



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:48 PM UTC

PDB ID : 8QPB / pdb_00008qpb
EMDB ID : EMD-18547
Title : Cryo-EM Structure of Pre-B+ATP Complex (core part)
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-01
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

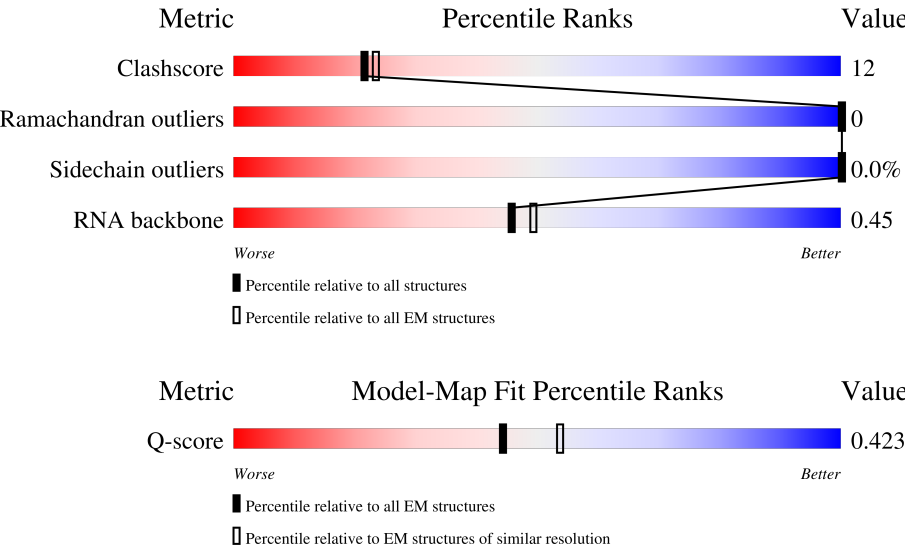
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	B	2136	99%
2	G	820	93%
3	J	683	88%

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Mol	Chain	Length	Quality of chain
4	L	499	
5	F	522	
6	N	941	
7	A	2335	
8	U	565	
9	S	800	
10	C	972	
11	M	128	
12	D	142	
13	5	117	
14	7	793	
15	4	144	
16	6	106	
17	z	13	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 43804 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	22	Total	C	N	O	S	0	0
			158	97	28	32	1		

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	57	Total	C	N	O	S	0	0
			484	304	88	91	1		

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	84	Total	C	N	O	S	0	0
			679	419	138	119	3		

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	376	Total	C	N	O	S	0	0
			2886	1796	526	552	12		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	61	Total	C	N	O	S	0	0
			488	297	97	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	457	Total	C	N	O	S	0	0
			3502	2191	655	644	12		

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1977	Total	C	N	O	S	0	0
			16409	10568	2864	2907	70		

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	456	Total	C	N	O	S	0	0
			3749	2427	635	673	14		

- Molecule 9 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	148	Total	C	N	O	S	0	0
			1164	724	216	222	2		

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	836	Total	C	N	O	S	0	0
			6592	4211	1110	1238	33		

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 12 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	141	Total	C	N	O	S	0	0
			1170	751	194	215	10		

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	79	Total	C	N	O	P	0	0
			1660	744	275	562	79		

- Molecule 14 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	107	Total	C	N	O	S	0	0
			846	522	152	169	3		

- Molecule 15 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	80	Total	C	N	O	P	0	0
			1699	760	297	562	80		

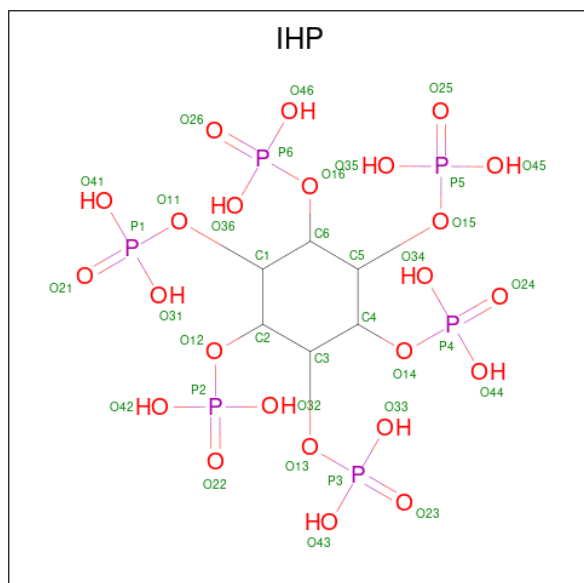
- Molecule 16 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	48	Total	C	N	O	P	0	0
			1034	462	196	328	48		

- Molecule 17 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	z	13	Total	C	N	O	P	0	0
			286	127	57	89	13		

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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



ALA	TYR	MET	GLY	CYS	ASP	GLN	GLU	TYR	LYS	PHE	SER	VAL	ASP	VAL	LYS	GLU	ALA	THR	TRP	TRP	VAL	ASP	VAL	GLY	ILE	ALA	ASP	PHE	GLY	ASP	GLY	GLN	VAL	GLY	THR	GLY	PRO	ASP	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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● Molecule 2: Probable ATP-dependent RNA helicase DDX23

Chain G: 5% 93%

MET	ALA	GLN	GLY	LEU	THR	HIS	LYS	ASN	LEU	GLY	THR	GLY	ASP	VAL	ALA	LYS	THR	LYS	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR	GLY	ASP	VAL	GLY	THR
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● Molecule 3: U4/U6 small nuclear ribonucleoprotein Prp3

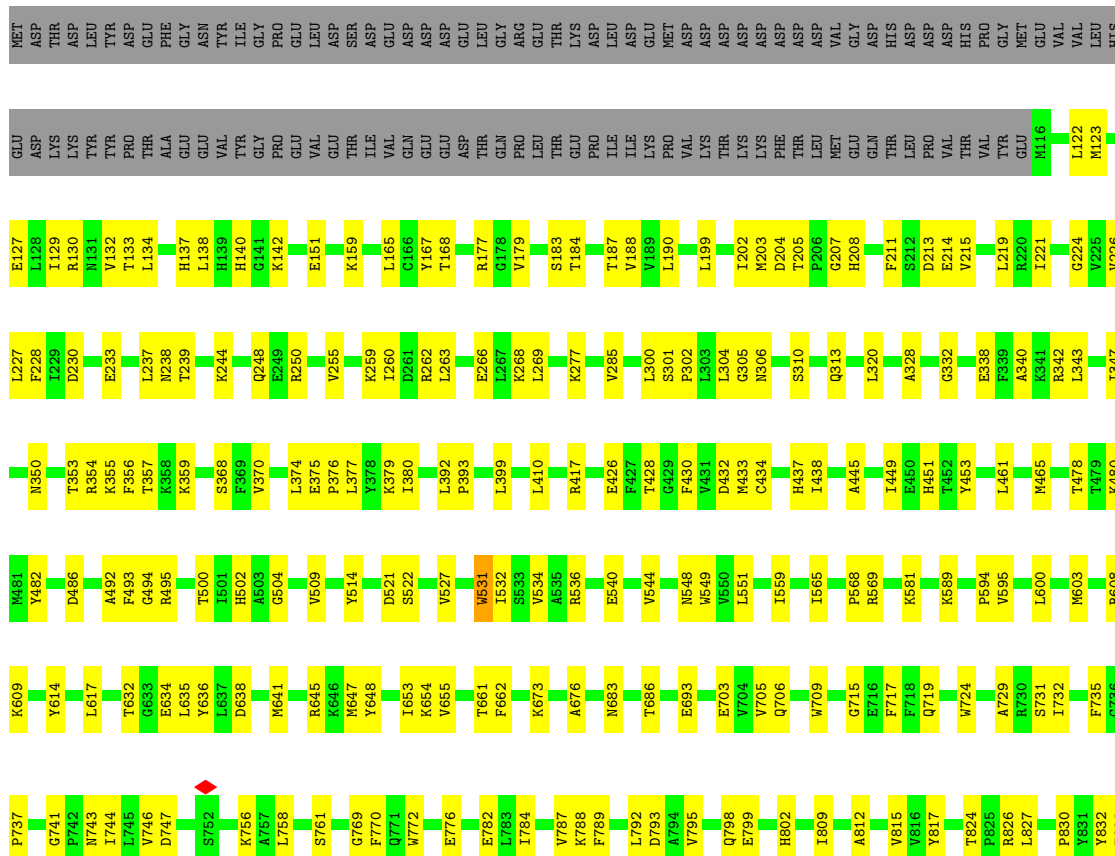
Chain J: 8% 5% 88%

ASP	R1941	K1838	L1747	W1637	K1517	L1403	C1291	F1187	P1084	N974	R861	H712
GLU	V1945	W1839	L1751	W1638	Q1522	T1404	E1292	M1188	I1085	V975	E862	A716
ILE		K1840	L1752	S1640	Q1522	S1411	M1293	M1189	R1086	N976	E863	L1086
THR	A1950	T1841	L1753	R1641	M1531	S1411	K1294	M1189	L1087		L864	L1087
SER				P1642		R1414	I1295	E1193	C1088	N984	G865	P732
THR	L1954	E1844	E1757	S1643	T1535	G1415	Q1296	E1193	G1089	N985	L866	G865
T2059	K1955	L1848	P1758	L1644	L1536	I1416	M1304	I1196	R1090	E986	L867	W738
S2060	P1956	L1849	T1759	L1645	W1537	I1417	S1305	L1197	Y1091	K987	L878	Y742
N2061	D1957	T1849	E1760	Y1660	P1540	T1421	P1308	P1198	I1097	L992	K882	W750
K1958	T1958	L1850	P1761	W1661	T1541	L1422	F1098	H1209	F1098	N993	R883	T751
E2062	T1959	S1851	Y1762	I1662	T1541	F1423	F1099	N994	N994	N994	N752	N752
T2064	T1960	K1859	L1763	D1663	R1544	Q1424	R1100	W1214	R1100	R995	Q888	
Q2065							F1101		F1101		R889	E759
	L1989	V1863	L1771	I1664	F1551	K1425	T1102	T1225	T1102	V1001	E760	R760
	K1994	T1864	F1772	Q1665	Q1552	L1426	A1103	A1103	A1103	I1005	E893	R763
		R1865	S1773	L1666	Q1552	L1426	E1105	G1228	E1105		R894	
	N1998	M1868	Q1775	W1668	L1555	T1429				T1010	F898	T766
V1999			L1776	G1669	L1556	K1434	R1231	R1231		A1011	M899	T770
	E2006	P1871	L1777	D1670	L1557	G1435	D1233	D1233		K1012	D900	C772
I2007	I2007	L1872	Y1671	Y1671	T1558	V1438	G1324	E1116	N1124	V1016	L905	L776
R2008	R2008	E1873	W1780	S1673	G1559	R1439	L1325	G1226	I1125	I1017	G906	G777
D2009	D2009	L1877	D1782	I1672	G1559	L1448	M1327	N1242	R1032	H1024	P907	R778
I2010	I2010	F1878	W1783	Y1687	L1573	P1452	L1328	V1244	R1245	G1033	Y909	L779
G2012	G2012	T1879	N1784	Y1687	L1573	K1463	M1330	Q1246	C1133	K1034	P913	T780
G2013	G2013	K1885	W1785	P1696	L1576	L1464	V1333		W1134		L914	R781
M2014	M2014	E1888	L1786	G1700	W1582	W1465	L1334	M1249	D1137	A1037	E915	L782
E2015	E2015	L1889	T1788	I1703	Q1583	Y1470	P1336	S1251	A1138	A1037	K916	Y783
I2016	I2016	P1892	L1790	I1703	Q1583	Y1470	P1336	S1251	R1139	I1040	E929	Q788
Q2022	Q2022	P1892	H1791	I1703	L1589	L1478	D1347	I1259	M1140	Y1044	R833	H792
A2027	A2027	L1897	K1792	D1706	V1590	I1484	M1357	V1280	R1141	G1045	R934	W816
GLU	GLU	K1898	E1795	N1710	M1591	T1488	L1364	N1284	D1146	D1049	L935	R820
ILE	ILE	V1899	G1796	A1714	D1592	L1489	L1365	T1265	V1147	L1050	V952	Y832
ASP	ASP	E1900	L1797	A1714	L1596	F1490	I1365	A1277	W939	V1052	P942	I825
THR	THR	K1901	L1798	N1717	V1596	K1491	Y1369	I1288	N1148		A943	P828
LEU	LEU	F1902	P1802	N1717	L1601	G1492	Y1369	M1271	L1149	L1055	D944	W816
GLY	GLY	L1905		K1723	L1601	T1493	I1372	R1275	W1155	H1056	R934	R820
THR	THR	L1906	G1805	Q1728	I1606	T1497	Q1373	E1276	D1156	R1057	L935	R820
GLN	GLN	K1908	A1806	A1729	P1616	E1498	P1374	A1277	I1157	E1060	V952	D835
LEU	LEU	M1914	I1807	M1730	P1616	E1499	W1375	V1278	R1160	M1061	Q857	K847
ILE	ILE	V1915	F1808	A1731	S1619	G1500	E1378	V1279	L1161	A1062	N960	N961
THR	THR	L1916	I1809	A1731	S1619	L1501	E1378	V1280	P1162	G1063	L962	K853
ALA	ALA	L1916	F1810	K1732	M1622	F1502	V1385	T1281	V1165	N1069	V965	S854
PRO	PRO	L1916	M1811	I1733	M1622	F1502	W1386	L1284	W1170	L1072	W966	R855
LYS	LYS	L1916	P1812	I1733	M1622	F1502	W1386	L1284	W1170	L1072	E972	Q858
ASN	ASN	L1916	R1813	N1737	I1629	E1504	W1386	L1284	W1170	L1072	C973	
VAL	VAL	L1916	L1817	N1737	I1629	E1504	W1386	L1284	W1170	L1072		
LEU	LEU	L1916	F1818	P1738	L1630	K1505	R1393	L1285	V1177	Q1075		
THR	THR	L1916	L1819	A1739	L1631	S1507	R1393	L1285	V1177	Q1075		
GLY	GLY	L1916	K1820	L1740	S1634	E1511	I1397	L1288	W1177	Q1075		
ASN	ASN	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
GLY	GLY	L1916	R1744	R1744	Y1635	E1511	I1397	L1288	W1177	Q1075		
THR	THR	L1916	R17									

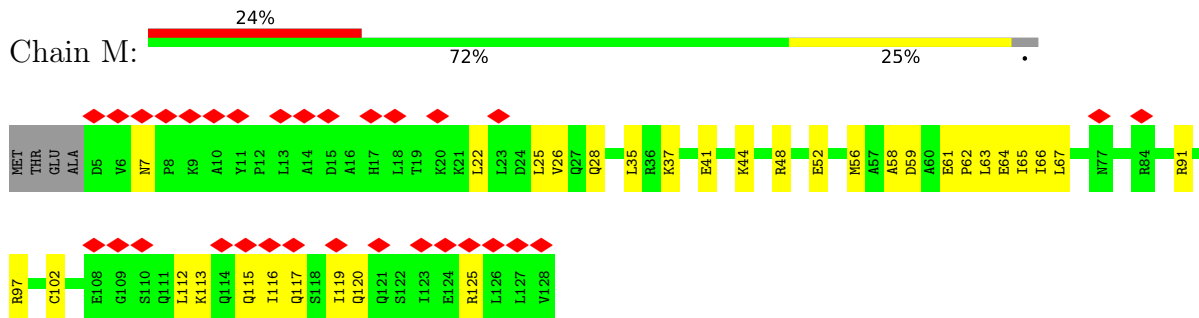
[illegible]

- Molecule 10: 116 kDa U5 small nuclear ribonucleoprotein component

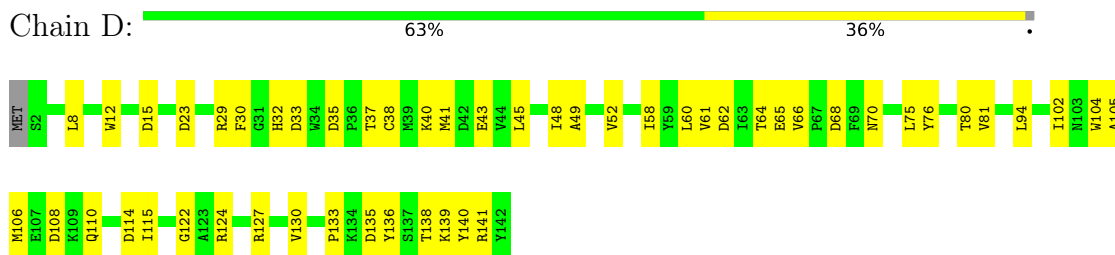
Chain C:  60% 26% 14%



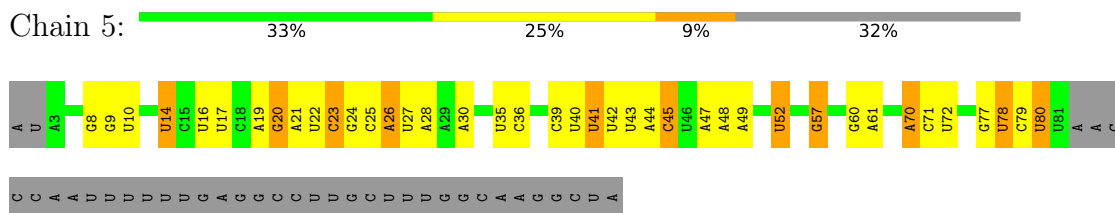
- Molecule 11: NHP2-like protein 1, N-terminally processed



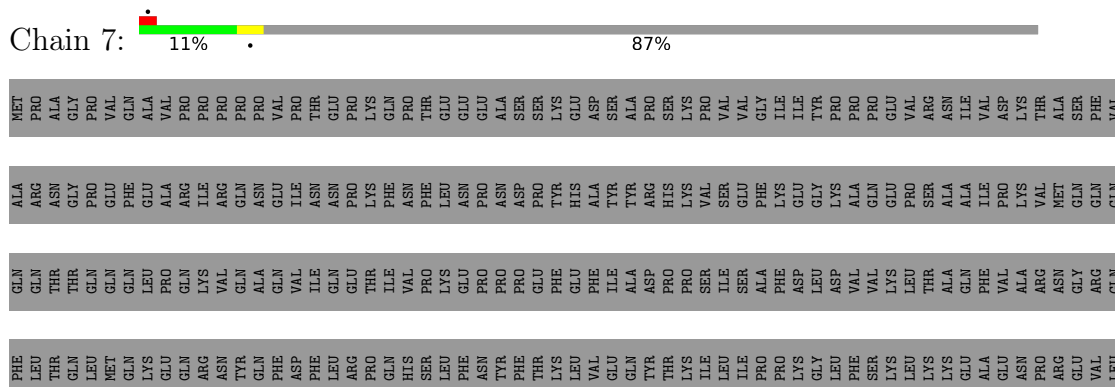
- Molecule 12: Thioredoxin-like protein 4A



- Molecule 13: U5 snRNA



- Molecule 14: Splicing factor 3A subunit 1



A-5	G-4	U-3	G-2	G-1	G1	U2	A3	A4	A5	A6	G7	C8
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94460	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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

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	B	0.13	0/158	0.36	0/209
2	G	0.08	0/493	0.23	0/659
3	J	0.12	0/686	0.27	0/914
4	L	0.12	0/2924	0.28	0/3938
5	F	0.10	0/491	0.27	0/657
6	N	0.11	0/3565	0.26	0/4818
7	A	0.14	0/16856	0.30	0/22865
8	U	0.10	0/3845	0.29	0/5208
9	S	0.11	0/1172	0.25	0/1567
10	C	0.13	0/6739	0.32	0/9151
11	M	0.13	0/974	0.34	0/1316
12	D	0.13	0/1199	0.26	0/1620
13	5	0.11	0/1850	0.20	0/2875
14	7	0.11	0/858	0.28	0/1152
15	4	0.10	0/1898	0.14	0/2954
16	6	0.10	0/1159	0.21	0/1806
17	z	0.11	0/321	0.14	0/500
All	All	0.12	0/45188	0.28	0/62209

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	158	0	166	8	0
2	G	484	0	469	18	0
3	J	679	0	728	32	0
4	L	2886	0	2885	75	0
5	F	488	0	499	13	0
6	N	3502	0	3379	110	0
7	A	16409	0	16326	422	0
8	U	3749	0	3769	100	0
9	S	1164	0	1173	23	0
10	C	6592	0	6615	175	0
11	M	962	0	1012	29	0
12	D	1170	0	1141	36	0
13	5	1660	0	842	25	0
14	7	846	0	837	22	0
15	4	1699	0	858	32	0
16	6	1034	0	521	21	0
17	z	286	0	142	8	0
18	A	36	0	6	0	0
All	All	43804	0	41368	980	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 12.

