



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 07:03 PM UTC

PDB ID : 6U5V / pdb_00006u5v
EMDB ID : EMD-20657
Title : Electron cryomicroscopy Structure of C. albicans FAS in the Apo 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 EMD 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

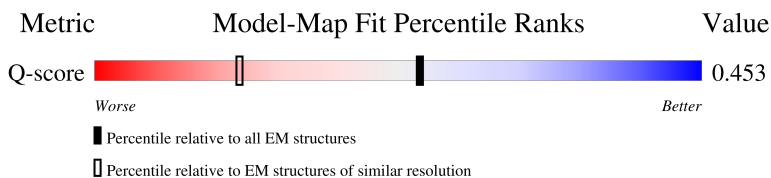
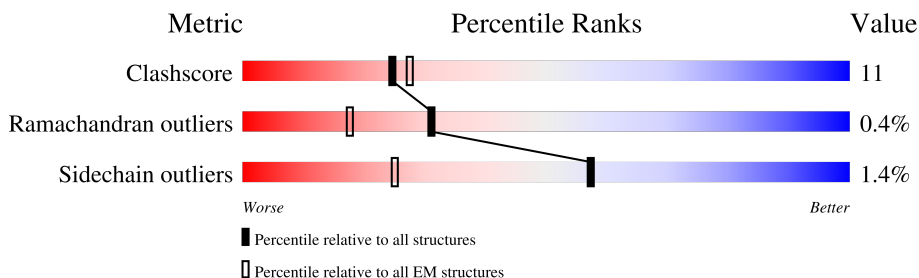
1 Overall quality at a glance

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	1885	
2	B	2037	

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
4	FMN	B	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28187 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	1596	Total	C	N	O	S	0	0
			12096	7645	2057	2349	45		

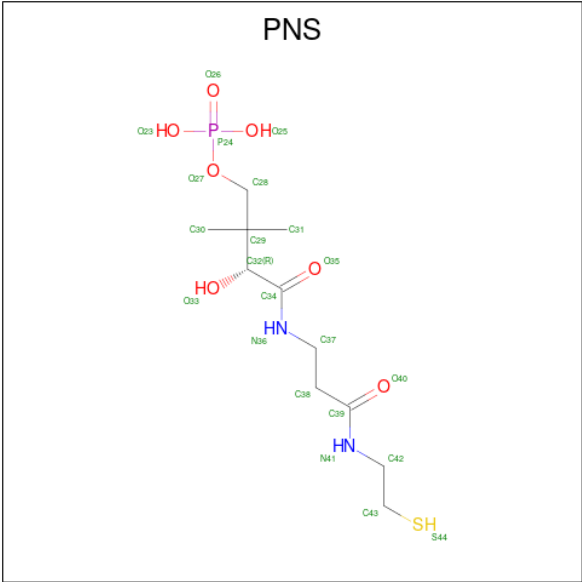
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	357	ALA	LEU	conflict	UNP P43098
A	814	THR	PRO	conflict	UNP P43098
A	1067	LYS	GLN	conflict	UNP P43098
A	1124	VAL	ILE	conflict	UNP P43098
A	1445	GLU	LYS	conflict	UNP P43098
A	1743	SER	ASN	conflict	UNP P43098

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

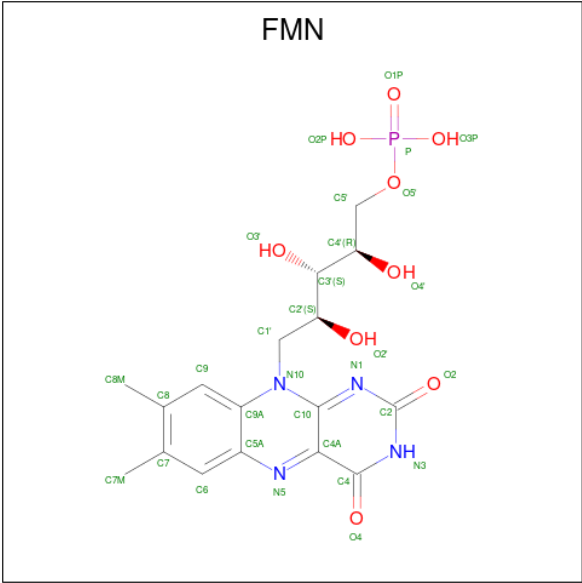
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2033	Total	C	N	O	S	1	0
			16054	10290	2665	3045	54		

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			6	2	3	1	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

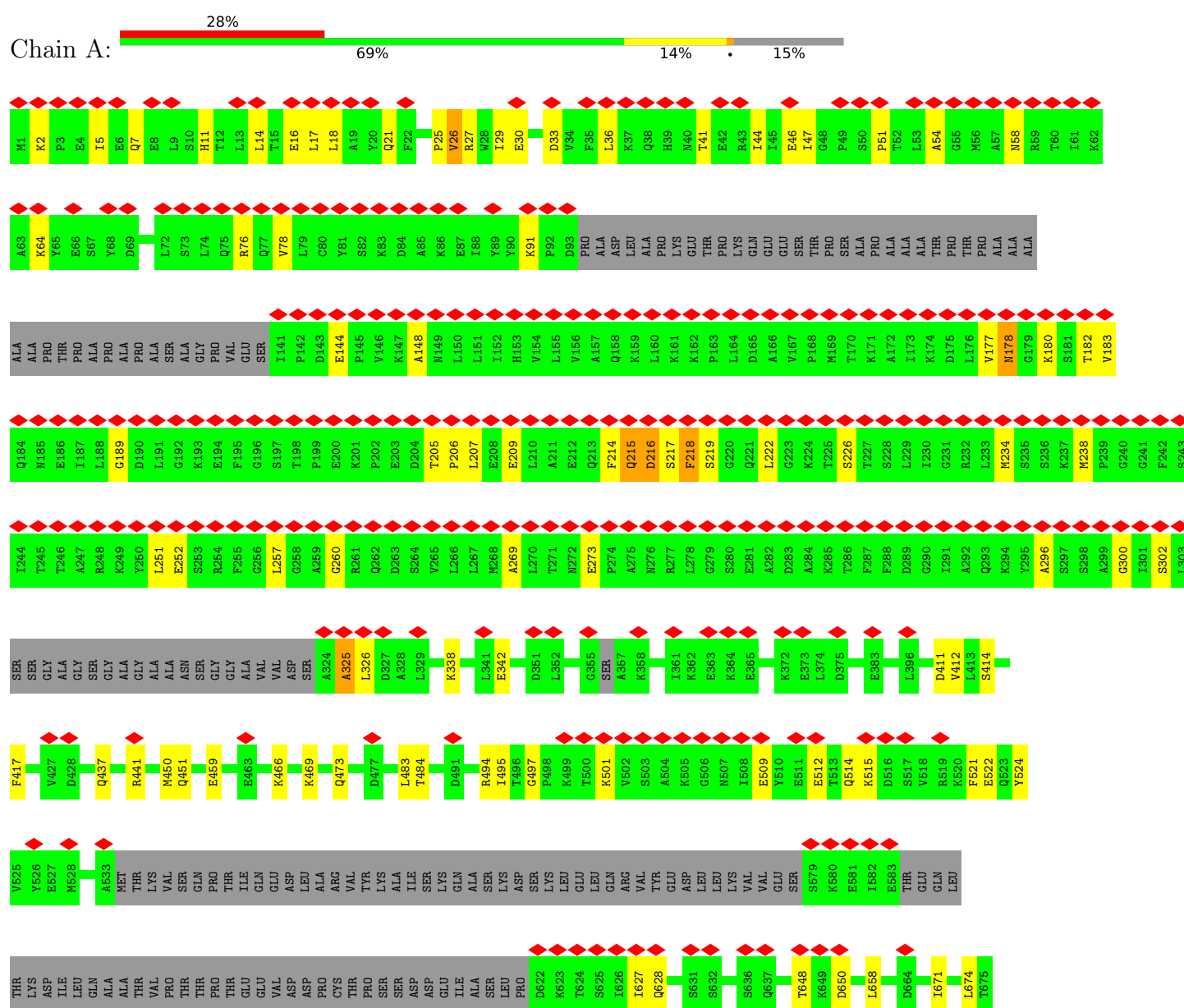


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

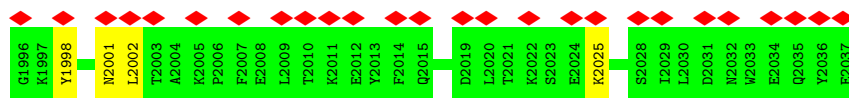
• Molecule 1: Fatty acid synthase subunit alpha







K1871	V1872	L1873	L1874	E1875	L1876	V1877	N1878	Y1879	N1880	V1881	E1882	N1883	Q1884	Q1885	V1886	V1887	A1888	A1889	D1890	D1891	L1892	R1893	A1894	L1895	D1896	T1897	L1898	T1899	N1900	V1901	L1902	N1903	V1904	L1905	K1906	I1907	N1908	K1909	I1910	D1911	I1912	V1913	K1914	L1915	Q1916	E1917	Q1918	M1919	S1920	I1921	E1922	K1923	V1924	K1925	E1926	H1927	Y1928	E1930
P1811	I1812	E1813	S1814	L1815	V1816	D1817	V1818	Y1819	R1822	G1823	M1824	T1825	M1826	Q1827	V1828	A1829	V1830	P1831	R1832	D1833	E1834	L1835	L1836	T1837	S1838	N1839	Y1840	G1841	M1842	V1843	A1844	V1845	P1847	S1848	R1849	V1850	S1851	A1852	T1853	F1854	D1855	D1856	S1857	A1858	L1859	R1860	F1861	V1862	V1863	D1864	E1865	V1866	K1868	K1869	T1870			
D1742	I1743	D1744	E1745	T1746	T1747	F1752	V1753	S1754	P1755	T1756	G1757	L1758	L1759	S1760	A1761	T1762	Q1763	F1764	T1765	Q1766	P1767	A1768	L1769	T1770	L1771	M1772	E1773	K1774	E1778	D1779	K1783	G1784	L1785	I1786	P1787	S1788	D1789	I1790	F1791	F1792	G1793	H1795	S1796	L1797	G1798	E1799	Y1800	S1801	A1802	L1803	S1804	S1805	L1806	A1807	N1808			
G1664	M1665	E1666	L1667	Y1668	N1669	S1670	S1671	E1672	V1673	A1674	T1675	E1676	D1682	R1683	V1686	N1687	N1688	Y1689	I1693	L1694	D1695	I1696	V1697	Q1698	M1699	N1700	P1701	N1702	E1703	R1714	R1717	D1718	N1719	Y1720	I1721	G1722	M1723	E1726	T1727	I1728	G1729	E1730	D1731	G1732	A1733	L1734	K1735	S1736	E1737	K1738	I1739	F1740	K1741					
F1598	V1599	G1600	M1601	V1602	L1603	P1604	M1605	D1606	T1607	L1608	Q1609	T1610	T1611	M1612	E1613	H1614	V1615	G1616	N1619	K1622	K1625	Y1626	E1627	T1628	R1629	M1630	V1631	E1632	T1633	E1634	L1635	L1638	I1639	G1640	E1643	T1644	E1645	T1648	T1649	T1650	Y1651	V1652	F1653	T1654	G1655	Q1656	S1658	Q1659	E1660	Q1661	G1662	M1663						
Q1443	F1444	D1445	V1446	F1449	R1450	G1451	E1452	K1458	S1459	A1460	N1461	V1462	Y1463	S1464	S1465	T1466	T1469	L1473	L1474	E1475	L1476	P1477	T1478	K1479	E1480	V1481	I1482	Q1483	V1484	G1485	S1486	V1487	D1488	Y1489	E1490	A1491	G1492	N1497	P1498	D1501	Y1502	L1503	S1504	R1505	N1506	G1507	T1509	I1510	E1511	E1512	S1513	V1514						
I1515	F1516	E1517	N1518	A1519	I1520	P1521	L1522	S1523	S1524	G1525	E1526	E1527	L1528	T1529	S1530	K1531	G1534	E1537	D1545	Y1546	N1547	P1548	I1549	H1550	V1551	S1552	R1553	V1554	K1560	T1564	I1565	D1568	M1569	Y1570	T1575	R1576	E1580	E1581	V1582	A1583	A1584	N1585	M1586	V1587	A1588	A1589	R1590	A1593	F1594	D1597								
A1362	E1363	I1364	L1368	M1369	Q1370	P1371	S1372	G1373	K1374	L1375	G1380	E1385	G1386	K1387	Q1395	F1396	R1399	G1400	E1401	Y1402	M1403	D1404	N1407	K1411	E1414	T1415	P1416	V1417	Q1418	V1419	A1420	F1421	K1422	S1423	A1424	K1425	D1426	L1427	A1428	V1429	L1430	R1431	E1434	H1437	L1438	E1439	K1440	D1441	V1442									
A1289	I1290	G1291	N1292	K1293	C1294	D1295	A1296	F1297	V1298	D1299	R1300	P1301	G1302	K1303	A1304	T1305	L1306	A1307	P1308	M1309	D1310	F1311	T1315	A1323	I1324	F1325	P1326	K1327	D1330	G1331	D1332	L1333	L1334	K1335	L1336	V1337	H1338	N1341	G1342	Y1343	T1347	G1348	A1349	A1350	P1351	L1352	K1353	K1354	G1355	D1356	V1357	S1358	S1359					
T1202	E1209	H1210	T1211	T1212	A1213	D1214	T1215	N1216	P1221	F1222	L1223	Y1224	K1225	D1230	E1237	I1238	M1239	E1240	E1244	R1245	I1246	K1247	G1256	S1257	S1258	V1259	P1260	Y1261	S1262	N1263	L1264	I1265	N1266	V1267	E1268	K1269	A1270	I1271	L1272	G1273	D1274	E1275	L1276	T1277	I1278	S1279	S1280	Q1281	T1282	I1283	S1284	H1288						
D1128	L1129	A1130	A1131	T1133	E1134	L1135	N1136	Q1139	T1144	D1145	R1146	K1152	N1156	P1157	L1158	H1159	I1161	L1162	T1163	P1164	A1165	K1166	H1167	K1168	K1169	K1174	K1175	T1176	K1177	L1179	T1180	A1181	F1182	E1183	N1184	T1185	G1186	G1187	D1188	L1189	L1190	P1191	V1192	V1193	E1194	L1197	V1198	K1199	P1200	M1201								
G1044	P1045	V1046	A1047	S1048	S1052	K1053	V1054	D1055	E1056	D1060	G1068	K1075	E1076	E1077	Y1078	A1079	G1080	D1081	E1082	S1083	K1084	E1089	K1094	K1095	P1096	A1097	S1098	S1099	S1100	A1101	T1102	S1103	V1104	M1105	T1106	T1107	D1108	G1109	M1110	Q1111	E1115	T1116	D1117	S1118	E1119	L1120	P1121	M1122	K1123	Q1124	L1127							



