Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 04:19 AM EST

PDB ID	:	6U5V
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:

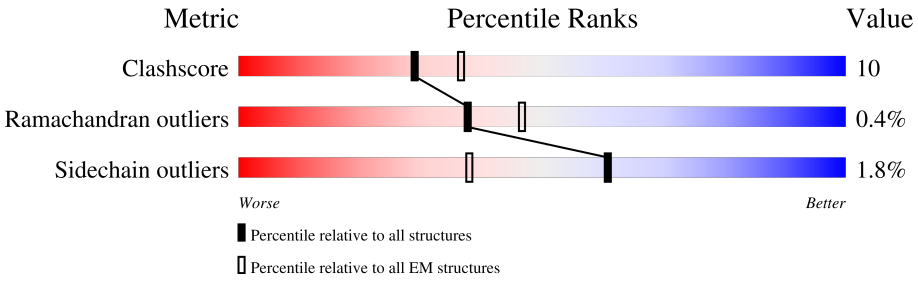
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	28% 69% 15% · 15%
2	B	2037	48% 78% 20% ·

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
			Total	C	N	O	S		
1	A	1596	12096	7645	2057	2349	45	0	0

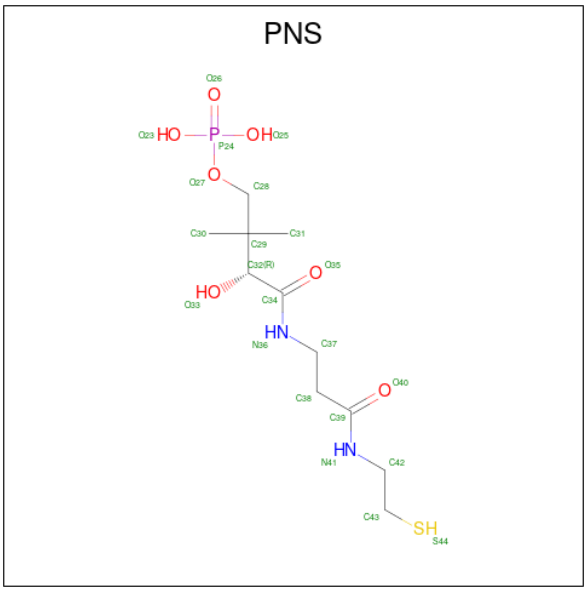
There are 10 discrepancies between the modelled and reference sequences:

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.

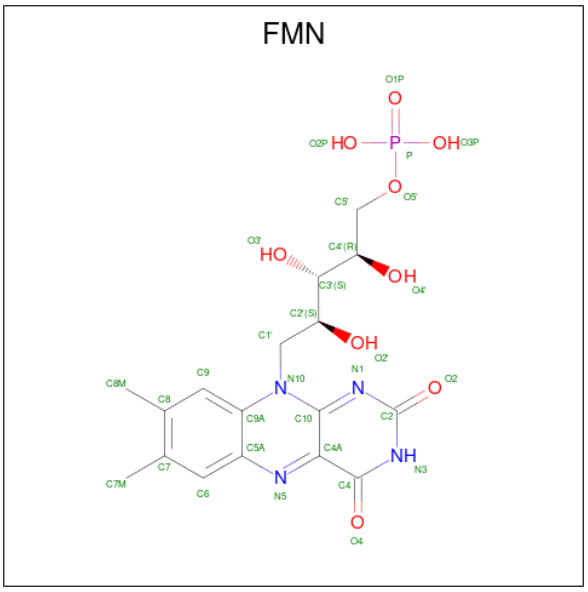
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	2033	16054	10290	2665	3045	54	1	0

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



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

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



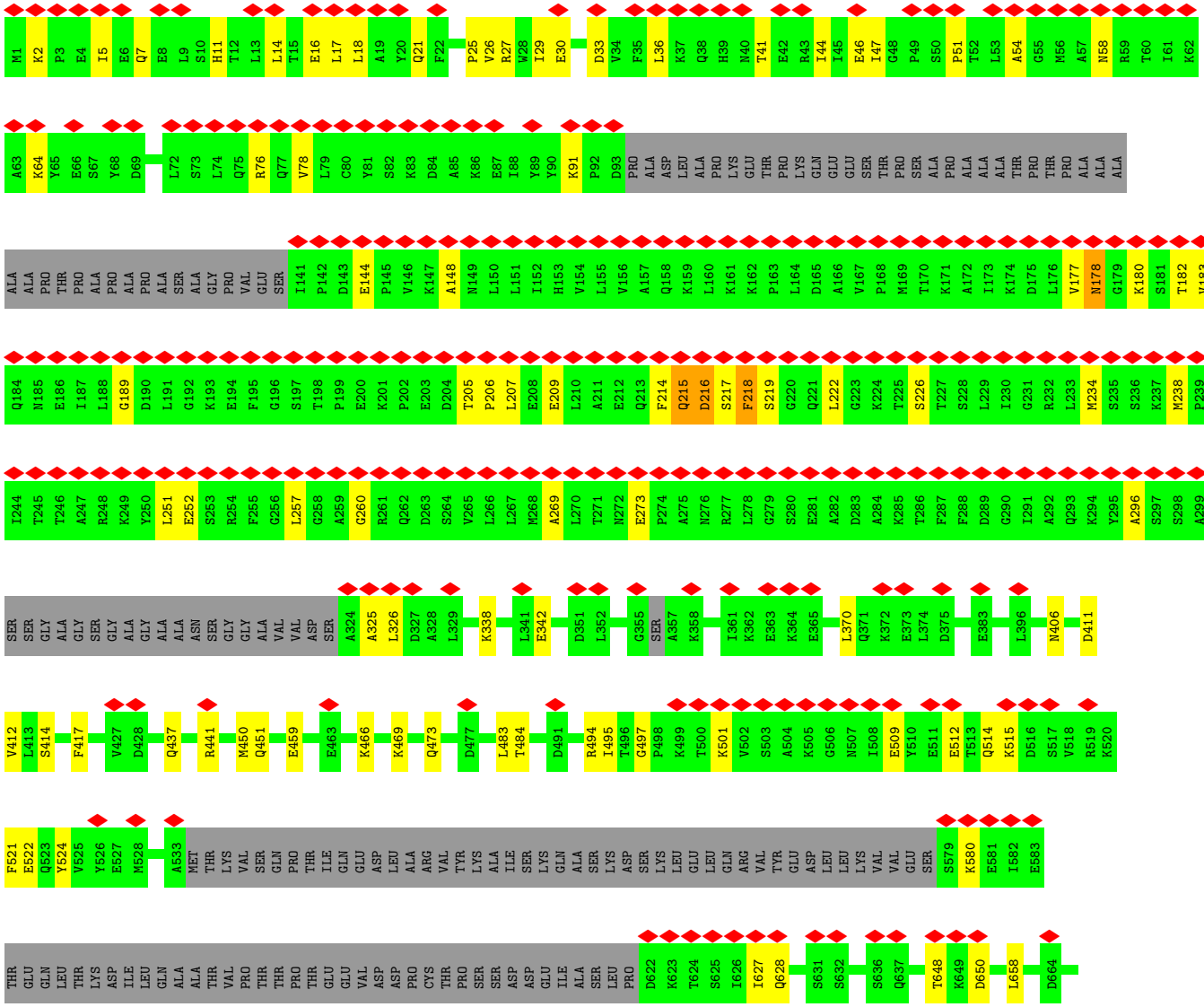
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	B	1	31	17	4	9	1	0

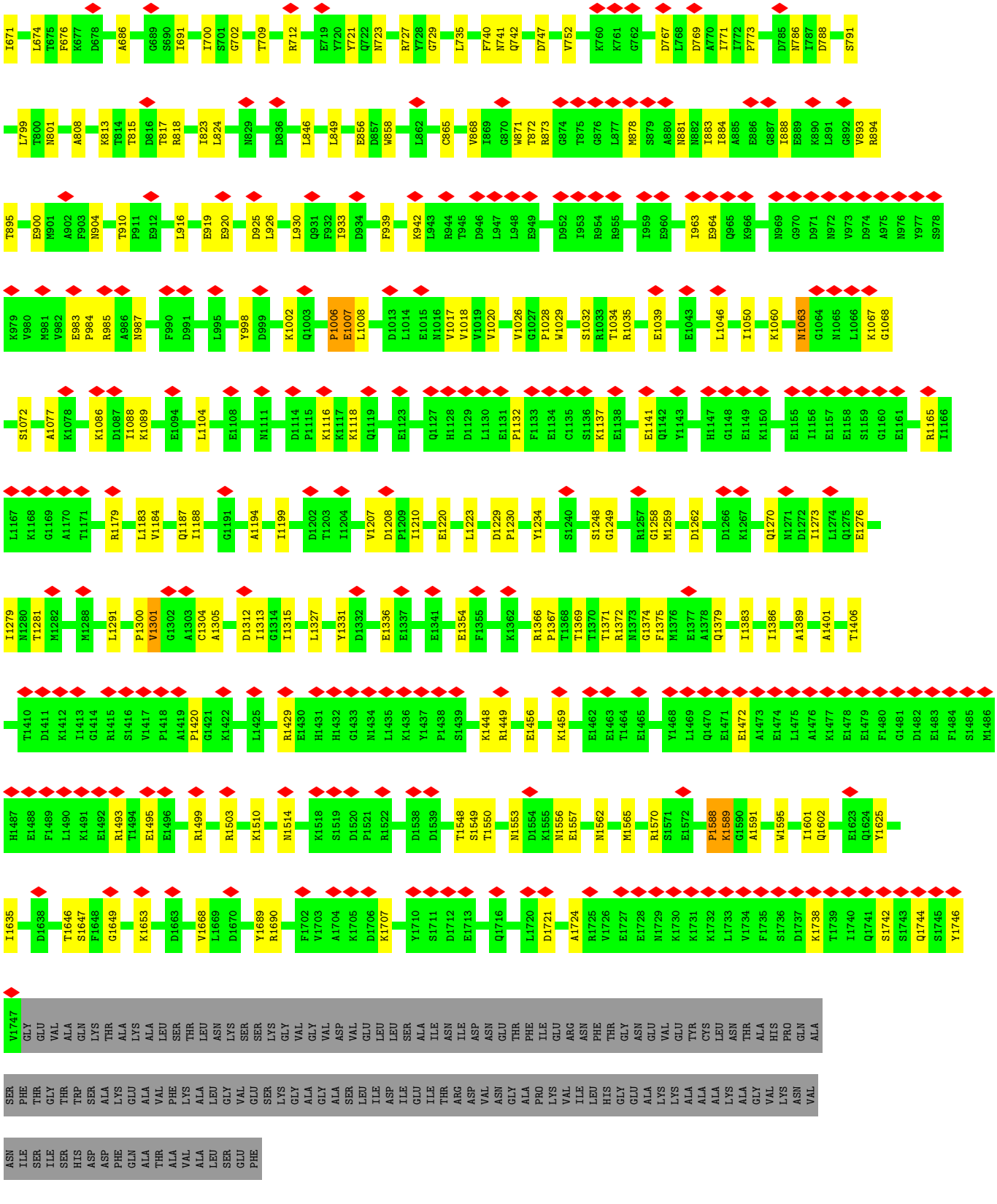
3 Residue-property plots (i)

