



Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 09:07 pm BST

PDB ID : 9FMD
EMDB ID : EMD-4525
Title : Integrative model of the human post-catalytic spliceosome (P-complex)
Authors : Rothe, P.; Plaschka, C.; Vorlaender, M.K.
Deposited on : 2024-06-05
Resolution : 3.30 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

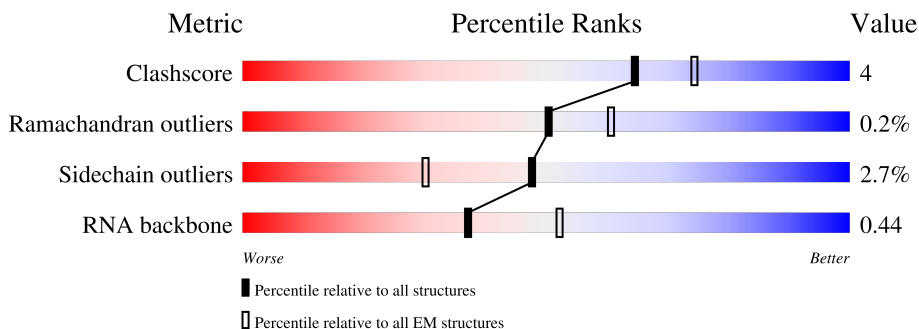
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



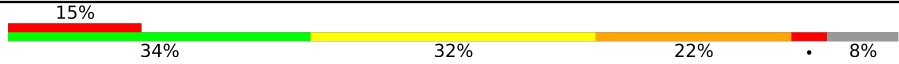
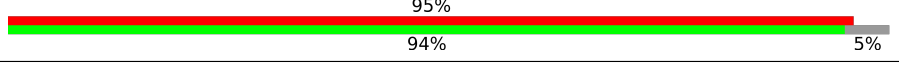
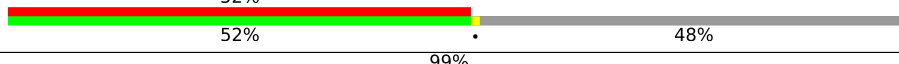
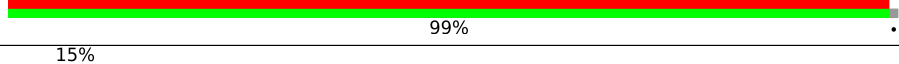

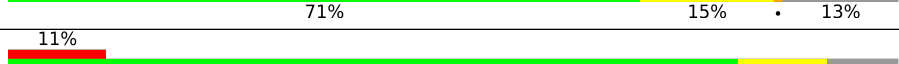

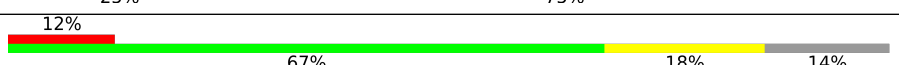


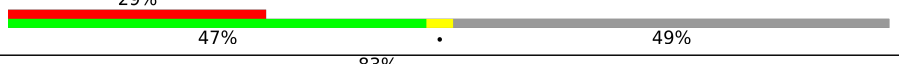



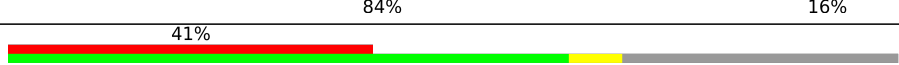




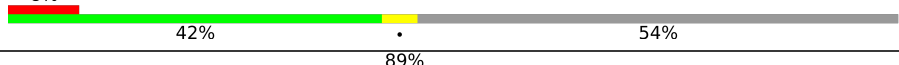
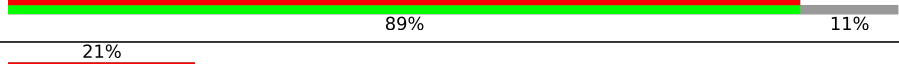




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	184	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">34%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">59%</div> <div style="text-align: center;">8%</div> <div style="text-align: center;">33%</div> </div>
2	2	187	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">36%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">31%</div> <div style="text-align: center;">26%</div> <div style="text-align: center;">6%</div> <div style="text-align: center;">36%</div> </div>
3	3	476	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">17%</div> <div style="text-align: center;">83%</div> </div>
4	32	112	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">9%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">44%</div> <div style="text-align: center;">9%</div> <div style="text-align: center;">46%</div> </div>
5	5	116	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">28%</div> <div style="text-align: center;">34%</div> <div style="text-align: center;">14%</div> <div style="text-align: center;">21%</div> </div>
6	50	339	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">62%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">61%</div> <div style="text-align: center;">37%</div> </div>
7	56	222	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">45%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">45%</div> <div style="text-align: center;">55%</div> </div>

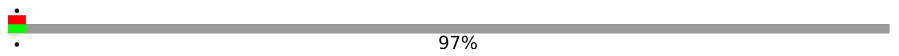
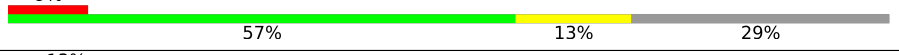
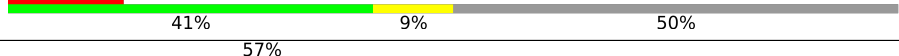
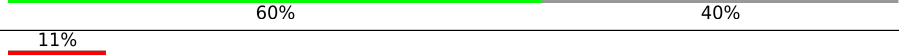
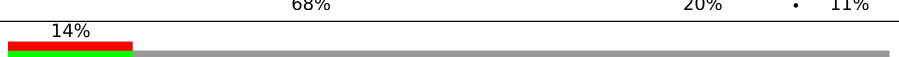
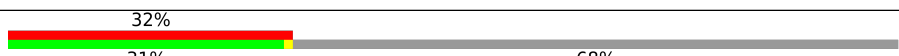








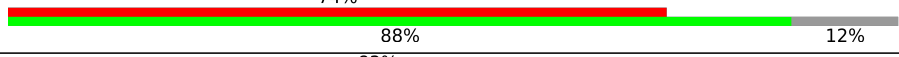


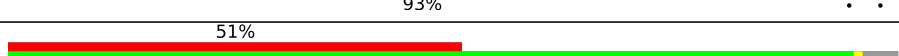

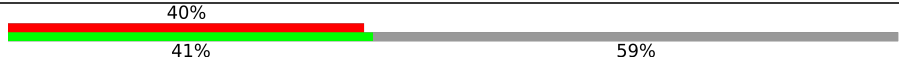





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Mol	Chain	Length	Quality of chain
8	6	106	
9	7	411	
10	8	174	
11	9	146	
12	A	2335	
13	B	2136	
14	C	972	
15	D	285	
16	E	357	
17	EX	14	
18	F	758	
19	H	908	
20	I	855	
21	IN	113	
22	J	848	
23	K	225	
24	L	802	
25	M	243	
26	N	144	
27	NO	301	
28	O	420	
29	P	229	
30	Q	1485	
31	R	536	
32	S	166	







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Mol	Chain	Length	Quality of chain
33	SR	2752	
34	T	514	
35	U	586	
36	V	1220	
37	W	579	
38	X	451	
39	Z	166	
40	a	126	
40	h	126	
41	b	240	
41	i	240	
42	c	119	
42	j	119	
43	d	118	
43	k	118	
44	e	92	
44	l	92	
45	f	86	
45	m	86	
46	g	76	
46	n	76	
47	o	255	
48	p	225	
49	q	504	
49	r	504	

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Mol	Chain	Length	Quality of chain
49	s	504	
49	t	504	
50	w	646	
51	x	289	
52	y	301	
53	z	415	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 120526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	123	1013	635	193	180	5	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	120	2535	1135	428	852	120	0	0

- Molecule 3 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	82	408	244	82	82	0	0

- Molecule 4 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	32	60	504	314	96	92	2	0	0

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	92	1936	867	322	655	92	0	0

- Molecule 6 is a protein called Protein FAM50A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
6	50	212	1053	629	212	212	0	0

- Molecule 7 is a protein called STING ER exit protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	56	101	498	296	101	101	0	0

- Molecule 8 is a DNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	6	97	2075	928	381	669	97	0	0

- Molecule 9 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	7	390	1928	1147	390	391	0	0

- Molecule 10 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	8	91	445	263	91	91	0	0

- Molecule 11 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	9	144	712	423	144	145	0	0

- Molecule 12 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	2250	17802	11405	3151	3176	70	0	0

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	1864	15004	9583	2569	2775	77	0	0

- Molecule 14 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	899	7116	4553	1184	1345	34	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	D	72	358	214	72	72	0	0

- Molecule 16 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	306	2394	1501	422	457	14	0	0

- Molecule 17 is a RNA chain called Exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	EX	14	296	132	52	98	14	0	0

- Molecule 18 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	122	1085	712	197	174	2	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	459	2932	1827	533	560	12	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	I	727	3610	2156	727	727	0	0

- Molecule 21 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	IN	42	Total	C	N	O	P	0	0
			893	400	158	293	42		

- Molecule 22 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	J	602	Total	C	N	O	0	0
			2998	1794	602	602		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	K	189	Total	C	N	O	0	0
			941	563	189	189		

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	555	Total	C	N	O	S	0	0
			3642	2233	706	695	8		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	M	224	Total	C	N	O	0	0
			1115	666	224	225		

- Molecule 26 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	144	Total	C	N	O	S	0	0
			1189	748	218	211	12		

- Molecule 27 is a protein called Nitric oxide synthase-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	NO	174	Total	C	N	O	0	0
			864	516	174	174		

- Molecule 28 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	289	2318	1455	416	428	19	0	0

- Molecule 29 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	P	106	889	544	174	169	2	0	0

- Molecule 30 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	Q	1322	6554	3910	1322	1322	0	0

- Molecule 31 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
31	R	328	2618	1634	479	489	2	14	0	0

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	164	1271	810	220	234	7	0	0

- Molecule 33 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	SR	70	412	251	80	80	1	0	0

- Molecule 34 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	T	363	2881	1820	525	526	10	0	0

- Molecule 35 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	U	295	Total	C	N	O	S	0	0
			2425	1525	431	461	8		

- Molecule 36 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	V	733	Total	C	N	O	0	0
			3629	2163	733	733		

- Molecule 37 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	513	Total	C	N	O	S	0	0
			4158	2643	719	772	24		

- Molecule 38 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	X	66	Total	C	N	O	0	0
			328	196	66	66		

- Molecule 39 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	84	Total	C	N	O	S	0	0
			658	412	116	124	6		
40	h	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	87	Total	C	N	O	S	0	0
			654	412	120	115	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	82	Total	C	N	O	S	0	0
			664	419	121	117	7		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	c	80	Total	C	N	O	S	0	0
			634	404	111	115	4		
42	j	80	Total	C	N	O	S	0	0
			634	404	111	115	4		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	89	Total	C	N	O	S	0	0
			723	454	133	131	5		
43	k	95	Total	C	N	O	S	0	0
			774	486	141	142	5		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	79	Total	C	N	O	S	0	0
			651	413	115	118	5		
44	l	81	Total	C	N	O	S	0	0
			669	424	119	121	5		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
45	m	72	Total	C	N	O	S	0	0
			562	364	93	100	5		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		
46	n	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

- Molecule 47 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	162	1282	820	219	240	3	0	0

- Molecule 48 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	p	92	745	480	130	130	5	0	0

- Molecule 49 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	q	103	514	308	103	103	0	0
49	r	119	594	356	119	119	0	0
49	s	132	659	395	132	132	0	0
49	t	103	514	308	103	103	0	0

- Molecule 50 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	538	2655	1578	538	539	0	0

- Molecule 51 is a protein called Splicing factor C9orf78.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	x	128	636	379	128	129	0	0

- Molecule 52 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	y	79	318	160	79	79	0	0

- Molecule 53 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	z	70	430	259	83	86	2	0	0

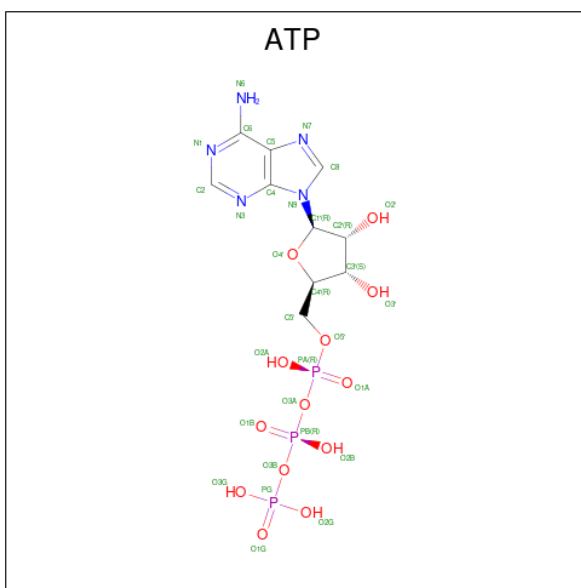
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	6	5	5	5	0
54	7	1	1	1	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
55	6	1	1	1	0

- Molecule 56 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



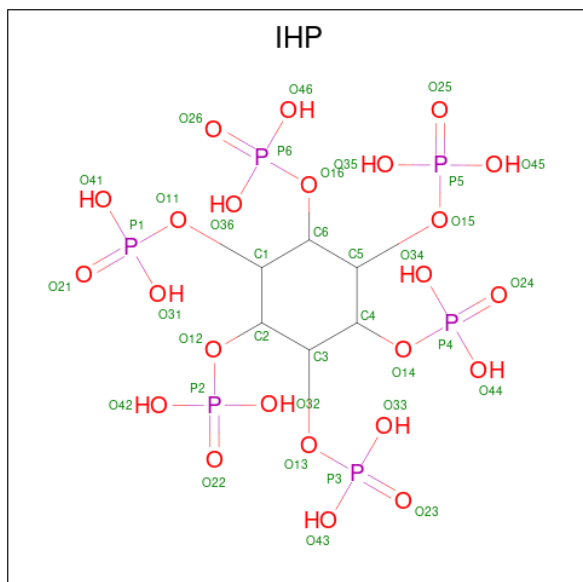


Mol	Chain	Residues	Atoms					AltConf
57	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

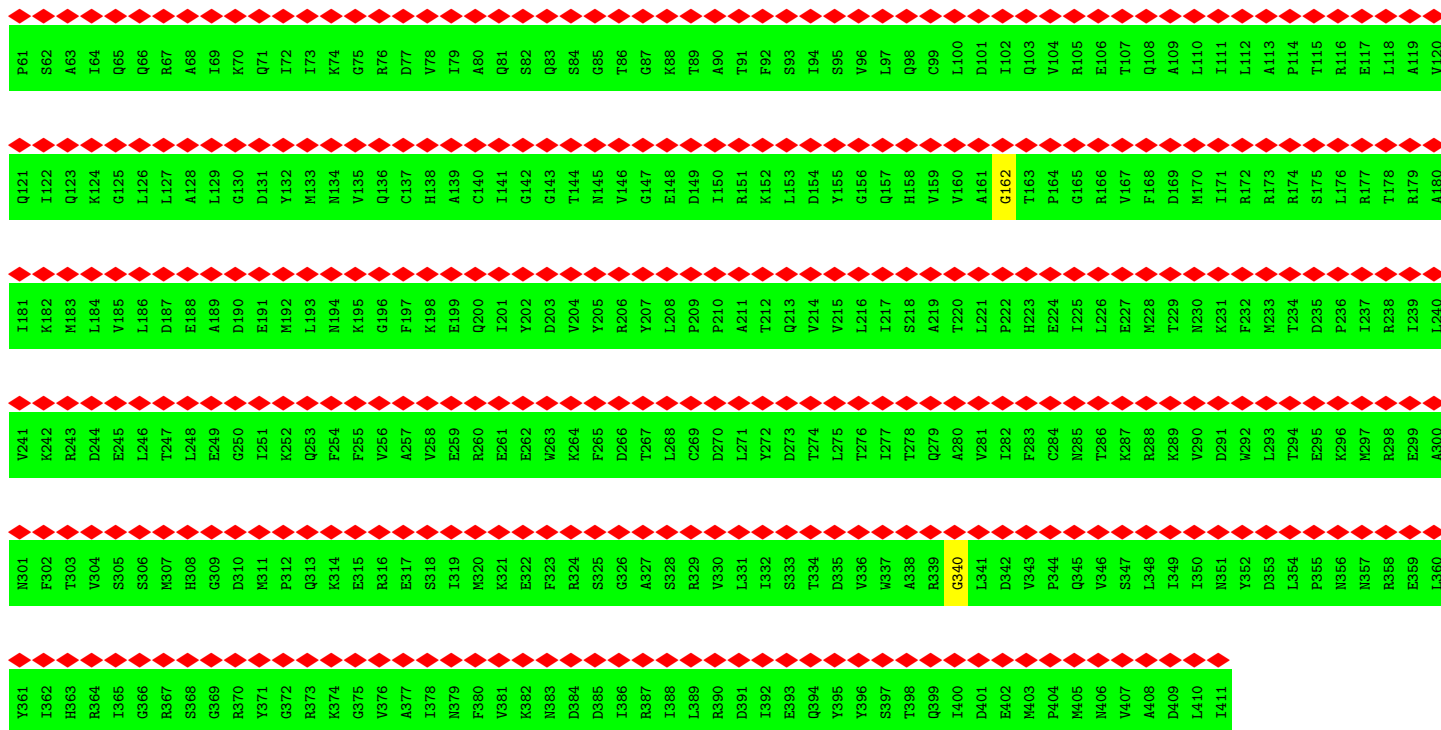
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	N	3	Total	Zn	0
			3	3	
58	O	3	Total	Zn	0
			3	3	

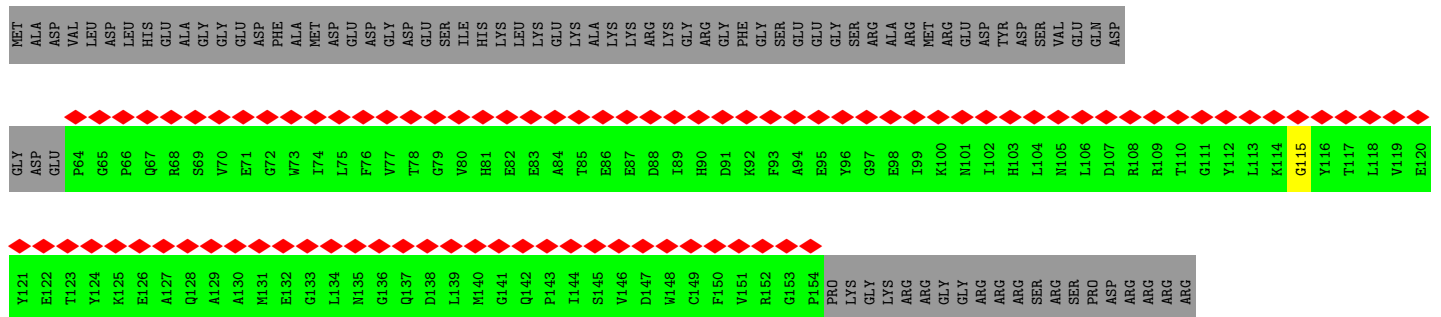
- Molecule 59 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



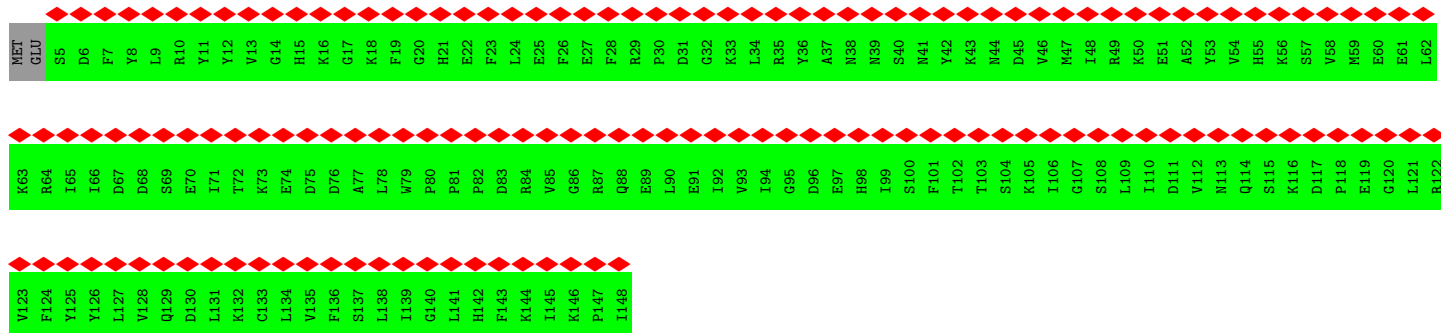
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	U	1	36	6	24	6	0



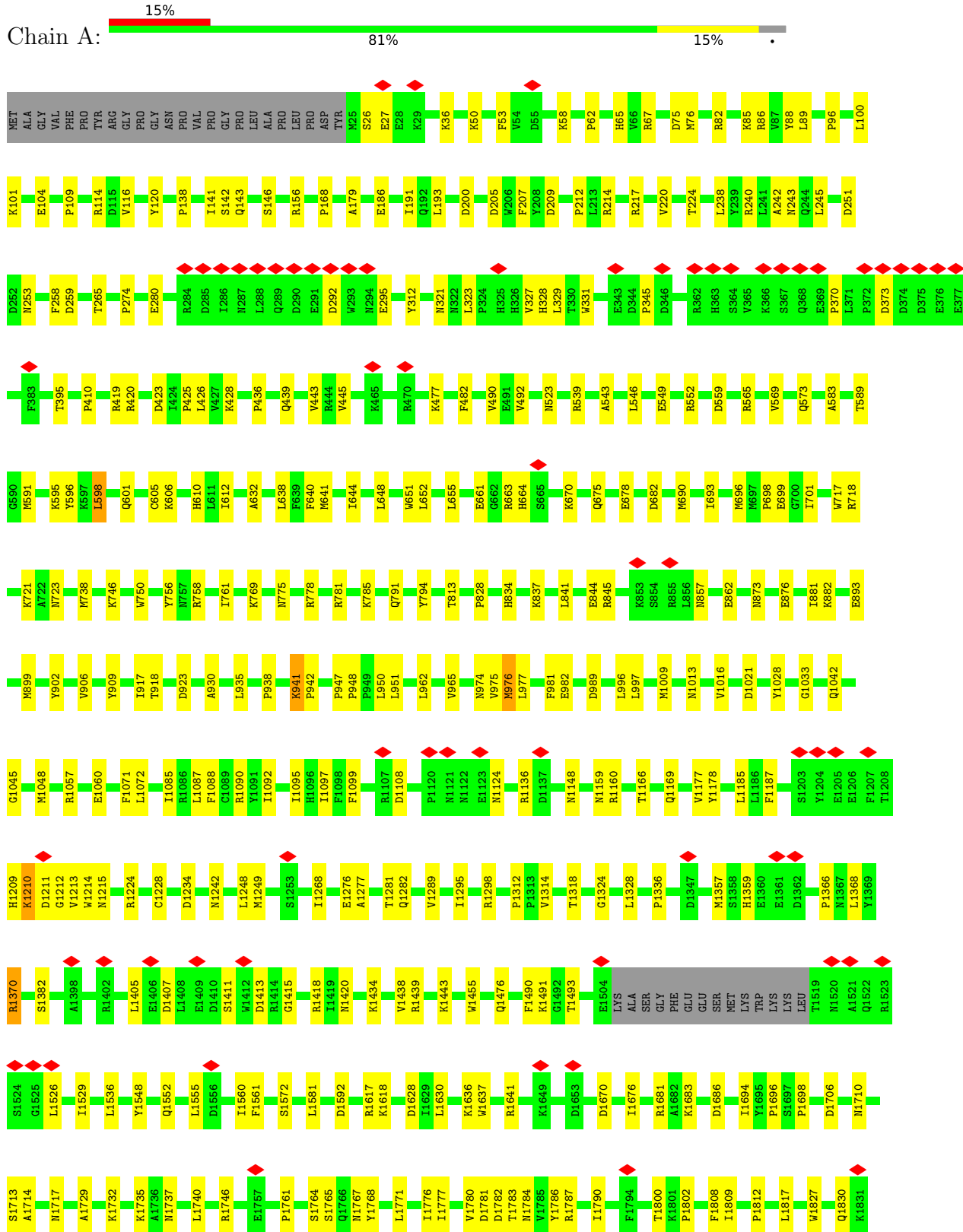
• Molecule 10: RNA-binding protein 8A



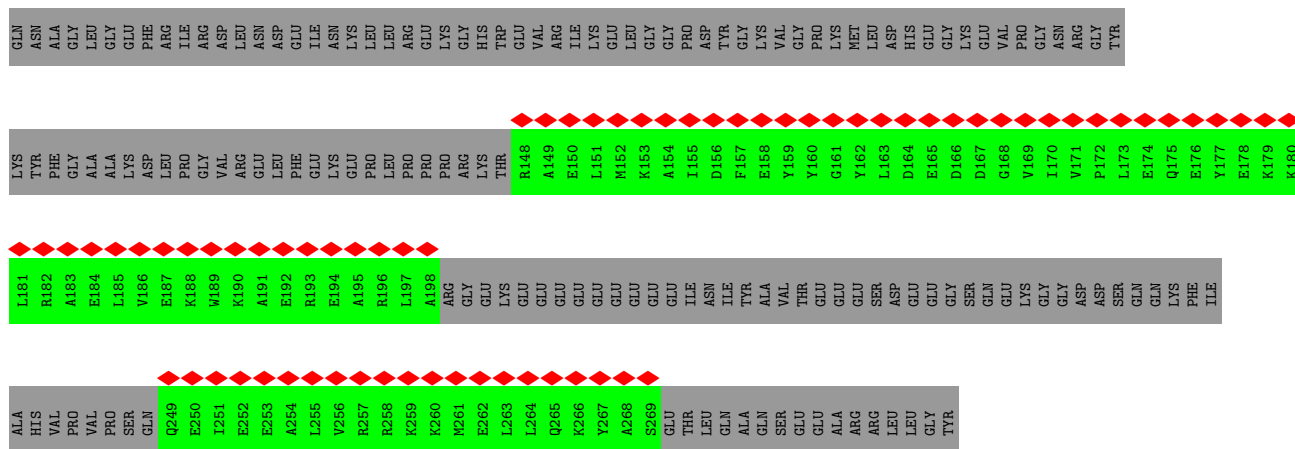
• Molecule 11: Protein mago nashi homolog



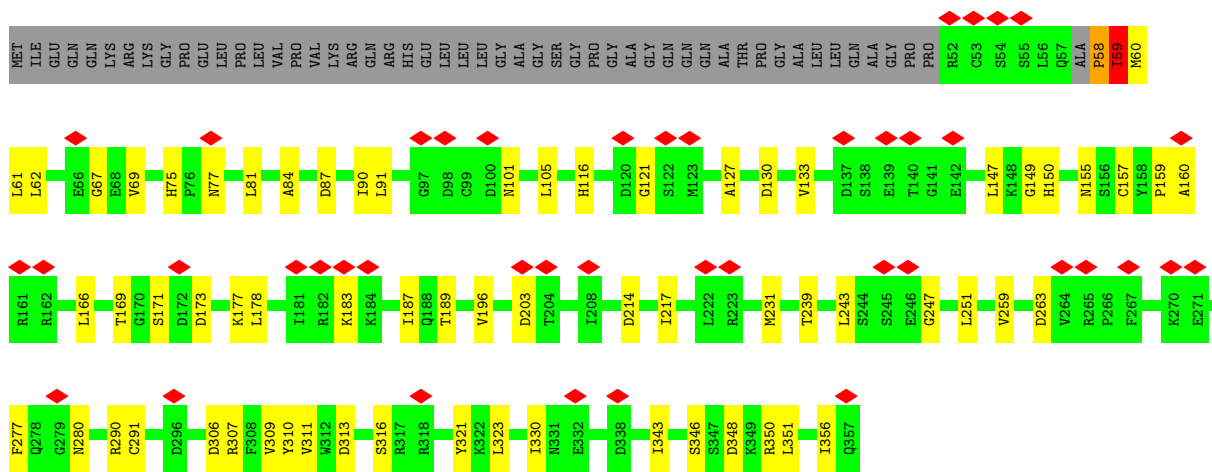
• Molecule 12: Pre-mRNA-processing-splicing factor 8



