



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:58 AM UTC

PDB ID : 8I0U / pdb_00008i0u
EMDB ID : EMD-35110
Title : The cryo-EM structure of human Bact-IV complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

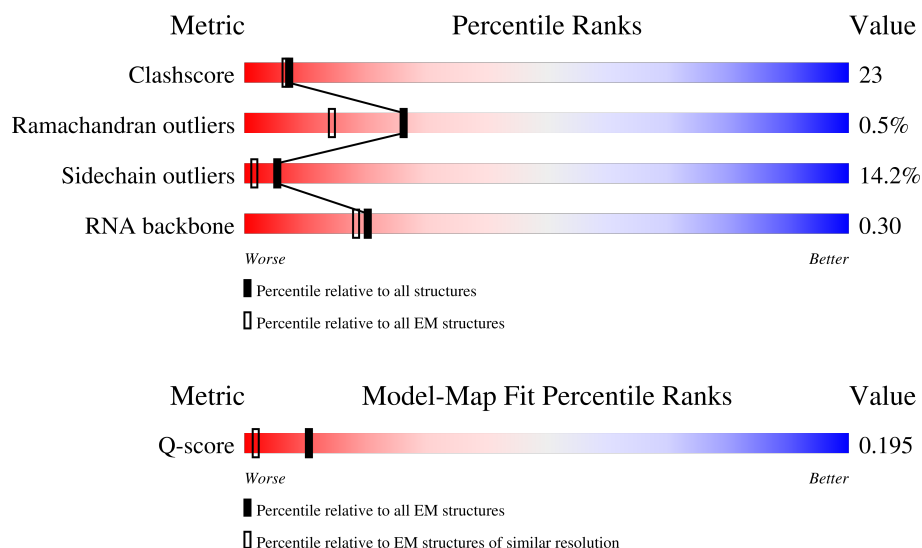
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2335	
2	B	117	
3	C	972	

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Mol	Chain	Length	Quality of chain
4	E	357	
5	F	107	
6	G	220	
7	H	188	
8	I	855	
9	J	848	
10	K	343	
11	L	802	
12	M	243	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	U	2752	
21	V	908	
22	W	579	
23	X	1041	
24	Y	492	
25	Z	225	
26	y	301	
27	a	240	
27	m	240	

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Mol	Chain	Length	Quality of chain
28	b	119	
28	n	119	
29	c	118	
29	h	118	
30	d	86	
30	i	86	
31	e	92	
31	j	92	
32	f	76	
32	k	76	
33	g	126	
33	l	126	
34	q	504	
34	r	504	
34	s	504	
34	t	504	
35	1	1304	
36	3	1217	
37	p	225	
38	w	501	
39	2	895	
40	4	424	
41	7	110	
42	5	86	
43	o	255	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 106396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1969	Total	C	N	O	S	0	0
			16331	10528	2863	2872	68		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2066	925	347	696	98		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	860	Total	C	N	O	S	0	0
			6724	4298	1122	1272	32		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 6 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	79	Total	C	N	O	P	0	0
			1587	708	248	552	79		

- Molecule 7 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	672	Total	C	N	O	0	0
			3387	2043	672	672		

- Molecule 9 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	561	Total	C	N	O	S	0	0
			3773	2350	709	708	6		

- Molecule 10 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	24	Total	C	N	O	S	0	0
			185	114	32	36	3		

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	387	Total	C	N	O	S	0	0
			2584	1596	494	489	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	114	Total	C	N	O	S	0	0
			971	605	181	183	2		

- Molecule 13 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total	C	N	O	0	0
			1447	862	292	293		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	101	Total	C	N	O	S	0	0
			876	537	175	162	2		

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1322	Total	C	N	O	0	0
			5288	2644	1322	1322		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	380	Total	C	N	O	P	S	0	0
			2915	1791	552	558	2	12		

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	158	Total	C	N	O	0	0
			770	454	158	158		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	462	Total	C	N	O	S	0	0
			2959	1842	537	567	13		

- Molecule 22 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	501	Total	C	N	O		0	0
			2473	1471	501	501			

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	786	Total	C	N	O	S	0	0
			6357	4010	1133	1184	30		

- Molecule 24 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	320	Total	C	N	O	S	0	0
			2556	1616	420	508	12		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	155	Total	C	N	O		0	0
			772	462	155	155			

- Molecule 26 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	79	Total	C	N	O		0	0
			316	158	79	79			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	86	Total	C	N	O		0	0
			344	172	86	86			
27	m	82	Total	C	N	O		0	0
			413	249	82	82			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	82	Total	C	N	O	0	0
			328	164	82	82		
28	n	80	Total	C	N	O	0	0
			402	242	80	80		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	97	Total	C	N	O	0	0
			388	194	97	97		
29	h	95	Total	C	N	O	0	0
			482	292	95	95		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	d	74	Total	C	N	O	0	0
			296	148	74	74		
30	i	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	79	Total	C	N	O	0	0
			316	158	79	79		
31	j	81	Total	C	N	O	0	0
			403	241	81	81		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	f	74	Total	C	N	O	0	0
			296	148	74	74		
32	k	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	g	81	Total	C	N	O	0	0
			324	162	81	81		
33	l	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	q	132	Total	C	N	O	0	0
			659	395	132	132		
34	r	131	Total	C	N	O	0	0
			654	392	131	131		
34	s	132	Total	C	N	O	0	0
			659	395	132	132		
34	t	131	Total	C	N	O	0	0
			654	392	131	131		

- Molecule 35 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	816	Total	C	N	O	S	0	0
			6486	4163	1119	1165	39		

- Molecule 36 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	167	Total	C	N	O	0	0
			841	507	167	167		

- Molecule 38 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	121	Total	C	N	O	S	0	0
			999	637	178	180	4		

- Molecule 39 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2	250	Total	C	N	O	S	0	0
			1803	1131	339	326	7		

- Molecule 40 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	151	Total	C	N	O		0	0
			743	441	151	151			

- Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	7	81	Total	C	N	O	S	0	0
			613	376	109	115	13		

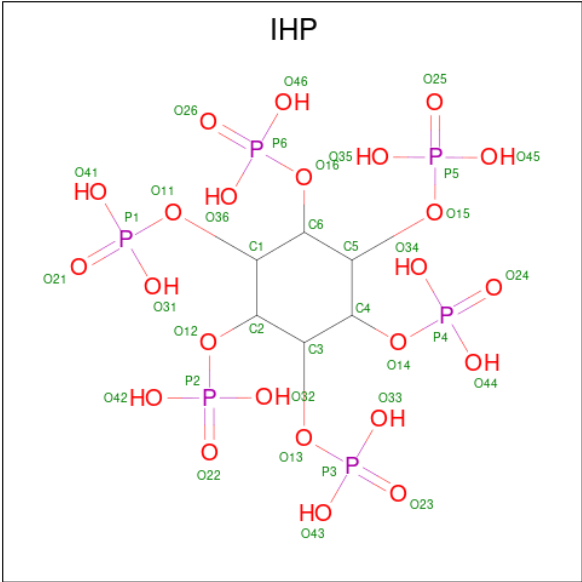
- Molecule 42 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5	77	Total	C	N	O	S	0	0
			635	403	110	117	5		

- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein A'.

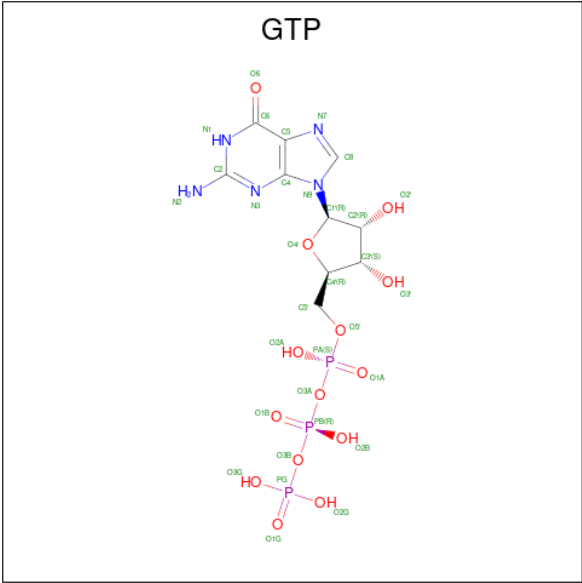
Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	162	Total	C	N	O		0	0
			816	492	162	162			

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
44	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	C	1	Total 1	Mg 1	0
46	F	6	Total 6	Mg 6	0

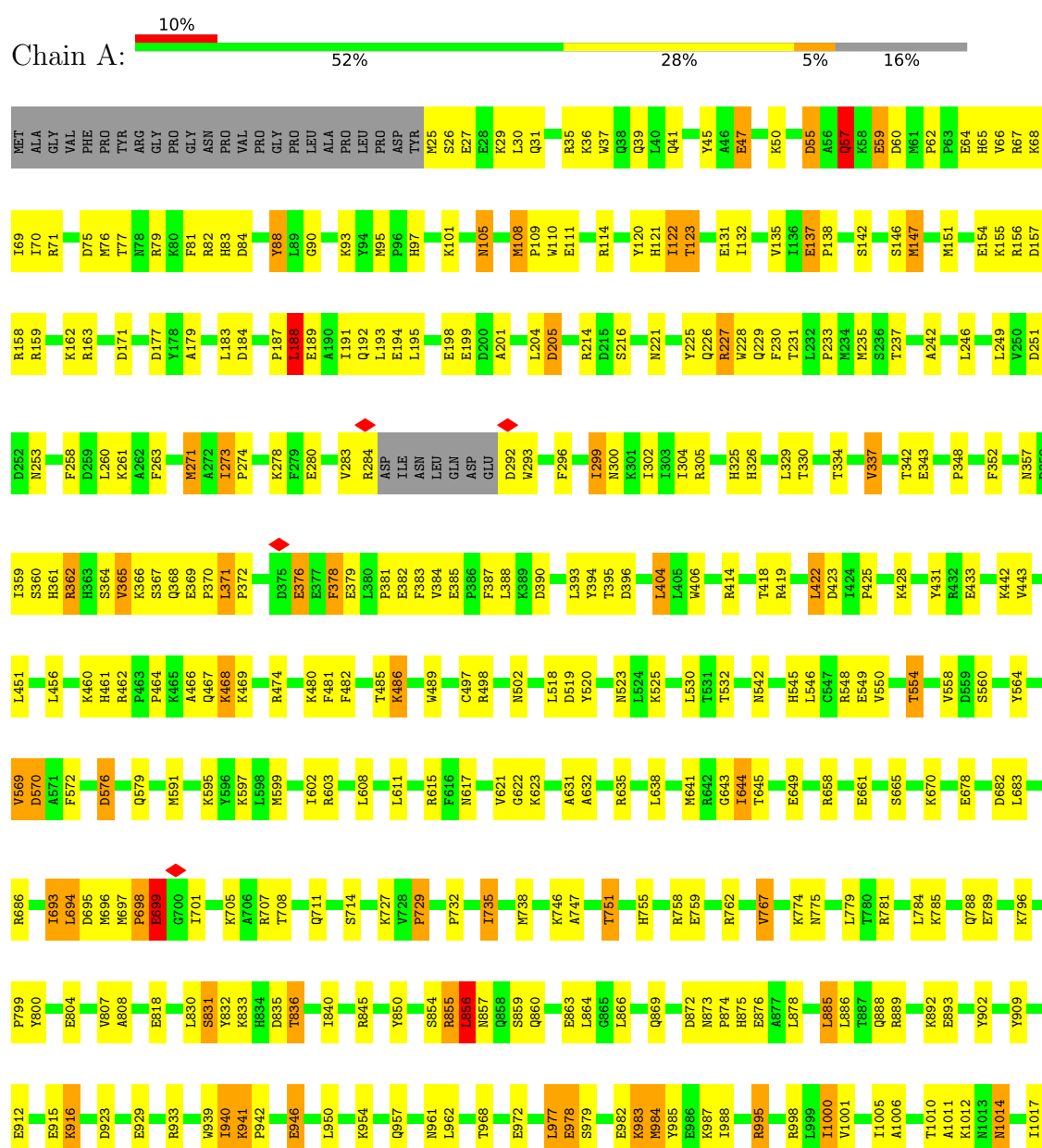
- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	K	1	Total 1	Zn 1	0
47	N	3	Total 3	Zn 3	0
47	7	3	Total 3	Zn 3	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Pre-mRNA-processing-splicing factor 8



VAL	LYS	HIS	D1990	Y1930	F1810	E1745	Y1659	T1568	K1463	Q1373	R1224	M143	Y1018
LEU	GLU	GLY	Y1991	T1931	M1811	R1746	Y1660	I1571	V1481	P1374	C1229	K1144	Y1019
LYS	GLU	ASP	G1992	A1932	P1812	K1749	W1661	S1572	E1482	F1229	F1229	M1147	K1020
PRO	PRO	ILE	K1993	F1933	R1813	S1755	D1663	L1573	E1489	E1377	S1251	V1147	D1021
LEU	LEU	ILE	N1994	S1934	G1815	S1756	I1664	R1578	F1490	E1378	G1252	M1148	N1023
GLY	TRP	THR	N1995	R1935	G1816	S1757	R1667	A1579	K1491	E1379	S1253	R1151	I1030
TRP	ILE	THR	N1996	L1936	L1817	P1758	D1670	H1580	G1492	T1254	G1254	A1152	G1033
HIS	THR	THR	V1997	I1937	L1818	T1759	V1671	W1582	T1493	S1382	T1255	R1160	Q1034
ASP	THR	THR	N1998	L1938	F1819	GLU	D1672	Q1583	W1498	V1385	I1268	R1163	Q1035
ARG	ASN	ASN	N1999	T1939	L1819	TVR	S1673	K1584	L1501	W1386	R1275	S1164	S1038
ALA	ALA	TYR	F1998	L1940	K1820	LEU	I1676	H1586	F1502	Y1389	E1276	V1165	Y1043
GLN	GLN	THR	N1999	L1941	I1821	SER	I1681	V1590	K1505	L1391	L1284	T1167	L1046
LEU	ALA	THR	L1999	I1942	I1822	Q1766	R1684	Q1599	ALA	E1390	N1293	V1168	V1047
GLN	GLN	THR	L2000	H1943	H1823	N1767	F1684	E1600	GLY	E1395	E1293	F1174	M1048
THR	THR	THR	T2003	V1945	T1824	Y1768	D1690	L1601	PHE	A1396	R1298	Q1169	L1050
GLY	GLY	THR	L2002	L1946	S1825	G1769	M1691	L1604	GLU	A1397	I1299	S1173	D1049
THR	THR	THR	S2005	N1947	V1826	Y1778	M1692	E1605	GLU	A1398	I1301	F1177	R1057
VAL	VAL	THR	E2006	D1948	W1827	E1770	S1693	E1606	SER	Q1399	K1300	V1177	E1060
PRO	VAL	THR	T2007	R1949	A1828	L1771	S1697	E1607	MET	Q1400	G1302	S1179	Q1075
ARG	PRO	ARG	R2008	R1950	G1829	F1772	T1698	T1608	LYS	L1403	L1303	D1181	D1076
THR	ASP	THR	D2009	K1951	Q1830	S1773	P1698	E1607	LYS	L1404	K1306	N1184	T1079
ASN	ASN	ARG	T2010	W1952	K1831	Q1774	T1699	E1607	LYS	L1405	F1311	L1185	R1090
ALA	ALA	ALA	L2011	L1953	R1832	Q1775	V1701	N1623	K1516	L1406	E1409	L1186	Y1091
ILE	ILE	THR	L2012	L1954	R1833	Q1776	I1702	S1625	K1517	L1407	M1327	C1190	I1092
LYS	LYS	SER	G2013	K1955	L1834	I1777	L1703	S1625	L1518	D1407	V1333	G1194	I1095
MET	ALA	ALA	M2014	P1956	Q1835	W1778	I1703	D1628	T1519	L1408	P1336	R1195	D1104
ALA	ASP	ASN	E2015	D1957	Q1836	F1778	D1706	E1628	N1520	E1409	Q1337	K1199	D1108
ASN	ASN	LEU	ILE	K1958	L1837	F1779	H1712	L1630	A1521	D1410	P1338	R1200	L1109
ARG	PRO	HIS	ALA	T1959	A1837	V1780	S1713	L1631	Q1522	L1328	S1329	R1201	T1202
LEU	LEU	ARG	ALA	K1898	K1838	D1781	A1714	F1632	R1523	W1412	V1333	G1194	S1203
THR	THR	THR	THR	V1960	W1839	D1782	T1715	A1633	S1524	R1414	P1336	R1195	D1104
ASN	ASN	ASN	GLN	I1961	E1900	T1783	G1716	S1634	G1525	G1415	Q1337	K1199	D1108
GLN	GLN	GLN	GLN	T1962	K1841	M1784	N1717	Y1635	L1526	I1416	P1338	R1201	L1109
GLN	GLN	GLN	GLN	E1963	A1942	V1785	W1718	K1636	N1527	P1417	S1338	R1201	T1202
GLN	GLN	GLN	GLN	P1964	E1943	Y1786	F1719	N1638	I1529	I1419	W1342	S1203	R1112
GLN	GLN	GLN	GLN	H1965	E1844	R1787	P1720	V1639	R1532	R1427	T1346	E1206	H1117
GLN	GLN	GLN	GLN	H1966	V1845	V1788	K1723	S1640	R1544	W1436	D1347	F1207	N1121
GLN	GLN	GLN	GLN	I1967	A1846	T1789	P1724	R1641	R1544	W1437	V1348	T1208	N1122
GLN	GLN	GLN	GLN	W1968	A1847	T1789	L1725	S1643	V1549	V1438	G1349	H1209	E1123
GLN	GLN	GLN	GLN	P1969	L1848	I1790	L1726	S1644	Q1552	R1439	T1351	K1210	G1127
GLN	GLN	GLN	GLN	T1970	I1849	H1791	I1726	L1644	V1553	T1440	H1352	G1212	W1213
GLN	GLN	GLN	GLN	L1971	R1850	K1792	W1730	S1648	Q1553	W1454	H1359	W1214	N1130
GLN	GLN	GLN	GLN	E1911	S1851	T1793	M1734	K1649	Q1554	W1559	E1360	E1361	K1131
GLN	GLN	GLN	GLN	P1912	L1852	F1794	M1737	D1650	L1555	T1568	H1362	L1216	W1134
GLN	GLN	GLN	GLN	Q1913	P1853	E1795	N1737	W1682	M1682	H1457	E1361	Q1217	R1139
GLN	GLN	GLN	GLN	M1914	V1854	G1796	P1738	T1655	I1589	Q1458	D1362	Q1217	M1140
GLN	GLN	GLN	GLN	V1915	V1855	N1797	A1739	T1656	I1560	R1459	D1362	Q1217	R1139
GLN	GLN	GLN	GLN	L1916	E1856	L1798	Y1741	T1657	F1561	H1460	Q1363	Q1217	M1140
GLN	GLN	GLN	GLN	F1917	E1857	T1799	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	N1918	Q1857	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	M1918	P1858	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	N1919	K1859	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	Y1920	K1860	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	D1921	I1861	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	L1922	I1862	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	W1923	V1863	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	L1924	T1864	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	K1925	R1865	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	T1926	K1866	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	T1927	G1867	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	S1928	M1868	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223
GLN	GLN	GLN	GLN	S1929	L1869	T1800	Y1741	T1657	F1561	D1461	L1368	K1222	E1223

[illegible]

- Molecule 2: U5 snRNA



G	C84	C85	C86	A87	A88	U89	U90	U91	U92	U93	U94	G95	A96	G97	G98	C99	C100	U101	U102	G103	C104	U105	U106	U107	G108	G109	C110	A111	A112	C115	U116	A117																												
A	U	C	C	U	U	U	U	C	C	A	U	G8	G9	U10	C13	U14	C15	U16	U17	C18	A19	G20	A21	U22	C23	G24	C25	A26	U27	A28	C39	U40	U41	U42	U43	A44	C45	U46	A47	A48	U52	U53	G57	U58	G59	A63	G64	G65	A66	A67	C68	A69	A70	C71	U	C	U	U	G	A

- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component



MET	ASP	THR	ASP	LEU	TYR	ASP	GLU	PHE	GLY	ASN	TYR	ILE	GLY	PRO	LEU	GLU	ASP	SER	ASP	GLU	ASP	ASP	ASP	ASP	GLU	GLY	LEU	ARG	GLU	THR	LYS	ASP	LEU	GLU	GLU	MET	ASP	ASP	ASP	ASP	ASP	VAL	GLY	ASP	HIS	ASP	ASP	HIS	PRO	GLY	MET	E56	V57	V58	L59	N60
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E61	D62	K63	K64	Y65		T68		E78	T79	I80	V81	Q82	E83	E84	D85	T86	Q87	P88	L89	T90		I93	T94	K95	P96		T99	LVS	LVS	PHE	THR	LEU	MET	GLU	GLN	THR	LEU	PRO	PRO	VAL	T112	V113	Y114	E115	D116	M117	F118	L119	A120	D121	L122	M123		S126		I129	R130	N131	V132	T133
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[illegible]

■ D213
 ■ T216
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 ■ A232
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 ■ P297

S298	S299	S300	S301	S302	S303	S304	S305	S306	S307	S308	S309	S310	S311	S312	Q313	S316	S320	S321	S322	S325	S326	S327	S328	S329	S330	S331	S332	S333	S334	S335	S336	S337	S338	S339	S340	S341	S342	S343	S344	S347	S348	S349	S350	S351	S352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000
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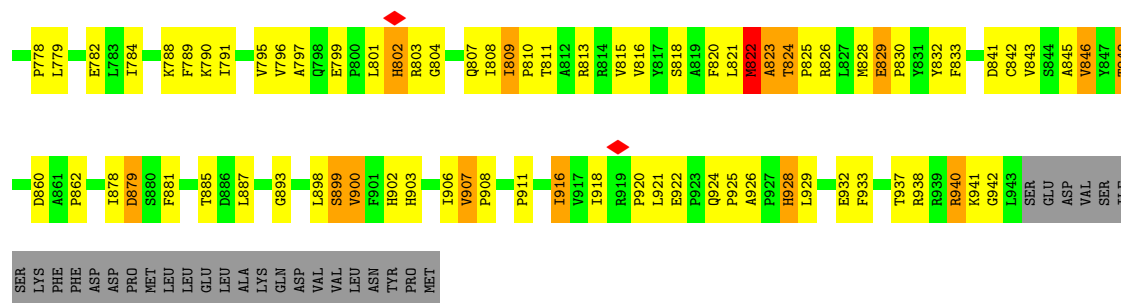
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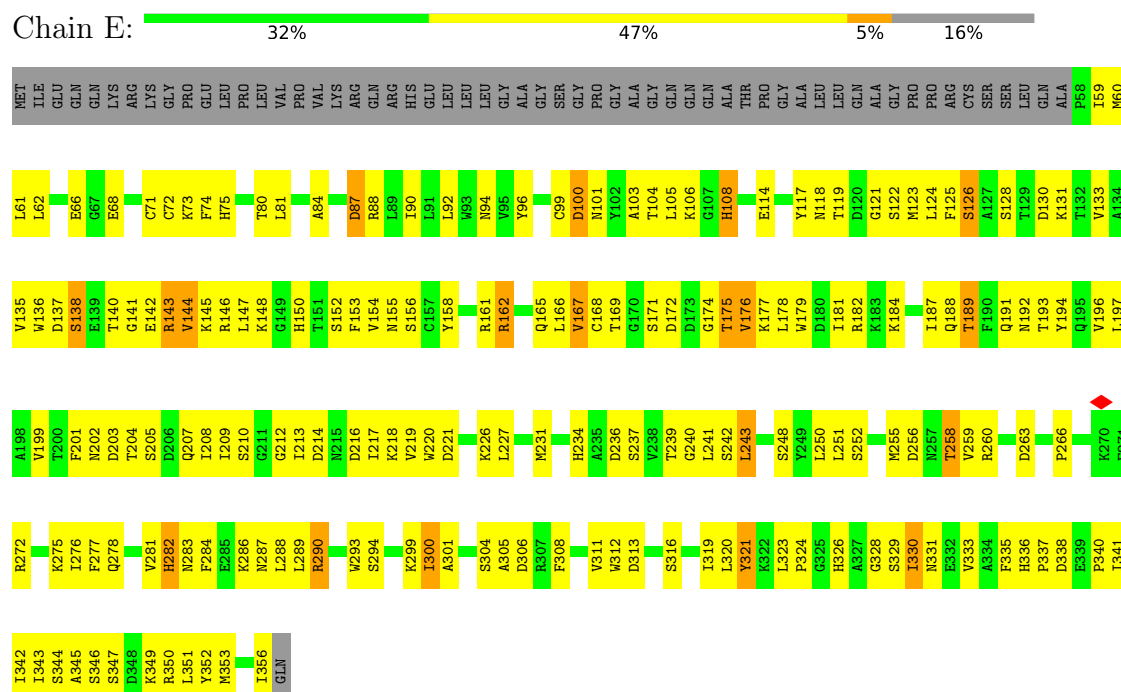
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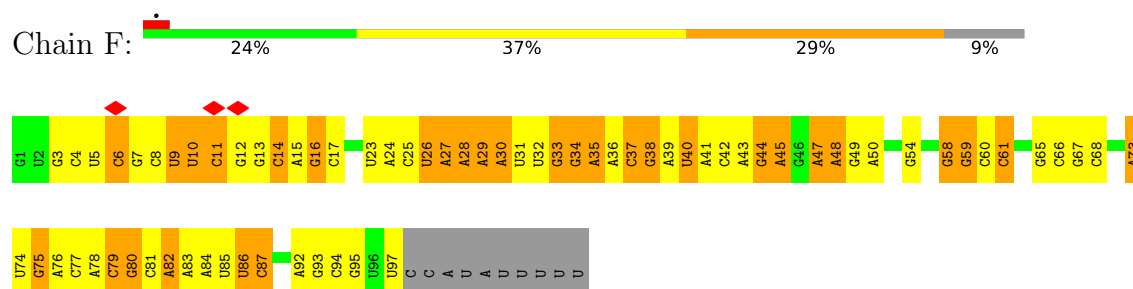
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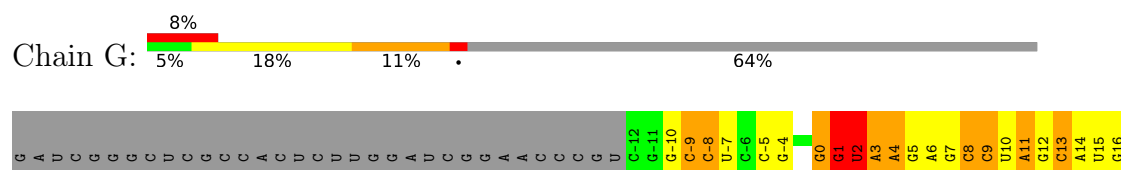
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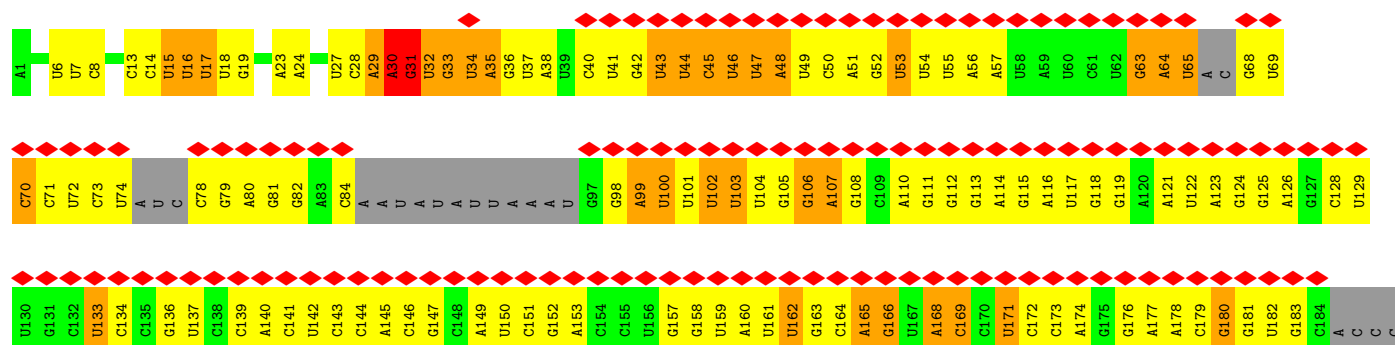
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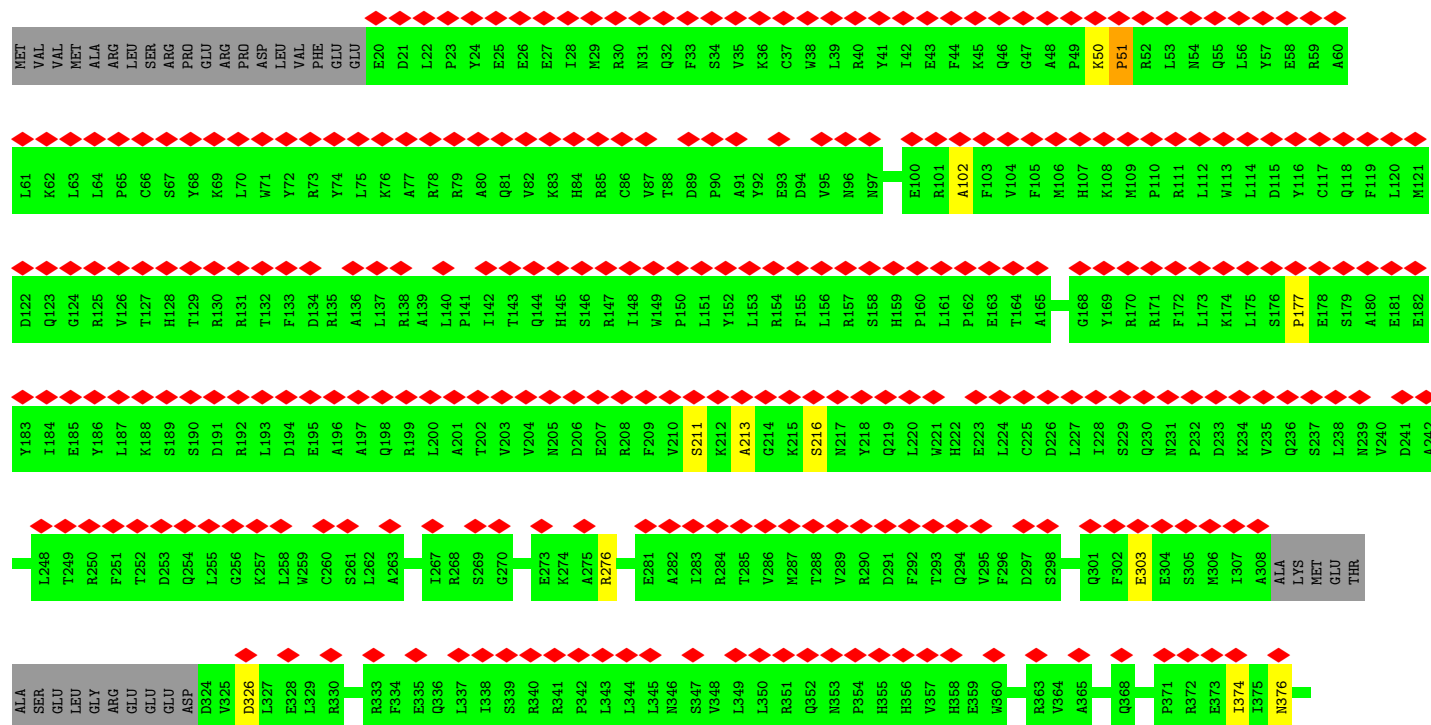
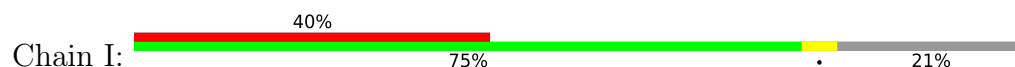
● Molecule 6: Pre-mRNA

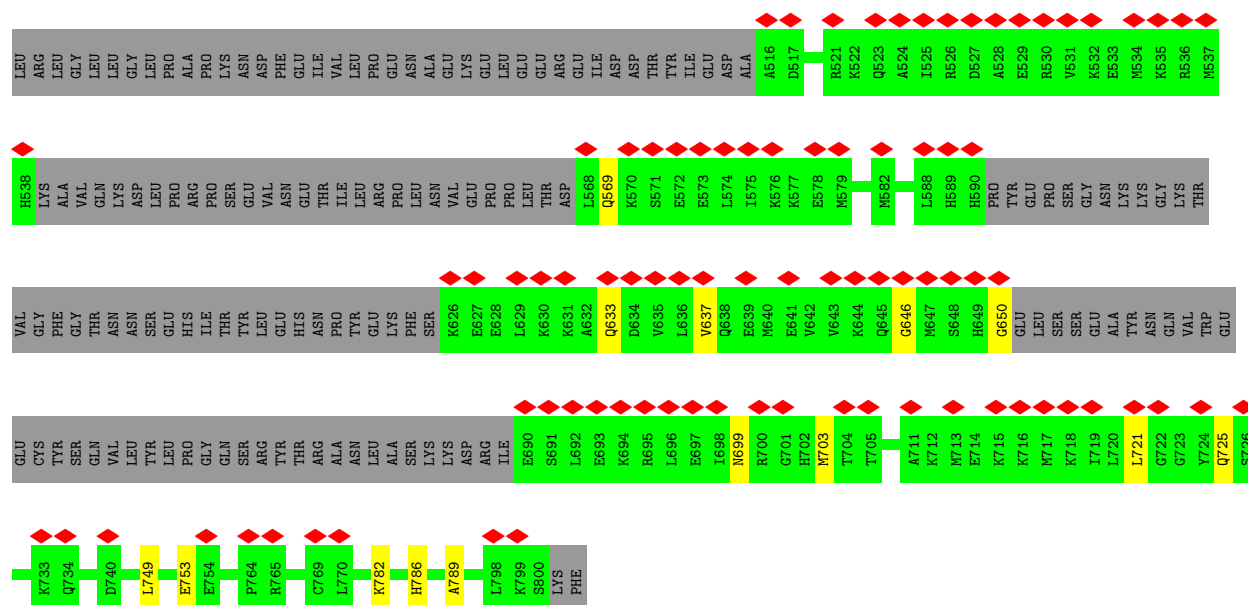


- Molecule 7: U2 snRNA

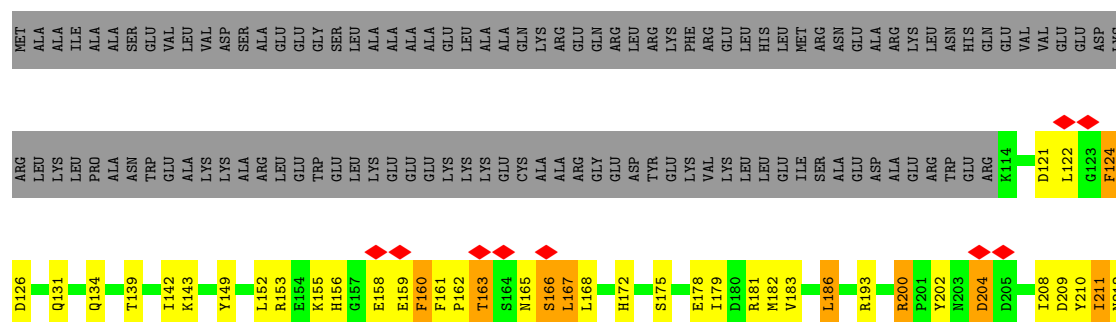


- Molecule 8: Pre-mRNA-splicing factor SYF1

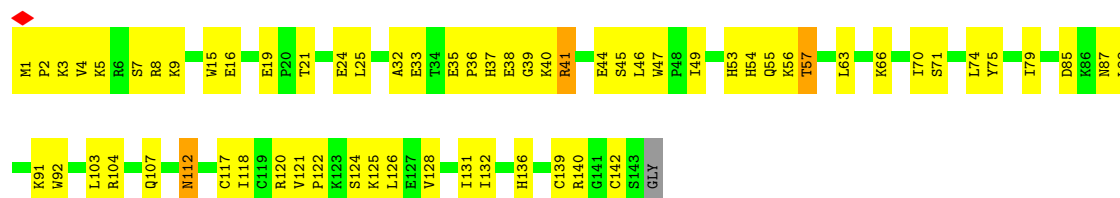




• Molecule 12: Pre-mRNA-splicing factor SYF2

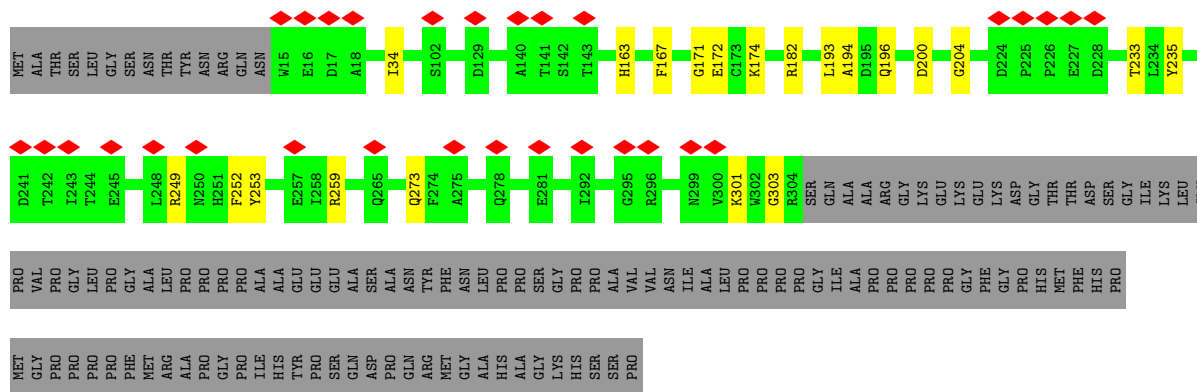


• Molecule 13: Protein BUD31 homolog

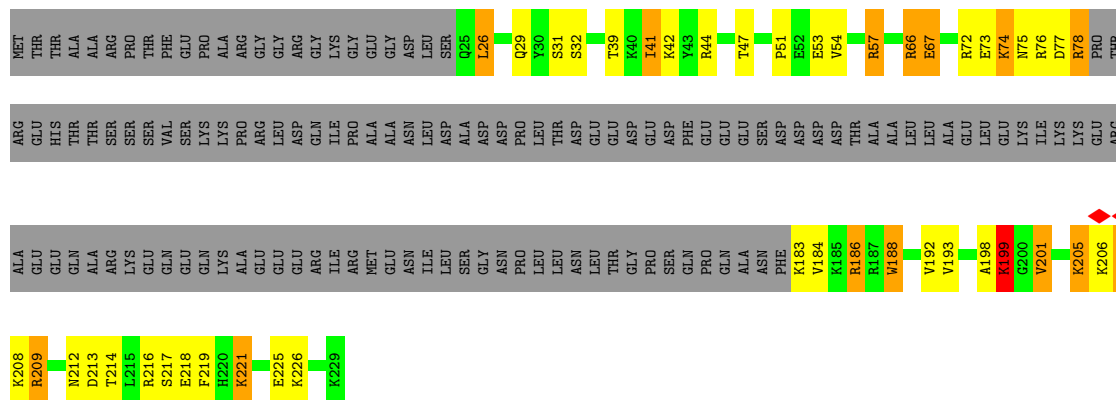
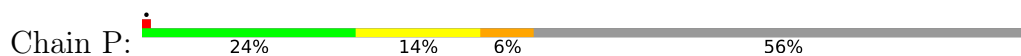


• Molecule 14: Pre-mRNA-splicing factor RBM22

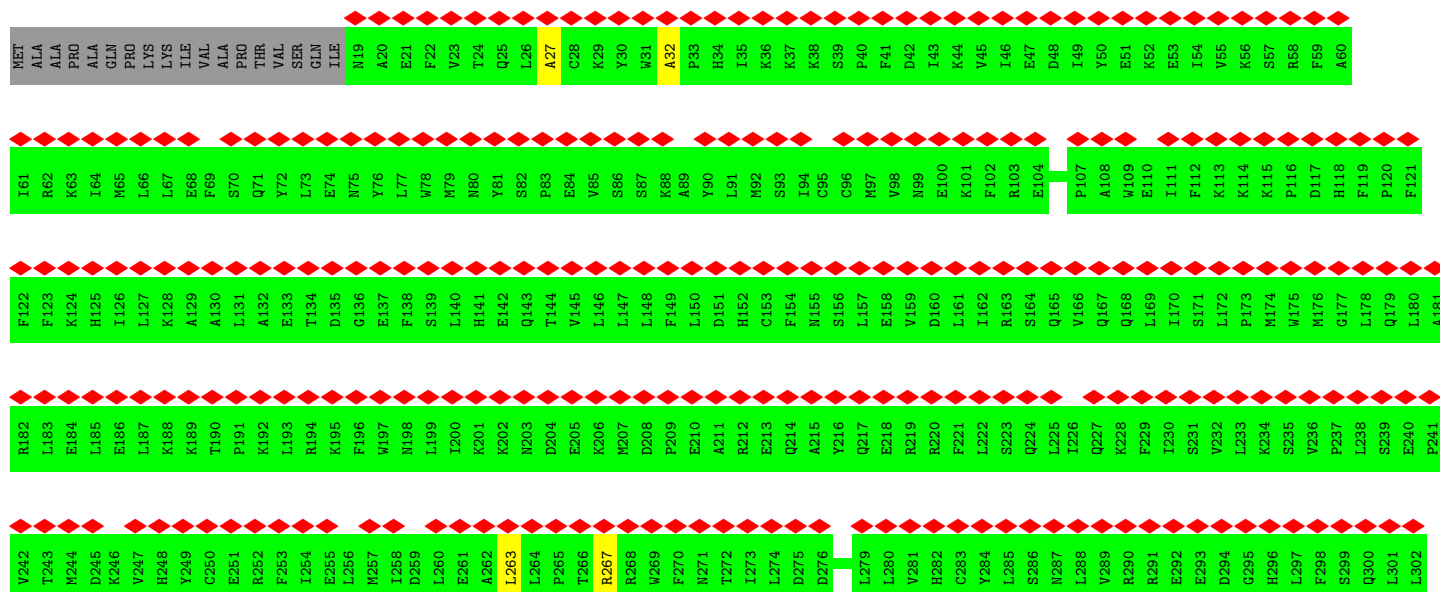
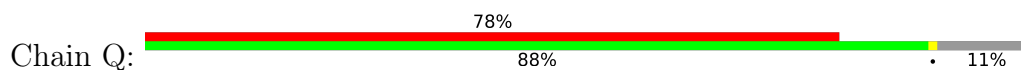




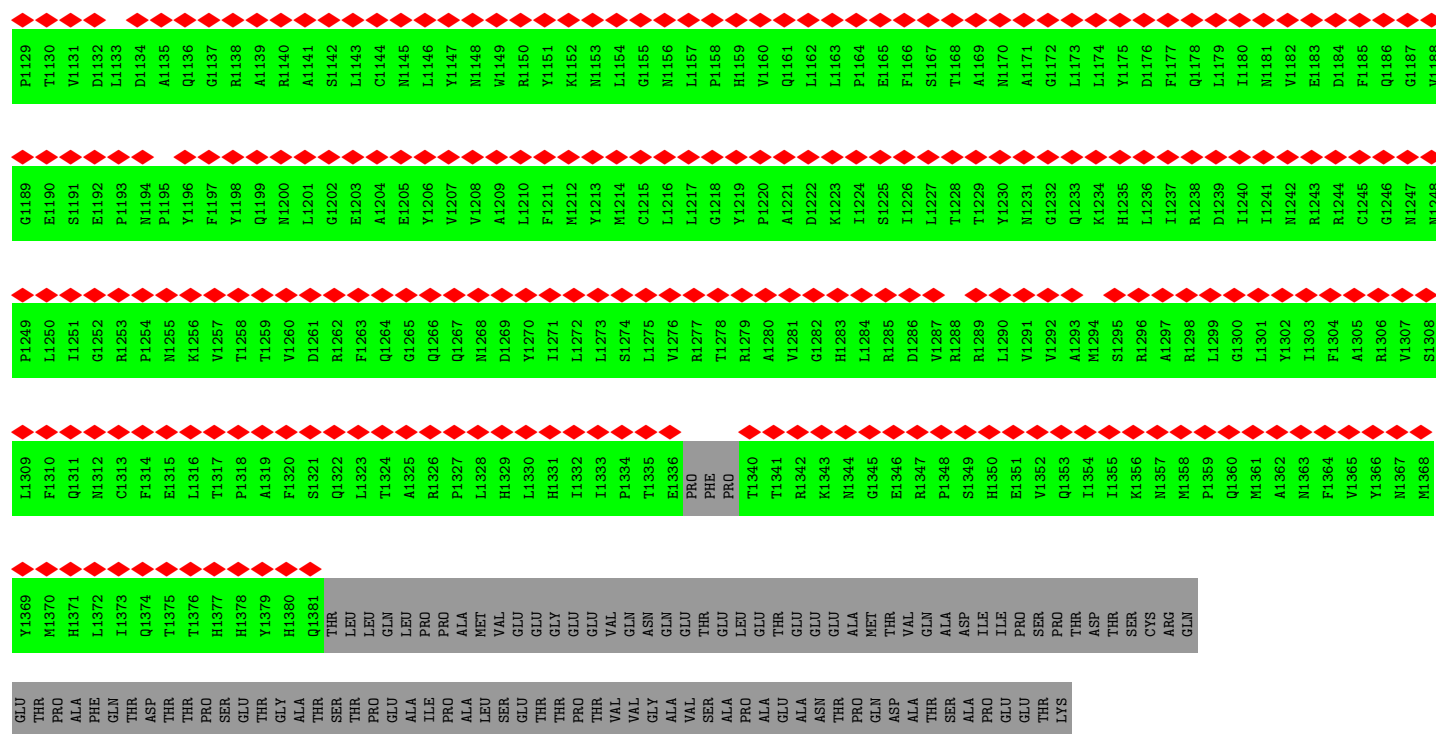
• Molecule 15: Spliceosome-associated protein CWC15 homolog



• Molecule 16: RNA helicase aquarius



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W753	ARG	SER	GLY	LYS	GLY	LYS	ARG	LYS	ASP	ALA	VAL	GLU	ASP	GLU	THR	GLU	E773	A774	K775	L776	L777	L778	W779	E780	S838	H782	W783	L784	P785	N786	R787	G788	P789	Y790	F791	Y792	N793	Q794	P795	K796	R797	W798	T799	I800	Q801	F802	T803	H804	T805	Q806	L807	E808	A809	I810	R811	A812		
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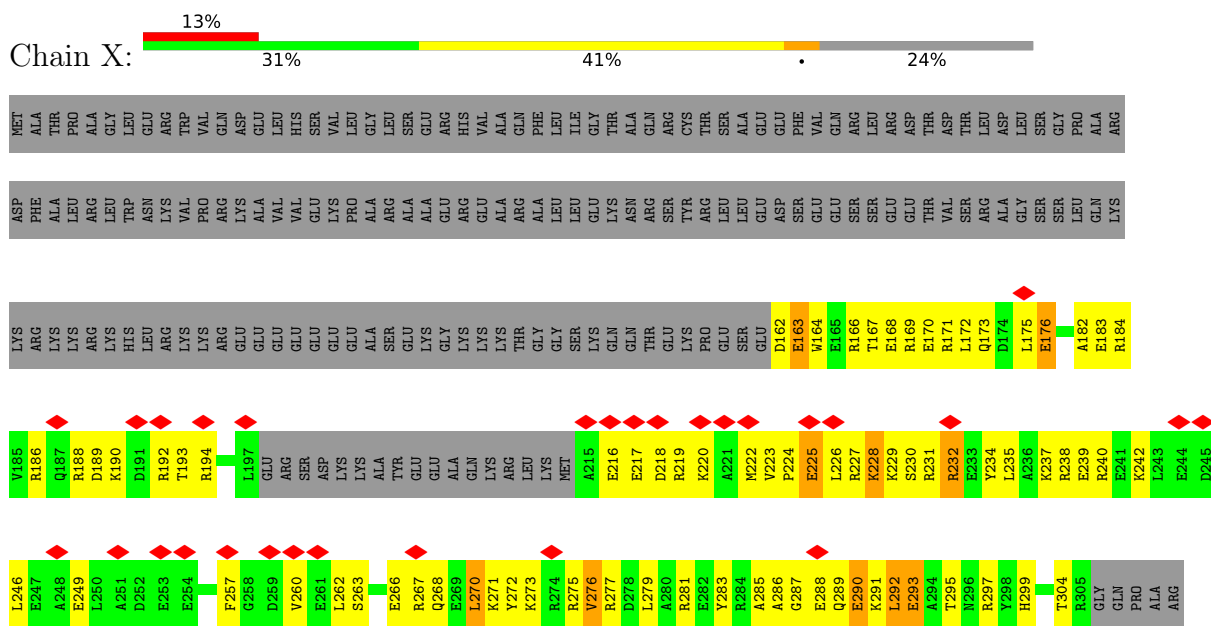
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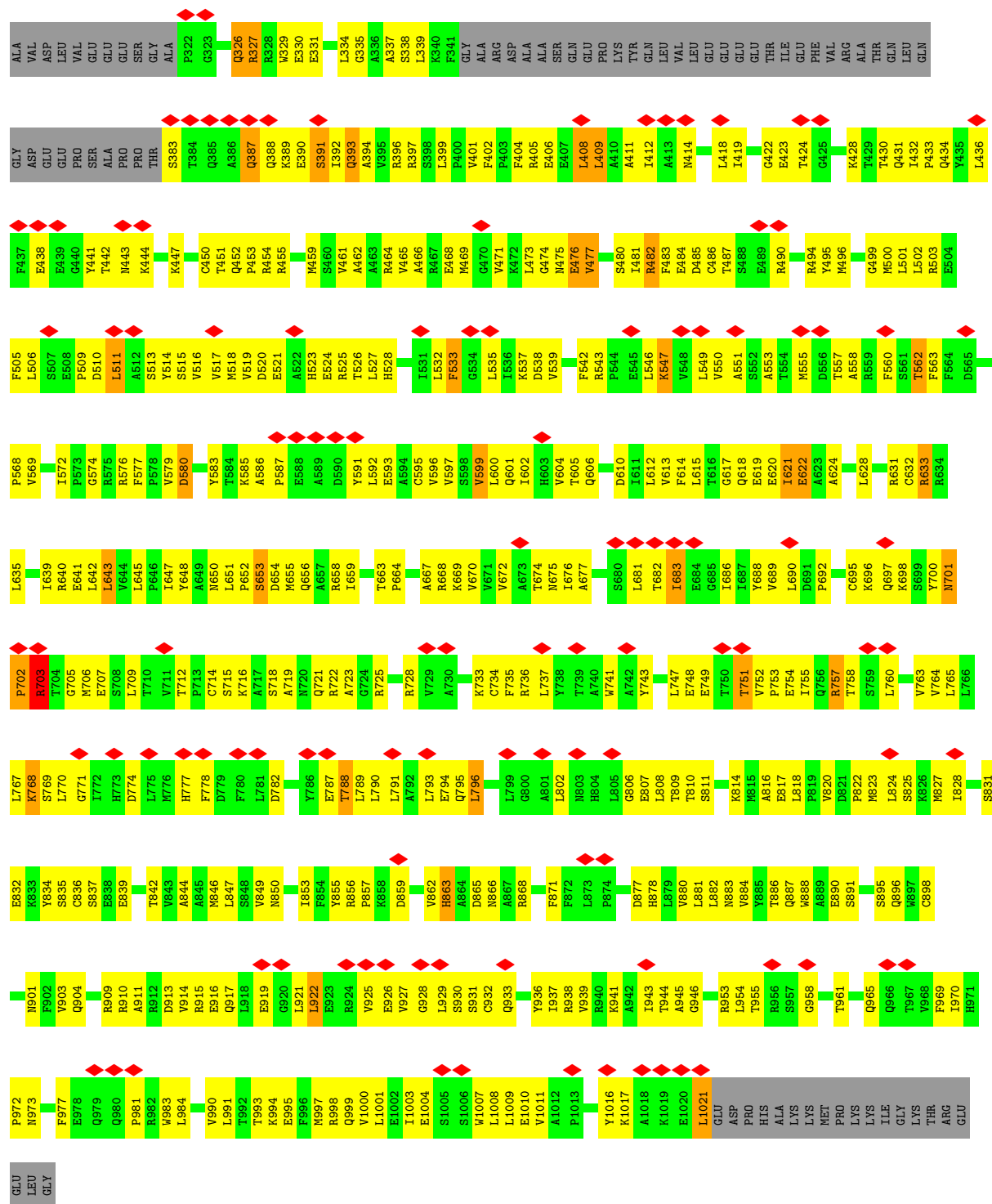




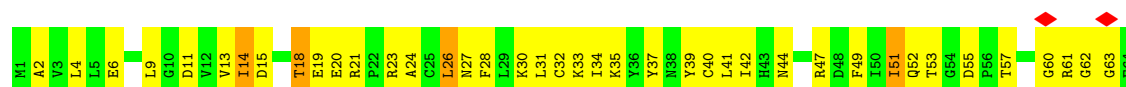
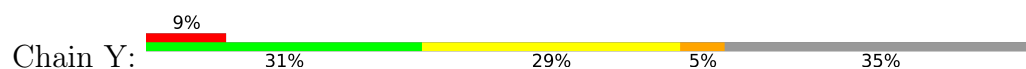
- Molecule 21: Pre-mRNA-splicing factor CWC22 homolog

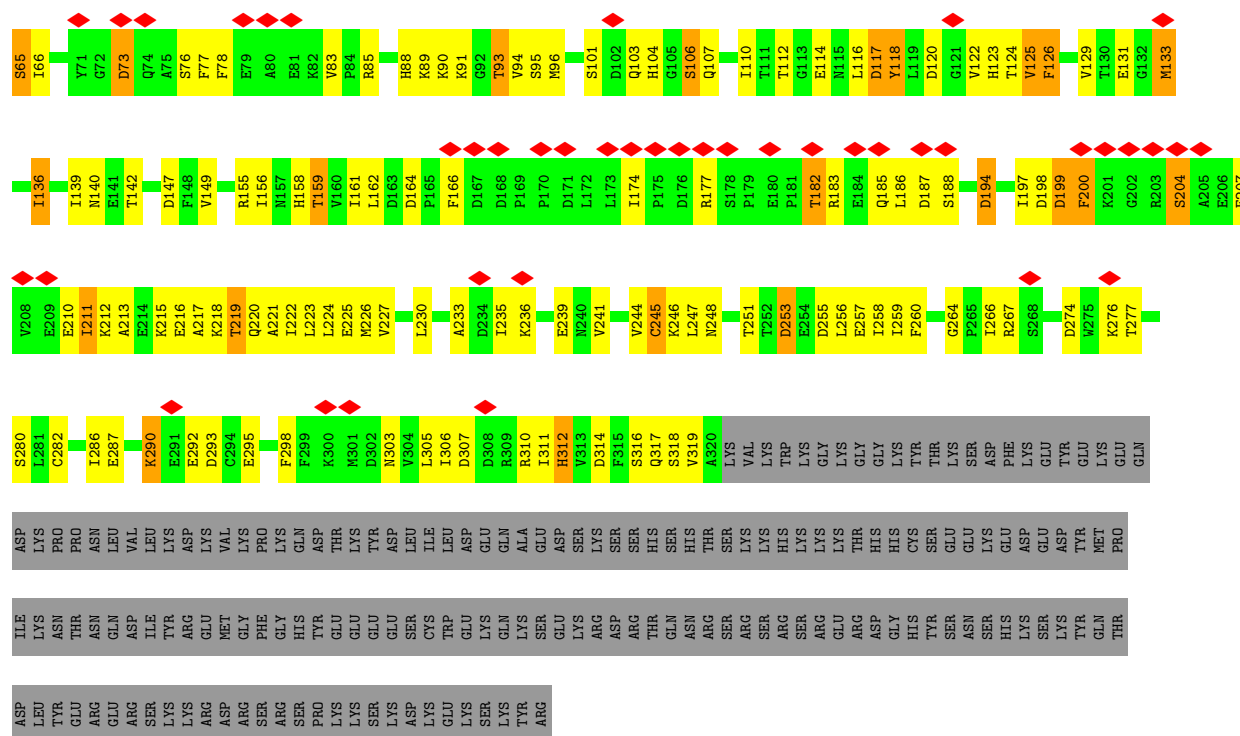




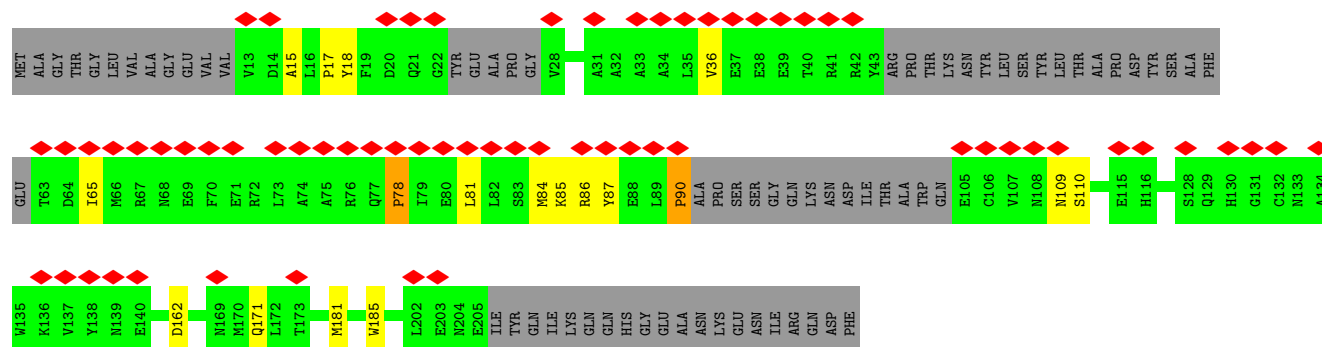


● Molecule 24: Peptidyl-prolyl cis-trans isomerase-like 4

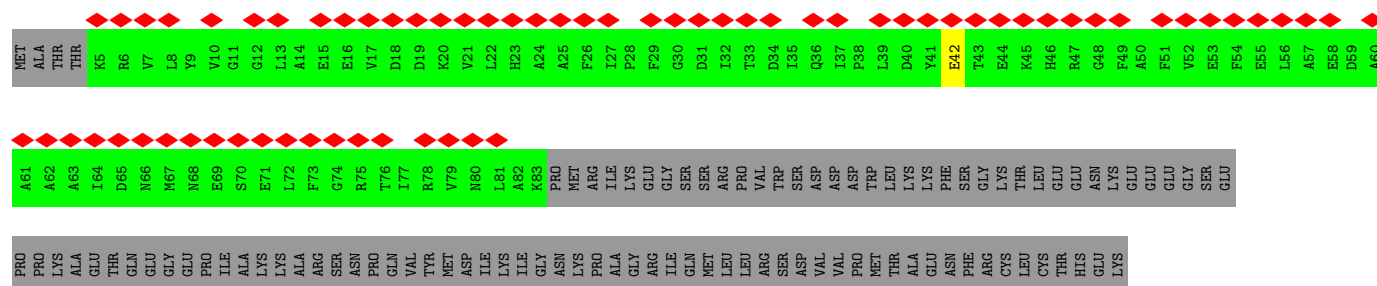


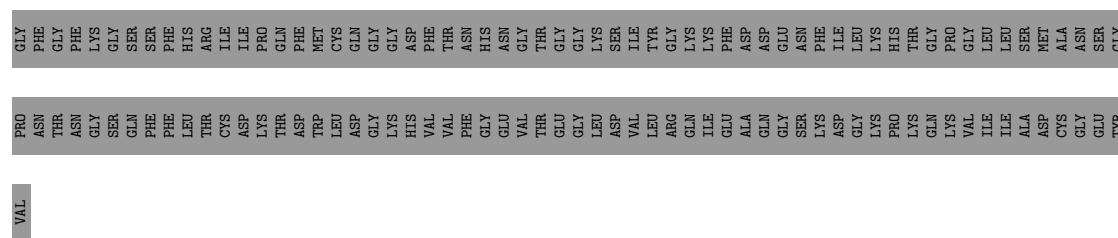


• Molecule 25: Pre-mRNA-splicing factor SPF27

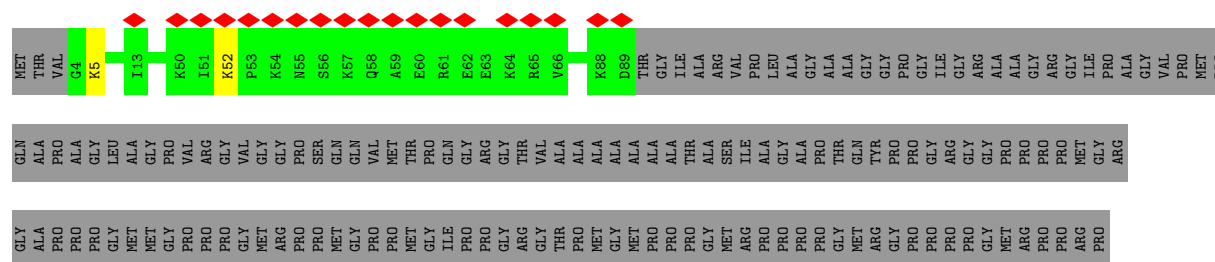


• Molecule 26: Peptidyl-prolyl cis-trans isomerase E

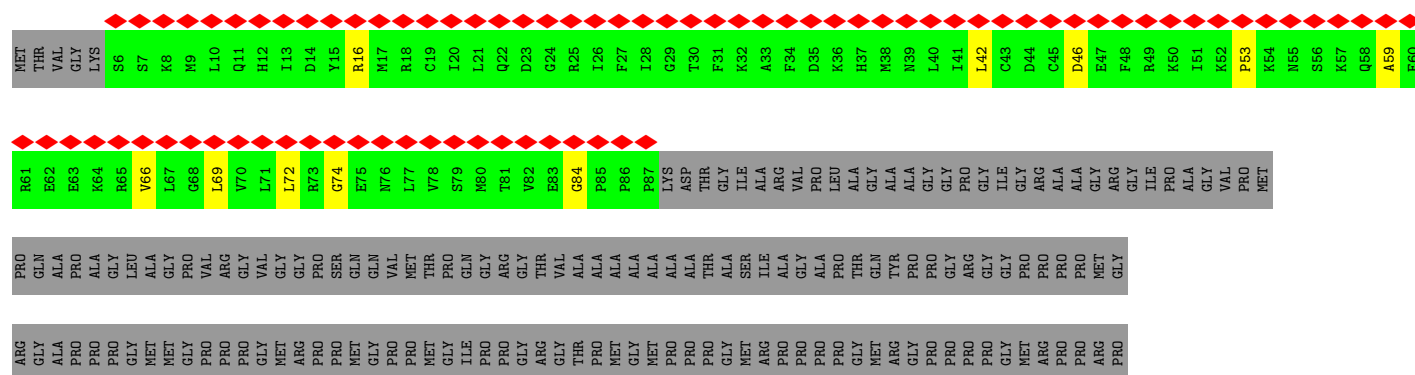




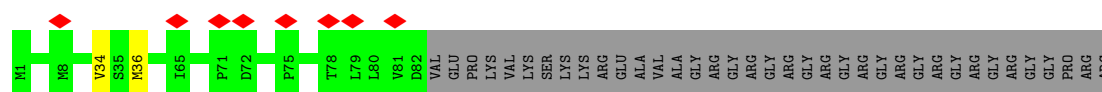
• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'



• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'

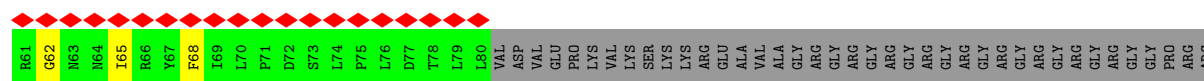


• Molecule 28: Small nuclear ribonucleoprotein Sm D1

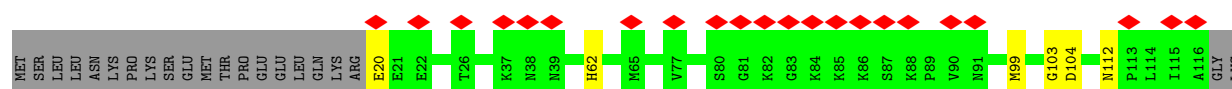


• Molecule 28: Small nuclear ribonucleoprotein Sm D1

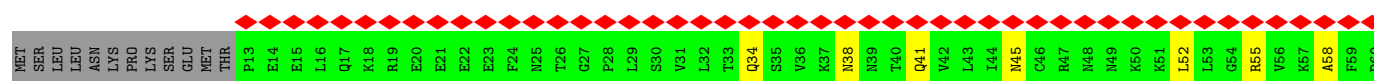
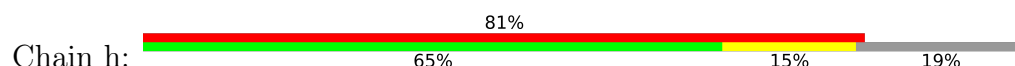




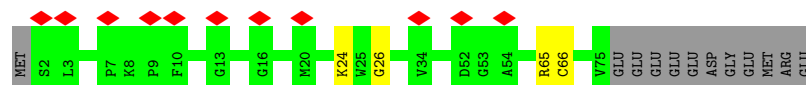
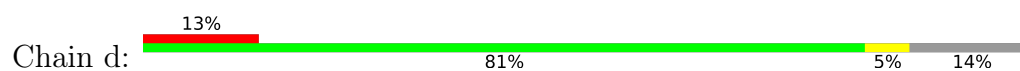
• Molecule 29: Small nuclear ribonucleoprotein Sm D2



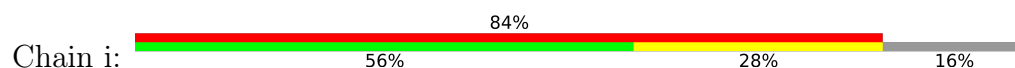
• Molecule 29: Small nuclear ribonucleoprotein Sm D2



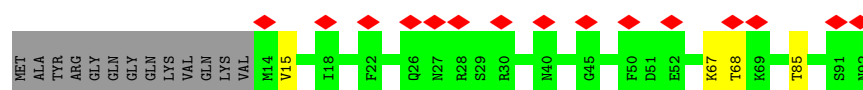
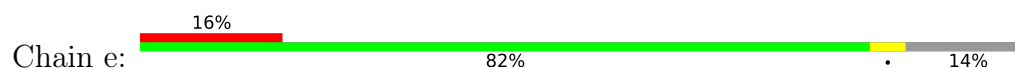
• Molecule 30: Small nuclear ribonucleoprotein F



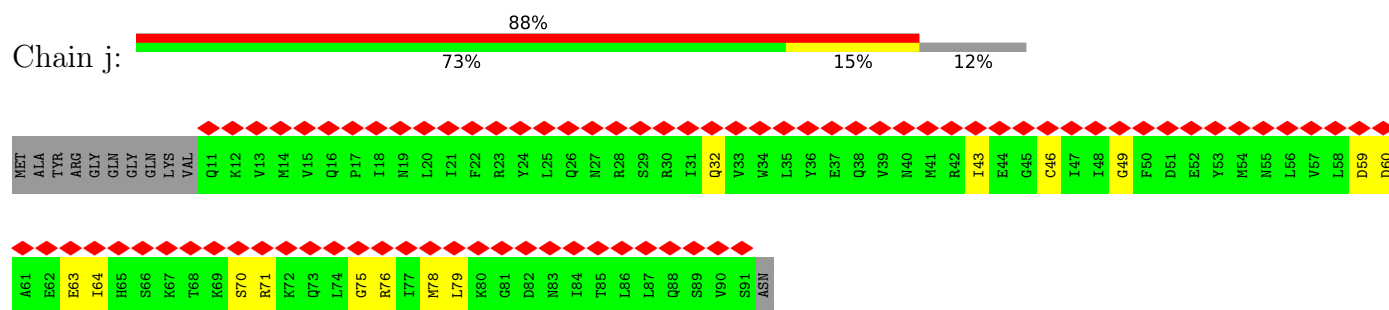
• Molecule 30: Small nuclear ribonucleoprotein F



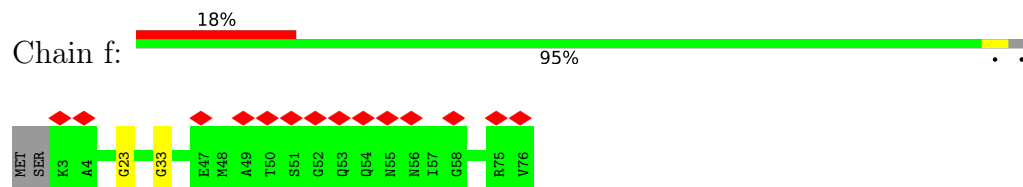
• Molecule 31: Small nuclear ribonucleoprotein E



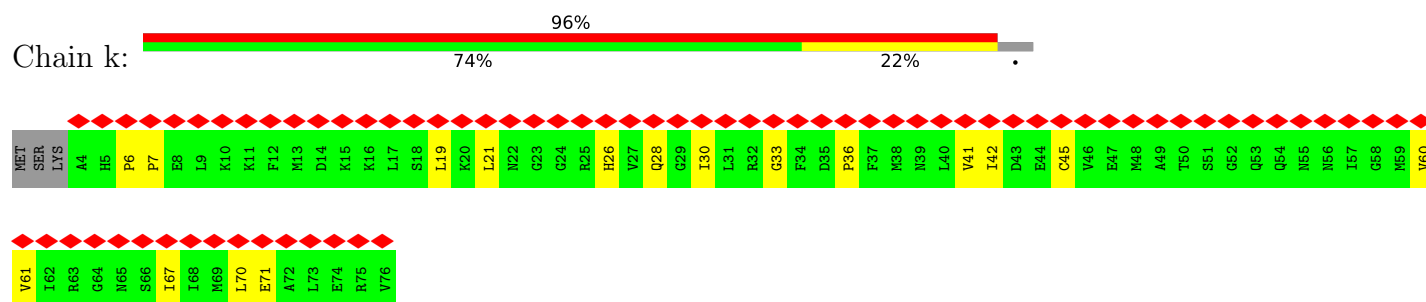
• Molecule 31: Small nuclear ribonucleoprotein E



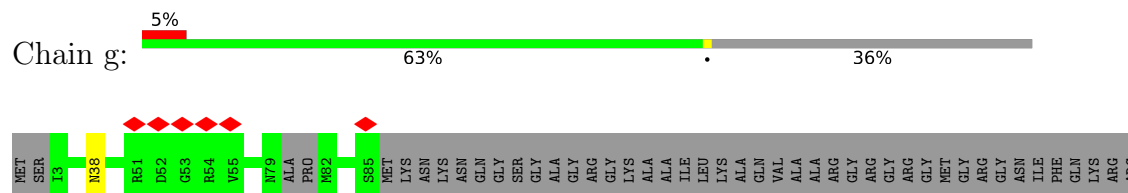
- Molecule 32: Small nuclear ribonucleoprotein G