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

- Molecule 1: Fatty acid synthase subunit alpha

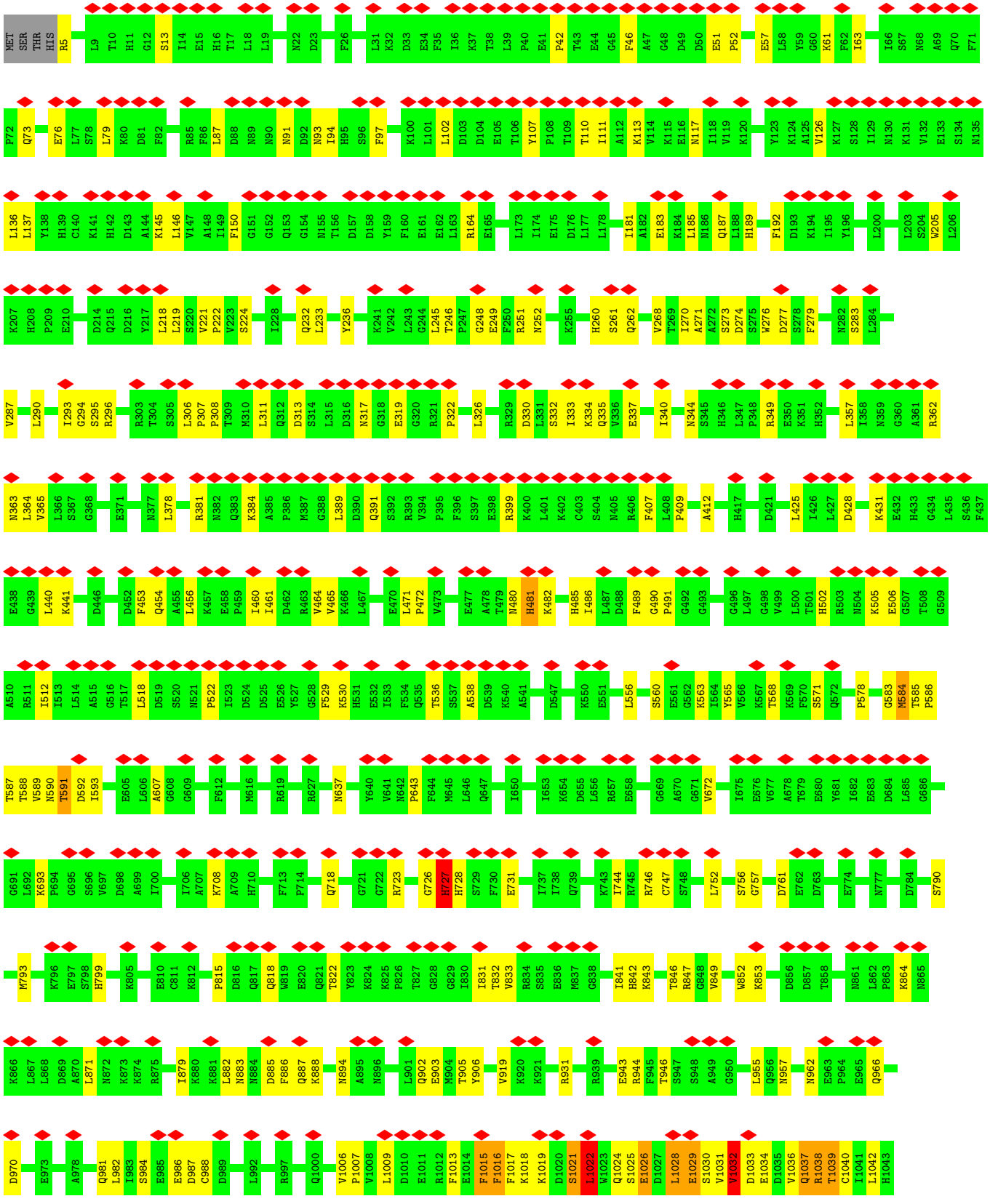
Chain A:

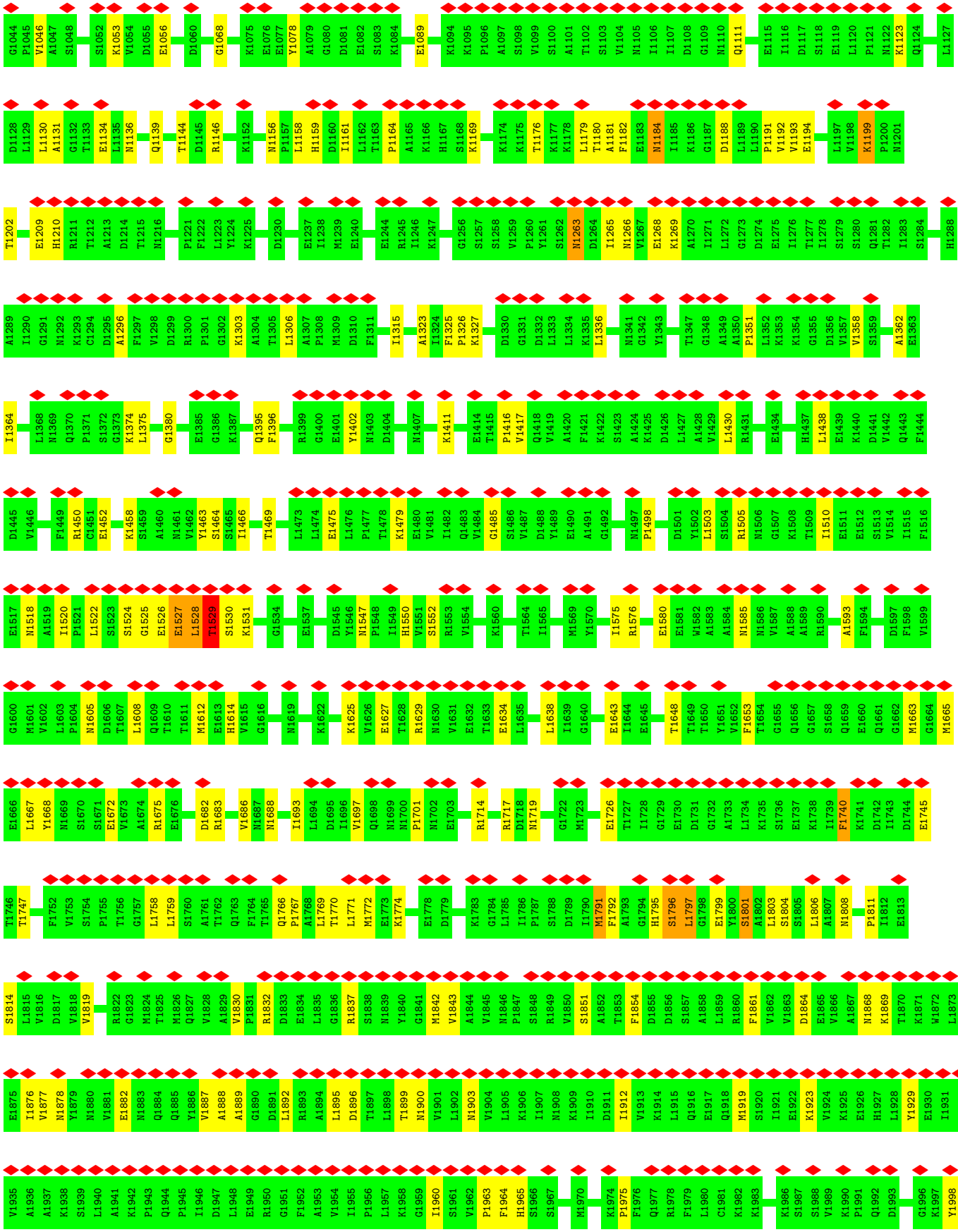




- Molecule 2: Fatty acid synthase subunit beta

Chain B:


MET SER THR HIS R5 L9 T10 H11 G12 S13 I14 E15 H16 T17 L18 L19 N22 D23 F26 L31 K32 D33 E34 F35 I36 K37 T38 L39 P40 E41 P42 T43 E44 G45 F46 A47 G48 D49 D50 E51 P52 E57 L58 Y59 G60 K61 F62 I63 I66 S67 N68 A69 Q70 F71
P72 Q73 E76 L77 S78 L79 K80 D81 F82 R85 F86 L87 D88 N89 N90 N91 D92 N93 I94 H95 S96 F97 K100 L101 L102 D103 D104 E105 T106 Y107 P108 T109 T110 I111 A112 K113 V114 K115 E116 N117 I118 V119 K120 Y123 K124 A125 V126 K127 S128 I129 N130 K131 V132 E133 S134 N135
L136 L137 Y138 H139 C140 K141 H142 D143 A144 K145 L146 V147 A148 I149 F150 G151 G152 Q153 G154 N155 T156 D157 D158 Y159 F160 E161 E162 L163 R164 E165 L173 I174 E175 D176 L177 L178 I181 A182 E183 K184 L185 N186 Q187 L188 H189 F192 D193 K194 I195 Y196 L200 L203 S204 W205 L206
K207 H208 P209 E210 D214 Q215 D216 Y217 L218 L219 S220 V221 P222 V223 S224 I228 Q232 L233 Y236 K241 V242 L243 G244 L245 T246 P247 G248 E249 F250 R251 N252 K255 H260 S261 Q262 V268 T269 I270 A271 A272 S273 D274 S275 W276 D277 S278 F279 N282 S283 L284
V287 L290 I293 G294 S295 R296 R303 T304 S305 L306 P307 P308 T309 M310 L311 Q312 D313 S314 L315 D316 N317 G318 E319 G320 R321 P322 L326 R329 D330 L331 S332 I333 K334 Q335 V336 E337 I340 N344 S345 H346 L347 P348 R349 E350 K351 H352 L357 I358 N359 G360 A361 R362
N363 L364 V365 L366 S367 G368 E371 N377 L378 R381 N382 Q383 K384 A385 P386 M387 G388 L389 D390 Q391 S392 R393 V394 P395 F396 S397 E398 R399 K400 L401 K402 C403 S404 N405 R406 F407 L408 P409 A412 H417 D421 L425 I426 L427 D428 K431 E432 H433 G434 L435 S436 F437
E438 G439 L440 K441 D446 D452 F453 Q454 A455 L456 K457 E458 P459 I460 I461 D462 R463 V464 V465 K466 L467 E470 L471 P472 V473 E477 A478 T479 N480 H481 K482 H485 I486 L487 D488 F489 G490 P491 G492 G493 G496 L497 G498 V499 L500 T501 H502 R503 N504 K505 E506 G507 T508 G509
A510 R511 I512 I513 L514 A515 G516 T517 L518 D519 S520 N521 P522 I523 D524 D525 E526 Y527 G528 F529 K530 H531 E532 I533 F534 Q535 T536 S537 A538 D539 K540 A541 D547 K550 E551 L556 S560 E561 G562 K563 I564 Y565 V566 K567 T568 K569 F570 S571 Q572 P578 G583 M584 T585 P586
T587 T588 V589 N590 T591 D592 I593 E605 L606 A607 G608 G609 F612 M616 R619 R627 N637 Y640 V641 N642 P643 F644 M645 L646 Q647 I650 I653 K654 D655 L656 R657 E658 G669 A670 G671 V672 I675 E676 V677 A678 T679 E680 Y681 I682 E683 D684 L685 G686
G691 L692 K693 P694 G695 S696 V697 D698 A699 I700 I706 A707 K708 A709 H710 F713 P714 Q718 G721 G722 R723 G726 H727 H728 S729 F730 E731 I737 I738 Q739 K743 I744 R745 R746 C747 S748 L752 S756 G757 D761 E762 D763 E774 N777 D784 S790
M793 K796 E797 S798 H799 K805 E810 C811 K812 P815 D816 Q817 Q818 W819 E820 Q821 T822 Y823 K824 K825 P826 T827 G828 G829 I830 I831 T832 V833 R834 S835 E836 M837 G838 I841 H842 K843 T846 R847 G848 V849 W852 K853 D856 D857 T858 N861 L862 P863 K864 N865
K866 L867 L868 D869 A870 L871 N872 K873 K874 R875 I879 K880 K881 L882 N883 N884 D885 F886 Q887 K888 N894 A895 N896 L901 Q902 E903 M904 T905 Y906 V919 K920 K921 R931 R939 E943 R944 F945 T946 S947 S948 A949 G950 L955 Q956 N957 N962 E963 P964 E965 Q966
D970 E973 A978 Q981 L982 I983 S984 E985 E986 D987 C988 D989 L992 R997 Q1000 V1006 P1007 V1008 L1009 D1010 E1011 R1012 F1013 E1014 F1015 F1016 F1017 K1018 K1019 D1020 S1021 L1022 W1023 Q1024 S1025 E1026 D1027 L1028 E1029 S1030 Y1031 V1032 D1033 E1034 D1035 V1036 Q1037 R1038 T1039 C1040 I1041 L1042 H1043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D1128 L1129 L1130 A1131 G1132 T1133 E1134 L1135 N1136 Q1139 T1144 D1145 R1146 K1152 N1156 P1157 L1158 H1159 D1160 I1161 L1162 T1163 P1164 A1165 K1166 H1167 S1168 K1169 K1174 K1175 T1176 K1177 K1178 L1179 T1180 A1181 F1182 E1183 N1184 I1185 K1186 G1187 D1188 L1189 L1190 P1191 V1192 V1193 E1194 L1197 V1198 K1199 P1200 N1201
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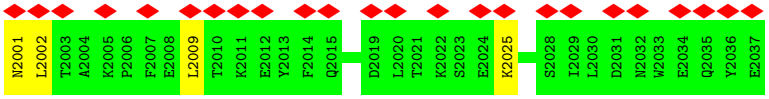
I1364 L1368 N1369 Q1370 P1371 S1372 G1373 K1374 L1375 G1380 E1385 G1386 K1387 Q1395 F1396 R1399 G1400 E1401 Y1402 N1403 D1404 N1407 K1411 E1414 T1415 P1416 V1417 Q1418 V1419 A1420 F1421 K1422 S1423 A1424 K1425 D1426 L1427 A1428 V1429 L1430 R1431 E1434 H1437 L1438 E1439 K1440 D1441 V1442 Q1443 F1444
D1445 V1446 F1449 R1450 C1451 E1452 K1458 S1459 A1460 N1461 V1462 Y1463 S1464 S1465 I1466 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 K1508 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 M1569 Y1570 I1575 R1576 E1580 E1581 W1582 A1583 A1584 N1585 N1586 V1587 A1588 A1589 R1590 A1593 F1594 D1597 F1598 V1599
G1600 M1601 V1602 L1603 P1604 N1605 D1606 T1607 L1608 Q1609 T1610 T1611 M1612 E1613 H1614 V1615 G1616 N1619 K1622 K1625 V1626 E1627 T1628 R1629 N1630 V1631 E1632 T1633 E1634 L1635 L1638 I1639 G1640 E1643 I1644 E1645 T1648 T1649 T1650 Y1651 V1652 F1653 T1654 G1655 Q1656 G1657 S1658 Q1659 E1660 Q1661 G1662 M1663 G1664 M1665
E1666 L1667 Y1668 N1669 S1670 S1671 E1672 V1673 A1674 R1675 E1676 D1682 R1683 V1686 N1687 N1688 I1693 L1694 D1695 I1696 V1697 Q1698 N1699 N1700 P1701 N1702 E1703 R1714 R1717 D1718 N1719 G1722 M1723 E1726 T1727 I1728 G1729 E1730 D1731 G1732 A1733 L1734 K1735 S1736 E1737 K1738 I1739 F1740 K1741 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 M1791 F1792 A1793 G1794 H1795 S1796 L1797 G1798 E1799 Y1800 S1801 A1802 L1803 S1804 S1805 L1806 A1807 N1808 P1811 I1812 E1813
S1814 L1815 V1816 D1817 V1818 V1819 R1822 G1823 M1824 T1825 M1826 Q1827 V1828 A1829 V1830 P1831 R1832 D1833 E1834 L1835 G1836 R1837 S1838 N1839 Y1840 G1841 M1842 V1843 A1844 V1845 N1846 P1847 S1848 R1849 V1850 S1851 A1852 T1853 F1854 D1855 D1856 S1857 A1858 L1859 R1860 F1861 V1862 L1863 D1864 E1865 V1866 A1867 N1868 K1869 T1870 K1871 W1872 L1873 L1874
E1875 I1876 V1877 N1878 Y1879 N1880 V1881 E1882 N1883 Q1884 Q1885 Y1886 V1887 A1888 A1889 G1890 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 L1928 Y1929 E1930 I1931 V1932 D1933 E1934
V1935 A1936 A1937 K1938 S1939 L1940 A1941 K1942 P1943 Q1944 P1945 I1946 D1947 L1948 E1949 R1950 G1951 F1952 A1953 V1954 I1955 P1956 L1957 K1958 G1959 I1960 S1961 V1962 P1963 F1964 H1965 S1966 S1967 H1970 K1974 P1975 F1976 Q1977 R1978 F1979 L1980 C1981 K1982 K1983 K1986 S1987 S1988 V1989 K1990 P1991 Q1992 D1993 G1996 K1997 Y1998


M2001
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T2003
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K2005
P2006
F2007
E2008
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K2011
E2012
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L2020
T2021
K2022
S2023
E2024
K2025
S2028
I2029
L2030
D2031
M2032
W2033
E2034
Q2035
Y2036
E2037

