



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 6U5U / pdb_00006u5u
EMDB ID : EMD-20656
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.80 Å (reported)
Based on initial model : 2UV8

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

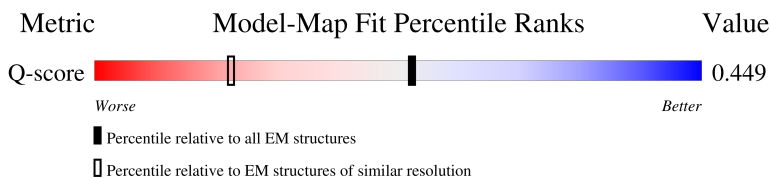
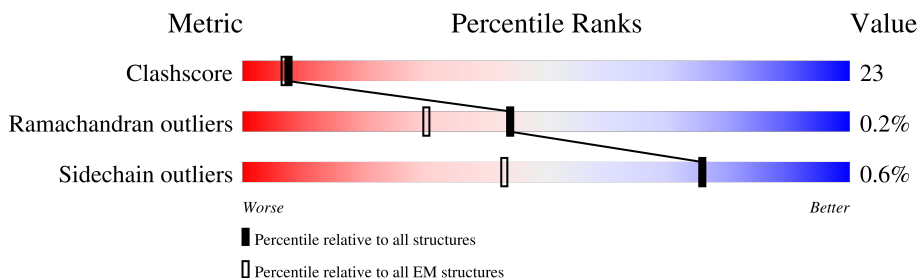
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	1887	25% 53% 32% 15%
2	G	2073	47% 52% 46% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	G	2102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28298 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1611	Total	C	N	O	S	0	0
			12171	7684	2081	2362	44		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0
			15995	10253	2660	3026	56		

There are 22 discrepancies between the modelled and reference sequences:

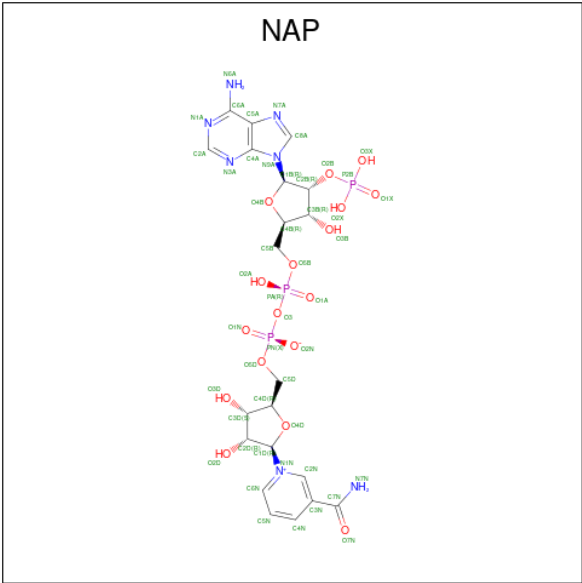
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression tag	UNP P07149
G	2059	ASP	-	expression tag	UNP P07149
G	2060	TYR	-	expression tag	UNP P07149
G	2061	LYS	-	expression tag	UNP P07149
G	2062	ASP	-	expression tag	UNP P07149
G	2063	HIS	-	expression tag	UNP P07149
G	2064	ASP	-	expression tag	UNP P07149
G	2065	ILE	-	expression tag	UNP P07149
G	2066	ASP	-	expression tag	UNP P07149
G	2067	TYR	-	expression tag	UNP P07149
G	2068	LYS	-	expression tag	UNP P07149
G	2069	ASP	-	expression tag	UNP P07149
G	2070	ASP	-	expression tag	UNP P07149
G	2071	ASP	-	expression tag	UNP P07149
G	2072	ASP	-	expression tag	UNP P07149

Continued on next page...

Continued from previous page...

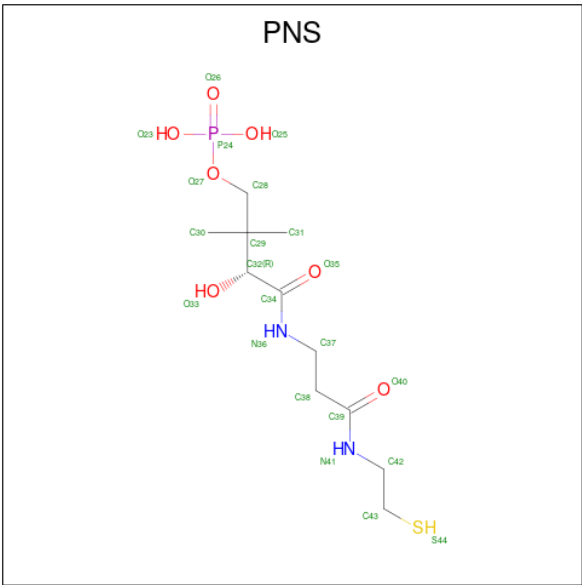
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



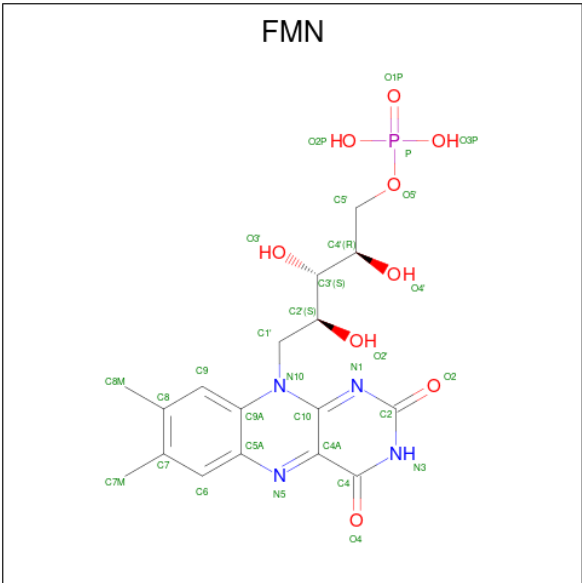
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			5	1	3	1	

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total	C	N	O	P	0
			31	17	4	9	1	



Q1529	G1394	F1457	G1394	V1329	W1267	T1189	ASP	Q1046	T969	K877	M906	F726	I663
K1530	S1397	D1458	S1397	G1330	K1268	T1193	SER	D1047	K962	N878	I807	P727	P664
V1531	R1398	L1459	R1398	W1331	L1269	L1197	SER	Q1049	L964	K879	A808	I728	L665
N1532	N1399	L1460	N1399	L1332	D1272	L1198	VAL	R1050	L964	V881	K809	A729	I666
L1533	G1400	K1461	G1400	L1335	P1274	L1199	SER	T1051	L967	P882	E810	L730	K667
E1534	K1401	K1462	K1401	I1336	P1275	P1200	GLU	C1052	L967	V881	V811	T733	E668
N1535	P1402	T1463	P1402	T1338	P1276	V1201	D1123	L1053	D974	E885	K812	G734	L669
P1536	V1403	L1464	V1403	F1339	E1273	Q1202	S1124	L1054	K975	A886	T813	G735	K671
T1537	M1404	T1465	M1404	P1340	N1274	G1203	A1125	H1055	P976	K887	S814	R736	S671
F1538	E1405	F1466	E1405	N1341	D1277	E1204	V1126	G1056	D977	R888	P815	G737	K672
I1539	V1406	E1467	V1406	L1205	F1278	L1204	F1127	P1057	E978	D889	D816	G738	G673
A1540	S1409	T1468	S1409	L1206	F1279	L1205	K1128	V1058	E979	Y890	A817	H740	Y674
L1542	F1410	T1470	F1410	K1206	P1281	D1280	A1129	Q1061	A979	I891	K818	H741	Q677
D1543	Y1411	K1475	Y1411	I1210	R1282	T1281	T1130	F1062	I980	E894	I821	H742	F678
S1544	R1413	N1476	R1413	L1213	L1283	P1284	S1131	T1063	E981	K894	A822	F743	L679
Y1545	G1414	A1477	G1414	L1214	V1284	V1284	S1132	K1064	K982	N896	T880	E744	T880
T1546	N1415	A1478	N1415	L1215	K1285	K1285	T1133	V1065	F984	A897	D829	D745	I681
S1547	Y1416	S1481	Y1416	K1216	K1286	K1286	E1135	D1067	Y887	D898	D830	A746	G682
S1548	T1417	K1484	T1417	E1217	G1287	G1287	D1134	E1068	R991	F899	K831	A747	A883
T1549	D1418	K1485	D1418	I1218	K1288	K1288	E1136	P1069	R991	Q901	K832	T748	G684
N1550	F1419	F1486	F1419	I1219	D1289	D1289	S1137	I1070	Q993	K901	E833	P749	V685
E1551	E1420	G1487	E1420	M1220	E1291	E1291	W1138	K1071	F994	P902	T835	H751	P686
P1552	N1421	G1488	N1421	M1221	E1292	E1292	L1142	M1074	D999	T906	Y836	L751	S687
Y1553	T1422	F1489	T1422	E1222	T1293	T1293	A1143	M1074	D1001	V907	K937	Y754	L688
A1554	Q1424	K1490	Q1424	M1223	L1294	L1294	E1146	H1078	I1000	N908	I843	Y757	E889
R1555	K1425	K1491	K1425	I1224	E1295	E1295	I1147	D1079	G909	Q910	V844	I757	V690
V1556	T1426	K1496	T1426	E1225	N1226	N1226	W1149	G1080	M1009	A911	E845	R758	A891
D1559	V1427	E1500	V1427	I1226	K1227	K1227	R1150	H1081	N1010	R912	R847	R759	E992
L1560	P1429	I1501	P1429	M1227	T1228	T1228	H1151	I1082	M1011	D913	S848	I763	E993
M1561	Y1430	G1502	Y1430	M1229	E1229	E1229	L1155	L1085	G1012	L914	E949	L765	Y694
P1562	Q1432	I1503	Q1432	D1230	K1231	K1231	F1158	H1087	V1018	M917	M950	L766	I694
I1563	H1434	D1504	H1434	D1231	K1232	K1232	L1158	L1086	K1013	T918	G851	I767	I695
H1564	Y1435	Y1506	Y1435	D1232	V1233	V1233	F1159	H1087	V1018	Y919	E952	F767	E696
R1567	K1436	E1507	K1436	L1233	P1234	P1234	D1162	G1091	D1022	R925	P853	G770	L698
H1568	T1437	G1510	T1437	L1239	F1242	F1242	K1163	E1094	R1023	L926	I854	F771	L700
F1569	S1438	S1511	S1438	Y1240	N1241	N1241	M1164	S1095	F1025	I932	K856	G772	L703
A1570	A1439	H1512	A1439	V1241	F1242	F1242	N1168	K1096	E1026	R933	R860	G773	G704
N1574	D1440	G1513	D1440	N1243	P1243	P1243	P1169	I1097	F1029	T935	G861	A774	L705
L1575	A1442	P1515	A1442	L1243	N1243	N1243	R1171	L1098	K1030	Q938	V862	D775	K706
G1577	V1443	V1516	V1443	P1250	M1255	M1255	K1172	P1098	D1032	F939	M863	D776	P707
T1578	L1444	V1517	L1444	D1257	E1256	E1256	N1176	E1099	S1033	D940	K866	W785	I710
I1579	R1445	F1518	R1445	L1251	Q1260	Q1260	P1177	V1100	L1034	R944	L864	M794	D711
T1580	S1446	F1519	S1446	I1251	R1261	R1261	Q1177	V1109	S1037	R952	W865	P795	A712
H1581	K1447	K1521	K1447	M1255	E1261	E1261	Q1178	VAL	E1038	R953	K867	F789	I713
G1582	P1385	R1522	P1385	D1257	K1263	K1263	M1180	ASP	H1039	T954	E870	M796	T716
M1583	T1386	E1523	T1386	Q1260	R1261	R1261	V1181	GLN	E1041	E955	T871	F796	I717
F1584	K1388	G1524	K1388	L1261	K1263	K1263	E1182	SER	E1041	E955	I872	D797	N718
S1585	T1389	S1525	T1389	Q1260	R1261	R1261	E1183	GLN	E1041	E955	F873	S803	I719
S1586	V1390	T1526	V1390	E1264	K1263	K1263	I1184	VAL	V1044	F958	N874	R804	A720
Y1589	D1391	L1527	Y1328	E1264	K1263	K1263	I1184	VAL	V1044	F958	N874	R804	A720
R1590	M1323	E1528	M1323	E1264	K1263	K1263	G1187	VAL	V1044	F958	N874	R804	A720
A1591	D1324	L1528	D1324	E1264	K1263	K1263	N1188	VAL	V1044	F958	N874	R804	A720
L1592	F1325	T1529	F1325	E1264	K1263	K1263	N1188	VAL	V1044	F958	N874	R804	A720
T1593	A1326	V1327	A1326	E1264	K1263	K1263	N1188	VAL	V1044	F958	N874	R804	A720
	V1328	V1328	V1328	E1264	K1263	K1263	N1188	VAL	V1044	F958	N874	R804	A720

V2029	A1965	R1905	D1845	M1784	L1719	E1654	E1594
Y2030	C1966	A1906	E1846	E1785	H1720	A1655	N1595
D2031	I1967	L1907	L1847	K1786	F1721	E1656	W1596
L2032	P1968	D1908	G1848	A1787	G1722	I1657	A1597
T2033	L1969	T1909	R1849	F1788		E1658	A1598
G2034	V1970	V1910	S1850	F1789	R1730	Q1659	D1599
S2035	G1971	T1911	N1851	E1790		P1660	S1600
E2036	I1972	N1912	Y1852	K1793	E1731	V1661	V1601
P2037	S1973	V1913	G1853	S1794	N1732	T1662	S1602
L2038	V1974	L1914	M1854	K1795	Y1733	T1663	S1603
K2039	P1975	N1915	I1855	G1796	A1735	F1664	R1604
E2040	F1976	F1916	A1856	L1797	M1736	V1665	V1605
I2041	H1977	I1917	I1857	I1798	I1737	F1666	R1606
L2042	S1978	K1918	N1858	P1799	F1738	T1667	G1607
D2043	T1979	L1919	P1859	A1800	E1739	G1668	Y1608
W2045		Q1920	G1860	D1801	T1740	Q1669	T1609
E2046	M1982	K1921	R1861	A1802	I1741	G1670	C1610
K2047	N1983	I1922	V1862	T1803	V1742	G1671	F1612
Y2048	G1984	D1923	A1863	F1804	D1743	Q1672	V1613
E2049	V1985	I1924	E1864	A1805	G1744	E1673	D1614
Q2050	K1986	I1925	S1865	G1806	K1745	Q1674	M1615
SER	P1987	T1925	F1866	H1807	L1746	G1675	V1616
	F1988	E1926	S1867	S1808	K1747	G1676	L1617
ASP	K1989	L1927	Q1868	L1809	T1748	M1676	P1618
TYR	S1990	Q1928	E1869	G1810	E1749	G1677	M1619
LYS	F1991	K1929	A1870	E1811	M1678	T1620	T1620
HIS	L1992	S1930	L1871	Y1812	K1750	D1679	A1621
ASP	K1993	L1931	Q1872	A1813	I1751	L1680	L1622
GLY	K1994	S1932	Y1873	A1814	F1752	Y1681	K1623
ASP	N1995	L1933	V1874	L1815	K1753	K1682	T1624
TYR	I1996	E1934	E1875	A1816	E1754	T1683	S1625
ASP	K1997	E1935	V1876	S1817	I1755	S1684	I1626
HIS	E1998	V1936	E1877	L1818	M1756	Q1627	Q1627
ASP	K1999	E1937	R1877	A1819	E1757	K1685	H1628
ILE	N2000	E1938	V1878	D1820	H1758	A1686	V1629
ASP	V2001	G1938	G1879	V1821	S1759	Q1688	G1630
LYS	K2002	H1939	K1880	M1822	Y1762	D1689	M1631
ASP	R2005	L1940	R1881	S1823	T1763	V1690	I1632
ASP		F1941	T1882	I1824	F1764	W1691	M1633
ASP	G2008	E1942	G1883	E1825	R1765		N1633
K2009	K2009	I1943	L1884	S1826	S1766	D1695	G1634
Y2010	Y2010	I1944	V1885	L1827		F1698	R1635
		D1945	L1886	V1828	E1767		K1636
N2013	N2013	E1946	L1885	E1829	K1768	T1701	L1637
L2014	L2014	A1947	E1887	V1830	G1769		I1638
T2015	T2015	S1948	I1888	V1831	L1770	F1704	K1639
A2016	A2016	K1949	V1889	F1832	L1771	S1705	F1640
K2017	K2017	K1950	N1890	Y1833	S1772	I1706	E1641
P2018	P2018	S1951	Y1891	G1834	A1773	L1707	T1642
F2019	F2019	I1951	N1892	R1835	T1774	D1708	R1643
Q2020	Q2020	A1952	G1893	M1836	Q1775	I1709	M1644
V2021	V2021	V1953	E1894	T1837	F1776	I1710	E1645
T2022	T2022	K1954	N1895	M1838	T1777	I1711	D1646
K2023	K2023	P1955	Q1896	Q1839	N1778	N1712	D1647
E2024	E2024	R1956	Q1897	V1840	Q1778	N1713	V1648
Y2025	Y2025	P1957	Y1898	A1841	P1779	V1649	V1649
F2026	F2026	L1958	R1899	V1842	A1780	V1715	V1650
Q2027	Q2027	K1959	V1899	P1843	L1781	N1716	L1651
D2028	D2028	L1960	A1900	R1844	T1782	L1717	T1652
		E1961	G1902		L1783	T1718	G1653
		R1962	D1903				
		G1963	L1904				
		F1964					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	594818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.727	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.706	Depositor
Map size ($\text{\AA}$)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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: NAP, PNS, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	1/12392 (0.0%)	0.72	12/16775 (0.1%)
2	G	0.40	0/16360	0.56	1/22198 (0.0%)
All	All	0.50	1/28752 (0.0%)	0.63	13/38973 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1033	ALA	CA-C	-5.79	1.44	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LYS	N-CA-C	7.98	120.44	109.11
1	A	1280	ILE	N-CA-C	-6.97	105.26	113.42
2	G	1278	ASP	N-CA-C	-6.21	106.39	112.97
1	A	1174	TYR	N-CA-C	5.90	117.49	109.11
1	A	142	ASP	CA-C-N	-5.86	111.63	122.06
1	A	142	ASP	C-N-CA	-5.86	111.63	122.06
1	A	806	VAL	N-CA-C	-5.59	105.17	113.39
1	A	1295	SER	N-CA-C	5.47	118.30	109.83
1	A	799	ILE	N-CA-C	-5.37	104.24	111.44
1	A	982	ILE	CA-C-N	5.23	130.88	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	ILE	C-N-CA	5.23	130.88	120.94
1	A	1173	LEU	N-CA-C	5.17	114.86	108.19
1	A	145	VAL	N-CA-C	5.13	116.02	109.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	GLU	Peptide
1	A	1173	LEU	Peptide
1	A	1584	PRO	Peptide
1	A	1716	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12171	0	11679	520	0
2	G	15995	0	15978	792	0
3	A	48	0	22	19	0
3	G	48	0	25	27	0
4	A	5	0	0	0	0
5	G	31	0	19	4	0
All	All	28298	0	27723	1290	0

