



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:02 AM UTC

PDB ID : 8H6L / pdb_00008h6l
EMDB ID : EMD-34508
Title : Cryo-EM structure of human exon-defined spliceosome in the early B state.
Authors : Zhang, W.; Zhan, X.; Zhang, X.; Bai, R.; Lei, J.; Yan, C.; Shi, Y.
Deposited on : 2022-10-18
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

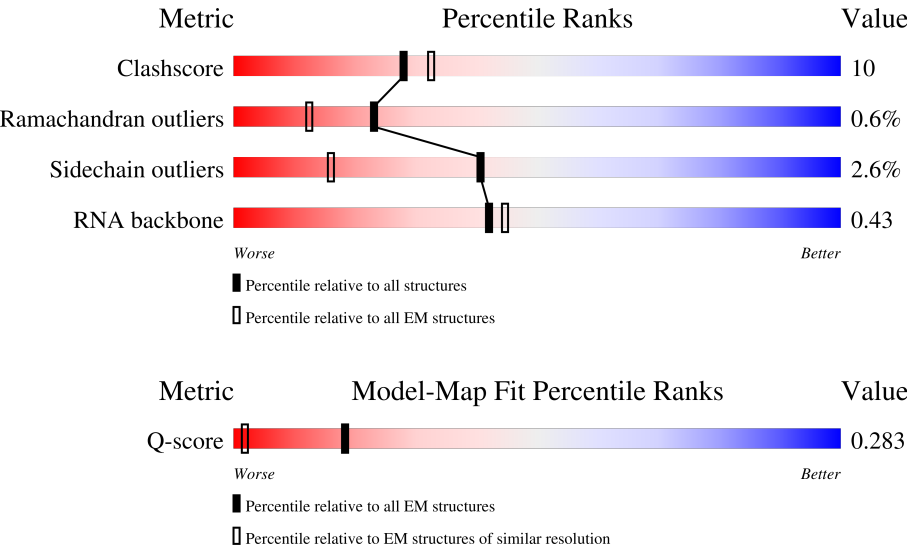
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 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	8728 (2.10 - 3.10)

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	144	29% 5% 13% 19% 60%
2	5A	117	38% 50% 33% 15%
3	5B	2335	84% 12%

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Mol	Chain	Length	Quality of chain
4	5C	972	
5	5D	2136	
6	5E	357	
7	2a	231	
7	4a	231	
7	5a	231	
8	2b	119	
8	4b	119	
8	5b	119	
9	2c	118	
9	4c	118	
9	5c	118	
10	2d	86	
10	4d	86	
10	5d	86	
11	2e	92	
11	4e	92	
11	5e	92	
12	2f	76	
12	4f	76	
12	5f	76	
13	2g	126	
13	4g	126	
13	5g	126	
14	6A	107	

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Mol	Chain	Length	Quality of chain
15	6a	95	
16	6b	102	
17	6c	139	
18	6d	91	
19	6e	80	
20	6f	103	
21	6g	96	
22	4A	145	
23	4B	683	
24	4C	522	
25	4D	499	
26	4E	128	
27	4F	142	
28	4G	941	
29	4H	177	
30	4I	376	
31	4J	800	
32	4Z	513	
33	2A	188	
34	2B	255	
35	2C	225	
36	2D	793	
37	2E	464	
38	2F	501	
39	2G	1304	

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Mol	Chain	Length	Quality of chain
40	2H	895	20%21%76%
41	2I	1217	96%83%13%
42	2J	424	18%17%82%
43	2K	125	86%74%12%14%
44	2L	110	81%73%8%19%
45	2M	86	77%53%22%23%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 94667 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 RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	57	Total	C	N	O	P	0	0
			1187	531	183	416	57		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	115	Total	C	N	O	P	0	0
			2420	1084	403	818	115		

- Molecule 3 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	2253	Total	C	N	O	S	0	0
			18642	11992	3250	3319	81		

- Molecule 4 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5C	818	Total	C	N	O	S	0	0
			6436	4114	1085	1205	32		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5D	1696	Total	C	N	O	S	0	0
			13633	8715	2329	2519	70		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5E	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 7 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5a	84	Total	C	N	O	0	0
			336	168	84	84		
7	4a	64	Total	C	N	O	0	0
			256	128	64	64		
7	2a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	5b	82	Total	C	N	O	0	0
			328	164	82	82		
8	4b	82	Total	C	N	O	0	0
			334	170	82	82		
8	2b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	5c	97	Total	C	N	O	0	0
			388	194	97	97		
9	4c	74	Total	C	N	O	0	0
			300	152	74	74		
9	2c	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	5d	74	Total	C	N	O	0	0
			296	148	74	74		
10	4d	71	Total	C	N	O	0	0
			292	150	71	71		
10	2d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	5e	79	Total	C	N	O	0	0
			316	158	79	79		
11	4e	78	Total	C	N	O	0	0
			314	158	78	78		
11	2e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	5f	72	Total	C	N	O	0	0
			288	144	72	72		
12	4f	73	Total	C	N	O	0	0
			298	152	73	73		
12	2f	68	Total	C	N	O	0	0
			272	136	68	68		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	5g	76	Total	C	N	O	0	0
			304	152	76	76		
13	4g	71	Total	C	N	O	0	0
			288	146	71	71		
13	2g	80	Total	C	N	O	0	0
			320	160	80	80		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6A	59	Total	C	N	O	P	0	0
			1251	558	230	404	59		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	6a	90	Total	C	N	O	0	0
			360	180	90	90		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	6b	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	6c	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	6d	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	6e	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6f	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	6g	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	129	Total	C	N	O	P	0	0
			2744	1225	472	917	130		

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4B	256	Total	C	N	O	S	0	0
			2076	1316	385	367	8		

- Molecule 24 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4C	426	Total	C	N	O	S	0	0
			3370	2118	612	620	20		

- Molecule 25 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4D	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 26 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4E	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 27 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4F	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 28 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4G	801	Total	C	N	O	S	0	0
			5504	3419	1043	1026	16		

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4H	169	Total	C	N	O		0	0
			844	506	169	169			

- Molecule 30 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4I	75	Total	C	N	O	S	0	0
			494	304	96	91	3		

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4J	153	Total	C	N	O	S	0	0
			1153	715	206	230	2		

- Molecule 32 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4Z	420	Total	C	N	O		0	0
			2093	1253	420	420			

- Molecule 33 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2A	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

- Molecule 34 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2B	162	Total	C	N	O		0	0
			648	324	162	162			

- Molecule 35 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2C	94	Total	C	N	O		0	0
			376	188	94	94			

- Molecule 36 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2D	236	Total	C	N	O	S	0	0
			1380	793	285	299	3		

- Molecule 37 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	2E	94	Total	C	N	O	0	0
			376	188	94	94		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2F	423	Total	C	N	O	0	0
			1693	847	423	423		

- Molecule 39 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2G	1048	Total	C	N	O	0	0
			4192	2096	1048	1048		

- Molecule 40 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2H	213	Total	C	N	O	S	0	0
			959	510	220	226	3		

- Molecule 41 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2I	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 42 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2J	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 43 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2K	108	Total	C	N	O	0	0
			432	216	108	108		

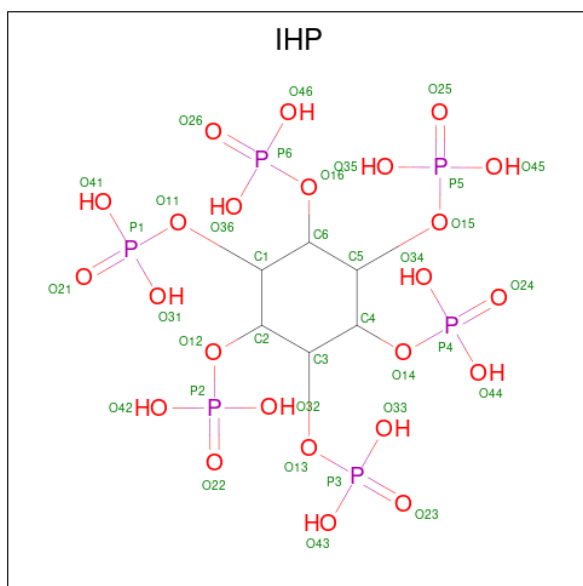
- Molecule 44 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2L	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 45 is a protein called Splicing factor 3B subunit 5.

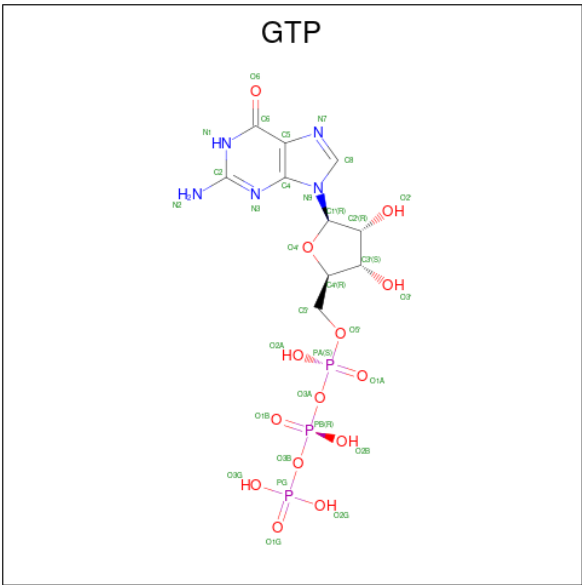
Mol	Chain	Residues	Atoms				AltConf	Trace
45	2M	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$).



Mol	Chain	Residues	Atoms				AltConf
46	5B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
47	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	5C	1	Total	Mg	0
			1	1	

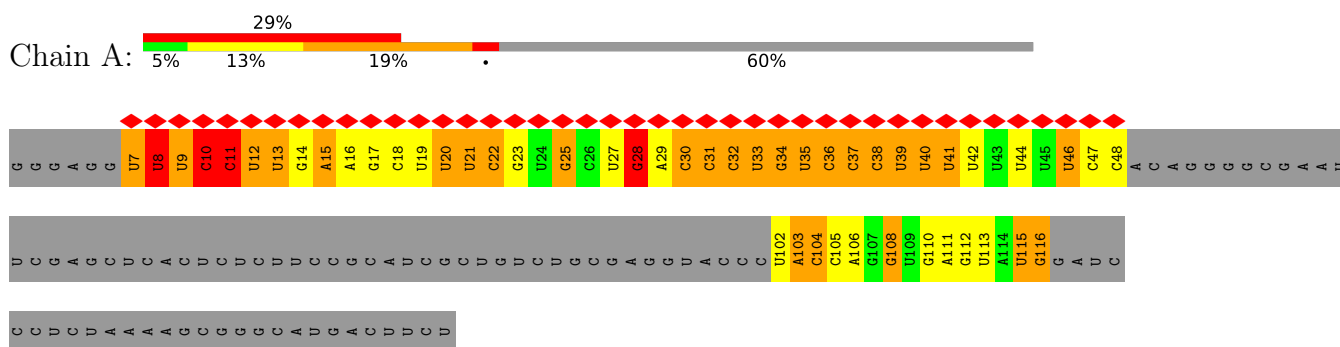
- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	4I	1	Total	Zn	0
			1	1	

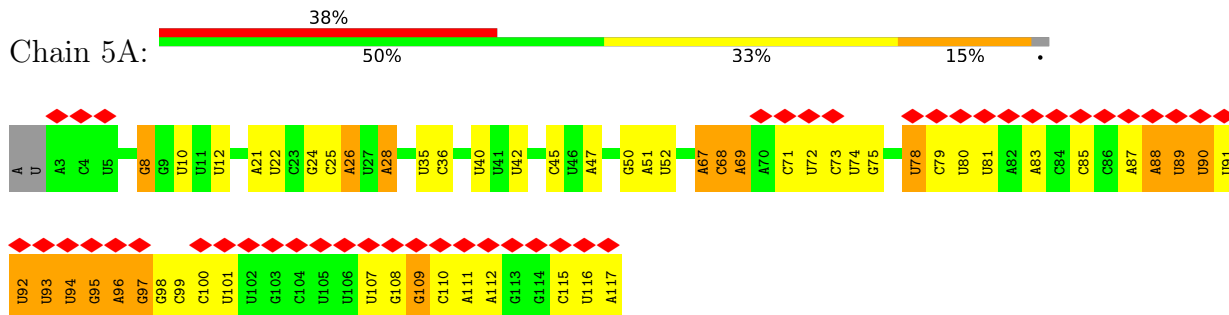
3 Residue-property plots [i](#)

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

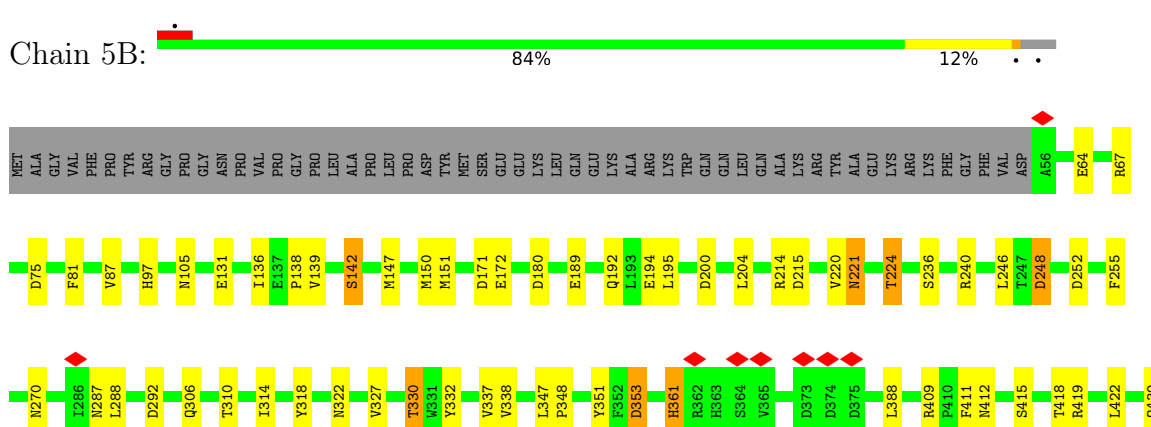
• Molecule 1: pre-mRNA

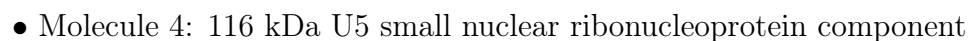


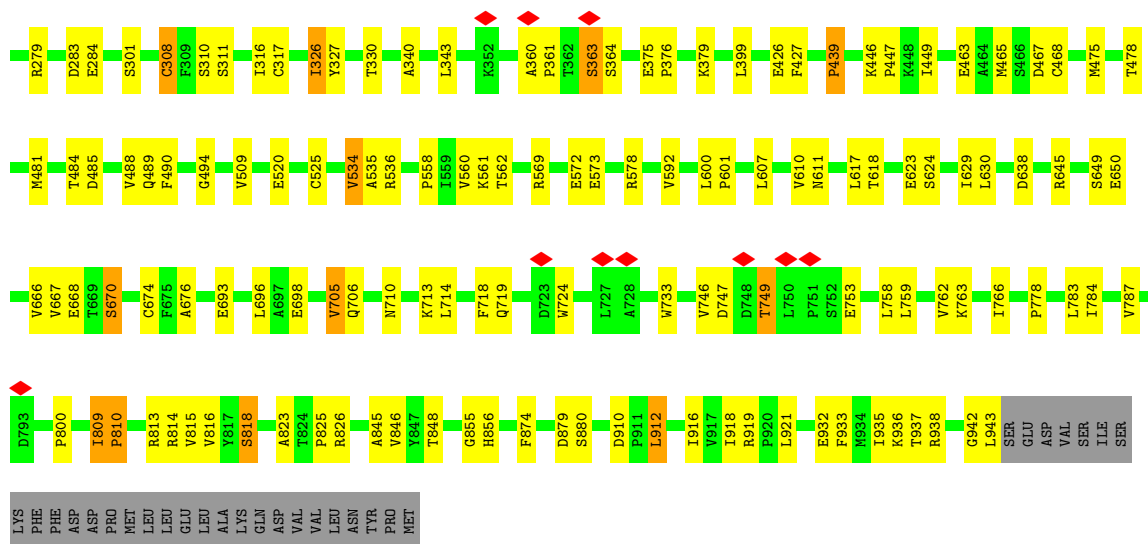
• Molecule 2: U5 snRNA



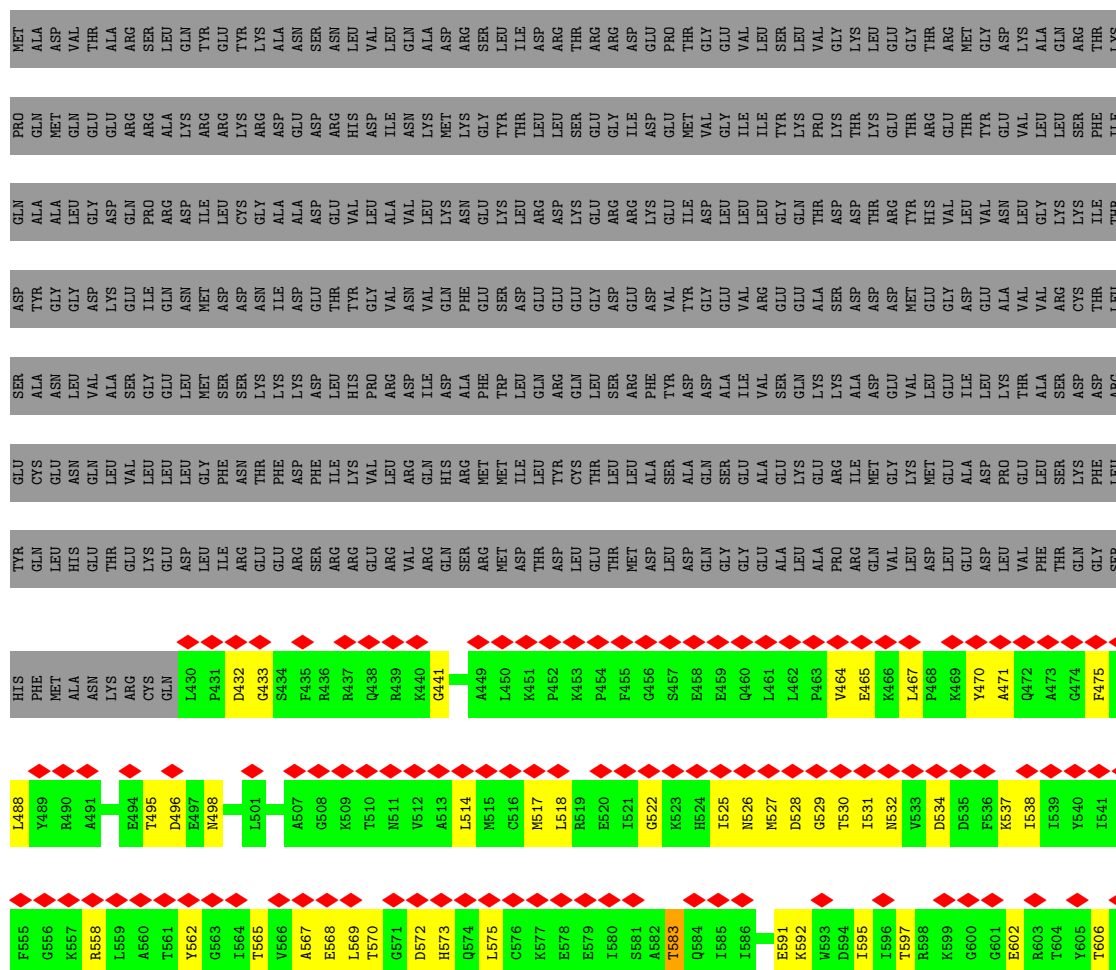
• Molecule 3: Pre-mRNA-processing-splicing factor 8







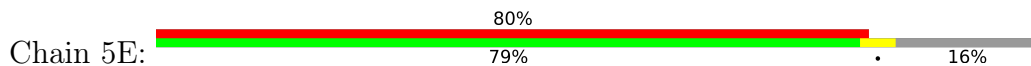
● Molecule 5: U5 small nuclear ribonucleoprotein 200 kDa helicase



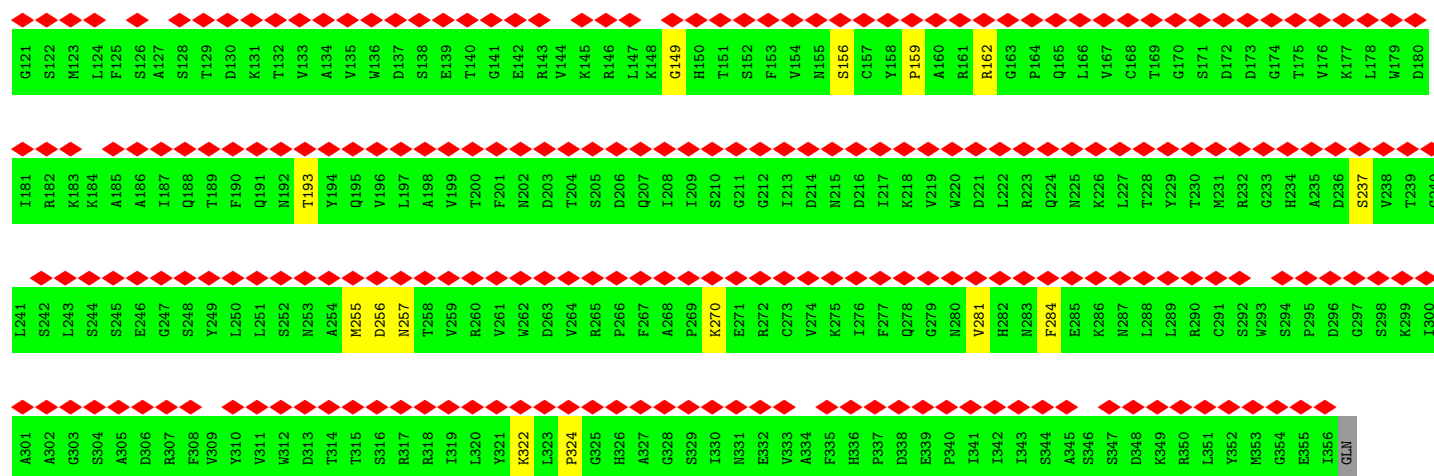


D1583	I1704	M1764	I1824	F1884	E1944	I2004	W2064	V2124
I1584	M1705	T1765	N1825	N1885	L1945	A2005	V2065	D2125
Q1585	C1706	Q1766	Y1826	D1886	A1946	D2006	V2066	VAL
R1586	Q1707	M1767	T1827	P1887	Q1947	V2007	V2067	GLU
Q1587	T1708	P1768	T1828	H1888	M1948	A2008	I2068	GLU
R1588	S1709	N1769	I1829	V1889	V1949	R2009	Q2069	ALA
F1589	M1710	Y1770	E1830	K1890	T1950	F2010	D2070	THR
L1590	K1711	Y1771	L1831	T1891	Q1951	C2011	A2071	ASP
H1591	D1712	M1772	F1832	N1892	A1952	R2012	K2072	SER
C1592	F1713	L1773	S1833	L1893	M1953	R2013	S2073	ASP
T1593	Q1774	G1775	M1834	L1894	W1954	Y2014	N2074	ASP
E1594	K1715	G1776	S1835	L1895	S1955	P2015	S2075	
K1595	K1716	I1776	L1836	Q1896	K1956	N2016	L2076	
D1596	F1717	S1777	N1837	A1897	D1957	T2017	I2077	
L1597	L1718	H1778	A1838	H1898	S1958	E2018	S2078	
I1598	Y1719	R1779	K1839	L1899	Y1959	L2019	I2079	
P1599	E1720	H1780	T1840	S1900	L1960	S2020	K2080	
Y1600	P1721	L1781	K1841	R1901	K1961	Y2021	R2081	
L1601	L1722	S1782	V1842	M1902	Q1962	E2022	L2082	
E1602	P1723	D1783	R1843	Q1903	L1963	V2023	T2083	
K1603	V1724	H1784	G1844	L1904	P1964	V2024	L2084	
L1604	E1725	L1785	L1845	S1905	H1965	D2025	Q2085	
S1605	S1726	T1786	L1846	A1906	F1966	K2026	Q2086	
D1606	H1727	E1787	I1847	A1907	P1967	D2027	K2087	
S1607	L1728	L1788	I1848	L1908	S1968	S2028	A2088	
T1608	D1729	V1789	I1849	Q1909	E1969	T2029	K2089	
L1609	H1730	E1790	S1850	S1910	H1970	R2030	V2090	
K1610	C1731	Q1791	N1851	D1911	I1971	S2031	K2091	
E1611	M1732	T1792	A1852	T1912	K1972	G2032	L2092	
T1612	H1733	L1793	A1853	E1913	R1973	G2033	D2093	
L1613	D1734	S1794	E1854	E1914	C1974	P2034	F2094	
L1614	A1675	D1795	Y1855	I1915	T1975	V2035	V2095	
N1615	Y1676	L1796	Y1856	L1916	D1976	V2036	A2096	
G1616	V1677	E1797	E1857	S1917	K1977	V2037	V2097	
V1617	D1678	Q1798	I1858	K1918	G1978	L2038	A2098	
G1618	P1679	S1799	P1859	A1919	V1979	V2039	T2099	
G1619	P1680	K1800	I1860	I1920	E1980	Q2040	G2100	
L1620	I1681	V1741	R1861	R1921	S1981	L2041	A2101	
H1621	Y1682	T1742	H1862	L1922	V1982	E2042	H2102	
E1622	D1683	K1743	H1863	I1923	F1983	R2043	N2103	
G1623	V1684	I1744	E1864	Q1924	D1984	E2044	Y2104	
L1624	L1685	I1745	A1865	A1925	I1985	E2045	T2105	
S1625	Q1686	E1746	D1866	C1926	M1986	E2046	L2106	
P1626	M1687	N1747	N1867	V1927	E1987	V2047	V2107	
M1627	V1688	K1748	L1868	I1928	M1988	T2048	F2108	
G1628	G1689	Q1749	R1869	V1929	E1989	G2049	M2109	
H1629	H1690	D1750	Q1870	L1930	D1990	P2050	S2110	
R1630	A1691	A1751	L1871	S1931	E1991	V2051	D2111	
L1631	N1692	V1752	P1872	S1932	E1992	I2052	A2112	
V1632	P1693	D1753	L1813	Q1873	R1993	A2053	T2113	
E1633	P1694	L1695	M1814	G1934	M1994	P2054	M2114	
Q1634	Q1696	L1754	L1815	V1935	A1995	L2055	G2115	
L1635	D1697	T1756	G1816	L1936	L1996	F2056	C2116	
F1636	D1698	W1757	M1817	S1937	L1997	P2057	T2117	
S1637	E1699	T1758	I1818	P1938	Q1998	Q2058	Q2118	
S1638	G1700	F1759	I1819	A1939	L1999	K2059	E2119	
G1639	R1701	L1760	A1820	L1940	T2000	R2060	Y2120	
I1640	C1702	Y1761	Y1821	A1941	D2001	E2061	K2121	
Q1642	V1703	R1762	Y1822	A1942	S2002	E2062	F2122	
				M1943	Q2003	G2063	S2123	

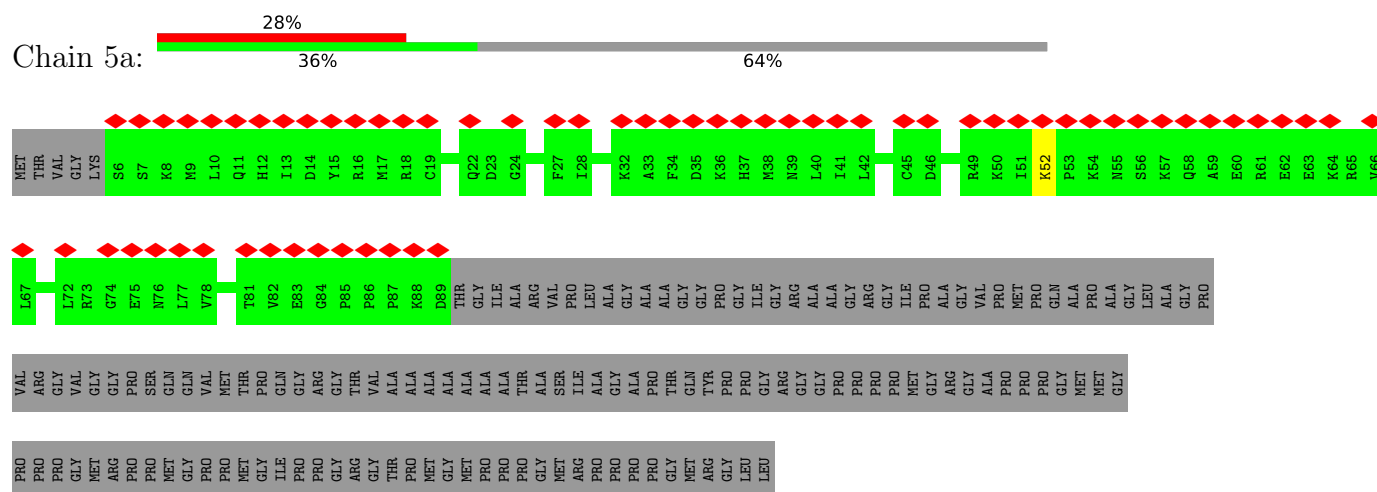
- Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein



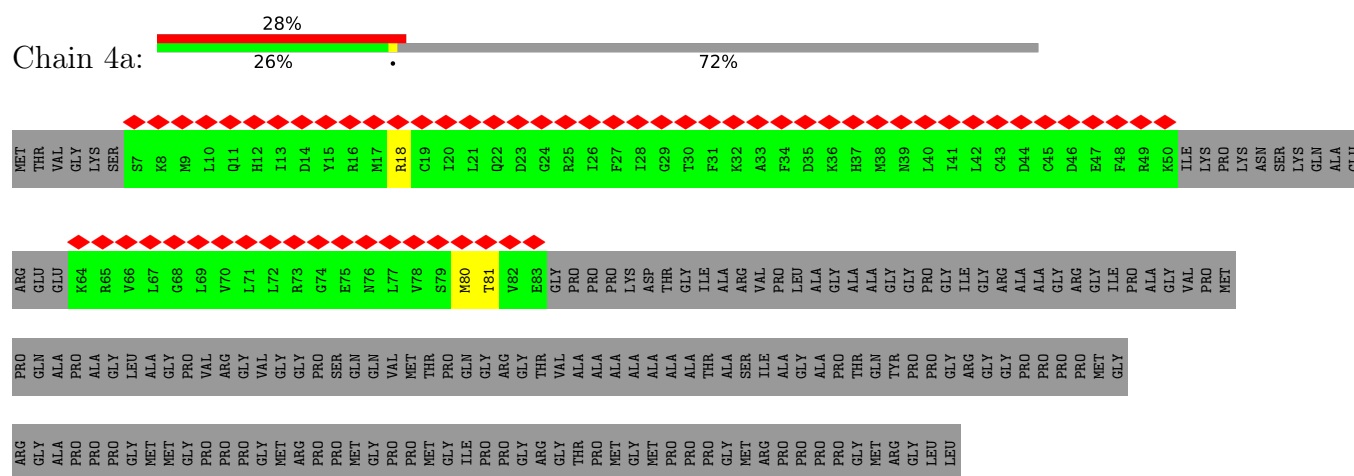
MET	P58	P59	M60
ILE			
GLU			
GLN			
GLN			
LYS			
ARG			
LYS			
GLY			
PRO			
GLU			
LEU			
PRO			
PRO			
LEU			
VAL			
PRO			
VAL			
LYS			
ARG			
GLN			
ARG			
GLU			
LEU			
LEU			
LEU			
LEU			
GLY			
ALA			
GLY			
GLY			
GLN			
GLN			
ALA			
THR			
PRO			
GLY			
ALA			
LEU			
LEU			
GLN			
ALA			
GLY			
GLY			
GLY			
LEU			
LEU			
GLN			
GLY			
PRO			
ARG			
CYS			
SER			
SER			
LEU			
GLN			
ALA			
L61			
L62			
S63			
G64			
H65			
E66			
G67			
E68			
V69			
Y70			
C71			
C72			
K73			
F74			
H75			
P76			
N77			
G78			
S79			
T80			
L81			
A82			
S83			
A84			
G85			
F86			
D87			
R88			
L89			
I90			
L91			
L92			
W93			
N94			
V95			
Y96			
G97			
D98			
C99			
D100			
N101			
Y102			
A103			
T104			
L105			
K106			
G107			
H108			
S109			
G110			
A111			
V112			
M113			
E114			
L115			
H116			
Y117			
N118			
T119			
D120			



- Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

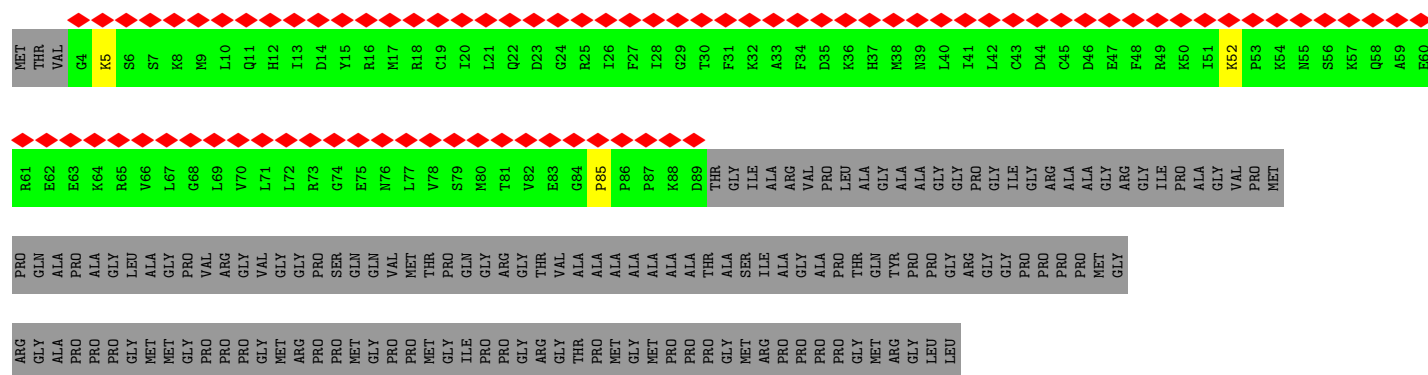


- Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

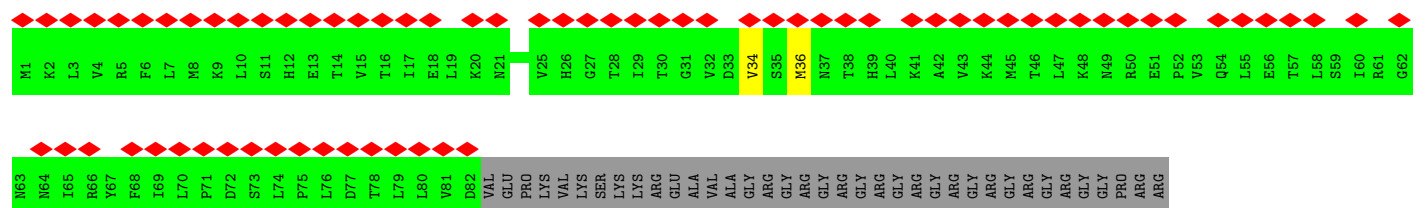


- Molecule 7: Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'

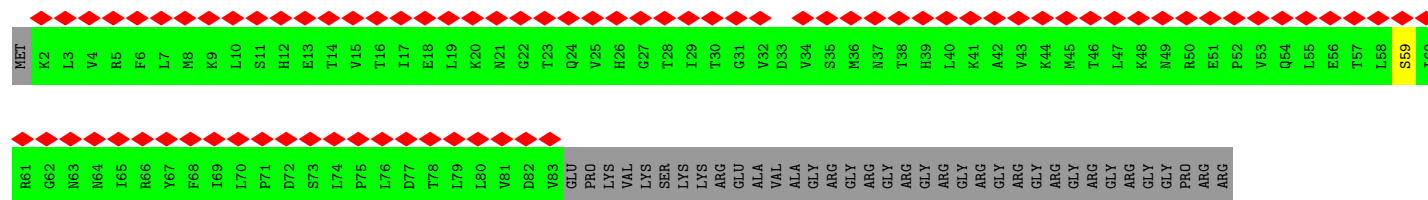




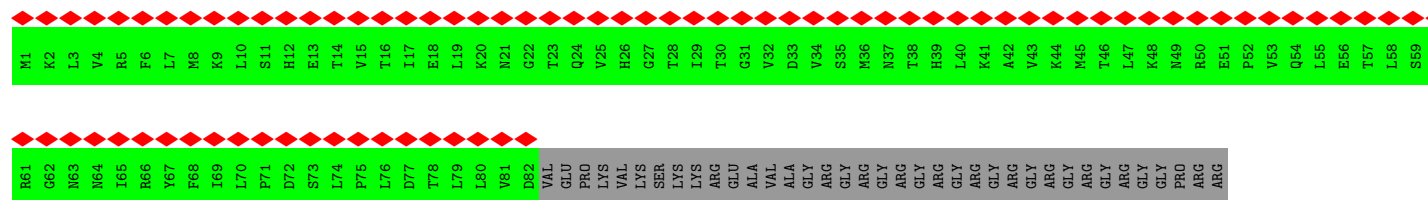
• Molecule 8: Small nuclear ribonucleoprotein Sm D1



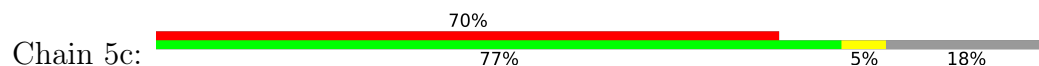
• Molecule 8: Small nuclear ribonucleoprotein Sm D1



• Molecule 8: Small nuclear ribonucleoprotein Sm D1

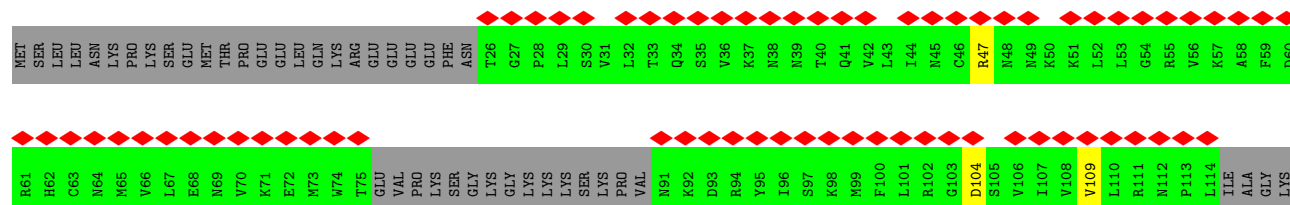


• Molecule 9: Small nuclear ribonucleoprotein Sm D2





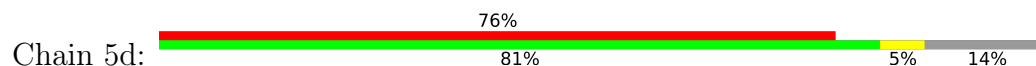
• Molecule 9: Small nuclear ribonucleoprotein Sm D2