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: FMN, PNS

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	0.49	1/12322 (0.0%)	0.61	2/16684 (0.0%)
2	B	0.42	0/16423	0.62	12/22279 (0.1%)
All	All	0.45	1/28745 (0.0%)	0.62	14/38963 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	VAL	CB-CG1	-5.10	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1529	THR	CB-CA-C	-6.29	94.61	111.60
2	B	1430	LEU	CA-CB-CG	6.26	129.71	115.30
2	B	1667	LEU	CA-CB-CG	6.15	129.44	115.30
2	B	2009	LEU	CA-CB-CG	5.85	128.76	115.30
2	B	1529	THR	N-CA-C	5.52	125.91	111.00
2	B	1430	LEU	CB-CG-CD2	-5.51	101.64	111.00
2	B	326	LEU	CA-CB-CG	5.45	127.83	115.30
2	B	1791	MET	CB-CG-SD	5.40	128.60	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	137	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	370	LEU	CA-CB-CG	5.22	127.32	115.30
2	B	1022	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	B	727[A]	HIS	CB-CA-C	5.06	120.52	110.40
2	B	727[B]	HIS	CB-CA-C	5.06	120.52	110.40
1	A	1327	LEU	CB-CG-CD2	-5.04	102.43	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12096	0	11589	197	0
2	B	16054	0	16016	406	0
3	A	6	0	2	0	0
4	B	31	0	19	32	0
All	All	28187	0	27626	576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (576) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:252:GLU:HA	1:A:257:LEU:CA	1.57	1.28
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: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
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
1:A:216:ASP:CB	1:A:1067:LYS:C	2.16	1.14
2:B:1524:SER:O	2:B:1527:GLU:OE2	1.65	1.12
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:793:MET:SD	4:B:2101:FMN:HM71	1.91	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
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	0.98
2:B:756:SER:HA	4:B:2101:FMN:O5'	1.65	0.96
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:790:SER:OG	4:B:2101:FMN:HM81	1.68	0.93
2:B:584:MET:HB3	4:B:2101:FMN:N5	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:252:GLU:C	1:A:257:LEU:H	1.74	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: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
1:A:189:GLY:HA2	2:B:643:PRO:CB	2.05	0.85
2:B:790:SER:OG	4:B:2101:FMN:C8M	2.24	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:1525:GLY:C	2:B:1527:GLU:OE1	2.17	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:587:THR:OG1	4:B:2101:FMN:HM73	1.80	0.82
2:B:793:MET:SD	4:B:2101:FMN:C7M	2.67	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
2:B:590:ASN:C	2:B:592:ASP:H	1.85	0.80
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:GLN:NE2	2:B:1796:SER:HA	2.07	0.70
1:A:252:GLU:CA	1:A:257:LEU:N	2.29	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
2:B:584:MET:HB2	2:B:587:THR:HB	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:215:GLN:C	1:A:217:SER:H	1.99	0.65
2:B:1007:PRO:CD	2:B:1016:PHE:CD2	2.72	0.65
2:B:1527:GLU:H	2:B:1527:GLU:CD	1.96	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: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
1:A:1060:LYS:HZ2	1:A:1077:ALA:HA	1.64	0.63
2:B:728:HIS:ND1	2:B:842:HIS:N	2.43	0.63
1:A:1366:ARG:NH1	1:A:1371:THR:O	2.30	0.62
2:B:590:ASN:C	2:B:592:ASP:N	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:790:SER:HG	4:B:2101:FMN:HM81	1.65	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
1:A:984:PRO:HD2	1:A:1086:LYS:HZ1	1.66	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
2:B:1717:ARG:NH1	2:B:1747:THR:O	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1799:GLU:OE2	2:B:1998:TYR:OH	2.16	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
1:A:1304:CYS:HB2	1:A:1649:GLY:HA2	1.87	0.56
1:A:1029:TRP:O	1:A:1034:THR:OG1	2.24	0.56
2:B:587:THR:HG1	4:B:2101:FMN:HM73	1.71	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1118:LYS:NZ	1:A:1336:GLU:OE2	2.31	0.55
2:B:232:GLN:HE21	2:B:491:PRO:HD3	1.72	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:52:PRO:HG3	2:B:61:LYS:NZ	2.21	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:1022:LEU:HD23	2:B:1022:LEU:C	2.20	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
1:A:215:GLN:C	1:A:217:SER:N	2.61	0.54
2:B:931:ARG:NH1	2:B:962:ASN:OD1	2.40	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
1:A:180:LYS:CB	1:A:183:VAL:CB	2.86	0.53
2:B:1792:PHE:CE2	2:B:1998:TYR:HD1	2.27	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
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:1037:GLN:C	2:B:1039:THR:H	2.12	0.52
2:B:1830:VAL:HB	2:B:1832:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1919:MET:HE2	2:B:1923:LYS:HE2	1.92	0.52
1:A:1565:MET:HB3	1:A:1570:ARG:HG3	1.91	0.51
2:B:1036:VAL:C	2:B:1039:THR:HG22	2.18	0.51
2:B:1811:PRO:HD2	2:B:1814:SER:HB2	1.92	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
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:1037:GLN:C	2:B:1039:THR:N	2.64	0.51
2:B:1191:PRO:O	2:B:1210:HIS:NE2	2.41	0.51
1:A:251:LEU:C	1:A:257:LEU:CB	2.79	0.51
2:B:843:LYS:HZ2	2:B:849:VAL:HG13	1.75	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:727[A]:HIS:C	2:B:727[A]:HIS:CD2	2.85	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
1:A:325:ALA:O	1:A:326:LEU:C	2.48	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
2:B:1015:PHE:C	2:B:1015:PHE:CD2	2.84	0.50
2:B:1672:GLU:CD	2:B:1675:ARG:HH12	2.14	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:1899:THR:O	2:B:1903:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:1169:LYS:HZ2	2:B:1182:PHE:HD2	1.58	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
1:A:58:ASN:HD21	1:A:78:VAL:HG11	1.78	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:1549:SER:O	1:A:1549:SER:OG	2.30	0.48
2:B:590:ASN:CG	2:B:799:HIS:CE1	2.86	0.48
1:A:14:LEU:HD21	2:B:1803:LEU:HD22	1.95	0.48
2:B:556:LEU:HB2	2:B:1078:TYR:HE2	1.78	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
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: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
1:A:1248:SER:OG	1:A:1249:GLY:N	2.47	0.47
2:B:146:LEU:HD23	2:B:485:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1524:SER:C	2:B:1527:GLU:OE2	2.47	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: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:790:SER:HA	4:B:2101:FMN:HM83	1.97	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
1:A:494:ARG:HD3	1:A:514:GLN:HG2	1.97	0.46
1:A:1367:PRO:O	1:A:1369:THR:OG1	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: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
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:939:PHE:HD1	1:A:942:LYS:HZ3	1.60	0.46
1:A:1118:LYS:HG3	1:A:1336:GLU:OE2	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1060:LYS:NZ	1:A:1077:ALA:HA	2.31	0.45
1:A:91:LYS:NZ	2:B:1518:ASN:HD22	2.15	0.45
1:A:1276:GLU:HA	1:A:1281:THR:HG21	1.98	0.45
2:B:727[A]:HIS:O	2:B:727[A]:HIS:CD2	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
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
2:B:1022:LEU:CD2	2:B:1022:LEU:C	2.85	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
2:B:1017:PHE:CD1	2:B:1017:PHE:C	2.84	0.44
2:B:590:ASN:O	2:B:591:THR:C	2.48	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:1268:GLU:OE2	2:B:1411:LYS:NZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:700:ILE:HG22	1:A:729:GLY:HA2	2.00	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
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
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:1229:ASP:OD1	1:A:1229:ASP:N	2.52	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:1266:ASN:HB3	2:B:1269:LYS:NZ	2.33	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
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: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: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
1:A:998:TYR:CZ	1:A:1002:LYS:NZ	2.87	0.42
2:B:333:ILE:HG13	2:B:364:LEU:HD21	2.01	0.42
2:B:1266:ASN:HB3	2:B:1269:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ARG:HH11	1:A:1371:THR:HG23	1.85	0.42
2:B:585:THR:N	4:B:2101:FMN:N5	2.67	0.42
1:A:216:ASP:CB	1:A:1067:LYS:CA	2.97	0.42
2:B:756:SER:CA	4:B:2101:FMN:H5'2	2.48	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
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
2:B:61:LYS:NZ	2:B:117:ASN:OD1	2.31	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
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.87	0.41
1:A:1305:ALA:HB2	1:A:1647:SER:C	2.40	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
1:A:1557:GLU:OE2	1:A:1646:THR:OG1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1199:LYS:O	2:B:1202:THR:OG1	2.30	0.41
2:B:181:ILE:HG23	2:B:287:VAL:HG21	2.03	0.41
2:B:833:VAL:HG11	2:B:843:LYS:HZ3	1.85	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
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:1208:ASP:N	1:A:1208:ASP:OD1	2.55	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: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:145:LYS:HZ3	2:B:482:LYS:HG3	1.87	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: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%)	25 56
2	B	2032/2037 (100%)	1924 (95%)	103 (5%)	5 (0%)	47 78
All	All	3618/3922 (92%)	3437 (95%)	167 (5%)	14 (0%)	38 66

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1221/1579 (77%)	1204 (99%)	17 (1%)	67 90
2	B	1780/1784 (100%)	1742 (98%)	38 (2%)	53 84
All	All	3001/3363 (89%)	2946 (98%)	55 (2%)	61 86

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	580	LYS
1	A	712	ARG
1	A	786	ASN
1	A	799	LEU
1	A	987	ASN
1	A	1063	ASN
1	A	1179	ARG
1	A	1383	ILE
1	A	1429	ARG
1	A	1449	ARG
1	A	1503	ARG
1	A	1553	ASN
1	A	1589	LYS
1	A	1690	ARG
1	A	1707	LYS
1	A	1738	LYS
2	B	5	ARG
2	B	252	ASN
2	B	277	ASP
2	B	334	LYS
2	B	363	ASN
2	B	480	ASN
2	B	584	MET
2	B	589	VAL
2	B	727[A]	HIS
2	B	727[B]	HIS
2	B	864	LYS
2	B	957	ASN
2	B	1015	PHE
2	B	1016	PHE
2	B	1021	SER
2	B	1022	LEU
2	B	1025	SER
2	B	1026	GLU

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Mol	Chain	Res	Type
2	B	1028	LEU
2	B	1029	GLU
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	1184	ASN
2	B	1263	ASN
2	B	1527	GLU
2	B	1528	LEU
2	B	1529	THR
2	B	1585	ASN
2	B	1714	ARG
2	B	1740	PHE
2	B	1791	MET
2	B	1797	LEU
2	B	1801	SER
2	B	1837	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	451	GLN
1	A	478	ASN
1	A	786	ASN
1	A	881	ASN
1	A	987	ASN
1	A	1016	ASN
1	A	1062	HIS
1	A	1063	ASN
1	A	1238	HIS
1	A	1379	GLN
1	A	1546	HIS
1	A	1553	ASN
2	B	187	GLN
2	B	252	ASN
2	B	262	GLN
2	B	282	ASN
2	B	335	GLN