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

All (1290) 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)
2:G:740:HIS:HB2	3:G:2102:NAP:C7N	1.22	1.59
1:A:147:ALA:CB	1:A:214:GLN:HA	1.50	1.41
2:G:740:HIS:HD2	3:G:2102:NAP:C2N	1.33	1.39
2:G:740:HIS:HD2	3:G:2102:NAP:C3N	1.40	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:740:HIS:CB	3:G:2102:NAP:C7N	2.06	1.32
1:A:147:ALA:HB2	1:A:214:GLN:CA	1.63	1.29
2:G:1034:LEU:HD13	3:G:2102:NAP:O1N	1.29	1.25
2:G:740:HIS:CD2	3:G:2102:NAP:C2N	2.19	1.24
1:A:147:ALA:CB	1:A:214:GLN:CA	2.14	1.23
2:G:740:HIS:HB2	3:G:2102:NAP:O7N	1.07	1.22
2:G:740:HIS:CD2	3:G:2102:NAP:C3N	2.22	1.20
2:G:1032:ASP:N	3:G:2102:NAP:O1A	1.74	1.20
1:A:688:ILE:CD1	3:A:1901:NAP:O4D	1.89	1.19
2:G:740:HIS:CB	3:G:2102:NAP:O7N	1.91	1.17
1:A:147:ALA:HB3	1:A:214:GLN:CB	1.78	1.12
1:A:688:ILE:HB	3:A:1901:NAP:H51N	1.30	1.10
2:G:740:HIS:HB2	3:G:2102:NAP:N7N	1.75	0.99
2:G:1034:LEU:CD1	3:G:2102:NAP:O1N	2.10	0.99
2:G:740:HIS:CG	3:G:2102:NAP:C7N	2.48	0.96
1:A:688:ILE:CB	3:A:1901:NAP:H51N	1.91	0.93
2:G:740:HIS:CD2	3:G:2102:NAP:C7N	2.52	0.92
1:A:1019:ILE:HG13	1:A:1316:VAL:HG23	1.52	0.92
1:A:688:ILE:HD13	3:A:1901:NAP:O4D	1.06	0.90
1:A:147:ALA:CB	1:A:214:GLN:CB	2.46	0.89
1:A:739:GLN:O	1:A:798:ASN:ND2	2.05	0.88
2:G:740:HIS:CB	3:G:2102:NAP:N7N	2.36	0.87
1:A:1125:VAL:HG12	1:A:1126:ILE:H	1.37	0.87
1:A:753:TYR:O	1:A:813:ARG:NH2	2.10	0.85
2:G:740:HIS:N	3:G:2102:NAP:O7N	2.10	0.84
1:A:771:PHE:HB3	3:A:1901:NAP:H52N	1.57	0.84
1:A:178:GLY:O	1:A:180:SER:N	2.12	0.83
1:A:971:ASN:HA	1:A:974:ASP:HB2	1.60	0.83
2:G:706:LYS:NZ	5:G:2101:FMN:O2'	2.11	0.83
2:G:1888:ILE:HD13	2:G:1900:ALA:HB2	1.60	0.82
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.44	0.82
1:A:709:ARG:NH2	3:A:1901:NAP:O2X	2.06	0.81
1:A:843:LYS:HE3	3:A:1901:NAP:O2D	1.80	0.81
2:G:1313:SER:N	2:G:1319:MET:SD	2.54	0.80
1:A:1123:GLN:HG2	1:A:1124:GLU:H	1.46	0.80
2:G:821:ILE:HG13	2:G:857:ILE:HD11	1.63	0.80
2:G:394:ARG:HA	2:G:397:LYS:HG3	1.64	0.80
2:G:1839:GLN:O	2:G:1844:ARG:NH1	2.15	0.79
2:G:907:VAL:HG23	2:G:917:MET:HE2	1.64	0.79
1:A:194:PHE:O	1:A:196:THR:N	2.15	0.79
2:G:610:THR:HB	2:G:617:ILE:HD11	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1430:VAL:HG13	2:G:1527:LEU:HB3	1.64	0.78
2:G:736:ARG:HD2	2:G:1058:VAL:HG11	1.65	0.78
1:A:520:ARG:HH12	1:A:521:LYS:HZ1	1.30	0.78
1:A:395:SER:HB3	1:A:398:LYS:HB2	1.66	0.77
1:A:1219:VAL:HG22	1:A:1384:ILE:HD13	1.67	0.77
1:A:490:TYR:OH	1:A:906:LEU:HB3	1.85	0.77
2:G:739:GLY:HA2	2:G:1054:LEU:HD13	1.67	0.77
2:G:881:VAL:HG13	2:G:882:PRO:HD3	1.67	0.77
2:G:1855:ILE:HD13	2:G:1960:LEU:HD21	1.64	0.77
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.65	0.76
1:A:41:THR:O	1:A:76:ARG:NH1	2.18	0.76
1:A:1183:ARG:NH1	1:A:1350:SER:O	2.19	0.76
2:G:456:GLN:O	2:G:469:ARG:NH2	2.18	0.76
2:G:688:LEU:HD22	2:G:715:GLN:HE22	1.50	0.76
2:G:1881:ARG:HH12	2:G:1949:LYS:HE3	1.50	0.76
1:A:1241:SER:HA	1:A:1295:SER:HB2	1.68	0.76
3:A:1901:NAP:O2X	3:A:1901:NAP:O3B	2.04	0.75
1:A:1067:LEU:HD23	1:A:1068:LYS:HG2	1.69	0.75
2:G:688:LEU:HD13	2:G:719:ILE:HD13	1.69	0.75
2:G:1842:VAL:O	2:G:1844:ARG:NH1	2.20	0.75
2:G:1890:ASN:HB2	2:G:1899:VAL:HG22	1.67	0.75
2:G:524:GLY:O	2:G:526:ARG:NH1	2.20	0.74
2:G:1319:MET:HB3	2:G:1368:VAL:HG21	1.68	0.74
2:G:1704:PHE:CE1	2:G:1709:ILE:HD11	2.22	0.74
2:G:914:LEU:HD23	2:G:1000:ILE:HG23	1.68	0.74
2:G:1623:LYS:HB2	2:G:1643:ARG:HB2	1.69	0.74
2:G:1636:LYS:HB2	2:G:1657:ILE:HG23	1.69	0.74
2:G:1037:SER:HB2	2:G:1053:ILE:HG22	1.69	0.74
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.19	0.74
2:G:952:ARG:NH2	2:G:967:ILE:O	2.21	0.74
2:G:1621:ALA:N	2:G:1645:GLU:OE1	2.19	0.73
2:G:1210:ILE:HB	2:G:1222:GLU:HB2	1.68	0.73
2:G:128:THR:O	2:G:132:MET:HB2	1.89	0.73
1:A:768:ILE:HG22	1:A:770:PRO:HD3	1.71	0.73
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.22	0.73
2:G:183:LEU:HD11	2:G:254:LYS:HG2	1.69	0.73
2:G:1022:ASP:OD2	2:G:1024:ARG:NH2	2.19	0.72
2:G:1704:PHE:HE1	2:G:1709:ILE:HD11	1.54	0.72
1:A:40:ASN:HA	1:A:76:ARG:HH22	1.53	0.72
1:A:1249:SER:OG	1:A:1250:GLY:N	2.21	0.72
2:G:896:ASN:O	2:G:1050:ARG:NH2	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1034:LEU:HD13	3:G:2102:NAP:PN	2.29	0.72
2:G:2047:LYS:O	2:G:2050:GLN:NE2	2.22	0.72
1:A:773:ALA:HB1	1:A:795:MET:HE2	1.72	0.72
2:G:716:VAL:HG21	2:G:730:LEU:HD21	1.71	0.72
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.70	0.72
2:G:1701:THR:O	2:G:1732:ASN:ND2	2.23	0.72
1:A:1182:ASP:OD2	1:A:1183:ARG:N	2.21	0.72
2:G:1904:LEU:HB3	2:G:1958:LEU:HD22	1.72	0.71
1:A:1123:GLN:O	1:A:1177:LYS:NZ	2.21	0.71
2:G:1031:LYS:HD2	3:G:2102:NAP:O5B	1.90	0.71
1:A:827:SER:OG	3:A:1901:NAP:C5N	2.38	0.71
2:G:1201:VAL:HG11	2:G:1226:ASN:HD21	1.54	0.71
2:G:175:ASP:O	2:G:179:THR:N	2.16	0.71
2:G:596:GLY:N	2:G:618:GLU:OE1	2.23	0.71
2:G:1279:PHE:HB3	2:G:1340:PRO:HB3	1.73	0.71
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.71	0.71
2:G:11:LEU:HB3	2:G:13:HIS:HE1	1.56	0.70
1:A:411:GLN:HE21	1:A:1629:LYS:HE2	1.56	0.70
2:G:56:THR:OG1	2:G:59:GLU:OE1	2.09	0.70
1:A:1077:ASP:OD2	1:A:1078:SER:N	2.24	0.70
2:G:1284:VAL:HG23	2:G:1377:VAL:HB	1.72	0.70
1:A:26:VAL:HG13	2:G:2013:ASN:HB3	1.74	0.70
2:G:326:ASP:O	2:G:330:ASN:ND2	2.22	0.70
2:G:1013:LYS:NZ	2:G:1032:ASP:OD2	2.24	0.70
1:A:507:GLY:O	1:A:955:LYS:NZ	2.19	0.70
2:G:1549:THR:HG23	2:G:1552:PRO:HD3	1.74	0.70
2:G:1180:MET:HG2	2:G:1199:GLU:HG2	1.74	0.69
2:G:1678:MET:HE3	2:G:1710:VAL:HG21	1.73	0.69
1:A:430:ARG:NH2	1:A:520:ARG:O	2.21	0.69
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.74	0.69
1:A:843:LYS:CE	3:A:1901:NAP:O2D	2.40	0.69
2:G:174:ARG:NH2	2:G:218:TRP:O	2.25	0.69
2:G:686:PRO:HB2	2:G:691:ALA:HB2	1.72	0.69
1:A:1545:SER:OG	1:A:1545:SER:O	2.10	0.69
2:G:596:GLY:HA3	2:G:650:ASN:HD22	1.57	0.69
2:G:2023:LYS:HD2	2:G:2045:TRP:CE2	2.28	0.69
1:A:1470:LEU:O	1:A:1474:ALA:N	2.26	0.69
2:G:1738:PHE:HB2	2:G:1751:ILE:HD13	1.73	0.69
2:G:1199:GLU:OE2	2:G:1567:ARG:NH2	2.24	0.69
1:A:1123:GLN:HB3	1:A:1177:LYS:HD3	1.75	0.69
2:G:218:TRP:HB3	2:G:225:THR:HG22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:740:HIS:CA	3:G:2102:NAP:O7N	2.40	0.68
1:A:1235:TYR:OH	1:A:1292:ILE:O	2.11	0.68
1:A:1414:ILE:O	1:A:1416:ARG:HG2	1.93	0.68
1:A:681:THR:HG21	1:A:802:MET:HE1	1.75	0.68
1:A:1186:ALA:O	1:A:1188:GLN:NE2	2.27	0.68
1:A:1373:ARG:HH11	1:A:1547:LYS:HA	1.57	0.68
2:G:1893:VAL:HG23	2:G:1896:GLN:HB3	1.74	0.68
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.26	0.67
2:G:626:SER:OG	2:G:627:ALA:N	2.26	0.67
1:A:479:ASN:ND2	1:A:613:VAL:O	2.26	0.67
2:G:517:HIS:HB2	2:G:527:VAL:HG11	1.74	0.67
1:A:332:THR:OG1	1:A:333:LYS:NZ	2.27	0.67
2:G:581:THR:H	2:G:584:SER:HG	1.39	0.67
1:A:1362:PRO:HA	1:A:1365:MET:HE3	1.77	0.67
2:G:56:THR:N	2:G:59:GLU:OE2	2.20	0.67
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.75	0.67
2:G:1319:MET:H	2:G:1368:VAL:HB	1.59	0.67
2:G:409:PHE:HA	2:G:412:ARG:HD2	1.77	0.67
1:A:985:ARG:N	2:G:956:GLU:O	2.27	0.67
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.75	0.67
1:A:147:ALA:HB2	1:A:214:GLN:HA	0.71	0.66
2:G:1878:VAL:HG22	2:G:1944:ILE:HD11	1.77	0.66
1:A:1138:LYS:NZ	1:A:1163:TYR:O	2.25	0.66
2:G:1135:GLU:HA	2:G:1176:PRO:HG2	1.77	0.66
1:A:21:GLN:NE2	2:G:1811:GLU:OE2	2.29	0.66
2:G:297:ARG:NH2	2:G:447:ASN:OD1	2.29	0.66
2:G:1126:VAL:HG12	2:G:1183:GLU:HG2	1.77	0.66
2:G:1629:VAL:HB	2:G:1639:LYS:HZ3	1.60	0.66
1:A:46:GLU:OE1	1:A:54:ALA:N	2.25	0.66
2:G:174:ARG:HA	2:G:177:TYR:CE1	2.31	0.66
2:G:362:ALA:HA	2:G:365:GLN:HG3	1.77	0.66
2:G:1863:ALA:HB3	2:G:1866:PHE:HB2	1.76	0.66
3:G:2102:NAP:O2N	3:G:2102:NAP:H3D	1.94	0.66
1:A:1034:ARG:NH2	1:A:1052:GLU:OE2	2.29	0.66
2:G:1424:GLN:HE22	2:G:1426:THR:HB	1.60	0.66
2:G:1767:GLU:HG2	2:G:1768:LYS:HG3	1.78	0.66
2:G:1550:ASN:ND2	2:G:1564:HIS:O	2.26	0.66
2:G:1742:VAL:HG23	2:G:1745:LYS:HB3	1.76	0.66
1:A:688:ILE:HB	3:A:1901:NAP:C5D	2.18	0.66
2:G:50:ALA:O	2:G:118:LYS:NZ	2.29	0.66
2:G:1877:ARG:HD3	2:G:1940:LEU:HD13	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:PRO:C	1:A:1177:LYS:HD2	2.21	0.65
2:G:130:ARG:NH2	2:G:136:PRO:O	2.27	0.65
2:G:1032:ASP:CA	3:G:2102:NAP:O1A	2.44	0.65
1:A:776:GLU:HB2	1:A:779:ILE:HD13	1.78	0.65
1:A:1203:ASP:OD2	1:A:1204:ILE:N	2.28	0.65
1:A:490:TYR:HB3	1:A:698:GLN:HB2	1.79	0.65
1:A:517:GLU:N	1:A:517:GLU:OE1	2.29	0.65
1:A:1403:ILE:HD11	1:A:1661:LEU:HB2	1.77	0.65
2:G:56:THR:HG21	2:G:108:LEU:HD11	1.79	0.65
2:G:818:LYS:HB3	2:G:1066:ILE:HD11	1.78	0.65
2:G:590:PRO:HB3	2:G:1078:HIS:CD2	2.31	0.65
1:A:852:ARG:NH1	1:A:856:GLU:OE2	2.29	0.65
2:G:1775:GLN:HE22	2:G:1836:MET:HB2	1.62	0.65
2:G:23:PRO:HD2	2:G:86:LEU:HD11	1.77	0.65
2:G:740:HIS:CD2	3:G:2102:NAP:H2N	2.27	0.64
2:G:1695:ASP:OD1	2:G:1707:LEU:N	2.21	0.64
1:A:36:LEU:O	1:A:76:ARG:NH2	2.31	0.64
1:A:1144:PHE:HZ	1:A:1174:TYR:CZ	2.15	0.64
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.30	0.64
2:G:343:ASN:HB2	2:G:416:PHE:HB3	1.80	0.64
2:G:1716:ASN:HD22	2:G:1765:ARG:HA	1.63	0.64
1:A:727:ALA:O	1:A:730:SER:OG	2.07	0.64
1:A:1584:PRO:O	1:A:1587:ALA:N	2.29	0.64
2:G:720:ALA:HB2	2:G:728:ILE:HD11	1.80	0.64
1:A:394:PHE:HB3	1:A:744:ASP:OD1	1.98	0.64
2:G:213:LEU:HD12	2:G:236:ILE:HG13	1.80	0.64
2:G:1041:GLU:HA	2:G:1046:GLN:HE22	1.62	0.64
2:G:1674:GLN:HE22	2:G:1713:ASN:HB2	1.63	0.64
2:G:707:PRO:HG3	2:G:730:LEU:HD22	1.79	0.63
1:A:464:GLU:OE2	1:A:465:ASN:ND2	2.32	0.63
2:G:993:GLN:NE2	2:G:994:PHE:O	2.32	0.63
1:A:445:ASP:OD1	1:A:445:ASP:N	2.31	0.63
1:A:529:MET:HE1	1:A:894:ARG:HG2	1.79	0.63
2:G:161:GLY:O	2:G:245:GLN:NE2	2.31	0.63
2:G:2036:GLU:HA	2:G:2039:LYS:HG2	1.80	0.63
1:A:32:GLN:HA	1:A:35:PHE:HE2	1.64	0.63
1:A:413:LEU:HB2	1:A:439:ILE:HD12	1.80	0.63
1:A:1102:GLY:O	1:A:1104:ARG:HG3	1.99	0.63
2:G:740:HIS:CG	3:G:2102:NAP:N7N	2.65	0.63
2:G:1885:LEU:O	2:G:1903:ASP:N	2.30	0.63
1:A:1121:MET:N	1:A:1177:LYS:O	2.23	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1040:LEU:HD21	2:G:1048:VAL:HB	1.81	0.63
2:G:1491:VAL:HB	2:G:1501:ILE:HD11	1.79	0.63
2:G:37:PHE:CE1	2:G:64:PHE:HA	2.34	0.62
1:A:843:LYS:NZ	3:A:1901:NAP:O2D	2.31	0.62
1:A:1414:ILE:HD13	1:A:1416:ARG:HH21	1.64	0.62
1:A:1070:ARG:HE	1:A:1071:PRO:HD2	1.62	0.62
2:G:54:PRO:HB3	2:G:59:GLU:HG2	1.80	0.62
2:G:148:ALA:HB1	2:G:153:ASN:HB3	1.81	0.62
2:G:259:THR:HG22	2:G:262:GLU:HB2	1.80	0.62
1:A:433:VAL:HG23	1:A:493:VAL:HG11	1.82	0.62
1:A:442:ARG:HD3	1:A:726:GLY:O	2.00	0.62
2:G:199:ILE:HD11	2:G:213:LEU:HD22	1.80	0.62
1:A:400:ARG:NH1	1:A:1367:ARG:HH22	1.97	0.62
1:A:1139:GLU:N	1:A:1139:GLU:OE1	2.33	0.62
2:G:1737:ILE:HG21	2:G:1748:THR:HG23	1.81	0.62
2:G:1866:PHE:HE2	2:G:1871:LEU:HG	1.64	0.62
1:A:1089:VAL:HG23	1:A:1093:TYR:HD2	1.64	0.62
2:G:1366:LEU:HD23	2:G:1366:LEU:H	1.65	0.62
1:A:251:GLN:HA	1:A:256:LEU:H	1.65	0.62
1:A:1120:GLU:OE1	1:A:1120:GLU:N	2.32	0.62
2:G:1172:LYS:NZ	2:G:1574:ASN:OD1	2.32	0.62
2:G:180:TYR:HB3	2:G:183:LEU:HB3	1.81	0.62
1:A:503:ILE:HG12	1:A:509:ILE:HG13	1.81	0.62
1:A:1134:PHE:HE1	1:A:1168:LEU:O	1.83	0.62
1:A:1334:ASP:OD1	1:A:1335:PHE:N	2.33	0.62
2:G:11:LEU:HD11	2:G:20:LEU:HB2	1.81	0.62
2:G:1550:ASN:ND2	2:G:1579:ILE:O	2.32	0.62
2:G:1685:LYS:NZ	2:G:1689:ASP:OD2	2.33	0.62
2:G:1546:THR:OG1	2:G:1620:THR:N	2.30	0.61
1:A:931:GLN:OE1	1:A:931:GLN:N	2.27	0.61
1:A:1268:GLU:N	1:A:1268:GLU:OE1	2.33	0.61
1:A:1367:ARG:NH1	1:A:1612:ASP:OD1	2.34	0.61
2:G:55:THR:HG23	2:G:56:THR:HG23	1.83	0.61
2:G:696:GLU:N	2:G:696:GLU:OE1	2.33	0.61
2:G:860:ARG:NH1	2:G:898:ASP:OD1	2.32	0.61
2:G:1189:THR:O	2:G:1193:THR:OG1	2.18	0.61
2:G:1468:THR:HA	2:G:1487:GLY:HA3	1.82	0.61
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.34	0.61
1:A:440:MET:HE3	1:A:479:ASN:HB3	1.81	0.61
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	1.83	0.61
1:A:1474:ALA:O	1:A:1482:GLN:NE2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1177:SER:H	2:G:1180:MET:HE2	1.65	0.61
2:G:1963:GLY:N	2:G:1966:CYS:SG	2.72	0.61
1:A:764:ASP:OD2	1:A:818:ARG:NH1	2.33	0.61
1:A:1604:ILE:HG12	1:A:1632:LYS:HG3	1.83	0.61
2:G:96:LEU:HD23	2:G:98:GLY:H	1.66	0.61
2:G:875:LEU:HG	2:G:876:PRO:HD2	1.82	0.61
2:G:723:HIS:HB3	2:G:726:PHE:CD2	2.36	0.61
2:G:1475:LYS:HB3	2:G:1481:SER:HB2	1.82	0.61
1:A:631:PRO:O	1:A:653:ARG:NH2	2.31	0.61
2:G:1667:THR:OG1	2:G:1785:GLU:OE2	2.16	0.61
1:A:191:GLY:O	1:A:195:GLY:N	2.33	0.61
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.34	0.61
1:A:1544:THR:HG23	1:A:1546:THR:H	1.65	0.61
2:G:953:ARG:HA	2:G:956:GLU:HB2	1.83	0.61
2:G:1828:VAL:HA	2:G:1831:VAL:HG12	1.83	0.60
1:A:1584:PRO:O	1:A:1586:GLY:N	2.35	0.60
2:G:569:LEU:HD21	2:G:1085:LEU:HB3	1.82	0.60
2:G:703:LEU:HB3	2:G:728:ILE:HG22	1.84	0.60
2:G:1877:ARG:HD2	2:G:1944:ILE:HB	1.82	0.60
2:G:2041:ILE:HG12	2:G:2047:LYS:HZ1	1.66	0.60
1:A:1505:GLN:O	1:A:1509:GLY:N	2.34	0.60
2:G:11:LEU:HB3	2:G:13:HIS:CE1	2.37	0.60
2:G:1277:LEU:HB3	2:G:1341:ASN:HB2	1.83	0.60
1:A:1183:ARG:NE	1:A:1349:THR:OG1	2.35	0.60
1:A:1337:GLU:OE1	1:A:1337:GLU:N	2.26	0.60
2:G:305:PHE:CD2	2:G:442:ASP:HB3	2.35	0.60
2:G:919:TYR:OH	2:G:999:ASP:OD2	2.13	0.60
1:A:56:MET:HG2	1:A:59:ARG:HH21	1.66	0.60
1:A:983:GLN:HB3	1:A:1087:LYS:HG3	1.82	0.60
1:A:1719:LEU:HD12	1:A:1744:TYR:HA	1.84	0.60
1:A:807:LYS:HD2	1:A:858:TRP:HB3	1.83	0.60
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.37	0.60
2:G:1227:ARG:HD3	2:G:1555:ARG:HH12	1.65	0.60
2:G:1844:ARG:HB3	2:G:1848:GLY:HA2	1.84	0.60
1:A:1718:PRO:HD2	1:A:1744:TYR:CE1	2.37	0.60
2:G:1142:LEU:O	2:G:1150:ARG:NE	2.29	0.60
1:A:739:GLN:HB2	1:A:794:ILE:HG23	1.83	0.59
1:A:1561:MET:HE3	1:A:1566:ARG:HD2	1.83	0.59
1:A:807:LYS:NZ	1:A:861:GLN:OE1	2.32	0.59
1:A:1550:ASP:O	1:A:1554:SER:OG	2.16	0.59
2:G:156:LEU:HD22	2:G:502:LEU:HD22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1925:ILE:H	2:G:1925:ILE:HD12	1.66	0.59
1:A:1035:THR:O	1:A:1035:THR:OG1	2.16	0.59
2:G:59:GLU:CB	2:G:122:LEU:HD21	2.32	0.59
2:G:121:GLU:OE2	2:G:125:ASN:ND2	2.35	0.59
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.85	0.59
1:A:1020:VAL:HG21	1:A:1400:ILE:HG12	1.84	0.59
2:G:879:LYS:C	2:G:882:PRO:HD2	2.26	0.59
1:A:1590:ALA:O	1:A:1594:ASN:HB2	2.02	0.59
2:G:37:PHE:CZ	2:G:67:TYR:HB3	2.37	0.59
2:G:459:VAL:HG23	2:G:468:LEU:HB2	1.85	0.59
2:G:515:LEU:O	2:G:519:ASN:ND2	2.35	0.59
1:A:1067:LEU:HB3	1:A:1072:TYR:CD2	2.38	0.59
2:G:408:PRO:HB2	2:G:411:GLU:HG2	1.85	0.59
2:G:1380:SER:HB2	2:G:1424:GLN:HA	1.85	0.59
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.85	0.59
2:G:241:ILE:HB	2:G:275:GLN:HE22	1.68	0.59
2:G:666:ILE:HG22	2:G:698:LEU:HD22	1.84	0.59
2:G:1243:ASN:N	2:G:1250:PRO:O	2.36	0.59
1:A:1301:PRO:HG3	1:A:1314:ILE:HD13	1.84	0.59
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.32	0.59
2:G:1034:LEU:CD1	3:G:2102:NAP:PN	2.88	0.59
2:G:1905:ARG:NH1	2:G:1955:PRO:O	2.36	0.59
1:A:81:TYR:HH	1:A:89:TYR:HH	1.50	0.58
2:G:580:GLU:OE2	2:G:585:LYS:HE2	2.03	0.58
1:A:413:LEU:HD22	1:A:451:MET:HE2	1.85	0.58
2:G:1037:SER:HA	2:G:1051:THR:HG21	1.84	0.58
1:A:194:PHE:C	1:A:196:THR:H	2.07	0.58
1:A:1168:LEU:HG	1:A:1169:LYS:H	1.68	0.58
2:G:745:ASP:OD1	2:G:746:ALA:N	2.35	0.58
2:G:1936:VAL:O	2:G:1940:LEU:HG	2.03	0.58
1:A:938:GLU:HA	1:A:941:ALA:HB3	1.85	0.58
1:A:1256:ALA:O	1:A:1259:GLY:N	2.36	0.58
2:G:1432:GLN:HG2	2:G:1465:THR:HG22	1.86	0.58
1:A:404:SER:O	1:A:404:SER:OG	2.16	0.58
1:A:1037:TRP:HB2	1:A:1598:GLN:NE2	2.19	0.58
1:A:1377:MET:O	1:A:1583:HIS:N	2.34	0.57
2:G:329:GLU:OE1	2:G:329:GLU:N	2.37	0.57
1:A:1014:ASP:HB2	1:A:1505:GLN:HB2	1.86	0.57
1:A:1137:SER:C	1:A:1138:LYS:HE2	2.29	0.57
1:A:1675:ALA:O	1:A:1678:SER:OG	2.22	0.57
2:G:1871:LEU:HA	2:G:1874:VAL:HG12	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:CB	1:A:214:GLN:N	2.67	0.57
1:A:329:GLU:O	1:A:333:LYS:NZ	2.34	0.57
1:A:1589:GLY:HA2	1:A:1592:MET:HG2	1.87	0.57
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.69	0.57
1:A:1360:ARG:HG2	1:A:1367:ARG:NH2	2.19	0.57
1:A:1499:SER:HA	1:A:1502:ARG:HG2	1.87	0.57
1:A:1542:HIS:HA	1:A:1592:MET:HE1	1.85	0.57
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.86	0.57
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.37	0.57
1:A:984:PRO:HG2	1:A:1087:LYS:HD3	1.87	0.57
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.86	0.57
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.86	0.57
2:G:1101:GLU:HB3	2:G:1147:ILE:HG22	1.86	0.57
1:A:442:ARG:HG3	1:A:727:ALA:HA	1.87	0.57
1:A:708:SER:OG	3:A:1901:NAP:O3X	2.22	0.57
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.20	0.57
2:G:571:LYS:HB2	2:G:1097:ILE:HG12	1.86	0.57
1:A:1247:SER:HG	1:A:1332:TYR:HE1	1.53	0.56
2:G:1859:PRO:HB3	2:G:1866:PHE:HD2	1.69	0.56
2:G:740:HIS:HA	2:G:854:ILE:HD13	1.87	0.56
1:A:1189:ILE:HG12	1:A:1380:GLN:HE21	1.71	0.56
2:G:130:ARG:NE	2:G:135:ARG:O	2.35	0.56
2:G:869:ASP:HA	2:G:873:PHE:HD2	1.70	0.56
1:A:986:ALA:HB1	1:A:1051:VAL:HG11	1.87	0.56
1:A:1139:GLU:HG2	1:A:1140:THR:H	1.69	0.56
2:G:161:GLY:H	2:G:505:GLY:HA3	1.70	0.56
1:A:984:PRO:HB3	2:G:959:THR:HG23	1.87	0.56
2:G:1138:TRP:O	2:G:1142:LEU:HG	2.06	0.56
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.41	0.56
2:G:1264:GLU:HA	2:G:1267:TRP:HD1	1.69	0.56
1:A:677:TYR:H	1:A:766:ASP:HB2	1.71	0.56
1:A:810:LYS:HB3	1:A:861:GLN:HG2	1.88	0.56
2:G:389:LEU:HA	2:G:392:THR:HG22	1.87	0.56
1:A:840:SER:OG	1:A:841:GLU:N	2.38	0.56
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.23	0.56
2:G:662:GLY:O	2:G:666:ILE:N	2.23	0.56
2:G:688:LEU:HD22	2:G:715:GLN:NE2	2.21	0.56
1:A:442:ARG:HA	1:A:728:LYS:HG3	1.87	0.56
1:A:1360:ARG:NH2	1:A:1372:THR:O	2.38	0.56
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.87	0.56
1:A:893:VAL:HG11	1:A:930:LEU:HD21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:HIS:CE1	1:A:1718:PRO:HA	2.41	0.55
1:A:1333:ASP:OD2	1:A:1334:ASP:N	2.37	0.55
2:G:220:GLU:HG2	2:G:221:ASN:N	2.21	0.55
2:G:404:GLN:NE2	2:G:413:LYS:H	2.05	0.55
2:G:586:LEU:HD21	2:G:1107:SER:HA	1.88	0.55
2:G:1227:ARG:NE	2:G:1551:GLU:OE2	2.30	0.55
2:G:1924:ILE:HA	2:G:1927:LEU:HD12	1.87	0.55
1:A:520:ARG:HH12	1:A:521:LYS:NZ	2.04	0.55
2:G:475:ILE:O	2:G:479:ILE:HG13	2.05	0.55
1:A:1137:SER:O	1:A:1138:LYS:HE2	2.06	0.55
1:A:1515:ARG:HH12	1:A:1517:PRO:HD3	1.72	0.55
2:G:1706:ILE:O	2:G:1709:ILE:N	2.39	0.55
1:A:339:ALA:HA	1:A:342:GLN:HG3	1.89	0.55
1:A:804:GLY:O	1:A:808:LYS:NZ	2.24	0.55
2:G:1789:PHE:CD2	2:G:1817:SER:HB2	2.42	0.55
1:A:484:LEU:HD23	1:A:485:ASP:HB2	1.89	0.55
1:A:625:THR:HG22	1:A:627:SER:H	1.72	0.55
1:A:1096:SER:HA	1:A:1099:GLU:HB3	1.87	0.55
2:G:1543:ASP:HA	2:G:1622:LEU:O	2.07	0.55
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.42	0.55
2:G:1637:LEU:O	2:G:1639:LYS:NZ	2.39	0.55
2:G:1914:LEU:HA	2:G:1917:ILE:HG22	1.89	0.55
1:A:960:GLU:O	1:A:964:GLU:N	2.28	0.55
1:A:960:GLU:OE1	2:G:1447:LYS:NZ	2.36	0.55
2:G:404:GLN:HB3	2:G:412:ARG:HG2	1.88	0.55
2:G:940:ASP:OD2	2:G:1013:LYS:HD2	2.07	0.55
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.71	0.55
2:G:528:ILE:HD12	2:G:547:ILE:HG12	1.88	0.55
2:G:529:VAL:HB	2:G:543:PHE:HD1	1.72	0.55
2:G:881:VAL:CG1	2:G:882:PRO:HD3	2.35	0.55
2:G:1830:VAL:HG12	2:G:1991:PHE:HE2	1.72	0.55
2:G:2041:ILE:HG12	2:G:2047:LYS:NZ	2.22	0.55
1:A:1104:ARG:NH2	1:A:1107:GLU:OE1	2.34	0.55
1:A:1148:HIS:ND1	1:A:1151:LYS:HD3	2.22	0.55
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.53	0.55
1:A:1286:TRP:HA	1:A:1289:MET:HB2	1.88	0.55
2:G:9:LEU:N	2:G:20:LEU:O	2.32	0.55
2:G:37:PHE:CZ	2:G:64:PHE:HA	2.42	0.55
2:G:1321:ALA:HB3	2:G:1366:LEU:HG	1.88	0.55
1:A:684:GLY:HA3	1:A:709:ARG:HH22	1.72	0.54
2:G:668:GLU:N	2:G:668:GLU:OE1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:695:ILE:HD11	2:G:723:HIS:CD2	2.42	0.54
2:G:582:LYS:HA	2:G:585:LYS:HE3	1.88	0.54
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.22	0.54
2:G:1433:MET:N	2:G:1464:LEU:O	2.39	0.54
2:G:1511:SER:OG	2:G:1512:HIS:N	2.40	0.54
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.89	0.54
2:G:669:LEU:HD22	2:G:674:TYR:CE2	2.42	0.54
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.40	0.54
1:A:460:GLU:OE1	1:A:470:LYS:NZ	2.41	0.54
1:A:1141:ALA:HB1	1:A:1145:LYS:HE2	1.90	0.54
1:A:1148:HIS:HB3	1:A:1151:LYS:HD3	1.90	0.54
1:A:1185:VAL:HG23	1:A:1377:MET:HE1	1.90	0.54
2:G:1431:TYR:HE1	2:G:1526:THR:HG22	1.71	0.54
1:A:777:GLN:N	1:A:777:GLN:OE1	2.41	0.54