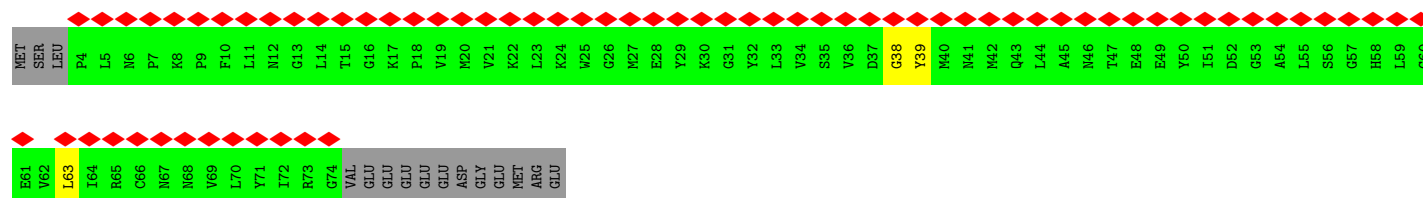
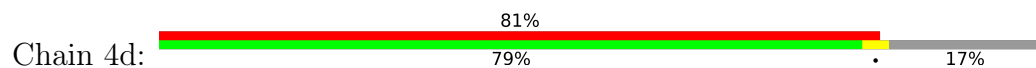
• Molecule 9: Small nuclear ribonucleoprotein Sm D2



• Molecule 10: Small nuclear ribonucleoprotein F

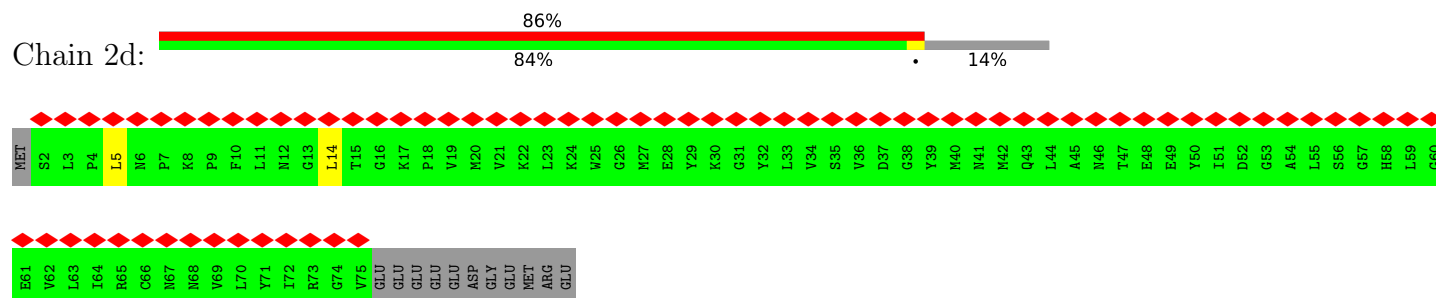


• Molecule 10: Small nuclear ribonucleoprotein F



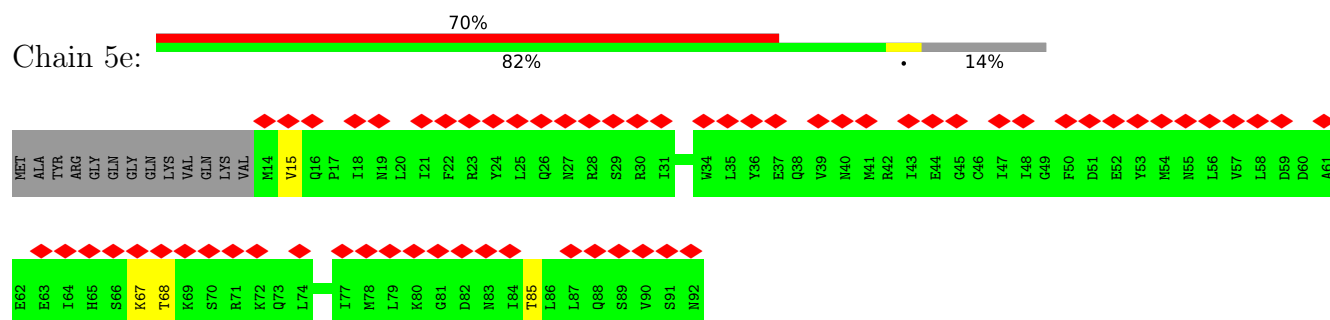
• Molecule 10: Small nuclear ribonucleoprotein F

Chain 2d:



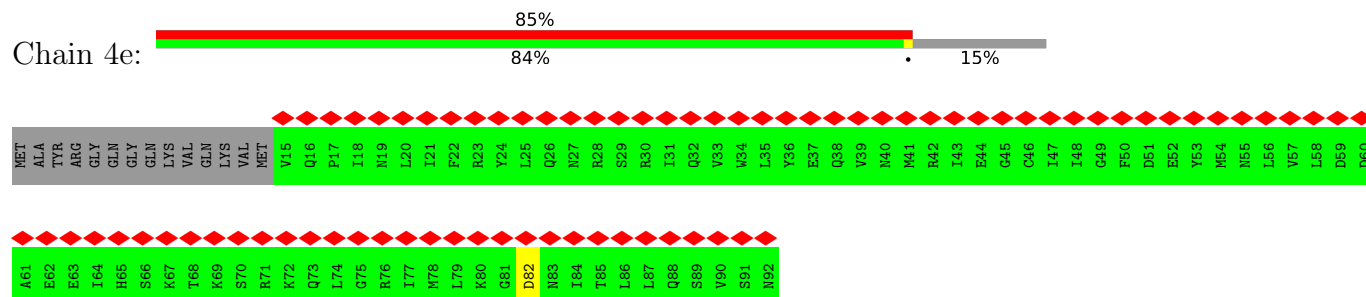
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 5e:



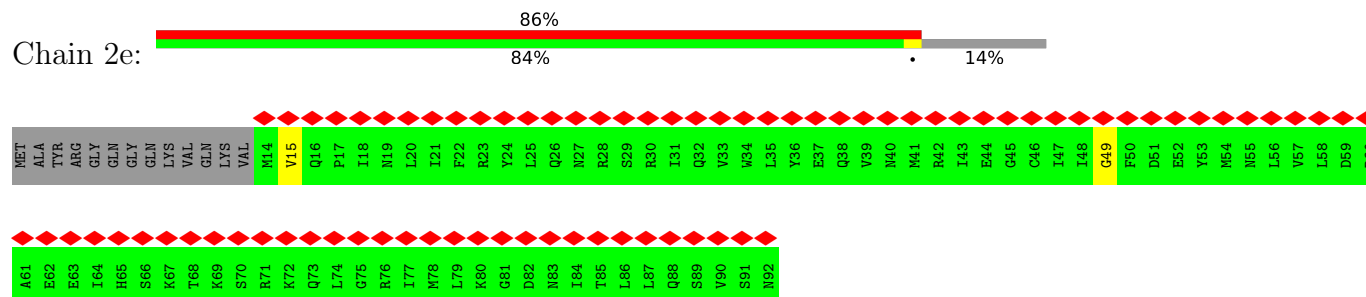
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 4e:



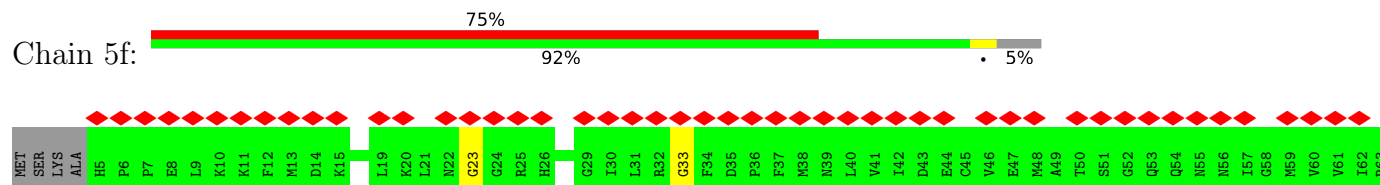
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 2e:

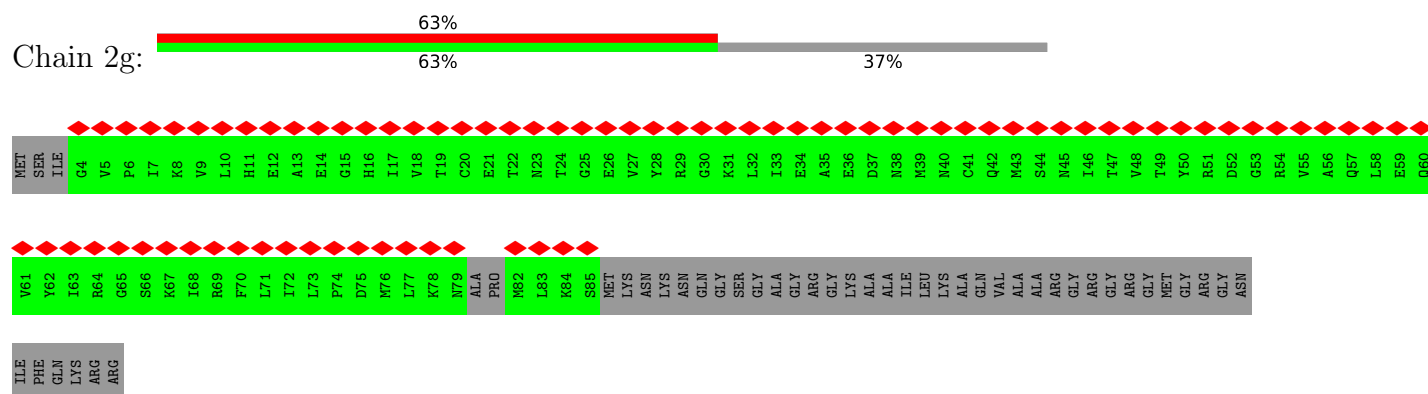


• Molecule 12: Small nuclear ribonucleoprotein G

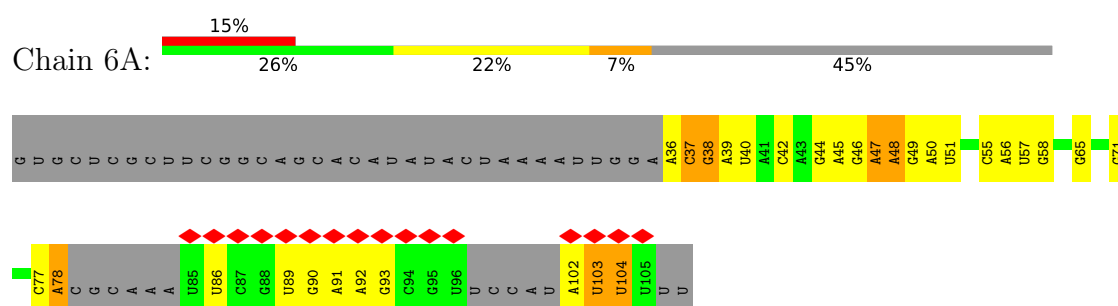
Chain 5f:



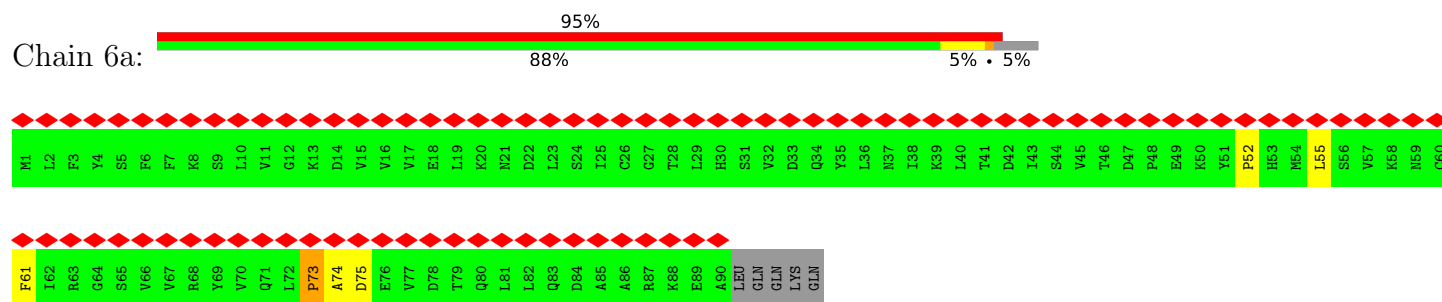
- Molecule 13: Small nuclear ribonucleoprotein Sm D3



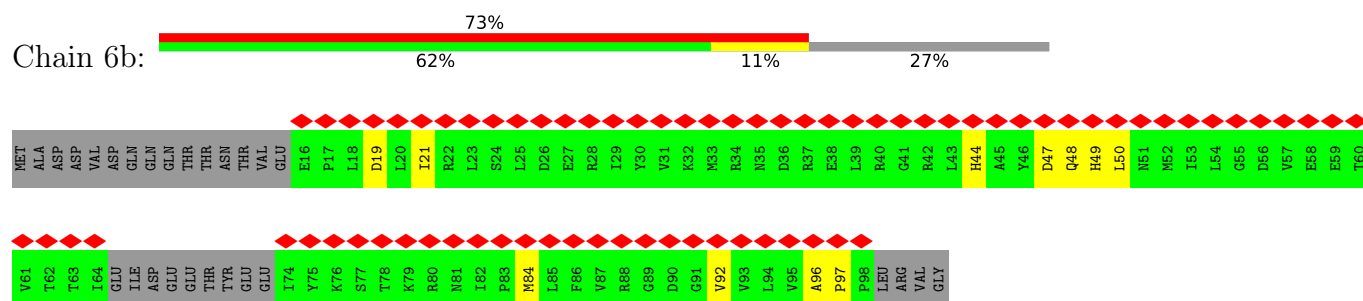
- Molecule 14: U6 snRNA



- Molecule 15: U6 snRNA-associated Sm-like protein LSm2

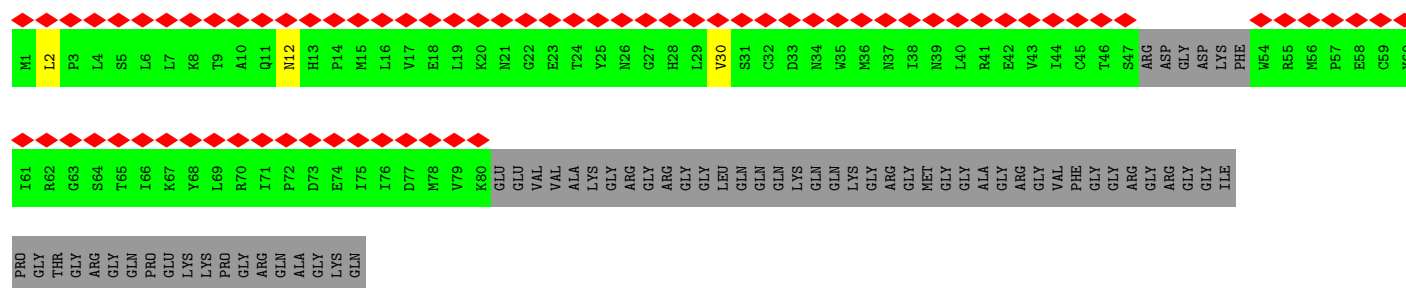


- Molecule 16: U6 snRNA-associated Sm-like protein LSm3

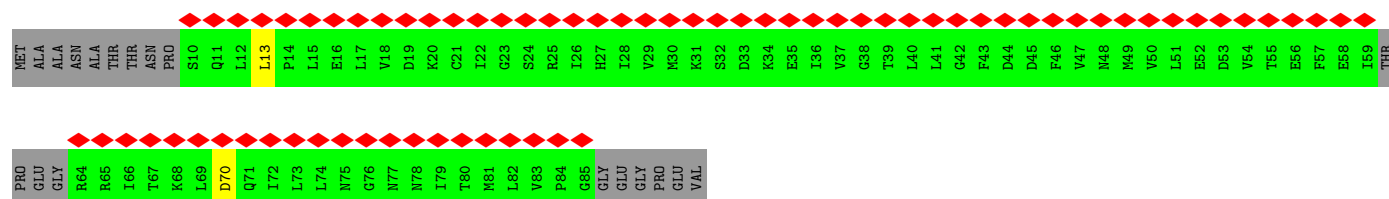
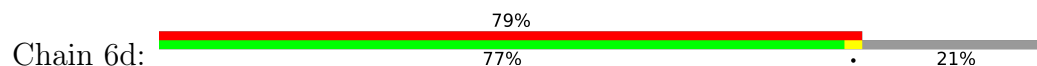


- Molecule 17: U6 snRNA-associated Sm-like protein LSm4

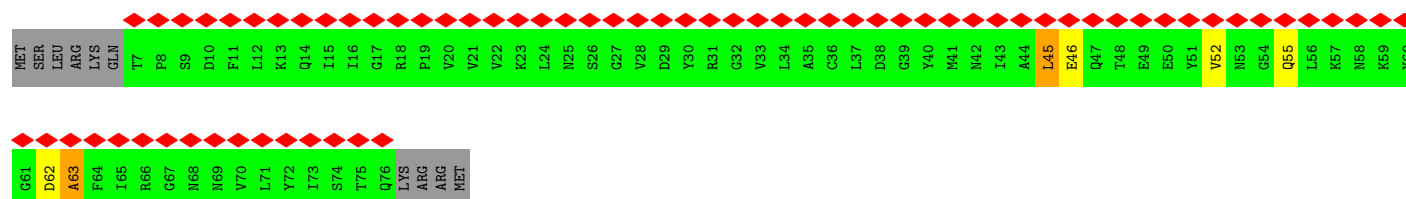
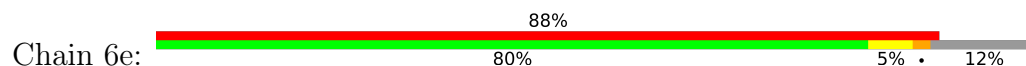




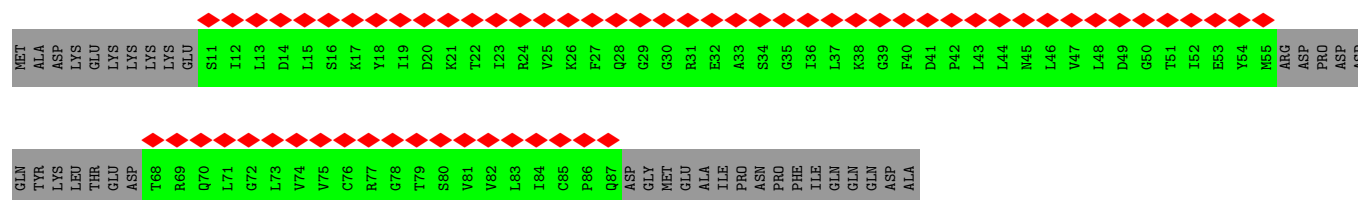
- Molecule 18: U6 snRNA-associated Sm-like protein LSm5



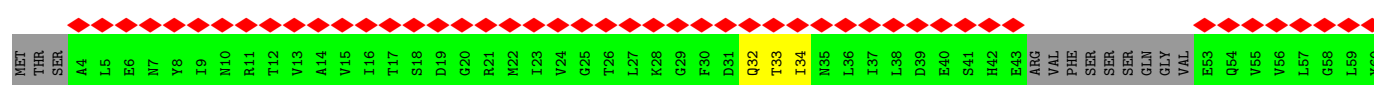
- Molecule 19: U6 snRNA-associated Sm-like protein LSm6

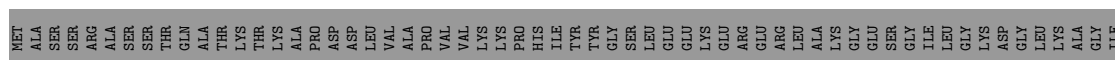


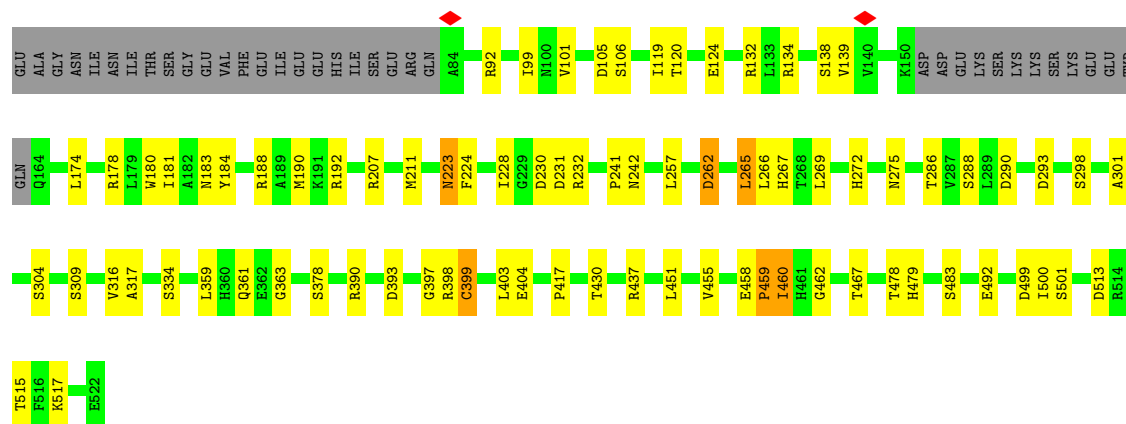
- Molecule 20: U6 snRNA-associated Sm-like protein LSm7



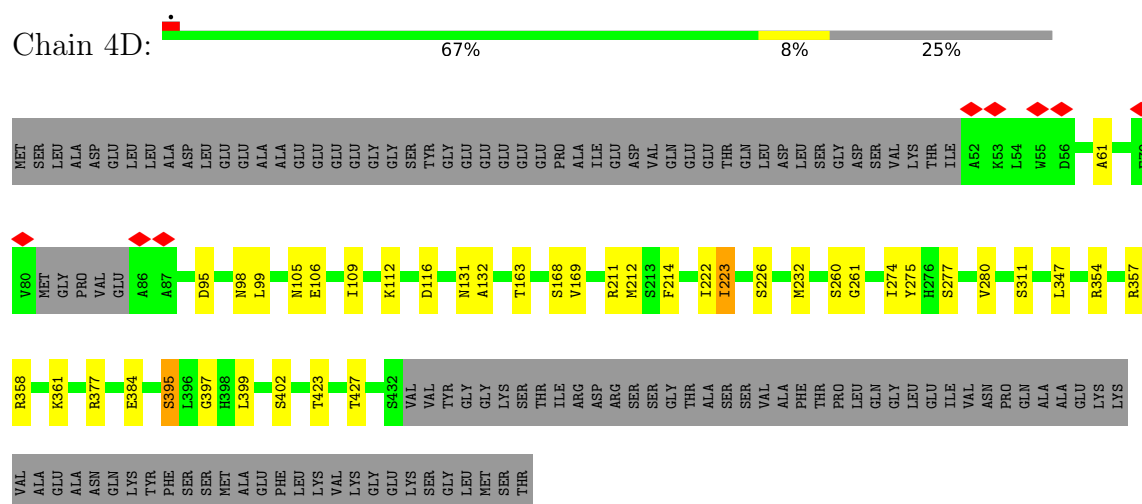
- Molecule 21: U6 snRNA-associated Sm-like protein LSm8



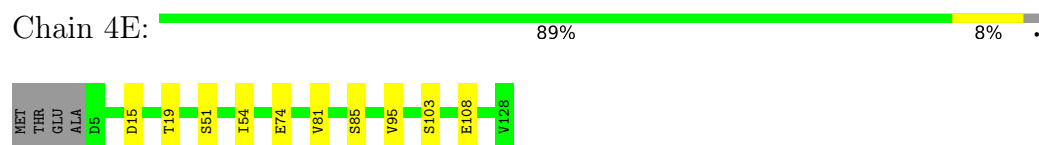




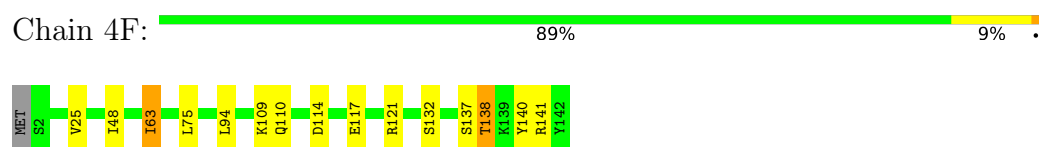
- Molecule 25: U4/U6 small nuclear ribonucleoprotein Prp31



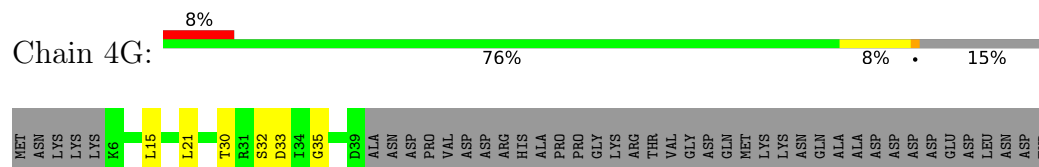
- Molecule 26: NHP2-like protein 1

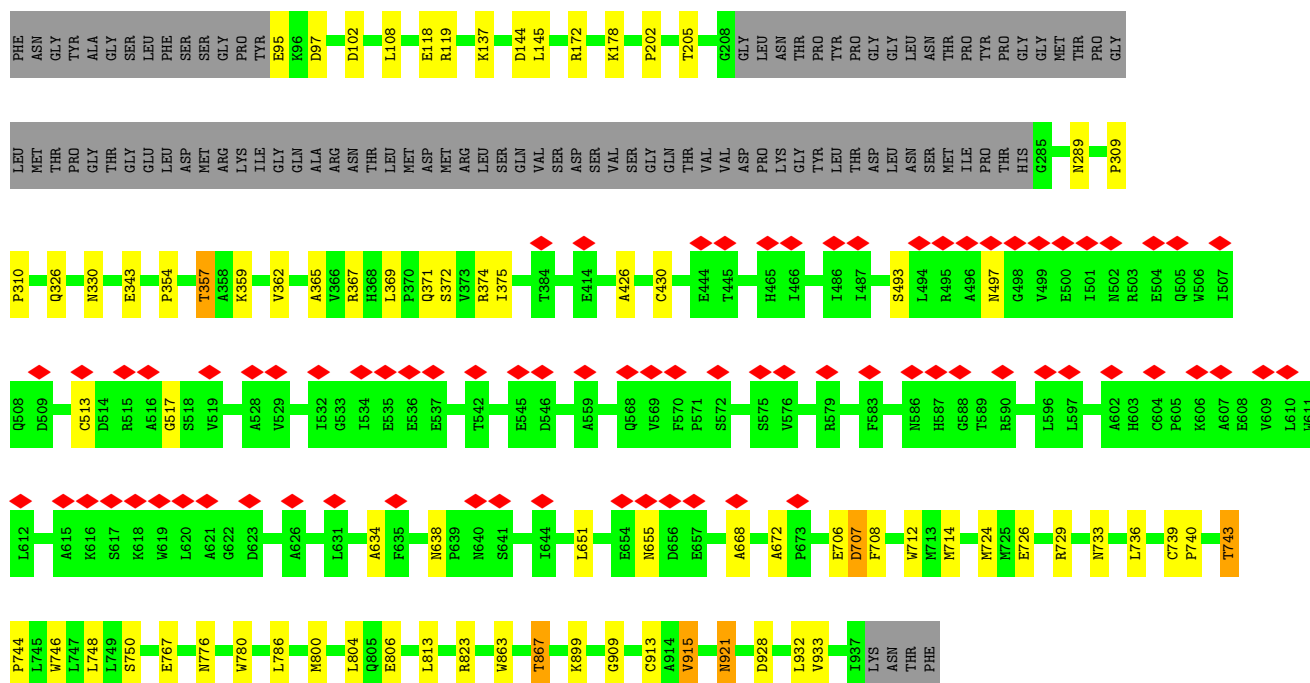


- Molecule 27: Thioredoxin-like protein 4A



- Molecule 28: Pre-mRNA-processing factor 6

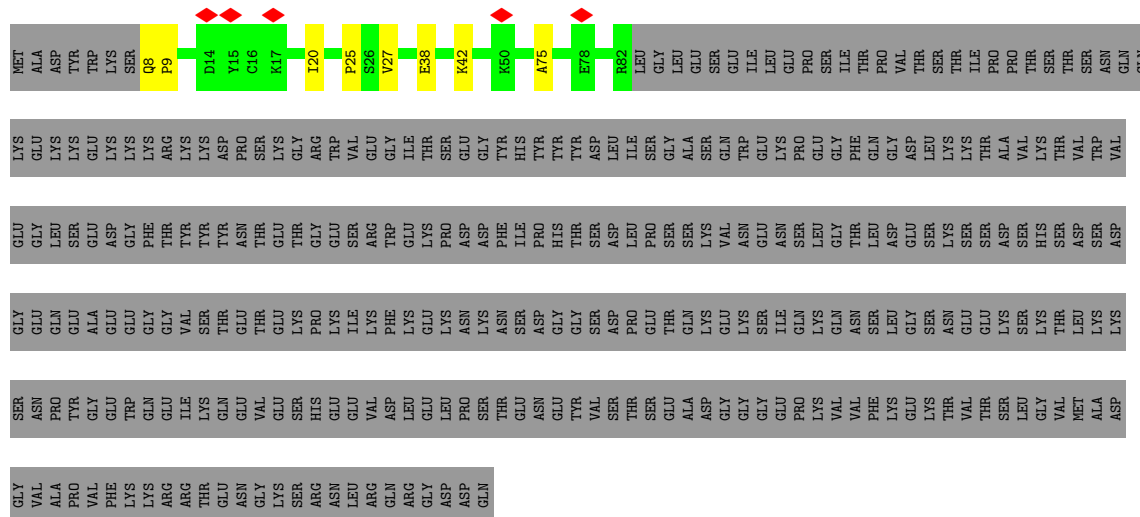




- Molecule 29: Peptidyl-prolyl cis-trans isomerase H



- Molecule 30: WW domain-binding protein 4



- Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1

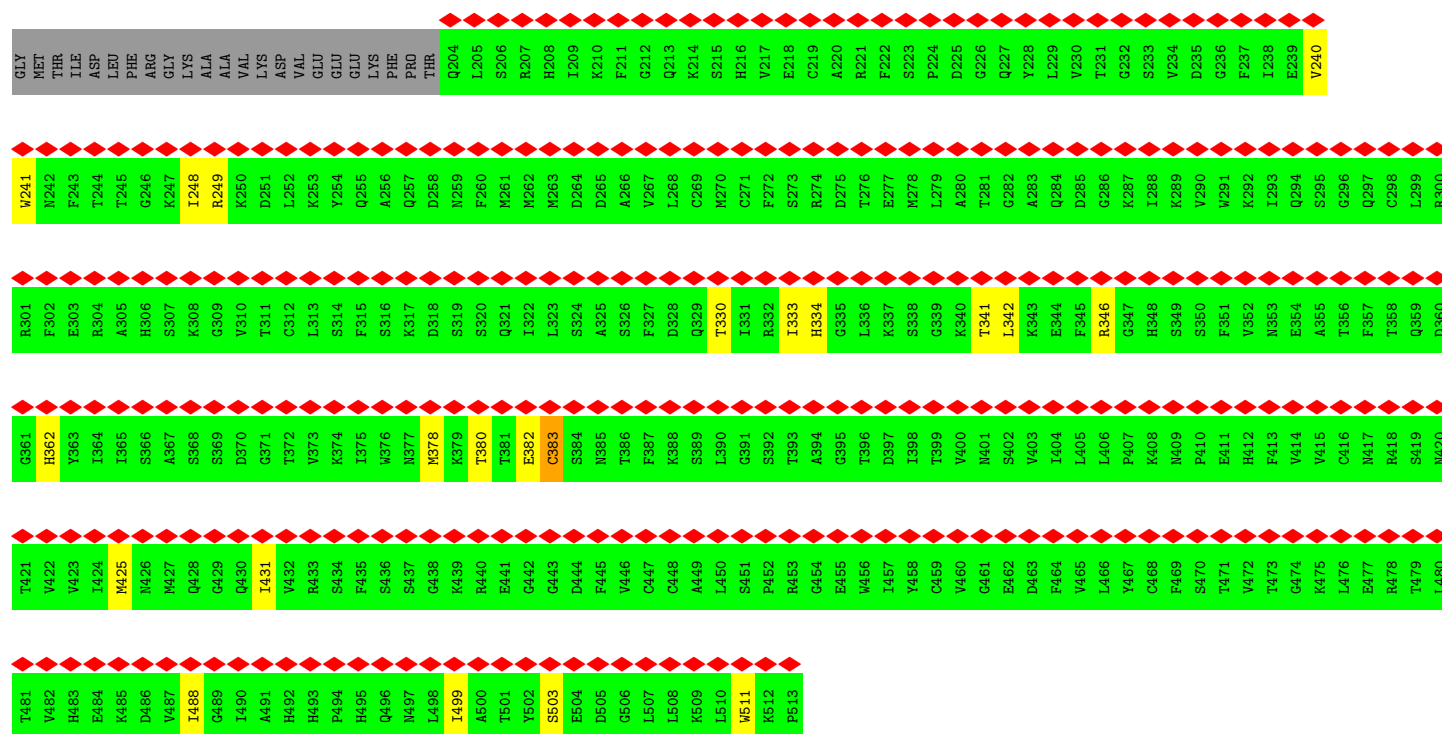
Satisfaction Level	Percentage
Very satisfied	17%
Satisfied	81%

[illegible]

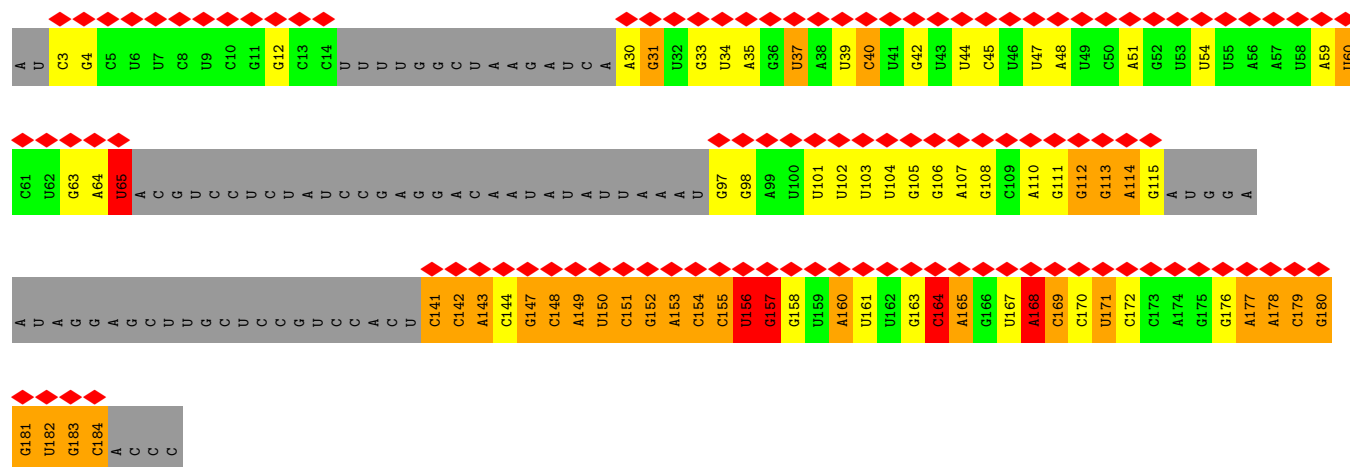
- Molecule 32: WD40 repeat-containing protein SMU1

Category	Percentage
Red Bar	82%
Green Bar	77%
Grey Bar	18%

MET	SER	ILE	GLU	ILE	GLU	SER	SER	ASP	VAL	ILE	ARG	LEU	ILE	MET	GLN	TYR	LEU	LYS	GLU	ASN	SER	SER	ASN	GLN	GLU	THR	THR	VAL	VAL	SER	LEU	ASN	THR	VAL	ASP	S43	I44	E45	S46	F47	V48	A49	D50	I51	N52	S53	G54	H55	M56	D57	T58	V59	L60						
Q61	A62	I63	Q64	S65	L66	K67	L68	P69	D70	K71	T72	L73	I74	D75	L76	Y77	E78	Q79	V80	V81	L82	E83	L84	I85	E86	L87	R88	E89	L90	G91	A92	A93	R94	S95	L96	L97	R98	Q99	T100	D101	P102	M103	I104	M105	L106	K107	Q108	T109	Q110	P111	E112	R113	Y114	I115	H116	L117	E118	N119	L120
L121	A122	A123	A124	Y125	F126	P127	A129	E130	A131	Y132	P133	D134	G135	SER	SER	K138	E139	K140	R141	R142	A143	A144	I145	A146	Q147	A148	L149	A150	G151	E152	V153	S154	VAL	VAL	PRO	PRO	SER	SER	ARG	LEU	LEU	MET	LEU	ALA	LEU	LEU	GLY	GLN	GLN	HIS	GLN	GLY	GLY	LEU	LEU	PRO			

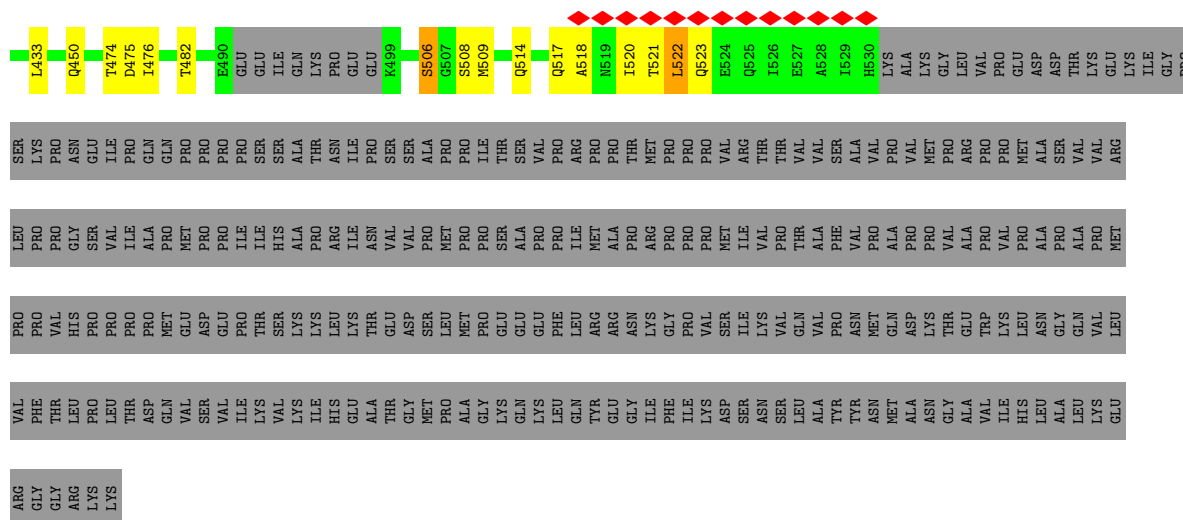


• Molecule 33: U2 snRNA

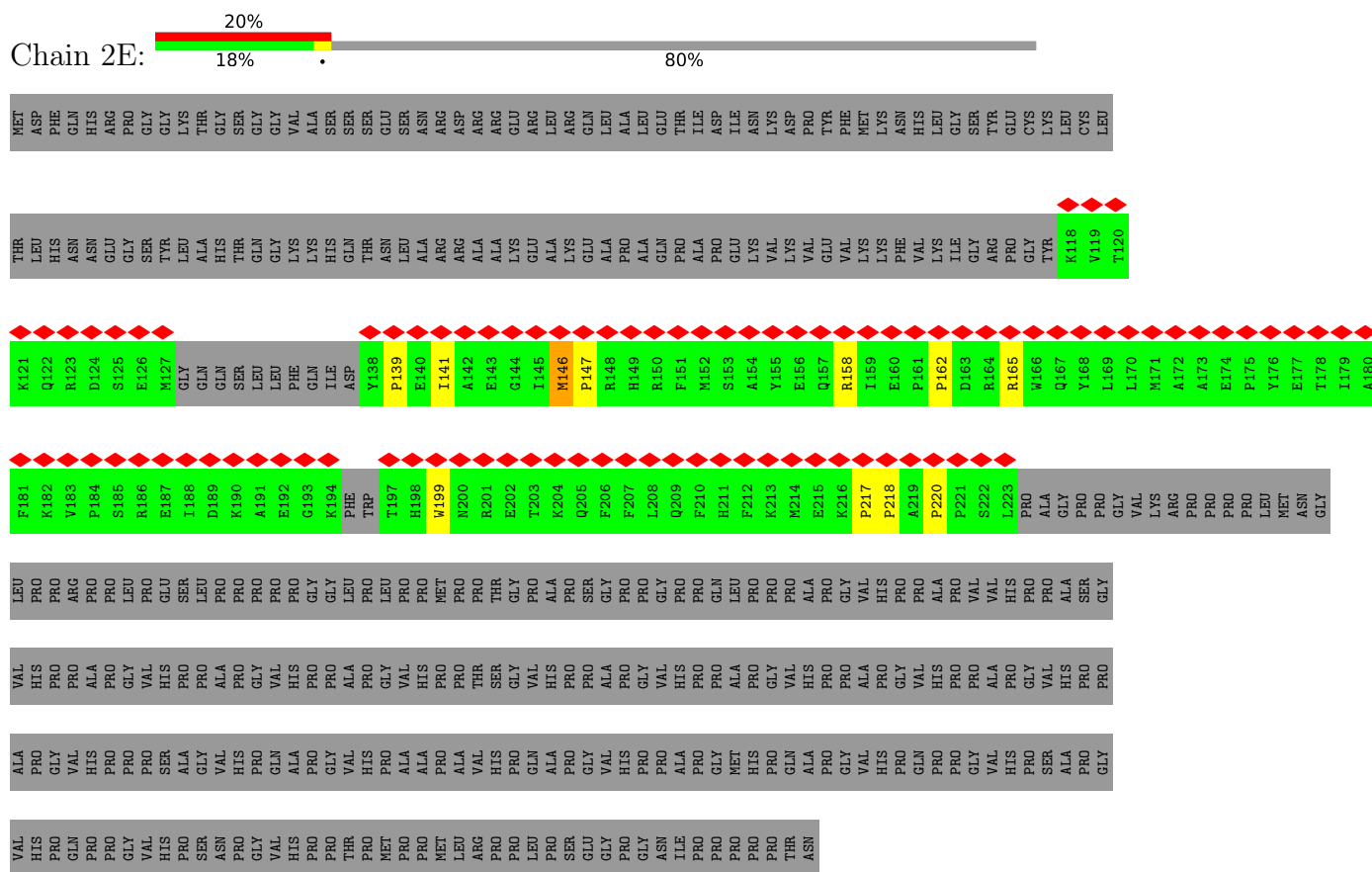


• Molecule 34: U2 small nuclear ribonucleoprotein A'

