Full wwPDB EM Validation Report ⓘ

Feb 27, 2023 – 05:41 pm GMT

PDB ID	:	8ALZ
EMDB ID	:	EMD-15521
Title	:	Cryo-EM structure of ASCC3 in complex with ASC1
Authors	:	Jia, J.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2022-08-01
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

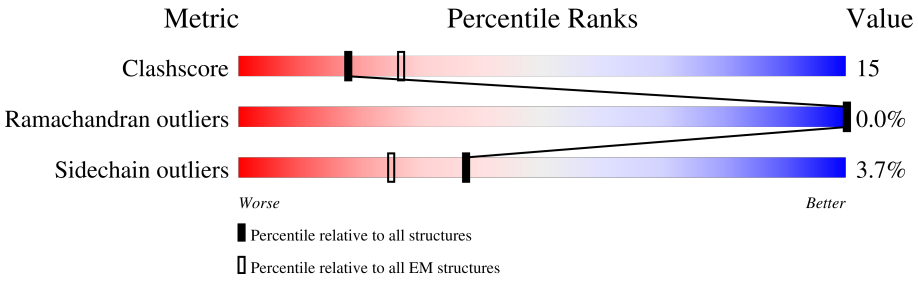
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	585	29% 15% 56%
2	B	1806	64% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16409 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 Activating signal cointegrator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	258	2052	1299	367	370	16	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q15650
A	-2	ALA	-	expression tag	UNP Q15650
A	-1	GLU	-	expression tag	UNP Q15650
A	0	PHE	-	expression tag	UNP Q15650

- Molecule 2 is a protein called Activating signal cointegrator 1 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1783	14355	9201	2482	2609	63	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	397	GLY	-	expression tag	UNP Q8N3C0
B	398	ALA	-	expression tag	UNP Q8N3C0
B	399	GLU	-	expression tag	UNP Q8N3C0
B	400	PHE	-	expression tag	UNP Q8N3C0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

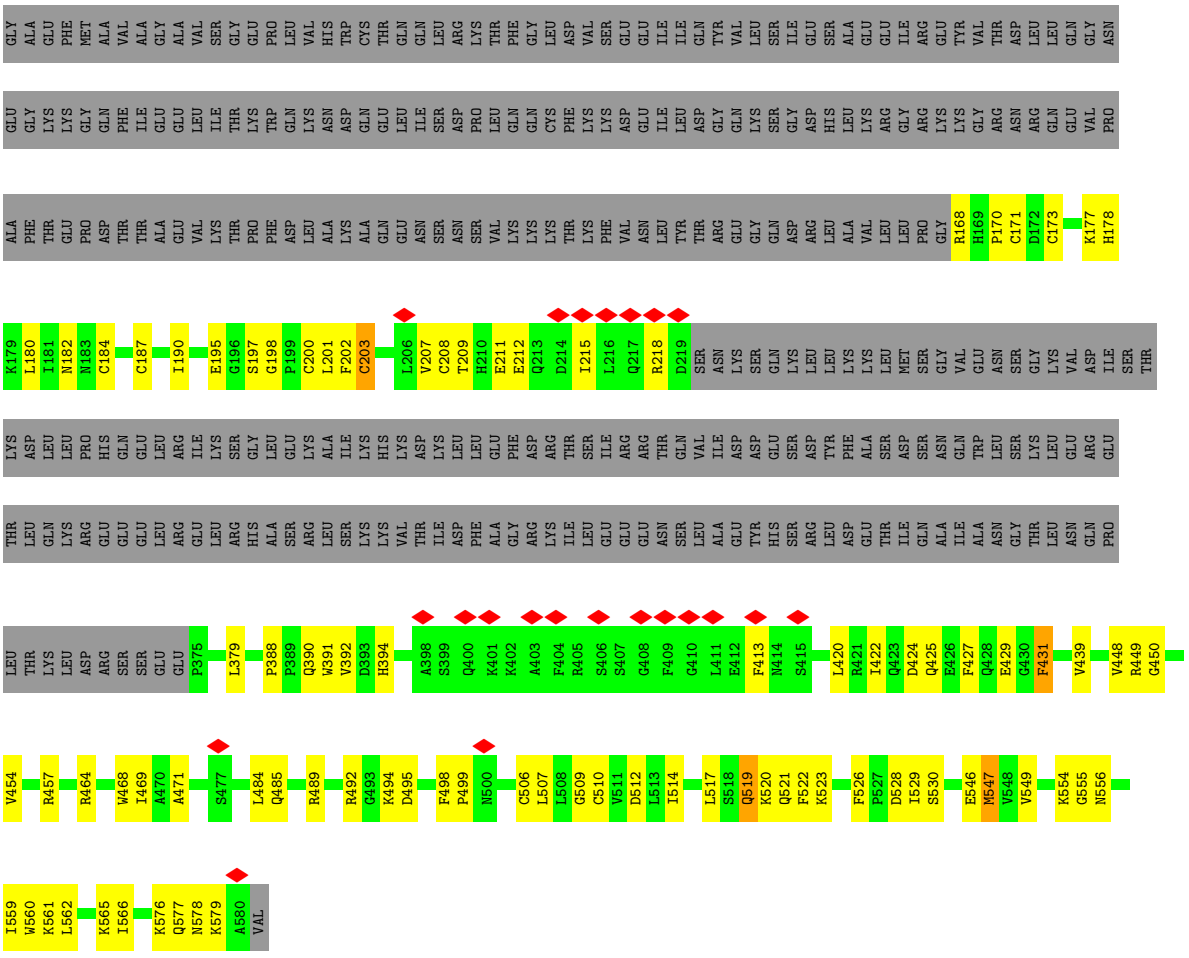
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	2	2	2	0

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.

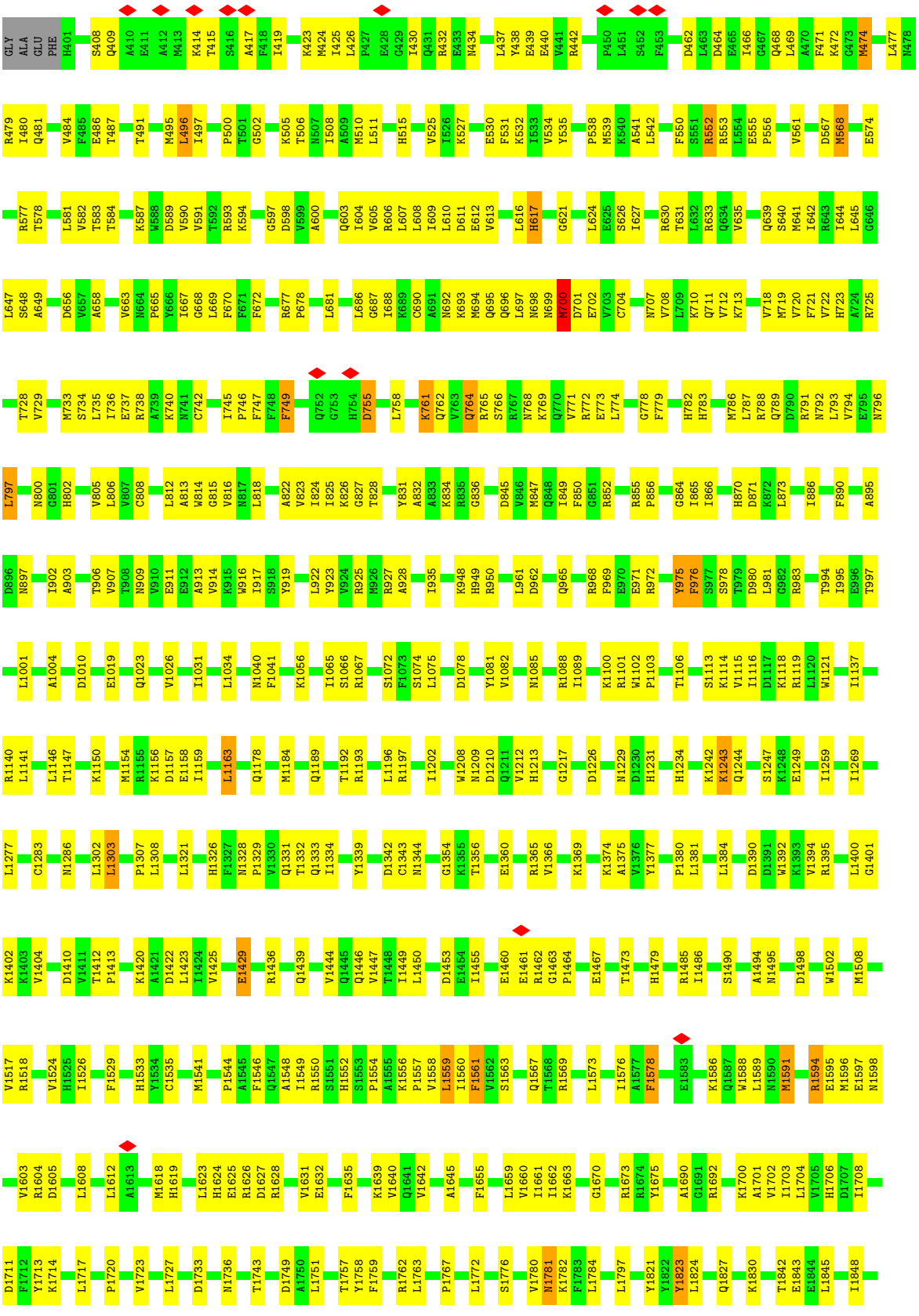
• Molecule 1: Activating signal cointegrator 1