All (980) 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)
10:C:168:THR:H	10:C:536:ARG:HH22	1.03	0.98
10:C:123:MET:HE1	10:C:532:ILE:HG21	1.61	0.83
3:J:489:ALA:HA	3:J:496:VAL:HG21	1.60	0.82
4:L:88:PRO:HD2	4:L:91:ARG:HE	1.44	0.82
7:A:152:ARG:HH22	7:A:619:GLY:H	1.29	0.81
8:U:174:CYS:O	8:U:178:ASN:HA	1.82	0.79
8:U:448:PRO:HA	8:U:554:ARG:HD2	1.65	0.79
7:A:1591:MET:HE1	7:A:2065:GLN:HG3	1.65	0.78
7:A:1590:VAL:HG13	7:A:1629:ILE:HD11	1.66	0.78
7:A:516:LEU:HD11	7:A:538:SER:HB2	1.67	0.75
7:A:465:LYS:O	13:5:23:C:N4	2.20	0.75
4:L:200:SER:HA	4:L:203:ARG:HE	1.51	0.74
7:A:1703:ILE:HG21	7:A:1730:MET:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:138:THR:HG22	12:D:140:TYR:H	1.53	0.73
8:U:246:VAL:HG12	8:U:248:PRO:HD2	1.71	0.72
7:A:1629:ILE:HB	7:A:1662:ILE:HB	1.71	0.72
7:A:1792:LYS:HB3	9:S:268:GLU:HA	1.71	0.72
6:N:108:LEU:HD21	7:A:476:PHE:HE1	1.55	0.71
8:U:174:CYS:O	8:U:178:ASN:CA	2.38	0.71
7:A:384:VAL:O	10:C:354:ARG:NH2	2.22	0.71
7:A:1411:SER:HA	7:A:1414:ARG:HD2	1.72	0.71
10:C:843:VAL:HG22	10:C:871:ILE:HD11	1.73	0.71
9:S:259:VAL:HG12	9:S:289:LEU:HB3	1.72	0.71
8:U:271:PHE:HA	8:U:274:VAL:HG12	1.73	0.70
12:D:37:THR:HG23	12:D:105:ALA:HB2	1.73	0.70
10:C:227:LEU:HD11	10:C:239:THR:HG23	1.74	0.70
7:A:1988:LEU:HD21	7:A:2007:ILE:HG23	1.74	0.69
8:U:270:MET:HG3	8:U:333:ALA:HB2	1.74	0.69
3:J:465:ARG:NH2	15:4:58:C:OP1	2.26	0.69
10:C:347:ILE:HD11	10:C:356:PHE:HB3	1.75	0.69
7:A:317:PRO:O	7:A:321:ASN:ND2	2.26	0.69
7:A:1809:ILE:HG21	7:A:1848:LEU:HD23	1.75	0.69
8:U:208:GLN:HE21	8:U:210:LYS:HG3	1.58	0.68
7:A:679:SER:HB2	12:D:40:LYS:HE3	1.75	0.68
3:J:451:GLN:NE2	14:7:433:LEU:O	2.26	0.68
7:A:112:GLN:HE21	7:A:190:ALA:H	1.41	0.68
8:U:316:GLN:HE22	8:U:511:GLU:HA	1.58	0.68
3:J:480:ASN:HD21	16:6:55:C:H5''	1.59	0.68
8:U:174:CYS:O	8:U:178:ASN:N	2.27	0.68
10:C:683:ASN:HA	10:C:795:VAL:O	1.94	0.68
7:A:474:ARG:HD3	13:5:14:U:H5'	1.75	0.67
10:C:632:THR:H	10:C:636:TYR:HD2	1.42	0.67
12:D:29:ARG:HH21	12:D:60:LEU:HD13	1.58	0.67
14:7:422:ALA:HA	14:7:425:MET:HB2	1.76	0.67
7:A:1146:ASP:OD2	7:A:1182:ASN:ND2	2.26	0.67
1:B:42:SER:HA	7:A:1289:VAL:HG11	1.76	0.67
7:A:103:LEU:HD11	7:A:554:THR:HG22	1.77	0.67
6:N:390:LYS:HA	6:N:413:LEU:HD21	1.77	0.67
10:C:301:SER:HB2	10:C:304:LEU:HD12	1.77	0.66
8:U:101:ARG:NH2	8:U:177:ASP:O	2.28	0.66
10:C:168:THR:H	10:C:536:ARG:NH2	1.85	0.66
7:A:150:MET:SD	7:A:153:ARG:NH2	2.66	0.66
4:L:131:ASN:HB3	4:L:134:ASP:HB2	1.77	0.66
7:A:593:ARG:NH2	7:A:594:TYR:OH	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:408:ARG:NH1	7:A:1879:PHE:O	2.28	0.66
7:A:907:PRO:HG2	7:A:1032:ARG:HH21	1.60	0.66
13:5:43:U:H3	17:z:-4:G:H22	1.41	0.66
4:L:376:ASN:HA	7:A:1505:LYS:HE3	1.79	0.65
6:N:825:GLN:HB3	6:N:829:LYS:HE3	1.76	0.65
6:N:250:LEU:HD23	7:A:1850:ARG:HE	1.61	0.65
7:A:419:ARG:NH2	7:A:423:ASP:O	2.29	0.65
7:A:99:VAL:HG13	7:A:554:THR:HG21	1.77	0.65
10:C:168:THR:N	10:C:536:ARG:HH22	1.87	0.65
4:L:257:LYS:HB2	4:L:267:VAL:HG13	1.76	0.65
7:A:281:PRO:O	7:A:284:ARG:NH2	2.29	0.65
10:C:595:VAL:HG22	10:C:654:LYS:HG3	1.78	0.65
7:A:863:GLU:HG2	7:A:913:PRO:HB3	1.79	0.65
8:U:262:ILE:O	8:U:264:ARG:NH1	2.30	0.65
8:U:358:LYS:HD3	8:U:438:LEU:HD23	1.79	0.65
7:A:281:PRO:HG2	7:A:284:ARG:HH21	1.60	0.65
7:A:974:ASN:OD1	7:A:1100:ARG:NH1	2.30	0.65
8:U:233:ASN:HD21	8:U:300:LEU:HD13	1.61	0.65
11:M:48:ARG:NH1	15:4:42:C:OP1	2.30	0.65
12:D:65:GLU:HG3	12:D:66:VAL:HG23	1.79	0.65
10:C:159:LYS:HB3	10:C:165:LEU:HB2	1.79	0.64
7:A:915:GLU:OE1	7:A:1012:LYS:NZ	2.29	0.64
7:A:1807:ILE:HB	7:A:1820:LYS:HB3	1.79	0.64
7:A:156:ARG:O	7:A:159:ARG:NH1	2.29	0.64
7:A:776:LEU:HD13	7:A:900:ASP:HB2	1.80	0.64
4:L:431:GLN:O	7:A:883:ARG:NH2	2.31	0.64
6:N:288:ILE:HD13	6:N:318:LEU:HD13	1.80	0.64
5:F:128:GLU:OE2	14:7:442:ARG:NH2	2.31	0.64
7:A:1737:ASN:HB3	7:A:1740:LEU:HB2	1.79	0.64
12:D:70:ASN:HA	12:D:75:LEU:HB2	1.78	0.63
6:N:916:SER:HA	6:N:921:ASN:H	1.61	0.63
8:U:515:ARG:HG2	8:U:530:GLN:HB2	1.80	0.63
10:C:183:SER:HA	10:C:204:ASP:O	1.99	0.63
3:J:462:GLU:HG3	5:F:90:PHE:HE1	1.62	0.63
3:J:444:GLU:OE1	11:M:91:ARG:NH2	2.32	0.63
4:L:222:ILE:HG22	4:L:223:ILE:HG23	1.80	0.63
4:L:141:GLU:OE1	4:L:154:ASN:ND2	2.32	0.63
7:A:142:SER:HA	7:A:242:ALA:HB2	1.80	0.63
7:A:694:LEU:HD12	14:7:466:LEU:HD12	1.80	0.63
7:A:1863:VAL:HG11	7:A:1868:MET:HB2	1.79	0.63
5:F:101:VAL:O	5:F:130:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:O	7:A:1209:HIS:NE2	2.31	0.62
9:S:160:ALA:HB1	9:S:164:ARG:HH21	1.62	0.62
13:5:8:G:H1	13:5:71:C:H5''	1.64	0.62
6:N:362:VAL:HG11	6:N:379:ALA:HB2	1.81	0.62
7:A:1069:ASN:ND2	7:A:1075:GLN:OE1	2.32	0.62
7:A:1072:LEU:HD22	7:A:1087:LEU:HD22	1.82	0.62
8:U:208:GLN:NE2	8:U:210:LYS:O	2.32	0.62
10:C:207:GLY:O	10:C:238:ASN:ND2	2.31	0.62
8:U:444:THR:HG23	8:U:488:VAL:HG11	1.80	0.62
14:7:430:ARG:NH1	15:4:25:A:OP2	2.33	0.62
10:C:531:TRP:HD1	10:C:540:GLU:HB2	1.64	0.62
7:A:888:GLN:O	7:A:889:ARG:NH1	2.33	0.62
7:A:2009:ASP:HB3	7:A:2014:MET:HB2	1.82	0.62
9:S:256:GLY:O	9:S:350:ARG:NH2	2.32	0.62
10:C:123:MET:HB3	10:C:548:ASN:HD21	1.65	0.62
10:C:259:LYS:NZ	10:C:313:GLN:OE1	2.33	0.62
10:C:504:GLY:N	10:C:527:VAL:O	2.33	0.62
7:A:909:TYR:HB2	7:A:1033:GLY:HA3	1.81	0.61
7:A:104:GLU:HB2	7:A:422:LEU:HD11	1.81	0.61
15:4:22:C:H2'	15:4:23:G:H8	1.64	0.61
8:U:127:SER:HB3	8:U:151:HIS:HE1	1.64	0.61
7:A:1661:TRP:CE2	7:A:1700:GLY:HA3	2.35	0.61
8:U:270:MET:HE1	8:U:273:LEU:HD23	1.83	0.61
6:N:329:ARG:HH21	6:N:354:PRO:HD3	1.65	0.61
7:A:357:ASN:ND2	10:C:866:SER:O	2.34	0.61
7:A:820:ARG:NH1	7:A:1063:GLY:O	2.23	0.61
7:A:847:LYS:HG3	7:A:867:ILE:HG21	1.83	0.61
12:D:62:ASP:HB3	12:D:65:GLU:HG2	1.81	0.61
6:N:132:ARG:NE	14:7:481:GLU:OE2	2.30	0.61
7:A:939:TRP:NE1	7:A:1049:ASP:OD2	2.32	0.60
7:A:1809:ILE:HB	7:A:1818:PHE:HB2	1.83	0.60
10:C:776:GLU:HA	10:C:782:GLU:HA	1.83	0.60
7:A:1762:TYR:CE2	7:A:1888:GLU:HB3	2.36	0.60
4:L:212:MET:HE2	4:L:220:SER:HB3	1.84	0.60
7:A:414:ARG:NH1	10:C:410:LEU:O	2.35	0.60
7:A:1378:GLU:HB3	7:A:1416:ILE:HD11	1.84	0.60
3:J:466:LEU:HD13	5:F:86:VAL:HG22	1.84	0.60
7:A:293:TRP:NE1	7:A:298:ASP:OD1	2.30	0.60
5:F:121:LEU:H	5:F:124:GLU:HG2	1.67	0.59
7:A:689:VAL:HG21	7:A:742:TYR:HB2	1.83	0.59
7:A:1386:TRP:HH2	7:A:1422:LEU:HD11	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1763:LEU:HD11	7:A:1771:LEU:HD12	1.84	0.59
8:U:276:ARG:HH11	8:U:302:ALA:HB2	1.67	0.59
3:J:457:GLN:NE2	16:6:57:U:O3'	2.34	0.59
7:A:143:GLN:O	7:A:147:MET:HG2	2.02	0.59
7:A:375:ASP:HB2	10:C:355:LYS:HD3	1.83	0.59
7:A:1187:PHE:HE2	7:A:1189:MET:HG2	1.67	0.59
14:7:429:MET:HE3	14:7:429:MET:HA	1.84	0.59
4:L:255:GLN:HB2	4:L:257:LYS:HE3	1.84	0.59
7:A:788:GLN:HG2	7:A:1024:HIS:HB3	1.83	0.59
3:J:481:LEU:HD12	3:J:500:VAL:HG21	1.83	0.59
7:A:641:MET:HA	7:A:644:ILE:HG22	1.83	0.59
7:A:1865:ARG:HD2	9:S:278:ASP:HB3	1.83	0.59
10:C:641:MET:HE2	10:C:655:VAL:HG22	1.82	0.59
7:A:595:LYS:NZ	13:5:45:C:OP2	2.36	0.59
8:U:113:ARG:NH1	8:U:188:ASP:OD2	2.35	0.59
7:A:342:THR:HG23	10:C:268:LYS:HZ3	1.68	0.59
10:C:167:TYR:CE2	10:C:536:ARG:HD2	2.37	0.59
10:C:277:LYS:NZ	10:C:864:PRO:O	2.33	0.59
7:A:1787:ARG:HH21	7:A:1906:ILE:HD11	1.68	0.59
7:A:682:ASP:OD1	7:A:683:LEU:N	2.34	0.59
7:A:1806:ALA:HB3	7:A:1897:LEU:HD11	1.85	0.59
8:U:358:LYS:HB2	8:U:381:GLU:HG2	1.84	0.59
10:C:478:THR:HG21	10:C:492:ALA:HB1	1.85	0.59
7:A:1116:GLU:OE2	7:A:1155:TRP:NE1	2.36	0.58
10:C:133:THR:HG21	10:C:219:LEU:HD12	1.84	0.58
10:C:703:GLU:O	10:C:706:GLN:NE2	2.33	0.58
11:M:28:GLN:HG2	11:M:112:LEU:HD11	1.84	0.58
6:N:202:PRO:O	7:A:1393:ARG:NH1	2.34	0.58
7:A:110:TRP:HE3	7:A:147:MET:HE2	1.69	0.58
7:A:1127:GLY:O	7:A:1170:TRP:NE1	2.28	0.58
7:A:1551:PHE:O	17:z:1:G:N1	2.36	0.58
7:A:952:VAL:HG22	7:A:1189:MET:HG3	1.85	0.58
8:U:156:SER:HB2	8:U:176:PRO:HD3	1.84	0.58
8:U:331:HIS:HD1	8:U:343:THR:HG1	1.51	0.58
8:U:481:ARG:O	8:U:489:GLN:NE2	2.34	0.58
7:A:783:TYR:OH	7:A:986:GLU:OE2	2.21	0.58
7:A:1290:LYS:O	7:A:1294:LYS:HG2	2.04	0.58
8:U:425:ILE:HG13	8:U:426:THR:HG23	1.86	0.58
6:N:33:ASP:OD2	7:A:541:GLY:N	2.37	0.58
4:L:122:PHE:CD2	4:L:125:LEU:HB2	2.38	0.58
7:A:139:VAL:HG11	7:A:212:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:444:ARG:NH2	14:7:448:GLU:OE1	2.36	0.58
4:L:165:MET:HE1	7:A:992:LEU:HB2	1.86	0.57
7:A:832:TYR:HB3	7:A:835:ASP:HB3	1.85	0.57
7:A:1556:ASP:OD2	16:6:44:G:N2	2.37	0.57
7:A:1818:PHE:HB3	7:A:1914:MET:HE3	1.86	0.57
8:U:221:LEU:HD13	8:U:520:HIS:HD2	1.69	0.57
7:A:1631:LEU:HB2	7:A:1660:TYR:HB3	1.85	0.57
7:A:1899:VAL:HG12	7:A:1901:LYS:H	1.69	0.57
10:C:187:THR:HG23	10:C:534:VAL:HG22	1.86	0.57
10:C:338:GLU:O	10:C:342:ARG:NH1	2.37	0.57
10:C:347:ILE:HG23	10:C:368:SER:HB3	1.86	0.57
15:4:63:U:H2'	15:4:64:G:C8	2.40	0.57
8:U:136:CYS:SG	8:U:161:HIS:ND1	2.76	0.57
10:C:177:ARG:NH2	10:C:638:ASP:OD2	2.34	0.57
11:M:61:GLU:CD	11:M:62:PRO:HD3	2.28	0.57
3:J:482:MET:HG3	7:A:1772:PHE:CD2	2.40	0.57
10:C:826:ARG:NH1	10:C:910:ASP:OD1	2.38	0.57
7:A:1775:GLN:HB2	7:A:1859:LYS:HD2	1.87	0.57
10:C:302:PRO:HB2	10:C:320:LEU:HD13	1.86	0.57
7:A:536:LYS:NZ	17:z:-1:G:OP1	2.36	0.57
10:C:770:PHE:HE1	10:C:789:PHE:HD2	1.52	0.57
7:A:1797:ASN:HB3	9:S:356:THR:O	2.05	0.56
4:L:105:ASN:OD1	6:N:823:ARG:NH1	2.38	0.56
5:F:112:LEU:HD23	5:F:119:ILE:HA	1.88	0.56
6:N:156:GLU:HG2	7:A:732:PRO:HG3	1.85	0.56
6:N:179:LEU:HD12	7:A:855:ARG:HB3	1.86	0.56
7:A:634:TRP:CE2	7:A:638:LEU:HD11	2.41	0.56
7:A:1102:THR:OG1	7:A:1104:ASP:OD1	2.20	0.56
7:A:1278:VAL:HG13	7:A:1284:LEU:HD23	1.87	0.56
7:A:1622:MET:O	7:A:1687:TYR:OH	2.21	0.56
10:C:137:HIS:O	10:C:142:LYS:NZ	2.38	0.56
10:C:509:VAL:O	10:C:522:SER:HA	2.06	0.56
6:N:343:GLU:HA	6:N:346:TRP:HD1	1.70	0.56
10:C:230:ASP:HB3	10:C:233:GLU:HB2	1.86	0.56
12:D:81:VAL:HB	12:D:102:ILE:HB	1.85	0.56
3:J:497:GLU:HG2	7:A:1927:ILE:HG22	1.88	0.56
7:A:96:PRO:HB2	7:A:645:THR:HG23	1.87	0.56
7:A:103:LEU:O	7:A:634:TRP:NE1	2.32	0.56
10:C:434:CYS:HA	10:C:438:ILE:HD12	1.86	0.56
10:C:776:GLU:O	10:C:817:TYR:OH	2.20	0.56
11:M:62:PRO:HG2	11:M:65:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:478:THR:HA	10:C:494:GLY:HA3	1.88	0.56
8:U:270:MET:SD	8:U:329:ALA:HB1	2.45	0.56
13:5:17:U:H3	13:5:60:G:H1	1.52	0.56
7:A:1275:ARG:HG2	7:A:1375:TRP:NE1	2.21	0.56
8:U:402:LYS:HE2	8:U:408:LEU:HG	1.88	0.56
6:N:158:LEU:HA	7:A:702:LYS:HZ1	1.71	0.56
7:A:1401:ARG:HH12	7:A:1403:LEU:HD13	1.70	0.56
7:A:901:LEU:O	7:A:1242:ASN:ND2	2.39	0.55
7:A:960:ASN:OD1	7:A:1225:THR:OG1	2.24	0.55
7:A:1730:MET:HA	7:A:1733:ILE:HG22	1.88	0.55
7:A:1761:PRO:HB2	7:A:1885:LYS:HG2	1.86	0.55
10:C:769:GLY:HA3	10:C:812:ALA:HB3	1.88	0.55
5:F:124:GLU:OE2	5:F:132:ARG:NH2	2.34	0.55
7:A:1871:PRO:HG3	9:S:281:VAL:HG21	1.89	0.55
10:C:693:GLU:OE2	10:C:724:TRP:NE1	2.35	0.55
16:6:64:U:H2'	16:6:65:G:C8	2.42	0.55
4:L:322:ASP:OD1	4:L:323:GLU:N	2.39	0.55
10:C:846:VAL:HG22	10:C:887:LEU:HD11	1.88	0.55
4:L:327:LYS:NZ	15:4:28:C:O3'	2.37	0.55
7:A:766:THR:HG22	12:D:141:ARG:HB3	1.87	0.55
7:A:828:PRO:HD3	7:A:1005:ILE:HD11	1.87	0.55
7:A:1667:ARG:HH12	7:A:1674:HIS:HA	1.72	0.55
7:A:2059:THR:OG1	16:6:42:C:OP1	2.24	0.55
6:N:393:LEU:HD13	6:N:413:LEU:HD22	1.88	0.55
6:N:247:ARG:HE	7:A:1877:LEU:HD23	1.72	0.55
7:A:792:HIS:NE2	8:U:408:LEU:O	2.40	0.55
10:C:514:TYR:HB2	10:C:521:ASP:HB3	1.87	0.55
11:M:25:LEU:HD22	11:M:119:ILE:HG13	1.89	0.55
7:A:550:VAL:O	7:A:554:THR:HG23	2.07	0.55
12:D:41:MET:HE3	12:D:106:MET:H	1.70	0.55
10:C:509:VAL:HG22	10:C:565:ILE:HG12	1.88	0.55
13:5:23:C:O2'	13:5:57:G:N2	2.40	0.55
7:A:1246:GLN:HA	7:A:1249:MET:HG2	1.88	0.55
8:U:312:GLN:HB3	8:U:315:LYS:HG2	1.88	0.55
7:A:188:LEU:HD11	7:A:567:GLY:HA2	1.90	0.54
7:A:1434:LYS:O	7:A:1439:ARG:NH2	2.40	0.54
10:C:647:MET:HE3	10:C:648:TYR:CZ	2.42	0.54
10:C:705:VAL:HG11	10:C:717:PHE:CD2	2.43	0.54
11:M:25:LEU:HD21	11:M:116:ILE:HD13	1.88	0.54
7:A:301:LYS:NZ	10:C:939:ARG:O	2.36	0.54
10:C:504:GLY:CA	10:C:527:VAL:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:251:LEU:HD13	15:4:40:U:H5'	1.88	0.54
7:A:1790:ILE:HD13	9:S:266:PHE:HE2	1.72	0.54
8:U:359:LYS:HB3	8:U:379:TYR:HA	1.89	0.54
2:G:320:TYR:HE1	10:C:840:ALA:HB3	1.72	0.54
7:A:158:ARG:HD2	7:A:161:PHE:HD1	1.72	0.54
8:U:206:ASP:OD1	8:U:250:ARG:NH2	2.41	0.54
8:U:274:VAL:HG23	8:U:330:LEU:HD22	1.88	0.54
9:S:274:LEU:HB3	9:S:289:LEU:HG	1.90	0.54
6:N:248:ASN:O	7:A:1850:ARG:NH2	2.40	0.54
7:A:1085:ILE:HG12	7:A:1099:PHE:CE1	2.42	0.54
8:U:504:VAL:HG21	8:U:545:SER:HB2	1.89	0.54
7:A:1314:VAL:HG23	7:A:1478:LEU:HD22	1.89	0.54
7:A:1773:SER:O	7:A:1813:ARG:NH1	2.41	0.54
3:J:457:GLN:OE1	16:6:57:U:O2'	2.25	0.54
7:A:425:PRO:HB2	7:A:428:LYS:HB2	1.89	0.54
4:L:97:ASN:ND2	4:L:237:GLY:HA2	2.23	0.54
6:N:119:ARG:NH1	13:5:19:A:OP2	2.38	0.54
7:A:1782:ASP:HB3	7:A:1841:THR:HG21	1.89	0.54
10:C:836:VAL:HG21	10:C:846:VAL:HG11	1.90	0.54
4:L:377:ARG:HB3	4:L:398:HIS:HD2	1.71	0.54
7:A:942:PRO:HD2	7:A:1438:VAL:HG22	1.90	0.54
7:A:1232:VAL:HG21	7:A:1284:LEU:HD22	1.90	0.54
7:A:1281:THR:HG22	7:A:1284:LEU:H	1.73	0.53
7:A:1393:ARG:O	7:A:1397:ILE:HG12	2.07	0.53
8:U:149:LYS:HZ3	10:C:772:TRP:HA	1.73	0.53
10:C:134:LEU:HD13	10:C:202:ILE:HG23	1.90	0.53
10:C:313:GLN:O	10:C:417:ARG:NH1	2.38	0.53
1:B:43:LEU:HD21	7:A:1285:LEU:HD12	1.90	0.53
10:C:357:THR:OG1	10:C:359:LYS:O	2.26	0.53
12:D:35:ASP:HB3	12:D:38:CYS:HB2	1.91	0.53
15:4:72:U:OP1	17:z:7:G:O2'	2.25	0.53
7:A:544:PHE:HB2	7:A:651:TRP:HH2	1.74	0.53
14:7:411:LEU:HD13	14:7:422:ALA:HB2	1.91	0.53
4:L:399:LEU:HG	6:N:191:LEU:HD22	1.90	0.53
7:A:1762:TYR:HE2	7:A:1888:GLU:HB3	1.74	0.53
7:A:2063:GLU:O	7:A:2063:GLU:HG3	2.09	0.53
10:C:151:GLU:OE1	10:C:417:ARG:NH2	2.36	0.53
10:C:715:GLY:HA2	10:C:729:ALA:HB1	1.89	0.53
6:N:401:PRO:O	6:N:407:TRP:NE1	2.34	0.53
7:A:164:MET:HE2	7:A:577:GLY:HA3	1.89	0.53
7:A:1090:ARG:NH1	7:A:1092:ILE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1237:MET:HG2	7:A:1284:LEU:HD13	1.89	0.53
7:A:1771:LEU:HD11	7:A:1779:PHE:HZ	1.74	0.53
10:C:304:LEU:O	10:C:437:HIS:NE2	2.37	0.53
6:N:247:ARG:NH1	6:N:314:ALA:O	2.32	0.53
6:N:818:ILE:HD11	6:N:834:LEU:HD13	1.89	0.53
10:C:165:LEU:HG	10:C:167:TYR:HB2	1.91	0.53
4:L:122:PHE:HD2	4:L:125:LEU:HB2	1.73	0.53
6:N:271:LYS:HE2	7:A:1914:MET:HG2	1.91	0.53
7:A:878:LEU:O	7:A:882:LYS:HG2	2.09	0.53
16:6:66:C:H2'	16:6:67:G:H8	1.73	0.53
2:G:304:ILE:HB	2:G:312:GLN:HE22	1.74	0.52
3:J:477:ARG:H	3:J:480:ASN:HB3	1.74	0.52
6:N:11:MET:HB2	12:D:12:TRP:HZ3	1.74	0.52
10:C:686:THR:HB	10:C:793:ASP:HB3	1.91	0.52
7:A:1522:GLN:NE2	16:6:49:G:OP1	2.25	0.52
7:A:1644:LEU:O	7:A:1723:LYS:NZ	2.39	0.52
10:C:188:VAL:HG13	10:C:190:LEU:HD11	1.91	0.52
6:N:394:ARG:HB2	9:S:203:TRP:CE2	2.44	0.52
4:L:348:ASP:HA	16:6:49:G:H22	1.74	0.52
5:F:108:VAL:HG13	5:F:133:LEU:HD13	1.91	0.52
6:N:827:ARG:HB2	6:N:850:LEU:HD21	1.91	0.52
7:A:1088:PHE:HD1	7:A:1097:ILE:HG12	1.75	0.52
11:M:52:GLU:HB2	11:M:120:GLN:NE2	2.24	0.52
4:L:148:LYS:O	4:L:152:ASN:ND2	2.43	0.52
6:N:35:GLY:O	7:A:510:ARG:NH2	2.39	0.52
6:N:350:ALA:HA	6:N:358:ALA:HB1	1.90	0.52
7:A:1061:MET:HE1	7:A:1088:PHE:HB3	1.90	0.52
7:A:1279:VAL:HG12	7:A:1369:TYR:HE1	1.75	0.52
8:U:146:ARG:HA	8:U:175:LEU:HD11	1.92	0.52
14:7:441:GLN:HA	14:7:444:ARG:HG2	1.92	0.52
6:N:394:ARG:HD2	6:N:395:LYS:N	2.25	0.52
7:A:95:MET:HE2	7:A:95:MET:HA	1.92	0.52
10:C:127:GLU:O	10:C:130:ARG:NH1	2.42	0.52
10:C:224:GLY:HA3	10:C:438:ILE:HG12	1.92	0.52
10:C:493:PHE:HB2	10:C:551:LEU:HD23	1.91	0.52
10:C:589:LYS:HE3	10:C:661:THR:HG22	1.90	0.52
6:N:335:GLY:O	6:N:339:CYS:N	2.40	0.52
7:A:850:TYR:HA	7:A:853:LYS:HG2	1.91	0.52