R1861	H1862	H1863	E1864	D1865	N1866	L1867	L1868	Q1869	Q1870	L1871	A1872	Q1873	K1874	V1875	P1876	H1877	K1878	L1879	N1880	M1881	P1882	K1883	F1884	D1885	N1886	P1887	H1888	V1889	K1890	T1891	N1892	L1893	L1894	L1895	Q1896	A1897	H1898	L1899	S1900	R1901	M1902	Q1903	L1904	S1905	A1906	E1907	L1908	Q1909	S1910	D1911	T1912	E1913	E1914	Y1915	L1916	S1917	K1918	A1919	I1920																																																											
C1801	I1802	S1803	I1804	E1805	D1806	E1807	M1808	L1809	V1810	A1811	P1812	L1813	M1814	L1815	G1816	M1817	L1818	A1819	Y1820	Y1821	Y1822	Y1823	I1824	M1825	D1826	T1827	L1828	I1829	E1830	L1831	F1832	S1833	M1834	S1835	L1836	M1837	A1838	K1839	T1840	K1841	V1842	R1843	G1844	L1845	I1846	E1847	L1848	I1849	S1850	M1851	A1852	E1853	E1854	Y1855	E1856	M1857	L1858	P1859	I1860																																																											
V1741	T1742	K1743	T1744	I1745	E1746	M1747	K1748	T1749	D1750	A1751	V1752	D1753	Y1754	L1755	T1756	M1757	T1758	F1759	L1760	Y1761	R1762	R1763	M1764	T1765	T1766	M1767	P1768	M1769	Y1770	Y1771	N1772	L1773	Q1774	G1775	I1776	S1777	H1778	R1779	H1780	L1781	V1782	D1783	H1784	L1785	V1786	E1787	L1788	V1789	E1790	Q1791	L1792	L1793	S1794	D1795	L1796	E1797	Q1798	S1799	K1800																																																											
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H1621	E1622	G1623	L1624	P1625	M1626	E1627	E1628	R1629	M1630	L1631	E1632	Q1633	L1634	L1635	F1636	S1637	M1638	G1639	A1640	I1641	Q1642	V1643	V1644	V1645	S1646	R1647	S1648	L1649	M1650	C1651	V1652	G1653	F1654	M1655	V1656	A1657	H1658	H1659	L1660	V1661	I1662	I1663	M1664	D1665	L1666	Q1667	Y1668	Y1669	M1670	E1671	K1672	L1673	H1674	A1675	V1676	V1677	Y1678	Y1679	P1680																																																											
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V1561	F1562	V1563	P1564	S1565	R1566	K1567	Q1568	T1569	R1570	L1571	T1572	A1573	I1574	D1575	I1576	L1577	T1578	T1579	C1580	A1581	A1582	D1583	I1584	Q1585	R1586	Q1587	R1588	F1589	L1590	H1591	C1592	T1593	S1594	E1595	K1596	D1596	L1597	I1598	P1599	L1600	L1601	E1602	K1603	L1604	S1605	D1606	S1607	T1608	L1609	K1610	E1611	T1612	L1613	L1614	M1615	G1616	V1617	G1618	Y1619	L1620																																																										
Q1441	R1442	K1443	M1444	L1445	Q1446	M1447	I1448	M1449	L1450	F1451	V1452	V1453	E1454	E1455	V1456	H1457	L1458	I1459	G1460	G1461	M1462	G1463	G1464	V1465	V1466	L1467	E1468	V1469	C1471	S1472	R1473	M1474	R1475	V1476	I1477	S1478	S1479	Q1480	I1481	E1482	R1483	P1484	I1485	R1486	I1487	V1488	L1489	L1490	S1491	S1492	S1493	I1494	S1495	N1496	A1497	R1498	D1499	V1500																																																												
P1381	M1382	E1383	A1384	L1385	A1386	E1387	Q1388	V1389	M1390	M1391	D1392	M1393	Y1394	E1395	K1396	F1397	Q1398	D1399	R1400	L1401	M1402	K1403	K1404	V1405	V1406	L1407	L1408	T1409	G1410	E1411	T1412	S1413	T1414	D1415	L1416	K1417	L1418	L1419	G1420	K1421	G1422	M1423	I1424	I1425	I1426	S1427	T1428	P1429	E1430	K1431	W1432	D1433	I1434	L1435	A1436	R1437	R1438	W1439	K1440																																																											
Y1321	Q1322	D1323	K1324	F1325	P1326	F1327	F1328	M1329	P1330	I1331	Q1332	T1333	Q1334	V1335	F1336	M1337	T1338	V1339	Y1340	M1341	S1342	D1343	D1344	M1345	V1346	F1347	V1348	G1349	L1350	P1351	T1352	G1353	K1354	G1355	L1356	T1357	I1358	C1359	A1360	E1361	F1362	A1363	I1364	L1365	P1366	M1367	L1368	L1369	Q1370	S1371	S1372	E1373	G1374	R1375	C1376	V1377	I1378	I1379	T1380																																																											
P1261	L1262	P1263	P1264	Q1265	Y1266	F1267	I1268	M1269	Q1269	V1270	V1271	S1272	D1273	R1274	M1275	L1276	S1277	C1278	E1279	T1280	L1281	L1282	P1283	V1284	S1285	V1286	M1287	H1288	L1289	I1290	L1291	P1292	E1293	K1294	Y1295	P1296	P1297	P1298	T1299	E1300	L1301	L1302	D1303	L1304	Q1305	P1306	L1307	P1308	V1309	S1310	A1311	L1312	R1313	M1314	S1315	A1316	F1317	E1318	S1319	L1320																																																										
E1201	L1202	T1203	I1204	T1205	P1206	D1207	F1208	Q1209	F1210	D1211	E1212	K1213	L1214	H1215	G1216	S1217	S1218	E1219	A1220	F1221	W1222	L1223	L1224	V1225	E1226	D1227	V1228	D1229	S1230	E1231	W1232	L1233	L1234	H1235	H1236	E1237	Y1238	F1239	L1240	L1241	K1242	A1243	K1244	Y1245	E1246	Q1247	D1248	E1249	H1250	L1251	I1252	T1253	F1254	F1255	S1256	P1257	F1259	E1260																																																												
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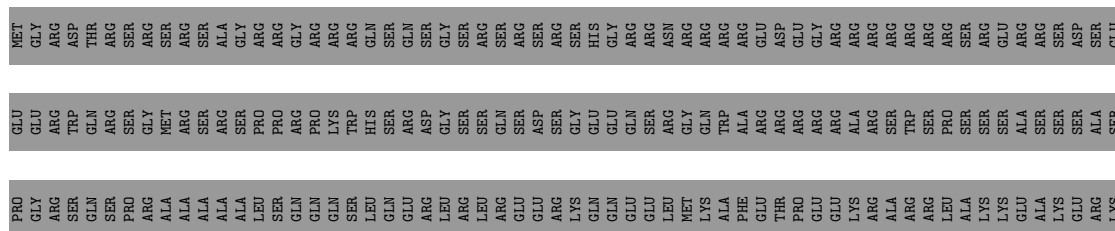
• Molecule 16: U5 small nuclear ribonucleoprotein 40 kDa protein

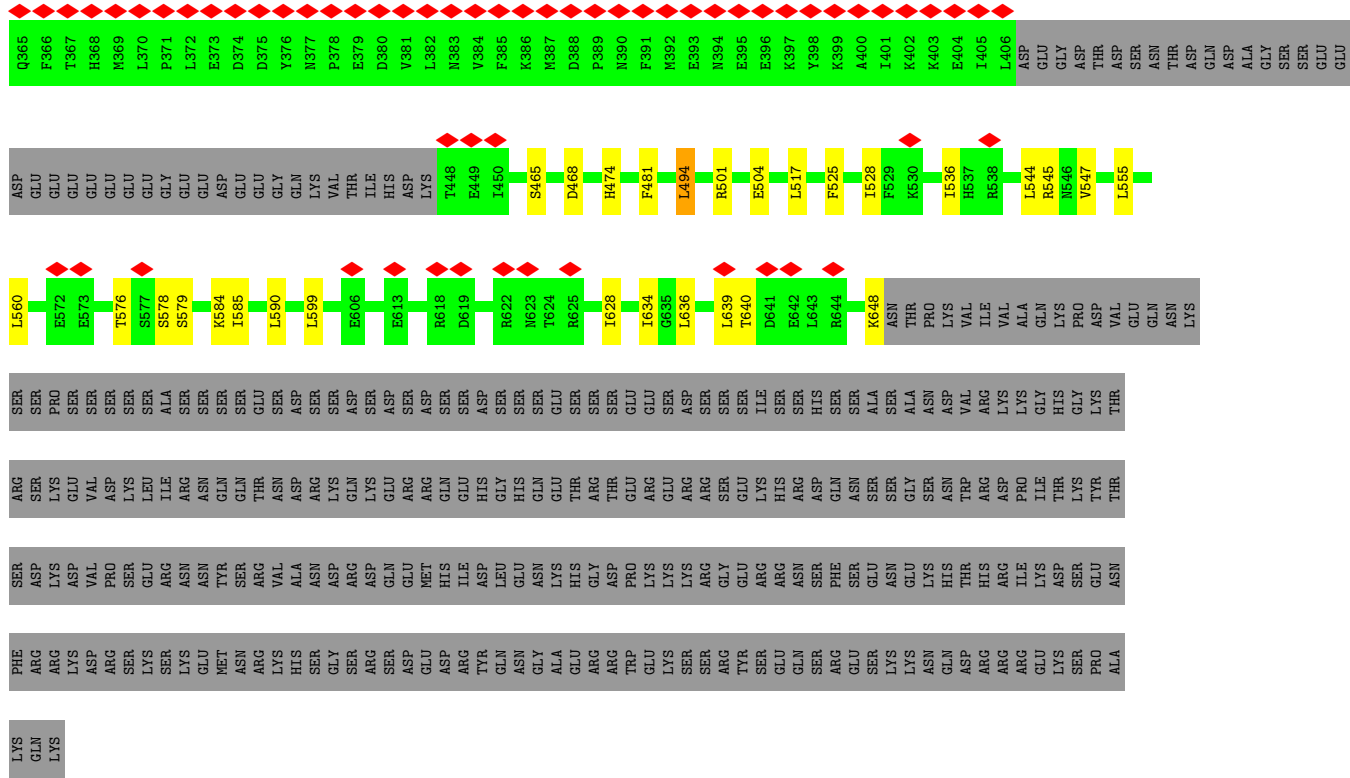


• Molecule 17: Exon

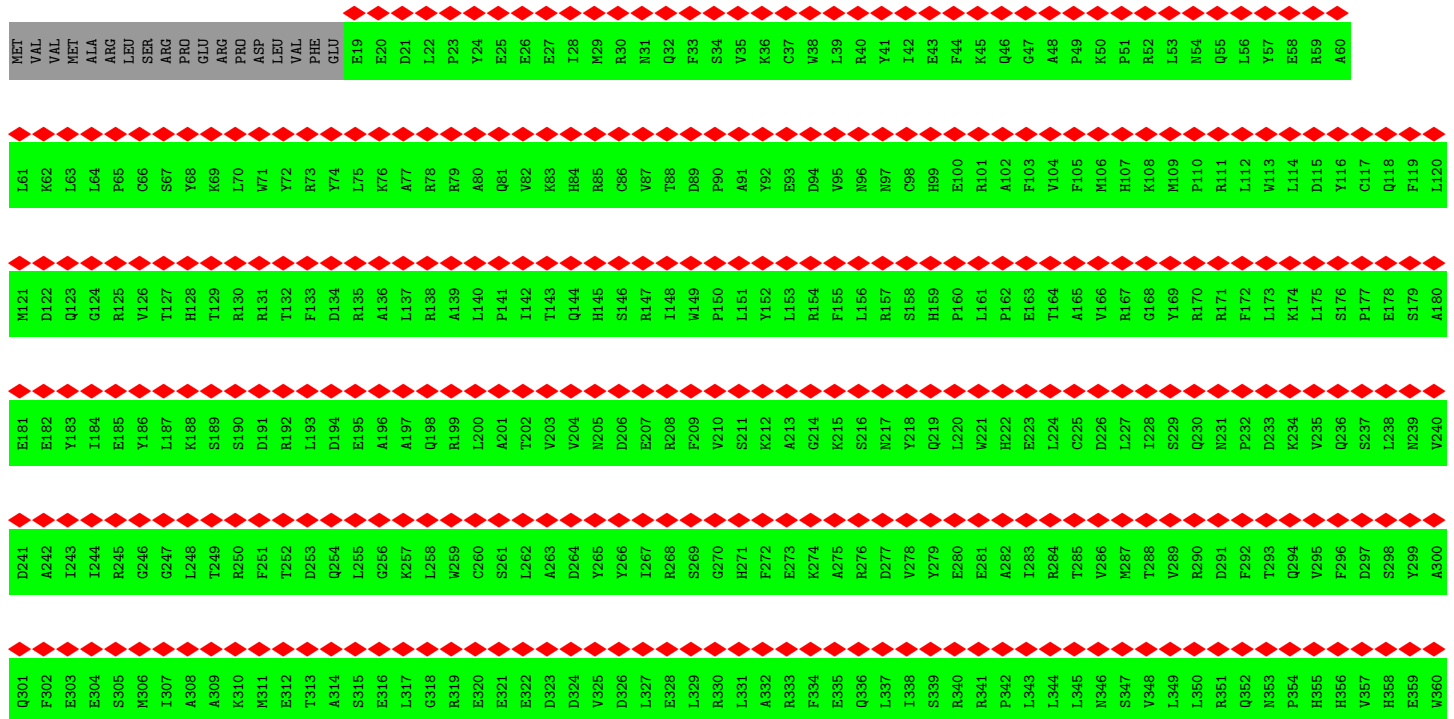
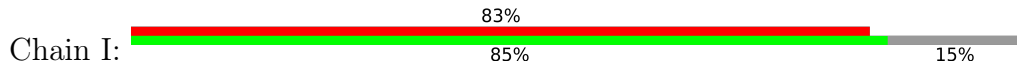


• Molecule 18: Splicing factor Cactin

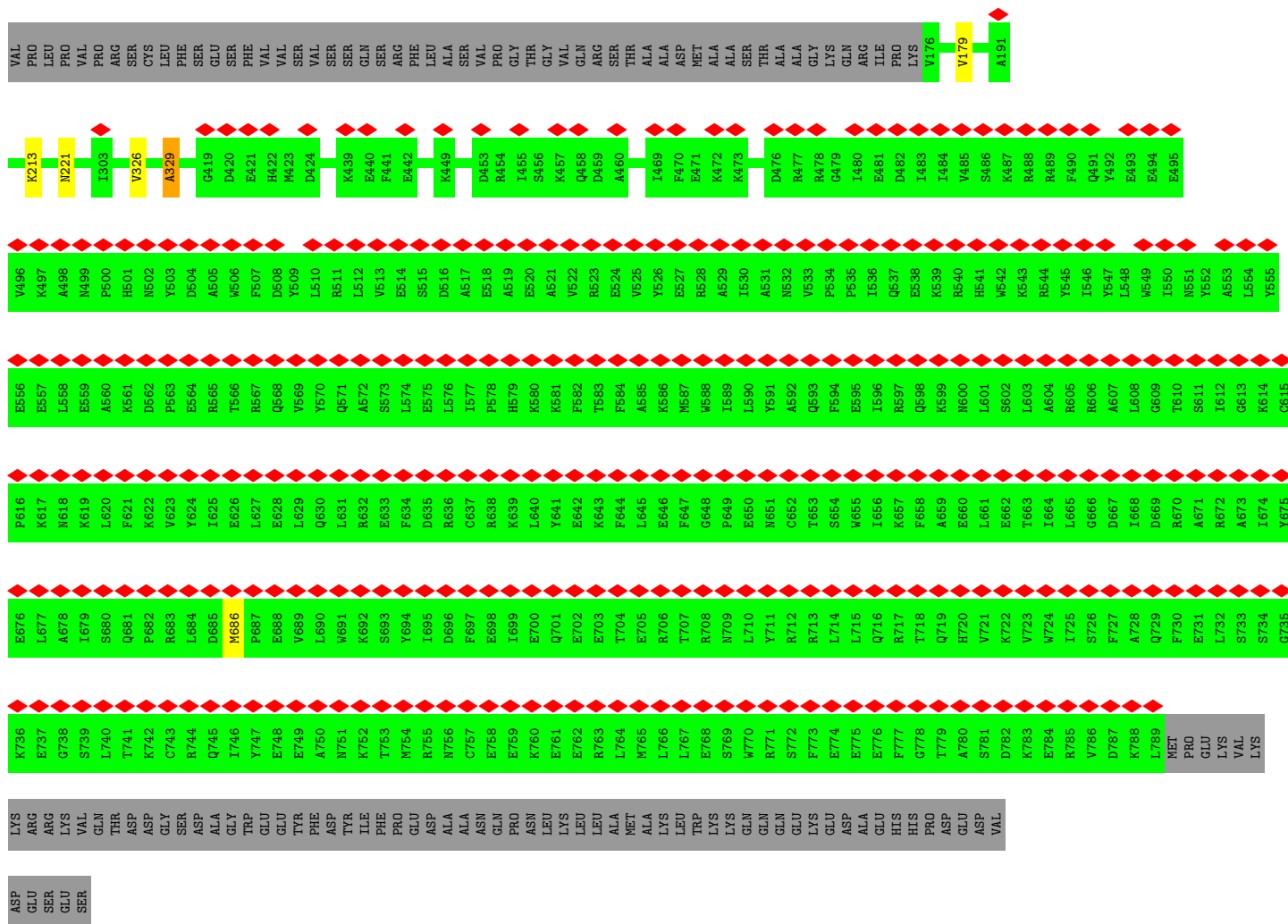




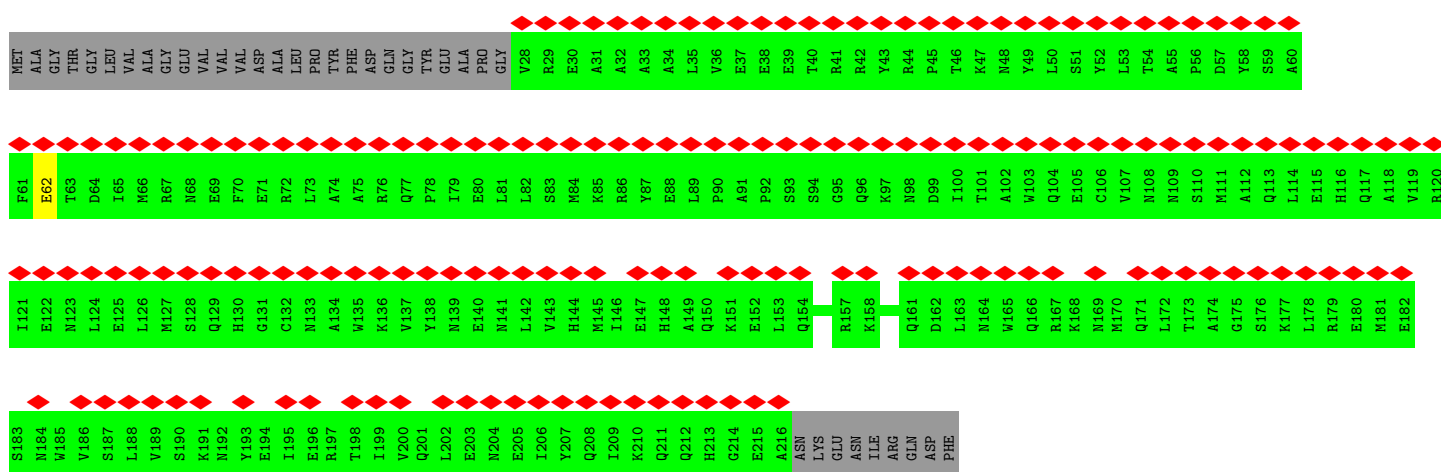
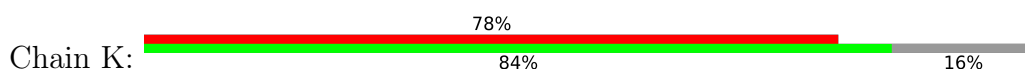
- Molecule 20: Pre-mRNA-splicing factor SYF1



H361	K362	R363	V364	A365	L366	H367	Q368	G369	R370	P371	R372	E373	I374	I375	N376	T377	Y378	T379	E380	A381	V382	Q383	T384	V385	D386	P387	F388	K389	A390	T391	G392	K393	P394	H395	T396	L397	W398	V399	A400	F401	A402	K403	F404	Y405	E406	D407	N408	G409	Q410	L411	D412	D413	A414	R415	V416	I417	L418	E419	K420																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A421	T422	K423	V424	N425	F426	K427	Q428	V429	D430	D431	L432	A433	S434	V435	W436	C437	Q438	C439	G440	E441	S442	E443	L444	R445	D446	E447	N448	Y449	D450	E451	A452	L453	R454	L455	L456	R457	K458	A459	T460	A461	P462	P463	A464	R465	R466	A467	E468	Y469	F470	D471	G472	S473	E474	P475	V476	Q477	N478	R479	V480																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Y481	K482	S483	L484	K485	V486	W487	S488	M489	L490	A491	D492	A493	E494	E495	S496	L497	G498	T499	F500	Q501	S502	T503	K504	A505	V506	Y507	D508	R509	I510	D512	L513	R514	I515	A516	T517	P518	Q519	I520	V521	I522	N523	Y524	A525	M526	F527	L528	E529	E530	D531	K532	Y533	F534	E535	E536	S537	F538	K539																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
E542	R543	G544	I545	S546	F548	R549	M550	P551	N552	V553	S554	D555	I556	W557	S558	T559	Y560	L561	A562	K563	F564	I565	A566	G569	G570	R571	K572	L573	R575	A576	R577	D578	L579	F580	E581	Q582	A583	L584	D585	G586	C587	P588	F589	K590	Y591	A592	K593	T594	L595	Y596	L597	L598	Y599	A600	Q601	L602																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
E603	E604	E605	W606	G607	L608	A609	R610	H611	A612	M613	V615	V616	E617	R618	A619	T620	R621	A622	V623	E624	P625	A626	Q627	Q628	Y629	D630	M631	L633	I634	Y635	I636	K637	R638	A639	E640	E641	A642	Y643	G644	V645	T646	H647	T648	R649	G650	I651	Y652	Q653	K654	A655	L656	E657	V658	L659	S660	D661	E662																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
H663	A664	R665	E666	M667	C668	L669	R670	F671	A672	D673	M674	E675	C676	K677	L678	G679	E680	I681	D682	R683	A684	R685	A686	I687	S688	F690	C691	S692	Q693	I694	C695	D696	P697	R698	T699	T700	G701	A702	F703	W704	Q705	T706	W707	K708	D709	F710	E711	W712	R713	H714	G715	N716	E717	D718	T719	L720	K721	E722																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
M723	L724	R725	I726	R727	R728	S729	W730	Q731	A732	T733	Y734	W735	T736	Q737	W738	N739	F740	M741	A742	S743	Q744	M745	L746	V747	S748	R749	A750	T751	R752	L753	P754	A755	G756	R757	T758	L759	M760	A761	S762	M763	L764	R765	T766	A767	S768	L769	M770	V771	S772	R773	A774	L775	S776	R777	L778	M779	V780	S781	R782	A783	L784	S785	R786	L787	M788	V789	S790	R791	A792	L793	S794	R795	L796	M797	V798	S799	R800	A801	L802	S803	R804	L805	M806	V807	S808	R809	A810	L811	S812	R813	L814	M815	V816	S817	R818	A819	L820	S821	R822	L823	M824	V825	S826	R827	A828	L829	M830	V831	S832	R833	L834	M835	V836	S837	R838	A839	L840	S841	R842	L843	M844	V845	S846	R847	A848	L849	S850	R851	L852	M853	V854	S855	R856	A857	L858	S859	R860	L861	M862	V863	S864	R865	A866	L867	S868	R869	L869	M870	V871	S872	R873	A874	L875	S876	R877	L878	M879	V880	S881	R882	A883	L884	S885	R886	L887	M888	V889	S890	R891	L892	M893	V894	S895	R896	A897	L898	S899	R900	L901	M902	V903	S904	R905	A906	L907	S908	R909	L909	M910	V911	S912	R913	A914	L915	S916	R917	L918	M919	V920	S921	R922	A923	L924	S925	R926	L927	M928	V929	S930	R931	A932	L933	S934	R935	L936	M937	V938	S939	R940	L941	M942	V943	S944	R945	L946	M947	V948	S949	R950	L951	M952	V953	S954	R955	L956	M957	V958	S959	R960	L961	M962	V963	S964	R965	L966	M967	V968	S969	R970	L971	M972	V973	S974	R975	L976	M977	V978	S979	R980	L981	M982	V983	S984	R985	L986	M987	V988	S989	R990	L991	M992	V993	S994	R995	L996	M997	V998	S999	R1000	L1001	M1002	V1003	S1004	R1005	L1006	M1007	V1008	S1009	R1010	L1011	M1012	V1013	S1014	R1015	L1016	M1017	V1018	S1019	R1020	L1021	M1022	V1023	S1024	R1025	L1026	M1027	V1028	S1029	R1030	L1031	M1032	V1033	S1034	R1035	L1036	M1037	V1038	S1039	R1040	L1041	M1042	V1043	S1044	R1045	L1046	M1047	V1048	S1049	R1050	L1051	M1052	V1053	S1054	R1055	L1056	M1057	V1058	S1059	R1060	L1061	M1062	V1063	S1064	R1065	L1066	M1067	V1068	S1069	R1070	L1071	M1072	V1073	S1074	R1075	L1076	M1077	V1078	S1079	R1080	L1081	M1082	V1083	S1084	R1085	L1086	M1087	V1088	S1089	R1090	L1091	M1092	V1093	S1094	R1095	L1096	M1097	V1098	S1099	R1100	L1101	M1102	V1103	S1104	R1105	L1106	M1107	V1108	S1109	R1110	L1111	M1112	V1113	S1114	R1115	L1116	M1117	V1118	S1119	R1120	L1121	M1122	V1123	S1124	R1125	L1126	M1127	V1128	S1129	R1130	L1131	M1132	V1133	S1134	R1135	L1136	M1137	V1138	S1139	R1140	L1141	M1142	V1143	S1144	R1145	L1146	M1147	V1148	S1149	R1150	L1151	M1152	V1153	S1154	R1155	L1156	M1157	V1158	S1159	R1160	L1161	M1162	V1163	S1164	R1165	L1166	M1167	V1168	S1169	R1170	L1171	M1172	V1173	S1174	R1175	L1176	M1177	V1178	S1179	R1180	L1181	M1182	V1183	S1184	R1185	L1186	M1187	V1188	S1189	R1190	L1191	M1192	V1193	S1194	R1195	L1196	M1197	V1198	S1199	R1200	L1201	M1202	V1203	S1204	R1205	L1206	M1207	V1208	S1209	R1210	L1211	M1212	V1213	S1214	R1215	L1216	M1217	V1218	S1219	R1220	L1221	M1222	V1223	S1224	R1225	L1226	M1227	V1228	S1229	R1230	L1231	M1232	V1233	S1234	R1235	L1236	M1237	V1238	S1239	R1240	L1241	M1242	V1243	S1244	R1245	L1246	M1247	V1248	S1249	R1250	L1251	M1252	V1253	S1254	R1255	L1256	M1257	V1258	S1259	R1260	L1261	M1262	V1263	S1264	R1265	L1266	M1267	V1268	S1269	R1270	L1271	M1272	V1273	S1274	R1275	L1276	M1277	V1278	S1279	R1280	L1281	M1282	V1283	S1284	R1285	L1286	M1287	V1288	S1289	R1290	L1291	M1292	V1293	S1294	R1295	L1296	M1297	V1298	S1299	R1300	L1301	M1302	V1303	S1304	R1305	L1306	M1307	V1308	S1309	R1310	L1311	M1312	V1313	S1314	R1315	L1316	M1317	V1318	S1319	R1320	L1321	M1322	V1323	S1324	R1325	L1326	M1327	V1328	S1329	R1330	L1331	M1332	V1333	S1334	R1335	L1336	M1337	V1338	S1339	R1340	L1341	M1342	V1343	S1344	R1345	L1346	M1347	V1348	S1349	R1350	L1351	M1352	V1353	S1354	R1355	L1356	M1357	V1358	S1359	R1360	L1361	M1362	V1363	S1364	R1365	L1366	M1367	V1368	S1369	R1370	L1371	M1372	V1373	S1374	R1375	L1376	M1377	V1378	S1379	R1380	L1381	M1382	V1383	S1384	R1385	L1386	M1387	V1388	S1389	R1390	L1391	M1392	V1393	S1394	R1395	L1396	M1397	V1398	S1399	R1400	L1401	M1402	V1403	S1404	R1405	L1406	M1407	V1408	S1409	R1410	L1411	M1412	V1413	S1414	R1415	L1416	M1417	V1418	S1419	R1420	L1421	M1422	V1423	S1424	R1425	L1426	M1427	V1428	S1429	R1430	L1431	M1432	V1433	S1434	R1435	L1436	M1437	V1438	S1439	R1440	L1441	M1442	V1443	S1444	R1445	L1446	M1447	V1448	S1449	R1450	L1451	M1452	V1453	S1454	R1455	L1456	M1457	V1458	S1459	R1460	L1461	M1462	V1463	S1464	R1465	L1466	M1467	V1468	S1469	R1470	L1471	M1472	V1473	S1474	R1475	L1476	M1477	V1478	S1479	R1480	L1481	M1482	V1483	S1484	R1485	L1486	M1487	V1488	S1489	R1490	L1491	M1492	V1493	S1494	R1495	L1496	M1497	V1498	S1499	R1500	L1501	M1502	V1503	S1504	R1505	L1506	M1507	V1508	S1509	R1510	L1511	M1512	V1513	S1514	R1515	L1516	M1517	V1518	S1519	R1520	L1521	M1522	V1523	S1524	R1525	L1526	M1527	V1528	S1529	R1530	L1531	M1532	V1533	S1534	R1535	L1536	M1537	V1538	S1539	R1540	L1541	M1542	V1543	S1544	R1545	L1546	M1547	V1548	S1549	R1550	L1551	M1552	V1553	S1554	R1555	L1556	M1557	V1558	S1559	R1560	L1561	M1562	V1563	S1564	R1565	L1566	M1567	V1568	S1569	R1570	L1571	M1572	V1573	S1574	R1575	L1576	M1577	V1578	S1579	R1580	L1581	M1582	V1583	S1584	R1585	L1586	M1587	V1588	S1589	R1590	L1591	M1592	V1593	S1594	R1595	L1596	M1597	V1598	S1599	R1600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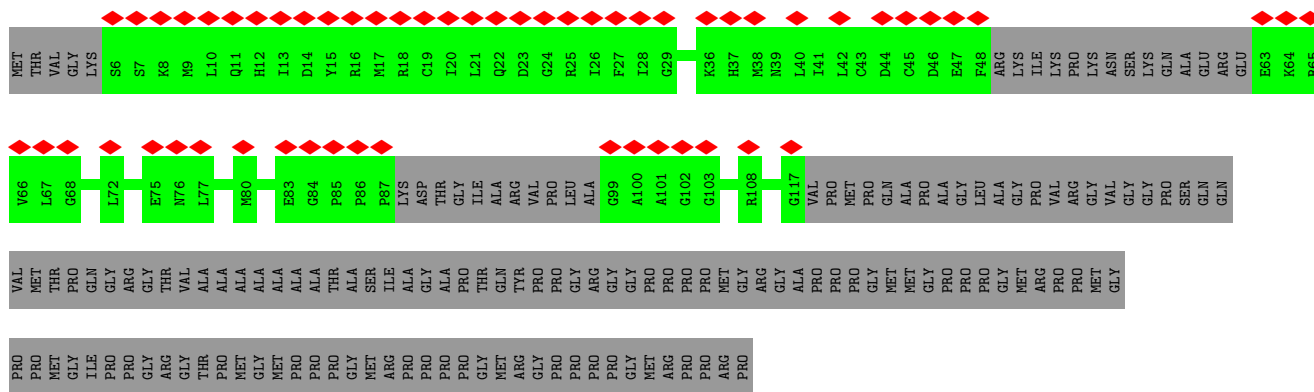