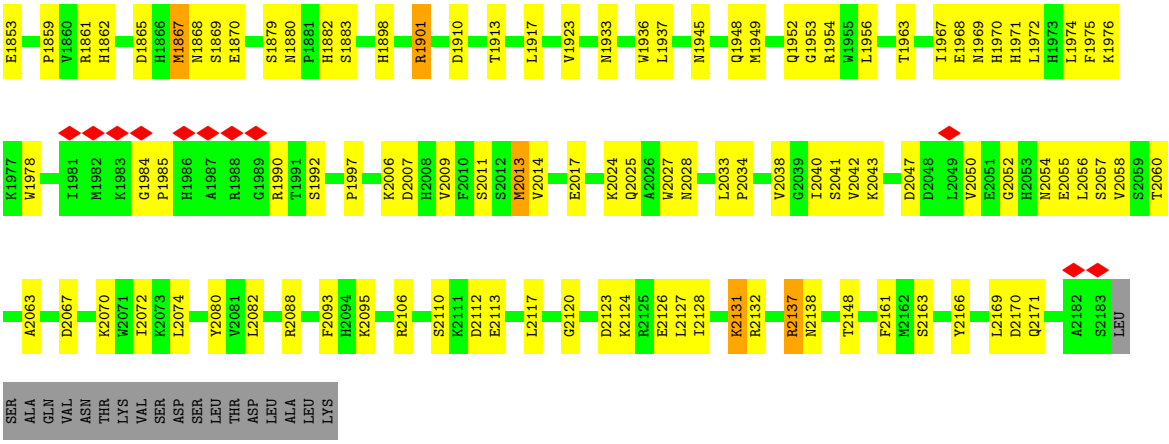
Chain A:



• Molecule 2: Activating signal cointegrator 1 complex subunit 3

Chain B:


GLY ALA GLU PHE H401 S408 Q409 A410 E411 A412 M413 K414 T415 S416 A417 F418 I419 K423 M424 I425 L426 P427 E428 G429 I430 Q431 R432 E433 N434 L437 Y438 E439 E440 V441 R442 P450 L451 S452 F453 D462 L463 D464 E465 I466 G467 Q468 L469 A470 F471 K472 G473 M474 L477 N478
R479 I480 Q481 V484 F485 E486 T487 T491 M495 L496 I497 P500 T501 G502 K505 T506 N507 I508 A509 M510 L511 H515 V525 I526 K527 E530 F531 K532 I533 V534 Y535 P538 M539 K540 A541 L542 F550 S551 R552 R553 L554 E555 P556 V561 D567 M568 E574
R577 T578 L581 V582 T583 T584 K587 W588 D589 V590 V591 T592 R593 K594 G597 D598 V599 A600 Q603 I604 V605 R606 L607 L608 I609 L610 D611 E612 V613 L616 H617 G621 L624 E625 S626 I627 R630 T631 L632 R633 Q634 V635 Q639 S640 M641 I642 R643 I644 L645 G646
L647 S648 A649 D656 V657 A658 V663 N664 P665 Y666 I667 G668 L669 F670 F671 F672 R677 P678 L681 L686 G687 I688 K689 C690 A691 N692 K693 M694 Q695 Q696 L697 N698 N699 M700 D701 E702 V703 C704 N707 V708 L709 K710 Q711 V712 K713 V718 M719 V720 F721 V722 H723 A724 R725
T728 V729 M733 S734 L735 I736 E737 R738 A739 K740 N741 C742 I745 P746 F747 F748 F749 Q752 G753 H754 D755 L758 K761 Q762 V763 Q764 R765 S766 R767 N768 K769 Q770 V771 R772 E773 L774 G778 F779 H782 H783 M786 L787 R788 D789 D790 R791 N792 L793 V794 E795 N796
L797 N800 G801 H802 V805 L806 V807 C808 L812 A813 W814 G815 V816 N817 L818 A822 V823 I824 I825 K826 G827 T828 Y831 A832 A833 K834 R835 G836 D845 V846 M847 Q848 I849 F850 G851 R852 R855 P856 G864 I865 I866 H870 D871 K872 L873 I886 F890 A895
D896 N897 I902 A903 T906 V907 T908 N909 V910 E911 E912 A913 V914 K915 W916 I917 S918 Y919 L922 Y923 V924 R925 M926 R927 A928 I935 K948 H949 R950 L961 D962 Q965 R968 F969 E970 E971 R972 Y975 F976 S977 S978 T979 D980 L981 G982 R983 T994 I995 E996 T997
L1001 A1004 D1010 E1019 Q1023 V1026 I1031 L1034 N1040 F1041 K1056 I1065 S1066 R1067 S1072 F1073 S1074 L1075 D1078 Y1081 V1082 N1085 R1088 I1089 K1100 R1101 W1102 P1103 T1106 S1113 K1114 V1115 I1116 D1117 K1118 R1119 L1120 W1121 I1137
R1140 L1141 L1146 T1147 K1150 M1154 R1155 K1156 D1157 E1158 I1159 L1163 Q1178 M1184 Q1189 T1192 R1193 L1196 R1197 I1202 W1208 N1209 D1210 Q1211 V1212 H1213 G1217 D1226 N1229 D1230 H1231 H1234 K1242 K1243 Q1244 S1247 K1248 E1249 I1259 I1269
L1277 C1283 N1286 L1302 L1303 P1307 L1308 L1321 H1326 F1327 N1328 P1329 V1330 Q1331 T1332 Q1333 I1334 Y1339 D1342 C1343 N1344 G1354 K1355 T1356 E1360 R1365 V1366 K1369 K1374 A1375 V1376 Y1377 P1380 L1381 L1384 D1390 D1391 W1392 K1393 V1394 R1395 L1400 G1401
K1402 K1403 V1404 D1410 V1411 T1412 P1413 K1420 A1421 D1422 L1423 I1424 V1425 E1429 R1436 Q1439 V1444 Q1445 Q1446 V1447 T1448 I1449 L1450 D1453 E1454 I1455 E1460 E1461 R1462 G1463 P1464 E1467 T1473 H1479 R1485 I1486 S1490 A1494 N1495 D1498 W1502 M1508
V1517 R1518 V1524 H1525 I1526 F1529 H1533 Y1534 C1535 M1541 P1544 A1545 F1546 Q1547 A1548 I1549 R1550 S1551 H1552 S1553 P1554 A1555 K1556 P1557 V1558 L1559 I1560 F1561 V1562 S1563 Q1567 T1568 R1569 L1573 I1576 A1577 F1578 E1583 K1586 Q1587 W1588 L1589 N1590 N1591 R1594 E1595 M1596 E1597 N1598
V1603 R1604 D1605 L1608 L1612 A1613 M1618 H1619 L1623 H1624 E1625 R1626 D1627 R1628 V1631 E1632 F1635 K1639 V1640 Q1641 V1642 A1645 F1655 L1659 V1660 I1661 I1662 K1663 G1670 R1673 R1674 Y1675 A1690 G1691 R1692 K1700 A1701 V1702 I1703 L1704 V1705 H1706 D1707 I1708
D1711 F1712 Y1713 K1714 L1717 P1720 V1723 L1727 D1733 N1736 T1743 D1749 A1750 L1751 T1757 Y1758 F1759 R1762 L1763 P1767 L1772 S1776 V1780 N1781 K1782 F1783 L1784 L1797 Y1821 Y1822 Y1823 L1824 Q1827 K1830 T1842 E1843 E1844 L1845 I1848


E1853 P1859 V1860 R1861 H1862 D1865 H1866 M1867 N1868 S1869 E1870 S1879 N1880 P1881 H1882 S1883 H1898 R1901 D1910 T1913 L1917 V1923 N1933 W1936 L1937 N1945 Q1948 M1949 Q1952 G1953 R1954 W1955 L1956 T1963 I1967 E1968 N1969 H1970 H1971 L1972 H1973 L1974 F1975 K1976
K1977 W1978 I1981 M1982 K1983 G1984 P1985 H1986 A1987 R1988 G1989 R1990 T1991 S1992 P1997 K2006 D2007 H2008 V2009 F2010 S2011 S2012 M2013 V2014 E2017 K2024 Q2025 A2026 W2027 N2028 L2033 P2034 V2038 G2039 I2040 S2041 V2042 K2043 D2047 D2048 L2049 V2050 E2051 G2052 H2053 N2054 E2055 L2056 S2057 V2058 S2059 T2060
A2063 D2067 K2070 W2071 I2072 K2073 L2074 Y2080 V2081 L2082 R2088 F2093 H2094 K2095 R2106 S2110 K2111 D2112 E2113 L2117 G2120 D2123 K2124 R2125 E2126 L2127 I2128 K2131 R2132 R2137 N2138 T2148 F2161 M2162 S2163 Y2166 L2169 D2170 Q2171 A2182 S2183 LEU
SER ALA GLN VAL ASN THR LYS VAL SER ASP SER LEU THR ASP LEU ALA LEU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	244064	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.657	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.157	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.25	0/2104	0.50	0/2838
2	B	0.25	0/14692	0.54	4/19926 (0.0%)
All	All	0.25	0/16796	0.53	4/22764 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	797	LEU	CA-CB-CG	5.77	128.58	115.30
2	B	1163	LEU	CA-CB-CG	5.53	128.02	115.30
2	B	665	PRO	CA-N-CD	-5.49	103.82	111.50
2	B	700	MET	CA-CB-CG	5.01	121.81	113.30

There are no chirality outliers.

There are no planarity outliers.

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	2052	0	2016	63	0
2	B	14355	0	14437	432	0
3	A	2	0	0	0	0
All	All	16409	0	16453	485	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 15.