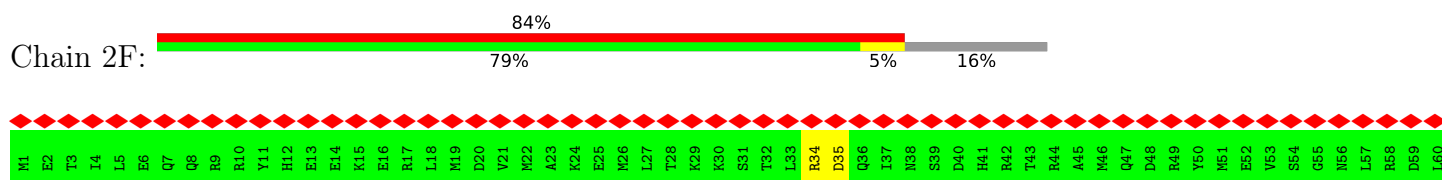




• Molecule 37: Splicing factor 3A subunit 2

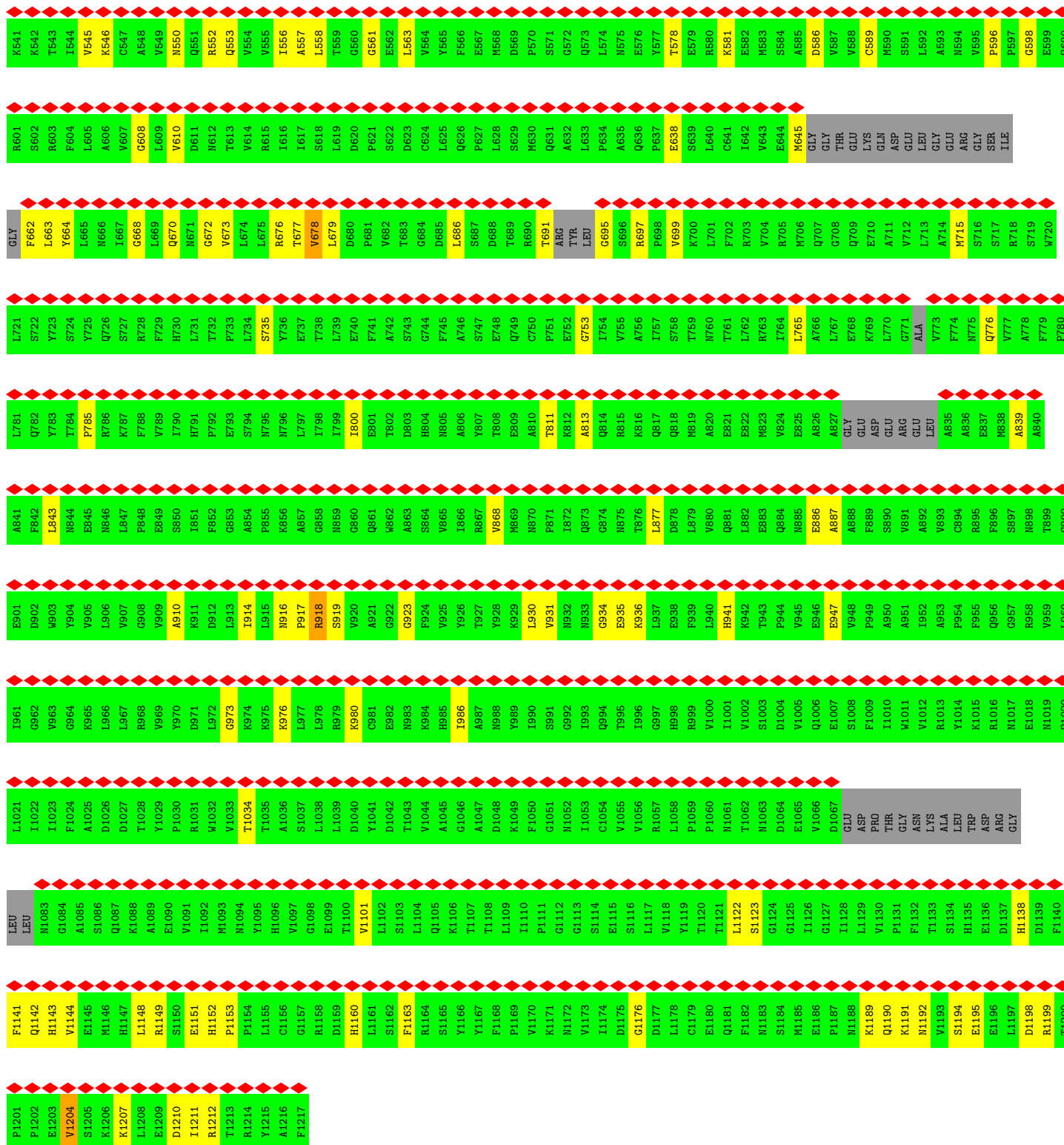


• Molecule 38: Splicing factor 3A subunit 3



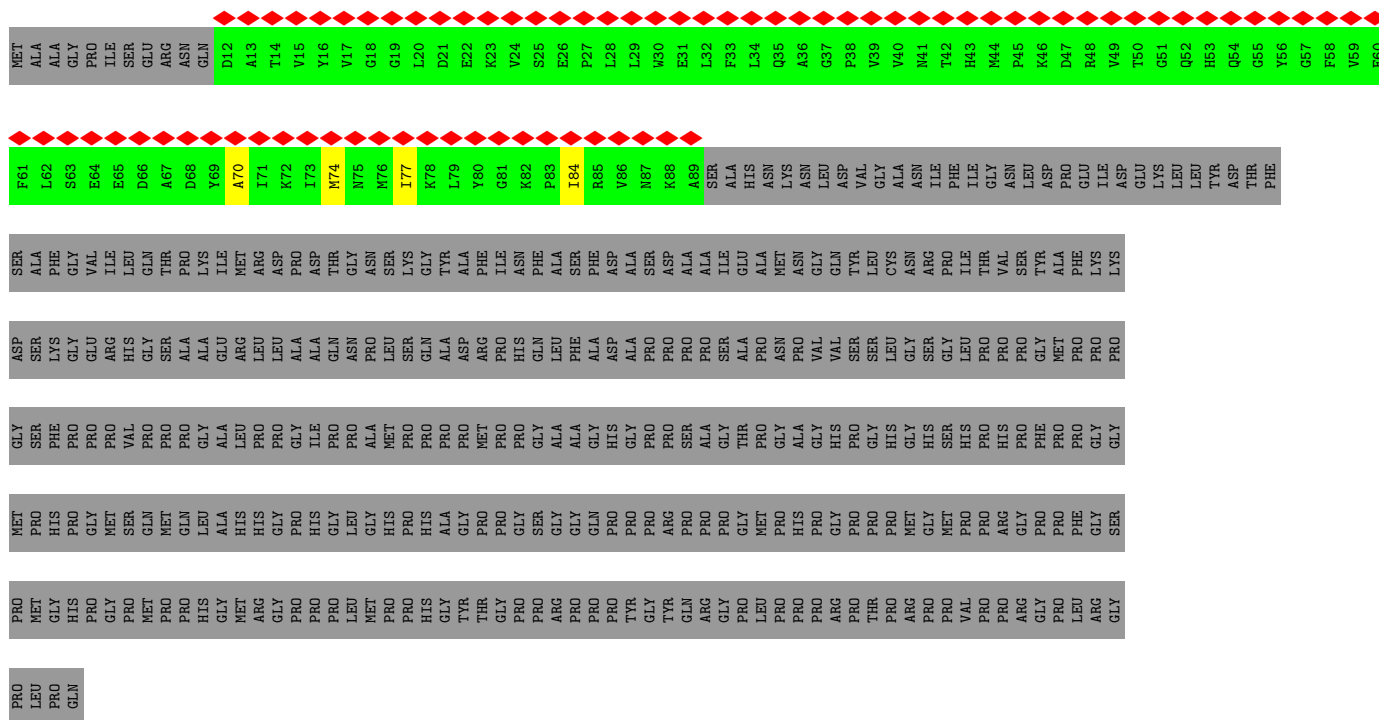




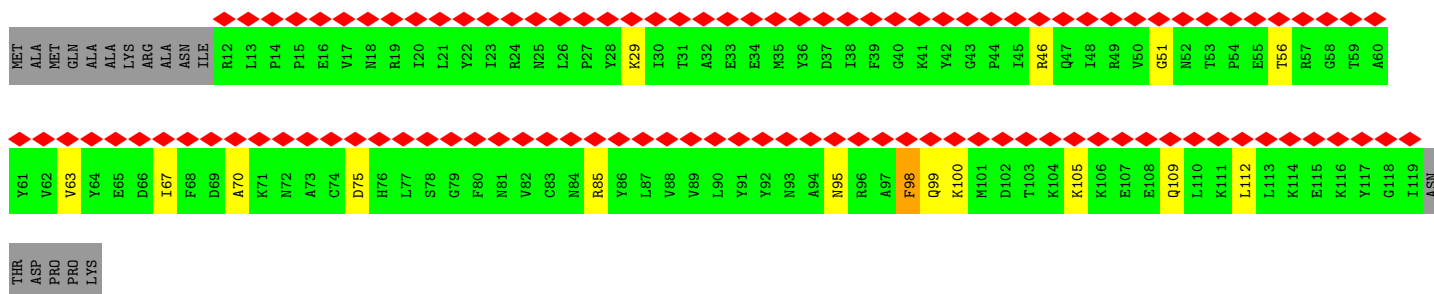
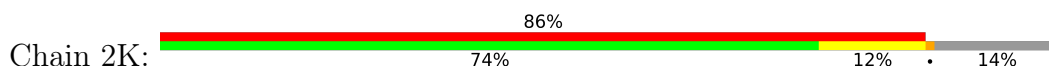


- Molecule 42: Splicing factor 3B subunit 4

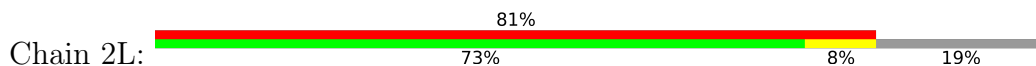




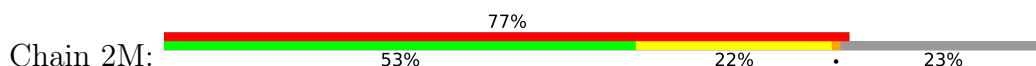
- Molecule 43: Splicing factor 3B subunit 6



- Molecule 44: PHD finger-like domain-containing protein 5A



- Molecule 45: Splicing factor 3B subunit 5



K61	A62	R63	Y64	R65	F66	N67	L68	M69	E70	K71	M72	L73	Q74	P75	C76	G77	P78	P79	A80	ASP	LYS	PRO	GLU	GLU	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	716083	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size ($\text{\AA}$)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M7M, IHP, ZN, MG, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	6/1317 (0.5%)	0.68	2/2042 (0.1%)
2	5A	0.20	0/2698	0.39	0/4195
3	5B	0.16	0/19157	0.32	2/26004 (0.0%)
4	5C	0.15	1/6580 (0.0%)	0.41	5/8938 (0.1%)
5	5D	0.15	0/13923	0.32	2/18868 (0.0%)
6	5E	1.08	0/1195	1.21	5/1492 (0.3%)
7	2a	0.86	0/343	1.21	3/427 (0.7%)
7	4a	0.13	0/254	0.39	0/314
7	5a	0.85	0/335	1.18	2/417 (0.5%)
8	2b	0.89	0/327	1.11	0/407
8	4b	0.15	0/333	0.46	0/416
8	5b	0.89	0/327	1.11	0/407
9	2c	1.18	0/338	1.20	1/419 (0.2%)
9	4c	0.16	0/298	0.49	0/370
9	5c	1.14	0/387	1.21	1/482 (0.2%)
10	2d	1.24	1/295 (0.3%)	1.26	0/367
10	4d	0.21	0/291	0.47	0/363
10	5d	1.23	0/295	1.26	0/367
11	2e	1.02	0/315	1.26	0/392
11	4e	0.17	0/313	0.47	0/390
11	5e	1.03	0/315	1.27	1/392 (0.3%)
12	2f	0.86	0/270	1.05	0/334
12	4f	0.24	0/297	0.59	0/371
12	5f	0.85	0/287	1.03	0/357
13	2g	0.81	0/318	1.01	0/394
13	4g	0.14	0/287	0.35	0/358
13	5g	0.78	0/302	1.02	0/374
14	6A	0.17	0/1398	0.34	0/2172
15	6a	0.69	0/359	1.28	0/447
16	6b	0.75	0/294	1.37	3/364 (0.8%)
17	6c	0.58	0/294	1.32	3/364 (0.8%)
18	6d	0.71	0/286	1.28	2/354 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	6e	0.71	0/279	1.40	2/347 (0.6%)
20	6f	0.60	0/258	1.14	0/319
21	6g	0.67	0/242	1.21	1/299 (0.3%)
22	4A	0.22	0/3025	0.37	0/4702
23	4B	0.12	0/2114	0.29	0/2836
24	4C	0.14	0/3452	0.33	0/4675
25	4D	0.15	0/2912	0.31	0/3924
26	4E	0.14	0/974	0.27	0/1316
27	4F	0.16	0/1198	0.32	0/1620
28	4G	0.11	0/5592	0.31	2/7615 (0.0%)
29	4H	0.09	0/853	0.26	0/1188
30	4I	0.19	0/502	0.55	2/683 (0.3%)
31	4J	0.12	0/1158	0.31	0/1553
32	4Z	0.17	0/2101	0.48	1/2928 (0.0%)
33	2A	0.71	12/2576 (0.5%)	1.11	27/4003 (0.7%)
34	2B	0.99	0/647	2.34	33/807 (4.1%)
35	2C	0.97	0/375	1.97	7/467 (1.5%)
36	2D	0.24	0/1388	0.62	2/1813 (0.1%)
37	2E	0.38	0/373	1.77	4/461 (0.9%)
38	2F	0.38	0/1688	0.92	3/2102 (0.1%)
39	2G	1.72	38/4184 (0.9%)	1.43	27/5216 (0.5%)
40	2H	1.02	0/957	1.09	2/1209 (0.2%)
41	2I	1.39	25/4664 (0.5%)	1.20	9/5816 (0.2%)
42	2J	1.02	0/311	0.99	0/387
43	2K	1.27	2/431 (0.5%)	1.27	1/537 (0.2%)
44	2L	1.16	0/355	1.12	0/442
45	2M	1.59	1/263 (0.4%)	1.23	0/327
All	All	0.61	86/96900 (0.1%)	0.70	155/130950 (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
3	5B	0	1
9	2c	0	1
9	5c	0	1
25	4D	0	1
38	2F	0	1
39	2G	0	11
40	2H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	2I	0	11
43	2K	0	1
45	2M	0	1
All	All	0	32

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2G	407	MET	N-CA	22.52	1.71	1.46
39	2G	406	ALA	C-N	14.95	1.52	1.33
39	2G	1243	PRO	N-CA	-9.49	1.35	1.47
39	2G	944	SER	N-CA	-8.41	1.34	1.46
41	2I	84	SER	CA-C	-7.80	1.42	1.53
33	2A	142	C	C1'-N1	7.52	1.59	1.48
41	2I	1101	VAL	CA-C	-7.22	1.44	1.52
39	2G	868	VAL	CA-C	-7.20	1.42	1.52
41	2I	110	SER	C-O	-7.20	1.15	1.23
41	2I	82	SER	CA-C	-7.15	1.44	1.52
33	2A	182	U	C1'-N1	7.14	1.59	1.48
41	2I	1101	VAL	C-O	-7.00	1.16	1.24
33	2A	150	U	C1'-N1	6.94	1.58	1.48
33	2A	151	C	C1'-N1	6.73	1.58	1.48
33	2A	97	G	C1'-N9	-6.71	1.37	1.48
39	2G	1273	TYR	CA-C	-6.71	1.43	1.52
33	2A	141	C	C1'-N1	6.58	1.58	1.48
39	2G	939	ARG	CA-C	-6.58	1.44	1.52
41	2I	289	CYS	C-O	-6.57	1.15	1.23
33	2A	184	C	C1'-N1	6.55	1.58	1.48
41	2I	141	VAL	C-O	-6.53	1.17	1.24
33	2A	148	C	C1'-N1	6.53	1.58	1.48
41	2I	64	SER	N-CA	-6.51	1.38	1.46
43	2K	98	PHE	N-CA	-6.49	1.37	1.46
39	2G	814	PHE	CA-C	-6.20	1.45	1.52
39	2G	678	ALA	N-CA	-6.05	1.38	1.46
41	2I	64	SER	C-O	-6.03	1.16	1.23
1	A	9	U	C1'-N1	6.01	1.56	1.47
1	A	8	U	C1'-N1	6.00	1.56	1.47
41	2I	213	LEU	CA-C	-6.00	1.45	1.52
1	A	7	U	C1'-N1	6.00	1.56	1.47
41	2I	302	LEU	C-O	-5.97	1.16	1.24
39	2G	945	ALA	CA-C	-5.97	1.44	1.52
39	2G	571	VAL	CA-C	-5.92	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2I	115	ILE	N-CA	-5.91	1.40	1.46
41	2I	167	VAL	CA-C	-5.89	1.46	1.52
39	2G	1167	TYR	CA-C	-5.89	1.45	1.52
41	2I	140	LEU	CA-C	-5.87	1.45	1.52
39	2G	893	ILE	N-CA	-5.85	1.39	1.46
33	2A	48	A	C1'-N9	-5.84	1.39	1.48
39	2G	940	LEU	CA-C	-5.81	1.45	1.52
33	2A	65	U	C1'-N1	5.74	1.57	1.48
39	2G	989	VAL	CA-C	-5.68	1.45	1.52
41	2I	1153	PRO	C-O	-5.67	1.18	1.24
39	2G	233	ASP	CA-C	-5.66	1.45	1.52
41	2I	104	GLN	CA-C	-5.66	1.46	1.52
41	2I	235	LEU	C-O	-5.66	1.16	1.23
39	2G	482	VAL	C-O	-5.64	1.17	1.24
39	2G	1177	LEU	C-O	-5.64	1.17	1.24
43	2K	95	ASN	N-CA	-5.64	1.39	1.46
39	2G	838	VAL	N-CA	-5.59	1.40	1.46
41	2I	80	VAL	C-O	-5.55	1.18	1.24
39	2G	235	THR	C-O	-5.53	1.19	1.24
1	A	11	C	C1'-N1	5.50	1.55	1.47
41	2I	1123	SER	CA-C	-5.50	1.45	1.52
33	2A	110	A	C1'-N9	-5.47	1.39	1.48
41	2I	134	ALA	C-O	-5.45	1.18	1.23
1	A	10	C	C1'-N1	5.45	1.55	1.47
41	2I	107	PHE	CA-C	-5.44	1.45	1.52
39	2G	439	GLY	CA-C	5.42	1.56	1.52
39	2G	738	HIS	N-CA	-5.41	1.39	1.45
41	2I	941	HIS	C-O	5.34	1.30	1.23
39	2G	627	THR	N-CA	-5.33	1.40	1.46
41	2I	38	LEU	CA-C	-5.32	1.46	1.52
1	A	46	U	C1'-N1	5.29	1.55	1.47
39	2G	680	LEU	C-O	-5.28	1.19	1.24
39	2G	721	ILE	N-CA	-5.25	1.40	1.46
39	2G	864	TYR	CA-C	-5.23	1.46	1.52
41	2I	1034	THR	CA-C	-5.20	1.47	1.53
39	2G	898	TYR	C-N	-5.18	1.27	1.33
39	2G	415	LEU	C-N	5.18	1.39	1.33
39	2G	672	ALA	CA-C	-5.17	1.46	1.52
39	2G	776	GLU	CA-C	-5.16	1.45	1.52
39	2G	407	MET	C-O	-5.16	1.18	1.23
45	2M	44	MET	C-O	-5.15	1.18	1.24
39	2G	601	ALA	N-CA	-5.14	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2A	60	U	C1'-N1	5.12	1.56	1.48
39	2G	1279	ALA	CA-C	-5.12	1.46	1.52
39	2G	1281	ILE	CA-C	-5.12	1.46	1.52
39	2G	944	SER	CA-C	5.09	1.59	1.53
39	2G	899	ALA	N-CA	-5.09	1.40	1.46
4	5C	810	PRO	CG-CD	-5.07	1.33	1.50
10	2d	14	LEU	CA-C	5.07	1.59	1.52
41	2I	68	PHE	N-CA	-5.05	1.40	1.46
39	2G	739	ARG	N-CA	-5.03	1.40	1.46
39	2G	1253	GLY	N-CA	-5.03	1.39	1.45

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2E	146	MET	CA-C-N	21.07	146.17	119.84
37	2E	146	MET	C-N-CA	21.07	146.17	119.84
39	2G	406	ALA	CA-C-N	17.67	147.39	120.89
39	2G	406	ALA	C-N-CA	17.67	147.39	120.89
4	5C	810	PRO	CA-N-CD	-14.59	91.58	112.00
39	2G	406	ALA	CA-C-O	-13.04	105.77	120.24
39	2G	108	ARG	CA-C-N	12.13	132.88	120.38
39	2G	108	ARG	C-N-CA	12.13	132.88	120.38
41	2I	916	ASN	CA-C-N	9.51	131.72	119.84
41	2I	916	ASN	C-N-CA	9.51	131.72	119.84
39	2G	114	ASP	N-CA-C	9.45	121.35	111.14
33	2A	180	G	O3'-P-O5'	-8.65	91.02	104.00
33	2A	149	A	O3'-P-O5'	-8.65	91.03	104.00
33	2A	182	U	O3'-P-O5'	-8.62	91.06	104.00
33	2A	183	G	O3'-P-O5'	-8.59	91.11	104.00
33	2A	148	C	O3'-P-O5'	-8.59	91.12	104.00
33	2A	141	C	O3'-P-O5'	-8.57	91.14	104.00
33	2A	150	U	O3'-P-O5'	-8.55	91.17	104.00
33	2A	113	G	O3'-P-O5'	-8.54	91.19	104.00
33	2A	181	G	O3'-P-O5'	-8.54	91.19	104.00
19	6e	45	LEU	N-CA-C	8.53	123.56	112.12
33	2A	114	A	O3'-P-O5'	-8.53	91.21	104.00
34	2B	16	THR	CA-C-O	-8.01	111.79	120.36
34	2B	99	SER	N-CA-C	8.01	122.84	112.26
28	4G	707	ASP	CA-C-N	7.86	135.84	121.70
28	4G	707	ASP	C-N-CA	7.86	135.84	121.70
5	5D	583	THR	CA-C-N	7.79	136.07	121.81
5	5D	583	THR	C-N-CA	7.79	136.07	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2B	117	TYR	CA-C-O	7.76	128.55	120.40
33	2A	168	A	P-O5'-C5'	-7.62	109.47	120.90
4	5C	810	PRO	N-CD-CG	-7.37	92.14	103.20
32	4Z	380	THR	N-CA-C	7.36	121.68	111.74
3	5B	1194	CYS	CA-CB-SG	7.31	131.21	114.40
33	2A	167	U	O3'-P-O5'	-7.27	93.09	104.00
34	2B	71	VAL	CA-C-N	7.19	131.60	120.75
34	2B	71	VAL	C-N-CA	7.19	131.60	120.75
39	2G	613	MET	N-CA-C	7.18	121.75	112.92
39	2G	1100	ASN	N-CA-C	7.16	119.22	110.41
39	2G	407	MET	N-CA-C	7.05	121.96	111.04
33	2A	170	C	C3'-C2'-O2'	-7.02	104.07	114.60
30	4I	25	PRO	N-CD-CG	-6.97	92.74	103.20
36	2D	199	ARG	CA-C-N	6.91	127.87	120.47
36	2D	199	ARG	C-N-CA	6.91	127.87	120.47
30	4I	25	PRO	CA-N-CD	-6.89	102.36	112.00
38	2F	290	GLY	N-CA-C	6.88	120.98	112.73
34	2B	121	LEU	CA-C-O	6.87	128.85	121.44
34	2B	4	LEU	N-CA-C	-6.85	98.05	108.67
35	2C	53	PHE	CA-C-O	-6.83	112.80	120.32
37	2E	158	ARG	N-CA-C	6.75	118.72	111.36
39	2G	1120	ALA	CA-C-N	-6.69	111.34	120.44
39	2G	1120	ALA	C-N-CA	-6.69	111.34	120.44
33	2A	164	C	C5'-C4'-O4'	-6.57	99.25	109.10
43	2K	85	ARG	N-CA-C	6.52	120.03	109.40
34	2B	87	LEU	CA-C-N	6.41	126.17	119.05
34	2B	87	LEU	C-N-CA	6.41	126.17	119.05
39	2G	406	ALA	O-C-N	6.41	130.56	122.23
33	2A	168	A	C5'-C4'-C3'	-6.33	106.51	116.00
34	2B	40	THR	CA-C-N	6.24	131.44	122.40
34	2B	40	THR	C-N-CA	6.24	131.44	122.40
39	2G	406	ALA	N-CA-C	6.23	119.35	111.69
33	2A	169	C	P-O3'-C3'	6.23	129.54	120.20
39	2G	1180	ARG	N-CA-C	-6.16	103.27	111.96
34	2B	73	ASN	N-CA-C	6.16	119.85	111.17
40	2H	559	PRO	N-CA-C	6.11	120.07	111.33
39	2G	1275	GLY	N-CA-C	-6.11	104.91	111.93
34	2B	79	ILE	CA-C-N	6.05	125.85	120.10
34	2B	79	ILE	C-N-CA	6.05	125.85	120.10
39	2G	415	LEU	O-C-N	-6.02	114.40	121.32
35	2C	46	MET	N-CA-C	-5.94	104.71	111.07
17	6c	2	LEU	CA-C-N	5.87	127.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6c	2	LEU	C-N-CA	5.87	127.17	119.84
34	2B	113	LYS	N-CA-C	5.85	118.41	111.33
33	2A	163	G	O3'-P-O5'	-5.85	95.23	104.00
39	2G	465	PRO	N-CA-C	-5.84	106.51	114.80
34	2B	50	SER	CA-C-O	5.83	127.73	121.55
18	6d	13	LEU	CA-C-N	5.82	125.95	119.32
18	6d	13	LEU	C-N-CA	5.82	125.95	119.32
34	2B	27	ARG	CA-C-N	5.74	128.78	120.11
34	2B	27	ARG	C-N-CA	5.74	128.78	120.11
41	2I	679	LEU	N-CA-C	5.73	119.43	110.32
19	6e	63	ALA	N-CA-C	5.71	118.08	109.23
33	2A	164	C	P-O3'-C3'	5.70	128.75	120.20
41	2I	887	ALA	N-CA-C	-5.68	101.64	110.10
39	2G	942	ASN	CA-C-N	-5.64	114.77	124.82
39	2G	942	ASN	C-N-CA	-5.64	114.77	124.82
7	2a	52	LYS	CA-C-N	-5.64	114.12	119.76
7	2a	52	LYS	C-N-CA	-5.64	114.12	119.76
33	2A	160	A	P-O5'-C5'	-5.62	112.46	120.90
34	2B	71	VAL	O-C-N	-5.62	115.54	122.57
39	2G	942	ASN	N-CA-C	-5.60	98.86	110.80
34	2B	32	PRO	CA-C-N	5.59	130.76	122.99
34	2B	32	PRO	C-N-CA	5.59	130.76	122.99
7	5a	52	LYS	CA-C-N	-5.56	114.20	119.76
7	5a	52	LYS	C-N-CA	-5.56	114.20	119.76
34	2B	34	ILE	CA-C-O	-5.53	114.21	120.74
6	5E	322	LYS	N-CA-C	-5.52	98.20	108.02
3	5B	1194	CYS	N-CA-CB	5.50	120.11	111.20
33	2A	168	A	O4'-C1'-C2'	-5.50	102.10	107.60
6	5E	284	PHE	N-CA-C	5.49	119.48	112.34
33	2A	157	G	P-O5'-C5'	-5.49	112.66	120.90
33	2A	165	A	N9-C1'-C2'	5.49	120.23	112.00
34	2B	159	GLU	N-CA-C	-5.48	104.95	111.69
7	2a	5	LYS	N-CA-C	5.48	118.17	111.82
6	5E	281	VAL	N-CA-C	5.46	116.17	108.36
34	2B	16	THR	O-C-N	5.45	129.43	123.22
16	6b	49	HIS	N-CA-C	-5.45	106.71	113.19
39	2G	1128	VAL	N-CA-C	5.45	117.90	111.09
40	2H	511	LEU	N-CA-C	5.44	117.53	108.99
39	2G	1105	GLU	N-CA-C	5.43	117.58	108.73
41	2I	488	GLY	N-CA-C	-5.42	106.37	115.80
1	A	28	G	C4'-C3'-O3'	-5.41	104.88	113.00
1	A	28	G	C2'-C3'-O3'	-5.41	105.59	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2B	40	THR	N-CA-C	-5.39	106.20	112.89
6	5E	156	SER	N-CA-C	5.38	116.70	108.42
6	5E	237	SER	N-CA-C	5.37	117.87	110.35
37	2E	199	TRP	N-CA-C	5.35	117.36	107.73
34	2B	125	VAL	CA-C-N	5.35	127.98	120.28
34	2B	125	VAL	C-N-CA	5.35	127.98	120.28
17	6c	30	VAL	N-CA-C	5.33	116.22	111.90
16	6b	92	VAL	N-CA-C	5.32	115.95	109.30
39	2G	1106	ARG	N-CA-C	5.28	118.86	111.74
34	2B	146	ASP	CA-C-N	5.26	130.03	122.40
34	2B	146	ASP	C-N-CA	5.26	130.03	122.40
41	2I	4	TYR	N-CA-C	-5.25	102.52	110.28
38	2F	289	LYS	N-CA-C	5.24	121.96	110.80
21	6g	69	VAL	N-CA-C	5.23	115.44	108.27
33	2A	171	U	C2'-C3'-O3'	-5.23	105.86	113.70
33	2A	170	C	O4'-C1'-C2'	-5.23	100.57	105.80
35	2C	20	LYS	N-CA-C	5.21	117.36	111.11
16	6b	44	HIS	N-CA-C	-5.18	107.02	113.55
4	5C	809	ILE	CA-CB-CG1	5.17	119.19	110.40
4	5C	308	CYS	CA-CB-SG	5.14	126.22	114.40
39	2G	415	LEU	CA-C-N	5.14	125.67	120.38
39	2G	415	LEU	C-N-CA	5.14	125.67	120.38
4	5C	810	PRO	CA-CB-CG	-5.14	94.74	104.50
9	5c	99	MET	N-CA-C	5.14	116.88	108.76
35	2C	51	GLN	N-CA-C	5.13	117.48	109.52
33	2A	155	C	P-O3'-C3'	5.12	127.88	120.20
35	2C	48	MET	N-CA-C	5.11	119.52	113.28
34	2B	90	LEU	O-C-N	5.11	129.39	122.59
11	5e	85	THR	N-CA-C	-5.11	105.89	112.68
35	2C	38	VAL	O-C-N	5.10	127.09	121.83
34	2B	90	LEU	CA-C-O	-5.10	113.22	120.51
33	2A	160	A	N9-C1'-C2'	5.10	119.65	112.00
34	2B	83	LEU	N-CA-C	5.09	117.50	111.33
9	2c	99	MET	N-CA-C	5.09	116.80	108.76
33	2A	156	U	C4'-C3'-C2'	5.08	107.69	102.60
35	2C	83	TYR	CA-C-O	-5.08	115.25	121.05
41	2I	404	LEU	N-CA-C	-5.08	105.82	111.36
41	2I	9	GLN	N-CA-C	-5.07	101.49	109.25
34	2B	81	GLU	N-CA-C	5.05	118.59	112.23
41	2I	445	SER	N-CA-C	-5.04	104.03	110.53
39	2G	1002	ASN	CA-C-N	-5.02	118.05	122.97
39	2G	1002	ASN	C-N-CA	-5.02	118.05	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2F	274	CYS	N-CA-C	5.01	116.56	111.14

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	2F	443	THR	Peptide
39	2G	1025	LYS	Peptide
39	2G	1122	THR	Peptide
39	2G	1127	THR	Peptide
39	2G	1179	ASP	Peptide
39	2G	1199	VAL	Peptide
39	2G	220	GLN	Peptide
39	2G	415	LEU	Mainchain,Peptide
39	2G	689	ILE	Peptide
39	2G	941	ASN	Peptide
39	2G	944	SER	Peptide
40	2H	553	MET	Peptide
40	2H	558	ARG	Peptide
40	2H	571	LEU	Peptide
41	2I	261	PHE	Peptide
41	2I	366	ASP	Peptide
41	2I	468	ASP	Peptide
41	2I	530	ASP	Peptide
41	2I	534	ASN	Peptide
41	2I	552	ARG	Peptide
41	2I	670	GLN	Peptide
41	2I	678	VAL	Peptide
41	2I	74	THR	Peptide
41	2I	980	LYS	Peptide
41	2I	986	ILE	Peptide
43	2K	29	LYS	Peptide
45	2M	74	GLN	Peptide
9	2c	112	ASN	Peptide
25	4D	358	ARG	Sidechain
3	5B	941	LYS	Peptide
9	5c	112	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1187	0	605	151	0
2	5A	2420	0	1226	77	0
3	5B	18642	0	18499	189	0
4	5C	6436	0	6453	105	0
5	5D	13633	0	13769	313	0
6	5E	1196	0	337	2	0
7	2a	344	0	93	4	0
7	4a	256	0	70	2	0
7	5a	336	0	89	0	0
8	2b	328	0	89	0	0
8	4b	334	0	92	1	0
8	5b	328	0	89	5	0
9	2c	340	0	87	1	0
9	4c	300	0	80	5	0
9	5c	388	0	102	7	0
10	2d	296	0	87	1	0
10	4d	292	0	93	7	0
10	5d	296	0	87	10	0
11	2e	316	0	85	2	0
11	4e	314	0	86	3	0
11	5e	316	0	85	4	0
12	2f	272	0	75	1	0
12	4f	298	0	89	5	0
12	5f	288	0	82	5	0
13	2g	320	0	88	0	0
13	4g	288	0	84	1	0
13	5g	304	0	82	6	0
14	6A	1251	0	630	25	0
15	6a	360	0	95	2	0
16	6b	296	0	76	5	0
17	6c	296	0	77	0	0
18	6d	288	0	78	0	0
19	6e	280	0	81	8	0
20	6f	260	0	75	0	0
21	6g	244	0	71	3	0
22	4A	2744	0	1395	67	0
23	4B	2076	0	2148	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4C	3370	0	3300	49	0
25	4D	2874	0	2856	24	0
26	4E	962	0	1012	5	0
27	4F	1169	0	1139	6	0
28	4G	5504	0	4772	57	0
29	4H	844	0	426	5	0
30	4I	494	0	384	6	0
31	4J	1153	0	1107	13	0
32	4Z	2093	0	993	15	0
33	2A	2311	0	1170	144	0
34	2B	648	0	167	1	0
35	2C	376	0	102	0	0
36	2D	1380	0	999	20	0
37	2E	376	0	85	0	0
38	2F	1693	0	454	22	0
39	2G	4192	0	1110	234	0
40	2H	959	0	417	11	0
41	2I	4672	0	1260	71	0
42	2J	312	0	87	3	0
43	2K	432	0	114	6	0
44	2L	356	0	105	5	0
45	2M	264	0	70	11	0
46	5B	36	0	6	1	0
47	5C	32	0	12	0	0
48	5C	1	0	0	0	0
49	4I	1	0	0	0	0
All	All	94667	0	69576	1572	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 10.