7:A:1087:LEU:HB2	7:A:1098:PHE:HB3	1.92	0.52
8:U:316:GLN:NE2	8:U:510:SER:O	2.42	0.52
7:A:1124:ASN:ND2	7:A:1148:ASN:OD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1251:SER:HB2	7:A:1259:ILE:HD11	1.91	0.52
8:U:270:MET:HE3	8:U:273:LEU:HB3	1.90	0.52
10:C:203:MET:HE2	10:C:203:MET:HA	1.92	0.52
10:C:603:MET:HG3	10:C:653:ILE:HD12	1.91	0.52
15:4:14:G:H2'	15:4:15:G:H8	1.74	0.52
6:N:168:ASN:OD1	6:N:171:GLN:NE2	2.33	0.52
7:A:452:LYS:NZ	13:5:48:A:OP2	2.42	0.52
7:A:1544:ARG:HD2	7:A:1672:ASP:H	1.75	0.52
1:B:43:LEU:HD23	1:B:43:LEU:H	1.74	0.51
4:L:386:ASP:O	7:A:1463:LYS:NZ	2.42	0.51
6:N:254:ARG:N	7:A:1851:SER:OG	2.41	0.51
7:A:1296:GLN:HG2	7:A:1327:MET:HE1	1.91	0.51
10:C:559:ILE:HD11	10:C:565:ILE:HD11	1.92	0.51
10:C:933:PHE:O	10:C:937:THR:OG1	2.22	0.51
12:D:8:LEU:HB2	12:D:61:VAL:HG22	1.92	0.51
4:L:408:ARG:HG2	7:A:1877:LEU:HD12	1.91	0.51
7:A:259:ASP:OD1	7:A:259:ASP:N	2.43	0.51
7:A:347:LEU:HD12	7:A:348:PRO:HD2	1.92	0.51
7:A:439:GLN:HB3	7:A:443:VAL:HG21	1.90	0.51
7:A:913:PRO:HA	7:A:916:LYS:HB2	1.91	0.51
7:A:1555:LEU:HB2	7:A:1558:THR:OG1	2.10	0.51
10:C:122:LEU:HD23	10:C:199:LEU:HB2	1.91	0.51
10:C:179:VAL:HG11	10:C:635:LEU:HD21	1.92	0.51
12:D:139:LYS:HB2	13:5:41:U:H5'	1.92	0.51
6:N:34:ILE:HD11	12:D:76:TYR:HB2	1.92	0.51
7:A:1560:ILE:HG12	7:A:1668:TRP:HB2	1.92	0.51
7:A:467:GLN:HG2	7:A:469:LYS:H	1.75	0.51
7:A:759:GLU:N	7:A:759:GLU:OE1	2.43	0.51
3:J:440:LEU:HA	11:M:91:ARG:HH21	1.75	0.51
7:A:269:LEU:HB3	7:A:271:MET:HE3	1.93	0.51
7:A:1057:ARG:NH1	7:A:1060:GLU:OE1	2.39	0.51
10:C:132:VAL:HG21	10:C:226:VAL:HG23	1.92	0.51
10:C:255:VAL:HG21	10:C:285:VAL:HG11	1.92	0.51
10:C:581:LYS:NZ	10:C:703:GLU:OE1	2.40	0.51
10:C:187:THR:CG2	10:C:534:VAL:HG22	2.40	0.51
2:G:324:MET:HG2	7:A:354:PRO:HG2	1.93	0.51
6:N:142:PHE:HB3	7:A:738:MET:HE1	1.93	0.51
7:A:1288:LEU:HD13	7:A:1330:MET:HG2	1.93	0.51
7:A:1634:SER:OG	7:A:1635:TYR:N	2.44	0.51
4:L:114:ILE:HG23	4:L:187:LEU:HD11	1.93	0.51
4:L:348:ASP:OD2	12:D:124:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:111:CYS:HB3	5:F:133:LEU:HD11	1.92	0.51
7:A:546:LEU:HD22	7:A:648:LEU:HD11	1.92	0.51
7:A:772:CYS:SG	7:A:1249:MET:HE1	2.51	0.51
4:L:121:ARG:HB2	4:L:179:LEU:HG	1.92	0.51
4:L:218:ASN:OD1	4:L:317:GLY:N	2.43	0.51
6:N:280:MET:HG3	6:N:317:ARG:NH2	2.26	0.51
7:A:1501:LEU:HD23	7:A:1753:LEU:HD12	1.93	0.51
7:A:1629:ILE:O	7:A:1662:ILE:N	2.43	0.51
10:C:634:GLU:OE2	10:C:882:GLY:N	2.35	0.51
11:M:44:LYS:NZ	15:4:43:G:N7	2.51	0.51
6:N:271:LYS:NZ	7:A:1916:LEU:HB2	2.26	0.50
7:A:137:GLU:HG2	7:A:138:PRO:HD3	1.92	0.50
7:A:143:GLN:O	7:A:146:SER:OG	2.21	0.50
7:A:962:LEU:HB2	7:A:965:VAL:HB	1.93	0.50
4:L:166:VAL:HG13	7:A:995:ARG:HD2	1.93	0.50
6:N:115:ARG:HG2	7:A:470:ARG:HB2	1.94	0.50
7:A:209:ASP:HB2	7:A:212:PRO:HA	1.92	0.50
7:A:1140:MET:HE3	7:A:1177:VAL:HG12	1.93	0.50
8:U:459:LYS:HA	8:U:464:VAL:HA	1.92	0.50
10:C:277:LYS:HD3	10:C:865:GLY:HA3	1.93	0.50
2:G:318:ARG:HE	2:G:321:GLY:HA3	1.75	0.50
8:U:391:LEU:HD12	8:U:452:PHE:HE1	1.75	0.50
10:C:328:ALA:O	10:C:332:GLY:N	2.43	0.50
7:A:1639:VAL:HG13	7:A:1717:ASN:HB3	1.92	0.50
8:U:134:TYR:CD1	8:U:145:GLY:HA2	2.46	0.50
13:5:70:A:H1'	13:5:71:C:C6	2.47	0.50
16:6:44:G:O2'	16:6:46:G:OP1	2.28	0.50
11:M:91:ARG:HH12	14:7:429:MET:HG3	1.75	0.50
12:D:127:ARG:NH2	16:6:47:A:OP1	2.45	0.50
5:F:119:ILE:O	5:F:132:ARG:NH2	2.45	0.50
7:A:102:LEU:HD22	7:A:493:GLY:HA2	1.93	0.50
15:4:4:U:H3	16:6:71:G:H1	1.57	0.50
3:J:462:GLU:HA	3:J:465:ARG:HD2	1.92	0.50
6:N:153:THR:HG23	6:N:156:GLU:H	1.75	0.50
8:U:356:PHE:HB2	8:U:440:ARG:HG3	1.94	0.50
8:U:459:LYS:HB2	8:U:464:VAL:HG22	1.94	0.50
8:U:134:TYR:OH	8:U:146:ARG:NH1	2.45	0.50
4:L:405:GLY:N	6:N:290:ASP:OD2	2.42	0.50
6:N:268:VAL:HG12	6:N:270:PRO:HD3	1.92	0.50
7:A:155:LYS:NZ	7:A:622:GLY:O	2.45	0.50
7:A:544:PHE:HB2	7:A:651:TRP:CH2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:285:PRO:HA	4:L:288:ARG:HG3	1.93	0.49
4:L:383:ILE:HD13	7:A:1321:GLU:HB2	1.94	0.49
7:A:716:ALA:O	8:U:401:TYR:OH	2.28	0.49
7:A:893:GLU:HG3	7:A:1016:VAL:HB	1.94	0.49
7:A:1214:TRP:HB2	7:A:1228:CYS:HB3	1.93	0.49
13:5:78:U:O2'	13:5:80:U:OP1	2.26	0.49
4:L:219:LEU:HD21	4:L:231:ILE:HD11	1.95	0.49
6:N:814:TRP:HE3	6:N:834:LEU:HD12	1.76	0.49
7:A:1706:ASP:O	7:A:1710:ASN:N	2.45	0.49
8:U:227:LEU:HG	8:U:241:GLN:HE21	1.78	0.49
10:C:263:LEU:HD22	10:C:269:LEU:HD12	1.93	0.49
3:J:475:LYS:O	3:J:480:ASN:ND2	2.45	0.49
4:L:278:ASP:OD1	4:L:278:ASP:N	2.42	0.49
4:L:343:LEU:HD12	4:L:344:PRO:HD2	1.94	0.49
4:L:384:GLU:HB3	4:L:401:LYS:HE3	1.92	0.49
4:L:421:SER:OG	15:4:20:A:OP1	2.28	0.49
7:A:1645:LEU:HB2	7:A:1714:ALA:H	1.77	0.49
2:G:289:LEU:HD11	10:C:852:ARG:HD3	1.94	0.49
2:G:310:LYS:HB3	2:G:314:ARG:HH12	1.78	0.49
10:C:832:TYR:CD2	10:C:899:SER:HB3	2.47	0.49
7:A:1052:VAL:O	7:A:1160:ARG:NH1	2.37	0.49
3:J:506:LYS:HA	3:J:509:LYS:HE2	1.94	0.49
4:L:358:ARG:NH2	15:4:18:G:O2'	2.27	0.49
10:C:832:TYR:HD2	10:C:899:SER:HB3	1.77	0.49
7:A:89:LEU:HA	7:A:92:LEU:HG	1.94	0.49
7:A:1576:ILE:HD13	7:A:1747:ILE:HG12	1.93	0.49
7:A:1667:ARG:HD2	7:A:1679:TYR:CE2	2.48	0.49
8:U:404:GLU:O	8:U:407:GLN:NE2	2.46	0.49
10:C:858:THR:OG1	10:C:872:LYS:O	2.29	0.49
2:G:307:ILE:HG23	7:A:618:THR:HG21	1.94	0.49
6:N:112:MET:O	6:N:115:ARG:HG3	2.13	0.48
7:A:1834:GLY:O	7:A:1838:LYS:HG2	2.13	0.48
7:A:1848:LEU:HD13	7:A:1914:MET:HE1	1.94	0.48
6:N:19:PRO:HG2	12:D:68:ASP:HB3	1.94	0.48
6:N:144:ASP:OD1	6:N:144:ASP:N	2.43	0.48
6:N:364:GLN:HE21	6:N:368:HIS:CE1	2.31	0.48
7:A:1294:LYS:HE3	13:5:40:U:OP2	2.13	0.48
10:C:732:ILE:HG12	10:C:746:VAL:HG22	1.94	0.48
16:6:64:U:H2'	16:6:65:G:H8	1.78	0.48
6:N:280:MET:HG3	6:N:317:ARG:HH22	1.79	0.48
6:N:833:ALA:HB2	11:M:48:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:191:ILE:HD11	7:A:572:PHE:HA	1.94	0.48
8:U:427:GLU:HA	8:U:440:ARG:HB3	1.96	0.48
7:A:1099:PHE:HZ	7:A:1157:ILE:HD11	1.78	0.48
7:A:1790:ILE:HD13	9:S:266:PHE:CE2	2.48	0.48
10:C:673:LYS:HG2	10:C:792:LEU:HD12	1.94	0.48
11:M:64:GLU:HG3	11:M:67:LEU:HD22	1.94	0.48
12:D:94:LEU:HD22	12:D:104:TRP:HH2	1.78	0.48
4:L:209:GLU:HG2	4:L:226:SER:HA	1.95	0.48
7:A:339:PHE:HZ	7:A:403:ALA:HA	1.78	0.48
7:A:1304:ASN:OD1	7:A:1305:SER:N	2.47	0.48
8:U:369:GLU:O	8:U:372:GLN:HG3	2.14	0.48
3:J:461:GLN:HB3	3:J:465:ARG:NH1	2.29	0.48
4:L:372:ARG:NH2	7:A:1511:GLU:OE2	2.43	0.48
7:A:206:TRP:HE3	7:A:212:PRO:HB3	1.78	0.48
7:A:985:TYR:HB3	7:A:1032:ARG:HH11	1.78	0.48
1:B:43:LEU:HD12	1:B:47:LEU:HD11	1.95	0.48
4:L:110:ILE:HG21	4:L:194:ALA:HB2	1.96	0.48
6:N:145:LEU:O	6:N:149:LEU:HG	2.14	0.48
7:A:1490:PHE:O	7:A:1493:THR:OG1	2.30	0.48
8:U:144:GLN:H	8:U:151:HIS:HB2	1.78	0.48
8:U:260:LYS:HG2	8:U:261:ASN:H	1.77	0.48
12:D:110:GLN:NE2	12:D:114:ASP:OD1	2.46	0.48
7:A:441:VAL:O	7:A:445:VAL:HG23	2.14	0.48
7:A:828:PRO:HB2	7:A:882:LYS:HE2	1.96	0.48
7:A:1892:PRO:HD2	7:A:1937:ILE:HD11	1.95	0.48
10:C:350:ASN:ND2	10:C:353:THR:OG1	2.46	0.48
7:A:1537:TRP:HE3	7:A:1751:LEU:HD23	1.79	0.48
8:U:101:ARG:H	8:U:101:ARG:HD3	1.79	0.48
12:D:23:ASP:OD1	12:D:23:ASP:N	2.47	0.48
7:A:1110:ILE:HD11	7:A:1149:LEU:HB2	1.96	0.48
7:A:1806:ALA:HB1	7:A:1819:LEU:HD12	1.96	0.48
8:U:198:THR:HG23	8:U:201:GLN:H	1.78	0.48
10:C:237:LEU:HD13	10:C:833:PHE:HE2	1.78	0.48
15:4:6:U:H2'	15:4:7:G:C8	2.49	0.48
7:A:1244:VAL:HG11	7:A:1291:CYS:HB3	1.95	0.47
8:U:172:PHE:HB2	8:U:181:ILE:HB	1.96	0.47
4:L:137:ARG:HE	4:L:158:ILE:HG23	1.79	0.47
7:A:1810:PHE:HB2	7:A:1817:LEU:HD13	1.95	0.47
5:F:99:ILE:O	5:F:134:ARG:NH1	2.38	0.47
6:N:152:VAL:HG13	6:N:156:GLU:HB3	1.94	0.47
6:N:800:MET:HE1	6:N:813:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:358:LYS:NZ	8:U:379:TYR:O	2.46	0.47
10:C:250:ARG:HH11	10:C:451:HIS:HB2	1.79	0.47
7:A:1583:GLN:NE2	7:A:1616:PRO:O	2.45	0.47
12:D:45:LEU:O	12:D:49:ALA:N	2.48	0.47
1:B:42:SER:HB2	7:A:1289:VAL:HG21	1.97	0.47
4:L:403:GLY:N	6:N:290:ASP:OD1	2.48	0.47
7:A:1265:THR:HG22	7:A:1452:PRO:HG3	1.96	0.47
7:A:1606:ILE:HG12	7:A:1637:TRP:HZ2	1.79	0.47
10:C:461:LEU:O	10:C:465:MET:HG2	2.15	0.47
6:N:814:TRP:CE3	6:N:834:LEU:HD12	2.49	0.47
6:N:814:TRP:HB3	6:N:834:LEU:CD1	2.44	0.47
7:A:1314:VAL:O	7:A:1318:THR:OG1	2.30	0.47
11:M:59:ASP:OD1	11:M:59:ASP:N	2.47	0.47
11:M:64:GLU:HA	11:M:67:LEU:HD13	1.95	0.47
15:4:20:A:H2'	15:4:21:U:C6	2.50	0.47
4:L:408:ARG:NE	7:A:1873:GLU:OE1	2.30	0.47
6:N:155:GLU:HA	6:N:158:LEU:HD12	1.97	0.47
6:N:169:LYS:NZ	15:4:50:G:O6	2.48	0.47
7:A:126:ILE:HD12	7:A:128:PHE:CZ	2.49	0.47
7:A:976:MET:HE2	7:A:1187:PHE:CB	2.45	0.47
8:U:164:PHE:CD1	8:U:175:LEU:HD23	2.49	0.47
10:C:609:LYS:HD2	10:C:648:TYR:HB3	1.97	0.47
10:C:830:PRO:HG2	10:C:877:ALA:HB3	1.96	0.47
12:D:32:HIS:CD2	12:D:64:THR:HG23	2.49	0.47
12:D:115:ILE:HD13	12:D:133:PRO:HD2	1.96	0.47
6:N:17:TYR:OH	12:D:15:ASP:OD2	2.28	0.47
6:N:271:LYS:HZ2	7:A:1916:LEU:HB2	1.79	0.47
7:A:112:GLN:NE2	7:A:190:ALA:H	2.10	0.47
7:A:293:TRP:HB3	7:A:1141:ARG:HA	1.96	0.47
7:A:339:PHE:CZ	7:A:403:ALA:HA	2.50	0.47
7:A:1541:THR:O	7:A:1544:ARG:NH1	2.48	0.47
7:A:1810:PHE:HD1	7:A:1817:LEU:HB2	1.78	0.47
10:C:213:ASP:OD1	10:C:214:GLU:N	2.48	0.47
3:J:497:GLU:OE1	7:A:1931:THR:OG1	2.27	0.47
7:A:1840:LYS:O	7:A:1844:GLU:HG2	2.15	0.47
8:U:286:ASN:ND2	8:U:289:ASN:OD1	2.48	0.47
9:S:298:GLU:O	9:S:301:GLU:HG3	2.14	0.47
10:C:743:ASN:HD21	10:C:784:ILE:C	2.23	0.47
10:C:798:GLN:HE21	10:C:799:GLU:HG2	1.79	0.47
6:N:844:LEU:HB3	6:N:867:THR:OG1	2.14	0.47
8:U:247:PRO:HD2	8:U:449:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:504:GLY:HA2	10:C:527:VAL:O	2.14	0.47
6:N:247:ARG:N	6:N:281:ILE:HB	2.30	0.46
7:A:66:VAL:HG11	7:A:487:LEU:HD11	1.97	0.46
9:S:274:LEU:HD23	9:S:291:ASN:HB2	1.96	0.46
10:C:531:TRP:HD1	10:C:540:GLU:CB	2.28	0.46
3:J:491:GLN:HE22	7:A:2007:ILE:HG21	1.80	0.46
4:L:100:THR:HG21	4:L:233:GLY:HA2	1.96	0.46
6:N:334:LYS:HD2	6:N:334:LYS:HA	1.74	0.46
7:A:1316:PHE:HB3	7:A:1327:MET:HE2	1.97	0.46
12:D:41:MET:CE	12:D:106:MET:H	2.28	0.46
6:N:299:LYS:HA	6:N:302:ARG:HH11	1.81	0.46
7:A:1777:ILE:O	7:A:1812:PRO:HD2	2.15	0.46
10:C:938:ARG:NH2	10:C:944:SER:OG	2.46	0.46
15:4:63:U:H2'	15:4:64:G:H8	1.79	0.46
7:A:595:LYS:NZ	13:5:30:A:OP1	2.48	0.46
7:A:975:VAL:HG13	7:A:1099:PHE:HB2	1.98	0.46
14:7:437:ARG:NH2	15:4:22:C:O2'	2.48	0.46
4:L:264:SER:O	4:L:269:PRO:HD3	2.16	0.46
6:N:269:ASP:HB2	7:A:1916:LEU:HB3	1.98	0.46
7:A:1162:PRO:HB2	7:A:1165:VAL:HG12	1.97	0.46
4:L:95:ASP:OD1	4:L:96:ALA:N	2.48	0.46
8:U:101:ARG:CZ	8:U:179:TYR:HB3	2.45	0.46
10:C:375:GLU:OE2	10:C:379:LYS:NZ	2.34	0.46
10:C:645:ARG:HH22	10:C:655:VAL:HG23	1.81	0.46
12:D:40:LYS:O	12:D:43:GLU:HG3	2.15	0.46
6:N:123:ARG:NH2	13:5:52:U:O2'	2.48	0.46
7:A:1276:GLU:OE2	7:A:1375:TRP:N	2.49	0.46
4:L:311:SER:OG	4:L:315:LYS:N	2.48	0.46
6:N:814:TRP:HB3	6:N:834:LEU:HD11	1.98	0.46
7:A:147:MET:O	7:A:151:MET:HG3	2.15	0.46
7:A:1507:SER:HB2	7:A:1752:GLN:NE2	2.30	0.46
15:4:6:U:H2'	15:4:7:G:H8	1.79	0.46
6:N:29:THR:HG23	16:6:37:C:H5	1.81	0.46
8:U:445:LYS:HA	8:U:492:HIS:CE1	2.51	0.46
10:C:140:HIS:NE2	10:C:233:GLU:OE1	2.40	0.46
14:7:510:ALA:O	14:7:514:GLN:HG2	2.16	0.46
3:J:441:THR:HG23	3:J:444:GLU:H	1.81	0.46
4:L:53:LYS:HA	4:L:53:LYS:HD3	1.76	0.46
6:N:394:ARG:HB2	9:S:203:TRP:NE1	2.31	0.46
6:N:821:GLU:O	6:N:826:ARG:NE	2.35	0.46
7:A:1738:PRO:HG2	7:A:2022:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1784:ASN:O	7:A:1806:ALA:N	2.39	0.46
13:5:48:A:H2'	13:5:49:A:H8	1.80	0.46
1:B:52:MET:HB2	7:A:1374:PRO:HG3	1.98	0.45
6:N:823:ARG:HA	6:N:826:ARG:HD2	1.98	0.45
7:A:1491:LYS:O	7:A:1710:ASN:ND2	2.49	0.45
10:C:140:HIS:CE1	10:C:230:ASP:H	2.35	0.45
13:5:47:A:O2'	13:5:48:A:H5''	2.15	0.45
7:A:109:PRO:HB2	7:A:147:MET:HE3	1.98	0.45
7:A:738:MET:HE3	7:A:738:MET:HA	1.98	0.45
7:A:1663:ASP:OD2	7:A:1665:GLN:NE2	2.49	0.45
10:C:137:HIS:CD2	10:C:138:LEU:H	2.34	0.45
7:A:168:PRO:HG2	7:A:559:ASP:HB3	1.98	0.45
7:A:1045:GLY:HA3	7:A:1090:ARG:CZ	2.45	0.45
7:A:1292:GLU:OE2	7:A:1317:TYR:OH	2.33	0.45
6:N:353:GLN:OE1	6:N:354:PRO:HD2	2.15	0.45
7:A:988:ILE:HG12	7:A:1044:TYR:CZ	2.50	0.45
7:A:1125:ILE:HG13	7:A:1147:VAL:HG11	1.99	0.45
7:A:1133:CYS:HB2	7:A:1231:ARG:NE	2.31	0.45
7:A:1321:GLU:O	7:A:1503:TRP:NE1	2.46	0.45
7:A:1902:PHE:O	7:A:1906:ILE:HG23	2.16	0.45
8:U:526:TRP:HD1	8:U:539:PRO:HG3	1.81	0.45
12:D:45:LEU:HD22	12:D:58:ILE:HD12	1.98	0.45
15:4:72:U:H3'	15:4:73:U:H5'	1.98	0.45
4:L:209:GLU:HA	4:L:212:MET:HG2	1.99	0.45
7:A:1134:TRP:O	7:A:1139:ARG:NH1	2.50	0.45
7:A:1308:PRO:HB2	7:A:1311:PHE:HB2	1.99	0.45
10:C:544:VAL:HG13	10:C:548:ASN:HD22	1.81	0.45
11:M:35:LEU:HD11	11:M:102:CYS:HB2	1.97	0.45
2:G:299:LEU:HA	2:G:320:TYR:CE2	2.50	0.45
4:L:117:LYS:HD3	4:L:117:LYS:HA	1.79	0.45
7:A:864:LEU:HD23	7:A:864:LEU:HA	1.82	0.45
7:A:898:PHE:CD1	7:A:905:LEU:HB3	2.51	0.45
7:A:1264:ASN:O	7:A:1268:ILE:HG12	2.17	0.45
7:A:1318:THR:HB	7:A:1324:GLY:HA3	1.98	0.45
8:U:137:LEU:HB2	8:U:163:VAL:HG13	1.99	0.45
10:C:862:PRO:HA	10:C:869:TYR:HA	1.98	0.45
4:L:304:ARG:HB3	11:M:65:ILE:HA	1.98	0.45
10:C:827:LEU:HD11	10:C:934:MET:HB3	1.99	0.45
7:A:97:HIS:ND1	7:A:649:GLU:OE2	2.45	0.45
7:A:1149:LEU:HD23	7:A:1177:VAL:HG21	1.97	0.45
7:A:1330:MET:HE1	7:A:1369:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1421:THR:HA	7:A:1424:GLN:HG3	1.99	0.45
10:C:123:MET:HA	10:C:129:ILE:HD11	1.98	0.45
10:C:320:LEU:HB3	10:C:340:ALA:HB1	1.98	0.45
11:M:22:LEU:O	11:M:26:VAL:HG23	2.17	0.45
12:D:94:LEU:HD11	12:D:102:ILE:HG12	1.98	0.45
15:4:45:G:H2'	15:4:46:G:C8	2.52	0.45
3:J:473:GLU:HG2	3:J:474:PRO:HD2	1.98	0.45
4:L:392:LEU:HD21	7:A:1465:TRP:HH2	1.82	0.45
6:N:297:LEU:O	6:N:301:VAL:HG23	2.17	0.45
7:A:114:ARG:HG3	7:A:210:HIS:CD2	2.52	0.45
7:A:303:ILE:HG21	10:C:878:ILE:HD11	1.98	0.45
7:A:420:ARG:NH2	7:A:423:ASP:OD1	2.42	0.45
7:A:993:LEU:HD11	7:A:1040:ILE:HG23	1.99	0.45
7:A:1034:LEU:HB2	7:A:1037:ALA:HB2	1.98	0.45
7:A:1593:LEU:HA	7:A:1596:VAL:HG12	1.97	0.45
7:A:1787:ARG:NH2	7:A:1906:ILE:HD11	2.31	0.45
7:A:2006:GLU:O	7:A:2010:ILE:HG12	2.17	0.45
10:C:340:ALA:HA	10:C:343:LEU:HD12	1.99	0.45
14:7:473:ARG:NH2	14:7:475:ASP:OD2	2.40	0.45
16:6:48:A:H2'	16:6:49:G:O4'	2.17	0.45
4:L:245:PRO:HG2	4:L:248:ASN:HB2	1.99	0.45
7:A:213:LEU:HD13	7:A:219:TYR:CD2	2.52	0.45
2:G:294:HIS:HB3	10:C:891:THR:HA	1.99	0.44
4:L:112:LYS:HE3	6:N:855:ARG:HG2	1.98	0.44
4:L:250:MET:HB3	4:L:296:ALA:HB2	1.99	0.44
6:N:112:MET:HE3	7:A:472:LEU:HD13	1.99	0.44
7:A:908:VAL:HG11	7:A:1448:LEU:HD22	1.98	0.44
7:A:957:GLN:HG3	7:A:961:ASN:ND2	2.32	0.44
7:A:972:GLU:HG3	7:A:1100:ARG:NH2	2.32	0.44
8:U:352:SER:HB3	8:U:445:LYS:HB3	1.99	0.44
10:C:370:VAL:HA	10:C:374:LEU:HB2	1.98	0.44
2:G:276:TRP:NE1	7:A:449:LYS:HG3	2.32	0.44
4:L:283:LEU:HD12	4:L:287:LEU:HD23	1.98	0.44
7:A:1781:ASP:HB3	7:A:1808:PHE:HB2	1.99	0.44
10:C:305:GLY:O	10:C:433:MET:HG3	2.17	0.44
10:C:744:ILE:HG22	10:C:788:LYS:HA	1.99	0.44
13:5:8:G:N2	13:5:70:A:O3'	2.48	0.44
16:6:66:C:H2'	16:6:67:G:C8	2.52	0.44
3:J:447:LYS:NZ	15:4:24:U:OP2	2.44	0.44
6:N:315:SER:O	6:N:319:GLU:HG2	2.17	0.44
7:A:825:ILE:HG23	7:A:929:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1937:ILE:HD12	7:A:1937:ILE:HA	1.89	0.44
6:N:833:ALA:HA	6:N:836:LYS:HE2	1.99	0.44
7:A:237:THR:HG23	7:A:240:ARG:NH2	2.33	0.44
7:A:387:PHE:HD1	10:C:399:LEU:HD22	1.81	0.44
7:A:1050:LEU:HD22	7:A:1055:LEU:HD23	1.99	0.44
7:A:1187:PHE:CE1	7:A:1196:ILE:HD11	2.52	0.44
7:A:1489:LEU:HG	7:A:1540:PRO:HD3	2.00	0.44
7:A:1497:THR:HG23	7:A:1499:GLU:H	1.81	0.44
8:U:166:ASN:ND2	8:U:169:THR:OG1	2.51	0.44
8:U:307:SER:O	8:U:310:THR:HG22	2.17	0.44