2:G:881:VAL:O	2:G:885:GLU:HG2	2.08	0.54
1:A:520:ARG:HH21	1:A:602:GLU:CD	2.15	0.54
2:G:1130:THR:N	2:G:1133:THR:OG1	2.28	0.54
2:G:1838:MET:HE3	2:G:1976:PHE:HB3	1.89	0.54
1:A:1173:LEU:HB2	1:A:1174:TYR:CD2	2.42	0.54
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.43	0.54
2:G:1738:PHE:O	2:G:1749:GLU:HG3	2.08	0.54
2:G:2024:GLU:O	2:G:2028:ASP:N	2.38	0.54
1:A:53:LEU:HD13	2:G:1665:VAL:HB	1.89	0.54
1:A:58:GLN:HB3	1:A:78:ILE:HD13	1.89	0.54
1:A:1175:ILE:O	1:A:1177:LYS:NZ	2.24	0.54
2:G:349:VAL:HG21	2:G:377:LEU:HD22	1.89	0.54
2:G:619:LEU:H	2:G:649:ILE:HA	1.73	0.54
2:G:1698:PHE:CZ	2:G:1828:VAL:HG22	2.43	0.54
1:A:79:LEU:HD21	1:A:87:GLU:HB2	1.89	0.54
1:A:1245:ASN:ND2	1:A:1284:SER:OG	2.41	0.54
2:G:9:LEU:O	2:G:20:LEU:N	2.32	0.54
1:A:439:ILE:HD11	1:A:451:MET:HE1	1.90	0.53
2:G:404:GLN:HE22	2:G:413:LYS:H	1.56	0.53
1:A:403:ASP:OD1	1:A:1613:ASN:ND2	2.28	0.53
2:G:259:THR:HG23	2:G:262:GLU:H	1.73	0.53
2:G:264:ARG:NH2	2:G:456:GLN:OE1	2.42	0.53
2:G:1138:TRP:CD1	2:G:1176:PRO:HG3	2.43	0.53
2:G:2026:PHE:HB3	2:G:2038:ILE:HG23	1.89	0.53
1:A:652:ASP:OD1	1:A:653:ARG:N	2.41	0.53
1:A:753:TYR:CE1	1:A:764:ASP:HA	2.43	0.53
2:G:1123:ASP:OD2	2:G:1187:GLY:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1539:ILE:HB	2:G:1626:ILE:HG22	1.89	0.53
1:A:329:GLU:O	1:A:332:THR:OG1	2.25	0.53
2:G:1691:TRP:HB3	2:G:1707:LEU:HD21	1.91	0.53
1:A:1105:LEU:HA	1:A:1185:VAL:HG12	1.91	0.53
1:A:1388:MET:HE1	1:A:1398:VAL:HG21	1.91	0.53
1:A:1595:GLY:HA2	1:A:1598:GLN:HG3	1.90	0.53
2:G:1148:ASN:H	2:G:1151:HIS:HB2	1.72	0.53
2:G:1607:GLY:O	2:G:1656:GLU:N	2.29	0.53
1:A:1239:HIS:HD2	1:A:1241:SER:H	1.57	0.53
2:G:55:THR:N	2:G:59:GLU:OE2	2.42	0.53
2:G:220:GLU:HG2	2:G:221:ASN:H	1.74	0.53
2:G:382:PRO:HD3	2:G:431:LEU:HD11	1.89	0.53
2:G:526:ARG:CG	2:G:558:ASN:H	2.22	0.53
2:G:1533:LEU:HD23	2:G:1534:GLU:N	2.23	0.53
2:G:1895:ASN:H	2:G:1898:TYR:HE2	1.57	0.53
2:G:2023:LYS:HD2	2:G:2045:TRP:CZ2	2.44	0.53
2:G:160:PHE:CE2	2:G:504:PHE:HB2	2.43	0.53
2:G:728:ILE:HG13	2:G:763:ILE:HD13	1.91	0.53
2:G:1517:VAL:O	2:G:1521:LYS:N	2.42	0.53
2:G:1754:GLU:OE1	2:G:1754:GLU:N	2.42	0.53
2:G:803:SER:N	5:G:2101:FMN:O1P	2.38	0.53
2:G:1226:ASN:HA	2:G:1233:PRO:HA	1.90	0.53
2:G:1866:PHE:HA	2:G:1925:ILE:HD11	1.91	0.53
2:G:1997:ILE:HG22	2:G:1999:GLU:H	1.74	0.53
1:A:1077:ASP:HB3	1:A:1082:GLU:H	1.73	0.53
1:A:1174:TYR:O	1:A:1175:ILE:HG13	2.09	0.53
1:A:1397:GLY:O	1:A:1680:ARG:NH1	2.42	0.53
2:G:461:ASP:HB3	2:G:465:GLY:H	1.74	0.53
2:G:1281:PRO:HG2	2:G:1342:THR:OG1	2.09	0.53
2:G:1356:GLY:HA2	2:G:1609:THR:HA	1.89	0.53
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.23	0.53
1:A:483:VAL:O	1:A:486:VAL:HG12	2.08	0.53
1:A:490:TYR:CZ	1:A:906:LEU:HD13	2.43	0.53
1:A:533:GLY:O	1:A:537:LYS:HG2	2.09	0.53
1:A:707:THR:HG21	1:A:718:TYR:HE2	1.74	0.53
2:G:720:ALA:HB2	2:G:763:ILE:HD11	1.90	0.53
2:G:847:ARG:HB3	2:G:851:GLY:HA2	1.89	0.53
2:G:1146:GLU:HG2	2:G:1148:ASN:ND2	2.24	0.53
2:G:1698:PHE:CD2	2:G:1706:ILE:HD11	2.43	0.53
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.90	0.52
2:G:873:PHE:CD1	2:G:1026:GLU:HB3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1830:VAL:HG12	2:G:1991:PHE:CE2	2.44	0.52
1:A:661:ASP:OD2	1:A:662:GLY:N	2.42	0.52
1:A:1334:ASP:CG	1:A:1335:PHE:H	2.17	0.52
2:G:145:LEU:HG	2:G:146:PHE:HD1	1.74	0.52
2:G:306:ILE:HD11	2:G:480:VAL:HG12	1.89	0.52
2:G:610:THR:HB	2:G:617:ILE:CD1	2.38	0.52
2:G:1323:MET:H	2:G:1590:ARG:NH2	2.06	0.52
1:A:42:GLU:N	1:A:42:GLU:OE2	2.42	0.52
1:A:87:GLU:OE2	1:A:87:GLU:N	2.33	0.52
1:A:774:ILE:CG2	3:A:1901:NAP:N7A	2.73	0.52
2:G:59:GLU:HB2	2:G:122:LEU:HD21	1.91	0.52
2:G:148:ALA:O	2:G:151:GLU:HG2	2.09	0.52
2:G:843:ILE:HG21	2:G:1057:PRO:HA	1.91	0.52
1:A:858:TRP:HE3	1:A:862:LEU:HB2	1.74	0.52
1:A:1247:SER:OG	1:A:1332:TYR:HE1	1.92	0.52
1:A:966:LYS:HD3	1:A:971:ASN:HB3	1.91	0.52
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.91	0.52
2:G:1234:VAL:HG11	2:G:1269:LEU:HD21	1.92	0.52
2:G:20:LEU:HD12	2:G:90:GLU:CD	2.35	0.52
2:G:1026:GLU:HA	2:G:1029:PHE:HB3	1.91	0.52
2:G:1709:ILE:HG22	2:G:1771:LEU:HD11	1.91	0.52
1:A:1360:ARG:NH1	1:A:1367:ARG:HG3	2.25	0.52
1:A:1544:THR:O	1:A:1545:SER:HB3	2.08	0.52
2:G:716:VAL:HG11	2:G:730:LEU:HD21	1.92	0.52
2:G:1614:ASP:OD1	2:G:1650:VAL:HG12	2.09	0.52
2:G:509:ALA:O	2:G:514:VAL:HG21	2.10	0.52
2:G:741:HIS:HB3	2:G:853:PRO:HG2	1.92	0.52
2:G:1338:ILE:HG22	2:G:1390:VAL:HG21	1.92	0.52
1:A:1211:ILE:HG21	1:A:1253:GLY:H	1.75	0.52
2:G:569:LEU:HB3	2:G:1097:ILE:CD1	2.40	0.52
2:G:1859:PRO:HG3	2:G:1871:LEU:HD21	1.91	0.52
1:A:490:TYR:HB3	1:A:698:GLN:CB	2.40	0.52
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.90	0.52
1:A:1037:TRP:HB2	1:A:1598:GLN:HE21	1.75	0.52
1:A:1139:GLU:HG2	1:A:1140:THR:N	2.25	0.52
2:G:37:PHE:CE2	2:G:67:TYR:HD2	2.28	0.52
2:G:116:LEU:O	2:G:119:THR:HG22	2.10	0.52
1:A:501:THR:HG21	1:A:883:ILE:O	2.10	0.51
1:A:1120:GLU:CD	1:A:1120:GLU:H	2.18	0.51
2:G:747:HIS:O	2:G:751:LEU:N	2.43	0.51
1:A:711:SER:OG	1:A:713:GLN:OE1	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:SER:OG	1:A:744:ASP:HB2	2.10	0.51
1:A:1104:ARG:HH22	1:A:1188:GLN:HB2	1.75	0.51
1:A:1132:GLU:O	1:A:1132:GLU:HG2	2.10	0.51
2:G:1311:PHE:HA	2:G:1320:LEU:HD21	1.92	0.51
2:G:1678:MET:HG3	2:G:1711:ILE:HG22	1.92	0.51
1:A:1136:ALA:O	1:A:1164:SER:OG	2.18	0.51
2:G:873:PHE:CE1	2:G:1026:GLU:HB3	2.45	0.51
1:A:77:GLU:HG3	1:A:79:LEU:CD1	2.40	0.51
1:A:953:VAL:HG12	2:G:1439:LYS:HB2	1.92	0.51
2:G:162:GLY:N	2:G:273:HIS:HB3	2.25	0.51
2:G:205:ALA:O	2:G:208:VAL:HG12	2.10	0.51
1:A:1115:ASN:HD22	1:A:1118:LYS:HB2	1.75	0.51
2:G:1911:THR:HG23	2:G:1966:CYS:SG	2.51	0.51
1:A:1718:PRO:HD2	1:A:1744:TYR:HE1	1.74	0.51
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.75	0.51
1:A:221:LEU:O	1:A:225:SER:CB	2.59	0.51
1:A:329:GLU:C	1:A:333:LYS:HZ3	2.17	0.51
1:A:430:ARG:NH2	1:A:606:ASP:OD2	2.42	0.51
1:A:1215:VAL:O	1:A:1219:VAL:HG23	2.10	0.51
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.92	0.51
1:A:1370:THR:HG22	1:A:1372:THR:H	1.76	0.51
2:G:785:TRP:NE1	2:G:794:MET:O	2.35	0.51
2:G:1519:PHE:O	2:G:1523:ASN:ND2	2.44	0.51
1:A:684:GLY:CA	1:A:709:ARG:HH22	2.23	0.51
1:A:1262:LYS:NZ	1:A:1338:GLU:OE2	2.38	0.51
1:A:1668:ASP:OD2	1:A:1668:ASP:N	2.43	0.51
1:A:608:ASP:OD2	1:A:611:LYS:HG2	2.11	0.51
2:G:1359:MET:HE2	2:G:1404:MET:HE2	1.93	0.51
1:A:1017:ARG:HH11	1:A:1320:LEU:HD12	1.74	0.51
1:A:1148:HIS:CD2	1:A:1167:LEU:HD22	2.46	0.51
2:G:116:LEU:HA	2:G:119:THR:HG22	1.93	0.51
2:G:1804:PHE:CD1	2:G:1818:LEU:HG	2.46	0.51
2:G:695:ILE:HD11	2:G:723:HIS:CG	2.46	0.50
2:G:2036:GLU:CD	2:G:2037:PRO:HD3	2.36	0.50
1:A:1425:ILE:CG1	1:A:1651:GLY:H	2.24	0.50
2:G:145:LEU:H	2:G:145:LEU:HD23	1.75	0.50
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.93	0.50
2:G:569:LEU:HD23	2:G:1090:TYR:HE1	1.75	0.50
2:G:1383:ASN:ND2	2:G:1416:TYR:HB2	2.25	0.50
2:G:1906:ALA:O	2:G:1910:VAL:HG23	2.12	0.50
1:A:416:LEU:HD22	1:A:420:ILE:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:GLU:CD	1:A:1135:GLU:H	2.19	0.50
2:G:619:LEU:N	2:G:648:GLY:O	2.44	0.50
2:G:694:TYR:O	2:G:698:LEU:HB2	2.12	0.50
2:G:737:GLY:O	2:G:855:HIS:ND1	2.32	0.50
2:G:740:HIS:CD2	3:G:2102:NAP:N7N	2.79	0.50
2:G:1452:LEU:HB3	2:G:1501:ILE:HG22	1.92	0.50
1:A:828:PRO:HG3	1:A:927:ASN:ND2	2.26	0.50
1:A:846:LEU:O	1:A:849:LEU:HB2	2.10	0.50
1:A:1226:SER:O	1:A:1226:SER:OG	2.23	0.50
2:G:480:VAL:O	2:G:484:ILE:HG12	2.11	0.50
2:G:625:PHE:HD2	3:G:2102:NAP:C6A	1.85	0.50
2:G:900:GLN:HE21	2:G:1052:CYS:H	1.60	0.50
2:G:1300:PHE:CZ	2:G:1304:VAL:HG21	2.46	0.50
2:G:1397:SER:HA	2:G:1403:VAL:HG23	1.93	0.50
2:G:1562:PRO:HB2	2:G:1569:PHE:CD2	2.46	0.50
1:A:609:SER:O	1:A:613:VAL:HG23	2.12	0.50
1:A:1360:ARG:HH21	1:A:1372:THR:HG23	1.77	0.50
2:G:9:LEU:HB3	2:G:20:LEU:HB3	1.94	0.50
2:G:1855:ILE:HB	2:G:1907:LEU:HD21	1.94	0.50
1:A:868:ILE:HG13	1:A:925:ASP:HA	1.94	0.50
1:A:1077:ASP:OD2	1:A:1079:LYS:N	2.39	0.50
1:A:1303:GLY:H	1:A:1307:THR:HB	1.77	0.50
2:G:72:VAL:HG21	2:G:84:LEU:HD22	1.93	0.50
2:G:1318:THR:OG1	2:G:1369:GLY:N	2.44	0.50
2:G:1668:GLY:HA2	2:G:1809:LEU:HB3	1.94	0.50
1:A:1355:GLU:CD	1:A:1360:ARG:HD2	2.37	0.50
2:G:118:LYS:O	2:G:122:LEU:HD23	2.10	0.50
2:G:1206:LYS:HD3	2:G:1226:ASN:HD22	1.76	0.50
2:G:1595:ASN:OD1	2:G:1596:TRP:N	2.44	0.50
1:A:42:GLU:OE2	2:G:1661:VAL:HB	2.11	0.50
1:A:403:ASP:O	1:A:405:SER:N	2.44	0.50
1:A:753:TYR:CB	1:A:809:GLN:HG2	2.42	0.50
2:G:1440:ASP:OD1	2:G:1441:ILE:N	2.45	0.50
2:G:1878:VAL:HG21	2:G:1910:VAL:HG22	1.92	0.50
1:A:1136:ALA:H	1:A:1164:SER:HB3	1.75	0.49
2:G:1320:LEU:H	2:G:1320:LEU:HD23	1.77	0.49
1:A:1373:ARG:HD2	1:A:1547:LYS:HA	1.92	0.49
2:G:139:LYS:NZ	2:G:140:LYS:O	2.38	0.49
2:G:426:PRO:HG3	2:G:431:LEU:HD12	1.95	0.49
2:G:670:ARG:HH11	2:G:670:ARG:HA	1.77	0.49
2:G:1884:TRP:HB2	2:G:1906:ALA:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2015:THR:OG1	2:G:2029:VAL:HG12	2.13	0.49
1:A:431:GLU:OE1	1:A:434:SER:OG	2.31	0.49
1:A:1476:GLU:OE2	1:A:1477:ILE:HG13	2.12	0.49
2:G:1294:ALA:HA	2:G:1368:VAL:HG11	1.94	0.49
1:A:47:ILE:HD13	1:A:81:TYR:HB2	1.93	0.49
1:A:168:MET:O	1:A:206:LEU:CB	2.60	0.49
1:A:475:GLN:O	1:A:479:ASN:N	2.40	0.49
1:A:1335:PHE:O	1:A:1336:GLN:HG2	2.12	0.49
2:G:368:ILE:HG22	2:G:379:VAL:HG12	1.93	0.49
2:G:1706:ILE:HA	2:G:1709:ILE:HD12	1.95	0.49
1:A:1207:GLN:NE2	1:A:1277:GLU:OE2	2.45	0.49
2:G:615:TYR:CZ	2:G:1074:MET:HB3	2.47	0.49
2:G:844:VAL:HG12	2:G:845:THR:N	2.27	0.49
2:G:1635:ARG:HD2	2:G:1656:GLU:OE1	2.12	0.49
2:G:1874:VAL:HA	2:G:1877:ARG:CZ	2.42	0.49
2:G:1941:PHE:HA	2:G:1944:ILE:HG22	1.94	0.49
1:A:994:GLU:OE1	1:A:994:GLU:N	2.46	0.49
1:A:1135:GLU:OE1	1:A:1135:GLU:N	2.44	0.49
2:G:818:LYS:O	2:G:821:ILE:HG22	2.13	0.49
1:A:1026:GLU:HB2	1:A:1594:ASN:ND2	2.28	0.49
2:G:435:ALA:O	2:G:439:ILE:HG13	2.12	0.49
2:G:1485:CYS:SG	2:G:1514:ASN:ND2	2.77	0.49
1:A:784:ILE:HD13	1:A:838:MET:HG3	1.93	0.49
2:G:31:SER:HA	2:G:34:GLN:HE21	1.78	0.49
2:G:59:GLU:HB3	2:G:122:LEU:HD21	1.95	0.49
2:G:691:ALA:HA	2:G:694:TYR:CD2	2.47	0.49
2:G:736:ARG:NE	2:G:769:SER:O	2.33	0.49
2:G:549:ASP:HB3	2:G:554:GLY:HA3	1.93	0.49
2:G:698:LEU:O	2:G:700:LEU:N	2.44	0.49
2:G:902:PRO:HG3	2:G:1044:VAL:HG11	1.93	0.49
2:G:1447:LYS:HG2	2:G:1449:TRP:CE2	2.46	0.49
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.94	0.49
1:A:1138:LYS:N	1:A:1139:GLU:OE1	2.46	0.49
2:G:202:THR:HG21	2:G:205:ALA:HB3	1.94	0.49
2:G:275:GLN:HE21	2:G:303:LEU:HD13	1.77	0.49
2:G:810:GLU:CD	2:G:1070:ILE:H	2.21	0.49
2:G:1215:LYS:O	2:G:1218:ILE:HG12	2.13	0.49
2:G:1695:ASP:OD1	2:G:1705:SER:OG	2.24	0.49
1:A:411:GLN:NE2	1:A:1629:LYS:HG2	2.27	0.48
1:A:727:ALA:N	1:A:730:SER:OG	2.46	0.48
1:A:1354:GLU:OE2	1:A:1374:ASN:ND2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:GLU:HA	2:G:122:LEU:HD11	1.95	0.48
2:G:610:THR:OG1	2:G:1070:ILE:HG12	2.12	0.48
2:G:1604:ARG:O	2:G:1657:ILE:HD12	2.13	0.48
2:G:1917:ILE:O	2:G:1921:LYS:N	2.43	0.48
1:A:1141:ALA:O	1:A:1145:LYS:HD3	2.13	0.48
2:G:35:GLU:HA	2:G:38:ASN:HD21	1.78	0.48
1:A:1189:ILE:HG12	1:A:1380:GLN:NE2	2.27	0.48
2:G:457:ILE:C	2:G:469:ARG:HH21	2.21	0.48
1:A:750:GLU:OE1	1:A:750:GLU:N	2.37	0.48
1:A:827:SER:HG	3:A:1901:NAP:C5N	2.25	0.48
2:G:1738:PHE:HB2	2:G:1751:ILE:CD1	2.43	0.48
1:A:159:LEU:O	1:A:161:LYS:N	2.45	0.48
1:A:1251:MET:HE2	1:A:1254:VAL:HG22	1.94	0.48
2:G:887:LYS:O	2:G:891:ILE:HG23	2.13	0.48
2:G:1359:MET:HG3	2:G:1606:ARG:HH21	1.79	0.48
2:G:1484:LYS:NZ	2:G:1507:GLU:HB2	2.28	0.48
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	1.95	0.48
1:A:30:GLU:HB2	2:G:2016:ALA:CB	2.43	0.48
1:A:974:ASP:HA	1:A:977:TYR:CD2	2.49	0.48
2:G:733:THR:OG1	2:G:769:SER:HB3	2.12	0.48
2:G:1224:ILE:O	2:G:1568:HIS:NE2	2.46	0.48
2:G:1373:SER:N	2:G:1397:SER:O	2.42	0.48
2:G:1454:ASP:OD1	2:G:1454:ASP:N	2.45	0.48
2:G:1822:MET:HG3	2:G:1827:LEU:HB2	1.94	0.48
1:A:27:ARG:HH21	2:G:2016:ALA:H	1.60	0.48
1:A:1317:GLU:O	1:A:1321:SER:HB3	2.13	0.48
2:G:214:ASN:HB3	2:G:217:GLU:OE2	2.13	0.48
2:G:1924:ILE:HD12	2:G:1924:ILE:H	1.77	0.48
2:G:215:ILE:HD12	2:G:240:LEU:HD21	1.94	0.48
2:G:646:THR:HG21	2:G:677:GLN:HB2	1.95	0.48
2:G:1079:ASP:OD2	2:G:1080:GLY:N	2.46	0.48
2:G:1129:ALA:HB2	2:G:1138:TRP:CH2	2.49	0.48
2:G:1845:ASP:CG	2:G:1849:ARG:HG2	2.39	0.48
2:G:1957:PRO:HB2	2:G:1959:LYS:HE2	1.95	0.48
1:A:1116:PRO:HB2	1:A:1184:LEU:HD13	1.96	0.48
2:G:45:THR:O	2:G:48:PHE:N	2.47	0.48
2:G:246:LEU:O	2:G:250:VAL:HG13	2.13	0.48
2:G:809:LYS:HB3	2:G:1067:ASP:O	2.13	0.48
2:G:1458:ASP:OD1	2:G:1458:ASP:N	2.44	0.48
2:G:2046:GLU:N	2:G:2046:GLU:OE1	2.46	0.48
1:A:421:ILE:HA	1:A:465:ASN:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.14	0.48
2:G:525:VAL:C	2:G:526:ARG:HD3	2.39	0.48
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.79	0.48
2:G:725:ASN:HA	2:G:1109:VAL:HG11	1.96	0.48
2:G:1839:GLN:HE21	2:G:1844:ARG:HD2	1.79	0.48
1:A:985:ARG:HG3	2:G:956:GLU:HB3	1.95	0.47
2:G:270:ALA:O	2:G:459:VAL:HA	2.13	0.47
1:A:1608:ASN:O	1:A:1610:ASN:N	2.47	0.47
2:G:16:LEU:HD23	2:G:48:PHE:CD2	2.50	0.47
2:G:155:GLN:HG2	2:G:499:THR:HG23	1.95	0.47
2:G:336:SER:OG	2:G:423:VAL:O	2.32	0.47
2:G:710:ILE:HD13	2:G:749:PRO:HB3	1.96	0.47
2:G:1889:VAL:HG23	2:G:1899:VAL:HG23	1.97	0.47
1:A:33:ASP:O	1:A:37:LYS:N	2.45	0.47
2:G:900:GLN:NE2	2:G:1052:CYS:H	2.11	0.47
2:G:1491:VAL:CB	2:G:1501:ILE:HD11	2.44	0.47
2:G:1908:ASP:OD2	2:G:1954:LYS:HD3	2.14	0.47
2:G:1976:PHE:HD1	2:G:1977:HIS:HD1	1.59	0.47
1:A:1125:VAL:CG1	1:A:1126:ILE:H	2.16	0.47
2:G:109:LEU:HG	2:G:114:THR:HG23	1.95	0.47
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.49	0.47
2:G:1038:GLU:H	2:G:1038:GLU:HG2	1.53	0.47
2:G:1485:CYS:HB2	2:G:1506:TYR:HB3	1.95	0.47
2:G:1850:SER:HB3	2:G:1973:SER:OG	2.14	0.47
1:A:385:PHE:CD2	1:A:787:LYS:HA	2.50	0.47
1:A:810:LYS:CB	1:A:861:GLN:HG2	2.45	0.47
1:A:1040:GLU:HA	1:A:1580:LEU:HD11	1.97	0.47
1:A:1390:ALA:O	1:A:1393:ALA:N	2.48	0.47
2:G:1310:ASP:OD1	2:G:1602:SER:N	2.45	0.47
2:G:1730:ARG:NH2	2:G:1757:GLU:O	2.47	0.47
1:A:745:VAL:C	1:A:747:ALA:H	2.23	0.47
1:A:1123:GLN:C	1:A:1177:LYS:HZ3	2.18	0.47
1:A:1377:MET:HB3	1:A:1377:MET:HE3	1.52	0.47
2:G:259:THR:HA	2:G:289:TRP:NE1	2.30	0.47
2:G:1058:VAL:O	2:G:1061:GLN:HG2	2.15	0.47
2:G:1517:VAL:O	2:G:1521:LYS:HG2	2.13	0.47
1:A:413:LEU:HD23	1:A:450:PHE:CD2	2.49	0.47
1:A:433:VAL:HG13	1:A:609:SER:HB2	1.95	0.47
1:A:1337:GLU:H	1:A:1337:GLU:CD	2.21	0.47
1:A:1584:PRO:HG2	1:A:1588:ALA:N	2.30	0.47
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:633:ALA:O	2:G:637:VAL:HG13	2.14	0.47
2:G:895:LEU:HD13	2:G:1018:VAL:HG21	1.95	0.47
2:G:1201:VAL:HG11	2:G:1226:ASN:ND2	2.27	0.47
2:G:1287:GLY:HA3	2:G:1374:THR:HG23	1.97	0.47
2:G:1718:THR:HA	2:G:1763:THR:HA	1.96	0.47
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.30	0.47
2:G:1960:LEU:HD23	2:G:1968:PRO:HB3	1.96	0.47
1:A:13:LEU:HD22	2:G:2026:PHE:CE1	2.50	0.47
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.97	0.47
2:G:530:ALA:HA	2:G:547:ILE:HD11	1.95	0.47
2:G:1263:LYS:HD3	2:G:1347:LEU:HD11	1.96	0.47
2:G:1323:MET:H	2:G:1590:ARG:HH22	1.60	0.47
2:G:1775:GLN:HE22	2:G:1836:MET:CB	2.26	0.47
2:G:1956:ARG:O	2:G:1956:ARG:NE	2.48	0.47
1:A:712:LYS:HB3	1:A:1361:THR:HG21	1.96	0.47
2:G:6:THR:HA	2:G:23:PRO:HA	1.96	0.47
2:G:421:LEU:O	2:G:423:VAL:N	2.48	0.47
2:G:589:ARG:HG2	2:G:590:PRO:HD2	1.96	0.47
2:G:1381:VAL:HG12	2:G:1390:VAL:HG12	1.97	0.47
2:G:1799:PRO:HD2	2:G:1802:ALA:HB2	1.96	0.47
1:A:440:MET:O	1:A:443:SER:OG	2.26	0.47
1:A:640:LEU:N	1:A:656:SER:OG	2.48	0.47
1:A:1059:PHE:HA	1:A:1079:LYS:NZ	2.30	0.47
1:A:1298:ILE:HD13	1:A:1298:ILE:HA	1.65	0.47
2:G:67:TYR:CZ	2:G:71:LEU:HD11	2.50	0.47
2:G:831:LYS:HE2	2:G:834:GLN:HG3	1.97	0.47
2:G:857:ILE:O	2:G:862:VAL:HG11	2.15	0.47
1:A:257:PRO:O	1:A:261:GLN:N	2.41	0.46
1:A:338:LEU:O	1:A:342:GLN:N	2.28	0.46
1:A:1064:ASN:HA	1:A:1072:TYR:O	2.15	0.46
2:G:1324:ASP:O	2:G:1327:ILE:HG22	2.15	0.46
2:G:1342:THR:O	2:G:1421:ASN:ND2	2.48	0.46
2:G:1351:VAL:HG21	2:G:1413:ARG:NH2	2.30	0.46
1:A:56:MET:HE1	2:G:1807:HIS:CD2	2.51	0.46
1:A:1152:VAL:HG11	1:A:1154:ILE:HG23	1.96	0.46
2:G:138:ASP:OD1	2:G:138:ASP:N	2.48	0.46
2:G:264:ARG:HH21	2:G:456:GLN:HB2	1.80	0.46
1:A:1119:LYS:HE3	1:A:1341:PHE:CD1	2.49	0.46
1:A:1397:GLY:O	1:A:1680:ARG:HG3	2.15	0.46
1:A:1446:LYS:O	1:A:1450:ARG:HG3	2.14	0.46
2:G:748:THR:HA	2:G:751:LEU:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:932:ILE:HD11	2:G:939:PHE:HB2	1.97	0.46
2:G:1550:ASN:HB3	2:G:1581:HIS:CE1	2.51	0.46
2:G:2030:TYR:HB2	2:G:2038:ILE:HG21	1.97	0.46
1:A:1360:ARG:NH2	1:A:1367:ARG:HD2	2.30	0.46
2:G:36:GLN:O	2:G:40:ILE:HG13	2.16	0.46
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.34	0.46
1:A:46:GLU:HB3	1:A:80:CYS:HA	1.97	0.46
1:A:693:LEU:HD13	1:A:705:VAL:HG11	1.97	0.46
1:A:858:TRP:CE3	1:A:862:LEU:HB2	2.50	0.46
2:G:273:HIS:CG	2:G:274:SER:H	2.34	0.46
2:G:338:MET:HE3	2:G:423:VAL:HG21	1.96	0.46
2:G:573:LYS:CG	2:G:1101:GLU:HA	2.45	0.46
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.37	0.46
2:G:1643:ARG:HB3	2:G:1647:ASP:HA	1.96	0.46
2:G:1812:TYR:OH	2:G:1834:ARG:NE	2.48	0.46
2:G:1924:ILE:O	2:G:1928:GLN:NE2	2.48	0.46
2:G:239:PRO:O	2:G:243:VAL:HG13	2.16	0.46
2:G:1093:ASP:OD1	2:G:1096:LYS:HB2	2.16	0.46
2:G:1138:TRP:NE1	2:G:1142:LEU:HD11	2.30	0.46
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.31	0.46
1:A:467:GLN:O	1:A:467:GLN:NE2	2.49	0.46
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.51	0.46
2:G:649:ILE:HD13	2:G:666:ILE:HD11	1.98	0.46
2:G:875:LEU:HD21	2:G:879:LYS:C	2.41	0.46
1:A:1029:PRO:HG3	1:A:1187:GLY:O	2.16	0.46
1:A:55:GLY:O	1:A:59:ARG:HG2	2.16	0.46
2:G:978:GLU:OE1	2:G:978:GLU:N	2.49	0.46
2:G:1149:TRP:HB2	2:G:1219:ILE:HD11	1.98	0.46
1:A:395:SER:HB3	1:A:398:LYS:HD2	1.97	0.46
1:A:440:MET:CE	1:A:479:ASN:HB3	2.43	0.46
1:A:452:GLU:O	1:A:456:SER:OG	2.29	0.46
1:A:521:LYS:HD2	1:A:523:SER:OG	2.15	0.46
1:A:527:GLN:HG2	1:A:626:VAL:HG21	1.96	0.46
1:A:1144:PHE:HZ	1:A:1174:TYR:HH	1.64	0.46
1:A:1461:ASP:O	1:A:1464:GLU:HG2	2.15	0.46
2:G:310:CYS:O	2:G:313:ALA:N	2.49	0.46
2:G:410:SER:OG	2:G:411:GLU:OE2	2.33	0.46
2:G:1455:GLU:CD	2:G:1455:GLU:H	2.22	0.46
2:G:1741:ILE:HD11	2:G:1986:LYS:HG2	1.97	0.46
1:A:1584:PRO:O	1:A:1585:LYS:C	2.58	0.45
2:G:142:ASN:HD21	2:G:147:ARG:NE	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:502:LEU:HD23	2:G:502:LEU:H	1.81	0.45
2:G:634:ILE:O	2:G:637:VAL:HG22	2.17	0.45
1:A:430:ARG:HG3	1:A:495:LYS:HG3	1.98	0.45
1:A:821:GLN:OE1	1:A:823:ILE:HD11	2.16	0.45
1:A:957:VAL:HG23	2:G:1443:VAL:HG12	1.99	0.45
1:A:1606:PRO:HA	1:A:1630:THR:HG23	1.99	0.45
2:G:540:ASP:OD1	2:G:540:ASP:N	2.49	0.45
2:G:646:THR:CG2	2:G:677:GLN:HB2	2.46	0.45
2:G:906:THR:OG1	2:G:925:ARG:NH2	2.49	0.45
2:G:1011:MET:C	3:G:2102:NAP:H2A	2.40	0.45
2:G:1488:PRO:HA	2:G:1503:ILE:HD13	1.98	0.45
2:G:1669:GLN:HB3	2:G:1809:LEU:HD13	1.99	0.45
2:G:1716:ASN:ND2	2:G:1765:ARG:HA	2.29	0.45
2:G:1819:ALA:HA	2:G:2005:ARG:HD2	1.98	0.45
2:G:273:HIS:HB2	2:G:512:LEU:HD22	1.98	0.45
2:G:479:ILE:O	2:G:483:ILE:HG13	2.16	0.45
2:G:865:TRP:CD1	2:G:865:TRP:C	2.93	0.45
2:G:938:TRP:CD2	2:G:944:ARG:HG3	2.51	0.45
2:G:1611:GLN:N	2:G:1652:THR:O	2.35	0.45
2:G:1644:ASN:HB3	2:G:1646:ASP:OD2	2.16	0.45
1:A:1001:VAL:HA	1:A:1004:ILE:HG22	1.98	0.45
1:A:1036:ARG:HH21	1:A:1598:GLN:HE21	1.65	0.45
1:A:1209:ASP:OD2	1:A:1253:GLY:HA2	2.17	0.45
1:A:1534:ASP:OD2	1:A:1567:SER:OG	2.32	0.45
2:G:430:HIS:HA	2:G:433:VAL:HG23	1.99	0.45
2:G:1641:GLU:OE2	2:G:1643:ARG:NE	2.48	0.45
2:G:1712:ASN:OD1	2:G:1712:ASN:N	2.50	0.45
1:A:1020:VAL:HG23	1:A:1402:GLY:O	2.16	0.45
1:A:1046:SER:OG	1:A:1047:LEU:N	2.48	0.45
1:A:1123:GLN:HB3	1:A:1177:LYS:CD	2.45	0.45
1:A:1182:ASP:O	1:A:1184:LEU:HB2	2.16	0.45
1:A:1207:GLN:HE22	1:A:1286:TRP:HZ2	1.65	0.45
1:A:1238:VAL:HG22	1:A:1242:GLU:HB2	1.98	0.45
2:G:126:TYR:HD2	2:G:127:ILE:HD13	1.80	0.45
2:G:1168:ASN:O	2:G:1172:LYS:HG2	2.17	0.45
2:G:1291:GLU:HA	2:G:1371:VAL:HA	1.98	0.45
2:G:1531:VAL:HG13	2:G:1631:MET:HB2	1.99	0.45
1:A:90:TYR:O	2:G:1533:LEU:HD21	2.17	0.45
1:A:1559:GLU:O	1:A:1563:HIS:N	2.39	0.45
2:G:1357:TYR:CD1	2:G:1406:VAL:HG12	2.52	0.45
2:G:1681:TYR:CE2	2:G:1691:TRP:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD23	1:A:450:PHE:CE2	2.52	0.45
1:A:739:GLN:HG3	1:A:772:ALA:HB3	1.98	0.45
1:A:803:MET:HE1	1:A:849:LEU:HD21	1.99	0.45
1:A:819:PRO:HB3	1:A:860:ASN:O	2.16	0.45