All (1572) 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)
39:2G:407:MET:N	39:2G:407:MET:CA	1.71	1.53
1:A:30:C:C2'	1:A:31:C:H5''	1.54	1.35
1:A:30:C:N4	1:A:31:C:C4	2.10	1.18
1:A:38:C:H4'	1:A:39:U:OP1	1.42	1.18
3:5B:2036:GLN:O	5:5D:1035:LEU:HD13	1.40	1.17
1:A:30:C:C4	1:A:31:C:C5	2.34	1.16
1:A:22:C:O2'	1:A:23:G:H5'	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:G:C8	1:A:35:U:C5	2.34	1.15
22:4A:119:A:H5''	10:4d:39:TYR:CA	1.75	1.14
1:A:30:C:H2'	1:A:31:C:C5'	1.78	1.13
4:5C:809:ILE:HD12	4:5C:810:PRO:HD2	1.32	1.12
33:2A:156:U:H6	33:2A:156:U:H5''	1.09	1.09
3:5B:2038:GLN:N	5:5D:1035:LEU:HD11	1.69	1.06
3:5B:2038:GLN:CB	5:5D:1035:LEU:CD1	2.33	1.06
33:2A:105:G:H2'	33:2A:106:G:H5''	1.37	1.06
2:5A:90:U:C5	13:5g:38:ASN:O	2.09	1.06
1:A:30:C:C3'	1:A:31:C:H5''	1.84	1.04
1:A:40:U:H4'	1:A:41:U:H5'	1.38	1.04
22:4A:118:A:C2	22:4A:119:A:N6	2.25	1.03
22:4A:126:A:C2	9:4c:104:ASP:CA	2.41	1.03
1:A:30:C:H2'	1:A:31:C:H5''	1.03	1.02
1:A:34:G:C8	1:A:35:U:C4	2.47	1.02
2:5A:95:G:H1'	10:5d:24:LYS:CA	1.90	1.01
1:A:30:C:C3'	1:A:31:C:C5'	2.40	1.00
3:5B:2036:GLN:C	5:5D:1035:LEU:HD13	1.86	0.99
3:5B:2038:GLN:N	5:5D:1035:LEU:CD1	2.27	0.98
22:4A:91:A:H2	22:4A:110:G:N2	1.61	0.98
3:5B:2038:GLN:CB	5:5D:1035:LEU:HD12	1.93	0.98
33:2A:168:A:C8	33:2A:168:A:H5''	1.98	0.97
1:A:31:C:C2	33:2A:33:G:N1	2.32	0.97
1:A:30:C:C2'	1:A:31:C:C5'	2.38	0.96
32:4Z:333:ILE:O	32:4Z:342:LEU:N	1.98	0.96
39:2G:501:LEU:O	39:2G:504:ILE:N	1.98	0.96
1:A:31:C:C2	33:2A:33:G:C6	2.53	0.95
1:A:31:C:O2	33:2A:33:G:C6	2.20	0.94
2:5A:93:U:H1'	9:5c:104:ASP:CA	1.96	0.94
33:2A:156:U:H5''	33:2A:156:U:C6	2.02	0.93
39:2G:86:ALA:O	39:2G:89:ALA:N	2.02	0.91
4:5C:196:LYS:HA	13:5g:33:ILE:O	1.71	0.91
2:5A:95:G:H21	2:5A:96:A:H5''	1.36	0.89
33:2A:54:U:OP1	38:2F:428:GLU:CA	2.20	0.89
1:A:23:G:H1	33:2A:39:U:H3	1.20	0.89
1:A:34:G:N7	1:A:35:U:C4	2.40	0.89
2:5A:93:U:O4	10:5d:66:CYS:N	2.06	0.89
1:A:40:U:O2'	1:A:41:U:OP2	1.89	0.88
39:2G:793:LYS:O	39:2G:797:GLY:HA3	1.72	0.88
3:5B:2038:GLN:H	5:5D:1035:LEU:CD1	1.86	0.88
3:5B:1412:TRP:O	3:5B:1420:ASN:ND2	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:U:H3'	1:A:103:A:H5''	1.55	0.87
22:4A:120:U:H2'	11:4e:82:ASP:CA	2.04	0.87
2:5A:93:U:C1'	9:5c:104:ASP:CA	2.52	0.87
33:2A:154:C:O2	33:2A:176:G:N2	2.07	0.87
1:A:12:U:OP2	1:A:12:U:H2'	1.74	0.87
3:5B:2036:GLN:O	5:5D:1035:LEU:CD1	2.23	0.86
5:5D:1519:ARG:NH2	5:5D:1691:ALA:O	2.07	0.86
27:4F:117:GLU:OE2	27:4F:121:ARG:NH1	2.08	0.86
33:2A:40:C:H5''	33:2A:40:C:H6	1.39	0.86
33:2A:156:U:H6	33:2A:156:U:C5'	1.89	0.86
2:5A:90:U:H5	13:5g:38:ASN:O	1.53	0.86
5:5D:1622:GLU:OE2	5:5D:1649:SER:OG	1.93	0.86
22:4A:118:A:H2	22:4A:119:A:H62	1.22	0.86
33:2A:168:A:H5''	33:2A:168:A:H8	1.36	0.86
1:A:38:C:OP1	1:A:39:U:P	2.34	0.85
4:5C:256:CYS:HA	4:5C:308:CYS:HB3	1.56	0.85
22:4A:121:U:H3	12:4f:63:ARG:CA	1.88	0.85
5:5D:471:ALA:HB1	5:5D:518:LEU:HD13	1.58	0.85
39:2G:728:LEU:O	39:2G:731:LEU:N	2.10	0.85
1:A:11:C:H2'	1:A:11:C:O2	1.75	0.84
1:A:30:C:H3'	1:A:31:C:C5'	2.04	0.84
22:4A:118:A:N3	22:4A:119:A:N6	2.23	0.84
22:4A:119:A:C5'	10:4d:39:TYR:CA	2.56	0.84
1:A:36:C:H1'	1:A:37:C:OP1	1.78	0.83
33:2A:152:G:N2	33:2A:153:A:N7	2.27	0.83
1:A:30:C:C5	1:A:31:C:C5	2.67	0.83
28:4G:354:PRO:O	28:4G:357:THR:OG1	1.95	0.83
24:4C:119:ILE:HG22	24:4C:120:THR:HG23	1.62	0.82
3:5B:2038:GLN:CB	5:5D:1035:LEU:HD11	2.08	0.82
19:6e:46:GLU:CA	19:6e:63:ALA:N	2.43	0.82
22:4A:49:C:OP1	28:4G:172:ARG:NH1	2.12	0.81
32:4Z:334:HIS:HA	32:4Z:341:THR:HA	1.62	0.81
33:2A:105:G:C2'	33:2A:106:G:H5''	2.10	0.81
39:2G:648:LEU:O	39:2G:651:VAL:N	2.13	0.81
41:2I:839:ALA:O	41:2I:843:LEU:N	2.13	0.81
1:A:31:C:O2	33:2A:33:G:N1	2.13	0.81
5:5D:991:TYR:OH	5:5D:1097:GLU:OE2	1.97	0.81
1:A:36:C:H4'	1:A:37:C:H5	1.44	0.81
33:2A:152:G:H5''	33:2A:153:A:OP2	1.80	0.81
1:A:34:G:C2	1:A:35:U:H2'	2.16	0.81
1:A:27:U:OP2	39:2G:1106:ARG:CA	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:U:O2	33:2A:42:G:C2	2.35	0.80
3:5B:1393:ARG:NH1	28:4G:202:PRO:O	2.15	0.80
2:5A:92:U:H3	8:5b:36:MET:CA	1.93	0.80
14:6A:65:G:O2'	23:4B:515:ASN:ND2	2.13	0.80
22:4A:108:C:O2'	22:4A:109:G:H5'	1.81	0.80
36:2D:418:GLU:N	36:2D:418:GLU:OE1	2.15	0.80
1:A:34:G:N9	1:A:35:U:C5	2.49	0.80
3:5B:1972:THR:OG1	3:5B:1975:GLU:OE1	1.99	0.80
1:A:112:G:N2	14:6A:42:C:O2	2.15	0.80
1:A:28:G:H5'	1:A:28:G:H8	1.45	0.79
1:A:32:C:O2	33:2A:31:G:N1	2.11	0.79
33:2A:101:U:H5''	33:2A:102:U:H5'	1.65	0.79
5:5D:1151:GLU:OE2	5:5D:1151:GLU:N	2.16	0.79
2:5A:94:U:H1'	2:5A:95:G:OP1	1.82	0.79
44:2L:56:GLY:O	44:2L:65:GLY:N	2.12	0.79
1:A:23:G:N2	33:2A:39:U:O2	2.14	0.79
33:2A:54:U:OP1	38:2F:424:ARG:O	2.00	0.79
39:2G:669:GLN:O	39:2G:672:ALA:N	2.16	0.79
1:A:28:G:H5'	1:A:28:G:C8	2.18	0.79
3:5B:292:ASP:OD1	3:5B:1139:ARG:NH1	2.16	0.79
1:A:30:C:N4	1:A:31:C:N4	2.31	0.78
1:A:31:C:H1'	33:2A:33:G:N2	1.99	0.78
1:A:34:G:H2'	1:A:35:U:C6	2.19	0.78
1:A:36:C:H4'	1:A:37:C:C5	2.18	0.78
3:5B:200:ASP:OD1	3:5B:240:ARG:NH2	2.16	0.78
41:2I:523:GLY:HA3	41:2I:536:TRP:O	1.83	0.78
5:5D:1090:ARG:NH1	22:4A:75:C:O2'	2.17	0.78
4:5C:569:ARG:O	4:5C:569:ARG:NH1	2.16	0.78
1:A:31:C:O2	33:2A:33:G:C2	2.37	0.77
41:2I:914:ILE:O	41:2I:918:ARG:CA	2.32	0.77
39:2G:428:ALA:O	39:2G:432:THR:N	2.17	0.77
4:5C:826:ARG:NH2	4:5C:910:ASP:OD2	2.18	0.77
3:5B:2188:LEU:O	3:5B:2251:TYR:OH	2.01	0.77
5:5D:880:LEU:O	5:5D:884:ASN:ND2	2.17	0.77
33:2A:177:A:H5''	33:2A:178:A:OP1	1.84	0.77
1:A:8:U:O2	1:A:8:U:H2'	1.84	0.77
33:2A:153:A:H2'	33:2A:154:C:H5'	1.65	0.76
39:2G:1246:MET:O	39:2G:1249:TYR:N	2.18	0.76
1:A:34:G:H3'	1:A:35:U:H5''	1.67	0.76
1:A:40:U:H4'	1:A:41:U:C5'	2.13	0.76
22:4A:121:U:N3	12:4f:63:ARG:CA	2.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:C:H1'	33:2A:33:G:C2	2.20	0.76
39:2G:531:LEU:O	39:2G:534:GLN:N	2.18	0.76
38:2F:276:GLY:C	38:2F:278:LEU:H	1.92	0.75
39:2G:1016:LEU:O	39:2G:1019:ARG:N	2.19	0.75
5:5D:1342:SER:O	5:5D:1486:ARG:NH2	2.20	0.75
1:A:17:G:H1	33:2A:44:U:H3	1.33	0.75
33:2A:153:A:C2'	33:2A:154:C:H5'	2.17	0.75
1:A:30:C:C4	1:A:31:C:C6	2.76	0.74
33:2A:143:A:H3'	33:2A:143:A:N3	2.01	0.74
23:4B:415:THR:HG23	23:4B:417:LEU:HD22	1.69	0.74
39:2G:1270:ASN:O	39:2G:1273:TYR:N	2.21	0.74
41:2I:304:GLN:CA	41:2I:309:ASP:O	2.36	0.74
38:2F:184:ARG:O	7:2a:85:PRO:N	2.21	0.74
1:A:31:C:O2	33:2A:33:G:C5	2.41	0.74
2:5A:93:U:O4	10:5d:65:ARG:CA	2.35	0.73
22:4A:91:A:H2	22:4A:110:G:H22	0.82	0.73
39:2G:874:LYS:O	39:2G:877:GLY:N	2.20	0.73
41:2I:442:LEU:O	41:2I:735:SER:N	2.19	0.73
1:A:38:C:OP1	1:A:39:U:OP1	2.06	0.73
4:5C:561:LYS:NZ	4:5C:611:ASN:O	2.20	0.73
1:A:34:G:H2'	1:A:35:U:H6	1.52	0.73
2:5A:117:A:N1	10:5d:26:GLY:HA3	2.03	0.73
22:4A:57:G:N7	25:4D:354:ARG:NH1	2.36	0.73
31:4J:352:GLU:N	31:4J:352:GLU:OE1	2.21	0.73
39:2G:660:ALA:O	39:2G:663:THR:N	2.22	0.73
3:5B:510:ARG:NH2	28:4G:35:GLY:O	2.22	0.73
5:5D:730:GLU:O	5:5D:734:THR:HG22	1.89	0.73
38:2F:276:GLY:O	38:2F:278:LEU:N	2.20	0.73
33:2A:179:C:H2'	33:2A:180:G:H8	1.54	0.72
33:2A:106:G:H21	33:2A:107:A:N6	1.87	0.72
19:6e:46:GLU:N	19:6e:63:ALA:H	1.87	0.72
36:2D:413:SER:OG	36:2D:416:THR:O	2.04	0.72
41:2I:753:GLY:HA3	41:2I:765:LEU:O	1.88	0.72
3:5B:2072:GLU:HG3	3:5B:2075:VAL:HG22	1.69	0.72
5:5D:441:GLY:O	5:5D:693:THR:OG1	2.08	0.72
5:5D:622:ASP:OD1	5:5D:623:ASP:N	2.22	0.72
28:4G:928:ASP:O	28:4G:932:LEU:HD12	1.88	0.72
39:2G:1055:TRP:O	39:2G:1058:ILE:N	2.22	0.72
2:5A:96:A:H61	12:5f:23:GLY:H	1.38	0.72
5:5D:1945:LEU:HA	5:5D:1948:MET:HE3	1.72	0.72
1:A:15:A:H2'	1:A:16:A:O4'	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:U:H3	33:2A:42:G:H1	1.37	0.72
39:2G:87:PRO:O	39:2G:91:LEU:N	2.21	0.72
39:2G:535:ILE:O	39:2G:538:LEU:N	2.23	0.72
1:A:21:U:H1'	1:A:22:C:OP1	1.90	0.72
39:2G:994:LEU:O	39:2G:997:LEU:N	2.22	0.71
3:5B:2295:GLU:OE2	3:5B:2295:GLU:N	2.22	0.71
39:2G:122:HIS:O	39:2G:125:THR:N	2.22	0.71
39:2G:791:VAL:O	39:2G:794:GLN:N	2.23	0.71
4:5C:130:ARG:NH2	4:5C:439:PRO:O	2.24	0.71
33:2A:106:G:H4'	33:2A:107:A:O4'	1.89	0.71
2:5A:96:A:H4'	2:5A:97:G:H5''	1.72	0.71
3:5B:1977:ILE:O	3:5B:1981:VAL:HG23	1.91	0.71
33:2A:153:A:H2'	33:2A:154:C:C5'	2.19	0.71
1:A:38:C:OP1	1:A:39:U:OP2	2.09	0.71
24:4C:262:ASP:OD1	24:4C:262:ASP:N	2.23	0.71
14:6A:86:U:H3	33:2A:12:G:H1	1.39	0.71
3:5B:715:GLU:OE1	3:5B:718:ARG:NH1	2.23	0.71
19:6e:46:GLU:N	19:6e:63:ALA:N	2.38	0.71
2:5A:92:U:N3	8:5b:36:MET:CA	2.53	0.70
3:5B:2278:SER:OG	3:5B:2309:HIS:NE2	2.22	0.70
25:4D:274:ILE:O	25:4D:277:SER:OG	2.08	0.70
2:5A:87:A:N6	2:5A:92:U:P	2.64	0.70
3:5B:105:ASN:ND2	3:5B:131:GLU:OE1	2.25	0.70
3:5B:2038:GLN:CA	5:5D:1035:LEU:HD11	2.21	0.70
24:4C:241:PRO:O	24:4C:286:THR:OG1	2.09	0.70
33:2A:54:U:OP1	38:2F:427:ALA:O	2.10	0.70
2:5A:94:U:C1'	2:5A:95:G:OP1	2.39	0.70
39:2G:700:LYS:O	39:2G:703:THR:N	2.24	0.70
40:2H:479:ASP:O	40:2H:482:ALA:N	2.25	0.70
5:5D:1041:LEU:HD23	5:5D:1041:LEU:O	1.90	0.70
5:5D:1699:GLU:OE2	5:5D:1701:ARG:NH1	2.25	0.70
14:6A:103:U:O4	21:6g:32:GLN:O	2.10	0.70
3:5B:861:ARG:NH2	28:4G:178:LYS:O	2.25	0.69
33:2A:40:C:H6	33:2A:40:C:C5'	2.05	0.69
41:2I:545:VAL:N	41:2I:557:ALA:O	2.25	0.69
33:2A:154:C:H2'	33:2A:155:C:C6	2.26	0.69
4:5C:310:SER:OG	4:5C:316:ILE:O	2.09	0.69
5:5D:1201:GLU:N	5:5D:1201:GLU:OE1	2.26	0.69
5:5D:731:THR:HG23	5:5D:810:VAL:HG12	1.74	0.69
5:5D:816:ALA:O	5:5D:855:ARG:NH2	2.26	0.69
33:2A:153:A:N6	33:2A:177:A:C2	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:93:U:O4	10:5d:65:ARG:C	2.36	0.69
44:2L:7:ASP:O	44:2L:91:LEU:N	2.25	0.69
1:A:30:C:H41	1:A:31:C:N4	1.91	0.69
5:5D:1186:LEU:HD21	5:5D:1270:VAL:HG23	1.75	0.69
23:4B:549:ARG:NH2	23:4B:680:GLU:OE2	2.25	0.69
41:2I:558:LEU:O	41:2I:561:GLY:N	2.24	0.69
22:4A:120:U:C2'	11:4e:82:ASP:CA	2.70	0.69
14:6A:102:A:O2'	21:6g:33:THR:CA	2.41	0.68
2:5A:87:A:N6	2:5A:92:U:OP2	2.26	0.68
33:2A:30:A:N3	33:2A:30:A:H2'	2.06	0.68
4:5C:215:VAL:HG11	4:5C:242:LEU:HD21	1.75	0.68
14:6A:103:U:H3'	14:6A:104:U:H5''	1.75	0.68
1:A:30:C:C4	1:A:31:C:C4	2.69	0.68
4:5C:173:THR:N	4:5C:176:GLU:OE1	2.27	0.67
5:5D:1980:GLU:N	5:5D:1980:GLU:OE1	2.27	0.67
28:4G:326:GLN:O	28:4G:330:ASN:ND2	2.26	0.67
33:2A:143:A:H2'	33:2A:144:C:H6	1.59	0.67
1:A:36:C:C4'	1:A:37:C:H5	2.07	0.67
5:5D:748:LEU:HD23	5:5D:748:LEU:O	1.94	0.67
40:2H:596:GLU:C	40:2H:598:GLU:H	2.00	0.67
2:5A:97:G:H1	2:5A:116:U:H3	1.41	0.67
33:2A:152:G:O3'	33:2A:153:A:O4'	2.11	0.67
1:A:22:C:O5'	1:A:22:C:H6	1.78	0.67
2:5A:95:G:H21	2:5A:96:A:C5'	2.06	0.67
3:5B:2237:TRP:NE1	3:5B:2250:GLY:O	2.28	0.67
28:4G:426:ALA:O	28:4G:430:CYS:N	2.28	0.67
41:2I:1148:LEU:O	41:2I:1152:HIS:N	2.27	0.67
1:A:31:C:H5'	1:A:31:C:H6	1.58	0.67
5:5D:569:LEU:HB2	5:5D:575:LEU:HD12	1.77	0.67
32:4Z:362:HIS:O	32:4Z:378:MET:N	2.26	0.67
33:2A:151:C:C2	33:2A:152:G:C8	2.83	0.67
1:A:30:C:N4	1:A:31:C:C5	2.50	0.67
22:4A:111:C:H6	22:4A:111:C:O5'	1.78	0.67
24:4C:190:MET:HA	24:4C:190:MET:HE2	1.76	0.67
4:5C:463:GLU:N	4:5C:463:GLU:OE1	2.28	0.66
33:2A:150:U:H3	33:2A:181:G:H1	1.41	0.66
5:5D:1218:SER:HB3	5:5D:1240:LEU:HD21	1.76	0.66
3:5B:919:ASP:OD2	3:5B:1012:LYS:NZ	2.28	0.66
3:5B:1217:GLN:OE1	3:5B:1224:ARG:NH2	2.28	0.66
3:5B:2278:SER:HG	3:5B:2309:HIS:HE2	1.37	0.66
5:5D:1943:MET:HE1	5:5D:2065:TRP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2A:151:C:H2'	33:2A:152:G:H8	1.60	0.66
39:2G:758:ASP:O	39:2G:762:ALA:N	2.28	0.66
39:2G:1280:LEU:O	39:2G:1283:HIS:N	2.22	0.66
39:2G:400:SER:O	39:2G:404:LEU:N	2.28	0.66
40:2H:487:LEU:O	40:2H:490:HIS:N	2.28	0.66
41:2I:753:GLY:CA	41:2I:765:LEU:O	2.44	0.66
33:2A:168:A:C8	33:2A:168:A:C5'	2.75	0.66
1:A:102:U:C3'	1:A:103:A:H5''	2.26	0.66
33:2A:151:C:O2	33:2A:152:G:C8	2.48	0.66
2:5A:93:U:O4'	9:5c:104:ASP:CA	2.42	0.66
39:2G:1243:PRO:O	39:2G:1246:MET:N	2.29	0.66
4:5C:573:GLU:OE1	4:5C:573:GLU:O	2.13	0.66
14:6A:103:U:H4'	14:6A:104:U:OP2	1.95	0.66
26:4E:15:ASP:O	26:4E:19:THR:OG1	2.10	0.66
1:A:36:C:H1'	1:A:37:C:P	2.36	0.66
33:2A:54:U:OP1	38:2F:427:ALA:C	2.39	0.65
1:A:8:U:O2	1:A:8:U:C2'	2.44	0.65
33:2A:153:A:C3'	33:2A:154:C:H5'	2.25	0.65
3:5B:598:LEU:HD11	3:5B:640:PHE:CE1	2.31	0.65
2:5A:67:A:H2'	2:5A:68:C:C5	2.32	0.65
39:2G:658:TRP:O	39:2G:661:ARG:N	2.30	0.65
1:A:32:C:OP2	1:A:32:C:H3'	1.96	0.65
5:5D:1538:ARG:NH1	5:5D:1665:ASP:OD1	2.30	0.65
5:5D:1948:MET:O	5:5D:1952:ALA:N	2.30	0.65
1:A:11:C:O2	1:A:11:C:C2'	2.45	0.64
2:5A:89:U:H2'	2:5A:90:U:H5''	1.79	0.64
5:5D:769:CYS:SG	5:5D:770:LYS:N	2.69	0.64
26:4E:108:GLU:OE2	26:4E:108:GLU:N	2.29	0.64
39:2G:886:HIS:O	39:2G:889:GLU:N	2.30	0.64
5:5D:488:LEU:HD12	5:5D:488:LEU:O	1.98	0.64
41:2I:325:ILE:O	41:2I:375:SER:N	2.30	0.64
1:A:36:C:C4'	1:A:37:C:C5	2.79	0.64
5:5D:526:ASN:O	5:5D:529:GLY:N	2.30	0.64
22:4A:117:C:O5'	22:4A:117:C:H6	1.80	0.64
33:2A:114:A:H61	33:2A:142:C:H42	1.44	0.64
2:5A:85:C:OP1	9:5c:20:GLU:CA	2.46	0.64
4:5C:177:ARG:NH1	4:5C:638:ASP:OD2	2.29	0.64
14:6A:36:A:O5'	36:2D:506:SER:OG	2.16	0.64
39:2G:1109:ARG:O	39:2G:1110:VAL:C	2.41	0.64
45:2M:40:TYR:O	45:2M:43:TYR:N	2.31	0.64
1:A:22:C:O2'	1:A:23:G:C5'	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:C:C2'	1:A:23:G:H5'	2.28	0.64
5:5D:1936:LEU:HD23	5:5D:1937:SER:N	2.12	0.64
22:4A:120:U:OP2	10:4d:39:TYR:O	2.16	0.64
32:4Z:334:HIS:CA	32:4Z:341:THR:HA	2.27	0.64
33:2A:147:G:H2'	33:2A:148:C:H6	1.63	0.64
40:2H:491:LEU:O	40:2H:494:THR:N	2.30	0.64
5:5D:1383:GLU:N	5:5D:1383:GLU:OE1	2.31	0.64
3:5B:858:GLN:OE1	3:5B:861:ARG:NH1	2.31	0.63
33:2A:154:C:H2'	33:2A:155:C:H6	1.63	0.63
41:2I:868:VAL:O	41:2I:877:LEU:N	2.30	0.63
1:A:35:U:OP1	44:2L:63:GLY:HA3	1.98	0.63
33:2A:152:G:C2	33:2A:153:A:C5	2.87	0.63
1:A:20:U:H5'	1:A:21:U:OP2	1.99	0.63
3:5B:138:PRO:O	3:5B:142:SER:OG	2.17	0.63
3:5B:1793:THR:OG1	3:5B:1797:ASN:OD1	2.11	0.63
39:2G:749:ALA:O	39:2G:752:TYR:N	2.31	0.63
39:2G:1018:PRO:O	39:2G:1021:THR:N	2.30	0.63
41:2I:563:LEU:N	41:2I:581:LYS:O	2.27	0.63
41:2I:645:MET:N	41:2I:662:PHE:O	2.28	0.63
22:4A:127:C:O2	9:4c:47:ARG:O	2.17	0.63
24:4C:417:PRO:HG3	24:4C:459:PRO:O	1.98	0.63
1:A:31:C:N3	33:2A:33:G:C6	2.66	0.63
33:2A:164:C:H6	33:2A:164:C:H5'	1.63	0.63
2:5A:88:A:H2'	2:5A:88:A:N3	2.14	0.63
5:5D:793:ASP:O	5:5D:797:VAL:HG23	1.98	0.63
22:4A:108:C:H2'	22:4A:109:G:H8	1.63	0.63
28:4G:744:PRO:O	28:4G:748:LEU:HD23	1.98	0.63
33:2A:153:A:H3'	33:2A:154:C:H5'	1.79	0.63
2:5A:90:U:H5	13:5g:38:ASN:C	2.06	0.63
5:5D:602:GLU:OE1	5:5D:606:THR:OG1	2.16	0.63
22:4A:89:U:C2'	22:4A:90:G:H5'	2.29	0.63
22:4A:89:U:O2'	22:4A:90:G:H5'	1.99	0.63
33:2A:156:U:C6	33:2A:156:U:C5'	2.72	0.63
22:4A:91:A:O5'	22:4A:91:A:H8	1.82	0.62
24:4C:265:LEU:O	24:4C:266:LEU:HD23	2.00	0.62
39:2G:1264:VAL:O	39:2G:1267:LYS:N	2.32	0.62
41:2I:1191:LYS:O	41:2I:1194:SER:N	2.32	0.62
4:5C:560:VAL:HG12	4:5C:561:LYS:H	1.64	0.62
5:5D:760:GLU:O	5:5D:764:THR:HG23	1.99	0.62
1:A:31:C:C2	1:A:32:C:C5	2.87	0.62
4:5C:340:ALA:HA	4:5C:343:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:537:LYS:N	5:5D:608:LEU:O	2.32	0.62
5:5D:1960:LEU:HD12	5:5D:1982:VAL:HG22	1.82	0.62
39:2G:179:GLY:O	39:2G:182:LYS:N	2.33	0.62
1:A:31:C:H2'	1:A:32:C:H6	1.65	0.62
4:5C:283:ASP:OD1	4:5C:284:GLU:N	2.33	0.62
33:2A:143:A:H2'	33:2A:144:C:C6	2.35	0.62
1:A:31:C:C2'	1:A:32:C:H5'	2.30	0.62
2:5A:95:G:N3	2:5A:95:G:H2'	2.15	0.62
3:5B:2231:THR:OG1	3:5B:2255:HIS:O	2.16	0.61
33:2A:112:G:H2'	33:2A:113:G:H8	1.65	0.61
39:2G:914:PHE:O	39:2G:917:VAL:N	2.32	0.61
41:2I:586:ASP:O	41:2I:610:VAL:N	2.32	0.61
42:2J:77:ILE:O	42:2J:84:ILE:N	2.32	0.61
3:5B:388:LEU:O	4:5C:379:LYS:NZ	2.19	0.61
5:5D:774:LEU:CD2	5:5D:778:LEU:HD11	2.30	0.61
36:2D:252:PHE:CA	38:2F:63:ASP:CA	2.79	0.61
39:2G:88:VAL:CA	39:2G:92:ASN:H	2.13	0.61
5:5D:1849:ILE:HD13	5:5D:1923:ILE:CD1	2.30	0.61
39:2G:784:MET:O	39:2G:787:ILE:N	2.34	0.61
2:5A:67:A:O2'	2:5A:68:C:OP1	2.18	0.61
5:5D:639:ILE:HD11	5:5D:646:VAL:HG22	1.83	0.61
33:2A:142:C:C2'	33:2A:143:A:H5'	2.30	0.61
39:2G:897:LEU:O	39:2G:900:PHE:N	2.34	0.61
1:A:31:C:O2'	1:A:32:C:H5'	2.00	0.61
3:5B:1208:THR:HG23	3:5B:1208:THR:O	1.99	0.61
5:5D:949:LEU:O	5:5D:953:ARG:NH1	2.34	0.61
41:2I:973:GLY:HA3	41:2I:976:LYS:O	2.00	0.61
1:A:40:U:H5''	1:A:41:U:H5''	1.82	0.61
3:5B:1592:ASP:OD2	31:4J:337:TYR:OH	2.11	0.61
33:2A:157:G:H5''	33:2A:157:G:H8	1.65	0.61
3:5B:1202:THR:HG23	3:5B:1204:TYR:CE2	2.36	0.61
3:5B:1901:LYS:NZ	3:5B:1966:HIS:O	2.32	0.61
3:5B:2038:GLN:CA	5:5D:1035:LEU:CD1	2.79	0.61
39:2G:895:GLY:O	39:2G:898:TYR:N	2.34	0.61
39:2G:981:TYR:O	39:2G:984:GLU:N	2.20	0.61
1:A:35:U:H4'	1:A:36:C:OP2	1.98	0.61
29:4H:20:GLY:N	29:4H:168:PRO:O	2.31	0.61
39:2G:173:ALA:C	39:2G:176:ALA:H	2.09	0.61
4:5C:215:VAL:HG11	4:5C:242:LEU:CD2	2.31	0.61
5:5D:1456:VAL:HG22	5:5D:1491:SER:HB3	1.83	0.61
5:5D:1428:THR:HG22	5:5D:1429:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2G:862:GLU:O	39:2G:865:ARG:N	2.33	0.60
3:5B:2141:GLU:OE1	3:5B:2143:ARG:NH2	2.34	0.60
23:4B:385:PRO:HG2	24:4C:437:ARG:NH1	2.17	0.60
24:4C:174:LEU:HD11	24:4C:178:ARG:HE	1.66	0.60
24:4C:404:GLU:N	24:4C:404:GLU:OE1	2.34	0.60
1:A:13:U:H2'	1:A:14:G:H8	1.66	0.60
4:5C:825:PRO:HG2	4:5C:912:LEU:HD11	1.83	0.60
5:5D:1078:MET:CE	5:5D:1082:VAL:HG23	2.30	0.60
39:2G:551:LEU:O	39:2G:554:LYS:N	2.34	0.60
41:2I:550:ASN:N	41:2I:553:GLN:O	2.27	0.60
1:A:10:C:O2'	1:A:11:C:OP2	2.16	0.60
5:5D:1604:LEU:HD13	5:5D:1609:LEU:HD22	1.83	0.60
1:A:31:C:H2'	1:A:32:C:C6	2.36	0.60
3:5B:270:ASN:ND2	3:5B:270:ASN:O	2.34	0.60
5:5D:789:MET:O	5:5D:794:ARG:NH1	2.35	0.60
39:2G:953:ASP:O	39:2G:956:SER:N	2.34	0.60
39:2G:1125:PRO:O	39:2G:1128:VAL:N	2.35	0.60
1:A:21:U:H1'	1:A:22:C:P	2.41	0.60
4:5C:607:LEU:O	4:5C:610:VAL:HG22	2.02	0.60
5:5D:1569:THR:OG1	5:5D:1645:VAL:HG12	2.02	0.60
5:5D:1037:LEU:HG	5:5D:1052:ILE:HD11	1.83	0.60
5:5D:1561:VAL:HG22	5:5D:1662:ILE:HB	1.84	0.60
28:4G:780:TRP:NE1	28:4G:806:GLU:OE2	2.32	0.60
22:4A:118:A:H2	22:4A:119:A:N6	1.84	0.60
23:4B:386:GLU:OE2	23:4B:386:GLU:N	2.32	0.60
39:2G:610:ILE:O	39:2G:613:MET:N	2.34	0.60
3:5B:1418:ARG:O	3:5B:1421:THR:OG1	2.17	0.60
33:2A:153:A:N6	33:2A:177:A:H2	1.98	0.60
41:2I:664:TYR:CA	41:2I:677:THR:O	2.50	0.60
1:A:13:U:O5'	1:A:13:U:H6	1.84	0.59
5:5D:696:LYS:NZ	22:4A:61:A:OP2	2.35	0.59
5:5D:1725:GLU:OE2	5:5D:1763:ARG:NH2	2.34	0.59
39:2G:929:LEU:O	39:2G:932:ILE:N	2.34	0.59
1:A:31:C:O2	33:2A:33:G:C4	2.56	0.59
3:5B:194:GLU:N	3:5B:194:GLU:OE1	2.35	0.59
19:6e:46:GLU:CA	19:6e:62:ASP:C	2.74	0.59
32:4Z:334:HIS:HA	32:4Z:342:LEU:H	1.67	0.59
33:2A:106:G:N2	33:2A:107:A:C6	2.67	0.59
41:2I:15:SER:N	41:2I:33:SER:O	2.35	0.59
5:5D:1248:ASP:OD1	5:5D:1248:ASP:N	2.35	0.59
2:5A:95:G:N2	2:5A:96:A:H5''	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:548:VAL:O	5:5D:552:VAL:HG23	2.02	0.59
4:5C:363:SER:O	4:5C:364:SER:OG	2.19	0.59
5:5D:551:MET:HA	5:5D:551:MET:HE2	1.84	0.59
39:2G:1109:ARG:O	39:2G:1112:THR:N	2.36	0.59
39:2G:1149:LYS:O	39:2G:1152:SER:N	2.36	0.59
3:5B:248:ASP:OD1	3:5B:248:ASP:N	2.34	0.59
3:5B:1169:GLN:O	3:5B:1173:SER:OG	2.20	0.59
39:2G:1182:LEU:O	39:2G:1185:ARG:N	2.35	0.59
23:4B:480:ASN:O	23:4B:480:ASN:ND2	2.36	0.59
25:4D:399:LEU:O	28:4G:289:ASN:ND2	2.36	0.59
32:4Z:334:HIS:CB	32:4Z:341:THR:HA	2.33	0.59
2:5A:95:G:O2'	10:5d:24:LYS:C	2.46	0.59
24:4C:458:GLU:HG2	24:4C:459:PRO:HD2	1.85	0.59
43:2K:67:ILE:O	43:2K:70:ALA:N	2.36	0.59
2:5A:87:A:N6	2:5A:91:U:O3'	2.36	0.58
3:5B:330:THR:O	3:5B:330:THR:OG1	2.19	0.58
14:6A:103:U:C3'	14:6A:104:U:H5''	2.31	0.58
28:4G:493:SER:O	28:4G:497:ASN:N	2.36	0.58
39:2G:745:ALA:O	39:2G:748:LYS:N	2.36	0.58
28:4G:137:LYS:NZ	36:2D:474:THR:O	2.25	0.58
29:4H:66:HIS:N	29:4H:75:GLN:O	2.35	0.58
1:A:22:C:HO2'	1:A:23:G:H5'	1.65	0.58
39:2G:811:LEU:O	39:2G:814:PHE:N	2.36	0.58
41:2I:931:VAL:O	41:2I:936:LYS:N	2.31	0.58
39:2G:424:ILE:O	39:2G:428:ALA:N	2.36	0.58
3:5B:2015:GLU:OE1	31:4J:299:ARG:NH2	2.37	0.58
5:5D:465:GLU:N	5:5D:465:GLU:OE1	2.36	0.58
19:6e:46:GLU:H	19:6e:63:ALA:N	2.01	0.58
24:4C:232:ARG:NH1	26:4E:74:GLU:OE1	2.36	0.58
1:A:30:C:H3'	1:A:31:C:H5'	1.83	0.58
4:5C:133:THR:HG21	4:5C:219:LEU:HD23	1.85	0.58
28:4G:95:GLU:OE1	28:4G:95:GLU:N	2.37	0.58
5:5D:552:VAL:HG21	5:5D:568:GLU:HB2	1.86	0.58
39:2G:929:LEU:O	39:2G:930:PRO:C	2.46	0.58
40:2H:596:GLU:O	40:2H:598:GLU:N	2.37	0.58
1:A:35:U:O2	1:A:35:U:O2'	2.22	0.58
22:4A:110:G:O5'	22:4A:110:G:H8	1.87	0.58
28:4G:513:CYS:O	28:4G:517:GLY:N	2.36	0.58
39:2G:308:SER:O	39:2G:311:ALA:N	2.35	0.58
1:A:30:C:N3	1:A:31:C:C6	2.72	0.58
22:4A:108:C:C2'	22:4A:109:G:H5'	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:675:TYR:OH	5:5D:885:GLN:OE1	2.10	0.58
5:5D:1197:THR:O	5:5D:1198:LEU:HD12	2.04	0.58
22:4A:111:C:H2'	22:4A:112:A:H8	1.69	0.58
41:2I:523:GLY:CA	41:2I:536:TRP:O	2.51	0.58
45:2M:48:ASP:O	45:2M:51:ASN:N	2.37	0.58
4:5C:759:LEU:HA	4:5C:762:VAL:HG22	1.86	0.57
27:4F:63:ILE:HD11	27:4F:75:LEU:HD13	1.86	0.57
39:2G:892:LEU:O	39:2G:895:GLY:N	2.37	0.57
32:4Z:382:GLU:O	32:4Z:383:CYS:CB	2.52	0.57
39:2G:491:GLU:O	39:2G:494:GLU:N	2.32	0.57
41:2I:1160:HIS:O	41:2I:1163:PHE:N	2.37	0.57
1:A:36:C:C5'	1:A:37:C:H5	2.17	0.57
4:5C:650:GLU:O	4:5C:650:GLU:OE1	2.23	0.57
5:5D:930:LEU:HD23	5:5D:949:LEU:HD12	1.86	0.57
23:4B:584:VAL:HG11	23:4B:594:PHE:CE2	2.39	0.57
38:2F:184:ARG:CA	7:2a:85:PRO:CA	2.82	0.57
41:2I:638:GLU:N	41:2I:668:GLY:O	2.32	0.57
33:2A:152:G:N2	33:2A:153:A:C5	2.73	0.57
1:A:34:G:C4	1:A:35:U:C6	2.93	0.57
5:5D:1071:LYS:HA	5:5D:1071:LYS:HE2	1.87	0.57
5:5D:1825:ASN:OD1	5:5D:1827:THR:N	2.38	0.57
5:5D:1828:THR:OG1	5:5D:1853:ALA:N	2.35	0.57
5:5D:1971:ILE:O	5:5D:1975:THR:HG23	2.05	0.57
41:2I:914:ILE:O	41:2I:918:ARG:C	2.47	0.57
3:5B:318:TYR:O	4:5C:645:ARG:NH1	2.36	0.57
22:4A:126:A:N1	9:4c:104:ASP:CA	2.67	0.57
1:A:34:G:N9	1:A:35:U:C6	2.72	0.57
22:4A:37:C:H1'	22:4A:38:U:H2'	1.86	0.57
2:5A:96:A:N6	12:5f:23:GLY:H	2.02	0.57
22:4A:121:U:C2	12:4f:63:ARG:CA	2.88	0.57
1:A:31:C:C1'	33:2A:33:G:N2	2.68	0.57
33:2A:152:G:N2	33:2A:153:A:C8	2.73	0.57
41:2I:1204:VAL:O	41:2I:1207:LYS:N	2.37	0.57
1:A:20:U:O2	33:2A:42:G:N2	2.38	0.56
5:5D:739:ARG:NE	5:5D:740:ASP:OD1	2.37	0.56
33:2A:141:C:C2	33:2A:142:C:C5	2.93	0.56
39:2G:937:LEU:O	39:2G:940:LEU:N	2.38	0.56
41:2I:973:GLY:HA3	41:2I:976:LYS:C	2.31	0.56
1:A:31:C:N4	1:A:32:C:H41	2.03	0.56
2:5A:81:U:H2'	2:5A:81:U:O2	2.05	0.56
2:5A:87:A:C6	2:5A:92:U:OP2	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:U:H2'	1:A:12:U:P	2.45	0.56
1:A:103:A:H2'	1:A:104:C:O4'	2.05	0.56
3:5B:306:GLN:NE2	4:5C:879:ASP:OD1	2.36	0.56
4:5C:520:GLU:N	4:5C:520:GLU:OE1	2.38	0.56
33:2A:154:C:O2'	33:2A:155:C:H5'	2.04	0.56
38:2F:184:ARG:O	7:2a:85:PRO:CA	2.53	0.56
1:A:10:C:O2'	1:A:11:C:P	2.64	0.56
4:5C:156:GLU:N	4:5C:156:GLU:OE1	2.39	0.56
2:5A:110:C:H2'	2:5A:111:A:H8	1.70	0.56
5:5D:544:MET:HE1	22:4A:73:U:H5''	1.87	0.56
27:4F:110:GLN:NE2	27:4F:114:ASP:OD1	2.38	0.56
41:2I:287:PHE:CA	41:2I:304:GLN:O	2.53	0.56
41:2I:931:VAL:O	41:2I:935:GLU:N	2.39	0.56
1:A:115:U:O2'	1:A:116:G:P	2.63	0.56
5:5D:470:TYR:O	5:5D:562:TYR:OH	2.12	0.56
33:2A:181:G:H2'	33:2A:182:U:H6	1.71	0.56
39:2G:968:GLU:O	39:2G:971:MET:N	2.39	0.56
3:5B:147:MET:O	3:5B:151:MET:HG3	2.06	0.56
3:5B:310:THR:HG22	3:5B:314:ILE:HD12	1.88	0.56
4:5C:719:GLN:NE2	4:5C:724:TRP:O	2.38	0.56
2:5A:8:G:H21	2:5A:71:C:H41	1.52	0.56
3:5B:136:ILE:HD13	3:5B:418:THR:HG22	1.88	0.56
5:5D:1725:GLU:OE1	5:5D:1763:ARG:NE	2.30	0.56
23:4B:579:VAL:HG23	23:4B:579:VAL:O	2.06	0.56
41:2I:42:ARG:N	41:2I:51:HIS:O	2.32	0.56
43:2K:98:PHE:O	43:2K:100:LYS:N	2.39	0.56
1:A:36:C:O2'	1:A:37:C:OP1	2.24	0.55
5:5D:774:LEU:HD21	5:5D:778:LEU:HD11	1.88	0.55
5:5D:1058:LYS:NZ	5:5D:1080:ASP:OD2	2.27	0.55
22:4A:58:C:OP1	23:4B:465:ARG:NH2	2.39	0.55
33:2A:149:A:H2'	33:2A:150:U:H6	1.70	0.55
1:A:21:U:C1'	1:A:22:C:P	2.94	0.55
5:5D:1402:ASN:O	5:5D:1402:ASN:ND2	2.37	0.55
22:4A:113:C:O5'	22:4A:113:C:H6	1.88	0.55
39:2G:1124:SER:O	39:2G:1127:THR:N	2.34	0.55
5:5D:1078:MET:HE1	5:5D:1082:VAL:HG23	1.88	0.55
5:5D:1092:MET:HE3	5:5D:1092:MET:O	2.07	0.55
19:6e:46:GLU:CA	19:6e:62:ASP:CA	2.85	0.55
36:2D:174:VAL:O	36:2D:178:GLY:HA2	2.05	0.55
1:A:34:G:C2'	1:A:35:U:C6	2.88	0.55
4:5C:763:LYS:HA	4:5C:766:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:877:GLN:OE1	5:5D:877:GLN:N	2.40	0.55
5:5D:1535:THR:HG21	5:5D:1676:TYR:CE2	2.42	0.55
41:2I:303:ALA:O	41:2I:310:ILE:CA	2.55	0.55
1:A:31:C:N3	33:2A:33:G:O6	2.40	0.55
1:A:36:C:O2'	1:A:36:C:O2	2.24	0.55
2:5A:110:C:H2'	2:5A:111:A:C8	2.42	0.55
5:5D:1186:LEU:HD21	5:5D:1270:VAL:CG2	2.36	0.55
5:5D:1636:PHE:HD2	5:5D:1656:VAL:HG21	1.70	0.55
5:5D:1943:MET:HE1	5:5D:2065:TRP:CB	2.37	0.55
33:2A:183:G:C4	33:2A:184:C:C5	2.94	0.55
39:2G:747:LEU:O	39:2G:748:LYS:C	2.48	0.55
43:2K:109:GLN:O	43:2K:112:LEU:N	2.39	0.55
1:A:36:C:C1'	1:A:37:C:P	2.94	0.55
1:A:113:U:H4'	30:4I:20:ILE:HD13	1.87	0.55
2:5A:117:A:C2	10:5d:26:GLY:HA3	2.41	0.55
3:5B:678:GLU:HA	3:5B:749:TRP:HZ2	1.72	0.55
4:5C:230:ASP:OD1	4:5C:233:GLU:N	2.34	0.55
5:5D:475:PHE:HE1	5:5D:514:LEU:HD23	1.72	0.55
33:2A:141:C:H2'	33:2A:142:C:H6	1.71	0.55
33:2A:150:U:C2	33:2A:151:C:C5	2.94	0.55
33:2A:150:U:H2'	33:2A:151:C:H6	1.71	0.55
39:2G:874:LYS:O	39:2G:877:GLY:CA	2.54	0.55
41:2I:1195:GLU:C	41:2I:1198:ASP:H	2.14	0.55
24:4C:458:GLU:CG	24:4C:459:PRO:HD2	2.36	0.55
3:5B:337:VAL:HG13	3:5B:337:VAL:O	2.06	0.55
5:5D:1802:ILE:HD12	5:5D:1810:VAL:CG1	2.36	0.55
39:2G:578:ILE:O	39:2G:581:LEU:N	2.39	0.55
3:5B:171:ASP:OD1	3:5B:171:ASP:N	2.37	0.55
3:5B:422:LEU:HD12	3:5B:422:LEU:H	1.71	0.55
5:5D:2037:VAL:HG13	5:5D:2092:LEU:CD2	2.37	0.55
28:4G:21:LEU:HD22	36:2D:509:MET:HG3	1.89	0.55
3:5B:442:LYS:NZ	46:5B:3000:IHP:O46	2.40	0.55
5:5D:1029:VAL:HG13	5:5D:1029:VAL:O	2.07	0.55
22:4A:73:U:O2'	22:4A:74:C:OP2	2.22	0.55
22:4A:108:C:H2'	22:4A:109:G:C8	2.41	0.55
33:2A:149:A:C4	33:2A:150:U:C5	2.95	0.55
33:2A:183:G:H2'	33:2A:184:C:H6	1.71	0.55
39:2G:86:ALA:C	39:2G:89:ALA:H	2.11	0.55
39:2G:557:ASP:O	39:2G:560:LEU:N	2.40	0.55
5:5D:1854:GLU:N	5:5D:1854:GLU:OE1	2.40	0.54
5:5D:1970:HIS:CE1	5:5D:1997:LEU:HD13	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2A:147:G:C4	33:2A:148:C:C5	2.95	0.54
3:5B:2046:THR:OG1	3:5B:2047:VAL:N	2.39	0.54
5:5D:2098:ALA:O	5:5D:2099:THR:HG22	2.06	0.54
39:2G:699:GLN:O	39:2G:700:LYS:C	2.48	0.54
39:2G:849:ILE:O	39:2G:852:ARG:N	2.38	0.54
3:5B:1673:SER:O	3:5B:1673:SER:OG	2.18	0.54
3:5B:1732:LYS:NZ	31:4J:338:ASP:OD1	2.38	0.54
5:5D:2037:VAL:HG13	5:5D:2092:LEU:HD21	1.90	0.54
24:4C:230:ASP:OD1	24:4C:231:ASP:N	2.36	0.54
25:4D:212:MET:HE1	25:4D:232:MET:CE	2.37	0.54
39:2G:517:ARG:O	39:2G:520:THR:N	2.41	0.54
39:2G:641:ILE:O	39:2G:644:LEU:N	2.40	0.54
41:2I:488:GLY:C	41:2I:490:THR:H	2.14	0.54
1:A:34:G:C3'	1:A:35:U:H5''	2.35	0.54
4:5C:918:ILE:HG13	4:5C:935:ILE:HD11	1.88	0.54
5:5D:687:GLN:OE1	5:5D:689:TYR:OH	2.24	0.54
24:4C:288:SER:O	24:4C:288:SER:OG	2.20	0.54
32:4Z:330:THR:HA	32:4Z:346:ARG:HA	1.88	0.54
39:2G:1205:GLU:O	39:2G:1208:LEU:N	2.41	0.54
41:2I:785:PRO:CA	41:2I:800:ILE:O	2.56	0.54
1:A:31:C:C2	33:2A:33:G:C2	2.95	0.54
3:5B:439:GLN:O	3:5B:444:ARG:NH1	2.40	0.54
19:6e:46:GLU:H	19:6e:63:ALA:CA	2.21	0.54
33:2A:181:G:C4	33:2A:182:U:C5	2.95	0.54
5:5D:1425:ILE:N	5:5D:1425:ILE:HD12	2.22	0.54
33:2A:179:C:H2'	33:2A:180:G:C8	2.39	0.54
3:5B:986:GLU:N	3:5B:986:GLU:OE1	2.41	0.54
3:5B:2135:ASP:CG	3:5B:2135:ASP:O	2.50	0.54
5:5D:1405:VAL:HG23	5:5D:1424:ILE:HB	1.89	0.54
31:4J:302:LYS:O	31:4J:302:LYS:HD3	2.08	0.54
3:5B:659:GLN:N	3:5B:659:GLN:OE1	2.41	0.54
5:5D:615:ASP:OD1	5:5D:616:GLU:N	2.41	0.54
28:4G:21:LEU:HD22	36:2D:509:MET:CG	2.38	0.54
28:4G:707:ASP:HA	28:4G:708:PHE:C	2.33	0.54
22:4A:119:A:H5''	10:4d:39:TYR:N	2.23	0.54
5:5D:1139:VAL:HG21	5:5D:1174:ILE:HD11	1.89	0.54
33:2A:147:G:H2'	33:2A:148:C:C6	2.43	0.54
4:5C:227:LEU:HD22	4:5C:243:ILE:CG2	2.38	0.53
5:5D:713:MET:HE3	5:5D:713:MET:HA	1.89	0.53
41:2I:589:CYS:O	41:2I:608:GLY:N	2.30	0.53
5:5D:1986:MET:O	5:5D:1993:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2A:153:A:H3'	33:2A:154:C:C5'	2.37	0.53
39:2G:1026:ASN:O	39:2G:1028:HIS:N	2.41	0.53
1:A:104:C:H42	2:5A:42:U:H3	1.56	0.53
5:5D:1736:PHE:HE1	5:5D:1751:ALA:HB1	1.73	0.53
33:2A:153:A:C3'	33:2A:154:C:C5'	2.85	0.53
39:2G:1132:LEU:O	39:2G:1135:GLU:N	2.41	0.53
1:A:10:C:HO2'	1:A:11:C:P	2.32	0.53
4:5C:467:ASP:OD1	4:5C:468:CYS:N	2.40	0.53
24:4C:228:ILE:HD13	24:4C:515:THR:HG22	1.91	0.53
39:2G:663:THR:O	39:2G:666:LYS:N	2.42	0.53
1:A:15:A:O2'	1:A:16:A:H5'	2.09	0.53
2:5A:99:C:H2'	2:5A:100:C:C6	2.43	0.53
2:5A:108:G:H3'	2:5A:109:G:H8	1.73	0.53
3:5B:195:LEU:HD23	3:5B:204:LEU:HA	1.90	0.53
3:5B:541:GLY:N	28:4G:33:ASP:OD2	2.41	0.53
14:6A:50:A:C2	25:4D:347:LEU:HD11	2.44	0.53
5:5D:696:LYS:HD2	22:4A:60:A:OP1	2.08	0.53
5:5D:1886:ASP:OD1	5:5D:1888:HIS:ND1	2.40	0.53
23:4B:518:ARG:HG3	23:4B:518:ARG:O	2.09	0.53
28:4G:800:MET:HE1	28:4G:813:LEU:HD22	1.89	0.53
39:2G:1280:LEU:O	39:2G:1282:ALA:N	2.42	0.53
30:4I:38:GLU:O	30:4I:42:LYS:HG2	2.08	0.53
1:A:22:C:C2'	1:A:23:G:C5'	2.87	0.53
5:5D:1157:ASN:OD1	5:5D:1159:ASN:N	2.41	0.53
33:2A:54:U:P	38:2F:424:ARG:O	2.67	0.53
41:2I:1195:GLU:O	41:2I:1198:ASP:N	2.41	0.53
3:5B:1957:ASP:O	3:5B:1960:THR:OG1	2.17	0.53
5:5D:1143:ILE:CD1	5:5D:1165:ILE:HD12	2.39	0.53
16:6b:47:ASP:O	16:6b:50:LEU:N	2.39	0.53
16:6b:48:GLN:C	16:6b:50:LEU:H	2.14	0.53
28:4G:634:ALA:O	28:4G:638:ASN:N	2.37	0.52
39:2G:244:THR:O	39:2G:247:ALA:N	2.43	0.52
1:A:41:U:H2'	1:A:41:U:O2	2.09	0.52
5:5D:890:GLU:OE2	5:5D:928:ARG:NH2	2.43	0.52
24:4C:513:ASP:OD1	24:4C:513:ASP:O	2.26	0.52
39:2G:1025:LYS:O	39:2G:1027:ARG:N	2.42	0.52
2:5A:95:G:N3	2:5A:95:G:C2'	2.73	0.52
5:5D:471:ALA:CB	5:5D:518:LEU:HD13	2.35	0.52
5:5D:785:HIS:HB3	5:5D:809:LEU:HD21	1.91	0.52
5:5D:824:HIS:ND1	5:5D:862:ASP:OD1	2.36	0.52
39:2G:978:LEU:O	39:2G:979:TYR:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2M:36:HIS:O	45:2M:37:ARG:C	2.53	0.52
1:A:36:C:C5'	1:A:37:C:C5	2.91	0.52
1:A:38:C:O2	1:A:38:C:H2'	2.08	0.52
3:5B:1832:ARG:NE	3:5B:1835:GLN:OE1	2.42	0.52
4:5C:698:GLU:CD	4:5C:698:GLU:H	2.17	0.52
22:4A:118:A:H8	22:4A:118:A:OP2	1.92	0.52
32:4Z:425:MET:HA	32:4Z:431:ILE:HA	1.92	0.52
39:2G:841:ALA:O	39:2G:843:LYS:N	2.41	0.52
23:4B:543:ILE:HD11	23:4B:638:ALA:HB3	1.92	0.52
2:5A:87:A:H61	2:5A:92:U:P	2.32	0.52
5:5D:1320:LEU:HD22	5:5D:1396:LYS:HG2	1.91	0.52
5:5D:1735:HIS:O	5:5D:1739:GLU:HG3	2.10	0.52
28:4G:118:GLU:OE2	28:4G:119:ARG:NH1	2.40	0.52
5:5D:933:PRO:HG3	5:5D:943:LEU:HD12	1.91	0.52
38:2F:411:CYS:O	38:2F:414:TYR:N	2.37	0.52
39:2G:407:MET:CA	39:2G:407:MET:H	2.06	0.52
39:2G:423:PRO:O	39:2G:427:PRO:N	2.43	0.52
39:2G:1280:LEU:O	39:2G:1281:ILE:C	2.51	0.52
3:5B:2183:ASN:OD1	3:5B:2183:ASN:C	2.52	0.52
4:5C:475:MET:HE2	4:5C:475:MET:HA	1.92	0.52
5:5D:1001:TYR:OH	5:5D:1091:LEU:HD12	2.09	0.52
39:2G:1207:SER:O	39:2G:1210:HIS:N	2.43	0.52
25:4D:105:ASN:OD1	28:4G:823:ARG:NH1	2.42	0.52
28:4G:739:CYS:HB3	28:4G:740:PRO:HA	1.92	0.52
33:2A:107:A:C6	33:2A:108:G:C5	2.98	0.52
4:5C:256:CYS:HA	4:5C:308:CYS:CB	2.34	0.51
3:5B:488:ASP:OD1	3:5B:489:TRP:N	2.43	0.51
3:5B:2184:GLU:OE1	3:5B:2217:SER:CB	2.59	0.51
4:5C:572:GLU:O	4:5C:573:GLU:HG3	2.10	0.51
5:5D:1127:CYS:SG	5:5D:1143:ILE:HG21	2.50	0.51
28:4G:724:MET:SD	28:4G:726:GLU:N	2.83	0.51
39:2G:1109:ARG:O	39:2G:1111:CYS:N	2.43	0.51
5:5D:597:THR:HG21	5:5D:634:ARG:HD2	1.91	0.51
5:5D:734:THR:HG23	5:5D:810:VAL:HG11	1.93	0.51
5:5D:1617:VAL:HG12	5:5D:1643:VAL:HB	1.93	0.51
5:5D:2084:LEU:HD23	5:5D:2084:LEU:H	1.76	0.51
25:4D:61:ALA:HB2	25:4D:106:GLU:OE2	2.11	0.51
39:2G:1129:LEU:O	39:2G:1132:LEU:N	2.44	0.51
41:2I:673:VAL:CA	41:2I:691:THR:H	2.24	0.51
1:A:115:U:H2'	1:A:116:G:O4'	2.10	0.51
5:5D:1819:ALA:HB2	5:5D:1829:ILE:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4A:120:U:O2'	11:4e:82:ASP:CA	2.58	0.51
39:2G:720:GLY:O	39:2G:721:ILE:C	2.54	0.51
39:2G:1094:LEU:O	39:2G:1098:LEU:N	2.41	0.51
39:2G:1110:VAL:O	39:2G:1113:THR:N	2.43	0.51
2:5A:96:A:N6	12:5f:23:GLY:N	2.58	0.51
3:5B:1305:SER:O	3:5B:1305:SER:OG	2.24	0.51
5:5D:1433:ASP:OD1	5:5D:1473:ARG:NH2	2.43	0.51
5:5D:1837:ASN:OD1	5:5D:1840:THR:N	2.43	0.51
28:4G:921:ASN:C	28:4G:921:ASN:ND2	2.68	0.51
33:2A:111:G:O3'	33:2A:112:G:O4'	2.29	0.51
39:2G:103:PRO:C	39:2G:106:GLU:H	2.18	0.51
5:5D:1295:TYR:OH	5:5D:1763:ARG:NH1	2.43	0.51
5:5D:1931:SER:HA	5:5D:2076:LEU:HD23	1.93	0.51
1:A:36:C:C1'	1:A:37:C:OP1	2.55	0.51
5:5D:1277:SER:O	5:5D:1277:SER:OG	2.28	0.51
23:4B:415:THR:CG2	23:4B:417:LEU:HD22	2.39	0.51
24:4C:119:ILE:CG2	24:4C:120:THR:HG23	2.38	0.51
41:2I:546:LYS:O	41:2I:556:ILE:CA	2.58	0.51
3:5B:832:TYR:OH	3:5B:929:GLU:OE2	2.24	0.51
3:5B:1154:PHE:CZ	3:5B:1168:VAL:HG12	2.46	0.51
4:5C:693:GLU:OE1	4:5C:693:GLU:N	2.41	0.51
25:4D:212:MET:HE1	25:4D:232:MET:HE2	1.92	0.51
41:2I:699:VAL:CA	41:2I:715:MET:O	2.59	0.51
2:5A:85:C:OP1	9:5c:20:GLU:N	2.44	0.51
4:5C:449:ILE:HD12	4:5C:465:MET:HE3	1.93	0.51
5:5D:1301:LEU:HD11	5:5D:1518:VAL:HG13	1.93	0.51
5:5D:1943:MET:HE1	5:5D:2065:TRP:CG	2.45	0.51
22:4A:111:C:H2'	22:4A:112:A:C8	2.46	0.51
3:5B:353:ASP:OD1	3:5B:353:ASP:N	2.44	0.51
5:5D:1222:TRP:NE1	5:5D:1273:ASP:OD1	2.36	0.51
5:5D:1622:GLU:N	5:5D:1622:GLU:OE1	2.44	0.51
25:4D:112:LYS:O	25:4D:116:ASP:OD1	2.29	0.51
39:2G:528:ALA:O	39:2G:531:LEU:N	2.44	0.51
43:2K:46:ARG:N	43:2K:63:VAL:O	2.44	0.51
45:2M:37:ARG:O	45:2M:40:TYR:N	2.44	0.51
1:A:31:C:H2'	1:A:32:C:H5'	1.91	0.50
24:4C:393:ASP:O	24:4C:397:GLY:N	2.44	0.50
30:4I:8:GLN:HB2	30:4I:9:PRO:HD3	1.93	0.50
33:2A:164:C:H5'	33:2A:164:C:C6	2.44	0.50
39:2G:629:ALA:O	39:2G:632:PHE:N	2.45	0.50
2:5A:98:G:H2'	2:5A:99:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:570:THR:HG23	5:5D:572:ASP:H	1.76	0.50
24:4C:207:ARG:O	24:4C:211:MET:HE2	2.11	0.50
3:5B:347:LEU:HD23	3:5B:348:PRO:HD2	1.93	0.50
5:5D:565:THR:O	5:5D:583:THR:OG1	2.26	0.50
39:2G:804:ASN:O	39:2G:807:LYS:N	2.44	0.50
39:2G:1243:PRO:O	39:2G:1244:CYS:C	2.55	0.50
4:5C:119:LEU:HD23	4:5C:119:LEU:O	2.11	0.50
5:5D:1345:ASN:OD1	5:5D:1487:ILE:HD12	2.11	0.50
7:4a:18:ARG:N	7:4a:81:THR:O	2.40	0.50
39:2G:771:LEU:O	39:2G:774:ILE:N	2.43	0.50
39:2G:939:ARG:O	39:2G:940:LEU:C	2.51	0.50
1:A:40:U:HO2'	1:A:41:U:P	2.24	0.50
2:5A:28:A:O2'	3:5B:643:GLY:HA3	2.12	0.50
3:5B:151:MET:SD	3:5B:628:GLY:O	2.69	0.50
5:5D:696:LYS:HZ1	22:4A:61:A:P	2.34	0.50
39:2G:862:GLU:O	39:2G:863:GLN:C	2.55	0.50
39:2G:892:LEU:O	39:2G:893:ILE:C	2.54	0.50
1:A:34:G:H21	1:A:35:U:H5'	1.77	0.50
1:A:37:C:H3'	1:A:37:C:H6	1.75	0.50
2:5A:100:C:H2'	2:5A:101:U:C6	2.46	0.50
5:5D:1947:GLN:NE2	5:5D:2114:MET:SD	2.85	0.50
28:4G:15:LEU:HB3	36:2D:520:ILE:HD11	1.93	0.50
39:2G:963:LYS:O	39:2G:966:GLN:N	2.30	0.50
39:2G:1035:CYS:O	39:2G:1038:LEU:N	2.44	0.50
39:2G:1188:ALA:O	39:2G:1191:VAL:N	2.45	0.50
3:5B:1091:TYR:O	3:5B:1092:ILE:C	2.53	0.50
5:5D:781:GLY:O	5:5D:806:ILE:HG23	2.11	0.50
5:5D:1767:ASN:OD1	5:5D:1770:TYR:HB2	2.12	0.50
5:5D:1899:LEU:HD22	5:5D:1948:MET:HG3	1.93	0.50
39:2G:1268:ILE:O	39:2G:1271:SER:N	2.44	0.50
1:A:25:G:H1	33:2A:37:U:H3	1.60	0.50
1:A:34:G:C2'	1:A:35:U:H6	2.23	0.50
4:5C:509:VAL:HG21	4:5C:558:PRO:HG2	1.94	0.50
5:5D:1092:MET:HE3	5:5D:1092:MET:HA	1.93	0.50
22:4A:143:U:H2'	22:4A:144:G:H5''	1.92	0.50
3:5B:1556:ASP:OD2	14:6A:44:G:N2	2.42	0.49
5:5D:1092:MET:HE3	5:5D:1092:MET:CA	2.41	0.49
11:5e:15:VAL:O	12:5f:33:GLY:HA3	2.12	0.49
22:4A:120:U:H3'	22:4A:120:U:H6	1.77	0.49
28:4G:15:LEU:HD12	36:2D:520:ILE:CD1	2.42	0.49
39:2G:708:ALA:O	39:2G:709:ILE:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2G:1080:THR:O	39:2G:1083:TYR:N	2.44	0.49
1:A:37:C:O2'	1:A:38:C:O5'	2.30	0.49
2:5A:50:G:O2'	2:5A:51:A:H5'	2.13	0.49
3:5B:1019:TYR:O	3:5B:1020:LYS:C	2.55	0.49
4:5C:360:ALA:N	4:5C:361:PRO:CD	2.76	0.49
5:5D:534:ASP:O	5:5D:534:ASP:OD1	2.30	0.49
5:5D:1609:LEU:C	5:5D:1609:LEU:HD23	2.37	0.49
33:2A:30:A:N3	33:2A:30:A:C2'	2.73	0.49
39:2G:501:LEU:O	39:2G:502:LEU:C	2.55	0.49
39:2G:665:ILE:O	39:2G:666:LYS:C	2.56	0.49
39:2G:974:LEU:O	39:2G:975:GLY:C	2.54	0.49
41:2I:1194:SER:O	41:2I:1199:ARG:N	2.35	0.49
3:5B:1179:SER:O	3:5B:1201:ARG:NH2	2.36	0.49
4:5C:118:PHE:O	4:5C:122:LEU:HD12	2.11	0.49
23:4B:570:THR:HG22	23:4B:571:GLY:N	2.27	0.49
24:4C:242:ASN:C	24:4C:242:ASN:OD1	2.56	0.49
5:5D:1411:GLU:OE2	5:5D:1413:SER:OG	2.21	0.49
25:4D:311:SER:O	25:4D:311:SER:OG	2.29	0.49
4:5C:617:LEU:HD11	4:5C:629:ILE:CG2	2.43	0.49
5:5D:642:THR:HG21	5:5D:644:GLU:OE2	2.12	0.49
16:6b:48:GLN:C	16:6b:50:LEU:N	2.69	0.49
28:4G:921:ASN:ND2	28:4G:921:ASN:O	2.39	0.49
33:2A:107:A:C2	33:2A:108:G:C4	3.01	0.49
39:2G:693:GLY:O	39:2G:694:LEU:C	2.55	0.49
39:2G:833:LEU:O	39:2G:834:VAL:C	2.56	0.49
41:2I:596:PRO:O	41:2I:598:GLY:N	2.46	0.49
5:5D:1624:LEU:O	5:5D:1629:ARG:NH1	2.46	0.49
5:5D:1830:GLU:OE2	5:5D:1830:GLU:HA	2.12	0.49
22:4A:138:G:OP2	13:4g:24:THR:O	2.31	0.49
11:2e:15:VAL:O	12:2f:33:GLY:HA3	2.12	0.49
2:5A:73:C:H2'	2:5A:74:U:C6	2.48	0.49
2:5A:115:C:OP1	11:5e:67:LYS:O	2.30	0.49
5:5D:815:LEU:HD23	5:5D:815:LEU:O	2.12	0.49
39:2G:553:VAL:O	39:2G:556:ILE:N	2.46	0.49
2:5A:98:G:H2'	2:5A:99:C:H6	1.77	0.49
5:5D:1462:GLU:O	5:5D:1463:ASN:OD1	2.31	0.49
5:5D:1628:GLU:CD	5:5D:1628:GLU:H	2.20	0.49
5:5D:2043:ARG:NE	5:5D:2045:GLU:O	2.44	0.49
24:4C:174:LEU:O	24:4C:174:LEU:HD12	2.12	0.49
39:2G:849:ILE:O	39:2G:850:ILE:C	2.54	0.49
45:2M:48:ASP:O	45:2M:49:LEU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:C:C2	1:A:32:C:H5	2.30	0.49
3:5B:1394:GLN:OE1	3:5B:1394:GLN:HA	2.12	0.49
3:5B:2072:GLU:OE1	3:5B:2074:ARG:HB2	2.11	0.49