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Mol	Chain	Res	Type
2	B	363	ASN
2	B	391	GLN
2	B	415	HIS
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
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	1518	ASN
2	B	1550	HIS
2	B	1567	HIS
2	B	1585	ASN
2	B	1614	HIS
2	B	1684	HIS
2	B	1868	ASN
2	B	1900	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 monosaccharides 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	6.33	21 (63%)	48,50,50	1.29	5 (10%)
3	PNS	A	1901	1	2,5,21	0.74	0	1,5,29	0.19	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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	12.56	1.58	1.39
4	B	2101	FMN	C9-C9A	12.30	1.59	1.39
4	B	2101	FMN	C6-C5A	12.01	1.58	1.40
4	B	2101	FMN	C9-C8	11.09	1.55	1.39
4	B	2101	FMN	C4A-N5	10.60	1.51	1.30
4	B	2101	FMN	O4-C4	9.92	1.42	1.23
4	B	2101	FMN	O2-C2	8.82	1.40	1.24
4	B	2101	FMN	C9A-C5A	8.33	1.55	1.41
4	B	2101	FMN	C10-N1	7.09	1.47	1.33
4	B	2101	FMN	C2-N1	7.06	1.53	1.36
4	B	2101	FMN	C8-C7	6.89	1.58	1.40
4	B	2101	FMN	C10-N10	6.52	1.51	1.37
4	B	2101	FMN	C4-N3	6.21	1.50	1.38
4	B	2101	FMN	C5A-N5	6.20	1.51	1.39
4	B	2101	FMN	C2-N3	5.79	1.52	1.39
4	B	2101	FMN	C9A-N10	5.15	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C4A-C10	3.63	1.54	1.44
4	B	2101	FMN	C1'-C2'	3.02	1.56	1.52
4	B	2101	FMN	P-O2P	2.91	1.66	1.54
4	B	2101	FMN	P-O3P	2.62	1.64	1.54
4	B	2101	FMN	C4A-C4	2.45	1.53	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2101	FMN	C4A-C10-N10	3.00	120.87	116.48
4	B	2101	FMN	C4'-C3'-C2'	-2.75	107.64	113.36
4	B	2101	FMN	C10-C4A-N5	-2.69	119.16	124.86
4	B	2101	FMN	C4-N3-C2	-2.34	121.31	125.64
4	B	2101	FMN	O2-C2-N1	-2.04	118.45	121.83

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.

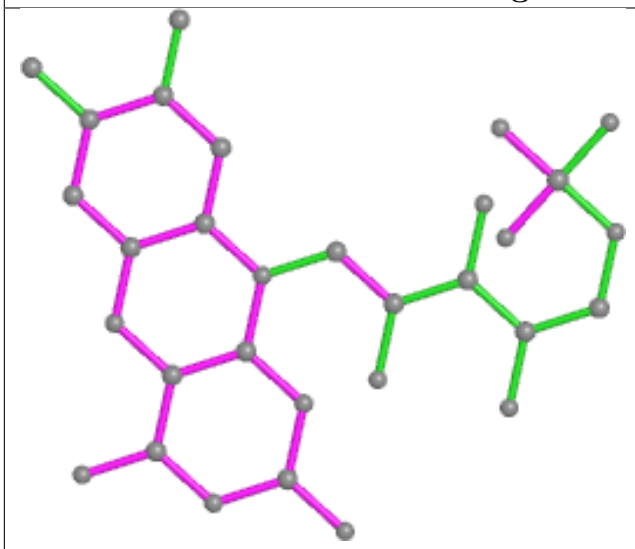
1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2101	FMN	32	0

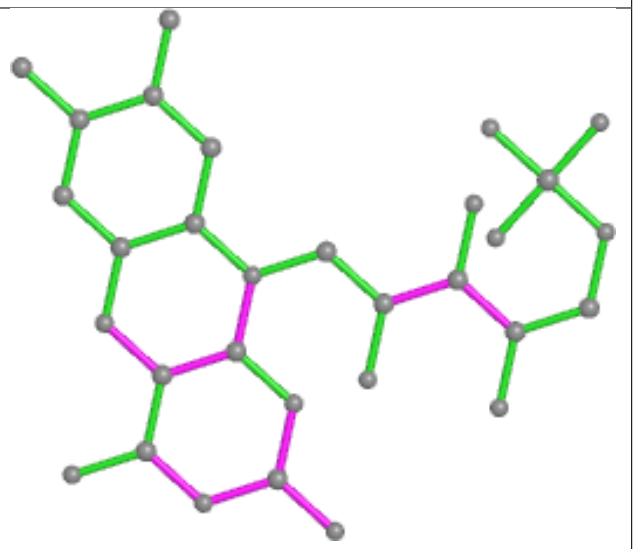
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

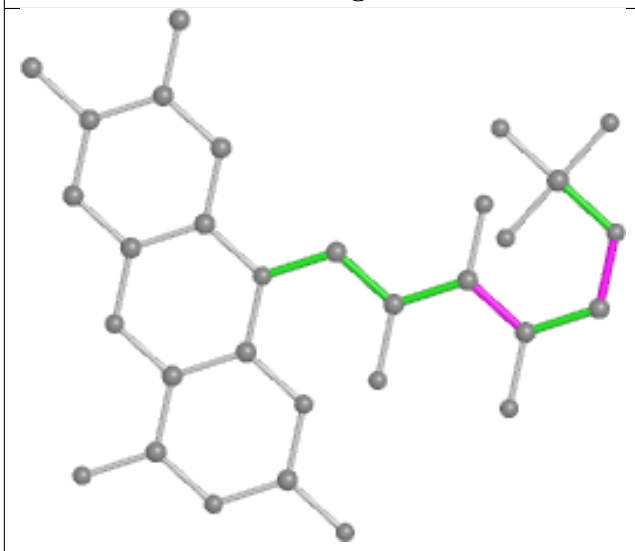
Ligand FMN B 2101



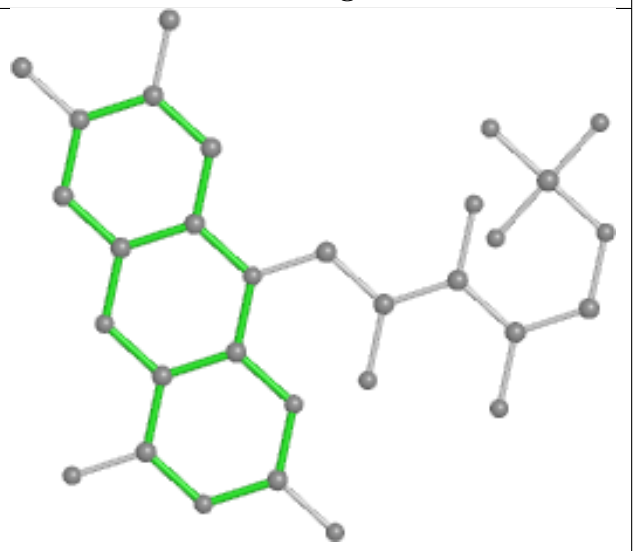
Bond lengths



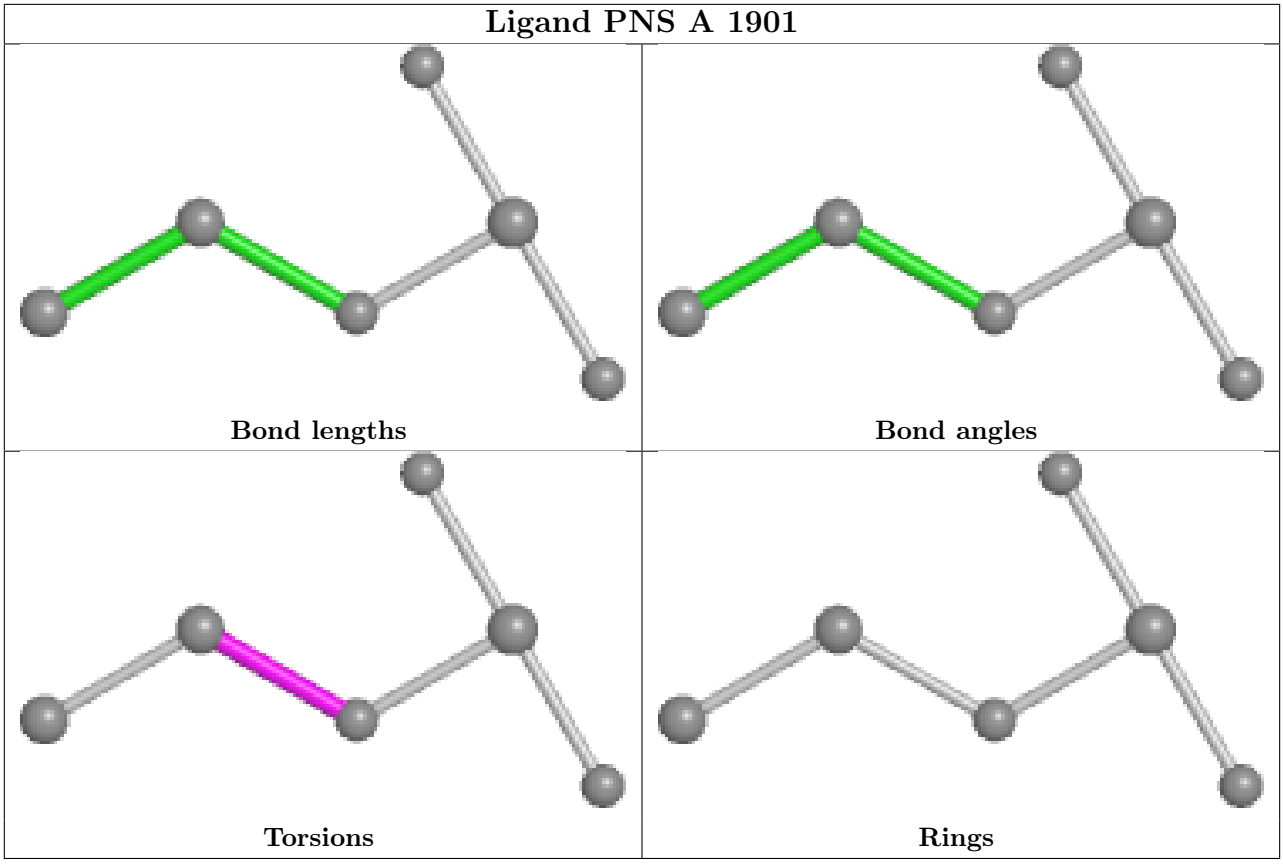
Bond angles



Torsions



Rings



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.