• Molecule 23: Pre-mRNA-splicing factor SPF27

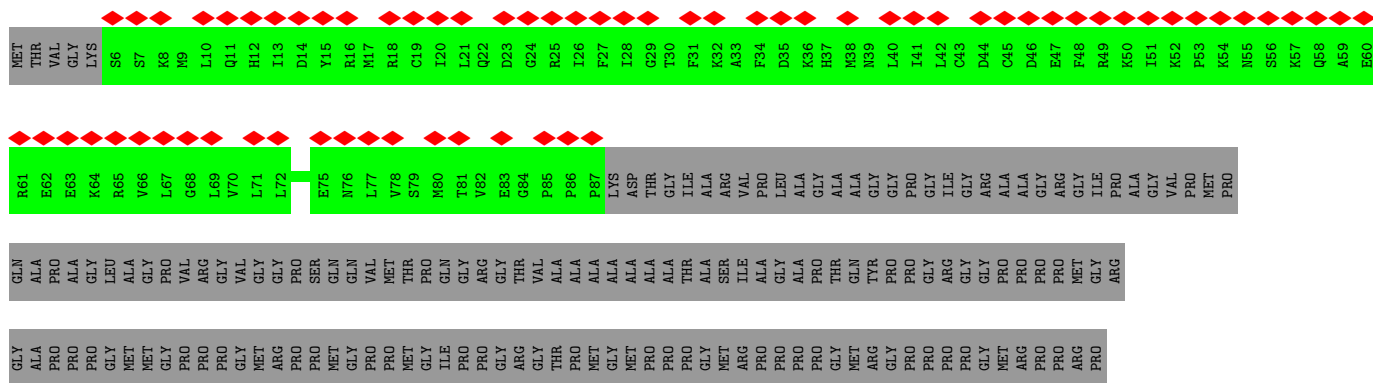


• Molecule 24: Cell division cycle 5-like protein

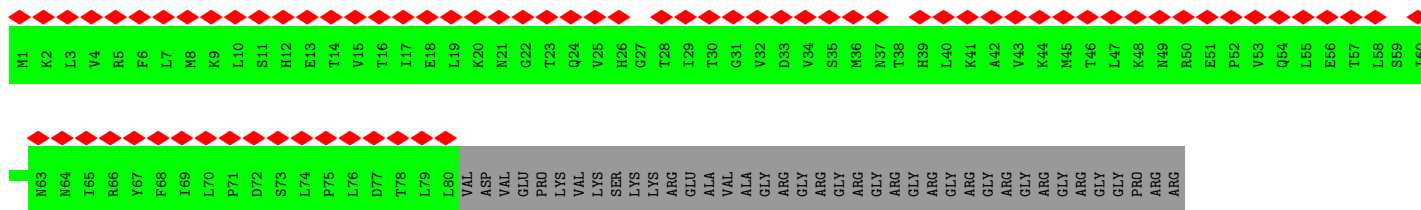
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V961	T962	E963	V964	S965	T966	F967	F968	P969	F970	H971	E972	Y973	F974	A975	N976	A977	P981	GLN	P982	I981	F982	K983	G984	R985	S986	Y987	E988	E989	D990	M991	E992	I993	A994	E995	G996	C997	F998	R999	H1000	I1001	M1002	K1003	X1004	F1005	T1006	Q1007	I1008	E1009	I1010	F1011	E1012	T1013	S1014	E1015	P1016	L1017	R1018	S1019	G1020	
Y841	H842	R843	F844	P845	E846	R847	R848	T849	L850	I851	V852	T853	H854	S855	N856	R857	A858	L859	N860	R861	L862	F863	E864	R865	L866	R867	A868	L869	D870	I871	D872	E873	R874	H875	L876	L877	R878	L879	C880	H881	GLY	E884	E885	L886	E887	T888	E889	K890	D891	F892	S893	R894	Y895	GLY	SER	THR	L897	V898	M899	Y900
P781	H782	V783	L784	P785	N786	R787	G788	P789	Y790	P791	Y792	M793	Q794	P795	K796	R797	N798	T799	I800	Q801	L802	F803	H804	T805	Q806	L807	E808	A809	L810	R811	A812	G813	H814	Q815	P816	G817	L818	T819	M820	H821	V822	G823	P824	P825	L826	T827	G828	R829	T830	D831	V832	A833	H834	Q835	L836	L837	R838	M839	L840	
I721	E722	H723	L724	K725	A726	S727	F728	P729	G730	H731	N732	V733	K734	V735	T736	V737	E738	D739	F740	A741	L742	L743	I744	F746	F747	R748	I749	T750	F751	P752	V753	ARG	SER	GLY	LYS	GLY	LYS	ARG	LYS	ASP	ALA	ASP	VAL	GLU	ASP	GLU	ASP	THR	GLU	E773	A774	K775	T776	L777	I778	V779	E780			
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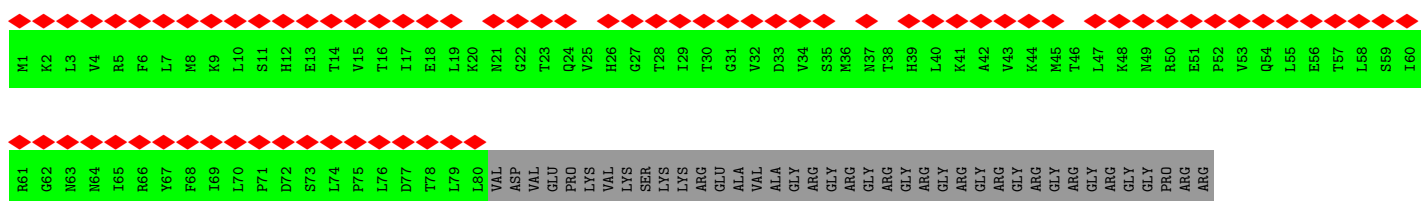
• Molecule 41: Small nuclear ribonucleoprotein-associated proteins B and B'



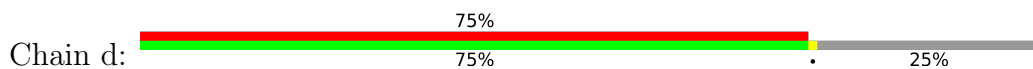
• Molecule 42: Small nuclear ribonucleoprotein Sm D1



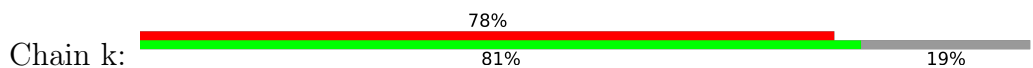
• Molecule 42: Small nuclear ribonucleoprotein Sm D1



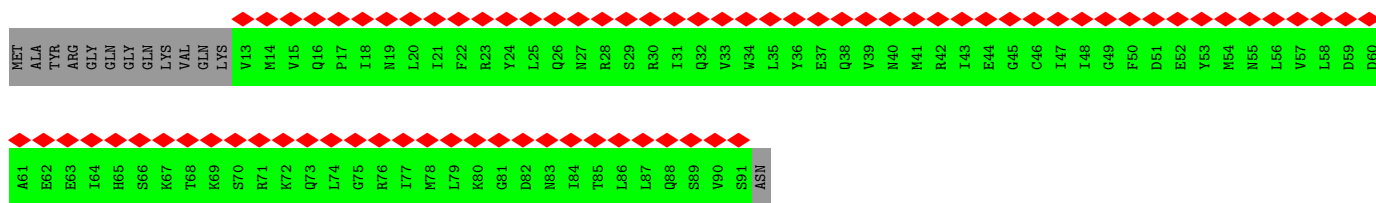
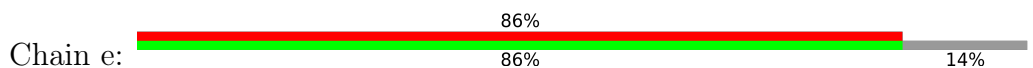
• Molecule 43: Small nuclear ribonucleoprotein Sm D2



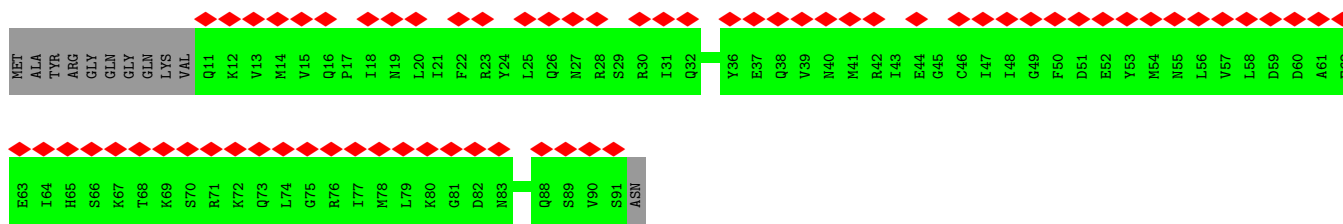
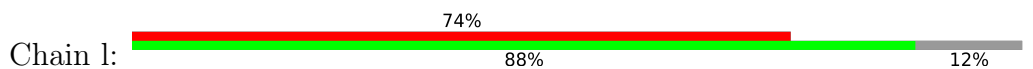
• Molecule 43: Small nuclear ribonucleoprotein Sm D2



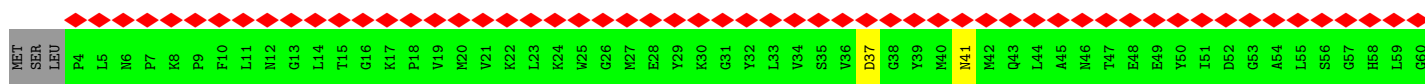
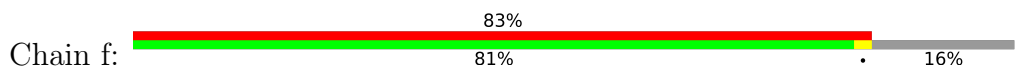
• Molecule 44: Small nuclear ribonucleoprotein E



• Molecule 44: Small nuclear ribonucleoprotein E

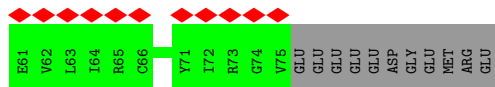
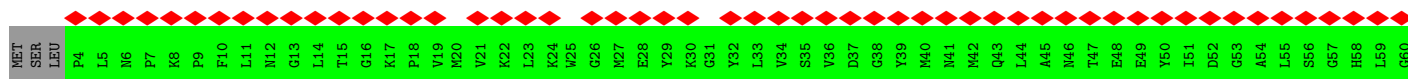
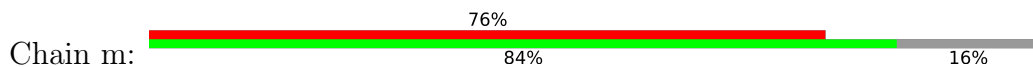


• Molecule 45: Small nuclear ribonucleoprotein F

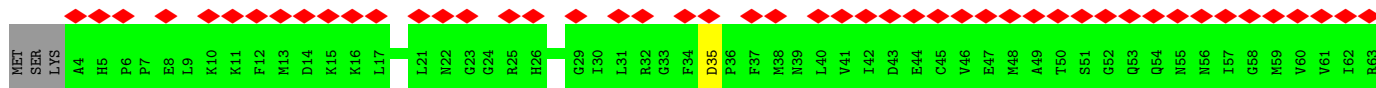
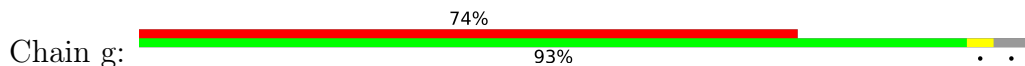




• Molecule 45: Small nuclear ribonucleoprotein F



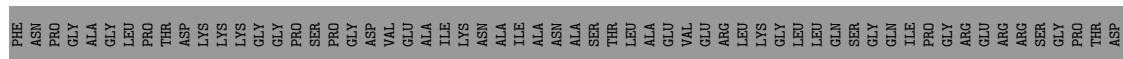
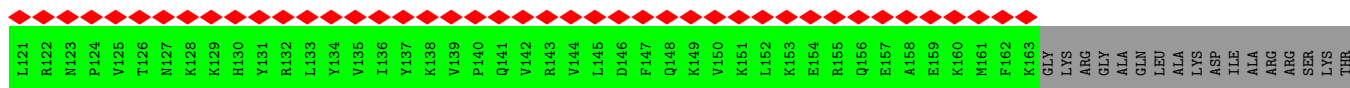
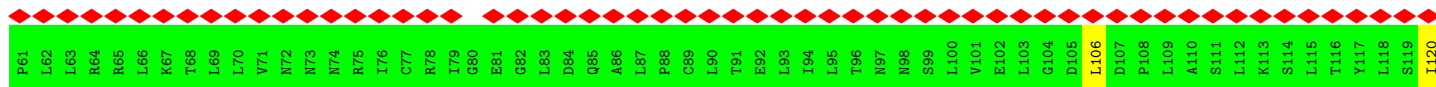
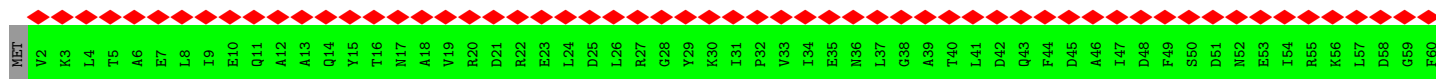
• Molecule 46: Small nuclear ribonucleoprotein G



• Molecule 46: Small nuclear ribonucleoprotein G

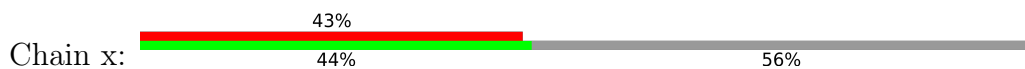


• Molecule 47: U2 small nuclear ribonucleoprotein A'



E181	E182	I183	Y184	C185	P186	G187	D188	A189	I190	S191	S192	V193	A194	A195	S196	E197	K198	S199	T200	K202	I203	F204	I205	Y206	D207	G208	R209	G210	D211	N212	Q213	Q214	L215	H216	L217	F218	D219	K220	L221	H222	T223	S224	P225	L226	T227	Q228	I229	R230	L231	N232	P233	V234	Y235	K236	A237	V238	V239	S240	
S241	D242	K243	S244	G245	M246	I247	E248	Y249	W250	T251	G252	P253	P254	H255	E256	Y257	K258	F259	P260	K261	N262	V263	N264	W265	E266	Y267	K268	T269	D270	T271	D272	L273	Y274	E275	F276	A277	K278	C279	K280	A281	Y282	P283	S284	S285	V286	C287	F288	S289	P290	L291	K292	K293	V294	I295	A296	T297	I298	G299	S300
D301	R302	K303	V304	I306	F307	R308	F309	V310	T311	G312	K313	L314	M315	R316	F317	F318	D319	E320	S321	L322	S323	M324	F325	T326	E327	L328	Q329	Q330	M331	R332	Q333	Q334	L335	P336	D337	M338	E339	F340	G341	R342	P343	M344	A345	V346	E347	R348	E349	L350	E351	K352	V353	A354	A355	V356	R357	L358	I359	N360	
I361	V362	F363	D364	E365	T366	G367	H368	F369	V370	L371	Y372	G373	T374	M375	L376	G377	I378	K379	V380	I381	N382	V383	E384	T385	N386	R387	C388	V389	R390	I391	L392	G393	K394	Q395	E396	N397	I398	R399	V400	M401	Q402	L403	A404	L405	F406	GLN	GLY	ILE	ALA	LYS	LYS	HIS	ARG	ALA	ALA	THR	THR	ILE	GLU
MET	LYS	ALA	SER	GLU	ASN	PRO	VAL	LEU	GLN	ASN	ASP	T437	I438	V439	C440	T441	S442	F443	K444	K445	N446	R447	F448	Y449	M450	F451	T452	K453	R454	E455	P456	E457	D458	T459	K460	S461	A462	D463	S464	D465	R466	D467	V468	F469	N470	E471	K472	P473	S474	K475	E476	E477	V478	M479	A480				
A481	T482	Q483	ALA	GLU	GLY	PRO	LYS	ARG	VAL	SER	ASP	S493	A494	I495	I496	H497	T498	S499	M500	G501	D502	I503	H504	T505	K506	L507	F508	P509	V510	E511	C512	P513	K514	T515	V516	E517	N518	F519	C520	V521	H522	S523	R524	N525	G526	Y527	E528	N529	G530	H531	T532	F533	H534	R535	I536	I537	K538	G539	F540
M541	Q543	T544	G545	D546	F547	T548	G549	T550	G551	M552	G553	G554	E555	S556	I557	M558	G559	G560	E561	F562	E563	D564	E565	F566	H567	S568	T569	L570	R571	H572	D573	D574	P575	Y576	T577	L578	S579	M580	A581	N582	A583	G584	S585	N586	T587	N588	G589	S590	Q591	F592	F593	I594	T595	V596	V597	P598	T599	P600	
M601	L602	D603	N604	K605	H606	T607	V608	F609	G610	R611	V612	T613	K614	G615	M616	E617	V618	V619	Q620	R621	I622	S623	N624	V625	K626	V627	N628	P629	K630	D632	T631	K633	P634	Y635	E636	D637	V638	S639	I640	I641	R642	K643	P644	N645	G646	V647	S648	A649	V650	A651	L652	L653	V654	G655	GLU	LYS	VAL	GLN	GLU

• Molecule 51: Splicing factor C9orf78



MET	PRO	VAL	R5	K6	I7	F8	R9	L10	R11	R12	G13	D14	S15	E16	S17	E18	E19	D20	E21	Q22	D23	S24	E25	E26	V27	R28	L29	K30	L31	E32	E33	T34	R35	E36	V37	Q38	N39	L40	R41	D42	R43	P44	N45	G46	V47	S48	A49	V50	A51	L52	L53	V54	G55	GLU	LYS	VAL	GLN	GLU
GLU	THR	LEU	VAL	ASP	PRO	PHE	GLN	MET	LYS	THR	GLY	MET	VAL	LYS	VAL	LYS	LEU	LYS	ARG	GLY	LYS	LYS	SER	GLU	GLU	GLU	ASP	LEU	HIS	THR	GLY	THR	ALA	GLU	GLU	THR	THR	THR	ASN	ARG	ARG	ASP	E111	D112	A113	D114	M115	M116	K117	Y118	I119	E120						
T121	E122	L123	K124	K125	R126	LYS	GLY	ILE	VAL	GLU	GLU	GLN	VAL	LYS	VAL	LYS	LYS	ASN	ALA	GLU	ASP	CYS	LEU	TYR	LEU	PRO	GLU	ASN	ILE	ARG	VAL	VAL	SER	ALA	ALA	ASN	TYR	E36	M164	L165	S166	N167	Q168	M169	L170	S171	G172	D177	L178	G179	I180	D181	A182	K183				
I184	K185	N186	I187	I188	S189	T190	E191	D192	A193	K194	A195	R196	L197	L198	A199	E200	Q201	Q202	N203	K204	K205	K206	D207	SER	GLU	THR	PHE	VAL	PRO	THR	ASN	ALA	ALA	ASN	TYR	VAL	GLN	HIS	ASN	ARG	ARG	PHE	TYR	HIS	ARG	ARG	ASN	ASN	PRO	ILE	ARG	ASN	LYS	GLU	GLU	PRO		
LYS	ALA	ARG	ARG	LEU	ARG	GLY	ASP	THR	GLU	LYS	PRO	GLU	GLU	ARG	SER	PRO	ASN	ARG	ARG	ALA	ALA	ASN	GLU	ALA	THR	D275	D276	Y277	H278	Y279	E280	K281	F282	K283	K284	M285	M286	R287	R288	Y289																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	492.00003, 492.00003, 492.00003	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1	0.38	0/1030	0.74	1/1371 (0.1%)
2	2	0.73	1/2827 (0.0%)	1.40	46/4393 (1.0%)
3	3	0.28	0/406	0.43	0/564
4	32	0.37	0/513	0.66	0/683
5	5	1.00	2/2157 (0.1%)	1.79	85/3351 (2.5%)
6	50	0.33	0/1050	0.69	0/1461
7	56	0.28	0/497	0.57	0/690
8	6	1.06	2/2323 (0.1%)	1.44	34/3619 (0.9%)
9	7	0.31	0/1927	0.65	1/2681 (0.0%)
10	8	0.28	0/444	0.67	0/614
11	9	0.31	0/711	0.62	0/987
12	A	0.61	1/18250 (0.0%)	0.71	9/24798 (0.0%)
13	B	0.36	0/15311	0.76	17/20733 (0.1%)
14	C	0.58	0/7277	0.87	15/9887 (0.2%)
15	D	0.30	0/356	0.52	0/494
16	E	0.41	0/2448	0.70	1/3316 (0.0%)
17	EX	1.43	0/329	2.62	36/510 (7.1%)
18	F	0.46	0/1130	0.68	1/1525 (0.1%)
19	H	0.40	0/2965	0.65	1/4049 (0.0%)
20	I	0.31	0/3609	0.57	0/5036
21	IN	0.73	0/996	1.71	36/1544 (2.3%)
22	J	0.34	1/2997 (0.0%)	0.63	0/4187
23	K	0.30	0/940	0.52	0/1312
24	L	0.41	0/3674	0.64	1/4988 (0.0%)
25	M	0.29	0/1114	0.53	0/1553
26	N	0.58	1/1215 (0.1%)	0.74	1/1627 (0.1%)
27	NO	0.31	0/861	0.58	0/1197
28	O	0.50	0/2366	0.67	0/3193
29	P	0.47	0/903	0.70	0/1201
30	Q	0.30	0/6545	0.57	0/9115
31	R	0.48	1/2647 (0.0%)	0.73	4/3554 (0.1%)
32	S	0.38	0/1305	0.65	0/1767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SR	0.59	2/414 (0.5%)	0.56	0/568
34	T	0.70	1/2957 (0.0%)	0.77	1/4023 (0.0%)
35	U	0.50	0/2483	0.68	0/3341
36	V	0.30	0/3626	0.57	0/5050
37	W	0.53	1/4266 (0.0%)	0.71	4/5761 (0.1%)
38	X	0.28	0/326	0.49	0/452
39	Z	0.28	0/263	0.53	0/365
40	a	0.34	0/666	0.68	0/897
40	h	0.36	0/660	0.68	0/889
41	b	0.31	0/663	0.65	0/885
41	i	0.31	0/674	0.62	0/899
42	c	0.29	0/642	0.59	0/867
42	j	0.28	0/642	0.60	0/867
43	d	0.29	0/732	0.66	0/984
43	k	0.32	0/784	0.64	0/1053
44	e	0.28	0/659	0.67	0/885
44	l	0.31	0/677	0.68	0/908
45	f	0.35	0/574	0.75	1/775 (0.1%)
45	m	0.34	0/574	0.65	0/775
46	g	0.34	0/575	0.72	2/768 (0.3%)
46	n	0.32	0/575	0.66	0/768
47	o	0.30	0/1299	0.71	1/1761 (0.1%)
48	p	0.30	0/759	0.57	0/1016
49	q	0.29	0/512	0.48	0/713
49	r	0.35	0/592	0.56	0/825
49	s	0.35	0/658	0.58	0/919
49	t	0.32	0/512	0.54	0/713
50	w	0.30	0/2652	0.65	0/3685
51	x	0.30	0/632	0.50	0/874
52	y	0.28	0/317	0.62	0/396
53	z	0.37	0/431	0.57	0/582
All	All	0.50	13/122919 (0.0%)	0.80	298/169264 (0.2%)

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
12	A	0	2
13	B	0	20
14	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	E	0	1
29	P	0	1
31	R	0	2
All	All	0	29

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	307	CYS	CB-SG	-7.01	1.70	1.82
34	T	220	VAL	CB-CG2	-6.64	1.38	1.52
8	6	58	G	N7-C5	-6.24	1.35	1.39
5	5	57	G	C2-N3	-5.78	1.28	1.32
12	A	492	VAL	CB-CG2	-5.66	1.41	1.52
33	SR	6	GLY	C-N	-5.62	1.21	1.34
33	SR	24	SER	CA-CB	-5.48	1.44	1.52
31	R	9	ALA	C-N	5.46	1.44	1.34
5	5	37	G	N9-C4	-5.38	1.33	1.38
2	2	20	G	N7-C5	-5.34	1.36	1.39
22	J	686	MET	C-N	5.32	1.44	1.34
26	N	142	CYS	CB-SG	-5.07	1.73	1.81
8	6	58	G	N9-C8	-5.05	1.34	1.37