All (485) 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)
1:A:187:CYS:SG	1:A:203:CYS:HB3	2.17	0.83
1:A:424:ASP:HA	2:B:2131:LYS:HZ2	1.47	0.79
2:B:690:CYS:HB2	2:B:696:GLN:HG3	1.65	0.78
2:B:825:ILE:HG23	2:B:827:GLY:H	1.50	0.77
2:B:500:PRO:HB2	2:B:677:ARG:HD3	1.68	0.76
2:B:1328:ASN:ND2	2:B:1331:GLN:OE1	2.24	0.71
2:B:723:HIS:HB3	2:B:828:THR:HB	1.73	0.71
2:B:414:LYS:HD2	2:B:417:ALA:HB2	1.74	0.70
2:B:591:VAL:HA	2:B:594:LYS:HG2	1.74	0.69
2:B:1321:LEU:HB3	2:B:1395:ARG:HH21	1.57	0.69
2:B:606:ARG:HH21	2:B:642:ILE:HD11	1.57	0.69
2:B:1969:ASN:HA	2:B:1972:LEU:HG	1.74	0.69
2:B:1366:VAL:HG11	2:B:1375:ALA:HB2	1.75	0.68
2:B:542:LEU:HD11	2:B:814:TRP:HE3	1.56	0.68
2:B:633:ARG:HD3	2:B:906:THR:HB	1.76	0.68
2:B:766:SER:O	2:B:772:ARG:NH1	2.26	0.67
2:B:1234:HIS:O	2:B:1234:HIS:ND1	2.29	0.66
2:B:484:VAL:HG11	2:B:508:ILE:HD12	1.77	0.65
2:B:1026:VAL:HG22	2:B:1056:LYS:HD2	1.78	0.65
2:B:1596:MET:SD	2:B:1596:MET:N	2.70	0.64
2:B:502:GLY:HA2	2:B:505:LYS:HD2	1.80	0.64
2:B:1936:TRP:HA	2:B:2126:GLU:HA	1.78	0.64
2:B:783:HIS:O	2:B:791:ARG:NH1	2.31	0.64
2:B:1954:ARG:NH2	2:B:1967:ILE:O	2.29	0.64
2:B:1997:PRO:HG3	2:B:2169:LEU:HD13	1.80	0.64
2:B:1861:ARG:O	2:B:1862:HIS:ND1	2.30	0.63
1:A:506:CYS:SG	1:A:507:LEU:N	2.71	0.63
2:B:782:HIS:HB2	2:B:806:LEU:HD11	1.80	0.63
2:B:1727:LEU:HD22	2:B:1757:THR:HG21	1.81	0.63
2:B:1945:ASN:HA	2:B:1948:GLN:HE21	1.63	0.63
2:B:1308:LEU:HD23	2:B:1332:THR:HG23	1.80	0.63
1:A:429:GLU:OE2	1:A:429:GLU:N	2.25	0.63
2:B:434:ASN:HB3	2:B:439:GLU:HG3	1.79	0.62
2:B:746:PRO:HA	2:B:749:PHE:HE1	1.64	0.62
2:B:1184:MET:HB2	2:B:1202:ILE:HG22	1.81	0.62
1:A:577:GLN:NE2	1:A:578:ASN:OD1	2.33	0.62
2:B:1608:LEU:HB3	2:B:1612:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1498:ASP:OD2	2:B:1762:ARG:NH1	2.32	0.62
2:B:1591:MET:HE3	2:B:1591:MET:H	1.65	0.61
2:B:1623:LEU:HG	2:B:1627:ASP:HB2	1.82	0.61
2:B:1380:PRO:HG2	2:B:1381:LEU:HD22	1.83	0.61
2:B:474:MET:SD	2:B:474:MET:N	2.69	0.61
2:B:695:GLN:HA	2:B:698:ASN:ND2	2.15	0.60
2:B:1661:ILE:HG22	2:B:1702:VAL:HG22	1.83	0.60
2:B:1949:MET:HE3	2:B:1956:LEU:HD23	1.83	0.60
2:B:471:PHE:HZ	2:B:477:LEU:HD21	1.67	0.60
2:B:612:GLU:N	2:B:647:LEU:O	2.35	0.60
2:B:1085:ASN:O	2:B:1089:ILE:HG12	2.01	0.60
2:B:1390:ASP:O	2:B:1394:VAL:HG22	2.01	0.59
2:B:1595:GLU:HG2	2:B:1596:MET:SD	2.43	0.59
1:A:528:ASP:OD1	1:A:528:ASP:N	2.36	0.59
1:A:168:ARG:HH22	1:A:198:GLY:HA3	1.68	0.59
2:B:707:ASN:HD22	2:B:865:ILE:HG21	1.68	0.59
2:B:1706:HIS:HD2	2:B:1708:ILE:HG12	1.68	0.59
2:B:426:LEU:HD11	2:B:430:ILE:HG12	1.85	0.58
2:B:1561:PHE:HE1	2:B:1662:ILE:HG22	1.68	0.58
2:B:1365:ARG:HE	2:B:1369:LYS:HG3	1.69	0.58
2:B:1843:GLU:OE2	2:B:1843:GLU:N	2.28	0.58
2:B:1824:LEU:HD21	2:B:1923:VAL:HG12	1.84	0.58
1:A:170:PRO:HG3	1:A:201:LEU:HG	1.85	0.58
1:A:190:ILE:HD11	2:B:1333:GLN:HA	1.84	0.58
2:B:1597:GLU:OE2	2:B:1598:ASN:ND2	2.36	0.58
2:B:762:GLN:HG2	2:B:765:ARG:HH21	1.69	0.58
2:B:1594:ARG:NH1	2:B:1595:GLU:HB3	2.18	0.58
2:B:1949:MET:O	2:B:1953:GLY:N	2.36	0.58
2:B:850:PHE:HE2	2:B:864:GLY:HA3	1.67	0.58
2:B:1114:LYS:O	2:B:1118:LYS:HB2	2.04	0.58
2:B:1502:TRP:CD2	2:B:1758:TYR:HB2	2.39	0.58
2:B:1040:ASN:OD1	2:B:1041:PHE:N	2.37	0.57
2:B:1563:SER:HA	2:B:1567:GLN:HB3	1.84	0.57
2:B:466:ILE:HD13	2:B:469:LEU:HD21	1.86	0.57
2:B:617:HIS:HB2	2:B:886:ILE:HG13	1.85	0.57
2:B:677:ARG:HD2	2:B:678:PRO:HD2	1.86	0.57
2:B:755:ASP:OD1	2:B:755:ASP:N	2.35	0.57
2:B:1157:ASP:OD1	2:B:1158:GLU:N	2.38	0.57
2:B:2067:ASP:H	2:B:2070:LYS:HZ3	1.51	0.57
1:A:468:TRP:HB3	1:A:507:LEU:HD11	1.87	0.57
2:B:720:VAL:HG22	2:B:824:ILE:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1560:ILE:O	2:B:1645:ALA:N	2.29	0.57
2:B:1749:ASP:OD1	2:B:1749:ASP:N	2.38	0.57
2:B:788:ARG:O	2:B:788:ARG:HD3	2.04	0.57
2:B:1533:HIS:ND1	2:B:1533:HIS:O	2.36	0.57
2:B:542:LEU:H	2:B:542:LEU:HD12	1.68	0.56
2:B:710:LYS:HA	2:B:713:LYS:HE2	1.86	0.56
2:B:423:LYS:HE3	2:B:425:ILE:HD13	1.86	0.56
2:B:479:ARG:NH1	2:B:480:ILE:HG13	2.20	0.56
2:B:923:TYR:O	2:B:927:ARG:HG2	2.05	0.56
2:B:1594:ARG:O	2:B:1597:GLU:HG3	2.05	0.56
2:B:626:SER:OG	2:B:630:ARG:NH2	2.38	0.56
2:B:711:GLN:HG3	2:B:718:VAL:HG11	1.88	0.56
2:B:1331:GLN:NE2	2:B:1354:GLY:O	2.39	0.56
2:B:1558:VAL:HG12	2:B:1659:LEU:H	1.70	0.56
2:B:535:TYR:HB3	2:B:582:VAL:HG22	1.87	0.55
2:B:855:ARG:HD3	2:B:856:PRO:HD2	1.87	0.55
2:B:1662:ILE:HG13	2:B:1703:ILE:HA	1.88	0.55
2:B:1972:LEU:O	2:B:1976:LYS:N	2.40	0.55
2:B:1518:ARG:NH2	2:B:1690:ALA:O	2.40	0.55
2:B:1067:ARG:HA	2:B:1119:ARG:HH21	1.72	0.55
2:B:471:PHE:HA	2:B:553:ARG:HH22	1.72	0.55
2:B:1550:ARG:HE	2:B:1554:PRO:HB3	1.72	0.55
2:B:902:ILE:HG22	2:B:978:SER:HB2	1.89	0.55
2:B:758:LEU:O	2:B:761:LYS:HG3	2.07	0.54
2:B:1974:LEU:HD13	2:B:2017:GLU:HG2	1.90	0.54
1:A:450:GLY:O	1:A:492:ARG:NH2	2.39	0.54
2:B:1661:ILE:HD12	2:B:1663:LYS:HB2	1.89	0.54
2:B:704:CYS:HB2	2:B:826:LYS:NZ	2.23	0.54
2:B:491:THR:O	2:B:515:HIS:NE2	2.36	0.54
1:A:173:CYS:HB2	1:A:177:LYS:HB3	1.88	0.54
1:A:469:ILE:HB	1:A:509:GLY:HA3	1.89	0.54
2:B:1247:SER:OG	2:B:1249:GLU:OE1	2.24	0.54
2:B:707:ASN:ND2	2:B:865:ILE:HG21	2.23	0.54
2:B:789:GLN:NE2	2:B:793:LEU:HD21	2.23	0.54
2:B:1767:PRO:HB3	2:B:1772:LEU:HD22	1.90	0.54
2:B:825:ILE:HG22	2:B:866:ILE:HA	1.90	0.53
2:B:733:MET:HA	2:B:736:ILE:HD12	1.90	0.53
2:B:1141:LEU:HB3	2:B:1146:LEU:HD11	1.89	0.53
2:B:1550:ARG:HH22	2:B:1588:TRP:HE1	1.53	0.53
2:B:1467:GLU:OE2	2:B:1759:PHE:N	2.40	0.53
2:B:1526:ILE:HG23	2:B:1703:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:THR:HG21	2:B:426:LEU:HB3	1.89	0.53
2:B:616:LEU:HA	2:B:621:GLY:HA3	1.90	0.53
2:B:746:PRO:HA	2:B:749:PHE:CE1	2.42	0.53
2:B:1226:ASP:OD1	2:B:1226:ASP:N	2.38	0.53
2:B:1342:ASP:HB2	2:B:1365:ARG:NH2	2.22	0.53
2:B:2050:VAL:HG12	2:B:2052:GLY:H	1.73	0.53
2:B:1078:ASP:O	2:B:1082:VAL:HG13	2.08	0.53
2:B:1868:ASN:OD1	2:B:1869:SER:N	2.41	0.53
2:B:589:ASP:OD2	2:B:593:ARG:NH2	2.40	0.53
2:B:1210:ASP:OD1	2:B:1242:LYS:NZ	2.39	0.53
2:B:1404:VAL:HG22	2:B:1423:LEU:HD22	1.91	0.53
2:B:677:ARG:HH21	2:B:681:LEU:HD11	1.73	0.53
2:B:1156:LYS:O	2:B:1159:ILE:HG12	2.09	0.53
2:B:786:MET:SD	2:B:787:LEU:N	2.82	0.53
2:B:1140:ARG:NH1	2:B:1163:LEU:O	2.42	0.53
2:B:1975:PHE:O	2:B:1978:TRP:NE1	2.42	0.52
2:B:2033:LEU:HD12	2:B:2034:PRO:HD2	1.91	0.52
2:B:495:MET:O	2:B:645:LEU:HA	2.09	0.52
2:B:913:ALA:O	2:B:917:ILE:HG12	2.10	0.52
2:B:419:ILE:HD13	2:B:424:MET:HB3	1.90	0.52
2:B:1952:GLN:NE2	2:B:1963:THR:OG1	2.42	0.52
2:B:567:ASP:OD2	2:B:568:MET:N	2.40	0.52
2:B:574:GLU:OE2	2:B:577:ARG:NH2	2.43	0.52
2:B:816:VAL:HG12	2:B:818:LEU:HD22	1.91	0.52
2:B:1865:ASP:O	2:B:1869:SER:OG	2.20	0.52
1:A:449:ARG:HD2	1:A:546:GLU:OE2	2.10	0.52
2:B:1140:ARG:HD2	2:B:1163:LEU:HG	1.90	0.52
2:B:2013:MET:SD	2:B:2013:MET:N	2.70	0.52
2:B:2040:ILE:HG13	2:B:2058:VAL:HG13	1.92	0.52
2:B:2123:ASP:OD1	2:B:2124:LYS:N	2.43	0.52
2:B:1552:HIS:HB3	2:B:1700:LYS:HD3	1.92	0.52
1:A:579:LYS:NZ	2:B:1479:HIS:HA	2.25	0.52
2:B:480:ILE:HG22	2:B:508:ILE:HD11	1.91	0.52
2:B:692:ASN:HB3	2:B:695:GLN:HG2	1.92	0.52
2:B:627:ILE:O	2:B:631:THR:HG22	2.10	0.52
1:A:495:ASP:OD1	1:A:495:ASP:N	2.43	0.51
2:B:711:GLN:HG3	2:B:718:VAL:CG1	2.39	0.51
2:B:2040:ILE:HB	2:B:2082:LEU:HD11	1.91	0.51
2:B:1494:ALA:HB2	2:B:1720:PRO:HB2	1.92	0.51
2:B:909:ASN:HB3	2:B:975:TYR:HD2	1.75	0.51
2:B:1101:ARG:HH22	2:B:1231:HIS:HD2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1209:ASN:HB3	2:B:1212:VAL:HB	1.92	0.51
2:B:610:LEU:O	2:B:647:LEU:HB3	2.09	0.51