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	92958	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	2.505	Depositor
Minimum map value	-1.098	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.744	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/12322	0.71	2/16684 (0.0%)
2	B	0.43	13/16423 (0.1%)	0.70	16/22279 (0.1%)
All	All	0.44	13/28745 (0.0%)	0.70	18/38963 (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	1
2	B	0	3
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1792	PHE	C-O	-8.03	1.14	1.23
2	B	1529	THR	CA-C	-7.50	1.43	1.52
2	B	1792	PHE	CA-C	-7.01	1.44	1.52
2	B	1529	THR	C-O	-6.65	1.15	1.23
2	B	1527	GLU	N-CA	-6.65	1.38	1.46
2	B	1528	LEU	C-O	-6.62	1.15	1.24
2	B	1035	ASP	CA-C	-6.12	1.45	1.52
2	B	1325	PHE	C-N	5.91	1.41	1.33
2	B	1528	LEU	CA-C	-5.84	1.44	1.52
2	B	1791	MET	C-O	-5.72	1.17	1.24
2	B	1791	MET	CA-C	-5.65	1.46	1.52
2	B	1017	PHE	CA-C	-5.51	1.48	1.53
2	B	1015	PHE	C-O	-5.19	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1529	THR	N-CA-C	11.44	125.91	110.35
2	B	1529	THR	CB-CA-C	-8.38	94.61	109.62
2	B	1528	LEU	N-CA-C	7.61	122.14	113.01
2	B	727[A]	HIS	CB-CA-C	7.20	120.52	110.16
2	B	727[B]	HIS	CB-CA-C	7.20	120.52	110.16
2	B	1038	ARG	CA-C-N	-6.81	111.38	122.82
2	B	1038	ARG	C-N-CA	-6.81	111.38	122.82
1	A	325	ALA	N-CA-C	-6.56	105.19	113.72
2	B	129	ILE	N-CA-C	-6.15	106.43	111.91
2	B	1526	GLU	O-C-N	6.11	129.63	122.24
2	B	1017	PHE	N-CA-C	5.88	121.97	110.56
2	B	1943	PRO	CA-C-N	5.55	127.90	120.58
2	B	1943	PRO	C-N-CA	5.55	127.90	120.58
2	B	1791	MET	CB-CG-SD	5.30	128.60	112.70
2	B	1016	PHE	N-CA-C	-5.30	105.96	112.90
2	B	1015	PHE	N-CA-C	-5.21	106.19	112.54
1	A	1303	ALA	CB-CA-C	-5.20	110.56	116.54
2	B	1019	LYS	N-CA-C	5.03	121.51	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1588	PRO	Peptide
2	B	1111	GLN	Peptide
2	B	1199	LYS	Peptide
2	B	481	HIS	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	12096	0	11589	202	0
2	B	16054	0	16016	417	0
3	A	6	0	2	0	0
4	B	31	0	19	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28187	0	27626	592	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 11.