8:U:501:ALA:HB3	8:U:551:ILE:HB	1.99	0.44
8:U:539:PRO:HA	8:U:542:ILE:HG12	1.99	0.44
10:C:614:TYR:HB2	10:C:617:LEU:HB2	1.99	0.44
2:G:299:LEU:HA	2:G:320:TYR:HE2	1.83	0.44
6:N:843:VAL:O	6:N:847:VAL:HG23	2.18	0.44
7:A:1601:LEU:HD23	7:A:1601:LEU:H	1.82	0.44
9:S:206:ARG:O	9:S:209:GLN:HG2	2.17	0.44
10:C:500:THR:OG1	10:C:502:HIS:NE2	2.50	0.44
11:M:97:ARG:NH1	15:4:29:A:N7	2.66	0.44
1:B:36:PRO:HB3	7:A:1336:PRO:HB3	1.98	0.44
4:L:207:TYR:O	4:L:210:SER:OG	2.30	0.44
6:N:31:ARG:NH2	6:N:33:ASP:OD2	2.50	0.44
6:N:197:HIS:CE1	7:A:1425:LYS:HA	2.53	0.44
6:N:326:GLN:HG3	9:S:173:ALA:HB1	1.99	0.44
7:A:106:MET:HE1	7:A:578:LEU:HD13	2.00	0.44
7:A:374:ASP:N	7:A:374:ASP:OD1	2.51	0.44
7:A:858:GLN:HA	7:A:861:ARG:HG2	2.00	0.44
7:A:889:ARG:HA	7:A:889:ARG:HD3	1.81	0.44
7:A:1630:LEU:HD12	7:A:1696:PRO:HG3	2.00	0.44
7:A:1740:LEU:O	7:A:1744:ARG:HD3	2.18	0.44
8:U:456:ARG:HG3	8:U:548:TYR:HD1	1.82	0.44
4:L:103:ILE:HA	4:L:106:GLU:HG2	1.99	0.44
7:A:449:LYS:HD3	7:A:449:LYS:HA	1.78	0.44
7:A:780:THR:HG22	7:A:898:PHE:CD2	2.53	0.44
7:A:1104:ASP:OD1	7:A:1105:GLU:N	2.50	0.44
7:A:1998:ASN:OD1	7:A:1999:VAL:N	2.51	0.44
10:C:731:SER:HB3	10:C:747:ASP:O	2.17	0.44
10:C:845:ALA:O	10:C:849:VAL:HG23	2.18	0.44
7:A:944:ASP:OD2	7:A:1435:GLY:N	2.41	0.44
7:A:1661:TRP:CD2	7:A:1700:GLY:HA3	2.53	0.44
7:A:1955:LYS:HD2	7:A:1955:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:244:LYS:O	10:C:248:GLN:HG2	2.18	0.44
10:C:374:LEU:HD23	10:C:374:LEU:HA	1.89	0.44
10:C:375:GLU:HB3	10:C:376:PRO:HD3	2.00	0.44
10:C:486:ASP:N	10:C:486:ASP:OD1	2.50	0.44
10:C:824:THR:HG22	10:C:826:ARG:HH12	1.81	0.44
10:C:832:TYR:CD1	10:C:901:PHE:HA	2.53	0.44
7:A:303:ILE:HG12	10:C:936:LYS:HD2	2.00	0.44
7:A:966:TRP:CG	7:A:1198:PRO:HB3	2.53	0.44
7:A:1233:ASP:OD1	7:A:1234:ASP:N	2.51	0.44
7:A:1328:LEU:HD23	7:A:1470:TYR:CE2	2.53	0.44
8:U:442:GLN:NE2	8:U:443:LEU:O	2.42	0.44
14:7:447:ARG:HA	14:7:447:ARG:NE	2.33	0.44
3:J:497:GLU:OE2	3:J:501:ARG:NE	2.51	0.43
4:L:358:ARG:HH22	15:4:54:A:H3'	1.83	0.43
7:A:1484:ILE:O	7:A:1488:THR:HG23	2.18	0.43
3:J:461:GLN:HB3	3:J:465:ARG:HH12	1.82	0.43
7:A:1788:VAL:HG12	7:A:1802:PRO:HA	2.01	0.43
10:C:221:ILE:HB	10:C:495:ARG:HB2	2.00	0.43
12:D:135:ASP:OD1	12:D:136:TYR:N	2.51	0.43
4:L:420:ILE:HG13	4:L:425:GLN:HG3	2.00	0.43
4:L:424:LEU:HD12	4:L:424:LEU:HA	1.81	0.43
7:A:1889:LEU:HD22	7:A:2012:LEU:HD13	1.99	0.43
10:C:300:LEU:HA	10:C:306:ASN:HD22	1.82	0.43
15:4:14:G:H2'	15:4:15:G:C8	2.52	0.43
7:A:219:TYR:CZ	7:A:234:MET:HE1	2.53	0.43
7:A:678:GLU:HG2	7:A:679:SER:N	2.32	0.43
7:A:1426:ASP:HB2	7:A:1429:THR:HG22	2.01	0.43
8:U:135:ALA:HB2	8:U:167:LEU:HD21	2.01	0.43
8:U:433:TYR:CZ	8:U:434:LYS:HG3	2.54	0.43
10:C:461:LEU:HG	10:C:465:MET:HE2	2.01	0.43
10:C:743:ASN:ND2	10:C:784:ILE:O	2.51	0.43
12:D:29:ARG:NH2	12:D:33:ASP:OD1	2.48	0.43
2:G:276:TRP:CE2	7:A:449:LYS:HG3	2.53	0.43
3:J:493:PRO:HB3	7:A:1934:SER:HB3	2.00	0.43
7:A:866:LEU:HD12	7:A:913:PRO:HB2	2.00	0.43
7:A:1536:LEU:HD22	7:A:1572:SER:HB3	1.99	0.43
8:U:111:ILE:HD13	8:U:186:LEU:HD11	1.99	0.43
10:C:568:PRO:HG2	10:C:569:ARG:NH1	2.34	0.43
6:N:199:SER:HB2	7:A:1404:THR:HG22	2.01	0.43
7:A:1589:ILE:HG22	7:A:1664:ILE:HD13	2.00	0.43
7:A:1667:ARG:HD2	7:A:1679:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:410:ILE:HD12	8:U:411:PRO:HD2	1.99	0.43
10:C:662:PHE:HB3	10:C:827:LEU:HD22	2.00	0.43
13:5:26:A:H2'	13:5:27:U:O4'	2.19	0.43
4:L:377:ARG:O	4:L:398:HIS:N	2.51	0.43
7:A:180:ASP:OD1	7:A:180:ASP:N	2.50	0.43
7:A:1335:ILE:HD11	7:A:1365:ILE:HG22	2.01	0.43
8:U:303:VAL:O	8:U:307:SER:OG	2.27	0.43
10:C:205:THR:HB	10:C:215:VAL:HG22	2.01	0.43
10:C:847:TYR:CE1	10:C:857:VAL:HG11	2.53	0.43
10:C:946:ASP:OD1	10:C:947:VAL:N	2.51	0.43
3:J:518:ARG:HB3	16:6:66:C:O2'	2.18	0.43
7:A:158:ARG:HD2	7:A:161:PHE:CD1	2.53	0.43
7:A:816:TRP:O	7:A:820:ARG:HG2	2.19	0.43
7:A:1260:VAL:HG21	7:A:1325:LEU:HB3	2.00	0.43
7:A:1950:ALA:O	7:A:1954:LEU:HG	2.19	0.43
8:U:123:LEU:HD22	10:C:608:ARG:HH21	1.84	0.43
8:U:540:GLN:OE1	8:U:540:GLN:N	2.52	0.43
13:5:9:G:OP2	13:5:9:G:N2	2.52	0.43
6:N:98:ASP:HB3	7:A:86:ARG:HG3	2.01	0.43
7:A:1582:TRP:HD1	7:A:1619:SER:HB3	1.84	0.43
8:U:262:ILE:HD11	8:U:271:PHE:HE1	1.83	0.43
10:C:743:ASN:OD1	10:C:787:VAL:N	2.46	0.43
12:D:30:PHE:HB2	12:D:80:THR:OG1	2.19	0.43
3:J:462:GLU:HG3	5:F:90:PHE:CE1	2.48	0.43
4:L:136:ILE:HD13	4:L:194:ALA:HB1	2.00	0.43
4:L:373:LYS:HB2	4:L:373:LYS:HE3	1.75	0.43
7:A:984:MET:HE3	7:A:984:MET:HB2	1.82	0.43
13:5:60:G:H2'	13:5:61:A:C8	2.54	0.43
17:z:3:A:H2'	17:z:4:A:C8	2.54	0.43
7:A:136:ILE:HG22	7:A:138:PRO:HD2	2.00	0.42
7:A:200:ASP:OD1	7:A:240:ARG:NH2	2.49	0.42
7:A:470:ARG:NH1	13:5:16:U:OP2	2.51	0.42
7:A:770:THR:HG21	12:D:108:ASP:HB2	2.00	0.42
7:A:1271:MET:SD	7:A:1278:VAL:HG21	2.59	0.42
10:C:262:ARG:O	10:C:266:GLU:HB2	2.19	0.42
2:G:299:LEU:HD13	7:A:340:ILE:HG12	2.00	0.42
2:G:301:ARG:NH2	7:A:353:ASP:OD1	2.52	0.42
4:L:305:VAL:HG13	4:L:310:GLU:HB2	2.02	0.42
6:N:268:VAL:HG13	7:A:1915:VAL:HG13	2.01	0.42
6:N:317:ARG:NH2	6:N:348:GLU:OE1	2.51	0.42
6:N:325:LEU:HB3	6:N:329:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:332:ILE:HG13	6:N:352:LEU:HD12	2.00	0.42
7:A:235:MET:HE3	7:A:235:MET:HB3	1.79	0.42
7:A:688:ALA:HA	14:7:477:PHE:CE2	2.54	0.42
8:U:177:ASP:HB3	8:U:179:TYR:CD1	2.53	0.42
9:S:209:GLN:O	9:S:212:LYS:HG3	2.18	0.42
10:C:747:ASP:OD2	10:C:756:LYS:NZ	2.51	0.42
14:7:430:ARG:HH12	15:4:25:A:H5'	1.85	0.42
6:N:146:LYS:O	7:A:696:MET:HE3	2.19	0.42
6:N:357:THR:O	6:N:361:VAL:HG23	2.19	0.42
7:A:336:ASN:OD1	10:C:837:GLN:NE2	2.28	0.42
7:A:682:ASP:OD1	7:A:683:LEU:HG	2.19	0.42
7:A:1385:VAL:HG21	7:A:1414:ARG:HB2	2.01	0.42
10:C:453:TYR:CE1	10:C:465:MET:HE1	2.55	0.42
7:A:1316:PHE:HD1	7:A:1325:LEU:HD12	1.84	0.42
7:A:1670:ASP:O	7:A:1674:HIS:HB3	2.19	0.42
10:C:377:LEU:HA	10:C:380:ILE:HG22	2.01	0.42
10:C:769:GLY:HA2	10:C:809:ILE:HG23	2.01	0.42
11:M:41:GLU:CD	15:4:32:G:H1	2.27	0.42
2:G:284:ILE:O	2:G:284:ILE:HG13	2.20	0.42
7:A:271:MET:SD	7:A:310:THR:HG23	2.60	0.42
7:A:965:VAL:O	7:A:974:ASN:ND2	2.39	0.42
7:A:1536:LEU:HD21	7:A:1576:ILE:HD11	2.01	0.42
10:C:480:LYS:HB2	10:C:493:PHE:HD2	1.84	0.42
10:C:705:VAL:HG12	10:C:709:TRP:CZ3	2.53	0.42
3:J:482:MET:HG3	7:A:1772:PHE:CG	2.54	0.42
7:A:427:VAL:HG12	7:A:430:TRP:CD2	2.54	0.42
7:A:517:HIS:HB2	7:A:527:VAL:HG12	2.00	0.42
7:A:1771:LEU:HD11	7:A:1779:PHE:CZ	2.53	0.42
10:C:208:HIS:HB3	10:C:211:PHE:HD2	1.83	0.42
10:C:432:ASP:OD1	10:C:433:MET:N	2.52	0.42
10:C:735:PHE:O	10:C:770:PHE:HE2	2.03	0.42
2:G:296:VAL:HG22	2:G:298:LEU:H	1.84	0.42
6:N:123:ARG:O	6:N:127:GLU:HG2	2.20	0.42
7:A:1994:LYS:HZ1	9:S:297:LYS:HE2	1.85	0.42
8:U:242:ALA:HB2	8:U:503:ILE:HD11	2.01	0.42
10:C:911:PRO:O	10:C:931:ARG:NH1	2.51	0.42
11:M:113:LYS:O	11:M:117:GLN:HG2	2.19	0.42
16:6:41:A:H61	17:z:6:A:H62	1.68	0.42
4:L:330:LYS:HE3	4:L:330:LYS:HB2	1.88	0.42
6:N:161:PRO:O	7:A:712:HIS:NE2	2.52	0.42
6:N:176:TYR:CZ	7:A:1517:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:319:GLU:HB2	6:N:328:ALA:HB2	2.01	0.42
7:A:760:ARG:HG2	7:A:763:ARG:HH21	1.85	0.42
8:U:119:ASP:OD1	8:U:283:LYS:NZ	2.38	0.42
8:U:500:ILE:HD13	8:U:519:LEU:HD23	2.02	0.42
15:4:64:G:C5	15:4:65:A:H1'	2.54	0.42
4:L:121:ARG:HA	4:L:177:GLN:O	2.20	0.42
4:L:130:PRO:HG3	4:L:258:THR:HG23	2.01	0.42
6:N:338:MET:HE2	6:N:338:MET:HB2	1.94	0.42
7:A:348:PRO:HG2	7:A:351:TYR:HB2	2.02	0.42
7:A:750:TRP:HH2	7:A:781:ARG:HB2	1.85	0.42
7:A:894:VAL:HG23	7:A:1017:ILE:HD13	2.02	0.42
7:A:1641:ARG:HG3	7:A:1642:PRO:HD2	2.02	0.42
8:U:366:PRO:HB2	8:U:369:GLU:HG3	2.01	0.42
14:7:430:ARG:NH1	15:4:25:A:H5'	2.34	0.42
7:A:441:VAL:HG22	7:A:444:ARG:HH21	1.85	0.42
7:A:752:ASN:HD22	8:U:462:PHE:HD2	1.67	0.42
10:C:445:ALA:O	10:C:449:ILE:HG12	2.20	0.42
10:C:493:PHE:CZ	10:C:549:TRP:HB3	2.55	0.42
12:D:127:ARG:NH1	16:6:47:A:OP2	2.53	0.42
3:J:478:ILE:HD13	3:J:478:ILE:HA	1.92	0.41
7:A:504:LEU:HD11	7:A:548:ARG:HA	2.02	0.41
7:A:1333:VAL:O	7:A:1364:LEU:HD12	2.20	0.41
10:C:799:GLU:HB2	10:C:802:HIS:ND1	2.35	0.41
11:M:56:MET:HE3	11:M:66:ILE:HD12	2.01	0.41
11:M:63:LEU:O	11:M:66:ILE:HG12	2.20	0.41
11:M:115:GLN:HE21	16:6:71:G:H4'	1.84	0.41
2:G:307:ILE:HD12	2:G:312:GLN:HE21	1.85	0.41
6:N:810:SER:HB2	6:N:813:LEU:HB2	2.02	0.41
7:A:547:CYS:O	7:A:550:VAL:HG12	2.20	0.41
7:A:933:ARG:O	7:A:935:LEU:N	2.53	0.41
7:A:1187:PHE:HE1	7:A:1196:ILE:HD11	1.86	0.41
7:A:1187:PHE:CE2	7:A:1189:MET:HG2	2.50	0.41
10:C:430:PHE:HA	10:C:433:MET:HE2	2.02	0.41
11:M:125:ARG:HD3	11:M:125:ARG:HA	1.80	0.41
3:J:438:VAL:HB	14:7:411:LEU:HD23	2.02	0.41
6:N:160:ILE:HD11	7:A:705:LYS:HB3	2.01	0.41
7:A:1083:HIS:CG	7:A:1084:PRO:HD2	2.55	0.41
7:A:1834:GLY:HA2	9:S:276:LEU:HD13	2.01	0.41
10:C:860:ASP:OD1	10:C:860:ASP:N	2.52	0.41
7:A:643:GLY:O	7:A:646:PRO:HD2	2.20	0.41
7:A:825:ILE:HB	7:A:1001:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1137:ASP:OD1	7:A:1138:ALA:N	2.53	0.41
10:C:168:THR:HG22	10:C:184:THR:HB	2.02	0.41
10:C:770:PHE:CE1	10:C:789:PHE:HD2	2.34	0.41
6:N:326:GLN:NE2	9:S:177:LYS:HD2	2.35	0.41
8:U:134:TYR:CE2	8:U:146:ARG:HB2	2.56	0.41
10:C:426:GLU:HB2	10:C:428:THR:HG23	2.02	0.41
13:5:60:G:H2'	13:5:61:A:H8	1.86	0.41
15:4:37:C:H3'	15:4:38:U:H2'	2.03	0.41
6:N:273:TYR:OH	7:A:1820:LYS:HE2	2.20	0.41
7:A:1188:ASN:ND2	7:A:1193:GLU:OE2	2.53	0.41
7:A:1416:ILE:HB	7:A:1417:PRO:HD3	2.02	0.41
8:U:408:LEU:HD23	8:U:408:LEU:HA	1.83	0.41
8:U:422:PHE:HB3	8:U:443:LEU:HG	2.03	0.41
10:C:834:VAL:HG11	10:C:883:PHE:HE2	1.86	0.41
11:M:7:ASN:HD22	11:M:58:ALA:HB1	1.85	0.41
11:M:61:GLU:OE2	11:M:62:PRO:HD3	2.20	0.41
4:L:204:ILE:O	4:L:208:VAL:HG23	2.21	0.41
6:N:148:LYS:HA	6:N:148:LYS:HD3	1.89	0.41
7:A:494:LEU:HD21	7:A:562:VAL:HG21	2.02	0.41
7:A:535:ARG:NH2	17:z:-2:G:H5'	2.36	0.41
7:A:1798:LEU:HD23	9:S:356:THR:O	2.20	0.41
7:A:1941:ARG:O	7:A:1945:VAL:HG23	2.21	0.41
8:U:197:PHE:HD2	8:U:254:LEU:HD13	1.85	0.41
8:U:503:ILE:O	8:U:548:TYR:N	2.45	0.41
4:L:406:ARG:O	6:N:289:ASN:HB3	2.21	0.41
7:A:182:ILE:HD11	7:A:562:VAL:HG13	2.01	0.41
7:A:390:ASP:OD1	7:A:390:ASP:N	2.54	0.41
7:A:750:TRP:NE1	7:A:778:ARG:HE	2.19	0.41
7:A:1956:PRO:HD2	7:A:1960:THR:HG21	2.03	0.41
4:L:249:ILE:HD12	4:L:300:THR:OG1	2.21	0.41
5:F:82:ARG:O	5:F:85:GLU:HG3	2.20	0.41
6:N:158:LEU:HD23	7:A:702:LYS:NZ	2.36	0.41
6:N:247:ARG:N	6:N:317:ARG:HH11	2.19	0.41
6:N:349:ALA:HB1	6:N:361:VAL:HG11	2.02	0.41
6:N:794:ASN:O	6:N:798:THR:HG23	2.20	0.41
7:A:858:GLN:O	7:A:862:GLU:HG2	2.20	0.41
7:A:1051:LEU:HD13	7:A:1162:PRO:HD2	2.02	0.41
7:A:1245:ARG:O	7:A:1249:MET:HG2	2.20	0.41
7:A:1264:ASN:ND2	7:A:1326:GLY:O	2.47	0.41
7:A:1560:ILE:HG21	7:A:1573:LEU:HD13	2.02	0.41
7:A:1785:VAL:O	7:A:1805:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:134:LEU:HG	10:C:228:PHE:HE1	1.85	0.41
10:C:676:ALA:HB3	10:C:815:VAL:HB	2.03	0.41
10:C:812:ALA:HA	10:C:815:VAL:HG12	2.03	0.41
11:M:64:GLU:CD	11:M:64:GLU:H	2.29	0.41
12:D:48:ILE:O	12:D:52:VAL:HG22	2.19	0.41
12:D:122:GLY:HA3	12:D:130:VAL:HG12	2.02	0.41
14:7:472:ARG:CZ	14:7:487:LYS:HG3	2.51	0.41
4:L:378:MET:HE3	7:A:1321:GLU:HA	2.01	0.41
7:A:1143:MET:HE3	7:A:1143:MET:HA	2.03	0.41
8:U:124:CYS:SG	8:U:151:HIS:ND1	2.90	0.41
8:U:133:ALA:HB3	8:U:167:LEU:HB2	2.03	0.41
8:U:189:ILE:HG12	8:U:290:PHE:HZ	1.86	0.41
8:U:548:TYR:CD2	8:U:549:ILE:HG13	2.56	0.41
10:C:359:LYS:HA	10:C:359:LYS:HD3	1.88	0.41
2:G:322:ASP:O	2:G:325:GLU:HG2	2.21	0.40
4:L:282:SER:O	4:L:282:SER:OG	2.34	0.40
6:N:197:HIS:CE1	7:A:1425:LYS:HD3	2.56	0.40
6:N:329:ARG:HB3	6:N:353:GLN:NE2	2.36	0.40
6:N:373:VAL:HA	6:N:376:TYR:HD2	1.86	0.40
7:A:155:LYS:HG3	7:A:626:GLY:HA3	2.03	0.40
7:A:464:PRO:HB2	13:5:23:C:C4	2.56	0.40
7:A:1905:LEU:HA	7:A:1908:LYS:HE2	2.03	0.40
6:N:254:ARG:HD3	7:A:1914:MET:SD	2.61	0.40
6:N:800:MET:HE2	6:N:804:LEU:HG	2.03	0.40
7:A:1086:ARG:O	7:A:1087:LEU:HD23	2.21	0.40
7:A:1552:GLN:HB3	7:A:1563:HIS:HD2	1.86	0.40
7:A:1728:GLN:O	7:A:1732:LYS:HD3	2.20	0.40
8:U:113:ARG:HD3	8:U:215:TYR:CE2	2.57	0.40
10:C:392:LEU:N	10:C:393:PRO:HD2	2.36	0.40
10:C:641:MET:HE3	10:C:641:MET:HB3	1.96	0.40
14:7:445:SER:O	14:7:448:GLU:HG2	2.20	0.40
3:J:510:ALA:O	3:J:513:GLU:HG3	2.22	0.40
6:N:288:ILE:HD11	7:A:1877:LEU:HD21	2.03	0.40
7:A:101:LYS:HB3	7:A:129:VAL:HB	2.03	0.40
7:A:239:TYR:HE1	7:A:408:PRO:HD2	1.86	0.40
7:A:382:GLU:HA	10:C:354:ARG:NE	2.35	0.40
7:A:407:ALA:O	7:A:412:ASN:ND2	2.46	0.40
7:A:684:GLU:OE2	14:7:473:ARG:NH2	2.54	0.40
7:A:1271:MET:HE3	7:A:1372:ILE:HD12	2.03	0.40
8:U:197:PHE:HZ	8:U:286:ASN:HA	1.86	0.40
8:U:231:LYS:HB2	8:U:313:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:353:MET:SD	8:U:354:ARG:N	2.95	0.40
8:U:460:ASN:ND2	8:U:465:GLU:OE1	2.55	0.40
9:S:329:LYS:HG3	9:S:330:PRO:HD3	2.04	0.40
10:C:449:ILE:HD12	10:C:465:MET:SD	2.61	0.40
10:C:758:LEU:O	10:C:761:SER:OG	2.34	0.40
15:4:11:A:H2'	15:4:12:G:C8	2.56	0.40
15:4:53:U:O2'	15:4:54:A:H5'	2.22	0.40
7:A:101:LYS:HA	7:A:101:LYS:HD2	1.69	0.40
7:A:507:LEU:O	7:A:510:ARG:HB2	2.22	0.40
7:A:994:ASN:HB2	7:A:1010:THR:HG21	2.04	0.40
8:U:254:LEU:HD23	8:U:254:LEU:HA	1.84	0.40
8:U:457:PHE:CD1	8:U:509:PRO:HB3	2.56	0.40
10:C:203:MET:HE3	10:C:549:TRP:CE3	2.56	0.40
10:C:260:ILE:HG12	10:C:310:SER:O	2.21	0.40
10:C:715:GLY:O	10:C:719:GLN:HG2	2.22	0.40
16:6:46:G:H5'	17:z:3:A:C2	2.57	0.40
6:N:118:GLU:HA	6:N:121:GLU:HG2	2.02	0.40
7:A:1531:ASN:O	7:A:1535:THR:HG23	2.21	0.40
9:S:297:LYS:HE3	9:S:297:LYS:HB2	1.92	0.40
10:C:183:SER:O	10:C:482:TYR:OH	2.33	0.40
10:C:594:PRO:HG3	10:C:600:LEU:HD13	2.04	0.40
10:C:737:PRO:HD2	10:C:741:GLY:HA3	2.04	0.40
11:M:37:LYS:HE2	11:M:37:LYS:HB2	1.97	0.40
13:5:19:A:H4'	13:5:20:G:C8	2.56	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	B	20/2136 (1%)	20 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	55/820 (7%)	53 (96%)	2 (4%)	0	100	100
3	J	82/683 (12%)	82 (100%)	0	0	100	100
4	L	372/499 (74%)	366 (98%)	6 (2%)	0	100	100
5	F	59/522 (11%)	59 (100%)	0	0	100	100
6	N	447/941 (48%)	437 (98%)	10 (2%)	0	100	100
7	A	1971/2335 (84%)	1890 (96%)	81 (4%)	0	100	100
8	U	454/565 (80%)	441 (97%)	13 (3%)	0	100	100
9	S	138/800 (17%)	136 (99%)	2 (1%)	0	100	100
10	C	834/972 (86%)	817 (98%)	17 (2%)	0	100	100
11	M	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
12	D	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
14	7	103/793 (13%)	98 (95%)	5 (5%)	0	100	100
All	All	4796/11336 (42%)	4651 (97%)	145 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	17/1908 (1%)	17 (100%)	0	100	100
2	G	51/721 (7%)	51 (100%)	0	100	100
3	J	72/599 (12%)	72 (100%)	0	100	100
4	L	303/424 (72%)	303 (100%)	0	100	100
5	F	52/442 (12%)	52 (100%)	0	100	100
6	N	341/792 (43%)	341 (100%)	0	100	100
7	A	1786/2108 (85%)	1786 (100%)	0	100	100
8	U	418/511 (82%)	418 (100%)	0	100	100
9	S	120/681 (18%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	738/866 (85%)	737 (100%)	1 (0%)	88	88
11	M	108/111 (97%)	108 (100%)	0	100	100
12	D	129/130 (99%)	129 (100%)	0	100	100
14	7	91/709 (13%)	91 (100%)	0	100	100
All	All	4226/10002 (42%)	4225 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	531	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	295	GLN
2	G	312	GLN
3	J	480	ASN
3	J	503	GLN
4	L	97	ASN
4	L	108	ASN
4	L	309	HIS
6	N	197	HIS
6	N	330	ASN
6	N	364	GLN
7	A	105	ASN
7	A	112	GLN
7	A	181	ASN
7	A	306	GLN
7	A	368	GLN
7	A	703	GLN
7	A	711	GLN
7	A	752	ASN
7	A	961	ASN
7	A	1003	HIS
7	A	1004	ASN
7	A	1014	ASN
7	A	1083	HIS
7	A	1242	ASN
7	A	1337	GLN
7	A	1450	GLN