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	IN	145	U	O4'-C1'-N1	14.47	119.78	108.20
17	EX	-2	C	O4'-C1'-N1	14.36	119.69	108.20
5	5	24	G	O4'-C1'-N9	-12.82	97.94	108.20
5	5	86	C	N1-C2-O2	12.72	126.53	118.90
2	2	50	C	N1-C2-O2	11.88	126.03	118.90
5	5	86	C	C2-N1-C1'	11.49	131.44	118.80
5	5	23	C	C2-N1-C1'	11.45	131.40	118.80
17	EX	-8	U	O4'-C1'-N1	11.12	117.10	108.20
17	EX	2	U	OP1-P-OP2	-11.01	103.09	119.60
14	C	486	ASP	CB-CG-OD1	10.79	128.01	118.30
12	A	598	LEU	CB-CG-CD1	-10.64	92.91	111.00
5	5	36	C	N1-C2-O2	10.46	125.18	118.90
5	5	11	U	C5-C6-N1	10.27	127.83	122.70
5	5	99	C	C6-N1-C2	-10.06	116.28	120.30
2	2	50	C	C2-N1-C1'	10.03	129.83	118.80
14	C	432	ASP	CB-CG-OD1	10.00	127.30	118.30
2	2	54	U	N3-C2-O2	-9.59	115.49	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	50	C	N3-C2-O2	-9.52	115.24	121.90
5	5	86	C	N3-C2-O2	-9.49	115.25	121.90
5	5	99	C	C2-N1-C1'	9.49	129.24	118.80
5	5	36	C	C2-N1-C1'	9.25	128.98	118.80
5	5	55	C	C6-N1-C2	-9.05	116.68	120.30
5	5	10	U	C5-C6-N1	8.96	127.18	122.70
8	6	61	C	C5-C6-N1	8.94	125.47	121.00
21	IN	13	C	C5-C6-N1	8.92	125.46	121.00
5	5	36	C	N3-C2-O2	-8.90	115.67	121.90
21	IN	13	C	C6-N1-C2	-8.83	116.77	120.30
8	6	61	C	C6-N1-C2	-8.80	116.78	120.30
21	IN	13	C	C2-N1-C1'	8.67	128.33	118.80
5	5	11	U	C2-N1-C1'	8.50	127.90	117.70
21	IN	1	G	O4'-C1'-N9	8.39	114.92	108.20
5	5	103	C	C6-N1-C2	-8.29	116.98	120.30
5	5	47	A	O4'-C1'-N9	8.25	114.80	108.20
8	6	58	G	N7-C8-N9	8.25	117.22	113.10
17	EX	-6	C	OP1-P-O3'	8.19	123.22	105.20
5	5	86	C	C6-N1-C1'	-8.14	111.03	120.80
2	2	54	U	N1-C2-O2	8.13	128.49	122.80
14	C	230	ASP	CB-CG-OD1	8.06	125.56	118.30
5	5	99	C	C5-C6-N1	8.03	125.01	121.00
13	B	501	LEU	CA-CB-CG	7.99	133.67	115.30
2	2	34	U	C5-C6-N1	7.98	126.69	122.70
21	IN	144	A	N9-C1'-C2'	-7.97	103.24	112.00
5	5	10	U	C2-N1-C1'	7.96	127.25	117.70
5	5	23	C	C6-N1-C2	-7.92	117.13	120.30
5	5	23	C	C6-N1-C1'	-7.84	111.39	120.80
8	6	58	G	C8-N9-C4	-7.80	103.28	106.40
14	C	910	ASP	CB-CG-OD1	7.77	125.29	118.30
13	B	467	LEU	CA-CB-CG	7.74	133.10	115.30
5	5	45	C	C6-N1-C2	-7.72	117.21	120.30
14	C	192	ASP	CB-CG-OD1	7.67	125.20	118.30
14	C	458	ASP	CB-CG-OD1	7.64	125.18	118.30
17	EX	2	U	O4'-C1'-N1	7.57	114.25	108.20
5	5	40	U	N1-C2-O2	7.45	128.01	122.80
21	IN	2	U	N3-C2-O2	-7.40	117.02	122.20
5	5	53	U	N3-C2-O2	-7.40	117.02	122.20
21	IN	142	U	P-O3'-C3'	7.38	128.56	119.70
12	A	329	LEU	CA-CB-CG	7.35	132.21	115.30
17	EX	-3	A	OP1-P-OP2	-7.29	108.66	119.60
2	2	102	U	P-O3'-C3'	7.27	128.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	638	LEU	CB-CG-CD1	-7.25	98.68	111.00
17	EX	-8	U	OP1-P-OP2	-7.24	108.73	119.60
5	5	103	C	C5-C6-N1	7.23	124.61	121.00
12	A	1405	LEU	CA-CB-CG	7.17	131.80	115.30
2	2	105	G	P-O3'-C3'	7.16	128.29	119.70
34	T	261	LEU	CA-CB-CG	7.12	131.68	115.30
13	B	1999	LEU	CA-CB-CG	7.11	131.65	115.30
13	B	1004	LEU	CB-CG-CD2	7.09	123.05	111.00
2	2	19	G	O4'-C1'-N9	-7.06	102.55	108.20
2	2	13	C	N1-C2-O2	7.04	123.13	118.90
26	N	118	ILE	CG1-CB-CG2	-7.04	95.91	111.40
8	6	60	C	C6-N1-C2	-7.01	117.49	120.30
17	EX	-7	C	O4'-C1'-N1	7.00	113.80	108.20
2	2	50	C	C6-N1-C2	-6.98	117.51	120.30
1	1	113	LEU	CA-CB-CG	6.94	131.27	115.30
5	5	86	C	C6-N1-C2	-6.94	117.53	120.30
21	IN	2	U	N1-C2-O2	6.89	127.63	122.80
5	5	38	C	C6-N1-C2	-6.88	117.55	120.30
21	IN	142	U	OP1-P-O3'	6.84	120.25	105.20
5	5	105	U	N3-C2-O2	-6.81	117.43	122.20
5	5	92	U	P-O3'-C3'	6.81	127.87	119.70
17	EX	-1	G	OP1-P-O3'	6.80	120.16	105.20
2	2	50	C	C6-N1-C1'	-6.79	112.65	120.80
17	EX	1	C	OP1-P-OP2	-6.79	109.41	119.60
13	B	1606	ASP	CB-CG-OD1	6.77	124.39	118.30
21	IN	11	A	OP1-P-OP2	-6.76	109.46	119.60
21	IN	12	G	OP1-P-OP2	-6.74	109.48	119.60
2	2	102	U	OP2-P-O3'	6.66	119.86	105.20
8	6	17	C	C5-C6-N1	6.66	124.33	121.00
17	EX	-10	C	OP1-P-OP2	-6.65	109.63	119.60
17	EX	-12	G	OP1-P-O3'	6.64	119.80	105.20
45	f	37	ASP	CB-CG-OD1	6.63	124.27	118.30
8	6	32	U	N3-C2-O2	-6.60	117.58	122.20
2	2	54	U	C2-N1-C1'	6.59	125.61	117.70
2	2	148	C	C5-C6-N1	6.58	124.29	121.00
5	5	95	G	P-O3'-C3'	6.57	127.59	119.70
17	EX	-11	G	OP1-P-OP2	-6.55	109.77	119.60
5	5	86	C	C5-C6-N1	6.55	124.28	121.00
5	5	36	C	C6-N1-C2	-6.54	117.69	120.30
17	EX	-9	C	OP1-P-OP2	-6.53	109.80	119.60
5	5	38	C	C5-C6-N1	6.52	124.26	121.00
21	IN	139	U	C5-C6-N1	6.50	125.95	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	g	35	ASP	CB-CG-OD1	6.50	124.15	118.30
17	EX	1	C	O4'-C1'-N1	6.46	113.37	108.20
8	6	87	C	C5-C6-N1	6.43	124.22	121.00
5	5	43	U	N1-C2-O2	6.40	127.28	122.80
21	IN	166	A	O4'-C1'-N9	-6.39	103.08	108.20
17	EX	1	C	OP1-P-O3'	6.37	119.21	105.20
2	2	32	U	N1-C2-O2	6.36	127.25	122.80
21	IN	147	C	C5-C6-N1	6.35	124.17	121.00
8	6	17	C	C6-N1-C2	-6.35	117.76	120.30
8	6	31	U	N1-C2-O2	6.32	127.22	122.80
2	2	13	C	N3-C2-O2	-6.29	117.50	121.90
5	5	36	C	C6-N1-C1'	-6.29	113.26	120.80
2	2	3	C	C5-C6-N1	6.26	124.13	121.00
2	2	30	A	C2-N3-C4	6.26	113.73	110.60
21	IN	142	U	N3-C2-O2	-6.25	117.83	122.20
2	2	54	U	C6-N1-C2	-6.24	117.25	121.00
2	2	55	U	N3-C2-O2	-6.23	117.84	122.20
13	B	969	LEU	CA-CB-CG	6.22	129.61	115.30
2	2	156	U	N1-C2-O2	6.20	127.14	122.80
13	B	500	LEU	CA-CB-CG	6.20	129.56	115.30
17	EX	-10	C	N3-C2-O2	-6.19	117.56	121.90
17	EX	-2	C	C6-N1-C2	-6.16	117.83	120.30
2	2	32	U	N3-C2-O2	-6.15	117.90	122.20
5	5	57	G	N3-C2-N2	-6.14	115.60	119.90
2	2	27	U	N3-C2-O2	-6.12	117.91	122.20
17	EX	-3	A	OP1-P-O3'	6.12	118.66	105.20
21	IN	146	C	C6-N1-C2	-6.12	117.85	120.30
21	IN	147	C	C6-N1-C2	-6.12	117.85	120.30
13	B	772	LEU	CA-CB-CG	6.11	129.34	115.30
8	6	31	U	N3-C2-O2	-6.10	117.93	122.20
5	5	55	C	C5-C6-N1	6.10	124.05	121.00
17	EX	-6	C	OP1-P-OP2	-6.10	110.46	119.60
17	EX	-5	G	OP1-P-OP2	-6.07	110.49	119.60
17	EX	-10	C	C1'-O4'-C4'	-6.06	105.05	109.90
5	5	32	C	C5-C6-N1	6.06	124.03	121.00
9	7	162	GLY	C-N-CA	6.05	136.83	121.70
5	5	13	C	C6-N1-C2	-6.03	117.89	120.30
8	6	31	U	C2-N1-C1'	6.03	124.94	117.70
21	IN	8	C	C5-C6-N1	6.03	124.02	121.00
5	5	105	U	N1-C2-O2	6.02	127.01	122.80
17	EX	1	C	C6-N1-C2	-6.00	117.90	120.30
21	IN	8	C	C6-N1-C2	-5.99	117.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	156	U	N3-C2-O2	-5.99	118.01	122.20
21	IN	17	U	N1-C2-O2	5.99	126.99	122.80
5	5	43	U	N3-C2-O2	-5.98	118.01	122.20
12	A	598	LEU	CA-CB-CG	5.98	129.05	115.30
14	C	860	ASP	CB-CG-OD1	5.97	123.67	118.30
5	5	9	G	C4-N9-C1'	5.97	134.26	126.50
17	EX	-4	A	OP1-P-O3'	5.96	118.31	105.20
5	5	55	C	N3-C2-O2	-5.96	117.73	121.90
8	6	15	A	N7-C8-N9	5.95	116.77	113.80
5	5	14	U	N3-C2-O2	-5.94	118.04	122.20
5	5	56	C	C5-C6-N1	5.92	123.96	121.00
5	5	32	C	C6-N1-C2	-5.91	117.94	120.30
5	5	109	C	C5-C6-N1	5.91	123.95	121.00
5	5	109	C	C6-N1-C2	-5.90	117.94	120.30
17	EX	-1	G	OP1-P-OP2	-5.90	110.75	119.60
8	6	8	C	C6-N1-C2	-5.90	117.94	120.30
5	5	99	C	C6-N1-C1'	-5.88	113.75	120.80
8	6	57	U	N3-C4-O4	5.87	123.51	119.40
5	5	53	U	N1-C2-O2	5.86	126.91	122.80
2	2	101	U	N1-C2-O2	5.85	126.89	122.80
5	5	54	U	C5-C6-N1	5.84	125.62	122.70
21	IN	139	U	C2-N1-C1'	5.84	124.71	117.70
5	5	10	U	N3-C4-O4	5.84	123.49	119.40
21	IN	17	U	C2-N1-C1'	5.83	124.69	117.70
2	2	95	A	P-O3'-C3'	5.82	126.68	119.70
8	6	62	C	C6-N1-C2	-5.82	117.97	120.30
21	IN	131	U	N1-C2-O2	5.81	126.87	122.80
21	IN	145	U	N1-C1'-C2'	-5.80	105.62	112.00
21	IN	17	U	N3-C2-O2	-5.79	118.15	122.20
5	5	40	U	N3-C2-O2	-5.78	118.16	122.20
5	5	104	C	O4'-C1'-N1	5.77	112.82	108.20
5	5	45	C	N3-C2-O2	-5.76	117.87	121.90
5	5	51	A	N9-C1'-C2'	5.76	121.48	114.00
5	5	15	C	C5-C6-N1	5.75	123.87	121.00
14	C	617	LEU	CB-CG-CD1	-5.75	101.23	111.00
17	EX	-12	G	OP1-P-OP2	-5.74	110.99	119.60
5	5	12	U	C5-C6-N1	5.73	125.57	122.70
5	5	46	U	N1-C1'-C2'	5.72	121.43	114.00
21	IN	131	U	N3-C2-O2	-5.72	118.20	122.20
21	IN	143	U	C5-C6-N1	5.69	125.54	122.70
17	EX	-6	C	C2-N1-C1'	5.68	125.05	118.80
2	2	50	C	C5-C6-N1	5.66	123.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	11	U	C6-N1-C2	-5.66	117.60	121.00
8	6	74	U	N3-C2-O2	-5.65	118.25	122.20
5	5	52	U	N1-C1'-C2'	5.64	121.33	114.00
17	EX	-7	C	OP1-P-OP2	-5.64	111.14	119.60
2	2	156	U	C2-N1-C1'	5.64	124.47	117.70
5	5	35	U	N3-C2-O2	-5.63	118.26	122.20
13	B	1240	LEU	CA-CB-CG	5.63	128.26	115.30
2	2	3	C	C6-N1-C2	-5.62	118.05	120.30
5	5	45	C	C5-C6-N1	5.62	123.81	121.00
5	5	18	C	C5-C6-N1	5.61	123.81	121.00
5	5	15	C	C6-N1-C2	-5.61	118.06	120.30
14	C	320	LEU	CB-CG-CD2	-5.61	101.47	111.00
8	6	8	C	C5-C6-N1	5.59	123.80	121.00
46	g	70	LEU	CA-CB-CG	5.58	128.15	115.30
12	A	331	TRP	CA-CB-CG	5.58	124.31	113.70
8	6	60	C	C5-C6-N1	5.58	123.79	121.00
17	EX	-2	C	C2-N1-C1'	5.57	124.93	118.80
2	2	155	C	O4'-C1'-N1	5.57	112.65	108.20
2	2	20	G	C8-N9-C1'	-5.56	119.78	127.00
5	5	12	U	C2-N1-C1'	5.55	124.36	117.70
8	6	52	U	C6-N1-C2	-5.54	117.68	121.00
17	EX	-9	C	OP1-P-O3'	5.54	117.38	105.20
8	6	37	C	C6-N1-C2	-5.53	118.09	120.30
8	6	87	C	C6-N1-C2	-5.53	118.09	120.30
2	2	55	U	N1-C2-O2	5.53	126.67	122.80
31	R	324	LEU	CA-CB-CG	5.53	128.01	115.30
13	B	1713	PHE	CB-CG-CD1	5.53	124.67	120.80
24	L	372	LEU	CA-CB-CG	5.53	128.01	115.30
5	5	103	C	C2-N1-C1'	5.51	124.87	118.80
13	B	619	LEU	CA-CB-CG	5.51	127.98	115.30
5	5	98	C	C5-C6-N1	5.51	123.75	121.00
8	6	34	G	C8-N9-C4	-5.48	104.21	106.40
13	B	2124	VAL	C-N-CA	5.46	135.36	121.70
8	6	23	U	N3-C2-O2	-5.46	118.38	122.20
21	IN	137	C	P-O3'-C3'	5.45	126.24	119.70
31	R	86	LEU	CA-CB-CG	5.45	127.83	115.30
14	C	381	LEU	CA-CB-CG	5.44	127.81	115.30
2	2	89	U	N3-C2-O2	-5.44	118.39	122.20
2	2	173	C	C6-N1-C2	-5.43	118.13	120.30
14	C	758	LEU	CA-CB-CG	5.43	127.79	115.30
13	B	2092	LEU	CA-CB-CG	5.42	127.77	115.30
14	C	696	LEU	CA-CB-CG	5.41	127.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	10	C	C6-N1-C2	-5.40	118.14	120.30
31	R	91	ASP	CB-CG-OD1	5.40	123.16	118.30
2	2	54	U	C5-C6-N1	5.39	125.40	122.70
5	5	13	C	C5-C6-N1	5.39	123.70	121.00
2	2	101	U	C2-N1-C1'	5.39	124.16	117.70
5	5	9	G	C8-N9-C1'	-5.38	120.00	127.00
5	5	105	U	C6-N1-C2	-5.38	117.77	121.00
2	2	21	C	O5'-P-OP1	-5.38	100.86	105.70
2	2	5	C	C6-N1-C2	-5.38	118.15	120.30
5	5	12	U	N3-C2-O2	-5.38	118.44	122.20
17	EX	-6	C	N1-C2-O2	5.37	122.12	118.90
8	6	50	A	P-O3'-C3'	5.36	126.14	119.70
21	IN	146	C	C5-C6-N1	5.36	123.68	121.00
8	6	55	C	C6-N1-C2	-5.36	118.16	120.30
12	A	976	MET	CG-SD-CE	-5.34	91.65	100.20
37	W	276	LEU	CA-CB-CG	5.34	127.58	115.30
37	W	506	MET	CA-CB-CG	5.33	122.36	113.30
21	IN	142	U	N1-C2-N3	5.31	118.09	114.90
5	5	35	U	N1-C2-O2	5.31	126.52	122.80
5	5	105	U	C5-C6-N1	5.31	125.35	122.70
17	EX	-12	G	C2'-C3'-O3'	5.30	122.19	113.70
8	6	41	A	N1-C2-N3	-5.30	126.65	129.30
16	E	59	ILE	CA-CB-CG2	5.29	121.49	110.90
13	B	1679	TYR	CA-CB-CG	5.29	123.46	113.40
2	2	148	C	C6-N1-C2	-5.29	118.19	120.30
8	6	57	U	C2-N1-C1'	5.28	124.03	117.70
21	IN	137	C	C6-N1-C2	-5.27	118.19	120.30
2	2	168	A	C4-N9-C1'	5.26	135.78	126.30
8	6	57	U	C5-C4-O4	-5.26	122.75	125.90
5	5	37	G	N9-C1'-C2'	5.23	120.80	114.00
2	2	5	C	C5-C6-N1	5.23	123.61	121.00
2	2	101	U	N3-C2-O2	-5.23	118.54	122.20
14	C	733	TRP	CA-CB-CG	5.23	123.63	113.70
18	F	708	LEU	CA-CB-CG	5.23	127.32	115.30
8	6	81	C	C6-N1-C2	-5.20	118.22	120.30
5	5	11	U	C6-N1-C1'	-5.20	113.92	121.20
21	IN	14	A	N7-C8-N9	5.19	116.39	113.80
5	5	34	U	C5-C6-N1	5.18	125.29	122.70
8	6	59	G	O4'-C1'-N9	5.18	112.35	108.20
14	C	474	LEU	CA-CB-CG	5.18	127.22	115.30
37	W	299	LEU	CA-CB-CG	5.17	127.19	115.30
13	B	821	LEU	CA-CB-CG	5.17	127.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	54	LEU	CA-CB-CG	5.16	127.16	115.30
37	W	305	LEU	CB-CG-CD1	-5.16	102.23	111.00
19	H	555	LEU	CB-CG-CD1	-5.16	102.23	111.00
5	5	98	C	C6-N1-C2	-5.13	118.25	120.30
5	5	22	U	C2-N1-C1'	5.13	123.86	117.70
8	6	38	G	O4'-C1'-N9	5.12	112.30	108.20
5	5	10	U	C6-N1-C2	-5.11	117.93	121.00
12	A	1108	ASP	CB-CG-OD1	5.09	122.89	118.30
5	5	11	U	N3-C4-O4	5.09	122.97	119.40
14	C	177	ARG	CA-CB-CG	5.09	124.60	113.40
5	5	56	C	C6-N1-C2	-5.09	118.27	120.30
17	EX	-3	A	N1-C2-N3	-5.08	126.76	129.30
17	EX	-2	C	N3-C2-O2	-5.08	118.35	121.90
13	B	2082	LEU	CA-CB-CG	5.08	126.98	115.30
21	IN	13	C	C6-N1-C1'	-5.08	114.71	120.80
8	6	37	C	C5-C6-N1	5.07	123.53	121.00
21	IN	146	C	O4'-C1'-N1	5.06	112.25	108.20
47	o	106	LEU	CA-CB-CG	5.06	126.94	115.30
17	EX	-6	C	N3-C2-O2	-5.06	118.36	121.90
2	2	168	A	C2-N3-C4	5.06	113.13	110.60
8	6	33	G	P-O3'-C3'	5.06	125.77	119.70
12	A	323	LEU	CA-CB-CG	5.05	126.92	115.30
17	EX	1	C	N1-C1'-C2'	5.05	120.57	114.00
5	5	95	G	OP2-P-O3'	5.04	116.30	105.20
5	5	10	U	C6-N1-C1'	-5.04	114.14	121.20
21	IN	13	C	N1-C2-O2	5.03	121.92	118.90
5	5	39	C	N1-C2-O2	5.03	121.92	118.90
2	2	152	G	N7-C8-N9	5.00	115.60	113.10
13	B	1276	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1418	ARG	Sidechain
12	A	941	LYS	Peptide
13	B	1030	ARG	Sidechain
13	B	1043	ARG	Sidechain
13	B	1274	ARG	Sidechain
13	B	129	ARG	Sidechain
13	B	1313	ARG	Sidechain
13	B	1375	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	B	1400	ARG	Sidechain
13	B	1438	ARG	Sidechain
13	B	1442	ARG	Sidechain
13	B	1566	ARG	Sidechain
13	B	1843	ARG	Sidechain
13	B	1901	ARG	Sidechain
13	B	2009	ARG	Sidechain
13	B	2013	ARG	Sidechain
13	B	2043	ARG	Sidechain
13	B	728	ARG	Sidechain
13	B	739	ARG	Sidechain
13	B	794	ARG	Sidechain
13	B	858	ARG	Sidechain
13	B	953	ARG	Sidechain
14	C	318	PHE	Peptide
14	C	342	ARG	Sidechain
14	C	813	ARG	Sidechain
16	E	307	ARG	Sidechain
29	P	16	ARG	Sidechain
31	R	332	ARG	Sidechain
31	R	9	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1013	0	1058	9	0
2	2	2535	0	1281	19	0
3	3	408	0	181	0	0
4	32	504	0	509	11	0
5	5	1936	0	982	19	0
6	50	1053	0	456	2	0
7	56	498	0	220	0	0
8	6	2075	0	1048	28	0
9	7	1928	0	855	0	0
10	8	445	0	203	0	0
11	9	712	0	299	0	0
12	A	17802	0	17006	229	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	15004	0	15162	104	0
14	C	7116	0	7128	32	0
15	D	358	0	167	0	0
16	E	2394	0	2329	42	0
17	EX	296	0	153	2	0
18	F	1085	0	1019	5	0
19	H	2932	0	2204	17	0
20	I	3610	0	1639	0	0
21	IN	893	0	453	13	0
22	J	2998	0	1333	3	0
23	K	941	0	424	0	0
24	L	3642	0	2904	31	0
25	M	1115	0	513	0	0
26	N	1189	0	1192	17	0
27	NO	864	0	371	1	0
28	O	2318	0	2298	38	0
29	P	889	0	865	8	0
30	Q	6554	0	2828	1	0
31	R	2618	0	2663	35	0
32	S	1271	0	1244	19	0
33	SR	412	0	287	5	0
34	T	2881	0	2836	40	0
35	U	2425	0	2370	39	0
36	V	3629	0	1603	0	0
37	W	4158	0	4060	75	0
38	X	328	0	156	1	0
39	Z	265	0	114	1	0
40	a	658	0	675	0	0
40	h	652	0	670	0	0
41	b	654	0	667	0	0
41	i	664	0	690	0	0
42	c	634	0	680	0	0
42	j	634	0	680	0	0
43	d	723	0	750	0	0
43	k	774	0	802	0	0
44	e	651	0	671	0	0
44	l	669	0	692	0	0
45	f	562	0	574	0	0
45	m	562	0	574	0	0
46	g	568	0	590	0	0
46	n	568	0	590	0	0
47	o	1282	0	1305	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	p	745	0	767	0	0
49	q	514	0	236	0	0
49	r	594	0	270	0	0
49	s	659	0	299	0	0
49	t	514	0	236	0	0
50	w	2655	0	1150	0	0
51	x	636	0	276	0	0
52	y	318	0	88	0	0
53	z	430	0	321	0	0
54	6	5	0	0	0	0
54	7	1	0	0	0	0
55	6	1	0	0	0	0
56	7	31	0	12	0	0
57	C	32	0	12	0	0
58	N	3	0	0	0	0
58	O	3	0	0	0	0
59	U	36	0	6	1	0
All	All	120526	0	96696	730	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 4.