2:B:718:VAL:O	2:B:805:VAL:HA	2.10	0.51
2:B:1661:ILE:HG22	2:B:1702:VAL:CG2	2.41	0.51
2:B:589:ASP:O	2:B:593:ARG:HG2	2.11	0.51
2:B:793:LEU:HA	2:B:796:ASN:HD21	1.76	0.51
2:B:981:LEU:HD11	2:B:995:ILE:HD11	1.92	0.51
2:B:1660:VAL:O	2:B:1701:ALA:HA	2.11	0.51
2:B:496:LEU:HD21	2:B:669:LEU:HD13	1.92	0.51
2:B:1374:LYS:HG2	2:B:1422:ASP:HA	1.93	0.51
2:B:1460:GLU:OE1	2:B:1462:ARG:N	2.43	0.51
1:A:392:VAL:HG12	1:A:394:HIS:H	1.75	0.51
2:B:909:ASN:HB3	2:B:975:TYR:CD2	2.47	0.51
2:B:1548:ALA:O	2:B:1552:HIS:ND1	2.33	0.51
2:B:439:GLU:O	2:B:687:GLY:N	2.45	0.50
2:B:965:GLN:HA	2:B:968:ARG:HH22	1.77	0.50
2:B:1541:MET:HB3	2:B:1704:LEU:HB3	1.93	0.50
2:B:2047:ASP:OD1	2:B:2047:ASP:N	2.45	0.50
2:B:1591:MET:H	2:B:1591:MET:CE	2.25	0.50
2:B:542:LEU:HD11	2:B:814:TRP:CE3	2.44	0.50
2:B:635:VAL:HG22	2:B:642:ILE:HD13	1.93	0.50
2:B:1229:ASN:HB3	2:B:1231:HIS:CE1	2.46	0.50
2:B:1937:LEU:HA	2:B:2127:LEU:HD23	1.93	0.50
2:B:1529:PHE:HZ	2:B:1544:PRO:HG2	1.75	0.50
2:B:1968:GLU:H	2:B:1971:HIS:HE1	1.60	0.50
1:A:449:ARG:HG3	1:A:499:PRO:HG3	1.93	0.50
2:B:1081:TYR:O	2:B:1085:ASN:ND2	2.44	0.50
2:B:1307:PRO:HB2	2:B:1326:HIS:HB3	1.94	0.50
2:B:1558:VAL:HG23	2:B:1642:VAL:HG23	1.94	0.50
2:B:2025:GLN:HA	2:B:2028:ASN:HD21	1.77	0.50
1:A:168:ARG:HD3	1:A:195:GLU:HB2	1.93	0.50
2:B:598:ASP:N	2:B:598:ASP:OD1	2.44	0.50
2:B:764:GLN:O	2:B:772:ARG:NH2	2.40	0.50
2:B:583:THR:OG1	2:B:584:THR:N	2.45	0.49
2:B:1711:ASP:OD1	2:B:1711:ASP:N	2.44	0.49
2:B:2161:PHE:HD2	2:B:2171:GLN:HE21	1.59	0.49
2:B:907:VAL:HG12	2:B:976:PHE:HE1	1.76	0.49
1:A:184:CYS:HA	1:A:207:VAL:HG21	1.94	0.49
1:A:379:LEU:HD13	2:B:1749:ASP:HB2	1.94	0.49
2:B:534:VAL:HG12	2:B:581:LEU:HB2	1.95	0.49
2:B:639:GLN:OE1	2:B:639:GLN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:935:ILE:HD11	2:B:949:HIS:CE1	2.47	0.49
1:A:448:VAL:HG21	1:A:509:GLY:HA2	1.93	0.49
2:B:612:GLU:HA	2:B:648:SER:HA	1.94	0.49
2:B:722:VAL:HG21	2:B:728:THR:HB	1.95	0.49
2:B:1495:ASN:ND2	2:B:1723:VAL:O	2.43	0.49
2:B:1879:SER:OG	2:B:1880:ASN:N	2.46	0.49
2:B:1971:HIS:HB2	2:B:1974:LEU:HD12	1.94	0.49
2:B:1910:ASP:O	2:B:1913:THR:HB	2.13	0.49
2:B:469:LEU:HD13	2:B:556:PRO:HB2	1.93	0.48
2:B:605:VAL:HG12	2:B:607:LEU:H	1.77	0.48
2:B:1781:ASN:OD1	2:B:1782:LYS:N	2.46	0.48
2:B:603:GLN:O	2:B:606:ARG:NH2	2.46	0.48
2:B:464:ASP:O	2:B:468:GLN:HG2	2.13	0.48
2:B:1561:PHE:HB3	2:B:1645:ALA:HB3	1.95	0.48
2:B:1524:VAL:HA	2:B:1701:ALA:O	2.13	0.48
2:B:782:HIS:HB3	2:B:808:CYS:HA	1.95	0.48
2:B:2043:LYS:HB2	2:B:2055:GLU:HG2	1.94	0.48
2:B:2131:LYS:HA	2:B:2131:LYS:HE3	1.94	0.48
1:A:182:ASN:H	1:A:209:THR:HG22	1.77	0.48
2:B:2163:SER:N	2:B:2170:ASP:OD1	2.44	0.48
2:B:825:ILE:HG21	2:B:866:ILE:HG22	1.96	0.48
2:B:721:PHE:HE2	2:B:849:ILE:HG23	1.79	0.48
2:B:1065:ILE:HD12	2:B:1115:VAL:HG12	1.94	0.48
2:B:1163:LEU:O	2:B:1163:LEU:HD23	2.14	0.48
2:B:1229:ASN:HB3	2:B:1231:HIS:HE1	1.79	0.48
2:B:2024:LYS:O	2:B:2028:ASN:ND2	2.46	0.48
2:B:735:LEU:HB3	2:B:779:PHE:HE2	1.78	0.48
2:B:1031:ILE:HD12	2:B:1034:LEU:HD23	1.96	0.48
2:B:1619:HIS:HB2	2:B:1628:ARG:HE	1.78	0.48
2:B:2117:LEU:HG	2:B:2131:LYS:HB2	1.96	0.48
2:B:1625:GLU:HA	2:B:1628:ARG:HD3	1.96	0.47
1:A:431:PHE:HZ	2:B:1821:TYR:HB2	1.78	0.47
2:B:1114:LYS:HE3	2:B:1277:LEU:HA	1.97	0.47
2:B:890:PHE:HB3	2:B:922:LEU:HD22	1.97	0.47
2:B:462:ASP:OD1	2:B:462:ASP:N	2.43	0.47
2:B:693:LYS:HB2	2:B:694:MET:HE1	1.96	0.47
2:B:774:LEU:HB3	2:B:779:PHE:O	2.14	0.47
2:B:962:ASP:OD1	2:B:968:ARG:NH2	2.44	0.47
2:B:1529:PHE:CZ	2:B:1544:PRO:HG2	2.49	0.47
2:B:1595:GLU:OE2	2:B:1595:GLU:N	2.24	0.47
2:B:486:GLU:OE1	2:B:486:GLU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:GLU:HG3	2:B:531:PHE:CD1	2.50	0.47
2:B:734:SER:O	2:B:737:GLU:HG3	2.14	0.47
2:B:1377:TYR:HD2	2:B:1425:VAL:HG12	1.79	0.47
2:B:1196:LEU:HD22	2:B:1259:ILE:HG21	1.95	0.47
2:B:1331:GLN:HA	2:B:1334:ILE:HG12	1.95	0.47
2:B:721:PHE:HD2	2:B:825:ILE:HA	1.79	0.47
2:B:408:SER:O	2:B:409:GLN:HG3	2.15	0.46
2:B:1137:ILE:O	2:B:1141:LEU:HG	2.15	0.46
2:B:1192:THR:HG22	2:B:1193:ARG:H	1.79	0.46
2:B:1460:GLU:OE1	2:B:1461:GLU:N	2.48	0.46
2:B:440:GLU:HB3	2:B:686:LEU:HD13	1.96	0.46
2:B:495:MET:HG3	2:B:668:GLY:HA3	1.97	0.46
2:B:663:VAL:HG23	2:B:667:ILE:HD11	1.97	0.46
2:B:702:GLU:HG3	2:B:738:ARG:HH22	1.79	0.46
2:B:786:MET:HE1	2:B:787:LEU:HB3	1.95	0.46
2:B:1243:LYS:HD2	2:B:1244:GLN:N	2.31	0.46
2:B:1586:LYS:HB3	2:B:1589:LEU:HB2	1.96	0.46
2:B:1901:ARG:HH12	2:B:2106:ARG:HG3	1.80	0.46
2:B:656:ASP:N	2:B:656:ASP:OD1	2.48	0.46
2:B:697:LEU:HA	2:B:700:MET:SD	2.56	0.46
2:B:1439:GLN:HG3	2:B:1743:THR:HG22	1.98	0.46
2:B:1605:ASP:HB3	2:B:1608:LEU:HG	1.97	0.46
2:B:745:ILE:N	2:B:746:PRO:HD2	2.30	0.46
2:B:1072:SER:HB3	2:B:1075:LEU:HB3	1.98	0.46
2:B:1286:ASN:N	2:B:1286:ASN:OD1	2.48	0.46
2:B:778:GLY:O	2:B:805:VAL:HG22	2.15	0.46
2:B:895:ALA:HB1	2:B:961:LEU:HD21	1.97	0.46
2:B:1619:HIS:O	2:B:1619:HIS:ND1	2.49	0.46
2:B:1969:ASN:OD1	2:B:1970:HIS:N	2.49	0.46
2:B:597:GLY:HA2	2:B:1535:CYS:SG	2.55	0.46
2:B:648:SER:OG	2:B:649:ALA:N	2.48	0.46
2:B:688:ILE:HD11	2:B:699:ASN:HB3	1.98	0.46
2:B:793:LEU:HA	2:B:796:ASN:ND2	2.31	0.46
2:B:1557:PRO:HD2	2:B:1692:ARG:HH22	1.81	0.46
2:B:1968:GLU:H	2:B:1971:HIS:CE1	2.33	0.46
2:B:718:VAL:CG1	2:B:822:ALA:HB3	2.46	0.46
2:B:1842:THR:HA	2:B:1845:LEU:HD23	1.98	0.46
2:B:698:ASN:HA	2:B:701:ASP:OD2	2.16	0.45
2:B:1450:LEU:HD22	2:B:1473:THR:HG21	1.98	0.45
2:B:2006:LYS:HB3	2:B:2009:VAL:HG22	1.99	0.45
2:B:725:ARG:O	2:B:728:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:925:ARG:HH12	2:B:928:ALA:HB3	1.80	0.45
2:B:2007:ASP:HB3	2:B:2027:TRP:NE1	2.32	0.45
2:B:480:ILE:HD12	2:B:480:ILE:H	1.82	0.45
2:B:738:ARG:HA	2:B:738:ARG:HD2	1.72	0.45
2:B:2042:VAL:HG12	2:B:2080:TYR:HD2	1.81	0.45
2:B:2042:VAL:HG22	2:B:2082:LEU:HD13	1.97	0.45
2:B:2056:LEU:HD12	2:B:2072:ILE:HG23	1.99	0.45
1:A:424:ASP:OD1	2:B:2132:ARG:HG2	2.15	0.45
2:B:417:ALA:HA	2:B:423:LYS:HD3	1.99	0.45
2:B:1670:GLY:O	2:B:1673:ARG:NH1	2.50	0.45
1:A:514:ILE:HD12	1:A:514:ILE:HA	1.87	0.45
1:A:177:LYS:HG2	1:A:178:HIS:HD1	1.81	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.16	0.45
2:B:466:ILE:HG13	2:B:525:VAL:HG11	1.99	0.45
2:B:672:PHE:CD1	2:B:672:PHE:N	2.85	0.45
2:B:1412:THR:OG1	2:B:1413:PRO:HD3	2.17	0.45
2:B:2041:SER:HA	2:B:2057:SER:HA	1.99	0.45
2:B:832:ALA:O	2:B:836:GLY:N	2.41	0.45
2:B:1269:ILE:HB	2:B:1283:CYS:SG	2.57	0.45
2:B:1449:ILE:HD12	2:B:1485:ARG:HB3	1.98	0.45
2:B:1576:ILE:HD12	2:B:1576:ILE:HA	1.88	0.45
1:A:180:LEU:HD22	2:B:1303:LEU:HD13	1.98	0.45
2:B:550:PHE:HB3	2:B:561:VAL:HG11	1.98	0.45
2:B:791:ARG:HA	2:B:794:VAL:HG12	1.99	0.45
2:B:1088:ARG:HG3	2:B:1089:ILE:HD13	1.99	0.45
2:B:1559:LEU:O	2:B:1560:ILE:HD13	2.17	0.45
2:B:1662:ILE:CG1	2:B:1703:ILE:HA	2.46	0.45
2:B:1845:LEU:HA	2:B:1848:ILE:HG22	1.99	0.45
1:A:413:PHE:HA	1:A:561:LYS:HB3	1.98	0.45
2:B:440:GLU:HB2	2:B:686:LEU:HD22	1.99	0.45
2:B:539:MET:SD	2:B:539:MET:N	2.90	0.45
1:A:439:VAL:HA	1:A:457:ARG:HH22	1.82	0.44
2:B:430:ILE:HB	2:B:442:ARG:HB2	1.99	0.44
2:B:1573:LEU:HA	2:B:1576:ILE:HG22	1.99	0.44
2:B:1356:THR:O	2:B:1360:GLU:HG3	2.18	0.44
2:B:1624:HIS:HD2	2:B:1626:ARG:HG2	1.82	0.44
1:A:211:GLU:OE2	1:A:211:GLU:N	2.30	0.44
1:A:388:PRO:HG2	1:A:390:GLN:NE2	2.32	0.44
1:A:391:TRP:CE3	2:B:1751:LEU:HD12	2.52	0.44
2:B:541:ALA:HB1	2:B:815:GLY:HA2	2.00	0.44
2:B:1189:GLN:HB2	2:B:1197:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:C	1:A:422:ILE:H	2.21	0.44
2:B:870:HIS:O	2:B:873:LEU:HG	2.18	0.44