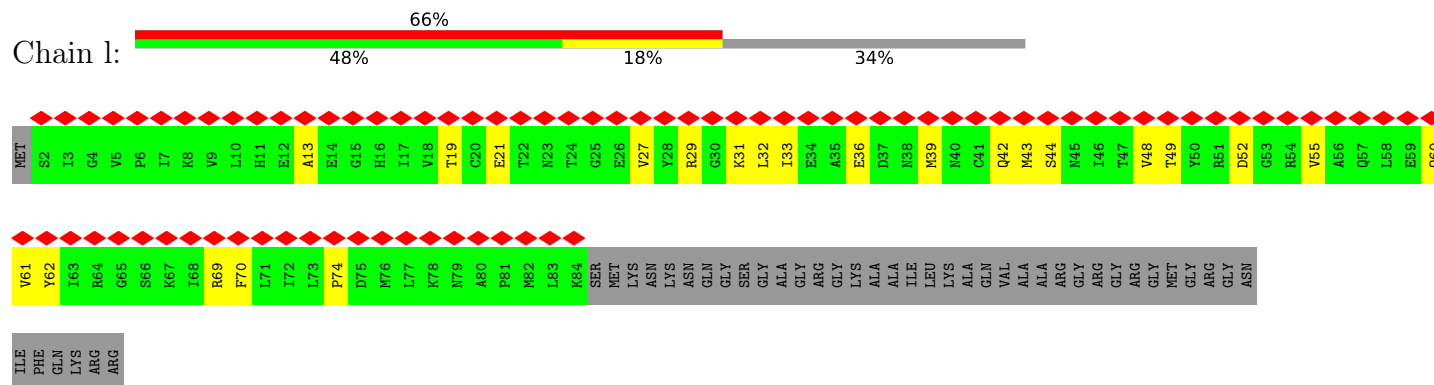
- Molecule 32: Small nuclear ribonucleoprotein G



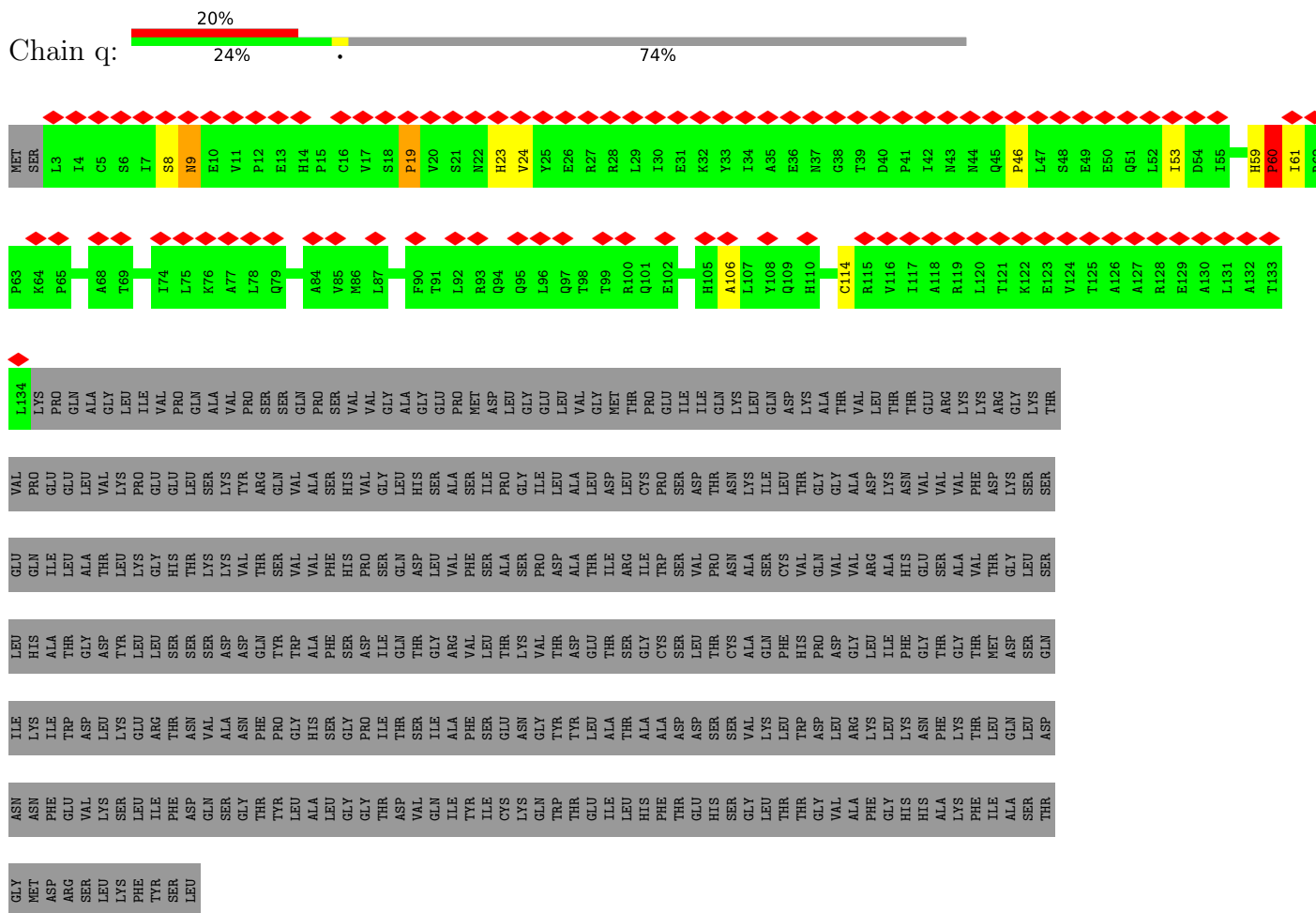
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



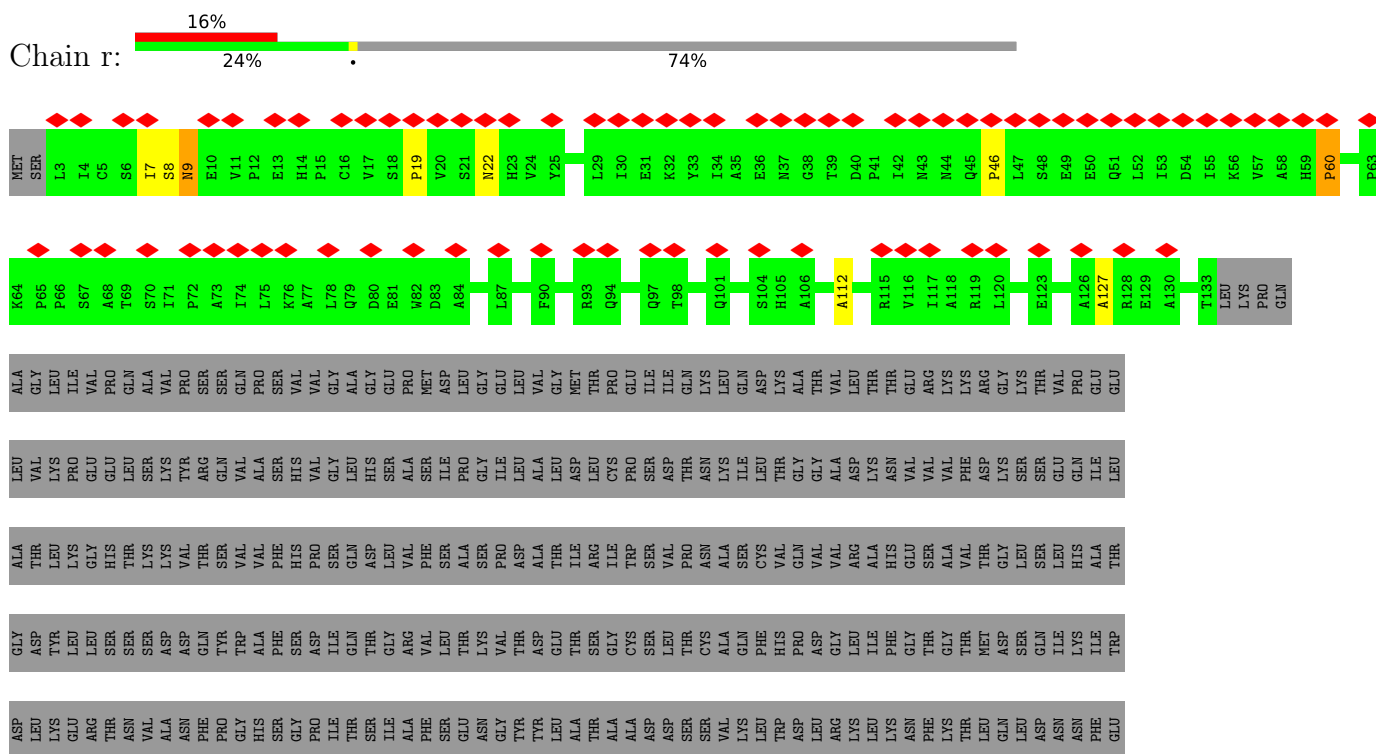
- Molecule 33: Small nuclear ribonucleoprotein Sm D3

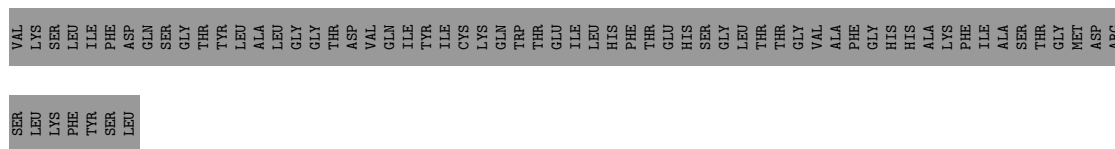


- Molecule 34: Pre-mRNA-processing factor 19

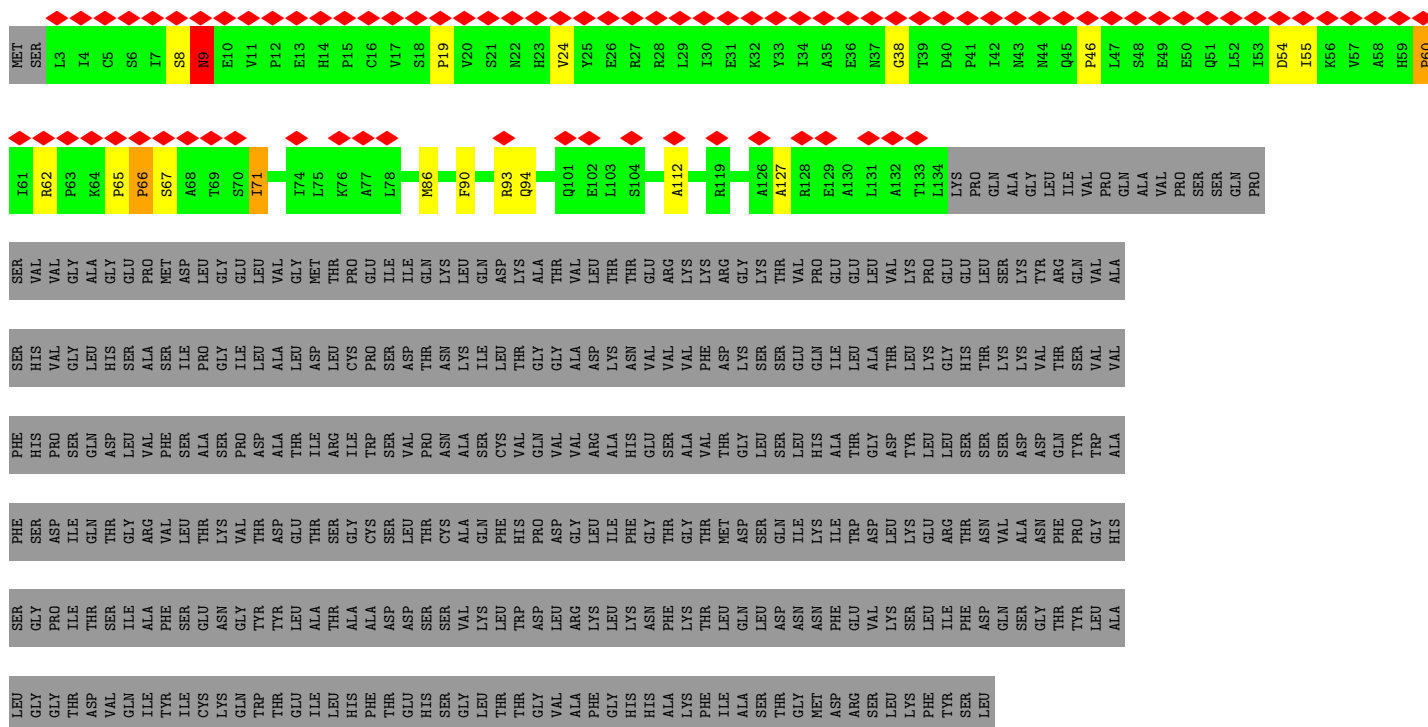


- Molecule 34: Pre-mRNA-processing factor 19

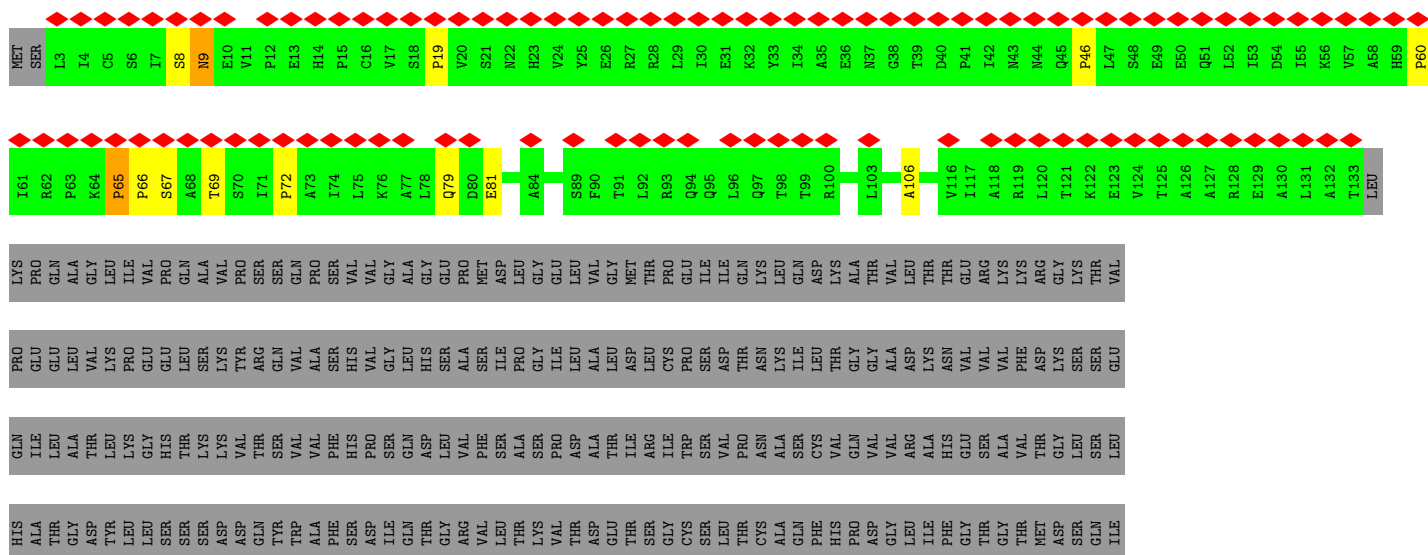




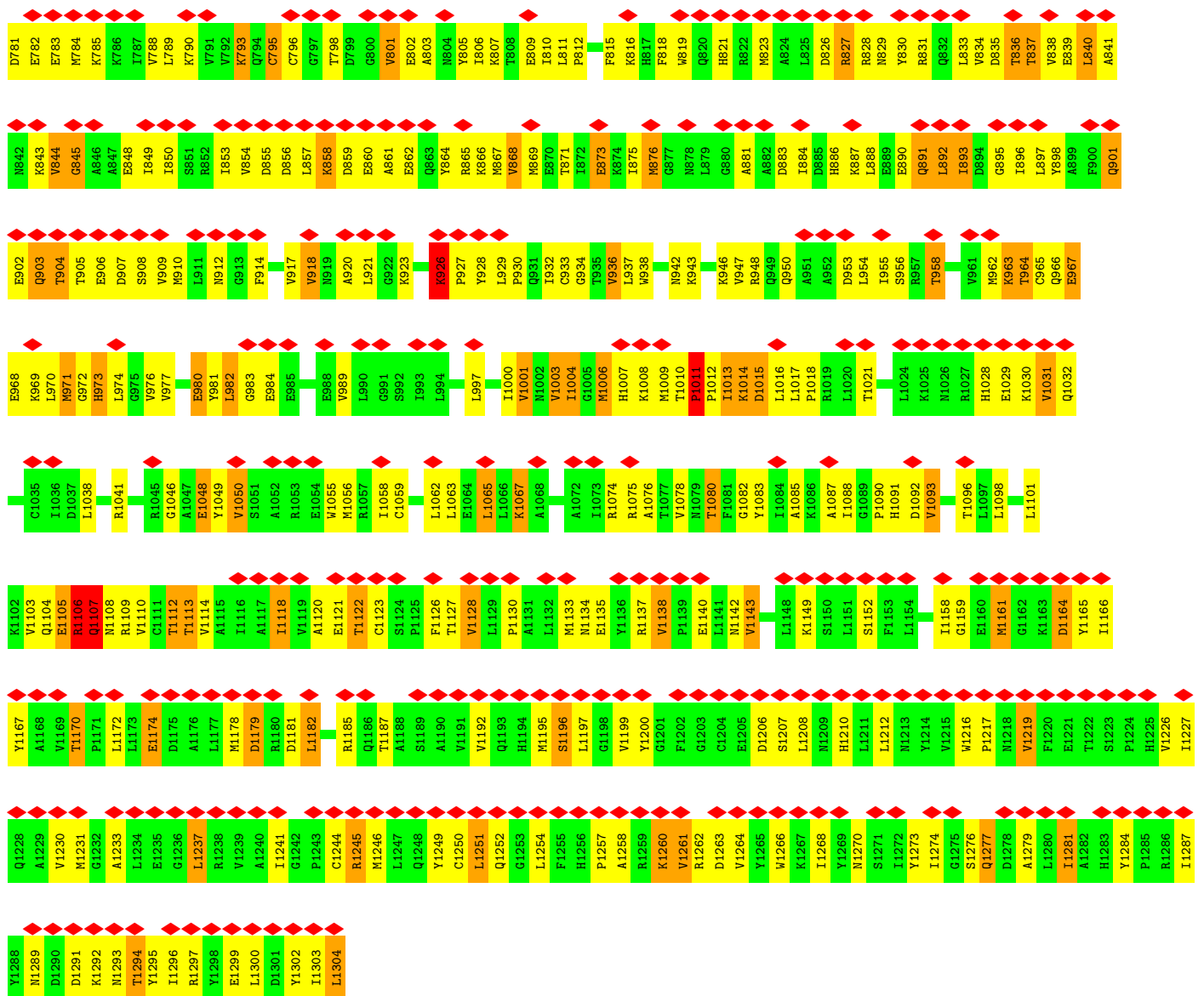
- Molecule 34: Pre-mRNA-processing factor 19



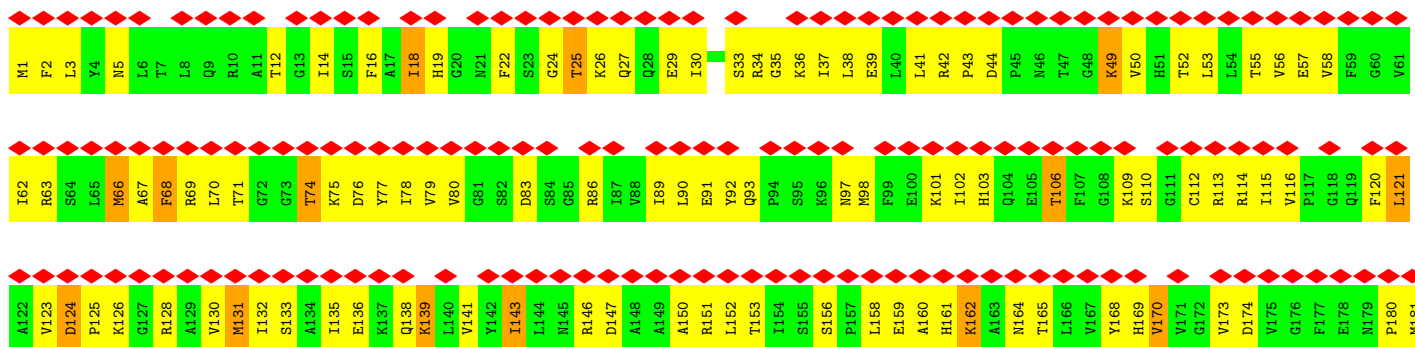
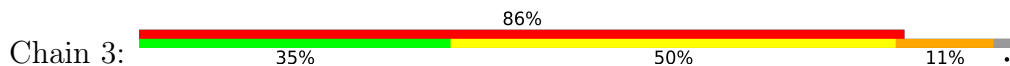
- Molecule 34: Pre-mRNA-processing factor 19



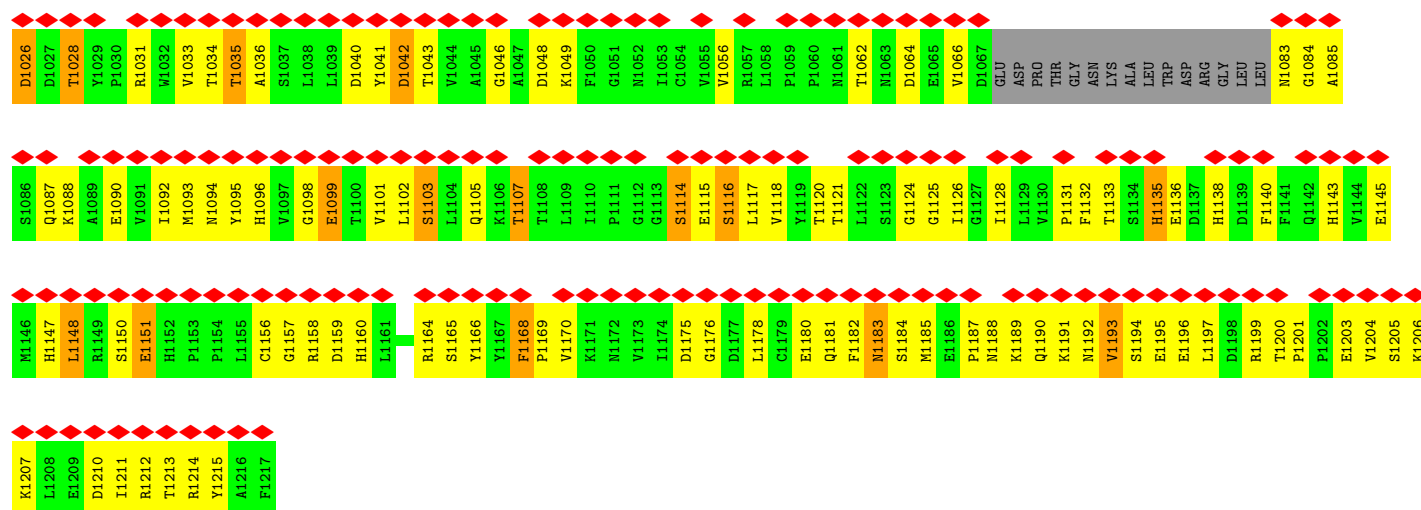




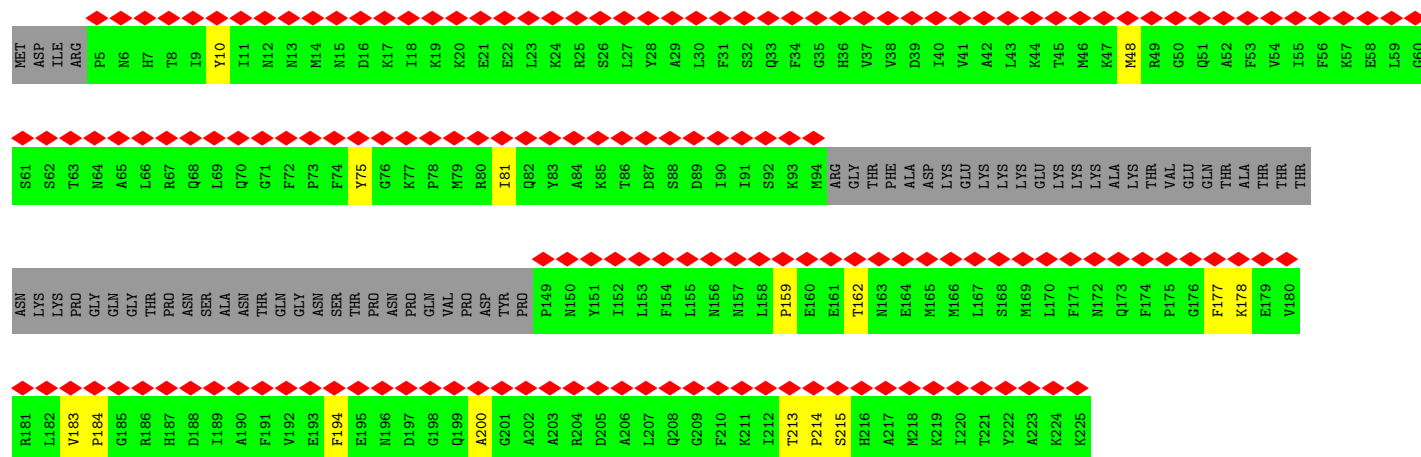
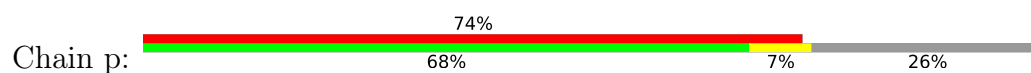
• Molecule 36: Splicing factor 3B subunit 3



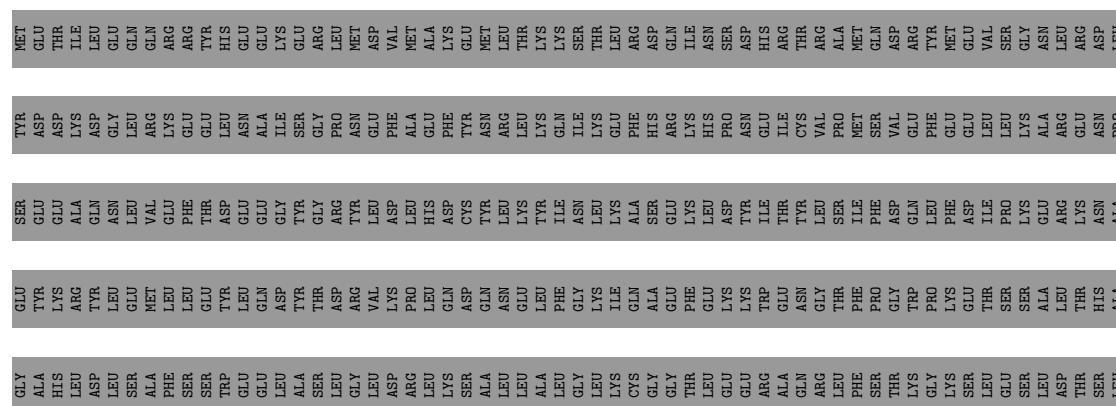


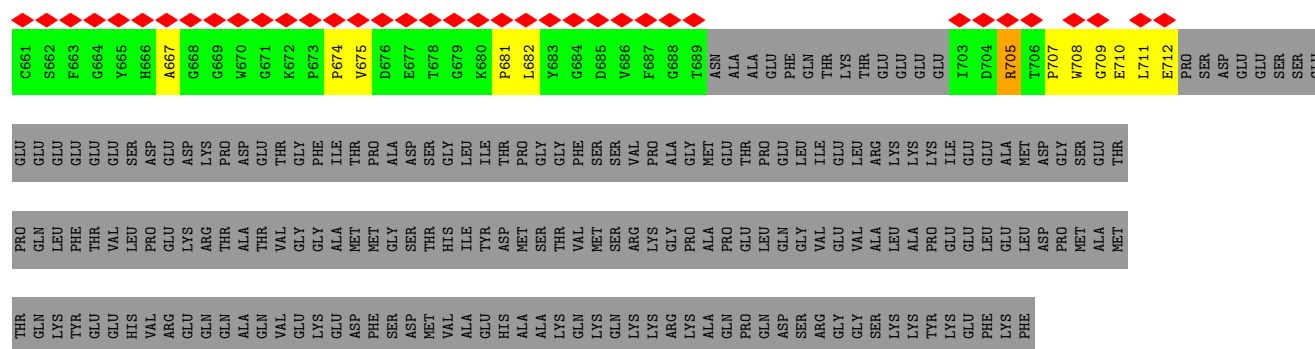


• Molecule 37: U2 small nuclear ribonucleoprotein B"

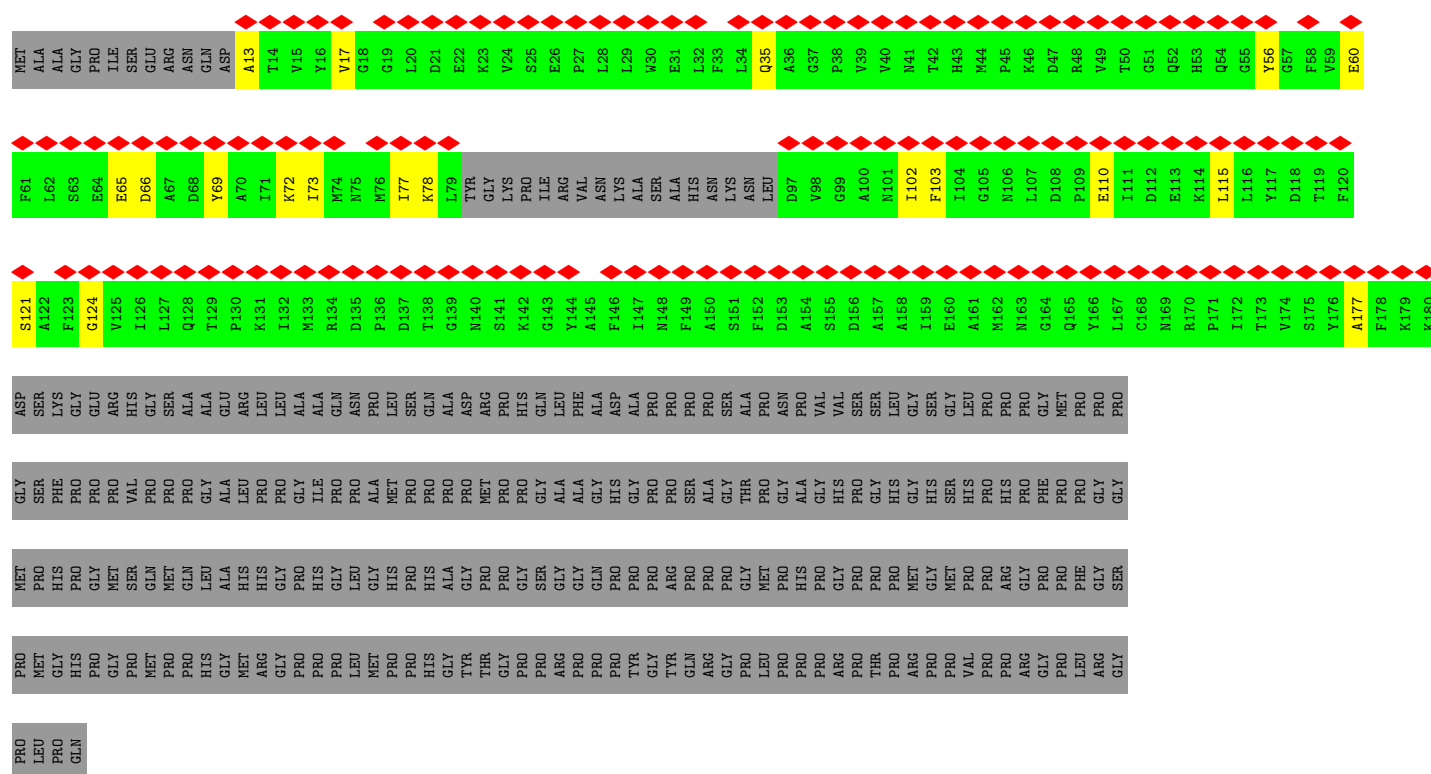


• Molecule 38: Splicing factor 3A subunit 3

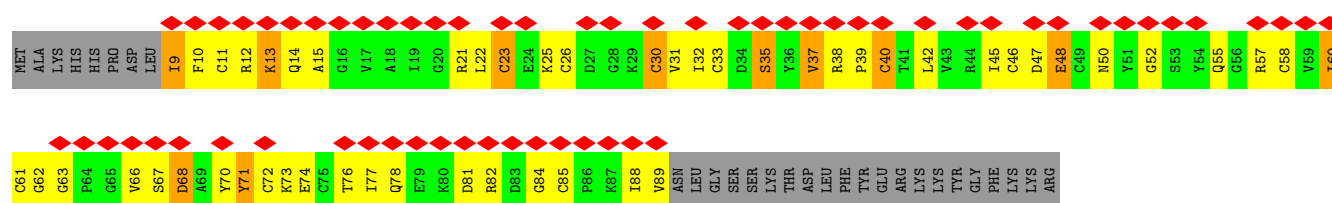
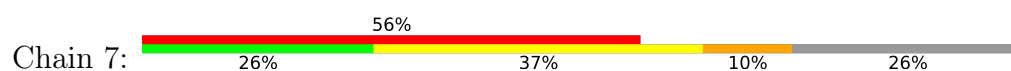




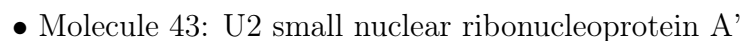
• Molecule 40: Splicing factor 3B subunit 4



• Molecule 41: PHD finger-like domain-containing protein 5A



• Molecule 42: Splicing factor 3B subunit 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.422	Depositor
Minimum map value	-1.073	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SEP, GTP, IHP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	2/16774 (0.0%)	0.71	9/22749 (0.0%)
2	B	0.53	0/2303	0.44	0/3579
3	C	0.49	0/6873	0.65	3/9346 (0.0%)
4	E	0.35	0/2392	0.62	0/3242
5	F	0.57	0/2323	0.52	0/3619
6	G	0.48	1/1764 (0.1%)	0.95	14/2737 (0.5%)
7	H	0.39	1/3947 (0.0%)	0.61	7/6138 (0.1%)
8	I	0.22	0/3406	0.46	0/4767
9	J	0.59	1/3817 (0.0%)	0.75	3/5184 (0.1%)
10	K	0.63	0/188	0.72	0/248
11	L	0.52	0/2612	0.75	4/3548 (0.1%)
12	M	0.56	0/991	0.98	1/1325 (0.1%)
13	N	0.56	0/1210	0.67	0/1622
14	O	0.29	0/1447	0.50	0/2013
15	P	0.71	0/888	0.95	1/1177 (0.1%)
16	Q	0.13	0/5279	0.30	0/6583
17	R	0.51	0/2937	0.73	1/3945 (0.0%)
18	S	0.21	0/769	0.41	0/1063
19	T	0.94	0/2574	0.73	0/3511
20	U	0.37	0/424	0.55	0/582
21	V	0.26	0/2993	0.48	0/4088
22	W	0.57	0/2471	1.03	0/3437
23	X	0.35	1/6479 (0.0%)	0.66	9/8747 (0.1%)
24	Y	0.26	0/2605	0.56	0/3522
25	Z	0.59	1/768 (0.1%)	0.99	2/1067 (0.2%)
26	y	0.16	0/315	0.30	0/392
27	a	0.86	0/343	1.21	3/427 (0.7%)
27	m	0.24	0/416	0.58	0/581
28	b	0.89	0/327	1.11	0/407
28	n	0.24	0/404	0.57	0/564
29	c	1.14	0/387	1.22	1/482 (0.2%)
29	h	0.22	0/485	0.47	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	1.23	0/295	1.26	0/367
30	i	0.23	0/362	0.52	0/502
31	e	1.04	0/315	1.27	1/392 (0.3%)
31	j	0.22	0/403	0.50	0/561
32	f	0.87	0/295	1.05	0/367
32	k	0.24	0/366	0.54	0/509
33	g	0.80	0/322	1.01	0/399
33	l	0.23	0/417	0.56	0/581
34	q	0.62	0/658	1.04	3/919 (0.3%)
34	r	0.57	0/653	0.99	3/912 (0.3%)
34	s	0.60	1/658 (0.2%)	1.11	4/919 (0.4%)
34	t	0.62	0/653	0.94	3/912 (0.3%)
35	1	0.71	5/6609 (0.1%)	0.94	15/8947 (0.2%)
36	3	0.47	0/9408	0.73	5/12767 (0.0%)
37	p	0.22	0/847	0.49	0/1181
38	w	0.29	0/1029	0.57	0/1393
39	2	0.73	5/1833 (0.3%)	1.27	10/2469 (0.4%)
40	4	0.36	0/741	0.65	0/1027
41	7	0.46	0/621	0.74	0/833
42	5	0.65	0/654	0.78	0/885
43	o	0.22	0/821	0.55	0/1149
All	All	0.54	18/108871 (0.0%)	0.72	102/149360 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	4
4	E	0	1
6	G	0	1
8	I	0	1
9	J	0	2
12	M	0	1
13	N	0	1
15	P	0	1
17	R	0	1
23	X	0	1
24	Y	0	1
29	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	1	0	5
36	3	0	5
39	2	0	1
41	7	0	1
42	5	0	1
All	All	0	40

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	207	PRO	C-N	19.22	1.50	1.33
35	1	718	PRO	N-CA	17.61	1.69	1.47
23	X	701	ASN	C-N	16.48	1.51	1.34
35	1	926	LYS	C-N	14.68	1.50	1.34
39	2	642	PRO	N-CA	11.64	1.70	1.46
39	2	641	PRO	N-CA	11.05	1.69	1.46
39	2	640	GLY	C-N	10.38	1.45	1.33
39	2	641	PRO	C-N	10.22	1.45	1.33
35	1	611	SER	C-O	8.45	1.34	1.24
7	H	32	U	O3'-P	6.62	1.71	1.61
39	2	645	TYR	C-N	6.56	1.49	1.33
1	A	985	TYR	CA-C	-6.13	1.42	1.52
6	G	1	G	O3'-P	5.46	1.69	1.61
25	Z	162	ASP	CA-CB	-5.38	1.44	1.53
35	1	611	SER	N-CA	5.25	1.52	1.46
1	A	352	PHE	C-N	-5.24	1.22	1.33
35	1	717	THR	C-N	5.12	1.45	1.33
34	s	9	ASN	CA-CB	-5.00	1.45	1.53

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	640	GLY	CA-C-N	22.18	143.22	120.38
39	2	640	GLY	C-N-CA	22.18	143.22	120.38
9	J	207	PRO	CA-C-N	21.57	135.41	119.66
9	J	207	PRO	C-N-CA	21.57	135.41	119.66
39	2	645	TYR	CA-C-N	20.38	145.31	119.84
39	2	645	TYR	C-N-CA	20.38	145.31	119.84
6	G	2	U	C4'-C3'-O3'	19.43	142.14	113.00
39	2	641	PRO	CA-C-N	18.28	139.21	120.38
39	2	641	PRO	C-N-CA	18.28	139.21	120.38
35	1	926	LYS	CA-C-N	17.61	138.18	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1	926	LYS	C-N-CA	17.61	138.18	119.87
35	1	717	THR	CA-C-N	17.17	141.30	119.84
35	1	717	THR	C-N-CA	17.17	141.30	119.84
39	2	567	ASP	CB-CA-C	13.35	136.32	109.76
23	X	701	ASN	CA-C-N	13.21	132.76	119.82
23	X	701	ASN	C-N-CA	13.21	132.76	119.82
6	G	1	G	C3'-C2'-O2'	13.16	134.34	114.60
7	H	32	U	C1'-C2'-O2'	-13.04	88.84	108.40
35	1	615	PRO	CA-N-CD	-12.08	95.08	112.00
35	1	718	PRO	CA-N-CD	-11.65	95.69	112.00
7	H	32	U	C4'-C3'-O3'	11.33	130.00	113.00
35	1	610	ILE	O-C-N	-11.10	108.70	122.57
35	1	1107	GLN	CA-C-N	-10.42	105.88	122.24
35	1	1107	GLN	C-N-CA	-10.42	105.88	122.24
35	1	619	ASN	CA-C-N	9.94	137.31	120.72
35	1	619	ASN	C-N-CA	9.94	137.31	120.72
36	3	568	MET	CA-C-N	9.85	134.09	120.39
36	3	568	MET	C-N-CA	9.85	134.09	120.39
34	s	46	PRO	N-CA-CB	9.45	111.20	103.36
6	G	1	G	C4'-C3'-O3'	-9.34	95.39	109.40
7	H	31	G	C4'-C3'-O3'	9.24	126.86	113.00
6	G	0	G	N9-C1'-C2'	-8.82	98.77	112.00
34	r	46	PRO	N-CA-CB	8.77	111.16	103.27
34	q	46	PRO	N-CA-CB	8.45	111.20	103.34
6	G	0	G	C4'-C3'-O3'	8.41	125.61	113.00
7	H	31	G	C2'-C3'-O3'	-8.32	101.22	113.70
34	s	60	PRO	N-CA-CB	8.16	111.81	103.25
12	M	200	ARG	CB-CA-C	7.96	119.09	109.31
7	H	31	G	C3'-C2'-O2'	7.84	122.47	110.70
34	q	60	PRO	N-CA-CB	7.38	111.00	103.25
39	2	642	PRO	CB-CA-C	7.35	119.88	110.92
7	H	30	A	C4'-C3'-O3'	7.34	120.42	109.40
25	Z	90	PRO	N-CA-CB	7.28	111.01	103.00
25	Z	78	PRO	N-CA-CB	7.21	110.82	103.25
15	P	188	TRP	CA-C-O	-7.18	113.54	121.87
34	t	60	PRO	N-CA-CB	7.18	111.34	103.30
35	1	619	ASN	N-CA-C	6.99	120.14	110.35
6	G	2	U	C1'-C2'-O2'	6.92	118.78	108.40
34	t	46	PRO	N-CA-CB	6.88	110.48	103.25
7	H	32	U	N1-C1'-C2'	-6.86	101.72	112.00
1	A	1516	LYS	CA-C-N	6.74	134.42	121.54
1	A	1516	LYS	C-N-CA	6.74	134.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	q	19	PRO	N-CA-CB	6.70	110.28	103.25
23	X	703	ARG	CA-C-N	6.65	132.02	121.44
23	X	703	ARG	C-N-CA	6.65	132.02	121.44
1	A	1303	LEU	CA-C-N	-6.64	112.03	123.25
1	A	1303	LEU	C-N-CA	-6.64	112.03	123.25
34	r	19	PRO	N-CA-CB	6.61	110.17	102.76
6	G	104	C	C4'-C3'-O3'	6.56	122.84	113.00
34	t	19	PRO	N-CA-CB	6.51	110.09	103.25
34	s	19	PRO	N-CA-CB	6.36	109.93	103.25
34	r	60	PRO	N-CA-CB	6.31	109.88	103.25
6	G	1	G	O4'-C1'-N9	6.17	117.46	108.20
35	1	1011	PRO	N-CA-C	-6.13	103.22	110.70
6	G	102	G	C1'-C2'-O2'	-5.97	99.44	108.40
23	X	702	PRO	CA-C-N	5.95	132.90	121.54
23	X	702	PRO	C-N-CA	5.95	132.90	121.54
3	C	155	PRO	N-CA-C	-5.94	108.51	114.68
23	X	701	ASN	CA-C-O	-5.91	114.39	119.36
35	1	592	GLU	CB-CA-C	5.88	121.47	110.70
6	G	2	U	C2'-C3'-O3'	-5.86	104.90	113.70
1	A	1700	GLY	N-CA-C	5.78	120.14	111.42
11	L	163	GLN	N-CA-C	5.73	118.58	110.50
1	A	57	GLN	CB-CG-CD	5.69	122.28	112.60
6	G	100	C	C4'-C3'-O3'	-5.67	100.89	109.40
27	a	52	LYS	CA-C-N	-5.58	114.18	119.76
27	a	52	LYS	C-N-CA	-5.58	114.18	119.76
1	A	1517	LYS	CA-CB-CG	5.56	125.22	114.10
11	L	164	GLY	CA-C-N	5.54	129.85	120.88
11	L	164	GLY	C-N-CA	5.54	129.85	120.88
35	1	845	GLY	CA-C-O	-5.54	118.47	122.45
3	C	822	MET	CA-C-N	-5.53	111.08	121.81
3	C	822	MET	C-N-CA	-5.53	111.08	121.81
17	R	325	ARG	N-CA-C	-5.48	105.00	110.97
1	A	105	ASN	CA-C-N	-5.35	111.23	123.15
1	A	105	ASN	C-N-CA	-5.35	111.23	123.15
27	a	5	LYS	N-CA-C	5.30	117.97	111.82
34	s	54	ASP	N-CA-CB	-5.28	102.28	110.46
23	X	703	ARG	N-CA-CB	-5.24	101.64	110.49
6	G	2	U	P-O3'-C3'	-5.23	112.36	120.20
39	2	566	ILE	CA-C-N	-5.19	110.42	121.32
39	2	566	ILE	C-N-CA	-5.19	110.42	121.32
6	G	1	G	O4'-C1'-C2'	5.19	110.99	105.80
36	3	1008	SER	N-CA-C	5.17	114.66	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	99	MET	N-CA-C	5.12	116.85	108.76
31	e	85	THR	N-CA-C	-5.11	105.88	112.68
36	3	498	GLY	N-CA-C	-5.11	108.19	115.64
9	J	207	PRO	N-CA-C	-5.08	104.51	110.70
23	X	617	GLY	N-CA-C	5.07	119.30	111.08
11	L	178	GLU	CB-CA-C	5.06	119.46	110.85
6	G	2	U	C5'-C4'-O4'	-5.02	102.27	109.80
36	3	917	PRO	N-CA-C	-5.02	102.13	112.47

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1	1105	GLU	Peptide
35	1	1107	GLN	Peptide
35	1	1179	ASP	Peptide
35	1	567	VAL	Peptide
35	1	610	ILE	Mainchain
39	2	502	ARG	Peptide
36	3	268	ARG	Peptide
36	3	342	LEU	Peptide
36	3	490	THR	Peptide
36	3	916	ASN	Peptide
36	3	971	ASP	Peptide
42	5	79	PRO	Peptide
41	7	13	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1416	ILE	Peptide
1	A	1516	LYS	Peptide
1	A	187	PRO	Peptide
1	A	365	VAL	Peptide
1	A	433	GLU	Peptide
1	A	699	GLU	Peptide
1	A	855	ARG	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
1	A	982	GLU	Peptide
3	C	443	VAL	Peptide
3	C	533	SER	Peptide
3	C	572	GLU	Peptide
3	C	823	ALA	Peptide
4	E	321	TYR	Peptide