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Mol	Chain	Res	Type
7	A	1476	GLN
7	A	1658	GLN
7	A	1875	HIS
7	A	1944	HIS
8	U	166	ASN
8	U	233	ASN
8	U	241	GLN
8	U	286	ASN
8	U	316	GLN
8	U	492	HIS
9	S	157	ASN
9	S	293	ASN
9	S	327	GLN
10	C	201	ASN
10	C	383	GLN
10	C	538	HIS
10	C	548	ASN
10	C	892	GLN
11	M	7	ASN
11	M	77	ASN
12	D	32	HIS
14	7	513	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	24 (30%)	2 (2%)
15	4	79/144 (54%)	24 (30%)	0
16	6	47/106 (44%)	8 (17%)	1 (2%)
17	z	12/13 (92%)	6 (50%)	0
All	All	216/380 (56%)	62 (28%)	3 (1%)

All (62) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	5	10	U
13	5	14	U
13	5	20	G
13	5	21	A
13	5	22	U
13	5	23	C

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Mol	Chain	Res	Type
13	5	24	G
13	5	25	C
13	5	26	A
13	5	28	A
13	5	35	U
13	5	36	C
13	5	39	C
13	5	41	U
13	5	42	U
13	5	44	A
13	5	45	C
13	5	52	U
13	5	57	G
13	5	70	A
13	5	72	U
13	5	78	U
13	5	79	C
13	5	80	U
15	4	11	A
15	4	18	G
15	4	19	U
15	4	25	A
15	4	26	G
15	4	36	U
15	4	38	U
15	4	39	A
15	4	40	U
15	4	41	C
15	4	42	C
15	4	44	A
15	4	45	G
15	4	53	U
15	4	55	U
15	4	58	C
15	4	65	A
15	4	68	A
15	4	69	C
15	4	70	U
15	4	71	U
15	4	72	U
15	4	73	U
15	4	74	C