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.45
1:A:27:ARG:NH2	2:G:2015:THR:HA	2.32	0.45
1:A:1103:ILE:HG23	1:A:1377:MET:HE2	1.99	0.45
2:G:109:LEU:HD12	2:G:119:THR:HG21	1.98	0.45
2:G:268:LYS:O	2:G:458:PRO:HD2	2.16	0.45
2:G:571:LYS:HD2	2:G:575:GLY:C	2.42	0.45
2:G:877:LYS:HG3	2:G:878:ASN:N	2.31	0.45
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.52	0.45
2:G:1745:LYS:NZ	2:G:1747:LYS:HA	2.32	0.45
1:A:333:LYS:O	1:A:337:VAL:HG13	2.16	0.45
1:A:847:GLU:C	1:A:849:LEU:H	2.25	0.45
1:A:853:TRP:CE3	1:A:921:PRO:HD3	2.51	0.45
1:A:1026:GLU:OE1	1:A:1594:ASN:ND2	2.47	0.45
1:A:1245:ASN:O	1:A:1298:ILE:HG23	2.17	0.45
1:A:1707:THR:O	1:A:1710:LEU:N	2.46	0.45
2:G:68:VAL:O	2:G:72:VAL:HG23	2.17	0.45
2:G:297:ARG:NE	2:G:447:ASN:HD21	2.15	0.45
2:G:391:LEU:O	2:G:394:ARG:N	2.42	0.45
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.82	0.45
2:G:872:ILE:O	2:G:875:LEU:HB3	2.17	0.45
2:G:1514:ASN:ND2	2:G:1516:VAL:HG22	2.32	0.45
1:A:891:MET:HE3	1:A:939:PHE:CZ	2.52	0.45
1:A:1418:VAL:HG12	1:A:1647:GLY:HA2	1.99	0.45
2:G:812:LYS:HD3	2:G:812:LYS:HA	1.56	0.45
2:G:1151:HIS:CD2	2:G:1155:LEU:HD12	2.51	0.45
2:G:1170:ILE:HG12	2:G:1221:MET:HE3	1.99	0.45
2:G:1669:GLN:HA	2:G:1781:LEU:HD13	1.99	0.45
2:G:1892:ASN:HB2	2:G:1897:GLN:HB3	1.99	0.45
1:A:945:LYS:O	1:A:949:GLU:HG2	2.17	0.44
1:A:981:GLU:OE2	2:G:962:LYS:HB2	2.17	0.44
1:A:1211:ILE:O	1:A:1215:VAL:HG23	2.17	0.44
1:A:1368:PRO:HG2	1:A:1608:ASN:ND2	2.31	0.44
1:A:1717:ASP:OD2	1:A:1739:GLN:HB2	2.17	0.44
2:G:408:PRO:HB3	2:G:833:GLU:OE2	2.17	0.44
2:G:1257:ASP:OD1	2:G:1260:GLN:HB2	2.18	0.44
2:G:1598:ALA:HB2	2:G:1657:ILE:HD11	1.98	0.44
2:G:1767:GLU:HG2	2:G:1768:LYS:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1804:PHE:CG	2:G:1818:LEU:HG	2.52	0.44
2:G:1854:MET:HA	2:G:1901:ALA:HA	1.98	0.44
1:A:330:GLU:HA	1:A:333:LYS:HG2	1.99	0.44
1:A:711:SER:H	1:A:714:VAL:HG12	1.82	0.44
2:G:230:TYR:O	2:G:236:ILE:HG21	2.17	0.44
2:G:437:ASP:OD1	2:G:437:ASP:N	2.50	0.44
2:G:587:ILE:HG13	2:G:589:ARG:H	1.82	0.44
2:G:665:LEU:HD21	2:G:669:LEU:HD12	1.99	0.44
2:G:734:GLY:H	2:G:769:SER:HB3	1.81	0.44
2:G:1214:LEU:HD21	2:G:1220:GLN:CD	2.42	0.44
2:G:1539:ILE:HD11	2:G:1628:HIS:HB2	1.97	0.44
2:G:1786:LYS:NZ	2:G:1816:ALA:O	2.50	0.44
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.53	0.44
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.77	0.44
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.71	0.44
2:G:124:LYS:HB2	2:G:179:THR:HA	1.99	0.44
2:G:423:VAL:HG12	2:G:424:ALA:H	1.81	0.44
2:G:1357:TYR:HD1	2:G:1406:VAL:HG12	1.82	0.44
2:G:1713:ASN:ND2	2:G:1771:LEU:HB2	2.33	0.44
2:G:169:TYR:OH	2:G:231:LEU:O	2.30	0.44
2:G:297:ARG:NH1	2:G:301:THR:HG21	2.32	0.44
2:G:330:ASN:HB3	2:G:394:ARG:HH12	1.83	0.44
2:G:543:PHE:HB2	2:G:545:GLN:NE2	2.32	0.44
2:G:1484:LYS:HZ3	2:G:1507:GLU:HB2	1.83	0.44
1:A:1123:GLN:HG2	1:A:1124:GLU:N	2.24	0.44
1:A:1254:VAL:HA	1:A:1257:LEU:HD12	1.99	0.44
1:A:1351:ASN:HB3	1:A:1354:GLU:HG2	2.00	0.44
1:A:1460:LYS:HE3	1:A:1460:LYS:HB3	1.87	0.44
2:G:597:MET:HB2	2:G:601:THR:HG23	2.00	0.44
2:G:604:PRO:HA	2:G:607:VAL:HG12	2.00	0.44
2:G:1277:LEU:C	2:G:1279:PHE:H	2.24	0.44
2:G:1624:THR:HA	2:G:1642:THR:HA	2.00	0.44
1:A:11:HIS:HB2	2:G:2001:VAL:HG11	2.00	0.44
1:A:843:LYS:CE	3:A:1901:NAP:HO2N	2.30	0.44
1:A:1086:ASP:O	1:A:1089:VAL:HG12	2.18	0.44
2:G:81:ASP:OD1	2:G:81:ASP:N	2.48	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.53	0.44
2:G:821:ILE:HD11	2:G:1055:HIS:ND1	2.32	0.44
2:G:861:GLY:HA2	2:G:898:ASP:O	2.17	0.44
1:A:774:ILE:HD11	1:A:791:ALA:HB2	2.00	0.44
1:A:1087:LYS:HA	1:A:1087:LYS:HD2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:MET:O	1:A:1238:VAL:HG12	2.18	0.44
2:G:148:ALA:O	2:G:153:ASN:N	2.50	0.44
2:G:368:ILE:HA	2:G:379:VAL:HG12	2.00	0.44
2:G:608:ALA:HA	2:G:611:THR:HG22	2.00	0.44
2:G:2037:PRO:HA	2:G:2040:GLU:OE2	2.17	0.44
1:A:477:ILE:O	1:A:481:LYS:HG3	2.18	0.44
1:A:985:ARG:HB2	2:G:957:ARG:HA	2.00	0.44
1:A:1125:VAL:HG12	1:A:1126:ILE:N	2.18	0.44
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.17	0.44
2:G:848:SER:OG	2:G:849:GLU:N	2.51	0.44
2:G:1001:ASP:OD2	2:G:1001:ASP:N	2.48	0.44
2:G:1213:LEU:C	2:G:1214:LEU:HD22	2.43	0.44
2:G:1297:VAL:HG23	2:G:1319:MET:HG2	2.00	0.44
2:G:1561:ASN:HD21	2:G:1563:ILE:HG12	1.82	0.44
2:G:1764:PHE:C	2:G:1765:ARG:HD2	2.42	0.44
1:A:658:LEU:HD11	1:A:916:LEU:HD22	1.99	0.44
1:A:1608:ASN:C	1:A:1610:ASN:H	2.26	0.44
2:G:66:GLY:O	2:G:69:SER:OG	2.22	0.44
2:G:686:PRO:HB3	2:G:690:VAL:HG13	2.00	0.44
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.86	0.44
2:G:1624:THR:OG1	2:G:1642:THR:HG22	2.18	0.44
1:A:8:GLU:O	1:A:12:ILE:HG12	2.18	0.43
1:A:448:ILE:HD13	1:A:481:LYS:HG2	2.00	0.43
2:G:394:ARG:HA	2:G:397:LYS:CG	2.43	0.43
2:G:461:ASP:OD2	2:G:478:ARG:HD3	2.18	0.43
2:G:736:ARG:NH1	2:G:829:ASP:OD2	2.51	0.43
2:G:1224:ILE:HA	2:G:1235:SER:HA	1.99	0.43
2:G:1299:ASP:OD2	2:G:1556:VAL:HG22	2.18	0.43
2:G:1594:GLU:HG2	2:G:1605:VAL:HG21	2.00	0.43
2:G:1672:GLN:CD	2:G:1672:GLN:H	2.24	0.43
1:A:402:PHE:HB2	1:A:732:LEU:CD2	2.48	0.43
1:A:1015:LEU:O	1:A:1390:ALA:HB3	2.18	0.43
2:G:123:ILE:HD12	2:G:123:ILE:H	1.82	0.43
2:G:240:LEU:HA	2:G:243:VAL:HG22	2.00	0.43
2:G:517:HIS:HB2	2:G:527:VAL:CG1	2.46	0.43
2:G:1078:HIS:O	2:G:1082:ILE:HG12	2.18	0.43
2:G:1533:LEU:HD23	2:G:1534:GLU:H	1.82	0.43
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.48	0.43
2:G:355:LYS:O	2:G:358:SER:OG	2.31	0.43
2:G:848:SER:C	2:G:851:GLY:H	2.25	0.43
2:G:856:LYS:HB2	2:G:862:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1353:LEU:HD23	2:G:1353:LEU:HA	1.84	0.43
1:A:46:GLU:HA	2:G:1665:VAL:HG23	1.99	0.43
1:A:83:LYS:HD2	1:A:84:ASP:OD1	2.18	0.43
1:A:724:LYS:HE3	1:A:725:TYR:CZ	2.53	0.43
1:A:960:GLU:OE2	1:A:961:THR:HG23	2.19	0.43
2:G:391:LEU:HD23	2:G:394:ARG:HE	1.83	0.43
2:G:1087:HIS:HA	2:G:1092:ASP:OD1	2.18	0.43
1:A:337:VAL:O	1:A:341:GLN:N	2.42	0.43
2:G:807:ILE:HD11	2:G:822:ALA:HB2	2.01	0.43
2:G:1225:GLU:OE1	2:G:1227:ARG:N	2.52	0.43
2:G:1434:HIS:CD2	2:G:1436:LYS:HE3	2.53	0.43
2:G:1448:GLU:H	2:G:1448:GLU:CD	2.26	0.43
2:G:1537:ILE:O	2:G:1537:ILE:HG13	2.19	0.43
2:G:1623:LYS:HA	2:G:1623:LYS:HE2	2.00	0.43
1:A:31:THR:HA	1:A:34:VAL:HG12	2.01	0.43
1:A:823:ILE:HD13	1:A:865:CYS:HB3	1.99	0.43
1:A:1101:SER:N	1:A:1104:ARG:HD3	2.32	0.43
2:G:45:THR:OG1	2:G:50:ALA:HB2	2.19	0.43
2:G:527:VAL:HG13	2:G:541:TYR:HB3	2.00	0.43
2:G:1045:ASP:OD1	2:G:1045:ASP:N	2.46	0.43
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.85	0.43
1:A:841:GLU:OE2	1:A:845:SER:OG	2.37	0.43
2:G:113:ASP:OD1	2:G:113:ASP:N	2.50	0.43
2:G:268:LYS:HE2	2:G:268:LYS:HB3	1.68	0.43
2:G:1869:GLU:HA	2:G:1872:GLN:HG2	2.00	0.43
2:G:2023:LYS:H	2:G:2023:LYS:HD3	1.83	0.43
2:G:256:LEU:HD23	2:G:256:LEU:HA	1.82	0.43
2:G:740:HIS:CE1	2:G:854:ILE:HD11	2.53	0.43
2:G:910:GLN:HE22	2:G:912:ARG:NH2	2.17	0.43
2:G:1428:GLU:OE2	2:G:1470:THR:OG1	2.23	0.43
2:G:1886:VAL:HA	2:G:1901:ALA:O	2.18	0.43
1:A:505:LYS:HA	1:A:954:ARG:HD2	2.01	0.43
1:A:883:ILE:HG13	1:A:884:ILE:HG23	2.01	0.43
2:G:767:PHE:HD2	2:G:771:PHE:CE2	2.37	0.43
2:G:1974:VAL:HG13	2:G:1976:PHE:HD2	1.83	0.43
1:A:430:ARG:CZ	1:A:605:LEU:HD13	2.49	0.43
1:A:694:GLN:O	1:A:698:GLN:HG3	2.19	0.43
1:A:1030:TRP:CZ2	1:A:1102:GLY:HA3	2.54	0.43
1:A:1140:THR:C	1:A:1142:GLU:H	2.27	0.43
1:A:1165:VAL:H	1:A:1165:VAL:HG22	1.63	0.43
1:A:1283:MET:HB2	1:A:1283:MET:HE3	1.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:571:LYS:HD3	2:G:571:LYS:HA	1.67	0.43
2:G:1614:ASP:OD1	2:G:1614:ASP:N	2.51	0.43
2:G:1775:GLN:NE2	2:G:1836:MET:SD	2.91	0.43
2:G:1821:VAL:HG23	2:G:1822:MET:HG2	2.00	0.43
2:G:1847:LEU:HD23	2:G:1847:LEU:O	2.19	0.43
1:A:712:LYS:NZ	1:A:716:ASP:OD1	2.51	0.42
1:A:774:ILE:HG22	3:A:1901:NAP:N7A	2.34	0.42
2:G:350:GLN:HA	2:G:353:VAL:HG22	2.00	0.42
2:G:1354:SER:OG	2:G:1409:SER:OG	2.35	0.42
2:G:1475:LYS:HG3	2:G:1476:ASN:HD22	1.85	0.42
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.53	0.42
1:A:413:LEU:CD2	1:A:451:MET:HB3	2.49	0.42
1:A:733:ILE:HG22	1:A:735:VAL:HG13	2.01	0.42
1:A:1312:VAL:O	1:A:1316:VAL:HG12	2.19	0.42
2:G:16:LEU:HB3	2:G:60:LEU:HD12	2.00	0.42
2:G:48:PHE:HD1	2:G:53:GLU:HB3	1.84	0.42
2:G:569:LEU:HD23	2:G:1090:TYR:CE1	2.52	0.42
2:G:1085:LEU:HA	2:G:1085:LEU:HD23	1.70	0.42
2:G:1383:ASN:HD22	2:G:1388:LYS:HB3	1.83	0.42
2:G:1685:LYS:HA	2:G:1688:GLN:CD	2.44	0.42
2:G:1762:TYR:HE2	2:G:1764:PHE:CE1	2.37	0.42
2:G:1923:ASP:HB2	2:G:1926:GLU:HG3	2.01	0.42
2:G:2039:LYS:HG3	2:G:2040:GLU:N	2.34	0.42
1:A:78:ILE:C	1:A:79:LEU:HD12	2.43	0.42
1:A:366:ASP:OD2	1:A:367:THR:N	2.52	0.42
1:A:1165:VAL:HB	1:A:1167:LEU:HD11	2.01	0.42
1:A:1323:LYS:HD3	1:A:1324:ALA:HB2	1.99	0.42
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.73	0.42
1:A:1538:VAL:HG12	1:A:1539:ALA:N	2.34	0.42
2:G:198:LEU:HA	2:G:201:THR:HG22	2.00	0.42
2:G:216:LEU:HD12	2:G:216:LEU:H	1.83	0.42
2:G:1181:VAL:O	2:G:1181:VAL:HG23	2.19	0.42
2:G:1447:LYS:HA	2:G:1447:LYS:HD3	1.81	0.42
2:G:1515:PRO:HB2	2:G:1519:PHE:CE2	2.54	0.42
2:G:1923:ASP:O	2:G:1927:LEU:HG	2.20	0.42
1:A:1260:MET:HG3	1:A:1261:PHE:N	2.34	0.42
1:A:1316:VAL:O	1:A:1320:LEU:HD23	2.19	0.42
1:A:1717:ASP:CG	1:A:1739:GLN:HB2	2.45	0.42
2:G:7:ARG:N	2:G:22:VAL:O	2.43	0.42
2:G:309:ARG:NE	2:G:442:ASP:OD2	2.28	0.42
2:G:346:GLN:HE21	2:G:368:ILE:HD13	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:370:LEU:HA	2:G:488:VAL:HG22	2.00	0.42
2:G:1420:GLU:H	2:G:1420:GLU:CD	2.26	0.42
2:G:1679:ASP:OD1	2:G:1680:LEU:N	2.47	0.42
1:A:338:LEU:HA	1:A:341:GLN:HB2	2.02	0.42
1:A:824:LEU:HB3	1:A:846:LEU:HD23	2.02	0.42
1:A:1070:ARG:HB3	1:A:1072:TYR:CE1	2.55	0.42
1:A:1557:ILE:O	1:A:1561:MET:HG2	2.19	0.42
1:A:1559:GLU:HA	1:A:1562:LYS:HB3	2.00	0.42
2:G:7:ARG:HG3	2:G:24:THR:HG22	2.01	0.42
2:G:159:ILE:HA	2:G:271:THR:O	2.20	0.42
2:G:1143:ALA:HB1	2:G:1151:HIS:HA	2.02	0.42
2:G:1514:ASN:HB3	2:G:1517:VAL:HG22	2.01	0.42
2:G:1902:GLY:H	2:G:1975:PRO:HB3	1.84	0.42
1:A:538:GLU:OE1	1:A:538:GLU:N	2.45	0.42
1:A:1115:ASN:O	1:A:1118:LYS:N	2.35	0.42
1:A:1223:PHE:HB3	1:A:1228:ILE:O	2.19	0.42
2:G:58:ALA:HA	2:G:95:TYR:CD1	2.54	0.42
2:G:526:ARG:HG2	2:G:558:ASN:H	1.85	0.42
2:G:607:VAL:HG11	2:G:619:LEU:HD13	2.01	0.42
2:G:1301:THR:HG23	2:G:1306:ASN:ND2	2.35	0.42
2:G:1311:PHE:CE1	2:G:1322:PRO:HA	2.54	0.42
2:G:1673:GLU:N	2:G:1673:GLU:OE1	2.52	0.42
1:A:393:SER:O	1:A:736:PRO:HB2	2.19	0.42
1:A:402:PHE:HB2	1:A:732:LEU:HD23	2.02	0.42
1:A:630:ILE:HG22	1:A:653:ARG:NH2	2.35	0.42
1:A:803:MET:CE	1:A:849:LEU:HD21	2.49	0.42
2:G:598:THR:HA	2:G:620:ALA:HB1	2.00	0.42
2:G:1197:LEU:HD12	2:G:1198:SER:N	2.35	0.42
2:G:1325:PHE:O	2:G:1329:VAL:HG12	2.20	0.42
2:G:1431:TYR:CE1	2:G:1526:THR:HG22	2.52	0.42
2:G:1537:ILE:HG13	2:G:1628:HIS:HB3	2.02	0.42
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.82	0.42
1:A:1152:VAL:CG1	1:A:1154:ILE:HG23	2.49	0.42
1:A:1307:THR:O	1:A:1311:SER:OG	2.33	0.42
1:A:1498:GLU:OE2	1:A:1502:ARG:HD3	2.19	0.42
2:G:14:GLY:HA3	2:G:48:PHE:HZ	1.84	0.42
2:G:217:GLU:HA	2:G:220:GLU:CD	2.44	0.42
2:G:670:ARG:NH1	2:G:674:TYR:O	2.53	0.42
2:G:1226:ASN:OD1	2:G:1226:ASN:N	2.48	0.42
2:G:1449:TRP:HZ2	2:G:1519:PHE:HD2	1.67	0.42
2:G:1632:ILE:O	2:G:1635:ARG:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:THR:HA	1:A:370:GLU:HG3	2.02	0.42
1:A:504:ASP:HB2	1:A:508:ASN:H	1.84	0.42
1:A:1592:MET:HG3	1:A:1641:ILE:HG23	2.02	0.42
2:G:677:GLN:O	2:G:678:PHE:HB3	2.20	0.42
2:G:680:THR:HA	2:G:704:GLY:O	2.20	0.42
2:G:1815:LEU:HB3	2:G:1821:VAL:HG21	2.01	0.42
2:G:1962:ARG:HB2	2:G:1968:PRO:HD3	2.02	0.42
1:A:82:SER:OG	1:A:83:LYS:N	2.53	0.42
1:A:1017:ARG:NH1	1:A:1320:LEU:HD12	2.35	0.42
1:A:1375:GLY:O	1:A:1545:SER:OG	2.29	0.42
1:A:1515:ARG:HA	1:A:1515:ARG:HD2	1.79	0.42
1:A:1516:ASP:OD1	1:A:1518:ARG:HG2	2.20	0.42
2:G:238:CYS:O	2:G:275:GLN:NE2	2.53	0.42
2:G:1475:LYS:HE3	2:G:1476:ASN:ND2	2.35	0.42
2:G:1765:ARG:HB3	2:G:1847:LEU:O	2.19	0.42
2:G:1778:GLN:HA	2:G:1809:LEU:HD11	2.01	0.42
2:G:1894:GLU:C	2:G:1896:GLN:H	2.27	0.42
1:A:431:GLU:O	1:A:435:GLU:N	2.53	0.41
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.55	0.41
1:A:1680:ARG:H	1:A:1680:ARG:HG2	1.71	0.41
1:A:1734:ASN:HB3	1:A:1736:LYS:HE2	2.00	0.41
2:G:440:ASN:HD21	2:G:477:GLU:HG2	1.83	0.41
2:G:730:LEU:HD23	2:G:730:LEU:HA	1.60	0.41
2:G:754:TYR:OH	2:G:795:PRO:O	2.30	0.41
2:G:1163:LYS:O	2:G:1164:MET:HG3	2.20	0.41
2:G:1263:LYS:NZ	2:G:1338:ILE:O	2.53	0.41
2:G:1306:ASN:OD1	2:G:1308:CYS:HB2	2.20	0.41
2:G:1322:PRO:HB2	2:G:1590:ARG:HH12	1.84	0.41
2:G:174:ARG:NH1	2:G:222:PRO:HG3	2.35	0.41
2:G:555:LEU:HD21	2:G:557:LYS:HE3	2.02	0.41
2:G:1319:MET:HB3	2:G:1368:VAL:CG2	2.46	0.41
1:A:2:LYS:HB2	1:A:2:LYS:HE2	1.78	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.87	0.41
1:A:807:LYS:HG3	1:A:861:GLN:OE1	2.21	0.41
1:A:1123:GLN:CB	1:A:1177:LYS:HD3	2.48	0.41
2:G:180:TYR:O	2:G:184:VAL:HG22	2.19	0.41
2:G:309:ARG:HB2	2:G:439:ILE:HG12	2.02	0.41
2:G:1011:MET:HE3	2:G:1011:MET:HB2	1.91	0.41
2:G:1127:PHE:HE2	2:G:1184:ILE:HD13	1.85	0.41
2:G:1381:VAL:O	2:G:1422:THR:HG23	2.20	0.41
2:G:1570:ALA:HA	2:G:1575:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2015:THR:HG23	2:G:2017:LYS:HE2	2.01	0.41
1:A:1:MET:HE1	2:G:2048:TYR:HA	2.02	0.41
1:A:251:GLN:O	1:A:255:GLY:HA2	2.20	0.41
1:A:417:TYR:OH	1:A:454:HIS:HB3	2.20	0.41
1:A:504:ASP:OD2	1:A:508:ASN:HB3	2.21	0.41
1:A:525:TYR:O	1:A:529:MET:HG2	2.21	0.41
1:A:1039:MET:HE2	1:A:1039:MET:HB3	1.80	0.41
1:A:1238:VAL:HG21	1:A:1325:ARG:HB2	2.02	0.41
2:G:268:LYS:NZ	2:G:497:LYS:O	2.45	0.41
2:G:765:LEU:HD12	2:G:765:LEU:HA	1.83	0.41
2:G:804:ARG:HD2	2:G:1063:THR:HG22	2.02	0.41
2:G:1066:ILE:HD12	2:G:1066:ILE:HA	1.94	0.41
2:G:1475:LYS:HG3	2:G:1476:ASN:ND2	2.35	0.41
1:A:191:GLY:O	1:A:195:GLY:HA2	2.21	0.41
1:A:1140:THR:HA	1:A:1142:GLU:OE1	2.21	0.41
1:A:1148:HIS:CD2	1:A:1167:LEU:CD2	3.03	0.41
1:A:1423:LYS:O	1:A:1424:GLY:C	2.64	0.41
1:A:1425:ILE:HD13	1:A:1425:ILE:HA	1.80	0.41
1:A:1740:SER:OG	1:A:1742:ASP:OD1	2.27	0.41
2:G:408:PRO:HB3	2:G:833:GLU:CD	2.46	0.41
2:G:673:GLY:O	2:G:1164:MET:HG2	2.20	0.41
2:G:1054:LEU:HB2	5:G:2101:FMN:HM73	2.01	0.41
2:G:1331:TRP:CD1	2:G:1335:ILE:HD13	2.55	0.41
2:G:1496:LYS:HB2	2:G:1496:LYS:HE3	1.79	0.41
2:G:1576:PRO:HB2	2:G:1617:LEU:HD21	2.00	0.41
2:G:1924:ILE:HG22	2:G:1928:GLN:HE22	1.85	0.41
2:G:748:THR:OG1	2:G:749:PRO:HD3	2.21	0.41
2:G:1445:ARG:H	2:G:1445:ARG:HG2	1.69	0.41
2:G:1739:GLU:HA	2:G:1747:LYS:O	2.21	0.41
2:G:1989:LYS:HE2	2:G:2037:PRO:HG2	2.03	0.41
1:A:156:ALA:HB1	1:A:161:LYS:O	2.20	0.41
1:A:1496:GLU:O	1:A:1500:GLN:HB2	2.21	0.41
3:A:1901:NAP:O2N	3:A:1901:NAP:C3D	2.69	0.41
2:G:31:SER:O	2:G:35:GLU:HG3	2.21	0.41
2:G:964:LEU:HD13	2:G:964:LEU:HA	1.93	0.41
2:G:1955:PRO:HB2	2:G:1957:PRO:HD2	2.02	0.41
1:A:79:LEU:HA	1:A:84:ASP:OD2	2.21	0.41
1:A:427:ASN:ND2	1:A:608:ASP:OD1	2.54	0.41
1:A:1676:LYS:O	1:A:1680:ARG:HG2	2.21	0.41
2:G:119:THR:O	2:G:123:ILE:HD12	2.21	0.41
2:G:1301:THR:HG22	2:G:1306:ASN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1638:ILE:O	2:G:1654:GLU:HA	2.21	0.41
2:G:1776:PHE:C	2:G:1779:PRO:HD2	2.46	0.41
1:A:34:VAL:HG23	1:A:38:ASP:OD2	2.20	0.41
1:A:61:LEU:HD11	1:A:76:ARG:HD2	2.03	0.41
1:A:439:ILE:HD11	1:A:451:MET:CE	2.50	0.41
1:A:460:GLU:HA	1:A:466:TYR:HB3	2.01	0.41
1:A:490:TYR:HE1	1:A:673:PHE:CE2	2.39	0.41
1:A:771:PHE:HB3	3:A:1901:NAP:C5D	2.40	0.41
1:A:1238:VAL:HG23	1:A:1325:ARG:HG3	2.01	0.41
2:G:74:PRO:HG3	2:G:132:MET:HG3	2.02	0.41
2:G:126:TYR:CD2	2:G:127:ILE:HD13	2.56	0.41
2:G:292:PHE:O	2:G:296:VAL:HG23	2.21	0.41
2:G:309:ARG:CB	2:G:439:ILE:HG12	2.51	0.41
2:G:323:ILE:HA	2:G:326:ASP:CG	2.46	0.41
2:G:326:ASP:OD1	2:G:326:ASP:C	2.64	0.41
2:G:597:MET:O	2:G:601:THR:N	2.54	0.41
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.85	0.41
2:G:803:SER:HB3	2:G:1055:HIS:CE1	2.56	0.41
2:G:926:LEU:HD23	2:G:926:LEU:HA	1.80	0.41
2:G:1313:SER:OG	2:G:1314:ARG:N	2.53	0.41
2:G:1484:LYS:HA	2:G:1484:LYS:HD3	1.82	0.41
2:G:1592:LEU:O	2:G:1592:LEU:HD23	2.21	0.41
2:G:1719:ILE:HG21	2:G:1733:TYR:HE2	1.85	0.41
2:G:1721:PHE:HE2	2:G:1755:ILE:HD11	1.86	0.41
2:G:1775:GLN:C	2:G:1776:PHE:HD2	2.29	0.41
2:G:1992:LEU:O	2:G:1996:ILE:HG12	2.21	0.41
1:A:473:GLY:O	1:A:477:ILE:HG23	2.21	0.41
1:A:881:ASN:CG	1:A:944:ARG:HH22	2.29	0.41
1:A:1024:PHE:HE1	1:A:1401:TYR:CD1	2.38	0.41
1:A:1034:ARG:HH21	1:A:1052:GLU:CD	2.29	0.41
1:A:1057:MET:HG2	1:A:1190:PRO:HB2	2.02	0.41
2:G:359:HIS:HB2	2:G:360:LEU:HD12	2.01	0.41
2:G:404:GLN:O	2:G:407:ILE:HG22	2.21	0.41
2:G:1123:ASP:OD1	2:G:1188:ASN:ND2	2.54	0.41
2:G:1680:LEU:HD21	2:G:1687:ALA:HB1	2.03	0.41
2:G:1979:THR:HA	2:G:1982:MET:HG2	2.03	0.41
1:A:419:GLU:O	1:A:424:VAL:N	2.51	0.40
1:A:850:PHE:C	1:A:852:ARG:H	2.29	0.40
1:A:910:THR:HG22	1:A:912:GLU:H	1.86	0.40
1:A:1065:GLY:O	1:A:1071:PRO:HA	2.20	0.40
1:A:1154:ILE:HD12	1:A:1156:GLU:OE1	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1737:ASN:HA	1:A:1740:SER:HB3	2.02	0.40
1:A:1742:ASP:OD1	1:A:1743:SER:N	2.54	0.40
2:G:322:SER:HA	2:G:325:GLU:OE2	2.21	0.40
2:G:666:ILE:HD13	2:G:666:ILE:HA	1.84	0.40
2:G:847:ARG:HH22	2:G:873:PHE:HB2	1.86	0.40
2:G:932:ILE:HG22	2:G:935:THR:H	1.86	0.40
2:G:980:ILE:HG23	2:G:984:PHE:CD1	2.56	0.40
2:G:1241:ASN:O	2:G:1251:ILE:HA	2.21	0.40
2:G:1290:PHE:HB3	2:G:1329:VAL:HG23	2.03	0.40
2:G:1544:SER:O	2:G:1621:ALA:HA	2.21	0.40
1:A:37:LYS:HB2	1:A:65:TYR:OH	2.22	0.40
2:G:89:THR:HG23	2:G:135:ARG:HH22	1.86	0.40
2:G:597:MET:HA	5:G:2101:FMN:N5	2.36	0.40
2:G:1610:CYS:HA	2:G:1653:GLY:HA3	2.03	0.40
1:A:30:GLU:HB2	2:G:2016:ALA:HB1	2.02	0.40
1:A:59:ARG:HH12	2:G:1897:GLN:HE21	1.69	0.40
1:A:630:ILE:HG22	1:A:653:ARG:HH21	1.86	0.40
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.83	0.40
1:A:1227:GLY:O	1:A:1680:ARG:NH2	2.42	0.40
1:A:1391:ASP:OD1	1:A:1392:LEU:N	2.54	0.40
2:G:814:SER:OG	2:G:1040:LEU:HD13	2.21	0.40
2:G:1564:HIS:ND1	2:G:1579:ILE:HG13	2.36	0.40
2:G:1669:GLN:HE22	2:G:1838:MET:HE1	1.85	0.40
2:G:1679:ASP:O	2:G:1683:THR:HG23	2.21	0.40
2:G:1773:ALA:O	2:G:1777:THR:HG23	2.21	0.40
2:G:1822:MET:HE2	2:G:1996:ILE:HG22	2.04	0.40
2:G:2045:TRP:CE2	2:G:2048:TYR:HB2	2.56	0.40
1:A:56:MET:HA	1:A:59:ARG:HE	1.86	0.40
1:A:455:ILE:HD13	1:A:455:ILE:HA	1.92	0.40
1:A:688:ILE:H	1:A:688:ILE:HG13	1.59	0.40
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	2.04	0.40
1:A:1089:VAL:HG23	1:A:1093:TYR:CD2	2.52	0.40
1:A:1305:CYS:HA	1:A:1585:LYS:O	2.21	0.40
1:A:1424:GLY:O	1:A:1427:THR:HG22	2.21	0.40
2:G:10:THR:HA	2:G:19:VAL:HA	2.03	0.40
2:G:408:PRO:HG3	2:G:836:TYR:CZ	2.57	0.40
2:G:602:VAL:HG21	2:G:623:GLY:HA3	2.04	0.40
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.56	0.40
2:G:738:GLY:HA2	2:G:1055:HIS:O	2.22	0.40
2:G:1756:ASN:OD1	2:G:1759:SER:N	2.54	0.40
2:G:1982:MET:O	2:G:1985:VAL:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:56:MET:HE3	2.03	0.40
1:A:460:GLU:H	1:A:460:GLU:CD	2.30	0.40
1:A:996:LYS:H	1:A:996:LYS:HG2	1.73	0.40
1:A:1056:ILE:HG21	1:A:1056:ILE:HD13	1.84	0.40
1:A:1064:ASN:HD22	2:G:1001:ASP:HB2	1.86	0.40
1:A:1142:GLU:N	1:A:1142:GLU:CD	2.80	0.40
1:A:1303:GLY:O	1:A:1304:ALA:C	2.64	0.40
2:G:85:ASN:HB2	2:G:135:ARG:NH2	2.36	0.40
2:G:757:ILE:O	2:G:759:ARG:N	2.54	0.40
2:G:788:LYS:HE2	2:G:789:PHE:HE1	1.86	0.40
2:G:832:TRP:CE3	2:G:833:GLU:HG2	2.56	0.40
2:G:1354:SER:N	2:G:1409:SER:OG	2.55	0.40
2:G:1618:PRO:HB2	2:G:1619:ASN:HD22	1.86	0.40
2:G:1685:LYS:HA	2:G:1688:GLN:NE2	2.37	0.40
2:G:1893:VAL:HG22	2:G:1897:GLN:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1601/1887 (85%)	1433 (90%)	161 (10%)	7 (0%)	30	60
2	G	2029/2073 (98%)	1883 (93%)	146 (7%)	0	100	100
All	All	3630/3960 (92%)	3316 (91%)	307 (8%)	7 (0%)	44	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	179	LYS
1	A	195	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1609	ARG
1	A	180	SER
1	A	851	ASN
1	A	1158	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1230/1566 (78%)	1220 (99%)	10 (1%)	73	90
2	G	1772/1810 (98%)	1765 (100%)	7 (0%)	84	94
All	All	3002/3376 (89%)	2985 (99%)	17 (1%)	76	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	A	439	ILE
1	A	680	ILE
1	A	933	VAL
1	A	1035	THR
1	A	1039	MET
1	A	1154	ILE
1	A	1298	ILE
1	A	1307	THR
1	A	1384	ILE
2	G	325	GLU
2	G	501	ILE
2	G	637	VAL
2	G	881	VAL
2	G	993	GLN
2	G	1378	ILE
2	G	1680	LEU