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Mol	Chain	Res	Type	Group
6	G	1	G	Sidechain
8	I	386	ASP	Peptide
9	J	201	ARG	Mainchain
9	J	240	THR	Peptide
12	M	124	PHE	Peptide
13	N	36	PRO	Peptide
15	P	29	GLN	Peptide
17	R	163	MET	Peptide
23	X	326	GLN	Peptide
24	Y	204	SER	Peptide
29	c	112	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16331	0	16276	650	0
2	B	2066	0	1047	93	0
3	C	6724	0	6696	332	0
4	E	2338	0	2275	158	0
5	F	2075	0	1048	86	0
6	G	1587	0	808	133	0
7	H	3539	0	1791	125	0
8	I	3387	0	1651	23	0
9	J	3773	0	2869	94	0
10	K	185	0	165	21	0
11	L	2584	0	2096	111	0
12	M	971	0	950	78	0
13	N	1184	0	1190	48	0
14	O	1447	0	638	31	0
15	P	876	0	875	53	0
16	Q	5288	0	1361	7	0
17	R	2915	0	2795	202	0
18	S	770	0	356	7	0
19	T	2507	0	2451	87	0
20	U	422	0	291	14	0
21	V	2959	0	2237	111	0
22	W	2473	0	1096	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	X	6357	0	6349	425	0
24	Y	2556	0	2492	150	0
25	Z	772	0	342	18	0
26	y	316	0	86	4	0
27	a	344	0	93	0	0
27	m	413	0	194	7	0
28	b	328	0	89	5	0
28	n	402	0	184	9	0
29	c	388	0	102	7	0
29	h	482	0	220	12	0
30	d	296	0	87	10	0
30	i	359	0	179	17	0
31	e	316	0	85	4	0
31	j	403	0	173	9	0
32	f	296	0	84	5	0
32	k	364	0	176	13	0
33	g	324	0	89	4	0
33	l	415	0	198	15	0
34	q	659	0	296	19	0
34	r	654	0	294	8	0
34	s	659	0	296	20	0
34	t	654	0	294	14	0
35	1	6486	0	6690	695	0
36	3	9220	0	9139	729	0
37	p	841	0	420	9	0
38	w	999	0	961	110	0
39	2	1803	0	1611	210	0
40	4	743	0	344	31	0
41	7	613	0	597	45	0
42	5	635	0	595	104	0
43	o	816	0	386	10	0
44	A	36	0	6	5	0
45	C	32	0	12	0	0
46	C	1	0	0	0	0
46	F	6	0	0	0	0
47	7	3	0	0	0	0
47	K	1	0	0	0	0
47	N	3	0	0	0	0
All	All	106396	0	84125	4419	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (4419) 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)
39:2:594:GLY:HA2	39:2:597:PHE:CE2	1.21	1.65
35:1:1056:MET:HG2	39:2:561:MET:SD	1.37	1.64
39:2:635:ALA:CB	40:4:73:ILE:HA	1.32	1.59
39:2:635:ALA:HB3	40:4:73:ILE:CA	1.10	1.55
39:2:641:PRO:N	39:2:641:PRO:CA	1.69	1.55
14:O:34:ILE:CB	17:R:197:ILE:HD11	1.36	1.54
39:2:594:GLY:HA2	39:2:597:PHE:CD2	1.39	1.54
35:1:540:MET:HE3	35:1:577:VAL:CG1	1.35	1.54
39:2:642:PRO:N	39:2:642:PRO:CA	1.70	1.51
35:1:564:ASP:HB3	35:1:603:ALA:CB	1.39	1.50
39:2:594:GLY:CA	39:2:597:PHE:CD2	1.90	1.50
35:1:718:PRO:N	35:1:718:PRO:CA	1.69	1.39
39:2:594:GLY:CA	39:2:597:PHE:CE2	1.95	1.38
14:O:34:ILE:CB	17:R:197:ILE:CD1	2.02	1.34
23:X:787:GLU:CG	35:1:542:PRO:HG2	1.58	1.33
35:1:557:ASP:CB	35:1:596:ILE:HG22	1.59	1.32
35:1:1056:MET:SD	39:2:561:MET:CE	2.17	1.32
35:1:557:ASP:HB2	35:1:596:ILE:CG2	1.59	1.30
6:G:1:G:N2	10:K:218:LYS:HG3	1.49	1.28
35:1:1056:MET:SD	39:2:561:MET:HE1	1.73	1.27
23:X:170:GLU:OE2	23:X:771:GLY:HA3	1.26	1.27
35:1:540:MET:CE	35:1:577:VAL:HG12	1.64	1.26
39:2:594:GLY:C	39:2:597:PHE:HD2	1.43	1.25
35:1:564:ASP:CB	35:1:603:ALA:HB1	1.66	1.24
11:L:162:THR:CG2	17:R:258:LYS:O	1.85	1.23
1:A:1741:TYR:OH	35:1:937:LEU:CD2	1.86	1.22
36:3:114:ARG:NH1	42:5:37:ARG:HB2	1.52	1.22
23:X:741:TRP:CE2	35:1:782:GLU:OE2	1.92	1.20
11:L:163:GLN:HB3	11:L:168:LYS:NZ	1.55	1.19
35:1:1056:MET:CG	39:2:561:MET:SD	2.30	1.18
8:I:433:ALA:HA	8:I:482:LYS:CB	1.72	1.18
39:2:635:ALA:CB	40:4:73:ILE:CA	2.01	1.18
35:1:819:TRP:HB3	35:1:864:TYR:OH	1.03	1.17
35:1:1001:VAL:CG2	35:1:1009:MET:HE1	1.74	1.17
11:L:162:THR:HG23	17:R:258:LYS:O	1.40	1.15
1:A:1741:TYR:OH	35:1:937:LEU:HD23	0.98	1.15
23:X:164:TRP:CZ2	23:X:539:VAL:HG22	1.83	1.13
35:1:819:TRP:CB	35:1:864:TYR:OH	1.97	1.13
38:w:399:LEU:HD11	39:2:507:LYS:HD3	1.17	1.13
35:1:1056:MET:CG	39:2:561:MET:CE	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:567:VAL:HG11	35:1:600:LEU:HD12	1.30	1.11
35:1:803:ALA:HA	35:1:843:LYS:NZ	1.67	1.10
1:A:1578:ARG:HD2	10:K:224:SER:HB3	1.34	1.09
35:1:1295:TYR:HH	42:5:29:TRP:CD1	1.69	1.09
6:G:19:G:N2	14:O:194:ALA:O	1.84	1.08
1:A:1741:TYR:CZ	35:1:937:LEU:HD23	1.89	1.08
17:R:325:ARG:HD3	24:Y:222:ILE:HG23	1.10	1.08
23:X:171:ARG:NH1	23:X:509:PRO:HB3	1.69	1.08
6:G:99:C:N4	7:H:32:U:H3	1.50	1.07
23:X:787:GLU:HG3	35:1:542:PRO:CG	1.84	1.07
35:1:1078:VAL:HG12	35:1:1118:ILE:HD12	1.09	1.07
35:1:528:ALA:H	35:1:566:LEU:HD23	1.14	1.07
36:3:616:ILE:HB	36:3:629:SER:O	1.54	1.07
39:2:635:ALA:CB	40:4:72:LYS:C	2.29	1.06
2:B:90:U:C5	33:g:38:ASN:O	2.09	1.05
6:G:1:G:H21	10:K:218:LYS:HG3	0.93	1.05
35:1:926:LYS:HB3	35:1:927:PRO:HD3	1.32	1.05
1:A:855:ARG:HG3	1:A:1520:ASN:HB3	1.09	1.05
1:A:1741:TYR:HE2	35:1:977:VAL:HG21	1.18	1.05
35:1:1056:MET:SD	39:2:561:MET:HE2	1.94	1.05
17:R:328:ALA:HB2	24:Y:226:MET:SD	1.95	1.05
35:1:540:MET:HE3	35:1:577:VAL:HG11	1.33	1.04
35:1:625:ARG:HB3	35:1:666:LYS:NZ	1.71	1.04
35:1:721:ILE:HG22	35:1:756:LEU:HD23	1.36	1.04
34:q:60:PRO:CB	34:s:93:ARG:C	2.30	1.04
35:1:721:ILE:CG2	35:1:756:LEU:HB3	1.87	1.04
34:s:71:ILE:CB	34:t:81:GLU:CB	2.35	1.04
39:2:606:PRO:HA	40:4:35:GLN:HA	1.35	1.04
39:2:635:ALA:HB3	40:4:73:ILE:N	1.73	1.04
39:2:594:GLY:O	39:2:597:PHE:HD2	1.37	1.03
22:W:321:GLU:CB	26:y:42:GLU:CA	2.37	1.03
23:X:787:GLU:CB	35:1:542:PRO:HG2	1.88	1.03
1:A:1756:SER:OG	35:1:943:LYS:CD	2.07	1.03
9:J:206:LEU:HB3	9:J:207:PRO:HD2	1.38	1.02
17:R:335:ARG:CB	23:X:272:TYR:HB2	1.88	1.02
35:1:803:ALA:CA	35:1:843:LYS:NZ	2.22	1.02
35:1:1056:MET:CG	39:2:561:MET:HE2	1.86	1.02
23:X:787:GLU:HG3	35:1:542:PRO:HG2	1.05	1.01
38:w:399:LEU:HD11	39:2:507:LYS:CD	1.90	1.01
43:o:46:ALA:HA	43:o:68:THR:O	1.60	1.01
36:3:982:GLU:HB3	38:w:476:GLU:OE2	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:15:ALA:HB1	34:s:112:ALA:O	1.60	1.01
36:3:984:LYS:HZ3	38:w:471:TRP:CA	1.72	1.01
35:1:1001:VAL:HG23	35:1:1009:MET:HE1	1.42	1.00
35:1:1078:VAL:CG1	35:1:1118:ILE:HD12	1.91	1.00
2:B:95:G:H1'	30:d:24:LYS:CA	1.91	1.00
35:1:1262:ARG:HD2	42:5:24:ALA:O	1.61	1.00
39:2:635:ALA:CB	40:4:73:ILE:N	2.22	1.00
11:L:163:GLN:HB3	11:L:168:LYS:HZ1	1.09	1.00
35:1:564:ASP:CB	35:1:603:ALA:CB	2.33	1.00
36:3:984:LYS:NZ	38:w:471:TRP:CA	2.25	1.00
1:A:1741:TYR:CZ	35:1:937:LEU:CD2	2.44	1.00
6:G:1:G:H21	10:K:218:LYS:CG	1.75	0.99
35:1:897:LEU:HD21	35:1:932:ILE:HG13	1.41	0.99
6:G:96:U:OP1	35:1:1149:LYS:HE2	1.61	0.99
35:1:1257:PRO:HD3	39:2:482:ALA:HB2	1.45	0.99
35:1:1001:VAL:HG22	35:1:1009:MET:HE1	1.44	0.99
35:1:1010:THR:OG1	35:1:1011:PRO:HD3	1.60	0.99
36:3:1116:SER:N	39:2:708:TRP:HZ2	1.61	0.99
36:3:106:THR:OG1	41:7:82:ARG:HD2	1.61	0.99
17:R:334:ARG:O	23:X:268:GLN:NE2	1.95	0.99
36:3:979:ARG:NH2	38:w:478:GLU:OE1	1.96	0.99
35:1:721:ILE:HG21	35:1:756:LEU:HB3	1.44	0.98
35:1:1137:ARG:NH1	39:2:522:PHE:O	1.95	0.98
39:2:594:GLY:HA3	39:2:597:PHE:CD2	1.95	0.98
39:2:635:ALA:HB3	40:4:73:ILE:CB	1.92	0.98
35:1:1056:MET:HG2	39:2:561:MET:CE	1.90	0.98
39:2:635:ALA:HB2	40:4:72:LYS:O	1.62	0.98
35:1:560:LEU:HD21	35:1:600:LEU:HA	1.46	0.98
5:F:38:G:H2'	5:F:39:A:H8	1.25	0.97
35:1:841:ALA:CB	35:1:875:ILE:HD13	1.94	0.97
43:o:13:ALA:O	43:o:24:LEU:HA	1.65	0.97
1:A:1738:PRO:HG3	35:1:969:LYS:HB3	1.46	0.96
35:1:1295:TYR:OH	42:5:29:TRP:HD1	1.47	0.96
25:Z:85:LYS:O	25:Z:87:TYR:N	1.98	0.96
1:A:1745:GLU:OE1	35:1:980:GLU:HG2	1.66	0.96
36:3:477:SER:HB2	36:3:505:THR:H	1.28	0.96
34:q:60:PRO:C	34:s:93:ARG:CB	2.39	0.96
36:3:189:TYR:HA	42:5:73:LEU:CD1	1.96	0.96
39:2:594:GLY:O	39:2:597:PHE:CD2	2.19	0.96
2:B:93:U:H1'	29:c:104:ASP:CA	1.96	0.95
17:R:335:ARG:O	23:X:268:GLN:HB3	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5:36:HIS:HD1	42:5:76:CYS:HG	1.07	0.95
12:M:215:ASN:ND2	17:R:260:TYR:HA	1.81	0.95
23:X:741:TRP:CD2	35:1:782:GLU:OE2	2.20	0.95
36:3:984:LYS:HZ3	38:w:471:TRP:N	1.64	0.95
11:L:16:ASP:HB2	11:L:54:LEU:HD21	1.47	0.94
23:X:741:TRP:CZ2	35:1:782:GLU:OE2	2.20	0.94
35:1:540:MET:CE	35:1:577:VAL:CG1	2.31	0.94
8:I:433:ALA:CA	8:I:482:LYS:CB	2.45	0.94
18:S:83:GLU:HA	18:S:106:ASP:HA	1.46	0.94
36:3:984:LYS:HZ3	38:w:470:ARG:C	1.75	0.94
11:L:163:GLN:CB	11:L:168:LYS:NZ	2.31	0.94
35:1:1167:TYR:CE2	39:2:581:LYS:HG2	2.03	0.94
39:2:594:GLY:CA	39:2:597:PHE:HD2	1.47	0.94
39:2:594:GLY:HA3	39:2:597:PHE:CE2	1.99	0.94
1:A:39:GLN:HE22	22:W:170:THR:N	1.66	0.94
35:1:528:ALA:H	35:1:566:LEU:CD2	1.80	0.94
1:A:372:PRO:O	3:C:342:ARG:NH2	2.01	0.93
36:3:189:TYR:CD1	42:5:37:ARG:NH2	2.36	0.93
35:1:1295:TYR:HH	42:5:29:TRP:HD1	1.01	0.93
5:F:59:G:H1	5:F:76:A:H61	1.09	0.93
17:R:325:ARG:HD3	24:Y:222:ILE:CG2	1.99	0.93
35:1:1164:ASP:O	39:2:579:GLN:NE2	2.01	0.93
25:Z:85:LYS:C	25:Z:87:TYR:H	1.72	0.93
6:G:99:C:H42	7:H:32:U:H3	0.95	0.92
23:X:480:SER:HB3	23:X:500:MET:HE2	1.50	0.92
2:B:20:G:O6	2:B:57:G:N1	2.02	0.92
36:3:459:VAL:HG21	36:3:757:ILE:HG21	1.51	0.92
36:3:193:ASP:C	42:5:79:PRO:HG2	1.94	0.92
3:C:461:LEU:HB3	3:C:465:MET:HE3	1.48	0.92
36:3:981:CYS:HA	38:w:471:TRP:CH2	2.04	0.92
35:1:1252:GLN:NE2	39:2:492:LYS:HA	1.84	0.92
17:R:325:ARG:CD	24:Y:222:ILE:HG23	2.00	0.92
25:Z:15:ALA:CB	34:s:112:ALA:O	2.18	0.91
39:2:635:ALA:HB1	40:4:72:LYS:C	1.94	0.91
39:2:635:ALA:CB	40:4:72:LYS:O	2.18	0.91
1:A:361:HIS:CE1	21:V:324:HIS:CB	2.53	0.91
1:A:467:GLN:OE1	2:B:20:G:N2	2.04	0.91
36:3:516:LEU:O	36:3:527:ILE:HB	1.70	0.91
23:X:170:GLU:OE2	23:X:771:GLY:CA	2.19	0.91
35:1:819:TRP:CB	35:1:864:TYR:HH	1.77	0.91
15:P:207:ASP:HB2	15:P:218:GLU:HB2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:206:LEU:HB3	9:J:207:PRO:CD	2.01	0.91
35:1:833:LEU:HD23	35:1:867:MET:SD	2.11	0.91
35:1:840:LEU:O	35:1:844:VAL:HG22	1.69	0.91
1:A:1741:TYR:CE2	35:1:977:VAL:HG21	2.04	0.90
2:B:95:G:H21	2:B:96:A:H5''	1.35	0.90
35:1:803:ALA:CA	35:1:843:LYS:HZ2	1.81	0.90
1:A:705:LYS:NZ	17:R:247:ILE:O	2.03	0.90
2:B:46:U:O2	20:U:11:ARG:NH2	2.03	0.90
36:3:114:ARG:CZ	42:5:37:ARG:HB2	2.01	0.90
3:C:350:ASN:HD22	3:C:353:THR:HG22	1.36	0.90
35:1:703:THR:HG22	35:1:745:ALA:HB3	1.51	0.90
36:3:984:LYS:NZ	38:w:471:TRP:HA	1.85	0.90
1:A:39:GLN:HE22	22:W:170:THR:H	0.97	0.90
22:W:321:GLU:HA	26:y:42:GLU:CA	2.01	0.90
23:X:164:TRP:CE2	23:X:539:VAL:HG22	2.07	0.90
39:2:635:ALA:HB2	40:4:73:ILE:HA	1.53	0.90
35:1:803:ALA:HA	35:1:843:LYS:HZ2	1.24	0.90
35:1:564:ASP:HB3	35:1:603:ALA:HB1	0.92	0.90
36:3:982:GLU:CB	38:w:476:GLU:OE2	2.20	0.90
14:O:34:ILE:CA	17:R:197:ILE:CD1	2.50	0.89
8:I:463:PRO:HG2	8:I:483:SER:CB	2.00	0.89
6:G:116:C:O4'	17:R:371:ARG:HA	1.73	0.89
2:B:93:U:O4	30:d:66:CYS:N	2.06	0.89
39:2:594:GLY:HA2	39:2:597:PHE:HE2	1.07	0.89
8:I:394:PRO:HG2	8:I:429:VAL:HA	1.53	0.89
35:1:540:MET:HE3	35:1:577:VAL:HG12	0.91	0.89
36:3:463:ARG:H	36:3:510:LEU:HD22	1.35	0.89
35:1:819:TRP:CZ3	35:1:867:MET:HE3	2.08	0.89
12:M:215:ASN:HD21	17:R:261:THR:N	1.70	0.88
3:C:614:TYR:OH	3:C:643:ASP:OD2	1.89	0.88
35:1:567:VAL:CG1	35:1:600:LEU:HD12	2.02	0.88
4:E:150:HIS:HE2	4:E:169:THR:HG1	1.17	0.88
1:A:31:GLN:OE1	4:E:194:TYR:OH	1.92	0.88
1:A:707:ARG:HH12	7:H:18:U:H5'	1.37	0.87
1:A:1756:SER:OG	35:1:943:LYS:HD3	1.74	0.87
35:1:1217:PRO:HD3	39:2:590:LEU:HD13	1.57	0.87
1:A:1526:LEU:HD13	1:A:1528:GLN:H	1.40	0.87
19:T:307:SER:OG	19:T:309:ASP:OD1	1.92	0.87
24:Y:246:LYS:HE3	24:Y:312:HIS:HB2	1.57	0.87
35:1:1179:ASP:HB2	39:2:511:LEU:HB2	1.56	0.87
9:J:199:LYS:O	9:J:199:LYS:NZ	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1006:MET:SD	35:1:1006:MET:N	2.48	0.87
2:B:93:U:C1'	29:c:104:ASP:CA	2.52	0.87
23:X:690:LEU:HD22	23:X:735:PHE:HB2	1.57	0.87
36:3:1115:GLU:CG	39:2:708:TRP:HE1	1.88	0.87
36:3:139:LYS:HG3	36:3:160:ALA:HB3	1.57	0.86
1:A:39:GLN:NE2	22:W:170:THR:H	1.73	0.86
17:R:360:ARG:HD2	24:Y:274:ASP:OD1	1.75	0.86
3:C:478:THR:HG21	3:C:492:ALA:HB1	1.56	0.86
5:F:36:A:H3'	5:F:37:C:H5''	1.55	0.86
35:1:821:HIS:HD2	35:1:861:ALA:CB	1.87	0.86
35:1:564:ASP:HB3	35:1:603:ALA:HB2	1.56	0.86
36:3:189:TYR:CB	42:5:73:LEU:HD12	2.06	0.86
6:G:1:G:OP2	6:G:1:G:H4'	1.76	0.86
2:B:90:U:H5	33:g:38:ASN:O	1.53	0.86
1:A:1755:SER:O	35:1:942:ASN:HA	1.75	0.85
19:T:349:SER:OG	19:T:351:ASP:OD1	1.92	0.85
43:o:23:GLU:HA	43:o:46:ALA:HB3	1.56	0.85
31:j:63:GLU:O	31:j:71:ARG:HA	1.75	0.85
35:1:803:ALA:N	35:1:843:LYS:NZ	2.24	0.85
35:1:1266:TRP:CZ3	42:5:22:GLY:HA3	2.11	0.85
35:1:528:ALA:N	35:1:566:LEU:HD23	1.91	0.85
5:F:38:G:H2'	5:F:39:A:C8	2.10	0.85
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.09	0.85
17:R:325:ARG:NH1	17:R:325:ARG:O	2.10	0.85
1:A:1578:ARG:HD2	10:K:224:SER:CB	2.05	0.85
36:3:668:GLY:HA3	36:3:699:VAL:HG11	1.57	0.85
36:3:806:ALA:HA	36:3:856:LYS:HB3	1.58	0.85
36:3:585:ALA:HB1	36:3:610:VAL:HG12	1.59	0.85
9:J:187:VAL:HG13	9:J:188:GLN:H	1.42	0.84
35:1:819:TRP:HB3	35:1:864:TYR:HH	1.03	0.84
11:L:162:THR:HG21	17:R:258:LYS:O	1.75	0.84
35:1:625:ARG:HB3	35:1:666:LYS:HZ1	1.39	0.84
36:3:984:LYS:HE2	38:w:476:GLU:OE1	1.78	0.84
38:w:399:LEU:CD1	39:2:507:LYS:HD3	2.05	0.84
3:C:117:ASP:N	3:C:117:ASP:OD1	2.11	0.84
23:X:991:LEU:HA	23:X:995:GLU:HA	1.60	0.84
35:1:821:HIS:CD2	35:1:861:ALA:HB2	2.13	0.84
3:C:488:VAL:HG13	3:C:609:LYS:HD3	1.59	0.84
22:W:321:GLU:CA	26:y:42:GLU:CA	2.56	0.83
39:2:643:PRO:CB	40:4:65:GLU:CB	2.56	0.83
23:X:171:ARG:HH22	23:X:509:PRO:HD3	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:556:ILE:HG23	35:1:596:ILE:HG21	1.58	0.83
36:3:1008:SER:OG	36:3:1009:PHE:N	2.07	0.83
23:X:787:GLU:HB2	35:1:542:PRO:HG2	1.60	0.83
36:3:984:LYS:HZ1	38:w:471:TRP:CB	1.91	0.83
1:A:1738:PRO:HA	35:1:973:HIS:NE2	1.92	0.83
4:E:92:LEU:HD12	4:E:103:ALA:HB3	1.61	0.83
39:2:606:PRO:HA	40:4:35:GLN:CA	2.07	0.83
42:5:36:HIS:ND1	42:5:76:CYS:SG	2.49	0.83
1:A:184:ASP:HB2	13:N:1:MET:HA	1.61	0.83
1:A:1636:LYS:HD3	1:A:1658:GLN:HE21	1.44	0.83
6:G:83:A:N6	38:w:400:HIS:HE2	1.76	0.83
35:1:1292:LYS:O	42:5:78:PRO:HD2	1.77	0.83
17:R:348:GLU:O	17:R:352:ARG:HB2	1.78	0.83
23:X:166:ARG:NH2	23:X:771:GLY:O	2.12	0.82
39:2:594:GLY:C	39:2:597:PHE:CD2	2.34	0.82
30:i:44:LEU:O	30:i:61:GLU:HA	1.79	0.82
1:A:1741:TYR:HB3	35:1:973:HIS:NE2	1.93	0.82
12:M:215:ASN:ND2	17:R:260:TYR:CA	2.40	0.82
23:X:162:ASP:HB2	23:X:542:PHE:HZ	1.42	0.82
23:X:272:TYR:OH	24:Y:227:VAL:O	1.96	0.82
35:1:1179:ASP:HB2	39:2:511:LEU:CB	2.09	0.82
36:3:352:GLU:OE2	36:3:429:ARG:NH1	2.12	0.82
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.25	0.82
36:3:280:ASP:HB3	36:3:283:ARG:HG3	1.60	0.82
38:w:388:ASP:OD2	38:w:390:LYS:NZ	2.10	0.82
32:k:21:LEU:HA	32:k:67:ILE:HA	1.61	0.82
1:A:1756:SER:OG	35:1:943:LYS:HB3	1.79	0.82
12:M:215:ASN:HD21	17:R:261:THR:H	1.24	0.82
35:1:560:LEU:CD2	35:1:600:LEU:HA	2.09	0.82
35:1:725:ASP:HA	35:1:728:LEU:HG	1.61	0.82
35:1:734:GLY:O	35:1:738:HIS:HB2	1.77	0.82
3:C:670:SER:HA	3:C:823:ALA:HB3	1.61	0.82
35:1:1266:TRP:CE3	42:5:22:GLY:HA3	2.14	0.82
7:H:30:A:H2'	7:H:30:A:N3	1.94	0.82
35:1:1056:MET:CB	39:2:561:MET:HE2	2.10	0.82
39:2:606:PRO:CA	40:4:35:GLN:HA	2.10	0.82
1:A:1402:ARG:HH22	23:X:641:GLU:CD	1.87	0.82
14:O:34:ILE:C	17:R:197:ILE:CD1	2.53	0.82
23:X:510:ASP:OD1	23:X:543:ARG:HD3	1.78	0.82
35:1:557:ASP:OD2	35:1:595:GLU:HB3	1.79	0.82
36:3:568:MET:HB3	36:3:574:LEU:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:7:40:CYS:SG	41:7:73:LYS:NZ	2.50	0.82
1:A:414:ARG:NH1	3:C:410:LEU:O	2.13	0.81
1:A:1741:TYR:HH	35:1:937:LEU:HD23	1.01	0.81
6:G:97:A:N1	35:1:1075:ARG:HG2	1.95	0.81
6:G:116:C:OP2	17:R:371:ARG:HD3	1.80	0.81
9:J:205:LEU:HD22	9:J:205:LEU:O	1.80	0.81
23:X:163:GLU:OE2	23:X:778:PHE:CD2	2.32	0.81
25:Z:84:MET:O	34:t:79:GLN:CB	2.28	0.81
35:1:665:ILE:HD13	35:1:705:SER:HB2	1.61	0.81
36:3:29:GLU:HG3	36:3:42:ARG:HG3	1.63	0.81
39:2:594:GLY:CA	39:2:597:PHE:HE2	1.59	0.81
5:F:59:G:H1	5:F:76:A:N6	1.76	0.81
1:A:1838:LYS:HB3	1:A:1868:MET:HG3	1.60	0.81
35:1:652:CYS:HB2	35:1:692:HIS:HE1	1.46	0.81
12:M:215:ASN:HD22	17:R:260:TYR:HA	1.45	0.81
25:Z:36:VAL:O	34:r:112:ALA:HB1	1.79	0.81
35:1:1287:ILE:HB	42:5:32:LEU:HD11	1.63	0.81
36:3:975:LYS:CB	38:w:484:GLY:O	2.28	0.81
4:E:87:ASP:OD1	4:E:87:ASP:N	2.13	0.81
17:R:367:ARG:NH1	24:Y:282:CYS:SG	2.54	0.81
35:1:1090:PRO:HA	35:1:1093:VAL:HG12	1.61	0.81
4:E:92:LEU:O	4:E:101:ASN:ND2	2.14	0.80
41:7:33:CYS:SG	41:7:35:SER:OG	2.31	0.80
1:A:701:ILE:HD11	17:R:237:MET:HG3	1.63	0.80
36:3:162:LYS:HE3	36:3:165:THR:HG21	1.62	0.80
1:A:1738:PRO:CG	35:1:969:LYS:HB3	2.11	0.80
4:E:197:LEU:HG	4:E:212:GLY:HA2	1.62	0.80
1:A:1402:ARG:NH2	23:X:641:GLU:OE2	2.14	0.80
1:A:1835:GLN:HA	1:A:1838:LYS:HG3	1.63	0.80
2:B:92:U:H3	28:b:36:MET:CA	1.93	0.80
35:1:532:PHE:CZ	35:1:574:ILE:HD11	2.16	0.80
35:1:757:MET:HB3	35:1:762:ALA:HB2	1.64	0.80
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.64	0.80
36:3:170:VAL:HG23	36:3:184:CYS:HB3	1.64	0.80
1:A:855:ARG:CG	1:A:1520:ASN:HB3	2.02	0.80
15:P:186:ARG:HH11	15:P:186:ARG:HG2	1.45	0.80
23:X:604:VAL:HG13	23:X:605:THR:HG23	1.64	0.80
35:1:805:TYR:O	35:1:809:GLU:HB2	1.82	0.80
1:A:474:ARG:NH1	2:B:15:C:OP2	2.15	0.79
9:J:204:GLU:OE1	9:J:204:GLU:HA	1.82	0.79
35:1:544:LEU:HD21	35:1:549:ARG:HG3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:614:ARG:C	35:1:614:ARG:HD3	2.08	0.79
1:A:1854:VAL:HG11	21:V:448:THR:HA	1.64	0.79
3:C:534:VAL:HG22	3:C:537:TYR:HB2	1.65	0.79
35:1:963:LYS:O	35:1:966:GLN:N	2.14	0.79
3:C:343:LEU:HD13	3:C:373:ILE:HD11	1.63	0.79
11:L:169:ARG:CZ	11:L:169:ARG:HB2	2.12	0.79
36:3:412:ILE:HG12	36:3:423:LEU:HD22	1.63	0.79
6:G:95:U:OP2	35:1:1106:ARG:CG	2.31	0.79
1:A:1738:PRO:HG3	35:1:969:LYS:CB	2.13	0.79
17:R:360:ARG:HD2	24:Y:274:ASP:CG	2.08	0.79
17:R:376:LYS:HA	17:R:379:LYS:HB2	1.65	0.79
36:3:114:ARG:NH1	42:5:37:ARG:CB	2.41	0.79
36:3:412:ILE:HD12	36:3:1107:THR:HG21	1.64	0.79
36:3:984:LYS:HZ3	38:w:471:TRP:HA	1.38	0.79
2:B:41:U:O4	6:G:0:G:N2	2.15	0.78
35:1:617:ILE:CD1	35:1:651:VAL:HB	2.13	0.78
35:1:926:LYS:CB	35:1:927:PRO:HD3	2.05	0.78
10:K:206:LYS:O	10:K:223:ARG:NH1	2.17	0.78
17:R:331:ALA:HA	23:X:275:ARG:NH1	1.98	0.78
35:1:598:SER:O	35:1:602:LYS:HB2	1.83	0.78
36:3:592:LEU:HD22	36:3:605:LEU:HD13	1.65	0.78
17:R:163:MET:O	17:R:165:VAL:N	2.14	0.78
19:T:191:HIS:NE2	19:T:440:ASP:OD1	2.16	0.78
1:A:55:ASP:OD1	1:A:55:ASP:N	2.17	0.78
36:3:929:LYS:HE3	36:3:938:GLU:HB2	1.65	0.78
36:3:984:LYS:NZ	38:w:471:TRP:N	2.31	0.78
1:A:1756:SER:OG	35:1:943:LYS:CB	2.32	0.78
10:K:223:ARG:HH21	35:1:1018:PRO:HB3	1.49	0.78
1:A:221:ASN:HB2	1:A:227:ARG:HB2	1.64	0.78
34:q:106:ALA:HB1	34:t:106:ALA:HB1	1.64	0.78
34:t:8:SER:O	34:t:9:ASN:CB	2.32	0.78
35:1:572:HIS:ND1	35:1:612:THR:HG21	1.99	0.78
2:B:94:U:H1'	2:B:95:G:OP1	1.82	0.78
6:G:1:G:N3	6:G:1:G:O2'	2.15	0.78
34:q:106:ALA:HB1	34:t:106:ALA:CB	2.14	0.78
1:A:1826:VAL:O	1:A:1830:GLN:NE2	2.17	0.77
17:R:308:VAL:HA	24:Y:197:ILE:HG21	1.65	0.77
23:X:171:ARG:NH1	23:X:509:PRO:CB	2.47	0.77
36:3:979:ARG:H	38:w:478:GLU:CG	1.97	0.77
1:A:1756:SER:OG	35:1:943:LYS:HD2	1.81	0.77
36:3:463:ARG:HB2	36:3:510:LEU:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:180:LYS:HA	22:W:200:VAL:H	1.49	0.77
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.13	0.77
17:R:314:GLN:HA	23:X:290:GLU:OE1	1.85	0.77
34:q:60:PRO:CB	34:s:93:ARG:O	2.32	0.77
36:3:136:GLU:OE2	36:3:189:TYR:OH	2.00	0.77
24:Y:245:CYS:SG	24:Y:246:LYS:N	2.58	0.77
36:3:464:ARG:HG2	36:3:516:LEU:HD11	1.67	0.77
6:G:95:U:OP2	35:1:1106:ARG:HG3	1.83	0.77
35:1:1300:LEU:HG	42:5:43:TYR:OH	1.84	0.77
35:1:625:ARG:CB	35:1:666:LYS:HZ1	1.97	0.77
1:A:923:ASP:OD2	1:A:1439:ARG:NH1	2.18	0.77
11:L:163:GLN:HB3	11:L:168:LYS:HZ3	1.49	0.77
15:P:186:ARG:HB2	24:Y:49:PHE:CD1	2.19	0.77
36:3:525:ARG:HG3	36:3:533:VAL:HG13	1.67	0.77
9:J:206:LEU:CD2	9:J:207:PRO:HD3	2.14	0.77
34:q:60:PRO:O	34:s:93:ARG:CB	2.32	0.77
1:A:1578:ARG:HB2	10:K:224:SER:OG	1.84	0.76
3:C:144:CYS:SG	3:C:313:GLN:NE2	2.58	0.76
9:J:205:LEU:HD22	9:J:205:LEU:C	2.10	0.76
35:1:549:ARG:HH22	35:1:586:ASP:CG	1.93	0.76
35:1:821:HIS:CD2	35:1:861:ALA:CB	2.67	0.76
35:1:1056:MET:HB2	39:2:561:MET:HE2	1.67	0.76
36:3:228:LEU:HD21	36:3:250:ILE:HG21	1.66	0.76
11:L:163:GLN:HA	11:L:163:GLN:NE2	2.00	0.76
23:X:480:SER:OG	23:X:485:ASP:OD1	2.04	0.76
28:n:32:VAL:HA	28:n:37:ASN:O	1.85	0.76
3:C:684:LYS:HB3	3:C:795:VAL:HB	1.67	0.76
23:X:242:LYS:O	23:X:246:LEU:HB2	1.86	0.76
36:3:115:ILE:HG21	42:5:19:ILE:HB	1.67	0.76
36:3:351:SER:H	36:3:356:HIS:HB3	1.50	0.76
4:E:135:VAL:HG13	4:E:144:VAL:HG23	1.68	0.76
8:I:621:ARG:O	8:I:625:PRO:HD2	1.85	0.76
4:E:216:ASP:OD2	4:E:218:LYS:NZ	2.18	0.76
23:X:961:THR:O	23:X:965:GLN:NE2	2.19	0.76
35:1:524:ARG:NH1	35:1:562:LYS:O	2.18	0.76
2:B:41:U:C4	6:G:0:G:N2	2.53	0.76
35:1:554:LYS:HA	35:1:558:ARG:HH21	1.50	0.76
35:1:703:THR:CG2	35:1:745:ALA:HB3	2.15	0.76
36:3:978:LEU:CD2	38:w:480:GLU:HB3	2.15	0.76
36:3:1115:GLU:HG2	39:2:708:TRP:HE1	1.49	0.76
39:2:646:PRO:O	39:2:648:LEU:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:303:GLU:CB	8:I:326:ASP:O	2.34	0.76
34:q:8:SER:O	34:q:9:ASN:CB	2.34	0.76
36:3:89:ILE:HD12	36:3:103:HIS:HB2	1.67	0.76
1:A:57:GLN:N	1:A:57:GLN:HE21	1.84	0.76
35:1:793:LYS:HE2	35:1:839:GLU:HG3	1.67	0.76
36:3:459:VAL:HG22	36:3:476:VAL:HA	1.68	0.76
21:V:576:THR:HB	21:V:579:SER:H	1.49	0.75
35:1:819:TRP:CZ3	35:1:867:MET:CE	2.68	0.75
36:3:325:ILE:N	36:3:375:SER:OG	2.20	0.75
6:G:96:U:OP1	35:1:1149:LYS:CE	2.33	0.75
35:1:1001:VAL:HG22	35:1:1009:MET:CE	2.15	0.75
2:B:18:C:O2	2:B:59:G:N2	2.19	0.75
7:H:28:C:O2'	7:H:29:A:N3	2.18	0.75
1:A:1830:GLN:HB3	1:A:1836:LEU:HD22	1.68	0.75
17:R:359:ARG:HB3	17:R:363:ARG:HH21	1.52	0.75
25:Z:90:PRO:CB	25:Z:109:ASN:CB	2.64	0.75
36:3:878:ASP:OD1	36:3:879:LEU:N	2.18	0.75
41:7:22:LEU:N	41:7:67:SER:O	2.18	0.75
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.19	0.75
4:E:312:TRP:HE1	4:E:319:ILE:HG12	1.50	0.75
35:1:710:ALA:HB1	35:1:752:TYR:CD1	2.20	0.75
35:1:1001:VAL:CG2	35:1:1009:MET:CE	2.61	0.75
36:3:412:ILE:H	36:3:1105:GLN:HE22	1.34	0.75
39:2:646:PRO:C	39:2:648:LEU:H	1.94	0.75
2:B:93:U:O4	30:d:65:ARG:CA	2.35	0.75
35:1:1130:PRO:HB3	39:2:528:ILE:HG23	1.68	0.75
24:Y:246:LYS:HB2	24:Y:311:ILE:HA	1.67	0.75
36:3:189:TYR:HA	42:5:73:LEU:HD12	1.68	0.75
36:3:1013:ARG:NH2	36:3:1064:ASP:OD1	2.19	0.75
1:A:1255:THR:HG22	1:A:1526:LEU:HD21	1.69	0.75
21:V:539:LEU:HD13	21:V:543:LYS:HB3	1.68	0.75
36:3:487:ILE:HA	36:3:491:VAL:HG13	1.69	0.75
36:3:978:LEU:HD22	38:w:480:GLU:HB3	1.69	0.75
18:S:18:THR:HA	18:S:159:ILE:HA	1.69	0.74
36:3:114:ARG:CZ	42:5:37:ARG:CB	2.65	0.74
1:A:362:ARG:NH1	21:V:323:LEU:C	2.46	0.74
35:1:694:LEU:HD13	35:1:727:VAL:HG21	1.68	0.74
36:3:228:LEU:HD12	36:3:229:GLU:H	1.52	0.74
36:3:1040:ASP:OD2	36:3:1043:THR:N	2.20	0.74
19:T:267:ASP:OD1	19:T:267:ASP:N	2.21	0.74
21:V:484:SER:O	21:V:487:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:641:PRO:N	39:2:641:PRO:CB	2.51	0.74
11:L:167:ALA:HA	11:L:170:LYS:HE3	1.68	0.74
13:N:53:HIS:NE2	13:N:85:ASP:OD2	2.19	0.74
15:P:206:LYS:HB3	15:P:218:GLU:HG2	1.69	0.74
23:X:219:ARG:NH2	24:Y:292:GLU:OE2	2.20	0.74
23:X:787:GLU:HB2	35:1:542:PRO:CG	2.18	0.74
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.05	0.74
35:1:625:ARG:HB3	35:1:666:LYS:HZ2	1.51	0.74
36:3:932:ASN:HB2	36:3:936:LYS:HE3	1.69	0.74
36:3:969:VAL:HB	36:3:981:CYS:HB2	1.69	0.74
1:A:658:ARG:NH1	5:F:67:G:OP2	2.20	0.74
23:X:919:GLU:HA	23:X:922:LEU:HB2	1.69	0.74
34:s:8:SER:O	34:s:9:ASN:CB	2.35	0.74
36:3:206:GLN:HG3	36:3:231:HIS:HD2	1.52	0.74
1:A:875:HIS:CE1	23:X:866:ASN:HB3	2.22	0.74
6:G:83:A:N6	38:w:400:HIS:NE2	2.35	0.74
35:1:840:LEU:O	35:1:844:VAL:CG2	2.35	0.74
36:3:511:LEU:HD23	36:3:512:GLY:H	1.53	0.74
1:A:1870:ASP:N	1:A:1870:ASP:OD1	2.20	0.74
6:G:1:G:C2	10:K:218:LYS:HG3	2.22	0.74
35:1:722:GLU:OE1	35:1:722:GLU:N	2.21	0.74
30:i:20:MET:HA	30:i:29:TYR:O	1.86	0.74
4:E:166:LEU:HD11	4:E:178:LEU:HG	1.70	0.73
7:H:181:G:N2	33:l:52:ASP:O	2.19	0.73
9:J:438:TYR:O	9:J:442:ARG:HB2	1.88	0.73
17:R:125:MET:N	17:R:125:MET:SD	2.61	0.73
23:X:428:LYS:HD2	23:X:551:ALA:HB1	1.70	0.73
35:1:610:ILE:HG22	35:1:647:PHE:CE1	2.23	0.73
39:2:642:PRO:HA	40:4:66:ASP:HA	1.70	0.73
1:A:1382:SER:HB2	1:A:1415:GLY:HA2	1.69	0.73
4:E:255:MET:HB2	4:E:282:HIS:HB3	1.71	0.73
14:O:34:ILE:O	17:R:197:ILE:HA	1.87	0.73
21:V:581:ILE:HA	21:V:584:LYS:HG2	1.71	0.73
23:X:242:LYS:NZ	24:Y:220:GLN:O	2.21	0.73
35:1:861:ALA:O	35:1:864:TYR:N	2.17	0.73
36:3:193:ASP:HA	42:5:79:PRO:CG	2.18	0.73
4:E:189:THR:OG1	4:E:191:GLN:OE1	2.06	0.73
35:1:821:HIS:HD2	35:1:861:ALA:HB3	1.50	0.73
12:M:165:ASN:HB2	17:R:95:LYS:HB3	1.70	0.73
17:R:328:ALA:CB	24:Y:226:MET:SD	2.76	0.73
41:7:21:ARG:NH1	41:7:68:ASP:OD1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:HIS:HE1	23:X:866:ASN:HB3	1.51	0.73
6:G:99:C:N4	7:H:32:U:N3	2.25	0.73
22:W:321:GLU:HA	26:y:42:GLU:N	2.02	0.73
35:1:841:ALA:HA	35:1:849:ILE:HG13	1.70	0.73
35:1:897:LEU:CD2	35:1:932:ILE:HG13	2.18	0.73
41:7:73:LYS:O	41:7:77:ILE:HG13	1.88	0.73
1:A:729:PRO:HG2	12:M:226:TYR:CE1	2.24	0.73
1:A:1011:ALA:HB2	11:L:80:THR:HB	1.71	0.73
23:X:752:VAL:O	23:X:757:ARG:NH2	2.21	0.73
7:H:43:U:O2'	7:H:44:U:O5'	2.05	0.73
14:O:34:ILE:CA	17:R:197:ILE:HD13	2.18	0.73
17:R:335:ARG:CB	23:X:272:TYR:CB	2.67	0.73
6:G:19:G:H22	14:O:194:ALA:C	1.96	0.72
12:M:224:ARG:HH11	12:M:224:ARG:CG	2.02	0.72
35:1:717:THR:HB	35:1:718:PRO:HD2	1.71	0.72
36:3:565:TYR:HE1	36:3:619:LEU:HB2	1.54	0.72
39:2:491:LEU:O	39:2:494:THR:OG1	2.06	0.72
14:O:34:ILE:O	17:R:197:ILE:HD13	1.89	0.72
35:1:1167:TYR:HE2	39:2:581:LYS:HG2	1.51	0.72
36:3:1026:ASP:OD1	36:3:1026:ASP:N	2.18	0.72
36:3:1160:HIS:NE2	36:3:1175:ASP:OD2	2.20	0.72
2:B:117:A:N1	30:d:26:GLY:HA3	2.03	0.72
23:X:741:TRP:CD1	35:1:782:GLU:HB3	2.24	0.72
36:3:1133:THR:O	39:2:712:GLU:CB	2.37	0.72
1:A:1652:MET:HG2	1:A:1719:PHE:HA	1.72	0.72
6:G:105:C:H4'	6:G:106:C:OP2	1.88	0.72
23:X:171:ARG:HH12	23:X:509:PRO:CG	2.01	0.72
29:h:73:MET:HA	29:h:92:LYS:O	1.89	0.72
1:A:888:GLN:O	1:A:889:ARG:NH1	2.22	0.72
17:R:321:GLU:HB2	23:X:283:TYR:CE2	2.25	0.72
19:T:188:PRO:HG2	19:T:502:VAL:HG11	1.70	0.72
23:X:689:VAL:O	23:X:734:CYS:HA	1.89	0.72
35:1:600:LEU:O	35:1:604:ALA:HB2	1.90	0.72
32:k:19:LEU:O	32:k:26:HIS:HA	1.90	0.72
3:C:778:PRO:HB2	3:C:821:LEU:HD21	1.71	0.72
4:E:128:SER:OG	4:E:130:ASP:OD1	2.03	0.72
35:1:819:TRP:HZ3	35:1:868:VAL:HG12	1.54	0.72
35:1:1276:SER:N	36:3:113:ARG:HH22	1.87	0.72
36:3:114:ARG:NH2	42:5:37:ARG:HD2	2.03	0.72
36:3:189:TYR:CA	42:5:73:LEU:HD12	2.19	0.72
36:3:581:LYS:HD2	36:3:625:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1838:LYS:O	1:A:1841:THR:OG1	2.07	0.72
19:T:223:SER:OG	19:T:225:ASP:OD2	2.03	0.72
35:1:528:ALA:HA	35:1:531:LEU:HB2	1.72	0.72
35:1:553:VAL:HA	35:1:556:ILE:HG22	1.72	0.72
35:1:613:MET:HB3	35:1:632:PHE:CE2	2.24	0.72
35:1:1292:LYS:NZ	42:5:79:PRO:O	2.23	0.72
38:w:480:GLU:HA	38:w:486:VAL:HA	1.70	0.72
1:A:159:ARG:NH1	1:A:159:ARG:HA	2.05	0.72
4:E:137:ASP:O	4:E:141:GLY:N	2.19	0.72
15:P:183:LYS:O	15:P:183:LYS:HD3	1.90	0.72
23:X:945:ALA:HA	23:X:1011:VAL:HG11	1.71	0.72
1:A:27:GLU:OE1	1:A:31:GLN:NE2	2.22	0.72
2:B:18:C:N3	2:B:59:G:N1	2.34	0.72
2:B:92:U:N3	28:b:36:MET:CA	2.53	0.72
17:R:160:ALA:HA	17:R:163:MET:HE3	1.71	0.72
17:R:327:MET:HB2	23:X:279:LEU:HD11	1.71	0.72
24:Y:51:ILE:HD11	24:Y:112:THR:HG23	1.72	0.72
1:A:1637:TRP:O	1:A:1656:THR:HA	1.89	0.72
24:Y:62:GLY:O	24:Y:107:GLN:NE2	2.23	0.72
35:1:617:ILE:HA	35:1:663:THR:HG21	1.72	0.72
29:h:108:VAL:HA	30:i:64:ILE:HA	1.71	0.72
1:A:855:ARG:HG3	1:A:1520:ASN:CB	2.03	0.71
7:H:43:U:H2'	7:H:44:U:C6	2.25	0.71
17:R:331:ALA:HA	23:X:275:ARG:HH12	1.55	0.71
24:Y:122:VAL:HB	24:Y:123:HIS:HD2	1.53	0.71
35:1:876:MET:HE3	35:1:920:ALA:HB3	1.72	0.71
1:A:419:ARG:NH2	1:A:423:ASP:O	2.23	0.71
9:J:363:ARG:NH1	9:J:386:GLU:OE2	2.23	0.71
35:1:582:LEU:HG	35:1:634:VAL:HG21	1.72	0.71
36:3:1116:SER:CA	39:2:708:TRP:HZ2	2.03	0.71
38:w:421:ALA:HA	38:w:424:ARG:HE	1.53	0.71
1:A:1992:GLY:HA2	1:A:1997:VAL:HG23	1.73	0.71
15:P:186:ARG:HG2	15:P:186:ARG:NH1	2.03	0.71
16:Q:497:SER:O	16:Q:500:GLY:N	2.23	0.71
35:1:802:GLU:HB2	35:1:805:TYR:H	1.55	0.71
41:7:71:TYR:CE2	41:7:81:ASP:HB2	2.25	0.71
2:B:96:A:H4'	2:B:97:G:H5''	1.72	0.71
2:B:96:A:H61	32:f:23:GLY:H	1.38	0.71
36:3:22:PHE:O	36:3:75:LYS:NZ	2.19	0.71
36:3:193:ASP:C	42:5:79:PRO:CG	2.63	0.71
14:O:34:ILE:CB	17:R:197:ILE:HD12	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:164:TRP:CE2	23:X:539:VAL:CG2	2.72	0.71
23:X:405:ARG:NH2	23:X:438:GLU:OE1	2.24	0.71
1:A:1571:ILE:HG23	10:K:220:LEU:HD22	1.72	0.71
3:C:258:ASN:OD1	3:C:259:LYS:N	2.24	0.71
5:F:5:U:H5'	5:F:6:C:H4'	1.73	0.71
6:G:111:U:H4'	6:G:112:U:OP2	1.90	0.71
12:M:215:ASN:ND2	17:R:261:THR:H	1.88	0.71
14:O:163:HIS:O	14:O:182:ARG:N	2.23	0.71
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.09	0.71
3:C:750:LEU:HD22	20:U:63:LYS:O	1.91	0.71
11:L:163:GLN:CB	11:L:168:LYS:HZ1	1.92	0.71
12:M:224:ARG:HH11	12:M:224:ARG:CB	2.04	0.71
33:l:62:TYR:N	32:k:70:LEU:O	2.22	0.71
35:1:1276:SER:H	36:3:113:ARG:HH22	1.39	0.71
36:3:902:ASP:OD1	36:3:902:ASP:N	2.20	0.71
36:3:1048:ASP:OD1	36:3:1049:LYS:N	2.24	0.71
1:A:1399:GLN:OE1	1:A:1401:ARG:NH1	2.24	0.71
7:H:18:U:OP2	12:M:221:LYS:NZ	2.22	0.71
35:1:841:ALA:HB2	35:1:875:ILE:HD13	1.72	0.71
36:3:487:ILE:HG13	36:3:491:VAL:HG22	1.73	0.71
1:A:468:LYS:HZ2	1:A:469:LYS:H	1.39	0.70
35:1:1294:THR:O	42:5:76:CYS:HA	1.90	0.70
14:O:34:ILE:C	17:R:197:ILE:HD12	2.15	0.70
42:5:62:ALA:HA	42:5:65:ARG:HH12	1.56	0.70
35:1:1090:PRO:HA	35:1:1093:VAL:CG1	2.21	0.70
35:1:1108:ASN:O	35:1:1112:THR:HG22	1.91	0.70
1:A:41:GLN:HE22	1:A:45:TYR:HD2	1.38	0.70
1:A:857:ASN:ND2	1:A:860:GLN:OE1	2.23	0.70
1:A:1889:LEU:HD11	1:A:2012:LEU:HD21	1.73	0.70
2:B:87:A:N6	2:B:92:U:P	2.64	0.70
39:2:675:VAL:HA	39:2:681:PRO:HA	1.73	0.70
43:o:116:THR:HA	43:o:142:VAL:HA	1.74	0.70
4:E:277:PHE:HE2	4:E:300:ILE:HG21	1.56	0.70
36:3:208:LEU:HD13	36:3:250:ILE:HD11	1.71	0.70
30:i:33:LEU:HA	30:i:44:LEU:HA	1.73	0.70
15:P:41:ILE:HG13	19:T:318:ARG:HG3	1.72	0.70
19:T:195:LYS:HZ3	19:T:490:ARG:HD2	1.56	0.70
23:X:231:ARG:O	23:X:235:LEU:HG	1.92	0.70
36:3:642:ILE:O	36:3:703:ARG:NE	2.24	0.70
17:R:328:ALA:HB1	24:Y:226:MET:HA	1.73	0.70
1:A:1935:ARG:NE	1:A:1980:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:U:C1'	2:B:95:G:OP1	2.39	0.70
9:J:225:LEU:HG	11:L:211:ASN:HB2	1.74	0.70
17:R:328:ALA:CB	24:Y:226:MET:HA	2.21	0.70
36:3:1116:SER:CA	39:2:708:TRP:CZ2	2.75	0.70
36:3:1194:SER:OG	36:3:1199:ARG:O	2.10	0.70
6:G:84:U:OP2	38:w:396:LEU:HD11	1.91	0.70
15:P:67:GLU:OE2	19:T:476:ARG:NH2	2.23	0.70
23:X:501:LEU:HB3	23:X:532:LEU:HD21	1.73	0.70
35:1:532:PHE:CE2	35:1:574:ILE:HD11	2.26	0.70
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.25	0.69
35:1:1181:ASP:OD1	35:1:1182:LEU:N	2.24	0.69
35:1:1276:SER:H	36:3:113:ARG:NH2	1.90	0.69
36:3:189:TYR:HA	42:5:73:LEU:HD11	1.74	0.69
1:A:1831:LYS:HG3	1:A:1832:ARG:N	2.07	0.69
6:G:1:G:N2	10:K:219:PHE:CD2	2.59	0.69
6:G:95:U:OP2	35:1:1106:ARG:CD	2.40	0.69
35:1:734:GLY:O	35:1:738:HIS:CB	2.40	0.69
35:1:1299:GLU:HA	35:1:1302:TYR:HE2	1.56	0.69
11:L:55:ASP:HB3	11:L:58:ILE:HD12	1.74	0.69
36:3:565:TYR:HB3	36:3:577:TYR:HB3	1.72	0.69
36:3:833:GLU:O	36:3:836:ALA:N	2.23	0.69
36:3:1182:PHE:O	36:3:1190:GLN:NE2	2.24	0.69
23:X:592:LEU:HD23	23:X:593:GLU:H	1.57	0.69
35:1:1179:ASP:H	39:2:511:LEU:HD13	1.55	0.69
36:3:812:LYS:HD2	36:3:856:LYS:HE3	1.74	0.69
1:A:705:LYS:HD3	17:R:247:ILE:HB	1.75	0.69
4:E:277:PHE:CE2	4:E:300:ILE:HG21	2.28	0.69
13:N:120:ARG:NH1	13:N:142:CYS:SG	2.66	0.69
23:X:510:ASP:OD2	23:X:543:ARG:HG3	1.93	0.69
35:1:827:ARG:HB2	35:1:827:ARG:NH2	2.08	0.69
35:1:948:ARG:NH2	35:1:984:GLU:OE2	2.25	0.69
36:3:189:TYR:HB3	42:5:73:LEU:HD12	1.73	0.69
36:3:984:LYS:NZ	38:w:470:ARG:C	2.51	0.69
42:5:62:ALA:HA	42:5:65:ARG:NH1	2.07	0.69
2:B:93:U:O4	30:d:65:ARG:C	2.36	0.69
3:C:137:HIS:CD2	3:C:138:LEU:H	2.11	0.69
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.74	0.69
23:X:835:SER:OG	23:X:938:ARG:NH1	2.26	0.69
35:1:586:ASP:OD1	35:1:589:ALA:N	2.24	0.69
35:1:803:ALA:HA	35:1:843:LYS:HZ3	1.53	0.69
35:1:841:ALA:HB1	35:1:875:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1178:MET:HG2	39:2:591:TYR:CZ	2.27	0.69
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.23	0.69
36:3:384:THR:OG1	36:3:385:PHE:O	2.08	0.69
5:F:82:A:H4'	5:F:82:A:OP2	1.92	0.69
5:F:86:U:OP2	12:M:193:ARG:NH1	2.25	0.69
8:I:433:ALA:CB	8:I:482:LYS:CB	2.71	0.69
23:X:164:TRP:CZ2	23:X:539:VAL:CG2	2.72	0.69
36:3:968:ARG:HB2	36:3:970:TYR:HE2	1.57	0.69
1:A:372:PRO:HG3	3:C:341:LYS:HB3	1.74	0.68
1:A:987:LYS:NZ	3:C:61:GLU:OE1	2.19	0.68
4:E:68:GLU:HG2	4:E:347:SER:HB2	1.75	0.68
35:1:498:MET:HE1	35:1:530:PRO:HB2	1.76	0.68
35:1:613:MET:HB3	35:1:632:PHE:CZ	2.28	0.68
35:1:1293:ASN:HA	42:5:77:GLY:HA3	1.74	0.68
36:3:434:SER:OG	36:3:436:ARG:NE	2.25	0.68
1:A:1807:ILE:HD11	1:A:1841:THR:HG22	1.75	0.68
3:C:131:ASN:HA	3:C:201:ASN:HB2	1.75	0.68
3:C:759:LEU:HA	3:C:762:VAL:HG12	1.74	0.68
4:E:146:ARG:HD2	4:E:148:LYS:HE2	1.75	0.68
12:M:217:LYS:HD2	12:M:217:LYS:O	1.93	0.68
23:X:167:THR:HG23	23:X:770:LEU:HB3	1.75	0.68
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.25	0.68
6:G:116:C:C1'	17:R:371:ARG:HA	2.23	0.68
38:w:422:PHE:O	38:w:425:HIS:ND1	2.20	0.68
9:J:330:ARG:NH2	12:M:149:TYR:OH	2.24	0.68
35:1:1012:PRO:HG2	35:1:1015:ASP:OD1	1.93	0.68
36:3:867:ARG:HD2	36:3:869:MET:HE3	1.76	0.68
1:A:1741:TYR:CB	35:1:973:HIS:NE2	2.56	0.68
11:L:67:GLU:OE1	11:L:91:ARG:NH2	2.26	0.68
35:1:503:LYS:HE2	35:1:511:MET:HG2	1.72	0.68
36:3:981:CYS:SG	36:3:1019:ASN:ND2	2.66	0.68
1:A:682:ASP:OD1	1:A:746:LYS:NZ	2.25	0.68
1:A:1544:ARG:NE	1:A:1672:ASP:OD2	2.26	0.68
7:H:173:C:H2'	7:H:174:A:C8	2.28	0.68
9:J:206:LEU:CB	9:J:207:PRO:CD	2.72	0.68
19:T:471:ASP:OD1	19:T:473:SER:OG	2.07	0.68
12:M:215:ASN:HD21	17:R:260:TYR:CA	2.07	0.68
13:N:25:LEU:HD13	13:N:56:LYS:HG2	1.76	0.68
23:X:281:ARG:NH1	23:X:281:ARG:HA	2.09	0.68
25:Z:85:LYS:C	25:Z:87:TYR:N	2.42	0.68
35:1:1010:THR:HG1	35:1:1011:PRO:HD3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:745:PHE:HB2	36:3:755:VAL:HG23	1.75	0.68
33:l:49:THR:HA	33:l:55:VAL:HA	1.74	0.68
1:A:1936:LEU:O	1:A:1940:LEU:HG	1.93	0.68
17:R:180:THR:HG23	17:R:194:GLN:HG2	1.76	0.68
35:1:803:ALA:N	35:1:843:LYS:HZ2	1.88	0.68
36:3:193:ASP:HA	42:5:79:PRO:HG3	1.74	0.68
36:3:215:LEU:H	36:3:215:LEU:HD12	1.59	0.68
17:R:327:MET:CB	23:X:279:LEU:HD11	2.23	0.68
35:1:819:TRP:CH2	35:1:867:MET:HE3	2.28	0.68
36:3:705:ARG:HA	36:3:710:GLU:HA	1.76	0.68
1:A:1578:ARG:HE	1:A:1746:ARG:NH2	1.91	0.68
2:B:8:G:H22	2:B:70:A:H1'	1.57	0.68
2:B:93:U:O4'	29:c:104:ASP:CA	2.42	0.68
2:B:95:G:H21	2:B:96:A:C5'	2.06	0.68
35:1:694:LEU:HD12	35:1:694:LEU:H	1.59	0.68
35:1:997:LEU:HD13	35:1:1016:LEU:HD21	1.75	0.68
36:3:328:LYS:NZ	36:3:370:GLU:OE2	2.26	0.68
1:A:532:THR:OG1	6:G:3:A:OP1	2.11	0.67
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.75	0.67
1:A:1962:THR:HG23	1:A:1966:HIS:HB2	1.75	0.67
35:1:621:ASP:HB3	35:1:624:VAL:HG22	1.75	0.67
35:1:926:LYS:HB3	35:1:927:PRO:CD	2.16	0.67
36:3:499:PHE:HZ	36:3:516:LEU:HD22	1.57	0.67
4:E:251:LEU:HD21	4:E:300:ILE:HG13	1.76	0.67
6:G:117:A:H2'	24:Y:246:LYS:HE2	1.76	0.67
21:V:543:LYS:HA	21:V:546:ASN:ND2	2.08	0.67
35:1:1257:PRO:CD	39:2:482:ALA:HB2	2.20	0.67
36:3:185:LEU:HG	36:3:235:LEU:HD11	1.77	0.67
39:2:635:ALA:HB3	40:4:73:ILE:HA	0.68	0.67
3:C:193:THR:HG23	3:C:194:LYS:HD2	1.75	0.67
9:J:311:GLN:OE1	9:J:311:GLN:N	2.24	0.67
34:q:53:ILE:CB	34:r:22:ASN:CB	2.73	0.67
35:1:617:ILE:HD13	35:1:651:VAL:HB	1.75	0.67
35:1:625:ARG:CB	35:1:666:LYS:NZ	2.51	0.67
35:1:680:LEU:HA	35:1:683:LEU:HB2	1.75	0.67
36:3:427:CYS:SG	36:3:428:GLY:N	2.66	0.67
1:A:59:GLU:OE1	13:N:87:ASN:HB2	1.93	0.67
17:R:332:ARG:HA	23:X:272:TYR:CD1	2.28	0.67
35:1:641:ILE:N	35:1:642:PRO:HD2	2.10	0.67
36:3:485:LEU:HD23	36:3:491:VAL:HG12	1.76	0.67
36:3:586:ASP:HB3	36:3:610:VAL:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:VAL:HG11	21:V:467:LEU:HD13	1.76	0.67
2:B:87:A:N6	2:B:92:U:OP2	2.26	0.67
2:B:97:G:H1	2:B:116:U:H3	1.41	0.67
4:E:217:ILE:HB	4:E:231:MET:HG3	1.74	0.67
17:R:389:SER:HA	17:R:392:ILE:HD12	1.75	0.67
36:3:434:SER:HG	36:3:436:ARG:HE	1.43	0.67
4:E:294:SER:OG	4:E:299:LYS:O	2.11	0.67
6:G:102:G:H2'	6:G:102:G:N3	2.08	0.67
36:3:39:GLU:OE2	36:3:55:THR:OG1	2.12	0.67
41:7:46:CYS:H	41:7:85:CYS:HB2	1.58	0.67
1:A:873:ASN:ND2	1:A:876:GLU:OE1	2.28	0.67
1:A:946:GLU:HB3	1:A:950:LEU:HD23	1.76	0.67
15:P:212:ASN:ND2	19:T:458:SER:OG	2.27	0.67
35:1:827:ARG:HH21	35:1:827:ARG:H	1.43	0.67
36:3:697:ARG:NH2	36:3:717:SER:OG	2.28	0.67
36:3:983:ASN:ND2	36:3:1021:LEU:O	2.25	0.67
5:F:43:A:H1'	6:G:5:G:N2	2.10	0.67
17:R:367:ARG:O	17:R:371:ARG:HG3	1.93	0.67
35:1:732:TRP:NE1	35:1:768:GLU:OE2	2.27	0.67
41:7:37:VAL:HB	41:7:38:ARG:HG3	1.75	0.67
28:n:23:THR:HA	28:n:47:LEU:HA	1.77	0.67
1:A:747:ALA:O	1:A:751:THR:HG22	1.94	0.67
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.77	0.67
23:X:430:THR:HG23	23:X:465:VAL:HG22	1.77	0.67
36:3:187:MET:HE2	42:5:73:LEU:HD22	1.77	0.67
36:3:603:ARG:HG3	36:3:604:PHE:CE1	2.29	0.67
36:3:620:ASP:N	36:3:620:ASP:OD1	2.27	0.67
36:3:775:ASN:HD22	36:3:775:ASN:H	1.40	0.67
36:3:840:ALA:O	36:3:844:ASN:ND2	2.27	0.67
9:J:411:MET:SD	9:J:416:TYR:HE2	2.18	0.67
35:1:1299:GLU:HA	35:1:1302:TYR:CE2	2.30	0.67
3:C:508:LYS:HG3	3:C:524:ILE:HG13	1.77	0.66
21:V:547:VAL:O	21:V:550:MET:HB2	1.95	0.66
35:1:1276:SER:O	35:1:1276:SER:OG	2.07	0.66
36:3:191:GLU:HA	36:3:194:ASN:HD22	1.59	0.66
32:k:42:ILE:N	32:k:60:VAL:O	2.27	0.66
3:C:213:ASP:OD1	3:C:616:SER:HB2	1.96	0.66
7:H:125:G:H2'	7:H:126:A:C8	2.30	0.66
11:L:201:LYS:HD2	11:L:202:ARG:H	1.58	0.66
14:O:34:ILE:O	17:R:197:ILE:CD1	2.43	0.66
3:C:758:LEU:HB3	3:C:796:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:628:ILE:O	21:V:632:THR:OG1	2.12	0.66
23:X:583:TYR:O	23:X:585:LYS:NZ	2.22	0.66
35:1:803:ALA:N	35:1:843:LYS:HZ1	1.92	0.66
36:3:984:LYS:HZ1	38:w:471:TRP:HB2	1.58	0.66
33:l:27:VAL:O	33:l:48:VAL:HA	1.96	0.66
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.78	0.66
23:X:234:TYR:O	23:X:238:ARG:HB2	1.96	0.66
35:1:1277:GLN:H	36:3:113:ARG:NH2	1.94	0.66
36:3:147:ASP:OD1	36:3:151:ARG:N	2.28	0.66
36:3:978:LEU:CD1	38:w:480:GLU:HG2	2.25	0.66
29:h:107:ILE:O	30:i:65:ARG:N	2.29	0.66
5:F:41:A:N1	6:G:6:A:N6	2.41	0.66
21:V:456:ARG:NE	21:V:492:MET:SD	2.68	0.66
36:3:521:PRO:O	36:3:543:THR:OG1	2.12	0.66
39:2:476:GLU:HG2	39:2:477:MET:H	1.61	0.66
6:G:105:C:OP1	23:X:993:THR:OG1	2.13	0.66
19:T:245:HIS:HE2	19:T:263:SER:HG	1.44	0.66
23:X:827:MET:HB3	23:X:946:GLY:HA3	1.78	0.66
35:1:758:ASP:O	35:1:762:ALA:N	2.15	0.66
36:3:121:LEU:HB2	36:3:132:ILE:HD12	1.78	0.66
36:3:979:ARG:CZ	38:w:478:GLU:OE1	2.43	0.66
36:3:1132:PHE:O	39:2:711:LEU:HD23	1.96	0.66
34:q:60:PRO:CB	34:s:94:GLN:N	2.57	0.66
35:1:702:ARG:HD2	35:1:746:PHE:CZ	2.30	0.66
36:3:449:VAL:HG13	36:3:763:ARG:HG2	1.76	0.66
38:w:473:PRO:O	38:w:477:GLU:HB3	1.95	0.66
41:7:26:CYS:SG	41:7:61:CYS:HB2	2.36	0.66
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	1.94	0.66
7:H:53:U:OP1	39:2:450:SER:OG	2.09	0.66
9:J:409:GLU:HG2	9:J:410:HIS:CD2	2.31	0.66
17:R:330:LYS:HZ2	23:X:275:ARG:HH22	1.44	0.66
36:3:189:TYR:CA	42:5:73:LEU:CD1	2.71	0.66
36:3:288:VAL:HG23	36:3:289:CYS:H	1.59	0.66
39:2:526:ASP:OD1	39:2:526:ASP:N	2.18	0.66
1:A:75:ASP:O	1:A:77:THR:N	2.29	0.66
1:A:1664:ILE:HG22	1:A:1703:ILE:HB	1.77	0.66
3:C:255:VAL:HB	3:C:307:VAL:HG12	1.77	0.66
36:3:511:LEU:HD21	36:3:517:VAL:HG23	1.78	0.66
36:3:635:ALA:HB3	36:3:669:LEU:HD13	1.78	0.66
36:3:700:LYS:HB3	36:3:702:PHE:CZ	2.30	0.66
39:2:642:PRO:N	39:2:642:PRO:CB	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:108:U:H5''	23:X:676:ILE:HB	1.78	0.66
11:L:173:GLU:OE1	11:L:173:GLU:HA	1.94	0.66
23:X:698:LYS:HD3	23:X:707:GLU:HG3	1.78	0.66
36:3:926:TYR:HB3	36:3:928:TYR:HE2	1.60	0.66
36:3:1116:SER:N	39:2:708:TRP:CZ2	2.54	0.66
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.76	0.65
23:X:769:SER:OG	23:X:816:ALA:HB1	1.96	0.65
1:A:163:ARG:NH2	1:A:576:ASP:OD1	2.30	0.65
3:C:192:ASP:CG	3:C:193:THR:H	2.04	0.65
15:P:186:ARG:HH11	15:P:186:ARG:CG	2.09	0.65
17:R:315:LYS:O	17:R:318:GLU:HG3	1.96	0.65
24:Y:104:HIS:CE1	24:Y:124:THR:HG1	2.14	0.65
35:1:862:GLU:OE1	35:1:904:THR:OG1	2.14	0.65
36:3:169:HIS:ND1	36:3:234:PHE:HB2	2.10	0.65
36:3:665:LEU:HD11	36:3:667:ILE:HG13	1.78	0.65
1:A:678:GLU:OE1	1:A:774:LYS:NZ	2.27	0.65
4:E:236:ASP:HB2	4:E:256:ASP:HB3	1.78	0.65
6:G:98:U:O4	7:H:33:G:N1	2.25	0.65
12:M:209:ASP:OD2	17:R:263:PRO:HG3	1.96	0.65
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.76	0.65
1:A:1776:ILE:HG22	1:A:1859:LYS:HZ3	1.61	0.65
24:Y:94:VAL:HG13	24:Y:110:ILE:HG13	1.77	0.65
35:1:699:GLN:HE22	35:1:738:HIS:CE1	2.12	0.65
35:1:1126:PHE:HB2	39:2:575:PHE:CD2	2.31	0.65
36:3:1133:THR:O	39:2:712:GLU:HB3	1.96	0.65
1:A:1703:ILE:HD13	1:A:1714:ALA:HB2	1.76	0.65
1:A:1809:ILE:HB	1:A:1818:PHE:HD2	1.62	0.65
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.31	0.65
35:1:712:LEU:O	35:1:716:ALA:HB3	1.97	0.65
35:1:721:ILE:C	35:1:721:ILE:HD12	2.21	0.65
36:3:1117:LEU:O	36:3:1128:ILE:HA	1.96	0.65
7:H:119:G:H8	7:H:119:G:O5'	1.80	0.65
36:3:568:MET:HA	36:3:574:LEU:HA	1.79	0.65
36:3:680:ASP:CG	36:3:681:PRO:HD2	2.21	0.65
1:A:47:GLU:H	1:A:47:GLU:CD	2.03	0.65
1:A:1778:TRP:HB2	1:A:1861:ILE:HD12	1.79	0.65
35:1:806:ILE:CD1	35:1:843:LYS:HE3	2.26	0.65
36:3:777:VAL:HG22	36:3:779:PHE:HE1	1.61	0.65
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.44	0.65
5:F:43:A:H2	6:G:4:A:H61	1.44	0.65
21:V:622:ARG:HA	21:V:625:ARG:HE	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:527:LEU:HD22	23:X:763:VAL:HG11	1.77	0.65
23:X:910:ARG:O	23:X:914:VAL:HG13	1.96	0.65
24:Y:253:ASP:OD1	24:Y:253:ASP:N	2.29	0.65
35:1:549:ARG:NH2	35:1:589:ALA:HB2	2.12	0.65
36:3:206:GLN:HG3	36:3:231:HIS:CD2	2.31	0.65
23:X:824:LEU:HD21	23:X:844:ALA:HB1	1.77	0.65
35:1:662:HIS:CE1	35:1:700:LYS:HB3	2.32	0.65
35:1:897:LEU:HD21	35:1:932:ILE:CG1	2.21	0.65
4:E:118:ASN:HD21	4:E:122:SER:H	1.45	0.65
23:X:164:TRP:NE1	23:X:539:VAL:HG23	2.12	0.65
23:X:510:ASP:CG	23:X:543:ARG:HD3	2.21	0.65
24:Y:267:ARG:N	24:Y:287:GLU:O	2.29	0.65
35:1:1276:SER:N	36:3:113:ARG:NH2	2.44	0.65
36:3:911:LYS:HB3	36:3:922:GLY:O	1.96	0.65
1:A:154:GLU:OE2	1:A:158:ARG:NE	2.29	0.64
6:G:88:G:O2'	6:G:89:U:H5'	1.98	0.64
23:X:618:GLN:HG2	23:X:648:TYR:CD2	2.32	0.64
24:Y:39:TYR:N	24:Y:156:ILE:O	2.28	0.64
35:1:770:MET:HE1	35:1:795:CYS:SG	2.36	0.64
35:1:1262:ARG:HB3	42:5:24:ALA:HB1	1.79	0.64
36:3:1009:PHE:HE1	36:3:1036:ALA:HB2	1.61	0.64
1:A:1201:ARG:O	1:A:1203:SER:N	2.30	0.64
35:1:662:HIS:CD2	35:1:704:ILE:HG21	2.32	0.64
35:1:696:ASP:O	35:1:702:ARG:NH1	2.29	0.64
1:A:382:GLU:HG3	3:C:354:ARG:HG3	1.77	0.64
3:C:926:ALA:HA	3:C:929:LEU:HG	1.80	0.64
11:L:149:LEU:HA	11:L:152:LEU:HD12	1.79	0.64
1:A:90:GLY:HA3	17:R:209:PRO:HD3	1.79	0.64
21:V:525:PHE:HB3	21:V:560:LEU:HD21	1.80	0.64
39:2:469:VAL:HG12	39:2:471:ARG:H	1.62	0.64
41:7:10:PHE:HB3	41:7:12:ARG:HG2	1.79	0.64
24:Y:32:CYS:SG	24:Y:159:THR:OG1	2.49	0.64
36:3:260:ASN:OD1	36:3:261:PHE:N	2.30	0.64
15:P:206:LYS:CB	15:P:218:GLU:HG2	2.27	0.64
35:1:613:MET:CA	35:1:613:MET:HE3	2.28	0.64
35:1:1006:MET:HA	35:1:1009:MET:HG3	1.80	0.64
1:A:57:GLN:HE21	1:A:57:GLN:H	1.45	0.64
1:A:1789:THR:HG22	1:A:1803:ILE:HD11	1.78	0.64
11:L:163:GLN:CB	11:L:168:LYS:CE	2.76	0.64
11:L:188:ARG:O	11:L:192:ARG:HG2	1.98	0.64
23:X:234:TYR:CE1	24:Y:317:GLN:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:490:GLU:O	35:1:494:GLU:HG2	1.98	0.64
36:3:384:THR:OG1	36:3:385:PHE:N	2.31	0.64
36:3:747:SER:N	36:3:750:CYS:O	2.31	0.64
1:A:201:ALA:HA	1:A:204:LEU:HD23	1.78	0.64
1:A:1948:ASP:HA	1:A:1951:LYS:HD3	1.80	0.64
4:E:153:PHE:HB2	4:E:172:ASP:HB2	1.79	0.64
5:F:82:A:H2'	7:H:17:U:OP1	1.97	0.64
14:O:34:ILE:C	17:R:197:ILE:HD13	2.20	0.64
23:X:171:ARG:HD2	23:X:770:LEU:HD22	1.80	0.64
36:3:114:ARG:NH1	42:5:38:ASP:OD1	2.30	0.64
36:3:979:ARG:H	38:w:478:GLU:HG3	1.61	0.64
36:3:1017:ASN:OD1	36:3:1018:GLU:N	2.31	0.64
1:A:1778:TRP:O	1:A:1862:ILE:HG13	1.98	0.64
3:C:737:PRO:HD2	3:C:741:GLY:HA3	1.78	0.64
17:R:357:HIS:CD2	17:R:361:LYS:HE2	2.33	0.64
23:X:232:ARG:HA	23:X:235:LEU:HD12	1.80	0.64
3:C:381:LEU:HD22	3:C:416:LEU:HD21	1.78	0.64
5:F:37:C:H4'	5:F:38:G:OP2	1.97	0.64
9:J:185:ALA:HA	11:L:142:ILE:HD13	1.79	0.64
13:N:112:ASN:N	13:N:112:ASN:OD1	2.28	0.64
15:P:186:ARG:HA	24:Y:49:PHE:CE1	2.34	0.64
23:X:937:ILE:HG22	23:X:941:LYS:HD2	1.78	0.64
35:1:796:CYS:HA	35:1:801:VAL:HG11	1.77	0.64
36:3:794:SER:O	36:3:796:ASN:ND2	2.31	0.64
36:3:1031:ARG:HG2	36:3:1031:ARG:HH11	1.63	0.64
36:3:1188:ASN:OD1	36:3:1189:LYS:N	2.28	0.64
3:C:493:PHE:HD2	3:C:551:LEU:HG	1.62	0.63
4:E:175:THR:HG22	4:E:191:GLN:HG3	1.80	0.63
21:V:609:GLN:HE22	21:V:616:LEU:HD21	1.63	0.63
23:X:619:GLU:HA	23:X:622:GLU:OE1	1.97	0.63
35:1:1206:ASP:OD2	39:2:581:LYS:NZ	2.32	0.63
38:w:429:TRP:HB3	38:w:430:ARG:HH12	1.63	0.63
33:l:61:VAL:HA	32:k:71:GLU:HA	1.80	0.63
1:A:1528:GLN:O	1:A:1532:ARG:HB2	1.99	0.63
6:G:116:C:C4	17:R:370:SER:HB3	2.33	0.63
9:J:206:LEU:HD22	9:J:207:PRO:HD3	1.78	0.63
9:J:296:ARG:NH1	9:J:320:GLU:OE2	2.29	0.63
35:1:613:MET:HE3	35:1:613:MET:HA	1.80	0.63
36:3:982:GLU:CG	38:w:476:GLU:OE2	2.45	0.63
37:p:178:LYS:H	37:p:194:PHE:HA	1.62	0.63
1:A:357:ASN:HD22	3:C:862:PRO:HB3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:C:OP1	29:c:20:GLU:CA	2.46	0.63
4:E:312:TRP:HD1	4:E:319:ILE:HA	1.63	0.63
4:E:313:ASP:OD1	4:E:316:SER:N	2.28	0.63
24:Y:303:ASN:O	24:Y:310:ARG:NH1	2.30	0.63
36:3:452:LEU:HD12	36:3:453:PRO:HD2	1.79	0.63
38:w:429:TRP:O	38:w:432:ALA:N	2.31	0.63
1:A:1741:TYR:CZ	35:1:937:LEU:HD22	2.29	0.63
34:r:8:SER:CB	34:s:86:MET:CB	2.77	0.63
35:1:859:ASP:O	35:1:865:ARG:NE	2.27	0.63
36:3:734:LEU:HD12	36:3:767:LEU:HD22	1.79	0.63
36:3:884:GLN:NE2	36:3:884:GLN:O	2.32	0.63
36:3:1201:PRO:HA	36:3:1204:VAL:HG22	1.80	0.63
38:w:460:ALA:O	38:w:464:LEU:HG	1.97	0.63
1:A:1854:VAL:CG1	21:V:448:THR:HA	2.28	0.63
35:1:613:MET:HE3	35:1:613:MET:N	2.13	0.63
35:1:1165:TYR:CD1	39:2:575:PHE:CD1	2.86	0.63
36:3:169:HIS:HD2	36:3:170:VAL:H	1.44	0.63
36:3:1136:GLU:OE1	36:3:1136:GLU:N	2.27	0.63
2:B:90:U:H5	33:g:38:ASN:C	2.06	0.63
5:F:79:C:H1'	5:F:82:A:H2	1.62	0.63
23:X:621:ILE:HG12	23:X:672:VAL:HG12	1.80	0.63
36:3:25:THR:OG1	36:3:27:GLN:N	2.31	0.63
36:3:114:ARG:HD3	42:5:38:ASP:OD1	1.99	0.63
36:3:545:VAL:HG12	36:3:546:LYS:HG2	1.79	0.63
36:3:958:ARG:NH2	36:3:1014:TYR:OH	2.31	0.63
36:3:1049:LYS:HE3	42:5:52:TYR:CZ	2.34	0.63
1:A:1222:LYS:O	21:V:592:GLU:HG3	1.99	0.63
3:C:64:LYS:HA	15:P:206:LYS:NZ	2.13	0.63
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.81	0.63
11:L:166:LYS:HG3	11:L:170:LYS:HE2	1.80	0.63
15:P:77:ASP:O	15:P:78:ARG:NE	2.32	0.63
35:1:1179:ASP:CB	39:2:511:LEU:CB	2.76	0.63
1:A:1014:ASN:ND2	1:A:1014:ASN:O	2.32	0.63
2:B:89:U:H2'	2:B:90:U:H5''	1.79	0.63
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.80	0.63
11:L:188:ARG:HE	11:L:191:LEU:HD12	1.64	0.63
24:Y:14:ILE:HD12	24:Y:94:VAL:HG21	1.80	0.63
35:1:710:ALA:HB1	35:1:752:TYR:HD1	1.61	0.63
36:3:512:GLY:HA3	36:3:515:ALA:HB3	1.79	0.63
36:3:928:TYR:HB3	36:3:937:LEU:HB3	1.81	0.63
38:w:399:LEU:CD1	39:2:507:LYS:CD	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:28:GLN:O	32:k:45:CYS:HA	1.98	0.63
5:F:79:C:H1'	5:F:82:A:C2	2.33	0.63
1:A:485:THR:HG22	1:A:486:LYS:H	1.63	0.62
3:C:64:LYS:HA	15:P:206:LYS:HZ3	1.64	0.62
11:L:163:GLN:HB2	11:L:168:LYS:CE	2.29	0.62
35:1:1174:GLU:OE2	35:1:1210:HIS:NE2	2.26	0.62
35:1:1212:LEU:HD13	35:1:1237:LEU:HD13	1.81	0.62
36:3:966:LEU:HB2	36:3:968:ARG:HD2	1.81	0.62
1:A:1014:ASN:HD21	11:L:83:ARG:HB2	1.64	0.62
1:A:1768:TYR:HA	1:A:1771:LEU:HB2	1.79	0.62
2:B:88:A:H2'	2:B:88:A:N3	2.14	0.62
3:C:560:VAL:HG22	3:C:561:LYS:H	1.64	0.62
5:F:49:G:H2'	5:F:50:A:H8	1.64	0.62
9:J:311:GLN:HG3	12:M:131:GLN:HG2	1.80	0.62
14:O:235:TYR:N	14:O:301:LYS:O	2.32	0.62
21:V:620:ASN:ND2	21:V:623:ASN:OD1	2.31	0.62
24:Y:27:ASN:O	24:Y:31:LEU:HD12	1.99	0.62
1:A:707:ARG:HH22	7:H:17:U:H4'	1.64	0.62
1:A:1578:ARG:HB2	10:K:224:SER:CB	2.29	0.62
14:O:171:GLY:O	22:W:207:LYS:HA	1.99	0.62
24:Y:39:TYR:O	24:Y:185:GLN:NE2	2.32	0.62
35:1:1013:ILE:HD11	35:1:1049:TYR:CD2	2.34	0.62
35:1:1277:GLN:HG2	36:3:113:ARG:HD3	1.81	0.62
36:3:1010:ILE:HG12	36:3:1026:ASP:HB3	1.80	0.62
39:2:674:PRO:O	39:2:682:LEU:N	2.24	0.62
41:7:46:CYS:O	41:7:50:ASN:HB2	1.99	0.62
3:C:750:LEU:HD23	3:C:751:PRO:HD3	1.82	0.62
36:3:70:LEU:HD11	36:3:152:LEU:HD13	1.80	0.62
36:3:565:TYR:CE1	36:3:619:LEU:HB2	2.33	0.62
38:w:434:GLY:O	38:w:438:LEU:HG	2.00	0.62
41:7:39:PRO:HB2	41:7:70:TYR:HD1	1.63	0.62
1:A:155:LYS:NZ	1:A:622:GLY:O	2.32	0.62
3:C:561:LYS:NZ	3:C:611:ASN:O	2.32	0.62
21:V:609:GLN:HA	21:V:612:PHE:HB2	1.80	0.62
23:X:163:GLU:OE2	23:X:778:PHE:CE2	2.53	0.62
23:X:580:ASP:OD2	23:X:733:LYS:NZ	2.31	0.62
9:J:330:ARG:HD3	9:J:361:ARG:HH22	1.64	0.62
34:r:8:SER:O	34:r:9:ASN:CB	2.47	0.62
36:3:387:PHE:HE1	36:3:389:PRO:HG3	1.64	0.62
1:A:957:GLN:O	1:A:961:ASN:ND2	2.26	0.62
6:G:95:U:P	35:1:1109:ARG:HH12	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:224:ARG:HH11	12:M:224:ARG:HG3	1.64	0.62
23:X:396:ARG:NH1	23:X:468:GLU:OE1	2.32	0.62
23:X:632:CYS:SG	23:X:642:LEU:HD13	2.39	0.62
35:1:742:GLY:O	35:1:746:PHE:HB2	1.99	0.62
35:1:1120:ALA:HB2	35:1:1128:VAL:HG21	1.80	0.62
36:3:293:HIS:NE2	36:3:295:THR:HB	2.15	0.62
36:3:1009:PHE:HZ	36:3:1046:GLY:HA3	1.65	0.62
41:7:30:CYS:SG	41:7:31:VAL:N	2.72	0.62
41:7:33:CYS:HB3	41:7:72:CYS:SG	2.39	0.62
1:A:758:ARG:HH21	1:A:775:ASN:HD22	1.45	0.62
2:B:63:A:H2'	2:B:64:G:H8	1.65	0.62
2:B:64:G:H2'	2:B:65:G:C8	2.34	0.62
2:B:95:G:H2'	2:B:95:G:N3	2.15	0.62
21:V:540:GLU:HG3	21:V:541:THR:H	1.65	0.62
23:X:249:GLU:HB3	23:X:273:LYS:HE2	1.82	0.62
24:Y:219:THR:O	24:Y:223:LEU:HB2	2.00	0.62
36:3:214:ASP:O	36:3:218:ASN:N	2.33	0.62
17:R:178:ARG:HD3	17:R:194:GLN:OE1	1.99	0.62
24:Y:40:CYS:O	24:Y:156:ILE:N	2.28	0.62
35:1:595:GLU:O	35:1:599:ASN:ND2	2.33	0.62
36:3:207:THR:O	36:3:209:THR:HG22	1.99	0.62
23:X:787:GLU:CG	35:1:542:PRO:CG	2.53	0.61
23:X:824:LEU:HD11	23:X:844:ALA:HA	1.82	0.61
24:Y:147:ASP:HB2	24:Y:149:VAL:HG12	1.80	0.61
36:3:325:ILE:O	36:3:374:SER:HA	2.00	0.61
9:J:344:GLN:N	9:J:344:GLN:OE1	2.33	0.61
17:R:320:HIS:O	17:R:323:LYS:HG2	1.99	0.61
23:X:167:THR:CG2	23:X:770:LEU:HB3	2.30	0.61
23:X:558:ALA:O	23:X:562:THR:OG1	2.17	0.61
35:1:1056:MET:HG2	39:2:561:MET:CG	2.29	0.61
36:3:233:ASN:ND2	36:3:233:ASN:H	1.95	0.61
1:A:231:THR:HG22	1:A:233:PRO:HD2	1.83	0.61
1:A:1181:ASP:OD1	1:A:1181:ASP:N	2.32	0.61
21:V:532:GLN:HE21	21:V:547:VAL:HG11	1.64	0.61
35:1:967:GLU:HG3	35:1:970:LEU:HB3	1.81	0.61
39:2:606:PRO:HA	40:4:35:GLN:CB	2.30	0.61
1:A:1276:GLU:OE1	1:A:1375:TRP:N	2.31	0.61
35:1:527:GLY:HA2	35:1:566:LEU:CD2	2.31	0.61
35:1:1055:TRP:CD1	35:1:1088:ILE:HD11	2.34	0.61
1:A:732:PRO:HG2	1:A:735:ILE:HD13	1.83	0.61
1:A:784:LEU:O	1:A:788:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:THR:HB	1:A:1632:PHE:HB2	1.83	0.61
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.01	0.61
5:F:50:A:OP1	11:L:165:LYS:NZ	2.23	0.61
35:1:550:HIS:HD2	35:1:551:LEU:HD22	1.64	0.61
36:3:330:PHE:O	36:3:390:ARG:NH2	2.32	0.61
36:3:1049:LYS:HE3	42:5:52:TYR:OH	2.00	0.61
1:A:81:PHE:O	1:A:83:HIS:N	2.34	0.61
1:A:1869:LEU:HD22	1:A:1884:ILE:HG22	1.83	0.61
36:3:1115:GLU:HB3	39:2:708:TRP:NE1	2.16	0.61
36:3:1193:VAL:HA	36:3:1196:GLU:HG2	1.81	0.61
1:A:988:ILE:HD12	1:A:1030:ILE:HG13	1.81	0.61
1:A:1336:PRO:HB2	1:A:1350:ILE:HG12	1.83	0.61
3:C:209:VAL:HG21	3:C:237:LEU:HD23	1.82	0.61
9:J:441:ASP:OD1	9:J:445:LYS:NZ	2.34	0.61
15:P:39:THR:O	19:T:318:ARG:HD3	2.00	0.61
21:V:511:ALA:HB1	21:V:525:PHE:HZ	1.64	0.61
23:X:651:LEU:HG	23:X:656:GLN:NE2	2.16	0.61
35:1:1028:HIS:O	35:1:1032:GLN:HB2	2.01	0.61
36:3:1180:GLU:CD	36:3:1212:ARG:HH21	2.08	0.61
41:7:52:GLY:H	41:7:55:GLN:HE21	1.47	0.61
3:C:463:GLU:H	3:C:463:GLU:CD	2.08	0.61
14:O:172:GLU:O	14:O:174:LYS:N	2.32	0.61
36:3:207:THR:O	36:3:207:THR:OG1	2.15	0.61
39:2:594:GLY:O	39:2:597:PHE:HB2	2.00	0.61
1:A:1969:PRO:HB2	1:A:1971:LEU:HD23	1.83	0.61
11:L:63:TRP:CD1	11:L:67:GLU:HB3	2.36	0.61
12:M:163:THR:HG23	12:M:166:SER:HB2	1.82	0.61
17:R:122:LYS:HG2	17:R:124:VAL:HG23	1.83	0.61
35:1:625:ARG:NE	35:1:666:LYS:HZ1	1.99	0.61
36:3:12:THR:O	36:3:34:ARG:NH1	2.34	0.61
2:B:63:A:H2'	2:B:64:G:C8	2.36	0.61
4:E:108:HIS:CD2	4:E:128:SER:HB2	2.36	0.61
35:1:815:PHE:CE1	35:1:853:ILE:CG2	2.84	0.61
35:1:834:VAL:O	35:1:838:VAL:HG23	2.01	0.61
35:1:1166:ILE:O	35:1:1170:THR:HG22	2.01	0.61
35:1:1258:ALA:HB3	35:1:1261:VAL:HG13	1.83	0.61
35:1:1274:ILE:HG22	36:3:109:LYS:CE	2.30	0.61
36:3:318:ASP:OD1	36:3:319:GLU:N	2.33	0.61
36:3:462:VAL:O	36:3:472:ALA:N	2.30	0.61
36:3:807:TYR:H	36:3:856:LYS:HD2	1.65	0.61
30:i:72:ILE:O	31:j:78:MET:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:15:A:H2'	5:F:16:G:C8	2.35	0.60
5:F:35:A:C8	6:G:12:G:C6	2.89	0.60
17:R:162:ALA:C	17:R:164:PRO:HD3	2.26	0.60
23:X:171:ARG:HH12	23:X:509:PRO:HG3	1.65	0.60
23:X:257:PHE:CZ	23:X:270:LEU:HB2	2.36	0.60
36:3:71:THR:O	36:3:146:ARG:NH2	2.33	0.60
36:3:138:GLN:HG2	36:3:161:HIS:CE1	2.36	0.60
36:3:139:LYS:NZ	36:3:160:ALA:O	2.34	0.60
36:3:1004:ASP:OD1	36:3:1006:GLN:N	2.28	0.60
1:A:1780:VAL:HB	1:A:1863:VAL:HG23	1.81	0.60
1:A:1862:ILE:HA	1:A:1885:LYS:O	2.01	0.60
3:C:64:LYS:HD3	15:P:209:ARG:HH12	1.66	0.60
23:X:677:ALA:O	23:X:725:ARG:NE	2.34	0.60
35:1:677:CYS:O	35:1:680:LEU:HD12	2.01	0.60
35:1:743:LEU:O	35:1:747:LEU:HB2	2.01	0.60
36:3:706:MET:HG3	36:3:707:GLN:HG2	1.83	0.60
39:2:487:LEU:HD22	42:5:28:LYS:HB2	1.82	0.60
1:A:641:MET:O	1:A:645:THR:HG23	1.99	0.60
4:E:203:ASP:N	4:E:203:ASP:OD1	2.32	0.60
5:F:36:A:H2'	5:F:38:G:OP2	2.02	0.60
35:1:590:ARG:O	35:1:594:ARG:HB2	2.02	0.60
36:3:947:GLU:HB3	36:3:963:VAL:HG13	1.82	0.60
40:4:17:VAL:O	40:4:56:TYR:HA	2.01	0.60
1:A:1892:PRO:HB3	1:A:1944:HIS:CD2	2.36	0.60
4:E:126:SER:OG	4:E:136:TRP:NE1	2.26	0.60
4:E:209:ILE:HG13	4:E:219:VAL:HG13	1.83	0.60
9:J:361:ARG:HD3	12:M:161:PHE:CE2	2.36	0.60
35:1:664:GLY:HA2	35:1:667:ILE:HD12	1.83	0.60
2:B:95:G:N2	2:B:96:A:H5''	2.12	0.60
11:L:79:PRO:O	11:L:80:THR:OG1	2.16	0.60
36:3:910:ALA:HB1	36:3:913:LEU:HD11	1.83	0.60
1:A:278:LYS:NZ	6:G:-8:C:OP1	2.35	0.60
1:A:755:HIS:CD2	15:P:219:PHE:HE2	2.20	0.60
1:A:892:LYS:HD2	1:A:912:GLU:OE1	2.00	0.60
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.19	0.60
4:E:135:VAL:HG12	4:E:145:LYS:HB2	1.82	0.60
7:H:106:G:N2	30:i:24:LYS:O	2.34	0.60
12:M:215:ASN:ND2	17:R:260:TYR:CB	2.65	0.60
23:X:765:LEU:HD22	23:X:822:PRO:HG3	1.82	0.60
24:Y:96:MET:HB2	24:Y:124:THR:HB	1.84	0.60
36:3:984:LYS:NZ	38:w:471:TRP:CB	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:477:MET:SD	39:2:478:HIS:ND1	2.75	0.60
15:P:44:ARG:NH2	19:T:255:SER:O	2.32	0.60
35:1:669:GLN:HB2	35:1:708:ALA:HA	1.83	0.60
35:1:1167:TYR:OH	39:2:581:LYS:HE2	2.02	0.60
40:4:78:LYS:CB	40:4:115:LEU:CB	2.79	0.60
1:A:972:GLU:OE1	1:A:972:GLU:N	2.30	0.60
1:A:1578:ARG:HE	1:A:1746:ARG:HH21	1.48	0.60
1:A:1663:ASP:O	1:A:1703:ILE:N	2.34	0.60
7:H:48:A:C2	7:H:65:U:H2'	2.37	0.60
15:P:42:LYS:O	19:T:258:SER:HB3	2.02	0.60
23:X:802:LEU:HB3	23:X:806:GLY:HA2	1.84	0.60
15:P:72:ARG:HA	15:P:75:ASN:ND2	2.17	0.60
18:S:99:ALA:HB2	18:S:128:ILE:HA	1.83	0.60
36:3:528:ARG:HG2	36:3:532:ARG:HH21	1.67	0.60
36:3:680:ASP:OD2	36:3:681:PRO:HD2	2.02	0.60
1:A:857:ASN:OD1	1:A:860:GLN:N	2.26	0.60
3:C:811:THR:O	3:C:815:VAL:HG23	2.00	0.60
15:P:186:ARG:O	15:P:186:ARG:HG3	2.01	0.60
19:T:271:LYS:HG2	19:T:280:VAL:HG11	1.84	0.60
23:X:406:GLU:HA	23:X:409:LEU:HD23	1.84	0.60
35:1:953:ASP:O	35:1:956:SER:OG	2.18	0.60
36:3:982:GLU:HG2	36:3:984:LYS:HE3	1.84	0.60
1:A:371:LEU:HD21	3:C:347:ILE:HD11	1.82	0.59
5:F:79:C:H4'	5:F:80:G:OP1	2.03	0.59
23:X:164:TRP:NE1	23:X:539:VAL:CG2	2.65	0.59
23:X:802:LEU:HA	23:X:807:GLU:O	2.02	0.59
24:Y:88:HIS:ND1	24:Y:120:ASP:OD1	2.35	0.59
34:r:7:ILE:O	34:s:90:PHE:CB	2.50	0.59
35:1:675:MET:HB3	35:1:678:ALA:HB3	1.84	0.59
35:1:698:GLN:HB3	35:1:701:VAL:HG12	1.84	0.59
35:1:850:ILE:O	35:1:854:VAL:HG13	2.01	0.59
35:1:1192:VAL:O	35:1:1196:SER:OG	2.20	0.59
36:3:329:TYR:CE2	36:3:389:PRO:HA	2.37	0.59
36:3:984:LYS:CE	38:w:471:TRP:HA	2.32	0.59
1:A:390:ASP:OD1	1:A:390:ASP:N	2.35	0.59
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.82	0.59
1:A:1527:ASN:O	1:A:1529:ILE:N	2.36	0.59
9:J:199:LYS:HD3	9:J:199:LYS:C	2.27	0.59
23:X:272:TYR:O	23:X:276:VAL:HB	2.02	0.59
35:1:819:TRP:CG	35:1:864:TYR:HH	2.20	0.59
35:1:1292:LYS:CD	42:5:78:PRO:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:193:ASP:O	42:5:79:PRO:CG	2.49	0.59
36:3:700:LYS:HE2	36:3:715:MET:HB3	1.84	0.59
1:A:280:GLU:HG3	20:U:9:THR:HG21	1.84	0.59
44:A:3000:IHP:H1	44:A:3000:IHP:O46	2.01	0.59
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.67	0.59
4:E:114:GLU:OE2	4:E:290:ARG:NH2	2.36	0.59
9:J:206:LEU:HD23	9:J:207:PRO:HD3	1.84	0.59
9:J:439:ALA:HA	9:J:442:ARG:HB3	1.84	0.59
23:X:225:GLU:O	23:X:229:LYS:HD3	2.03	0.59
24:Y:42:ILE:HA	24:Y:53:THR:HG22	1.82	0.59
24:Y:77:PHE:HB3	24:Y:103:GLN:HB3	1.83	0.59
24:Y:91:LYS:HG3	24:Y:114:GLU:HG3	1.84	0.59
36:3:212:GLU:HB2	36:3:223:LYS:HG3	1.84	0.59
36:3:435:LEU:HD13	36:3:799:ILE:HD11	1.84	0.59
36:3:1115:GLU:CB	39:2:708:TRP:HE1	2.14	0.59
42:5:65:ARG:HB3	42:5:65:ARG:CZ	2.32	0.59
1:A:384:VAL:HG12	3:C:331:PHE:HB3	1.83	0.59
4:E:300:ILE:HG23	4:E:312:TRP:HB2	1.83	0.59
5:F:28:A:O2'	13:N:39:GLY:O	2.19	0.59
13:N:121:VAL:HG11	13:N:126:LEU:HD21	1.83	0.59
35:1:508:THR:HB	35:1:510:PRO:HD2	1.84	0.59
2:B:87:A:N6	2:B:91:U:O3'	2.35	0.59
4:E:202:ASN:ND2	4:E:204:THR:OG1	2.36	0.59
6:G:85:G:H2'	6:G:86:A:C8	2.38	0.59
13:N:70:ILE:HB	13:N:74:LEU:HD23	1.83	0.59
35:1:854:VAL:HG23	35:1:855:ASP:H	1.68	0.59
36:3:615:ARG:NH2	36:3:630:MET:HB3	2.17	0.59
29:h:109:VAL:N	30:i:63:LEU:O	2.27	0.59
1:A:1841:THR:O	1:A:1845:VAL:HG23	2.02	0.59
1:A:1919:LEU:HD12	1:A:1936:LEU:HD11	1.83	0.59
3:C:137:HIS:O	3:C:142:LYS:NZ	2.26	0.59
24:Y:161:ILE:HG21	24:Y:164:ASP:HB2	1.84	0.59
36:3:607:VAL:HB	36:3:615:ARG:HB2	1.85	0.59
36:3:982:GLU:HB3	38:w:471:TRP:CE3	2.37	0.59
3:C:724:TRP:HH2	3:C:788:LYS:HZ2	1.51	0.59
23:X:612:LEU:O	23:X:689:VAL:HA	2.03	0.59
23:X:698:LYS:NZ	23:X:758:THR:HA	2.17	0.59
36:3:982:GLU:HB3	38:w:471:TRP:HE3	1.67	0.59
36:3:1133:THR:O	39:2:712:GLU:HB2	2.01	0.59
31:j:46:CYS:O	31:j:59:ASP:N	2.35	0.59
4:E:105:LEU:HD11	4:E:136:TRP:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:150:HIS:NE2	4:E:169:THR:OG1	2.19	0.59
4:E:312:TRP:CD1	4:E:319:ILE:HA	2.37	0.59
36:3:246:SER:OG	36:3:247:GLY:N	2.35	0.59
1:A:729:PRO:HG2	12:M:226:TYR:HE1	1.65	0.59
4:E:218:LYS:HD2	4:E:220:TRP:CZ2	2.38	0.59
5:F:59:G:N2	5:F:76:A:N1	2.42	0.59
7:H:46:U:O2'	7:H:47:U:OP2	2.16	0.59
7:H:180:G:H2'	7:H:181:G:C8	2.38	0.59
19:T:455:GLN:HG2	19:T:456:PRO:HD2	1.85	0.59
21:V:545:ARG:HG3	21:V:585:ILE:HG21	1.85	0.59
23:X:557:THR:HA	23:X:560:PHE:HB2	1.85	0.59
38:w:454:ASP:CG	39:2:463:ALA:HB1	2.28	0.59
1:A:47:GLU:HA	1:A:50:LYS:HG3	1.83	0.59
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.38	0.59
4:E:251:LEU:HB2	4:E:293:TRP:CE2	2.38	0.59
35:1:495:ARG:HH21	35:1:530:PRO:HB3	1.66	0.59
35:1:610:ILE:CG2	35:1:647:PHE:CD1	2.86	0.59
30:i:30:LYS:O	30:i:47:THR:HA	2.02	0.59
1:A:425:PRO:HB2	1:A:428:LYS:HG3	1.85	0.58
1:A:1558:THR:OG1	1:A:1559:GLY:N	2.33	0.58
3:C:617:LEU:HD11	3:C:629:ILE:HG23	1.85	0.58
9:J:443:ILE:HG13	9:J:444:SER:N	2.18	0.58
12:M:224:ARG:NH1	12:M:224:ARG:O	2.36	0.58
17:R:373:ALA:HB3	17:R:376:LYS:HB3	1.84	0.58
23:X:526:THR:HG22	23:X:528:HIS:H	1.68	0.58
35:1:1270:ASN:OD1	42:5:21:THR:HB	2.03	0.58
1:A:263:PHE:HE1	1:A:273:ILE:HD11	1.68	0.58
1:A:362:ARG:HH11	21:V:323:LEU:C	2.11	0.58
1:A:498:ARG:O	1:A:502:ASN:ND2	2.35	0.58
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.85	0.58
1:A:1427:ARG:HE	23:X:326:GLN:CD	2.09	0.58
13:N:38:GLU:C	13:N:40:LYS:H	2.10	0.58
17:R:332:ARG:HA	23:X:272:TYR:HD1	1.65	0.58
21:V:497:CYS:HB3	21:V:507:PHE:CG	2.37	0.58
35:1:1074:ARG:O	35:1:1078:VAL:HG23	2.03	0.58
35:1:1110:VAL:O	35:1:1113:THR:HG22	2.02	0.58
38:w:432:ALA:O	38:w:436:ARG:HD3	2.01	0.58
43:o:64:ARG:HA	43:o:88:PRO:HD2	1.85	0.58
1:A:41:GLN:NE2	4:E:153:PHE:HE2	2.02	0.58
1:A:1298:ARG:HH11	1:A:1298:ARG:HB2	1.68	0.58
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:THR:OG1	1:A:1522:GLN:HB2	2.04	0.58
6:G:19:G:N2	14:O:194:ALA:C	2.59	0.58
7:H:50:C:H2'	7:H:51:A:C8	2.38	0.58
9:J:433:ARG:O	9:J:437:LYS:HG2	2.03	0.58
17:R:330:LYS:NZ	23:X:275:ARG:NH2	2.51	0.58
21:V:606:GLU:HA	21:V:609:GLN:CG	2.33	0.58
36:3:525:ARG:HD3	36:3:533:VAL:HG22	1.85	0.58
36:3:583:MET:HE2	36:3:583:MET:HA	1.85	0.58
36:3:695:GLY:O	36:3:697:ARG:NE	2.30	0.58
36:3:994:GLN:HE22	36:3:1036:ALA:C	2.10	0.58
38:w:461:LYS:HA	38:w:464:LEU:HD12	1.85	0.58
38:w:464:LEU:O	38:w:468:SER:OG	2.18	0.58
2:B:95:G:O2'	30:d:24:LYS:C	2.46	0.58
4:E:140:THR:HB	4:E:142:GLU:HG2	1.85	0.58
35:1:652:CYS:HB2	35:1:692:HIS:CE1	2.35	0.58
35:1:747:LEU:HA	35:1:750:ILE:HG12	1.85	0.58
38:w:425:HIS:HA	38:w:428:GLU:HB2	1.85	0.58
32:k:19:LEU:HA	32:k:70:LEU:HA	1.83	0.58
1:A:909:TYR:HB2	1:A:1033:GLY:HA3	1.85	0.58
1:A:1571:ILE:HG23	10:K:220:LEU:HD13	1.84	0.58
2:B:14:U:H2'	2:B:15:C:H6	1.69	0.58
6:G:83:A:N6	38:w:400:HIS:CE1	2.71	0.58
35:1:641:ILE:HB	35:1:682:HIS:CE1	2.38	0.58
35:1:898:TYR:OH	35:1:902:GLU:HG2	2.03	0.58
36:3:326:ARG:NE	36:3:372:GLU:OE2	2.19	0.58
36:3:387:PHE:CE1	36:3:389:PRO:HG3	2.38	0.58
36:3:447:MET:HE2	36:3:766:ALA:HB2	1.86	0.58
36:3:883:GLU:OE2	36:3:884:GLN:N	2.33	0.58
36:3:1147:HIS:O	36:3:1151:GLU:HG3	2.03	0.58
38:w:445:HIS:CD2	39:2:473:ASP:OD2	2.56	0.58
7:H:99:A:O2'	7:H:100:U:OP2	2.18	0.58
23:X:546:LEU:HD22	23:X:547:LYS:H	1.69	0.58
24:Y:13:VAL:HB	24:Y:131:GLU:HB3	1.85	0.58
35:1:512:ARG:O	35:1:516:LEU:HB2	2.04	0.58
1:A:1768:TYR:HA	1:A:1771:LEU:CB	2.34	0.58
3:C:879:ASP:OD1	3:C:879:ASP:N	2.36	0.58
7:H:70:C:H2'	7:H:71:C:C6	2.39	0.58
13:N:32:ALA:HA	13:N:35:GLU:HG2	1.85	0.58
1:A:707:ARG:NH1	7:H:18:U:H5'	2.13	0.58
5:F:35:A:C2	5:F:36:A:C6	2.91	0.58
11:L:49:ARG:NH1	11:L:133:GLU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:328:ALA:HB1	24:Y:226:MET:CA	2.34	0.58
35:1:843:LYS:C	35:1:843:LYS:HD3	2.29	0.58
35:1:1110:VAL:O	35:1:1114:VAL:HG23	2.03	0.58
36:3:310:ILE:O	36:3:311:PHE:HD2	1.87	0.58
1:A:1779:PHE:HB2	1:A:1810:PHE:HB3	1.85	0.58
21:V:491:ASN:HA	21:V:528:ILE:HD11	1.85	0.58
23:X:653:SER:HA	23:X:656:GLN:HG3	1.85	0.58
25:Z:181:MET:O	25:Z:185:TRP:N	2.36	0.58
36:3:195:ASP:OD2	36:3:198:GLY:N	2.36	0.58
1:A:1749:LYS:HG3	35:1:980:GLU:HG2	1.85	0.58
3:C:250:ARG:NH1	3:C:447:PRO:O	2.36	0.58
4:E:158:TYR:HB3	4:E:168:CYS:SG	2.44	0.58
6:G:88:G:H4'	6:G:89:U:OP1	2.04	0.58
12:M:179:ILE:O	12:M:183:VAL:HG23	2.04	0.58
23:X:664:PRO:HG2	23:X:667:ALA:HB3	1.85	0.58
23:X:850:ASN:O	23:X:853:ILE:HG12	2.03	0.58
35:1:1179:ASP:H	39:2:511:LEU:CD1	2.15	0.58
36:3:642:ILE:H	36:3:703:ARG:HE	1.52	0.58
1:A:194:GLU:HA	1:A:194:GLU:OE2	2.03	0.57
3:C:444:GLY:O	3:C:447:PRO:HD2	2.04	0.57
12:M:215:ASN:HD21	17:R:260:TYR:C	2.11	0.57
13:N:57:THR:HG21	13:N:88:LEU:HD23	1.86	0.57
18:S:14:VAL:O	18:S:24:VAL:HA	2.04	0.57
21:V:543:LYS:HA	21:V:546:ASN:HD21	1.69	0.57
23:X:283:TYR:OH	24:Y:219:THR:HA	2.04	0.57
23:X:650:ASN:O	23:X:904:GLN:NE2	2.37	0.57
23:X:714:CYS:SG	23:X:718:SER:OG	2.61	0.57
36:3:25:THR:OG1	36:3:26:LYS:N	2.35	0.57
36:3:1115:GLU:HB3	39:2:708:TRP:HE1	1.69	0.57
38:w:411:CYS:SG	38:w:416:TYR:OH	2.61	0.57
42:5:7:ILE:HG13	42:5:8:HIS:N	2.18	0.57
42:5:14:LEU:HA	42:5:17:LYS:HB2	1.86	0.57
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.04	0.57
12:M:165:ASN:HD22	17:R:95:LYS:HE2	1.69	0.57
21:V:471:GLU:OE1	21:V:475:LYS:NZ	2.33	0.57
23:X:192:ARG:HG2	23:X:192:ARG:HH11	1.68	0.57
35:1:759:ALA:O	35:1:763:ASN:N	2.35	0.57
35:1:826:ASP:HB3	35:1:829:ASN:HB2	1.86	0.57
36:3:115:ILE:HD13	42:5:19:ILE:H	1.69	0.57
36:3:169:HIS:CD2	36:3:170:VAL:H	2.22	0.57
36:3:449:VAL:HG22	36:3:763:ARG:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:538:THR:OG1	36:3:542:LYS:O	2.22	0.57
36:3:791:HIS:HD2	36:3:794:SER:OG	1.87	0.57
39:2:542:GLU:O	39:2:546:GLN:HG2	2.03	0.57
3:C:113:VAL:HG23	3:C:114:TYR:H	1.68	0.57
3:C:711:ARG:NH2	3:C:732:ILE:O	2.38	0.57
9:J:206:LEU:HD22	9:J:207:PRO:CD	2.34	0.57
11:L:11:TRP:CE2	11:L:49:ARG:HD3	2.39	0.57
17:R:161:ALA:HA	17:R:166:ARG:HH12	1.69	0.57
19:T:195:LYS:NZ	19:T:490:ARG:HD2	2.19	0.57
35:1:717:THR:CB	35:1:718:PRO:HD2	2.35	0.57
35:1:819:TRP:HE3	35:1:864:TYR:HH	1.53	0.57
35:1:1001:VAL:HG23	35:1:1009:MET:CE	2.26	0.57
36:3:365:GLY:HA2	36:3:394:ASN:ND2	2.19	0.57
36:3:638:GLU:OE2	36:3:698:PRO:HB3	2.04	0.57
41:7:33:CYS:HB2	41:7:74:GLU:OE1	2.04	0.57
1:A:665:SER:O	1:A:665:SER:OG	2.18	0.57
1:A:1676:ILE:HD12	1:A:1706:ASP:HB2	1.86	0.57
3:C:176:GLU:H	3:C:176:GLU:CD	2.13	0.57
3:C:779:LEU:O	3:C:938:ARG:HD2	2.04	0.57
7:H:41:U:H2'	7:H:42:G:C8	2.39	0.57
23:X:707:GLU:O	23:X:990:VAL:HA	2.03	0.57
24:Y:2:ALA:HA	24:Y:15:ASP:HA	1.86	0.57
36:3:69:ARG:NH1	36:3:74:THR:HA	2.18	0.57
36:3:329:TYR:HE2	36:3:389:PRO:HA	1.69	0.57
36:3:552:ARG:HH21	36:3:567:GLU:HB3	1.69	0.57
36:3:758:SER:N	36:3:761:THR:O	2.25	0.57
36:3:1148:LEU:HA	36:3:1151:GLU:OE2	2.05	0.57
36:3:1200:THR:O	36:3:1203:GLU:N	2.38	0.57
37:p:213:THR:O	37:p:215:SER:N	2.38	0.57
7:H:68:G:H2'	7:H:69:U:C6	2.39	0.57
11:L:699:ASN:CB	25:Z:110:SER:CB	2.81	0.57
14:O:34:ILE:H	17:R:197:ILE:HD13	1.69	0.57
23:X:394:ALA:HA	23:X:397:ARG:HD2	1.86	0.57
23:X:1009:LEU:HD21	23:X:1021:LEU:HD11	1.85	0.57
24:Y:55:ASP:OD2	24:Y:60:GLY:N	2.37	0.57
35:1:1098:LEU:HD12	35:1:1135:GLU:HG2	1.87	0.57
35:1:1165:TYR:CE1	39:2:575:PHE:CD1	2.92	0.57
36:3:510:LEU:HD23	36:3:510:LEU:H	1.70	0.57
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.36	0.57
1:A:1604:LEU:HD21	1:A:1725:LEU:HD22	1.85	0.57
7:H:125:G:H2'	7:H:126:A:H8	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:593:GLU:O	23:X:597:VAL:HG22	2.04	0.57
35:1:1299:GLU:OE2	42:5:40:TYR:OH	2.14	0.57
41:7:68:ASP:OD1	41:7:68:ASP:N	2.38	0.57
33:l:31:LYS:O	33:l:44:SER:N	2.38	0.57
1:A:1160:ARG:HD3	15:P:192:VAL:HG11	1.87	0.57
4:E:282:HIS:NE2	22:W:150:ALA:HB2	2.18	0.57
23:X:760:LEU:O	23:X:764:VAL:HG23	2.05	0.57
24:Y:24:ALA:HA	24:Y:78:PHE:HZ	1.69	0.57
24:Y:139:ILE:HA	24:Y:142:THR:HG23	1.86	0.57
36:3:1140:PHE:HE1	36:3:1197:LEU:HD13	1.68	0.57
3:C:261:ASP:OD2	3:C:261:ASP:N	2.35	0.57
12:M:163:THR:OG1	12:M:165:ASN:OD1	2.21	0.57
17:R:175:GLN:OE1	17:R:176:TYR:N	2.33	0.57
17:R:335:ARG:O	23:X:268:GLN:CB	2.49	0.57
21:V:491:ASN:O	21:V:494:LEU:HB3	2.05	0.57
21:V:636:LEU:O	21:V:640:THR:OG1	2.18	0.57
23:X:587:PRO:HB2	35:1:827:ARG:HH12	1.69	0.57
23:X:640:ARG:HH22	23:X:668:ARG:HB2	1.70	0.57
24:Y:33:LYS:HG3	24:Y:174:ILE:HD13	1.85	0.57
1:A:1815:GLY:O	1:A:1918:ASN:HA	2.04	0.57
1:A:1927:ILE:HD12	1:A:1931:THR:HG22	1.87	0.57
6:G:1:G:N1	10:K:217:CYS:SG	2.74	0.57
6:G:85:G:N2	7:H:45:C:N3	2.51	0.57
9:J:334:GLU:OE2	9:J:349:TYR:OH	2.10	0.57
21:V:551:PHE:HD1	21:V:554:LEU:HD12	1.69	0.57
23:X:462:ALA:HB1	23:X:473:LEU:HD11	1.87	0.57
24:Y:23:ARG:O	24:Y:26:LEU:HD23	2.05	0.57
35:1:631:ALA:O	35:1:635:VAL:HG13	2.05	0.57
1:A:171:ASP:O	1:A:520:TYR:HB2	2.04	0.57
4:E:260:ARG:HD3	4:E:276:ILE:HG12	1.87	0.57
10:K:205:TYR:O	10:K:209:GLY:N	2.36	0.57
18:S:14:VAL:HA	18:S:164:PRO:HA	1.87	0.57
35:1:1104:GLN:O	35:1:1105:GLU:HB3	2.03	0.57
39:2:632:TRP:O	40:4:73:ILE:CB	2.53	0.57
1:A:30:LEU:HD22	4:E:214:ASP:OD2	2.04	0.56
1:A:1635:TYR:CZ	1:A:1636:LYS:HB2	2.40	0.56
1:A:1839:TRP:CZ3	1:A:1871:PRO:HA	2.40	0.56
2:B:87:A:C6	2:B:92:U:OP2	2.59	0.56
14:O:34:ILE:N	17:R:197:ILE:HD13	2.20	0.56
23:X:171:ARG:HH12	23:X:509:PRO:CB	2.18	0.56
23:X:234:TYR:CZ	24:Y:317:GLN:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:616:ILE:HG22	36:3:628:LEU:HB3	1.86	0.56
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.38	0.56
1:A:1978:LYS:O	1:A:1981:VAL:HG12	2.05	0.56
15:P:209:ARG:O	15:P:209:ARG:HG2	2.05	0.56
23:X:511:LEU:HG	23:X:514:TYR:HB2	1.86	0.56
35:1:556:ILE:CG2	35:1:596:ILE:HG21	2.32	0.56
35:1:850:ILE:HG22	35:1:888:LEU:HD11	1.85	0.56
36:3:92:TYR:OH	36:3:97:ASN:OD1	2.18	0.56
36:3:876:THR:O	36:3:876:THR:OG1	2.12	0.56
39:2:457:MET:HE3	39:2:457:MET:HA	1.86	0.56
33:l:43:MET:O	33:l:60:GLN:HA	2.05	0.56
1:A:1817:LEU:HD23	1:A:1919:LEU:HD21	1.87	0.56
3:C:490:PHE:O	3:C:491:HIS:ND1	2.33	0.56
6:G:85:G:H1	7:H:45:C:H42	1.53	0.56
13:N:16:GLU:N	13:N:16:GLU:OE1	2.33	0.56
16:Q:27:ALA:O	16:Q:32:ALA:N	2.32	0.56
23:X:217:GLU:HA	23:X:220:LYS:HB2	1.87	0.56
23:X:519:VAL:HB	23:X:550:VAL:HG13	1.87	0.56
24:Y:104:HIS:NE2	24:Y:124:THR:OG1	2.38	0.56
24:Y:224:LEU:HD11	24:Y:230:LEU:HD23	1.86	0.56
34:r:127:ALA:HB1	34:s:127:ALA:HB3	1.87	0.56
35:1:549:ARG:NH2	35:1:586:ASP:OD1	2.38	0.56
36:3:978:LEU:HD13	38:w:480:GLU:HG2	1.87	0.56
1:A:711:GLN:HE22	7:H:18:U:H5"	1.71	0.56