All (730) 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)
5:5:36:C:H42	5:5:46:U:H3	1.09	0.90
2:2:25:G:N1	8:6:52:U:O2	2.15	0.76
2:2:153:A:H62	2:2:177:A:H2	1.32	0.75
2:2:153:A:N6	2:2:177:A:C2	2.57	0.73
5:5:36:C:N4	5:5:46:U:H3	1.85	0.73
34:T:216:ASN:HD21	34:T:472:GLN:H	1.37	0.73
8:6:40:U:H3	21:IN:7:G:H22	1.41	0.68
28:O:24:CYS:SG	28:O:81:CYS:HB2	2.34	0.68
2:2:153:A:N6	2:2:177:A:H2	1.91	0.67
12:A:67:ARG:HD3	12:A:179:ALA:HB2	1.78	0.66
34:T:314:ILE:HD12	34:T:324:HIS:HB2	1.76	0.66
12:A:1476:GLN:NE2	35:U:85:GLN:OE1	2.30	0.65
16:E:259:VAL:HB	16:E:277:PHE:HB2	1.79	0.65
12:A:156:ARG:HD3	35:U:153:GLU:HG2	1.79	0.65
32:S:15:TYR:HB2	32:S:163:TYR:HB2	1.79	0.64
26:N:101:CYS:SG	26:N:102:CYS:N	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R:62:GLY:HA3	32:S:131:ARG:HH11	1.63	0.63
16:E:62:LEU:HB2	16:E:351:LEU:HB2	1.82	0.62
22:J:213:LYS:O	24:L:189:ARG:NH2	2.33	0.62
12:A:209:ASP:HB2	12:A:212:PRO:HA	1.82	0.62
12:A:1771:LEU:HD22	12:A:1812:PRO:HG2	1.81	0.61
13:B:1819:ALA:HB2	13:B:1829:ILE:HD13	1.82	0.61
5:5:45:C:H4'	12:A:596:TYR:HB3	1.83	0.61
13:B:1353:GLY:O	13:B:1692:ASN:ND2	2.34	0.61
24:L:145:ASP:OD1	24:L:145:ASP:N	2.34	0.60
29:P:23:LEU:HA	29:P:26:LEU:HD23	1.83	0.60
12:A:909:TYR:HB2	12:A:1033:GLY:HA3	1.83	0.60
13:B:415:VAL:HG12	13:B:894:VAL:HB	1.84	0.60
16:E:91:LEU:HD22	16:E:101:ASN:HD21	1.65	0.60
37:W:524:ILE:HG22	37:W:534:ILE:HG12	1.83	0.60
8:6:21:U:O2'	37:W:130:ARG:NH2	2.35	0.60
12:A:443:VAL:HG12	12:A:610:HIS:HB3	1.83	0.60
35:U:51:GLU:HB2	35:U:59:ILE:HB	1.83	0.60
24:L:65:ARG:HG3	24:L:362:ILE:HD11	1.83	0.59
34:T:349:SER:OG	34:T:351:ASP:OD1	2.19	0.59
2:2:22:U:OP1	12:A:717:TRP:NE1	2.35	0.59
32:S:52:LYS:HA	32:S:158:LYS:HA	1.84	0.59
12:A:549:GLU:OE1	12:A:552:ARG:NH1	2.35	0.59
12:A:82:ARG:NH2	21:IN:16:G:N7	2.51	0.59
12:A:1581:LEU:HD22	12:A:1746:ARG:HH11	1.68	0.59
13:B:569:LEU:HD13	13:B:580:ILE:HG21	1.85	0.59
35:U:67:ILE:HG23	35:U:85:GLN:HE21	1.68	0.59
8:6:64:U:OP2	12:A:663:ARG:NH2	2.33	0.58
8:6:49:G:OP1	24:L:33:ARG:NH1	2.35	0.58
13:B:686:GLU:HB2	13:B:866:GLU:HG2	1.86	0.58
31:R:205:ASP:HB3	31:R:208:GLU:HB2	1.86	0.58
37:W:552:VAL:HG13	37:W:571:TRP:HD1	1.67	0.58
4:32:72:ARG:NH2	12:A:186:GLU:O	2.37	0.58
28:O:64:ARG:HG3	28:O:162:PRO:HA	1.84	0.58
14:C:300:LEU:HD13	14:C:306:ASN:HB3	1.86	0.58
1:1:68:MET:HA	18:F:757:ARG:HE	1.69	0.57
8:6:21:U:OP1	26:N:116:ASN:ND2	2.37	0.57
12:A:205:ASP:N	12:A:205:ASP:OD1	2.35	0.57
31:R:189:ASN:HD21	31:R:195:ARG:HB3	1.69	0.57
12:A:321:ASN:O	14:C:645:ARG:NH2	2.36	0.57
2:2:37:U:OP1	37:W:454:LYS:NZ	2.36	0.57
8:6:10:U:O2'	8:6:12:G:N7	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:479:GLN:NE2	37:W:525:SER:OG	2.37	0.57
16:E:203:ASP:HB3	16:E:247:GLY:HA3	1.86	0.57
13:B:493:LEU:O	13:B:519:ARG:NH1	2.37	0.57
37:W:432:ARG:NH2	37:W:446:GLU:OE2	2.37	0.57
5:5:12:U:H3	5:5:65:G:H1	1.52	0.57
8:6:14:C:H2'	8:6:15:A:H8	1.68	0.57
12:A:200:ASP:OD1	12:A:240:ARG:NH2	2.36	0.57
12:A:1214:TRP:HB2	12:A:1228:CYS:HB3	1.87	0.57
12:A:1984:LYS:HG3	35:U:345:ALA:HB1	1.85	0.57
16:E:177:LYS:HG2	16:E:189:THR:HG22	1.87	0.57
26:N:105:CYS:HB3	26:N:119:CYS:SG	2.45	0.57
6:50:126:GLU:O	13:B:1442:ARG:NH1	2.37	0.57
34:T:294:LEU:HD12	34:T:303:LEU:HD11	1.86	0.57
8:6:2:U:O2	26:N:95:GLN:NE2	2.38	0.57
37:W:434:VAL:HG22	37:W:444:VAL:HG22	1.85	0.57
12:A:873:ASN:ND2	12:A:876:GLU:OE1	2.38	0.57
31:R:178:ARG:HB2	37:W:118:ALA:HB2	1.87	0.56
37:W:435:SER:HB3	37:W:445:TRP:HE1	1.70	0.56
6:50:316:LYS:HA	6:50:321:ALA:HB3	1.86	0.56
34:T:399:LYS:HB3	34:T:404:SER:HB2	1.85	0.56
2:2:32:U:O4	21:IN:146:C:N3	2.38	0.56
13:B:128:PRO:HD2	13:B:131:ILE:HD12	1.88	0.56
28:O:56:ARG:HG2	28:O:67:LYS:HB3	1.86	0.56
34:T:210:ILE:HG13	34:T:480:ALA:HB2	1.88	0.56
37:W:333:LYS:H	37:W:353:ASP:HB3	1.71	0.56
16:E:346:SER:OG	16:E:348:ASP:OD1	2.23	0.56
12:A:243:ASN:O	35:U:131:LYS:NZ	2.36	0.56
12:A:1124:ASN:ND2	12:A:1148:ASN:OD1	2.37	0.56
12:A:981:PHE:O	12:A:1166:THR:OG1	2.24	0.56
16:E:59:ILE:HD11	37:W:82:ASN:H	1.71	0.56
12:A:280:GLU:OE2	33:SR:11:ARG:NH1	2.39	0.55
37:W:436:THR:HG21	37:W:464:MET:HB2	1.88	0.55
5:5:46:U:O2	33:SR:11:ARG:NH2	2.38	0.55
8:6:20:A:O2'	26:N:120:ARG:NH2	2.39	0.55
28:O:131:THR:O	37:W:108:ARG:NH1	2.39	0.55
37:W:257:ILE:HD12	37:W:266:ARG:HE	1.71	0.55
12:A:678:GLU:OE2	12:A:778:ARG:NH2	2.39	0.55
12:A:1214:TRP:NE1	12:A:1276:GLU:OE1	2.39	0.55
24:L:37:LEU:HD13	24:L:158:ARG:HD3	1.88	0.55
31:R:44:TYR:HA	31:R:47:ARG:HD2	1.87	0.55
12:A:601:GLN:HG2	12:A:640:PHE:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:881:ILE:HG23	12:A:918:THR:HG23	1.87	0.55
12:A:1366:PRO:HA	19:H:465:SER:HA	1.89	0.55
24:L:147:ASP:OD1	24:L:147:ASP:N	2.36	0.55
12:A:976:MET:HG2	12:A:1187:PHE:HB3	1.88	0.55
14:C:177:ARG:NH2	14:C:638:ASP:OD2	2.39	0.55
31:R:265:ASP:OD1	31:R:265:ASP:N	2.38	0.55
13:B:1093:ARG:NH2	13:B:1273:ASP:OD1	2.40	0.55
13:B:1456:VAL:HG22	13:B:1491:SER:HB2	1.89	0.55
12:A:546:LEU:HD11	12:A:595:LYS:HB2	1.89	0.55
28:O:240:GLY:H	28:O:268:GLN:HB2	1.71	0.55
12:A:552:ARG:NH1	12:A:589:THR:O	2.40	0.55
16:E:311:VAL:HB	16:E:321:TYR:HB2	1.89	0.55
28:O:78:LYS:O	28:O:97:ARG:NH2	2.40	0.55
37:W:390:LEU:HD22	37:W:402:GLN:HE21	1.72	0.55
12:A:141:ILE:HD12	12:A:410:PRO:HG3	1.89	0.54
12:A:1042:GLN:HE22	12:A:1092:ILE:HA	1.72	0.54
19:H:525:PHE:HA	19:H:528:ILE:HG22	1.89	0.54
35:U:122:ASN:ND2	35:U:133:CYS:SG	2.74	0.54
4:32:99:LEU:HD22	12:A:1617:ARG:HD2	1.89	0.54
12:A:723:ASN:OD1	12:A:785:LYS:NZ	2.39	0.54
32:S:25:LEU:HD23	32:S:98:LEU:HD21	1.88	0.54
37:W:126:GLU:HA	37:W:129:ARG:HG2	1.89	0.54
22:J:221:ASN:O	24:L:211:ASN:ND2	2.41	0.54
32:S:156:ASP:N	32:S:156:ASP:OD1	2.39	0.54
12:A:1009:MET:O	12:A:1013:ASN:ND2	2.41	0.54
35:U:342:HIS:HB3	35:U:345:ALA:HB3	1.89	0.54
12:A:523:ASN:OD1	12:A:552:ARG:NH2	2.41	0.54
12:A:1215:ASN:HB3	12:A:1224:ARG:HD3	1.90	0.54
34:T:210:ILE:HG12	34:T:221:THR:HG22	1.90	0.54
31:R:238:THR:HG23	31:R:241:GLU:H	1.74	0.53
12:A:143:GLN:NE2	12:A:207:PHE:O	2.33	0.53
28:O:162:PRO:HG2	28:O:182:ARG:HG3	1.91	0.53
37:W:255:LEU:HD21	37:W:362:GLU:HB3	1.90	0.53
12:A:1411:SER:O	12:A:1411:SER:OG	2.26	0.53
19:H:517:LEU:HD21	33:SR:24:SER:HA	1.89	0.53
32:S:26:GLU:OE1	32:S:131:ARG:NH2	2.41	0.53
12:A:1536:LEU:HG	12:A:1572:SER:HB3	1.90	0.53
16:E:81:LEU:HD21	16:E:343:ILE:HD12	1.90	0.53
13:B:1855:TYR:HB3	13:B:1891:THR:HG21	1.90	0.53
5:5:11:U:O2'	12:A:217:ARG:NH2	2.42	0.53
12:A:1090:ARG:NH2	12:A:1092:ILE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R:47:ARG:HA	31:R:50:TRP:HE1	1.73	0.53
12:A:214:ARG:HA	12:A:220:VAL:HG21	1.91	0.53
37:W:404:ASP:HB3	37:W:407:SER:HB3	1.91	0.53
12:A:1021:ASP:OD1	12:A:1021:ASP:N	2.39	0.53
12:A:1618:LYS:NZ	12:A:1628:ASP:OD2	2.36	0.53
12:A:109:PRO:HB2	12:A:191:ILE:HD12	1.90	0.53
12:A:698:PRO:HD2	12:A:701:ILE:HG13	1.90	0.53
13:B:844:LEU:HD11	13:B:849:ILE:HG23	1.90	0.53
24:L:178:GLU:OE2	24:L:181:ARG:NH1	2.42	0.53
24:L:250:GLU:OE1	24:L:258:ARG:NH2	2.42	0.53
37:W:304:LEU:HD11	37:W:567:ILE:HG21	1.90	0.53
24:L:33:ARG:O	24:L:158:ARG:NH2	2.41	0.53
31:R:61:GLY:HA3	32:S:136:ILE:HG21	1.91	0.53
12:A:36:LYS:NZ	37:W:163:GLN:O	2.42	0.52
12:A:641:MET:HA	12:A:644:ILE:HG22	1.90	0.52
12:A:1904:ASP:HB3	12:A:1908:LYS:HE2	1.90	0.52
12:A:1946:ASN:HD22	12:A:1986:LEU:HD11	1.73	0.52
12:A:997:LEU:HD22	12:A:1009:MET:HE3	1.92	0.52
12:A:1042:GLN:HA	12:A:1090:ARG:HH12	1.72	0.52
13:B:1985:ILE:HA	13:B:1988:MET:HG3	1.92	0.52
8:6:35:A:N6	21:IN:11:A:OP2	2.42	0.52
12:A:58:LYS:NZ	12:A:477:LYS:O	2.43	0.52
12:A:1860:GLN:HG2	12:A:1883:VAL:HB	1.91	0.52
13:B:537:LYS:NZ	13:B:581:SER:O	2.42	0.52
12:A:721:LYS:HB3	12:A:781:ARG:HD3	1.90	0.52
13:B:1570:ARG:HH11	13:B:1608:THR:HG21	1.73	0.52
34:T:305:THR:OG1	34:T:315:TRP:NE1	2.40	0.52
37:W:173:LYS:NZ	37:W:175:THR:O	2.41	0.52
12:A:1085:ILE:HD11	12:A:1160:ARG:HH12	1.74	0.52
12:A:1780:VAL:HG22	12:A:1809:ILE:HG12	1.90	0.52
35:U:189:ASP:HA	35:U:192:LYS:HB2	1.90	0.52
12:A:490:VAL:HG21	12:A:565:ARG:HG3	1.92	0.52
12:A:962:LEU:HB3	12:A:965:VAL:HB	1.92	0.52
12:A:1491:LYS:O	12:A:1710:ASN:ND2	2.41	0.52
13:B:967:ASN:ND2	13:B:995:ASN:O	2.41	0.52
24:L:176:LEU:HD22	37:W:440:LYS:HD3	1.90	0.52
37:W:301:GLY:O	37:W:559:HIS:NE2	2.41	0.52
2:2:151:C:H2'	2:2:152:G:H8	1.75	0.52
5:5:67:A:H5''	26:N:90:ALA:HB1	1.90	0.52
31:R:107:SER:OG	31:R:108:LYS:N	2.43	0.52
34:T:347:THR:HG22	34:T:357:TRP:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1777:ILE:HG12	12:A:1860:GLN:HB2	1.91	0.52
29:P:16:ARG:NH2	31:R:218:ILE:O	2.43	0.52
4:32:80:LYS:NZ	35:U:184:GLU:OE2	2.40	0.51
12:A:26:SER:OG	12:A:27:GLU:N	2.43	0.51
13:B:425:ASN:ND2	13:B:886:GLN:O	2.42	0.51
16:E:67:GLY:N	16:E:87:ASP:OD1	2.44	0.51
34:T:365:ARG:HH22	34:T:401:PRO:HB2	1.75	0.51
2:2:166:G:OP2	2:2:166:G:N2	2.37	0.51
8:6:58:G:H2'	8:6:59:G:C8	2.45	0.51
12:A:761:ILE:HD12	12:A:775:ASN:HD22	1.76	0.51
12:A:857:ASN:N	12:A:857:ASN:OD1	2.43	0.51
13:B:1099:VAL:HG13	13:B:1108:THR:HG22	1.92	0.51
13:B:1564:PRO:O	13:B:1648:ARG:NH1	2.44	0.51
28:O:176:GLY:HA2	37:W:206:ALA:HB2	1.93	0.51
12:A:664:HIS:HE1	31:R:214:ILE:HG22	1.76	0.51
13:B:1083:TYR:O	13:B:1087:SER:OG	2.28	0.51
13:B:1950:THR:OG1	13:B:2060:ARG:NH2	2.42	0.51
19:H:545:ARG:HA	19:H:585:ILE:HG21	1.93	0.51
28:O:97:ARG:HA	28:O:147:LEU:HD11	1.93	0.51
31:R:177:ILE:HG22	37:W:117:PRO:HA	1.92	0.51
34:T:371:HIS:NE2	34:T:389:SER:OG	2.37	0.51
5:5:12:U:H5'	12:A:224:THR:HG23	1.93	0.51
8:6:65:G:N7	12:A:663:ARG:NH1	2.50	0.51
12:A:86:ARG:HH21	21:IN:14:A:H5'	1.75	0.51
13:B:1360:ALA:HB2	13:B:1490:LEU:HD11	1.93	0.51
37:W:103:GLN:NE2	37:W:111:LEU:O	2.43	0.51
13:B:548:VAL:HG22	13:B:587:VAL:HG12	1.93	0.51
12:A:1776:ILE:HB	12:A:1858:PRO:HA	1.92	0.51
13:B:1130:ARG:HG3	13:B:1140:VAL:HG11	1.91	0.51
19:H:590:LEU:HD22	19:H:599:LEU:HD13	1.93	0.51
37:W:572:ASP:OD1	37:W:572:ASP:N	2.42	0.51
34:T:392:PRO:HG3	34:T:415:ILE:HA	1.93	0.51
12:A:923:ASP:OD2	12:A:1439:ARG:NH1	2.44	0.50
28:O:22:ILE:HD13	37:W:111:LEU:HD23	1.93	0.50
34:T:270:VAL:HB	34:T:284:TYR:HB2	1.93	0.50
1:1:123:GLN:HB3	1:1:127:ARG:HH12	1.75	0.50
12:A:539:ARG:NH1	17:EX:-3:A:O2'	2.44	0.50
13:B:639:ILE:HD11	13:B:646:VAL:HB	1.94	0.50
32:S:17:GLU:HB3	32:S:22:ILE:HG12	1.91	0.50
12:A:65:HIS:ND1	12:A:120:TYR:OH	2.42	0.50
12:A:975:VAL:HB	12:A:1099:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1045:GLY:HA2	12:A:1048:MET:HE2	1.94	0.50
13:B:999:GLN:NE2	13:B:1003:GLN:OE1	2.41	0.50
12:A:445:VAL:HG21	17:EX:-9:C:H2'	1.93	0.50
12:A:1382:SER:HA	12:A:1415:GLY:HA2	1.93	0.50
14:C:151:GLU:O	14:C:158:ARG:NH1	2.44	0.50
37:W:286:GLY:HA3	37:W:316:TRP:HH2	1.76	0.50
16:E:166:LEU:HD23	16:E:178:LEU:HD11	1.94	0.50
34:T:312:ALA:HB3	34:T:326:LEU:HB2	1.92	0.50
29:P:213:ASP:OD2	29:P:216:ARG:NH1	2.41	0.50
31:R:122:LYS:HD2	34:T:406:ILE:HD13	1.94	0.50
12:A:1268:ILE:HG22	12:A:1368:LEU:HD21	1.93	0.50
12:A:1686:ASP:OD1	35:U:169:ARG:NH1	2.45	0.50
12:A:1782:ASP:OD2	12:A:1865:ARG:NH1	2.45	0.50
13:B:790:THR:HG21	13:B:793:ASP:HB2	1.93	0.50
28:O:75:SER:OG	28:O:80:VAL:O	2.29	0.50
5:5:56:C:H4'	12:A:100:LEU:HD21	1.94	0.50
13:B:2105:THR:HG23	13:B:2121:LYS:HG3	1.94	0.50
31:R:320:HIS:HA	31:R:323:LYS:HB3	1.94	0.50
12:A:769:LYS:HD3	12:A:1249:MET:HG2	1.93	0.50
12:A:1555:LEU:HD22	12:A:1560:ILE:HD12	1.94	0.50
19:H:474:HIS:HD2	33:SR:23:LEU:H	1.59	0.50
34:T:221:THR:HG21	34:T:486:ILE:HG12	1.94	0.50
34:T:223:SER:OG	34:T:224:ALA:N	2.44	0.50
13:B:1329:ASN:ND2	13:B:1354:SER:O	2.45	0.49
12:A:974:ASN:HB2	12:A:1178:TYR:HB3	1.94	0.49
12:A:1926:THR:O	35:U:355:LYS:NZ	2.40	0.49
12:A:690:MET:HA	12:A:693:ILE:HG12	1.94	0.49
12:A:1312:PRO:HG2	12:A:1314:VAL:HG12	1.94	0.49
13:B:569:LEU:HD22	13:B:586:ILE:HD12	1.93	0.49
14:C:564:THR:HG21	14:C:576:ILE:HA	1.95	0.49
28:O:87:ASP:OD1	28:O:88:LEU:N	2.44	0.49
37:W:121:ASN:HB3	37:W:124:MET:HG2	1.93	0.49
8:6:24:A:N3	8:6:26:U:O2'	2.39	0.49
28:O:175:ARG:HB2	28:O:179:CYS:HB2	1.93	0.49
28:O:261:ILE:HG12	28:O:272:ILE:HG23	1.94	0.49
31:R:192:ALA:O	37:W:142:SER:OG	2.29	0.49
34:T:406:ILE:HG22	34:T:407:GLN:HB2	1.93	0.49
13:B:143:LEU:O	13:B:153:ARG:NH1	2.46	0.49
2:2:150:U:H3	2:2:181:G:H1	1.60	0.49
12:A:1210:LYS:NZ	12:A:1211:ASP:OD1	2.33	0.49
12:A:1832:ARG:NH1	21:IN:2:U:OP1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:183:LYS:HG3	16:E:187:ILE:HD11	1.93	0.49
19:H:636:LEU:HB3	19:H:639:LEU:HD13	1.94	0.49
26:N:64:PHE:HZ	26:N:72:ARG:HD2	1.77	0.49
5:5:23:C:H5'	5:5:24:G:H5''	1.95	0.49
12:A:75:ASP:N	12:A:75:ASP:OD1	2.43	0.49
12:A:1042:GLN:OE1	12:A:1090:ARG:NH1	2.46	0.49
26:N:51:ARG:NH2	37:W:192:PHE:O	2.46	0.49
12:A:245:LEU:HD13	12:A:426:LEU:HB3	1.93	0.49
12:A:862:GLU:HG3	24:L:6:ILE:HG23	1.94	0.49
13:B:739:ARG:NH2	13:B:776:ASP:OD2	2.45	0.49
14:C:676:ALA:HB2	14:C:815:VAL:HB	1.95	0.49
21:IN:18:A:O2'	28:O:83:THR:O	2.28	0.49
28:O:106:ASP:OD1	28:O:106:ASP:N	2.45	0.49
16:E:214:ASP:N	16:E:214:ASP:OD1	2.45	0.49
24:L:59:LYS:O	24:L:91:ARG:NH1	2.46	0.49
32:S:87:HIS:ND1	32:S:89:ASP:OD1	2.45	0.49
2:2:161:U:O2	2:2:163:G:N2	2.46	0.49
12:A:1641:ARG:HD2	35:U:175:PRO:HB2	1.94	0.49
12:A:1942:ALA:HB1	12:A:1986:LEU:HD23	1.93	0.49
13:B:538:ILE:HB	13:B:585:ILE:HG12	1.94	0.49
37:W:484:GLN:HG2	37:W:503:LYS:HB3	1.95	0.49
12:A:948:PRO:HD2	12:A:1455:TRP:HB2	1.95	0.48
12:A:2328:ALA:HB3	13:B:788:GLY:HA2	1.93	0.48
13:B:1538:ARG:NH1	13:B:1665:ASP:OD1	2.46	0.48
28:O:94:ILE:HD12	28:O:202:TYR:HA	1.93	0.48
29:P:57:ARG:NH2	34:T:215:GLY:O	2.46	0.48
31:R:52:PRO:HG2	31:R:71:GLN:HG2	1.95	0.48
1:1:125:ALA:HA	1:1:128:ARG:HB2	1.95	0.48
8:6:57:U:H2'	8:6:58:G:C8	2.48	0.48
12:A:146:SER:HB2	12:A:193:LEU:HD22	1.95	0.48
12:A:698:PRO:HB2	31:R:237:MET:HE1	1.95	0.48
12:A:938:PRO:HB2	12:A:1071:PHE:HA	1.94	0.48
12:A:1095:ILE:HD12	12:A:1097:ILE:HD11	1.93	0.48
12:A:1670:ASP:OD1	12:A:1670:ASP:N	2.44	0.48
35:U:102:TYR:HB3	35:U:156:GLN:HE21	1.78	0.48
12:A:425:PRO:HB2	12:A:428:LYS:HB2	1.95	0.48
12:A:1552:GLN:HG2	12:A:1561:PHE:HB3	1.95	0.48
13:B:1186:LEU:HD13	13:B:1282:LEU:HD22	1.94	0.48
13:B:1998:GLN:NE2	13:B:2003:GLN:OE1	2.46	0.48
16:E:133:VAL:HG21	16:E:169:THR:HG21	1.94	0.48
24:L:15:GLU:HG2	24:L:151:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:150:GLU:HA	24:L:153:SER:HB2	1.95	0.48
8:6:29:A:N6	21:IN:16:G:O2'	2.42	0.48
28:O:40:LYS:HA	28:O:53:THR:HG23	1.96	0.48
32:S:149:SER:O	37:W:100:ARG:NH2	2.46	0.48
37:W:258:PRO:HD2	37:W:265:LEU:HD12	1.96	0.48
8:6:14:C:H2'	8:6:15:A:C8	2.49	0.48
12:A:1212:GLY:HA2	12:A:1276:GLU:HB3	1.95	0.48
13:B:1837:ASN:O	13:B:1840:THR:OG1	2.31	0.48
35:U:102:TYR:HD1	35:U:156:GLN:HB3	1.78	0.48
12:A:841:LEU:HA	12:A:844:GLU:HG2	1.95	0.48
13:B:964:LEU:HD22	13:B:969:LEU:HG	1.94	0.48
19:H:536:ILE:HG23	19:H:544:LEU:HD21	1.96	0.48
37:W:210:GLU:HA	37:W:213:GLN:HB2	1.95	0.48
12:A:1413:ASP:OD1	12:A:1420:ASN:ND2	2.47	0.48
12:A:2328:ALA:HB1	13:B:791:ARG:HH22	1.78	0.48
31:R:53:ARG:N	31:R:57:ASP:OD2	2.45	0.48
34:T:419:LEU:HD22	34:T:427:LEU:HD11	1.96	0.48
37:W:422:ASN:N	37:W:436:THR:O	2.45	0.48
37:W:442:LEU:HB2	37:W:456:ILE:HB	1.94	0.48
4:32:88:ARG:HB3	12:A:1694:ILE:HG12	1.95	0.48
12:A:1630:LEU:HD11	12:A:1696:PRO:HG3	1.94	0.48
12:A:2015:GLU:OE1	18:F:758:ARG:NE	2.41	0.48
13:B:1456:VAL:HG11	13:B:1489:ALA:HB1	1.96	0.48
14:C:474:LEU:HA	14:C:499:GLY:HA3	1.95	0.48
12:A:251:ASP:HB3	12:A:253:ASN:H	1.79	0.48
13:B:782:PHE:HB3	13:B:808:VAL:HB	1.94	0.48
13:B:2067:VAL:HB	13:B:2107:TYR:HB2	1.94	0.48
37:W:534:ILE:HB	37:W:544:SER:HB3	1.96	0.48
16:E:90:ILE:HB	16:E:105:LEU:HB2	1.96	0.47
31:R:69:VAL:O	31:R:71:GLN:NE2	2.47	0.47
37:W:280:GLN:NE2	37:W:282:HIS:O	2.46	0.47
37:W:384:ASP:O	37:W:388:GLN:NE2	2.45	0.47
5:5:12:U:O2	5:5:65:G:N2	2.43	0.47
12:A:76:MET:HB3	12:A:85:LYS:HG2	1.97	0.47
12:A:975:VAL:HG22	12:A:1177:VAL:HG22	1.97	0.47
13:B:603:ARG:HH22	13:B:907:LEU:HD22	1.79	0.47
14:C:86:THR:HG21	34:T:237:LYS:HE3	1.95	0.47
1:1:133:LYS:NZ	2:2:175:G:OP2	2.38	0.47
4:32:80:LYS:HA	4:32:88:ARG:HH22	1.80	0.47
12:A:265:THR:OG1	12:A:328:HIS:O	2.32	0.47
12:A:569:VAL:HG13	12:A:573:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1072:LEU:HD13	12:A:1087:LEU:HD13	1.95	0.47
12:A:1956:PRO:HD2	12:A:1960:THR:HG21	1.96	0.47
26:N:107:GLN:OE1	26:N:109:ARG:NH1	2.43	0.47
4:32:58:ARG:HD2	4:32:62:GLN:HB3	1.96	0.47
12:A:652:LEU:HD23	12:A:655:LEU:HD23	1.96	0.47
12:A:58:LYS:NZ	12:A:482:PHE:O	2.44	0.47
12:A:312:TYR:OH	14:C:853:ARG:NH2	2.47	0.47
12:A:1407:ASP:OD1	12:A:1407:ASP:N	2.44	0.47
13:B:505:THR:HG22	13:B:509:LYS:HZ1	1.78	0.47
28:O:169:VAL:HA	37:W:216:LEU:HD13	1.97	0.47
1:1:62:GLU:O	12:A:1949:ARG:NH1	2.48	0.47
2:2:19:G:H21	29:P:9:PHE:HD2	1.62	0.47
12:A:1592:ASP:OD2	35:U:274:TYR:OH	2.33	0.47
12:A:1790:ILE:HG22	12:A:1800:THR:HG22	1.97	0.47
13:B:986:ARG:O	13:B:990:HIS:ND1	2.47	0.47
8:6:34:G:N2	21:IN:13:C:O2	2.47	0.47
14:C:250:ARG:NH1	14:C:295:ASP:OD2	2.48	0.47
16:E:171:SER:OG	16:E:173:ASP:OD1	2.32	0.47
2:2:151:C:H2'	2:2:152:G:C8	2.49	0.47
12:A:682:ASP:OD2	12:A:746:LYS:NZ	2.40	0.47
13:B:142:VAL:HG12	13:B:153:ARG:HG2	1.96	0.47
14:C:686:THR:HG23	14:C:793:ASP:HB2	1.97	0.47
16:E:155:ASN:ND2	16:E:196:VAL:O	2.46	0.47
35:U:307:VAL:HG12	35:U:309:TYR:H	1.80	0.47
12:A:606:LYS:NZ	12:A:1548:TYR:O	2.41	0.47
12:A:794:TYR:OH	12:A:989:ASP:OD1	2.29	0.47
12:A:1209:HIS:HB3	12:A:1213:VAL:HG21	1.97	0.47
13:B:730:GLU:HA	13:B:733:LYS:HB2	1.97	0.47
14:C:137:HIS:HD2	14:C:238:ASN:H	1.63	0.47
16:E:149:GLY:O	16:E:177:LYS:NZ	2.42	0.47
37:W:428:ASP:OD2	37:W:431:ARG:NH1	2.45	0.47
12:A:893:GLU:HG2	12:A:1016:VAL:HB	1.96	0.46
13:B:300:ARG:O	13:B:304:ASN:ND2	2.47	0.46
14:C:814:ARG:NH1	14:C:951:PHE:O	2.48	0.46
34:T:246:ILE:HG13	34:T:269:GLN:HE22	1.80	0.46
12:A:1159:ASN:ND2	29:P:197:CYS:O	2.49	0.46
16:E:84:ALA:HB2	16:E:90:ILE:HG23	1.97	0.46
26:N:51:ARG:HH21	37:W:193:LEU:HD23	1.80	0.46
34:T:307:SER:OG	34:T:308:ARG:N	2.48	0.46
5:5:58:U:H2'	5:5:59:G:H8	1.81	0.46
37:W:358:LEU:HD23	37:W:367:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:240:ARG:HG2	35:U:137:PRO:HB2	1.98	0.46
12:A:899:MET:HB3	12:A:906:VAL:HB	1.98	0.46
12:A:1282:GLN:NE2	12:A:1336:PRO:O	2.46	0.46
13:B:1671:GLY:HA3	13:B:1860:ILE:HB	1.96	0.46
14:C:507:VAL:HA	14:C:568:PRO:HD3	1.96	0.46
28:O:150:LEU:HD13	28:O:213:LEU:HD23	1.96	0.46
28:O:188:ASP:N	28:O:188:ASP:OD1	2.43	0.46
12:A:419:ARG:NH2	12:A:423:ASP:O	2.49	0.46
13:B:720:GLN:HG2	13:B:807:GLN:HA	1.97	0.46
13:B:987:ILE:HG12	13:B:1097:GLU:HB3	1.97	0.46
16:E:330:ILE:HG12	16:E:346:SER:HB3	1.97	0.46
32:S:56:ILE:HG12	32:S:62:ILE:HG23	1.98	0.46
12:A:930:ALA:HB1	12:A:935:LEU:HB3	1.97	0.46