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	11	HIS
1	A	21	GLN
1	A	411	GLN
1	A	465	ASN
1	A	669	ASN
1	A	830	HIS
1	A	854	HIS
1	A	969	ASN
1	A	989	GLN
1	A	1115	ASN
1	A	1146	HIS
1	A	1188	GLN
1	A	1207	GLN
1	A	1239	HIS
1	A	1272	ASN
1	A	1380	GLN
1	A	1507	GLN
1	A	1598	GLN
1	A	1601	ASN
1	A	1689	HIS
1	A	1734	ASN
2	G	34	GLN
2	G	99	ASN
2	G	142	ASN
2	G	178	GLN
2	G	273	HIS
2	G	275	GLN
2	G	350	GLN
2	G	354	ASN
2	G	428	HIS
2	G	440	ASN
2	G	612	ASN
2	G	650	ASN
2	G	715	GLN
2	G	723	HIS
2	G	740	HIS
2	G	741	HIS
2	G	747	HIS
2	G	985	ASN
2	G	993	GLN
2	G	1046	GLN
2	G	1148	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	1260	GLN
2	G	1302	HIS
2	G	1352	HIS
2	G	1355	ASN
2	G	1383	ASN
2	G	1424	GLN
2	G	1476	ASN
2	G	1514	ASN
2	G	1535	ASN
2	G	1564	HIS
2	G	1611	GLN
2	G	1619	ASN
2	G	1669	GLN
2	G	1674	GLN
2	G	1696	ASN
2	G	1716	ASN
2	G	1807	HIS
2	G	1839	GLN
2	G	1868	GLN
2	G	1890	ASN
2	G	1897	GLN
2	G	1920	GLN
2	G	1928	GLN
2	G	1939	HIS
2	G	2027	GLN
2	G	2050	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands 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
3	NAP	G	2102	-	50,52,52	1.17	5 (10%)	71,80,80	1.55	9 (12%)
5	FMN	G	2101	-	33,33,33	1.23	5 (15%)	48,50,50	1.28	8 (16%)
4	PNS	A	1902	1	1,4,21	0.65	0	0,4,29	-	-
3	NAP	A	1901	-	50,52,52	2.66	27 (54%)	71,80,80	2.43	24 (33%)