2:B:96:A:N6	32:f:23:GLY:H	2.02	0.56
3:C:829:GLU:HG2	3:C:907:VAL:HB	1.86	0.56
6:G:90:C:O5'	6:G:90:C:H6	1.89	0.56
8:I:463:PRO:CG	8:I:483:SER:CB	2.80	0.56
35:1:833:LEU:CD2	35:1:867:MET:SD	2.91	0.56
36:3:141:VAL:HB	36:3:158:LEU:HD12	1.86	0.56
36:3:345:GLY:O	36:3:360:GLN:HG3	2.04	0.56
36:3:527:ILE:HG12	36:3:532:ARG:O	2.06	0.56
1:A:378:PHE:O	3:C:355:LYS:HG3	2.05	0.56
1:A:381:PRO:O	1:A:383:PHE:N	2.32	0.56
1:A:1410:ASP:OD2	1:A:1411:SER:N	2.38	0.56
2:B:110:C:H2'	2:B:111:A:H8	1.70	0.56
23:X:246:LEU:HG	23:X:277:ARG:NE	2.20	0.56
23:X:716:LYS:HG3	23:X:747:LEU:HB3	1.87	0.56
24:Y:216:GLU:HA	24:Y:219:THR:HG23	1.86	0.56
35:1:815:PHE:HE1	35:1:853:ILE:CG2	2.18	0.56
35:1:1165:TYR:HD1	39:2:575:PHE:CD1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:w:454:ASP:OD2	39:2:463:ALA:CB	2.53	0.56
31:j:59:ASP:HA	31:j:76:ARG:HA	1.88	0.56
1:A:1006:ALA:O	1:A:1010:THR:HG22	2.05	0.56
3:C:713:LYS:HA	3:C:716:GLU:CD	2.30	0.56
3:C:833:PHE:HB3	3:C:900:VAL:HG23	1.88	0.56
4:E:243:LEU:HG	4:E:250:LEU:HB2	1.87	0.56
11:L:28:LYS:HE2	17:R:268:LEU:HD23	1.88	0.56
23:X:430:THR:O	23:X:434:GLN:HG3	2.06	0.56
24:Y:247:LEU:HD11	24:Y:256:LEU:HD11	1.86	0.56
36:3:86:ARG:NH1	36:3:1157:GLY:O	2.38	0.56
36:3:193:ASP:CA	42:5:79:PRO:CG	2.83	0.56
36:3:342:LEU:HB3	36:3:343:LYS:O	2.06	0.56
36:3:373:PHE:HE1	36:3:385:PHE:HB3	1.70	0.56
36:3:1143:HIS:O	36:3:1147:HIS:ND1	2.39	0.56
39:2:594:GLY:N	39:2:597:PHE:HE2	2.02	0.56
28:n:39:HIS:HA	28:n:59:SER:HA	1.87	0.56
1:A:431:TYR:HB3	1:A:611:LEU:HD21	1.88	0.56
1:A:854:SER:OG	1:A:855:ARG:N	2.37	0.56
4:E:197:LEU:HD11	4:E:213:ILE:HD13	1.87	0.56
7:H:72:U:H2'	7:H:73:C:C6	2.41	0.56
9:J:200:GLU:C	9:J:202:GLU:H	2.13	0.56
11:L:147:ASP:HA	11:L:150:GLU:HG3	1.88	0.56
17:R:317:LYS:HG3	23:X:286:ALA:HB1	1.88	0.56
24:Y:246:LYS:HD2	24:Y:310:ARG:O	2.06	0.56
35:1:970:LEU:O	35:1:973:HIS:HB2	2.06	0.56
35:1:1299:GLU:CB	42:5:43:TYR:HE2	2.18	0.56
36:3:68:PHE:CE2	36:3:77:TYR:HB2	2.41	0.56
41:7:13:LYS:NZ	41:7:48:GLU:OE1	2.26	0.56
2:B:15:C:H2'	2:B:16:U:H6	1.71	0.56
3:C:401:ILE:HD11	3:C:423:PHE:HB2	1.88	0.56
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.87	0.56
4:E:239:THR:OG1	4:E:289:LEU:O	2.22	0.56
6:G:95:U:P	35:1:1106:ARG:HD2	2.46	0.56
9:J:321:GLU:OE1	9:J:355:ARG:NH1	2.39	0.56
35:1:954:LEU:O	35:1:958:THR:HG22	2.05	0.56
35:1:1178:MET:HG2	39:2:591:TYR:CE2	2.39	0.56
35:1:1179:ASP:CB	39:2:511:LEU:HB2	2.32	0.56
1:A:1980:GLU:O	1:A:1984:LYS:HG2	2.06	0.56
3:C:529:ARG:NH2	3:C:540:GLU:HB2	2.20	0.56
17:R:357:HIS:O	17:R:361:LYS:HD2	2.06	0.56
23:X:430:THR:HG22	23:X:434:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1293:ASN:OD1	42:5:77:GLY:HA3	2.06	0.56
28:n:40:LEU:N	28:n:58:LEU:O	2.39	0.56
11:L:66:GLU:O	11:L:69:GLU:HG3	2.05	0.56
11:L:223:GLY:HA2	17:R:86:LEU:CD2	2.36	0.56
23:X:171:ARG:NH2	23:X:505:PHE:O	2.39	0.56
23:X:331:GLU:O	23:X:335:GLY:N	2.39	0.56
23:X:476:GLU:HG3	23:X:477:VAL:H	1.70	0.56
23:X:580:ASP:HB2	23:X:733:LYS:HG3	1.88	0.56
23:X:698:LYS:O	23:X:757:ARG:HD3	2.06	0.56
35:1:605:GLY:O	35:1:608:THR:OG1	2.16	0.56
36:3:418:GLU:OE1	36:3:419:ASP:N	2.28	0.56
38:w:399:LEU:HD11	39:2:507:LYS:CG	2.36	0.56
42:5:14:LEU:HD23	42:5:17:LYS:HD2	1.88	0.56
1:A:35:ARG:O	1:A:39:GLN:HG3	2.06	0.55
1:A:984:MET:HE3	1:A:1048:MET:HE2	1.89	0.55
1:A:1636:LYS:HD3	1:A:1658:GLN:NE2	2.18	0.55
3:C:678:THR:HG22	3:C:679:PRO:HD2	1.88	0.55
23:X:518:MET:HA	23:X:549:LEU:O	2.06	0.55
24:Y:257:GLU:OE2	24:Y:266:ILE:HG21	2.06	0.55
35:1:735:ILE:HD12	35:1:747:LEU:HD12	1.88	0.55
35:1:739:ARG:HA	35:1:743:LEU:HD22	1.88	0.55
36:3:477:SER:HB2	36:3:505:THR:N	2.11	0.55
36:3:479:VAL:HG23	36:3:480:ASN:ND2	2.20	0.55
36:3:703:ARG:HH11	36:3:703:ARG:HB2	1.70	0.55
40:4:13:ALA:O	40:4:60:GLU:HA	2.06	0.55
33:l:21:GLU:O	33:l:69:ARG:N	2.39	0.55
1:A:729:PRO:HG2	12:M:226:TYR:CD1	2.41	0.55
1:A:762:ARG:NH2	15:P:226:LYS:HZ3	2.05	0.55
1:A:1382:SER:CB	1:A:1415:GLY:HA2	2.36	0.55
6:G:94:C:OP1	35:1:1142:ASN:OD1	2.24	0.55
6:G:111:U:O2'	23:X:482:ARG:HD2	2.06	0.55
7:H:27:U:O2'	7:H:28:C:H5'	2.06	0.55
7:H:57:A:H5'	39:2:481:THR:HG21	1.88	0.55
7:H:78:C:H2'	7:H:79:G:H8	1.71	0.55
15:P:198:ALA:O	15:P:201:VAL:HG23	2.06	0.55
23:X:164:TRP:HB2	23:X:538:ASP:HB3	1.88	0.55
23:X:602:ILE:O	23:X:606:GLN:HB2	2.06	0.55
23:X:700:TYR:HA	23:X:706:MET:O	2.07	0.55
23:X:811:SER:HA	23:X:814:LYS:NZ	2.21	0.55
35:1:703:THR:HG22	35:1:745:ALA:CB	2.30	0.55
35:1:818:PHE:HD1	35:1:823:MET:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1295:TYR:CE1	42:5:76:CYS:HB3	2.42	0.55
36:3:819:MET:HA	36:3:822:GLU:CD	2.31	0.55
1:A:758:ARG:HH21	1:A:775:ASN:ND2	2.03	0.55
2:B:117:A:C2	30:d:26:GLY:HA3	2.41	0.55
4:E:150:HIS:HA	4:E:177:LYS:HZ3	1.71	0.55
7:H:6:U:H2'	7:H:7:U:H6	1.70	0.55
7:H:50:C:H2'	7:H:51:A:H8	1.71	0.55
11:L:176:LEU:HD13	11:L:176:LEU:O	2.07	0.55
16:Q:543:LEU:N	16:Q:621:GLU:O	2.35	0.55
17:R:160:ALA:O	17:R:166:ARG:NH1	2.40	0.55
35:1:754:ILE:HG22	35:1:755:PRO:HD3	1.88	0.55
35:1:784:MET:O	35:1:788:VAL:HG12	2.05	0.55
35:1:926:LYS:O	35:1:929:LEU:HG	2.06	0.55
36:3:542:LYS:HB2	36:3:558:LEU:HD11	1.89	0.55
36:3:718:ARG:HB2	36:3:720:TRP:NE1	2.21	0.55
36:3:1015:LYS:O	36:3:1019:ASN:N	2.40	0.55
1:A:406:TRP:CZ2	3:C:266:GLU:HG3	2.41	0.55
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.41	0.55
4:E:165:GLN:HG3	4:E:181:ILE:HD13	1.89	0.55
35:1:819:TRP:HZ2	35:1:837:THR:HG21	1.71	0.55
36:3:69:ARG:HH12	36:3:74:THR:HA	1.71	0.55
36:3:1083:ASN:OD1	36:3:1084:GLY:N	2.39	0.55
1:A:548:ARG:HG2	1:A:548:ARG:HH21	1.72	0.55
1:A:831:SER:O	1:A:831:SER:OG	2.18	0.55
1:A:1795:GLU:HG2	1:A:1797:ASN:H	1.71	0.55
3:C:441:PRO:HB3	3:C:495:ARG:HH21	1.72	0.55
23:X:443:ASN:O	23:X:444:LYS:HB2	2.05	0.55
23:X:647:ILE:HA	23:X:651:LEU:HD21	1.88	0.55
36:3:978:LEU:HD11	38:w:480:GLU:HG2	1.88	0.55
3:C:86:THR:OG1	3:C:87:GLN:N	2.38	0.55
3:C:360:ALA:H	3:C:361:PRO:HD3	1.71	0.55
3:C:711:ARG:HB3	3:C:730:ARG:HH22	1.72	0.55
4:E:105:LEU:HD11	4:E:136:TRP:CG	2.42	0.55
4:E:201:PHE:CD1	4:E:208:ILE:HD13	2.42	0.55
5:F:35:A:H8	6:G:12:G:C6	2.23	0.55
6:G:1:G:N3	6:G:1:G:C2'	2.70	0.55
23:X:275:ARG:O	23:X:279:LEU:HD23	2.07	0.55
24:Y:122:VAL:HB	24:Y:123:HIS:CD2	2.39	0.55
36:3:294:LYS:HZ2	36:3:294:LYS:C	2.13	0.55
39:2:451:LYS:HB2	39:2:455:ARG:NH1	2.22	0.55
1:A:214:ARG:HH12	1:A:225:TYR:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HH22	1:A:229:GLN:HE21	1.54	0.55
1:A:1502:PHE:HZ	1:A:1505:LYS:HG3	1.72	0.55
3:C:529:ARG:HH22	3:C:540:GLU:HB2	1.71	0.55
5:F:42:C:H2'	5:F:43:A:O4'	2.06	0.55
7:H:36:G:H2'	7:H:37:U:C6	2.42	0.55
12:M:218:PHE:CD1	12:M:218:PHE:C	2.85	0.55
19:T:349:SER:OG	19:T:350:HIS:N	2.39	0.55
35:1:1062:LEU:HA	35:1:1065:LEU:HD12	1.88	0.55
36:3:233:ASN:HD21	36:3:286:ILE:CG2	2.19	0.55
36:3:791:HIS:NE2	36:3:934:GLY:HA3	2.22	0.55
36:3:1041:TYR:HB3	39:2:705:ARG:HG3	1.87	0.55
36:3:1145:GLU:HA	36:3:1148:LEU:HB2	1.87	0.55
38:w:429:TRP:HB3	38:w:430:ARG:NH1	2.22	0.55
3:C:506:PRO:HB2	3:C:569:ARG:NH2	2.22	0.55
3:C:632:THR:H	3:C:636:TYR:HD2	1.55	0.55
13:N:131:ILE:H	13:N:131:ILE:HD12	1.72	0.55
23:X:640:ARG:HG3	23:X:640:ARG:HH11	1.71	0.55
35:1:807:LYS:HG3	35:1:844:VAL:HG12	1.88	0.55
35:1:1130:PRO:HB2	39:2:533:ILE:HG21	1.89	0.55
35:1:1167:TYR:OH	39:2:581:LYS:CE	2.54	0.55
36:3:206:GLN:NE2	36:3:231:HIS:HA	2.21	0.55
36:3:1191:LYS:O	36:3:1195:GLU:HG3	2.06	0.55
42:5:27:THR:HG23	42:5:30:GLU:HG3	1.88	0.55
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.42	0.55
6:G:85:G:N1	7:H:44:U:N3	2.55	0.55
7:H:107:A:H2'	7:H:108:G:C8	2.42	0.55
7:H:165:A:O2'	7:H:166:G:O5'	2.24	0.55
23:X:537:LYS:HD2	23:X:563:PHE:CZ	2.41	0.55
23:X:1008:LEU:HB3	23:X:1016:TYR:HD2	1.71	0.55
35:1:1274:ILE:HG22	36:3:109:LYS:HE2	1.89	0.55
39:2:646:PRO:C	39:2:648:LEU:N	2.59	0.55
41:7:33:CYS:HG	41:7:35:SER:HG	1.07	0.55
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.21	0.55
1:A:1975:GLU:O	1:A:1979:VAL:HG22	2.07	0.55
6:G:107:U:O2	23:X:709:LEU:HD22	2.05	0.55
11:L:159:LEU:O	12:M:211:ILE:CD1	2.54	0.55
17:R:196:VAL:HG13	17:R:196:VAL:O	2.07	0.55
21:V:606:GLU:OE2	21:V:609:GLN:HG3	2.06	0.55
23:X:412:ILE:HB	23:X:418:LEU:HD22	1.88	0.55
35:1:769:VAL:HA	35:1:772:ILE:HD13	1.89	0.55
36:3:911:LYS:CB	36:3:922:GLY:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:926:TYR:HB3	36:3:928:TYR:CE2	2.41	0.55
37:p:177:PHE:HA	37:p:194:PHE:HA	1.89	0.55
42:5:8:HIS:NE2	42:5:12:GLU:OE2	2.37	0.55
1:A:36:LYS:NZ	22:W:163:GLN:O	2.37	0.54
1:A:135:VAL:O	1:A:418:THR:OG1	2.22	0.54
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.20	0.54
9:J:438:TYR:O	9:J:442:ARG:CB	2.55	0.54
11:L:176:LEU:HD13	11:L:176:LEU:C	2.32	0.54
11:L:782:LYS:O	11:L:786:HIS:N	2.39	0.54
17:R:408:ASP:OD1	17:R:410:ARG:N	2.28	0.54
19:T:371:HIS:CE1	19:T:396:LYS:HG3	2.42	0.54
23:X:515:SER:O	23:X:547:LYS:HB2	2.07	0.54
23:X:631:ARG:HG3	23:X:635:LEU:HD23	1.88	0.54
35:1:1297:ARG:NH1	42:5:39:SER:OG	2.40	0.54
36:3:592:LEU:HD11	36:3:619:LEU:HD21	1.88	0.54
1:A:1108:ASP:O	1:A:1112:ARG:HG3	2.06	0.54
3:C:514:TYR:HE2	3:C:522:SER:HB3	1.72	0.54
4:E:188:GLN:NE2	4:E:189:THR:H	2.05	0.54
5:F:38:G:P	5:F:38:G:H8	2.29	0.54
19:T:429:SER:HB3	19:T:439:TRP:HE1	1.72	0.54
35:1:728:LEU:HB3	35:1:765:TYR:OH	2.08	0.54
35:1:1277:GLN:CG	36:3:113:ARG:HD3	2.37	0.54
36:3:189:TYR:CG	42:5:37:ARG:NH2	2.75	0.54
36:3:406:PRO:HG2	36:3:408:LEU:HD11	1.89	0.54
36:3:642:ILE:N	36:3:703:ARG:HE	2.06	0.54
36:3:979:ARG:H	38:w:478:GLU:CD	2.15	0.54
3:C:112:THR:OG1	3:C:116:MET:N	2.41	0.54
4:E:90:ILE:HD12	4:E:105:LEU:HD22	1.90	0.54
5:F:41:A:H2'	5:F:42:C:C6	2.43	0.54
7:H:43:U:HO2'	7:H:44:U:P	2.29	0.54
11:L:224:PHE:H	17:R:86:LEU:HD23	1.72	0.54
12:M:204:ASP:OD2	12:M:204:ASP:N	2.40	0.54
23:X:471:VAL:HG21	23:X:476:GLU:CD	2.33	0.54
23:X:695:CYS:HB3	23:X:722:ARG:HH22	1.73	0.54
35:1:833:LEU:O	35:1:837:THR:OG1	2.23	0.54
36:3:191:GLU:O	36:3:194:ASN:N	2.26	0.54
36:3:567:GLU:OE2	36:3:601:ARG:NH2	2.40	0.54
1:A:41:GLN:NE2	1:A:41:GLN:O	2.41	0.54
1:A:1519:THR:HG23	1:A:1519:THR:O	2.08	0.54
2:B:8:G:H1	2:B:70:A:H1'	1.71	0.54
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:713:LYS:HA	3:C:716:GLU:OE2	2.07	0.54
5:F:16:G:H2'	5:F:17:C:C6	2.42	0.54
19:T:371:HIS:NE2	19:T:389:SER:OG	2.37	0.54
36:3:168:TYR:OH	42:5:70:GLU:OE2	2.26	0.54
36:3:226:GLU:OE1	36:3:259:LYS:HD3	2.06	0.54
36:3:526:HIS:CG	36:3:573:GLN:HE21	2.25	0.54
38:w:429:TRP:CE3	38:w:430:ARG:HG3	2.43	0.54
29:h:69:ASN:N	29:h:97:SER:O	2.41	0.54
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.08	0.54
1:A:1861:ILE:HG22	1:A:1882:ILE:HG12	1.89	0.54
3:C:297:ASN:N	3:C:297:ASN:OD1	2.37	0.54
4:E:166:LEU:HD12	4:E:167:VAL:H	1.73	0.54
7:H:7:U:H2'	7:H:8:C:C6	2.42	0.54
21:V:584:LYS:HG3	21:V:585:ILE:N	2.21	0.54
36:3:193:ASP:CA	42:5:79:PRO:HG3	2.37	0.54
36:3:234:PHE:C	36:3:235:LEU:HD12	2.33	0.54
39:2:640:GLY:O	40:4:69:TYR:CB	2.56	0.54
40:4:121:SER:HA	40:4:124:GLY:O	2.07	0.54
41:7:57:ARG:NH1	41:7:62:GLY:O	2.39	0.54
1:A:701:ILE:H	1:A:701:ILE:HD12	1.72	0.54
1:A:1756:SER:HG	35:1:943:LYS:HD2	1.70	0.54
9:J:216:ASP:HB3	9:J:217:GLU:OE1	2.08	0.54
11:L:205:LYS:H	11:L:205:LYS:HD3	1.71	0.54
20:U:71:LEU:O	20:U:75:GLU:N	2.38	0.54
23:X:620:GLU:CD	23:X:620:GLU:H	2.15	0.54
23:X:937:ILE:HD12	23:X:937:ILE:H	1.72	0.54
24:Y:4:LEU:HD11	24:Y:11:ASP:HB3	1.90	0.54
24:Y:255:ASP:HA	24:Y:258:ILE:HD12	1.89	0.54
25:Z:85:LYS:HA	34:t:79:GLN:CB	2.38	0.54
35:1:785:LYS:O	35:1:789:LEU:HD12	2.07	0.54
35:1:933:CYS:SG	35:1:970:LEU:HD21	2.48	0.54
36:3:269:CYS:SG	36:3:327:LEU:HD11	2.48	0.54
36:3:717:SER:HB2	36:3:718:ARG:NH1	2.20	0.54
1:A:1130:ASN:OD1	1:A:1139:ARG:HB3	2.07	0.54
1:A:1164:SER:HB3	3:C:59:LEU:HD21	1.90	0.54
2:B:110:C:H2'	2:B:111:A:C8	2.41	0.54
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.90	0.54
5:F:15:A:H2'	5:F:16:G:H8	1.73	0.54
35:1:652:CYS:SG	35:1:689:ILE:HG23	2.48	0.54
35:1:815:PHE:HE1	35:1:853:ILE:HG21	1.72	0.54
35:1:819:TRP:CZ3	35:1:868:VAL:HG12	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:933:CYS:O	35:1:936:VAL:N	2.41	0.54
36:3:312:LYS:HB2	36:3:330:PHE:HD1	1.72	0.54
1:A:122:ILE:HD12	1:A:123:THR:HG22	1.90	0.54
4:E:202:ASN:ND2	4:E:207:GLN:OE1	2.41	0.54
9:J:238:ASN:C	9:J:240:THR:H	2.15	0.54
9:J:568:LYS:HA	9:J:601:GLY:HA3	1.89	0.54
12:M:178:GLU:HA	12:M:181:ARG:HD3	1.90	0.54
15:P:208:LYS:O	15:P:208:LYS:NZ	2.29	0.54
21:V:609:GLN:NE2	21:V:616:LEU:HD21	2.23	0.54
23:X:648:TYR:O	23:X:656:GLN:NE2	2.40	0.54
23:X:837:SER:HB2	23:X:930:SER:O	2.08	0.54
34:q:106:ALA:HB1	34:t:106:ALA:HB3	1.89	0.54
35:1:1103:VAL:O	35:1:1109:ARG:HD3	2.07	0.54
36:3:2:PHE:C	36:3:3:LEU:HD23	2.32	0.54
36:3:18:ILE:HG21	36:3:67:ALA:H	1.72	0.54
1:A:1681:ARG:NH1	1:A:1681:ARG:HB3	2.23	0.54
1:A:1979:VAL:HA	1:A:1982:GLN:HB2	1.88	0.54
3:C:119:LEU:O	3:C:123:MET:HG3	2.08	0.54
3:C:699:ASP:OD1	3:C:722:TYR:OH	2.24	0.54
4:E:62:LEU:O	4:E:350:ARG:HB2	2.07	0.54
21:V:589:GLU:O	21:V:593:TYR:HB2	2.07	0.54
23:X:635:LEU:HB2	23:X:639:ILE:HD11	1.89	0.54
23:X:793:LEU:HA	23:X:796:LEU:HD12	1.90	0.54
35:1:614:ARG:O	35:1:614:ARG:NH1	2.34	0.54
35:1:849:ILE:O	35:1:853:ILE:HG12	2.08	0.54
39:2:495:ARG:O	39:2:497:SER:N	2.41	0.54
3:C:126:SER:O	3:C:126:SER:OG	2.22	0.54
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.90	0.54
3:C:928:HIS:ND1	3:C:928:HIS:N	2.55	0.54
6:G:88:G:O6	7:H:40:C:N4	2.41	0.54
19:T:346:ILE:HD13	19:T:380:LEU:HD21	1.89	0.54
23:X:639:ILE:HG22	23:X:640:ARG:H	1.73	0.54
35:1:896:ILE:HD12	35:1:917:VAL:HG11	1.90	0.54
35:1:1206:ASP:OD1	35:1:1207:SER:N	2.41	0.54
35:1:1257:PRO:HD3	39:2:482:ALA:CB	2.27	0.54
36:3:234:PHE:CE1	36:3:236:ILE:HG12	2.42	0.54
36:3:943:THR:HG23	36:3:976:LYS:HB3	1.89	0.54
39:2:530:ARG:HH12	39:2:578:TRP:CD1	2.26	0.54
29:h:58:ALA:O	29:h:65:MET:HA	2.07	0.54
1:A:57:GLN:HE21	1:A:57:GLN:CA	2.20	0.53
1:A:395:THR:HG22	1:A:396:ASP:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.73	0.53
3:C:349:PHE:HB2	3:C:356:PHE:CD1	2.43	0.53
7:H:151:C:H2'	7:H:152:G:C8	2.43	0.53
23:X:696:LYS:HB3	23:X:709:LEU:HD11	1.90	0.53
35:1:806:ILE:HG23	35:1:810:ILE:HB	1.91	0.53
35:1:1092:ASP:O	35:1:1096:THR:HG23	2.08	0.53
35:1:1274:ILE:HG22	36:3:109:LYS:HE3	1.90	0.53
36:3:289:CYS:SG	36:3:338:ALA:HA	2.48	0.53
36:3:747:SER:OG	36:3:748:GLU:N	2.40	0.53
3:C:220:ARG:NH1	3:C:578:ARG:O	2.38	0.53
3:C:818:SER:O	3:C:822:MET:HB2	2.09	0.53
4:E:260:ARG:CD	4:E:276:ILE:HG12	2.39	0.53
11:L:39:HIS:H	11:L:151:MET:HE3	1.73	0.53
12:M:224:ARG:CB	12:M:224:ARG:NH1	2.72	0.53
23:X:527:LEU:HD23	23:X:755:ILE:HD13	1.90	0.53
35:1:693:GLY:HA2	35:1:696:ASP:HB2	1.90	0.53
35:1:778:GLN:N	35:1:778:GLN:OE1	2.41	0.53
36:3:164:ASN:HA	36:3:189:TYR:CZ	2.43	0.53
1:A:263:PHE:CE1	1:A:273:ILE:HD11	2.43	0.53
1:A:1189:MET:HG2	1:A:1190:CYS:H	1.72	0.53
3:C:187:THR:HA	3:C:200:PHE:O	2.08	0.53
7:H:118:G:H2'	7:H:119:G:C8	2.44	0.53
9:J:443:ILE:HG13	9:J:444:SER:H	1.72	0.53
11:L:569:GLN:HA	34:q:114:CYS:O	2.07	0.53
17:R:328:ALA:HB1	24:Y:226:MET:O	2.07	0.53
19:T:351:ASP:O	19:T:352:THR:OG1	2.25	0.53
21:V:628:ILE:HD11	21:V:643:LEU:HB2	1.90	0.53
23:X:164:TRP:CZ3	23:X:168:GLU:OE2	2.62	0.53
23:X:455:ARG:NE	23:X:481:ILE:HD13	2.23	0.53
24:Y:118:TYR:N	24:Y:118:TYR:CD1	2.77	0.53
35:1:731:LEU:O	35:1:735:ILE:HG12	2.08	0.53
35:1:883:ASP:OD2	35:1:883:ASP:N	2.35	0.53
36:3:803:ASP:OD1	36:3:804:HIS:N	2.41	0.53
36:3:978:LEU:HD21	38:w:480:GLU:HB3	1.87	0.53
38:w:440:ILE:HG12	38:w:459:TRP:CG	2.44	0.53
1:A:214:ARG:NH1	1:A:225:TYR:HB2	2.24	0.53
1:A:836:THR:O	1:A:840:ILE:HG12	2.07	0.53
2:B:108:G:H3'	2:B:109:G:H8	1.73	0.53
3:C:825:PRO:O	3:C:826:ARG:HG2	2.08	0.53
11:L:184:ALA:O	11:L:188:ARG:N	2.31	0.53
17:R:386:ARG:NH1	17:R:391:VAL:HG21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:250:ARG:HD2	19:T:266:GLU:HG3	1.90	0.53
23:X:700:TYR:HE2	23:X:705:GLY:HA2	1.73	0.53
23:X:842:THR:HB	23:X:882:LEU:HD23	1.91	0.53
24:Y:21:ARG:HH12	24:Y:83:VAL:N	2.07	0.53
35:1:815:PHE:HA	35:1:819:TRP:CD1	2.43	0.53
35:1:1252:GLN:CD	39:2:492:LYS:HA	2.33	0.53
36:3:623:ASP:OD2	36:3:626:GLN:NE2	2.41	0.53
41:7:46:CYS:N	41:7:85:CYS:HB2	2.22	0.53
1:A:1817:LEU:CD2	1:A:1919:LEU:HD21	2.39	0.53
1:A:1920:TYR:HE1	1:A:1936:LEU:HD22	1.72	0.53
3:C:112:THR:OG1	3:C:112:THR:O	2.25	0.53
3:C:725:ASP:HB3	3:C:728:ALA:H	1.74	0.53
6:G:12:G:H3'	6:G:13:C:C6	2.44	0.53
7:H:36:G:H2'	7:H:37:U:H6	1.73	0.53
9:J:397:LYS:O	9:J:400:GLU:HG3	2.09	0.53
23:X:643:LEU:HG	23:X:669:LYS:HA	1.89	0.53
35:1:572:HIS:CE1	35:1:612:THR:HB	2.44	0.53
36:3:34:ARG:HB2	36:3:37:ILE:HB	1.91	0.53
1:A:1352:HIS:CD2	20:U:5:ILE:HG21	2.43	0.53
1:A:1771:LEU:HD21	1:A:1779:PHE:HE2	1.74	0.53
2:B:87:A:H61	2:B:92:U:P	2.32	0.53
3:C:441:PRO:O	3:C:444:GLY:HA3	2.09	0.53
3:C:453:TYR:CE1	3:C:465:MET:HE1	2.43	0.53
6:G:83:A:P	6:G:83:A:H8	2.31	0.53
11:L:201:LYS:NZ	11:L:203:LYS:HG2	2.23	0.53
12:M:125:SER:O	17:R:242:GLN:NE2	2.42	0.53
17:R:150:ALA:O	17:R:153:LYS:HG3	2.09	0.53
17:R:351:GLU:O	17:R:355:ILE:HG13	2.08	0.53
17:R:413:ASN:O	23:X:633:ARG:HD3	2.09	0.53
19:T:287:HIS:NE2	19:T:305:THR:OG1	2.33	0.53
23:X:640:ARG:HH12	23:X:668:ARG:HB2	1.74	0.53
23:X:787:GLU:HG3	35:1:542:PRO:CD	2.39	0.53
24:Y:306:ILE:HG12	24:Y:311:ILE:HD13	1.89	0.53
36:3:193:ASP:O	42:5:79:PRO:HG2	2.08	0.53
36:3:530:ASP:O	36:3:532:ARG:N	2.40	0.53
36:3:979:ARG:N	38:w:478:GLU:HG3	2.24	0.53
1:A:142:SER:HA	1:A:242:ALA:HB2	1.91	0.53
1:A:1831:LYS:NZ	1:A:1832:ARG:HB2	2.24	0.53
2:B:99:C:H2'	2:B:100:C:C6	2.43	0.53
3:C:279:ARG:NH1	21:V:324:HIS:O	2.41	0.53
4:E:240:GLY:O	4:E:252:SER:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:159:LEU:O	12:M:211:ILE:HD13	2.08	0.53
13:N:63:LEU:O	13:N:70:ILE:HG12	2.09	0.53
35:1:523:ALA:C	35:1:563:LEU:HD11	2.33	0.53
36:3:442:LEU:HD13	36:3:770:LEU:HD23	1.91	0.53
36:3:607:VAL:N	36:3:615:ARG:O	2.29	0.53
36:3:632:ALA:O	36:3:633:LEU:HD23	2.09	0.53
36:3:674:LEU:C	36:3:675:LEU:HD12	2.34	0.53
1:A:41:GLN:HE22	1:A:45:TYR:HB2	1.74	0.53
1:A:83:HIS:NE2	6:G:16:G:O6	2.42	0.53
1:A:1143:MET:SD	1:A:1143:MET:N	2.81	0.53
3:C:439:PRO:O	3:C:443:VAL:HB	2.09	0.53
3:C:460:ASP:OD2	3:C:461:LEU:N	2.41	0.53
3:C:481:MET:SD	3:C:612:LYS:HG3	2.48	0.53
3:C:938:ARG:HG2	3:C:942:GLY:HA3	1.91	0.53
10:K:209:GLY:HA2	10:K:223:ARG:HD3	1.90	0.53
35:1:609:MET:HE1	35:1:635:VAL:HG11	1.91	0.53
36:3:940:LEU:HB3	36:3:941:HIS:CE1	2.43	0.53
1:A:225:TYR:O	1:A:418:THR:HG21	2.09	0.53
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.16	0.53
1:A:1019:TYR:O	1:A:1020:LYS:C	2.52	0.53
3:C:514:TYR:CE2	3:C:522:SER:HB3	2.44	0.53
4:E:208:ILE:HG23	4:E:220:TRP:HD1	1.74	0.53
4:E:311:VAL:HB	4:E:321:TYR:HB2	1.90	0.53
6:G:1:G:C2	6:G:2:U:H1'	2.43	0.53
19:T:203:HIS:CE1	19:T:229:LYS:HG3	2.44	0.53
23:X:725:ARG:HD3	23:X:728:ARG:NH1	2.23	0.53
23:X:787:GLU:CB	35:1:542:PRO:CG	2.72	0.53
35:1:557:ASP:HB2	35:1:596:ILE:HG22	0.70	0.53
35:1:1006:MET:HB3	35:1:1013:ILE:HG12	1.90	0.53
42:5:63:ARG:O	42:5:67:ASN:ND2	2.42	0.53
23:X:741:TRP:CH2	35:1:782:GLU:OE2	2.61	0.53
35:1:557:ASP:CA	35:1:596:ILE:HG22	2.36	0.53
35:1:1274:ILE:O	36:3:113:ARG:NH1	2.26	0.53
36:3:229:GLU:HB2	36:3:230:GLU:OE1	2.09	0.53
36:3:883:GLU:HB3	36:3:886:GLU:HG3	1.89	0.53
36:3:939:PHE:CZ	36:3:942:LYS:HG2	2.44	0.53
36:3:1015:LYS:HZ2	36:3:1016:ARG:N	2.07	0.53
39:2:460:PHE:HB3	39:2:464:GLU:HG2	1.91	0.53
40:4:102:ILE:C	40:4:177:ALA:HB2	2.33	0.53
1:A:65:HIS:O	1:A:69:ILE:HG13	2.10	0.52
1:A:1737:ASN:OD1	1:A:1739:ALA:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:258:THR:HG23	4:E:278:GLN:HE22	1.73	0.52
4:E:283:ASN:N	4:E:283:ASN:OD1	2.41	0.52
6:G:8:C:H2'	6:G:9:C:C2	2.45	0.52
19:T:468:CYS:HB3	19:T:479:THR:HG22	1.89	0.52
23:X:167:THR:O	23:X:171:ARG:HG3	2.08	0.52
23:X:390:GLU:O	23:X:393:GLN:HG3	2.09	0.52
35:1:515:ALA:O	35:1:519:ILE:HG22	2.09	0.52
35:1:796:CYS:C	35:1:801:VAL:HG21	2.34	0.52
35:1:1058:ILE:O	35:1:1062:LEU:HG	2.08	0.52
36:3:278:LEU:HD21	36:3:816:LYS:HZ3	1.74	0.52
36:3:769:LYS:HD3	36:3:769:LYS:N	2.24	0.52
1:A:274:PRO:HG3	20:U:1:MET:HE3	1.91	0.52
1:A:1381:ASP:OD1	1:A:1414:ARG:HG2	2.09	0.52
3:C:750:LEU:HA	3:C:753:GLU:HB2	1.91	0.52
6:G:85:G:H2'	6:G:86:A:N9	2.25	0.52
9:J:375:ASP:OD1	9:J:376:VAL:N	2.42	0.52
21:V:490:CYS:SG	21:V:521:TYR:HB3	2.49	0.52
23:X:936:TYR:HA	23:X:939:VAL:HG22	1.91	0.52
24:Y:6:GLU:HG3	24:Y:158:HIS:HB3	1.91	0.52
35:1:1260:LYS:O	35:1:1264:VAL:HG22	2.09	0.52
36:3:484:VAL:C	36:3:485:LEU:HD12	2.34	0.52
36:3:978:LEU:HA	38:w:478:GLU:OE2	2.09	0.52
38:w:430:ARG:HH11	38:w:430:ARG:H	1.56	0.52
41:7:21:ARG:NH1	41:7:66:VAL:O	2.27	0.52
1:A:233:PRO:O	1:A:237:THR:HG23	2.10	0.52
1:A:885:LEU:HD23	1:A:1005:ILE:HG12	1.91	0.52
1:A:1844:GLU:O	1:A:1848:LEU:HD23	2.10	0.52
4:E:100:ASP:N	4:E:100:ASP:OD1	2.42	0.52
6:G:102:G:N3	6:G:102:G:C2'	2.71	0.52
9:J:443:ILE:HG23	9:J:444:SER:O	2.10	0.52
17:R:325:ARG:NH1	17:R:328:ALA:HB3	2.24	0.52
25:Z:15:ALA:CB	34:s:112:ALA:C	2.82	0.52
35:1:740:GLY:H	35:1:743:LEU:HD22	1.74	0.52
35:1:1127:THR:HA	39:2:571:LEU:HD13	1.92	0.52
1:A:1819:LEU:HD21	1:A:1906:ILE:HD11	1.91	0.52
2:B:64:G:H2'	2:B:65:G:H8	1.74	0.52
3:C:559:ILE:HD12	3:C:560:VAL:O	2.09	0.52
8:I:433:ALA:HB1	8:I:482:LYS:CB	2.38	0.52
14:O:249:ARG:O	14:O:252:PHE:N	2.43	0.52
23:X:162:ASP:HB2	23:X:542:PHE:CZ	2.33	0.52
36:3:1025:ALA:HA	36:3:1087:GLN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:41:GLN:HA	29:h:55:ARG:HA	1.92	0.52
31:j:60:ASP:N	31:j:75:GLY:O	2.42	0.52
1:A:845:ARG:HH11	1:A:1440:THR:HG22	1.74	0.52
1:A:1283:GLU:OE1	1:A:1283:GLU:N	2.42	0.52
4:E:145:LYS:NZ	4:E:184:LYS:HG3	2.24	0.52
12:M:224:ARG:NH1	12:M:224:ARG:HB2	2.25	0.52
35:1:1080:THR:HA	35:1:1083:TYR:HD2	1.74	0.52
36:3:477:SER:CB	36:3:505:THR:H	2.11	0.52
41:7:39:PRO:HB2	41:7:70:TYR:CD1	2.44	0.52
1:A:832:TYR:OH	1:A:929:GLU:OE2	2.25	0.52
1:A:1211:ASP:C	1:A:1213:VAL:H	2.18	0.52
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.23	0.52
1:A:1894:GLN:HE21	1:A:1944:HIS:CE1	2.26	0.52
4:E:108:HIS:NE2	4:E:128:SER:HB2	2.24	0.52
4:E:281:VAL:HG21	4:E:306:ASP:HB2	1.91	0.52
6:G:85:G:O6	7:H:44:U:O4	2.28	0.52
7:H:172:C:N4	7:H:173:C:H41	2.07	0.52
23:X:164:TRP:HB2	23:X:538:ASP:CB	2.39	0.52
23:X:276:VAL:CG2	24:Y:227:VAL:HA	2.40	0.52
25:Z:36:VAL:O	34:r:112:ALA:CB	2.55	0.52
35:1:560:LEU:HD11	35:1:600:LEU:HD13	1.92	0.52
35:1:1274:ILE:CG2	36:3:109:LYS:HE2	2.40	0.52
36:3:120:PHE:HB2	36:3:133:SER:OG	2.09	0.52
36:3:206:GLN:NE2	36:3:232:GLY:H	2.07	0.52
27:m:72:LEU:HA	33:l:70:PHE:HA	1.91	0.52
1:A:1972:THR:O	1:A:1976:TRP:HB2	2.09	0.52
2:B:95:G:N3	2:B:95:G:C2'	2.73	0.52
3:C:497:LEU:O	3:C:546:ALA:HB1	2.10	0.52
4:E:135:VAL:CG1	4:E:145:LYS:HB2	2.40	0.52
35:1:547:GLN:HA	35:1:550:HIS:HB3	1.92	0.52
35:1:1007:HIS:CD2	35:1:1008:LYS:HG3	2.45	0.52
36:3:147:ASP:OD1	36:3:150:ALA:N	2.43	0.52
36:3:233:ASN:HD21	36:3:286:ILE:HG22	1.75	0.52
36:3:819:MET:HA	36:3:822:GLU:OE1	2.10	0.52
30:i:21:VAL:O	30:i:28:GLU:HA	2.09	0.52
1:A:75:ASP:O	1:A:77:THR:HG22	2.10	0.52
1:A:1650:ASP:OD1	1:A:1718:TRP:HB2	2.10	0.52
23:X:223:VAL:HA	23:X:226:LEU:HG	1.92	0.52
35:1:1231:MET:HE1	35:1:1268:ILE:HG12	1.90	0.52
36:3:642:ILE:HB	36:3:703:ARG:HH21	1.73	0.52
36:3:777:VAL:HG22	36:3:779:PHE:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:1125:GLY:C	36:3:1126:ILE:HG13	2.35	0.52
1:A:872:ASP:O	1:A:874:PRO:HD3	2.10	0.52
1:A:1786:TYR:CD1	1:A:1833:LEU:HB2	2.45	0.52
3:C:750:LEU:CD2	20:U:63:LYS:O	2.56	0.52
7:H:103:U:H4'	7:H:104:U:H5'	1.92	0.52
17:R:91:ASP:OD1	17:R:95:LYS:N	2.27	0.52
35:1:545:GLU:HG2	35:1:548:GLU:HG3	1.91	0.52
35:1:1167:TYR:OH	39:2:581:LYS:CD	2.57	0.52
35:1:1291:ASP:OD1	35:1:1292:LYS:N	2.43	0.52
35:1:1297:ARG:HG2	42:5:36:HIS:NE2	2.25	0.52
36:3:390:ARG:HD3	36:3:393:LYS:HE3	1.91	0.52
36:3:519:VAL:HB	36:3:524:ILE:HG23	1.91	0.52
39:2:531:THR:O	39:2:531:THR:OG1	2.25	0.52
29:h:100:PHE:N	28:n:68:PHE:O	2.43	0.52
1:A:1785:VAL:O	1:A:1805:GLY:HA3	2.10	0.52
3:C:320:LEU:HD13	3:C:343:LEU:HB2	1.92	0.52
3:C:333:ASP:OD1	3:C:333:ASP:N	2.43	0.52
4:E:145:LYS:HE2	4:E:184:LYS:HE2	1.92	0.52
4:E:208:ILE:O	4:E:219:VAL:HA	2.10	0.52
11:L:63:TRP:HB3	11:L:68:GLU:HG3	1.91	0.52
15:P:67:GLU:CD	19:T:476:ARG:HH21	2.15	0.52
23:X:287:GLY:O	23:X:291:LYS:HG2	2.10	0.52
23:X:432:ILE:HB	23:X:433:PRO:HD3	1.91	0.52
24:Y:27:ASN:HD21	24:Y:65:SER:HA	1.75	0.52
36:3:317:THR:HB	36:3:322:VAL:HA	1.92	0.52
36:3:413:ALA:HB1	36:3:415:LEU:HD13	1.92	0.52
1:A:1973:ASP:OD1	1:A:1973:ASP:N	2.42	0.51
3:C:131:ASN:OD1	3:C:201:ASN:ND2	2.43	0.51
3:C:209:VAL:HG23	3:C:898:LEU:HD13	1.92	0.51
5:F:41:A:C2	6:G:7:G:N1	2.78	0.51
6:G:116:C:H2'	6:G:117:A:H5'	1.91	0.51
15:P:213:ASP:OD2	15:P:216:ARG:HB2	2.10	0.51
17:R:319:LYS:O	17:R:322:GLU:HG3	2.10	0.51
21:V:511:ALA:HB1	21:V:525:PHE:CZ	2.43	0.51
23:X:401:VAL:HG12	23:X:572:ILE:HD12	1.91	0.51
23:X:700:TYR:HB3	23:X:757:ARG:O	2.09	0.51
35:1:1289:ASN:HB3	35:1:1295:TYR:H	1.75	0.51
36:3:515:ALA:HB2	36:3:528:ARG:CZ	2.40	0.51
36:3:872:ILE:HD12	36:3:872:ILE:H	1.75	0.51
36:3:984:LYS:NZ	38:w:470:ARG:O	2.43	0.51
39:2:451:LYS:O	39:2:455:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:ARG:HB3	23:X:329:TRP:CE3	2.45	0.51
1:A:1718:TRP:CZ3	1:A:1726:ILE:HD11	2.45	0.51
2:B:69:A:H3'	2:B:70:A:C8	2.45	0.51
17:R:243:GLN:O	17:R:246:LYS:HG2	2.09	0.51
23:X:455:ARG:C	23:X:459:MET:HE3	2.34	0.51
23:X:683:ILE:HD13	23:X:686:ILE:HG13	1.91	0.51
35:1:886:HIS:HD2	35:1:887:LYS:HD3	1.74	0.51
36:3:91:GLU:HG2	36:3:92:TYR:N	2.25	0.51
36:3:266:ASP:OD1	36:3:266:ASP:N	2.40	0.51
36:3:424:TYR:CD1	36:3:437:VAL:HG22	2.46	0.51
1:A:59:GLU:CD	13:N:87:ASN:HB2	2.35	0.51
23:X:424:THR:HG21	23:X:728:ARG:NH2	2.25	0.51
23:X:441:TYR:OH	23:X:547:LYS:NZ	2.39	0.51
23:X:586:ALA:HB1	35:1:826:ASP:HA	1.92	0.51
23:X:877:ASP:O	23:X:881:LEU:HG	2.10	0.51
35:1:648:LEU:HA	35:1:651:VAL:HG22	1.92	0.51
35:1:972:GLY:O	35:1:976:VAL:HG12	2.10	0.51
36:3:991:SER:O	36:3:991:SER:OG	2.28	0.51
1:A:59:GLU:HB3	13:N:103:LEU:HD21	1.92	0.51
2:B:85:C:OP1	29:c:20:GLU:N	2.44	0.51
3:C:213:ASP:OD2	3:C:213:ASP:N	2.42	0.51
3:C:514:TYR:HD1	3:C:514:TYR:C	2.19	0.51
3:C:750:LEU:HD13	20:U:67:GLU:HA	1.92	0.51
5:F:40:U:H2'	5:F:41:A:C8	2.45	0.51
6:G:116:C:C5	17:R:370:SER:HB2	2.45	0.51
19:T:381:HIS:HD2	19:T:441:TRP:CE2	2.29	0.51
23:X:289:GLN:HG2	23:X:293:GLU:OE1	2.11	0.51
23:X:882:LEU:O	23:X:886:THR:OG1	2.20	0.51
24:Y:213:ALA:HA	24:Y:216:GLU:HG3	1.92	0.51
25:Z:90:PRO:CB	25:Z:109:ASN:C	2.83	0.51
35:1:1056:MET:HE3	35:1:1059:CYS:HB2	1.92	0.51
36:3:356:HIS:CD2	36:3:403:SER:HG	2.28	0.51
36:3:1168:PHE:N	36:3:1168:PHE:CD2	2.77	0.51
1:A:357:ASN:ND2	3:C:862:PRO:HB3	2.25	0.51
1:A:384:VAL:HA	3:C:331:PHE:HD2	1.75	0.51
3:C:514:TYR:C	3:C:514:TYR:CD1	2.89	0.51
15:P:74:LYS:O	15:P:77:ASP:HB3	2.11	0.51
17:R:148:ARG:O	17:R:152:GLU:HG3	2.11	0.51
17:R:367:ARG:HH11	17:R:371:ARG:NH1	2.09	0.51
23:X:412:ILE:HD13	23:X:418:LEU:HB2	1.91	0.51
24:Y:95:SER:OG	24:Y:125:VAL:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:661:ARG:HG2	35:1:692:HIS:NE2	2.25	0.51
35:1:1122:THR:OG1	35:1:1123:CYS:N	2.41	0.51
35:1:1179:ASP:HB2	39:2:511:LEU:CD1	2.40	0.51
35:1:1179:ASP:HB2	39:2:511:LEU:HD12	1.93	0.51
36:3:605:LEU:O	36:3:617:ILE:N	2.42	0.51
36:3:695:GLY:HA3	36:3:717:SER:OG	2.10	0.51
36:3:833:GLU:C	36:3:836:ALA:H	2.13	0.51
38:w:458:LEU:HD11	39:2:466:LYS:CB	2.41	0.51
41:7:58:CYS:HB3	41:7:62:GLY:N	2.25	0.51
33:l:33:ILE:N	33:l:42:GLN:O	2.43	0.51
1:A:71:ARG:NH1	1:A:177:ASP:OD1	2.43	0.51
1:A:1502:PHE:CZ	1:A:1505:LYS:HG3	2.46	0.51
1:A:1516:LYS:O	1:A:1517:LYS:HD2	2.10	0.51
7:H:181:G:H2'	7:H:182:U:C6	2.46	0.51
10:K:223:ARG:HH21	35:1:1018:PRO:CB	2.22	0.51
12:M:165:ASN:HB2	17:R:95:LYS:CB	2.38	0.51
17:R:321:GLU:HB2	23:X:283:TYR:CD2	2.46	0.51
19:T:272:CYS:HB3	19:T:282:ARG:HB3	1.92	0.51
24:Y:244:VAL:HG13	24:Y:312:HIS:O	2.11	0.51
35:1:712:LEU:O	35:1:716:ALA:CB	2.58	0.51
36:3:43:PRO:HB3	36:3:50:VAL:HG22	1.93	0.51
36:3:614:VAL:HG23	36:3:633:LEU:HD11	1.93	0.51
36:3:628:LEU:HD21	36:3:681:PRO:HA	1.92	0.51
38:w:440:ILE:HG12	38:w:459:TRP:CD2	2.45	0.51
38:w:472:GLN:O	38:w:476:GLU:HG3	2.10	0.51
38:w:478:GLU:HA	38:w:488:ASN:HA	1.92	0.51
39:2:534:GLN:O	39:2:538:GLU:HG3	2.11	0.51
1:A:1121:ASN:HB2	1:A:1123:GLU:OE2	2.11	0.51
13:N:38:GLU:CD	13:N:38:GLU:H	2.18	0.51
20:U:1:MET:O	20:U:3:ASN:N	2.44	0.51
24:Y:215:LYS:O	24:Y:218:LYS:N	2.44	0.51
36:3:1:MET:CG	39:2:709:GLY:O	2.59	0.51
36:3:379:LEU:HD12	36:3:380:GLU:H	1.76	0.51
36:3:451:GLU:HA	36:3:761:THR:HG22	1.92	0.51
36:3:663:LEU:HD23	36:3:679:LEU:HB3	1.92	0.51
1:A:26:SER:HB3	1:A:29:LYS:HB2	1.93	0.51
1:A:81:PHE:C	1:A:83:HIS:H	2.19	0.51
1:A:93:LYS:O	1:A:649:GLU:HG2	2.10	0.51
1:A:661:GLU:HB3	17:R:214:ILE:HG12	1.93	0.51
1:A:693:ILE:O	1:A:695:ASP:N	2.43	0.51
1:A:1091:TYR:O	1:A:1092:ILE:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.46	0.51
1:A:1935:ARG:O	1:A:1938:LEU:HG	2.11	0.51
4:E:72:CYS:SG	4:E:81:LEU:HD11	2.51	0.51
4:E:84:ALA:HB2	4:E:90:ILE:HG12	1.93	0.51
5:F:40:U:H3	6:G:7:G:H1	1.59	0.51
6:G:95:U:OP2	35:1:1106:ARG:HD2	2.10	0.51
13:N:54:HIS:CE1	13:N:92:TRP:HZ2	2.28	0.51
19:T:274:ASP:HB2	19:T:281:ILE:HD13	1.92	0.51
23:X:418:LEU:HD12	23:X:568:PRO:HG2	1.92	0.51
35:1:663:THR:HA	35:1:666:LYS:HE3	1.93	0.51
35:1:687:VAL:O	35:1:690:ILE:HG13	2.11	0.51
35:1:906:GLU:N	35:1:906:GLU:OE1	2.44	0.51
36:3:606:ALA:HA	36:3:616:ILE:HA	1.92	0.51
36:3:613:THR:HB	36:3:630:MET:HE1	1.93	0.51
39:2:453:LYS:HB3	39:2:456:ARG:HH21	1.74	0.51
27:m:46:ASP:HA	27:m:66:VAL:HA	1.93	0.51
1:A:1375:TRP:O	1:A:1378:GLU:N	2.44	0.51
3:C:782:GLU:OE2	3:C:941:LYS:NZ	2.44	0.51
7:H:133:U:H2'	7:H:134:C:C6	2.46	0.51
7:H:173:C:H2'	7:H:174:A:H8	1.76	0.51
11:L:166:LYS:HA	11:L:166:LYS:HE3	1.93	0.51
23:X:330:GLU:O	23:X:334:LEU:HD12	2.11	0.51
23:X:451:THR:HA	23:X:496:MET:O	2.10	0.51
35:1:848:GLU:OE2	35:1:848:GLU:HA	2.10	0.51
36:3:146:ARG:HB3	36:3:150:ALA:HA	1.93	0.51
36:3:233:ASN:ND2	36:3:233:ASN:N	2.59	0.51
36:3:288:VAL:HG12	42:5:62:ALA:HB3	1.93	0.51
36:3:458:ALA:HB1	36:3:460:TRP:HZ3	1.76	0.51
36:3:720:TRP:CE3	36:3:731:LEU:HG	2.45	0.51
1:A:422:LEU:HD22	1:A:638:LEU:HD13	1.93	0.51
1:A:1590:VAL:HG21	1:A:1628:ASP:OD1	2.11	0.51
5:F:45:A:C6	6:G:3:A:C5	2.99	0.51
7:H:165:A:O2'	7:H:166:G:O4'	2.29	0.51
8:I:393:LYS:N	8:I:394:PRO:HD3	2.26	0.51
12:M:159:GLU:OE2	12:M:167:LEU:HB3	2.11	0.51
13:N:104:ARG:HD3	13:N:136:HIS:HB3	1.92	0.51
17:R:189:ASN:HA	17:R:195:ARG:NH2	2.25	0.51
23:X:257:PHE:CE1	23:X:270:LEU:HB2	2.47	0.51
23:X:483:PHE:HE1	23:X:917:GLN:HB2	1.76	0.51
36:3:168:TYR:CE1	42:5:70:GLU:OE2	2.64	0.51
36:3:169:HIS:HD2	36:3:170:VAL:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:292:THR:HG1	36:3:301:PHE:HD1	1.57	0.51
36:3:700:LYS:O	36:3:714:ALA:HA	2.11	0.51
36:3:932:ASN:O	36:3:933:ASN:ND2	2.44	0.51
36:3:1131:PRO:HD3	39:2:708:TRP:CH2	2.46	0.51
31:j:32:GLN:HA	31:j:43:ILE:O	2.10	0.51
1:A:362:ARG:HG2	21:V:333:GLN:HA	1.93	0.50
1:A:1599:GLN:HB2	1:A:1600:GLU:OE1	2.10	0.50
2:B:96:A:H61	32:f:23:GLY:N	2.07	0.50
11:L:192:ARG:NH1	11:L:198:ILE:HB	2.26	0.50
21:V:550:MET:O	21:V:554:LEU:HG	2.11	0.50
23:X:171:ARG:NH2	23:X:509:PRO:HD3	2.21	0.50
23:X:596:VAL:O	23:X:600:LEU:HG	2.12	0.50
23:X:721:GLN:O	23:X:725:ARG:N	2.43	0.50
23:X:880:VAL:O	23:X:884:VAL:HG23	2.11	0.50
35:1:731:LEU:HD23	35:1:746:PHE:CD1	2.46	0.50
36:3:159:GLU:CD	36:3:161:HIS:H	2.19	0.50
36:3:185:LEU:HD13	36:3:206:GLN:OE1	2.11	0.50
36:3:550:ASN:HD22	36:3:553:GLN:HB2	1.75	0.50
36:3:776:GLN:HG2	36:3:777:VAL:N	2.26	0.50
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.35	0.50
1:A:1770:GLU:O	1:A:1773:SER:OG	2.29	0.50
3:C:343:LEU:HA	3:C:368:SER:OG	2.11	0.50
3:C:534:VAL:CG2	3:C:537:TYR:HB2	2.38	0.50
4:E:152:SER:OG	4:E:153:PHE:N	2.43	0.50
4:E:308:PHE:HE1	4:E:324:PRO:HB3	1.76	0.50
6:G:84:U:OP2	38:w:396:LEU:CD1	2.59	0.50
6:G:85:G:H2'	6:G:86:A:C4	2.46	0.50
7:H:102:U:O2	27:m:74:GLY:N	2.44	0.50
11:L:26:TYR:OH	11:L:158:ARG:NH1	2.36	0.50
21:V:536:ILE:HG21	21:V:579:SER:OG	2.11	0.50
23:X:430:THR:HG22	23:X:434:GLN:HE21	1.77	0.50
23:X:697:GLN:NE2	23:X:751:THR:OG1	2.42	0.50
23:X:774:ASP:CG	23:X:777:HIS:HD1	2.18	0.50
23:X:810:THR:O	23:X:814:LYS:HG3	2.11	0.50
24:Y:198:ASP:CG	24:Y:199:ASP:H	2.19	0.50
35:1:1134:ASN:ND2	39:2:534:GLN:HG3	2.26	0.50
36:3:259:LYS:HE2	36:3:266:ASP:HB3	1.94	0.50
36:3:677:THR:HA	36:3:685:ASP:O	2.12	0.50
1:A:467:GLN:HG3	2:B:19:A:N7	2.26	0.50
1:A:1845:VAL:O	1:A:1849:ILE:HG12	2.11	0.50
5:F:30:A:H61	6:G:16:G:H1'	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:386:ASP:O	8:I:388:PHE:N	2.44	0.50
9:J:330:ARG:HH22	12:M:149:TYR:HH	1.51	0.50
9:J:429:PHE:O	9:J:432:VAL:HG22	2.11	0.50
13:N:139:CYS:SG	13:N:140:ARG:N	2.84	0.50
19:T:309:ASP:OD1	19:T:309:ASP:N	2.43	0.50
23:X:944:THR:HG23	23:X:1003:ILE:HD11	1.93	0.50
35:1:830:TYR:O	35:1:834:VAL:HG23	2.11	0.50
35:1:908:SER:OG	35:1:912:ASN:OD1	2.28	0.50
36:3:929:LYS:HG3	36:3:931:VAL:HG22	1.93	0.50
36:3:940:LEU:HB3	36:3:941:HIS:ND1	2.26	0.50
36:3:984:LYS:CE	38:w:476:GLU:OE1	2.53	0.50
1:A:916:LYS:HD2	1:A:1035:GLN:NE2	2.26	0.50
1:A:1712:HIS:ND1	1:A:1734:MET:HG3	2.26	0.50
1:A:1866:LYS:HG3	1:A:1886:GLY:HA3	1.94	0.50
2:B:90:U:C5	33:g:38:ASN:C	2.85	0.50
2:B:98:G:H2'	2:B:99:C:C6	2.47	0.50
3:C:192:ASP:CG	3:C:193:THR:N	2.67	0.50
3:C:300:LEU:HD23	3:C:306:ASN:HB3	1.92	0.50
3:C:465:MET:HE2	3:C:475:MET:HG3	1.93	0.50
4:E:243:LEU:HA	4:E:250:LEU:HA	1.93	0.50
7:H:41:U:H2'	7:H:42:G:H8	1.75	0.50
7:H:152:G:H2'	7:H:153:A:C8	2.47	0.50
12:M:224:ARG:HH11	12:M:224:ARG:C	2.20	0.50
23:X:230:SER:O	23:X:234:TYR:HB2	2.11	0.50
23:X:601:GLN:HA	23:X:604:VAL:HG12	1.93	0.50
23:X:856:ARG:NH2	23:X:865:ASP:OD1	2.44	0.50
24:Y:217:ALA:O	24:Y:220:GLN:HG3	2.12	0.50
35:1:573:LYS:H	35:1:573:LYS:HD2	1.75	0.50
35:1:862:GLU:HA	35:1:865:ARG:NH1	2.27	0.50
36:3:642:ILE:H	36:3:703:ARG:NE	2.09	0.50
36:3:644:GLU:HG2	36:3:645:MET:N	2.25	0.50
41:7:71:TYR:CD2	41:7:81:ASP:HB2	2.46	0.50
1:A:1251:SER:O	1:A:1251:SER:OG	2.17	0.50
1:A:1397:ILE:HD11	17:R:405:VAL:HA	1.94	0.50
4:E:60:MET:CB	4:E:353:MET:HB3	2.41	0.50
23:X:741:TRP:CE3	35:1:782:GLU:OE2	2.65	0.50
34:q:106:ALA:CB	34:t:106:ALA:CB	2.87	0.50
36:3:275:ARG:HB3	36:3:275:ARG:HH21	1.75	0.50
38:w:496:LYS:HA	38:w:501:LEU:HB2	1.92	0.50
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.26	0.50
1:A:216:SER:O	1:A:216:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:PHE:HB2	1:A:1209:HIS:CD2	2.47	0.50
1:A:1745:GLU:OE1	35:1:980:GLU:CG	2.51	0.50
3:C:709:TRP:HA	3:C:713:LYS:HZ2	1.76	0.50
19:T:231:TRP:CZ3	19:T:238:LEU:HB2	2.46	0.50
23:X:184:ARG:O	23:X:188:ARG:HG3	2.12	0.50
35:1:831:ARG:O	35:1:834:VAL:HB	2.11	0.50
36:3:209:THR:OG1	36:3:210:PHE:N	2.45	0.50
36:3:469:GLU:HG2	36:3:470:PHE:CD1	2.47	0.50
36:3:823:MET:SD	36:3:838:MET:HG3	2.52	0.50
36:3:1031:ARG:HG2	36:3:1031:ARG:NH1	2.27	0.50
36:3:1114:SER:HB2	36:3:1215:TYR:CE1	2.46	0.50
33:l:36:GLU:O	33:l:39:MET:N	2.24	0.50
1:A:1785:VAL:O	1:A:1822:ILE:HD11	2.11	0.50
3:C:115:GLU:OE1	3:C:115:GLU:N	2.45	0.50
3:C:406:GLU:OE1	3:C:406:GLU:N	2.39	0.50
3:C:726:LEU:O	3:C:730:ARG:HG2	2.11	0.50
5:F:35:A:H8	6:G:12:G:O6	1.93	0.50
7:H:151:C:H2'	7:H:152:G:H8	1.76	0.50
9:J:222:ASP:OD1	9:J:226:ARG:NH1	2.44	0.50
17:R:235:ARG:NE	17:R:235:ARG:H	2.10	0.50
17:R:246:LYS:NZ	17:R:246:LYS:HB3	2.26	0.50
19:T:422:ASN:OD1	19:T:474:GLU:HB3	2.11	0.50
22:W:459:PRO:CB	39:2:567:ASP:HB3	2.42	0.50
23:X:834:TYR:CZ	23:X:941:LYS:HB3	2.47	0.50
24:Y:274:ASP:HB3	24:Y:277:THR:OG1	2.12	0.50
25:Z:81:LEU:CB	34:t:72:PRO:CB	2.90	0.50
31:e:15:VAL:O	32:f:33:GLY:HA3	2.12	0.50
35:1:819:TRP:HE3	35:1:864:TYR:CZ	2.30	0.50
35:1:1292:LYS:HD3	42:5:78:PRO:HG2	1.93	0.50
36:3:181:MET:HB3	36:3:212:GLU:HA	1.92	0.50
36:3:463:ARG:HD3	36:3:468:ASP:HB3	1.94	0.50
36:3:700:LYS:HB3	36:3:702:PHE:HZ	1.74	0.50
36:3:1116:SER:C	39:2:708:TRP:CZ2	2.90	0.50
2:B:115:C:OP1	31:e:67:LYS:O	2.30	0.50
3:C:177:ARG:C	3:C:179:VAL:H	2.20	0.50
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.27	0.50
3:C:710:ASN:OD1	3:C:712:LYS:HB3	2.12	0.50
11:L:19:LEU:HD23	11:L:54:LEU:HD22	1.92	0.50
11:L:63:TRP:HD1	11:L:67:GLU:HB3	1.77	0.50
11:L:178:GLU:O	11:L:182:LEU:HB2	2.12	0.50
19:T:497:GLU:OE1	19:T:497:GLU:N	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:217:ALA:HB2	21:V:357:LEU:HA	1.94	0.50
21:V:540:GLU:O	21:V:544:LEU:HB2	2.12	0.50
21:V:553:HIS:CD2	21:V:556:TYR:HE1	2.30	0.50
21:V:571:SER:OG	21:V:573:GLU:OE2	2.29	0.50
23:X:171:ARG:NE	23:X:505:PHE:O	2.43	0.50
23:X:612:LEU:HB2	23:X:686:ILE:HD12	1.93	0.50
23:X:652:PRO:HG2	23:X:655:MET:HE2	1.94	0.50
23:X:715:SER:O	23:X:718:SER:OG	2.29	0.50
24:Y:37:TYR:O	24:Y:40:CYS:HB2	2.10	0.50
25:Z:18:TYR:CB	25:Z:171:GLN:CB	2.90	0.50
36:3:704:VAL:C	36:3:710:GLU:HG3	2.37	0.50
36:3:945:VAL:HG21	36:3:963:VAL:HG21	1.93	0.50
36:3:1207:LYS:O	36:3:1211:ILE:HG12	2.12	0.50
2:B:96:A:N6	32:f:23:GLY:N	2.58	0.50
3:C:687:MET:HA	3:C:790:LYS:O	2.12	0.50
6:G:90:C:H42	7:H:40:C:H42	1.60	0.50
8:I:460:THR:CB	8:I:487:TRP:CB	2.90	0.50
23:X:698:LYS:HZ2	23:X:758:THR:HA	1.77	0.50
24:Y:298:PHE:HE2	24:Y:314:ASP:HA	1.77	0.50
35:1:1076:ALA:O	35:1:1080:THR:HG23	2.12	0.50
35:1:1287:ILE:HB	42:5:32:LEU:CD1	2.38	0.50
36:3:616:ILE:O	36:3:628:LEU:N	2.45	0.50
36:3:979:ARG:N	38:w:478:GLU:CG	2.73	0.50
28:n:30:THR:N	28:n:39:HIS:O	2.31	0.50
1:A:550:VAL:O	1:A:554:THR:HG23	2.12	0.49
2:B:39:C:H4'	2:B:40:U:OP1	2.12	0.49
4:E:66:GLU:N	4:E:87:ASP:OD2	2.45	0.49
8:I:102:ALA:HB1	16:Q:934:TYR:O	2.11	0.49
11:L:176:LEU:C	11:L:176:LEU:CD1	2.85	0.49
24:Y:183:ARG:HA	24:Y:183:ARG:NE	2.26	0.49
24:Y:305:LEU:HD23	24:Y:305:LEU:H	1.77	0.49
35:1:1010:THR:N	35:1:1011:PRO:CD	2.74	0.49
36:3:713:LEU:HD13	36:3:714:ALA:N	2.27	0.49
36:3:1040:ASP:OD2	36:3:1042:ASP:N	2.45	0.49
1:A:1014:ASN:ND2	11:L:83:ARG:HB2	2.28	0.49
1:A:1418:ARG:HB2	1:A:1462:GLY:HA3	1.94	0.49
1:A:1571:ILE:CG2	10:K:220:LEU:HD13	2.42	0.49
2:B:98:G:H2'	2:B:99:C:H6	1.77	0.49
3:C:536:ARG:O	3:C:536:ARG:HD3	2.12	0.49
4:E:105:LEU:HD21	4:E:136:TRP:CE2	2.48	0.49
4:E:181:ILE:H	4:E:181:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:248:SER:HB2	4:E:263:ASP:OD2	2.12	0.49
6:G:24:G:O2'	6:G:25:G:OP1	2.28	0.49
19:T:243:THR:O	19:T:243:THR:OG1	2.23	0.49
35:1:581:LEU:O	35:1:584:ASP:HB3	2.12	0.49
35:1:1003:VAL:HG22	35:1:1004:ILE:N	2.27	0.49
35:1:1126:PHE:HD2	39:2:571:LEU:HB3	1.76	0.49
38:w:421:ALA:HA	38:w:424:ARG:NE	2.24	0.49
41:7:15:ALA:HB2	41:7:84:GLY:HA2	1.94	0.49
1:A:525:LYS:HB2	1:A:525:LYS:HZ3	1.76	0.49
1:A:597:LYS:N	2:B:45:C:OP1	2.45	0.49
1:A:800:TYR:HB3	3:C:59:LEU:HD23	1.93	0.49
1:A:1771:LEU:HD21	1:A:1779:PHE:CE2	2.47	0.49
1:A:1785:VAL:HG23	1:A:1786:TYR:CD2	2.47	0.49
2:B:100:C:H2'	2:B:101:U:C6	2.46	0.49
6:G:111:U:H5'	23:X:499:GLY:HA3	1.94	0.49
7:H:33:G:C6	7:H:34:U:C4	3.01	0.49
17:R:263:PRO:HB2	17:R:265:ASP:OD1	2.12	0.49
21:V:503:TYR:CD1	21:V:549:LYS:HD2	2.47	0.49
24:Y:211:ILE:O	24:Y:215:LYS:HG2	2.13	0.49
35:1:702:ARG:HD2	35:1:746:PHE:CE2	2.48	0.49
35:1:1012:PRO:O	35:1:1015:ASP:OD1	2.30	0.49
35:1:1159:GLY:O	35:1:1161:MET:N	2.46	0.49
36:3:639:SER:OG	36:3:699:VAL:O	2.14	0.49
1:A:1914:MET:HE2	1:A:1915:VAL:C	2.37	0.49
2:B:13:C:H2'	2:B:14:U:C6	2.48	0.49
3:C:404:THR:O	3:C:408:LEU:HD12	2.12	0.49
3:C:474:LEU:HA	3:C:498:SER:O	2.11	0.49
3:C:832:TYR:CD2	3:C:899:SER:HB2	2.46	0.49
4:E:237:SER:OG	4:E:255:MET:HE2	2.13	0.49
5:F:49:G:N2	7:H:29:A:N7	2.60	0.49
5:F:86:U:H5''	12:M:134:GLN:HE22	1.77	0.49
9:J:320:GLU:OE1	9:J:325:ASN:HB3	2.13	0.49
9:J:330:ARG:CZ	9:J:361:ARG:HH12	2.26	0.49
11:L:79:PRO:C	11:L:80:THR:HG1	2.18	0.49
11:L:86:ALA:HB1	11:L:91:ARG:O	2.12	0.49
11:L:169:ARG:CZ	11:L:169:ARG:CB	2.88	0.49
19:T:201:SER:HB3	19:T:485:THR:HG22	1.95	0.49
19:T:297:HIS:HA	19:T:338:CYS:SG	2.53	0.49
23:X:163:GLU:OE2	23:X:778:PHE:HD2	1.89	0.49
23:X:164:TRP:CB	23:X:538:ASP:HB3	2.43	0.49
23:X:856:ARG:HD2	23:X:868:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:1007:TRP:HA	23:X:1010:GLU:HB2	1.94	0.49
35:1:517:ARG:HB3	35:1:517:ARG:CZ	2.43	0.49
35:1:933:CYS:SG	35:1:970:LEU:HD11	2.52	0.49
35:1:1012:PRO:C	35:1:1014:LYS:N	2.68	0.49
36:3:1187:PRO:O	36:3:1191:LYS:HG3	2.12	0.49
3:C:132:VAL:HG11	3:C:226:VAL:HG23	1.93	0.49
4:E:75:HIS:CE1	4:E:121:GLY:HA3	2.47	0.49
4:E:75:HIS:HB2	4:E:80:THR:H	1.78	0.49
7:H:57:A:OP1	39:2:459:ARG:NH1	2.37	0.49
9:J:185:ALA:HB2	11:L:141:PRO:O	2.13	0.49
11:L:166:LYS:HE3	11:L:166:LYS:CA	2.42	0.49
17:R:89:GLN:OE1	17:R:90:VAL:N	2.39	0.49
17:R:104:GLN:HE21	17:R:225:PRO:HB3	1.77	0.49
21:V:596:LEU:N	21:V:597:PRO:HD2	2.27	0.49
23:X:419:ILE:HD11	23:X:560:PHE:HB3	1.95	0.49
23:X:496:MET:HB2	23:X:500:MET:HB3	1.95	0.49
24:Y:290:LYS:HB3	24:Y:293:ASP:H	1.78	0.49
35:1:823:MET:HE3	35:1:829:ASN:HB3	1.93	0.49
36:3:388:GLN:NE2	36:3:845:GLU:OE1	2.46	0.49
36:3:979:ARG:O	38:w:478:GLU:HG2	2.11	0.49
36:3:1011:TRP:HB2	36:3:1025:ALA:O	2.11	0.49
1:A:162:LYS:HE2	1:A:163:ARG:O	2.13	0.49
1:A:1953:ILE:O	1:A:1956:PRO:HD3	2.13	0.49
2:B:92:U:H3'	2:B:92:U:H6	1.77	0.49
3:C:447:PRO:HA	3:C:450:GLU:OE1	2.13	0.49
3:C:767:VAL:O	3:C:771:GLN:HG3	2.12	0.49
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.30	0.49
4:E:182:ARG:NE	4:E:182:ARG:HA	2.28	0.49
4:E:337:PRO:HG2	4:E:338:ASP:OD2	2.12	0.49
5:F:80:G:H22	9:J:209:PRO:HD3	1.78	0.49
7:H:54:U:H2'	7:H:55:U:C6	2.48	0.49
9:J:189:ILE:HG22	9:J:189:ILE:O	2.12	0.49
9:J:205:LEU:C	9:J:205:LEU:CD2	2.84	0.49
12:M:155:LYS:HD2	12:M:156:HIS:NE2	2.27	0.49
19:T:213:GLU:HG2	19:T:214:PRO:N	2.26	0.49
19:T:460:ASP:OD2	19:T:460:ASP:N	2.45	0.49
23:X:743:TYR:O	23:X:747:LEU:HB2	2.12	0.49
23:X:972:PRO:HA	23:X:977:PHE:CD2	2.47	0.49
35:1:495:ARG:HA	35:1:498:MET:HE3	1.94	0.49
35:1:528:ALA:N	35:1:566:LEU:CD2	2.59	0.49
35:1:610:ILE:HG22	35:1:647:PHE:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:841:ALA:CA	35:1:849:ILE:HG13	2.39	0.49
35:1:898:TYR:CZ	35:1:902:GLU:HG2	2.47	0.49
36:3:22:PHE:HA	36:3:76:ASP:HB2	1.95	0.49
36:3:22:PHE:N	36:3:29:GLU:OE1	2.45	0.49
36:3:581:LYS:HB2	36:3:625:LEU:HD22	1.94	0.49
36:3:968:ARG:HG2	36:3:982:GLU:OE1	2.12	0.49
1:A:292:ASP:CG	1:A:293:TRP:H	2.20	0.49
1:A:485:THR:HG22	1:A:486:LYS:N	2.27	0.49
2:B:14:U:H2'	2:B:15:C:C6	2.46	0.49
3:C:480:LYS:HB2	3:C:493:PHE:HB3	1.93	0.49
3:C:514:TYR:OH	3:C:519:GLU:HG2	2.13	0.49
11:L:233:GLN:H	11:L:233:GLN:CD	2.19	0.49
23:X:227:ARG:NE	24:Y:239:GLU:OE2	2.44	0.49
23:X:828:ILE:O	23:X:831:SER:OG	2.29	0.49
24:Y:89:LYS:HB3	24:Y:90:LYS:HD3	1.95	0.49
24:Y:246:LYS:CE	24:Y:312:HIS:HB2	2.38	0.49
35:1:970:LEU:O	35:1:974:LEU:HG	2.13	0.49
35:1:1273:TYR:OH	42:5:38:ASP:OD2	2.28	0.49
36:3:488:GLY:C	36:3:490:THR:H	2.20	0.49
36:3:757:ILE:HG22	36:3:762:LEU:HG	1.94	0.49
36:3:982:GLU:N	38:w:471:TRP:CZ3	2.80	0.49
31:j:64:ILE:HA	31:j:70:SER:O	2.11	0.49
1:A:226:GLN:HA	1:A:418:THR:HG22	1.94	0.49
1:A:278:LYS:NZ	6:G:-9:C:O3'	2.46	0.49
1:A:1661:TRP:NE1	1:A:1697:SER:O	2.41	0.49
1:A:1738:PRO:CA	35:1:973:HIS:NE2	2.70	0.49
3:C:114:TYR:N	3:C:115:GLU:OE1	2.46	0.49
9:J:286:GLU:HG3	9:J:298:ILE:HD12	1.94	0.49
19:T:220:VAL:HG13	19:T:252:VAL:HG21	1.95	0.49
19:T:396:LYS:HD3	19:T:405:PHE:HE1	1.78	0.49
21:V:391:PHE:O	21:V:395:GLU:CB	2.61	0.49
23:X:855:TYR:CE2	23:X:857:PRO:HG3	2.46	0.49
24:Y:77:PHE:O	24:Y:103:GLN:NE2	2.46	0.49
36:3:181:MET:HB2	36:3:211:TYR:O	2.13	0.49
36:3:503:THR:HG22	36:3:504:PRO:HD2	1.95	0.49
36:3:543:THR:C	36:3:558:LEU:HD12	2.38	0.49
41:7:52:GLY:N	41:7:55:GLN:HE21	2.10	0.49
1:A:1786:TYR:HD1	1:A:1833:LEU:HB2	1.78	0.49
3:C:538:HIS:CE1	3:C:551:LEU:HD13	2.47	0.49
5:F:31:U:H3'	5:F:32:U:H6	1.76	0.49
7:H:16:U:H6	7:H:16:U:OP1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:142:ILE:HD12	12:M:143:LYS:H	1.78	0.49
21:V:473:ALA:O	21:V:477:LEU:HG	2.12	0.49
34:q:60:PRO:CB	34:s:94:GLN:HA	2.43	0.49
35:1:721:ILE:C	35:1:721:ILE:CD1	2.85	0.49
36:3:42:ARG:HB2	36:3:53:LEU:HD11	1.93	0.49
36:3:112:CYS:SG	42:5:46:HIS:CD2	3.06	0.49
36:3:612:ASN:HA	36:3:636:GLN:HA	1.95	0.49
36:3:1098:GLY:C	36:3:1099:GLU:HG3	2.38	0.49
38:w:453:GLU:HA	38:w:456:VAL:HG22	1.93	0.49
38:w:479:TYR:N	38:w:487:VAL:O	2.40	0.49
42:5:60:SER:O	42:5:63:ARG:N	2.46	0.49
1:A:983:LYS:HE3	1:A:983:LYS:HB3	1.52	0.49
1:A:1524:SER:HB3	10:K:215:ASP:HB2	1.95	0.49
3:C:302:PRO:HB2	3:C:320:LEU:HG	1.94	0.49
4:E:94:ASN:O	4:E:99:CYS:HA	2.13	0.49
6:G:11:A:H2'	6:G:12:G:O4'	2.12	0.49
7:H:163:G:O2'	37:p:48:MET:HA	2.13	0.49
9:J:286:GLU:HG3	9:J:298:ILE:CD1	2.43	0.49
9:J:399:TYR:O	9:J:403:VAL:HG23	2.13	0.49
12:M:160:PHE:C	12:M:161:PHE:HD1	2.20	0.49
17:R:123:GLU:HB3	17:R:125:MET:CE	2.43	0.49
19:T:424:ASP:OD1	19:T:424:ASP:N	2.46	0.49
23:X:618:GLN:HG2	23:X:648:TYR:CG	2.48	0.49
35:1:796:CYS:HB3	35:1:806:ILE:HG12	1.95	0.49
35:1:869:MET:HE2	35:1:896:ILE:HD13	1.95	0.49
36:3:249:LEU:HA	36:3:257:THR:O	2.12	0.49
36:3:331:ASP:CG	36:3:390:ARG:HH21	2.20	0.49
36:3:914:ILE:HD12	36:3:919:SER:HB3	1.95	0.49
41:7:42:LEU:HG	41:7:70:TYR:CE2	2.48	0.49
1:A:156:ARG:NH2	1:A:157:ASP:OD2	2.46	0.48
1:A:1301:ILE:HD11	1:A:1306:LYS:HD3	1.95	0.48
3:C:476:CYS:SG	3:C:496:VAL:HG12	2.53	0.48
3:C:843:VAL:O	3:C:846:VAL:HG13	2.13	0.48
4:E:156:SER:HB2	4:E:199:VAL:HG12	1.95	0.48
7:H:105:G:O2'	7:H:107:A:OP1	2.23	0.48
7:H:106:G:N3	7:H:107:A:C6	2.81	0.48
9:J:206:LEU:CD2	9:J:207:PRO:CD	2.86	0.48
11:L:48:ALA:O	11:L:52:GLU:HG2	2.12	0.48
23:X:281:ARG:HA	23:X:281:ARG:CZ	2.42	0.48
23:X:447:LYS:HB2	23:X:514:TYR:CD1	2.47	0.48
23:X:533:PHE:CE1	23:X:550:VAL:HG11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:126:PHE:C	24:Y:126:PHE:CD2	2.91	0.48
24:Y:241:VAL:HG22	24:Y:287:GLU:HA	1.95	0.48
35:1:522:LYS:HD3	35:1:526:PHE:CE2	2.48	0.48
35:1:610:ILE:CG2	35:1:647:PHE:CE1	2.95	0.48
35:1:632:PHE:O	35:1:635:VAL:HG22	2.13	0.48
35:1:1082:GLY:O	35:1:1085:ALA:HB3	2.13	0.48
38:w:410:ILE:HD12	38:w:438:LEU:HD11	1.95	0.48
39:2:594:GLY:O	39:2:597:PHE:CB	2.61	0.48
1:A:251:ASP:N	1:A:251:ASP:OD2	2.45	0.48
1:A:1749:LYS:HG3	35:1:980:GLU:CG	2.43	0.48
1:A:1812:PRO:O	1:A:1920:TYR:OH	2.22	0.48
1:A:1866:LYS:HE2	1:A:1886:GLY:H	1.79	0.48
3:C:325:LYS:HG2	3:C:329:ASP:OD2	2.14	0.48
3:C:453:TYR:CZ	3:C:465:MET:HE1	2.48	0.48
3:C:471:ASP:H	3:C:499:GLY:HA2	1.78	0.48
3:C:724:TRP:HA	3:C:724:TRP:CE3	2.48	0.48
7:H:64:A:H2'	7:H:65:U:C6	2.48	0.48
12:M:165:ASN:HB2	17:R:95:LYS:HA	1.95	0.48
17:R:256:ASN:ND2	17:R:259:GLY:HA2	2.28	0.48
17:R:408:ASP:OD1	17:R:409:GLN:N	2.46	0.48
19:T:220:VAL:HG23	19:T:230:ILE:HG12	1.95	0.48
23:X:648:TYR:CE2	23:X:651:LEU:HB3	2.48	0.48
23:X:741:TRP:NE1	35:1:783:GLU:H	2.11	0.48
23:X:768:LYS:HE3	23:X:802:LEU:HD21	1.94	0.48
35:1:770:MET:HA	35:1:773:LEU:HG	1.95	0.48
35:1:1010:THR:OG1	35:1:1011:PRO:CD	2.48	0.48
36:3:407:ILE:HD11	36:3:1124:GLY:CA	2.43	0.48
36:3:594:ASN:OD1	36:3:594:ASN:N	2.46	0.48
36:3:1165:SER:HB2	36:3:1169:PRO:HA	1.94	0.48
38:w:454:ASP:OD2	39:2:463:ALA:HB1	2.12	0.48
42:5:51:ASN:OD1	42:5:51:ASN:N	2.46	0.48
1:A:111:GLU:OE2	1:A:114:ARG:NH2	2.41	0.48
1:A:147:MET:O	1:A:151:MET:HG2	2.13	0.48
1:A:643:GLY:HA3	2:B:28:A:O2'	2.13	0.48
1:A:1738:PRO:HA	35:1:973:HIS:CE1	2.48	0.48
4:E:242:SER:O	4:E:293:TRP:NE1	2.45	0.48
9:J:199:LYS:C	9:J:199:LYS:CD	2.84	0.48
19:T:355:ARG:HH11	19:T:364:THR:HG21	1.78	0.48
23:X:701:ASN:ND2	23:X:703:ARG:HD3	2.28	0.48
34:q:60:PRO:CB	34:s:93:ARG:CB	2.91	0.48
35:1:702:ARG:HG2	35:1:746:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:346:PHE:HA	36:3:360:GLN:HA	1.95	0.48
36:3:357:TYR:HE1	36:3:400:GLU:HG3	1.77	0.48
36:3:804:HIS:NE2	36:3:859:ASN:O	2.46	0.48
30:i:71:TYR:HA	31:j:79:LEU:HA	1.96	0.48
1:A:82:ARG:NH2	6:G:16:G:H1	2.11	0.48
3:C:764:ASP:OD2	3:C:764:ASP:N	2.46	0.48
3:C:820:PHE:HD1	3:C:821:LEU:HD23	1.77	0.48
5:F:77:C:H2'	5:F:78:A:O4'	2.13	0.48
15:P:26:LEU:HD13	15:P:26:LEU:HA	1.68	0.48
25:Z:85:LYS:CB	34:t:79:GLN:CB	2.92	0.48
35:1:556:ILE:HG23	35:1:596:ILE:CG2	2.39	0.48
35:1:717:THR:HB	35:1:718:PRO:CD	2.41	0.48
35:1:796:CYS:HA	35:1:801:VAL:HG21	1.94	0.48
35:1:1006:MET:HB2	35:1:1049:TYR:CZ	2.49	0.48
35:1:1126:PHE:CB	39:2:575:PHE:CD2	2.96	0.48
36:3:49:LYS:HD3	36:3:49:LYS:HA	1.59	0.48
36:3:238:VAL:HB	36:3:247:GLY:O	2.12	0.48
36:3:745:PHE:CB	36:3:755:VAL:HG23	2.43	0.48
36:3:823:MET:HE2	36:3:823:MET:HB3	1.70	0.48
36:3:1095:TYR:CE1	36:3:1164:ARG:HD2	2.48	0.48
38:w:405:ASN:HA	38:w:416:TYR:O	2.13	0.48
1:A:1874:VAL:O	1:A:1877:LEU:HG	2.13	0.48
3:C:719:GLN:NE2	3:C:726:LEU:HA	2.28	0.48
3:C:746:VAL:O	3:C:791:ILE:HG13	2.13	0.48
4:E:255:MET:HB2	4:E:282:HIS:CB	2.43	0.48
14:O:259:ARG:N	14:O:273:GLN:O	2.39	0.48
17:R:358:ASP:O	17:R:362:GLU:HB2	2.13	0.48
17:R:369:LEU:HG	17:R:376:LYS:HG3	1.95	0.48
23:X:818:LEU:HD21	23:X:925:VAL:HG21	1.95	0.48
35:1:495:ARG:HA	35:1:498:MET:HB3	1.95	0.48
36:3:636:GLN:HG2	36:3:637:PRO:HD2	1.96	0.48
36:3:665:LEU:HD21	36:3:667:ILE:HD11	1.94	0.48
36:3:706:MET:HG2	36:3:770:LEU:HD12	1.94	0.48
38:w:383:LEU:CD1	38:w:391:PRO:HB3	2.43	0.48
39:2:530:ARG:HH12	39:2:578:TRP:CG	2.32	0.48
1:A:205:ASP:OD2	1:A:205:ASP:N	2.43	0.48
1:A:1635:TYR:CE1	1:A:1636:LYS:HB2	2.48	0.48
3:C:230:ASP:OD2	3:C:259:LYS:HD2	2.13	0.48
3:C:589:LYS:HD2	3:C:661:THR:HG22	1.96	0.48
4:E:328:GLY:O	4:E:346:SER:OG	2.31	0.48
6:G:95:U:O5'	35:1:1106:ARG:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:182:U:H2'	7:H:183:G:C8	2.48	0.48
9:J:230:THR:HA	9:J:233:ASP:OD2	2.14	0.48
11:L:569:GLN:CB	34:q:114:CYS:C	2.86	0.48
13:N:21:THR:O	13:N:24:GLU:HG3	2.13	0.48
21:V:535:THR:HB	21:V:538:ARG:HG3	1.95	0.48
23:X:190:LYS:HG2	24:Y:310:ARG:HH21	1.79	0.48
23:X:461:VAL:O	23:X:465:VAL:HG23	2.14	0.48
23:X:461:VAL:HA	23:X:464:ARG:HE	1.78	0.48
23:X:527:LEU:HG	23:X:754:GLU:OE1	2.13	0.48
23:X:618:GLN:HG2	23:X:648:TYR:CE2	2.48	0.48
23:X:820:VAL:HG21	23:X:824:LEU:HD22	1.94	0.48
35:1:1140:GLU:HB2	35:1:1143:VAL:CG1	2.44	0.48
36:3:24:GLY:HA2	36:3:74:THR:O	2.14	0.48
36:3:595:VAL:HG21	36:3:600:GLN:C	2.39	0.48
39:2:617:LEU:HA	40:4:78:LYS:O	2.13	0.48
39:2:705:ARG:N	39:2:705:ARG:HD2	2.28	0.48
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.48	0.48
1:A:835:ASP:HB3	1:A:878:LEU:HD13	1.95	0.48
1:A:1831:LYS:HG3	1:A:1832:ARG:H	1.75	0.48
2:B:111:A:H2'	2:B:112:A:C8	2.49	0.48
7:H:139:C:H2'	7:H:140:A:H8	1.78	0.48
11:L:19:LEU:HD23	11:L:54:LEU:CD2	2.44	0.48
23:X:811:SER:HA	23:X:814:LYS:HZ2	1.77	0.48
24:Y:241:VAL:HA	24:Y:286:ILE:O	2.12	0.48
35:1:815:PHE:O	35:1:819:TRP:HB2	2.13	0.48
36:3:19:HIS:ND1	36:3:19:HIS:O	2.46	0.48
36:3:302:LEU:HA	36:3:311:PHE:O	2.14	0.48
36:3:617:ILE:HG12	36:3:627:PRO:HA	1.95	0.48
41:7:58:CYS:HB3	41:7:62:GLY:H	1.79	0.48
30:i:19:VAL:HA	30:i:73:ARG:O	2.14	0.48
1:A:1303:LEU:HD12	1:A:1311:PHE:HE1	1.78	0.48
1:A:1498:TRP:CD1	1:A:1498:TRP:H	2.30	0.48
4:E:308:PHE:CE1	4:E:324:PRO:HB3	2.49	0.48
11:L:162:THR:HG23	17:R:258:LYS:C	2.31	0.48
11:L:176:LEU:HD12	11:L:180:ARG:HD2	1.95	0.48
11:L:201:LYS:HD2	11:L:202:ARG:N	2.28	0.48
17:R:235:ARG:HB3	17:R:235:ARG:CZ	2.43	0.48
23:X:878:HIS:CE1	23:X:1001:LEU:HB2	2.48	0.48
24:Y:133:MET:HA	24:Y:136:ILE:HB	1.96	0.48
36:3:143:ILE:H	36:3:143:ILE:HD12	1.79	0.48
36:3:436:ARG:HD3	36:3:776:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:740:GLU:HB2	36:3:758:SER:HA	1.95	0.48
36:3:926:TYR:CZ	36:3:942:LYS:HD2	2.48	0.48
41:7:30:CYS:SG	41:7:33:CYS:HB3	2.53	0.48
43:o:100:LEU:O	43:o:124:PRO:HD2	2.13	0.48
1:A:1210:LYS:HD3	1:A:1210:LYS:N	2.29	0.48
3:C:118:PHE:HA	3:C:121:ASP:OD2	2.14	0.48
3:C:918:ILE:HG23	3:C:924:GLN:NE2	2.29	0.48
4:E:105:LEU:HD21	4:E:136:TRP:CZ2	2.49	0.48
5:F:13:G:H8	5:F:13:G:O5'	1.97	0.48
13:N:132:ILE:O	13:N:140:ARG:HG3	2.13	0.48
19:T:493:ASP:OD1	19:T:493:ASP:N	2.34	0.48
23:X:224:PRO:O	23:X:228:LYS:HD2	2.14	0.48
23:X:285:ALA:HA	23:X:288:GLU:OE2	2.13	0.48
24:Y:90:LYS:O	24:Y:93:THR:OG1	2.25	0.48
34:q:61:ILE:N	34:s:93:ARG:CB	2.75	0.48
36:3:664:TYR:CG	36:3:729:PHE:HZ	2.32	0.48
36:3:757:ILE:HA	36:3:762:LEU:HA	1.94	0.48
1:A:41:GLN:NE2	1:A:45:TYR:HB2	2.28	0.48
1:A:381:PRO:C	1:A:383:PHE:H	2.21	0.48
1:A:845:ARG:NH1	1:A:1440:THR:HG22	2.29	0.48
1:A:1352:HIS:HD2	20:U:5:ILE:HG21	1.79	0.48
1:A:1664:ILE:HG13	1:A:1664:ILE:O	2.13	0.48
3:C:181:ILE:O	3:C:206:PRO:HG3	2.14	0.48
3:C:592:VAL:O	3:C:593:GLU:HG2	2.14	0.48
3:C:826:ARG:NH1	3:C:911:PRO:HD2	2.29	0.48
7:H:34:U:H2'	7:H:35:A:C8	2.49	0.48
7:H:106:G:H1'	7:H:107:A:N7	2.29	0.48
11:L:206:ARG:HD2	11:L:206:ARG:O	2.13	0.48
12:M:200:ARG:HD2	12:M:200:ARG:N	2.28	0.48
12:M:222:ALA:HB1	17:R:266:LYS:HE3	1.96	0.48
23:X:503:ARG:NH2	23:X:817:GLU:O	2.47	0.48
23:X:835:SER:OG	23:X:835:SER:O	2.31	0.48
35:1:524:ARG:HD3	35:1:563:LEU:HD12	1.96	0.48
36:3:1:MET:HG2	39:2:709:GLY:O	2.14	0.48
36:3:16:PHE:HE2	36:3:63:ARG:C	2.22	0.48
36:3:18:ILE:HD12	36:3:67:ALA:HB2	1.95	0.48
36:3:347:LEU:CD2	36:3:359:TYR:HB2	2.44	0.48
36:3:373:PHE:CE1	36:3:385:PHE:HB3	2.48	0.48
36:3:642:ILE:H	36:3:703:ARG:HH21	1.61	0.48
1:A:105:ASN:O	1:A:489:TRP:NE1	2.47	0.47
1:A:235:MET:HB3	1:A:404:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:C:H2'	2:B:16:U:C6	2.49	0.47
8:I:564:PHE:O	8:I:568:TYR:N	2.44	0.47
17:R:123:GLU:HB3	17:R:125:MET:HE3	1.96	0.47
21:V:606:GLU:HA	21:V:609:GLN:HG2	1.96	0.47
23:X:503:ARG:O	23:X:506:LEU:HB3	2.14	0.47
23:X:997:MET:HE2	23:X:997:MET:HB3	1.59	0.47
35:1:841:ALA:HB2	35:1:875:ILE:CD1	2.40	0.47
35:1:1299:GLU:O	35:1:1302:TYR:HD2	1.97	0.47
36:3:316:GLU:O	36:3:323:THR:OG1	2.29	0.47
36:3:457:ASN:ND2	36:3:479:VAL:HG12	2.29	0.47
36:3:477:SER:HA	36:3:482:THR:HG23	1.95	0.47
36:3:603:ARG:HD2	36:3:603:ARG:O	2.13	0.47
39:2:461:THR:OG1	39:2:464:GLU:N	2.26	0.47
30:i:50:TYR:HA	30:i:54:ALA:O	2.14	0.47
1:A:64:GLU:H	1:A:64:GLU:CD	2.21	0.47
1:A:123:THR:O	1:A:123:THR:OG1	2.30	0.47
1:A:1352:HIS:HD1	20:U:21:ARG:HA	1.79	0.47
1:A:1792:LYS:HE2	1:A:1798:LEU:HG	1.95	0.47
1:A:1836:LEU:HA	1:A:1839:TRP:HD1	1.79	0.47
1:A:1838:LYS:HE2	1:A:1868:MET:CE	2.44	0.47
4:E:145:LYS:HZ3	4:E:184:LYS:HG3	1.79	0.47
11:L:204:ARG:HE	11:L:207:GLY:HA3	1.78	0.47
35:1:663:THR:HA	35:1:666:LYS:CE	2.43	0.47
35:1:789:LEU:HB3	35:1:836:THR:HG21	1.96	0.47
35:1:819:TRP:CE3	35:1:867:MET:CE	2.96	0.47
35:1:854:VAL:HG11	35:1:891:GLN:HE21	1.79	0.47
35:1:967:GLU:CG	35:1:970:LEU:HB3	2.43	0.47
35:1:1006:MET:CB	35:1:1013:ILE:HG12	2.44	0.47
35:1:1197:LEU:CD2	41:7:78:GLN:HE21	2.26	0.47
36:3:415:LEU:HB2	36:3:424:TYR:CE2	2.49	0.47
36:3:484:VAL:O	36:3:485:LEU:HD12	2.13	0.47
1:A:41:GLN:NE2	4:E:153:PHE:CE2	2.81	0.47
1:A:482:PHE:HZ	17:R:207:MET:HE3	1.79	0.47
1:A:767:VAL:HG21	2:B:39:C:O2'	2.15	0.47
1:A:1391:LEU:O	1:A:1394:GLN:HG3	2.13	0.47
1:A:1684:PHE:HD1	1:A:1702:LEU:HG	1.78	0.47
3:C:153:THR:O	3:C:155:PRO:HD3	2.14	0.47
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.96	0.47
6:G:85:G:N2	7:H:45:C:C2	2.80	0.47
7:H:6:U:H2'	7:H:7:U:C6	2.48	0.47
7:H:70:C:H2'	7:H:71:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:222:ALA:CB	17:R:266:LYS:HE3	2.44	0.47
21:V:497:CYS:HB3	21:V:507:PHE:CB	2.44	0.47
21:V:549:LYS:O	21:V:549:LYS:HD3	2.13	0.47
35:1:647:PHE:O	35:1:651:VAL:HG13	2.15	0.47
35:1:770:MET:O	35:1:774:ILE:HG12	2.14	0.47
35:1:795:CYS:O	35:1:798:THR:HG23	2.13	0.47
35:1:893:ILE:HD13	35:1:893:ILE:HA	1.67	0.47
35:1:914:PHE:O	35:1:918:VAL:HG23	2.14	0.47
40:4:103:PHE:N	40:4:177:ALA:HB2	2.29	0.47
41:7:21:ARG:HH11	41:7:66:VAL:C	2.19	0.47
1:A:253:ASN:O	3:C:893:GLY:HA3	2.15	0.47
1:A:1491:LYS:HE3	1:A:1491:LYS:HB2	1.49	0.47
3:C:116:MET:HA	3:C:119:LEU:HD12	1.95	0.47
3:C:737:PRO:HD3	3:C:743:ASN:HD22	1.80	0.47
4:E:60:MET:HB3	4:E:353:MET:HB3	1.96	0.47
6:G:116:C:OP2	17:R:371:ARG:HB3	2.15	0.47
17:R:328:ALA:HB2	24:Y:226:MET:CG	2.44	0.47
17:R:348:GLU:HB2	23:X:263:SER:H	1.79	0.47
17:R:360:ARG:CD	24:Y:274:ASP:OD1	2.55	0.47
19:T:213:GLU:HG2	19:T:214:PRO:HD2	1.97	0.47
19:T:295:ASP:OD1	19:T:296:LEU:N	2.40	0.47
24:Y:44:ASN:OD1	24:Y:52:GLN:HB3	2.13	0.47
24:Y:183:ARG:HH21	24:Y:187:ASP:CG	2.21	0.47
35:1:864:TYR:O	35:1:868:VAL:HG13	2.15	0.47
36:3:169:HIS:CD2	36:3:170:VAL:N	2.82	0.47
36:3:558:LEU:HG	36:3:559:THR:N	2.30	0.47
38:w:426:PHE:CZ	38:w:448:ASN:HA	2.49	0.47
41:7:73:LYS:HA	41:7:76:THR:HG22	1.95	0.47
1:A:762:ARG:HA	1:A:902:TYR:O	2.15	0.47
1:A:1776:ILE:HD11	1:A:1778:TRP:NE1	2.29	0.47
3:C:352:LYS:HE2	3:C:352:LYS:H	1.80	0.47
3:C:667:VAL:HG13	3:C:826:ARG:HG3	1.97	0.47
4:E:124:LEU:O	4:E:135:VAL:HA	2.14	0.47
4:E:131:LYS:HA	4:E:152:SER:O	2.15	0.47
4:E:150:HIS:HA	4:E:177:LYS:NZ	2.29	0.47
5:F:49:G:H2'	5:F:50:A:C8	2.47	0.47
13:N:44:GLU:HB2	13:N:47:TRP:CE3	2.49	0.47
17:R:124:VAL:O	17:R:124:VAL:HG12	2.13	0.47
17:R:235:ARG:H	17:R:235:ARG:HE	1.62	0.47
21:V:556:TYR:HB2	21:V:594:MET:SD	2.54	0.47
23:X:597:VAL:HA	23:X:600:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:616:ASP:HA	35:1:619:ASN:ND2	2.30	0.47
35:1:699:GLN:NE2	35:1:738:HIS:CE1	2.82	0.47
36:3:75:LYS:HE3	36:3:76:ASP:H	1.79	0.47
36:3:839:ALA:O	36:3:843:LEU:HD12	2.14	0.47
41:7:13:LYS:HD2	41:7:48:GLU:OE2	2.15	0.47
1:A:179:ALA:HA	1:A:183:LEU:HB2	1.96	0.47
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.96	0.47
1:A:818:GLU:OE2	17:R:305:ARG:HD2	2.14	0.47
1:A:1624:SER:OG	1:A:1625:SER:N	2.47	0.47
1:A:1630:LEU:HA	1:A:1660:TYR:O	2.14	0.47
2:B:117:A:C2	30:d:26:GLY:O	2.68	0.47
7:H:171:U:N3	7:H:172:C:C4	2.83	0.47
9:J:189:ILE:HD12	11:L:140:ASP:OD2	2.13	0.47
23:X:183:GLU:HA	23:X:186:ARG:HD2	1.96	0.47
23:X:291:LYS:O	23:X:295:THR:HG22	2.15	0.47
23:X:618:GLN:HA	23:X:648:TYR:CE1	2.50	0.47
23:X:970:ILE:HD12	23:X:977:PHE:O	2.14	0.47
24:Y:27:ASN:OD1	24:Y:66:ILE:N	2.36	0.47
36:3:70:LEU:HD13	36:3:146:ARG:HG2	1.96	0.47
36:3:698:PRO:O	36:3:700:LYS:NZ	2.34	0.47
39:2:631:PRO:CB	40:4:77:ILE:HA	2.44	0.47
32:k:30:ILE:O	32:k:42:ILE:HA	2.15	0.47
1:A:137:GLU:HG2	1:A:419:ARG:HD3	1.97	0.47
1:A:376:GLU:H	1:A:376:GLU:HG3	1.49	0.47
1:A:464:PRO:O	1:A:466:ALA:N	2.47	0.47
1:A:697:MET:N	1:A:698:PRO:HD3	2.29	0.47
1:A:833:LYS:O	1:A:833:LYS:HD3	2.14	0.47
1:A:1779:PHE:CG	1:A:1862:ILE:HD11	2.49	0.47
1:A:1862:ILE:HG22	1:A:1885:LYS:HB3	1.95	0.47
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.14	0.47
1:A:1943:LEU:HD12	1:A:1950:ALA:HB1	1.97	0.47
3:C:154:HIS:C	3:C:156:GLU:H	2.22	0.47
3:C:311:SER:HB2	3:C:316:ILE:HG23	1.96	0.47
3:C:496:VAL:HG23	3:C:546:ALA:HA	1.97	0.47
4:E:161:ARG:HH12	4:E:203:ASP:HB3	1.79	0.47
4:E:241:LEU:HA	4:E:251:LEU:O	2.14	0.47
4:E:343:ILE:HA	4:E:352:TYR:O	2.14	0.47
7:H:51:A:H2'	7:H:52:G:O4'	2.15	0.47
7:H:107:A:C6	7:H:108:G:C6	3.02	0.47
7:H:176:G:H8	7:H:176:G:O5'	1.97	0.47
12:M:165:ASN:ND2	17:R:95:LYS:HE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:233:THR:O	14:O:303:GLY:N	2.41	0.47
17:R:328:ALA:HB1	24:Y:226:MET:C	2.40	0.47
21:V:577:SER:O	21:V:581:ILE:HG12	2.14	0.47
23:X:189:ASP:O	23:X:193:THR:HG22	2.15	0.47
23:X:824:LEU:O	23:X:828:ILE:HG13	2.15	0.47
23:X:832:GLU:CD	23:X:928:GLY:H	2.23	0.47
23:X:911:ALA:HA	23:X:914:VAL:HG22	1.97	0.47
24:Y:212:LYS:O	24:Y:216:GLU:HG3	2.15	0.47
35:1:854:VAL:HG12	35:1:892:LEU:CD2	2.45	0.47
35:1:860:GLU:O	35:1:865:ARG:NH2	2.48	0.47
35:1:933:CYS:O	35:1:934:GLY:C	2.58	0.47
35:1:1165:TYR:HD1	39:2:575:PHE:CE1	2.33	0.47
35:1:1197:LEU:HD21	41:7:78:GLN:HE21	1.79	0.47
35:1:1249:TYR:CE2	39:2:587:HIS:CE1	3.03	0.47
36:3:329:TYR:HB3	36:3:370:GLU:CD	2.39	0.47
36:3:524:ILE:O	36:3:535:GLU:HA	2.15	0.47
36:3:605:LEU:HD23	36:3:617:ILE:HG22	1.95	0.47
36:3:945:VAL:HG23	36:3:968:ARG:HH12	1.79	0.47
36:3:1158:ARG:HG3	36:3:1159:ASP:H	1.79	0.47
38:w:397:TYR:HE2	38:w:402:LEU:HB2	1.80	0.47
38:w:445:HIS:CD2	38:w:445:HIS:N	2.82	0.47
39:2:514:LYS:NZ	39:2:596:GLU:OE1	2.43	0.47
39:2:553:MET:HE3	39:2:553:MET:HB2	1.75	0.47
29:h:45:ASN:O	29:h:107:ILE:N	2.39	0.47
3:C:320:LEU:HD11	3:C:344:TRP:HB2	1.96	0.47
3:C:350:ASN:HD22	3:C:353:THR:H	1.63	0.47
4:E:259:VAL:HG22	4:E:277:PHE:HB2	1.97	0.47
4:E:341:ILE:C	4:E:342:ILE:HD13	2.39	0.47
11:L:98:GLU:O	11:L:101:GLU:HG3	2.15	0.47
13:N:1:MET:N	13:N:2:PRO:HD2	2.30	0.47
21:V:562:TRP:CE2	21:V:602:ARG:HD3	2.50	0.47
23:X:702:PRO:HG2	23:X:788:THR:HB	1.96	0.47
23:X:842:THR:O	23:X:846:MET:HG2	2.15	0.47
24:Y:182:THR:OG1	24:Y:183:ARG:N	2.45	0.47
35:1:746:PHE:O	35:1:750:ILE:HG23	2.15	0.47
35:1:982:LEU:HD21	35:1:1016:LEU:HD11	1.95	0.47
35:1:1277:GLN:NE2	35:1:1277:GLN:O	2.48	0.47
36:3:232:GLY:HA3	36:3:252:SER:HA	1.97	0.47
36:3:334:PRO:HB3	36:3:432:ARG:NH1	2.30	0.47
36:3:867:ARG:NH1	36:3:879:LEU:HD13	2.30	0.47
36:3:1116:SER:HA	39:2:708:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:1199:ARG:HH21	36:3:1207:LYS:HD3	1.80	0.47
1:A:693:ILE:HB	1:A:738:MET:SD	2.55	0.47
1:A:1413:ASP:O	1:A:1414:ARG:HG3	2.14	0.47
1:A:1901:LYS:NZ	1:A:1967:ILE:HA	2.30	0.47
3:C:200:PHE:HE1	3:C:434:CYS:SG	2.37	0.47
3:C:243:ILE:O	3:C:247:VAL:HG13	2.14	0.47
3:C:284:GLU:O	3:C:288:LEU:HG	2.14	0.47
3:C:702:ASN:HB2	3:C:704:VAL:HG23	1.95	0.47
3:C:801:LEU:HD13	3:C:802:HIS:NE2	2.30	0.47
3:C:804:GLY:O	3:C:808:ILE:HG12	2.15	0.47
7:H:166:G:N3	7:H:166:G:H2'	2.29	0.47
9:J:325:ASN:HB2	12:M:172:HIS:HD2	1.80	0.47
12:M:121:ASP:OD2	12:M:122:LEU:N	2.47	0.47
12:M:224:ARG:NH1	12:M:224:ARG:C	2.73	0.47
15:P:186:ARG:CA	24:Y:49:PHE:CE1	2.97	0.47
23:X:606:GLN:HG3	23:X:688:TYR:CE1	2.50	0.47
34:r:127:ALA:HB1	34:s:127:ALA:CB	2.44	0.47
35:1:573:LYS:O	35:1:577:VAL:HG23	2.15	0.47
35:1:1299:GLU:HB3	42:5:43:TYR:HE2	1.78	0.47
36:3:193:ASP:HB3	42:5:29:TRP:HH2	1.79	0.47
36:3:563:LEU:O	36:3:580:ARG:HB3	2.14	0.47
36:3:604:PHE:HA	36:3:618:SER:HA	1.96	0.47
36:3:665:LEU:CB	36:3:679:LEU:HD23	2.45	0.47
36:3:952:ILE:HG12	36:3:961:ILE:HG12	1.95	0.47
1:A:682:ASP:O	1:A:686:ARG:HG2	2.14	0.47
1:A:1090:ARG:HG2	1:A:1091:TYR:O	2.15	0.47
3:C:239:THR:O	3:C:243:ILE:HG23	2.14	0.47
4:E:124:LEU:HD21	4:E:138:SER:HB3	1.97	0.47
4:E:137:ASP:HB2	4:E:140:THR:OG1	2.14	0.47
5:F:3:G:H2'	5:F:4:C:C6	2.50	0.47
7:H:181:G:H21	33:l:52:ASP:C	2.19	0.47
19:T:221:THR:OG1	19:T:231:TRP:NE1	2.46	0.47
23:X:267:ARG:O	23:X:271:LYS:HD3	2.14	0.47
23:X:591:TYR:HB2	23:X:737:LEU:HD23	1.97	0.47
23:X:871:PHE:HZ	23:X:901:ASN:HB3	1.80	0.47
35:1:540:MET:CE	35:1:577:VAL:HG11	2.23	0.47
35:1:560:LEU:CD2	35:1:600:LEU:CA	2.87	0.47
36:3:565:TYR:HE1	36:3:619:LEU:HD12	1.80	0.47
36:3:592:LEU:HD11	36:3:619:LEU:HD11	1.97	0.47
36:3:633:LEU:HD12	36:3:637:PRO:HG3	1.97	0.47
1:A:296:PHE:O	1:A:302:ILE:HD11	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:LEU:HD23	1:A:1857:GLN:HA	1.97	0.46
3:C:693:GLU:OE1	3:C:695:GLY:N	2.38	0.46
13:N:117:CYS:SG	13:N:136:HIS:ND1	2.87	0.46
14:O:167:PHE:O	14:O:171:GLY:N	2.48	0.46
15:P:53:GLU:HB3	15:P:57:ARG:HH12	1.80	0.46
16:Q:263:LEU:O	16:Q:267:ARG:N	2.47	0.46
17:R:314:GLN:HA	23:X:290:GLU:CD	2.39	0.46
19:T:315:TRP:CZ3	19:T:322:SER:HB2	2.51	0.46
24:Y:65:SER:N	24:Y:76:SER:O	2.27	0.46
35:1:527:GLY:CA	35:1:566:LEU:CD2	2.93	0.46
35:1:570:TYR:HA	35:1:573:LYS:HD3	1.96	0.46
35:1:823:MET:O	35:1:829:ASN:HB2	2.14	0.46
35:1:871:THR:O	35:1:875:ILE:HG13	2.15	0.46
35:1:1179:ASP:CB	39:2:511:LEU:HB3	2.45	0.46
35:1:1233:ALA:O	35:1:1237:LEU:HB2	2.15	0.46
36:3:272:PRO:HD3	36:3:327:LEU:HD13	1.97	0.46
36:3:449:VAL:HG11	36:3:763:ARG:NH1	2.29	0.46
36:3:511:LEU:HD21	36:3:517:VAL:CG2	2.44	0.46
38:w:397:TYR:CE2	38:w:402:LEU:HB2	2.50	0.46
39:2:529:LYS:HB2	39:2:529:LYS:HE2	1.61	0.46
1:A:362:ARG:HD3	1:A:362:ARG:HA	1.69	0.46
1:A:497:CYS:SG	1:A:558:VAL:HG11	2.55	0.46
1:A:781:ARG:O	1:A:785:LYS:HG3	2.14	0.46
2:B:21:A:H2'	2:B:21:A:N3	2.31	0.46
3:C:137:HIS:CG	3:C:138:LEU:H	2.33	0.46
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.68	0.46
3:C:668:GLU:HG3	3:C:824:THR:HG21	1.97	0.46
5:F:29:A:H2'	5:F:30:A:O4'	2.14	0.46
7:H:18:U:C5	12:M:218:PHE:CE2	3.02	0.46
12:M:125:SER:HA	17:R:242:GLN:OE1	2.14	0.46
24:Y:21:ARG:NH1	24:Y:83:VAL:O	2.48	0.46
35:1:898:TYR:HA	35:1:901:GLN:OE1	2.15	0.46
38:w:408:CYS:HB2	38:w:416:TYR:CE2	2.50	0.46
42:5:8:HIS:HA	42:5:11:LEU:HB2	1.97	0.46
1:A:1629:ILE:O	1:A:1661:TRP:HA	2.14	0.46
2:B:99:C:H2'	2:B:100:C:H6	1.80	0.46
3:C:480:LYS:C	3:C:481:MET:HG3	2.40	0.46
3:C:749:THR:O	3:C:753:GLU:HB2	2.16	0.46
3:C:916:ILE:HG21	3:C:928:HIS:HB3	1.97	0.46
5:F:86:U:H5''	12:M:134:GLN:NE2	2.30	0.46
6:G:1:G:H21	10:K:218:LYS:CD	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:90:C:H42	7:H:40:C:N4	2.14	0.46
9:J:297:ASN:OD1	11:L:225:TYR:HB2	2.15	0.46
13:N:7:SER:C	13:N:9:LYS:H	2.22	0.46
21:V:594:MET:O	21:V:598:LYS:HE3	2.15	0.46
23:X:172:LEU:HD12	23:X:173:GLN:N	2.31	0.46
23:X:941:LYS:HE2	23:X:1007:TRP:NE1	2.31	0.46
23:X:998:ARG:O	23:X:999:GLN:HG2	2.16	0.46
34:t:65:PRO:O	34:t:66:PRO:C	2.58	0.46
35:1:1279:ALA:O	35:1:1281:ILE:N	2.48	0.46
36:3:451:GLU:HG3	36:3:760:ASN:O	2.16	0.46
36:3:1117:LEU:HD12	36:3:1117:LEU:HA	1.60	0.46
36:3:1191:LYS:O	36:3:1192:ASN:C	2.57	0.46
1:A:371:LEU:HD22	1:A:371:LEU:HA	1.74	0.46
1:A:699:GLU:HB3	17:R:237:MET:HE2	1.97	0.46
1:A:1019:TYR:CG	1:A:1020:LYS:N	2.83	0.46
1:A:1919:LEU:N	1:A:1919:LEU:HD23	2.29	0.46
1:A:1998:ASN:OD1	1:A:2001:SER:N	2.48	0.46
6:G:95:U:P	35:1:1106:ARG:HG3	2.54	0.46
12:M:175:SER:N	12:M:178:GLU:OE2	2.49	0.46
17:R:377:ARG:HE	23:X:240:ARG:HH22	1.61	0.46
19:T:393:ASP:OD2	19:T:393:ASP:N	2.40	0.46
23:X:474:GLY:HA2	23:X:486:CYS:O	2.15	0.46
35:1:549:ARG:NH2	35:1:586:ASP:CG	2.69	0.46
35:1:554:LYS:HD2	35:1:558:ARG:HE	1.80	0.46
35:1:666:LYS:HB3	35:1:704:ILE:HD13	1.96	0.46
35:1:923:LYS:O	35:1:923:LYS:HG2	2.15	0.46
35:1:967:GLU:HB3	35:1:970:LEU:HB3	1.98	0.46
35:1:1000:ILE:O	35:1:1003:VAL:HG13	2.16	0.46
36:3:115:ILE:CD1	42:5:19:ILE:H	2.28	0.46
36:3:910:ALA:CB	36:3:913:LEU:HD11	2.45	0.46
36:3:1041:TYR:CD2	39:2:705:ARG:HG3	2.51	0.46
36:3:1181:GLN:O	36:3:1185:MET:HG3	2.14	0.46
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.46
1:A:1892:PRO:HG2	1:A:1940:LEU:CB	2.45	0.46
3:C:281:ILE:O	3:C:285:VAL:HG12	2.15	0.46
3:C:622:GLU:O	3:C:625:GLY:N	2.41	0.46
4:E:345:ALA:HA	4:E:351:LEU:HD23	1.97	0.46
5:F:41:A:H2	6:G:6:A:N1	2.14	0.46
6:G:116:C:C2	17:R:370:SER:O	2.68	0.46
21:V:540:GLU:HG3	21:V:541:THR:N	2.28	0.46
21:V:618:ARG:HB3	21:V:646:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:249:GLU:CB	23:X:273:LYS:HE2	2.45	0.46
24:Y:236:LYS:HA	24:Y:236:LYS:HD3	1.69	0.46
35:1:641:ILE:N	35:1:642:PRO:CD	2.78	0.46
35:1:662:HIS:HE1	35:1:700:LYS:HB3	1.81	0.46
35:1:1006:MET:HA	35:1:1009:MET:CG	2.44	0.46
36:3:69:ARG:HG3	36:3:75:LYS:O	2.15	0.46
36:3:809:GLU:O	36:3:812:LYS:HB2	2.15	0.46
38:w:433:HIS:O	38:w:434:GLY:C	2.59	0.46
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.64	0.46
1:A:1000:ILE:HD12	1:A:1000:ILE:HA	1.59	0.46
3:C:532:ILE:HB	3:C:539:ILE:HD11	1.97	0.46
3:C:841:ASP:OD1	3:C:842:CYS:N	2.49	0.46
4:E:147:LEU:HA	4:E:147:LEU:HD23	1.72	0.46
6:G:9:C:O2'	6:G:10:U:O4'	2.25	0.46
17:R:251:ILE:O	17:R:251:ILE:HG12	2.15	0.46
21:V:609:GLN:HE21	21:V:612:PHE:HD2	1.64	0.46
23:X:257:PHE:CZ	23:X:266:GLU:HG3	2.50	0.46
23:X:663:THR:HG23	23:X:669:LYS:HB2	1.98	0.46
23:X:818:LEU:HD12	23:X:825:SER:OG	2.15	0.46
35:1:567:VAL:CG1	35:1:600:LEU:CD1	2.85	0.46
35:1:614:ARG:HB3	35:1:615:PRO:HD2	1.98	0.46
35:1:644:LEU:HB3	35:1:648:LEU:CD1	2.46	0.46
35:1:907:ASP:OD2	35:1:909:VAL:HB	2.16	0.46
35:1:1195:MET:O	35:1:1199:VAL:HG23	2.16	0.46
36:3:226:GLU:HB3	36:3:261:PHE:CE2	2.51	0.46
36:3:1102:LEU:HD12	36:3:1102:LEU:HA	1.66	0.46
36:3:1204:VAL:HG23	36:3:1205:SER:N	2.30	0.46
41:7:12:ARG:NH1	41:7:84:GLY:O	2.48	0.46
42:5:13:HIS:ND1	42:5:17:LYS:HE3	2.30	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.70	0.46
1:A:464:PRO:HG2	2:B:20:G:C5	2.51	0.46
1:A:1638:ASN:O	1:A:1652:MET:HB3	2.15	0.46
1:A:1660:TYR:CE1	1:A:1699:THR:HG22	2.51	0.46
1:A:1778:TRP:C	1:A:1779:PHE:HD2	2.24	0.46
1:A:1865:ARG:HD2	1:A:1865:ARG:HA	1.76	0.46
3:C:283:ASP:OD2	3:C:284:GLU:N	2.48	0.46
4:E:62:LEU:HD21	4:E:99:CYS:HB2	1.98	0.46
9:J:325:ASN:HB2	12:M:172:HIS:CD2	2.51	0.46
12:M:214:ARG:HB3	17:R:260:TYR:OH	2.14	0.46
15:P:205:LYS:CB	15:P:208:LYS:HB3	2.45	0.46
35:1:586:ASP:O	35:1:590:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1135:GLU:O	35:1:1138:VAL:HG12	2.15	0.46
35:1:1263:ASP:HA	42:5:24:ALA:HB2	1.97	0.46
35:1:1304:LEU:HD12	42:5:52:TYR:CD2	2.50	0.46
36:3:2:PHE:CD2	39:2:711:LEU:HG	2.51	0.46
36:3:184:CYS:HG	36:3:211:TYR:HE1	1.63	0.46
36:3:864:SER:O	36:3:865:VAL:HG23	2.15	0.46
1:A:845:ARG:HA	1:A:845:ARG:HD2	1.61	0.46
1:A:1169:GLN:O	1:A:1173:SER:OG	2.24	0.46
1:A:1199:LYS:HE2	1:A:1206:GLU:HG3	1.97	0.46
1:A:1275:ARG:O	1:A:1369:TYR:HE1	1.99	0.46
2:B:8:G:N2	2:B:70:A:H1'	2.26	0.46
3:C:465:MET:O	3:C:468:CYS:N	2.46	0.46
3:C:604:LEU:HD21	3:C:627:HIS:HE1	1.80	0.46
3:C:710:ASN:O	3:C:714:LEU:HD13	2.16	0.46
5:F:23:U:H2'	5:F:24:A:O4'	2.15	0.46
6:G:99:C:C2'	6:G:100:C:H5'	2.46	0.46
13:N:25:LEU:HD23	13:N:25:LEU:HA	1.70	0.46
17:R:91:ASP:HA	17:R:97:LYS:NZ	2.31	0.46
17:R:382:ARG:NH2	17:R:385:ASN:HB2	2.31	0.46