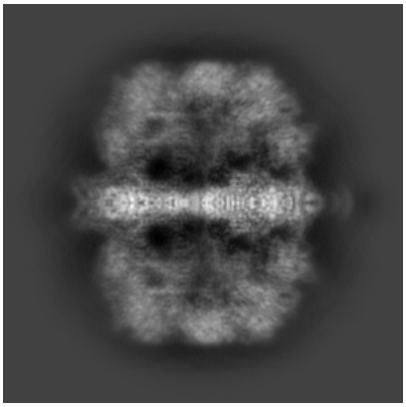
6 Map visualisation

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.

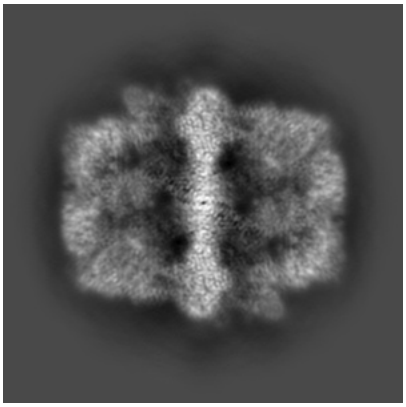
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

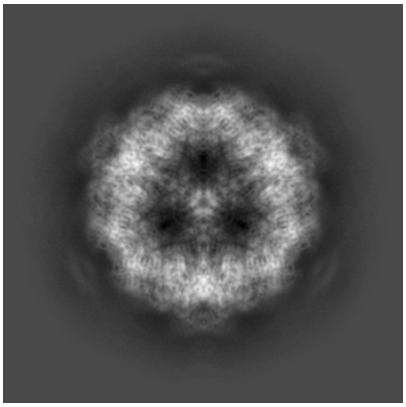
6.1.1 Primary map



X



Y

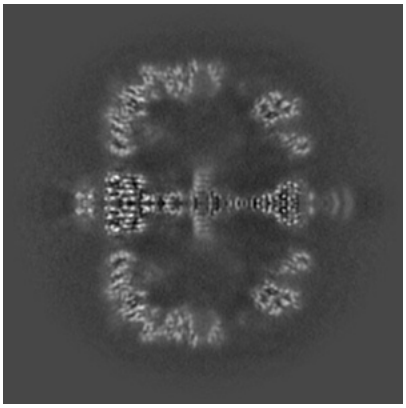


Z

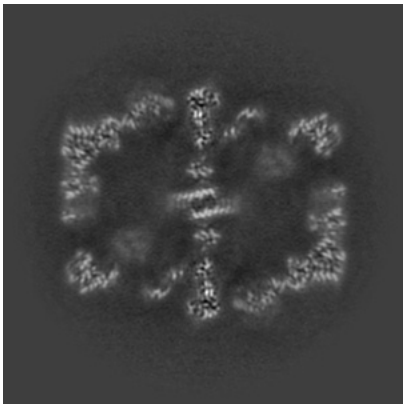
The images above show the map projected in three orthogonal directions.

6.2 Central slices

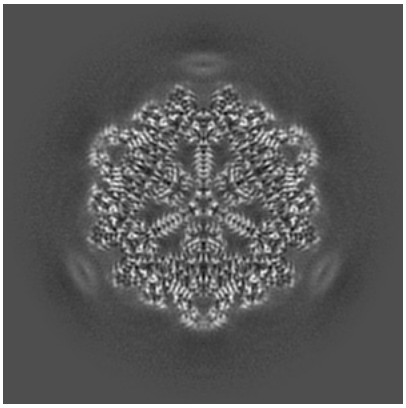
6.2.1 Primary map



X Index: 176



Y Index: 176

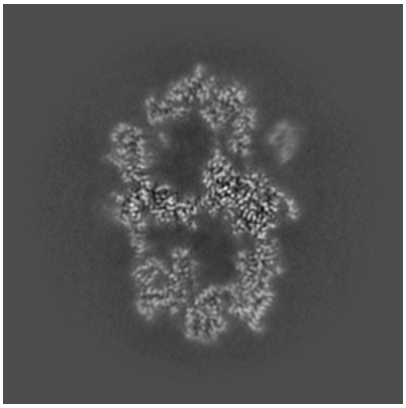


Z Index: 176

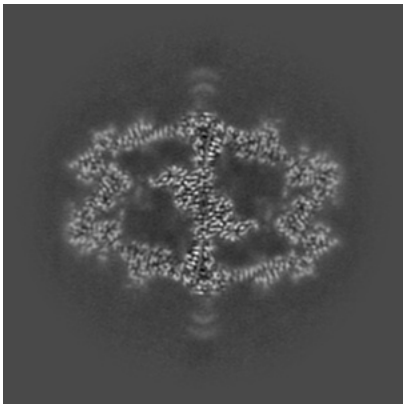
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

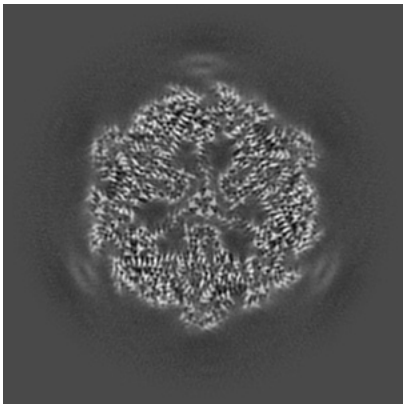
6.3.1 Primary map



X Index: 237



Y Index: 120

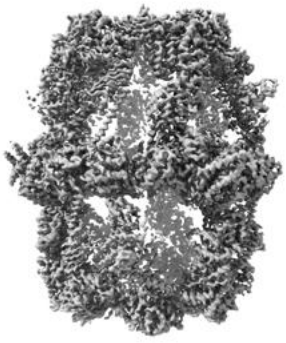


Z Index: 172

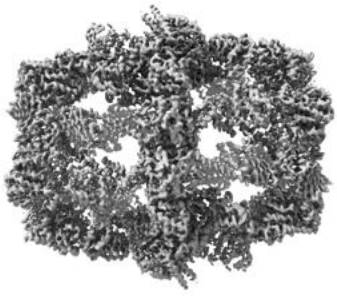
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

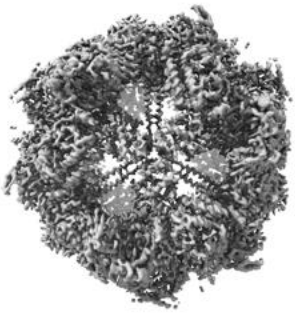
6.4.1 Primary map



X



Y



Z

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.

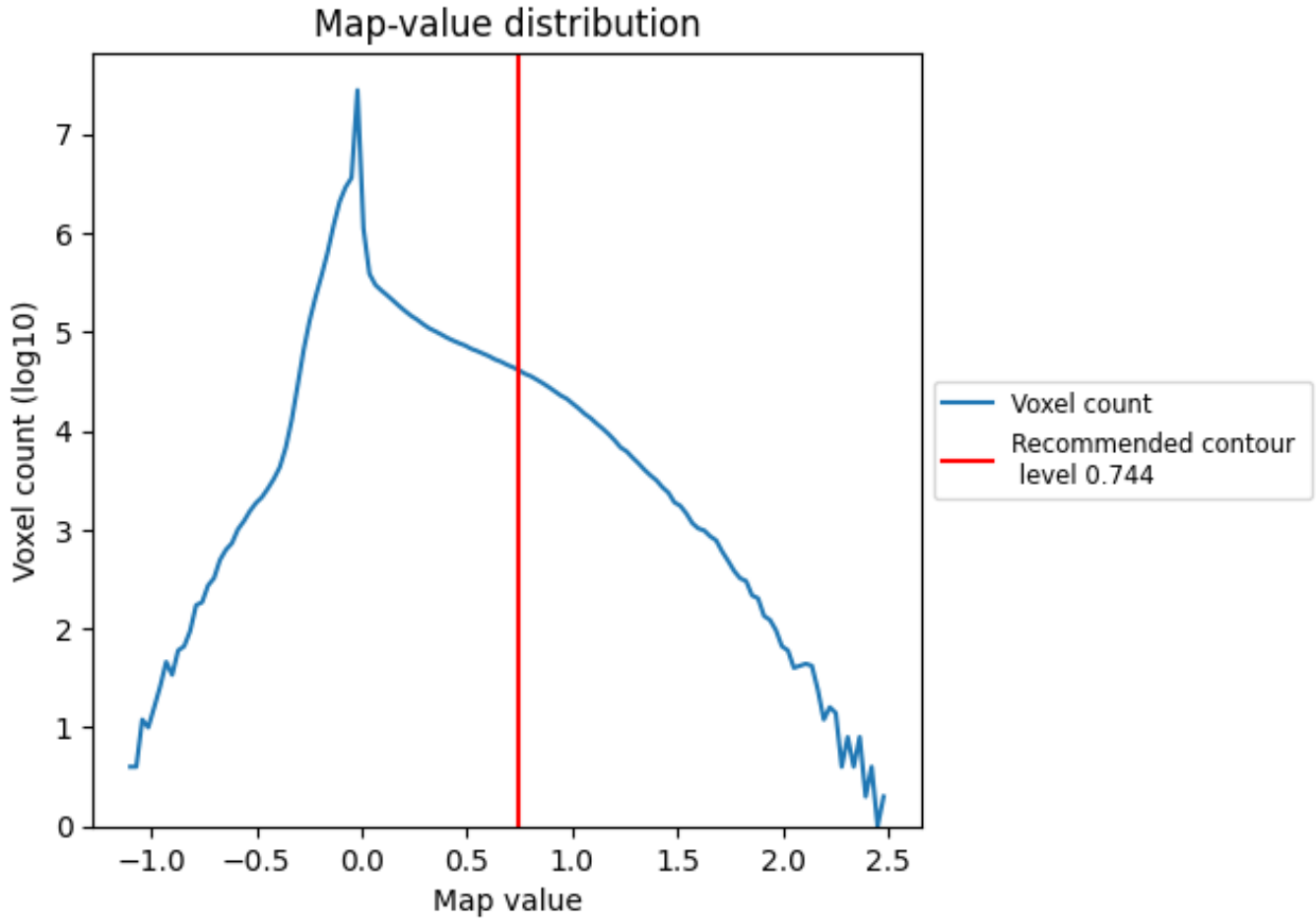
6.5 Mask visualisation (i)