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
3	NAP	G	2102	-	-	6/35/67/67	0/5/5/5
5	FMN	G	2101	-	-	3/18/18/18	0/3/3/3
4	PNS	A	1902	1	-	0/0/2/27	-
3	NAP	A	1901	-	-	6/35/67/67	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	C3N-C7N	-5.46	1.42	1.50
3	A	1901	NAP	C5A-N7A	-5.29	1.29	1.39
3	A	1901	NAP	PN-O3	-4.93	1.54	1.59
3	A	1901	NAP	O4D-C4D	-4.91	1.34	1.45
3	G	2102	NAP	C5A-C4A	4.76	1.47	1.39
3	A	1901	NAP	C8A-N9A	-4.57	1.29	1.37
3	A	1901	NAP	C4A-N9A	-4.41	1.28	1.37
3	A	1901	NAP	C2N-N1N	-4.21	1.30	1.35
3	A	1901	NAP	C4N-C3N	-4.07	1.33	1.39
3	A	1901	NAP	O7N-C7N	-4.02	1.16	1.24
3	A	1901	NAP	C2N-C3N	-3.72	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	P2B-O2B	-3.15	1.54	1.59
5	G	2101	FMN	C4A-N5	2.99	1.37	1.30
3	A	1901	NAP	PN-O2N	-2.80	1.42	1.55
3	A	1901	NAP	C2A-N1A	-2.78	1.29	1.33
3	G	2102	NAP	C5A-C6A	2.76	1.48	1.41
3	A	1901	NAP	P2B-O3X	-2.72	1.44	1.54
3	A	1901	NAP	C6A-N1A	-2.71	1.28	1.35
3	A	1901	NAP	P2B-O2X	-2.71	1.44	1.54
3	A	1901	NAP	C3D-C4D	-2.53	1.46	1.53
3	A	1901	NAP	C7N-N7N	-2.53	1.28	1.33
3	A	1901	NAP	O4B-C4B	-2.48	1.39	1.45
3	A	1901	NAP	C3B-C4B	-2.43	1.46	1.53
3	G	2102	NAP	C8A-N7A	2.39	1.36	1.31
3	A	1901	NAP	C4A-N3A	-2.37	1.30	1.34
3	A	1901	NAP	C6A-N6A	-2.36	1.28	1.34
3	A	1901	NAP	PN-O5D	-2.35	1.50	1.59
5	G	2101	FMN	C9A-N10	-2.29	1.37	1.41
3	A	1901	NAP	PN-O1N	-2.28	1.42	1.50
3	G	2102	NAP	C5A-N7A	-2.25	1.35	1.39
5	G	2101	FMN	C10-N1	2.17	1.37	1.33
5	G	2101	FMN	C4A-C10	-2.13	1.37	1.44
3	A	1901	NAP	C6N-N1N	-2.11	1.30	1.35
5	G	2101	FMN	C9A-C5A	-2.10	1.37	1.41
3	A	1901	NAP	C2A-N3A	-2.07	1.30	1.33
3	A	1901	NAP	O5D-C5D	-2.06	1.36	1.44
3	G	2102	NAP	O4D-C1D	2.00	1.43	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	C4D-O4D-C1D	-9.30	101.40	109.92
3	G	2102	NAP	C5A-C4A-N3A	-5.86	118.65	126.72
3	A	1901	NAP	C5A-C4A-N3A	-5.78	118.76	126.72
3	A	1901	NAP	O3D-C3D-C4D	-5.30	95.86	111.08
3	A	1901	NAP	C6N-N1N-C2N	-5.22	117.44	121.88
3	A	1901	NAP	P2B-O2B-C2B	-4.64	111.04	123.43
3	G	2102	NAP	N3A-C4A-N9A	4.63	135.04	127.17
3	A	1901	NAP	N3A-C4A-N9A	4.50	134.82	127.17
3	A	1901	NAP	O4B-C4B-C3B	-4.40	96.42	105.15
3	A	1901	NAP	O4B-C1B-C2B	-4.09	99.54	106.59
3	G	2102	NAP	C2A-N3A-C4A	3.70	120.87	111.83
3	A	1901	NAP	C2A-N3A-C4A	3.68	120.82	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2101	FMN	C4-N3-C2	-3.50	119.42	125.64
3	G	2102	NAP	C4A-C5A-N7A	-3.47	106.62	110.58
3	A	1901	NAP	C4A-N9A-C8A	3.46	109.37	105.74
3	A	1901	NAP	O2A-PA-O3	3.34	116.30	107.27
3	A	1901	NAP	N3A-C2A-N1A	-3.32	123.55	128.58
3	G	2102	NAP	N3A-C2A-N1A	-3.22	123.71	128.58
3	A	1901	NAP	N9A-C8A-N7A	-3.01	109.67	113.94
3	A	1901	NAP	O4B-C1B-N9A	-2.95	102.43	108.09
3	A	1901	NAP	C5B-C4B-C3B	-2.81	105.08	115.21
5	G	2101	FMN	C4A-C4-N3	2.79	120.34	113.25
3	A	1901	NAP	O3X-P2B-O2B	-2.71	95.30	105.85
3	G	2102	NAP	C4A-N9A-C8A	2.62	108.48	105.74
3	A	1901	NAP	C5N-C4N-C3N	-2.61	117.80	120.36
5	G	2101	FMN	O4-C4-C4A	-2.59	119.69	126.53
3	A	1901	NAP	C4A-C5A-N7A	-2.54	107.68	110.58
3	G	2102	NAP	C2B-C1B-N9A	-2.52	109.60	113.75
3	G	2102	NAP	C5A-N7A-C8A	2.52	107.42	103.45
5	G	2101	FMN	C5A-C9A-N10	2.47	120.20	117.97
3	A	1901	NAP	O3X-P2B-O2X	2.44	116.93	107.80
3	A	1901	NAP	O5B-PA-O1A	-2.36	99.57	108.94
5	G	2101	FMN	C9A-C5A-N5	-2.30	120.01	122.45
5	G	2101	FMN	C4'-C3'-C2'	-2.28	109.78	113.57
5	G	2101	FMN	C4A-C10-N10	2.25	119.70	116.48
3	A	1901	NAP	O5B-C5B-C4B	2.22	116.54	108.99
3	A	1901	NAP	O3-PA-O1A	-2.20	104.08	110.70
3	A	1901	NAP	C5A-N7A-C8A	2.17	106.86	103.45
5	G	2101	FMN	C10-C4A-N5	-2.13	120.46	124.81
3	A	1901	NAP	C6A-C5A-N7A	2.08	136.10	132.09
3	G	2102	NAP	C6A-C5A-N7A	2.06	136.06	132.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C5D-O5D-PN-O3
3	A	1901	NAP	C5D-O5D-PN-O2N
3	A	1901	NAP	C4D-C5D-O5D-PN
3	G	2102	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	C3B-C4B-C5B-O5B
3	A	1901	NAP	O4B-C4B-C5B-O5B
5	G	2101	FMN	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