5:5D:877:GLN:HA	5:5D:880:LEU:HD12	1.95	0.49
39:2G:793:LYS:O	39:2G:797:GLY:CA	2.54	0.49
3:5B:214:ARG:NH2	3:5B:215:ASP:OD1	2.46	0.49
3:5B:2275:ALA:HB2	3:5B:2297:GLN:HB2	1.95	0.49
5:5D:694:GLU:O	5:5D:700:ARG:NH2	2.46	0.49
6:5E:255:MET:C	6:5E:257:ASN:H	2.21	0.49
22:4A:18:G:H1	25:4D:357:ARG:HH21	1.61	0.49
25:4D:98:ASN:OD1	25:4D:99:LEU:N	2.45	0.49
33:2A:143:A:N3	33:2A:143:A:C3'	2.73	0.49
39:2G:177:LYS:O	39:2G:180:GLU:N	2.46	0.49
39:2G:663:THR:O	39:2G:664:GLY:C	2.56	0.49
41:2I:430:GLY:O	41:2I:433:SER:N	2.31	0.49
3:5B:1957:ASP:OD1	3:5B:1958:LYS:N	2.46	0.48
3:5B:2111:LEU:HD21	3:5B:2225:LEU:HD11	1.95	0.48
5:5D:995:ASN:O	5:5D:998:VAL:HG22	2.12	0.48
14:6A:57:U:C2	14:6A:58:G:C8	3.01	0.48
39:2G:1227:ILE:O	39:2G:1230:VAL:N	2.46	0.48
2:5A:92:U:H3'	2:5A:92:U:H6	1.77	0.48
5:5D:1946:ALA:O	5:5D:1949:VAL:HG12	2.14	0.48
39:2G:237:GLY:O	39:2G:239:ALA:N	2.45	0.48
39:2G:944:SER:O	39:2G:946:LYS:N	2.38	0.48
41:2I:930:LEU:C	41:2I:934:GLY:HA2	2.38	0.48
5:5D:525:ILE:O	5:5D:526:ASN:OD1	2.31	0.48
39:2G:955:ILE:O	39:2G:956:SER:C	2.57	0.48
40:2H:491:LEU:O	40:2H:493:ALA:N	2.46	0.48
41:2I:672:GLY:O	41:2I:695:GLY:N	2.46	0.48
3:5B:1200:CYS:SG	3:5B:1201:ARG:N	2.85	0.48
3:5B:1953:ILE:HD12	3:5B:1986:LEU:HD12	1.95	0.48
5:5D:938:ILE:HD13	5:5D:949:LEU:HD21	1.95	0.48
5:5D:1693:ARG:NH2	5:5D:1697:ASP:OD1	2.47	0.48
5:5D:1815:LEU:HD12	5:5D:1829:ILE:HG13	1.95	0.48
39:2G:953:ASP:O	39:2G:954:LEU:C	2.56	0.48
1:A:34:G:H3'	1:A:34:G:N3	2.28	0.48
22:4A:17:A:H2'	22:4A:18:G:C8	2.49	0.48
33:2A:54:U:C5'	38:2F:424:ARG:O	2.62	0.48
39:2G:226:HIS:O	39:2G:229:SER:N	2.46	0.48
39:2G:625:ARG:O	39:2G:628:THR:N	2.46	0.48
39:2G:631:ALA:O	39:2G:634:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:287:ASN:OD1	3:5B:288:LEU:N	2.46	0.48
3:5B:2074:ARG:NH2	5:5D:1044:VAL:O	2.41	0.48
5:5D:528:ASP:OD1	5:5D:528:ASP:N	2.45	0.48
5:5D:1369:LEU:HD23	5:5D:1369:LEU:O	2.14	0.48
5:5D:1970:HIS:HE1	5:5D:1996:LEU:HD23	1.77	0.48
24:4C:455:VAL:HG12	24:4C:467:THR:HG22	1.96	0.48
39:2G:994:LEU:O	39:2G:995:GLY:C	2.56	0.48
43:2K:98:PHE:C	43:2K:100:LYS:N	2.72	0.48
3:5B:1010:THR:HG22	25:4D:261:GLY:O	2.14	0.48
3:5B:2184:GLU:OE1	3:5B:2217:SER:OG	2.26	0.48
5:5D:1777:SER:OG	5:5D:1780:HIS:ND1	2.45	0.48
26:4E:15:ASP:OD1	26:4E:15:ASP:N	2.46	0.48
33:2A:153:A:C2'	33:2A:154:C:C5'	2.86	0.48
1:A:17:G:H2'	1:A:18:C:H6	1.78	0.48
3:5B:933:ARG:O	3:5B:935:LEU:N	2.46	0.48
4:5C:932:GLU:OE2	4:5C:936:LYS:NZ	2.25	0.48
5:5D:1358:ILE:HG22	5:5D:1362:PHE:CE1	2.48	0.48
15:6a:61:PHE:N	21:6g:70:ILE:O	2.45	0.48
24:4C:138:SER:OG	24:4C:139:VAL:HG23	2.13	0.48
25:4D:211:ARG:HA	25:4D:211:ARG:NE	2.28	0.48
28:4G:909:GLY:N	28:4G:913:CYS:SG	2.85	0.48
39:2G:667:ILE:O	39:2G:668:VAL:C	2.53	0.48
3:5B:682:ASP:OD1	3:5B:749:TRP:CZ3	2.66	0.48
3:5B:1139:ARG:HA	3:5B:1186:LEU:HD11	1.96	0.48
3:5B:2128:LEU:HD11	3:5B:2214:ILE:HD12	1.96	0.48
4:5C:174:GLU:O	4:5C:178:GLY:N	2.47	0.48
22:4A:61:A:H2'	22:4A:62:U:O4'	2.14	0.48
39:2G:705:SER:O	39:2G:706:ALA:C	2.54	0.48
1:A:38:C:H4'	1:A:38:C:OP1	2.14	0.48
4:5C:845:ALA:O	4:5C:848:THR:HG22	2.14	0.48
5:5D:1787:GLU:C	5:5D:1787:GLU:OE1	2.56	0.48
39:2G:803:ALA:O	39:2G:804:ASN:C	2.54	0.48
5:5D:517:MET:HG2	5:5D:538:ILE:HD13	1.96	0.47
5:5D:713:MET:HA	5:5D:716:ALA:HB2	1.95	0.47
5:5D:996:ASP:OD1	5:5D:997:THR:N	2.46	0.47
5:5D:1625:SER:HB3	5:5D:1628:GLU:OE1	2.14	0.47
2:5A:111:A:H2'	2:5A:112:A:C8	2.49	0.47
5:5D:641:MET:HG2	5:5D:1582:ALA:HB1	1.95	0.47
5:5D:1968:SER:HA	5:5D:1971:ILE:HD12	1.95	0.47
22:4A:110:G:H2'	22:4A:111:C:C6	2.49	0.47
33:2A:151:C:C2	33:2A:152:G:N7	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5C:196:LYS:CA	13:5g:33:ILE:O	2.53	0.47
5:5D:1739:GLU:OE2	5:5D:1754:TYR:CZ	2.67	0.47
32:4Z:499:ILE:N	32:4Z:511:TRP:O	2.43	0.47
1:A:28:G:H22	33:2A:34:U:H3	1.61	0.47
4:5C:481:MET:HE2	4:5C:490:PHE:HB3	1.97	0.47
5:5D:1737:ASN:O	5:5D:1740:ILE:HG22	2.14	0.47
5:5D:1740:ILE:HD12	5:5D:1745:ILE:HG22	1.96	0.47
5:5D:1849:ILE:HD13	5:5D:1923:ILE:HD12	1.96	0.47
23:4B:388:GLU:OE1	24:4C:192:ARG:NH2	2.47	0.47
24:4C:293:ASP:O	24:4C:309:SER:OG	2.31	0.47
33:2A:150:U:H2'	33:2A:151:C:C6	2.50	0.47
39:2G:1110:VAL:O	39:2G:1111:CYS:C	2.57	0.47
40:2H:573:ASP:O	40:2H:577:LYS:N	2.44	0.47
4:5C:152:GLN:NE2	4:5C:426:GLU:O	2.47	0.47
5:5D:467:LEU:HD12	5:5D:467:LEU:N	2.30	0.47
5:5D:1424:ILE:C	5:5D:1425:ILE:HD12	2.40	0.47
39:2G:660:ALA:O	39:2G:661:ARG:C	2.53	0.47
41:2I:558:LEU:O	41:2I:561:GLY:CA	2.63	0.47
3:5B:758:ARG:NH2	3:5B:900:ASP:OD1	2.36	0.47
3:5B:1233:ASP:C	3:5B:1233:ASP:OD1	2.58	0.47
4:5C:746:VAL:HG22	4:5C:747:ASP:H	1.79	0.47
5:5D:1845:LEU:O	5:5D:1849:ILE:HD12	2.15	0.47
5:5D:1961:LYS:HD3	5:5D:1971:ILE:HD11	1.97	0.47
5:5D:2041:LEU:O	5:5D:2087:LYS:HA	2.15	0.47
41:2I:923:GLY:HA3	41:2I:947:GLU:O	2.14	0.47
45:2M:42:SER:O	45:2M:45:GLY:N	2.48	0.47
2:5A:117:A:C2	10:5d:26:GLY:O	2.68	0.47
3:5B:1130:ASN:N	3:5B:1130:ASN:OD1	2.48	0.47
5:5D:716:ALA:HB1	5:5D:751:PHE:CE1	2.50	0.47
5:5D:1027:ILE:HG21	5:5D:1059:ILE:HD11	1.95	0.47
5:5D:1157:ASN:O	5:5D:1161:ILE:N	2.39	0.47
24:4C:265:LEU:C	24:4C:266:LEU:HD23	2.40	0.47
29:4H:110:LEU:O	29:4H:141:PHE:N	2.47	0.47
33:2A:153:A:C8	33:2A:154:C:H5'	2.50	0.47
33:2A:183:G:H2'	33:2A:184:C:C6	2.50	0.47
39:2G:993:ILE:O	39:2G:994:LEU:C	2.56	0.47
39:2G:1264:VAL:O	39:2G:1265:TYR:C	2.56	0.47
3:5B:941:LYS:HG2	3:5B:951:LEU:HD13	1.96	0.47
5:5D:1357:THR:O	5:5D:1361:GLU:HG3	2.15	0.47
5:5D:2052:ILE:HG22	5:5D:2054:PRO:HD3	1.96	0.47
24:4C:101:VAL:HG21	24:4C:134:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2D:514:GLN:O	36:2D:518:ALA:N	2.39	0.47
3:5B:1959:THR:O	3:5B:1960:THR:C	2.57	0.47
5:5D:1561:VAL:HB	5:5D:1645:VAL:HG22	1.97	0.47
22:4A:109:G:H2'	22:4A:110:G:C8	2.50	0.47
28:4G:800:MET:HE2	28:4G:804:LEU:HG	1.97	0.47
31:4J:184:LEU:HD12	31:4J:184:LEU:C	2.40	0.47
39:2G:567:VAL:O	39:2G:568:ARG:C	2.58	0.47
39:2G:865:ARG:O	39:2G:866:LYS:C	2.56	0.47
41:2I:44:ASP:O	41:2I:48:GLY:HA2	2.15	0.47
42:2J:70:ALA:O	42:2J:74:MET:N	2.40	0.47
3:5B:1357:MET:SD	3:5B:1358:SER:N	2.88	0.47
5:5D:1920:ILE:HD11	5:5D:1950:THR:CG2	2.45	0.47
24:4C:458:GLU:OE1	24:4C:462:GLY:N	2.48	0.47
39:2G:471:ASP:O	39:2G:472:ILE:C	2.57	0.47
39:2G:645:LEU:O	39:2G:646:PRO:C	2.56	0.47
41:2I:1148:LEU:O	41:2I:1149:ARG:C	2.57	0.47
3:5B:1545:ALA:HB2	3:5B:1563:HIS:CD2	2.49	0.46
4:5C:710:ASN:H	4:5C:713:LYS:HZ3	1.63	0.46
14:6A:78:A:N3	14:6A:78:A:H2'	2.30	0.46
28:4G:369:LEU:O	28:4G:371:GLN:N	2.45	0.46
3:5B:1341:ARG:HE	3:5B:1354:ARG:NH2	2.14	0.46
33:2A:141:C:H2'	33:2A:142:C:C6	2.50	0.46
39:2G:952:ALA:O	39:2G:953:ASP:C	2.57	0.46
5:5D:591:GLU:OE1	5:5D:992:TYR:CE2	2.68	0.46
5:5D:1432:TRP:HE1	5:5D:1474:MET:HE2	1.80	0.46
5:5D:1802:ILE:HD12	5:5D:1810:VAL:HG13	1.97	0.46
24:4C:266:LEU:O	24:4C:267:HIS:ND1	2.48	0.46
33:2A:107:A:C6	33:2A:108:G:C6	3.04	0.46
39:2G:693:GLY:O	39:2G:695:VAL:N	2.48	0.46
39:2G:810:ILE:O	39:2G:811:LEU:C	2.59	0.46
39:2G:872:ILE:O	39:2G:873:GLU:C	2.57	0.46
1:A:7:U:H4'	1:A:8:U:OP1	2.15	0.46
3:5B:1910:THR:C	3:5B:1911:GLU:HG3	2.39	0.46
4:5C:534:VAL:O	4:5C:535:ALA:C	2.58	0.46
5:5D:1455:GLU:N	5:5D:1490:LEU:O	2.47	0.46
5:5D:1672:LYS:HD2	5:5D:1672:LYS:N	2.30	0.46
2:5A:74:U:H2'	2:5A:75:G:C8	2.51	0.46
2:5A:99:C:H2'	2:5A:100:C:H6	1.79	0.46
3:5B:441:VAL:O	3:5B:445:VAL:HG23	2.16	0.46
3:5B:1090:ARG:HG2	3:5B:1091:TYR:O	2.16	0.46
5:5D:935:LEU:H	5:5D:935:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2G:745:ALA:O	39:2G:746:PHE:C	2.59	0.46
39:2G:867:MET:O	39:2G:868:VAL:C	2.57	0.46
39:2G:1165:TYR:O	39:2G:1166:ILE:C	2.59	0.46
3:5B:252:ASP:OD1	3:5B:252:ASP:N	2.38	0.46
4:5C:125:ASN:OD1	4:5C:127:GLU:N	2.38	0.46
5:5D:639:ILE:HD11	5:5D:646:VAL:CG2	2.46	0.46
5:5D:617:ILE:HD12	5:5D:628:LEU:HD13	1.98	0.46
5:5D:1183:LYS:O	5:5D:1184:LEU:HD12	2.15	0.46
5:5D:1914:GLU:O	5:5D:1917:SER:OG	2.30	0.46
16:6b:19:ASP:C	16:6b:21:ILE:H	2.23	0.46
33:2A:3:C:H2'	33:2A:4:G:C8	2.51	0.46
39:2G:429:ARG:O	39:2G:432:THR:N	2.46	0.46
39:2G:1119:VAL:O	39:2G:1122:THR:N	2.49	0.46
39:2G:1129:LEU:O	39:2G:1130:PRO:C	2.59	0.46
39:2G:1256:HIS:O	39:2G:1257:PRO:C	2.58	0.46
2:5A:67:A:O2'	2:5A:68:C:P	2.73	0.46
3:5B:75:ASP:OD1	3:5B:75:ASP:N	2.47	0.46
3:5B:835:ASP:OD1	3:5B:835:ASP:N	2.48	0.46
3:5B:1618:LYS:NZ	3:5B:1628:ASP:OD2	2.49	0.46
5:5D:475:PHE:CE1	5:5D:514:LEU:HD23	2.51	0.46
5:5D:531:ILE:HD12	5:5D:531:ILE:N	2.31	0.46
5:5D:757:ALA:O	5:5D:761:VAL:HG23	2.16	0.46
5:5D:1825:ASN:N	5:5D:1854:GLU:OE2	2.37	0.46
33:2A:149:A:H2'	33:2A:150:U:C6	2.50	0.46
39:2G:257:THR:O	39:2G:259:SER:N	2.49	0.46
1:A:28:G:C2	33:2A:35:A:C2	3.04	0.46
4:5C:375:GLU:HB2	4:5C:376:PRO:HD3	1.97	0.46
5:5D:2003:GLN:O	5:5D:2007:VAL:HG23	2.16	0.46
15:6a:73:PRO:O	15:6a:75:ASP:N	2.49	0.46
22:4A:20:A:H2'	22:4A:21:U:C6	2.51	0.46
38:2F:403:ASN:N	38:2F:417:ARG:O	2.49	0.46
39:2G:210:ALA:O	39:2G:213:LYS:N	2.48	0.46
2:5A:78:U:H5''	2:5A:78:U:O2	2.16	0.46
3:5B:857:ASN:ND2	3:5B:860:GLN:OE1	2.49	0.46
3:5B:1592:ASP:O	3:5B:1596:VAL:HG23	2.15	0.46
3:5B:2020:SER:HA	31:4J:306:LEU:HD22	1.97	0.46
5:5D:1868:LEU:HD11	5:5D:1890:LYS:HE3	1.97	0.46
28:4G:776:ASN:OD1	28:4G:776:ASN:O	2.34	0.46
31:4J:302:LYS:HD3	31:4J:302:LYS:C	2.41	0.46
2:5A:96:A:H61	12:5f:23:GLY:N	2.07	0.45
3:5B:1480:GLY:HA3	31:4J:155:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:1490:PHE:O	3:5B:1493:THR:OG1	2.31	0.45
3:5B:2174:PRO:O	3:5B:2210:LYS:NZ	2.44	0.45
4:5C:560:VAL:O	4:5C:561:LYS:C	2.59	0.45
5:5D:1742:THR:O	5:5D:1742:THR:HG22	2.16	0.45
5:5D:1920:ILE:HD11	5:5D:1950:THR:HG23	1.99	0.45
24:4C:290:ASP:N	24:4C:290:ASP:OD1	2.46	0.45
39:2G:841:ALA:C	39:2G:843:LYS:N	2.73	0.45
45:2M:62:ALA:O	45:2M:65:ARG:N	2.50	0.45
4:5C:283:ASP:OD1	4:5C:283:ASP:C	2.59	0.45
5:5D:1672:LYS:NZ	5:5D:1860:ILE:HG21	2.32	0.45
5:5D:1753:ASP:O	5:5D:1756:THR:HG22	2.16	0.45
33:2A:152:G:O2'	33:2A:153:A:H1'	2.16	0.45
38:2F:394:TYR:C	38:2F:396:LEU:H	2.24	0.45
1:A:34:G:N3	1:A:35:U:H5''	2.31	0.45
5:5D:1768:PRO:HG3	5:5D:1776:ILE:HG22	1.98	0.45
39:2G:914:PHE:O	39:2G:915:GLY:C	2.58	0.45
45:2M:46:HIS:O	45:2M:47:PHE:C	2.59	0.45
1:A:38:C:C4'	1:A:39:U:OP1	2.35	0.45
3:5B:1434:LYS:O	3:5B:1439:ARG:NH2	2.45	0.45
5:5D:2084:LEU:HD12	5:5D:2086:GLN:O	2.17	0.45
38:2F:276:GLY:C	38:2F:278:LEU:N	2.60	0.45
4:5C:240:GLU:O	4:5C:243:ILE:HG13	2.17	0.45
5:5D:567:ALA:HB1	5:5D:575:LEU:HD21	1.98	0.45
24:4C:359:LEU:HD21	24:4C:361:GLN:HB2	1.98	0.45
33:2A:180:G:H2'	33:2A:181:G:H8	1.81	0.45
39:2G:1031:VAL:O	39:2G:1032:GLN:C	2.60	0.45
3:5B:64:GLU:OE2	3:5B:67:ARG:NH1	2.50	0.45
4:5C:710:ASN:O	4:5C:714:LEU:HD12	2.17	0.45
39:2G:687:VAL:O	39:2G:690:ILE:N	2.50	0.45
39:2G:889:GLU:O	39:2G:890:GLU:C	2.57	0.45
41:2I:672:GLY:O	41:2I:691:THR:N	2.49	0.45
1:A:31:C:C4	1:A:32:C:N4	2.73	0.45
1:A:32:C:N3	33:2A:31:G:O6	2.50	0.45
2:5A:92:U:N3	8:5b:36:MET:N	2.64	0.45
3:5B:1347:ASP:OD1	3:5B:1348:VAL:HG13	2.17	0.45
3:5B:1996:ASN:O	3:5B:1996:ASN:ND2	2.50	0.45
3:5B:2064:THR:O	3:5B:2064:THR:OG1	2.34	0.45
5:5D:801:PHE:HB3	5:5D:821:LEU:HD21	1.98	0.45
5:5D:1167:MET:HA	5:5D:1167:MET:HE3	1.98	0.45
5:5D:1290:ILE:HG23	5:5D:1290:ILE:O	2.17	0.45
5:5D:1425:ILE:N	5:5D:1425:ILE:CD1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:1868:LEU:HD13	5:5D:1890:LYS:HG2	1.98	0.45
39:2G:830:TYR:O	39:2G:831:ARG:C	2.57	0.45
41:2I:1141:PHE:O	41:2I:1144:VAL:N	2.49	0.45
44:2L:46:CYS:O	44:2L:50:ASN:N	2.43	0.45
3:5B:758:ARG:HD3	3:5B:779:LEU:HD11	1.99	0.45
5:5D:1300:GLU:OE1	5:5D:1300:GLU:N	2.36	0.45
5:5D:2036:VAL:HG23	5:5D:2093:ASP:OD1	2.17	0.45
22:4A:115:G:H2'	22:4A:116:G:C8	2.52	0.45
33:2A:114:A:H2'	33:2A:115:G:H8	1.81	0.45
36:2D:450:GLN:HG2	36:2D:450:GLN:O	2.17	0.45
39:2G:1078:VAL:O	39:2G:1081:PHE:N	2.50	0.45
30:4I:8:GLN:HB2	30:4I:9:PRO:CD	2.47	0.45
38:2F:394:TYR:C	38:2F:396:LEU:N	2.75	0.45
39:2G:708:ALA:O	39:2G:711:ALA:N	2.49	0.45
41:2I:663:LEU:O	41:2I:678:VAL:CA	2.65	0.45
4:5C:943:LEU:N	4:5C:943:LEU:HD22	2.30	0.45
5:5D:1464:GLY:N	5:5D:1465:PRO:CD	2.80	0.45
22:4A:118:A:OP2	22:4A:118:A:C8	2.70	0.45
24:4C:459:PRO:HD3	24:4C:500:ILE:HG21	1.99	0.45
33:2A:59:A:H2'	33:2A:60:U:O4'	2.17	0.45
39:2G:629:ALA:O	39:2G:630:ARG:C	2.56	0.45
39:2G:791:VAL:O	39:2G:792:VAL:C	2.60	0.45
41:2I:215:LEU:O	41:2I:218:ASN:N	2.50	0.45
41:2I:1141:PHE:O	41:2I:1142:GLN:C	2.60	0.45
41:2I:1191:LYS:O	41:2I:1192:ASN:C	2.59	0.45
3:5B:189:GLU:O	3:5B:564:TYR:OH	2.24	0.44
3:5B:1189:MET:O	3:5B:1191:GLY:N	2.51	0.44
5:5D:1037:LEU:CG	5:5D:1052:ILE:HD11	2.47	0.44
28:4G:921:ASN:C	28:4G:921:ASN:HD22	2.23	0.44
39:2G:1013:ILE:O	39:2G:1014:LYS:C	2.60	0.44
39:2G:1128:VAL:O	39:2G:1129:LEU:C	2.60	0.44
41:2I:672:GLY:C	41:2I:691:THR:H	2.25	0.44
1:A:33:U:O3'	1:A:34:G:O4'	2.35	0.44
14:6A:91:A:H2'	14:6A:92:A:H8	1.82	0.44
22:4A:91:A:H2'	22:4A:92:C:C6	2.53	0.44
23:4B:388:GLU:OE2	23:4B:388:GLU:N	2.50	0.44
24:4C:124:GLU:OE1	24:4C:132:ARG:NH2	2.42	0.44
25:4D:377:ARG:O	25:4D:397:GLY:HA3	2.17	0.44
28:4G:15:LEU:HD12	36:2D:520:ILE:HD11	1.99	0.44
28:4G:651:LEU:O	28:4G:655:ASN:N	2.50	0.44
33:2A:54:U:H5'	38:2F:424:ARG:CA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2G:658:TRP:O	39:2G:659:GLN:C	2.60	0.44
39:2G:669:GLN:O	39:2G:670:GLN:C	2.60	0.44
39:2G:749:ALA:O	39:2G:750:ILE:C	2.60	0.44
39:2G:937:LEU:O	39:2G:938:TRP:C	2.59	0.44
2:5A:81:U:O5'	2:5A:81:U:C6	2.70	0.44
5:5D:597:THR:HG21	5:5D:634:ARG:CD	2.48	0.44
7:4a:80:MET:O	8:4b:59:SER:N	2.44	0.44
33:2A:143:A:OP2	33:2A:143:A:C2	2.71	0.44
39:2G:935:THR:O	39:2G:936:VAL:C	2.58	0.44
39:2G:1246:MET:O	39:2G:1247:LEU:C	2.59	0.44
2:5A:117:A:C6	10:5d:26:GLY:HA3	2.52	0.44
5:5D:569:LEU:HD13	5:5D:575:LEU:HB2	1.98	0.44
5:5D:1015:PHE:CE2	5:5D:1063:LEU:HD23	2.53	0.44
5:5D:1499:ASP:OD2	5:5D:1763:ARG:NH1	2.42	0.44
14:6A:90:G:H2'	14:6A:91:A:H8	1.82	0.44
14:6A:91:A:H2'	14:6A:92:A:C8	2.53	0.44
22:4A:122:U:H1'	12:4f:65:ASN:CA	2.47	0.44
12:4f:22:ASN:N	12:4f:66:SER:O	2.49	0.44
1:A:108:G:N1	3:5B:1551:PHE:O	2.46	0.44
2:5A:92:U:C4	8:5b:36:MET:N	2.85	0.44
3:5B:2298:LEU:CD2	5:5D:1265:GLN:OE1	2.66	0.44
4:5C:488:VAL:HG23	4:5C:489:GLN:N	2.33	0.44
22:4A:127:C:H1'	9:4c:47:ARG:C	2.42	0.44
28:4G:863:TRP:O	28:4G:867:THR:OG1	2.31	0.44
39:2G:834:VAL:O	39:2G:835:ASP:C	2.60	0.44
39:2G:874:LYS:O	39:2G:875:ILE:C	2.60	0.44
1:A:113:U:C4'	30:4I:20:ILE:HD13	2.48	0.44
3:5B:1220:VAL:HG23	3:5B:1221:THR:HG23	1.98	0.44
3:5B:2072:GLU:OE1	3:5B:2075:VAL:HG13	2.17	0.44
5:5D:783:ALA:HB3	5:5D:806:ILE:HG21	2.00	0.44
5:5D:1845:LEU:HA	5:5D:1848:ILE:HG22	2.00	0.44
5:5D:1846:ILE:HG22	5:5D:1892:ASN:OD1	2.18	0.44
5:5D:1919:ALA:O	5:5D:1923:ILE:HG12	2.18	0.44
5:5D:2041:LEU:HD23	5:5D:2108:PHE:CZ	2.52	0.44
24:4C:223:ASN:OD1	24:4C:224:PHE:N	2.50	0.44
27:4F:138:THR:HG22	27:4F:140:TYR:H	1.83	0.44
33:2A:112:G:H2'	33:2A:113:G:C8	2.50	0.44
39:2G:429:ARG:C	39:2G:432:THR:H	2.26	0.44
39:2G:631:ALA:O	39:2G:632:PHE:C	2.58	0.44
39:2G:831:ARG:O	39:2G:832:GLN:C	2.58	0.44
4:5C:446:LYS:HB3	4:5C:447:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:1784:HIS:O	5:5D:1788:LEU:HG	2.18	0.44
22:4A:127:C:O5'	22:4A:127:C:C6	2.70	0.44
24:4C:316:VAL:O	24:4C:317:ALA:C	2.60	0.44
25:4D:131:ASN:OD1	25:4D:132:ALA:N	2.51	0.44
28:4G:714:MET:O	28:4G:714:MET:SD	2.75	0.44
9:4c:109:VAL:N	10:4d:63:LEU:O	2.42	0.44
33:2A:40:C:C5'	33:2A:40:C:C6	2.92	0.44
33:2A:113:G:H2'	33:2A:114:A:H8	1.82	0.44
33:2A:153:A:H2'	33:2A:154:C:H5''	1.99	0.44
39:2G:1223:SER:O	39:2G:1224:PRO:C	2.60	0.44
3:5B:361:HIS:O	3:5B:361:HIS:ND1	2.50	0.44
4:5C:623:GLU:OE2	4:5C:624:SER:OG	2.18	0.44
4:5C:670:SER:HA	4:5C:823:ALA:HA	1.99	0.44
4:5C:813:ARG:O	4:5C:816:VAL:HG12	2.17	0.44
33:2A:182:U:H2'	33:2A:183:G:H8	1.81	0.44
39:2G:578:ILE:O	39:2G:579:GLU:C	2.57	0.44
39:2G:606:LEU:O	39:2G:609:MET:N	2.51	0.44
41:2I:406:PRO:CA	41:2I:1122:LEU:O	2.65	0.44
4:5C:126:SER:O	4:5C:126:SER:OG	2.33	0.44
5:5D:616:GLU:HA	5:5D:616:GLU:OE1	2.18	0.44
5:5D:1604:LEU:HD13	5:5D:1609:LEU:CD2	2.47	0.44
5:5D:2039:VAL:HB	5:5D:2090:VAL:HG13	2.00	0.44
24:4C:92:ARG:HA	24:4C:92:ARG:NE	2.32	0.44
24:4C:517:LYS:NZ	28:4G:767:GLU:OE1	2.51	0.44
39:2G:1029:GLU:O	39:2G:1032:GLN:N	2.51	0.44
41:2I:676:ARG:O	41:2I:686:LEU:CA	2.65	0.44
1:A:34:G:C5	1:A:35:U:C4	3.05	0.43
1:A:35:U:O2'	1:A:36:C:C5	2.71	0.43
3:5B:337:VAL:HG23	4:5C:266:GLU:OE1	2.18	0.43
4:5C:317:CYS:HB3	4:5C:427:PHE:CD1	2.53	0.43
5:5D:765:GLU:N	5:5D:765:GLU:OE1	2.51	0.43
39:2G:1230:VAL:O	39:2G:1233:ALA:N	2.51	0.43
3:5B:2162:GLN:O	3:5B:2294:TYR:OH	2.18	0.43
3:5B:2317:PHE:CE2	5:5D:1070:LEU:HD11	2.52	0.43
4:5C:509:VAL:HG21	4:5C:558:PRO:CG	2.48	0.43
4:5C:749:THR:O	4:5C:753:GLU:HB3	2.18	0.43
5:5D:526:ASN:ND2	5:5D:531:ILE:O	2.51	0.43
5:5D:815:LEU:HD21	5:5D:821:LEU:HB3	2.00	0.43
14:6A:37:C:H4'	14:6A:38:G:OP2	2.17	0.43
40:2H:805:ILE:HG12	40:2H:806:TYR:N	2.34	0.43
41:2I:1148:LEU:O	41:2I:1151:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:684:GLU:HG2	36:2D:476:ILE:HD11	2.00	0.43
3:5B:2072:GLU:CD	3:5B:2074:ARG:HB2	2.43	0.43
5:5D:1360:ALA:HB2	5:5D:1490:LEU:HD11	2.00	0.43
14:6A:92:A:H2'	14:6A:93:G:H8	1.83	0.43
24:4C:363:GLY:O	24:4C:390:ARG:NH2	2.51	0.43
28:4G:144:ASP:OD1	28:4G:145:LEU:N	2.51	0.43
29:4H:152:ARG:CB	30:4I:75:ALA:HB2	2.48	0.43
33:2A:98:G:H5'	33:2A:104:U:OP2	2.19	0.43
33:2A:154:C:O2'	33:2A:155:C:C5'	2.66	0.43
33:2A:181:G:H2'	33:2A:182:U:C6	2.50	0.43
39:2G:792:VAL:O	39:2G:793:LYS:C	2.59	0.43
3:5B:1635:TYR:CD1	3:5B:1635:TYR:C	2.95	0.43
5:5D:1628:GLU:CD	5:5D:1628:GLU:N	2.76	0.43
5:5D:1844:GLY:O	5:5D:1848:ILE:HG22	2.18	0.43
31:4J:149:GLU:O	31:4J:149:GLU:CG	2.67	0.43
1:A:17:G:H2'	1:A:18:C:C6	2.53	0.43
2:5A:92:U:O4	8:5b:34:VAL:O	2.37	0.43
3:5B:2275:ALA:HB3	3:5B:2295:GLU:OE1	2.19	0.43
4:5C:856:HIS:O	4:5C:856:HIS:CG	2.70	0.43
25:4D:95:ASP:O	25:4D:98:ASN:OD1	2.35	0.43
28:4G:367:ARG:CZ	28:4G:367:ARG:HB2	2.48	0.43
45:2M:64:VAL:O	45:2M:65:ARG:C	2.59	0.43
1:A:20:U:C2	33:2A:42:G:C2	3.04	0.43
3:5B:1108:ASP:OD1	3:5B:1108:ASP:N	2.50	0.43
3:5B:1268:ILE:O	3:5B:1272:THR:OG1	2.31	0.43
5:5D:1518:VAL:O	5:5D:1518:VAL:CG1	2.67	0.43
14:6A:45:A:C6	14:6A:47:A:N6	2.86	0.43
14:6A:55:C:H2'	14:6A:56:A:O4'	2.19	0.43
32:4Z:488:ILE:H	32:4Z:503:SER:HA	1.83	0.43
33:2A:40:C:H5''	33:2A:40:C:C6	2.32	0.43
33:2A:148:C:H2'	33:2A:149:A:H8	1.82	0.43
39:2G:82:PRO:O	39:2G:86:ALA:N	2.42	0.43
39:2G:310:TRP:O	39:2G:311:ALA:C	2.62	0.43
39:2G:625:ARG:O	39:2G:626:ASN:C	2.61	0.43
39:2G:1262:ARG:O	39:2G:1263:ASP:C	2.61	0.43
2:5A:89:U:C2'	2:5A:90:U:H5''	2.47	0.43
5:5D:530:THR:CB	5:5D:531:ILE:HD12	2.48	0.43
5:5D:595:ILE:HD12	5:5D:992:TYR:HB2	2.01	0.43
24:4C:499:ASP:OD1	24:4C:500:ILE:N	2.52	0.43
27:4F:48:ILE:CG2	27:4F:109:LYS:HB2	2.49	0.43
33:2A:142:C:H2'	33:2A:143:A:H5'	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2G:665:ILE:O	39:2G:668:VAL:N	2.52	0.43
41:2I:318:ASP:N	41:2I:321:MET:O	2.27	0.43
3:5B:533:LYS:O	3:5B:537:LYS:HG3	2.18	0.43
5:5D:1518:VAL:O	5:5D:1518:VAL:HG12	2.17	0.43
5:5D:1960:LEU:CD1	5:5D:1982:VAL:HG22	2.48	0.43
14:6A:89:U:H2'	14:6A:90:G:C8	2.53	0.43
23:4B:580:ASN:OD1	23:4B:580:ASN:N	2.52	0.43
24:4C:275:ASN:O	24:4C:301:ALA:N	2.51	0.43
28:4G:800:MET:HE3	28:4G:800:MET:HA	2.01	0.43
39:2G:782:GLU:O	39:2G:783:GLU:C	2.62	0.43
39:2G:889:GLU:O	39:2G:892:LEU:N	2.51	0.43
39:2G:916:THR:O	39:2G:917:VAL:C	2.61	0.43
39:2G:981:TYR:C	39:2G:983:GLY:N	2.75	0.43
41:2I:147:ASP:N	41:2I:151:ARG:O	2.42	0.43
3:5B:783:TYR:CD1	3:5B:783:TYR:C	2.96	0.43
16:6b:19:ASP:C	16:6b:21:ILE:N	2.77	0.43
23:4B:447:LYS:NZ	36:2D:433:LEU:O	2.44	0.43
28:4G:365:ALA:HB1	28:4G:375:ILE:HD13	2.00	0.43
41:2I:430:GLY:O	41:2I:431:PRO:C	2.61	0.43
41:2I:886:GLU:CA	41:2I:910:ALA:O	2.67	0.43
3:5B:677:VAL:HA	3:5B:680:HIS:HB2	2.01	0.43
3:5B:1202:THR:HG23	3:5B:1204:TYR:CD2	2.54	0.43
4:5C:133:THR:HG23	4:5C:225:VAL:HG23	2.00	0.43
4:5C:478:THR:HA	4:5C:494:GLY:HA3	1.99	0.43
5:5D:534:ASP:OD1	5:5D:534:ASP:C	2.62	0.43
5:5D:831:THR:CG2	5:5D:869:LEU:HD11	2.48	0.43
14:6A:89:U:H2'	14:6A:90:G:H8	1.84	0.43
22:4A:120:U:C6	22:4A:120:U:C3'	3.01	0.43
39:2G:627:THR:O	39:2G:630:ARG:N	2.52	0.43
41:2I:5:ASN:O	41:2I:1176:GLY:HA3	2.19	0.43
4:5C:666:VAL:HG22	4:5C:787:VAL:HG22	2.01	0.42
5:5D:1196:SER:O	5:5D:1196:SER:OG	2.34	0.42
5:5D:1923:ILE:HG21	5:5D:1946:ALA:HB2	2.01	0.42
14:6A:47:A:O2'	14:6A:48:A:C8	2.72	0.42
24:4C:478:THR:HG22	24:4C:479:HIS:N	2.33	0.42
33:2A:178:A:N3	33:2A:178:A:H2'	2.34	0.42
39:2G:854:VAL:O	39:2G:856:ASP:N	2.52	0.42
39:2G:928:TYR:O	39:2G:929:LEU:C	2.61	0.42
39:2G:1016:LEU:O	39:2G:1017:LEU:C	2.62	0.42
39:2G:1090:PRO:O	39:2G:1091:HIS:C	2.62	0.42
1:A:37:C:C2'	1:A:38:C:O5'	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:464:VAL:HA	5:5D:467:LEU:HD13	2.02	0.42
5:5D:696:LYS:NZ	22:4A:61:A:P	2.92	0.42
5:5D:848:ASP:O	5:5D:852:MET:HG3	2.20	0.42
5:5D:1569:THR:CG2	5:5D:1570:ARG:N	2.82	0.42
14:6A:92:A:H2'	14:6A:93:G:C8	2.54	0.42
22:4A:90:G:H2'	22:4A:91:A:C8	2.55	0.42
28:4G:97:ASP:OD1	28:4G:97:ASP:N	2.45	0.42
28:4G:371:GLN:N	28:4G:371:GLN:OE1	2.52	0.42
28:4G:786:LEU:HD13	28:4G:786:LEU:C	2.45	0.42
31:4J:285:GLU:N	31:4J:285:GLU:OE1	2.51	0.42
33:2A:64:A:H2'	33:2A:65:U:C6	2.54	0.42
39:2G:682:HIS:O	39:2G:683:LEU:C	2.61	0.42
39:2G:723:SER:C	39:2G:725:ASP:H	2.26	0.42
39:2G:948:ARG:O	39:2G:949:GLN:C	2.60	0.42
41:2I:1189:LYS:O	41:2I:1190:GLN:C	2.62	0.42
3:5B:220:VAL:HG12	3:5B:221:ASN:N	2.35	0.42
3:5B:1502:PHE:O	3:5B:1503:TRP:C	2.63	0.42
4:5C:484:THR:OG1	4:5C:485:ASP:N	2.52	0.42
4:5C:919:ARG:HE	4:5C:919:ARG:N	2.17	0.42
5:5D:525:ILE:O	5:5D:526:ASN:C	2.62	0.42
33:2A:107:A:N1	33:2A:108:G:C5	2.88	0.42
39:2G:981:TYR:O	39:2G:983:GLY:N	2.53	0.42
43:2K:51:GLY:HA3	43:2K:56:THR:O	2.19	0.42
45:2M:62:ALA:O	45:2M:63:ARG:C	2.62	0.42
3:5B:1194:CYS:HA	3:5B:1229:PHE:O	2.19	0.42
4:5C:747:ASP:CG	4:5C:749:THR:HG1	2.28	0.42
5:5D:495:THR:HG22	5:5D:496:ASP:N	2.35	0.42
5:5D:642:THR:O	5:5D:642:THR:HG22	2.19	0.42
5:5D:1857:ASN:OD1	5:5D:1857:ASN:C	2.62	0.42
22:4A:110:G:O5'	22:4A:110:G:C8	2.70	0.42
22:4A:119:A:H5''	10:4d:38:GLY:O	2.19	0.42
28:4G:899:LYS:HD3	28:4G:899:LYS:N	2.35	0.42
33:2A:142:C:O2'	33:2A:143:A:H5'	2.18	0.42
39:2G:632:PHE:O	39:2G:633:ALA:C	2.59	0.42
39:2G:950:GLN:O	39:2G:951:ALA:C	2.61	0.42
1:A:37:C:O2'	1:A:38:C:O4'	2.38	0.42
3:5B:337:VAL:O	3:5B:337:VAL:CG1	2.66	0.42
3:5B:988:ILE:O	3:5B:1028:TYR:O	2.37	0.42
3:5B:2298:LEU:HD21	5:5D:1265:GLN:OE1	2.19	0.42
4:5C:747:ASP:OD1	4:5C:749:THR:HG23	2.19	0.42
22:4A:119:A:H5''	10:4d:38:GLY:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2B:160:LYS:O	34:2B:161:MET:C	2.63	0.42
2:5A:95:G:C1'	10:5d:24:LYS:CA	2.80	0.42
3:5B:784:LEU:O	3:5B:788:GLN:HG3	2.19	0.42
5:5D:1936:LEU:HD23	5:5D:1936:LEU:C	2.43	0.42
5:5D:2098:ALA:C	5:5D:2099:THR:HG22	2.45	0.42
25:4D:274:ILE:C	25:4D:277:SER:HG	2.23	0.42
28:4G:343:GLU:OE2	28:4G:374:ARG:NE	2.52	0.42
28:4G:668:ALA:O	28:4G:672:ALA:N	2.47	0.42
33:2A:157:G:H2'	33:2A:158:G:O4'	2.19	0.42
39:2G:574:ILE:O	39:2G:575:LEU:C	2.63	0.42
39:2G:1205:GLU:O	39:2G:1206:ASP:C	2.61	0.42
39:2G:1279:ALA:O	39:2G:1280:LEU:C	2.60	0.42
1:A:33:U:O2'	1:A:34:G:C8	2.70	0.42
2:5A:71:C:H2'	2:5A:72:U:O4'	2.19	0.42
3:5B:2233:SER:O	3:5B:2236:GLU:HG3	2.20	0.42
5:5D:467:LEU:HD12	5:5D:467:LEU:H	1.84	0.42
5:5D:1613:LEU:CD1	5:5D:1641:ILE:HG21	2.50	0.42
5:5D:1943:MET:HE3	5:5D:2109:MET:HB2	2.01	0.42
28:4G:309:PRO:N	28:4G:310:PRO:CD	2.83	0.42
39:2G:710:ALA:O	39:2G:711:ALA:C	2.61	0.42
39:2G:1078:VAL:O	39:2G:1079:ASN:C	2.63	0.42
39:2G:1115:ALA:O	39:2G:1116:ILE:C	2.61	0.42
1:A:22:C:H2'	1:A:23:G:C5'	2.49	0.42
2:5A:12:U:OP1	3:5B:224:THR:OG1	2.34	0.42
3:5B:984:MET:HE3	3:5B:1048:MET:CE	2.50	0.42
5:5D:514:LEU:HD22	5:5D:558:ARG:HD3	2.01	0.42
5:5D:938:ILE:HD11	5:5D:952:ARG:HG2	2.01	0.42
5:5D:1369:LEU:HD23	5:5D:1369:LEU:C	2.45	0.42
5:5D:1847:GLU:OE1	5:5D:1847:GLU:C	2.63	0.42
27:4F:63:ILE:HD12	27:4F:63:ILE:HA	1.85	0.42
33:2A:155:C:H2'	33:2A:156:U:H5''	2.02	0.42
39:2G:854:VAL:C	39:2G:856:ASP:H	2.28	0.42
39:2G:997:LEU:O	39:2G:998:LYS:C	2.62	0.42
1:A:20:U:H5''	1:A:20:U:H6	1.85	0.42
2:5A:67:A:C2'	2:5A:68:C:OP1	2.68	0.42
3:5B:150:MET:HE2	3:5B:192:GLN:O	2.20	0.42
3:5B:1021:ASP:N	3:5B:1021:ASP:OD1	2.53	0.42
5:5D:625:GLY:N	5:5D:626:PRO:CD	2.83	0.42
29:4H:45:GLN:O	29:4H:49:GLY:N	2.53	0.42
32:4Z:334:HIS:HA	32:4Z:342:LEU:N	2.34	0.42
39:2G:887:LYS:O	39:2G:888:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2I:1211:ILE:O	41:2I:1212:ARG:C	2.62	0.42
1:A:10:C:C2	1:A:10:C:OP2	2.73	0.42
3:5B:1911:GLU:O	3:5B:1912:PRO:C	2.63	0.42
3:5B:2286:VAL:O	3:5B:2286:VAL:HG22	2.20	0.42
4:5C:733:TRP:CZ3	4:5C:747:ASP:HB2	2.55	0.42
4:5C:921:LEU:HD12	4:5C:921:LEU:O	2.20	0.42
5:5D:573:HIS:C	5:5D:575:LEU:H	2.27	0.42
5:5D:690:VAL:HG11	5:5D:707:ILE:HD13	2.01	0.42
5:5D:692:ILE:HG21	5:5D:700:ARG:HG3	2.02	0.42
22:4A:74:C:N3	22:4A:75:C:N4	2.68	0.42
28:4G:367:ARG:HB2	28:4G:367:ARG:NH1	2.34	0.42
32:4Z:241:TRP:HA	32:4Z:248:ILE:HA	2.01	0.42
36:2D:506:SER:HA	36:2D:509:MET:SD	2.59	0.42
38:2F:34:ARG:O	38:2F:35:ASP:C	2.62	0.42
39:2G:704:ILE:O	39:2G:705:SER:C	2.61	0.42
39:2G:806:ILE:O	39:2G:807:LYS:C	2.62	0.42
42:2J:77:ILE:O	42:2J:84:ILE:CA	2.68	0.42
1:A:115:U:HO2'	1:A:116:G:P	2.41	0.41
2:5A:93:U:C4'	9:5c:104:ASP:CA	2.97	0.41
2:5A:116:U:OP2	11:5e:68:THR:CA	2.67	0.41
3:5B:388:LEU:HD21	4:5C:399:LEU:HD21	2.02	0.41
3:5B:2306:HIS:CD2	3:5B:2308:VAL:HG22	2.55	0.41
4:5C:326:ILE:O	4:5C:330:THR:HG23	2.20	0.41
4:5C:845:ALA:O	4:5C:846:VAL:C	2.62	0.41
4:5C:855:GLY:O	4:5C:874:PHE:O	2.38	0.41
28:4G:915:VAL:HG11	28:4G:933:VAL:HG12	2.02	0.41
33:2A:103:U:C3'	33:2A:104:U:H5'	2.50	0.41
39:2G:91:LEU:O	39:2G:94:ILE:N	2.53	0.41
39:2G:862:GLU:O	39:2G:864:TYR:N	2.53	0.41
39:2G:1038:LEU:O	39:2G:1039:VAL:C	2.62	0.41
1:A:30:C:C5	1:A:31:C:H5	2.32	0.41
3:5B:679:SER:O	3:5B:680:HIS:C	2.62	0.41
3:5B:2190:PRO:HA	3:5B:2193:VAL:HG12	2.01	0.41
4:5C:778:PRO:HD3	4:5C:784:ILE:HD11	2.03	0.41
5:5D:641:MET:HG2	5:5D:1582:ALA:CB	2.50	0.41
5:5D:1166:ARG:CZ	5:5D:1166:ARG:HB2	2.49	0.41
5:5D:1536:GLN:O	5:5D:1540:LEU:HG	2.20	0.41
5:5D:1970:HIS:ND1	5:5D:1974:CYS:SG	2.89	0.41
22:4A:107:U:H2'	22:4A:108:C:H6	1.85	0.41
32:4Z:146:ALA:O	32:4Z:150:ALA:CB	2.67	0.41
32:4Z:240:VAL:O	32:4Z:249:ARG:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2A:153:A:H62	33:2A:177:A:H2	1.67	0.41
39:2G:318:ARG:O	39:2G:321:ASP:N	2.52	0.41
39:2G:1169:VAL:O	39:2G:1172:LEU:N	2.54	0.41
3:5B:1189:MET:O	3:5B:1190:CYS:C	2.63	0.41
3:5B:1920:TYR:O	3:5B:1921:ASP:C	2.62	0.41
4:5C:243:ILE:O	4:5C:247:VAL:HG12	2.20	0.41
4:5C:933:PHE:O	4:5C:937:THR:OG1	2.14	0.41
5:5D:592:LYS:O	5:5D:595:ILE:HG22	2.19	0.41
24:4C:184:TYR:OH	24:4C:188:ARG:NH1	2.49	0.41
24:4C:257:LEU:HD13	24:4C:269:LEU:HD11	2.01	0.41
33:2A:54:U:H5'	38:2F:424:ARG:C	2.45	0.41
38:2F:404:ILE:N	38:2F:417:ARG:O	2.44	0.41
39:2G:600:LEU:O	39:2G:604:ALA:N	2.35	0.41
39:2G:998:LYS:O	39:2G:1001:VAL:N	2.51	0.41
39:2G:1082:GLY:O	39:2G:1083:TYR:C	2.61	0.41
40:2H:504:TRP:C	40:2H:506:PHE:H	2.27	0.41
41:2I:127:GLY:O	41:2I:128:ARG:C	2.63	0.41
2:5A:115:C:OP1	11:5e:67:LYS:CA	2.67	0.41
4:5C:705:VAL:O	4:5C:706:GLN:C	2.62	0.41
4:5C:758:LEU:N	4:5C:758:LEU:HD22	2.35	0.41
5:5D:1936:LEU:HD21	5:5D:1940:LEU:HD11	2.02	0.41
5:5D:2042:GLU:HA	5:5D:2087:LYS:HB3	2.02	0.41
14:6A:50:A:N3	25:4D:347:LEU:HD11	2.35	0.41
25:4D:275:TYR:HA	25:4D:280:VAL:HG11	2.02	0.41
31:4J:264:ASP:OD1	31:4J:264:ASP:C	2.62	0.41
33:2A:63:G:H2'	33:2A:64:A:C8	2.56	0.41
3:5B:97:HIS:ND1	3:5B:649:GLU:OE1	2.53	0.41
3:5B:246:LEU:HD11	3:5B:411:PHE:CE2	2.55	0.41
3:5B:255:PHE:O	3:5B:332:TYR:OH	2.38	0.41
4:5C:600:LEU:N	4:5C:601:PRO:HD2	2.35	0.41
5:5D:1351:PRO:HG3	5:5D:1516:PRO:HA	2.01	0.41
5:5D:1492:SER:OG	5:5D:1493:SER:N	2.53	0.41
5:5D:1665:ASP:O	5:5D:1667:GLN:N	2.48	0.41
24:4C:460:ILE:H	24:4C:460:ILE:HG13	1.55	0.41
28:4G:736:LEU:HD22	28:4G:746:TRP:CE2	2.56	0.41
39:2G:86:ALA:O	39:2G:89:ALA:CA	2.67	0.41
39:2G:1040:GLY:O	39:2G:1041:ARG:C	2.63	0.41
1:A:40:U:O4'	1:A:41:U:C5	2.72	0.41
2:5A:68:C:H2'	2:5A:69:A:C4'	2.50	0.41
2:5A:90:U:C5	13:5g:38:ASN:C	2.85	0.41
4:5C:676:ALA:HB3	4:5C:815:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5D:573:HIS:O	5:5D:575:LEU:N	2.53	0.41
5:5D:769:CYS:SG	5:5D:771:ASN:N	2.93	0.41
33:2A:152:G:H2'	33:2A:153:A:C1'	2.51	0.41
41:2I:1210:ASP:O	41:2I:1211:ILE:C	2.64	0.41
3:5B:172:GLU:HA	3:5B:172:GLU:OE2	2.20	0.41
3:5B:659:GLN:N	3:5B:659:GLN:CD	2.78	0.41
3:5B:1863:VAL:HG11	3:5B:1868:MET:HB3	2.03	0.41
3:5B:2119:ASP:OD2	3:5B:2305:TYR:OH	2.39	0.41
4:5C:535:ALA:HB3	4:5C:536:ARG:NH1	2.35	0.41
39:2G:301:ARG:O	39:2G:302:ASP:C	2.63	0.41
39:2G:594:ARG:O	39:2G:595:GLU:C	2.61	0.41
44:2L:93:SER:O	44:2L:94:SER:C	2.64	0.41
3:5B:579:GLN:HG3	3:5B:629:PHE:H	1.86	0.41
4:5C:256:CYS:CA	4:5C:308:CYS:HB3	2.38	0.41
5:5D:699:LYS:HD2	5:5D:699:LYS:HA	1.92	0.41
22:4A:33:A:H2'	22:4A:34:G:O4'	2.21	0.41
25:4D:106:GLU:HA	25:4D:109:ILE:HG12	2.02	0.41
28:4G:706:GLU:O	28:4G:712:TRP:NE1	2.50	0.41
33:2A:112:G:O5'	33:2A:112:G:H8	2.04	0.41
36:2D:517:GLN:HA	36:2D:520:ILE:HG22	2.03	0.41
39:2G:1182:LEU:O	39:2G:1183:VAL:C	2.63	0.41
41:2I:1143:HIS:O	41:2I:1144:VAL:C	2.64	0.41
1:A:102:U:H2'	1:A:103:A:O4'	2.20	0.41
2:5A:26:A:OP1	3:5B:419:ARG:NH1	2.48	0.41
3:5B:338:VAL:N	4:5C:266:GLU:OE2	2.53	0.41
3:5B:409:ARG:HA	3:5B:412:ASN:OD1	2.21	0.41
3:5B:598:LEU:HD11	3:5B:640:PHE:CZ	2.55	0.41
3:5B:1609:VAL:HG12	3:5B:1631:LEU:HD22	2.02	0.41
3:5B:2123:GLN:HB2	3:5B:2157:VAL:HG13	2.03	0.41
4:5C:122:LEU:O	4:5C:125:ASN:HB3	2.21	0.41
5:5D:488:LEU:HD12	5:5D:488:LEU:C	2.46	0.41
5:5D:1375:ARG:NH1	5:5D:1447:ASN:O	2.54	0.41
5:5D:1631:LEU:HD23	5:5D:1631:LEU:C	2.46	0.41
5:5D:1748:LYS:NZ	5:5D:1790:GLU:OE1	2.46	0.41
5:5D:1920:ILE:HG22	5:5D:1924:GLN:OE1	2.21	0.41
5:5D:1943:MET:HE3	5:5D:2109:MET:CB	2.51	0.41
5:5D:2098:ALA:O	5:5D:2099:THR:CG2	2.68	0.41
6:5E:255:MET:O	6:5E:257:ASN:N	2.54	0.41
19:6e:45:LEU:N	19:6e:63:ALA:O	2.37	0.41
24:4C:180:TRP:O	24:4C:183:ASN:OD1	2.39	0.41
24:4C:458:GLU:HG2	24:4C:459:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4E:54:ILE:HD13	26:4E:103:SER:HB2	2.03	0.41
33:2A:152:G:H2'	33:2A:152:G:N3	2.36	0.41
33:2A:171:U:H2'	33:2A:172:C:O4'	2.21	0.41
39:2G:647:PHE:O	39:2G:648:LEU:C	2.63	0.41
39:2G:712:LEU:O	39:2G:713:ALA:C	2.64	0.41
39:2G:750:ILE:O	39:2G:751:GLY:C	2.63	0.41
39:2G:1018:PRO:O	39:2G:1019:ARG:C	2.63	0.41
41:2I:811:THR:C	41:2I:813:ALA:N	2.78	0.41
3:5B:831:SER:O	3:5B:831:SER:OG	2.37	0.41
3:5B:930:ALA:O	3:5B:933:ARG:O	2.39	0.41
3:5B:1997:VAL:HG12	3:5B:1998:ASN:N	2.36	0.41
4:5C:375:GLU:HA	4:5C:375:GLU:OE2	2.21	0.41
4:5C:465:MET:SD	4:5C:475:MET:HG3	2.61	0.41
4:5C:938:ARG:O	4:5C:942:GLY:N	2.54	0.41
5:5D:526:ASN:O	5:5D:527:MET:C	2.64	0.41
5:5D:1036:GLU:OE1	5:5D:1075:PHE:HA	2.21	0.41
24:4C:272:HIS:NE2	24:4C:298:SER:OG	2.52	0.41
33:2A:149:A:C6	33:2A:150:U:C4	3.09	0.41
39:2G:758:ASP:O	39:2G:761:TYR:N	2.54	0.41
40:2H:596:GLU:C	40:2H:598:GLU:N	2.67	0.41
41:2I:437:VAL:O	41:2I:776:GLN:CA	2.69	0.41
4:5C:916:ILE:N	4:5C:916:ILE:HD13	2.35	0.40
5:5D:730:GLU:OE2	5:5D:829:LYS:NZ	2.50	0.40
5:5D:1006:LYS:O	5:5D:1107:LEU:HD22	2.21	0.40
5:5D:1165:ILE:O	5:5D:1165:ILE:HG22	2.22	0.40
25:4D:384:GLU:OE2	25:4D:395:SER:OG	2.39	0.40
28:4G:729:ARG:O	28:4G:733:ASN:OD1	2.39	0.40
38:2F:184:ARG:CA	7:2a:85:PRO:C	2.94	0.40
39:2G:301:ARG:O	39:2G:304:PRO:N	2.54	0.40
39:2G:771:LEU:O	39:2G:772:ILE:C	2.65	0.40
39:2G:1149:LYS:O	39:2G:1150:SER:C	2.63	0.40
41:2I:672:GLY:N	41:2I:697:ARG:O	2.54	0.40
3:5B:180:ASP:OD1	3:5B:180:ASP:N	2.53	0.40
3:5B:1456:THR:OG1	3:5B:1457:HIS:N	2.54	0.40
4:5C:618:THR:HB	4:5C:630:LEU:HB2	2.03	0.40
4:5C:714:LEU:O	4:5C:718:PHE:HD2	2.03	0.40
5:5D:782:PHE:N	5:5D:782:PHE:CD1	2.89	0.40
5:5D:1382:MET:HE2	5:5D:1652:TRP:CG	2.56	0.40
5:5D:1598:ILE:N	5:5D:1599:PRO:CD	2.85	0.40
25:4D:423:THR:O	25:4D:427:THR:HG23	2.20	0.40
28:4G:743:THR:N	28:4G:744:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2D:522:LEU:HD23	36:2D:523:GLN:OE1	2.21	0.40
39:2G:706:ALA:O	39:2G:707:LEU:C	2.61	0.40
45:2M:52:TYR:O	45:2M:53:PHE:C	2.62	0.40
3:5B:1981:VAL:O	3:5B:1985:ASP:OD1	2.40	0.40
3:5B:2083:LEU:HD21	3:5B:2218:PHE:CE2	2.56	0.40
5:5D:537:LYS:NZ	5:5D:583:THR:O	2.53	0.40
5:5D:1437:ARG:CD	5:5D:1738:ALA:HB1	2.52	0.40
5:5D:1559:VAL:N	5:5D:1642:GLN:O	2.49	0.40
5:5D:1962:GLN:OE1	5:5D:2114:MET:N	2.48	0.40
5:5D:1988:MET:HE1	5:5D:1996:LEU:HD13	2.03	0.40
24:4C:99:ILE:HG22	24:4C:101:VAL:HG23	2.02	0.40
31:4J:187:ILE:HD12	31:4J:187:ILE:O	2.21	0.40
36:2D:475:ASP:OD1	36:2D:475:ASP:N	2.54	0.40
39:2G:951:ALA:O	39:2G:952:ALA:C	2.61	0.40
39:2G:1169:VAL:O	39:2G:1170:THR:C	2.65	0.40
9:2c:62:HIS:O	9:2c:103:GLY:HA3	2.21	0.40
4:5C:758:LEU:HD12	4:5C:800:PRO:HD3	2.03	0.40
5:5D:518:LEU:O	5:5D:522:GLY:N	2.52	0.40
5:5D:530:THR:HB	5:5D:531:ILE:HD12	2.03	0.40
5:5D:531:ILE:HG22	5:5D:532:ASN:N	2.37	0.40
5:5D:792:VAL:O	5:5D:795:THR:HG22	2.22	0.40
5:5D:1946:ALA:O	5:5D:1950:THR:HG23	2.20	0.40
33:2A:183:G:C6	33:2A:184:C:N4	2.89	0.40
39:2G:899:ALA:O	39:2G:900:PHE:C	2.64	0.40
10:2d:5:LEU:O	11:2e:49:GLY:HA3	2.21	0.40
2:5A:107:U:H2'	2:5A:108:G:O4'	2.22	0.40
3:5B:1204:TYR:N	3:5B:1204:TYR:CD1	2.89	0.40
3:5B:1521:ALA:O	3:5B:1524:SER:OG	2.34	0.40
3:5B:1850:ARG:NH2	40:2H:800:MET:O	2.50	0.40
4:5C:668:GLU:HA	4:5C:668:GLU:OE2	2.21	0.40
4:5C:814:ARG:O	4:5C:818:SER:OG	2.38	0.40
5:5D:432:ASP:OD1	5:5D:433:GLY:N	2.52	0.40
5:5D:498:ASN:OD1	5:5D:498:ASN:N	2.55	0.40
5:5D:1214:VAL:HG23	5:5D:1215:HIS:N	2.36	0.40
5:5D:1240:LEU:C	5:5D:1240:LEU:HD23	2.47	0.40
5:5D:1860:ILE:HD12	5:5D:1890:LYS:HD3	2.04	0.40
9:5c:62:HIS:O	9:5c:103:GLY:HA3	2.21	0.40
23:4B:536:ASP:O	23:4B:538:SER:N	2.54	0.40
24:4C:398:ARG:O	24:4C:399:CYS:C	2.64	0.40
25:4D:222:ILE:HG22	25:4D:223:ILE:HG23	2.03	0.40
28:4G:359:LYS:HA	28:4G:362:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2A:160:A:H2'	33:2A:161:U:O4'	2.22	0.40
36:2D:411:LEU:N	36:2D:419:LYS:HZ2	2.20	0.40
39:2G:705:SER:O	39:2G:708:ALA:N	2.55	0.40
39:2G:750:ILE:O	39:2G:753:LEU:N	2.54	0.40
39:2G:1062:LEU:O	39:2G:1064:GLU:N	2.54	0.40
39:2G:1187:THR:O	39:2G:1188:ALA:C	2.64	0.40
39:2G:1188:ALA:O	39:2G:1189:SER:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	5B	2249/2335 (96%)	2145 (95%)	104 (5%)	0	100	100
4	5C	814/972 (84%)	745 (92%)	68 (8%)	1 (0%)	48	70
5	5D	1694/2136 (79%)	1618 (96%)	75 (4%)	1 (0%)	48	70
6	5E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	6
7	2a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
7	4a	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
7	5a	82/231 (36%)	80 (98%)	2 (2%)	0	100	100
8	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
8	4b	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
8	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
9	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
9	4c	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
9	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
10	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	4d	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
10	5d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
11	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
11	4e	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
11	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
12	2f	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
12	4f	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
12	5f	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
13	2g	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
13	4g	69/126 (55%)	69 (100%)	0	0	100	100
13	5g	72/126 (57%)	70 (97%)	2 (3%)	0	100	100
15	6a	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	2
16	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	2
17	6c	70/139 (50%)	63 (90%)	6 (9%)	1 (1%)	9	19
18	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	8	18
19	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	3	6
20	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
21	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	14
23	4B	248/683 (36%)	229 (92%)	19 (8%)	0	100	100
24	4C	422/522 (81%)	388 (92%)	33 (8%)	1 (0%)	43	66
25	4D	372/499 (74%)	354 (95%)	18 (5%)	0	100	100
26	4E	122/128 (95%)	112 (92%)	10 (8%)	0	100	100
27	4F	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
28	4G	795/941 (84%)	745 (94%)	50 (6%)	0	100	100
29	4H	167/177 (94%)	156 (93%)	11 (7%)	0	100	100
30	4I	73/376 (19%)	71 (97%)	2 (3%)	0	100	100
31	4J	143/800 (18%)	136 (95%)	7 (5%)	0	100	100
32	4Z	414/513 (81%)	401 (97%)	12 (3%)	1 (0%)	43	66
34	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	21
35	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
36	2D	226/793 (28%)	208 (92%)	12 (5%)	6 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	0
38	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	10	23
39	2G	1032/1304 (79%)	844 (82%)	166 (16%)	22 (2%)	5	11
40	2H	199/895 (22%)	179 (90%)	16 (8%)	4 (2%)	6	12
41	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	14	30
42	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100	100
43	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	4	6
44	2L	87/110 (79%)	74 (85%)	13 (15%)	0	100	100
45	2M	64/86 (74%)	55 (86%)	7 (11%)	2 (3%)	3	5
All	All	13703/20230 (68%)	12707 (93%)	908 (7%)	88 (1%)	23	42