2:B:903:ALA:O	2:B:983:ARG:NH2	2.39	0.44
2:B:1004:ALA:HB2	2:B:1102:TRP:CE2	2.53	0.44
2:B:1827:GLN:HG3	2:B:1853:GLU:HG2	2.00	0.44
2:B:1867:MET:HA	2:B:1870:GLU:HG3	1.99	0.44
2:B:1990:ARG:NH2	2:B:1992:SER:O	2.49	0.44
1:A:468:TRP:CE3	1:A:510:CYS:HB3	2.53	0.44
2:B:608:LEU:HB3	2:B:644:ILE:HD13	1.98	0.44
2:B:1113:SER:HA	2:B:1116:ILE:HG22	1.98	0.44
2:B:1556:LYS:HB2	2:B:1556:LYS:HE2	1.69	0.44
2:B:695:GLN:HA	2:B:698:ASN:HD21	1.79	0.44
2:B:1591:MET:HB3	2:B:1639:LYS:HD3	2.00	0.44
2:B:506:THR:O	2:B:510:MET:HE2	2.17	0.44
2:B:789:GLN:O	2:B:793:LEU:HG	2.18	0.44
2:B:1154:MET:SD	2:B:1159:ILE:HG22	2.57	0.44
2:B:1533:HIS:ND1	2:B:1535:CYS:SG	2.90	0.44
2:B:1635:PHE:HD1	2:B:1640:VAL:HB	1.82	0.44
2:B:505:LYS:HG2	2:B:647:LEU:HD11	2.00	0.44
2:B:1178:GLN:O	2:B:1213:HIS:NE2	2.51	0.44
2:B:1429:GLU:HB2	2:B:1823:TYR:HE2	1.82	0.44
2:B:1541:MET:HB2	2:B:1663:LYS:HG3	2.00	0.44
2:B:1603:VAL:HG13	2:B:1623:LEU:HD11	1.98	0.44
2:B:611:ASP:HA	2:B:647:LEU:HB3	1.99	0.43
2:B:761:LYS:O	2:B:765:ARG:HG3	2.18	0.43
2:B:1302:LEU:HD22	2:B:1517:VAL:HG13	1.99	0.43
2:B:897:ASN:HB3	2:B:916:TRP:HH2	1.83	0.43
2:B:1628:ARG:O	2:B:1631:VAL:HG22	2.19	0.43
2:B:1628:ARG:NH2	2:B:1632:GLU:OE2	2.51	0.43
1:A:425:GLN:OE1	2:B:2131:LYS:NZ	2.29	0.43
2:B:534:VAL:HG23	2:B:608:LEU:HD13	1.99	0.43
2:B:2038:VAL:HG23	2:B:2060:THR:HG21	2.00	0.43
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.84	0.43
1:A:526:PHE:HE2	1:A:529:ILE:HB	1.83	0.43
2:B:616:LEU:HD21	2:B:624:LEU:HB3	2.01	0.43
2:B:667:ILE:HG13	2:B:668:GLY:N	2.33	0.43
2:B:1733:ASP:O	2:B:1736:ASN:HB3	2.18	0.43
2:B:2074:LEU:HD13	2:B:2148:THR:HG21	2.01	0.43
1:A:208:CYS:HB3	1:A:212:GLU:HG3	1.99	0.43
1:A:562:LEU:HD21	1:A:566:ILE:HG22	2.00	0.43
2:B:497:ILE:O	2:B:647:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:ALA:H	2:B:603:GLN:HE22	1.67	0.43
2:B:1339:TYR:O	2:B:1365:ARG:HD3	2.18	0.43
2:B:2137:ARG:HG2	2:B:2138:ASN:N	2.34	0.43
2:B:471:PHE:CZ	2:B:477:LEU:HD21	2.51	0.43
2:B:768:ASN:HB3	2:B:771:VAL:HG12	2.00	0.43
2:B:997:THR:O	2:B:1001:LEU:HB2	2.19	0.43
1:A:424:ASP:HB3	1:A:427:PHE:CD1	2.54	0.43
2:B:437:LEU:HD23	2:B:437:LEU:H	1.84	0.43
2:B:613:VAL:HG22	2:B:648:SER:HB2	2.00	0.43
2:B:729:VAL:O	2:B:733:MET:SD	2.77	0.43
2:B:1381:LEU:HB2	2:B:1384:LEU:HB2	2.00	0.43
2:B:1546:PHE:CG	2:B:1578:PHE:HE2	2.36	0.43
1:A:494:LYS:HA	1:A:494:LYS:HD3	1.78	0.43
1:A:579:LYS:HZ3	2:B:1479:HIS:HA	1.83	0.43
2:B:2067:ASP:H	2:B:2070:LYS:NZ	2.17	0.43
1:A:182:ASN:HB2	1:A:209:THR:HA	2.00	0.42
1:A:454:VAL:HG11	1:A:522:PHE:HZ	1.84	0.42
2:B:2011:SER:HA	2:B:2014:VAL:HG22	1.99	0.42
2:B:1560:ILE:HD12	2:B:1661:ILE:HG13	2.01	0.42
2:B:1619:HIS:HB2	2:B:1628:ARG:HH21	1.85	0.42
2:B:871:ASP:OD1	2:B:871:ASP:N	2.52	0.42
2:B:1328:ASN:HB2	2:B:1329:PRO:HD2	2.00	0.42
2:B:1360:GLU:HG2	2:B:1392:TRP:CH2	2.55	0.42
2:B:1450:LEU:HD12	2:B:1450:LEU:HA	1.87	0.42
2:B:437:LEU:HG	2:B:438:TYR:CD2	2.54	0.42
1:A:177:LYS:HG2	1:A:178:HIS:ND1	2.35	0.42
2:B:497:ILE:HD11	2:B:672:PHE:CZ	2.54	0.42
2:B:1763:LEU:HD21	2:B:1772:LEU:HD13	2.00	0.42
1:A:517:LEU:HD12	1:A:521:GLN:HB3	2.01	0.42
1:A:547:MET:HG2	1:A:549:VAL:H	1.85	0.42
2:B:603:GLN:HG2	2:B:604:ILE:HG23	2.00	0.42
2:B:616:LEU:HD22	2:B:621:GLY:HA2	2.01	0.42
2:B:1526:ILE:HG21	2:B:1714:LYS:HD2	2.01	0.42
2:B:1546:PHE:HA	2:B:1549:ILE:HD12	2.00	0.42
2:B:2113:GLU:HG3	2:B:2166:TYR:HE2	1.84	0.42
2:B:812:LEU:HD22	2:B:818:LEU:HD21	2.02	0.42
2:B:914:VAL:HG22	2:B:950:ARG:HB3	2.02	0.42
2:B:969:PHE:CE2	2:B:971:GLU:HG2	2.54	0.42
2:B:1460:GLU:OE1	2:B:1462:ARG:HG3	2.20	0.42
2:B:2054:ASN:OD1	2:B:2054:ASN:N	2.50	0.42
2:B:2063:ALA:O	2:B:2070:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:VAL:HG11	1:A:522:PHE:CZ	2.55	0.42
1:A:529:ILE:HG22	1:A:529:ILE:O	2.19	0.42
2:B:477:LEU:HD22	2:B:481:GLN:HG3	2.01	0.42
2:B:909:ASN:OD1	2:B:911:GLU:HG2	2.20	0.42
2:B:1560:ILE:HD12	2:B:1661:ILE:CG1	2.49	0.42
1:A:554:LYS:NZ	1:A:555:GLY:O	2.50	0.42
2:B:1569:ARG:O	2:B:1573:LEU:HD13	2.19	0.42
1:A:485:GLN:HB3	1:A:489:ARG:HH12	1.84	0.42
2:B:479:ARG:HD2	2:B:480:ILE:N	2.35	0.42
2:B:2095:LYS:HA	2:B:2095:LYS:HD3	1.81	0.42
2:B:677:ARG:HH11	2:B:678:PRO:HD2	1.83	0.41
2:B:737:GLU:HA	2:B:740:LYS:HE2	2.01	0.41
2:B:788:ARG:HH11	2:B:792:ASN:ND2	2.18	0.41
2:B:1420:LYS:HA	2:B:1420:LYS:HD2	1.83	0.41
2:B:1446:GLN:H	2:B:1446:GLN:HG3	1.73	0.41
2:B:1937:LEU:HB3	2:B:2127:LEU:HB3	2.02	0.41
2:B:1776:SER:O	2:B:1780:VAL:HG12	2.20	0.41
2:B:1859:PRO:HG2	2:B:1861:ARG:HH12	1.85	0.41
2:B:1898:HIS:NE2	2:B:1917:LEU:HD11	2.34	0.41
1:A:215:ILE:HG13	1:A:218:ARG:HH12	1.85	0.41
1:A:485:GLN:O	1:A:489:ARG:HG2	2.21	0.41
1:A:565:LYS:HB2	1:A:565:LYS:HE2	1.81	0.41
2:B:812:LEU:HB2	2:B:818:LEU:HD21	2.02	0.41
2:B:1713:TYR:O	2:B:1717:LEU:N	2.46	0.41
2:B:831:TYR:CD2	2:B:1074:SER:HB2	2.55	0.41
2:B:1984:GLY:N	2:B:1985:PRO:HD2	2.35	0.41
2:B:2120:GLY:HA2	2:B:2128:ILE:HG13	2.02	0.41
2:B:1066:SER:HB3	2:B:1121:TRP:HE1	1.86	0.41
2:B:1147:THR:HG23	2:B:1150:LYS:H	1.86	0.41
2:B:1404:VAL:HG13	2:B:1423:LEU:HD22	2.03	0.41
2:B:1444:VAL:O	2:B:1447:VAL:HG12	2.21	0.41
2:B:1529:PHE:HE2	2:B:1704:LEU:HD22	1.86	0.41
2:B:1797:LEU:O	2:B:1830:LYS:NZ	2.45	0.41
2:B:1880:ASN:HD22	2:B:1883:SER:HB3	1.85	0.41
2:B:2024:LYS:HB2	2:B:2024:LYS:HE2	1.85	0.41
1:A:471:ALA:HB3	1:A:506:CYS:H	1.85	0.41
1:A:519:GLN:O	1:A:523:LYS:HG2	2.21	0.41
2:B:495:MET:HG2	2:B:496:LEU:N	2.35	0.41
2:B:719:MET:HE1	2:B:823:VAL:HG13	2.02	0.41
2:B:1010:ASP:OD1	2:B:1010:ASP:N	2.52	0.41
2:B:1784:LEU:HD23	2:B:1784:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:ALA:HB2	2:B:669:LEU:HD11	2.03	0.41
2:B:914:VAL:HG13	2:B:950:ARG:HD2	2.03	0.41
2:B:1400:LEU:HD23	2:B:1401:GLY:N	2.35	0.41
1:A:187:CYS:SG	1:A:202:PHE:HB3	2.61	0.41
1:A:526:PHE:O	1:A:530:SER:OG	2.25	0.41
2:B:1439:GLN:HE21	2:B:1743:THR:HG22	1.85	0.41
2:B:487:THR:O	2:B:491:THR:OG1	2.32	0.41
2:B:640:SER:OG	2:B:641:MET:N	2.54	0.41
2:B:708:VAL:O	2:B:712:VAL:HG13	2.19	0.41
2:B:812:LEU:HD12	2:B:813:ALA:N	2.35	0.41
2:B:1344:ASN:HB3	2:B:1486:ILE:H	1.85	0.41
2:B:1410:ASP:HB3	2:B:1413:PRO:HD2	2.03	0.41
2:B:1463:GLY:N	2:B:1464:PRO:HD3	2.36	0.41
1:A:485:GLN:HB3	1:A:489:ARG:NH1	2.35	0.41
1:A:485:GLN:HG2	1:A:498:PHE:CE2	2.55	0.41
2:B:532:LYS:O	2:B:605:VAL:HA	2.20	0.41
2:B:718:VAL:HG12	2:B:822:ALA:HB3	2.03	0.41
2:B:552:ARG:O	2:B:552:ARG:HG2	2.21	0.40
2:B:794:VAL:HA	2:B:797:LEU:HG	2.04	0.40
2:B:845:ASP:O	2:B:849:ILE:HG12	2.21	0.40
2:B:1529:PHE:CD2	2:B:1541:MET:HG2	2.56	0.40
2:B:2006:LYS:HG3	2:B:2093:PHE:CE2	2.56	0.40
2:B:532:LYS:HE2	2:B:578:THR:O	2.22	0.40
2:B:1208:TRP:HH2	2:B:1217:GLY:HA2	1.86	0.40
2:B:472:LYS:NZ	2:B:555:GLU:OE2	2.41	0.40
2:B:609:ILE:HD13	2:B:609:ILE:HA	1.90	0.40
2:B:994:THR:N	2:B:1019:GLU:OE2	2.54	0.40
2:B:1455:ILE:H	2:B:1490:SER:HB3	1.85	0.40
1:A:556:ASN:HB2	1:A:560:TRP:CD2	2.56	0.40
2:B:1321:LEU:HD23	2:B:1395:ARG:HB3	2.04	0.40
2:B:481:GLN:HE22	2:B:511:LEU:HD23	1.85	0.40
2:B:538:PRO:HD2	2:B:542:LEU:HD22	2.04	0.40
2:B:587:LYS:HA	2:B:590:VAL:HG22	2.04	0.40
2:B:670:PHE:HB3	2:B:672:PHE:HE1	1.86	0.40
2:B:834:LYS:O	2:B:1023:GLN:NE2	2.37	0.40
2:B:1103:PRO:HA	2:B:1106:THR:HG22	2.04	0.40
2:B:1400:LEU:HD22	2:B:1402:LYS:HG2	2.04	0.40
2:B:2067:ASP:O	2:B:2070:LYS:HG2	2.21	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	254/585 (43%)	243 (96%)	10 (4%)	1 (0%)	34 67
2	B	1781/1806 (99%)	1699 (95%)	82 (5%)	0	100 100
All	All	2035/2391 (85%)	1942 (95%)	92 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	ILE