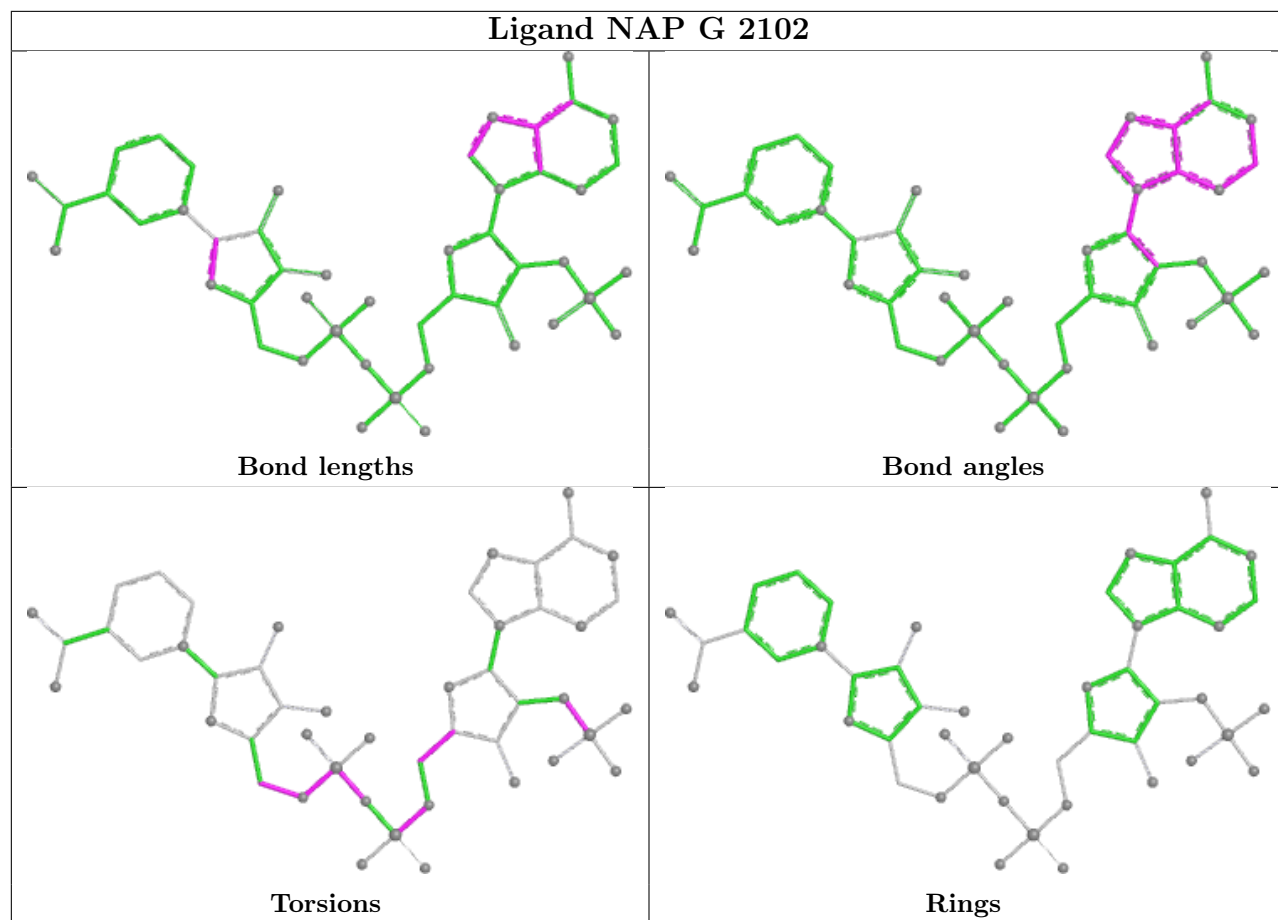
Mol	Chain	Res	Type	Atoms
3	G	2102	NAP	C3B-C4B-C5B-O5B
3	G	2102	NAP	C5B-O5B-PA-O3
3	G	2102	NAP	C4D-C5D-O5D-PN
5	G	2101	FMN	C4'-C5'-O5'-P
5	G	2101	FMN	C5'-O5'-P-O2P
3	G	2102	NAP	PA-O3-PN-O2N
3	G	2102	NAP	C2B-O2B-P2B-O1X

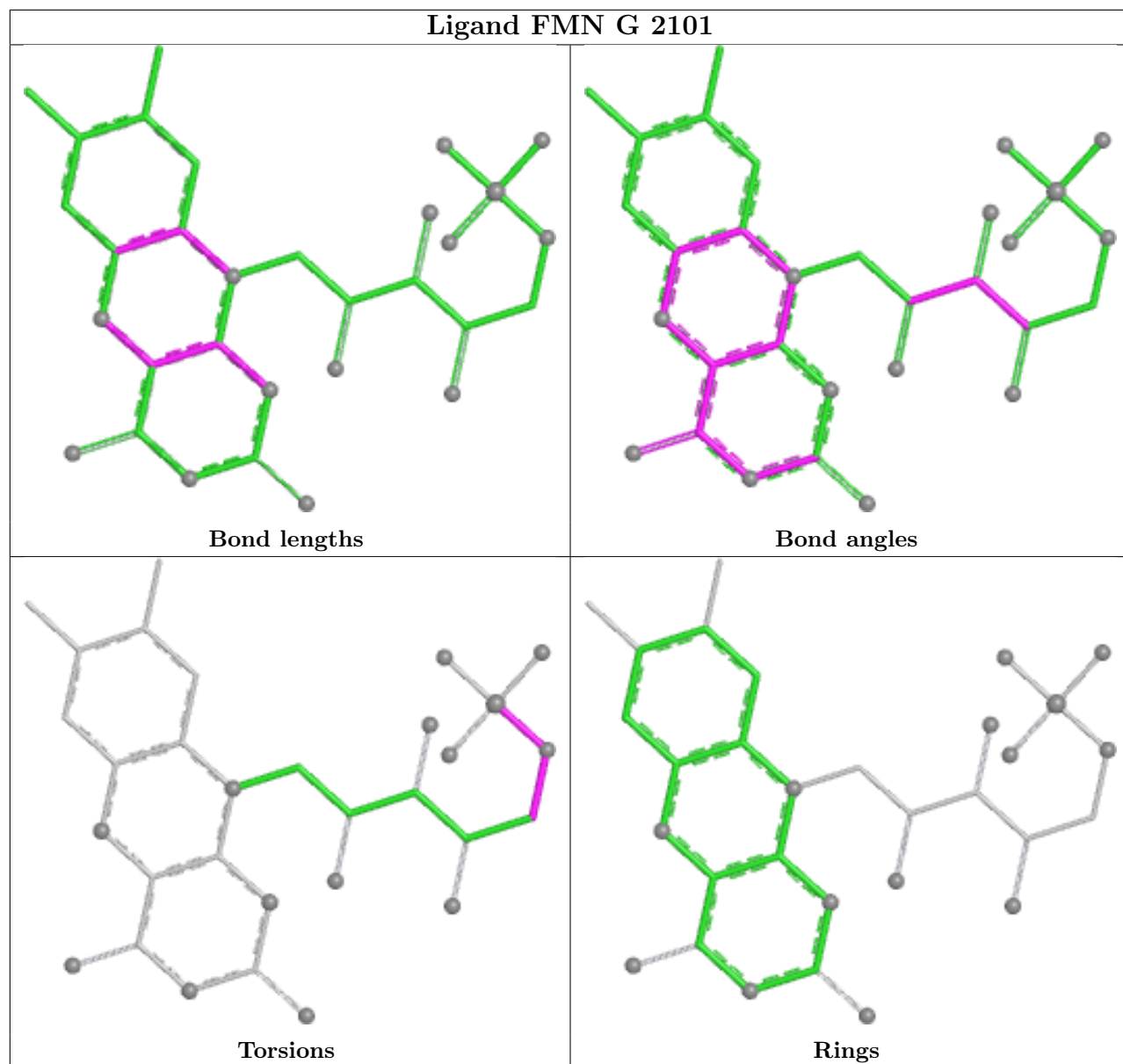
There are no ring outliers.

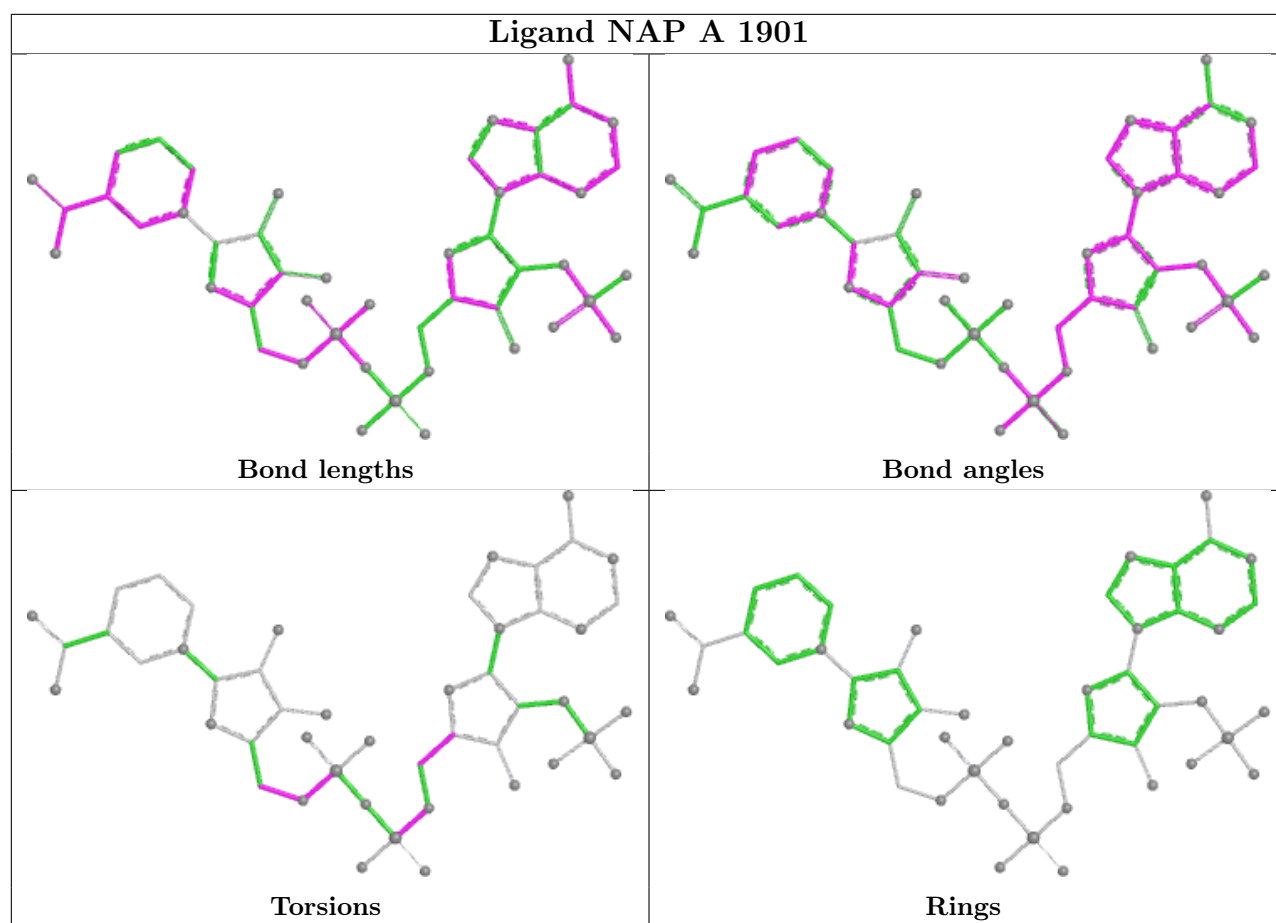
3 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2102	NAP	27	0
5	G	2101	FMN	4	0
3	A	1901	NAP	19	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

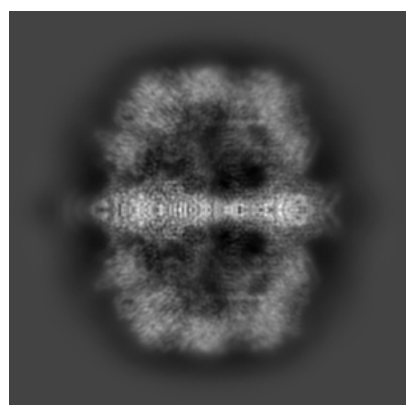
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20656. These allow visual inspection of the internal detail of the map and identification of artifacts.

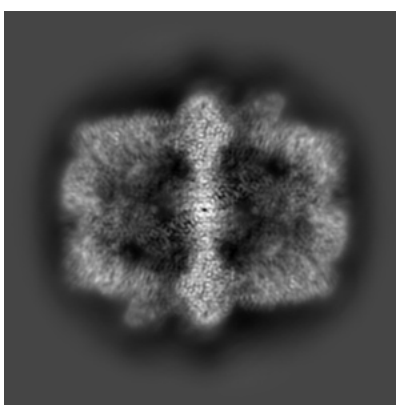
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

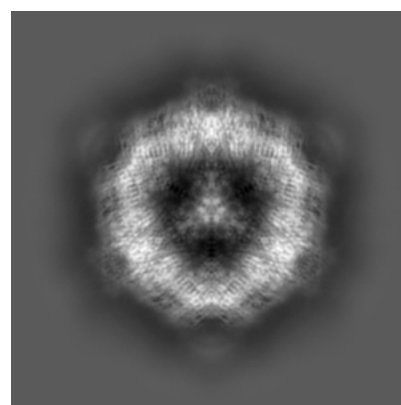
6.1.1 Primary map



X



Y

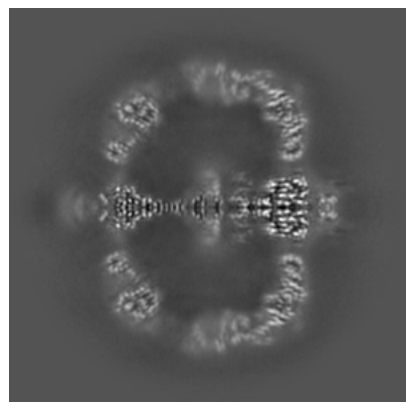


Z

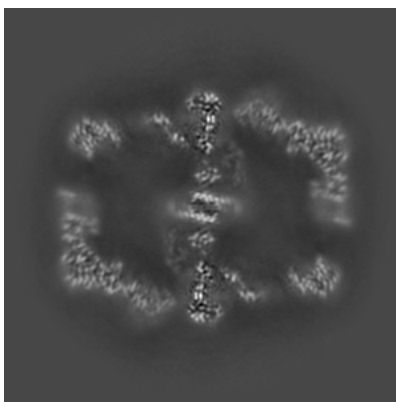
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

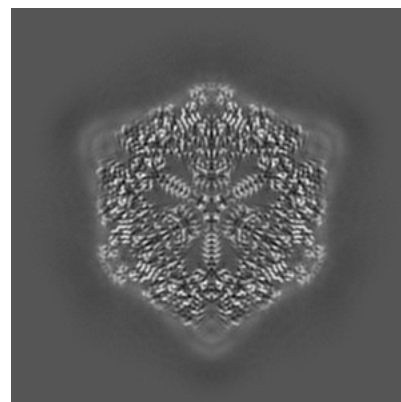
6.2.1 Primary map



X Index: 176



Y Index: 176

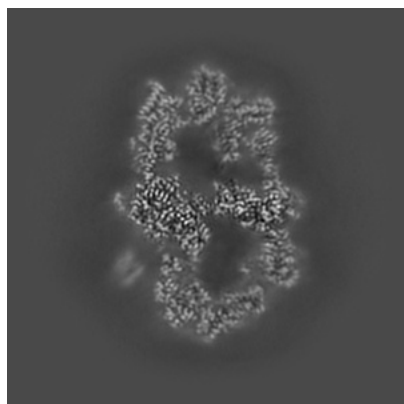


Z Index: 176

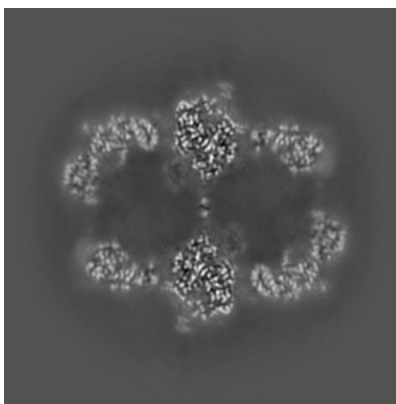
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

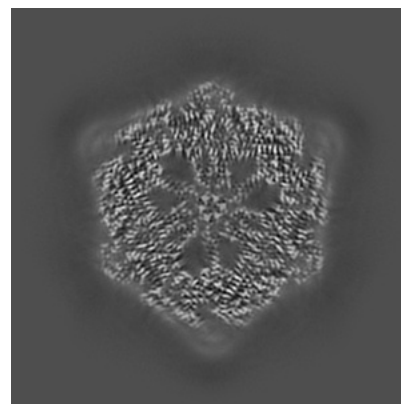
6.3.1 Primary map



X Index: 237



Y Index: 140

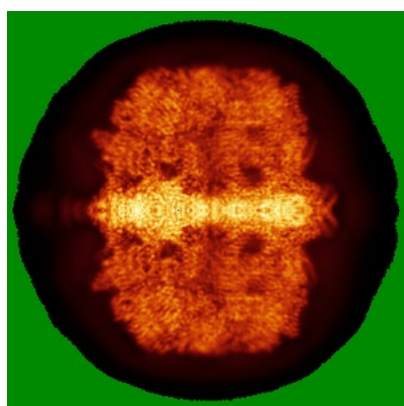


Z Index: 172

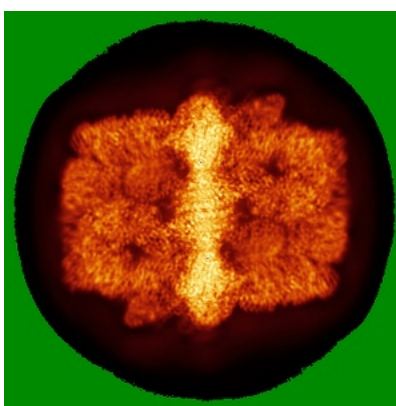
The images above show the largest variance slices of the map in three orthogonal directions.