12:A:1248:LEU:O	12:A:1298:ARG:NH2	2.49	0.46
13:B:987:ILE:HG21	13:B:1098:ILE:HG13	1.97	0.46
14:C:500:THR:OG1	14:C:502:HIS:NE2	2.48	0.46
16:E:127:ALA:HB2	16:E:157:CYS:HB3	1.97	0.46
31:R:251:ILE:HG21	31:R:262:ILE:HG21	1.98	0.46
12:A:1764:SER:H	12:A:1767:ASN:HB2	1.80	0.46
13:B:827:ILE:HD11	13:B:870:ILE:HD11	1.97	0.46
31:R:3:LEU:HA	31:R:6:PHE:HB2	1.97	0.46
34:T:354:ILE:HB	34:T:368:LEU:HB2	1.98	0.46
12:A:834:HIS:HA	12:A:837:LYS:HE3	1.98	0.46
12:A:1808:PHE:HE2	12:A:1893:PHE:HB3	1.80	0.46
13:B:1992:GLU:HA	13:B:1995:ALA:HB3	1.97	0.46
16:E:173:ASP:OD1	16:E:173:ASP:N	2.47	0.46
37:W:397:ASP:OD1	37:W:397:ASP:N	2.47	0.46
5:5:23:C:H5''	5:5:24:G:H8	1.80	0.46
8:6:56:A:OP1	12:A:675:GLN:NE2	2.49	0.46
12:A:1277:ALA:O	12:A:1281:THR:OG1	2.27	0.46
12:A:1827:TRP:O	12:A:1830:GLN:NE2	2.39	0.46
14:C:313:GLN:O	14:C:417:ARG:NH1	2.48	0.46
21:IN:19:G:H21	28:O:196:GLN:HG3	1.79	0.46
35:U:125:ALA:HB2	35:U:150:ALA:HB3	1.97	0.46
13:B:807:GLN:H	13:B:807:GLN:HG2	1.53	0.46
14:C:401:ILE:HD11	14:C:423:PHE:HB2	1.97	0.46
28:O:24:CYS:SG	28:O:81:CYS:CB	3.01	0.46
34:T:373:LYS:HD2	34:T:392:PRO:HB2	1.98	0.46
13:B:1499:ASP:OD2	13:B:1763:ARG:NH1	2.45	0.45
4:32:54:GLY:O	35:U:174:ASN:ND2	2.47	0.45
8:6:25:C:N4	28:O:39:GLU:OE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:2041:LEU:HB2	13:B:2088:ALA:HB3	1.97	0.45
24:L:276:PRO:HA	24:L:279:ILE:HG12	1.98	0.45
12:A:1784:ASN:HD22	12:A:1897:LEU:HD12	1.82	0.45
12:A:1808:PHE:HB2	12:A:1817:LEU:HD11	1.98	0.45
24:L:192:ARG:NH2	24:L:197:GLU:OE2	2.50	0.45
8:6:19:C:H1'	26:N:95:GLN:HG3	1.99	0.45
13:B:1338:THR:O	13:B:1342:SER:OG	2.31	0.45
14:C:85:ASP:OD1	14:C:85:ASP:N	2.49	0.45
19:H:494:LEU:HD11	19:H:547:VAL:HG13	1.98	0.45
35:U:161:PHE:HB2	35:U:166:LYS:HG3	1.99	0.45
1:1:78:GLU:HA	1:1:81:VAL:HG22	1.99	0.45
13:B:1382:MET:HG3	13:B:1652:TRP:CG	2.51	0.45
14:C:924:GLN:HB3	14:C:928:HIS:HB2	1.98	0.45
19:H:544:LEU:HD11	19:H:578:SER:HB2	1.99	0.45
24:L:28:LYS:HB2	24:L:28:LYS:HE3	1.71	0.45
24:L:67:GLU:OE1	24:L:91:ARG:NH2	2.45	0.45
35:U:124:GLY:HA3	35:U:149:ILE:HG23	1.99	0.45
12:A:750:TRP:HH2	12:A:781:ARG:HB3	1.82	0.45
12:A:976:MET:HB2	12:A:976:MET:HE2	1.78	0.45
31:R:179:TYR:OH	37:W:112:SER:OG	2.29	0.45
32:S:23:ILE:HD13	32:S:139:VAL:HG12	1.99	0.45
13:B:641:MET:HG3	13:B:1582:ALA:HB2	1.98	0.45
13:B:785:HIS:HB2	13:B:797:VAL:HG11	1.98	0.45
24:L:8:GLY:N	24:L:40:ARG:O	2.49	0.45
27:NO:108:GLN:O	27:NO:112:ARG:N	2.41	0.45
34:T:435:THR:HG23	34:T:451:HIS:HD2	1.82	0.45
8:6:73:A:OP1	8:6:75:G:O2'	2.35	0.45
13:B:1678:ASP:OD1	13:B:1710:LYS:NZ	2.46	0.45
16:E:306:ASP:HA	37:W:143:LEU:HD22	1.99	0.45
4:32:83:LYS:HB2	4:32:83:LYS:HE3	1.81	0.45
4:32:91:ASP:OD1	4:32:94:ARG:NH2	2.44	0.45
14:C:295:ASP:N	14:C:295:ASP:OD1	2.50	0.45
37:W:505:HIS:HB2	37:W:527:ASP:HB3	1.98	0.45
26:N:5:LYS:NZ	26:N:83:TYR:OH	2.49	0.45
28:O:169:VAL:HG13	37:W:216:LEU:HD22	1.98	0.45
31:R:159:VAL:HG12	31:R:163:MET:HB2	1.99	0.45
39:Z:124:LEU:O	39:Z:128:LYS:N	2.49	0.45
12:A:1781:ASP:OD1	12:A:1864:THR:OG1	2.35	0.44
13:B:294:LYS:HE3	13:B:333:LEU:HD11	1.99	0.44
13:B:1527:ILE:HD13	13:B:1715:LYS:HG2	1.98	0.44
16:E:309:VAL:HB	16:E:323:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R:235:ARG:NH1	31:R:241:GLU:OE1	2.42	0.44
12:A:50:LYS:HB3	12:A:53:PHE:HB2	1.99	0.44
12:A:738:MET:HE3	12:A:738:MET:HB3	1.88	0.44
12:A:1057:ARG:NH1	12:A:1060:GLU:OE1	2.50	0.44
31:R:58:PHE:HZ	31:R:71:GLN:HB3	1.82	0.44
38:X:99:GLU:O	38:X:110:ARG:N	2.49	0.44
8:6:46:G:OP1	24:L:169:ARG:NH1	2.45	0.44
13:B:1432:TRP:HD1	13:B:1470:ILE:HD12	1.82	0.44
13:B:1530:PHE:O	13:B:1708:GLY:N	2.41	0.44
14:C:362:THR:O	14:C:364:SER:N	2.49	0.44
5:5:29:A:H2'	5:5:30:A:H8	1.82	0.44
12:A:718:ARG:NH1	31:R:252:SER:OG	2.50	0.44
12:A:758:ARG:HA	12:A:758:ARG:HD2	1.69	0.44
12:A:1234:ASP:N	12:A:1234:ASP:OD1	2.48	0.44
12:A:1717:ASN:HD21	35:U:178:HIS:CE1	2.36	0.44
13:B:1120:LYS:HG2	13:B:1131:GLN:HG2	1.99	0.44
14:C:208:HIS:HB3	14:C:211:PHE:HD2	1.81	0.44
12:A:265:THR:HG23	12:A:327:VAL:HG13	1.99	0.44
12:A:699:GLU:HG2	34:T:372:LYS:HD3	2.00	0.44
12:A:1676:ILE:HD13	12:A:1706:ASP:HB2	2.00	0.44
13:B:1455:GLU:HG3	13:B:1457:HIS:CE1	2.52	0.44
31:R:182:SER:O	31:R:182:SER:OG	2.34	0.44
12:A:62:PRO:HG3	26:N:53:HIS:CG	2.53	0.44
12:A:1328:LEU:HB3	12:A:1368:LEU:HD13	2.00	0.44
14:C:920:PRO:O	14:C:936:LYS:NZ	2.50	0.44
28:O:196:GLN:HE22	28:O:209:VAL:HG23	1.83	0.44
32:S:93:THR:O	32:S:93:THR:OG1	2.35	0.44
5:5:17:U:H3	5:5:60:G:H1	1.66	0.44
12:A:168:PRO:HG2	12:A:559:ASP:HB3	1.99	0.44
13:B:787:ALA:HA	13:B:794:ARG:HD3	2.00	0.44
16:E:69:VAL:HG11	16:E:351:LEU:HD21	2.00	0.44
16:E:160:ALA:HB3	16:E:166:LEU:H	1.83	0.44
29:P:42:LYS:HZ1	34:T:276:GLU:HB3	1.83	0.44
12:A:138:PRO:HB2	12:A:238:LEU:HD13	2.00	0.44
12:A:292:ASP:HB2	12:A:1136:ARG:HE	1.82	0.44
13:B:1180:LEU:O	13:B:1215:HIS:NE2	2.49	0.44
13:B:1342:SER:O	13:B:1486:ARG:NH2	2.51	0.44
13:B:1979:VAL:HG13	13:B:1984:ASP:HB2	2.00	0.44
16:E:75:HIS:ND1	16:E:77:ASN:OD1	2.51	0.44
28:O:232:THR:HB	28:O:274:PHE:HB2	2.00	0.44
37:W:307:CYS:HB3	37:W:335:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:610:HIS:NE2	59:U:601:IHP:O21	2.50	0.44
12:A:1248:LEU:HD21	12:A:1295:ILE:HD13	2.00	0.44
12:A:1681:ARG:NH2	35:U:170:TRP:O	2.45	0.44
12:A:1737:ASN:HB3	12:A:1740:LEU:HB2	2.00	0.44
12:A:1800:THR:HG21	21:IN:145:U:H5'	1.99	0.44
37:W:527:ASP:OD1	37:W:531:LYS:N	2.51	0.44
12:A:612:ILE:HD11	12:A:632:ALA:HB3	1.99	0.43
13:B:1313:ARG:HA	13:B:1313:ARG:HD2	1.91	0.43
24:L:270:LYS:HG3	24:L:278:ALA:HB2	2.00	0.43
13:B:1824:ILE:HD13	13:B:1922:LEU:HD23	2.00	0.43
14:C:496:VAL:O	14:C:547:GLY:N	2.47	0.43
16:E:130:ASP:N	16:E:130:ASP:OD1	2.47	0.43
16:E:239:THR:O	16:E:290:ARG:NH1	2.50	0.43
35:U:318:THR:O	35:U:321:THR:OG1	2.36	0.43
5:5:64:G:H2'	5:5:65:G:H8	1.83	0.43
12:A:58:LYS:HE2	12:A:58:LYS:HB3	1.83	0.43
12:A:813:THR:HG21	12:A:996:LEU:HD22	2.01	0.43
13:B:905:ILE:HG22	13:B:981:VAL:HG22	1.99	0.43
26:N:94:LYS:HA	26:N:94:LYS:HD3	1.76	0.43
2:2:15:U:H5'	2:2:16:U:H2'	2.00	0.43
5:5:37:G:H2'	5:5:38:C:C6	2.53	0.43
12:A:1892:PRO:HD3	12:A:1941:ARG:HH21	1.83	0.43
16:E:217:ILE:HB	16:E:231:MET:HB2	2.00	0.43
28:O:259:ARG:HD2	28:O:273:GLN:HB3	2.00	0.43
13:B:1936:LEU:HD23	13:B:1936:LEU:HA	1.89	0.43
14:C:311:SER:HB3	14:C:316:ILE:HB	2.00	0.43
16:E:251:LEU:HD23	16:E:291:CYS:HB3	1.99	0.43
28:O:261:ILE:HG23	28:O:272:ILE:HG12	2.00	0.43
31:R:103:ARG:NH1	31:R:110:LYS:O	2.51	0.43
37:W:188:ASN:OD1	37:W:188:ASN:N	2.48	0.43
37:W:386:ASP:OD2	37:W:387:LYS:NZ	2.52	0.43
12:A:1318:THR:HB	12:A:1324:GLY:HA3	2.01	0.43
14:C:485:ASP:OD1	14:C:485:ASP:N	2.47	0.43
2:2:25:G:C6	8:6:52:U:O2	2.72	0.43
12:A:420:ARG:NH2	12:A:423:ASP:OD1	2.51	0.43
13:B:328:ILE:O	13:B:332:THR:OG1	2.37	0.43
24:L:130:PRO:HB2	24:L:131:ASN:H	1.69	0.43
24:L:192:ARG:HA	24:L:192:ARG:HD3	1.82	0.43
31:R:60:ASP:HB3	32:S:134:GLN:HA	2.01	0.43
37:W:313:ILE:HB	37:W:328:PHE:HB2	2.00	0.43
12:A:259:ASP:OD1	12:A:259:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:349:PHE:HZ	14:C:354:ARG:HD3	1.84	0.43
34:T:267:ASP:HB3	34:T:269:GLN:HG2	1.99	0.43
37:W:190:ASP:OD1	37:W:190:ASP:N	2.42	0.43
37:W:270:PRO:HB3	37:W:518:PRO:HB3	2.01	0.43
12:A:1210:LYS:HE2	19:H:468:ASP:HA	2.01	0.43
12:A:1490:PHE:O	12:A:1493:THR:OG1	2.36	0.43
28:O:129:ASP:OD1	28:O:129:ASP:N	2.46	0.43
32:S:91:LYS:HA	32:S:91:LYS:HD3	1.92	0.43
34:T:320:LYS:HE3	34:T:320:LYS:HB2	1.91	0.43
35:U:106:VAL:HB	35:U:151:PRO:HB2	2.00	0.43
37:W:208:PRO:HG2	37:W:213:GLN:HG2	2.01	0.43
1:1:123:GLN:O	1:1:127:ARG:NH1	2.51	0.43
8:6:23:U:C5	26:N:118:ILE:HD12	2.54	0.43
12:A:947:PRO:HD2	12:A:950:LEU:HD23	2.01	0.43
12:A:1782:ASP:HB3	12:A:1841:THR:HG21	2.01	0.43
12:A:1838:LYS:HB3	12:A:1871:PRO:HG2	2.00	0.43
13:B:1590:LEU:HD11	13:B:1597:LEU:HD11	2.01	0.43
14:C:255:VAL:HG21	14:C:285:VAL:HG11	2.01	0.43
24:L:10:VAL:HG11	24:L:138:ARG:HD3	2.01	0.43
37:W:103:GLN:HG2	37:W:108:ARG:HD3	2.01	0.43
4:32:79:LYS:O	4:32:88:ARG:NH2	2.50	0.42
12:A:982:GLU:HG3	12:A:1169:GLN:H	1.84	0.42
13:B:442:TYR:HA	13:B:693:THR:H	1.84	0.42
16:E:313:ASP:HB3	16:E:316:SER:HB3	2.01	0.42
37:W:228:LYS:HD2	37:W:228:LYS:HA	1.86	0.42
12:A:101:LYS:NZ	12:A:104:GLU:OE2	2.41	0.42
12:A:373:ASP:OD1	12:A:373:ASP:N	2.52	0.42
12:A:965:VAL:O	12:A:974:ASN:ND2	2.49	0.42
12:A:977:LEU:HD22	12:A:1097:ILE:HD12	2.01	0.42
12:A:1088:PHE:HD1	12:A:1097:ILE:HG23	1.84	0.42
12:A:1370:ARG:NH1	19:H:504:GLU:OE1	2.52	0.42
12:A:1783:THR:HG22	12:A:1865:ARG:HD2	2.01	0.42
37:W:239:THR:HG21	37:W:364:GLY:HA3	2.01	0.42
12:A:292:ASP:HB2	12:A:1136:ARG:HH21	1.84	0.42
12:A:845:ARG:HD3	12:A:845:ARG:HA	1.83	0.42
13:B:1346:VAL:HG12	13:B:1510:SER:HB2	2.01	0.42
31:R:272:GLY:O	31:R:276:GLN:NE2	2.50	0.42
37:W:398:LYS:HD2	37:W:418:LEU:HA	2.02	0.42
16:E:116:HIS:HB3	16:E:159:PRO:HD3	2.01	0.42
26:N:131:ILE:HD12	28:O:177:GLU:HB3	2.02	0.42
30:Q:827:THR:HA	30:Q:1136:GLN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:284:TRP:HE1	37:W:322:ARG:HB3	1.84	0.42
35:U:122:ASN:HB2	35:U:130:LYS:HG3	2.02	0.42
12:A:436:PRO:HG2	12:A:439:GLN:HG3	2.01	0.42
4:32:58:ARG:NH2	35:U:177:GLU:OE1	2.52	0.42
12:A:696:MET:HE3	12:A:696:MET:HB2	1.86	0.42
12:A:1698:PRO:HB2	35:U:182:VAL:HG22	2.01	0.42
12:A:1761:PRO:HD2	35:U:293:ARG:HH12	1.83	0.42
14:C:221:ILE:O	14:C:549:TRP:NE1	2.51	0.42
16:E:133:VAL:HB	16:E:147:LEU:HB2	2.01	0.42
19:H:628:ILE:HA	19:H:640:THR:HG21	2.01	0.42
32:S:76:SER:OG	32:S:77:ILE:N	2.53	0.42
34:T:214:PRO:HG3	34:T:256:THR:HG22	2.02	0.42
35:U:86:ARG:HA	35:U:86:ARG:HD3	1.81	0.42
37:W:137:TYR:OH	37:W:165:LEU:N	2.53	0.42
37:W:297:PHE:HB2	37:W:303:LEU:HB2	2.01	0.42
37:W:392:VAL:HG22	37:W:400:ILE:HG22	2.02	0.42
5:5:100:U:H2'	5:5:101:U:H6	1.85	0.42
14:C:559:ILE:HD13	14:C:559:ILE:HG21	1.88	0.42
34:T:213:GLU:HG3	34:T:218:TRP:CE2	2.54	0.42
34:T:257:ARG:NE	34:T:301:ASP:OD2	2.51	0.42
34:T:270:VAL:HG21	34:T:305:THR:HG21	2.01	0.42
12:A:1786:TYR:HE1	12:A:1802:PRO:HB3	1.85	0.42
12:A:1889:LEU:HD23	12:A:1891:LEU:HD11	2.00	0.42
13:B:711:LYS:HE2	13:B:868:ILE:HG12	2.00	0.42
14:C:137:HIS:HA	14:C:238:ASN:HB3	2.01	0.42
16:E:58:PRO:O	16:E:60:MET:N	2.46	0.42
18:F:655:TRP:HB3	18:F:660:GLN:HE21	1.85	0.42
18:F:686:ILE:HG12	18:F:715:PRO:HB3	2.01	0.42
28:O:22:ILE:H	28:O:82:GLN:HE21	1.68	0.42
35:U:135:GLU:OE1	35:U:138:ARG:NH1	2.52	0.42
12:A:670:LYS:HB3	12:A:670:LYS:HE2	1.83	0.42
12:A:1764:SER:OG	12:A:1765:SER:N	2.52	0.42
13:B:606:THR:HA	13:B:609:VAL:HG22	2.01	0.42
13:B:690:VAL:HG13	13:B:870:ILE:HA	2.01	0.42
13:B:1651:CYS:O	13:B:1690:HIS:NE2	2.46	0.42
16:E:61:LEU:HD11	16:E:350:ARG:HD2	2.02	0.42
34:T:346:ILE:HD12	34:T:356:LEU:HG	2.01	0.42
37:W:296:LEU:HD23	37:W:296:LEU:HA	1.90	0.42
12:A:881:ILE:HD11	12:A:917:ILE:HG22	2.02	0.41
12:A:941:LYS:HG3	12:A:951:LEU:HD22	2.02	0.41
12:A:1784:ASN:HB3	12:A:1787:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1572:THR:HB	13:B:1645:VAL:HG11	2.02	0.41
13:B:1777:SER:OG	13:B:1778:HIS:N	2.52	0.41
12:A:583:ALA:HA	12:A:605:CYS:HB3	2.01	0.41
13:B:1005:LEU:HD22	13:B:1107:LEU:HD21	2.02	0.41
16:E:75:HIS:NE2	16:E:121:GLY:O	2.52	0.41
34:T:295:ASP:OD2	34:T:338:CYS:N	2.52	0.41
34:T:399:LYS:HB2	34:T:406:ILE:HD11	2.02	0.41
1:1:130:LYS:HB2	1:1:130:LYS:HE2	1.86	0.41
12:A:345:PRO:HG3	35:U:140:VAL:HG22	2.03	0.41
12:A:1526:LEU:HD12	12:A:1529:ILE:HD12	2.02	0.41
12:A:1768:TYR:OH	35:U:344:GLN:NE2	2.44	0.41
13:B:729:LYS:HD2	13:B:729:LYS:HA	1.88	0.41
13:B:1072:LEU:HB2	13:B:1078:MET:HG2	2.02	0.41
14:C:476:CYS:HB3	14:C:565:ILE:HB	2.02	0.41
16:E:155:ASN:O	16:E:290:ARG:NH2	2.53	0.41
26:N:8:ARG:HD2	26:N:8:ARG:HA	1.93	0.41
28:O:74:CYS:O	28:O:202:TYR:OH	2.32	0.41
2:2:159:U:H2'	2:2:160:A:H8	1.85	0.41
12:A:591:MET:HE2	12:A:598:LEU:HD11	2.02	0.41
12:A:942:PRO:HG2	12:A:1438:VAL:HG22	2.03	0.41
13:B:307:VAL:HG22	13:B:318:ILE:HD13	2.02	0.41
24:L:24:MET:HB3	31:R:261:THR:HG23	2.02	0.41
29:P:187:ARG:HA	29:P:187:ARG:HD3	1.90	0.41
34:T:216:ASN:HD22	34:T:216:ASN:HA	1.62	0.41
12:A:89:LEU:HD23	12:A:89:LEU:HA	1.84	0.41
12:A:791:GLN:OE1	12:A:1028:TYR:N	2.51	0.41
12:A:828:PRO:HB2	12:A:882:LYS:HE2	2.03	0.41
13:B:1034:LYS:HA	13:B:1037:LEU:HB2	2.02	0.41
13:B:2043:ARG:HB3	13:B:2086:GLN:HA	2.02	0.41
28:O:73:THR:HG23	28:O:125:ILE:HD12	2.01	0.41
35:U:130:LYS:HB3	35:U:130:LYS:HE2	1.85	0.41
37:W:443:ARG:NH1	37:W:452:ASP:OD2	2.50	0.41
12:A:274:PRO:HG3	33:SR:1:MET:HB3	2.02	0.41
12:A:1434:LYS:O	12:A:1439:ARG:NH2	2.51	0.41
13:B:502:CYS:HB3	13:B:654:THR:HA	2.02	0.41
13:B:898:PRO:HA	13:B:960:ALA:HB1	2.03	0.41
19:H:576:THR:H	19:H:579:SER:HB3	1.86	0.41
37:W:552:VAL:HG13	37:W:571:TRP:CD1	2.52	0.41
12:A:661:GLU:HA	31:R:213:LYS:HA	2.02	0.41
12:A:775:ASN:HA	12:A:778:ARG:HB2	2.02	0.41
16:E:280:ASN:HA	16:E:310:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:648:LYS:HA	19:H:648:LYS:HD3	1.89	0.41
28:O:114:LYS:HB3	28:O:114:LYS:HE2	1.88	0.41
32:S:58:LYS:HE2	32:S:144:MET:HG2	2.02	0.41
12:A:1443:LYS:HA	12:A:1443:LYS:HD3	1.87	0.41
16:E:150:HIS:CG	16:E:171:SER:HG	2.35	0.41
24:L:214:ILE:HB	24:L:217:GLU:HB3	2.03	0.41
31:R:158:LYS:NZ	34:T:322:SER:O	2.54	0.41
32:S:6:PRO:O	32:S:37:LYS:NZ	2.54	0.41
37:W:477:ALA:HA	37:W:487:ILE:HD13	2.03	0.41
12:A:96:PRO:HG3	12:A:648:LEU:HB3	2.02	0.41
12:A:114:ARG:HG2	12:A:116:VAL:HG13	2.02	0.41
12:A:1713:SER:OG	12:A:1714:ALA:N	2.54	0.41
13:B:1011:GLU:HG2	13:B:1110:LYS:HG2	2.03	0.41
16:E:321:TYR:OH	16:E:356:ILE:O	2.33	0.41
18:F:682:TYR:CZ	18:F:712:ALA:HB2	2.56	0.41
19:H:584:LYS:HG3	19:H:634:ILE:HG23	2.02	0.41
28:O:239:LEU:HD22	28:O:270:ALA:HB2	2.02	0.41
37:W:476:LEU:HG	37:W:490:ALA:HB2	2.02	0.41
12:A:976:MET:HE2	12:A:1185:LEU:HD21	2.02	0.41
24:L:49:ARG:NH1	24:L:133:GLU:O	2.44	0.41
24:L:49:ARG:NH1	24:L:135:LYS:O	2.44	0.41
31:R:152:GLU:HA	31:R:155:VAL:HG22	2.03	0.41
32:S:165:SER:OG	32:S:166:GLY:N	2.54	0.41
12:A:1729:ALA:HA	35:U:278:LEU:HD22	2.03	0.40
12:A:1732:LYS:HG2	35:U:278:LEU:HA	2.02	0.40
12:A:1735:LYS:HE2	12:A:1735:LYS:HB3	1.89	0.40
16:E:263:ASP:OD1	16:E:263:ASP:N	2.43	0.40
21:IN:18:A:OP2	28:O:163:HIS:NE2	2.46	0.40
22:J:326:VAL:HA	22:J:329:ALA:HB3	2.03	0.40
28:O:173:CYS:HB3	37:W:206:ALA:HB3	2.02	0.40
35:U:121:GLU:HG2	35:U:130:LYS:HD3	2.03	0.40
1:1:90:TYR:O	1:1:94:ASP:N	2.53	0.40
2:2:22:U:H3	8:6:53:A:H61	1.69	0.40
5:5:24:G:O2'	5:5:26:A:N7	2.54	0.40
12:A:1289:VAL:HG13	12:A:1357:MET:HG3	2.02	0.40
13:B:725:VAL:HG12	13:B:727:SER:H	1.86	0.40
13:B:1534:HIS:CE1	13:B:1536:GLN:HB2	2.56	0.40
13:B:1550:ILE:HG23	13:B:1559:VAL:HG21	2.03	0.40
19:H:560:LEU:HD23	19:H:560:LEU:HA	1.91	0.40
21:IN:135:G:N7	21:IN:136:U:N3	2.69	0.40
37:W:434:VAL:HG21	37:W:476:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:24:A:H8	2:2:24:A:H2'	1.79	0.40
8:6:40:U:H2'	8:6:41:A:H8	1.85	0.40
8:6:48:A:OP2	24:L:33:ARG:NH2	2.52	0.40
12:A:142:SER:HA	12:A:242:ALA:HB2	2.02	0.40
12:A:543:ALA:HB2	12:A:651:TRP:HB3	2.03	0.40
12:A:902:TYR:HB2	12:A:1242:ASN:HB3	2.03	0.40
12:A:1683:LYS:HD3	12:A:1683:LYS:HA	1.74	0.40
13:B:1815:LEU:HD11	13:B:1833:SER:HB2	2.03	0.40
13:B:696:LYS:HB3	13:B:698:ILE:HG12	2.04	0.40
13:B:1737:ASN:HB2	13:B:1796:LEU:HD21	2.04	0.40
13:B:1923:ILE:HD13	13:B:1946:ALA:HA	2.03	0.40
34:T:261:LEU:HB2	34:T:275:LEU:HD11	2.03	0.40
37:W:513:GLN:HE22	37:W:557:VAL:HG22	1.87	0.40
13:B:1201:GLU:HB3	13:B:1251:LEU:HD11	2.03	0.40
24:L:16:ASP:OD2	24:L:49:ARG:NH2	2.49	0.40
35:U:370:GLU:O	35:U:374:GLU:N	2.39	0.40
37:W:218:GLU:HG2	37:W:222:LYS:HE3	2.04	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	
1	1	121/184 (66%)	113 (93%)	7 (6%)	1 (1%)	19	51
3	3	78/476 (16%)	78 (100%)	0	0	100	100
4	32	58/112 (52%)	56 (97%)	2 (3%)	0	100	100
6	50	206/339 (61%)	194 (94%)	10 (5%)	2 (1%)	15	46
7	56	99/222 (45%)	98 (99%)	1 (1%)	0	100	100
9	7	388/411 (94%)	377 (97%)	10 (3%)	1 (0%)	41	71
10	8	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	9	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
12	A	2244/2335 (96%)	2109 (94%)	132 (6%)	3 (0%)	51	81
13	B	1856/2136 (87%)	1786 (96%)	67 (4%)	3 (0%)	47	77
14	C	897/972 (92%)	821 (92%)	72 (8%)	4 (0%)	34	66
15	D	68/285 (24%)	67 (98%)	1 (2%)	0	100	100
16	E	304/357 (85%)	281 (92%)	21 (7%)	2 (1%)	22	54
18	F	120/758 (16%)	109 (91%)	11 (9%)	0	100	100
19	H	455/908 (50%)	439 (96%)	15 (3%)	1 (0%)	47	77
20	I	725/855 (85%)	710 (98%)	15 (2%)	0	100	100
22	J	600/848 (71%)	572 (95%)	26 (4%)	2 (0%)	41	71
23	K	187/225 (83%)	174 (93%)	12 (6%)	1 (0%)	29	61
24	L	545/802 (68%)	524 (96%)	20 (4%)	1 (0%)	47	77
25	M	222/243 (91%)	215 (97%)	6 (3%)	1 (0%)	29	61
26	N	142/144 (99%)	131 (92%)	9 (6%)	2 (1%)	11	38
27	NO	168/301 (56%)	158 (94%)	8 (5%)	2 (1%)	13	42
28	O	287/420 (68%)	272 (95%)	15 (5%)	0	100	100
29	P	100/229 (44%)	94 (94%)	6 (6%)	0	100	100
30	Q	1304/1485 (88%)	1267 (97%)	34 (3%)	3 (0%)	47	77
31	R	322/536 (60%)	296 (92%)	25 (8%)	1 (0%)	41	71
32	S	162/166 (98%)	148 (91%)	14 (9%)	0	100	100
33	SR	66/2752 (2%)	59 (89%)	7 (11%)	0	100	100
34	T	359/514 (70%)	340 (95%)	16 (4%)	3 (1%)	19	51
35	U	291/586 (50%)	272 (94%)	18 (6%)	1 (0%)	41	71
36	V	727/1220 (60%)	708 (97%)	18 (2%)	1 (0%)	51	81
37	W	511/579 (88%)	460 (90%)	51 (10%)	0	100	100
38	X	62/451 (14%)	59 (95%)	3 (5%)	0	100	100
39	Z	49/166 (30%)	49 (100%)	0	0	100	100
40	a	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
40	h	81/126 (64%)	75 (93%)	6 (7%)	0	100	100
41	b	81/240 (34%)	80 (99%)	1 (1%)	0	100	100
41	i	80/240 (33%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	c	78/119 (66%)	73 (94%)	5 (6%)	0	100	100
42	j	78/119 (66%)	76 (97%)	2 (3%)	0	100	100
43	d	85/118 (72%)	82 (96%)	3 (4%)	0	100	100
43	k	91/118 (77%)	88 (97%)	3 (3%)	0	100	100
44	e	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
44	l	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
45	f	70/86 (81%)	70 (100%)	0	0	100	100
45	m	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
46	g	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
46	n	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
47	o	160/255 (63%)	146 (91%)	14 (9%)	0	100	100
48	p	90/225 (40%)	88 (98%)	2 (2%)	0	100	100
49	q	99/504 (20%)	98 (99%)	1 (1%)	0	100	100
49	r	115/504 (23%)	111 (96%)	4 (4%)	0	100	100
49	s	130/504 (26%)	125 (96%)	4 (3%)	1 (1%)	19	51
49	t	99/504 (20%)	96 (97%)	2 (2%)	1 (1%)	15	46
50	w	532/646 (82%)	514 (97%)	18 (3%)	0	100	100
51	x	120/289 (42%)	118 (98%)	2 (2%)	0	100	100
52	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
53	z	66/415 (16%)	64 (97%)	1 (2%)	1 (2%)	10	38
All	All	16536/28198 (59%)	15749 (95%)	748 (4%)	39 (0%)	50	77