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	227/519 (44%)	216 (95%)	11 (5%)	25 56
2	B	1579/1598 (99%)	1524 (96%)	55 (4%)	36 65
All	All	1806/2117 (85%)	1740 (96%)	66 (4%)	37 62

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	CYS
1	A	197	SER
1	A	200	CYS
1	A	203	CYS
1	A	431	PHE

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Mol	Chain	Res	Type
1	A	464	ARG
1	A	512	ASP
1	A	519	GLN
1	A	520	LYS
1	A	547	MET
1	A	576	LYS
2	B	432	ARG
2	B	474	MET
2	B	496	LEU
2	B	527	LYS
2	B	552	ARG
2	B	568	MET
2	B	617	HIS
2	B	700	MET
2	B	742	CYS
2	B	747	PHE
2	B	749	PHE
2	B	755	ASP
2	B	761	LYS
2	B	764	GLN
2	B	769	LYS
2	B	773	GLU
2	B	800	ASN
2	B	802	HIS
2	B	847	MET
2	B	852	ARG
2	B	919	TYR
2	B	948	LYS
2	B	972	ARG
2	B	975	TYR
2	B	976	PHE
2	B	980	ASP
2	B	1100	LYS
2	B	1243	LYS
2	B	1303	LEU
2	B	1343	CYS
2	B	1429	GLU
2	B	1436	ARG
2	B	1453	ASP
2	B	1508	MET
2	B	1559	LEU
2	B	1561	PHE