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

7 Map analysis

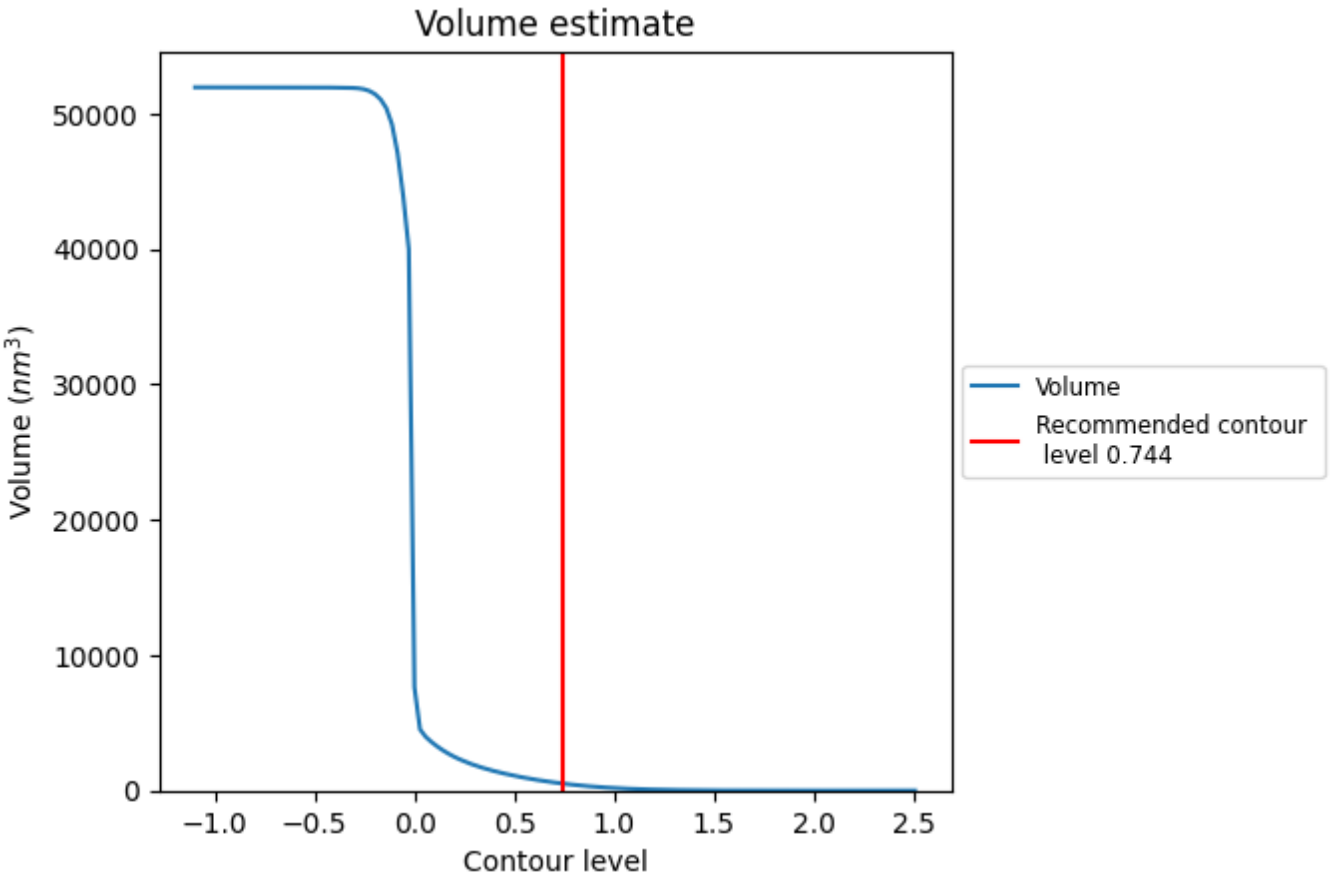
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

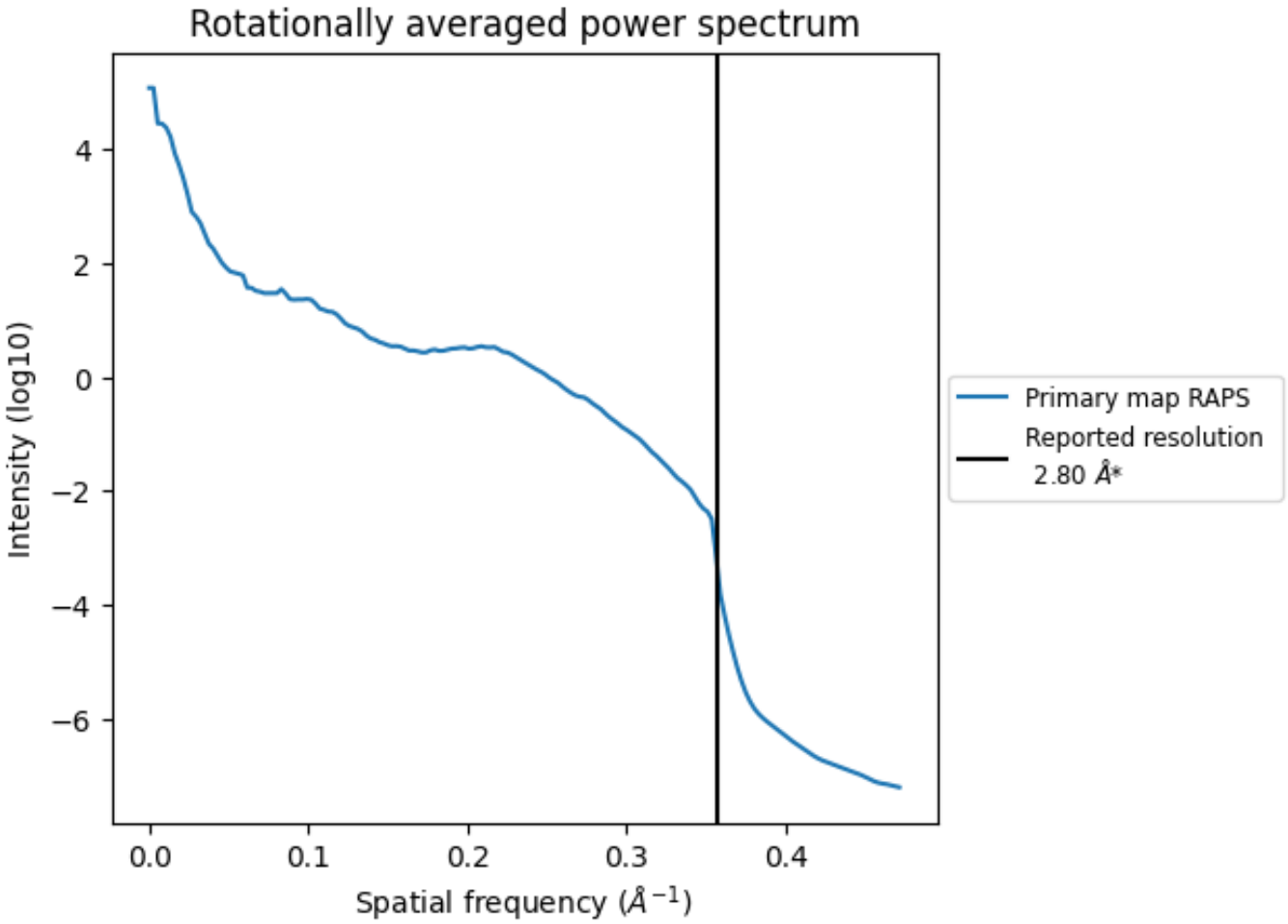
7.2 Volume estimate



The volume at the recommended contour level is 515 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation (i)

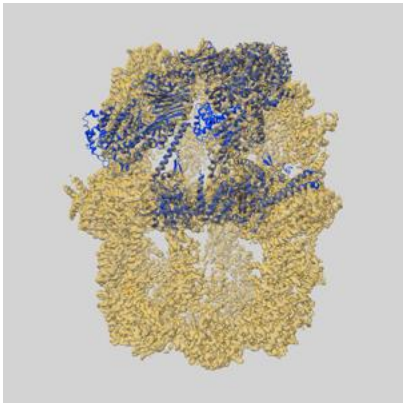
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