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	B	1584	ILE
16	E	59	ILE
30	Q	1078	LEU
49	s	65	PRO
6	50	322	SER
9	7	340	GLY
10	8	115	GLY
13	B	957	VAL
16	E	58	PRO
22	J	329	ALA

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Mol	Chain	Res	Type
26	N	135	THR
27	NO	126	LEU
30	Q	279	LEU
30	Q	406	LEU
12	A	1636	LYS
13	B	831	THR
14	C	363	SER
22	J	179	VAL
24	L	215	PRO
34	T	456	PRO
14	C	702	ASN
27	NO	50	LEU
31	R	10	PRO
34	T	458	SER
6	50	295	THR
14	C	821	LEU
19	H	501	ARG
23	K	62	GLU
53	z	411	GLY
12	A	295	GLU
12	A	370	PRO
25	M	117	ARG
26	N	128	VAL
36	V	640	GLN
49	t	15	PRO
14	C	97	VAL
1	1	47	PRO
35	U	267	ILE
34	T	32	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	106/157 (68%)	105 (99%)	1 (1%)	78 87
4	32	54/99 (54%)	53 (98%)	1 (2%)	57 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	A	1792/2108 (85%)	1783 (100%)	9 (0%)	88	93
13	B	1668/1908 (87%)	1513 (91%)	155 (9%)	9	30
14	C	799/866 (92%)	770 (96%)	29 (4%)	35	63
16	E	263/300 (88%)	262 (100%)	1 (0%)	91	95
18	F	110/655 (17%)	109 (99%)	1 (1%)	78	87
19	H	182/838 (22%)	180 (99%)	2 (1%)	73	85
24	L	233/709 (33%)	232 (100%)	1 (0%)	91	95
26	N	130/130 (100%)	129 (99%)	1 (1%)	81	89
28	O	254/361 (70%)	253 (100%)	1 (0%)	91	95
29	P	94/203 (46%)	94 (100%)	0	100	100
31	R	275/457 (60%)	274 (100%)	1 (0%)	91	95
32	S	133/134 (99%)	132 (99%)	1 (1%)	81	89
33	SR	21/2432 (1%)	20 (95%)	1 (5%)	25	56
34	T	316/441 (72%)	312 (99%)	4 (1%)	69	82
35	U	258/520 (50%)	253 (98%)	5 (2%)	57	77
37	W	451/502 (90%)	445 (99%)	6 (1%)	69	82
40	a	74/101 (73%)	74 (100%)	0	100	100
40	h	73/101 (72%)	73 (100%)	0	100	100
41	b	68/177 (38%)	68 (100%)	0	100	100
41	i	75/177 (42%)	75 (100%)	0	100	100
42	c	75/101 (74%)	75 (100%)	0	100	100
42	j	75/101 (74%)	75 (100%)	0	100	100
43	d	85/110 (77%)	84 (99%)	1 (1%)	71	83
43	k	91/110 (83%)	91 (100%)	0	100	100
44	e	74/84 (88%)	74 (100%)	0	100	100
44	l	76/84 (90%)	76 (100%)	0	100	100
45	f	61/74 (82%)	60 (98%)	1 (2%)	62	79
45	m	61/74 (82%)	61 (100%)	0	100	100
46	g	63/66 (96%)	63 (100%)	0	100	100
46	n	63/66 (96%)	62 (98%)	1 (2%)	62	79
47	o	139/218 (64%)	138 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	p	81/195 (42%)	81 (100%)	0	100	100
53	z	25/366 (7%)	25 (100%)	0	100	100
All	All	8398/15025 (56%)	8174 (97%)	224 (3%)	48	71

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	102	LYS
4	32	79	LYS
12	A	88	TYR
12	A	258	PHE
12	A	395	THR
12	A	756	TYR
12	A	1210	LYS
12	A	1359	HIS
12	A	1370	ARG
12	A	1637	TRP
12	A	1868	MET
13	B	130	ASP
13	B	159	LEU
13	B	164	THR
13	B	290	LEU
13	B	300	ARG
13	B	332	THR
13	B	334	LEU
13	B	406	ARG
13	B	409	LEU
13	B	410	ASP
13	B	414	LEU
13	B	420	SER
13	B	432	ASP
13	B	436	ARG
13	B	446	HIS
13	B	447	VAL
13	B	451	LYS
13	B	467	LEU
13	B	488	LEU
13	B	489	TYR
13	B	495	THR
13	B	500	LEU
13	B	505	THR

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Mol	Chain	Res	Type
13	B	533	VAL
13	B	547	LEU
13	B	550	GLU
13	B	572	ASP
13	B	576	CYS
13	B	584	GLN
13	B	591	GLU
13	B	595	ILE
13	B	602	GLU
13	B	610	ARG
13	B	623	ASP
13	B	637	ARG
13	B	643	GLN
13	B	673	LEU
13	B	690	VAL
13	B	701	PHE
13	B	712	ILE
13	B	728	ARG
13	B	743	LEU
13	B	759	THR
13	B	772	LEU
13	B	773	GLU
13	B	775	LYS
13	B	782	PHE
13	B	786	HIS
13	B	791	ARG
13	B	807	GLN
13	B	810	VAL
13	B	820	ASN
13	B	837	GLU
13	B	849	ILE
13	B	850	LEU
13	B	852	MET
13	B	855	ARG
13	B	869	LEU
13	B	877	GLN
13	B	885	GLN
13	B	887	LEU
13	B	894	VAL
13	B	897	LEU
13	B	900	MET
13	B	901	LEU

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Mol	Chain	Res	Type
13	B	910	VAL
13	B	920	LEU
13	B	941	ASP
13	B	942	ASP
13	B	957	VAL
13	B	972	TYR
13	B	975	LYS
13	B	992	TYR
13	B	1016	ARG
13	B	1020	LEU
13	B	1030	ARG
13	B	1053	GLU
13	B	1063	LEU
13	B	1087	SER
13	B	1100	LEU
13	B	1102	ARG
13	B	1135	LEU
13	B	1143	ILE
13	B	1165	ILE
13	B	1166	ARG
13	B	1186	LEU
13	B	1224	LEU
13	B	1225	VAL
13	B	1228	VAL
13	B	1234	LEU
13	B	1241	LEU
13	B	1244	LYS
13	B	1301	LEU
13	B	1312	LEU
13	B	1320	LEU
13	B	1343	ASP
13	B	1375	ARG
13	B	1399	ASP
13	B	1408	LEU
13	B	1413	SER
13	B	1419	LEU
13	B	1421	LYS
13	B	1430	GLU
13	B	1436	SER
13	B	1442	ARG
13	B	1443	LYS
13	B	1455	GLU

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Mol	Chain	Res	Type
13	B	1456	VAL
13	B	1474	MET
13	B	1477	ILE
13	B	1480	GLN
13	B	1482	GLU
13	B	1492	SER
13	B	1567	LYS
13	B	1655	ASN
13	B	1682	TYR
13	B	1707	GLN
13	B	1728	LEU
13	B	1731	CYS
13	B	1734	ASP
13	B	1742	THR
13	B	1750	ASP
13	B	1762	ARG
13	B	1779	ARG
13	B	1788	LEU
13	B	1817	MET
13	B	1823	TYR
13	B	1826	TYR
13	B	1834	MET
13	B	1840	THR
13	B	1865	ASP
13	B	1880	ASN
13	B	1956	LYS
13	B	1969	GLU
13	B	1970	HIS
13	B	1996	LEU
13	B	1997	LEU
13	B	1999	LEU
13	B	2000	THR
13	B	2017	ILE
13	B	2027	ASP
13	B	2029	ILE
13	B	2030	ARG
13	B	2031	SER
13	B	2047	VAL
13	B	2055	LEU
13	B	2070	ASP
13	B	2082	LEU
13	B	2084	LEU

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Mol	Chain	Res	Type
13	B	2092	LEU
13	B	2102	HIS
13	B	2105	THR
13	B	2109	MET
13	B	2121	LYS
13	B	2125	ASP
14	C	129	ILE
14	C	165	LEU
14	C	215	VAL
14	C	325	LYS
14	C	381	LEU
14	C	474	LEU
14	C	475	MET
14	C	476	CYS
14	C	480	LYS
14	C	531	TRP
14	C	556	ASP
14	C	593	GLU
14	C	624	SER
14	C	650	GLU
14	C	655	VAL
14	C	733	TRP
14	C	740	THR
14	C	749	THR
14	C	753	GLU
14	C	776	GLU
14	C	785	ARG
14	C	792	LEU
14	C	798	GLN
14	C	811	THR
14	C	824	THR
14	C	878	ILE
14	C	903	HIS
14	C	907	VAL
14	C	952	PHE
16	E	243	LEU
18	F	739	GLN
19	H	481	PHE
19	H	494	LEU
24	L	261	LYS
26	N	80	LYS
28	O	222	ARG

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Mol	Chain	Res	Type
31	R	315	LYS
32	S	139	VAL
33	SR	1	MET
34	T	29	ASN
34	T	302	VAL
34	T	364	THR
34	T	456	PRO
35	U	34	ARG
35	U	321	THR
35	U	329	LEU
35	U	352	LEU
35	U	390	LEU
37	W	255	LEU
37	W	336	ARG
37	W	436	THR
37	W	440	LYS
37	W	515	ASP
37	W	552	VAL
43	d	110	LEU
45	f	41	ASN
46	n	43	ASP
47	o	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
12	A	160	HIS
12	A	270	ASN
12	A	434	HIS
12	A	483	GLN
12	A	505	ASN
12	A	512	ASN
12	A	664	HIS
12	A	755	HIS
12	A	775	ASN
12	A	792	HIS
12	A	834	HIS
12	A	994	ASN
12	A	1014	ASN
12	A	1018	ASN
12	A	1023	ASN
12	A	1066	GLN

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Mol	Chain	Res	Type
12	A	1096	HIS
12	A	1159	ASN
12	A	1169	GLN
12	A	1337	GLN
12	A	1468	ASN
12	A	1476	GLN
12	A	1586	HIS
12	A	1615	HIS
12	A	1658	GLN
12	A	1717	ASN
12	A	1946	ASN
12	A	1947	ASN
13	B	425	ASN
13	B	805	HIS
13	B	951	GLN
13	B	1101	ASN
13	B	1337	ASN
13	B	1659	HIS
13	B	1686	GLN
13	B	1880	ASN
13	B	1898	HIS
14	C	82	GLN
14	C	154	HIS
16	E	101	ASN
16	E	165	GLN
16	E	225	ASN
18	F	660	GLN
19	H	474	HIS
19	H	499	GLN
19	H	600	ASN
24	L	245	GLN
26	N	116	ASN
28	O	82	GLN
29	P	56	ASN
31	R	84	ASN
31	R	320	HIS
32	S	31	HIS
32	S	148	ASN
34	T	50	ASN
34	T	191	HIS
34	T	216	ASN
34	T	269	GLN

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Mol	Chain	Res	Type
34	T	417	ASN
34	T	446	ASN
34	T	451	HIS
34	T	500	HIS
35	U	84	HIS
35	U	85	GLN
35	U	122	ASN
35	U	154	HIS
35	U	156	GLN
35	U	171	ASN
37	W	145	ASN
37	W	147	GLN
37	W	250	GLN
37	W	402	GLN
37	W	462	HIS
37	W	479	GLN
40	a	42	GLN
41	b	76	ASN
43	d	39	ASN
43	d	69	ASN
43	d	91	ASN
45	f	68	ASN
40	h	16	HIS
40	h	40	ASN
40	h	45	ASN
40	h	60	GLN
41	i	76	ASN
42	j	64	ASN
43	k	49	ASN
44	l	19	ASN
45	m	58	HIS
45	m	68	ASN
46	n	26	HIS
47	o	14	GLN
47	o	72	ASN
48	p	15	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	EX	14/14 (100%)	5 (35%)	1 (7%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	117/187 (62%)	30 (25%)	5 (4%)
21	IN	39/113 (34%)	19 (48%)	3 (7%)
5	5	90/116 (77%)	23 (25%)	2 (2%)
All	All	260/430 (60%)	77 (29%)	11 (4%)

All (77) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	16	U
2	2	17	U
2	2	19	G
2	2	20	G
2	2	24	A
2	2	25	G
2	2	29	A
2	2	30	A
2	2	32	U
2	2	40	C
2	2	41	U
2	2	46	U
2	2	47	U
2	2	51	A
2	2	53	U
2	2	54	U
2	2	96	A
2	2	97	G
2	2	99	U
2	2	100	U
2	2	101	U
2	2	102	U
2	2	103	U
2	2	104	G
2	2	105	G
2	2	106	A
2	2	109	U
2	2	157	G
2	2	171	U
2	2	178	A
5	5	10	U
5	5	11	U
5	5	20	G
5	5	35	U

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Mol	Chain	Res	Type
5	5	36	C
5	5	38	C
5	5	39	C
5	5	42	U
5	5	45	C
5	5	47	A
5	5	52	U
5	5	53	U
5	5	57	G
5	5	69	A
5	5	89	U
5	5	91	U
5	5	92	U
5	5	93	U
5	5	94	U
5	5	95	G
5	5	96	A
5	5	104	C
5	5	115	U
17	EX	-11	G
17	EX	-7	C
17	EX	-6	C
17	EX	1	C
17	EX	2	U
21	IN	5	G
21	IN	14	A
21	IN	16	G
21	IN	17	U
21	IN	21	A
21	IN	134	U
21	IN	135	G
21	IN	136	U
21	IN	137	C
21	IN	138	A
21	IN	139	U
21	IN	140	A
21	IN	142	U
21	IN	143	U
21	IN	144	A
21	IN	145	U
21	IN	146	C
21	IN	166	A

Continued on next page...

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Mol	Chain	Res	Type
21	IN	167	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	39	U
2	2	46	U
2	2	95	A
2	2	102	U
2	2	105	G
5	5	92	U
5	5	95	G
17	EX	-12	G
21	IN	137	C
21	IN	142	U
21	IN	145	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SEP	R	232	31	8,9,10	1.58	1 (12%)	8,12,14	1.37	1 (12%)
31	SEP	R	224	31	8,9,10	1.45	1 (12%)	8,12,14	1.88	1 (12%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SEP	R	232	31	-	3/5/8/10	-
31	SEP	R	224	31	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	232	SEP	P-O1P	3.39	1.61	1.50
31	R	224	SEP	P-O1P	3.07	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	224	SEP	P-OG-CB	-4.78	105.13	118.30
31	R	232	SEP	P-OG-CB	-2.74	110.76	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	R	232	SEP	CB-OG-P-O1P
31	R	232	SEP	CB-OG-P-O2P
31	R	232	SEP	CB-OG-P-O3P
31	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 13 are monoatomic - leaving 3 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	$\# Z > 2$
59	IHP	U	601	-	36,36,36	1.33	6 (16%)	54,60,60	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	GTP	C	1500	-	26,34,34	1.43	2 (7%)	32,54,54	1.68	8 (25%)
56	ATP	7	702	54	26,33,33	0.64	0	31,52,52	1.06	2 (6%)

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
59	IHP	U	601	-	-	6/30/54/54	0/1/1/1
57	GTP	C	1500	-	-	0/18/38/38	0/3/3/3
56	ATP	7	702	54	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	C	1500	GTP	C5-C6	-4.98	1.37	1.47
59	U	601	IHP	P3-O13	2.68	1.64	1.59
59	U	601	IHP	P6-O16	2.58	1.64	1.59
59	U	601	IHP	P2-O12	2.37	1.63	1.59
57	C	1500	GTP	C5-C4	-2.29	1.37	1.43
59	U	601	IHP	P5-O15	2.23	1.63	1.59
59	U	601	IHP	P1-O11	2.19	1.63	1.59
59	U	601	IHP	P4-O14	2.06	1.63	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	C	1500	GTP	C5-C6-N1	3.66	120.41	113.95
57	C	1500	GTP	PA-O3A-PB	-3.42	121.10	132.83
57	C	1500	GTP	C2-N1-C6	-3.24	119.14	125.10
57	C	1500	GTP	C8-N7-C5	3.07	108.84	102.99
59	U	601	IHP	C6-C1-C2	-3.02	103.80	110.41
57	C	1500	GTP	O2G-PG-O3B	2.98	114.64	104.64
59	U	601	IHP	C5-C4-C3	2.97	116.91	110.41
56	7	702	ATP	O5'-PA-O1A	-2.87	97.85	109.07
57	C	1500	GTP	PB-O3B-PG	-2.83	123.12	132.83
57	C	1500	GTP	O6-C6-C5	-2.82	118.87	124.37
57	C	1500	GTP	C3'-C2'-C1'	2.80	105.19	100.98
56	7	702	ATP	C5-C6-N6	2.26	123.79	120.35
59	U	601	IHP	C4-C3-C2	2.07	114.94	110.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

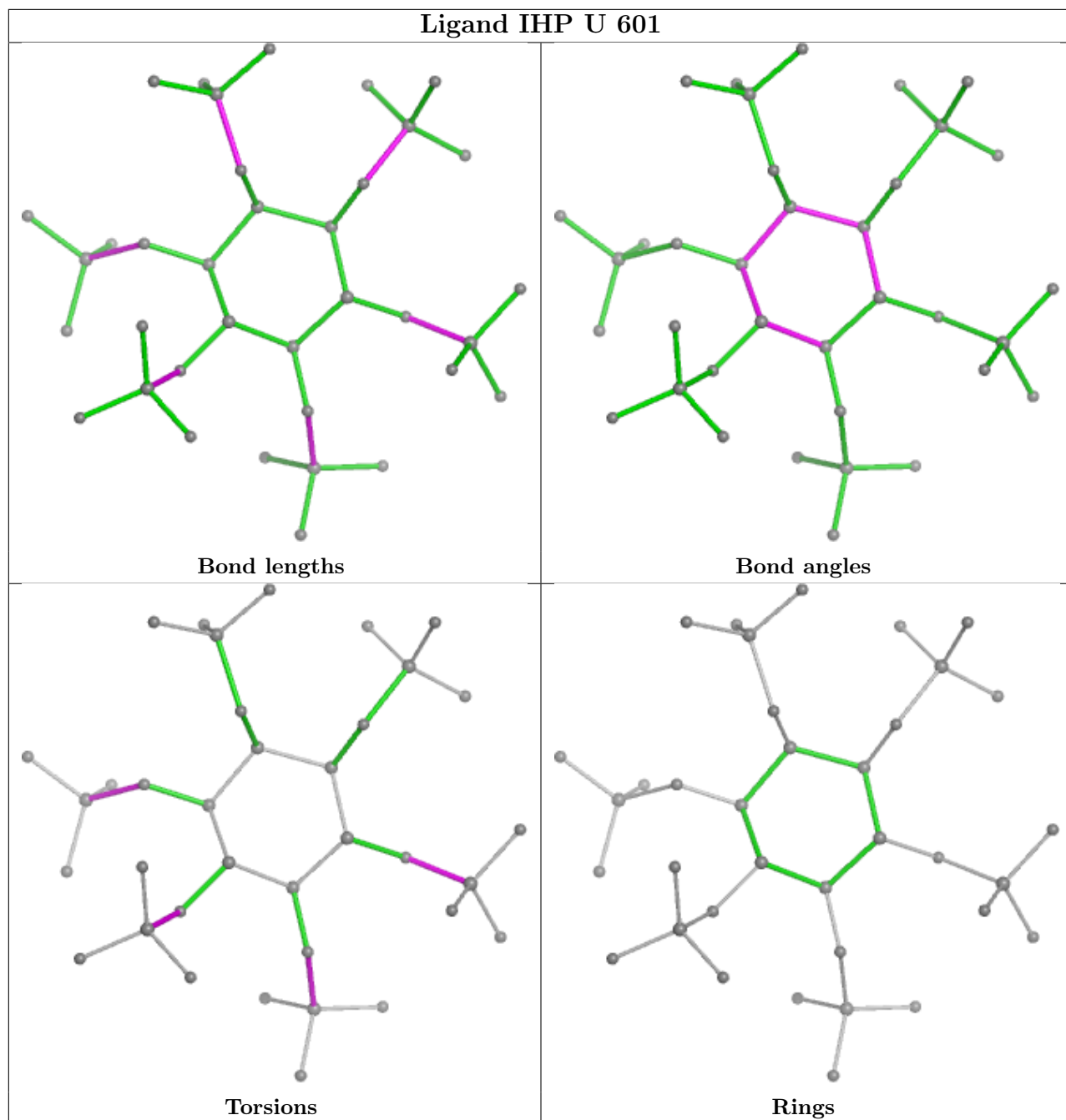
Mol	Chain	Res	Type	Atoms
59	U	601	IHP	C2-O12-P2-O42
59	U	601	IHP	C5-O15-P5-O25
59	U	601	IHP	C6-O16-P6-O26
59	U	601	IHP	C1-O11-P1-O31
59	U	601	IHP	C1-O11-P1-O41
59	U	601	IHP	C6-O16-P6-O46

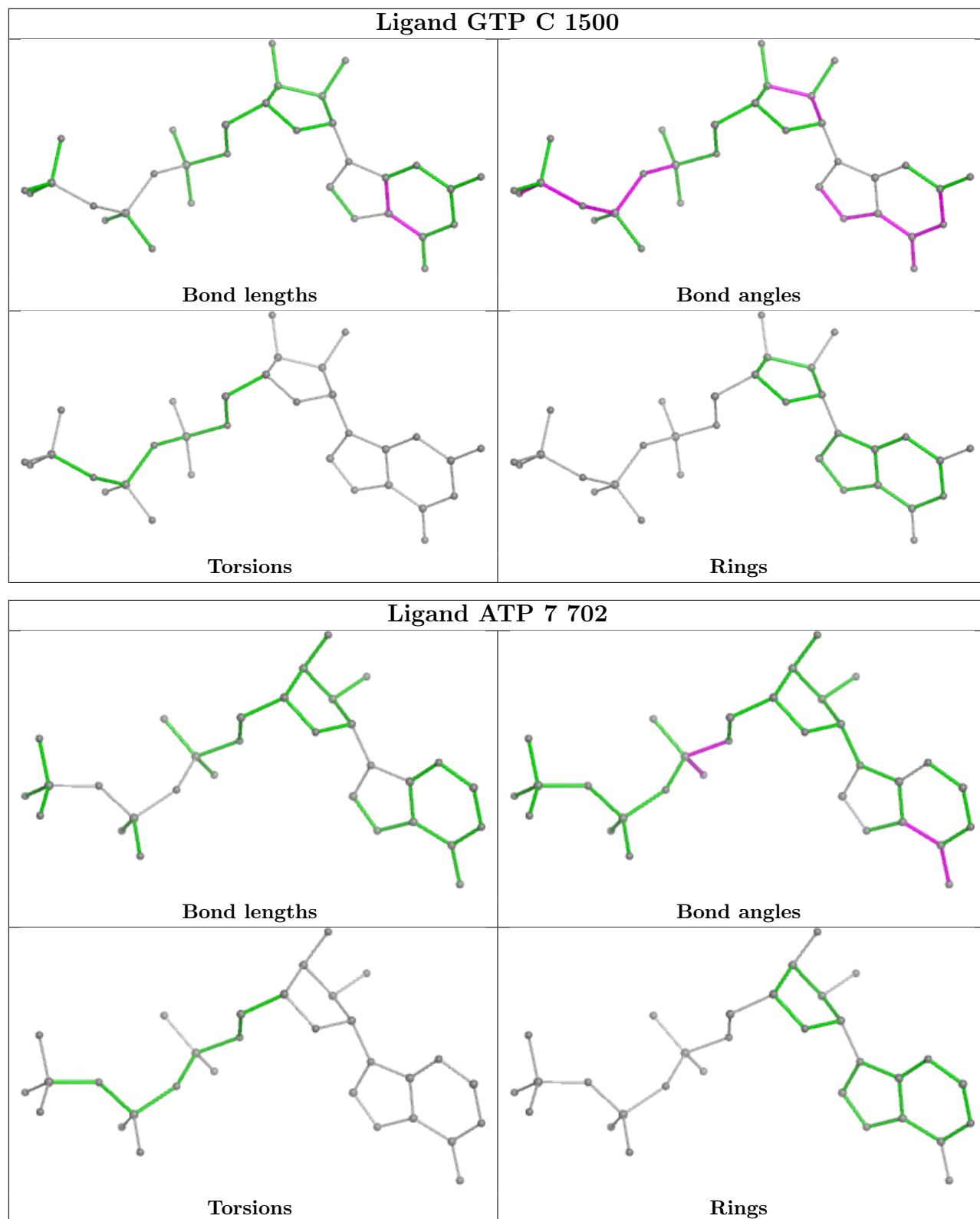
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	U	601	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

There are no chain breaks in this entry.

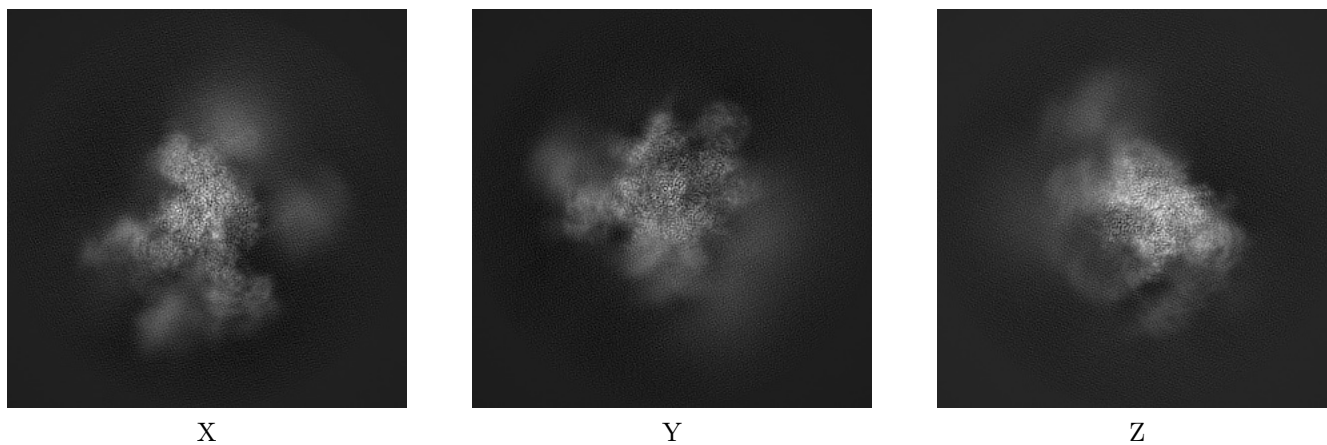
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4525. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

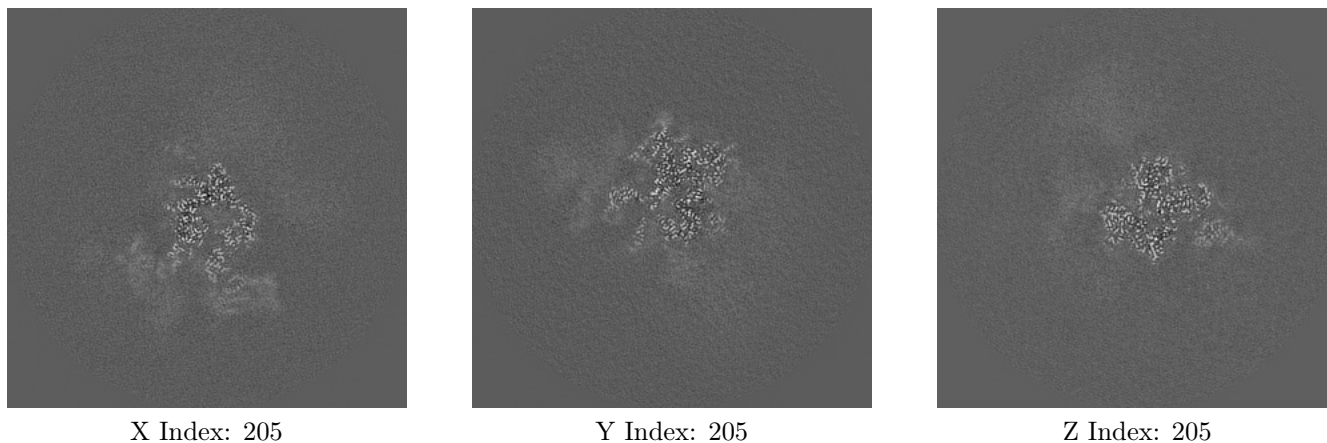
6.1.1 Primary map



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

6.2 Central slices [i](#)

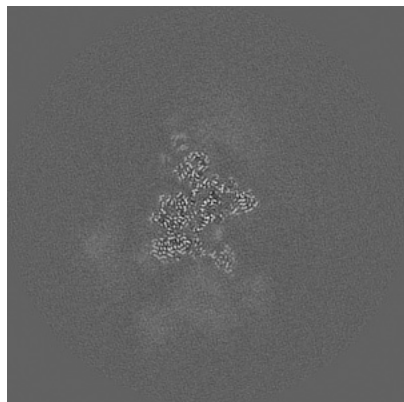
6.2.1 Primary map



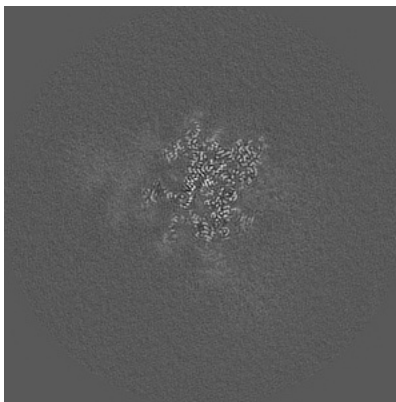
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

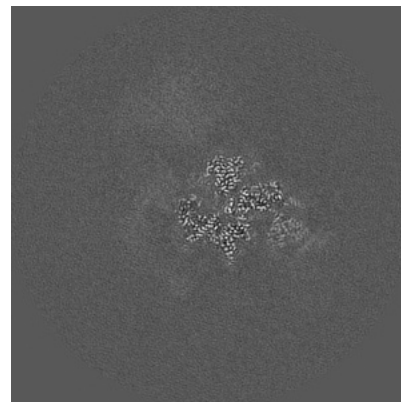
6.3.1 Primary map



X Index: 231



Y Index: 203

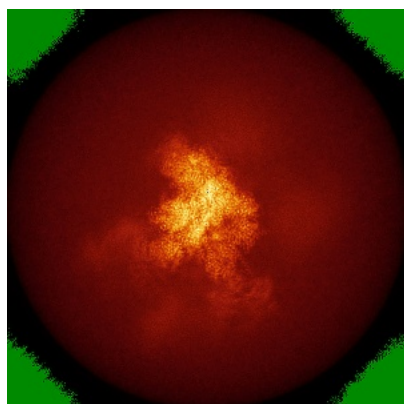


Z Index: 202

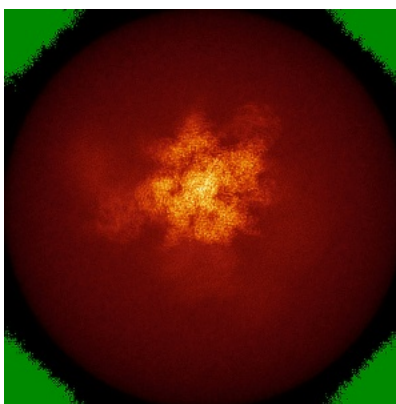
The images above show the largest variance slices of the map in three orthogonal directions.