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5D	1086	GLN
6	5E	193	THR
15	6a	55	LEU
16	6b	84	MET
18	6d	70	ASP
19	6e	52	VAL
19	6e	55	GLN
24	4C	459	PRO
32	4Z	383	CYS
36	2D	301	PRO
37	2E	139	PRO
37	2E	141	ILE
37	2E	146	MET
37	2E	162	PRO
37	2E	165	ARG
37	2E	218	PRO
38	2F	284	ARG
39	2G	208	PRO
39	2G	416	PRO
39	2G	418	PRO
39	2G	456	VAL
39	2G	717	THR
39	2G	941	ASN
39	2G	1107	GLN
41	2I	405	SER

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Mol	Chain	Res	Type
41	2I	919	SER
43	2K	99	GLN
43	2K	105	LYS
15	6a	74	ALA
16	6b	97	PRO
17	6c	12	ASN
34	2B	160	LYS
36	2D	223	LYS
36	2D	280	VAL
38	2F	277	THR
39	2G	113	ALA
39	2G	1110	VAL
40	2H	597	PHE
41	2I	917	PRO
6	5E	60	MET
6	5E	88	ARG
6	5E	256	ASP
38	2F	177	ARG
38	2F	393	PRO
40	2H	510	TYR
6	5E	162	ARG
16	6b	96	ALA
34	2B	32	PRO
36	2D	300	THR
39	2G	112	ILE
39	2G	437	PRO
39	2G	523	ALA
39	2G	909	VAL
39	2G	1006	MET
40	2H	463	ALA
40	2H	574	ALA
41	2I	529	ALA
41	2I	578	THR
43	2K	75	ASP
6	5E	159	PRO
15	6a	73	PRO
37	2E	147	PRO
37	2E	217	PRO
39	2G	1047	ALA
39	2G	1075	ARG
39	2G	1186	GLN
41	2I	95	SER