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Mol	Chain	Res	Type
16	6	35	A
16	6	37	C
16	6	40	U
16	6	46	G
16	6	50	A
16	6	70	A
16	6	77	C
16	6	78	A
17	z	-2	G
17	z	1	G
17	z	2	U
17	z	3	A
17	z	4	A
17	z	7	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	77	G
13	5	78	U
16	6	77	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
18	IHP	A	2401	-	36,36,36	0.70	0	60,60,60	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	IHP	A	2401	-	-	4/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

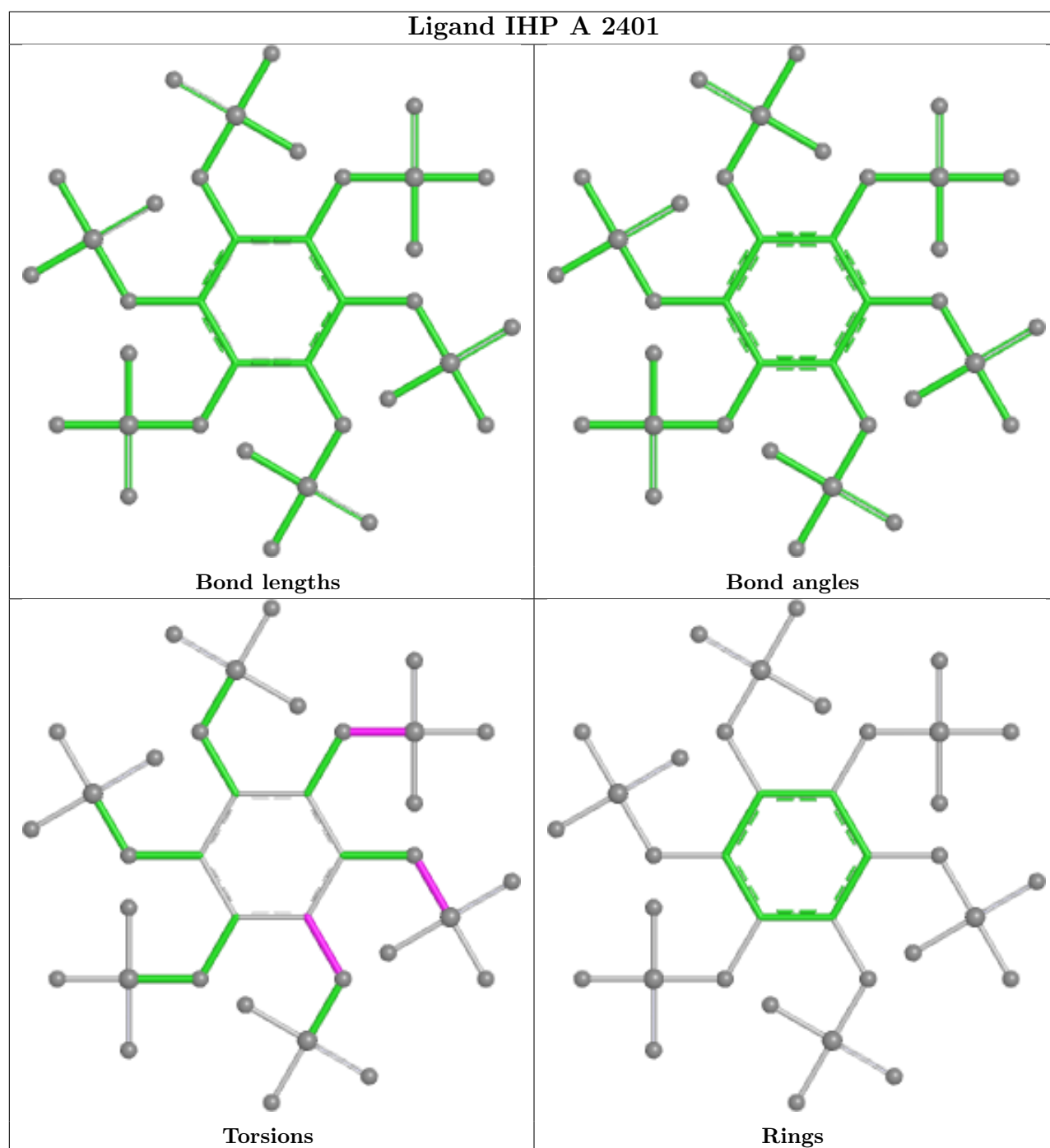
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C1-C6-O16-P6
18	A	2401	IHP	C5-C6-O16-P6
18	A	2401	IHP	C4-O14-P4-O44
18	A	2401	IHP	C5-O15-P5-O35

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

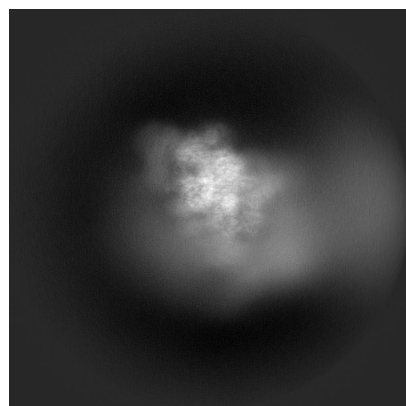
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18547. These allow visual inspection of the internal detail of the map and identification of artifacts.