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

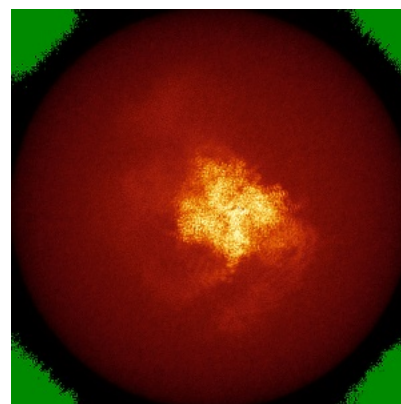
6.4.1 Primary map



X



Y

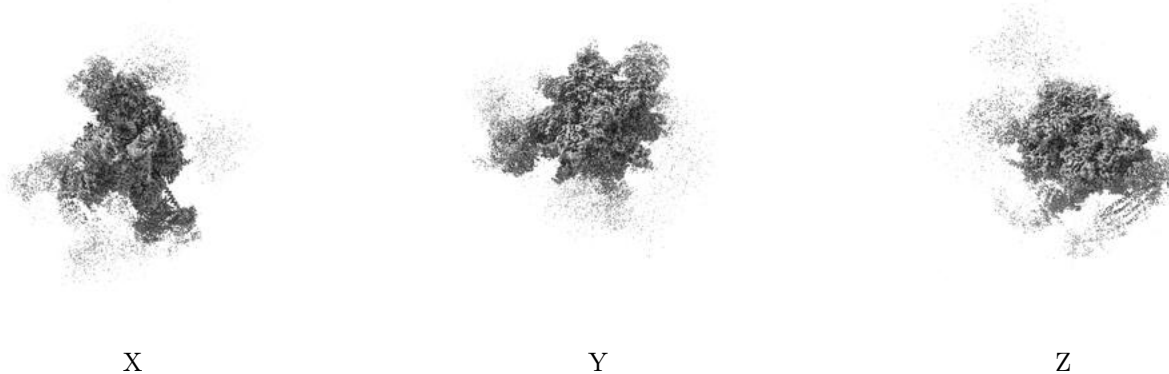


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

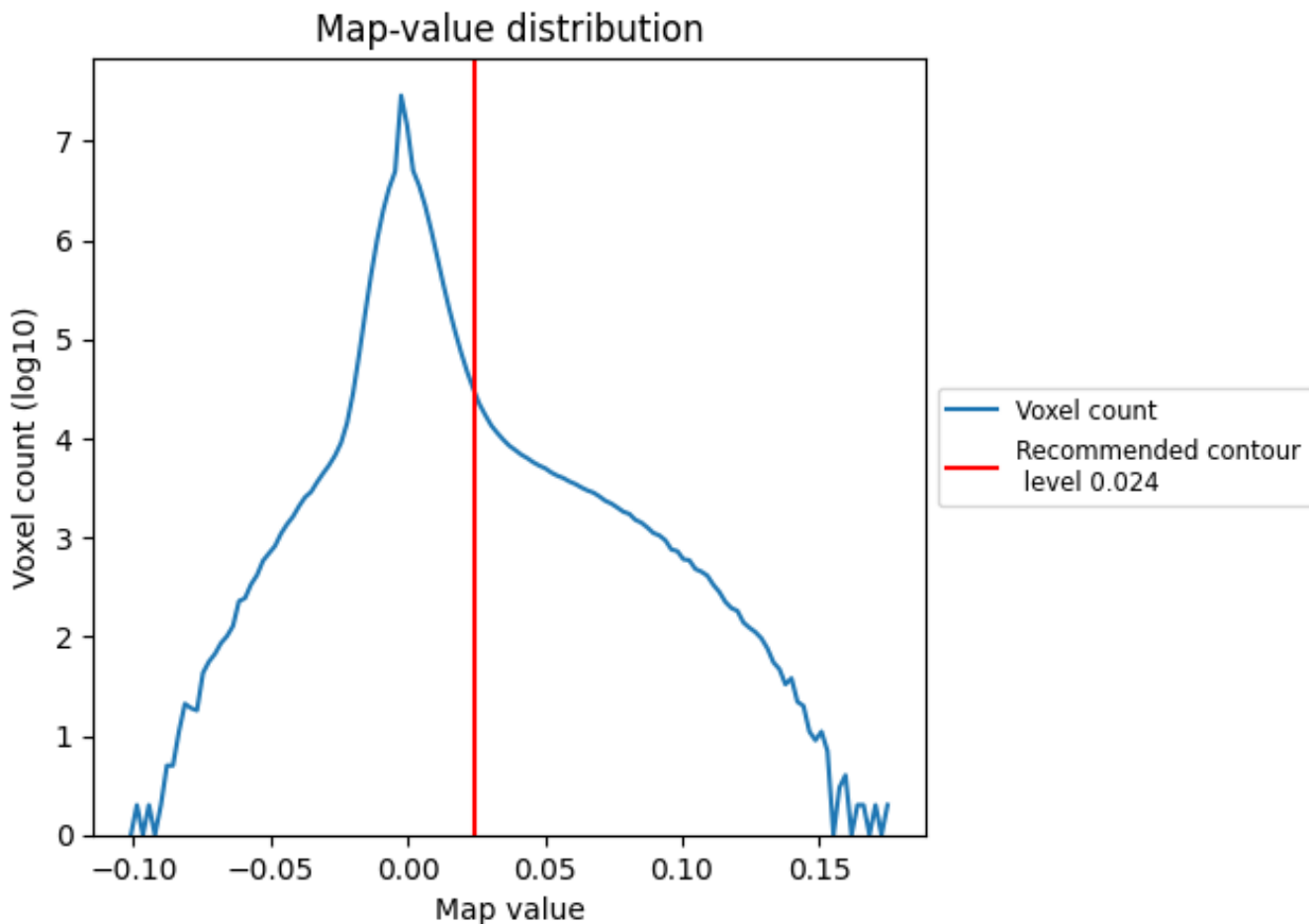
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

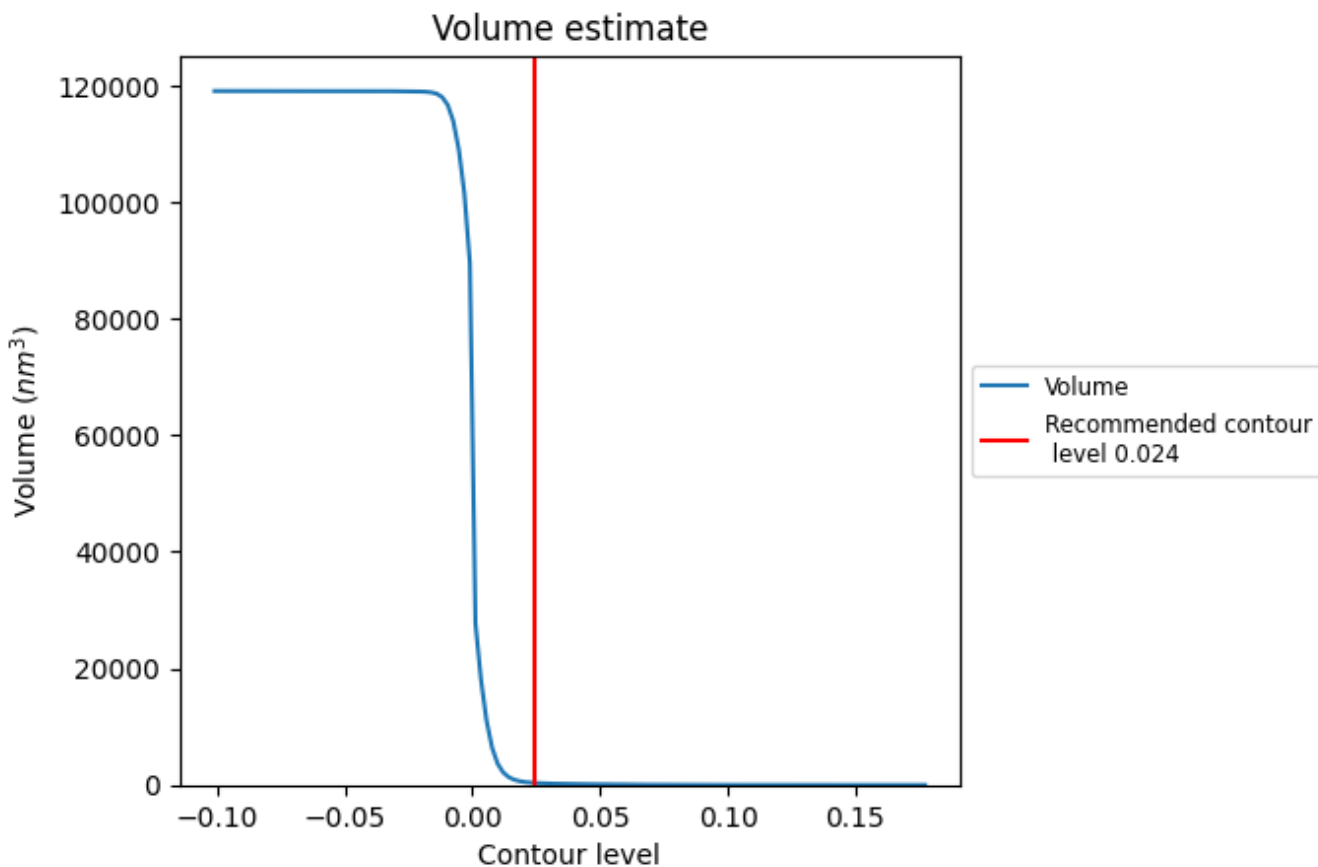
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

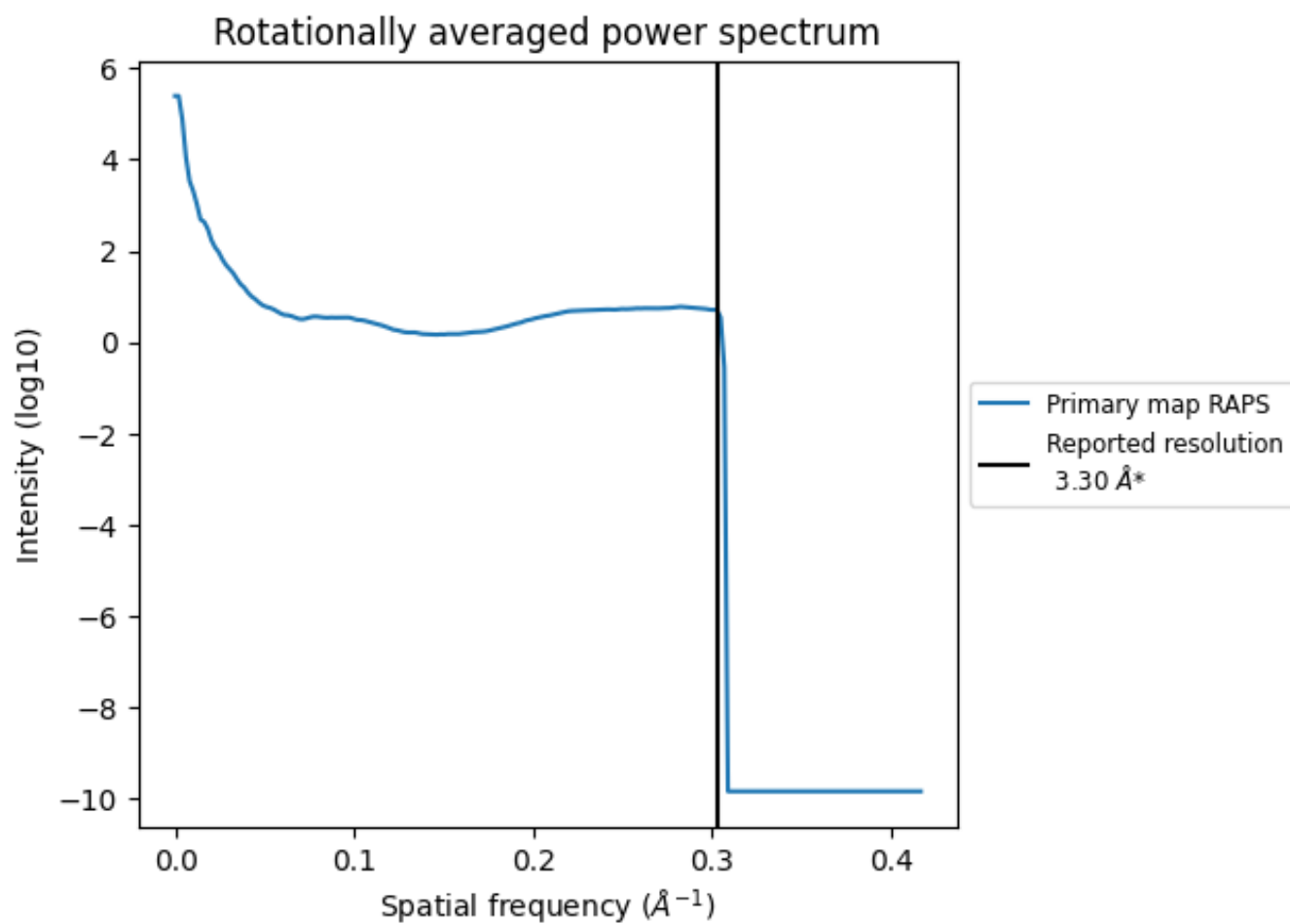
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm^3 ; this corresponds to an approximate mass of 321 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 [\(i\)](#)

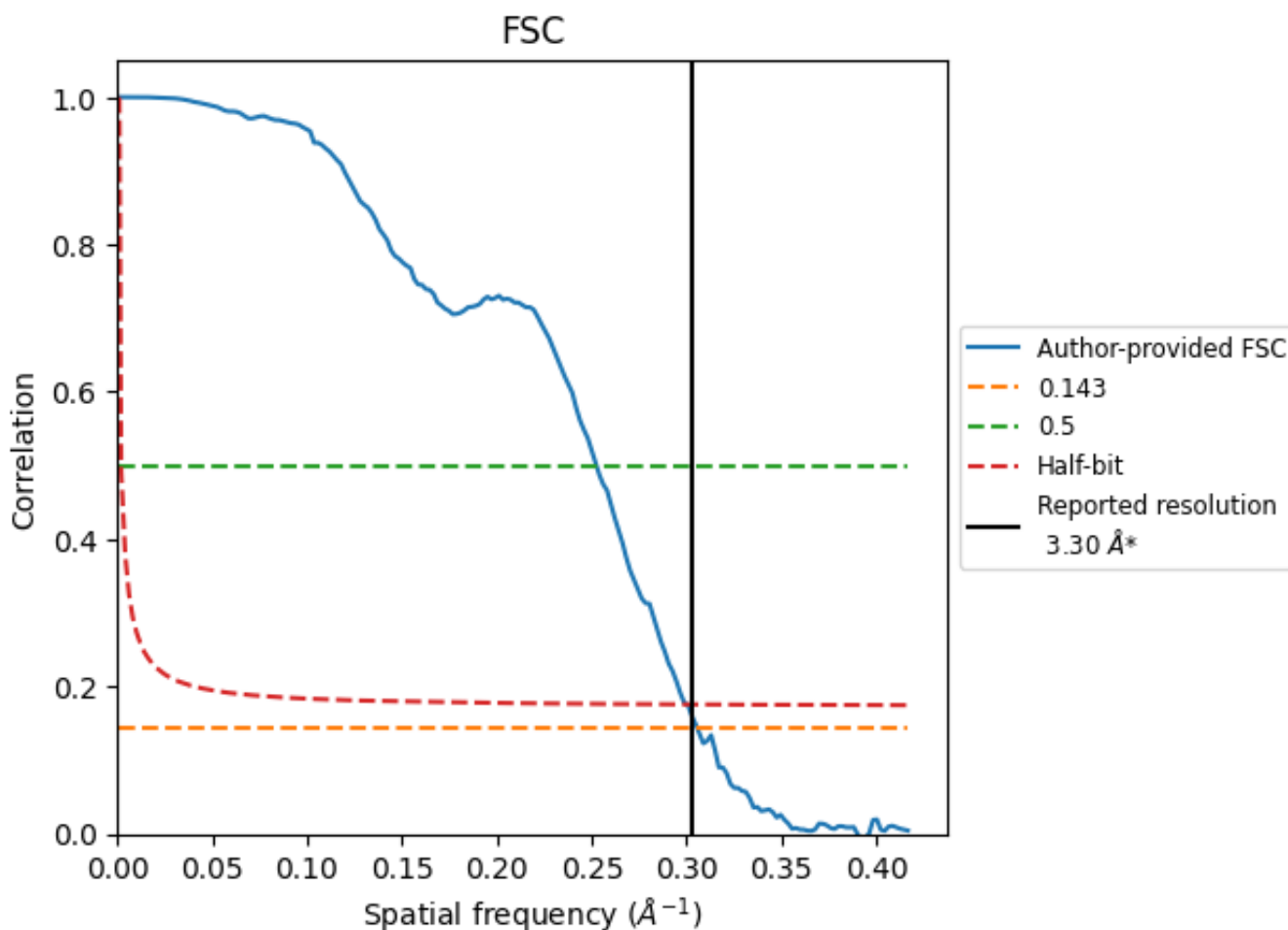


*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

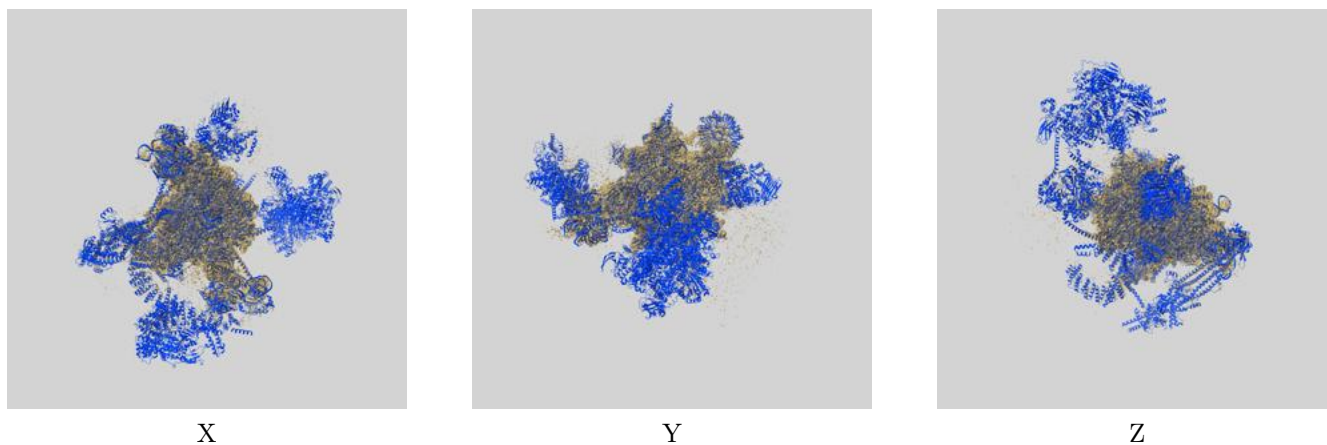
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.96	3.33
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

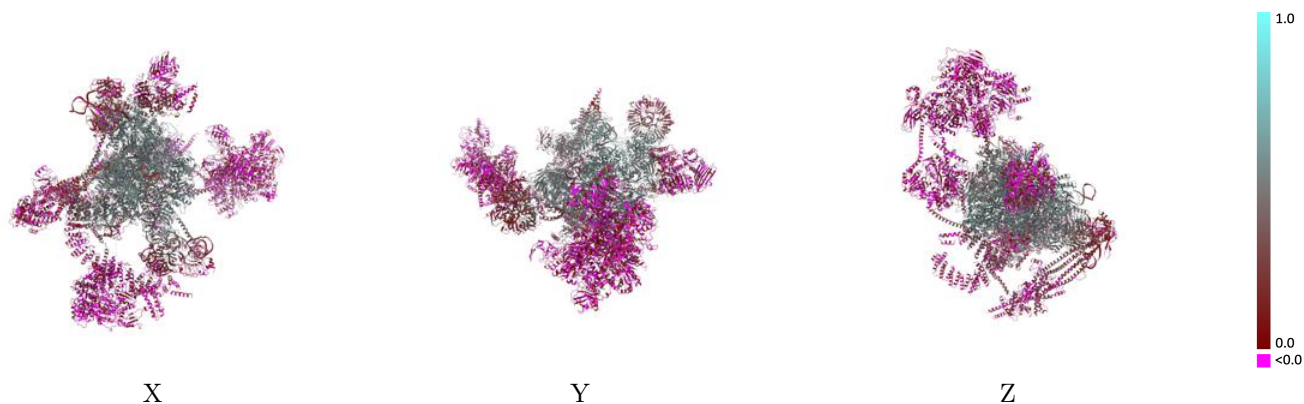
This section contains information regarding the fit between EMDB map EMD-4525 and PDB model 9FMD. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



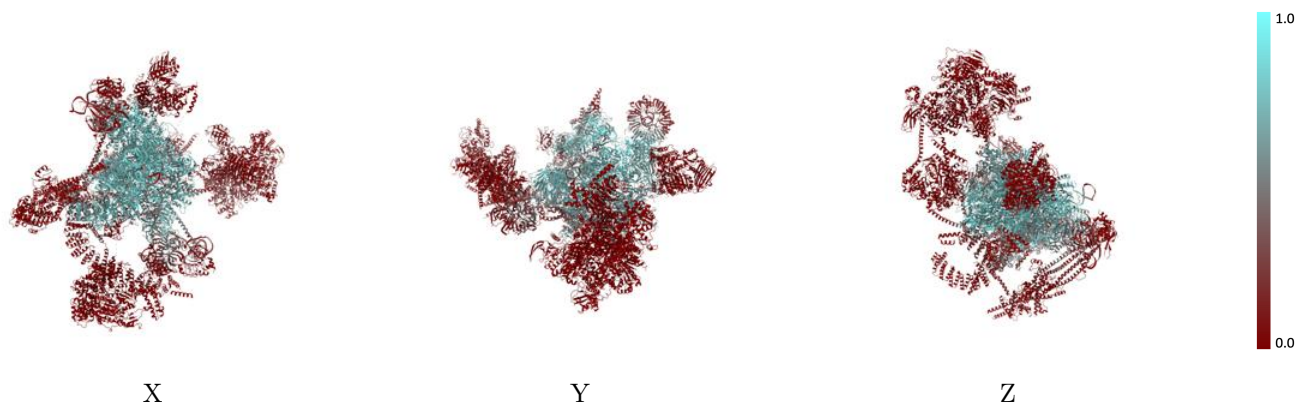
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



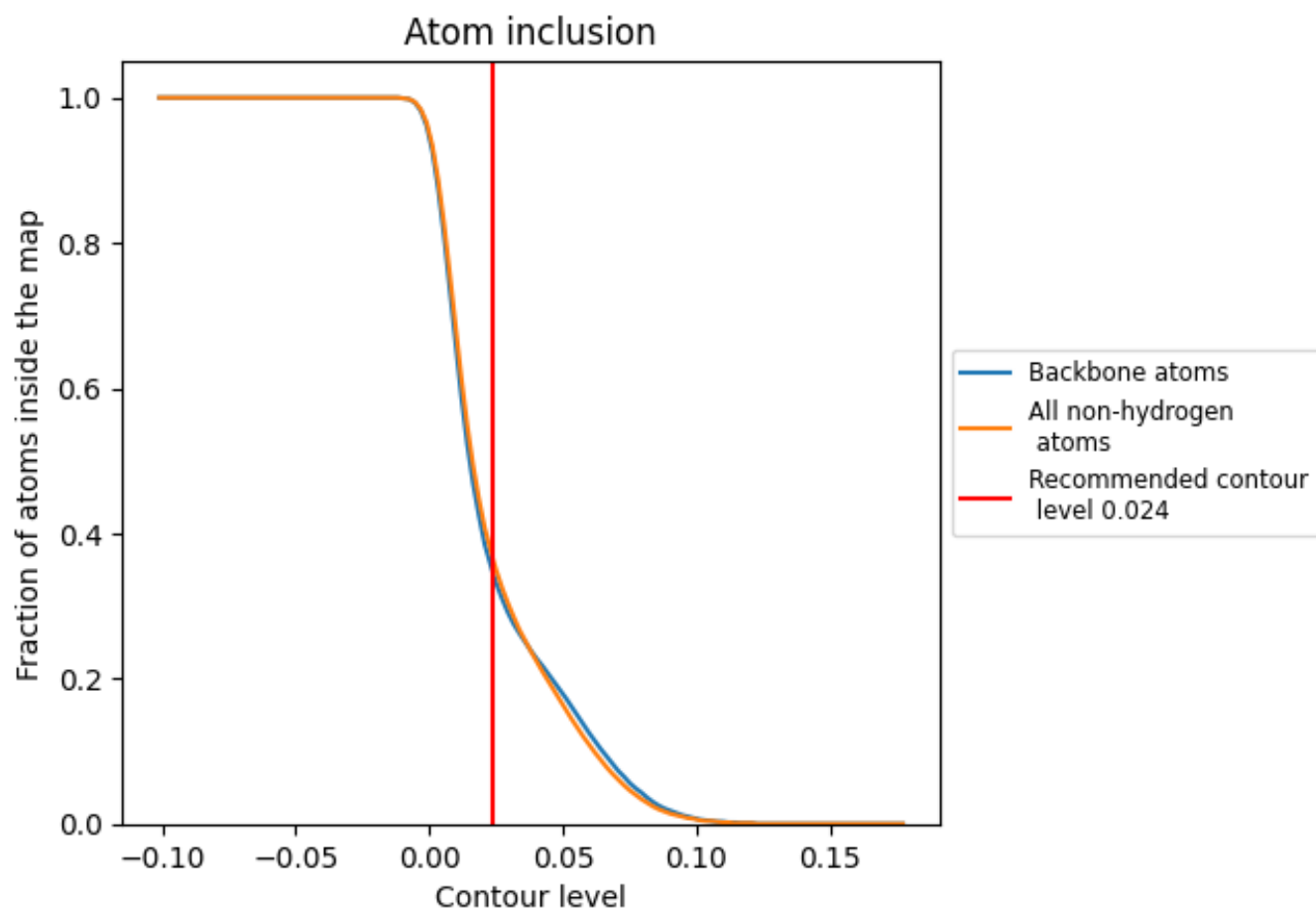
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).






































































9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 36% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3620	 0.2980
1	 0.4130	 0.3810
2	 0.4200	 0.3000
3	 0.1450	 0.2540
32	 0.5850	 0.5110
5	 0.6150	 0.3810
50	 0.0100	 0.1010
56	 0.0000	 -0.0090
6	 0.7350	 0.4580
7	 0.0070	 0.1140
8	 0.0000	 0.0490
9	 0.0000	 0.0430
A	 0.7240	 0.5090
B	 0.0010	 0.0500
C	 0.6900	 0.4910
D	 0.0000	 0.0950
E	 0.6280	 0.4780
EX	 0.8180	 0.5330
F	 0.6330	 0.4700
H	 0.4150	 0.3570
I	 0.0520	 0.1020
IN	 0.5710	 0.3790
J	 0.3960	 0.2850
K	 0.1190	 0.1860
L	 0.4040	 0.3650
M	 0.4970	 0.3810
N	 0.7490	 0.5370
NO	 0.0010	 0.1270
O	 0.5200	 0.4490
P	 0.6510	 0.5200
Q	 0.0020	 0.0530
R	 0.5330	 0.4400
S	 0.5800	 0.4560
SR	 0.4040	 0.3320
T	 0.7390	 0.5090



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Chain	Atom inclusion	Q-score
U	 0.5870	 0.4570
V	 0.0510	 0.0800
W	 0.6730	 0.5020
X	 0.0150	 0.1550
Z	 0.0150	 0.0570
a	 0.4310	 0.4160
b	 0.3380	 0.3350
c	 0.1330	 0.2070
d	 0.0620	 0.1480
e	 0.0850	 0.1950
f	 0.0470	 0.1550
g	 0.2210	 0.3340
h	 0.3960	 0.3520
i	 0.2430	 0.2910
j	 0.1220	 0.2030
k	 0.0780	 0.1560
l	 0.2420	 0.2790
m	 0.1360	 0.1820
n	 0.3660	 0.3690
o	 0.0260	 0.1130
p	 0.0600	 0.1370
q	 0.0410	 0.1150
r	 0.0200	 0.0850
s	 0.0290	 0.1460
t	 0.0100	 0.0890
w	 0.0000	 0.0380
x	 0.0300	 0.1330
y	 0.0030	 0.1230
z	 0.3510	 0.3010