All (592) 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:B:1007:PRO:HD2	2:B:1016:PHE:CE2	1.08	1.59
2:B:886:PHE:CE2	2:B:1017:PHE:CE1	1.83	1.58
2:B:886:PHE:CE2	2:B:1017:PHE:HE1	0.92	1.56
2:B:886:PHE:CZ	2:B:1017:PHE:CE1	1.93	1.54
2:B:1007:PRO:CD	2:B:1016:PHE:HE2	0.89	1.52
2:B:584:MET:HB3	4:B:2101:FMN:C5A	1.43	1.47
2:B:1032:VAL:CG2	2:B:1038:ARG:HD2	1.42	1.46
2:B:1032:VAL:CG2	2:B:1038:ARG:HH11	1.16	1.37
2:B:251:ARG:NH2	2:B:274:ASP:OD1	1.62	1.30
2:B:1036:VAL:O	2:B:1039:THR:HG22	1.20	1.24
1:A:252:GLU:HA	1:A:257:LEU:N	1.49	1.23
2:B:793:MET:SD	4:B:2101:FMN:HM71	1.77	1.23
2:B:1007:PRO:CD	2:B:1016:PHE:CE2	1.82	1.21
2:B:886:PHE:CZ	2:B:1017:PHE:HE1	1.39	1.21
1:A:216:ASP:CB	1:A:1067:LYS:C	2.16	1.19
2:B:1036:VAL:O	2:B:1039:THR:CG2	1.90	1.18
2:B:1032:VAL:HG23	2:B:1038:ARG:CD	1.75	1.16
1:A:214:PHE:CB	1:A:218:PHE:CB	2.22	1.16
2:B:1032:VAL:CG2	2:B:1038:ARG:CD	2.23	1.16
2:B:1524:SER:O	2:B:1527:GLU:OE2	1.65	1.12
1:A:252:GLU:HA	1:A:257:LEU:CA	1.57	1.11
2:B:887:GLN:HB3	2:B:1038:ARG:O	1.50	1.11
1:A:252:GLU:CA	1:A:257:LEU:H	1.65	1.10
2:B:886:PHE:CD2	2:B:1017:PHE:HE1	1.70	1.09
2:B:727[A]:HIS:HB2	2:B:841:ILE:HD13	1.35	1.07
2:B:1032:VAL:HG22	2:B:1038:ARG:HH11	1.11	1.06
2:B:590:ASN:O	2:B:592:ASP:N	1.88	1.05
2:B:588:THR:O	2:B:607:ALA:HB3	1.54	1.05
2:B:1032:VAL:HG22	2:B:1038:ARG:NH1	1.62	1.05
2:B:1007:PRO:HD3	2:B:1016:PHE:CE2	1.87	1.04
2:B:1032:VAL:CG2	2:B:1038:ARG:NH1	1.98	1.03
1:A:205:THR:CB	1:A:209:GLU:CB	2.40	1.00
2:B:584:MET:HB3	4:B:2101:FMN:C6	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:727[A]:HIS:HB2	2:B:841:ILE:CD1	1.93	0.99
2:B:1032:VAL:HG23	2:B:1038:ARG:HD2	1.31	0.99
2:B:584:MET:CB	4:B:2101:FMN:C5A	2.40	0.98
2:B:886:PHE:CD2	2:B:1017:PHE:CE1	2.48	0.98
2:B:1529:THR:HG22	2:B:1530:SER:N	1.75	0.97
2:B:756:SER:HA	4:B:2101:FMN:O5'	1.65	0.96
1:A:252:GLU:C	1:A:257:LEU:H	1.74	0.95
1:A:252:GLU:HA	1:A:257:LEU:H	1.15	0.95
2:B:1032:VAL:HG22	2:B:1038:ARG:HD2	1.46	0.94
2:B:757:GLY:N	4:B:2101:FMN:P	2.41	0.93
2:B:584:MET:HB3	4:B:2101:FMN:N5	1.82	0.93
1:A:216:ASP:CB	1:A:1067:LYS:O	2.17	0.93
1:A:1137:LYS:NZ	1:A:1141:GLU:OE2	2.02	0.93
2:B:757:GLY:H	4:B:2101:FMN:P	1.91	0.93
1:A:177:VAL:O	1:A:178:ASN:CB	2.17	0.92
2:B:1032:VAL:HG21	2:B:1038:ARG:HD2	1.51	0.91
2:B:1007:PRO:HD2	2:B:1016:PHE:CZ	2.03	0.90
2:B:919:VAL:CG2	2:B:1030:SER:HB2	2.01	0.90
2:B:585:THR:HB	2:B:586:PRO:HD3	1.53	0.90
1:A:501:LYS:NZ	1:A:509:GLU:OE2	2.06	0.89
2:B:886:PHE:CZ	2:B:1017:PHE:CZ	2.60	0.89
2:B:886:PHE:CE1	2:B:1017:PHE:CZ	2.61	0.89
2:B:1527:GLU:N	2:B:1527:GLU:OE1	2.06	0.88
1:A:27:ARG:NH1	1:A:30:GLU:OE2	2.07	0.88
2:B:1525:GLY:C	2:B:1527:GLU:OE1	2.17	0.87
2:B:919:VAL:HG22	2:B:1030:SER:HB2	1.55	0.87
2:B:886:PHE:CE1	2:B:1017:PHE:CE1	2.63	0.87
2:B:1526:GLU:N	2:B:1527:GLU:OE1	2.08	0.86
2:B:790:SER:OG	4:B:2101:FMN:C8M	2.24	0.85
1:A:189:GLY:HA2	2:B:643:PRO:CB	2.05	0.85
2:B:590:ASN:C	2:B:592:ASP:H	1.85	0.84
2:B:790:SER:OG	4:B:2101:FMN:HM83	1.78	0.84
1:A:767:ASP:O	1:A:818:ARG:NH1	2.11	0.84
2:B:847:ARG:NH1	2:B:885:ASP:OD1	2.10	0.83
2:B:1774:LYS:NZ	2:B:1804:SER:OG	2.11	0.83
2:B:757:GLY:HA2	4:B:2101:FMN:O1P	1.77	0.83
2:B:847:ARG:H	2:B:1037:GLN:HG3	1.43	0.83
2:B:248:GLY:N	2:B:274:ASP:O	2.13	0.82
2:B:846:THR:HB	2:B:1037:GLN:HA	1.61	0.81
2:B:756:SER:HA	4:B:2101:FMN:C5'	2.11	0.81
2:B:1022:LEU:HD23	2:B:1022:LEU:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLU:O	1:A:466:LYS:NZ	2.14	0.80
2:B:584:MET:HA	4:B:2101:FMN:C4A	2.11	0.80
2:B:886:PHE:CE2	2:B:1017:PHE:CD1	2.68	0.79
2:B:793:MET:SD	4:B:2101:FMN:C7M	2.67	0.79
2:B:1797:LEU:HD22	2:B:1797:LEU:O	1.83	0.78
1:A:512:GLU:OE2	1:A:873:ARG:NH1	2.16	0.78
2:B:757:GLY:CA	4:B:2101:FMN:O1P	2.32	0.78
2:B:588:THR:HB	2:B:607:ALA:HB2	1.66	0.78
1:A:144:GLU:O	1:A:260:GLY:O	2.00	0.77
2:B:1032:VAL:HG22	2:B:1038:ARG:CZ	2.15	0.77
1:A:252:GLU:HA	1:A:257:LEU:CB	2.15	0.77
2:B:585:THR:HB	2:B:586:PRO:CD	2.14	0.77
2:B:757:GLY:N	4:B:2101:FMN:O2P	2.15	0.76
1:A:338:LYS:NZ	1:A:342:GLU:OE2	2.18	0.76
2:B:251:ARG:NH1	2:B:271:ALA:O	2.18	0.76
2:B:586:PRO:HB3	2:B:1022:LEU:CD2	2.15	0.76
1:A:217:SER:O	1:A:219:SER:N	2.19	0.75
2:B:584:MET:HA	4:B:2101:FMN:N5	2.02	0.75
2:B:887:GLN:NE2	2:B:1021:SER:CB	2.50	0.75
1:A:894:ARG:NH1	1:A:895:THR:O	2.21	0.74
2:B:757:GLY:N	4:B:2101:FMN:O1P	2.20	0.74
1:A:26:VAL:HG21	2:B:1795:HIS:HD2	1.52	0.74
2:B:584:MET:CB	4:B:2101:FMN:N5	2.51	0.74
2:B:1672:GLU:OE1	2:B:1675:ARG:NH1	2.21	0.74
2:B:506:GLU:OE2	2:B:746:ARG:NH2	2.21	0.74
2:B:588:THR:O	2:B:607:ALA:CB	2.34	0.73
2:B:330:ASP:O	2:B:362:ARG:NH1	2.22	0.73
2:B:966:GLN:NE2	2:B:970:ASP:OD2	2.22	0.73
2:B:1032:VAL:HG23	2:B:1038:ARG:HH11	1.45	0.72
2:B:584:MET:CB	4:B:2101:FMN:C6	2.65	0.72
2:B:584:MET:CA	4:B:2101:FMN:N5	2.53	0.72
2:B:1134:GLU:OE2	2:B:1136:ASN:ND2	2.23	0.72
2:B:183:GLU:OE2	2:B:187:GLN:NE2	2.23	0.71
2:B:296:ARG:HH11	2:B:425:LEU:HB3	1.56	0.70
1:A:252:GLU:CA	1:A:257:LEU:CA	2.52	0.70
2:B:727[A]:HIS:CB	2:B:841:ILE:HD13	2.03	0.70
2:B:1032:VAL:HG23	2:B:1038:ARG:HD3	1.70	0.70
1:A:214:PHE:CA	1:A:218:PHE:CB	2.68	0.70
2:B:1529:THR:HG22	2:B:1530:SER:H	1.54	0.70
1:A:215:GLN:C	1:A:217:SER:H	1.99	0.70
1:A:21:GLN:NE2	2:B:1796:SER:HA	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:CA	1:A:257:LEU:N	2.29	0.70
2:B:1527:GLU:H	2:B:1527:GLU:CD	1.96	0.70
2:B:887:GLN:NE2	2:B:1021:SER:HB2	2.06	0.70
2:B:1032:VAL:CG2	2:B:1038:ARG:CZ	2.70	0.69
2:B:563:LYS:HZ2	2:B:565:TYR:HE1	1.40	0.69
2:B:727[A]:HIS:HA	2:B:841:ILE:HD13	1.75	0.69
2:B:1452:GLU:OE2	2:B:1469:THR:OG1	2.11	0.69
1:A:33:ASP:OD2	1:A:64:LYS:NZ	2.26	0.69
1:A:1060:LYS:HZ2	1:A:1077:ALA:HA	1.56	0.69
2:B:584:MET:HB2	2:B:587:THR:HB	1.74	0.68
2:B:1023:TRP:CD1	2:B:1023:TRP:H	2.09	0.68
2:B:888:LYS:NZ	2:B:1019:LYS:O	2.25	0.67
2:B:1663:MET:HB3	2:B:1772:MET:HG3	1.77	0.67
2:B:378:LEU:HD23	2:B:381:ARG:HH12	1.60	0.67
2:B:887:GLN:HE22	2:B:1021:SER:CB	2.07	0.67
2:B:887:GLN:CB	2:B:1038:ARG:O	2.35	0.67
1:A:983:GLU:OE2	1:A:1086:LYS:NZ	2.27	0.66
1:A:216:ASP:CB	1:A:1068:GLY:N	2.57	0.66
2:B:1650:THR:OG1	2:B:1791:MET:O	2.12	0.66
2:B:799:HIS:CB	2:B:1026:GLU:HG3	2.25	0.66
2:B:1792:PHE:CZ	2:B:1998:TYR:HB2	2.31	0.66
2:B:902:GLN:NE2	2:B:988:CYS:SG	2.68	0.66
2:B:1683:ARG:HA	2:B:1686:VAL:HG12	1.78	0.65
2:B:1007:PRO:CD	2:B:1016:PHE:CD2	2.72	0.65
1:A:1270:GLN:HB3	1:A:1273:ILE:HG23	1.79	0.65
2:B:52:PRO:HG3	2:B:61:LYS:HZ2	1.60	0.65
1:A:215:GLN:O	1:A:217:SER:N	2.28	0.65
2:B:344:ASN:HB3	2:B:349:ARG:HH12	1.62	0.65
2:B:571:SER:HB3	2:B:578:PRO:HG3	1.78	0.65
2:B:1529:THR:CG2	2:B:1530:SER:N	2.48	0.64
2:B:164:ARG:NH1	2:B:205:TRP:O	2.31	0.64
1:A:1188:ILE:H	1:A:1379:GLN:HE21	1.43	0.64
1:A:1007:GLU:O	1:A:1448:LYS:NZ	2.27	0.64
1:A:674:LEU:HD21	1:A:910:THR:HG22	1.79	0.64
2:B:1022:LEU:HD23	2:B:1022:LEU:C	2.20	0.64
2:B:1024:GLN:N	2:B:1024:GLN:OE1	2.29	0.64
2:B:1006:VAL:HA	2:B:1016:PHE:HD2	1.62	0.64
1:A:189:GLY:CA	2:B:643:PRO:CB	2.76	0.63
2:B:887:GLN:NE2	2:B:1021:SER:OG	2.31	0.63
1:A:26:VAL:HG21	2:B:1795:HIS:CD2	2.33	0.63
2:B:728:HIS:ND1	2:B:842:HIS:N	2.43	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ARG:NH1	1:A:1371:THR:O	2.30	0.62
2:B:1792:PHE:HB3	2:B:1806:LEU:HD22	1.79	0.62
1:A:824:LEU:HD23	1:A:846:LEU:HB3	1.81	0.62
2:B:906:TYR:OH	2:B:987:ASP:OD2	2.14	0.62
2:B:919:VAL:HG21	2:B:1030:SER:HB2	1.78	0.62
1:A:658:LEU:HD22	1:A:916:LEU:HD11	1.81	0.62
2:B:1263:ASN:ND2	2:B:1325:PHE:O	2.31	0.62
2:B:357:LEU:HB2	2:B:365:VAL:HB	1.82	0.62
1:A:251:LEU:O	1:A:257:LEU:CB	2.48	0.62
1:A:1188:ILE:HG12	1:A:1379:GLN:HG3	1.82	0.62
2:B:799:HIS:O	2:B:1026:GLU:HA	2.00	0.61
2:B:887:GLN:HE21	2:B:1021:SER:HB2	1.62	0.61
1:A:36:LEU:O	1:A:76:ARG:NH2	2.34	0.61
1:A:700:ILE:HG13	1:A:735:LEU:HD12	1.82	0.61
1:A:985:ARG:HG2	2:B:943:GLU:HG2	1.81	0.61
2:B:1306:LEU:HD11	2:B:1351:PRO:HB2	1.82	0.61
1:A:148:ALA:HB2	1:A:214:PHE:CB	2.30	0.61
1:A:483:LEU:HD23	1:A:484:THR:HG23	1.82	0.61
2:B:886:PHE:CD1	2:B:1017:PHE:CZ	2.89	0.61
2:B:1006:VAL:HG12	2:B:1016:PHE:HB3	1.83	0.61
1:A:742:GLN:O	1:A:801:ASN:ND2	2.34	0.61
1:A:1369:THR:O	1:A:1372:ARG:NH1	2.33	0.61
2:B:268:VAL:HG21	2:B:460:ILE:HG21	1.82	0.61
1:A:824:LEU:HD21	1:A:849:LEU:HD12	1.82	0.61
2:B:1796:SER:HB2	2:B:1965:HIS:CE1	2.36	0.61
1:A:296:ALA:HB1	1:A:302:SER:HA	1.82	0.61
2:B:727[A]:HIS:CB	2:B:841:ILE:CD1	2.66	0.61
2:B:756:SER:HA	4:B:2101:FMN:H5'2	1.83	0.61
2:B:344:ASN:O	2:B:349:ARG:NH1	2.34	0.61
2:B:1799:GLU:OE1	2:B:2001:ASN:ND2	2.33	0.61
2:B:1006:VAL:HA	2:B:1016:PHE:CD2	2.35	0.60
2:B:886:PHE:CD1	2:B:1017:PHE:HZ	2.19	0.60
2:B:1416:PRO:HB3	2:B:1450:ARG:HG2	1.84	0.60
1:A:1499:ARG:NH1	1:A:1746:TYR:OH	2.35	0.60
2:B:296:ARG:NH1	2:B:425:LEU:HB3	2.15	0.60
2:B:586:PRO:HB3	2:B:1022:LEU:HD21	1.83	0.59
1:A:1026:VAL:HG12	1:A:1188:ILE:HD12	1.84	0.59
1:A:1194:ALA:HB1	1:A:1199:ILE:HD12	1.84	0.59
2:B:1336:LEU:HD11	2:B:1396:PHE:HB3	1.84	0.59
2:B:1522:LEU:HD12	2:B:1612:MET:HG2	1.85	0.59
2:B:1576:ARG:NH1	2:B:1580:GLU:OE1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1717:ARG:NH1	2:B:1747:THR:O	2.35	0.59
1:A:215:GLN:C	1:A:217:SER:N	2.61	0.59
1:A:1300:PRO:HG3	1:A:1313:ILE:HD12	1.85	0.58
2:B:583:GLY:O	2:B:637:ASN:ND2	2.36	0.58
2:B:337:GLU:HA	2:B:340:ILE:HG12	1.84	0.58
2:B:1028:LEU:O	2:B:1028:LEU:HG	2.04	0.58
2:B:1131:ALA:HB1	2:B:1139:GLN:HG2	1.84	0.58
1:A:17:LEU:HD23	2:B:2002:LEU:HD23	1.84	0.58
1:A:1374:GLY:HA2	1:A:1550:THR:HG22	1.85	0.58
2:B:13:SER:H	2:B:46:PHE:HZ	1.51	0.58
2:B:1416:PRO:HB2	2:B:1510:ILE:HD12	1.85	0.58
2:B:1799:GLU:OE2	2:B:1998:TYR:OH	2.16	0.58
2:B:1375:LEU:HD11	2:B:1395:GLN:HE21	1.68	0.58
1:A:648:THR:OG1	1:A:650:ASP:OD1	2.22	0.58
2:B:728:HIS:HD1	2:B:842:HIS:N	2.02	0.58
2:B:1184:ASN:ND2	2:B:1188:ASP:O	2.37	0.58
1:A:984:PRO:HD2	1:A:1086:LYS:NZ	2.19	0.58
2:B:399:ARG:HH22	2:B:731:GLU:HG2	1.68	0.58
2:B:885:ASP:O	2:B:1038:ARG:HA	2.05	0.57
1:A:919:GLU:HG3	1:A:920:GLU:HG2	1.85	0.57
2:B:1796:SER:HB2	2:B:1965:HIS:HE1	1.68	0.57
2:B:232:GLN:HG2	2:B:490:GLY:HA2	1.86	0.57
2:B:587:THR:OG1	4:B:2101:FMN:HM73	2.04	0.57
1:A:878:MET:HG3	1:A:881:ASN:HD22	1.70	0.57
2:B:1770:THR:HG22	2:B:1801:SER:OG	2.05	0.57
2:B:905:THR:HA	2:B:982:LEU:HA	1.86	0.57
1:A:1032:SER:O	1:A:1602:GLN:NE2	2.36	0.56
2:B:1036:VAL:O	2:B:1039:THR:HG23	1.96	0.56
2:B:1037:GLN:C	2:B:1039:THR:H	2.12	0.56
1:A:18:LEU:CD2	2:B:1799:GLU:HG2	2.35	0.56
2:B:727[B]:HIS:HA	2:B:841:ILE:HA	1.87	0.56
2:B:1726:GLU:H	2:B:1975:PRO:HG3	1.70	0.56
1:A:771:ILE:HG22	1:A:773:PRO:HD3	1.87	0.56
2:B:136:LEU:HD21	2:B:538:ALA:HA	1.88	0.56
2:B:1130:LEU:HD23	2:B:1179:LEU:HD11	1.86	0.56
2:B:1529:THR:HG23	2:B:1608:LEU:O	2.05	0.56
1:A:963:ILE:HG21	2:B:1505:ARG:HH12	1.71	0.56
2:B:1036:VAL:C	2:B:1039:THR:HG22	2.18	0.56
1:A:1304:CYS:HB2	1:A:1649:GLY:HA2	1.87	0.56
2:B:1032:VAL:HG23	2:B:1038:ARG:NH1	2.11	0.56
2:B:1136:ASN:ND2	2:B:1176:THR:OG1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:ASP:OD1	1:A:813:LYS:NZ	2.39	0.56
1:A:1248:SER:HB3	1:A:1279:ILE:HG23	1.86	0.56
2:B:882:LEU:HD13	2:B:1006:VAL:HG21	1.88	0.56
2:B:815:PRO:HD2	2:B:818:GLN:HE21	1.71	0.56
2:B:1458:LYS:HB2	2:B:1464:SER:HB2	1.88	0.56
1:A:18:LEU:HD21	2:B:1803:LEU:HD21	1.88	0.55
1:A:1118:LYS:NZ	1:A:1336:GLU:OE2	2.31	0.55
2:B:1037:GLN:C	2:B:1039:THR:N	2.64	0.55
1:A:251:LEU:C	1:A:257:LEU:CB	2.79	0.55
1:A:767:ASP:HB3	1:A:818:ARG:NH1	2.21	0.55
1:A:1063:ASN:ND2	1:A:1072:SER:OG	2.38	0.55
1:A:1562:ASN:HD22	1:A:1625:TYR:HD1	1.52	0.55
2:B:1263:ASN:HB3	2:B:1327:LYS:NZ	2.20	0.55
2:B:1851:SER:HB3	2:B:1854:PHE:HB2	1.87	0.55
2:B:293:ILE:HD11	2:B:465:VAL:HG12	1.89	0.55
2:B:847:ARG:HG3	2:B:1037:GLN:HG2	1.88	0.55
2:B:799:HIS:HB2	2:B:1026:GLU:HG3	1.87	0.55
1:A:1420:PRO:HB2	1:A:1556:ASN:HD22	1.71	0.55
2:B:590:ASN:O	2:B:591:THR:C	2.48	0.55
2:B:727[A]:HIS:C	2:B:727[A]:HIS:CD2	2.85	0.55
2:B:232:GLN:HE21	2:B:491:PRO:HD3	1.72	0.55
1:A:325:ALA:O	1:A:326:LEU:C	2.48	0.55
1:A:437:GLN:O	1:A:441:ARG:NE	2.35	0.55
1:A:1689:TYR:OH	2:B:981:GLN:NE2	2.34	0.55
2:B:107:TYR:OH	2:B:110:THR:O	2.24	0.55
2:B:590:ASN:OD1	2:B:799:HIS:CE1	2.59	0.55
2:B:1672:GLU:CD	2:B:1675:ARG:HH12	2.14	0.55
2:B:52:PRO:HG3	2:B:61:LYS:NZ	2.21	0.55
2:B:1015:PHE:C	2:B:1015:PHE:CD2	2.84	0.55
2:B:1479:LYS:NZ	2:B:1808:ASN:HB2	2.21	0.55
2:B:831:ILE:HD11	2:B:849:VAL:HG12	1.89	0.54
2:B:453:PHE:HD1	2:B:456:LEU:HD11	1.72	0.54
2:B:1156:ASN:HB3	2:B:1159:HIS:HB2	1.89	0.54
2:B:42:PRO:HB3	2:B:46:PHE:HE1	1.72	0.54
1:A:883:ILE:HG13	1:A:884:ILE:HG23	1.90	0.54
1:A:44:ILE:HG23	1:A:78:VAL:HA	1.89	0.54
2:B:586:PRO:HG2	4:B:2101:FMN:H6	1.89	0.54
2:B:931:ARG:NH1	2:B:962:ASN:OD1	2.40	0.54
2:B:1266:ASN:HB3	2:B:1269:LYS:HZ2	1.73	0.54
1:A:522:GLU:HG2	1:A:671:ILE:HG22	1.89	0.54
2:B:245:LEU:HD12	2:B:249:GLU:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:CB	1:A:183:VAL:CB	2.86	0.53
2:B:790:SER:HA	4:B:2101:FMN:HM82	1.90	0.53
2:B:1792:PHE:CE2	2:B:1998:TYR:HD1	2.27	0.53
2:B:590:ASN:CG	2:B:799:HIS:CE1	2.86	0.53
2:B:1181:ALA:HB3	2:B:1193:VAL:HB	1.89	0.53
1:A:769:ASP:OD1	1:A:818:ARG:NE	2.41	0.53
2:B:590:ASN:ND2	2:B:799:HIS:CD2	2.77	0.53
1:A:21:GLN:HE21	2:B:1796:SER:HA	1.73	0.53
1:A:269:ALA:O	1:A:273:GLU:N	2.42	0.53
1:A:46:GLU:OE1	1:A:54:ALA:N	2.40	0.53
2:B:708:LYS:NZ	2:B:747:CYS:SG	2.76	0.53
2:B:919:VAL:HG21	2:B:1030:SER:CB	2.37	0.53
2:B:1688:ASN:O	2:B:1719:ASN:ND2	2.41	0.53
1:A:1456:GLU:HA	1:A:1459:LYS:HG2	1.90	0.53
2:B:1593:ALA:HB3	2:B:1643:GLU:HB2	1.91	0.53
2:B:727[B]:HIS:HD2	2:B:841:ILE:HG23	1.73	0.53
2:B:1263:ASN:HB3	2:B:1327:LYS:HZ1	1.73	0.53
1:A:412:VAL:HG11	1:A:450:MET:HG2	1.90	0.52
2:B:727[A]:HIS:HD2	2:B:727[A]:HIS:O	1.93	0.52
2:B:1830:VAL:HB	2:B:1832:ARG:HH12	1.75	0.52
1:A:25:PRO:HA	2:B:1965:HIS:HB3	1.92	0.52
1:A:676:PHE:HD2	1:A:702:GLY:HA3	1.74	0.52
2:B:219:LEU:HD21	2:B:409:PRO:HB3	1.91	0.52
2:B:1032:VAL:HG22	2:B:1038:ARG:CD	2.17	0.52
1:A:1472:GLU:OE1	1:A:1493:ARG:NH1	2.42	0.52
2:B:57:GLU:OE2	2:B:113:LYS:HB3	2.09	0.52
2:B:726:GLY:HA2	2:B:1042:LEU:HD23	1.92	0.52
2:B:1529:THR:HG22	2:B:1530:SER:O	2.10	0.52
1:A:16:GLU:OE2	2:B:2025:LYS:HE2	2.10	0.52
2:B:1524:SER:C	2:B:1527:GLU:OE2	2.47	0.52
1:A:1565:MET:HB3	1:A:1570:ARG:HG3	1.91	0.51
2:B:1811:PRO:HD2	2:B:1814:SER:HB2	1.92	0.51
2:B:843:LYS:HZ3	2:B:849:VAL:HG13	1.74	0.51
2:B:871:LEU:HD22	2:B:1009:LEU:HD12	1.92	0.51
2:B:1876:ILE:HA	2:B:1888:ALA:HA	1.93	0.51
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.35	0.51
2:B:563:LYS:NZ	2:B:565:TYR:HE1	2.07	0.51
2:B:87:LEU:HB3	2:B:91:ASN:HA	1.92	0.51
2:B:727[A]:HIS:HA	2:B:841:ILE:HA	1.91	0.51
2:B:886:PHE:CE1	2:B:1017:PHE:HZ	2.21	0.51
1:A:1305:ALA:HB1	1:A:1647:SER:OG	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1588:PRO:HB2	1:A:1591:ALA:HB3	1.93	0.51
2:B:1037:GLN:N	2:B:1037:GLN:OE1	2.43	0.51
2:B:1191:PRO:O	2:B:1210:HIS:NE2	2.41	0.51
1:A:1279:ILE:HG21	1:A:1301:VAL:HG22	1.92	0.50
1:A:815:THR:HG22	1:A:817:THR:H	1.76	0.50
2:B:1169:LYS:HZ2	2:B:1182:PHE:HD2	1.57	0.50
2:B:93:ASN:HD21	2:B:536:THR:HG23	1.75	0.50
2:B:894:ASN:ND2	2:B:903:GLU:O	2.44	0.50
2:B:984:SER:OG	2:B:986:GLU:OE1	2.30	0.50
2:B:1896:ASP:O	2:B:1900:ASN:ND2	2.45	0.50
1:A:1366:ARG:NH1	1:A:1371:THR:HG23	2.27	0.50
1:A:868:VAL:HB	1:A:925:ASP:HA	1.92	0.50
2:B:518:LEU:HD13	2:B:530:LYS:HB3	1.93	0.50
2:B:590:ASN:C	2:B:592:ASP:N	2.44	0.50
1:A:1029:TRP:O	1:A:1034:THR:OG1	2.24	0.50
2:B:1899:THR:O	2:B:1903:ASN:ND2	2.45	0.50
2:B:1529:THR:CG2	2:B:1530:SER:H	2.21	0.49
2:B:1869:LYS:HG3	2:B:1929:TYR:HE1	1.77	0.49
2:B:723:ARG:HD2	2:B:1046:VAL:HG11	1.93	0.49
2:B:1877:VAL:HB	2:B:1965:HIS:HB2	1.93	0.49
2:B:585:THR:N	4:B:2101:FMN:O4	2.45	0.49
2:B:1842:MET:HB2	2:B:1960:ILE:HG21	1.94	0.49
1:A:723:ASN:OD1	1:A:727:ARG:NH2	2.45	0.49
2:B:1022:LEU:CD2	2:B:1022:LEU:C	2.85	0.49
2:B:1180:THR:HG23	2:B:1194:GLU:HG2	1.94	0.49
1:A:1649:GLY:N	1:A:1653:LYS:O	2.44	0.49
2:B:756:SER:H	4:B:2101:FMN:H5'2	1.77	0.49
1:A:686:ALA:O	1:A:721:TYR:OH	2.29	0.49
2:B:1209:GLU:OE1	2:B:1552:SER:OG	2.25	0.49
2:B:1774:LYS:HZ1	2:B:1804:SER:CB	2.23	0.49
1:A:252:GLU:CA	1:A:257:LEU:CB	2.89	0.49
1:A:984:PRO:HB3	2:B:946:THR:HG23	1.95	0.49
2:B:344:ASN:HB3	2:B:349:ARG:NH1	2.27	0.49
1:A:1104:LEU:HA	1:A:1184:VAL:HA	1.95	0.49
2:B:1919:MET:HE2	2:B:1923:LYS:HG3	1.94	0.49
1:A:58:ASN:HD21	1:A:78:VAL:HG11	1.78	0.49
1:A:1367:PRO:O	1:A:1369:THR:OG1	2.30	0.49
2:B:1682:ASP:HB3	2:B:1693:ILE:HG22	1.95	0.49
1:A:91:LYS:NZ	2:B:1518:ASN:HB2	2.27	0.48
1:A:1354:GLU:OE1	1:A:1366:ARG:NH2	2.46	0.48
1:A:14:LEU:HD21	2:B:1803:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:LEU:HB2	2:B:1078:TYR:HE2	1.78	0.48
2:B:145:LYS:HZ2	2:B:482:LYS:HG3	1.79	0.48
2:B:1017:PHE:CD1	2:B:1017:PHE:C	2.84	0.48
2:B:1878:ASN:HB2	2:B:1887:VAL:HB	1.95	0.48
1:A:234:MET:O	1:A:238:MET:CB	2.61	0.48
2:B:79:LEU:HD21	2:B:126:VAL:HG23	1.94	0.48
2:B:1266:ASN:HD22	2:B:1269:LYS:HE3	1.77	0.48
1:A:1018:VAL:HG11	1:A:1315:ILE:HG12	1.95	0.48
2:B:584:MET:O	2:B:607:ALA:HB2	2.14	0.48
2:B:1479:LYS:HZ2	2:B:1808:ASN:HB2	1.77	0.48
1:A:888:ILE:HD13	1:A:930:LEU:HD21	1.96	0.48
2:B:222:PRO:HG3	2:B:295:SER:HA	1.96	0.48
1:A:148:ALA:CB	1:A:214:PHE:CB	2.92	0.48
1:A:411:ASP:HA	1:A:414:SER:HB3	1.96	0.48
1:A:871:TRP:HB2	1:A:930:LEU:HD11	1.95	0.48
1:A:1557:GLU:OE2	1:A:1646:THR:OG1	2.21	0.47
2:B:790:SER:OG	4:B:2101:FMN:HM82	2.12	0.47
1:A:1234:TYR:OH	1:A:1291:LEU:O	2.22	0.47
2:B:693:LYS:HG2	2:B:718:GLN:HB2	1.96	0.47
2:B:146:LEU:HD23	2:B:485:HIS:HB2	1.96	0.47
2:B:790:SER:CA	4:B:2101:FMN:HM82	2.45	0.47
2:B:1192:VAL:HG23	2:B:1193:VAL:HG23	1.96	0.47
2:B:1032:VAL:CG2	2:B:1038:ARG:NE	2.75	0.47
2:B:1717:ARG:NH2	2:B:1745:GLU:O	2.47	0.47
2:B:522:PRO:HD3	2:B:529:PHE:HE2	1.80	0.47
2:B:590:ASN:O	2:B:593:ILE:N	2.45	0.47
2:B:1689:TYR:O	2:B:1720:TYR:OH	2.28	0.47
2:B:481:HIS:HD2	2:B:505:LYS:NZ	2.12	0.47
1:A:984:PRO:HG2	1:A:1086:LYS:HD3	1.96	0.47
1:A:1304:CYS:HA	1:A:1589:LYS:O	2.15	0.47
2:B:246:THR:HG22	2:B:248:GLY:H	1.79	0.47
2:B:831:ILE:HD13	2:B:853:LYS:HE2	1.96	0.47
2:B:1531:LYS:NZ	2:B:1605:ASN:O	2.46	0.47
2:B:1792:PHE:O	2:B:1792:PHE:CD2	2.67	0.47
1:A:939:PHE:HD1	1:A:942:LYS:HZ3	1.59	0.47
1:A:1035:ARG:NH1	1:A:1039:GLU:OE1	2.47	0.47
2:B:761:ASP:OD2	2:B:1068:GLY:HA3	2.15	0.47
2:B:1374:LYS:HB2	2:B:1402:TYR:HD2	1.80	0.47
2:B:440:LEU:HB3	2:B:454:GLN:HG2	1.96	0.46
2:B:1053:LYS:HE3	2:B:1056:GLU:HB3	1.97	0.46
2:B:1792:PHE:O	2:B:1792:PHE:CG	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ARG:HD3	1:A:514:GLN:HG2	1.97	0.46
1:A:1549:SER:O	1:A:1549:SER:OG	2.30	0.46
2:B:728:HIS:HD1	2:B:842:HIS:H	1.63	0.46
2:B:799:HIS:O	2:B:1026:GLU:CA	2.40	0.46
1:A:1220:GLU:HA	1:A:1223:LEU:HB2	1.98	0.46
2:B:738:ILE:HA	2:B:781:MET:HE1	1.97	0.46
2:B:1032:VAL:HG22	2:B:1038:ARG:NE	2.30	0.46
1:A:214:PHE:HA	1:A:218:PHE:CB	2.45	0.46
1:A:1008:LEU:HG	1:A:1668:VAL:HG12	1.97	0.46
1:A:1305:ALA:HB2	1:A:1647:SER:C	2.40	0.46
2:B:1767:PRO:HG3	2:B:1819:VAL:HG13	1.98	0.46
2:B:42:PRO:HA	2:B:51:GLU:OE2	2.16	0.46
2:B:233:LEU:HD13	2:B:283:SER:HB2	1.97	0.46
1:A:1118:LYS:HG3	1:A:1336:GLU:OE2	2.16	0.46
1:A:988:MET:HE3	1:A:1050:ILE:HG13	1.97	0.46
1:A:1401:ALA:HB2	1:A:1601:ILE:HG12	1.98	0.46
1:A:1510:LYS:HA	1:A:1514:ASN:HB2	1.97	0.46
2:B:192:PHE:HE1	2:B:296:ARG:HE	1.63	0.46
1:A:1248:SER:OG	1:A:1249:GLY:N	2.47	0.46
2:B:1026:GLU:HA	2:B:1026:GLU:OE1	2.16	0.46
2:B:1792:PHE:CE2	2:B:1998:TYR:CD1	3.03	0.46
2:B:1795:HIS:CE1	2:B:1878:ASN:ND2	2.84	0.46
2:B:1795:HIS:NE2	2:B:1878:ASN:ND2	2.63	0.46
1:A:985:ARG:HB2	2:B:944:ARG:HA	1.98	0.45
2:B:560:SER:HB2	2:B:1089:GLU:HA	1.98	0.45
1:A:963:ILE:HG21	2:B:1505:ARG:NH1	2.30	0.45
1:A:1230:PRO:HB3	1:A:1291:LEU:HD23	1.98	0.45
2:B:727[A]:HIS:HB2	2:B:841:ILE:HD11	1.88	0.45
1:A:1495:GLU:OE1	1:A:1499:ARG:NH2	2.49	0.45
2:B:94:ILE:HA	2:B:97:PHE:HB3	1.97	0.45
2:B:273:SER:HB2	2:B:279:PHE:HA	1.98	0.45
2:B:313:ASP:OD1	2:B:317:ASN:ND2	2.49	0.45
2:B:381:ARG:HA	2:B:384:LYS:HG2	1.98	0.45
1:A:893:VAL:HG21	1:A:933:ILE:HD11	1.99	0.45
1:A:91:LYS:NZ	2:B:1518:ASN:HD22	2.15	0.45
1:A:869:ILE:HG23	1:A:901:MET:HE2	1.99	0.45
1:A:984:PRO:HD2	1:A:1086:LYS:HZ1	1.80	0.45
1:A:1276:GLU:HA	1:A:1281:THR:HG21	1.98	0.45
2:B:727[A]:HIS:CD2	2:B:727[A]:HIS:O	2.70	0.45
2:B:1665:MET:HA	2:B:1668:TYR:HB3	1.98	0.45
1:A:752:VAL:HG21	1:A:808:ALA:HB1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:GLY:HA2	1:A:1262:ASP:HB2	1.98	0.45
2:B:1864:ASP:O	2:B:1868:ASN:ND2	2.50	0.45
2:B:102:LEU:HD11	2:B:111:ILE:HD13	1.99	0.45
2:B:584:MET:O	2:B:607:ALA:CB	2.65	0.45
2:B:723:ARG:HH11	2:B:1046:VAL:HG11	1.82	0.45
2:B:236:TYR:CG	2:B:270:ILE:HD11	2.52	0.45
2:B:389:LEU:HD23	2:B:391:GLN:HE21	1.82	0.45
2:B:847:ARG:N	2:B:1037:GLN:HG3	2.23	0.45
1:A:41:THR:HG22	2:B:1648:THR:HG22	1.99	0.44
1:A:47:ILE:HD12	2:B:1653:PHE:HE1	1.83	0.44
1:A:1721:ASP:OD2	1:A:1724:ALA:HB2	2.17	0.44
2:B:502:HIS:HB2	2:B:512:ILE:HG13	1.98	0.44
2:B:1529:THR:CG2	2:B:1608:LEU:O	2.65	0.44
2:B:63:ILE:HD11	2:B:79:LEU:HA	1.99	0.44
1:A:182:THR:CB	2:B:672:VAL:O	2.66	0.44
1:A:459:GLU:OE2	1:A:469:LYS:HD2	2.18	0.44
2:B:727[B]:HIS:HA	2:B:841:ILE:HD13	1.75	0.44
2:B:847:ARG:H	2:B:1037:GLN:CG	2.24	0.44
2:B:1031:VAL:HG13	2:B:1032:VAL:HG22	1.98	0.44
2:B:1315:ILE:HD13	2:B:1358:VAL:HG11	1.99	0.44
2:B:1547:ASN:HB3	2:B:1550:HIS:CD2	2.52	0.44
1:A:1187:GLN:H	1:A:1187:GLN:HG2	1.53	0.44
2:B:251:ARG:NH1	2:B:441:LYS:HB2	2.33	0.44
2:B:1013:PHE:O	2:B:1017:PHE:N	2.51	0.44
2:B:1158:LEU:HA	2:B:1161:ILE:HG12	2.00	0.44
2:B:1199:LYS:O	2:B:1202:THR:OG1	2.30	0.44
1:A:2:LYS:HE2	1:A:5:ILE:HD12	2.00	0.43
1:A:1259:MET:HB3	1:A:1273:ILE:HD13	2.00	0.43
1:A:1361:PRO:HA	1:A:1364:MET:HE3	2.00	0.43
1:A:700:ILE:HG22	1:A:729:GLY:HA2	2.00	0.43
1:A:1596:MET:HE2	1:A:1645:VAL:HG13	1.99	0.43
2:B:846:THR:CB	2:B:1037:GLN:HA	2.42	0.43
2:B:1463:TYR:HD2	2:B:1466:ILE:HD11	1.83	0.43
2:B:1629:ARG:NH2	2:B:1634:GLU:OE1	2.50	0.43
1:A:691:ILE:HD11	1:A:872:THR:HG21	2.00	0.43
1:A:709:THR:HG23	1:A:740:PHE:HB3	1.99	0.43
2:B:145:LYS:HZ2	2:B:482:LYS:CG	2.30	0.43
2:B:1338:HIS:CE1	2:B:1569:MET:HE3	2.53	0.43
1:A:741:ASN:HB3	1:A:747:ASP:OD2	2.18	0.43
1:A:1210:ILE:HD11	1:A:1331:TYR:HD2	1.84	0.43
2:B:1701:PRO:HD2	2:B:1758:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1792:PHE:HZ	2:B:1998:TYR:HB2	1.81	0.43
2:B:1889:ALA:HB1	2:B:1963:PRO:HB3	2.00	0.43
2:B:1960:ILE:HD11	2:B:1964:PHE:HE1	1.83	0.43
1:A:1472:GLU:CD	1:A:1493:ARG:HH12	2.27	0.43
2:B:727[B]:HIS:HD2	2:B:841:ILE:CG2	2.25	0.43
2:B:1037:GLN:O	2:B:1039:THR:N	2.52	0.43
2:B:1861:PHE:HD2	2:B:1912:ILE:HD13	1.83	0.43
1:A:222:LEU:O	1:A:226:SER:CB	2.67	0.43
2:B:221:VAL:HG21	2:B:412:ALA:HB2	1.99	0.43
2:B:221:VAL:HG12	2:B:294:GLY:HA2	2.00	0.43
2:B:1362:ALA:HA	2:B:1380:GLY:HA2	2.01	0.43
2:B:1438:LEU:HA	2:B:1485:GLY:HA3	2.01	0.43
1:A:1300:PRO:C	1:A:1301:VAL:HG23	2.44	0.43
2:B:586:PRO:HD2	4:B:2101:FMN:H6	2.01	0.43
2:B:1528:LEU:HA	2:B:1528:LEU:HD22	1.64	0.43
1:A:18:LEU:HD23	2:B:1799:GLU:HG2	2.00	0.42
2:B:590:ASN:ND2	2:B:592:ASP:HB3	2.33	0.42
2:B:919:VAL:HG11	2:B:1029:GLU:OE1	2.19	0.42
1:A:788:ASP:O	1:A:791:SER:OG	2.30	0.42
1:A:998:TYR:CZ	1:A:1002:LYS:NZ	2.87	0.42
1:A:1006:PRO:O	1:A:1008:LEU:N	2.51	0.42
2:B:260:HIS:CG	2:B:261:SER:H	2.37	0.42
2:B:1266:ASN:HB3	2:B:1269:LYS:NZ	2.33	0.42
2:B:1843:VAL:O	2:B:1888:ALA:N	2.47	0.42
1:A:823:ILE:HD13	1:A:865:CYS:HB3	2.01	0.42
2:B:333:ILE:HG13	2:B:364:LEU:HD21	2.01	0.42
1:A:1366:ARG:HH11	1:A:1371:THR:HG23	1.85	0.42
1:A:1229:ASP:OD1	1:A:1229:ASP:N	2.52	0.42
2:B:585:THR:N	4:B:2101:FMN:N5	2.67	0.42
2:B:756:SER:CA	4:B:2101:FMN:H5'2	2.48	0.42
2:B:833:VAL:HG11	2:B:843:LYS:HZ1	1.83	0.42
2:B:879:ILE:O	2:B:883:ASN:ND2	2.53	0.42
2:B:1520:ILE:HG13	2:B:1614:HIS:HB3	2.01	0.42
1:A:30:GLU:HA	1:A:33:ASP:HB2	2.02	0.42
1:A:1028:PRO:HD3	1:A:1595:TRP:CH2	2.55	0.42
2:B:428:ASP:OD1	2:B:431:LYS:NZ	2.53	0.42
2:B:481:HIS:HD2	2:B:505:LYS:HZ2	1.68	0.42
1:A:451:GLN:HE22	1:A:473:GLN:HE22	1.68	0.42
1:A:904:ASN:HB3	1:A:926:LEU:HD13	2.02	0.42
1:A:964:GLU:HG2	2:B:1498:PRO:HB3	2.01	0.42
1:A:1017:VAL:O	1:A:1389:ALA:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:PHE:HB3	1:A:1548:THR:O	2.20	0.42
2:B:185:LEU:O	2:B:189:HIS:N	2.53	0.42
2:B:822:THR:HG22	2:B:832:THR:H	1.85	0.42
1:A:51:PRO:HB3	1:A:54:ALA:HB3	2.02	0.42
1:A:495:ILE:HG23	1:A:900:GLU:OE2	2.19	0.42
2:B:276:TRP:CE3	2:B:276:TRP:HA	2.54	0.42
2:B:306:LEU:HD23	2:B:311:LEU:HB3	2.01	0.42
2:B:1475:GLU:OE2	2:B:1479:LYS:HA	2.19	0.42
1:A:521:PHE:HA	1:A:524:TYR:HB3	2.01	0.41
1:A:1060:LYS:NZ	1:A:1077:ALA:HA	2.31	0.41
2:B:61:LYS:NZ	2:B:117:ASN:OD1	2.31	0.41
2:B:790:SER:HG	4:B:2101:FMN:HM83	1.80	0.41
2:B:1265:ILE:HB	2:B:1326:PRO:HG3	2.00	0.41
1:A:1132:PRO:HG3	1:A:1165:ARG:HB2	2.02	0.41
1:A:1537:ILE:HD11	1:A:1565:MET:HE1	2.02	0.41
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.87	0.41
2:B:218:LEU:O	2:B:224:SER:OG	2.38	0.41
2:B:1017:PHE:CD1	2:B:1017:PHE:O	2.74	0.41
2:B:1771:LEU:HD23	2:B:1771:LEU:HA	1.89	0.41
1:A:296:ALA:O	1:A:300:GLY:N	2.53	0.41
2:B:461:ILE:HA	2:B:464:VAL:HG12	2.02	0.41
2:B:486:ILE:HB	2:B:512:ILE:HD13	2.01	0.41
2:B:568:THR:N	2:B:571:SER:OG	2.44	0.41
2:B:1575:ILE:HG13	2:B:1638:LEU:HD12	2.01	0.41
2:B:262:GLN:HE21	2:B:290:LEU:HD23	1.84	0.41
2:B:744:ILE:HG21	2:B:752:LEU:HD12	2.01	0.41
2:B:73:GLN:HA	2:B:76:GLU:OE2	2.21	0.41
2:B:319:GLU:OE2	2:B:381:ARG:NH2	2.53	0.41
2:B:1417:VAL:HG11	2:B:1503:LEU:HB3	2.03	0.41
2:B:1697:VAL:HA	2:B:1759:LEU:HD22	2.03	0.41
1:A:1116:LYS:HD3	1:A:1183:LEU:HD21	2.02	0.41
2:B:727[A]:HIS:C	2:B:727[A]:HIS:HD2	2.28	0.41
2:B:181:ILE:HG23	2:B:287:VAL:HG21	2.03	0.41
2:B:1296:ALA:HA	2:B:1303:LYS:NZ	2.35	0.41
2:B:1525:GLY:CA	2:B:1527:GLU:OE1	2.68	0.41
1:A:497:GLY:HA3	1:A:515:LYS:HD3	2.02	0.41
1:A:1050:ILE:HG22	1:A:1088:ILE:HG21	2.02	0.41
1:A:1375:PHE:HA	1:A:1549:SER:HB3	2.02	0.41
2:B:471:LEU:HA	2:B:472:PRO:HD3	1.94	0.41
2:B:1144:THR:HG22	2:B:1146:ARG:H	1.85	0.41
1:A:417:PHE:HD2	1:A:1635:ILE:HD11	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:LEU:HD23	1:A:933:ILE:HD12	2.03	0.41
1:A:1020:VAL:HG22	1:A:1386:ILE:HG22	2.03	0.41
2:B:1144:THR:O	2:B:1156:ASN:ND2	2.54	0.41
1:A:7:GLN:O	1:A:11:HIS:N	2.46	0.40
1:A:1312:ASP:HA	1:A:1406:THR:HG21	2.02	0.40
2:B:332:SER:H	2:B:335:GLN:HE21	1.68	0.40
2:B:1766:GLN:HG3	2:B:1819:VAL:HG22	2.02	0.40
1:A:29:ILE:HG21	2:B:1882:GLU:OE2	2.21	0.40
1:A:983:GLU:O	2:B:943:GLU:HG3	2.22	0.40
1:A:1046:LEU:HD23	1:A:1089:LYS:HE2	2.03	0.40
2:B:150:PHE:HE1	2:B:489:PHE:HB2	1.85	0.40
2:B:843:LYS:NZ	2:B:849:VAL:HG13	2.35	0.40
2:B:1769:LEU:HD23	2:B:1769:LEU:HA	1.95	0.40
1:A:1742:SER:HB3	1:A:1744:GLN:HG2	2.03	0.40
2:B:322:PRO:HA	2:B:407:PHE:CG	2.56	0.40
2:B:1033:ASP:O	2:B:1034:GLU:C	2.64	0.40
2:B:1323:ALA:HB1	2:B:1364:ILE:HD12	2.04	0.40
2:B:1740:PHE:HD1	2:B:1740:PHE:HA	1.75	0.40
2:B:852:TRP:CH2	2:B:1018:LYS:HA	2.56	0.40
2:B:955:LEU:HD12	2:B:955:LEU:HA	1.92	0.40
1:A:627:ILE:HD12	1:A:628:GLN:HG2	2.04	0.40
2:B:587:THR:OG1	4:B:2101:FMN:C7M	2.69	0.40
2:B:846:THR:HB	2:B:1037:GLN:CA	2.42	0.40
2:B:1123:LYS:HA	2:B:1164:PRO:HG2	2.03	0.40
2:B:1625:LYS:HD3	2:B:1627:GLU:OE2	2.21	0.40
2:B:1892:LEU:HD23	2:B:1895:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1586/1885 (84%)	1513 (95%)	64 (4%)	9 (1%)	21	51
2	B	2032/2037 (100%)	1924 (95%)	103 (5%)	5 (0%)	43	72
All	All	3618/3922 (92%)	3437 (95%)	167 (5%)	14 (0%)	31	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	PHE
2	B	591	THR
2	B	1032	VAL
1	A	178	ASN
2	B	1038	ARG
2	B	1796	SER
1	A	206	PRO
1	A	207	LEU
1	A	216	ASP
1	A	1301	VAL
1	A	215	GLN
1	A	1007	GLU
2	B	1022	LEU
1	A	1006	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	1221/1579 (77%)	1213 (99%)	8 (1%)	76	91
2	B	1780/1784 (100%)	1745 (98%)	35 (2%)	48	80
All	All	3001/3363 (89%)	2958 (99%)	43 (1%)	57	85