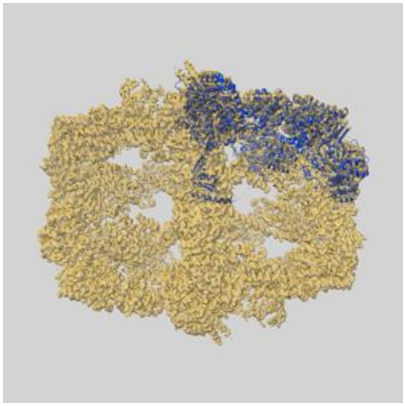
This section contains information regarding the fit between EMDB map EMD-20657 and PDB model 6U5V. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

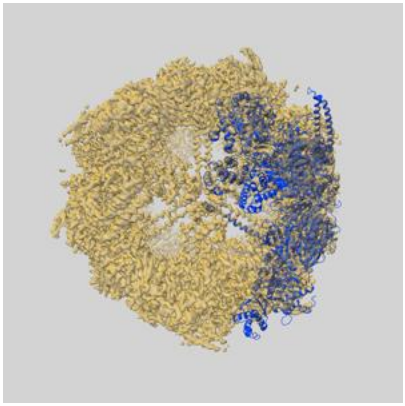
9.1.1 Map-model overlay



X

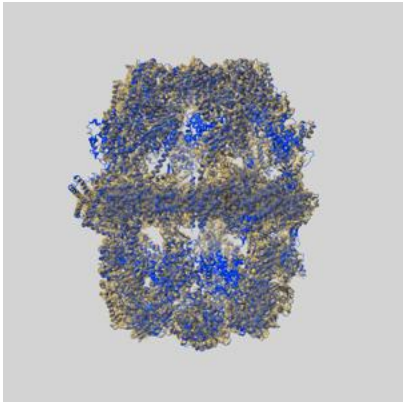


Y

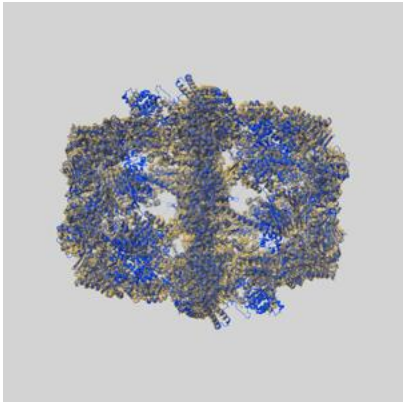


Z

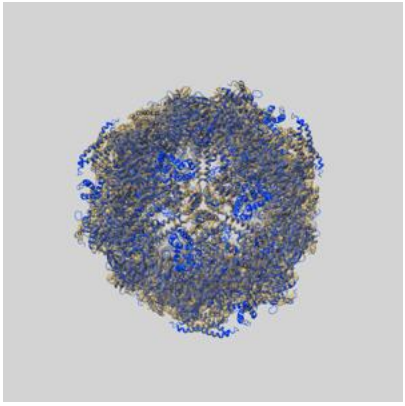
9.1.2 Map-model assembly overlay



X



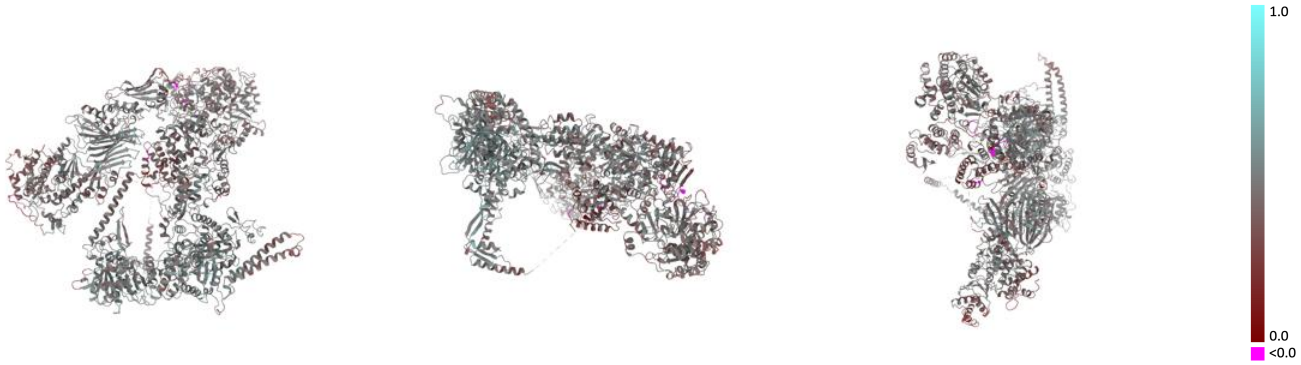
Y



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.

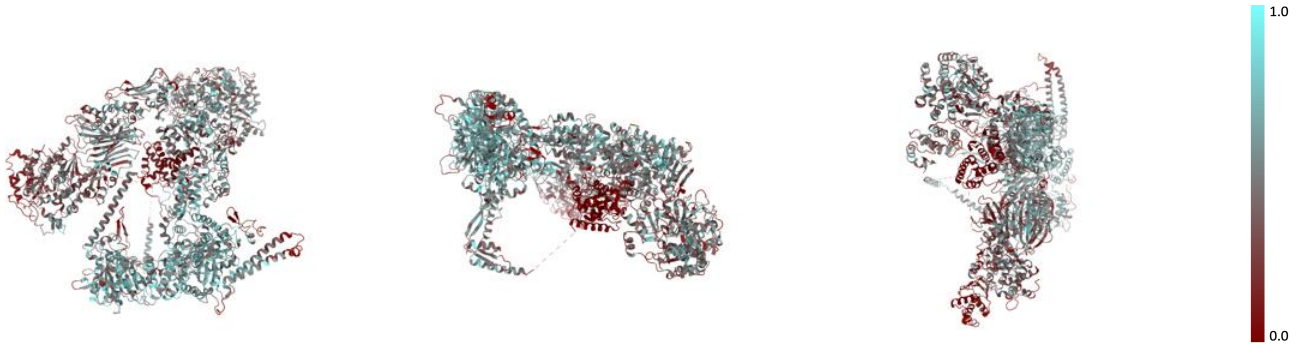
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

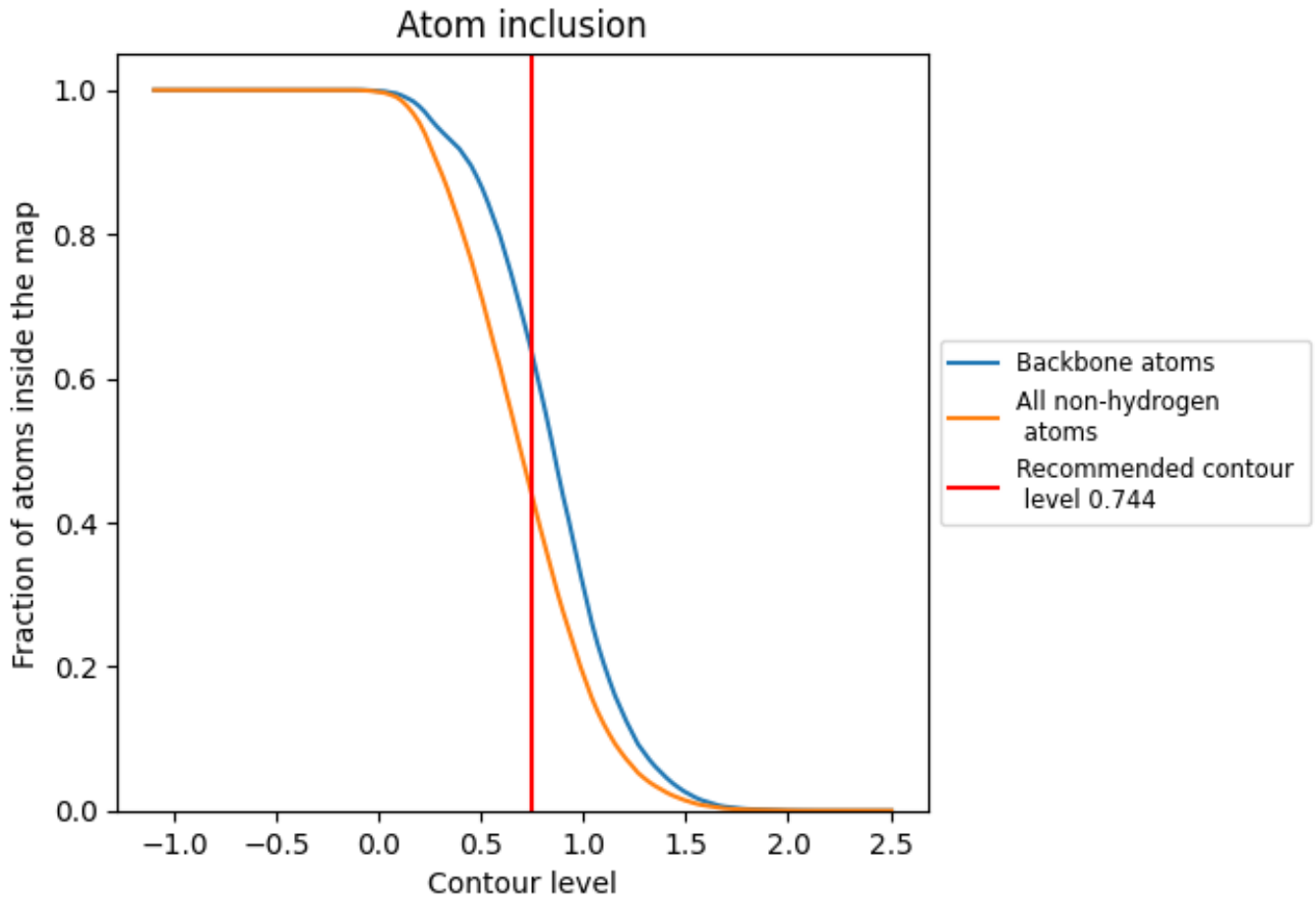
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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	0.4422	0.4530
A	0.4987	0.4750
B	0.3998	0.4360