19:T:412:HIS:ND1	19:T:429:SER:OG	2.47	0.46
23:X:487:THR:HG21	23:X:494:ARG:HD2	1.98	0.46
23:X:520:ASP:HB3	23:X:521:GLU:OE1	2.15	0.46
23:X:953:ARG:HB3	23:X:983:TRP:CZ3	2.51	0.46
35:1:582:LEU:HA	35:1:590:ARG:HA	1.97	0.46
35:1:826:ASP:OD1	35:1:828:ARG:N	2.42	0.46
35:1:929:LEU:N	35:1:930:PRO:HD2	2.30	0.46
36:3:1034:THR:HG22	36:3:1049:LYS:HG3	1.96	0.46
37:p:75:TYR:N	43:o:147:PHE:O	2.49	0.46
39:2:635:ALA:CA	40:4:73:ILE:HA	2.31	0.46
41:7:47:ASP:HA	41:7:50:ASN:HB3	1.97	0.46
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.47	0.46
1:A:191:ILE:O	1:A:191:ILE:HG22	2.16	0.46
1:A:361:HIS:HD1	1:A:361:HIS:N	2.14	0.46
1:A:1868:MET:O	1:A:1871:PRO:HD2	2.15	0.46
3:C:406:GLU:H	3:C:406:GLU:CD	2.22	0.46
3:C:433:MET:HE2	3:C:433:MET:HB3	1.81	0.46
3:C:921:LEU:HD23	3:C:921:LEU:HA	1.78	0.46
4:E:143:ARG:CZ	4:E:146:ARG:HE	2.28	0.46
5:F:31:U:H3'	5:F:32:U:C6	2.51	0.46
5:F:38:G:OP2	5:F:38:G:H8	1.99	0.46
9:J:191:ALA:O	9:J:194:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:15:TRP:NE1	13:N:19:GLU:OE1	2.49	0.46
13:N:122:PRO:HB2	13:N:125:LYS:HD3	1.98	0.46
17:R:377:ARG:HH21	17:R:377:ARG:HG2	1.81	0.46
23:X:640:ARG:HG3	23:X:640:ARG:NH1	2.30	0.46
34:s:65:PRO:O	34:s:66:PRO:C	2.59	0.46
35:1:567:VAL:HG23	35:1:568:ARG:HA	1.98	0.46
36:3:164:ASN:HA	36:3:189:TYR:OH	2.15	0.46
36:3:676:ARG:HD2	36:3:729:PHE:CD2	2.51	0.46
36:3:1200:THR:OG1	36:3:1203:GLU:OE1	2.28	0.46
38:w:496:LYS:HG3	38:w:501:LEU:C	2.41	0.46
39:2:542:GLU:HA	39:2:545:GLU:HG2	1.98	0.46
41:7:23:CYS:N	41:7:58:CYS:SG	2.73	0.46
1:A:57:GLN:HE21	1:A:57:GLN:C	2.23	0.46
1:A:888:GLN:C	1:A:889:ARG:HG2	2.41	0.46
1:A:1552:GLN:OE1	1:A:1563:HIS:NE2	2.48	0.46
3:C:351:PRO:O	3:C:354:ARG:HD3	2.16	0.46
4:E:117:TYR:CD1	4:E:121:GLY:HA2	2.52	0.46
7:H:158:G:H2'	7:H:159:U:O4'	2.17	0.46
8:I:569:GLY:HA3	8:I:576:ALA:HB2	1.97	0.46
9:J:537:TRP:O	9:J:541:ALA:N	2.48	0.46
11:L:223:GLY:HA2	17:R:86:LEU:HD21	1.98	0.46
23:X:576:ARG:HB3	23:X:577:PHE:CD2	2.51	0.46
23:X:624:ALA:O	23:X:628:LEU:HG	2.16	0.46
25:Z:85:LYS:CA	34:t:79:GLN:CB	2.93	0.46
35:1:881:ALA:HB1	35:1:884:ILE:HG12	1.97	0.46
35:1:903:GLN:HG2	35:1:910:MET:HG3	1.98	0.46
35:1:1284:TYR:CE2	42:5:35:GLN:HB2	2.51	0.46
36:3:185:LEU:O	36:3:186:GLU:HG3	2.16	0.46
36:3:304:GLN:HE21	36:3:308:GLY:HA2	1.80	0.46
36:3:569:ASP:O	36:3:572:GLY:N	2.45	0.46
36:3:817:GLN:HG3	36:3:818:GLN:OE1	2.15	0.46
36:3:1210:ASP:HA	36:3:1213:THR:OG1	2.15	0.46
1:A:84:ASP:O	1:A:88:TYR:HB2	2.16	0.45
1:A:198:GLU:HG2	1:A:199:GLU:H	1.82	0.45
1:A:1144:LYS:O	1:A:1148:ASN:HB2	2.16	0.45
1:A:1359:HIS:HD2	1:A:1361:GLU:O	1.99	0.45
1:A:1362:ASP:CG	1:A:1363:GLN:H	2.24	0.45
1:A:1391:LEU:O	1:A:1395:GLU:HG2	2.16	0.45
1:A:1870:ASP:HA	1:A:1873:GLU:OE1	2.16	0.45
3:C:350:ASN:HD21	3:C:352:LYS:HB2	1.80	0.45
3:C:510:LEU:HB3	3:C:576:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:711:ARG:HB3	3:C:730:ARG:NH2	2.31	0.45
4:E:171:SER:H	4:E:196:VAL:HG13	1.81	0.45
4:E:207:GLN:HB3	4:E:219:VAL:HG12	1.98	0.45
6:G:99:C:N3	7:H:33:G:C4	2.84	0.45
11:L:94:ALA:O	11:L:98:GLU:HG3	2.16	0.45
12:M:210:TYR:O	12:M:210:TYR:CG	2.69	0.45
23:X:228:LYS:HA	23:X:231:ARG:HD3	1.99	0.45
23:X:741:TRP:CG	35:1:782:GLU:HB3	2.50	0.45
23:X:1008:LEU:HB3	23:X:1016:TYR:CD2	2.50	0.45
35:1:581:LEU:HD13	35:1:589:ALA:HB1	1.98	0.45
35:1:706:ALA:O	35:1:749:ALA:HB2	2.16	0.45
35:1:1090:PRO:CA	35:1:1093:VAL:CG1	2.92	0.45
35:1:1165:TYR:CD1	39:2:575:PHE:CE1	3.04	0.45
36:3:288:VAL:HG23	36:3:289:CYS:N	2.30	0.45
36:3:515:ALA:HA	36:3:528:ARG:HA	1.97	0.45
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.76	0.45
1:A:1361:GLU:HG3	1:A:1362:ASP:OD2	2.17	0.45
1:A:1977:ILE:HG22	1:A:1978:LYS:HD2	1.98	0.45
4:E:118:ASN:ND2	4:E:122:SER:H	2.10	0.45
6:G:13:C:C2	6:G:14:A:C8	3.04	0.45
7:H:56:A:O2'	39:2:481:THR:OG1	2.20	0.45
9:J:322:MET:HE1	12:M:142:ILE:HG12	1.97	0.45
21:V:562:TRP:CD2	21:V:602:ARG:HD3	2.51	0.45
21:V:569:LYS:HD2	21:V:614:GLY:HA3	1.98	0.45
23:X:171:ARG:CZ	23:X:509:PRO:HB3	2.42	0.45
23:X:715:SER:HB3	23:X:718:SER:HB3	1.98	0.45
23:X:787:GLU:HB2	35:1:542:PRO:HG3	1.98	0.45
34:s:65:PRO:O	34:s:67:SER:N	2.49	0.45
36:3:184:CYS:SG	36:3:211:TYR:HE1	2.40	0.45
36:3:259:LYS:HB2	36:3:259:LYS:HE3	1.69	0.45
36:3:503:THR:OG1	36:3:522:ASP:OD2	2.21	0.45
36:3:528:ARG:NH1	36:3:572:GLY:O	2.49	0.45
36:3:565:TYR:CE1	36:3:619:LEU:HD12	2.51	0.45
36:3:615:ARG:C	36:3:616:ILE:HD12	2.41	0.45
36:3:745:PHE:CG	36:3:755:VAL:HG23	2.51	0.45
36:3:788:PHE:HB2	36:3:799:ILE:HA	1.98	0.45
36:3:910:ALA:HB2	36:3:948:VAL:HG23	1.98	0.45
36:3:911:LYS:HG3	36:3:912:ASP:CG	2.42	0.45
36:3:1159:ASP:OD1	36:3:1160:HIS:N	2.50	0.45
1:A:362:ARG:NH1	21:V:324:HIS:N	2.63	0.45
1:A:977:LEU:HG	1:A:978:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1831:LYS:HZ3	1:A:1832:ARG:HB2	1.79	0.45
3:C:845:ALA:O	3:C:848:THR:OG1	2.31	0.45
5:F:36:A:N1	6:G:10:U:C4	2.84	0.45
6:G:97:A:C2	35:1:1075:ARG:HG2	2.51	0.45
12:M:160:PHE:HB3	12:M:161:PHE:CD1	2.51	0.45
19:T:341:ALA:O	19:T:344:GLN:HG3	2.16	0.45
23:X:790:LEU:O	23:X:794:GLU:HG2	2.16	0.45
35:1:662:HIS:HB2	35:1:701:VAL:HB	1.98	0.45
35:1:997:LEU:HA	35:1:997:LEU:HD23	1.84	0.45
35:1:1226:VAL:O	35:1:1230:VAL:HG23	2.17	0.45
36:3:185:LEU:HD23	36:3:185:LEU:HA	1.69	0.45
36:3:234:PHE:HE1	36:3:236:ILE:HG12	1.81	0.45
36:3:590:MET:HE3	36:3:607:VAL:HG22	1.99	0.45
36:3:604:PHE:CE1	36:3:681:PRO:HD3	2.51	0.45
1:A:1127:GLY:HA3	1:A:1151:ARG:HH22	1.81	0.45
1:A:1526:LEU:HD22	1:A:1527:ASN:H	1.81	0.45
1:A:1868:MET:C	1:A:1871:PRO:HD2	2.41	0.45
3:C:860:ASP:N	3:C:860:ASP:OD1	2.49	0.45
5:F:33:G:C2	5:F:34:G:C8	3.05	0.45
6:G:99:C:N4	7:H:32:U:C4	2.84	0.45
7:H:150:U:H3	7:H:181:G:H22	1.64	0.45
12:M:139:THR:O	12:M:142:ILE:HG22	2.17	0.45
12:M:210:TYR:O	12:M:210:TYR:CD2	2.69	0.45
15:P:186:ARG:HB2	24:Y:49:PHE:CE1	2.50	0.45
19:T:203:HIS:CE1	19:T:223:SER:HB3	2.51	0.45
19:T:329:HIS:CE1	19:T:349:SER:HB3	2.51	0.45
23:X:235:LEU:HD22	24:Y:217:ALA:HA	1.97	0.45
24:Y:73:ASP:OD1	24:Y:73:ASP:N	2.48	0.45
35:1:1017:LEU:HD22	35:1:1050:VAL:HG11	1.98	0.45
35:1:1135:GLU:O	35:1:1135:GLU:HG3	2.15	0.45
35:1:1216:TRP:O	35:1:1219:VAL:HB	2.16	0.45
36:3:5:ASN:O	36:3:1176:GLY:HA3	2.16	0.45
36:3:193:ASP:HB3	42:5:29:TRP:CH2	2.51	0.45
36:3:343:LYS:C	36:3:345:GLY:H	2.24	0.45
36:3:404:LEU:HD12	36:3:404:LEU:HA	1.77	0.45
36:3:1203:GLU:HG3	36:3:1206:LYS:HZ1	1.81	0.45
43:o:52:ASN:O	43:o:74:ASN:HA	2.17	0.45
32:k:41:VAL:HA	32:k:61:VAL:HA	1.98	0.45
1:A:1571:ILE:HG23	10:K:220:LEU:CD2	2.41	0.45
1:A:1817:LEU:O	1:A:1916:LEU:HA	2.17	0.45
2:B:92:U:N3	28:b:36:MET:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.51	0.45
3:C:662:PHE:CE1	3:C:829:GLU:HB3	2.51	0.45
3:C:918:ILE:HG21	3:C:932:GLU:OE2	2.16	0.45
6:G:15:U:C2	6:G:16:G:C8	3.05	0.45
6:G:107:U:O2	23:X:709:LEU:CD2	2.65	0.45
11:L:749:LEU:O	11:L:753:GLU:N	2.45	0.45
17:R:309:GLU:OE1	17:R:309:GLU:HA	2.17	0.45
19:T:391:SER:OG	19:T:393:ASP:OD2	2.26	0.45
21:V:560:LEU:HD23	21:V:560:LEU:HA	1.80	0.45
23:X:592:LEU:O	23:X:596:VAL:HG23	2.16	0.45
35:1:869:MET:O	35:1:873:GLU:HB3	2.15	0.45
36:3:14:ILE:HD11	36:3:356:HIS:CD2	2.51	0.45
36:3:93:GLN:O	36:3:97:ASN:N	2.50	0.45
36:3:249:LEU:HD23	36:3:256:ILE:HD11	1.98	0.45
36:3:333:VAL:HG21	36:3:349:VAL:HG21	1.97	0.45
36:3:458:ALA:O	36:3:459:VAL:HG23	2.16	0.45
36:3:642:ILE:H	36:3:703:ARG:NH2	2.13	0.45
36:3:986:ILE:HG21	36:3:990:ILE:HG12	1.99	0.45
38:w:466:LYS:HE3	38:w:466:LYS:HB2	1.73	0.45
43:o:14:GLN:HA	43:o:23:GLU:O	2.15	0.45
27:m:16:ARG:O	27:m:84:GLY:N	2.44	0.45
1:A:699:GLU:OE1	1:A:699:GLU:HA	2.14	0.45
1:A:727:LYS:HE2	1:A:727:LYS:HB3	1.70	0.45
2:B:53:U:OP1	15:P:39:THR:OG1	2.34	0.45
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.70	0.45
3:C:755:ASP:O	3:C:758:LEU:N	2.48	0.45
4:E:209:ILE:HG23	4:E:219:VAL:HG22	1.99	0.45
5:F:10:U:H2'	5:F:11:C:H4'	1.99	0.45
7:H:43:U:H2'	7:H:44:U:C5	2.51	0.45
7:H:105:G:N2	7:H:107:A:H5'	2.32	0.45
11:L:163:GLN:CB	11:L:168:LYS:HZ3	2.16	0.45
35:1:508:THR:HB	35:1:510:PRO:CD	2.46	0.45
35:1:761:TYR:O	35:1:765:TYR:HB2	2.17	0.45
36:3:147:ASP:OD2	36:3:151:ARG:HG2	2.16	0.45
36:3:601:ARG:HD3	36:3:620:ASP:HB3	1.98	0.45
36:3:725:TYR:O	36:3:728:ARG:HB2	2.16	0.45
36:3:741:PHE:HB3	36:3:757:ILE:HG13	1.99	0.45
36:3:996:ILE:HG21	36:3:1041:TYR:CD1	2.52	0.45
39:2:526:ASP:O	39:2:528:ILE:N	2.50	0.45
39:2:569:GLN:O	39:2:573:ASP:HB2	2.17	0.45
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ASN:O	1:A:546:LEU:HB2	2.17	0.45
1:A:832:TYR:HB3	1:A:835:ASP:OD1	2.17	0.45
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.48	0.45
1:A:1785:VAL:HG11	1:A:1807:ILE:HD13	1.99	0.45
2:B:92:U:C4	28:b:36:MET:N	2.85	0.45
9:J:200:GLU:C	9:J:202:GLU:N	2.74	0.45
11:L:201:LYS:HZ2	11:L:203:LYS:HG2	1.81	0.45
15:P:51:PRO:HA	15:P:54:VAL:HG22	1.99	0.45
21:V:490:CYS:HA	21:V:493:ILE:HD12	1.99	0.45
23:X:172:LEU:HA	23:X:175:LEU:HD23	1.99	0.45
23:X:725:ARG:HD3	23:X:728:ARG:HH12	1.82	0.45
23:X:871:PHE:HB3	23:X:883:ASN:HD22	1.82	0.45
35:1:1015:ASP:OD1	35:1:1015:ASP:N	2.49	0.45
35:1:1167:TYR:CZ	39:2:581:LYS:HG2	2.49	0.45
35:1:1244:CYS:O	35:1:1245:ARG:C	2.60	0.45
36:3:528:ARG:HG3	36:3:529:ALA:N	2.31	0.45
36:3:1085:ALA:HB3	36:3:1088:LYS:HE2	1.97	0.45
42:5:33:VAL:CG2	42:5:76:CYS:HB2	2.47	0.45
1:A:1458:GLN:NE2	1:A:1463:LYS:HD3	2.32	0.45
3:C:188:VAL:HG23	3:C:190:LEU:HD11	1.98	0.45
3:C:678:THR:HB	3:C:680:ASN:O	2.17	0.45
9:J:357:LYS:N	9:J:357:LYS:HD2	2.31	0.45
14:O:167:PHE:O	14:O:172:GLU:N	2.48	0.45
14:O:249:ARG:O	14:O:253:TYR:N	2.50	0.45
15:P:73:GLU:HG2	15:P:76:ARG:HH21	1.81	0.45
17:R:184:GLN:HE21	17:R:184:GLN:HB3	1.46	0.45
19:T:399:LYS:HB2	19:T:406:ILE:HD11	1.98	0.45
19:T:478:LEU:HD23	19:T:488:VAL:HG22	1.98	0.45
21:V:503:TYR:CE2	21:V:550:MET:HG2	2.52	0.45
21:V:647:LEU:O	21:V:651:PRO:HD3	2.17	0.45
23:X:475:ASN:ND2	23:X:490:ARG:HD3	2.32	0.45
23:X:502:LEU:O	23:X:505:PHE:HB2	2.17	0.45
23:X:718:SER:OG	23:X:719:ALA:N	2.47	0.45
35:1:625:ARG:HH21	35:1:662:HIS:CG	2.35	0.45
35:1:694:LEU:HD22	35:1:727:VAL:CG2	2.47	0.45
35:1:802:GLU:C	35:1:843:LYS:HZ2	2.24	0.45
35:1:826:ASP:OD1	35:1:827:ARG:N	2.50	0.45
36:3:27:GLN:OE1	36:3:42:ARG:NH1	2.50	0.45
36:3:164:ASN:HD22	36:3:190:GLU:HG2	1.82	0.45
36:3:1116:SER:HA	39:2:708:TRP:CZ2	2.50	0.45
1:A:108:MET:O	1:A:110:TRP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HH22	21:V:320:ARG:HA	1.82	0.45
1:A:1359:HIS:CD2	1:A:1361:GLU:O	2.70	0.45
1:A:1661:TRP:HH2	1:A:1684:PHE:CE1	2.35	0.45
3:C:685:ILE:HB	3:C:815:VAL:HG21	1.99	0.45
3:C:803:ARG:O	3:C:807:GLN:HG3	2.17	0.45
4:E:108:HIS:CE1	4:E:128:SER:HB2	2.52	0.45
4:E:176:VAL:O	4:E:189:THR:HA	2.17	0.45
11:L:14:THR:HG23	11:L:152:LEU:HD21	1.99	0.45
11:L:699:ASN:O	11:L:703:MET:N	2.50	0.45
17:R:147:THR:O	17:R:151:LEU:HB2	2.17	0.45
17:R:360:ARG:HD2	24:Y:274:ASP:OD2	2.16	0.45
17:R:434:ASP:OD2	17:R:434:ASP:N	2.48	0.45
23:X:674:THR:HG22	23:X:675:ASN:N	2.32	0.45
23:X:984:LEU:HD21	23:X:1000:VAL:HG21	1.97	0.45
35:1:550:HIS:CD2	35:1:551:LEU:HD22	2.49	0.45
35:1:854:VAL:HG11	35:1:891:GLN:HG3	1.97	0.45
35:1:1017:LEU:HD21	35:1:1058:ILE:HD11	1.99	0.45
35:1:1080:THR:HA	35:1:1083:TYR:CD2	2.52	0.45
35:1:1231:MET:HE1	35:1:1268:ILE:CG1	2.46	0.45
36:3:243:ASP:OD1	36:3:244:GLY:N	2.50	0.45
36:3:407:ILE:HD11	36:3:1124:GLY:HA2	1.99	0.45
36:3:442:LEU:HD23	36:3:442:LEU:HA	1.71	0.45
41:7:9:ILE:O	41:7:88:ILE:HG22	2.17	0.45
1:A:76:MET:HE1	1:A:84:ASP:HB2	1.98	0.45
1:A:995:ARG:HH11	1:A:998:ARG:HH11	1.64	0.45
1:A:1346:THR:O	1:A:1346:THR:OG1	2.22	0.45
1:A:1799:THR:O	1:A:1801:LYS:NZ	2.42	0.45
1:A:1820:LYS:NZ	1:A:1914:MET:HB2	2.32	0.45
2:B:26:A:H2'	2:B:27:U:O4'	2.17	0.45
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.99	0.45
9:J:187:VAL:CG1	9:J:188:GLN:H	2.23	0.45
9:J:367:GLU:OE1	9:J:382:TYR:CZ	2.70	0.45
13:N:9:LYS:HE2	13:N:9:LYS:HB3	1.57	0.45
15:P:184:VAL:HG13	15:P:184:VAL:O	2.16	0.45
17:R:386:ARG:NE	17:R:386:ARG:HA	2.29	0.45
21:V:539:LEU:HB3	21:V:543:LYS:HB2	1.99	0.45
21:V:551:PHE:HA	21:V:554:LEU:HD12	1.98	0.45
23:X:689:VAL:C	23:X:690:LEU:HD23	2.42	0.45
35:1:685:SER:O	35:1:689:ILE:HG12	2.17	0.45
35:1:856:ASP:HB3	35:1:864:TYR:CE2	2.51	0.45
35:1:963:LYS:O	35:1:965:CYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1063:LEU:HA	35:1:1063:LEU:HD23	1.64	0.45
36:3:312:LYS:HB2	36:3:330:PHE:CD1	2.50	0.45
36:3:485:LEU:HA	36:3:494:VAL:HB	1.98	0.45
36:3:558:LEU:HD23	36:3:562:GLU:HB3	1.99	0.45
36:3:717:SER:HB2	36:3:718:ARG:HH12	1.81	0.45
36:3:1021:LEU:HD23	36:3:1021:LEU:HA	1.77	0.45
36:3:1041:TYR:HD2	39:2:705:ARG:HG3	1.81	0.45
37:p:10:TYR:O	37:p:81:ILE:HA	2.17	0.45
39:2:541:GLN:O	39:2:545:GLU:HG2	2.17	0.45
1:A:64:GLU:OE1	1:A:64:GLU:N	2.35	0.44
1:A:367:SER:OG	1:A:368:GLN:N	2.50	0.44
1:A:1189:MET:CG	1:A:1190:CYS:H	2.30	0.44
1:A:1606:ILE:HD11	1:A:1631:LEU:HD13	1.98	0.44
1:A:2007:ILE:HA	1:A:2010:ILE:HG22	1.99	0.44
2:B:67:A:H2'	2:B:68:C:O4'	2.17	0.44
6:G:1:G:C6	6:G:2:U:H1'	2.52	0.44
6:G:99:C:N3	7:H:33:G:C5	2.86	0.44
7:H:106:G:N3	7:H:107:A:N6	2.65	0.44
17:R:411:LEU:HD13	17:R:411:LEU:HA	1.74	0.44
35:1:536:LEU:O	35:1:540:MET:HG2	2.16	0.44
35:1:721:ILE:CG2	35:1:756:LEU:HD23	2.26	0.44
35:1:1046:GLY:O	35:1:1048:GLU:N	2.50	0.44
35:1:1304:LEU:HD21	42:5:55:ILE:HG22	1.99	0.44
36:3:38:LEU:HD12	36:3:38:LEU:HA	1.79	0.44
36:3:965:LYS:HB3	36:3:965:LYS:HE2	1.69	0.44
36:3:1156:CYS:O	36:3:1158:ARG:N	2.50	0.44
39:2:596:GLU:N	39:2:596:GLU:OE2	2.50	0.44
1:A:67:ARG:HD2	13:N:33:GLU:OE2	2.17	0.44
3:C:260:ILE:CD1	3:C:309:PHE:HB3	2.47	0.44
3:C:536:ARG:HD3	3:C:536:ARG:C	2.43	0.44
3:C:719:GLN:HG3	3:C:724:TRP:O	2.17	0.44
4:E:266:PRO:CG	11:L:789:ALA:HA	2.47	0.44
7:H:114:A:H2'	7:H:115:G:C8	2.53	0.44
15:P:188:TRP:O	15:P:188:TRP:CD1	2.70	0.44
15:P:205:LYS:HG2	15:P:208:LYS:HB3	1.98	0.44
17:R:404:GLU:OE1	23:X:327:ARG:NE	2.42	0.44
23:X:182:ALA:HB1	23:X:186:ARG:HH21	1.82	0.44
23:X:388:GLN:O	23:X:392:ILE:HG13	2.17	0.44
23:X:719:ALA:HB1	23:X:736:ARG:HE	1.82	0.44
24:Y:221:ALA:O	24:Y:225:GLU:HG2	2.17	0.44
35:1:645:LEU:HD13	35:1:682:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:721:ILE:C	35:1:723:SER:N	2.75	0.44
35:1:1277:GLN:H	36:3:113:ARG:CZ	2.30	0.44
35:1:1299:GLU:HB3	42:5:43:TYR:CE2	2.52	0.44
36:3:1:MET:HE3	36:3:3:LEU:HD21	1.99	0.44
36:3:101:LYS:HB2	36:3:101:LYS:HE3	1.65	0.44
36:3:275:ARG:HH21	36:3:275:ARG:CB	2.31	0.44
36:3:925:VAL:O	36:3:942:LYS:HA	2.18	0.44
36:3:988:ASN:ND2	36:3:1004:ASP:OD1	2.50	0.44
36:3:1211:ILE:HD12	36:3:1214:ARG:HE	1.82	0.44
1:A:122:ILE:HG13	1:A:481:PHE:O	2.17	0.44
1:A:305:ARG:HG3	3:C:878:ILE:HG21	1.98	0.44
1:A:329:LEU:HD23	1:A:329:LEU:H	1.83	0.44
1:A:644:ILE:HD12	1:A:644:ILE:HA	1.80	0.44
1:A:1117:HIS:CE1	15:P:199:LYS:HG3	2.53	0.44
1:A:1498:TRP:O	1:A:1501:LEU:HG	2.16	0.44
3:C:304:LEU:H	3:C:304:LEU:HD12	1.82	0.44
3:C:585:THR:O	3:C:587:VAL:HG23	2.17	0.44
3:C:687:MET:HB3	3:C:815:VAL:CG1	2.47	0.44
4:E:263:ASP:O	4:E:272:ARG:HD2	2.16	0.44
5:F:30:A:H2'	5:F:31:U:O4'	2.17	0.44
5:F:58:G:HO2'	5:F:59:G:P	2.38	0.44
5:F:93:G:H2'	5:F:94:C:C6	2.52	0.44
7:H:18:U:O2	17:R:258:LYS:HB2	2.17	0.44
13:N:16:GLU:N	13:N:16:GLU:CD	2.74	0.44
17:R:184:GLN:H	17:R:184:GLN:HG2	1.50	0.44
17:R:383:ASN:N	17:R:383:ASN:OD1	2.51	0.44
19:T:435:THR:HB	19:T:451:HIS:CE1	2.53	0.44
21:V:503:TYR:HE2	21:V:550:MET:HG2	1.82	0.44
21:V:532:GLN:HE22	21:V:539:LEU:HD11	1.82	0.44
23:X:1017:LYS:HE2	23:X:1017:LYS:HB2	1.76	0.44
24:Y:246:LYS:HE3	24:Y:312:HIS:CB	2.40	0.44
34:q:106:ALA:CB	34:t:106:ALA:HB1	2.43	0.44
35:1:658:TRP:CZ3	35:1:698:GLN:HG2	2.52	0.44
35:1:946:LYS:O	35:1:950:GLN:HG3	2.17	0.44
35:1:1158:ILE:HG13	35:1:1159:GLY:N	2.32	0.44
36:3:341:VAL:HG12	36:3:347:LEU:HB2	2.00	0.44
39:2:477:MET:SD	39:2:478:HIS:CE1	3.10	0.44
39:2:535:GLU:H	39:2:535:GLU:CD	2.26	0.44
1:A:159:ARG:HA	1:A:159:ARG:CZ	2.48	0.44
1:A:1140:MET:HE3	1:A:1177:VAL:H	1.82	0.44
1:A:1554:GLN:HG3	1:A:1561:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:461:LEU:HD21	3:C:572:GLU:OE2	2.18	0.44
3:C:642:HIS:O	3:C:646:LYS:HB2	2.18	0.44
3:C:711:ARG:HA	3:C:714:LEU:HD22	1.99	0.44
4:E:181:ILE:HG22	4:E:182:ARG:NH1	2.32	0.44
7:H:160:A:C2	7:H:171:U:C2	3.05	0.44
12:M:215:ASN:ND2	17:R:261:THR:N	2.49	0.44
23:X:289:GLN:HA	23:X:292:LEU:HD23	2.00	0.44
35:1:781:ASP:O	35:1:785:LYS:HG3	2.17	0.44
35:1:857:LEU:HA	35:1:865:ARG:HB3	1.98	0.44
35:1:1142:ASN:H	35:1:1142:ASN:HD22	1.64	0.44
35:1:1200:TYR:C	35:1:1200:TYR:CD1	2.95	0.44
36:3:124:ASP:OD2	36:3:128:ARG:HG3	2.17	0.44
36:3:125:PRO:HG2	36:3:174:ASP:HA	1.99	0.44
36:3:278:LEU:HD21	36:3:816:LYS:NZ	2.32	0.44
36:3:924:PHE:HA	36:3:943:THR:O	2.18	0.44
36:3:993:ILE:HG23	36:3:1002:VAL:HG23	1.99	0.44
36:3:1151:GLU:OE2	36:3:1193:VAL:HG21	2.18	0.44
38:w:383:LEU:HD13	38:w:391:PRO:HB3	1.98	0.44
1:A:120:TYR:HE1	1:A:485:THR:OG1	2.01	0.44
1:A:758:ARG:HD2	1:A:775:ASN:HD21	1.83	0.44
1:A:1284:LEU:HA	1:A:1284:LEU:HD23	1.72	0.44
3:C:118:PHE:O	3:C:122:LEU:HD12	2.17	0.44
3:C:514:TYR:HB2	3:C:521:ASP:HB2	1.99	0.44
5:F:44:G:H8	5:F:44:G:OP2	2.00	0.44
5:F:61:C:OP1	17:R:217:LYS:NZ	2.45	0.44
5:F:79:C:O2'	5:F:80:G:O5'	2.32	0.44
12:M:125:SER:HB2	17:R:237:MET:O	2.18	0.44
15:P:78:ARG:HD3	15:P:78:ARG:HA	1.72	0.44
17:R:86:LEU:HD23	17:R:86:LEU:H	1.81	0.44
21:V:468:ASP:OD1	21:V:468:ASP:N	2.49	0.44
21:V:497:CYS:HB3	21:V:507:PHE:HB2	1.99	0.44
21:V:622:ARG:NH2	21:V:623:ASN:HB3	2.32	0.44
23:X:461:VAL:HA	23:X:464:ARG:NE	2.33	0.44
23:X:461:VAL:HG22	23:X:464:ARG:HH21	1.83	0.44
23:X:807:GLU:OE2	23:X:807:GLU:HA	2.17	0.44
24:Y:33:LYS:HD3	24:Y:33:LYS:HA	1.67	0.44
24:Y:117:ASP:N	24:Y:117:ASP:OD1	2.48	0.44
24:Y:186:LEU:HD23	24:Y:186:LEU:HA	1.71	0.44
35:1:1167:TYR:OH	39:2:581:LYS:HD3	2.18	0.44
36:3:1:MET:SD	39:2:709:GLY:O	2.76	0.44
36:3:404:LEU:HB3	36:3:407:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:485:LEU:CD2	36:3:491:VAL:HG12	2.46	0.44
36:3:753:GLY:O	36:3:754:ILE:HD13	2.17	0.44
38:w:408:CYS:SG	38:w:431:HIS:CE1	3.10	0.44
42:5:71:LYS:C	42:5:73:LEU:H	2.26	0.44
1:A:369:GLU:OE1	1:A:370:PRO:HD2	2.18	0.44
1:A:564:TYR:HA	1:A:569:VAL:HG23	1.99	0.44
1:A:1043:TYR:O	1:A:1046:LEU:HB3	2.18	0.44
4:E:181:ILE:HD12	4:E:181:ILE:N	2.32	0.44
5:F:26:U:H3'	5:F:27:A:H5''	2.00	0.44
9:J:333:PHE:O	9:J:337:MET:HG2	2.18	0.44
11:L:223:GLY:O	11:L:225:TYR:N	2.51	0.44
15:P:218:GLU:HA	15:P:221:LYS:HG3	2.00	0.44
17:R:330:LYS:NZ	23:X:275:ARG:HH22	2.07	0.44
19:T:191:HIS:CD2	19:T:440:ASP:OD1	2.70	0.44
21:V:617:PRO:HB3	21:V:623:ASN:ND2	2.32	0.44
35:1:566:LEU:HD12	35:1:566:LEU:HA	1.89	0.44
35:1:668:VAL:HG22	35:1:686:LEU:HD23	1.99	0.44
36:3:114:ARG:NH1	42:5:34:ASN:O	2.51	0.44
36:3:190:GLU:CD	36:3:194:ASN:HD21	2.26	0.44
36:3:590:MET:HB2	36:3:606:ALA:O	2.18	0.44
36:3:1136:GLU:H	36:3:1136:GLU:CD	2.21	0.44
36:3:1191:LYS:HB2	36:3:1191:LYS:HZ3	1.82	0.44
39:2:504:TRP:CD1	39:2:504:TRP:H	2.34	0.44
42:5:50:LEU:HA	42:5:50:LEU:HD12	1.54	0.44
42:5:72:MET:HE2	42:5:72:MET:HB3	1.88	0.44
29:h:34:GLN:O	29:h:38:ASN:CB	2.66	0.44
1:A:946:GLU:HG2	1:A:954:LYS:NZ	2.33	0.44
2:B:117:A:C6	30:d:26:GLY:HA3	2.52	0.44
3:C:349:PHE:HE1	3:C:354:ARG:HA	1.83	0.44
3:C:485:ASP:OD2	3:C:485:ASP:N	2.47	0.44
4:E:304:SER:O	4:E:330:ILE:HD12	2.17	0.44
4:E:340:PRO:HB2	4:E:356:ILE:C	2.43	0.44
9:J:428:GLU:O	9:J:432:VAL:HG13	2.18	0.44
17:R:348:GLU:OE1	23:X:263:SER:HB3	2.17	0.44
21:V:554:LEU:HA	21:V:559:SER:OG	2.18	0.44
23:X:659:ILE:O	23:X:669:LYS:NZ	2.50	0.44
35:1:769:VAL:HG13	35:1:773:LEU:HD21	1.98	0.44
35:1:843:LYS:C	35:1:843:LYS:CD	2.90	0.44
36:3:595:VAL:HG22	36:3:596:PRO:O	2.17	0.44
36:3:613:THR:CB	36:3:630:MET:HE1	2.48	0.44
30:i:24:LYS:N	30:i:68:ASN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1635:TYR:CE2	1:A:1636:LYS:HB2	2.52	0.44
1:A:1813:ARG:HA	1:A:1929:SER:HB2	1.99	0.44
1:A:1963:GLU:O	1:A:1965:HIS:N	2.51	0.44
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.99	0.44
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.53	0.44
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.16	0.44
5:F:32:U:H2'	5:F:33:G:C8	2.53	0.44
17:R:325:ARG:HA	17:R:325:ARG:HD2	1.50	0.44
21:V:570:LEU:HD23	21:V:570:LEU:HA	1.86	0.44
21:V:573:GLU:H	21:V:573:GLU:CD	2.25	0.44
23:X:824:LEU:HA	23:X:827:MET:HG2	1.99	0.44
24:Y:39:TYR:HB3	24:Y:185:GLN:HE22	1.82	0.44
24:Y:264:GLY:HA3	24:Y:293:ASP:CG	2.43	0.44
35:1:575:LEU:HD11	35:1:613:MET:SD	2.58	0.44
35:1:666:LYS:HB3	35:1:704:ILE:CD1	2.48	0.44
36:3:528:ARG:HG3	36:3:529:ALA:H	1.83	0.44
36:3:554:VAL:HG12	36:3:556:ILE:HG23	2.00	0.44
38:w:410:ILE:HG23	38:w:438:LEU:HD11	1.98	0.44
1:A:929:GLU:OE1	1:A:933:ARG:NH2	2.51	0.44
1:A:1527:ASN:O	1:A:1529:ILE:HD12	2.17	0.44
1:A:1854:VAL:HA	1:A:1857:GLN:OE1	2.17	0.44
1:A:1865:ARG:HA	1:A:1865:ARG:NH2	2.33	0.44
3:C:78:GLU:HG3	3:C:79:THR:N	2.33	0.44
3:C:267:LEU:HD23	3:C:267:LEU:HA	1.80	0.44
3:C:305:GLY:O	3:C:433:MET:HG3	2.18	0.44
3:C:470:PRO:HA	3:C:499:GLY:O	2.18	0.44
4:E:287:ASN:OD1	4:E:288:LEU:N	2.51	0.44
6:G:99:C:C4	7:H:33:G:C5	3.05	0.44
6:G:99:C:C4	7:H:33:G:C6	3.05	0.44
13:N:124:SER:OG	13:N:125:LYS:HD2	2.18	0.44
17:R:311:LYS:HG3	24:Y:200:PHE:HZ	1.83	0.44
35:1:750:ILE:HG13	35:1:751:GLY:N	2.32	0.44
35:1:807:LYS:CG	35:1:844:VAL:HG12	2.47	0.44
35:1:1212:LEU:HD12	35:1:1212:LEU:HA	1.76	0.44
35:1:1281:ILE:HD11	42:5:38:ASP:HB3	2.00	0.44
36:3:325:ILE:HB	36:3:375:SER:HB3	1.99	0.44
36:3:565:TYR:HB3	36:3:577:TYR:CB	2.46	0.44
36:3:770:LEU:HD23	36:3:770:LEU:HA	1.82	0.44
39:2:534:GLN:HG2	39:2:538:GLU:OE1	2.18	0.44
33:l:32:LEU:HA	33:l:43:MET:HA	1.99	0.44
1:A:599:MET:O	1:A:603:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:SER:OG	3:C:480:LYS:NZ	2.39	0.43
5:F:13:G:H2'	5:F:14:C:C6	2.53	0.43
5:F:36:A:C3'	5:F:37:C:H5''	2.37	0.43
5:F:58:G:O2'	5:F:59:G:H5'	2.17	0.43
5:F:87:C:OP2	12:M:193:ARG:HA	2.18	0.43
8:I:50:LYS:CB	8:I:51:PRO:HD3	2.47	0.43
9:J:440:LEU:O	9:J:445:LYS:HD2	2.17	0.43
19:T:266:GLU:HG2	19:T:290:ALA:HB1	2.00	0.43
23:X:681:LEU:O	23:X:725:ARG:NH2	2.50	0.43
23:X:1003:ILE:HG13	23:X:1004:GLU:N	2.33	0.43
24:Y:28:PHE:O	24:Y:32:CYS:HB2	2.18	0.43
35:1:827:ARG:HB2	35:1:827:ARG:CZ	2.47	0.43
35:1:967:GLU:HB3	35:1:971:MET:H	1.83	0.43
36:3:187:MET:HE3	36:3:231:HIS:NE2	2.32	0.43
36:3:234:PHE:CD1	36:3:235:LEU:N	2.86	0.43
36:3:543:THR:O	36:3:558:LEU:HD12	2.17	0.43
1:A:818:GLU:CD	17:R:305:ARG:HH11	2.26	0.43
1:A:1963:GLU:O	1:A:1966:HIS:N	2.50	0.43
3:C:436:GLN:HB3	3:C:437:HIS:HD2	1.82	0.43
5:F:34:G:H2'	5:F:35:A:C8	2.54	0.43
6:G:88:G:H2'	6:G:88:G:N3	2.33	0.43
7:H:161:U:H2'	7:H:163:G:N2	2.32	0.43
13:N:38:GLU:C	13:N:40:LYS:N	2.77	0.43
13:N:120:ARG:HA	13:N:120:ARG:HD2	1.66	0.43
17:R:320:HIS:HA	17:R:323:LYS:CE	2.48	0.43
19:T:333:VAL:HA	19:T:349:SER:HB2	1.99	0.43
21:V:470:GLU:CD	21:V:513:ARG:HH21	2.26	0.43
21:V:496:CYS:HA	21:V:499:GLN:OE1	2.17	0.43
23:X:555:MET:C	23:X:557:THR:H	2.27	0.43
23:X:871:PHE:HB3	23:X:883:ASN:ND2	2.33	0.43
35:1:892:LEU:HD22	35:1:892:LEU:HA	1.70	0.43
35:1:1108:ASN:N	35:1:1108:ASN:OD1	2.51	0.43
38:w:383:LEU:HA	38:w:383:LEU:HD23	1.67	0.43
39:2:451:LYS:O	39:2:454:LEU:HG	2.18	0.43
39:2:469:VAL:HG12	39:2:471:ARG:N	2.31	0.43
1:A:37:TRP:CD1	1:A:37:TRP:C	2.96	0.43
1:A:1401:ARG:HG2	1:A:1401:ARG:HH11	1.82	0.43
1:A:1690:ASP:OD1	1:A:1693:SER:OG	2.29	0.43
1:A:1779:PHE:CD2	1:A:1862:ILE:HD11	2.53	0.43
3:C:660:VAL:HG22	3:C:878:ILE:HD11	2.01	0.43
3:C:682:LYS:HB3	3:C:797:ALA:CB	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:283:ASN:O	4:E:286:LYS:HD2	2.19	0.43
18:S:96:GLY:O	18:S:131:ARG:HA	2.19	0.43
23:X:915:ARG:O	23:X:919:GLU:HG3	2.18	0.43
35:1:617:ILE:CA	35:1:663:THR:HG21	2.46	0.43
35:1:1254:LEU:O	35:1:1262:ARG:HG2	2.19	0.43
36:3:549:VAL:HG12	36:3:550:ASN:O	2.18	0.43
36:3:604:PHE:CZ	36:3:681:PRO:HD3	2.53	0.43
36:3:779:PHE:N	36:3:779:PHE:CD1	2.86	0.43
36:3:788:PHE:C	36:3:788:PHE:CD1	2.96	0.43
32:k:7:PRO:HD3	32:k:36:PRO:HA	2.00	0.43
1:A:41:GLN:NE2	1:A:45:TYR:HD2	2.09	0.43
1:A:1211:ASP:C	1:A:1213:VAL:N	2.77	0.43
1:A:1527:ASN:C	1:A:1529:ILE:H	2.25	0.43
3:C:173:THR:O	3:C:177:ARG:HB2	2.18	0.43
4:E:96:TYR:OH	4:E:336:HIS:NE2	2.49	0.43
6:G:116:C:C5	17:R:370:SER:CB	3.01	0.43
7:H:56:A:HO2'	39:2:481:THR:HG1	1.50	0.43
12:M:210:TYR:CD2	12:M:210:TYR:C	2.95	0.43
19:T:288:LEU:O	19:T:289:SER:OG	2.34	0.43
21:V:515:CYS:HA	21:V:521:TYR:HB2	2.00	0.43
21:V:546:ASN:OD1	21:V:547:VAL:N	2.51	0.43
23:X:297:ARG:HE	23:X:297:ARG:HB3	1.60	0.43
23:X:743:TYR:HA	23:X:747:LEU:HD23	2.00	0.43
24:Y:194:ASP:OD1	24:Y:194:ASP:N	2.50	0.43
35:1:721:ILE:HG22	35:1:756:LEU:CD2	2.26	0.43
35:1:969:LYS:HD2	35:1:969:LYS:H	1.83	0.43
35:1:1252:GLN:NE2	39:2:497:SER:OG	2.51	0.43
36:3:249:LEU:HD12	36:3:249:LEU:N	2.33	0.43
36:3:424:TYR:HD1	36:3:437:VAL:HG22	1.82	0.43
36:3:955:PHE:HZ	36:3:1014:TYR:CD2	2.36	0.43
39:2:487:LEU:O	39:2:488:LEU:C	2.61	0.43
39:2:528:ILE:O	39:2:531:THR:HG23	2.18	0.43
41:7:74:GLU:O	41:7:78:GLN:HG3	2.18	0.43
1:A:1580:HIS:HB3	1:A:1583:GLN:NE2	2.33	0.43
3:C:392:LEU:HB3	3:C:393:PRO:HD3	2.01	0.43
4:E:301:ALA:HB2	4:E:335:PHE:CZ	2.53	0.43
4:E:326:HIS:CE1	4:E:346:SER:HB2	2.52	0.43
6:G:90:C:H2'	6:G:91:A:C8	2.53	0.43
7:H:35:A:H3'	7:H:36:G:H8	1.83	0.43
12:M:153:ARG:HB2	12:M:160:PHE:HE2	1.83	0.43
13:N:7:SER:O	13:N:8:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:353:ASP:O	17:R:357:HIS:HB2	2.19	0.43
24:Y:290:LYS:HB2	24:Y:293:ASP:CG	2.43	0.43
35:1:806:ILE:HA	35:1:810:ILE:HD12	2.00	0.43
35:1:834:VAL:O	35:1:835:ASP:C	2.60	0.43
36:3:705:ARG:NH2	36:3:746:ALA:HB2	2.34	0.43
38:w:419:PRO:O	38:w:422:PHE:HB3	2.18	0.43
39:2:512:GLN:N	39:2:512:GLN:OE1	2.51	0.43
42:5:63:ARG:HD3	42:5:63:ARG:HA	1.77	0.43
30:i:43:GLN:HA	30:i:63:LEU:HA	2.01	0.43
1:A:696:MET:C	1:A:698:PRO:HD3	2.43	0.43
1:A:1109:LEU:HG	1:A:1152:ALA:HB1	2.00	0.43
1:A:1586:HIS:NE2	1:A:1664:ILE:HG13	2.34	0.43
2:B:92:U:O4	28:b:34:VAL:O	2.37	0.43
3:C:231:ALA:O	3:C:277:LYS:HE3	2.18	0.43
4:E:133:VAL:HG22	4:E:154:VAL:HG21	2.00	0.43
8:I:276:ARG:CB	16:Q:357:ALA:CA	2.97	0.43
9:J:240:THR:HG22	9:J:241:VAL:N	2.33	0.43
9:J:400:GLU:O	9:J:404:GLU:HG2	2.19	0.43
19:T:213:GLU:HG2	19:T:214:PRO:CD	2.48	0.43
19:T:269:GLN:HE21	19:T:269:GLN:HB3	1.60	0.43
23:X:523:HIS:O	23:X:525:ARG:HG2	2.18	0.43
23:X:586:ALA:CB	35:1:826:ASP:HA	2.49	0.43
23:X:654:ASP:OD1	23:X:655:MET:N	2.52	0.43
24:Y:225:GLU:OE1	24:Y:233:ALA:HA	2.18	0.43
35:1:503:LYS:HE2	35:1:511:MET:CG	2.44	0.43
35:1:781:ASP:HB3	35:1:784:MET:HB2	2.00	0.43
35:1:1106:ARG:H	35:1:1109:ARG:HG3	1.84	0.43
36:3:35:GLY:HA3	42:5:47:PHE:CZ	2.54	0.43
36:3:131:MET:HB2	36:3:141:VAL:HG22	2.01	0.43
36:3:412:ILE:H	36:3:1105:GLN:NE2	2.09	0.43
36:3:526:HIS:HB2	36:3:574:LEU:CD2	2.48	0.43
36:3:791:HIS:NE2	36:3:793:GLU:HB2	2.34	0.43
36:3:1114:SER:HB2	36:3:1215:TYR:HE1	1.83	0.43
39:2:511:LEU:HA	39:2:511:LEU:HD23	1.73	0.43
39:2:707:PRO:HG2	39:2:710:GLU:HG2	2.00	0.43
1:A:82:ARG:HE	1:A:82:ARG:HB3	1.70	0.43
1:A:785:LYS:HB3	1:A:785:LYS:HE3	1.67	0.43
1:A:1436:TRP:CD1	1:A:1436:TRP:H	2.36	0.43
1:A:1661:TRP:HH2	1:A:1684:PHE:HE1	1.67	0.43
1:A:1799:THR:O	1:A:1801:LYS:HG3	2.19	0.43
1:A:1969:PRO:HB2	1:A:1971:LEU:CD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:ARG:HG3	3:C:179:VAL:HB	2.01	0.43
3:C:461:LEU:HB3	3:C:465:MET:CE	2.35	0.43
3:C:665:THR:HG21	3:C:828:MET:HG3	2.01	0.43
4:E:335:PHE:CE1	4:E:342:ILE:HD12	2.54	0.43
6:G:90:C:H2'	6:G:91:A:C4	2.54	0.43
6:G:107:U:C2	23:X:709:LEU:HD13	2.54	0.43
7:H:118:G:C6	7:H:140:A:N6	2.87	0.43
9:J:429:PHE:HA	9:J:432:VAL:HG22	1.99	0.43
11:L:92:THR:OG1	11:L:95:GLN:HG3	2.19	0.43
17:R:428:GLU:O	17:R:429:ILE:HD13	2.19	0.43
21:V:609:GLN:N	21:V:610:PRO:HD2	2.33	0.43
23:X:268:GLN:HA	23:X:271:LYS:HE2	2.00	0.43
23:X:289:GLN:NE2	23:X:293:GLU:OE2	2.51	0.43
24:Y:183:ARG:HA	24:Y:183:ARG:CZ	2.48	0.43
35:1:551:LEU:O	35:1:555:VAL:HG23	2.19	0.43
35:1:641:ILE:CG2	35:1:682:HIS:NE2	2.82	0.43
35:1:962:MET:O	35:1:967:GLU:HB2	2.18	0.43
36:3:169:HIS:HD2	36:3:170:VAL:O	2.02	0.43
36:3:373:PHE:HD1	36:3:385:PHE:CD2	2.36	0.43
36:3:641:CYS:H	36:3:701:LEU:HD23	1.83	0.43
36:3:769:LYS:HD3	36:3:769:LYS:H	1.81	0.43
39:2:472:PRO:O	39:2:475:VAL:HG23	2.19	0.43
39:2:483:GLN:OE1	39:2:483:GLN:N	2.51	0.43
29:h:52:LEU:HA	29:h:71:LYS:O	2.19	0.43
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.69	0.43
1:A:305:ARG:HG3	3:C:878:ILE:CG2	2.48	0.43
1:A:1213:VAL:HG22	1:A:1229:PHE:CD1	2.54	0.43
1:A:1623:ASN:H	1:A:1623:ASN:ND2	2.17	0.43
1:A:1652:MET:HE2	1:A:1652:MET:HB2	1.97	0.43
1:A:1718:TRP:HZ3	1:A:1726:ILE:HD11	1.84	0.43
1:A:1781:ASP:HB2	1:A:1808:PHE:HB3	2.01	0.43
3:C:607:LEU:O	3:C:608:ARG:C	2.60	0.43
3:C:641:MET:HE2	3:C:641:MET:HB3	1.91	0.43
6:G:88:G:H1'	7:H:42:G:N2	2.33	0.43
6:G:112:U:OP1	23:X:503:ARG:HG2	2.19	0.43
7:H:162:U:H4'	7:H:163:G:O4'	2.18	0.43
9:J:354:LEU:HA	9:J:354:LEU:HD23	1.81	0.43
17:R:230:MET:HB3	17:R:230:MET:HE3	1.71	0.43
19:T:356:LEU:HD13	19:T:366:VAL:HB	2.00	0.43
19:T:394:ASN:OD1	19:T:394:ASN:N	2.51	0.43
21:V:547:VAL:HA	21:V:550:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:399:LEU:HD23	23:X:399:LEU:HA	1.84	0.43
23:X:868:ARG:NH2	23:X:973:ASN:HD21	2.16	0.43
23:X:888:TRP:O	23:X:891:SER:OG	2.24	0.43
34:q:106:ALA:CB	34:t:106:ALA:HB3	2.48	0.43
36:3:331:ASP:OD2	36:3:393:LYS:N	2.39	0.43
36:3:1035:THR:HG21	36:3:1103:SER:HA	2.01	0.43
38:w:477:GLU:HG2	38:w:479:TYR:HE2	1.83	0.43
1:A:1050:LEU:HD23	1:A:1050:LEU:HA	1.83	0.43
1:A:1224:ARG:HG2	21:V:592:GLU:O	2.19	0.43
1:A:1975:GLU:HG2	1:A:1979:VAL:HG13	2.00	0.43
2:B:115:C:OP1	31:e:67:LYS:CA	2.67	0.43
3:C:193:THR:HB	3:C:428:THR:CG2	2.49	0.43
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.68	0.43
3:C:283:ASP:OD2	3:C:283:ASP:C	2.62	0.43
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.84	0.43
4:E:305:ALA:HA	4:E:329:SER:HB2	1.99	0.43
5:F:80:G:N2	9:J:209:PRO:HD3	2.34	0.43
12:M:160:PHE:C	12:M:162:PRO:HD3	2.44	0.43
12:M:182:MET:HE3	12:M:182:MET:HB2	1.86	0.43
17:R:391:VAL:HG13	17:R:396:VAL:HB	2.01	0.43
21:V:502:THR:HG22	21:V:503:TYR:H	1.84	0.43
23:X:419:ILE:HG21	23:X:557:THR:OG1	2.19	0.43
23:X:535:LEU:O	23:X:539:VAL:HG23	2.19	0.43
23:X:587:PRO:HB2	35:1:827:ARG:NH1	2.32	0.43
35:1:493:LYS:O	35:1:496:LYS:N	2.52	0.43
35:1:1167:TYR:CE2	39:2:581:LYS:HA	2.53	0.43
35:1:1273:TYR:O	35:1:1277:GLN:HB3	2.19	0.43
36:3:192:ALA:HA	36:3:200:ALA:HB3	2.01	0.43
36:3:638:GLU:O	36:3:638:GLU:HG3	2.19	0.43
36:3:1183:ASN:OD1	36:3:1183:ASN:N	2.51	0.43
39:2:517:ILE:H	39:2:517:ILE:HG13	1.27	0.43
42:5:20:GLY:HA2	42:5:34:ASN:ND2	2.33	0.43
1:A:138:PRO:HG3	1:A:235:MET:HE1	2.00	0.43
1:A:1581:LEU:HD22	1:A:1746:ARG:HH11	1.84	0.43
3:C:200:PHE:CE1	3:C:434:CYS:SG	3.12	0.43
3:C:478:THR:CG2	3:C:492:ALA:HB1	2.37	0.43
3:C:624:SER:OG	3:C:941:LYS:HA	2.19	0.43
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.54	0.43
3:C:673:LYS:HB3	3:C:688:ILE:CG2	2.49	0.43
5:F:37:C:H6	5:F:37:C:H2'	1.48	0.43
5:F:97:U:O5'	5:F:97:U:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:20:A:HI'	14:O:193:LEU:O	2.19	0.43
9:J:260:ARG:NH1	11:L:215:PRO:HD3	2.33	0.43
11:L:178:GLU:HA	11:L:181:ARG:CG	2.49	0.43
11:L:646:GLY:O	11:L:650:GLY:N	2.52	0.43
12:M:165:ASN:O	17:R:95:LYS:HA	2.19	0.43
15:P:72:ARG:HA	15:P:75:ASN:HD21	1.83	0.43
17:R:327:MET:HB3	23:X:279:LEU:HD11	1.99	0.43
21:V:545:ARG:HG3	21:V:585:ILE:HD13	2.00	0.43
23:X:516:VAL:HG13	23:X:549:LEU:HD13	2.01	0.43
23:X:913:ASP:O	23:X:916:GLU:HG3	2.19	0.43
35:1:548:GLU:O	35:1:552:LEU:HG	2.19	0.43
35:1:606:LEU:HD12	35:1:606:LEU:HA	1.75	0.43
35:1:1172:LEU:HD12	39:2:522:PHE:CE1	2.54	0.43
35:1:1178:MET:O	35:1:1179:ASP:C	2.62	0.43
36:3:123:VAL:HG22	36:3:124:ASP:H	1.84	0.43
36:3:595:VAL:HG21	36:3:601:ARG:N	2.34	0.43
36:3:665:LEU:HB2	36:3:679:LEU:HD23	2.00	0.43
36:3:882:LEU:HD13	36:3:882:LEU:HA	1.73	0.43
1:A:75:ASP:OD1	1:A:75:ASP:N	2.47	0.42
1:A:387:PHE:HZ	3:C:330:THR:HG21	1.83	0.42
1:A:1397:ILE:HA	1:A:1397:ILE:HD13	1.72	0.42
1:A:1719:PHE:HB2	1:A:1720:PRO:HD2	2.01	0.42
2:B:93:U:C4'	29:c:104:ASP:CA	2.97	0.42
3:C:189:VAL:HA	3:C:198:TYR:O	2.19	0.42
3:C:506:PRO:HB2	3:C:569:ARG:HH22	1.84	0.42
3:C:938:ARG:O	3:C:942:GLY:N	2.50	0.42
7:H:152:G:C6	7:H:153:A:N6	2.87	0.42
9:J:197:GLU:OE2	11:L:156:ARG:HD3	2.19	0.42
11:L:57:SER:O	11:L:57:SER:OG	2.36	0.42
17:R:155:VAL:O	17:R:159:VAL:HG12	2.18	0.42
19:T:253:ILE:O	19:T:261:LEU:HD12	2.19	0.42
19:T:471:ASP:OD2	19:T:472:GLN:N	2.48	0.42
19:T:471:ASP:CG	19:T:472:GLN:N	2.77	0.42
23:X:257:PHE:CE2	23:X:262:LEU:HD21	2.54	0.42
23:X:396:ARG:NE	23:X:431:GLN:HE22	2.17	0.42
23:X:397:ARG:HA	23:X:402:PHE:CD1	2.54	0.42
23:X:991:LEU:HB2	23:X:995:GLU:OE1	2.19	0.42
35:1:666:LYS:O	35:1:670:GLN:HG2	2.19	0.42
35:1:1149:LYS:O	35:1:1152:SER:HB3	2.17	0.42
35:1:1294:THR:O	42:5:76:CYS:CA	2.65	0.42
36:3:611:ASP:O	36:3:612:ASN:HB2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:804:HIS:O	42:5:58:ASN:ND2	2.52	0.42
29:h:71:LYS:HA	29:h:95:TYR:HA	2.01	0.42
1:A:382:GLU:N	1:A:382:GLU:OE1	2.52	0.42
1:A:1076:ASP:OD1	1:A:1076:ASP:N	2.52	0.42
1:A:1555:LEU:HD22	1:A:1555:LEU:HA	1.71	0.42
1:A:1673:SER:O	1:A:1673:SER:OG	2.36	0.42
1:A:1756:SER:HA	35:1:943:LYS:HB3	2.01	0.42
1:A:1935:ARG:HE	1:A:1980:GLU:CD	2.24	0.42
3:C:89:LEU:HD12	19:T:240:LEU:HD11	2.01	0.42
3:C:193:THR:HB	3:C:428:THR:HG21	2.01	0.42
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.42
3:C:933:PHE:O	3:C:937:THR:HG22	2.18	0.42
5:F:35:A:H2	5:F:36:A:N6	2.16	0.42
5:F:42:C:H3'	5:F:43:A:C8	2.54	0.42
6:G:90:C:N4	7:H:40:C:H42	2.16	0.42
12:M:220:LYS:HA	12:M:223:GLU:CD	2.44	0.42
13:N:54:HIS:O	13:N:55:GLN:C	2.62	0.42
17:R:367:ARG:HD2	17:R:368:ASN:N	2.35	0.42
19:T:394:ASN:ND2	19:T:408:ASN:HD22	2.17	0.42
23:X:419:ILE:HG21	23:X:569:VAL:HG22	2.01	0.42
24:Y:207:GLU:HA	24:Y:210:GLU:HB3	2.01	0.42
35:1:815:PHE:HA	35:1:819:TRP:HD1	1.83	0.42
35:1:903:GLN:OE1	35:1:910:MET:HB2	2.19	0.42
35:1:963:LYS:HG3	35:1:964:THR:N	2.33	0.42
35:1:1199:VAL:HG12	35:1:1199:VAL:O	2.19	0.42
35:1:1227:ILE:O	35:1:1231:MET:HG2	2.19	0.42
36:3:77:TYR:HE2	36:3:152:LEU:HD22	1.84	0.42
36:3:115:ILE:HD11	42:5:18:TYR:HA	2.02	0.42
36:3:483:LEU:HD11	36:3:493:GLU:OE2	2.19	0.42
36:3:499:PHE:CZ	36:3:516:LEU:HD22	2.46	0.42
36:3:514:ASP:OD1	36:3:514:ASP:N	2.52	0.42
36:3:1028:THR:O	39:2:496:ASN:ND2	2.52	0.42
36:3:1158:ARG:HG3	36:3:1159:ASP:N	2.34	0.42
36:3:1175:ASP:OD1	36:3:1178:LEU:N	2.52	0.42
42:5:12:GLU:HA	42:5:15:GLN:HB3	2.01	0.42
1:A:57:GLN:O	1:A:57:GLN:NE2	2.52	0.42
1:A:758:ARG:NH2	1:A:775:ASN:HD22	2.15	0.42
3:C:505:GLN:HG3	3:C:507:VAL:HG13	2.00	0.42
3:C:665:THR:OG1	3:C:666:VAL:N	2.52	0.42
4:E:192:ASN:CG	4:E:193:THR:H	2.28	0.42
4:E:218:LYS:HE2	4:E:218:LYS:HB2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:A:C5	6:G:11:A:N1	2.87	0.42
5:F:73:A:OP1	5:F:75:G:O2'	2.32	0.42
9:J:183:ALA:O	11:L:142:ILE:HG12	2.19	0.42
11:L:131:ASN:O	11:L:135:LYS:NZ	2.53	0.42
13:N:75:TYR:CZ	13:N:79:ILE:HD11	2.54	0.42
19:T:351:ASP:OD1	19:T:351:ASP:N	2.37	0.42
21:V:474:HIS:ND1	21:V:474:HIS:C	2.77	0.42
21:V:590:LEU:HB3	21:V:599:LEU:HD22	2.00	0.42
23:X:277:ARG:O	23:X:281:ARG:HG2	2.20	0.42
23:X:431:GLN:HA	23:X:434:GLN:NE2	2.35	0.42
23:X:658:ARG:HE	23:X:658:ARG:HB3	1.73	0.42
23:X:839:GLU:H	23:X:839:GLU:CD	2.27	0.42
24:Y:260:PHE:C	24:Y:266:ILE:HD11	2.44	0.42
35:1:501:LEU:HD23	35:1:501:LEU:HA	1.72	0.42
35:1:823:MET:SD	35:1:829:ASN:ND2	2.92	0.42
35:1:857:LEU:HD13	35:1:895:GLY:C	2.44	0.42
35:1:974:LEU:HG	35:1:974:LEU:H	1.46	0.42
35:1:1101:LEU:HD23	35:1:1101:LEU:HA	1.92	0.42
35:1:1165:TYR:CD1	39:2:575:PHE:HD1	2.34	0.42
36:3:83:ASP:OD1	36:3:83:ASP:C	2.62	0.42
36:3:182:PHE:O	36:3:210:PHE:HA	2.19	0.42
36:3:484:VAL:O	36:3:494:VAL:HB	2.20	0.42
36:3:582:GLU:H	36:3:582:GLU:CD	2.27	0.42
39:2:456:ARG:HE	39:2:456:ARG:HB3	1.79	0.42
1:A:299:ILE:HD12	3:C:920:PRO:HB2	2.01	0.42
1:A:364:SER:O	1:A:366:LYS:HD3	2.19	0.42
1:A:693:ILE:C	1:A:695:ASP:N	2.76	0.42
2:B:46:U:C2'	2:B:47:A:H5'	2.49	0.42
3:C:80:ILE:HG22	3:C:82:GLN:HG2	2.01	0.42
3:C:603:MET:O	3:C:607:LEU:HD12	2.18	0.42
3:C:668:GLU:O	3:C:824:THR:OG1	2.37	0.42
3:C:763:LYS:O	3:C:767:VAL:HG22	2.20	0.42
4:E:299:LYS:HE2	4:E:299:LYS:HB2	1.79	0.42
5:F:36:A:H5''	5:F:37:C:OP2	2.20	0.42
5:F:92:A:H2'	5:F:93:G:C8	2.54	0.42
7:H:44:U:OP2	7:H:44:U:H6	2.02	0.42
8:I:177:PRO:HB3	8:I:211:SER:HA	2.01	0.42
23:X:192:ARG:HG2	23:X:192:ARG:NH1	2.30	0.42
23:X:218:ASP:O	23:X:222:MET:HG2	2.19	0.42
23:X:823:MET:HE3	23:X:946:GLY:O	2.19	0.42
23:X:862:VAL:HG13	23:X:863:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:267:ARG:HB3	24:Y:287:GLU:HG2	2.02	0.42
35:1:936:VAL:HG12	35:1:937:LEU:HD12	2.01	0.42
35:1:1012:PRO:C	35:1:1014:LYS:H	2.27	0.42
35:1:1087:ALA:HB3	35:1:1088:ILE:HD12	2.01	0.42
36:3:206:GLN:HE22	36:3:232:GLY:H	1.66	0.42
36:3:423:LEU:HB2	36:3:438:LEU:HB2	2.02	0.42
36:3:462:VAL:HG11	36:3:516:LEU:HD23	2.00	0.42
36:3:576:GLU:OE1	36:3:580:ARG:NH2	2.52	0.42
36:3:947:GLU:HG3	36:3:948:VAL:H	1.84	0.42
36:3:1015:LYS:HD2	36:3:1015:LYS:HA	1.79	0.42
38:w:445:HIS:CD2	38:w:445:HIS:H	2.37	0.42
1:A:251:ASP:HB3	1:A:337:VAL:HG13	2.01	0.42
1:A:808:ALA:HB1	15:P:193:VAL:HG11	2.01	0.42
1:A:856:LEU:H	1:A:856:LEU:HG	1.36	0.42
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	2.00	0.42
1:A:1436:TRP:CZ3	1:A:1457:HIS:HB2	2.54	0.42
1:A:1826:VAL:HB	1:A:1830:GLN:HE22	1.85	0.42
3:C:602:LYS:HE2	3:C:602:LYS:HB3	1.84	0.42
3:C:762:VAL:HG23	3:C:808:ILE:HD12	2.02	0.42
4:E:74:PHE:CZ	4:E:343:ILE:HG13	2.55	0.42
4:E:287:ASN:ND2	4:E:331:ASN:OD1	2.52	0.42
4:E:313:ASP:OD1	4:E:316:SER:OG	2.32	0.42
6:G:1:G:C8	6:G:2:U:H4'	2.55	0.42
11:L:205:LYS:H	11:L:205:LYS:CD	2.33	0.42
12:M:186:LEU:HA	12:M:186:LEU:HD22	1.82	0.42
13:N:37:HIS:O	13:N:37:HIS:CG	2.72	0.42
17:R:163:MET:C	17:R:165:VAL:N	2.77	0.42
19:T:309:ASP:O	19:T:310:SER:OG	2.26	0.42
21:V:584:LYS:HE2	21:V:584:LYS:HB2	1.92	0.42
23:X:787:GLU:O	23:X:790:LEU:HB3	2.19	0.42
23:X:814:LYS:NZ	23:X:814:LYS:HB2	2.34	0.42
23:X:898:CYS:HB3	23:X:903:VAL:O	2.19	0.42
24:Y:35:LYS:NZ	24:Y:159:THR:O	2.50	0.42
24:Y:224:LEU:CD1	24:Y:230:LEU:HD23	2.50	0.42
34:q:60:PRO:CB	34:s:94:GLN:CA	2.97	0.42
35:1:609:MET:HE1	35:1:635:VAL:CG1	2.49	0.42
35:1:981:TYR:C	35:1:983:GLY:H	2.27	0.42
35:1:1090:PRO:CA	35:1:1093:VAL:HG12	2.43	0.42
36:3:577:TYR:HE2	36:3:579:GLU:HB3	1.85	0.42
36:3:675:LEU:HB3	36:3:686:LEU:HD12	2.02	0.42
36:3:996:ILE:O	36:3:998:HIS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:19:THR:HA	33:I:29:ARG:HA	2.02	0.42
1:A:110:TRP:O	1:A:192:GLN:NE2	2.53	0.42
1:A:278:LYS:NZ	6:G:-8:C:P	2.93	0.42
1:A:1352:HIS:CD2	20:U:5:ILE:HG12	2.55	0.42
1:A:1397:ILE:CG1	17:R:405:VAL:HG22	2.50	0.42
3:C:299:ILE:HD13	3:C:299:ILE:HA	1.79	0.42
3:C:522:SER:O	3:C:522:SER:OG	2.36	0.42
3:C:809:ILE:CG1	3:C:810:PRO:HD3	2.49	0.42
3:C:809:ILE:H	3:C:809:ILE:HG12	1.46	0.42
3:C:810:PRO:HA	3:C:813:ARG:HG2	2.01	0.42
4:E:162:ARG:HE	4:E:162:ARG:HB2	1.52	0.42
4:E:208:ILE:HA	4:E:208:ILE:HD12	1.81	0.42
9:J:268:ALA:HB1	9:J:278:LEU:HD21	2.01	0.42
11:L:721:LEU:O	11:L:725:GLN:N	2.39	0.42
17:R:330:LYS:HZ1	23:X:275:ARG:NH2	2.17	0.42
17:R:356:ARG:O	17:R:360:ARG:HB2	2.19	0.42
21:V:646:HIS:ND1	21:V:646:HIS:C	2.77	0.42
35:1:753:LEU:HD23	35:1:753:LEU:HA	1.81	0.42
36:3:58:VAL:HG21	36:3:62:ILE:CD1	2.49	0.42
36:3:212:GLU:CB	36:3:223:LYS:HG3	2.49	0.42
36:3:630:MET:HE2	36:3:630:MET:HB2	1.48	0.42
39:2:526:ASP:HA	39:2:529:LYS:NZ	2.34	0.42
39:2:547:LYS:NZ	39:2:555:GLU:HG2	2.35	0.42
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.84	0.42
1:A:1217:GLN:OE1	1:A:1224:ARG:NE	2.52	0.42
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.55	0.42
1:A:1640:SER:HB3	1:A:1652:MET:HA	2.01	0.42
8:I:512:ASP:O	8:I:514:ARG:N	2.52	0.42
9:J:238:ASN:O	9:J:239:ARG:HB3	2.20	0.42
9:J:256:LYS:HG3	11:L:235:LEU:HD23	2.01	0.42
12:M:208:ILE:O	12:M:208:ILE:HG22	2.20	0.42
15:P:73:GLU:HG2	15:P:76:ARG:NH2	2.34	0.42
17:R:352:ARG:HG2	17:R:356:ARG:NH2	2.35	0.42
21:V:452:LEU:HD11	21:V:456:ARG:CZ	2.49	0.42
21:V:487:LYS:H	21:V:487:LYS:HD3	1.85	0.42
23:X:450:CYS:O	23:X:495:TYR:HA	2.20	0.42
23:X:595:CYS:O	23:X:599:VAL:HG22	2.20	0.42
23:X:1004:GLU:HB2	23:X:1007:TRP:CD2	2.55	0.42
24:Y:30:LYS:O	24:Y:34:ILE:HG23	2.19	0.42
24:Y:31:LEU:HD11	24:Y:66:ILE:N	2.35	0.42
24:Y:147:ASP:OD2	24:Y:147:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:721:ILE:C	35:1:723:SER:H	2.28	0.42
35:1:1029:GLU:H	35:1:1029:GLU:HG3	1.73	0.42
36:3:724:SER:HB2	36:3:727:SER:HA	2.01	0.42
36:3:789:VAL:HG13	36:3:891:VAL:HG13	2.01	0.42
36:3:1199:ARG:HH21	36:3:1207:LYS:NZ	2.18	0.42
42:5:61:LYS:HB3	42:5:65:ARG:HH22	1.83	0.42
42:5:69:MET:HE2	42:5:69:MET:HB2	1.52	0.42
1:A:525:LYS:HB2	1:A:525:LYS:NZ	2.34	0.42
1:A:1838:LYS:HE2	1:A:1868:MET:HE2	2.01	0.42
3:C:243:ILE:HG13	3:C:244:LYS:N	2.33	0.42
3:C:440:SER:O	3:C:442:LYS:N	2.52	0.42
3:C:736:GLY:HA2	3:C:771:GLN:HG2	2.02	0.42
3:C:907:VAL:HA	3:C:908:PRO:HD3	1.84	0.42
4:E:329:SER:C	4:E:346:SER:HG	2.21	0.42
9:J:189:ILE:HA	9:J:193:GLN:OE1	2.20	0.42
9:J:278:LEU:HD12	9:J:278:LEU:HA	1.69	0.42
9:J:299:TRP:O	9:J:303:ILE:HG23	2.19	0.42
24:Y:24:ALA:HA	24:Y:78:PHE:CZ	2.53	0.42
35:1:876:MET:HE1	35:1:917:VAL:HG23	2.01	0.42
36:3:311:PHE:HZ	36:3:387:PHE:CE2	2.38	0.42
36:3:690:ARG:HH12	36:3:696:SER:H	1.67	0.42
36:3:791:HIS:CB	36:3:796:ASN:O	2.68	0.42
37:p:183:VAL:HA	37:p:184:PRO:HD3	1.90	0.42
39:2:465:LEU:HB3	39:2:475:VAL:HG11	2.01	0.42
39:2:550:LYS:HG2	39:2:554:ARG:HH21	1.84	0.42
43:o:92:GLU:HA	43:o:117:TYR:O	2.19	0.42
1:A:68:LYS:NZ	13:N:45:SER:O	2.53	0.42
1:A:271:MET:HB2	1:A:271:MET:HE3	1.58	0.42
1:A:1489:LEU:HD12	1:A:1489:LEU:HA	1.77	0.42
1:A:1857:GLN:HE21	1:A:1857:GLN:HB2	1.53	0.42
3:C:381:LEU:CD2	3:C:416:LEU:HD21	2.49	0.42
4:E:179:TRP:HA	4:E:187:ILE:HG12	2.02	0.42
5:F:45:A:N6	6:G:3:A:C8	2.88	0.42
7:H:63:G:N1	7:H:64:A:N6	2.67	0.42
7:H:182:U:H2'	7:H:183:G:H8	1.85	0.42
8:I:213:ALA:HA	8:I:216:SER:O	2.20	0.42
11:L:633:GLN:O	11:L:637:VAL:N	2.50	0.42
13:N:2:PRO:O	13:N:4:VAL:N	2.53	0.42
17:R:91:ASP:CG	17:R:93:GLU:H	2.27	0.42
17:R:352:ARG:HG2	17:R:356:ARG:HH21	1.85	0.42
19:T:423:SER:HB3	19:T:474:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:506:PHE:CD1	21:V:506:PHE:C	2.98	0.42
21:V:600:ASN:OD1	21:V:639:LEU:HB2	2.20	0.42
21:V:617:PRO:HB2	21:V:624:THR:OG1	2.19	0.42
23:X:406:GLU:HA	23:X:409:LEU:CD2	2.48	0.42
23:X:692:PRO:HA	23:X:737:LEU:HB2	2.02	0.42
23:X:698:LYS:HZ1	23:X:758:THR:HA	1.84	0.42
23:X:832:GLU:HG2	23:X:927:VAL:HG22	2.02	0.42
23:X:887:GLN:O	23:X:890:GLU:HB3	2.19	0.42
35:1:664:GLY:O	35:1:668:VAL:HG23	2.20	0.42
36:3:43:PRO:HA	36:3:50:VAL:HA	2.01	0.42
36:3:275:ARG:HB3	36:3:386:PHE:HB3	2.02	0.42
36:3:701:LEU:C	36:3:702:PHE:CG	2.98	0.42
38:w:471:TRP:CZ3	38:w:476:GLU:HB2	2.55	0.42
39:2:461:THR:HG1	39:2:464:GLU:H	1.60	0.42
41:7:58:CYS:N	41:7:63:GLY:O	2.52	0.42
42:5:11:LEU:O	42:5:14:LEU:HB2	2.19	0.42
1:A:47:GLU:OE1	1:A:47:GLU:N	2.52	0.42
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.55	0.42
1:A:1755:SER:OG	35:1:938:TRP:CZ2	2.67	0.42
44:A:3000:IHP:O12	44:A:3000:IHP:P1	2.78	0.42
2:B:116:U:OP2	31:e:68:THR:CA	2.67	0.42
4:E:174:GLY:HA2	4:E:194:TYR:C	2.45	0.42
4:E:308:PHE:N	4:E:330:ILE:HD11	2.35	0.42
5:F:86:U:O2'	5:F:87:C:O5'	2.36	0.42
5:F:92:A:H2'	5:F:93:G:H8	1.85	0.42
6:G:83:A:H61	38:w:400:HIS:CE1	2.38	0.42
6:G:86:A:H2	7:H:44:U:O2	2.02	0.42
11:L:177:GLU:HA	11:L:180:ARG:CD	2.50	0.42
12:M:160:PHE:O	12:M:162:PRO:HD3	2.19	0.42
17:R:352:ARG:HA	17:R:355:ILE:HD12	2.02	0.42
18:S:150:GLN:C	18:S:152:ARG:H	2.28	0.42
24:Y:41:LEU:HD23	24:Y:155:ARG:HH12	1.85	0.42
24:Y:204:SER:OG	24:Y:207:GLU:HG2	2.20	0.42
24:Y:292:GLU:HA	24:Y:295:GLU:CD	2.45	0.42
35:1:630:ARG:O	35:1:634:VAL:HG23	2.19	0.42
35:1:807:LYS:HD3	35:1:848:GLU:HG3	2.02	0.42
35:1:1249:TYR:HE2	39:2:587:HIS:CE1	2.38	0.42
36:3:1:MET:HG3	36:3:1092:ILE:HD12	2.02	0.42
36:3:70:LEU:HA	36:3:70:LEU:HD23	1.78	0.42
36:3:896:PHE:H	36:3:896:PHE:HD2	1.68	0.42
36:3:1200:THR:N	36:3:1203:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:456:ARG:HA	39:2:459:ARG:HB2	2.02	0.42
32:k:33:GLY:O	32:k:41:VAL:N	2.49	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.82	0.41
1:A:296:PHE:HZ	3:C:593:GLU:HB2	1.85	0.41
1:A:569:VAL:O	1:A:570:ASP:HB2	2.19	0.41
1:A:599:MET:HA	1:A:602:ILE:HB	2.01	0.41
1:A:1604:LEU:HB3	1:A:1606:ILE:CD1	2.50	0.41
1:A:1885:LYS:HG2	1:A:1886:GLY:N	2.35	0.41
3:C:121:ASP:OD1	3:C:122:LEU:N	2.53	0.41
3:C:137:HIS:CE1	3:C:236:MET:HE2	2.55	0.41
3:C:420:CYS:O	3:C:424:PHE:HB2	2.20	0.41
3:C:662:PHE:HE1	3:C:829:GLU:HB3	1.84	0.41
5:F:10:U:H2'	5:F:11:C:C4'	2.50	0.41
6:G:117:A:C2'	24:Y:246:LYS:HE2	2.49	0.41
7:H:41:U:C2	7:H:42:G:C8	3.08	0.41
8:I:374:ILE:O	8:I:376:ASN:N	2.52	0.41
19:T:331:ASN:O	19:T:332:ALA:C	2.63	0.41
24:Y:317:GLN:NE2	24:Y:317:GLN:HA	2.35	0.41
35:1:608:THR:O	35:1:611:SER:HB3	2.20	0.41
35:1:620:MET:HE3	35:1:620:MET:HB3	1.90	0.41
35:1:902:GLU:O	35:1:903:GLN:C	2.62	0.41
36:3:436:ARG:HG2	36:3:778:ALA:CB	2.49	0.41
36:3:610:VAL:HA	36:3:636:GLN:HE21	1.85	0.41
37:p:159:PRO:HB2	37:p:162:THR:H	1.85	0.41
37:p:194:PHE:CB	37:p:200:ALA:HB2	2.50	0.41
38:w:408:CYS:SG	38:w:425:HIS:NE2	2.77	0.41
39:2:572:HIS:O	39:2:576:PHE:HB2	2.20	0.41
1:A:79:ARG:HG2	1:A:82:ARG:HG3	2.02	0.41
1:A:857:ASN:OD1	1:A:859:SER:N	2.53	0.41
1:A:1385:VAL:HG12	1:A:1419:ILE:HD11	2.01	0.41
1:A:1633:ALA:HB3	1:A:1658:GLN:HA	2.02	0.41
3:C:174:GLU:OE1	3:C:182:LYS:NZ	2.52	0.41
3:C:529:ARG:HH12	3:C:540:GLU:HG3	1.86	0.41
3:C:801:LEU:HD13	3:C:802:HIS:CE1	2.56	0.41
3:C:940:ARG:H	3:C:940:ARG:HG2	1.71	0.41
4:E:290:ARG:HG3	4:E:331:ASN:O	2.20	0.41
12:M:153:ARG:HA	12:M:160:PHE:CE2	2.55	0.41
13:N:41:ARG:HB3	13:N:44:GLU:HG2	2.02	0.41
14:O:34:ILE:O	17:R:197:ILE:HD12	2.18	0.41
17:R:348:GLU:CD	23:X:263:SER:HB3	2.45	0.41
17:R:387:ASP:OD1	17:R:388:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:344:GLN:C	19:T:345:ILE:HG13	2.45	0.41
21:V:612:PHE:O	21:V:616:LEU:HG	2.20	0.41
21:V:630:PHE:HD1	21:V:631:PHE:HD2	1.68	0.41
23:X:587:PRO:HB2	35:1:827:ARG:HH22	1.85	0.41
23:X:932:CYS:HB2	23:X:938:ARG:HD2	2.02	0.41
35:1:551:LEU:O	35:1:554:LYS:HB3	2.19	0.41
35:1:556:ILE:O	35:1:560:LEU:HB2	2.21	0.41
35:1:564:ASP:HB2	35:1:603:ALA:HB1	1.80	0.41
35:1:613:MET:HB3	35:1:632:PHE:HE2	1.80	0.41
35:1:632:PHE:HA	35:1:635:VAL:HG22	2.01	0.41
35:1:769:VAL:O	35:1:772:ILE:HB	2.21	0.41
35:1:858:LYS:HB3	35:1:858:LYS:HE2	1.67	0.41
35:1:1028:HIS:HB3	35:1:1031:VAL:HG13	2.02	0.41
35:1:1130:PRO:HB3	39:2:528:ILE:CG2	2.46	0.41
36:3:25:THR:HG1	36:3:27:GLN:N	2.18	0.41
36:3:91:GLU:OE1	36:3:102:ILE:HD11	2.20	0.41
36:3:715:MET:HE3	36:3:739:LEU:H	1.86	0.41
38:w:429:TRP:O	38:w:430:ARG:C	2.62	0.41
33:l:13:ALA:HA	33:l:74:PRO:HD2	2.03	0.41
1:A:1019:TYR:O	1:A:1021:ASP:N	2.53	0.41
1:A:1122:ASN:OD1	1:A:1122:ASN:N	2.53	0.41
1:A:1381:ASP:CG	1:A:1414:ARG:HE	2.28	0.41
1:A:1684:PHE:HB2	1:A:1702:LEU:HD11	2.03	0.41
1:A:1802:PRO:HB3	1:A:1827:TRP:CZ3	2.55	0.41
44:A:3000:IHP:P3	44:A:3000:IHP:O24	2.79	0.41
2:B:9:G:H2'	2:B:10:U:C6	2.55	0.41
3:C:493:PHE:CD2	3:C:551:LEU:HG	2.50	0.41
3:C:696:LEU:O	3:C:700:ILE:HG12	2.20	0.41
3:C:833:PHE:O	3:C:899:SER:HA	2.20	0.41
3:C:846:VAL:HB	3:C:887:LEU:HD11	2.02	0.41
4:E:145:LYS:NZ	4:E:181:ILE:O	2.44	0.41
4:E:266:PRO:HG3	11:L:789:ALA:HA	2.01	0.41
6:G:18:A:C2	14:O:196:GLN:O	2.73	0.41
9:J:400:GLU:OE2	9:J:401:ARG:HG3	2.20	0.41
11:L:138:ARG:HA	11:L:139:PRO:HD3	1.96	0.41
11:L:169:ARG:HH21	11:L:169:ARG:HG3	1.85	0.41
23:X:535:LEU:HA	23:X:535:LEU:HD23	1.78	0.41
23:X:610:ASP:HB2	23:X:686:ILE:HA	2.01	0.41
24:Y:41:LEU:HD23	24:Y:155:ARG:NH1	2.34	0.41
24:Y:241:VAL:O	24:Y:316:SER:HB3	2.20	0.41
35:1:527:GLY:HA2	35:1:566:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:609:MET:HE2	35:1:609:MET:HB3	1.51	0.41
35:1:729:LYS:O	35:1:733:LYS:HG2	2.21	0.41
35:1:1055:TRP:HA	35:1:1055:TRP:CE3	2.55	0.41
35:1:1109:ARG:O	35:1:1112:THR:HG23	2.20	0.41
36:3:898:ASN:OD1	36:3:899:THR:N	2.52	0.41
36:3:914:ILE:HG22	36:3:917:PRO:HD2	2.02	0.41
32:k:42:ILE:O	32:k:60:VAL:N	2.48	0.41
28:n:62:GLY:O	28:n:65:ILE:N	2.54	0.41
1:A:796:LYS:HB3	1:A:796:LYS:HE3	1.80	0.41
1:A:1638:ASN:HA	1:A:1655:THR:O	2.20	0.41
1:A:1730:MET:HE2	1:A:1730:MET:HA	2.02	0.41
1:A:1776:ILE:HG23	1:A:1859:LYS:HG3	2.02	0.41
3:C:183:SER:HG	3:C:480:LYS:HZ1	1.60	0.41
3:C:436:GLN:C	3:C:437:HIS:HD2	2.29	0.41
4:E:251:LEU:HB2	4:E:293:TRP:NE1	2.34	0.41
4:E:313:ASP:HB3	4:E:320:LEU:HD11	2.02	0.41
4:E:321:TYR:HB3	4:E:323:LEU:HG	2.02	0.41
5:F:23:U:C4	13:N:118:ILE:HD13	2.55	0.41
7:H:55:U:H2'	7:H:57:A:OP2	2.21	0.41
9:J:189:ILE:HG21	11:L:152:LEU:HD22	2.02	0.41
11:L:169:ARG:HH21	11:L:169:ARG:CG	2.34	0.41
15:P:212:ASN:O	15:P:212:ASN:CG	2.63	0.41
21:V:458:THR:HG21	21:V:479:MET:HE1	2.03	0.41
23:X:169:ARG:O	23:X:173:GLN:HG3	2.20	0.41
24:Y:18:THR:HB	24:Y:166:PHE:CE2	2.55	0.41
35:1:646:PRO:O	35:1:649:LYS:HB2	2.20	0.41
35:1:802:GLU:HG2	35:1:805:TYR:HB2	2.02	0.41
36:3:199:GLU:OE2	36:3:199:GLU:HA	2.19	0.41
36:3:289:CYS:SG	36:3:290:SER:N	2.93	0.41
36:3:1015:LYS:NZ	36:3:1016:ARG:H	2.18	0.41
36:3:1022:ILE:HA	36:3:1022:ILE:HD13	1.77	0.41
38:w:407:ASN:O	38:w:407:ASN:ND2	2.54	0.41
38:w:414:TYR:HD1	38:w:416:TYR:CE1	2.38	0.41
38:w:453:GLU:OE1	38:w:454:ASP:N	2.44	0.41
39:2:451:LYS:HA	39:2:454:LEU:HD23	2.02	0.41
39:2:459:ARG:HD2	39:2:481:THR:HA	2.03	0.41
32:k:6:PRO:HA	32:k:7:PRO:HD3	1.90	0.41
1:A:300:ASN:OD1	1:A:300:ASN:N	2.45	0.41
1:A:379:GLU:HA	3:C:354:ARG:O	2.21	0.41
1:A:623:LYS:O	44:A:3000:IHP:O44	2.39	0.41
1:A:939:TRP:CD1	1:A:939:TRP:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:TRP:CD1	23:X:337:ALA:HB1	2.55	0.41
1:A:1847:ALA:O	1:A:1850:ARG:HB3	2.21	0.41
1:A:1978:LYS:HA	1:A:1978:LYS:HE3	2.03	0.41
3:C:286:ASN:ND2	3:C:299:ILE:HG23	2.35	0.41
3:C:759:LEU:HA	3:C:759:LEU:HD12	1.83	0.41
6:G:97:A:C6	35:1:1075:ARG:HG2	2.54	0.41
6:G:104:C:O2	6:G:104:C:C2'	2.68	0.41
7:H:34:U:H2'	7:H:35:A:C1'	2.51	0.41
9:J:344:GLN:H	9:J:344:GLN:CD	2.25	0.41
17:R:265:ASP:OD1	17:R:265:ASP:N	2.52	0.41
17:R:377:ARG:HG2	17:R:377:ARG:NH2	2.35	0.41
19:T:257:ARG:HH21	19:T:301:ASP:CG	2.29	0.41
19:T:423:SER:N	19:T:474:GLU:OE2	2.52	0.41
23:X:411:ALA:HA	23:X:414:ASN:ND2	2.36	0.41
23:X:969:PHE:CD2	23:X:994:LYS:HG2	2.55	0.41
35:1:500:LEU:C	35:1:502:LEU:N	2.76	0.41
35:1:621:ASP:CG	35:1:623:TYR:HB3	2.45	0.41
35:1:694:LEU:CD1	35:1:727:VAL:HG21	2.44	0.41
35:1:699:GLN:HE22	35:1:738:HIS:HE1	1.60	0.41
35:1:862:GLU:O	35:1:866:LYS:HB2	2.21	0.41
35:1:912:ASN:OD1	35:1:912:ASN:N	2.53	0.41
35:1:1133:MET:HE1	39:2:525:PRO:CD	2.50	0.41
36:3:497:SER:OG	36:3:499:PHE:HB2	2.21	0.41
36:3:671:ASN:HA	36:3:696:SER:C	2.44	0.41
36:3:1004:ASP:OD2	36:3:1007:GLU:HB2	2.21	0.41
36:3:1040:ASP:OD2	36:3:1040:ASP:C	2.63	0.41
38:w:413:ASN:HD22	38:w:413:ASN:HA	1.61	0.41
39:2:536:MET:HE2	39:2:536:MET:HB3	1.76	0.41
27:m:42:LEU:O	27:m:69:LEU:HA	2.21	0.41
1:A:329:LEU:HB2	3:C:177:ARG:NH2	2.36	0.41
1:A:456:LEU:HD22	1:A:460:LYS:NZ	2.35	0.41
1:A:599:MET:HE3	1:A:599:MET:HB3	1.82	0.41
1:A:1389:TYR:CD2	1:A:1389:TYR:C	2.97	0.41
1:A:1636:LYS:HE3	1:A:1656:THR:HG23	2.01	0.41
3:C:828:MET:HG2	3:C:906:ILE:HD13	2.03	0.41
7:H:31:G:N3	7:H:31:G:C2'	2.83	0.41
9:J:323:LEU:HA	9:J:323:LEU:HD23	1.77	0.41
11:L:130:PRO:HB2	11:L:131:ASN:H	1.62	0.41
21:V:469:PHE:CZ	21:V:509:LEU:HD22	2.55	0.41
21:V:476:LEU:O	21:V:479:MET:HB2	2.21	0.41
23:X:234:TYR:CD1	24:Y:317:GLN:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:910:ARG:HA	23:X:913:ASP:OD2	2.20	0.41
35:1:504:ILE:HG13	35:1:515:ALA:HB3	2.03	0.41
35:1:682:HIS:C	35:1:684:ARG:H	2.29	0.41
35:1:806:ILE:HD12	35:1:843:LYS:HE3	1.99	0.41
36:3:164:ASN:N	36:3:164:ASN:OD1	2.53	0.41
36:3:299:PHE:CD1	36:3:299:PHE:C	2.99	0.41
38:w:400:HIS:HB3	38:w:402:LEU:HD22	2.02	0.41
39:2:510:TYR:O	39:2:511:LEU:HD23	2.20	0.41
39:2:667:ALA:HB2	40:4:110:GLU:CB	2.50	0.41
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.90	0.41
1:A:1130:ASN:HD21	1:A:1140:MET:CB	2.33	0.41
1:A:1457:HIS:O	1:A:1461:ASP:HB2	2.20	0.41
1:A:1482:GLU:N	1:A:1482:GLU:OE2	2.54	0.41
3:C:95:LYS:HA	3:C:96:PRO:HD3	1.90	0.41
3:C:353:THR:HG23	3:C:355:LYS:H	1.84	0.41
3:C:736:GLY:O	3:C:738:ASP:N	2.53	0.41
4:E:81:LEU:O	4:E:92:LEU:HA	2.21	0.41
7:H:28:C:O2'	7:H:29:A:C4	2.69	0.41
13:N:55:GLN:HE21	13:N:55:GLN:HB2	1.75	0.41
17:R:159:VAL:O	17:R:162:ALA:N	2.54	0.41
17:R:355:ILE:HD11	23:X:266:GLU:CD	2.45	0.41
21:V:603:LEU:HA	21:V:603:LEU:HD12	1.78	0.41
21:V:650:THR:HB	21:V:651:PRO:HD3	2.03	0.41
23:X:483:PHE:HB2	23:X:484:GLU:OE1	2.20	0.41
23:X:955:THR:OG1	23:X:958:GLY:O	2.24	0.41
23:X:981:PRO:HD2	23:X:984:LEU:HD13	2.02	0.41
35:1:625:ARG:HB3	35:1:666:LYS:CE	2.49	0.41
35:1:867:MET:HE2	35:1:867:MET:HB3	1.82	0.41
36:3:438:LEU:HD23	36:3:438:LEU:HA	1.72	0.41
36:3:610:VAL:HG23	36:3:636:GLN:NE2	2.36	0.41
36:3:855:PRO:O	36:3:856:LYS:HD3	2.20	0.41
42:5:74:GLN:NE2	42:5:78:PRO:HA	2.36	0.41
30:i:23:LEU:N	30:i:27:MET:O	2.42	0.41
1:A:228:TRP:CD1	1:A:228:TRP:H	2.37	0.41
1:A:385:GLU:O	3:C:327:TYR:OH	2.32	0.41
1:A:615:ARG:HE	1:A:615:ARG:HB2	1.69	0.41
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.51	0.41
1:A:1454:TRP:CD1	1:A:1454:TRP:H	2.39	0.41
1:A:2002:LEU:HD22	1:A:2006:GLU:OE1	2.21	0.41
3:C:363:SER:O	3:C:364:SER:OG	2.28	0.41
6:G:90:C:H4'	9:J:181:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7:U:H2'	7:H:8:C:H6	1.82	0.41
8:I:626:ALA:C	8:I:628:GLN:H	2.29	0.41
11:L:26:TYR:CE1	11:L:33:ARG:HB3	2.56	0.41
15:P:188:TRP:O	15:P:188:TRP:CG	2.70	0.41
17:R:114:SER:HB3	17:R:228:PRO:HG2	2.02	0.41
17:R:213:LYS:NZ	17:R:215:ASN:OD1	2.48	0.41
17:R:325:ARG:HH12	17:R:329:GLN:N	2.18	0.41
19:T:223:SER:OG	19:T:224:ALA:N	2.52	0.41
19:T:306:CYS:HB2	19:T:333:VAL:HG12	2.02	0.41
21:V:617:PRO:HB3	21:V:623:ASN:HD22	1.86	0.41
23:X:173:GLN:HA	23:X:176:GLU:OE2	2.21	0.41
23:X:246:LEU:HG	23:X:277:ARG:CZ	2.51	0.41
23:X:533:PHE:HE1	23:X:550:VAL:HG11	1.86	0.41
23:X:614:PHE:O	23:X:615:LEU:HD12	2.21	0.41
23:X:645:LEU:HB3	23:X:659:ILE:HG22	2.02	0.41
23:X:790:LEU:HD23	23:X:791:LEU:N	2.35	0.41
24:Y:2:ALA:O	24:Y:162:LEU:HB3	2.20	0.41
24:Y:212:LYS:HA	24:Y:212:LYS:HD2	1.80	0.41
35:1:699:GLN:NE2	35:1:738:HIS:HE1	2.17	0.41
35:1:816:LYS:HB3	35:1:816:LYS:HE3	1.82	0.41
35:1:841:ALA:O	35:1:845:GLY:N	2.50	0.41
35:1:1251:LEU:HA	35:1:1251:LEU:HD23	1.68	0.41
36:3:615:ARG:O	36:3:616:ILE:HD12	2.21	0.41
36:3:637:PRO:HB3	36:3:640:LEU:HD21	2.03	0.41
38:w:411:CYS:O	38:w:414:TYR:HB2	2.21	0.41
39:2:506:PHE:N	39:2:506:PHE:CD1	2.88	0.41
1:A:62:PRO:HB2	1:A:64:GLU:OE1	2.20	0.41
1:A:65:HIS:CD2	13:N:46:LEU:HD13	2.56	0.41
1:A:131:GLU:HG2	1:A:132:ILE:N	2.35	0.41
1:A:519:ASP:OD2	1:A:523:ASN:HB2	2.20	0.41
1:A:631:ALA:O	1:A:635:ARG:HG3	2.21	0.41
1:A:799:PRO:HD3	17:R:284:PHE:CE1	2.56	0.41
1:A:1194:CYS:HB3	1:A:1228:CYS:SG	2.60	0.41
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.20	0.41
1:A:1631:LEU:HD23	1:A:1631:LEU:HA	1.79	0.41
1:A:1965:HIS:N	1:A:1965:HIS:CD2	2.87	0.41
3:C:129:ILE:HA	3:C:199:LEU:O	2.21	0.41
3:C:177:ARG:HA	3:C:177:ARG:HE	1.86	0.41
3:C:441:PRO:C	3:C:444:GLY:HA3	2.45	0.41
3:C:501:ILE:HG22	3:C:530:LEU:HD11	2.01	0.41
3:C:516:LEU:HD23	3:C:516:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:VAL:HB	3:C:717:PHE:CZ	2.55	0.41
4:E:125:PHE:CD2	4:E:125:PHE:N	2.89	0.41
4:E:168:CYS:SG	4:E:208:ILE:HD11	2.60	0.41
5:F:33:G:C2	5:F:34:G:H8	2.39	0.41
6:G:18:A:H2	14:O:196:GLN:O	2.03	0.41
6:G:90:C:N3	7:H:40:C:N3	2.68	0.41
6:G:93:A:C2	7:H:38:A:C2	3.08	0.41
6:G:109:U:H5''	23:X:454:ARG:HD3	2.02	0.41
7:H:168:A:H5''	7:H:169:C:C6	2.56	0.41
9:J:190:THR:HA	11:L:17:GLU:CD	2.46	0.41
9:J:203:LEU:CD2	9:J:203:LEU:O	2.69	0.41
9:J:294:HIS:CE1	11:L:227:THR:OG1	2.73	0.41
9:J:394:HIS:O	9:J:398:VAL:HG23	2.21	0.41
12:M:218:PHE:C	12:M:218:PHE:HD1	2.27	0.41
14:O:200:ASP:O	14:O:204:GLY:N	2.46	0.41
17:R:246:LYS:NZ	17:R:246:LYS:CB	2.84	0.41
17:R:408:ASP:HB3	17:R:411:LEU:HD23	2.02	0.41
19:T:207:VAL:HG12	19:T:480:ALA:HB1	2.03	0.41
21:V:402:LYS:O	21:V:406:LEU:N	2.53	0.41
21:V:495:ASP:O	21:V:498:ALA:HB3	2.21	0.41
23:X:246:LEU:HG	23:X:277:ARG:HE	1.84	0.41
23:X:276:VAL:HG22	24:Y:227:VAL:HA	2.03	0.41
23:X:387:GLN:NE2	23:X:391:SER:OG	2.54	0.41
23:X:389:LYS:NZ	23:X:390:GLU:HG3	2.35	0.41
23:X:393:GLN:HA	23:X:396:ARG:HB2	2.02	0.41
23:X:422:GLY:O	23:X:553:ALA:HA	2.19	0.41
23:X:453:PRO:HB3	23:X:524:GLU:CD	2.46	0.41
23:X:595:CYS:SG	23:X:613:VAL:HG11	2.61	0.41
23:X:716:LYS:HB2	23:X:748:GLU:O	2.21	0.41
23:X:741:TRP:HE1	35:1:783:GLU:H	1.67	0.41
23:X:931:SER:O	23:X:933:GLN:NE2	2.54	0.41
24:Y:41:LEU:HA	24:Y:155:ARG:HA	2.02	0.41
24:Y:255:ASP:OD2	24:Y:259:ILE:HD11	2.21	0.41
35:1:534:GLN:O	35:1:538:LEU:HD12	2.20	0.41
35:1:563:LEU:HB3	35:1:566:LEU:HB2	2.02	0.41
35:1:686:LEU:HA	35:1:689:ILE:HG12	2.03	0.41
35:1:1208:LEU:HB3	35:1:1237:LEU:HD21	2.03	0.41
35:1:1246:MET:HE2	35:1:1246:MET:HB3	1.75	0.41
35:1:1292:LYS:HD2	42:5:78:PRO:HG2	2.01	0.41
36:3:128:ARG:HH21	36:3:180:PRO:HG3	1.85	0.41
36:3:184:CYS:SG	36:3:211:TYR:CE1	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:212:GLU:HG2	36:3:213:LEU:N	2.35	0.41
36:3:469:GLU:OE1	36:3:469:GLU:N	2.53	0.41
36:3:515:ALA:HB2	36:3:528:ARG:NE	2.36	0.41
36:3:605:LEU:HB3	36:3:619:LEU:HD22	2.02	0.41
36:3:665:LEU:O	36:3:676:ARG:HA	2.21	0.41
36:3:671:ASN:HB3	36:3:696:SER:HA	2.01	0.41
36:3:998:HIS:HE1	36:3:1041:TYR:OH	2.04	0.41
36:3:1140:PHE:CE1	36:3:1197:LEU:HD13	2.53	0.41
36:3:1185:MET:HE3	36:3:1185:MET:HB3	1.93	0.41
38:w:381:LYS:HE2	38:w:381:LYS:HB2	1.70	0.41
27:m:53:PRO:HG3	27:m:59:ALA:C	2.46	0.41
1:A:27:GLU:O	1:A:31:GLN:HG2	2.21	0.41
1:A:1402:ARG:HD2	17:R:406:GLN:OE1	2.21	0.41
1:A:1868:MET:O	1:A:1868:MET:HG2	2.21	0.41
1:A:1939:ILE:HD11	1:A:1976:TRP:HH2	1.86	0.41
3:C:680:ASN:O	3:C:682:LYS:N	2.53	0.41
5:F:8:C:H3'	5:F:9:U:O4'	2.20	0.41
7:H:15:U:O3'	7:H:16:U:H2'	2.21	0.41
7:H:42:G:C6	7:H:43:U:C4	3.09	0.41
12:M:158:GLU:CD	12:M:158:GLU:N	2.79	0.41
13:N:91:LYS:HA	13:N:91:LYS:HD3	1.80	0.41
15:P:66:ARG:HE	15:P:66:ARG:HB2	1.49	0.41
17:R:238:THR:OG1	17:R:239:VAL:N	2.53	0.41
19:T:297:HIS:CG	19:T:298:PRO:HD2	2.56	0.41
23:X:674:THR:HG22	23:X:675:ASN:H	1.86	0.41
35:1:510:PRO:HA	35:1:513:LYS:HE2	2.03	0.41
35:1:758:ASP:OD2	35:1:761:TYR:HB2	2.21	0.41
35:1:1067:LYS:HB3	35:1:1067:LYS:HE2	1.67	0.41
36:3:164:ASN:ND2	36:3:190:GLU:HG2	2.35	0.41
36:3:192:ALA:O	42:5:74:GLN:NE2	2.35	0.41
36:3:334:PRO:HG2	36:3:357:TYR:CD2	2.56	0.41
36:3:941:HIS:CE1	36:3:974:LYS:HA	2.56	0.41
36:3:1001:ILE:HD12	36:3:1011:TRP:NE1	2.36	0.41
39:2:641:PRO:N	39:2:641:PRO:C	2.67	0.41
41:7:26:CYS:SG	41:7:60:ILE:HG13	2.61	0.41
27:m:53:PRO:HG3	27:m:59:ALA:O	2.21	0.41
1:A:461:HIS:O	1:A:462:ARG:NH1	2.54	0.40
1:A:850:TYR:HD2	1:A:864:LEU:HD21	1.85	0.40
1:A:1012:LYS:O	1:A:1012:LYS:HG3	2.20	0.40
2:B:95:G:Cl'	30:d:24:LYS:CA	2.80	0.40
3:C:717:PHE:CE1	3:C:721:LYS:HE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:94:C:H2'	5:F:95:G:C8	2.56	0.40
6:G:-8:C:O4'	20:U:18:TYR:HB2	2.21	0.40
6:G:7:G:C2	6:G:8:C:C2	3.09	0.40
6:G:8:C:H2'	6:G:9:C:C4	2.57	0.40
19:T:405:PHE:HZ	19:T:408:ASN:OD1	2.04	0.40
21:V:461:LEU:HA	21:V:461:LEU:HD23	1.88	0.40
21:V:529:PHE:CE1	21:V:564:VAL:HB	2.56	0.40
23:X:466:ALA:HA	23:X:469:MET:HB2	2.03	0.40
23:X:856:ARG:HB3	23:X:856:ARG:CZ	2.51	0.40
23:X:868:ARG:HH22	23:X:973:ASN:HD21	1.69	0.40
23:X:909:ARG:HG2	23:X:909:ARG:HH11	1.86	0.40
24:Y:26:LEU:HB2	24:Y:166:PHE:CG	2.56	0.40
24:Y:55:ASP:OD1	24:Y:57:THR:OG1	2.39	0.40
35:1:563:LEU:HB3	35:1:566:LEU:CB	2.51	0.40
35:1:835:ASP:O	35:1:839:GLU:HG2	2.22	0.40
35:1:897:LEU:HD21	35:1:932:ILE:CD1	2.51	0.40
35:1:914:PHE:O	35:1:917:VAL:HG12	2.21	0.40
35:1:1142:ASN:HD22	35:1:1142:ASN:N	2.19	0.40
35:1:1179:ASP:HB3	39:2:511:LEU:HB3	2.03	0.40
36:3:541:LYS:HD3	36:3:541:LYS:HA	1.87	0.40
36:3:768:GLU:HB3	36:3:769:LYS:H	1.63	0.40
36:3:926:TYR:CD1	36:3:942:LYS:HB3	2.56	0.40
36:3:1041:TYR:CB	39:2:705:ARG:HG3	2.51	0.40
41:7:12:ARG:HA	41:7:12:ARG:HD2	1.68	0.40
42:5:53:PHE:O	42:5:57:GLU:HG2	2.21	0.40
28:n:25:VAL:HA	28:n:44:LYS:O	2.22	0.40
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.86	0.40
1:A:617:ASN:HA	1:A:621:VAL:HB	2.02	0.40
1:A:833:LYS:HD3	1:A:833:LYS:C	2.45	0.40
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.80	0.40
1:A:1268:ILE:HD13	1:A:1268:ILE:HG21	1.87	0.40
1:A:1684:PHE:N	1:A:1702:LEU:HD21	2.36	0.40
2:B:13:C:H2'	2:B:14:U:H6	1.86	0.40
3:C:415:LEU:HD12	3:C:415:LEU:HA	1.83	0.40
3:C:736:GLY:O	3:C:737:PRO:C	2.64	0.40
4:E:136:TRP:CZ3	4:E:143:ARG:HG2	2.56	0.40
4:E:323:LEU:HD21	22:W:83:PRO:O	2.22	0.40
7:H:13:C:H5''	7:H:14:C:C5	2.56	0.40
7:H:57:A:C5'	39:2:481:THR:HG21	2.51	0.40
7:H:160:A:H2'	7:H:161:U:O4'	2.21	0.40
8:I:479:ARG:O	8:I:483:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:24:MET:HE2	11:L:24:MET:HB2	1.79	0.40
11:L:55:ASP:OD2	11:L:57:SER:HB3	2.22	0.40
11:L:141:PRO:HG2	11:L:144:MET:HA	2.03	0.40
11:L:186:GLN:HG3	11:L:189:ARG:HH12	1.87	0.40
13:N:66:LYS:HD2	13:N:66:LYS:HA	1.84	0.40
15:P:206:LYS:O	15:P:209:ARG:O	2.39	0.40
16:Q:514:ILE:N	16:Q:654:ASN:O	2.31	0.40
17:R:412:PHE:HE2	23:X:326:GLN:HE22	1.69	0.40
19:T:320:LYS:HE2	19:T:320:LYS:HB2	1.64	0.40
23:X:173:GLN:O	23:X:176:GLU:HG2	2.21	0.40
23:X:716:LYS:N	23:X:747:LEU:HD12	2.36	0.40
23:X:832:GLU:OE1	23:X:927:VAL:HG13	2.21	0.40
29:c:62:HIS:O	29:c:103:GLY:HA3	2.21	0.40
35:1:555:VAL:HG12	35:1:559:ILE:HD13	2.02	0.40
35:1:641:ILE:HG22	35:1:682:HIS:NE2	2.37	0.40
35:1:642:PRO:C	35:1:644:LEU:H	2.28	0.40
35:1:840:LEU:HD13	35:1:840:LEU:HA	1.80	0.40
35:1:841:ALA:CB	35:1:875:ILE:CD1	2.82	0.40
35:1:1277:GLN:HG3	36:3:113:ARG:CD	2.51	0.40
36:3:174:ASP:HB3	36:3:240:GLY:H	1.86	0.40
36:3:180:PRO:HD2	36:3:215:LEU:HD11	2.03	0.40
36:3:280:ASP:H	36:3:857:ALA:CB	2.33	0.40
36:3:373:PHE:HD1	36:3:385:PHE:CG	2.40	0.40
36:3:408:LEU:HD12	36:3:427:CYS:HA	2.02	0.40
36:3:459:VAL:HA	36:3:475:ILE:O	2.21	0.40
36:3:706:MET:HG2	36:3:770:LEU:CD1	2.51	0.40
36:3:755:VAL:HG22	36:3:764:ILE:CD1	2.52	0.40
42:5:44:MET:HB2	42:5:44:MET:HE2	1.75	0.40
30:i:5:LEU:H	31:j:49:GLY:HA3	1.87	0.40
1:A:229:GLN:O	1:A:230:PHE:HD1	2.03	0.40
1:A:442:LYS:NZ	44:A:3000:IHP:O33	2.54	0.40
1:A:1130:ASN:HD21	1:A:1140:MET:HB2	1.87	0.40
1:A:1215:ASN:HB3	1:A:1224:ARG:HH11	1.85	0.40
1:A:1409:GLU:OE2	1:A:1409:GLU:HA	2.20	0.40
1:A:1924:LEU:HD12	1:A:1924:LEU:HA	1.85	0.40
3:C:62:ASP:O	3:C:63:LYS:C	2.64	0.40
3:C:368:SER:O	3:C:372:PHE:HB2	2.21	0.40
3:C:572:GLU:HG3	3:C:573:GLU:H	1.86	0.40
3:C:618:THR:OG1	3:C:630:LEU:HB3	2.21	0.40
3:C:823:ALA:O	3:C:824:THR:OG1	2.35	0.40
4:E:197:LEU:HD21	4:E:213:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:5:G:N1	6:G:6:A:N6	2.69	0.40
6:G:7:G:C5	6:G:8:C:C4	3.10	0.40
6:G:96:U:H5''	6:G:97:A:OP2	2.21	0.40
7:H:99:A:HO2'	7:H:100:U:P	2.43	0.40
7:H:142:U:C2	7:H:143:C:C5	3.09	0.40
11:L:11:TRP:CD2	11:L:49:ARG:HD3	2.56	0.40
11:L:154:GLU:HG3	11:L:155:ALA:N	2.35	0.40
17:R:151:LEU:HD22	17:R:151:LEU:HA	1.87	0.40
23:X:216:GLU:HG2	23:X:217:GLU:N	2.37	0.40
23:X:423:GLU:HB2	23:X:574:GLY:O	2.22	0.40
23:X:723:ALA:HA	23:X:734:CYS:SG	2.61	0.40
23:X:929:LEU:HD23	23:X:929:LEU:HA	1.89	0.40
24:Y:47:ARG:HA	24:Y:140:ASN:HD21	1.85	0.40
24:Y:247:LEU:HG	24:Y:248:ASN:N	2.36	0.40
35:1:540:MET:SD	35:1:577:VAL:HG12	2.58	0.40
35:1:669:GLN:NE2	35:1:707:LEU:HD22	2.37	0.40
35:1:811:LEU:HB2	35:1:812:PRO:HD3	2.03	0.40
35:1:1179:ASP:CB	39:2:511:LEU:CD1	3.00	0.40
35:1:1216:TRP:CH2	35:1:1268:ILE:HD13	2.56	0.40
35:1:1304:LEU:HD12	42:5:52:TYR:CE2	2.57	0.40
36:3:327:LEU:O	36:3:373:PHE:HB2	2.22	0.40
36:3:719:SER:OG	36:3:734:LEU:HB2	2.22	0.40
36:3:739:LEU:HD23	36:3:739:LEU:HA	1.71	0.40
36:3:998:HIS:CE1	36:3:1041:TYR:OH	2.75	0.40
39:2:568:TYR:O	39:2:569:GLN:HB2	2.22	0.40
28:n:18:GLU:HA	28:n:23:THR:O	2.21	0.40
1:A:154:GLU:HG2	1:A:572:PHE:CD1	2.56	0.40
1:A:545:HIS:O	1:A:549:GLU:HG2	2.21	0.40
1:A:1342:TRP:HB2	1:A:1348:VAL:HG21	2.03	0.40
1:A:1636:LYS:HE3	1:A:1656:THR:CG2	2.51	0.40
1:A:1741:TYR:HH	35:1:937:LEU:CD2	1.95	0.40
3:C:672:LEU:HG	3:C:673:LYS:H	1.86	0.40
4:E:137:ASP:OD1	4:E:137:ASP:N	2.54	0.40
4:E:221:ASP:OD1	4:E:226:LYS:HE3	2.22	0.40
4:E:323:LEU:HD23	4:E:323:LEU:HA	1.92	0.40
5:F:47:A:H4'	5:F:48:A:OP1	2.21	0.40
17:R:124:VAL:O	17:R:124:VAL:CG1	2.69	0.40
19:T:412:HIS:NE2	19:T:431:ALA:HB2	2.37	0.40
23:X:681:LEU:H	23:X:725:ARG:NH2	2.19	0.40
23:X:753:PRO:HG2	23:X:782:ASP:OD2	2.22	0.40
35:1:614:ARG:HD3	35:1:615:PRO:CD	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:933:CYS:CB	35:1:970:LEU:HD11	2.51	0.40
36:3:2:PHE:CE2	39:2:711:LEU:HD12	2.56	0.40
36:3:66:MET:HE3	36:3:123:VAL:HG12	2.03	0.40
36:3:151:ARG:O	36:3:151:ARG:HG3	2.21	0.40
36:3:883:GLU:CD	36:3:884:GLN:H	2.30	0.40
36:3:1096:HIS:ND1	36:3:1166:TYR:HB2	2.36	0.40
38:w:398:LYS:HD3	38:w:398:LYS:HA	1.80	0.40
38:w:429:TRP:HE3	38:w:430:ARG:NH1	2.19	0.40
38:w:493:GLU:HA	38:w:496:LYS:HB3	2.03	0.40
1:A:1131:LYS:HE2	1:A:1174:PHE:CE2	2.55	0.40
1:A:1573:LEU:HA	1:A:1573:LEU:HD23	1.89	0.40
1:A:1885:LYS:HE2	1:A:1887:SER:HA	2.04	0.40
2:B:89:U:C2'	2:B:90:U:H5''	2.47	0.40
3:C:878:ILE:HD12	3:C:878:ILE:HG23	1.90	0.40
5:F:39:A:C2'	5:F:40:U:H5'	2.51	0.40
9:J:401:ARG:HA	9:J:404:GLU:HG2	2.03	0.40
11:L:186:GLN:HG3	11:L:189:ARG:NH1	2.37	0.40
17:R:376:LYS:CA	17:R:379:LYS:HB2	2.42	0.40
20:U:5:ILE:O	20:U:5:ILE:HD12	2.22	0.40
23:X:404:PHE:O	23:X:408:LEU:HD23	2.22	0.40
23:X:719:ALA:C	23:X:736:ARG:HH21	2.30	0.40
23:X:859:ASP:OD2	23:X:859:ASP:N	2.52	0.40
24:Y:63:GLY:C	24:Y:106:SER:H	2.29	0.40
24:Y:136:ILE:O	24:Y:140:ASN:HB2	2.22	0.40
35:1:1217:PRO:C	35:1:1219:VAL:H	2.30	0.40
36:3:168:TYR:OH	36:3:187:MET:SD	2.63	0.40
36:3:258:TYR:HB3	36:3:267:ILE:HB	2.04	0.40
36:3:258:TYR:CG	36:3:259:LYS:N	2.90	0.40
36:3:278:LEU:HA	36:3:815:ARG:NH1	2.37	0.40
36:3:592:LEU:HD13	36:3:592:LEU:HA	1.64	0.40
36:3:1135:HIS:HA	36:3:1138:HIS:HB3	2.03	0.40
39:2:635:ALA:HB1	40:4:73:ILE:N	2.12	0.40
41:7:23:CYS:HB3	41:7:58:CYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1961/2335 (84%)	1760 (90%)	186 (10%)	15 (1%)	16	45
3	C	854/972 (88%)	751 (88%)	100 (12%)	3 (0%)	30	60
4	E	297/357 (83%)	270 (91%)	27 (9%)	0	100	100
8	I	662/855 (77%)	575 (87%)	86 (13%)	1 (0%)	43	71
9	J	525/848 (62%)	487 (93%)	33 (6%)	5 (1%)	12	40
10	K	22/343 (6%)	18 (82%)	4 (18%)	0	100	100
11	L	375/802 (47%)	358 (96%)	16 (4%)	1 (0%)	36	65
12	M	112/243 (46%)	105 (94%)	5 (4%)	2 (2%)	6	29
13	N	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
14	O	288/420 (69%)	262 (91%)	26 (9%)	0	100	100
15	P	97/229 (42%)	89 (92%)	7 (7%)	1 (1%)	12	40
16	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100	100
17	R	370/536 (69%)	336 (91%)	31 (8%)	3 (1%)	16	45
18	S	156/166 (94%)	144 (92%)	12 (8%)	0	100	100
19	T	318/514 (62%)	300 (94%)	18 (6%)	0	100	100
20	U	68/2752 (2%)	63 (93%)	4 (6%)	1 (2%)	8	32
21	V	458/908 (50%)	433 (94%)	25 (6%)	0	100	100
22	W	497/579 (86%)	473 (95%)	24 (5%)	0	100	100
23	X	778/1041 (75%)	728 (94%)	49 (6%)	1 (0%)	48	75
24	Y	318/492 (65%)	296 (93%)	22 (7%)	0	100	100
25	Z	147/225 (65%)	138 (94%)	5 (3%)	4 (3%)	4	22
26	y	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
27	a	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
27	m	80/240 (33%)	72 (90%)	8 (10%)	0	100	100
28	b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	n	78/119 (66%)	67 (86%)	11 (14%)	0	100	100
29	c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
29	h	91/118 (77%)	82 (90%)	9 (10%)	0	100	100
30	d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
30	i	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
31	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
31	j	79/92 (86%)	73 (92%)	6 (8%)	0	100	100
32	f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
32	k	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
33	g	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
33	l	81/126 (64%)	70 (86%)	11 (14%)	0	100	100
34	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2	13
34	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	7	31
34	s	130/504 (26%)	114 (88%)	8 (6%)	8 (6%)	1	9
34	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3	20
35	1	814/1304 (62%)	703 (86%)	101 (12%)	10 (1%)	10	37
36	3	1165/1217 (96%)	992 (85%)	172 (15%)	1 (0%)	48	75
37	p	163/225 (72%)	147 (90%)	15 (9%)	1 (1%)	21	52
38	w	119/501 (24%)	107 (90%)	12 (10%)	0	100	100
39	2	246/895 (28%)	208 (85%)	34 (14%)	4 (2%)	7	31
40	4	147/424 (35%)	129 (88%)	18 (12%)	0	100	100
41	7	79/110 (72%)	65 (82%)	14 (18%)	0	100	100
42	5	75/86 (87%)	64 (85%)	11 (15%)	0	100	100
43	o	160/255 (63%)	136 (85%)	24 (15%)	0	100	100
All	All	14418/25294 (57%)	13114 (91%)	1231 (8%)	73 (0%)	26	55