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	709	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	712	ARG
1	A	1046	LEU
1	A	1105	ILE
1	A	1273	ILE
1	A	1383	ILE
1	A	1429	ARG
2	B	74	ILE
2	B	270	ILE
2	B	277	ASP
2	B	293	ILE
2	B	552	LEU
2	B	584	MET
2	B	589	VAL
2	B	685	LEU
2	B	727[A]	HIS
2	B	727[B]	HIS
2	B	831	ILE
2	B	859	ILE
2	B	1015	PHE
2	B	1016	PHE
2	B	1021	SER
2	B	1022	LEU
2	B	1025	SER
2	B	1026	GLU
2	B	1028	LEU
2	B	1031	VAL
2	B	1032	VAL
2	B	1033	ASP
2	B	1034	GLU
2	B	1037	GLN
2	B	1039	THR
2	B	1040	CYS
2	B	1514	VAL
2	B	1527	GLU
2	B	1528	LEU
2	B	1529	THR
2	B	1549	ILE
2	B	1740	PHE
2	B	1791	MET
2	B	1797	LEU
2	B	1801	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	21	GLN
1	A	39	HIS
1	A	381	HIS
1	A	451	GLN
1	A	474	GLN
1	A	530	GLN
1	A	637	GLN
1	A	722	GLN
1	A	782	ASN
1	A	786	ASN
1	A	881	ASN
1	A	969	ASN
1	A	987	ASN
1	A	1016	ASN
1	A	1063	ASN
1	A	1080	GLN
1	A	1147	HIS
1	A	1238	HIS
1	A	1344	ASN
1	A	1379	GLN
1	A	1470	GLN
1	A	1656	GLN
2	B	68	ASN
2	B	187	GLN
2	B	232	GLN
2	B	252	ASN
2	B	262	GLN
2	B	335	GLN
2	B	363	ASN
2	B	391	GLN
2	B	480	ASN
2	B	481	HIS
2	B	572	GLN
2	B	590	ASN
2	B	734	HIS
2	B	799	HIS
2	B	818	GLN
2	B	872	ASN
2	B	887	GLN
2	B	902	GLN
2	B	957	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	960	GLN
2	B	981	GLN
2	B	1069	HIS
2	B	1136	ASN
2	B	1153	HIS
2	B	1184	ASN
2	B	1338	HIS
2	B	1370	GLN
2	B	1506	ASN
2	B	1518	ASN
2	B	1550	HIS
2	B	1567	HIS
2	B	1585	ASN
2	B	1614	HIS
2	B	1630	ASN
2	B	1707	HIS
2	B	1839	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
4	FMN	B	2101	-	33,33,33	6.45	22 (66%)	48,50,50	1.35	6 (12%)
3	PNS	A	1901	1	2,5,21	0.59	0	1,5,29	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	B	2101	-	-	5/18/18/18	0/3/3/3
3	PNS	A	1901	1	-	1/1/3/27	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	13.49	1.58	1.39
4	B	2101	FMN	C6-C5A	12.40	1.58	1.40
4	B	2101	FMN	C9-C9A	12.37	1.59	1.39
4	B	2101	FMN	C9-C8	11.90	1.55	1.39
4	B	2101	FMN	O4-C4	9.96	1.42	1.23
4	B	2101	FMN	C4A-N5	9.56	1.51	1.30
4	B	2101	FMN	C9A-C5A	8.70	1.55	1.41
4	B	2101	FMN	O2-C2	8.20	1.40	1.24
4	B	2101	FMN	C2-N1	7.47	1.53	1.36
4	B	2101	FMN	C10-N1	7.19	1.47	1.33
4	B	2101	FMN	C8-C7	7.09	1.58	1.40
4	B	2101	FMN	C10-N10	6.61	1.51	1.37
4	B	2101	FMN	C5A-N5	6.53	1.51	1.39
4	B	2101	FMN	C2-N3	6.16	1.52	1.39
4	B	2101	FMN	C4-N3	6.15	1.50	1.38
4	B	2101	FMN	C9A-N10	5.22	1.50	1.41
4	B	2101	FMN	C4A-C10	3.64	1.54	1.44
4	B	2101	FMN	C1'-C2'	3.06	1.56	1.52
4	B	2101	FMN	P-O2P	3.03	1.66	1.54
4	B	2101	FMN	P-O3P	2.73	1.64	1.54
4	B	2101	FMN	C4A-C4	2.43	1.53	1.44
4	B	2101	FMN	C7M-C7	2.03	1.54	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2101	FMN	C4'-C3'-C2'	-3.56	107.64	113.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2101	FMN	C4A-C10-N10	3.07	120.87	116.48
4	B	2101	FMN	C10-C4A-N5	-2.77	119.16	124.81
4	B	2101	FMN	C4-N3-C2	-2.44	121.31	125.64
4	B	2101	FMN	C5A-C9A-N10	2.03	119.81	117.97
4	B	2101	FMN	O2-C2-N1	-2.01	118.45	121.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