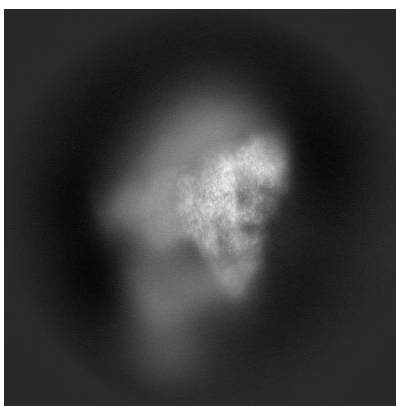
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

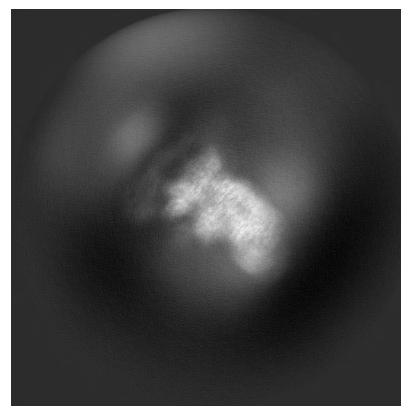
6.1.1 Primary map



X

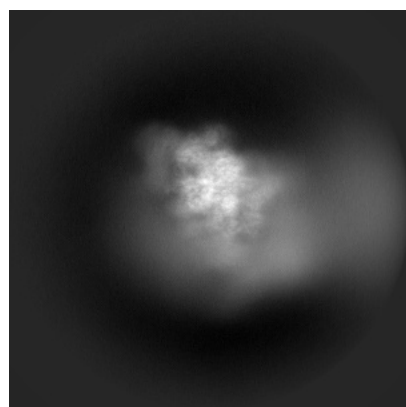


Y

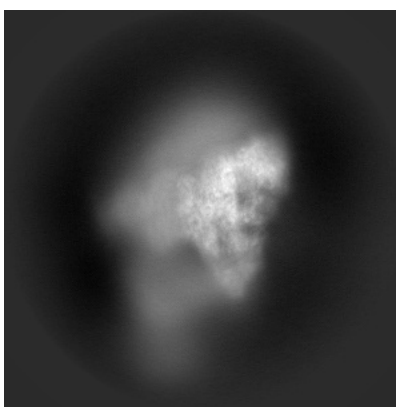


Z

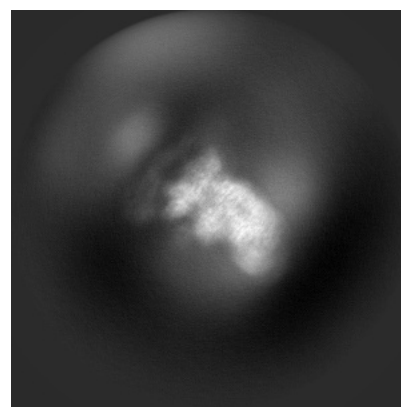
6.1.2 Raw map



X



Y

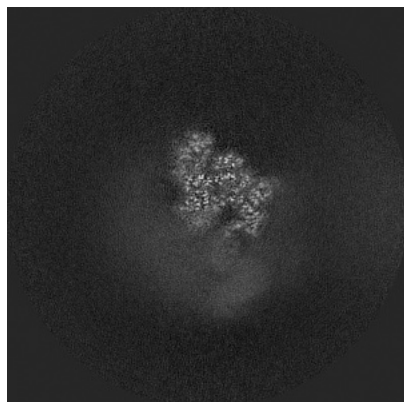


Z

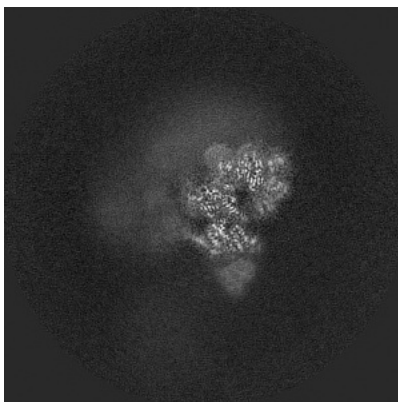
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

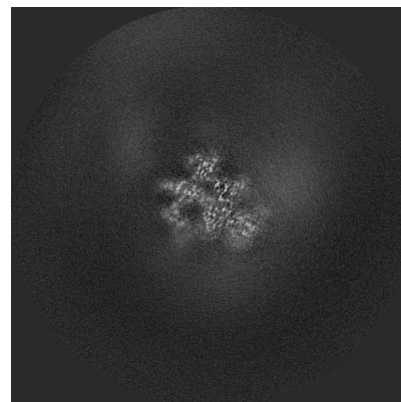
6.2.1 Primary map



X Index: 240

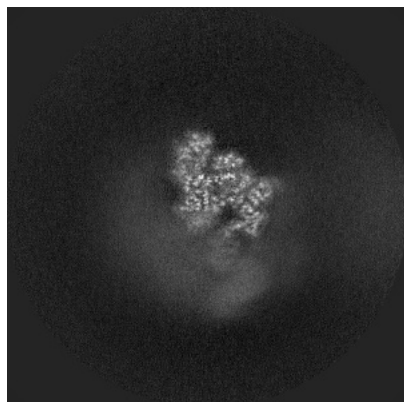


Y Index: 240

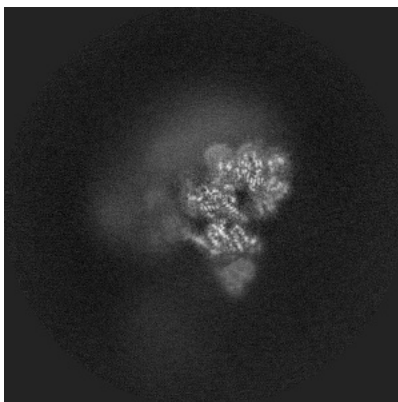


Z Index: 240

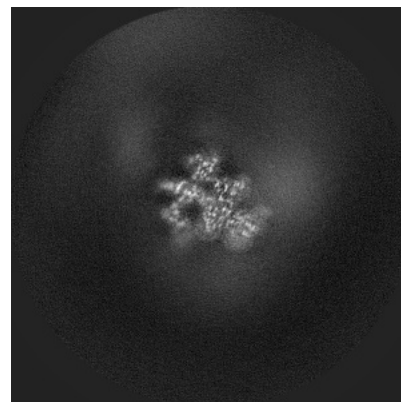
6.2.2 Raw map



X Index: 240



Y Index: 240

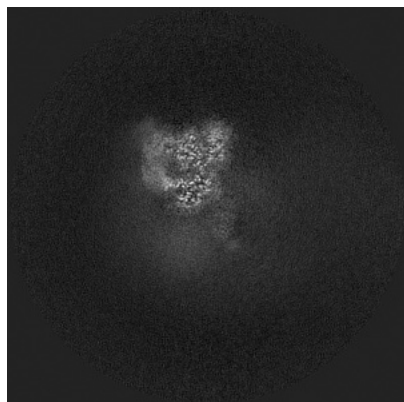


Z Index: 240

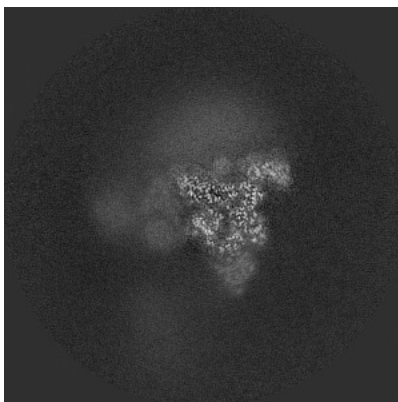
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

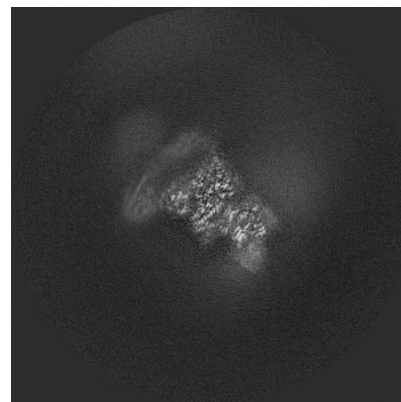
6.3.1 Primary map



X Index: 287

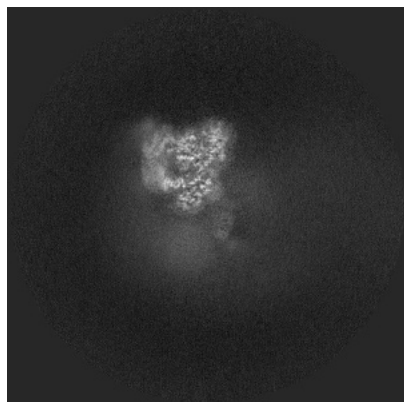


Y Index: 255

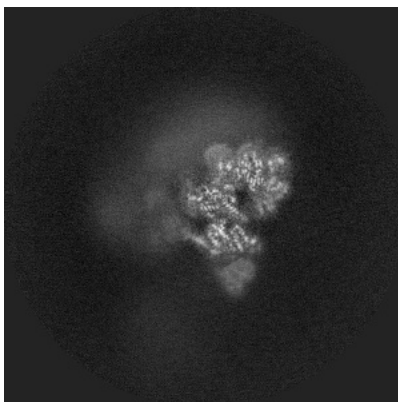


Z Index: 274

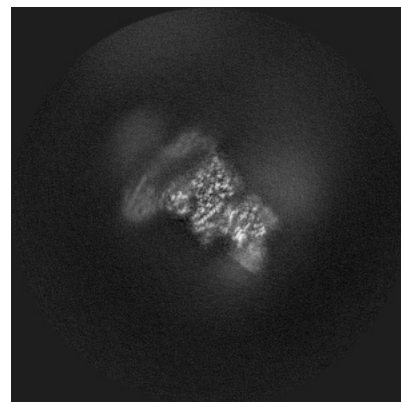
6.3.2 Raw map



X Index: 288



Y Index: 240

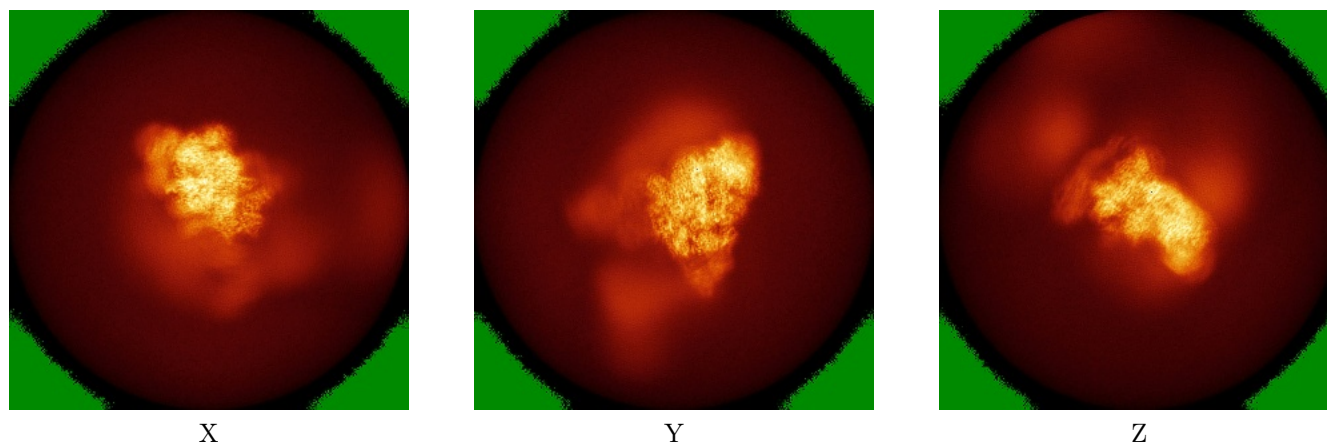


Z Index: 274

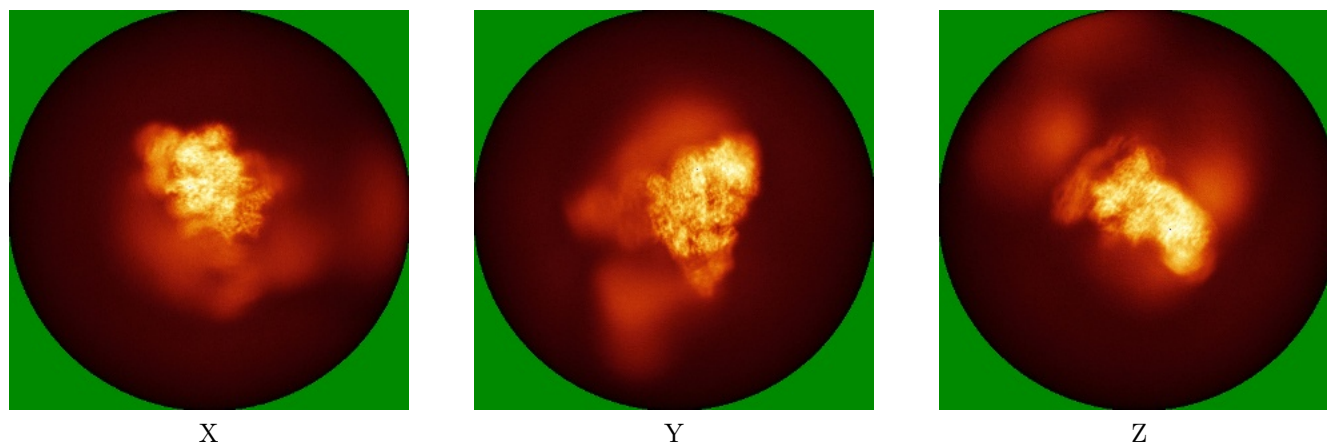
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

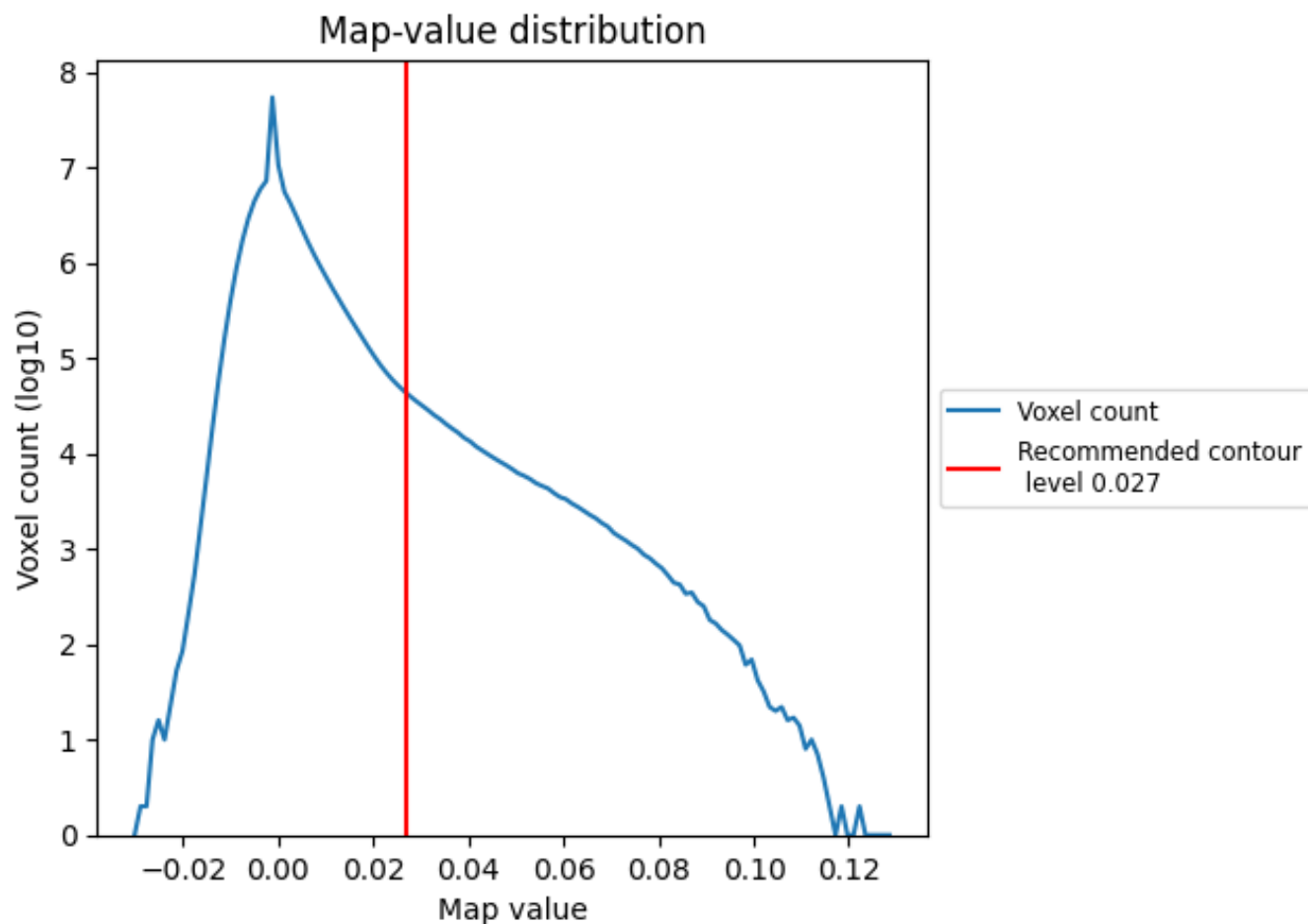
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

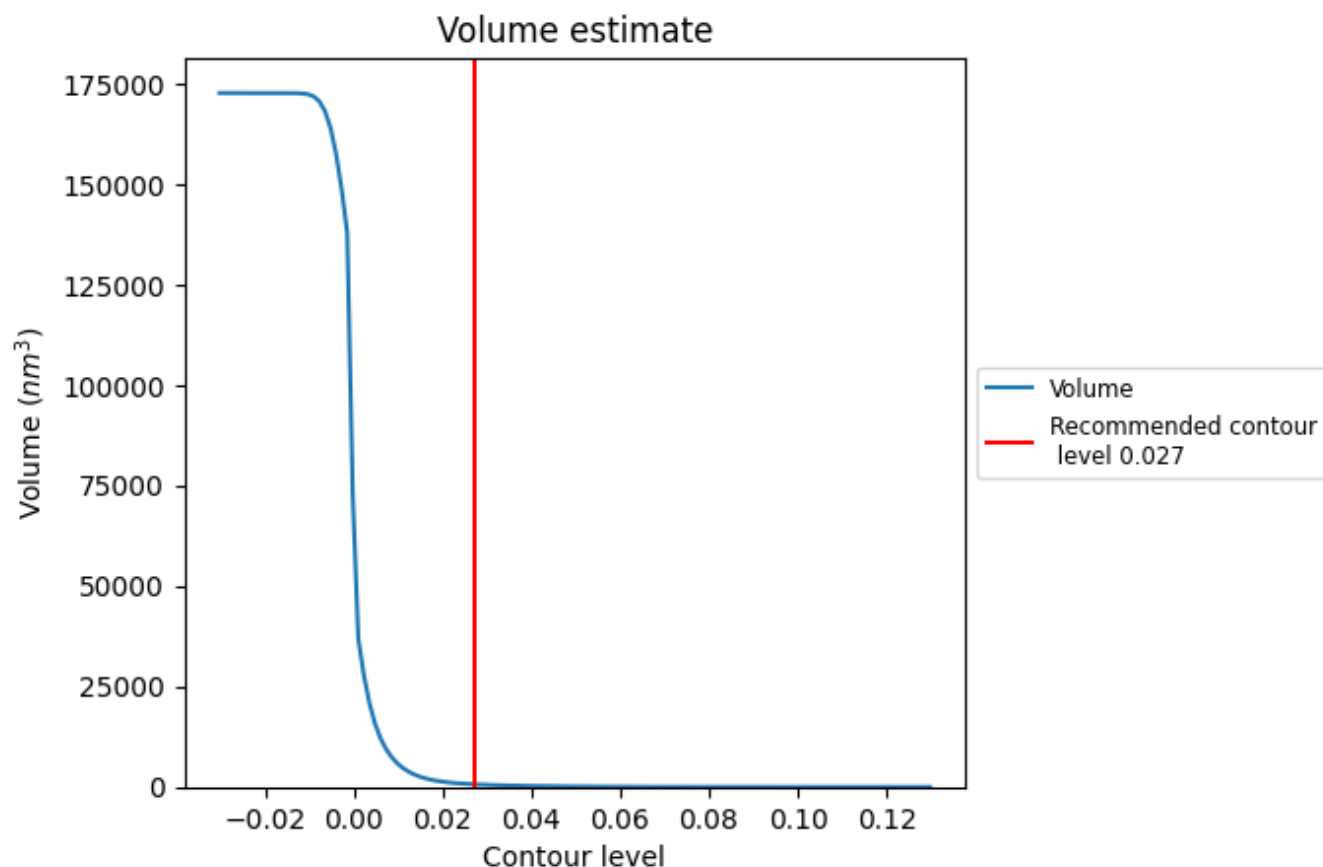
This section contains the results of statistical analysis of the map.