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1417	PRO
9	J	202	GLU
17	R	164	PRO
25	Z	78	PRO
25	Z	86	ARG

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Mol	Chain	Res	Type
34	q	24	VAL
34	q	59	HIS
34	q	60	PRO
34	s	9	ASN
34	s	55	ILE
34	s	60	PRO
34	s	66	PRO
34	s	71	ILE
34	t	9	ASN
34	t	69	THR
35	1	718	PRO
39	2	642	PRO
39	2	646	PRO
39	2	647	ASN
1	A	699	GLU
1	A	856	LEU
1	A	1517	LYS
3	C	84	GLU
9	J	241	VAL
12	M	202	TYR
15	P	199	LYS
23	X	703	ARG
34	q	9	ASN
34	s	24	VAL
35	1	1013	ILE
35	1	1107	GLN
39	2	641	PRO
1	A	1418	ARG
1	A	1528	GLN
9	J	206	LEU
12	M	124	PHE
34	q	19	PRO
34	q	23	HIS
34	r	9	ASN
34	t	67	SER
35	1	722	GLU
35	1	926	LYS
35	1	1106	ARG
1	A	378	PHE
1	A	570	ASP
1	A	698	PRO
3	C	358	LYS

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Mol	Chain	Res	Type
9	J	188	GLN
11	L	146	GLU
17	R	428	GLU
20	U	2	TYR
25	Z	65	ILE
34	t	65	PRO
35	1	611	SER
35	1	717	THR
1	A	188	LEU
9	J	341	PRO
34	s	62	ARG
35	1	1011	PRO
35	1	1091	HIS
1	A	108	MET
1	A	227	ARG
17	R	223	PRO
37	p	214	PRO
1	A	942	PRO
3	C	440	SER
25	Z	17	PRO
1	A	109	PRO
8	I	51	PRO
34	s	38	GLY
36	3	672	GLY
1	A	729	PRO
34	r	60	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1768/2108 (84%)	1578 (89%)	190 (11%)	6	24
3	C	747/866 (86%)	652 (87%)	95 (13%)	4	18
4	E	256/300 (85%)	219 (86%)	37 (14%)	3	14
8	I	24/749 (3%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	239/751 (32%)	222 (93%)	17 (7%)	13	40
10	K	20/294 (7%)	16 (80%)	4 (20%)	1	6
11	L	171/709 (24%)	149 (87%)	22 (13%)	4	17
12	M	104/209 (50%)	92 (88%)	12 (12%)	5	21
13	N	130/130 (100%)	121 (93%)	9 (7%)	14	41
14	O	3/361 (1%)	3 (100%)	0	100	100
15	P	95/203 (47%)	75 (79%)	20 (21%)	1	5
17	R	282/457 (62%)	242 (86%)	40 (14%)	3	14
19	T	273/441 (62%)	244 (89%)	29 (11%)	6	24
20	U	21/2432 (1%)	17 (81%)	4 (19%)	1	7
21	V	188/838 (22%)	155 (82%)	33 (18%)	2	9
23	X	682/897 (76%)	610 (89%)	72 (11%)	6	24
24	Y	286/451 (63%)	244 (85%)	42 (15%)	3	14
27	m	4/177 (2%)	4 (100%)	0	100	100
28	n	3/101 (3%)	3 (100%)	0	100	100
29	h	5/110 (4%)	5 (100%)	0	100	100
30	i	4/74 (5%)	4 (100%)	0	100	100
31	j	1/84 (1%)	1 (100%)	0	100	100
32	k	3/66 (4%)	3 (100%)	0	100	100
33	l	3/101 (3%)	3 (100%)	0	100	100
35	1	700/1104 (63%)	577 (82%)	123 (18%)	2	9
36	3	1018/1051 (97%)	791 (78%)	227 (22%)	1	5
37	p	8/195 (4%)	8 (100%)	0	100	100
38	w	104/446 (23%)	87 (84%)	17 (16%)	2	11
39	2	151/776 (20%)	126 (83%)	25 (17%)	2	11
41	7	69/95 (73%)	53 (77%)	16 (23%)	1	4
42	5	68/77 (88%)	48 (71%)	20 (29%)	0	2
43	o	6/218 (3%)	6 (100%)	0	100	100
All	All	7436/16871 (44%)	6382 (86%)	1054 (14%)	5	14