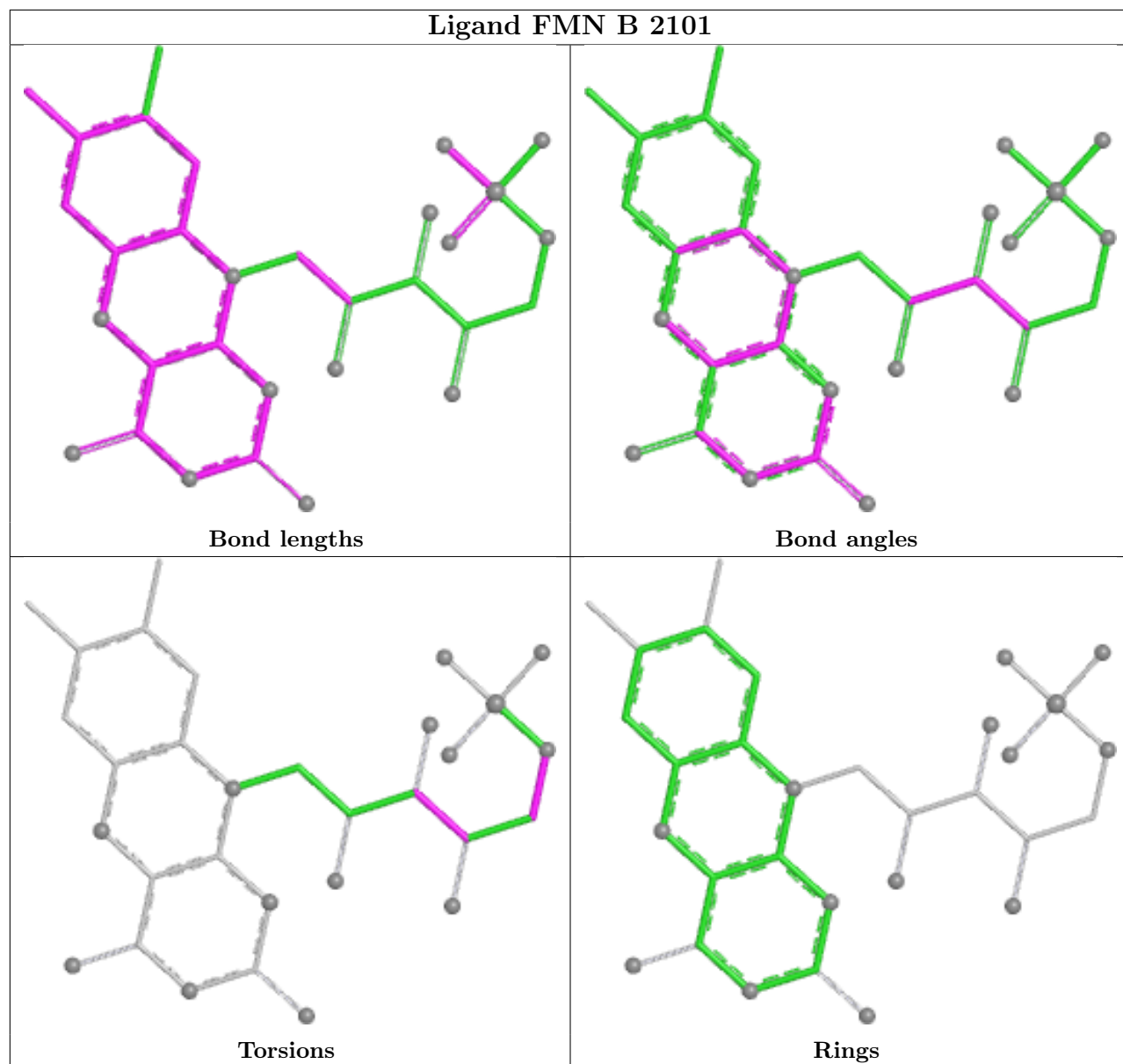
Mol	Chain	Res	Type	Atoms
3	A	1901	PNS	C29-C28-O27-P24
4	B	2101	FMN	C2'-C3'-C4'-C5'
4	B	2101	FMN	O3'-C3'-C4'-C5'
4	B	2101	FMN	C2'-C3'-C4'-O4'
4	B	2101	FMN	O3'-C3'-C4'-O4'
4	B	2101	FMN	C4'-C5'-O5'-P