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Mol	Chain	Res	Type
41	2I	229	GLU
6	5E	270	LYS
21	6g	34	ILE
37	2E	220	PRO
39	2G	326	THR
39	2G	932	ILE
41	2I	918	ARG
41	2I	1138	HIS
45	2M	56	ALA
6	5E	149	GLY
39	2G	417	PRO
36	2D	221	PRO
39	2G	223	THR
4	5C	439	PRO
38	2F	229	TRP
41	2I	1204	VAL
6	5E	324	PRO
36	2D	298	PRO
39	2G	1031	VAL
45	2M	64	VAL
15	6a	52	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	
3	5B	2034/2108 (96%)	1974 (97%)	60 (3%)	37	65
4	5C	718/866 (83%)	693 (96%)	25 (4%)	32	59
5	5D	1517/1908 (80%)	1514 (100%)	3 (0%)	87	95
23	4B	225/599 (38%)	216 (96%)	9 (4%)	28	55
24	4C	362/442 (82%)	345 (95%)	17 (5%)	23	48
25	4D	299/424 (70%)	289 (97%)	10 (3%)	33	61
26	4E	108/111 (97%)	104 (96%)	4 (4%)	30	57
27	4F	129/130 (99%)	122 (95%)	7 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	4G	417/792 (53%)	405 (97%)	12 (3%)	37	65
29	4H	10/148 (7%)	10 (100%)	0	100	100
30	4I	32/333 (10%)	31 (97%)	1 (3%)	35	63
31	4J	113/681 (17%)	107 (95%)	6 (5%)	20	43
32	4Z	11/450 (2%)	11 (100%)	0	100	100
36	2D	95/709 (13%)	89 (94%)	6 (6%)	16	36
40	2H	26/776 (3%)	26 (100%)	0	100	100
All	All	6096/10477 (58%)	5936 (97%)	160 (3%)	41	68

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5B	81	PHE
3	5B	87	VAL
3	5B	139	VAL
3	5B	142	SER
3	5B	221	ASN
3	5B	224	THR
3	5B	236	SER
3	5B	248	ASP
3	5B	322	ASN
3	5B	327	VAL
3	5B	330	THR
3	5B	351	TYR
3	5B	353	ASP
3	5B	361	HIS
3	5B	415	SER
3	5B	468	LYS
3	5B	661	GLU
3	5B	679	SER
3	5B	680	HIS
3	5B	721	LYS
3	5B	724	ILE
3	5B	801	ILE
3	5B	812	THR
3	5B	859	SER
3	5B	866	LEU
3	5B	873	ASN
3	5B	912	GLU
3	5B	945	THR

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Mol	Chain	Res	Type
3	5B	991	THR
3	5B	1089	CYS
3	5B	1129	ASN
3	5B	1168	VAL
3	5B	1173	SER
3	5B	1176	SER
3	5B	1218	ASN
3	5B	1303	LEU
3	5B	1362	ASP
3	5B	1377	SER
3	5B	1384	ARG
3	5B	1385	VAL
3	5B	1393	ARG
3	5B	1413	ASP
3	5B	1420	ASN
3	5B	1438	VAL
3	5B	1634	SER
3	5B	1673	SER
3	5B	1697	SER
3	5B	1765	SER
3	5B	1767	ASN
3	5B	1775	GLN
3	5B	1799	THR
3	5B	1813	ARG
3	5B	1872	LEU
3	5B	1911	GLU
3	5B	2003	THR
3	5B	2046	THR
3	5B	2056	THR
3	5B	2068	SER
3	5B	2072	GLU
3	5B	2231	THR
4	5C	177	ARG
4	5C	193	THR
4	5C	269	LEU
4	5C	279	ARG
4	5C	301	SER
4	5C	311	SER
4	5C	326	ILE
4	5C	327	TYR
4	5C	363	SER
4	5C	525	CYS

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Mol	Chain	Res	Type
4	5C	534	VAL
4	5C	562	THR
4	5C	578	ARG
4	5C	592	VAL
4	5C	649	SER
4	5C	667	VAL
4	5C	670	SER
4	5C	674	CYS
4	5C	696	LEU
4	5C	705	VAL
4	5C	749	THR
4	5C	783	LEU
4	5C	818	SER
4	5C	880	SER
4	5C	912	LEU
5	5D	778	LEU
5	5D	984	LEU
5	5D	1705	MET
23	4B	414	ILE
23	4B	424	LEU
23	4B	434	VAL
23	4B	466	LEU
23	4B	538	SER
23	4B	548	VAL
23	4B	580	ASN
23	4B	653	THR
23	4B	658	ARG
24	4C	105	ASP
24	4C	106	SER
24	4C	181	ILE
24	4C	223	ASN
24	4C	262	ASP
24	4C	265	LEU
24	4C	304	SER
24	4C	334	SER
24	4C	378	SER
24	4C	399	CYS
24	4C	403	LEU
24	4C	430	THR
24	4C	451	LEU
24	4C	460	ILE
24	4C	483	SER

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Mol	Chain	Res	Type
24	4C	492	GLU
24	4C	501	SER
25	4D	163	THR
25	4D	168	SER
25	4D	169	VAL
25	4D	214	PHE
25	4D	223	ILE
25	4D	226	SER
25	4D	260	SER
25	4D	361	LYS
25	4D	395	SER
25	4D	402	SER
26	4E	51	SER
26	4E	81	VAL
26	4E	85	SER
26	4E	95	VAL
27	4F	25	VAL
27	4F	63	ILE
27	4F	94	LEU
27	4F	132	SER
27	4F	137	SER
27	4F	138	THR
27	4F	141	ARG
28	4G	30	THR
28	4G	32	SER
28	4G	102	ASP
28	4G	108	LEU
28	4G	205	THR
28	4G	357	THR
28	4G	372	SER
28	4G	743	THR
28	4G	750	SER
28	4G	867	THR
28	4G	915	VAL
28	4G	921	ASN
30	4I	27	VAL
31	4J	265	SER
31	4J	284	GLU
31	4J	288	VAL
31	4J	290	VAL
31	4J	332	SER
31	4J	347	HIS

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Mol	Chain	Res	Type
36	2D	423	SER
36	2D	482	THR
36	2D	506	SER
36	2D	508	SER
36	2D	521	THR
36	2D	522	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	5B	73	HIS
3	5B	83	HIS
3	5B	105	ASN
3	5B	326	HIS
3	5B	357	ASN
3	5B	363	HIS
3	5B	517	HIS
3	5B	545	HIS
3	5B	587	GLN
3	5B	680	HIS
3	5B	1042	GLN
3	5B	1457	HIS
3	5B	1487	HIS
3	5B	1563	HIS
3	5B	1638	ASN
3	5B	1737	ASN
3	5B	1791	HIS
3	5B	1890	GLN
3	5B	1996	ASN
3	5B	2032	GLN
3	5B	2089	HIS
3	5B	2241	ASN
3	5B	2255	HIS
3	5B	2288	HIS
4	5C	280	HIS
4	5C	313	GLN
4	5C	335	ASN
4	5C	502	HIS
4	5C	627	HIS
4	5C	642	HIS
5	5D	715	HIS
5	5D	785	HIS

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Mol	Chain	Res	Type
5	5D	902	ASN
5	5D	911	GLN
5	5D	1002	ASN
5	5D	1288	HIS
5	5D	1515	HIS
5	5D	1553	HIS
5	5D	1655	ASN
5	5D	1667	GLN
5	5D	1690	HIS
5	5D	1733	HIS
5	5D	1784	HIS
5	5D	1896	GLN
5	5D	2003	GLN
23	4B	480	ASN
23	4B	511	HIS
23	4B	515	ASN
24	4C	135	ASN
24	4C	282	HIS
24	4C	322	HIS
24	4C	364	HIS
24	4C	421	HIS
25	4D	177	GLN
25	4D	270	HIS
25	4D	376	ASN
26	4E	17	HIS
26	4E	77	ASN
27	4F	89	HIS
28	4G	173	ASN
28	4G	190	HIS
28	4G	308	HIS
28	4G	368	HIS
28	4G	794	ASN
28	4G	805	GLN
31	4J	261	HIS
31	4J	293	ASN
36	2D	505	HIS
40	2H	804	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	55/144 (38%)	35 (63%)	10 (18%)
14	6A	55/107 (51%)	14 (25%)	2 (3%)
2	5A	114/117 (97%)	30 (26%)	5 (4%)
22	4A	124/145 (85%)	35 (28%)	4 (3%)
33	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	453/701 (64%)	136 (30%)	24 (5%)

All (136) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	C
1	A	11	C
1	A	12	U
1	A	13	U
1	A	15	A
1	A	20	U
1	A	21	U
1	A	22	C
1	A	25	G
1	A	29	A
1	A	30	C
1	A	31	C
1	A	32	C
1	A	33	U
1	A	34	G
1	A	35	U
1	A	36	C
1	A	37	C
1	A	39	U
1	A	41	U
1	A	42	U
1	A	44	U
1	A	46	U
1	A	47	C
1	A	48	C
1	A	103	A
1	A	104	C
1	A	105	C
1	A	106	A

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Mol	Chain	Res	Type
1	A	108	G
1	A	110	G
1	A	111	A
1	A	116	G
2	5A	8	G
2	5A	10	U
2	5A	21	A
2	5A	22	U
2	5A	24	G
2	5A	25	C
2	5A	26	A
2	5A	28	A
2	5A	35	U
2	5A	36	C
2	5A	40	U
2	5A	45	C
2	5A	47	A
2	5A	52	U
2	5A	68	C
2	5A	69	A
2	5A	78	U
2	5A	79	C
2	5A	80	U
2	5A	83	A
2	5A	88	A
2	5A	89	U
2	5A	90	U
2	5A	92	U
2	5A	93	U
2	5A	94	U
2	5A	95	G
2	5A	96	A
2	5A	97	G
2	5A	109	G
14	6A	37	C
14	6A	38	G
14	6A	39	A
14	6A	40	U
14	6A	46	G
14	6A	47	A
14	6A	48	A
14	6A	49	G

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Mol	Chain	Res	Type
14	6A	51	U
14	6A	71	G
14	6A	77	C
14	6A	78	A
14	6A	103	U
14	6A	104	U
22	4A	2	G
22	4A	17	A
22	4A	18	G
22	4A	19	U
22	4A	25	A
22	4A	26	G
22	4A	37	C
22	4A	38	U
22	4A	39	A
22	4A	40	U
22	4A	45	G
22	4A	53	U
22	4A	54	A
22	4A	71	U
22	4A	73	U
22	4A	74	C
22	4A	75	C
22	4A	76	C
22	4A	84	C
22	4A	85	G
22	4A	90	G
22	4A	100	A
22	4A	103	A
22	4A	109	G
22	4A	114	U
22	4A	115	G
22	4A	118	A
22	4A	119	A
22	4A	120	U
22	4A	121	U
22	4A	124	U
22	4A	125	G
22	4A	126	A
22	4A	127	C
22	4A	144	G
33	2A	31	G

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Mol	Chain	Res	Type
33	2A	37	U
33	2A	40	C
33	2A	45	C
33	2A	47	U
33	2A	51	A
33	2A	65	U
33	2A	112	G
33	2A	143	A
33	2A	147	G
33	2A	152	G
33	2A	153	A
33	2A	154	C
33	2A	156	U
33	2A	157	G
33	2A	164	C
33	2A	165	A
33	2A	168	A
33	2A	169	C
33	2A	177	A
33	2A	178	A
33	2A	179	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	21	U
1	A	28	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	C
1	A	40	U
1	A	41	U
1	A	115	U
2	5A	67	A
2	5A	78	U
2	5A	79	C
2	5A	94	U
2	5A	96	A
14	6A	37	C
14	6A	77	C

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Mol	Chain	Res	Type
22	4A	18	G
22	4A	38	U
22	4A	99	C
22	4A	114	U
33	2A	156	U
33	2A	164	C
33	2A	168	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
47	GTP	5C	1500	48	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
46	IHP	5B	3000	-	36,36,36	0.73	0	60,60,60	1.12	2 (3%)

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
47	GTP	5C	1500	48	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	IHP	5B	3000	-	-	3/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	5C	1500	GTP	C2-N3	2.08	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5C	1500	GTP	C5-C4-N3	-4.92	120.56	128.39
47	5C	1500	GTP	C2-N3-C4	4.64	120.30	112.30
47	5C	1500	GTP	N9-C4-N3	3.04	132.04	125.95
47	5C	1500	GTP	C2-N1-C6	-2.93	119.80	125.11
47	5C	1500	GTP	N9-C8-N7	-2.67	108.45	113.40
47	5C	1500	GTP	C5-C6-N1	2.54	119.72	113.25
47	5C	1500	GTP	C8-N7-C5	2.50	108.72	104.26
47	5C	1500	GTP	O6-C6-C5	-2.47	120.01	126.53
46	5B	3000	IHP	C6-C5-C4	2.07	114.96	110.43
46	5B	3000	IHP	C5-C4-C3	2.00	114.82	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

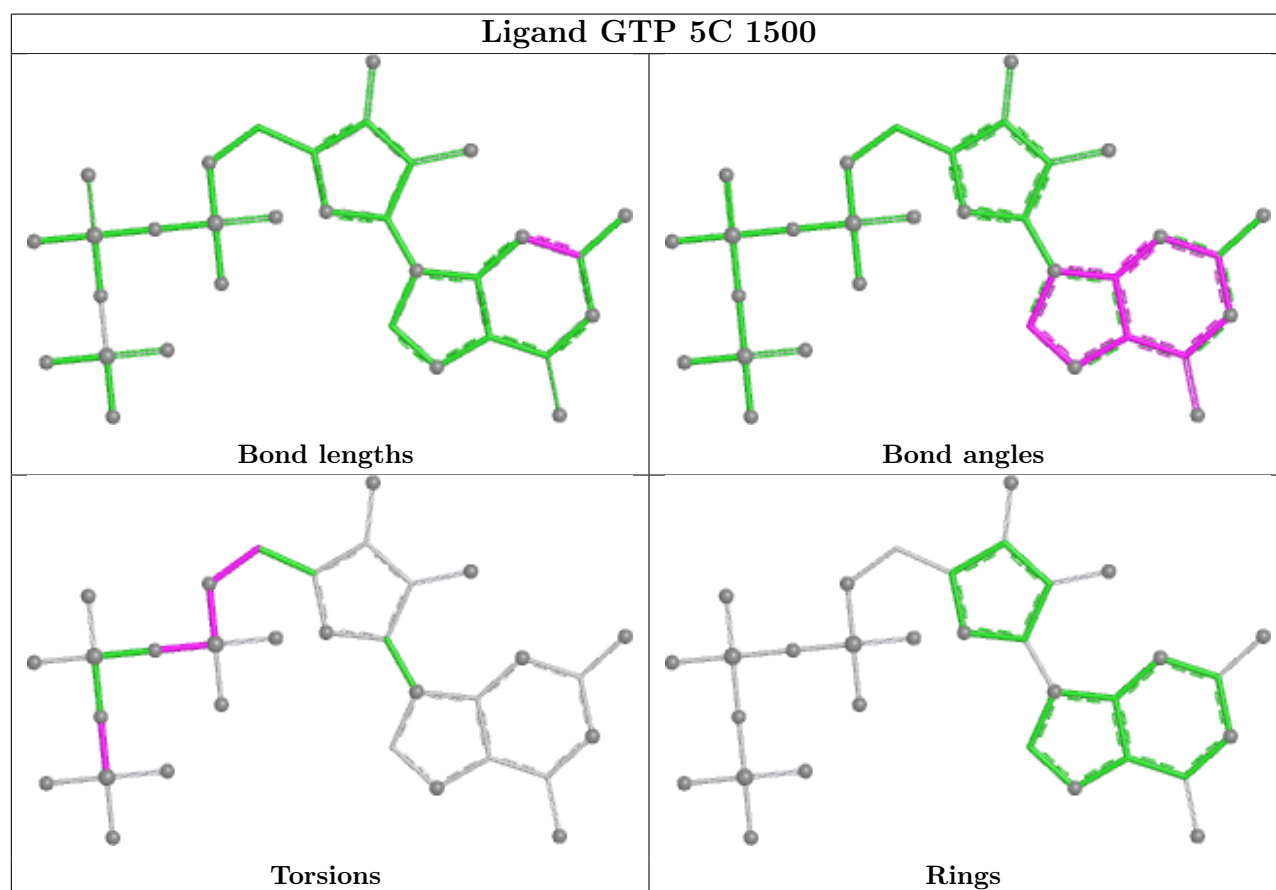
Mol	Chain	Res	Type	Atoms
47	5C	1500	GTP	PB-O3B-PG-O3G
47	5C	1500	GTP	C5'-O5'-PA-O3A
47	5C	1500	GTP	C5'-O5'-PA-O1A
47	5C	1500	GTP	PB-O3A-PA-O5'
47	5C	1500	GTP	C5'-O5'-PA-O2A
46	5B	3000	IHP	C2-O12-P2-O42
46	5B	3000	IHP	C4-O14-P4-O44
46	5B	3000	IHP	C5-O15-P5-O25
47	5C	1500	GTP	C4'-C5'-O5'-PA

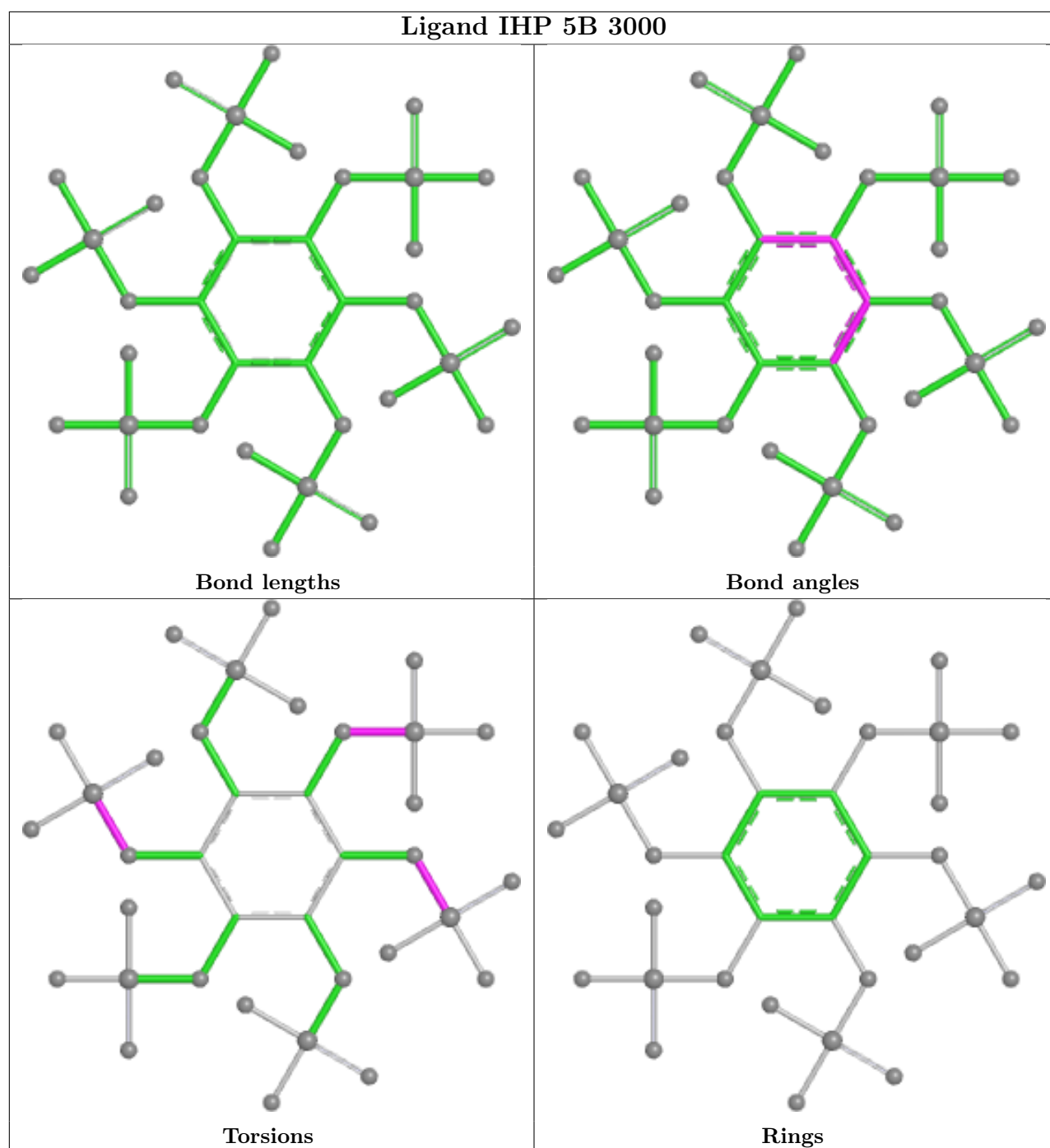
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	5B	3000	IHP	1	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.

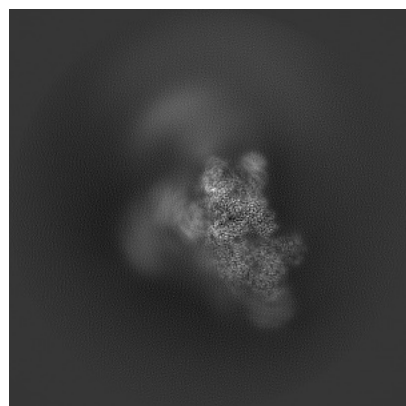
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34508. These allow visual inspection of the internal detail of the map and identification of artifacts.