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

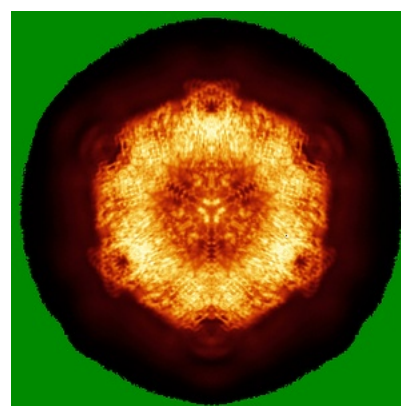
6.4.1 Primary map



X



Y

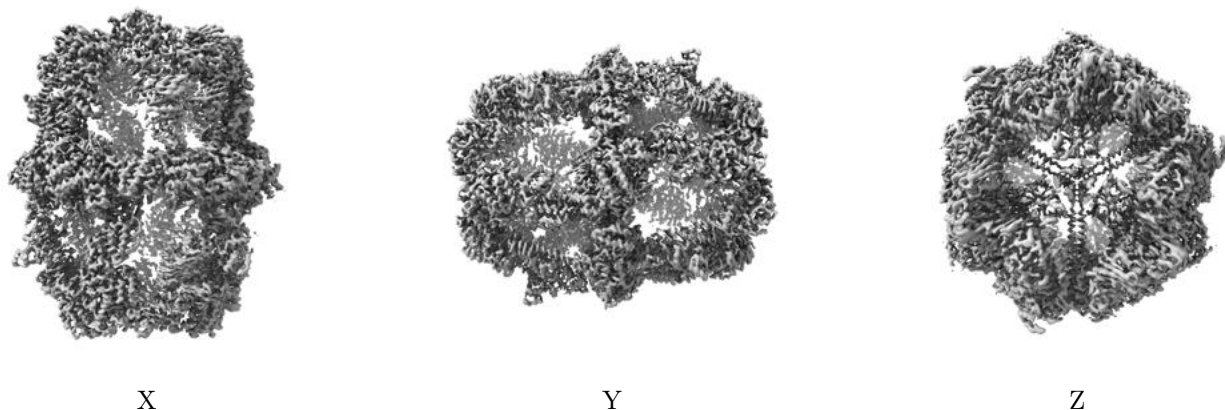


Z

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

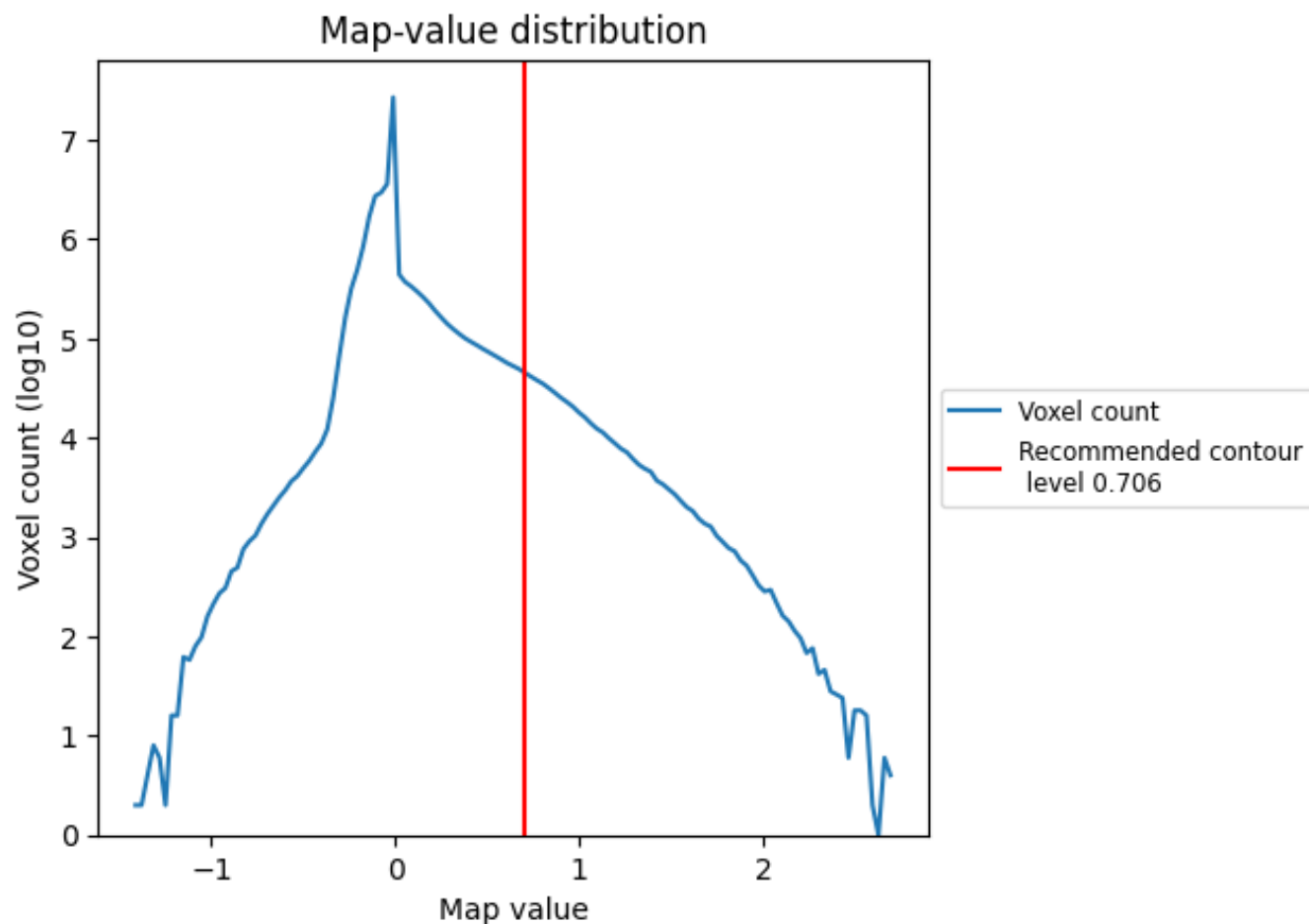
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

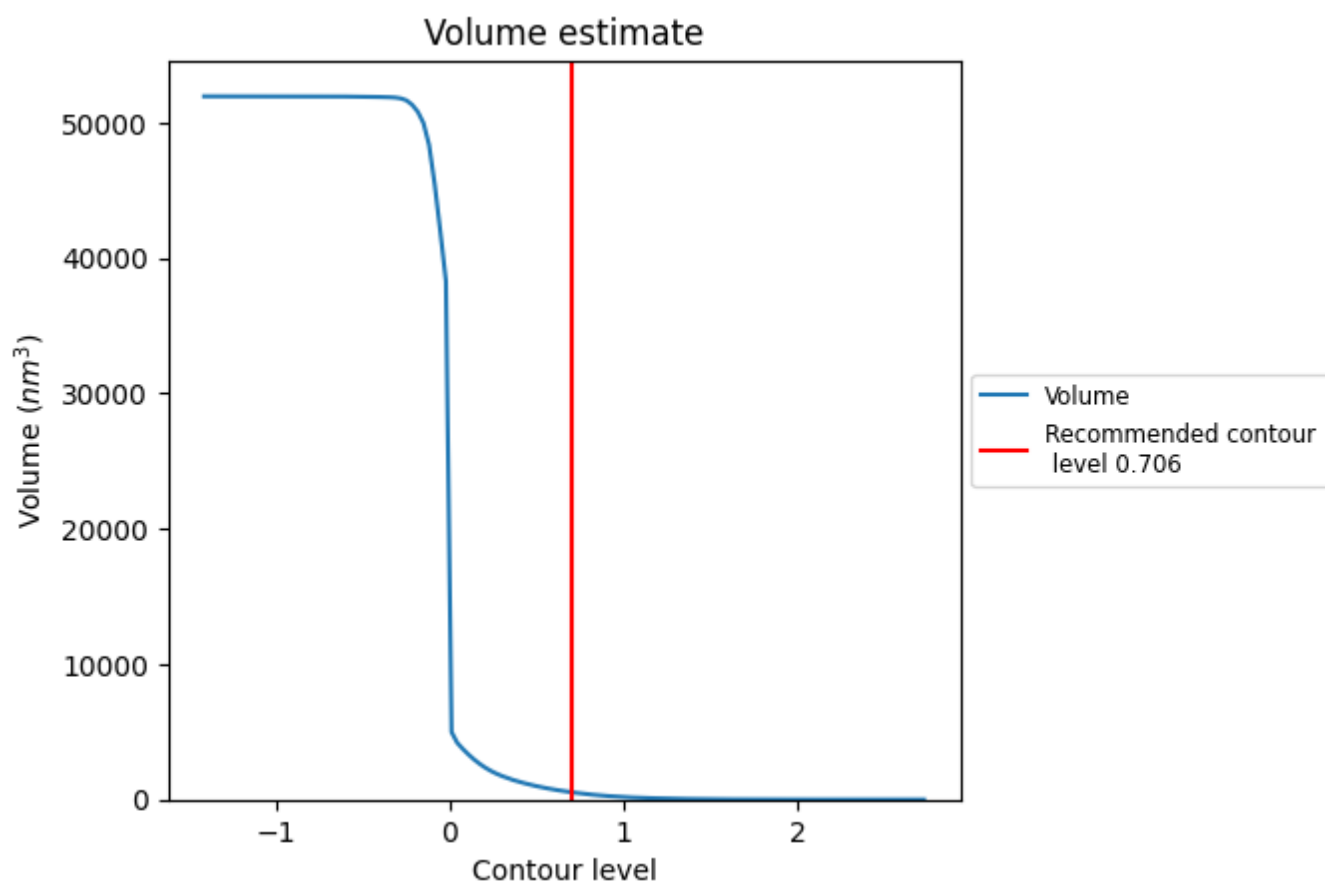
This section contains the results of statistical analysis of the map.

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.

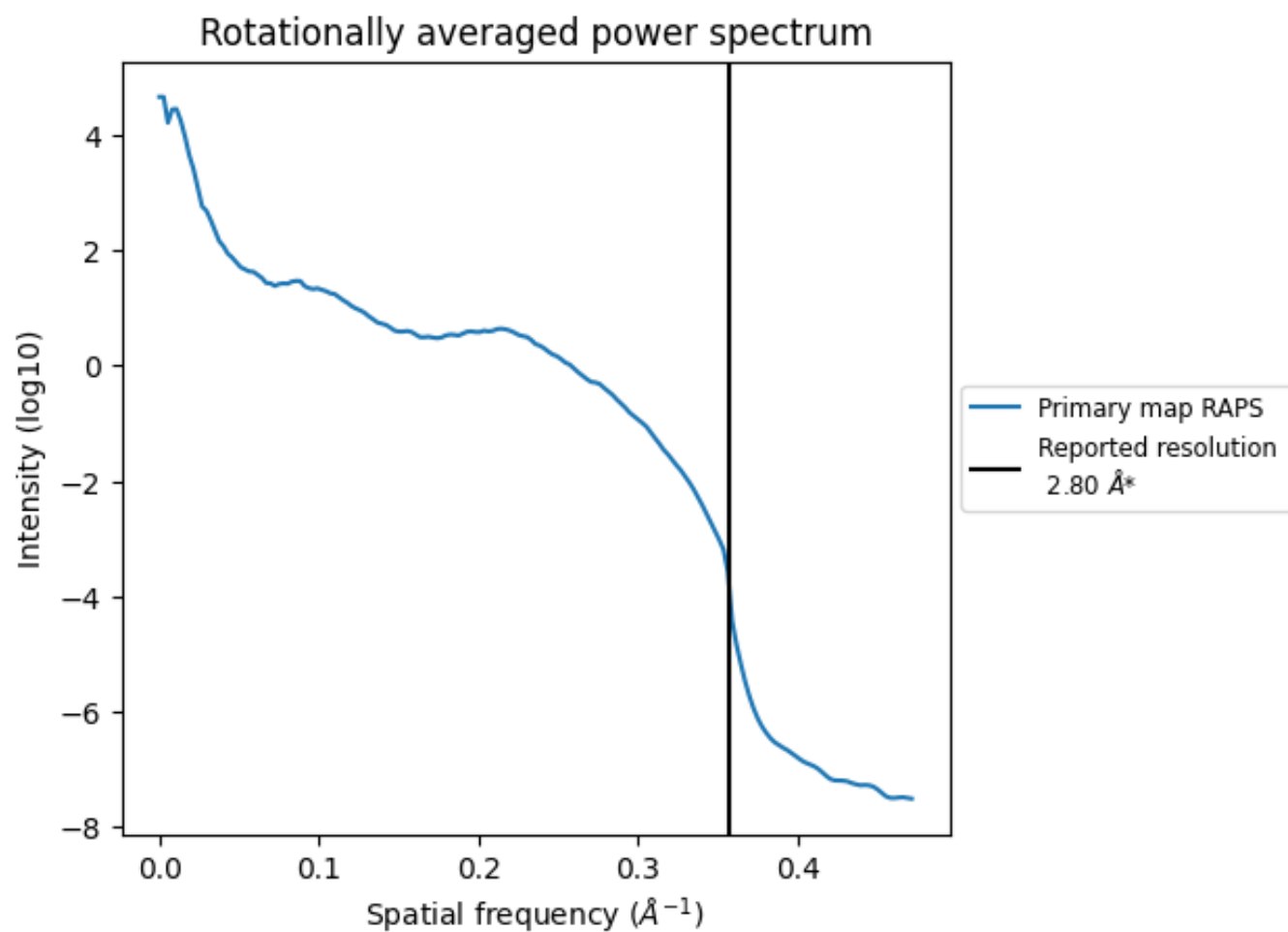
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 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 0.357 Å⁻¹

8 Fourier-Shell correlation ⓘ

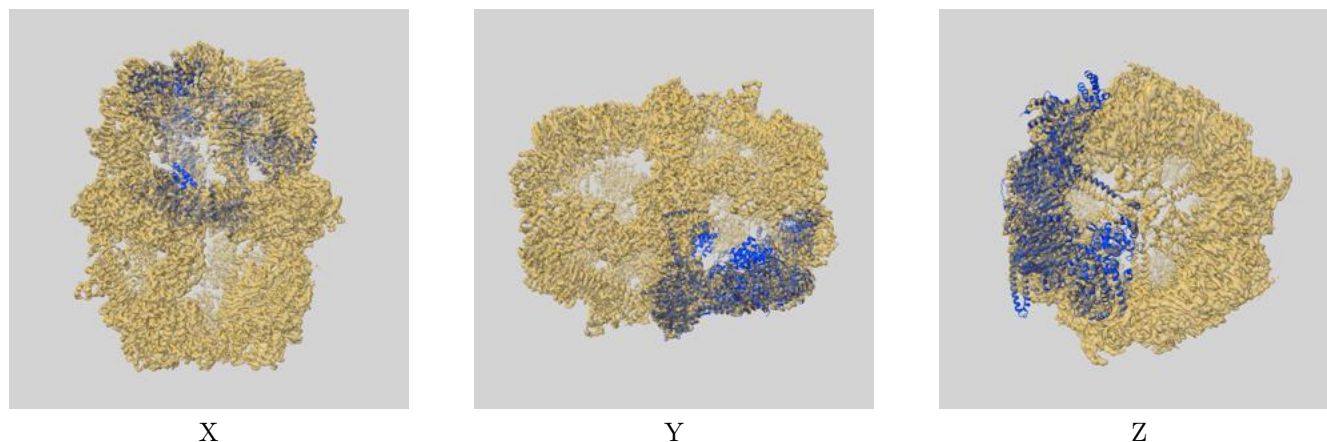
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20656 and PDB model 6U5U. Per-residue inclusion information can be found in section 3 on page 7.

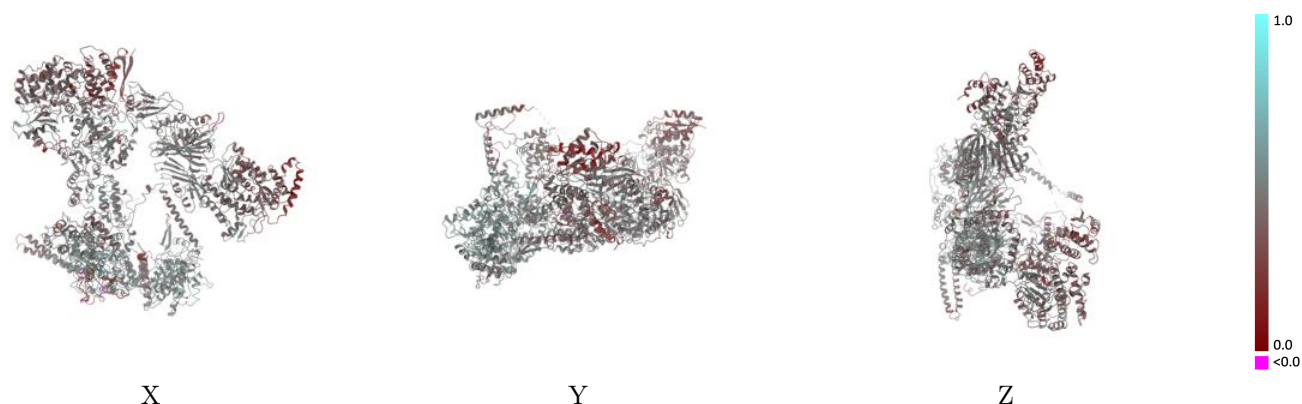
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



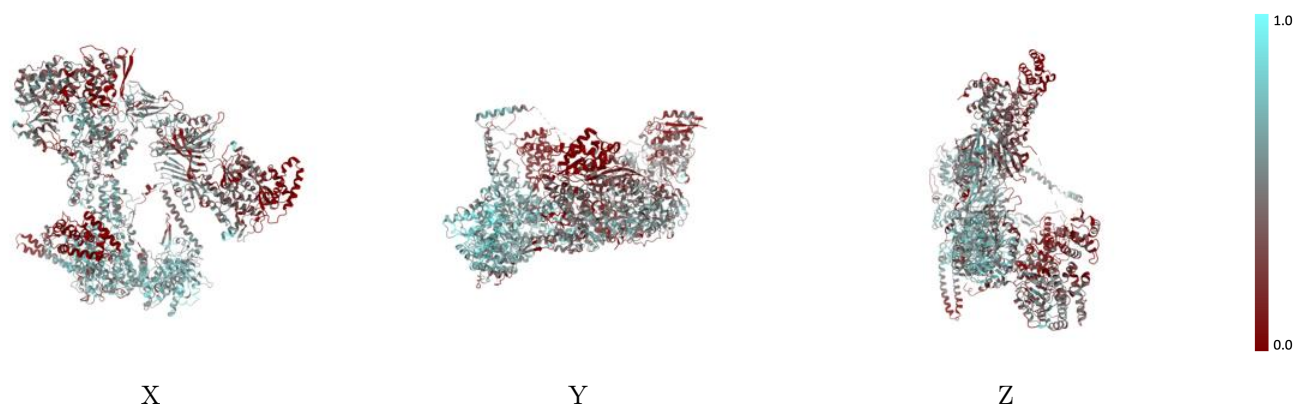
The images above show the 3D surface view of the map at the recommended contour level 0.706 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



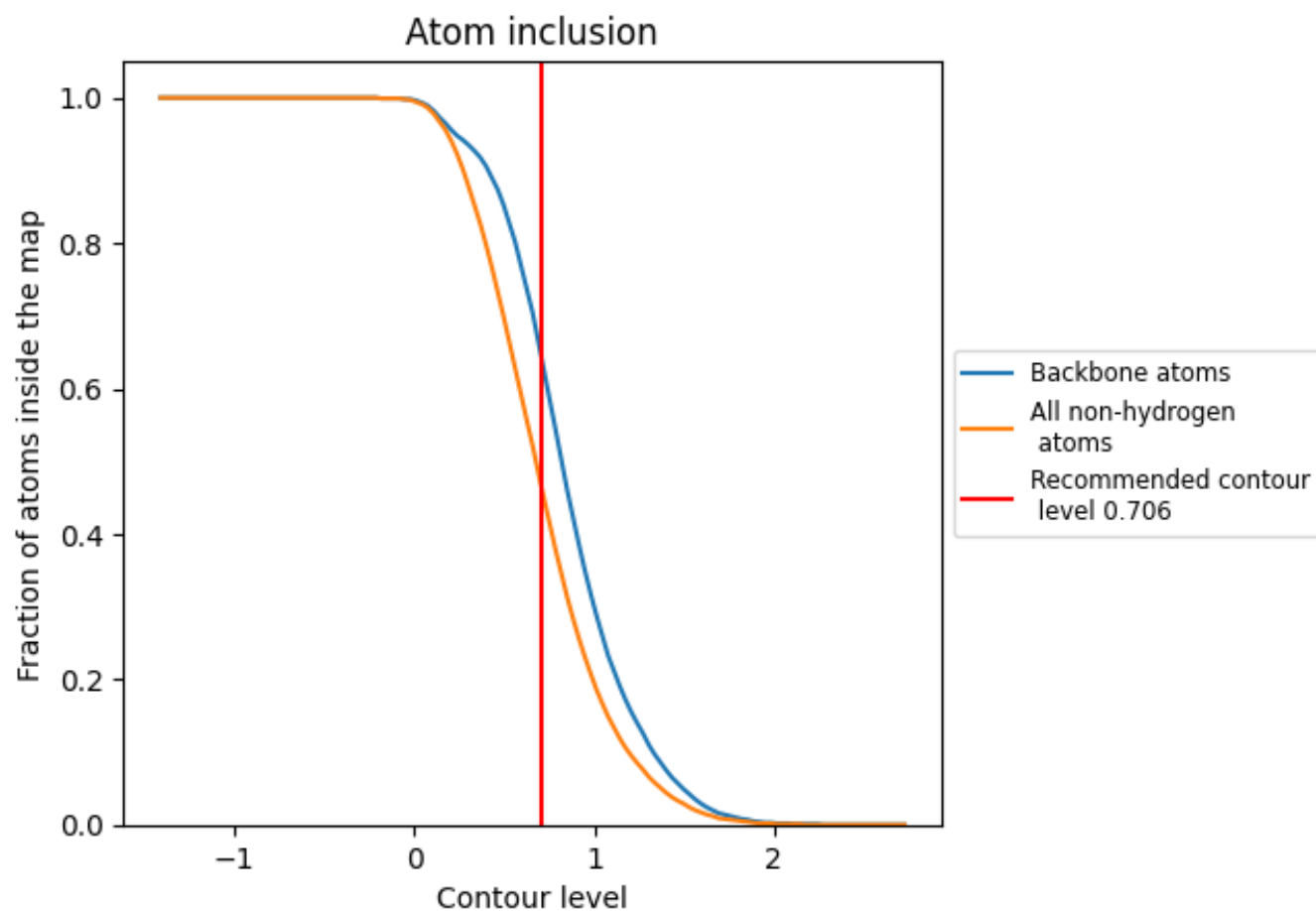
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.706).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 46% 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 (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4650	0.4490
A	0.5460	0.4800
G	0.4030	0.4260