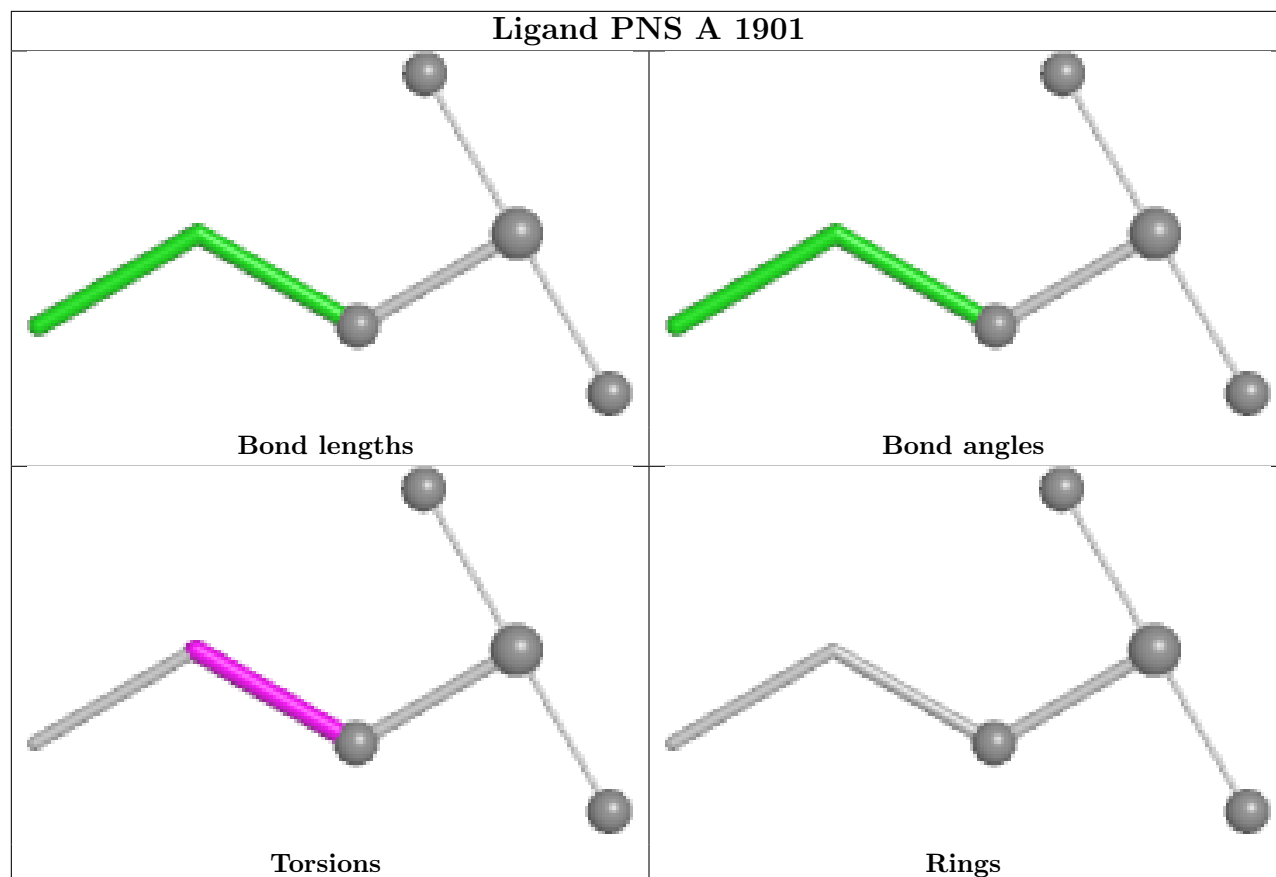
There are no ring outliers.

1 monomer is involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2101	FMN	34	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.

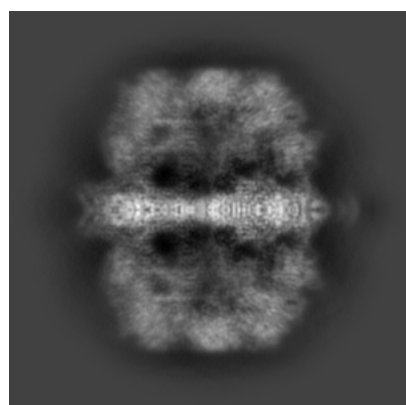
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20657. These allow visual inspection of the internal detail of the map and identification of artifacts.

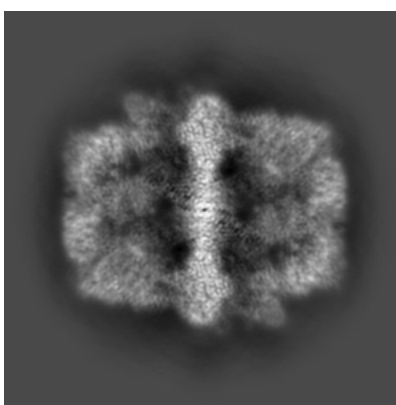
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

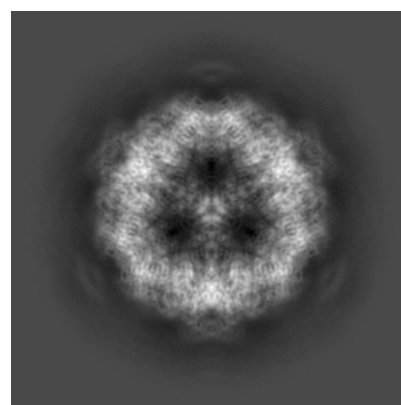
6.1.1 Primary map



X



Y

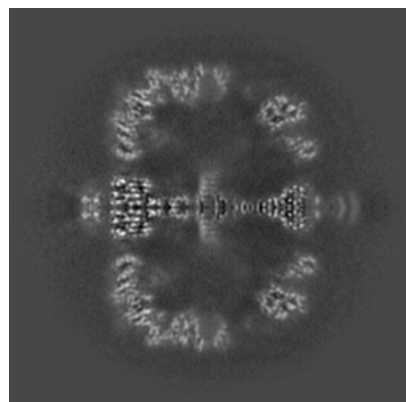


Z

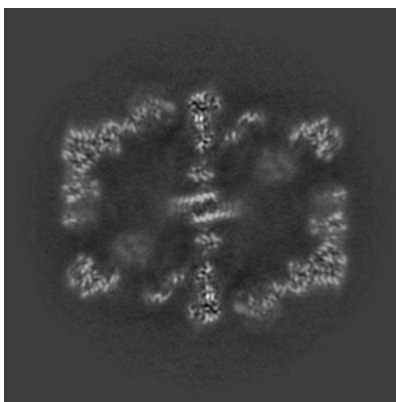
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