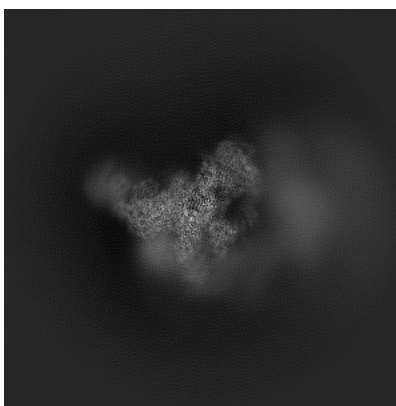
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

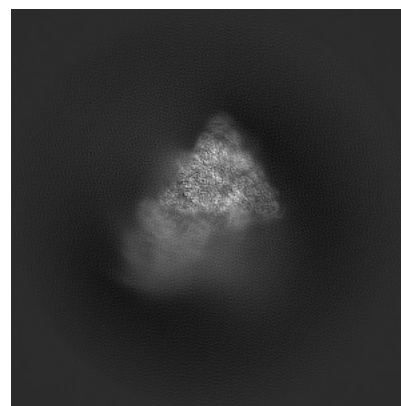
6.1.1 Primary map



X

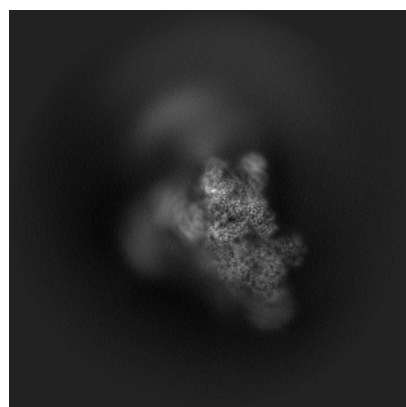


Y

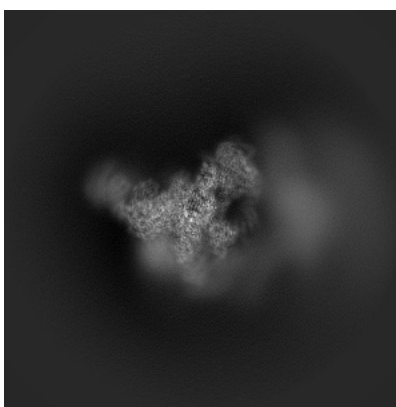


Z

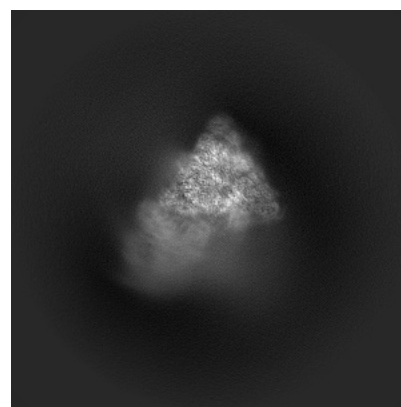
6.1.2 Raw map



X



Y

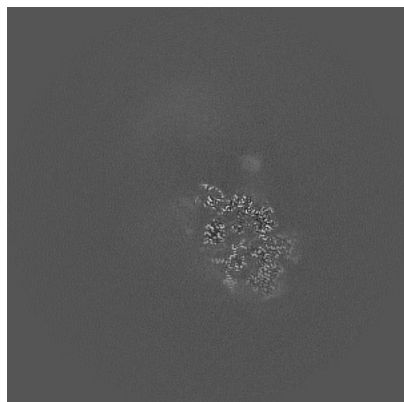


Z

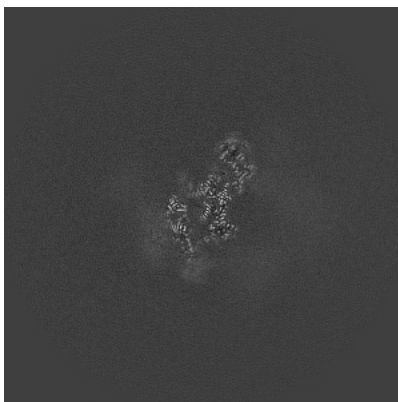
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

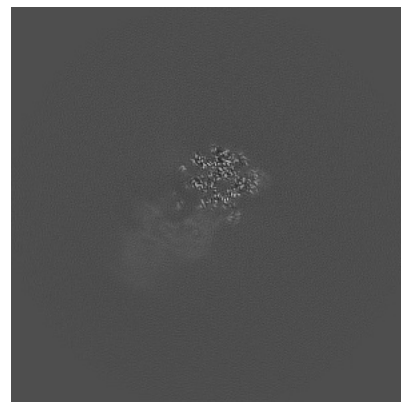
6.2.1 Primary map



X Index: 256

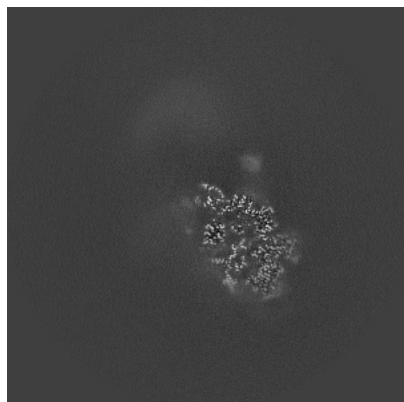


Y Index: 256

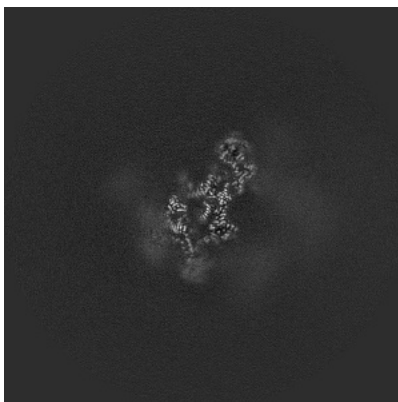


Z Index: 256

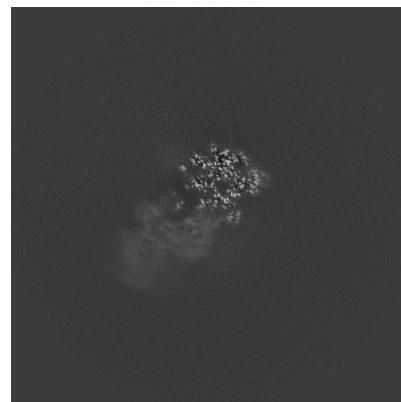
6.2.2 Raw map



X Index: 256



Y Index: 256

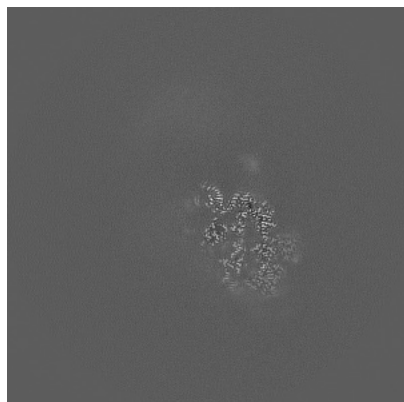


Z Index: 256

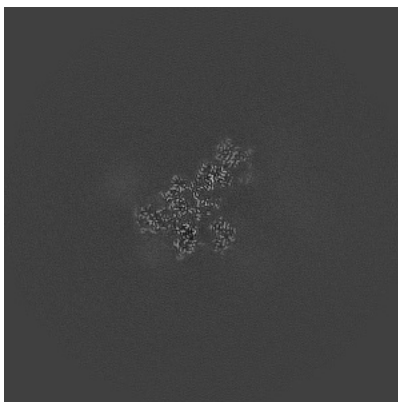
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

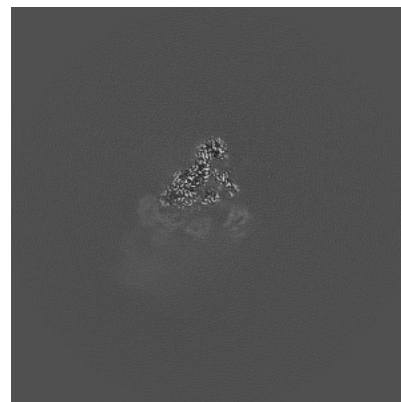
6.3.1 Primary map



X Index: 259

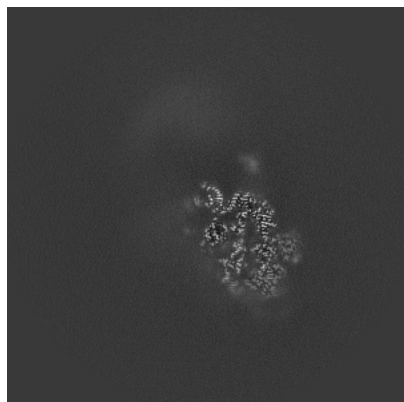


Y Index: 274

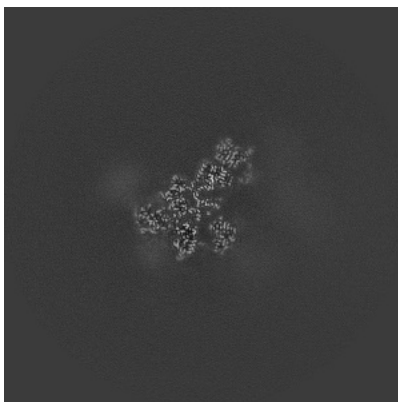


Z Index: 234

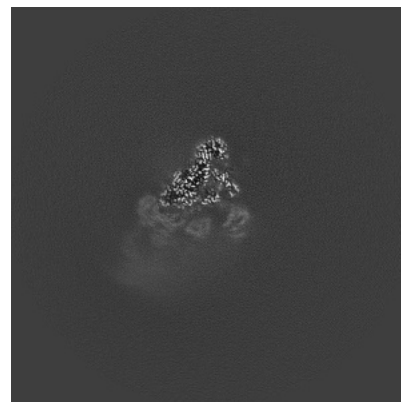
6.3.2 Raw map



X Index: 259



Y Index: 274

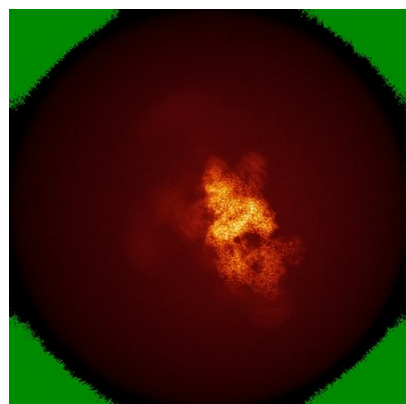


Z Index: 234

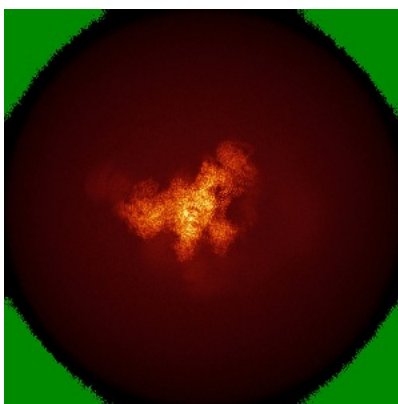
The images above show the largest variance slices of the map in three orthogonal directions.

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

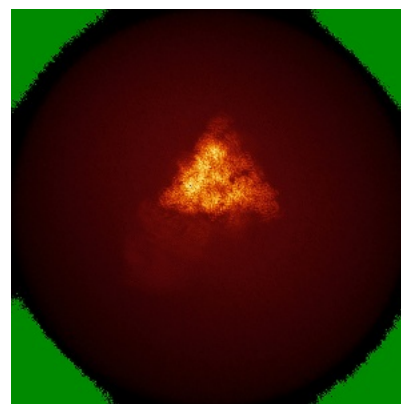
6.4.1 Primary map



X

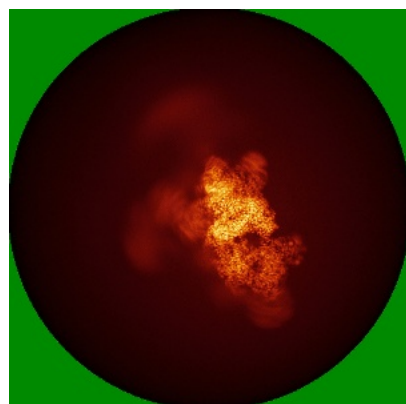


Y

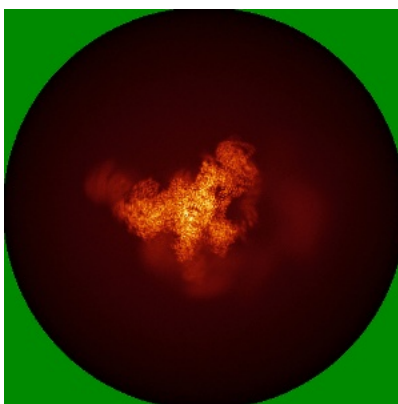


Z

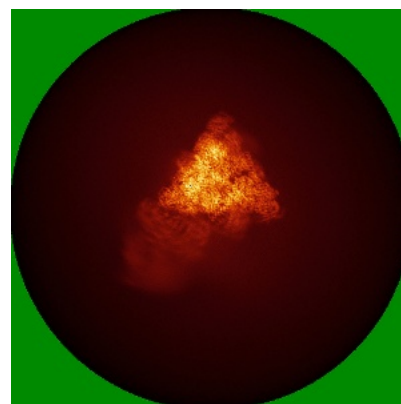
6.4.2 Raw map



X



Y

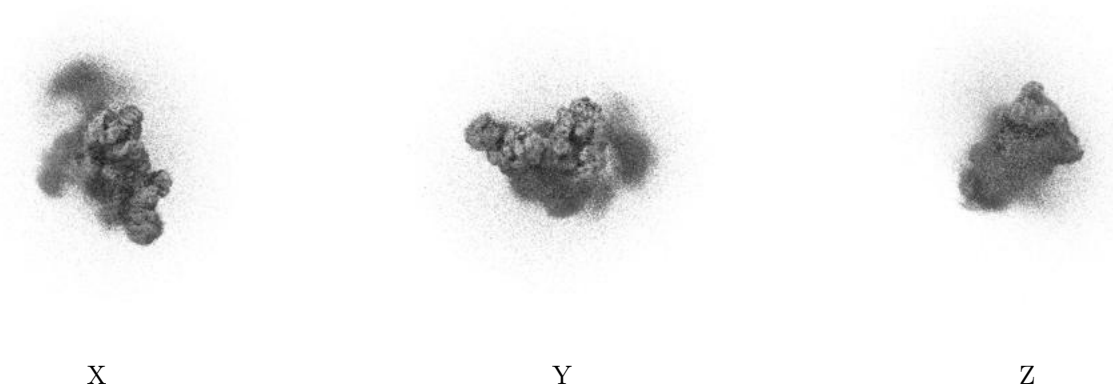


Z

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.

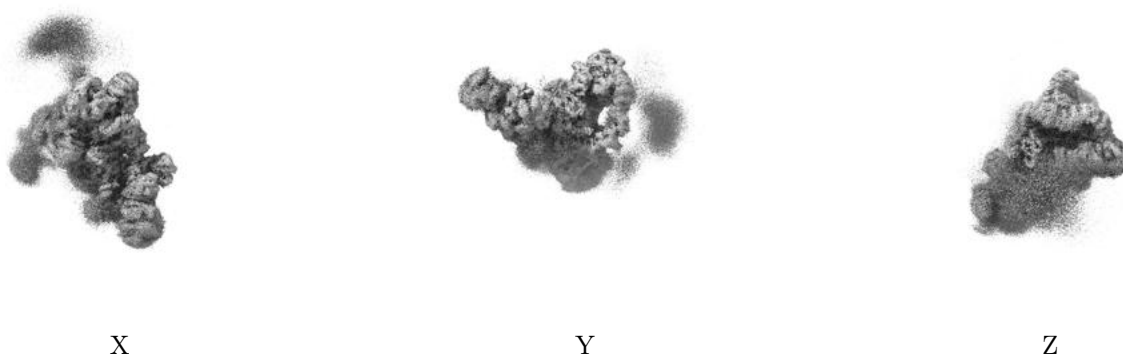
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

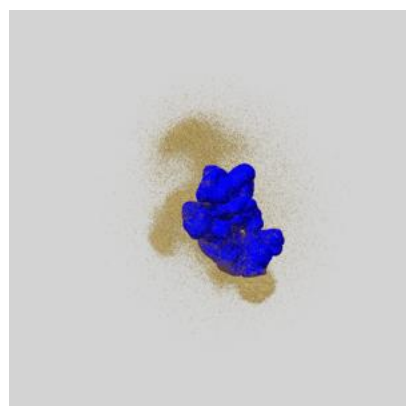
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

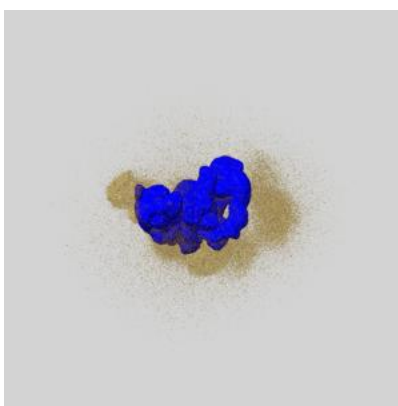
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

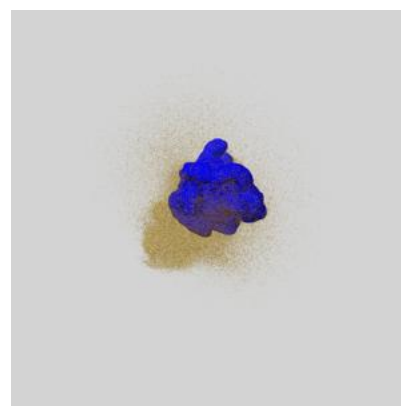
6.6.1 emd_34508_msk_1.map [i](#)



X



Y

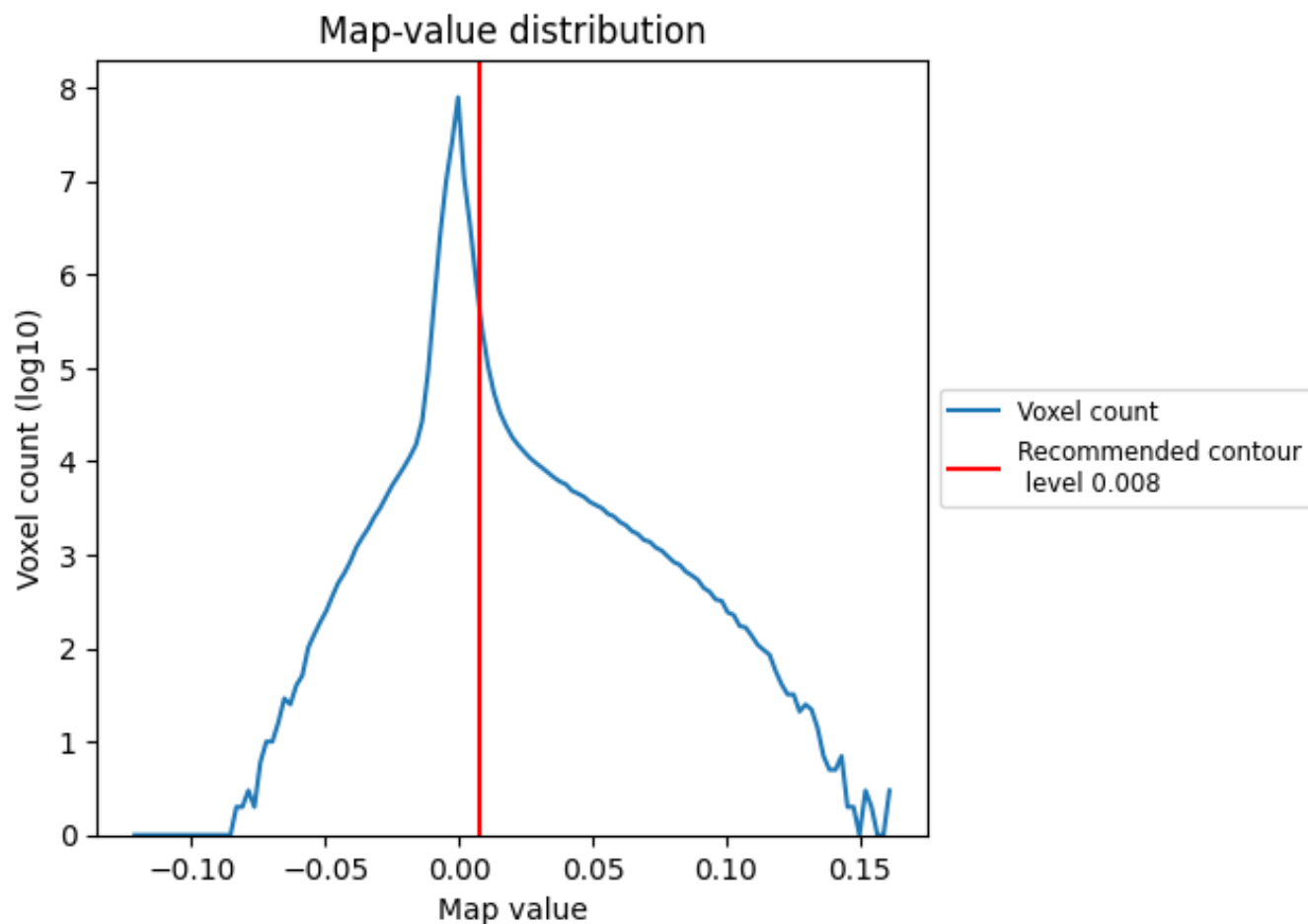


Z

7 Map analysis [i](#)

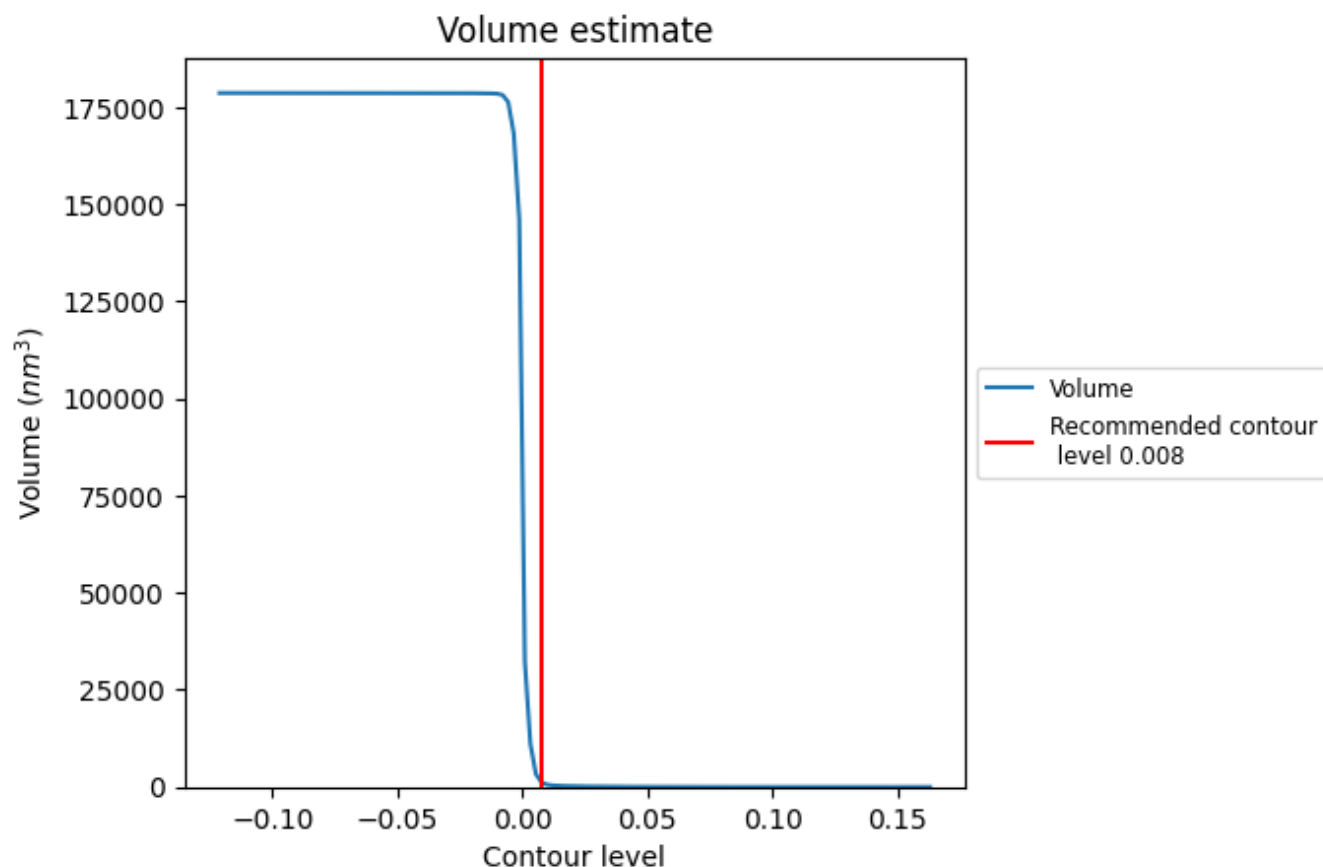
This section contains the results of statistical analysis of the map.

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.

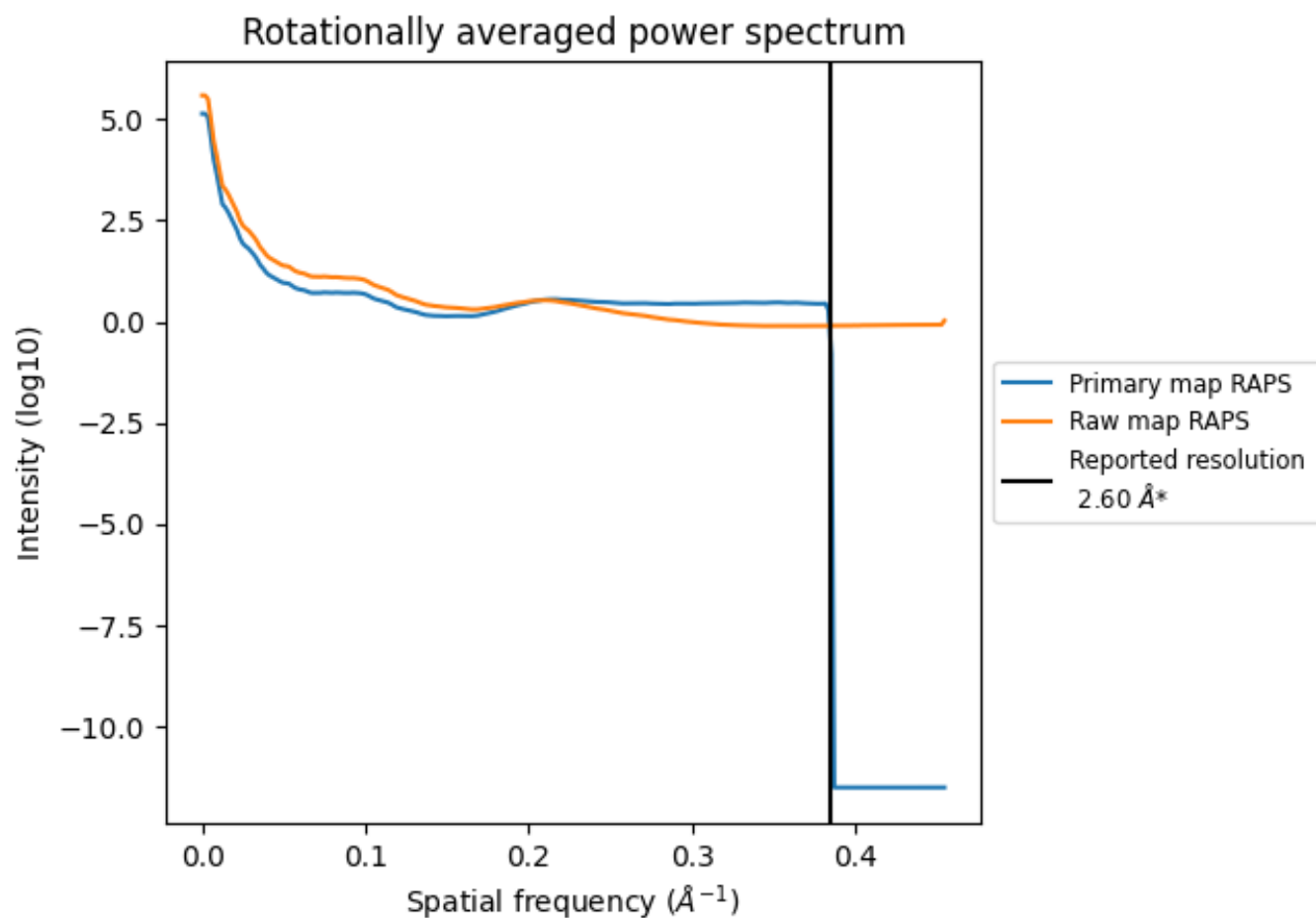
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1104 nm^3 ; this corresponds to an approximate mass of 997 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 ⓘ

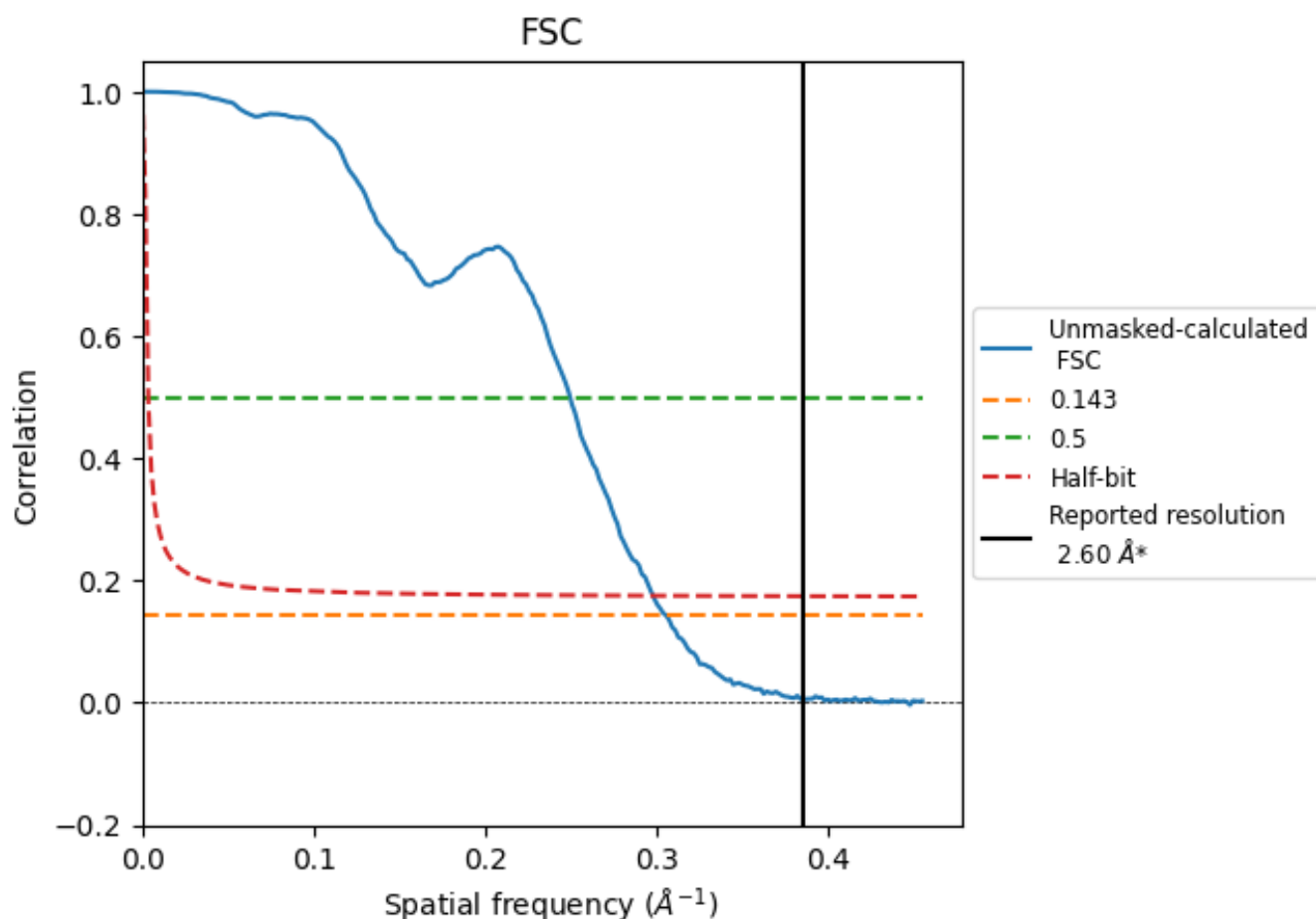


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

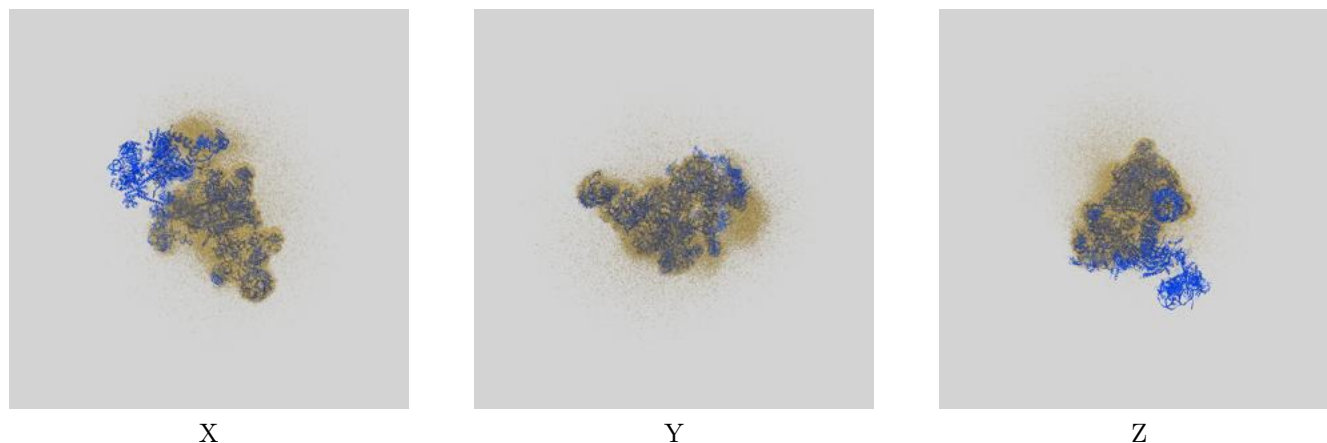
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.01	3.36

*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 3.28 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34508 and PDB model 8H6L. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



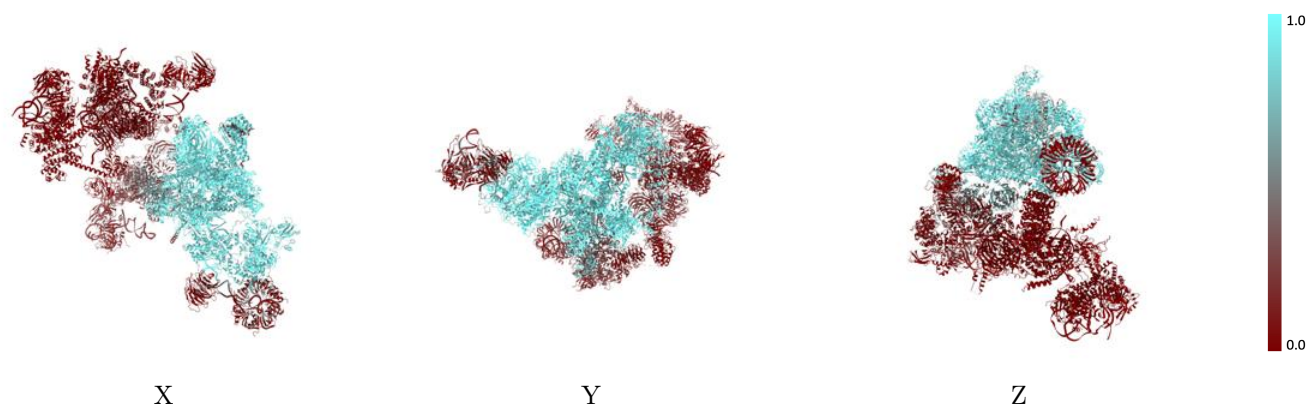
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



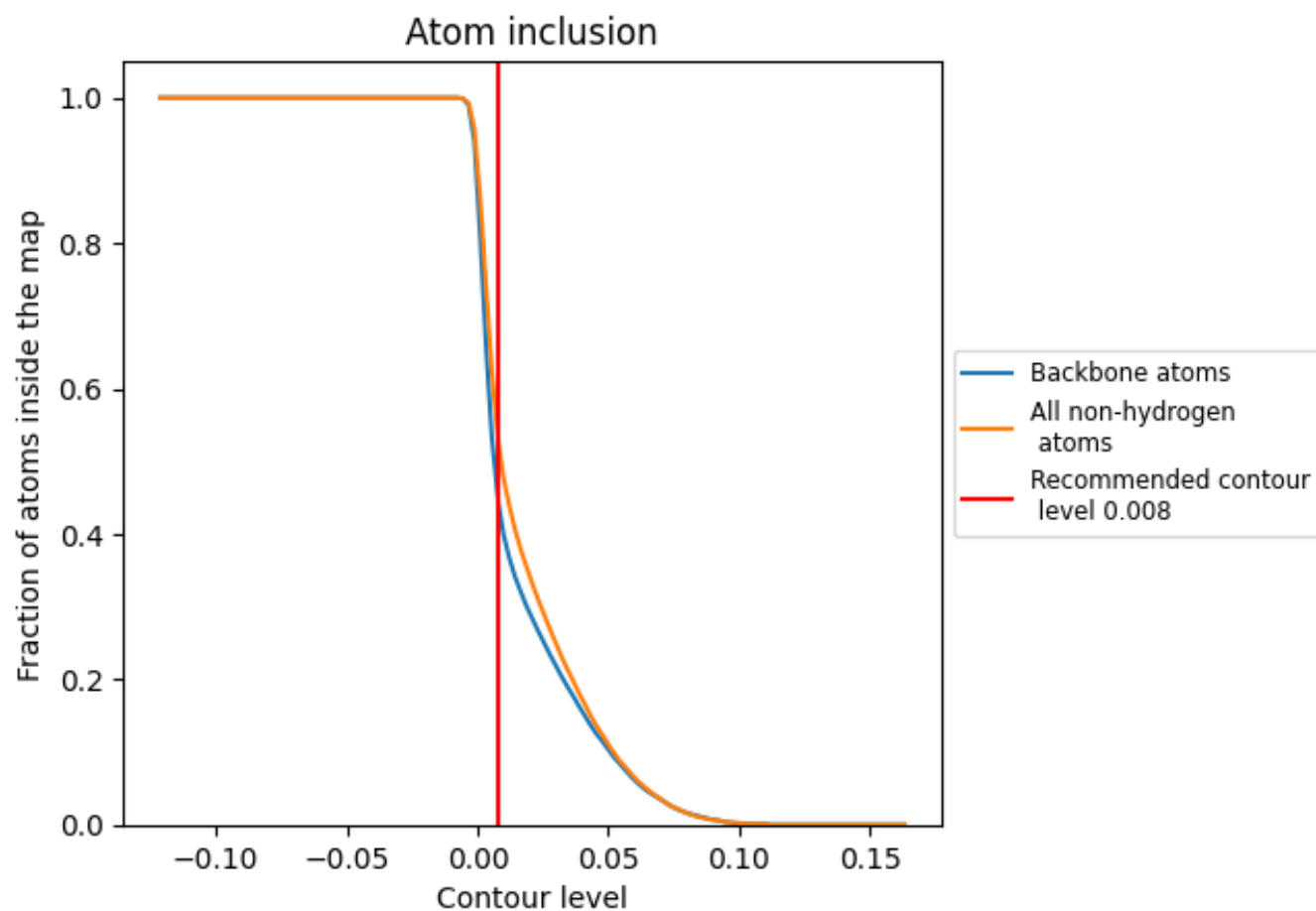
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 53% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.2830
2A	 0.0030	 0.0080
2B	 0.0000	 0.0230
2C	 0.0000	 0.0180
2D	 0.5430	 0.3300
2E	 0.0000	 0.0370
2F	 0.0000	 0.0030
2G	 0.0050	 0.0040
2H	 0.2340	 0.1520
2I	 0.0010	 0.0030
2J	 0.0030	 -0.0330
2K	 0.0000	 0.0130
2L	 0.0000	 -0.0350
2M	 0.0110	 0.0050
2a	 0.0000	 0.0390
2b	 0.0000	 -0.0010
2c	 0.0000	 -0.0030
2d	 0.0000	 0.0150
2e	 0.0000	 -0.0110
2f	 0.0000	 0.0220
2g	 0.0000	 -0.0050
4A	 0.5380	 0.3160
4B	 0.9470	 0.5370
4C	 0.9600	 0.5400
4D	 0.9580	 0.5830
4E	 0.9860	 0.6400
4F	 0.9950	 0.6570
4G	 0.8880	 0.4510
4H	 0.9260	 0.3380
4I	 0.7670	 0.3290
4J	 0.9200	 0.5340
4Z	 0.0570	 -0.0000
4a	 0.0190	 -0.0450
4b	 0.0240	 -0.0130
4c	 0.0730	 -0.0240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
4d	 0.0580	 -0.0190
4e	 0.0450	 -0.0350
4f	 0.0600	 0.0000
4g	 0.0620	 0.0350
5A	 0.6410	 0.3220
5B	 0.9230	 0.5570
5C	 0.9400	 0.5080
5D	 0.2680	 0.0360
5E	 0.0720	 0.0020
5a	 0.2230	 -0.0220
5b	 0.1550	 -0.0160
5c	 0.1470	 0.0070
5d	 0.1350	 0.0090
5e	 0.1610	 -0.0140
5f	 0.1980	 -0.0280
5g	 0.2570	 -0.0050
6A	 0.7150	 0.4220
6a	 0.0060	 0.0080
6b	 0.0030	 -0.0140
6c	 0.0030	 0.0150
6d	 0.0070	 0.0160
6e	 0.0210	 0.0620
6f	 0.0040	 0.0110
6g	 0.0080	 -0.0300
A	 0.2650	 0.1630