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.

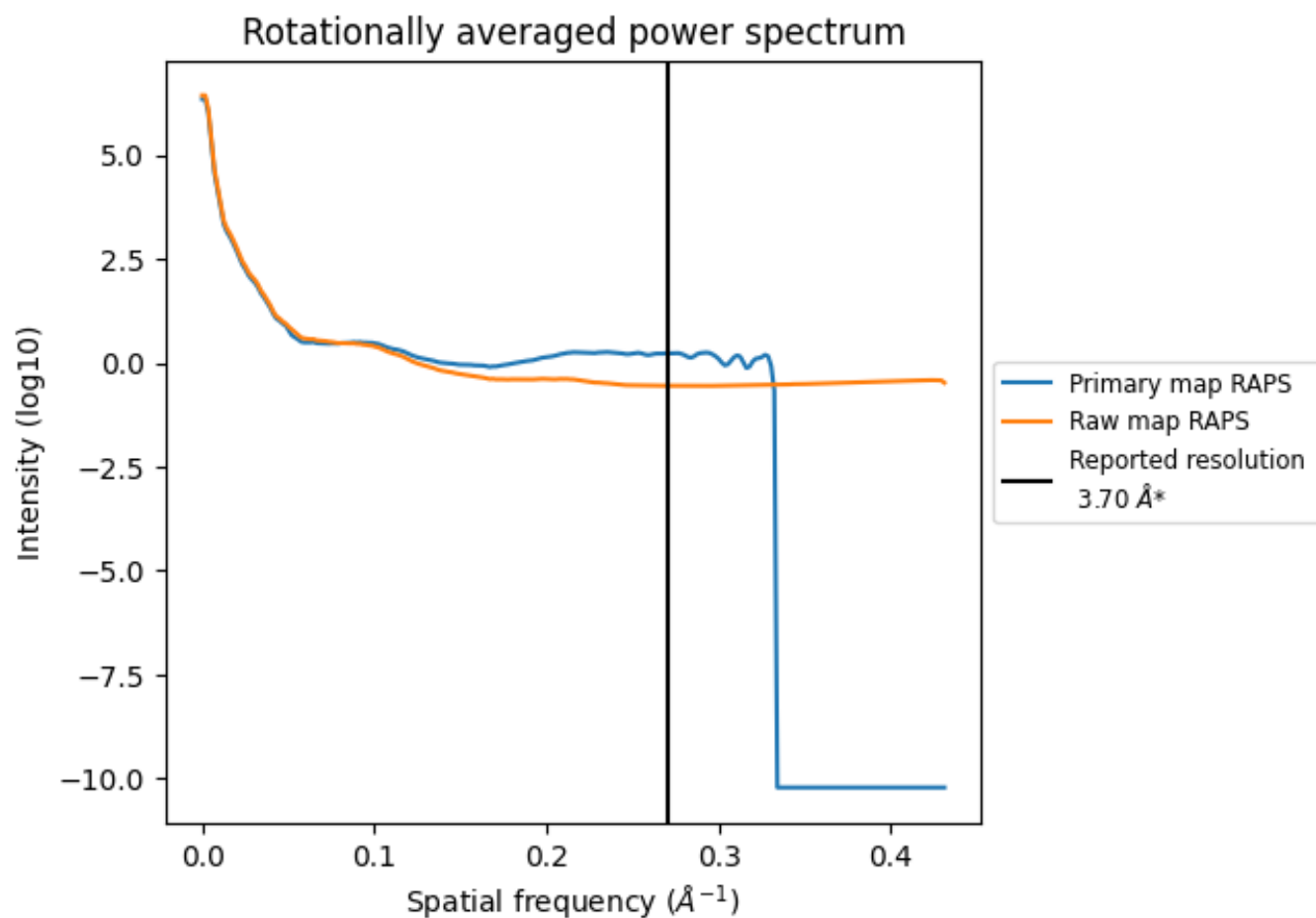
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 667 nm^3 ; this corresponds to an approximate mass of 602 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

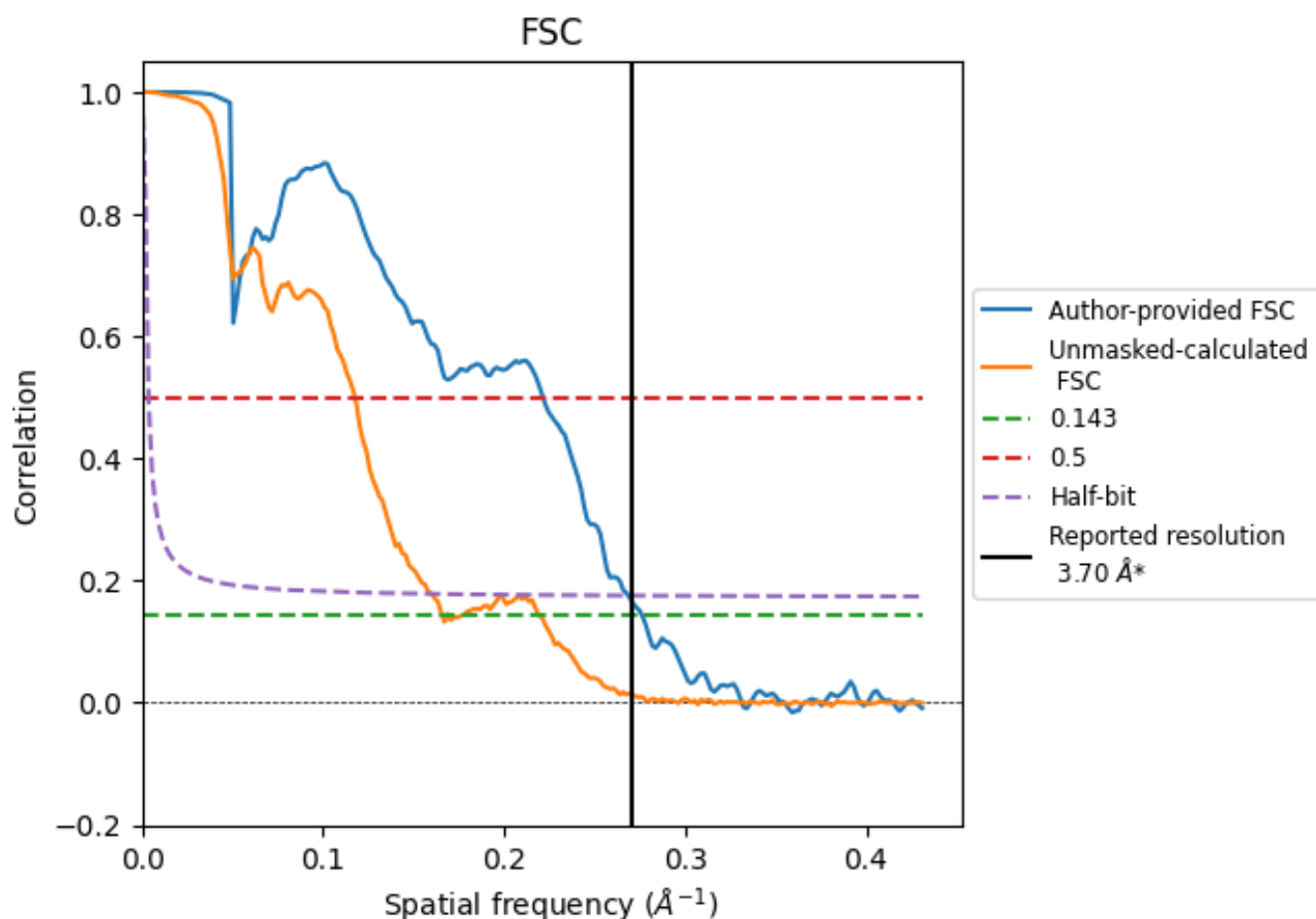


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

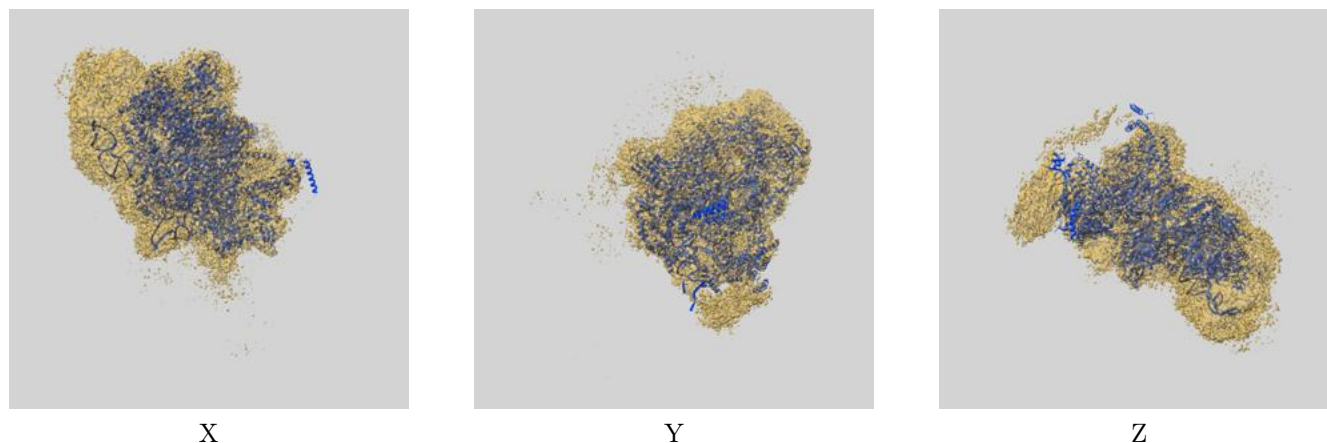
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.62	4.51	3.72
Unmasked-calculated*	6.03	8.50	6.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.03 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

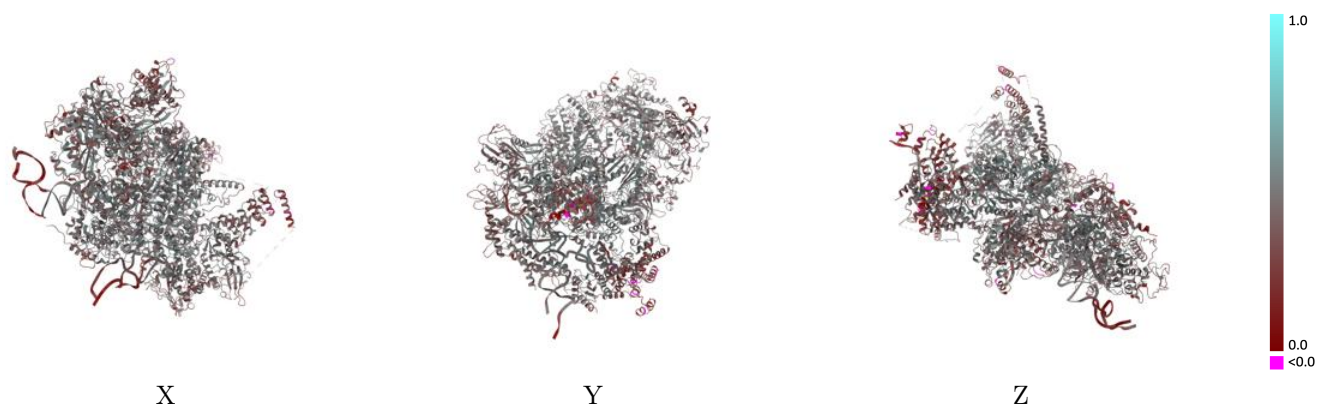
This section contains information regarding the fit between EMDB map EMD-18547 and PDB model 8QPB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



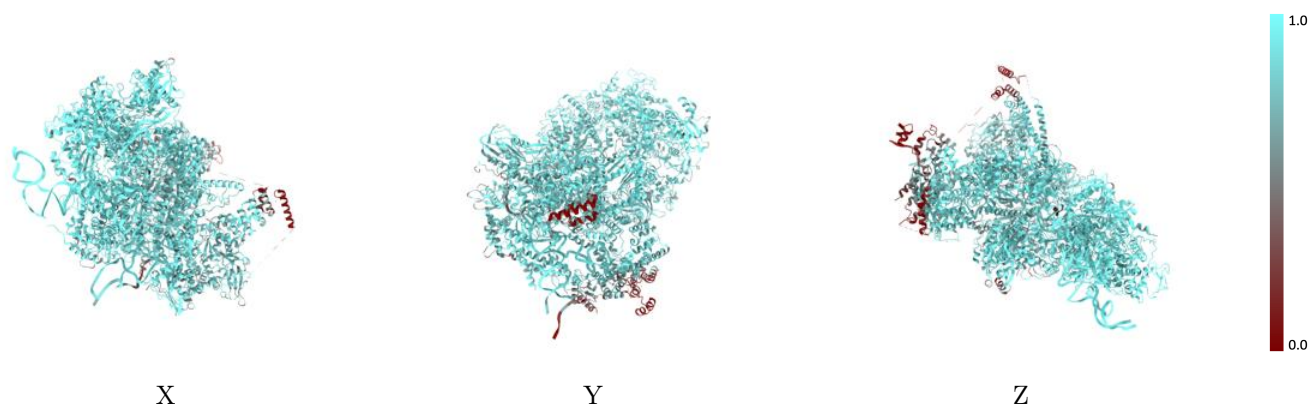
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



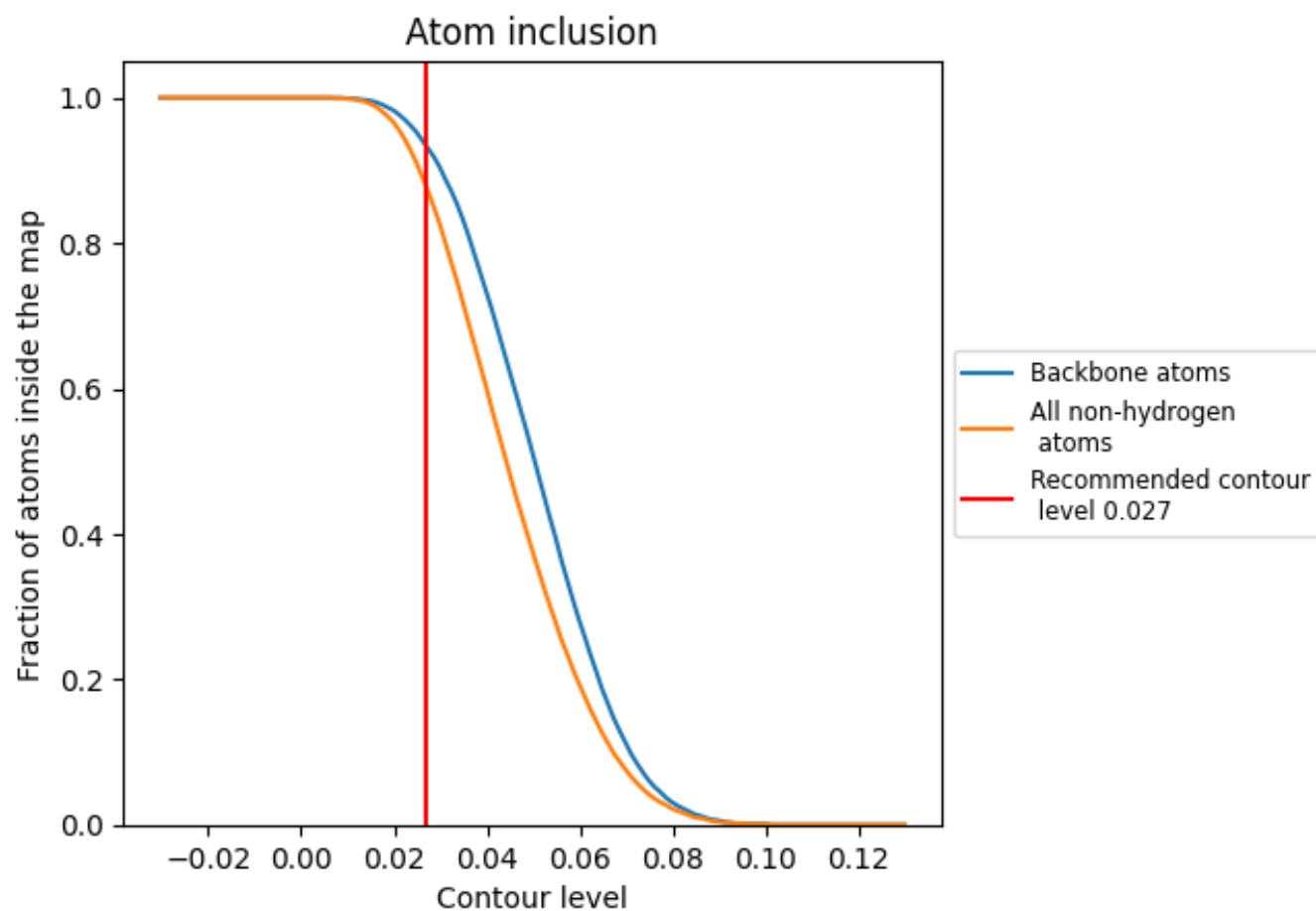
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.4230
4	0.8890	0.3960
5	0.9860	0.4040
6	0.8720	0.3990
7	0.7700	0.3800
A	0.9090	0.4570
B	0.8530	0.4010
C	0.9590	0.4230
D	0.9340	0.5000
F	0.8120	0.3510
G	0.9000	0.3210
J	0.9150	0.4390
L	0.8180	0.4070
M	0.6360	0.4180
N	0.7370	0.3710
S	0.6410	0.3590
U	0.8440	0.3830
z	0.9790	0.4300