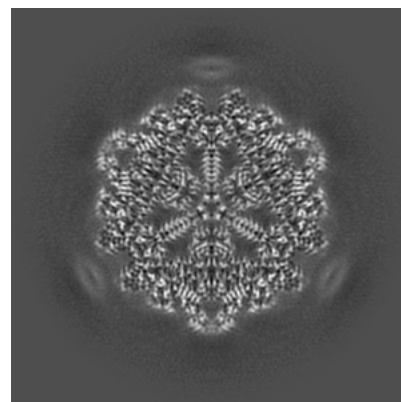
6.2.1 Primary map



X Index: 176



Y Index: 176

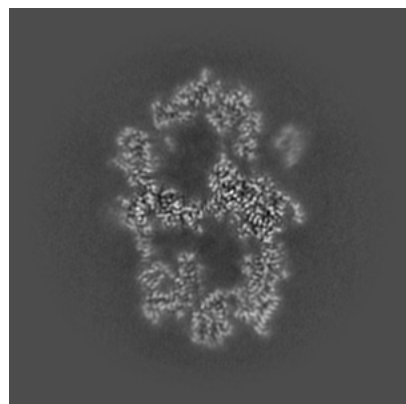


Z Index: 176

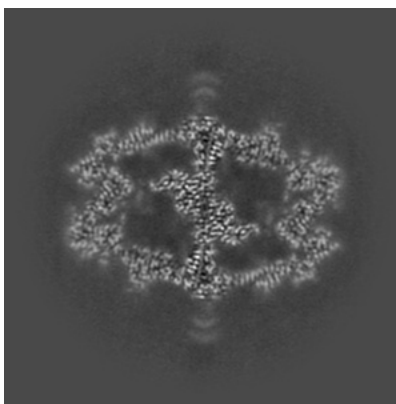
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

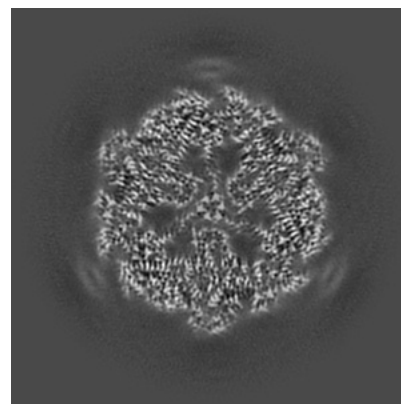
6.3.1 Primary map



X Index: 237



Y Index: 120

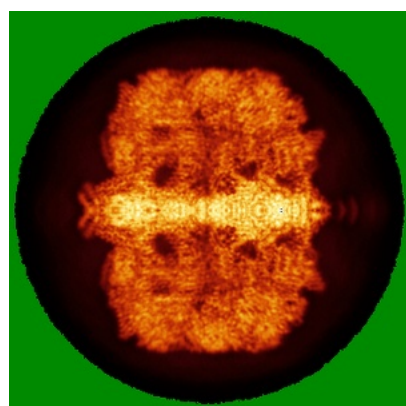


Z Index: 172

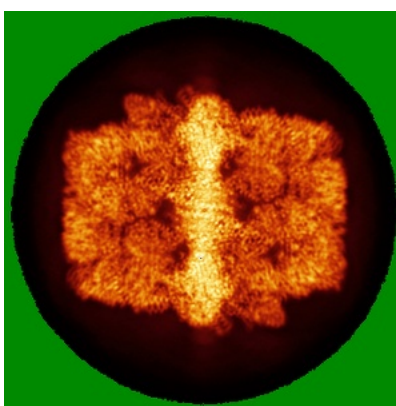
The images above show the largest variance slices of the map in three orthogonal directions.

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

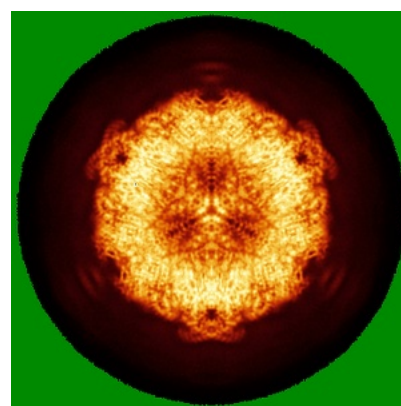
6.4.1 Primary map



X



Y

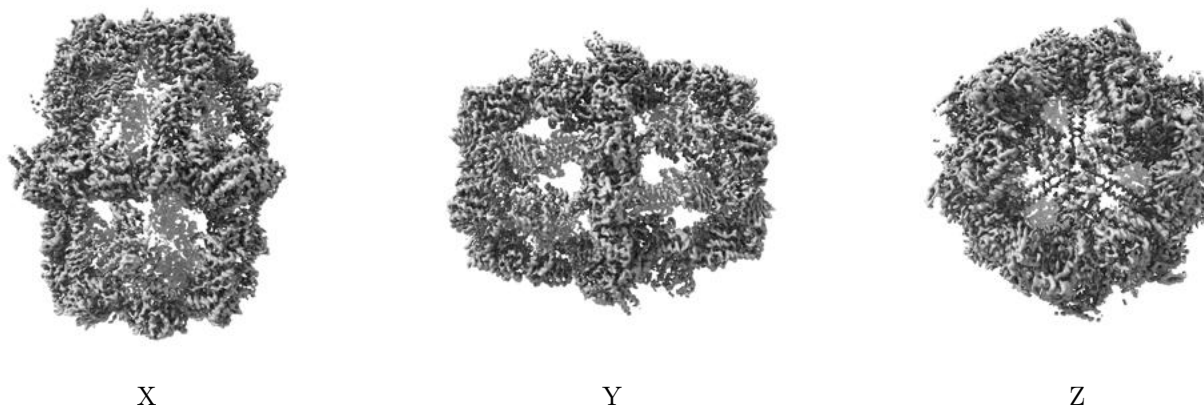


Z

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

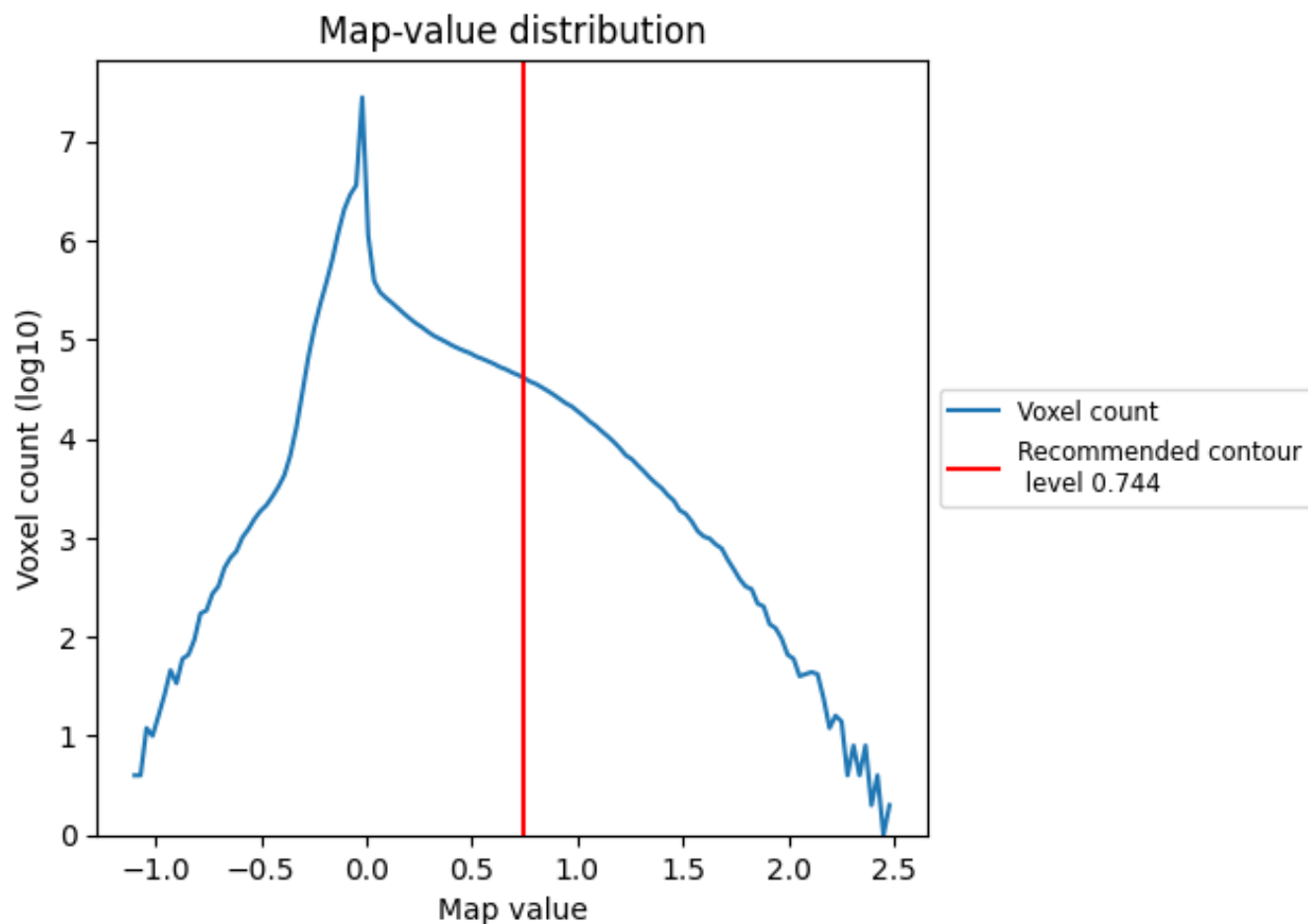
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

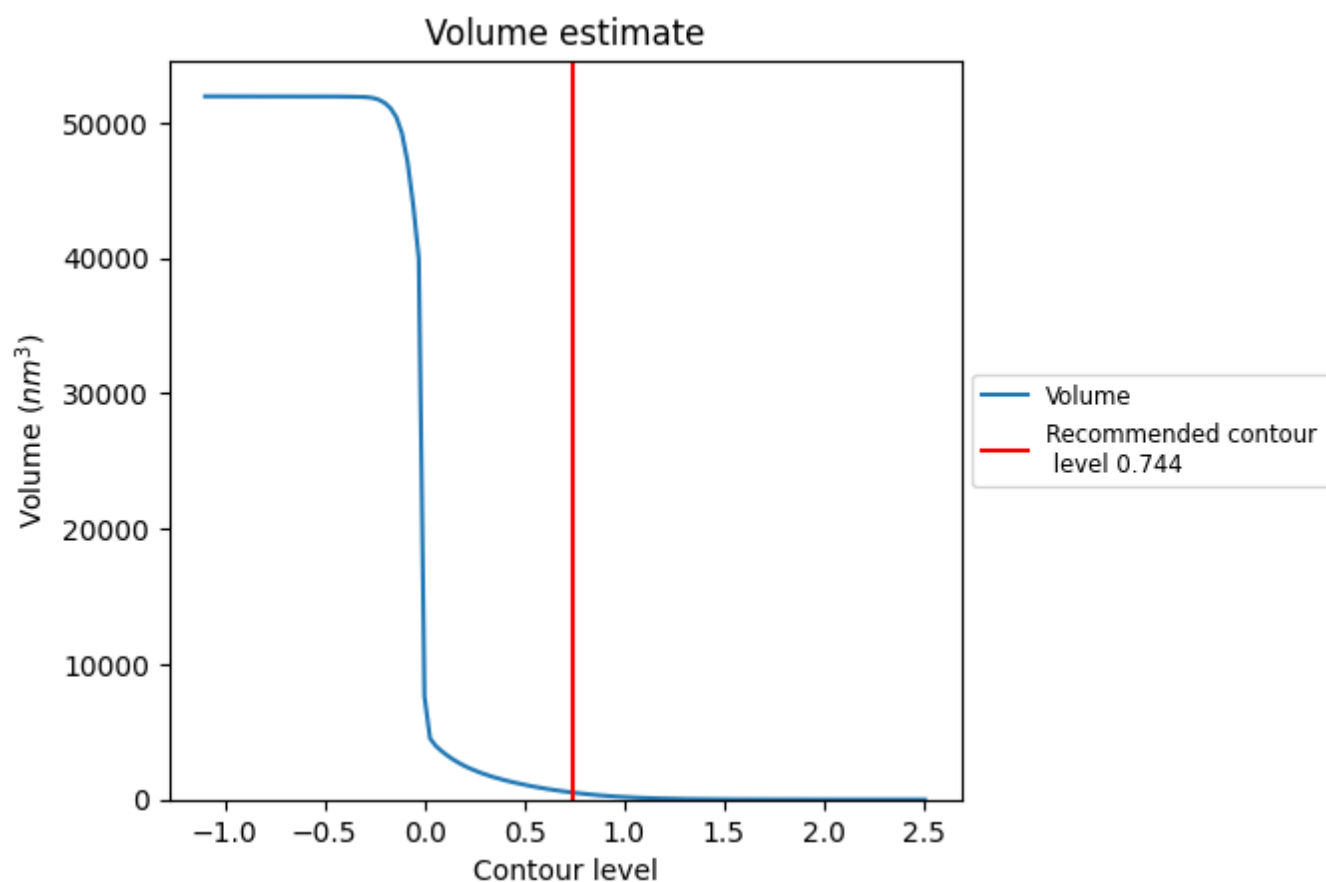
This section contains the results of statistical analysis of the map.

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.