All (1054) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	47	GLU
1	A	55	ASP
1	A	57	GLN
1	A	59	GLU
1	A	60	ASP
1	A	66	VAL
1	A	70	ILE
1	A	88	TYR
1	A	95	MET
1	A	97	HIS
1	A	122	ILE
1	A	123	THR
1	A	137	GLU
1	A	146	SER
1	A	147	MET
1	A	188	LEU
1	A	189	GLU
1	A	193	LEU
1	A	195	LEU
1	A	205	ASP
1	A	249	LEU
1	A	258	PHE
1	A	261	LYS
1	A	271	MET
1	A	273	ILE
1	A	283	VAL
1	A	284	ARG
1	A	299	ILE
1	A	304	ILE
1	A	330	THR
1	A	334	THR
1	A	337	VAL
1	A	342	THR
1	A	343	GLU
1	A	359	ILE
1	A	360	SER
1	A	362	ARG
1	A	365	VAL
1	A	371	LEU
1	A	376	GLU
1	A	388	LEU
1	A	393	LEU

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	422	LEU
1	A	443	VAL
1	A	468	LYS
1	A	480	LYS
1	A	486	LYS
1	A	518	LEU
1	A	530	LEU
1	A	554	THR
1	A	560	SER
1	A	569	VAL
1	A	576	ASP
1	A	579	GLN
1	A	591	MET
1	A	595	LYS
1	A	644	ILE
1	A	670	LYS
1	A	683	LEU
1	A	693	ILE
1	A	694	LEU
1	A	708	THR
1	A	714	SER
1	A	735	ILE
1	A	751	THR
1	A	759	GLU
1	A	767	VAL
1	A	789	GLU
1	A	804	GLU
1	A	807	VAL
1	A	830	LEU
1	A	831	SER
1	A	836	THR
1	A	856	LEU
1	A	866	LEU
1	A	869	GLN
1	A	885	LEU
1	A	886	LEU
1	A	893	GLU
1	A	915	GLU
1	A	916	LYS
1	A	940	ILE
1	A	941	LYS

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Mol	Chain	Res	Type
1	A	946	GLU
1	A	968	THR
1	A	977	LEU
1	A	978	GLU
1	A	979	SER
1	A	983	LYS
1	A	984	MET
1	A	995	ARG
1	A	1000	ILE
1	A	1014	ASN
1	A	1017	ILE
1	A	1038	SER
1	A	1075	GLN
1	A	1076	ASP
1	A	1079	THR
1	A	1095	ILE
1	A	1104	ASP
1	A	1112	ARG
1	A	1130	ASN
1	A	1147	VAL
1	A	1163	ARG
1	A	1166	THR
1	A	1181	ASP
1	A	1186	LEU
1	A	1194	CYS
1	A	1210	LYS
1	A	1217	GLN
1	A	1253	SER
1	A	1255	THR
1	A	1276	GLU
1	A	1293	ASN
1	A	1298	ARG
1	A	1299	ILE
1	A	1327	MET
1	A	1329	SER
1	A	1348	VAL
1	A	1359	HIS
1	A	1368	LEU
1	A	1376	GLU
1	A	1382	SER
1	A	1404	THR
1	A	1407	ASP

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Mol	Chain	Res	Type
1	A	1427	ARG
1	A	1438	VAL
1	A	1459	ARG
1	A	1481	VAL
1	A	1491	LYS
1	A	1517	LYS
1	A	1519	THR
1	A	1523	ARG
1	A	1524	SER
1	A	1526	LEU
1	A	1529	ILE
1	A	1549	VAL
1	A	1553	VAL
1	A	1554	GLN
1	A	1555	LEU
1	A	1558	THR
1	A	1568	THR
1	A	1601	LEU
1	A	1606	ILE
1	A	1608	THR
1	A	1623	ASN
1	A	1628	ASP
1	A	1635	TYR
1	A	1639	VAL
1	A	1640	SER
1	A	1644	LEU
1	A	1648	SER
1	A	1649	LYS
1	A	1667	ARG
1	A	1672	ASP
1	A	1681	ARG
1	A	1692	MET
1	A	1697	SER
1	A	1702	LEU
1	A	1773	SER
1	A	1776	ILE
1	A	1783	THR
1	A	1800	THR
1	A	1825	SER
1	A	1836	LEU
1	A	1852	LEU
1	A	1857	GLN

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Mol	Chain	Res	Type
1	A	1870	ASP
1	A	1878	ASP
1	A	1884	ILE
1	A	1887	SER
1	A	1889	LEU
1	A	1910	THR
1	A	1913	GLN
1	A	1919	LEU
1	A	1924	LEU
1	A	1926	THR
1	A	1938	LEU
1	A	1961	ILE
1	A	1970	THR
1	A	1973	ASP
1	A	1975	GLU
1	A	1977	ILE
1	A	1986	LEU
1	A	1997	VAL
1	A	2005	SER
1	A	2012	LEU
1	A	2015	GLU
3	C	58	VAL
3	C	65	TYR
3	C	68	THR
3	C	86	THR
3	C	90	THR
3	C	93	ILE
3	C	112	THR
3	C	117	ASP
3	C	122	LEU
3	C	132	VAL
3	C	134	LEU
3	C	173	THR
3	C	179	VAL
3	C	213	ASP
3	C	223	ASP
3	C	233	GLU
3	C	248	GLN
3	C	282	VAL
3	C	283	ASP
3	C	293	SER
3	C	295	ASP

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Mol	Chain	Res	Type
3	C	299	ILE
3	C	308	CYS
3	C	312	SER
3	C	313	GLN
3	C	316	ILE
3	C	322	SER
3	C	326	ILE
3	C	327	TYR
3	C	333	ASP
3	C	359	LYS
3	C	363	SER
3	C	385	VAL
3	C	394	ARG
3	C	417	ARG
3	C	436	GLN
3	C	440	SER
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	479	THR
3	C	483	SER
3	C	485	ASP
3	C	500	THR
3	C	507	VAL
3	C	509	VAL
3	C	510	LEU
3	C	514	TYR
3	C	536	ARG
3	C	538	HIS
3	C	539	ILE
3	C	544	VAL
3	C	559	ILE
3	C	562	THR
3	C	571	ASN
3	C	572	GLU
3	C	573	GLU
3	C	578	ARG
3	C	599	GLU
3	C	607	LEU
3	C	608	ARG
3	C	612	LYS
3	C	622	GLU

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Mol	Chain	Res	Type
3	C	632	THR
3	C	639	CYS
3	C	661	THR
3	C	675	PHE
3	C	677	GLU
3	C	678	THR
3	C	696	LEU
3	C	716	GLU
3	C	724	TRP
3	C	749	THR
3	C	750	LEU
3	C	753	GLU
3	C	754	VAL
3	C	759	LEU
3	C	766	ILE
3	C	799	GLU
3	C	802	HIS
3	C	809	ILE
3	C	822	MET
3	C	824	THR
3	C	829	GLU
3	C	846	VAL
3	C	848	THR
3	C	879	ASP
3	C	885	THR
3	C	899	SER
3	C	900	VAL
3	C	907	VAL
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
3	C	940	ARG
4	E	59	ILE
4	E	61	LEU
4	E	71	CYS
4	E	73	LYS
4	E	87	ASP
4	E	88	ARG
4	E	100	ASP
4	E	104	THR
4	E	106	LYS
4	E	108	HIS

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Mol	Chain	Res	Type
4	E	119	THR
4	E	123	MET
4	E	126	SER
4	E	138	SER
4	E	143	ARG
4	E	144	VAL
4	E	155	ASN
4	E	162	ARG
4	E	167	VAL
4	E	175	THR
4	E	176	VAL
4	E	189	THR
4	E	205	SER
4	E	210	SER
4	E	227	LEU
4	E	234	HIS
4	E	243	LEU
4	E	258	THR
4	E	275	LYS
4	E	282	HIS
4	E	284	PHE
4	E	290	ARG
4	E	300	ILE
4	E	330	ILE
4	E	333	VAL
4	E	344	SER
4	E	349	LYS
9	J	186	GLU
9	J	195	LEU
9	J	199	LYS
9	J	203	LEU
9	J	204	GLU
9	J	205	LEU
9	J	214	ILE
9	J	220	LEU
9	J	225	LEU
9	J	238	ASN
9	J	258	ILE
9	J	276	ILE
9	J	292	VAL
9	J	367	GLU
9	J	376	VAL

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Mol	Chain	Res	Type
9	J	408	ASP
9	J	411	MET
10	K	208	THR
10	K	215	ASP
10	K	218	LYS
10	K	222	ASP
11	L	18	ILE
11	L	24	MET
11	L	64	SER
11	L	89	ILE
11	L	138	ARG
11	L	146	GLU
11	L	154	GLU
11	L	166	LYS
11	L	168	LYS
11	L	169	ARG
11	L	170	LYS
11	L	173	GLU
11	L	176	LEU
11	L	177	GLU
11	L	178	GLU
11	L	182	LEU
11	L	201	LYS
11	L	205	LYS
11	L	218	LYS
11	L	219	LYS
11	L	222	LEU
11	L	235	LEU
12	M	126	ASP
12	M	152	LEU
12	M	160	PHE
12	M	163	THR
12	M	166	SER
12	M	167	LEU
12	M	168	LEU
12	M	186	LEU
12	M	204	ASP
12	M	211	ILE
12	M	212	ASN
12	M	224	ARG
13	N	3	LYS
13	N	5	LYS

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Mol	Chain	Res	Type
13	N	41	ARG
13	N	49	ILE
13	N	57	THR
13	N	71	SER
13	N	107	GLN
13	N	112	ASN
13	N	128	VAL
15	P	26	LEU
15	P	31	SER
15	P	32	SER
15	P	41	ILE
15	P	47	THR
15	P	57	ARG
15	P	66	ARG
15	P	67	GLU
15	P	74	LYS
15	P	78	ARG
15	P	186	ARG
15	P	199	LYS
15	P	201	VAL
15	P	205	LYS
15	P	207	ASP
15	P	209	ARG
15	P	214	THR
15	P	217	SER
15	P	221	LYS
15	P	225	GLU
17	R	111	VAL
17	R	115	LYS
17	R	125	MET
17	R	131	ASP
17	R	132	LEU
17	R	136	ASP
17	R	151	LEU
17	R	165	VAL
17	R	170	LYS
17	R	171	LEU
17	R	175	GLN
17	R	180	THR
17	R	183	GLN
17	R	184	GLN
17	R	188	PHE

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Mol	Chain	Res	Type
17	R	197	ILE
17	R	218	ILE
17	R	220	ARG
17	R	235	ARG
17	R	238	THR
17	R	243	GLN
17	R	246	LYS
17	R	251	ILE
17	R	289	GLU
17	R	295	ASP
17	R	300	GLU
17	R	325	ARG
17	R	326	GLU
17	R	348	GLU
17	R	352	ARG
17	R	357	HIS
17	R	370	SER
17	R	383	ASN
17	R	386	ARG
17	R	405	VAL
17	R	407	TYR
17	R	409	GLN
17	R	411	LEU
17	R	415	SER
17	R	416	LYS
19	T	221	THR
19	T	223	SER
19	T	235	SER
19	T	247	SER
19	T	258	SER
19	T	263	SER
19	T	264	CYS
19	T	267	ASP
19	T	280	VAL
19	T	294	LEU
19	T	304	VAL
19	T	307	SER
19	T	319	THR
19	T	323	VAL
19	T	326	LEU
19	T	338	CYS
19	T	349	SER

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Mol	Chain	Res	Type
19	T	360	VAL
19	T	365	ARG
19	T	384	HIS
19	T	389	SER
19	T	393	ASP
19	T	394	ASN
19	T	410	SER
19	T	424	ASP
19	T	429	SER
19	T	443	THR
19	T	478	LEU
19	T	499	THR
20	U	1	MET
20	U	2	TYR
20	U	5	ILE
20	U	25	LEU
21	V	458	THR
21	V	459	ILE
21	V	465	SER
21	V	481	PHE
21	V	483	GLU
21	V	486	THR
21	V	494	LEU
21	V	504	GLU
21	V	517	LEU
21	V	518	LYS
21	V	522	MET
21	V	523	GLU
21	V	528	ILE
21	V	530	LYS
21	V	544	LEU
21	V	556	TYR
21	V	571	SER
21	V	576	THR
21	V	584	LYS
21	V	588	GLN
21	V	590	LEU
21	V	593	TYR
21	V	603	LEU
21	V	606	GLU
21	V	616	LEU
21	V	619	ASP

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Mol	Chain	Res	Type
21	V	628	ILE
21	V	633	SER
21	V	639	LEU
21	V	640	THR
21	V	645	GLU
21	V	646	HIS
21	V	648	LYS
23	X	163	GLU
23	X	176	GLU
23	X	194	ARG
23	X	225	GLU
23	X	228	LYS
23	X	232	ARG
23	X	237	LYS
23	X	239	GLU
23	X	260	VAL
23	X	270	LEU
23	X	276	VAL
23	X	290	GLU
23	X	292	LEU
23	X	293	GLU
23	X	299	HIS
23	X	304	THR
23	X	327	ARG
23	X	338	SER
23	X	339	LEU
23	X	383	SER
23	X	387	GLN
23	X	391	SER
23	X	393	GLN
23	X	408	LEU
23	X	409	LEU
23	X	436	LEU
23	X	442	THR
23	X	452	GLN
23	X	476	GLU
23	X	477	VAL
23	X	482	ARG
23	X	511	LEU
23	X	513	SER
23	X	517	VAL
23	X	533	PHE

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Mol	Chain	Res	Type
23	X	547	LYS
23	X	562	THR
23	X	579	VAL
23	X	580	ASP
23	X	599	VAL
23	X	621	ILE
23	X	622	GLU
23	X	633	ARG
23	X	643	LEU
23	X	653	SER
23	X	670	VAL
23	X	682	THR
23	X	683	ILE
23	X	712	THR
23	X	749	GLU
23	X	751	THR
23	X	757	ARG
23	X	767	LEU
23	X	768	LYS
23	X	788	THR
23	X	789	LEU
23	X	795	GLN
23	X	796	LEU
23	X	808	LEU
23	X	809	THR
23	X	836	CYS
23	X	847	LEU
23	X	849	VAL
23	X	863	HIS
23	X	895	SER
23	X	896	GLN
23	X	921	LEU
23	X	922	LEU
23	X	926	GLU
23	X	943	ILE
23	X	954	LEU
23	X	1021	LEU
24	Y	9	LEU
24	Y	14	ILE
24	Y	18	THR
24	Y	19	GLU
24	Y	20	GLU

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Mol	Chain	Res	Type
24	Y	26	LEU
24	Y	51	ILE
24	Y	61	ARG
24	Y	65	SER
24	Y	73	ASP
24	Y	85	ARG
24	Y	93	THR
24	Y	101	SER
24	Y	106	SER
24	Y	116	LEU
24	Y	117	ASP
24	Y	118	TYR
24	Y	125	VAL
24	Y	126	PHE
24	Y	129	VAL
24	Y	133	MET
24	Y	136	ILE
24	Y	159	THR
24	Y	177	ARG
24	Y	182	THR
24	Y	188	SER
24	Y	194	ASP
24	Y	199	ASP
24	Y	200	PHE
24	Y	211	ILE
24	Y	219	THR
24	Y	235	ILE
24	Y	245	CYS
24	Y	251	THR
24	Y	253	ASP
24	Y	276	LYS
24	Y	280	SER
24	Y	290	LYS
24	Y	307	ASP
24	Y	312	HIS
24	Y	318	SER
24	Y	319	VAL
35	1	493	LYS
35	1	498	MET
35	1	544	LEU
35	1	545	GLU
35	1	560	LEU