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Mol	Chain	Res	Type
2	B	1578	PHE
2	B	1591	MET
2	B	1594	ARG
2	B	1604	ARG
2	B	1618	MET
2	B	1655	PHE
2	B	1675	TYR
2	B	1781	ASN
2	B	1823	TYR
2	B	1867	MET
2	B	1882	HIS
2	B	1901	ARG
2	B	1933	ASN
2	B	2013	MET
2	B	2088	ARG
2	B	2110	SER
2	B	2112	ASP
2	B	2131	LYS
2	B	2137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	GLN
1	A	577	GLN
2	B	1231	HIS
2	B	1948	GLN
2	B	1971	HIS
2	B	2028	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

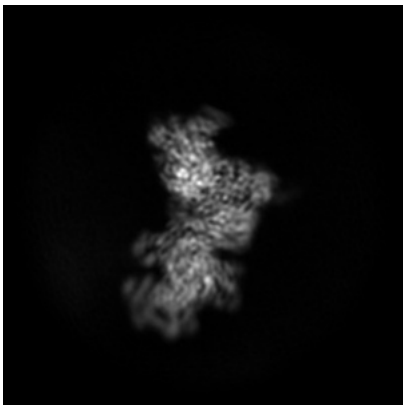
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15521. These allow visual inspection of the internal detail of the map and identification of artifacts.

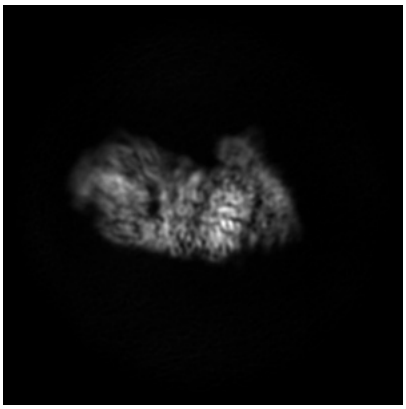
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

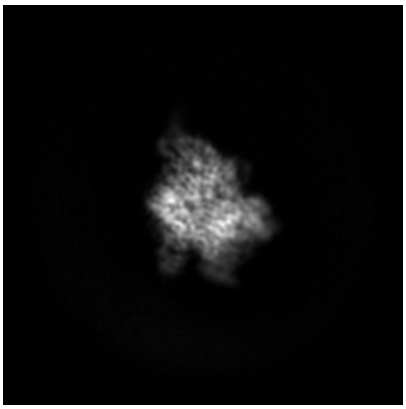
6.1.1 Primary map



X

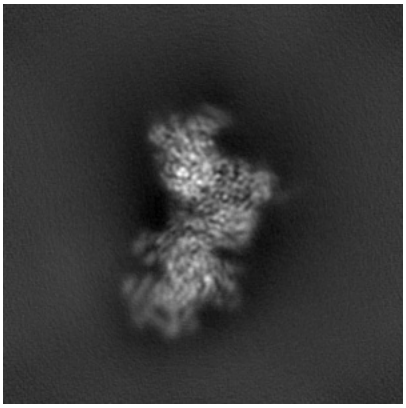


Y

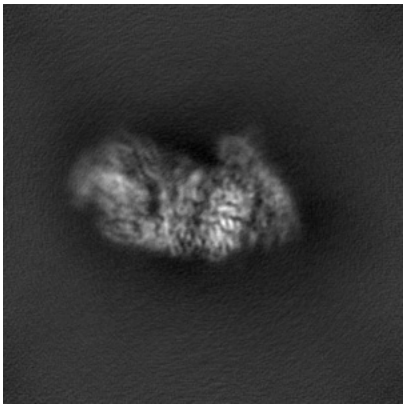


Z

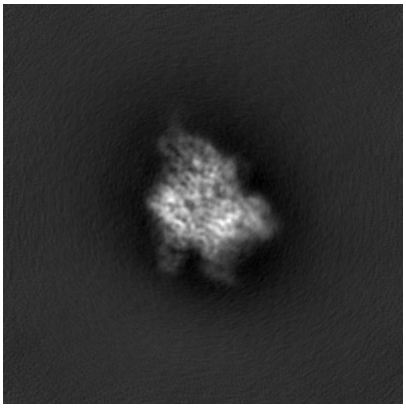
6.1.2 Raw map



X



Y

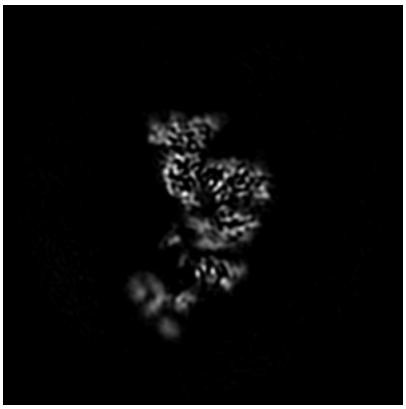


Z

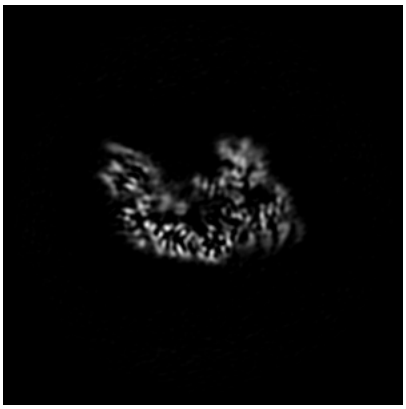
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

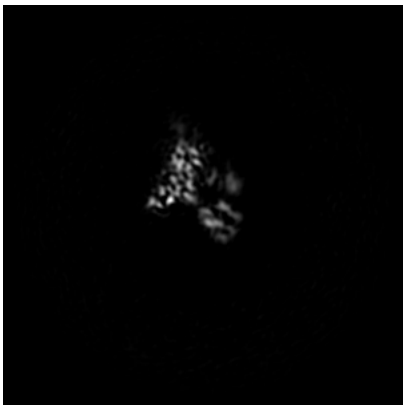
6.2.1 Primary map



X Index: 160

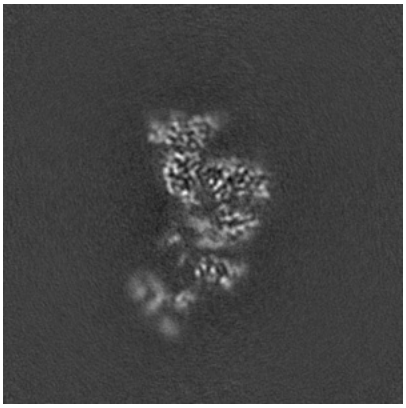


Y Index: 160

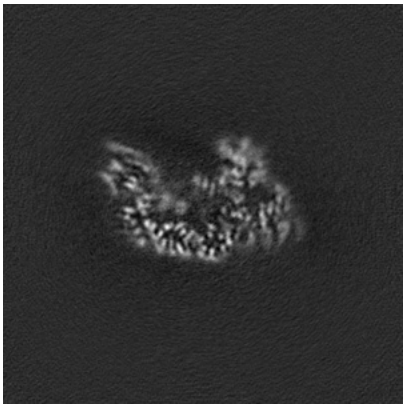


Z Index: 160

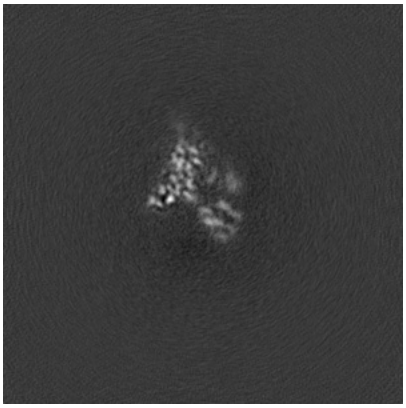
6.2.2 Raw map



X Index: 160



Y Index: 160

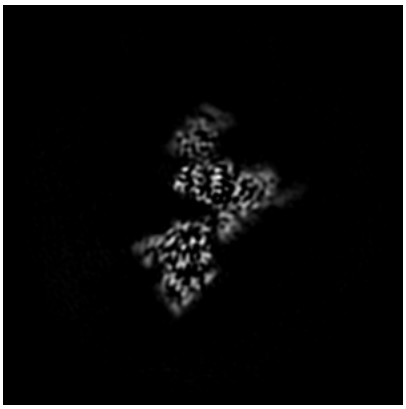


Z Index: 160

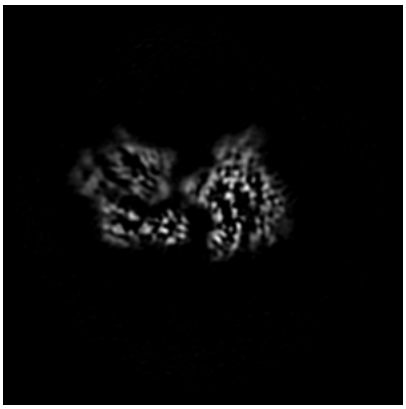
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