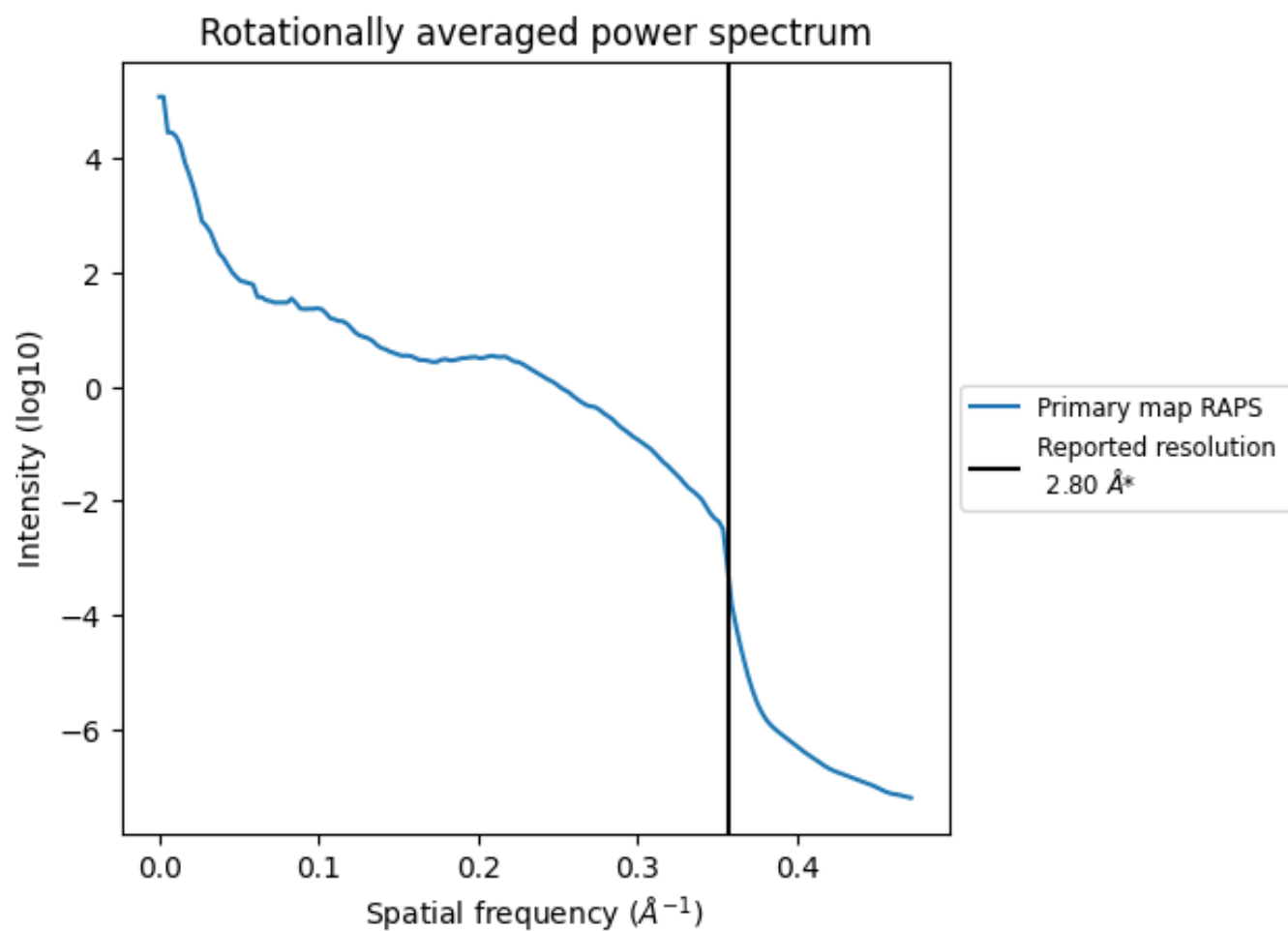
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm³; this corresponds to an approximate mass of 465 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 ⓘ

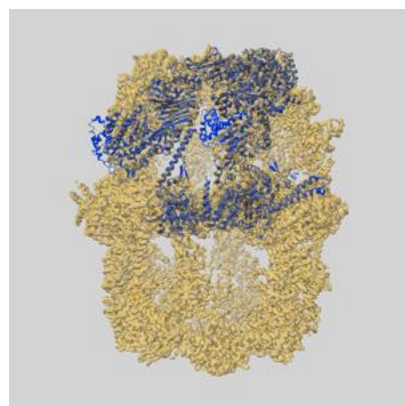
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

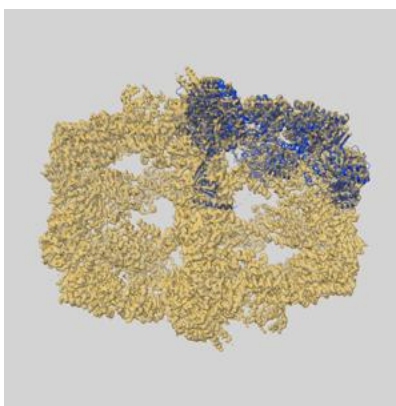
This section contains information regarding the fit between EMDB map EMD-20657 and PDB model 6U5V. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

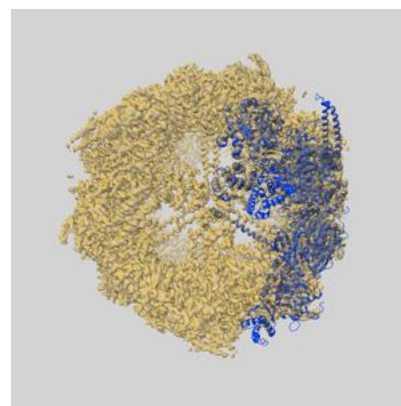
9.1.1 Map-model overlay [i](#)



X

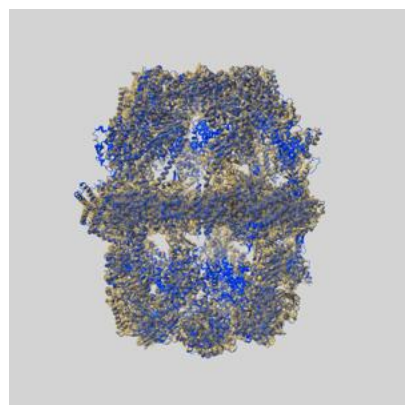


Y

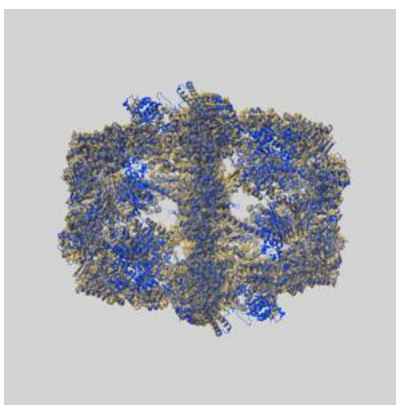


Z

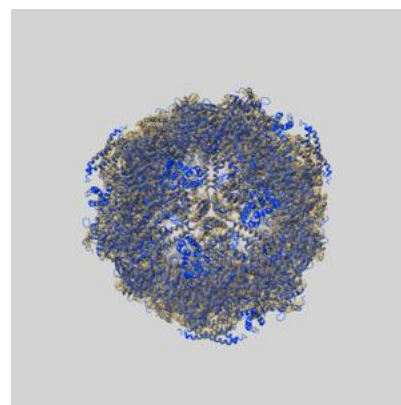
9.1.2 Map-model assembly overlay [i](#)



X



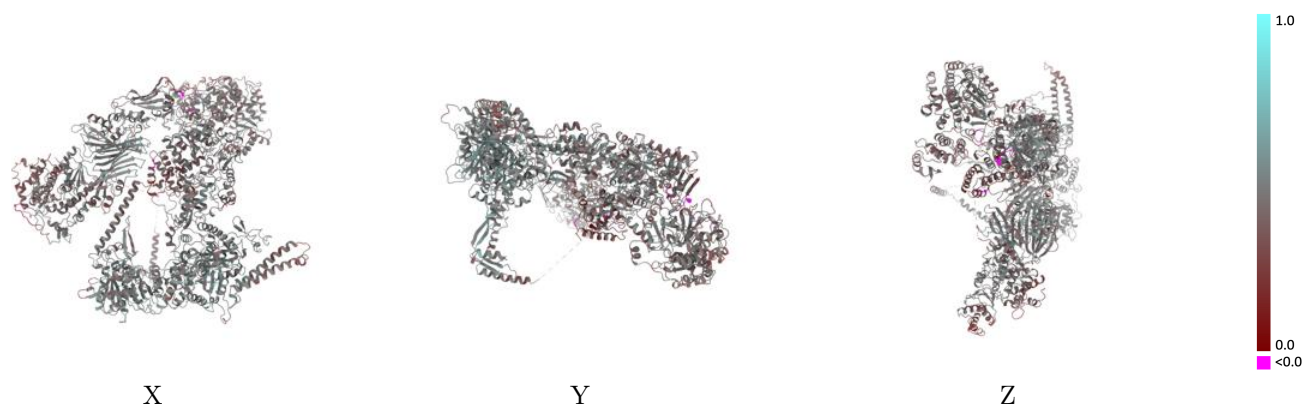
Y



Z

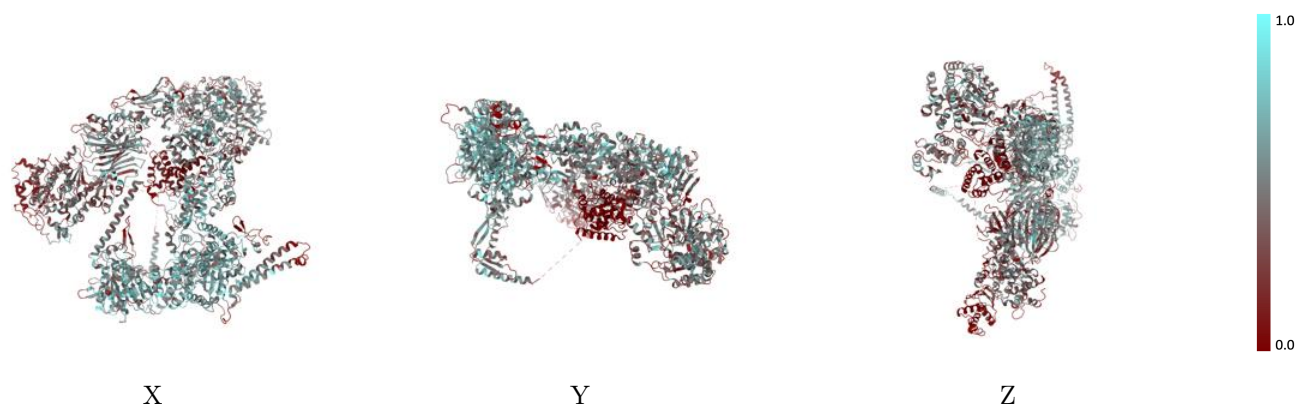
The images above show the 3D surface view of the map at the recommended contour level 0.744 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



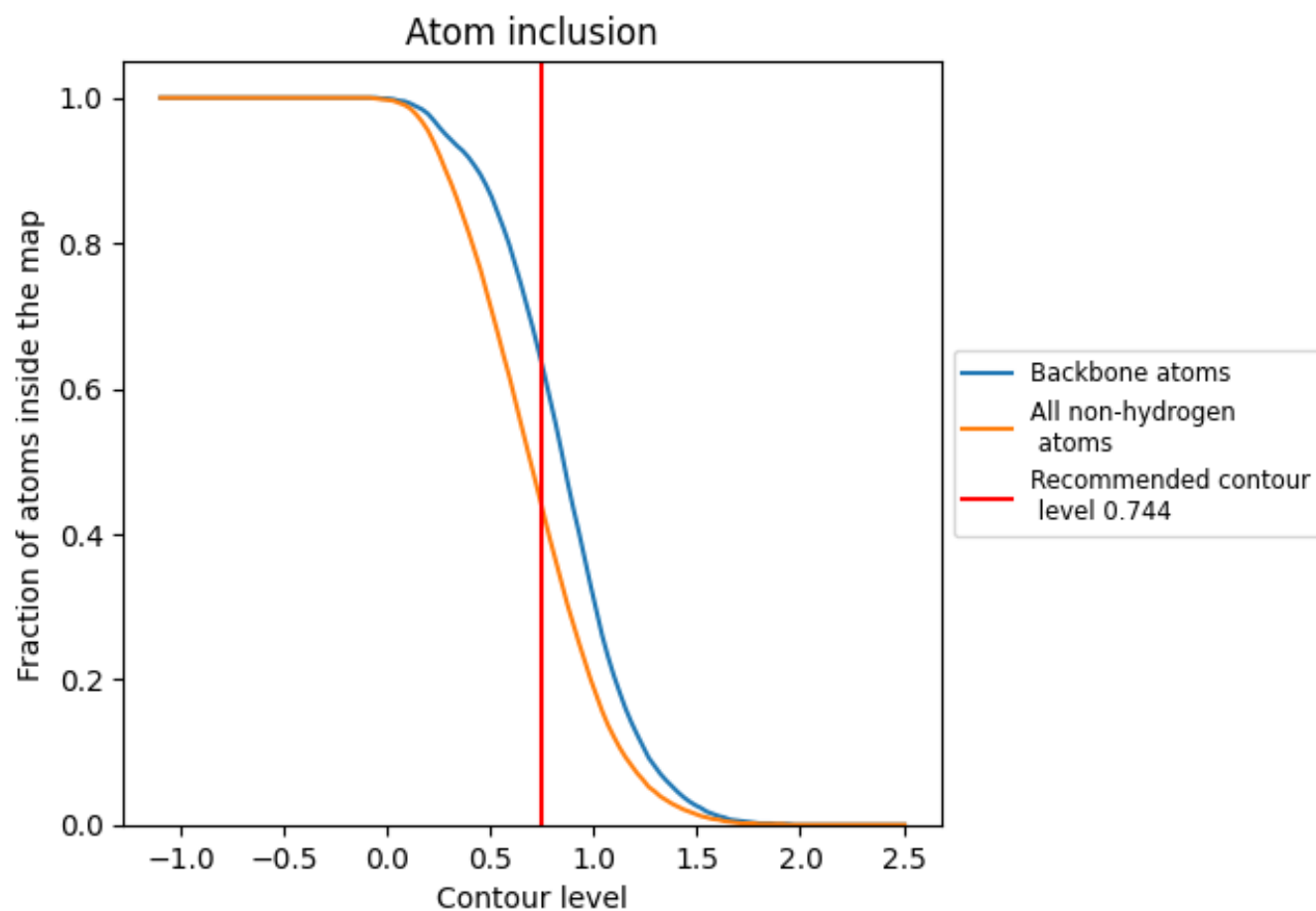
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.744).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 44% 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 (0.744) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4420	0.4530
A	0.4990	0.4750
B	0.4000	0.4360

