	E	47	LYS	2.1
46	n	36	LYS	2.1
46	n	122	LYS	2.1
19	Q	44	ALA	2.1
19	Q	86	LEU	2.1
4	B	45	ASN	2.1
4	B	108	PRO	2.1
53	u	49	ALA	2.1
36	d	39	ILE	2.1
31	y	88	C	2.1
45	m	26	LEU	2.1
49	q	1	MET	2.1
41	i	90	GLY	2.1
7	E	51	ARG	2.1
49	q	23	ASP	2.1
31	y	776	G	2.1
1	w	1095	A	2.1
1	w	2755	C	2.1
31	y	240	C	2.1
35	c	240	GLN	2.1
31	y	1166	G	2.1
19	Q	14	PRO	2.1
31	y	136(A)	C	2.1
15	M	83	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
24	V	59	THR	2.0
4	B	95	LEU	2.0
5	C	199	ARG	2.0
53	u	48	LYS	2.0
1	w	1500	G	2.0
1	w	1666	G	2.0
1	w	1763	G	2.0
1	w	2731	G	2.0
5	C	114	ALA	2.0
15	M	37	ALA	2.0
16	N	70	VAL	2.0
12	J	37	GLY	2.0
18	P	31	ALA	2.0
1	w	1633	G	2.0
5	C	196	VAL	2.0
1	w	820	A	2.0
53	u	9	ASN	2.0
15	M	28	VAL	2.0
29	a	5	LYS	2.0
11	I	13	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	PSU	2	55	20/21	0.82	0.24	-	1,1,1,1	0
31	5MC	y	1400	21/22	0.97	0.24	-	1,1,1,1	0
31	5MC	y	1407	21/22	0.93	0.16	-	1,1,1,1	0
31	2MG	y	1207	24/25	0.95	0.16	-	1,1,1,1	0
31	5MC	y	967	21/22	0.94	0.14	-	1,1,1,1	0
31	PSU	y	516	20/21	0.92	0.17	-	1,1,1,1	0
31	MA6	y	1518	24/25	0.93	0.17	-	1,1,1,1	0
31	M2G	y	966	25/26	0.92	0.14	-	1,1,1,1	0
31	MA6	y	1519	24/25	0.93	0.16	-	1,1,1,1	0
31	5MC	y	1404	21/22	0.94	0.20	-	1,1,1,1	0
31	7MG	y	527	24/25	0.93	0.23	-	1,1,1,1	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.