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Mol	Chain	Res	Type
35	1	562	LYS
35	1	563	LEU
35	1	564	ASP
35	1	571	VAL
35	1	581	LEU
35	1	582	LEU
35	1	585	GLU
35	1	591	VAL
35	1	592	GLU
35	1	596	ILE
35	1	598	SER
35	1	609	MET
35	1	610	ILE
35	1	613	MET
35	1	616	ASP
35	1	617	ILE
35	1	630	ARG
35	1	635	VAL
35	1	645	LEU
35	1	673	ILE
35	1	685	SER
35	1	687	VAL
35	1	691	GLU
35	1	698	GLN
35	1	701	VAL
35	1	707	LEU
35	1	736	ARG
35	1	754	ILE
35	1	760	GLU
35	1	768	GLU
35	1	769	VAL
35	1	771	LEU
35	1	779	SER
35	1	790	LYS
35	1	793	LYS
35	1	795	CYS
35	1	801	VAL
35	1	827	ARG
35	1	836	THR
35	1	837	THR
35	1	840	LEU
35	1	844	VAL

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Mol	Chain	Res	Type
35	1	858	LYS
35	1	868	VAL
35	1	873	GLU
35	1	876	MET
35	1	890	GLU
35	1	891	GLN
35	1	892	LEU
35	1	893	ILE
35	1	901	GLN
35	1	903	GLN
35	1	904	THR
35	1	905	THR
35	1	918	VAL
35	1	921	LEU
35	1	928	TYR
35	1	936	VAL
35	1	947	VAL
35	1	955	ILE
35	1	958	THR
35	1	963	LYS
35	1	964	THR
35	1	967	GLU
35	1	968	GLU
35	1	971	MET
35	1	973	HIS
35	1	980	GLU
35	1	982	LEU
35	1	989	VAL
35	1	1001	VAL
35	1	1003	VAL
35	1	1004	ILE
35	1	1006	MET
35	1	1014	LYS
35	1	1015	ASP
35	1	1021	THR
35	1	1030	LYS
35	1	1031	VAL
35	1	1038	LEU
35	1	1041	ARG
35	1	1048	GLU
35	1	1050	VAL
35	1	1065	LEU

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Mol	Chain	Res	Type
35	1	1067	LYS
35	1	1080	THR
35	1	1093	VAL
35	1	1106	ARG
35	1	1112	THR
35	1	1113	THR
35	1	1118	ILE
35	1	1121	GLU
35	1	1122	THR
35	1	1128	VAL
35	1	1138	VAL
35	1	1143	VAL
35	1	1161	MET
35	1	1164	ASP
35	1	1170	THR
35	1	1174	GLU
35	1	1182	LEU
35	1	1185	ARG
35	1	1187	THR
35	1	1196	SER
35	1	1219	VAL
35	1	1237	LEU
35	1	1241	ILE
35	1	1245	ARG
35	1	1250	CYS
35	1	1251	LEU
35	1	1260	LYS
35	1	1261	VAL
35	1	1277	GLN
35	1	1281	ILE
35	1	1294	THR
35	1	1296	ILE
35	1	1303	ILE
35	1	1304	LEU
36	3	18	ILE
36	3	25	THR
36	3	30	ILE
36	3	33	SER
36	3	36	LYS
36	3	41	LEU
36	3	44	ASP
36	3	49	LYS

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Mol	Chain	Res	Type
36	3	52	THR
36	3	56	VAL
36	3	57	GLU
36	3	66	MET
36	3	68	PHE
36	3	74	THR
36	3	78	ILE
36	3	79	VAL
36	3	80	VAL
36	3	90	LEU
36	3	98	MET
36	3	106	THR
36	3	110	SER
36	3	116	VAL
36	3	121	LEU
36	3	124	ASP
36	3	126	LYS
36	3	130	VAL
36	3	131	MET
36	3	135	ILE
36	3	139	LYS
36	3	143	ILE
36	3	153	THR
36	3	156	SER
36	3	162	LYS
36	3	170	VAL
36	3	173	VAL
36	3	188	ASP
36	3	195	ASP
36	3	204	THR
36	3	207	THR
36	3	209	THR
36	3	221	VAL
36	3	225	SER
36	3	226	GLU
36	3	230	GLU
36	3	233	ASN
36	3	235	LEU
36	3	236	ILE
36	3	237	THR
36	3	242	SER
36	3	256	ILE

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Mol	Chain	Res	Type
36	3	257	THR
36	3	261	PHE
36	3	264	GLN
36	3	266	ASP
36	3	271	ILE
36	3	273	ARG
36	3	275	ARG
36	3	286	ILE
36	3	294	LYS
36	3	297	SER
36	3	310	ILE
36	3	315	LEU
36	3	317	THR
36	3	320	ASP
36	3	321	MET
36	3	327	LEU
36	3	332	THR
36	3	333	VAL
36	3	335	VAL
36	3	340	CYS
36	3	343	LYS
36	3	344	THR
36	3	347	LEU
36	3	355	ASN
36	3	356	HIS
36	3	364	LEU
36	3	370	GLU
36	3	384	THR
36	3	390	ARG
36	3	392	LEU
36	3	403	SER
36	3	404	LEU
36	3	412	ILE
36	3	427	CYS
36	3	433	SER
36	3	435	LEU
36	3	439	ARG
36	3	443	GLU
36	3	459	VAL
36	3	461	THR
36	3	462	VAL
36	3	464	ARG

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Mol	Chain	Res	Type
36	3	465	HIS
36	3	466	ILE
36	3	469	GLU
36	3	471	ASP
36	3	474	ILE
36	3	475	ILE
36	3	482	THR
36	3	492	GLU
36	3	511	LEU
36	3	514	ASP
36	3	527	ILE
36	3	537	LYS
36	3	541	LYS
36	3	543	THR
36	3	544	ILE
36	3	555	VAL
36	3	556	ILE
36	3	563	LEU
36	3	564	VAL
36	3	568	MET
36	3	574	LEU
36	3	578	THR
36	3	584	SER
36	3	592	LEU
36	3	594	ASN
36	3	595	VAL
36	3	603	ARG
36	3	604	PHE
36	3	605	LEU
36	3	614	VAL
36	3	617	ILE
36	3	620	ASP
36	3	626	GLN
36	3	630	MET
36	3	642	ILE
36	3	643	VAL
36	3	665	LEU
36	3	669	LEU
36	3	675	LEU
36	3	676	ARG
36	3	677	THR
36	3	678	VAL

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Mol	Chain	Res	Type
36	3	679	LEU
36	3	685	ASP
36	3	689	THR
36	3	697	ARG
36	3	703	ARG
36	3	704	VAL
36	3	715	MET
36	3	721	LEU
36	3	726	GLN
36	3	727	SER
36	3	732	THR
36	3	738	THR
36	3	758	SER
36	3	761	THR
36	3	775	ASN
36	3	776	GLN
36	3	797	LEU
36	3	798	ILE
36	3	802	THR
36	3	818	GLN
36	3	821	GLU
36	3	822	GLU
36	3	834	LEU
36	3	837	GLU
36	3	850	SER
36	3	851	ILE
36	3	865	VAL
36	3	867	ARG
36	3	868	VAL
36	3	876	THR
36	3	882	LEU
36	3	883	GLU
36	3	897	SER
36	3	901	GLU
36	3	902	ASP
36	3	920	VAL
36	3	925	VAL
36	3	927	THR
36	3	931	VAL
36	3	937	LEU
36	3	941	HIS
36	3	942	LYS

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Mol	Chain	Res	Type
36	3	943	THR
36	3	945	VAL
36	3	948	VAL
36	3	958	ARG
36	3	959	VAL
36	3	960	LEU
36	3	961	ILE
36	3	966	LEU
36	3	968	ARG
36	3	969	VAL
36	3	978	LEU
36	3	981	CYS
36	3	988	ASN
36	3	991	SER
36	3	993	ILE
36	3	995	THR
36	3	996	ILE
36	3	998	HIS
36	3	1000	VAL
36	3	1002	VAL
36	3	1012	VAL
36	3	1022	ILE
36	3	1026	ASP
36	3	1028	THR
36	3	1033	VAL
36	3	1035	THR
36	3	1042	ASP
36	3	1056	VAL
36	3	1062	THR
36	3	1066	VAL
36	3	1090	GLU
36	3	1093	MET
36	3	1094	ASN
36	3	1099	GLU
36	3	1101	VAL
36	3	1103	SER
36	3	1107	THR
36	3	1114	SER
36	3	1116	SER
36	3	1118	VAL
36	3	1120	THR
36	3	1121	THR

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Mol	Chain	Res	Type
36	3	1135	HIS
36	3	1148	LEU
36	3	1150	SER
36	3	1151	GLU
36	3	1168	PHE
36	3	1170	VAL
36	3	1183	ASN
36	3	1184	SER
36	3	1193	VAL
38	w	390	LYS
38	w	400	HIS
38	w	403	ASN
38	w	414	TYR
38	w	415	THR
38	w	425	HIS
38	w	430	ARG
38	w	437	CYS
38	w	446	PHE
38	w	453	GLU
38	w	458	LEU
38	w	463	LYS
38	w	468	SER
38	w	471	TRP
38	w	475	THR
38	w	487	VAL
38	w	500	LEU
39	2	451	LYS
39	2	460	PHE
39	2	461	THR
39	2	465	LEU
39	2	471	ARG
39	2	474	VAL
39	2	475	VAL
39	2	477	MET
39	2	488	LEU
39	2	494	THR
39	2	505	CYS
39	2	509	LYS
39	2	512	GLN
39	2	517	ILE
39	2	524	LEU
39	2	526	ASP

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Mol	Chain	Res	Type
39	2	528	ILE
39	2	531	THR
39	2	543	LYS
39	2	557	VAL
39	2	561	MET
39	2	564	ILE
39	2	590	LEU
39	2	595	LYS
39	2	705	ARG
41	7	9	ILE
41	7	11	CYS
41	7	14	GLN
41	7	23	CYS
41	7	25	LYS
41	7	30	CYS
41	7	32	ILE
41	7	35	SER
41	7	37	VAL
41	7	40	CYS
41	7	45	ILE
41	7	48	GLU
41	7	60	ILE
41	7	68	ASP
41	7	71	TYR
41	7	89	VAL
42	5	5	TYR
42	5	11	LEU
42	5	12	GLU
42	5	23	HIS
42	5	25	ASP
42	5	26	THR
42	5	27	THR
42	5	32	LEU
42	5	33	VAL
42	5	35	GLN
42	5	36	HIS
42	5	42	SER
42	5	51	ASN
42	5	57	GLU
42	5	60	SER
42	5	63	ARG
42	5	65	ARG

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Mol	Chain	Res	Type
42	5	69	MET
42	5	72	MET
42	5	74	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	41	GLN
1	A	57	GLN
1	A	73	HIS
1	A	78	ASN
1	A	105	ASN
1	A	143	GLN
1	A	181	ASN
1	A	321	ASN
1	A	322	ASN
1	A	325	HIS
1	A	326	HIS
1	A	439	GLN
1	A	461	HIS
1	A	495	GLN
1	A	502	ASN
1	A	654	ASN
1	A	659	GLN
1	A	664	HIS
1	A	711	GLN
1	A	755	HIS
1	A	775	ASN
1	A	788	GLN
1	A	1013	ASN
1	A	1014	ASN
1	A	1056	HIS
1	A	1117	HIS
1	A	1121	ASN
1	A	1293	ASN
1	A	1337	GLN
1	A	1424	GLN
1	A	1460	HIS
1	A	1520	ASN
1	A	1546	ASN
1	A	1552	GLN

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Mol	Chain	Res	Type
1	A	1554	GLN
1	A	1583	GLN
1	A	1623	ASN
1	A	1658	GLN
1	A	1710	ASN
1	A	1774	ASN
1	A	1804	ASN
1	A	1816	GLN
1	A	1823	HIS
1	A	1830	GLN
1	A	1835	GLN
1	A	1857	GLN
1	A	1894	GLN
1	A	1944	HIS
3	C	82	GLN
3	C	306	ASN
3	C	313	GLN
3	C	350	ASN
3	C	402	HIS
3	C	437	HIS
3	C	538	HIS
3	C	627	HIS
3	C	903	HIS
3	C	924	GLN
3	C	928	HIS
4	E	108	HIS
4	E	188	GLN
4	E	225	ASN
4	E	257	ASN
4	E	278	GLN
9	J	181	ASN
9	J	238	ASN
9	J	410	HIS
11	L	30	GLN
11	L	45	GLN
11	L	81	GLN
11	L	163	GLN
12	M	134	GLN
12	M	172	HIS
12	M	189	GLN
12	M	215	ASN
12	M	219	ASN

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Mol	Chain	Res	Type
13	N	37	HIS
13	N	95	GLN
14	O	120	ASN
15	P	45	GLN
15	P	212	ASN
17	R	104	GLN
17	R	184	GLN
17	R	243	GLN
17	R	279	HIS
17	R	357	HIS
17	R	364	GLN
17	R	381	GLN
17	R	398	ASN
17	R	431	ASN
19	T	203	HIS
19	T	216	ASN
19	T	269	GLN
19	T	344	GLN
19	T	407	GLN
19	T	408	ASN
19	T	446	ASN
21	V	451	ASN
21	V	532	GLN
21	V	542	ASN
21	V	553	HIS
21	V	609	GLN
23	X	173	GLN
23	X	387	GLN
23	X	414	ASN
23	X	475	ASN
23	X	523	HIS
23	X	675	ASN
23	X	697	GLN
23	X	745	HIS
23	X	803	ASN
23	X	850	ASN
23	X	863	HIS
23	X	904	GLN
23	X	917	GLN
24	Y	52	GLN
24	Y	74	GLN
24	Y	99	ASN

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Mol	Chain	Res	Type
24	Y	115	ASN
24	Y	123	HIS
24	Y	140	ASN
24	Y	240	ASN
35	1	550	HIS
35	1	599	ASN
35	1	669	GLN
35	1	682	HIS
35	1	817	HIS
35	1	821	HIS
35	1	829	ASN
35	1	886	HIS
35	1	1007	HIS
35	1	1026	ASN
35	1	1028	HIS
35	1	1032	GLN
35	1	1134	ASN
35	1	1225	HIS
35	1	1277	GLN
36	3	5	ASN
36	3	19	HIS
36	3	46	ASN
36	3	145	ASN
36	3	169	HIS
36	3	179	ASN
36	3	194	ASN
36	3	205	GLN
36	3	206	GLN
36	3	219	HIS
36	3	231	HIS
36	3	233	ASN
36	3	264	GLN
36	3	304	GLN
36	3	411	GLN
36	3	440	HIS
36	3	480	ASN
36	3	518	GLN
36	3	550	ASN
36	3	573	GLN
36	3	612	ASN
36	3	636	GLN
36	3	671	ASN

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Mol	Chain	Res	Type
36	3	709	GLN
36	3	730	HIS
36	3	775	ASN
36	3	796	ASN
36	3	844	ASN
36	3	861	GLN
36	3	881	GLN
36	3	933	ASN
36	3	994	GLN
36	3	1019	ASN
36	3	1052	ASN
36	3	1105	GLN
38	w	407	ASN
38	w	413	ASN
38	w	445	HIS
39	2	546	GLN
39	2	587	HIS
41	7	55	GLN
41	7	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	28 (29%)	3 (3%)
5	F	96/107 (89%)	42 (43%)	6 (6%)
6	G	77/220 (35%)	44 (57%)	12 (15%)
7	H	163/188 (86%)	69 (42%)	9 (5%)
All	All	432/632 (68%)	183 (42%)	30 (6%)

All (183) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	U
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	26	A

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Mol	Chain	Res	Type
2	B	40	U
2	B	43	U
2	B	45	C
2	B	47	A
2	B	48	A
2	B	52	U
2	B	65	G
2	B	70	A
2	B	71	C
2	B	88	A
2	B	89	U
2	B	90	U
2	B	92	U
2	B	93	U
2	B	94	U
2	B	95	G
2	B	96	A
2	B	97	G
2	B	109	G
5	F	6	C
5	F	7	G
5	F	9	U
5	F	10	U
5	F	11	C
5	F	12	G
5	F	14	C
5	F	16	G
5	F	25	C
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	30	A
5	F	33	G
5	F	34	G
5	F	35	A
5	F	37	C
5	F	38	G
5	F	40	U
5	F	44	G
5	F	45	A
5	F	48	A

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Mol	Chain	Res	Type
5	F	54	G
5	F	59	G
5	F	60	C
5	F	61	C
5	F	65	G
5	F	66	C
5	F	68	C
5	F	73	A
5	F	74	U
5	F	75	G
5	F	79	C
5	F	80	G
5	F	81	C
5	F	82	A
5	F	83	A
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	C
6	G	-10	G
6	G	-9	C
6	G	-8	C
6	G	-7	U
6	G	-5	C
6	G	-4	G
6	G	1	G
6	G	2	U
6	G	3	A
6	G	4	A
6	G	8	C
6	G	9	C
6	G	11	A
6	G	13	C
6	G	17	U
6	G	21	A
6	G	22	C
6	G	23	U
6	G	25	G
6	G	26	U
6	G	27	U
6	G	30	C
6	G	84	U

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Mol	Chain	Res	Type
6	G	85	G
6	G	88	G
6	G	89	U
6	G	90	C
6	G	92	U
6	G	97	A
6	G	98	U
6	G	100	C
6	G	101	U
6	G	102	G
6	G	103	U
6	G	104	C
6	G	106	C
6	G	107	U
6	G	111	U
6	G	112	U
6	G	113	U
6	G	114	U
6	G	115	C
6	G	116	C
6	G	117	A
7	H	15	U
7	H	16	U
7	H	17	U
7	H	19	G
7	H	23	A
7	H	24	A
7	H	29	A
7	H	30	A
7	H	31	G
7	H	33	G
7	H	34	U
7	H	35	A
7	H	44	U
7	H	45	C
7	H	46	U
7	H	47	U
7	H	48	A
7	H	49	U
7	H	53	U
7	H	63	G
7	H	64	A

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Mol	Chain	Res	Type
7	H	65	U
7	H	70	C
7	H	74	U
7	H	80	A
7	H	81	G
7	H	82	G
7	H	84	C
7	H	98	G
7	H	99	A
7	H	100	U
7	H	101	U
7	H	102	U
7	H	103	U
7	H	106	G
7	H	107	A
7	H	110	A
7	H	111	G
7	H	112	G
7	H	113	G
7	H	116	A
7	H	117	U
7	H	121	A
7	H	122	U
7	H	123	A
7	H	124	G
7	H	128	C
7	H	129	U
7	H	133	U
7	H	136	G
7	H	137	U
7	H	141	C
7	H	144	C
7	H	145	A
7	H	146	C
7	H	147	G
7	H	149	A
7	H	157	G
7	H	162	U
7	H	164	C
7	H	165	A
7	H	166	G
7	H	168	A

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Mol	Chain	Res	Type
7	H	169	C
7	H	171	U
7	H	177	A
7	H	178	A
7	H	179	C
7	H	180	G

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C
2	B	94	U
2	B	96	A
5	F	37	C
5	F	47	A
5	F	58	G
5	F	79	C
5	F	84	A
5	F	86	U
6	G	1	G
6	G	21	A
6	G	84	U
6	G	88	G
6	G	89	U
6	G	100	C
6	G	101	U
6	G	102	G
6	G	103	U
6	G	105	C
6	G	111	U
6	G	113	U
7	H	15	U
7	H	16	U
7	H	29	A
7	H	30	A
7	H	31	G
7	H	43	U
7	H	45	C
7	H	47	U
7	H	165	A

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

2 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	$\# Z > 2$
17	SEP	R	232	17	8,9,10	1.57	1 (12%)	7,12,14	1.14	0
17	SEP	R	224	17	8,9,10	1.47	1 (12%)	7,12,14	1.25	1 (14%)

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
17	SEP	R	232	17	-	3/6/8/10	-
17	SEP	R	224	17	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	232	SEP	P-O1P	3.35	1.60	1.50
17	R	224	SEP	P-O1P	3.26	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	224	SEP	OG-CB-CA	2.44	110.52	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	R	224	SEP	N-CA-CB-OG
17	R	224	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
17	R	232	SEP	C-CA-CB-OG
17	R	232	SEP	CB-OG-P-O2P
17	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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$
45	GTP	C	1500	46	33,34,34	1.12	3 (9%)	50,54,54	1.96	12 (24%)
44	IHP	A	3000	-	36,36,36	1.02	1 (2%)	60,60,60	2.04	15 (25%)

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
45	GTP	C	1500	46	-	5/22/38/38	0/3/3/3
44	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C5-N7	-2.35	1.34	1.39
44	A	3000	IHP	P5-O15	2.17	1.63	1.59
45	C	1500	GTP	C5-C6	-2.03	1.37	1.44
45	C	1500	GTP	O4'-C4'	-2.01	1.40	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1500	GTP	C5-C4-N3	-6.08	118.72	128.39
45	C	1500	GTP	C2-N3-C4	4.85	120.65	112.30
44	A	3000	IHP	O41-P1-O31	4.76	125.65	107.80
44	A	3000	IHP	O15-C5-C4	4.72	118.81	108.76
44	A	3000	IHP	C5-C4-C3	4.57	120.46	110.43
44	A	3000	IHP	O41-P1-O11	-4.46	88.48	105.85
45	C	1500	GTP	N9-C4-N3	4.43	134.80	125.95
44	A	3000	IHP	P3-O13-C3	-4.41	111.67	123.43
44	A	3000	IHP	C5-C6-C1	4.37	120.02	110.43
44	A	3000	IHP	P6-O16-C6	-4.35	111.83	123.43
45	C	1500	GTP	C2-N1-C6	-3.79	118.23	125.11
44	A	3000	IHP	C4-C3-C2	3.14	117.31	110.43
45	C	1500	GTP	C5-C6-N1	3.05	121.03	113.25
44	A	3000	IHP	O16-C6-C5	3.04	115.22	108.76
45	C	1500	GTP	N9-C8-N7	-2.95	107.94	113.40
44	A	3000	IHP	O15-C5-C6	2.93	114.99	108.76
45	C	1500	GTP	O2G-PG-O3B	2.89	114.31	104.64
44	A	3000	IHP	C6-C1-C2	2.67	116.29	110.43
45	C	1500	GTP	C8-N7-C5	2.65	108.98	104.26
44	A	3000	IHP	P1-O11-C1	-2.62	116.43	123.43
45	C	1500	GTP	O6-C6-C5	-2.60	119.66	126.53
44	A	3000	IHP	O36-P6-O26	2.49	120.54	110.83
44	A	3000	IHP	O12-P2-O22	-2.45	100.61	109.33
45	C	1500	GTP	O5'-C5'-C4'	2.28	116.76	108.99
45	C	1500	GTP	O2A-PA-O3A	2.17	113.14	107.27
44	A	3000	IHP	O13-C3-C4	2.11	113.24	108.76
45	C	1500	GTP	O2'-C2'-C1'	-2.01	103.17	110.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C3-C4-O14-P4
45	C	1500	GTP	C4'-C5'-O5'-PA

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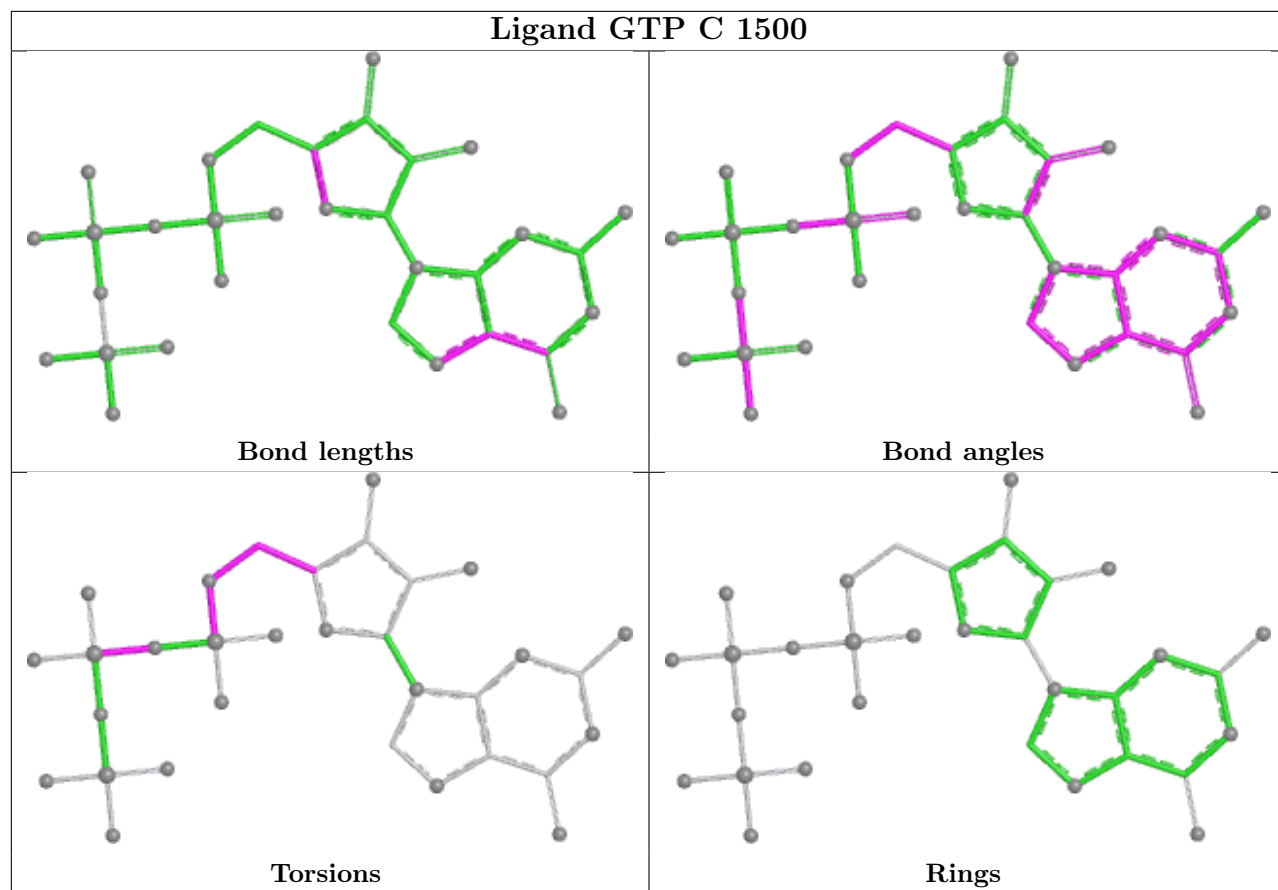
Mol	Chain	Res	Type	Atoms
45	C	1500	GTP	C3'-C4'-C5'-O5'
45	C	1500	GTP	O4'-C4'-C5'-O5'
44	A	3000	IHP	C1-C6-O16-P6
45	C	1500	GTP	C5'-O5'-PA-O1A
44	A	3000	IHP	C3-O13-P3-O23
44	A	3000	IHP	C5-O15-P5-O25
44	A	3000	IHP	C3-O13-P3-O43
44	A	3000	IHP	C1-O11-P1-O21
45	C	1500	GTP	PA-O3A-PB-O2B

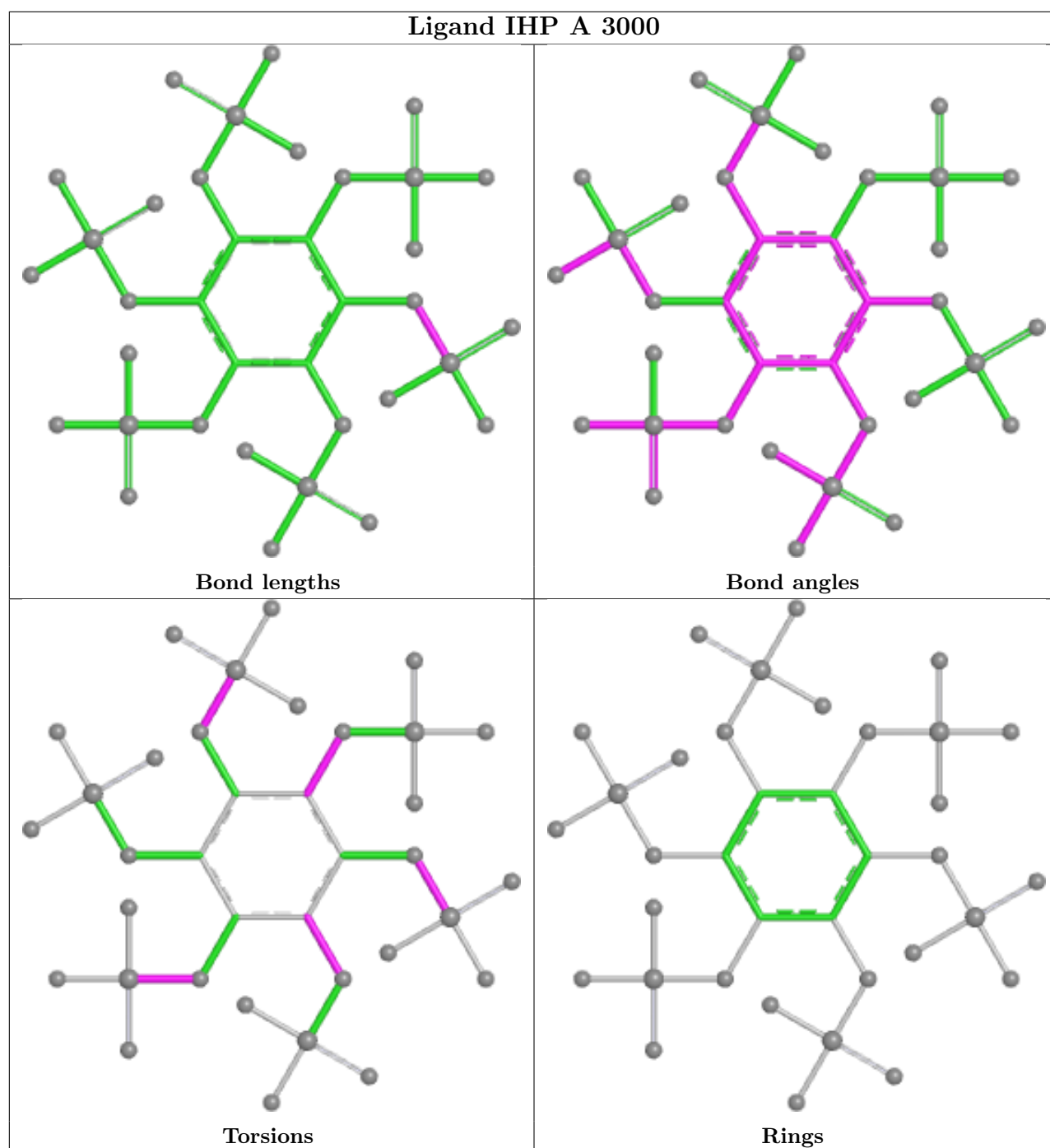
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	3000	IHP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

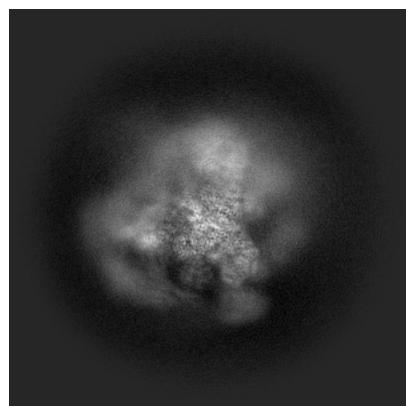
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35110. These allow visual inspection of the internal detail of the map and identification of artifacts.

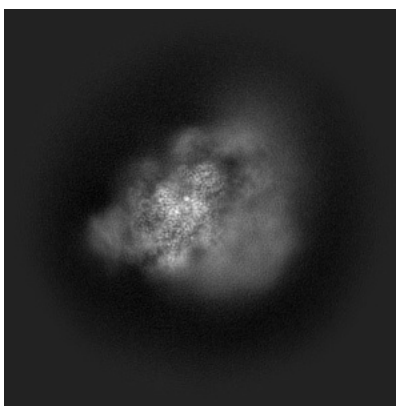
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

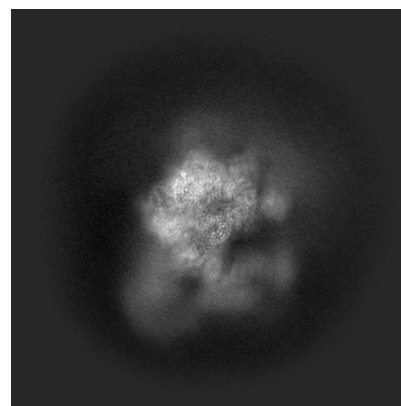
6.1.1 Primary map



X

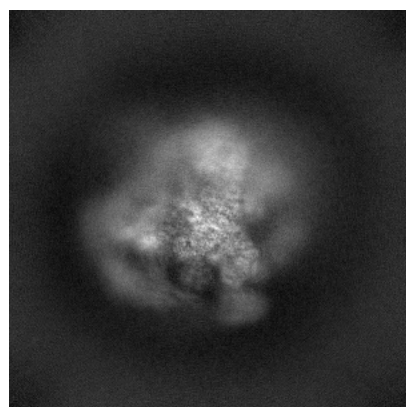


Y

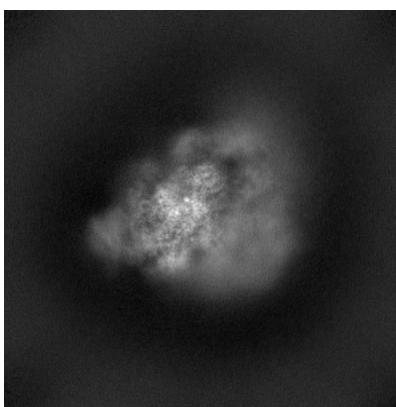


Z

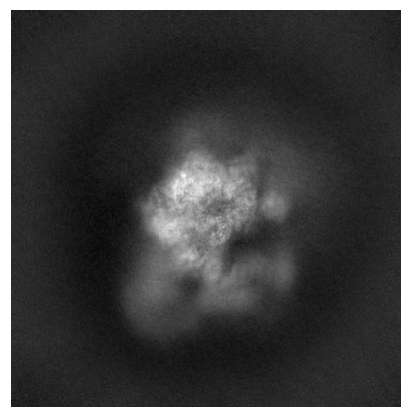
6.1.2 Raw map



X



Y

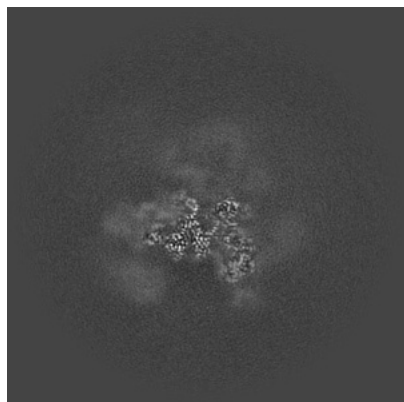


Z

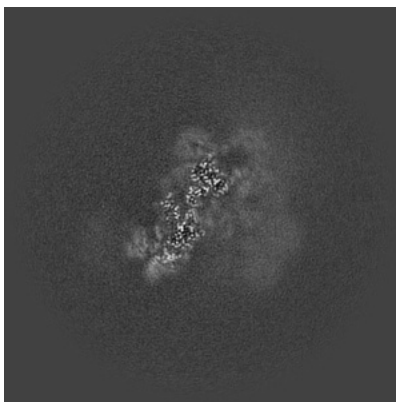
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

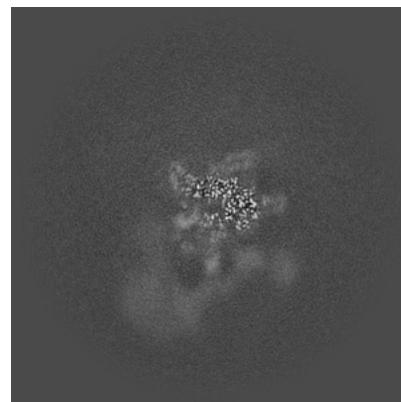
6.2.1 Primary map



X Index: 240

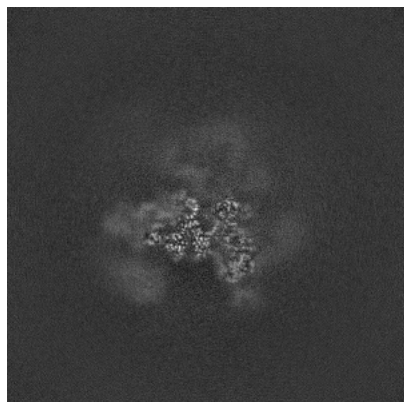


Y Index: 240

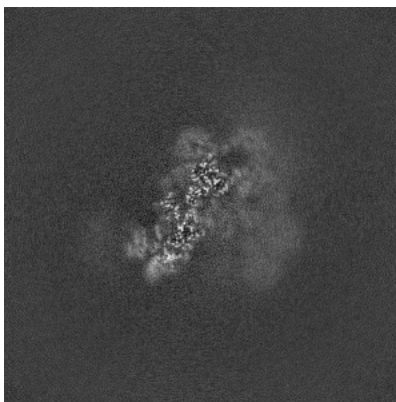


Z Index: 240

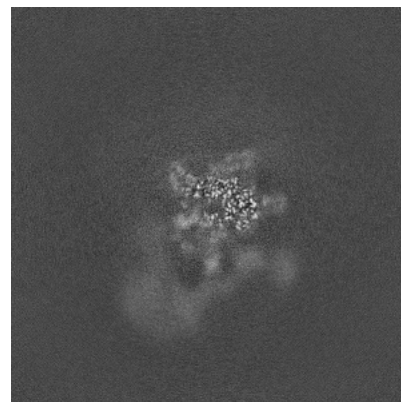
6.2.2 Raw map



X Index: 240



Y Index: 240

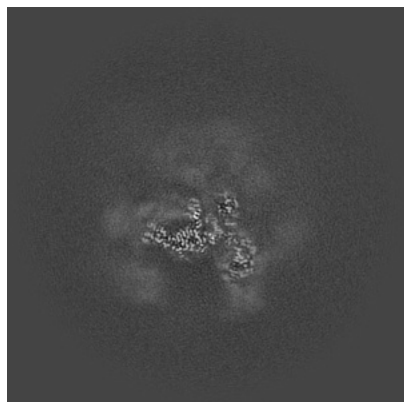


Z Index: 240

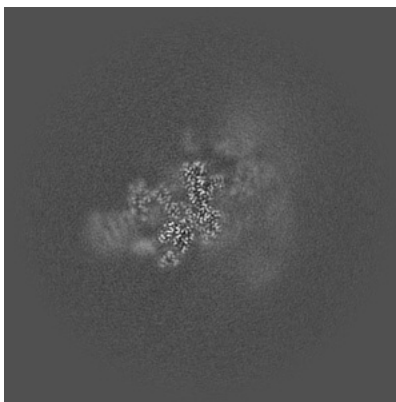
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

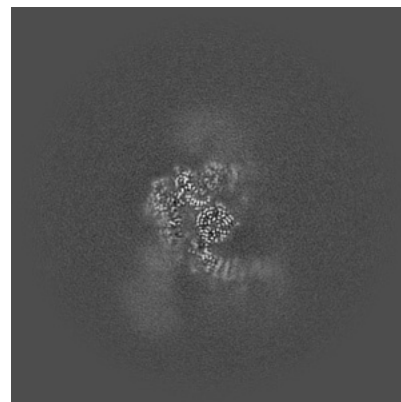
6.3.1 Primary map



X Index: 235

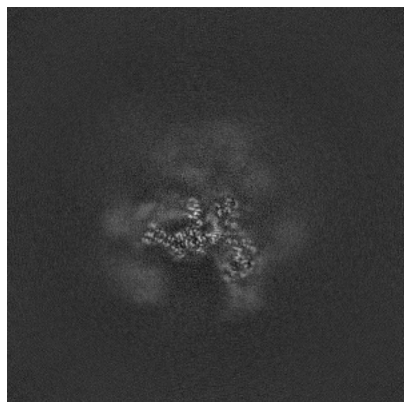


Y Index: 262

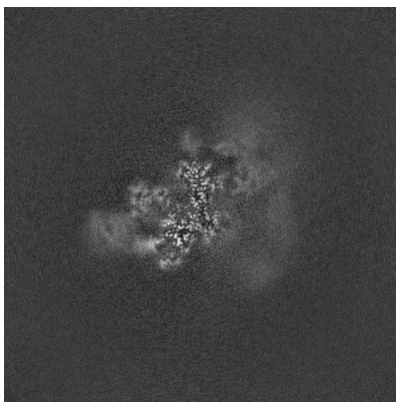


Z Index: 200

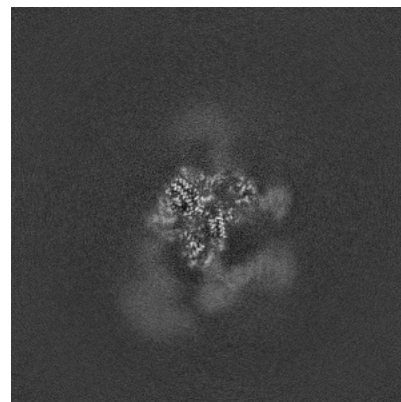
6.3.2 Raw map



X Index: 236



Y Index: 259

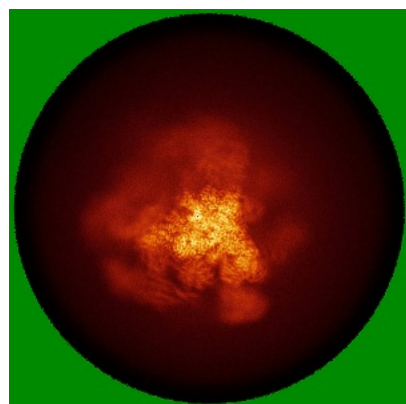


Z Index: 218

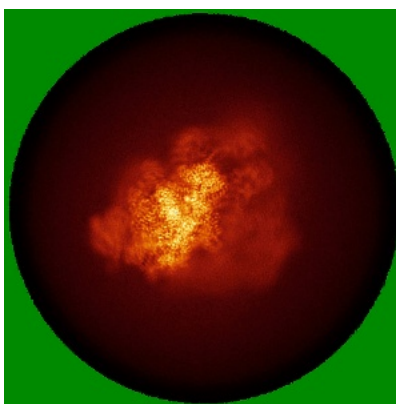
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

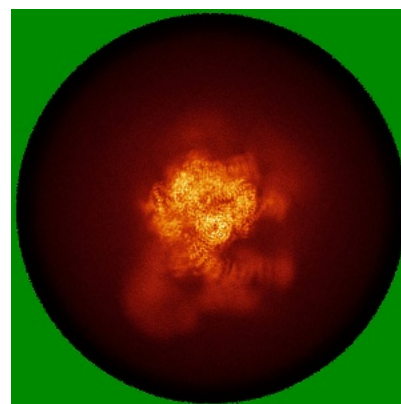
6.4.1 Primary map



X

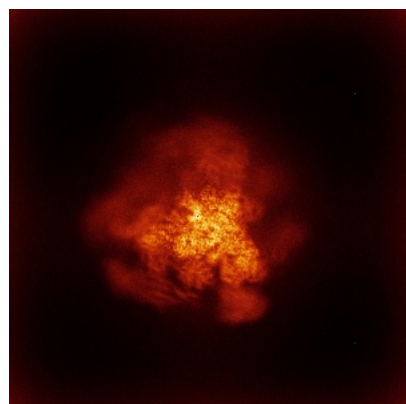


Y

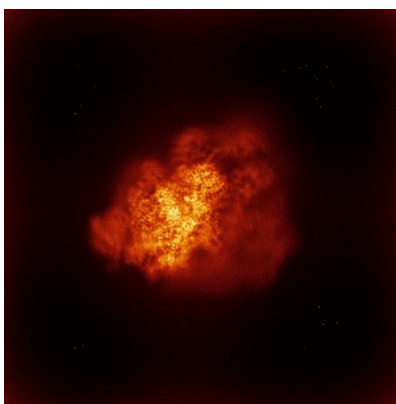


Z

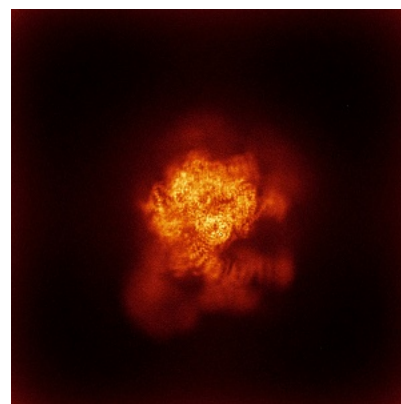
6.4.2 Raw map



X



Y

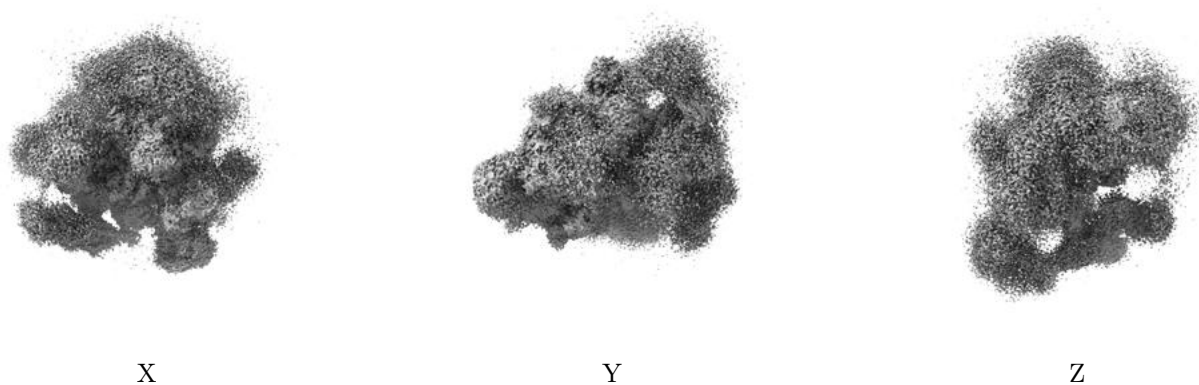


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

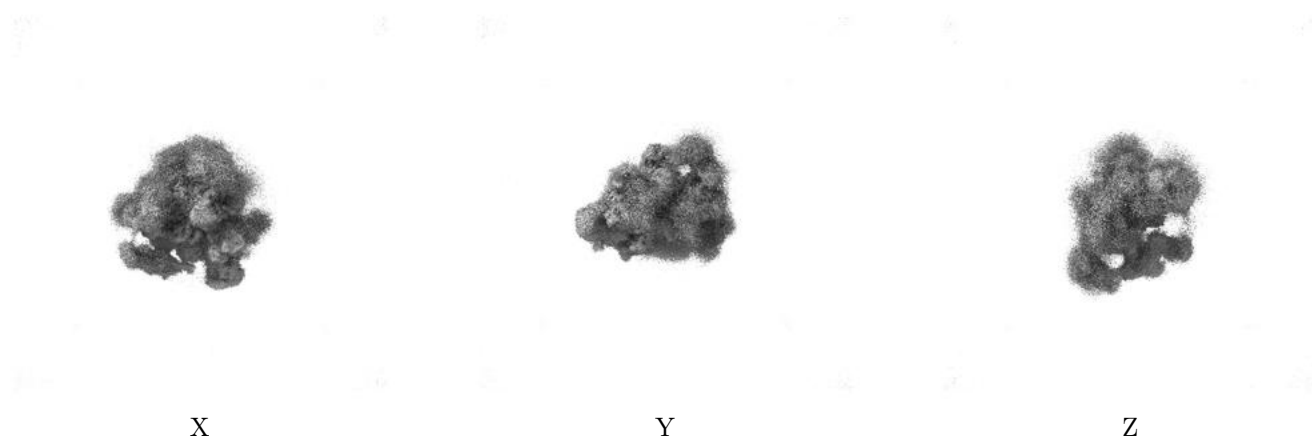
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

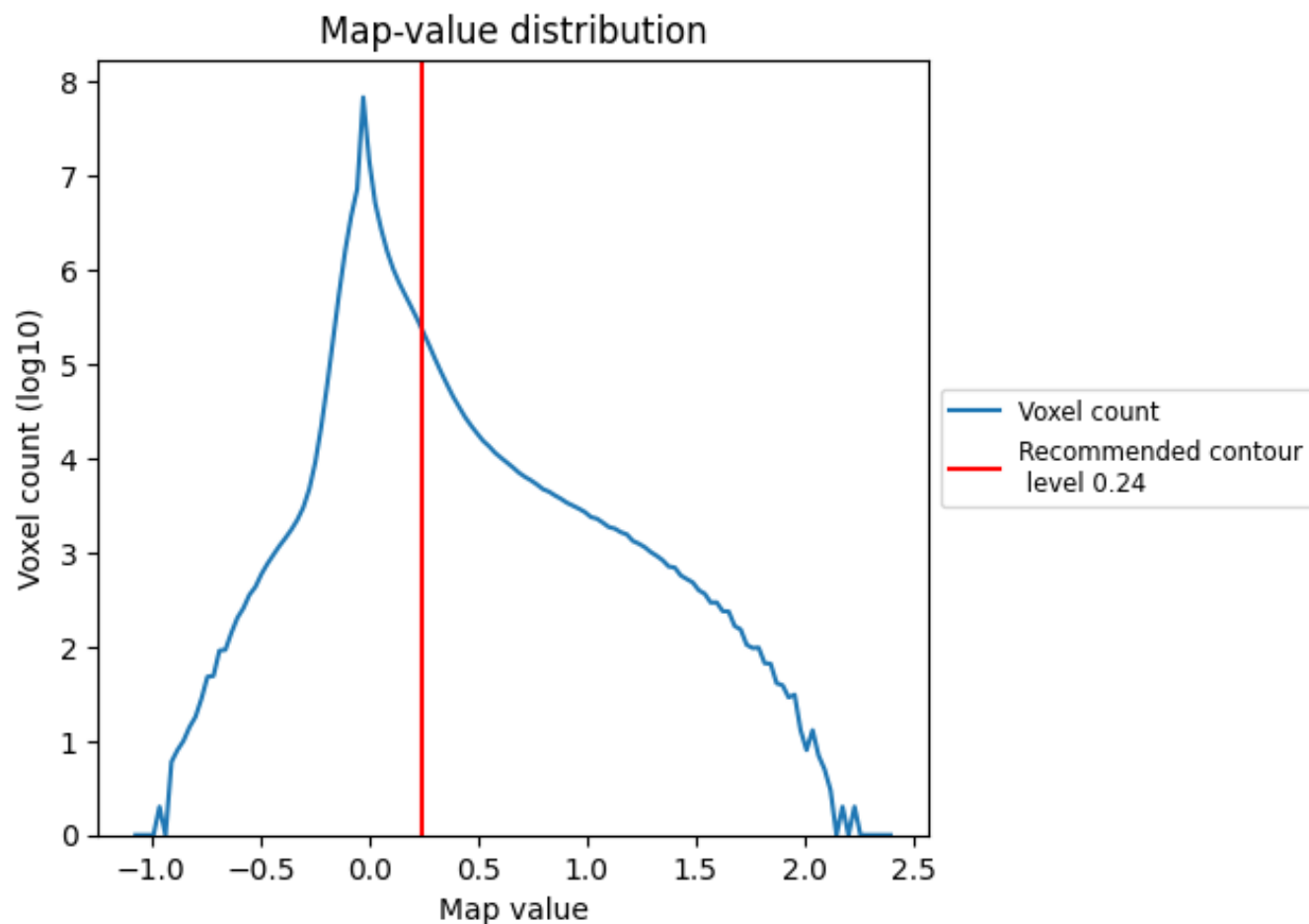
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

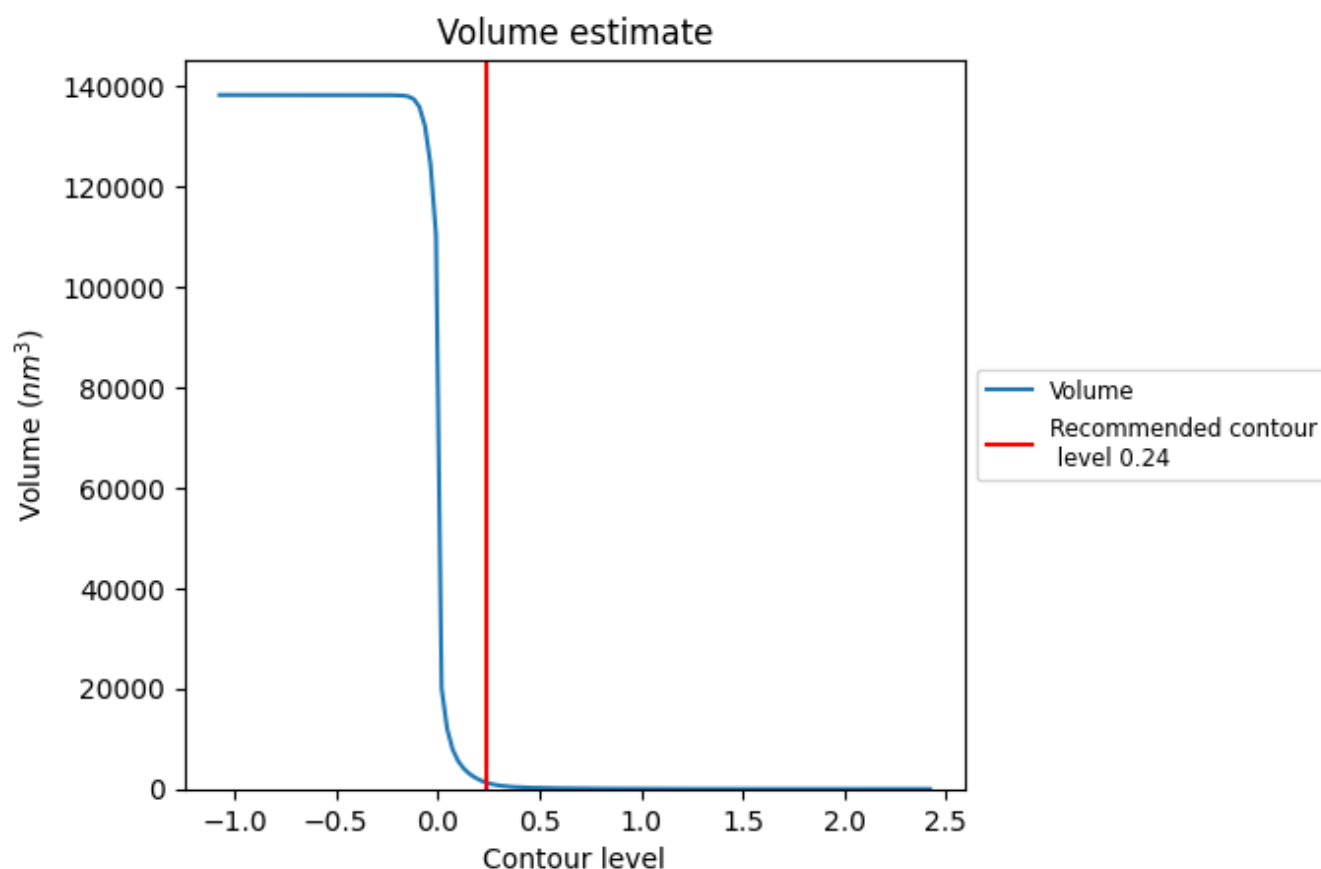
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

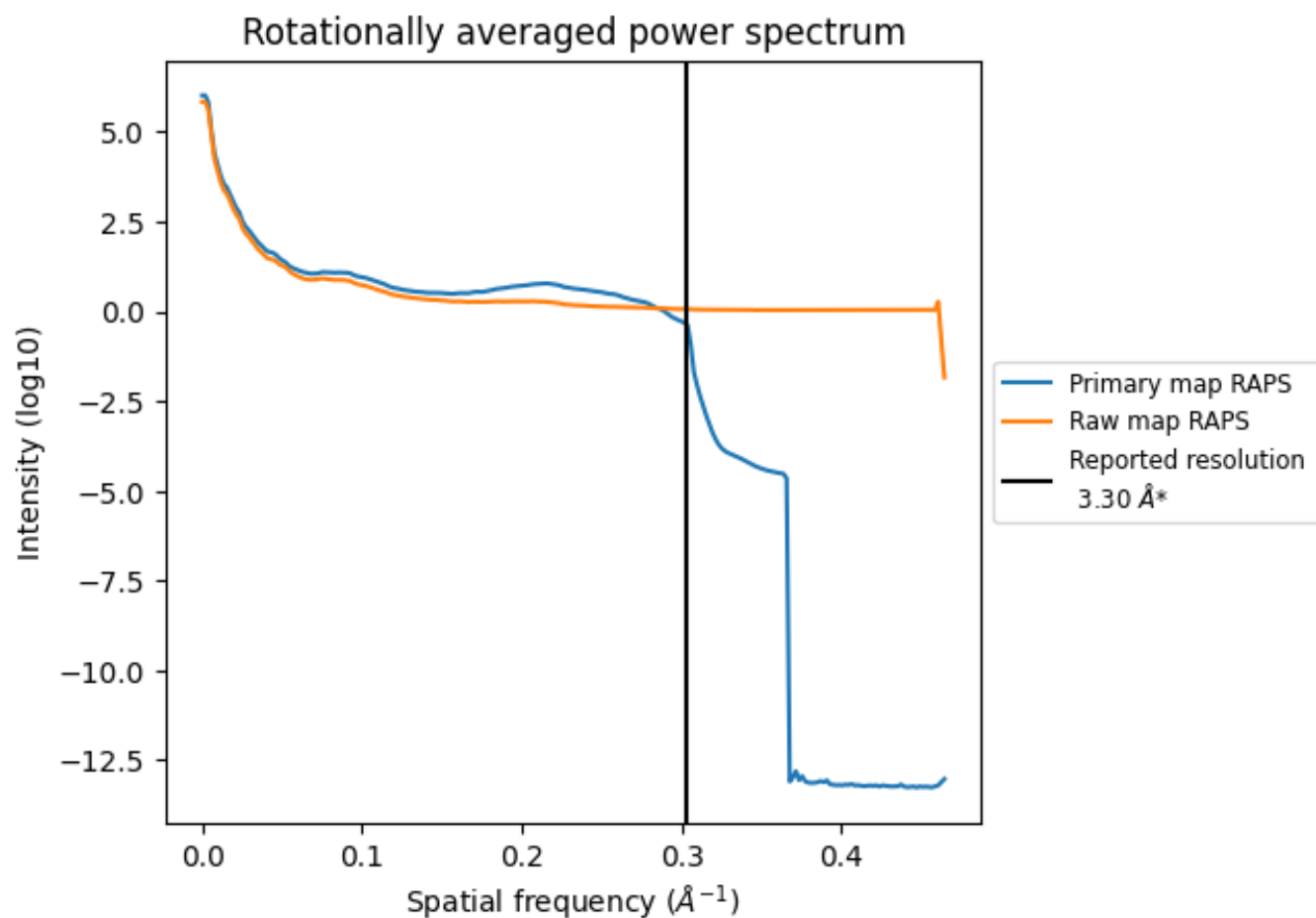
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1270 nm^3 ; this corresponds to an approximate mass of 1147 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

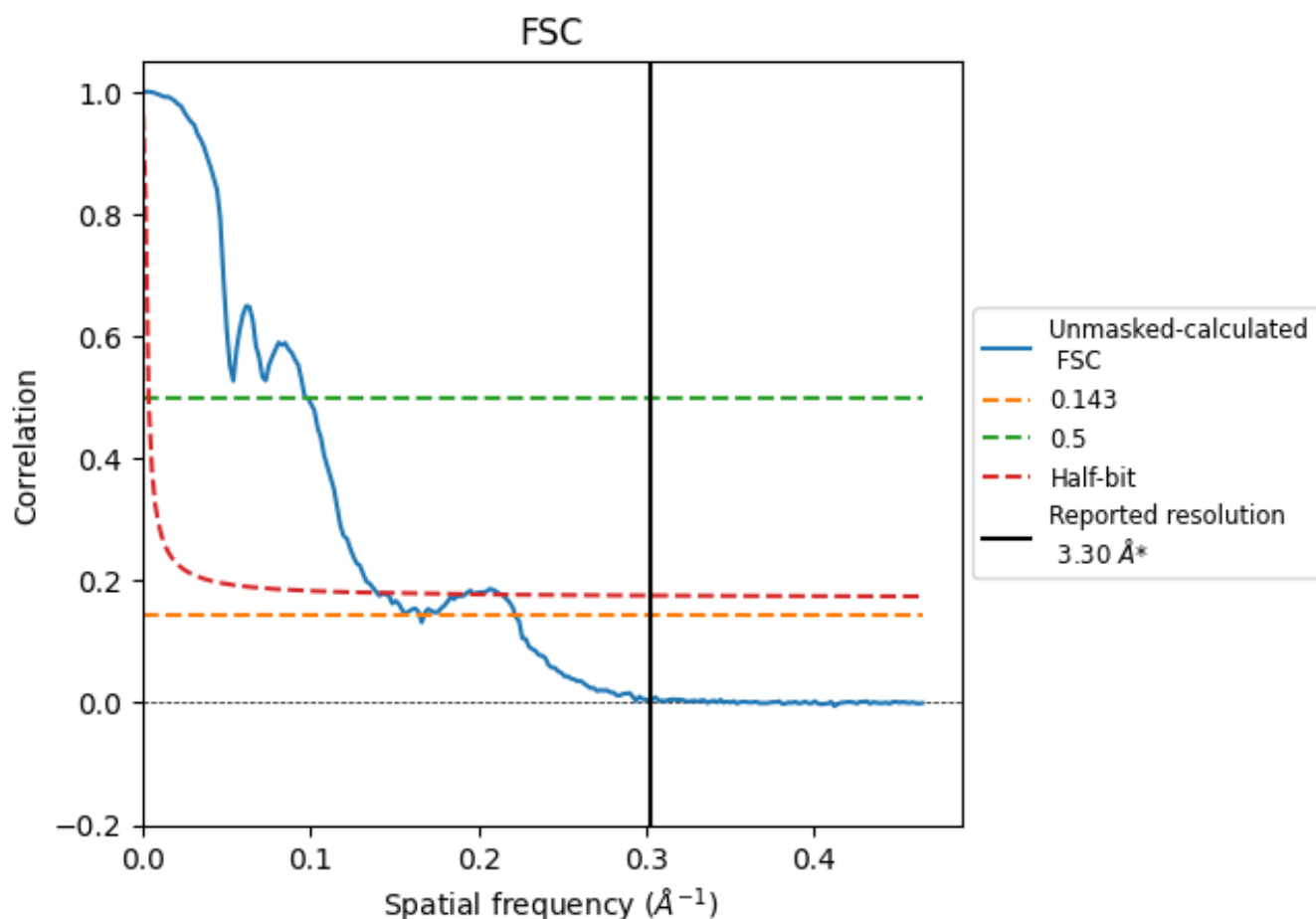


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

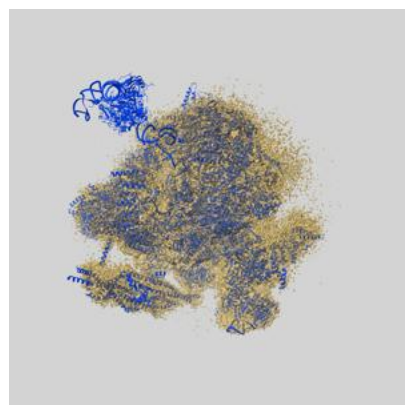
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.06	10.25	7.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.06 differs from the reported value 3.3 by more than 10 %

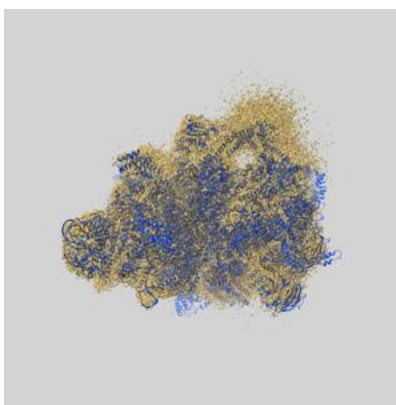
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35110 and PDB model 8I0U. Per-residue inclusion information can be found in section 3 on page 14.

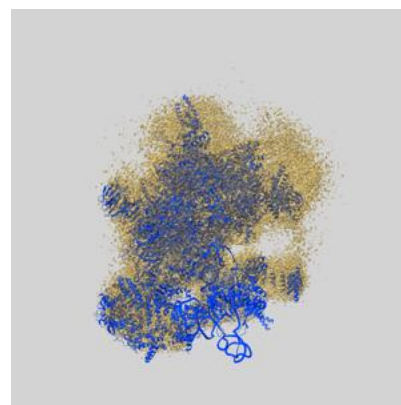
9.1 Map-model overlay [i](#)



X



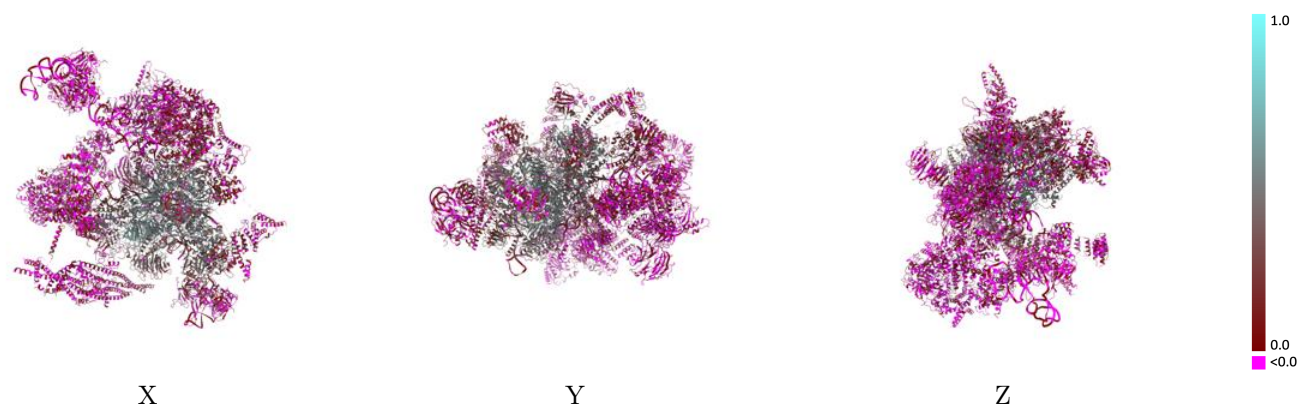
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

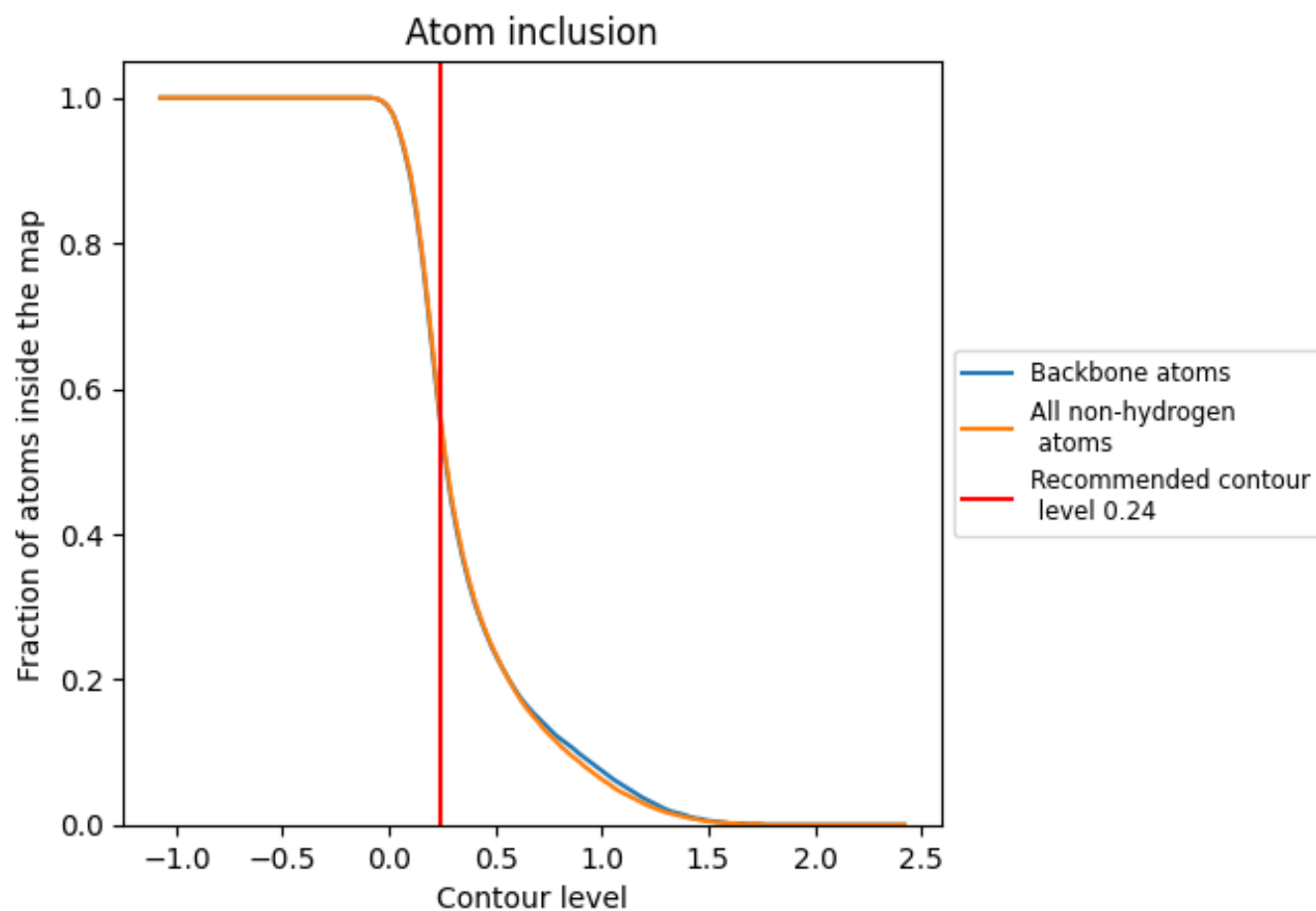


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5640	 0.1950
1	 0.3010	 0.0610
2	 0.1370	 0.0270
3	 0.1540	 0.0140
4	 0.0820	 0.0730
5	 0.1900	 0.0420
7	 0.2500	 0.0280
A	 0.8410	 0.4130
B	 0.8840	 0.2950
C	 0.9260	 0.3690
E	 0.9220	 0.3010
F	 0.8990	 0.3120
G	 0.7160	 0.1670
H	 0.2260	 0.0480
I	 0.4770	 0.0620
J	 0.7680	 0.2640
K	 0.5190	 0.1250
L	 0.7490	 0.2670
M	 0.7880	 0.2730
N	 0.9310	 0.4230
O	 0.8600	 0.3210
P	 0.8790	 0.4120
Q	 0.1160	 0.0130
R	 0.8110	 0.3270
S	 0.8680	 0.1710
T	 0.9810	 0.5470
U	 0.6150	 0.2860
V	 0.5210	 0.1380
W	 0.3650	 0.0840
X	 0.6580	 0.1520
Y	 0.7070	 0.1480
Z	 0.5870	 0.0830
a	 0.7410	 0.1220
b	 0.8170	 0.0700
c	 0.6830	 0.0420



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Chain	Atom inclusion	Q-score
d	 0.7370	 0.0720
e	 0.7220	 0.0200
f	 0.7030	 0.0640
g	 0.8890	 0.1830
h	 0.0000	 -0.0280
i	 0.0000	 0.0130
j	 0.0000	 0.0080
k	 0.0000	 -0.0330
l	 0.0020	 0.0010
m	 0.0000	 0.0040
n	 0.0000	 0.0480
o	 0.0000	 -0.0050
p	 0.0020	 0.0130
q	 0.2560	 0.0050
r	 0.4110	 0.0430
s	 0.3380	 0.0280
t	 0.2160	 0.0160
w	 0.1590	 0.0060
y	 0.1270	 0.0130