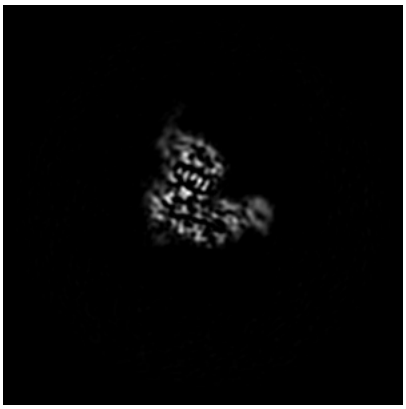
6.3.1 Primary map



X Index: 142

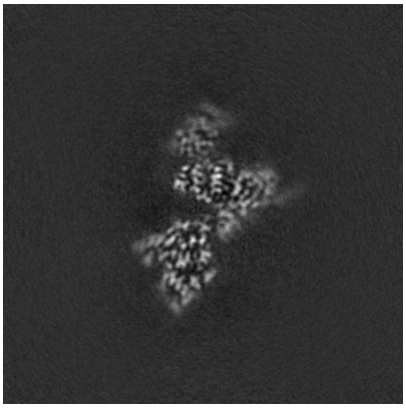


Y Index: 146

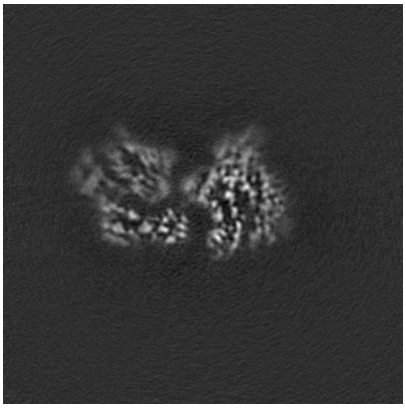


Z Index: 176

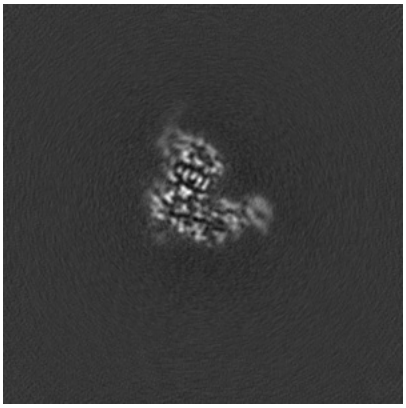
6.3.2 Raw map



X Index: 142



Y Index: 146



Z Index: 176

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

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

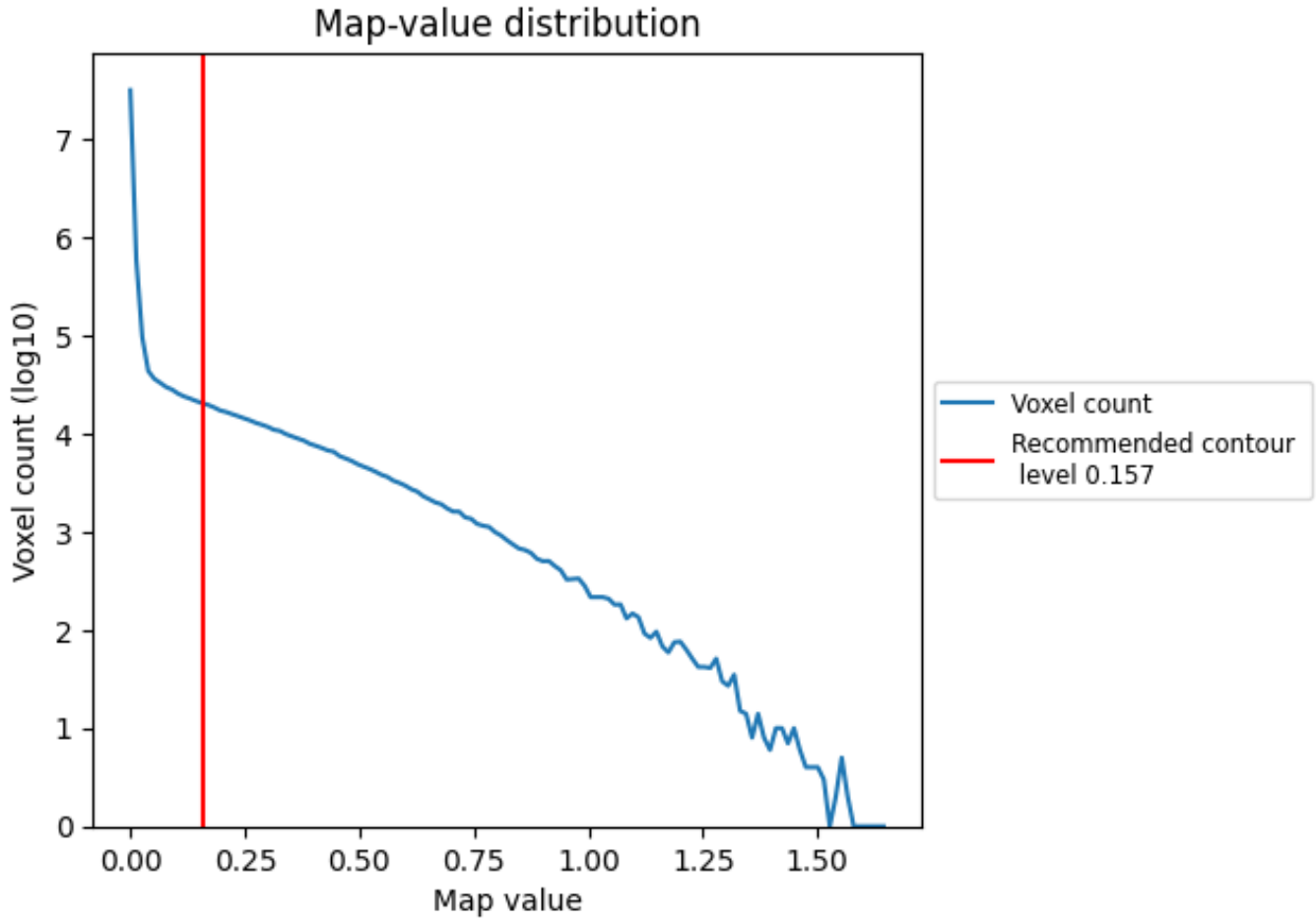
6.5 Mask visualisation (i)

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

7 Map analysis

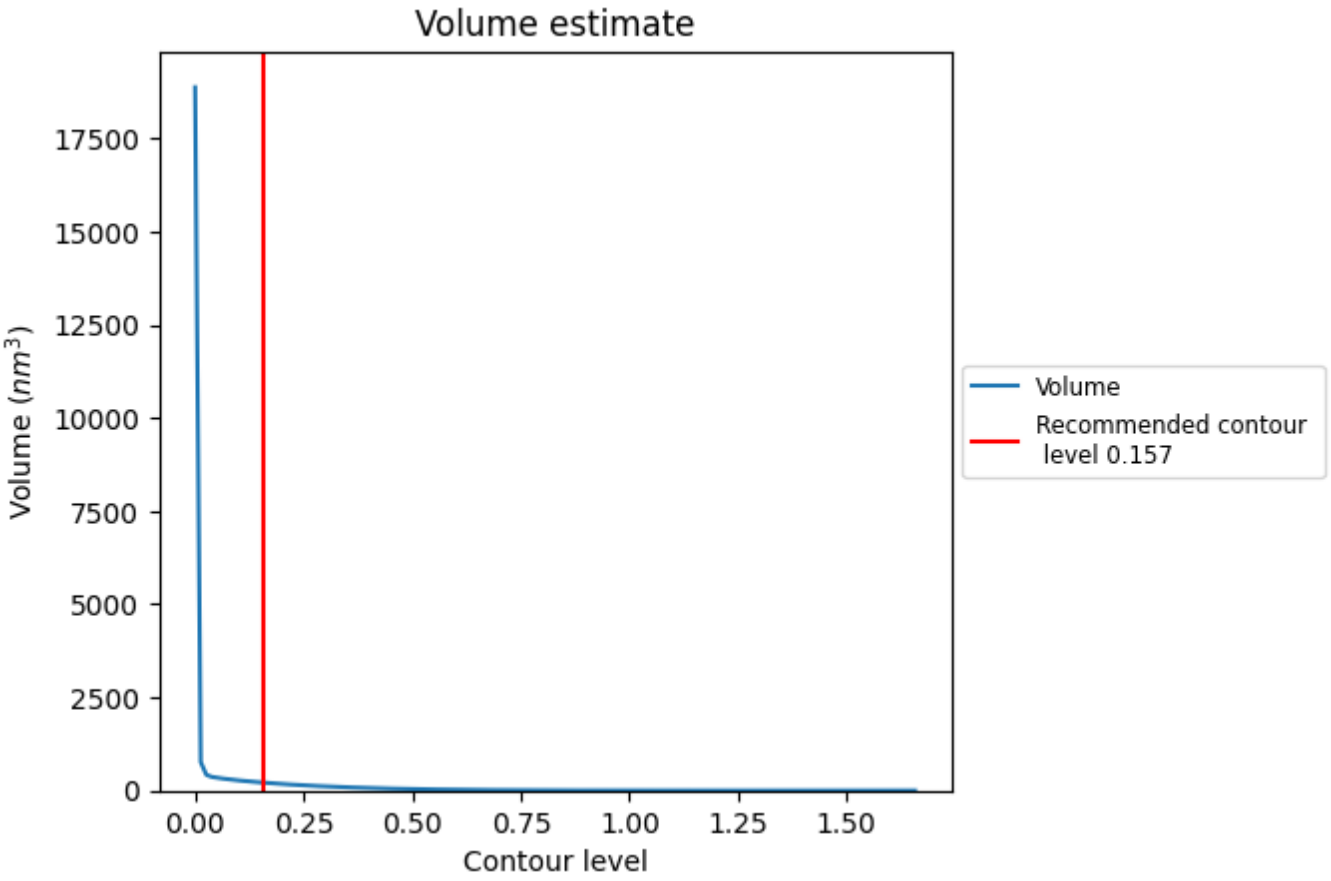
This section contains the results of statistical analysis of the map.

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.

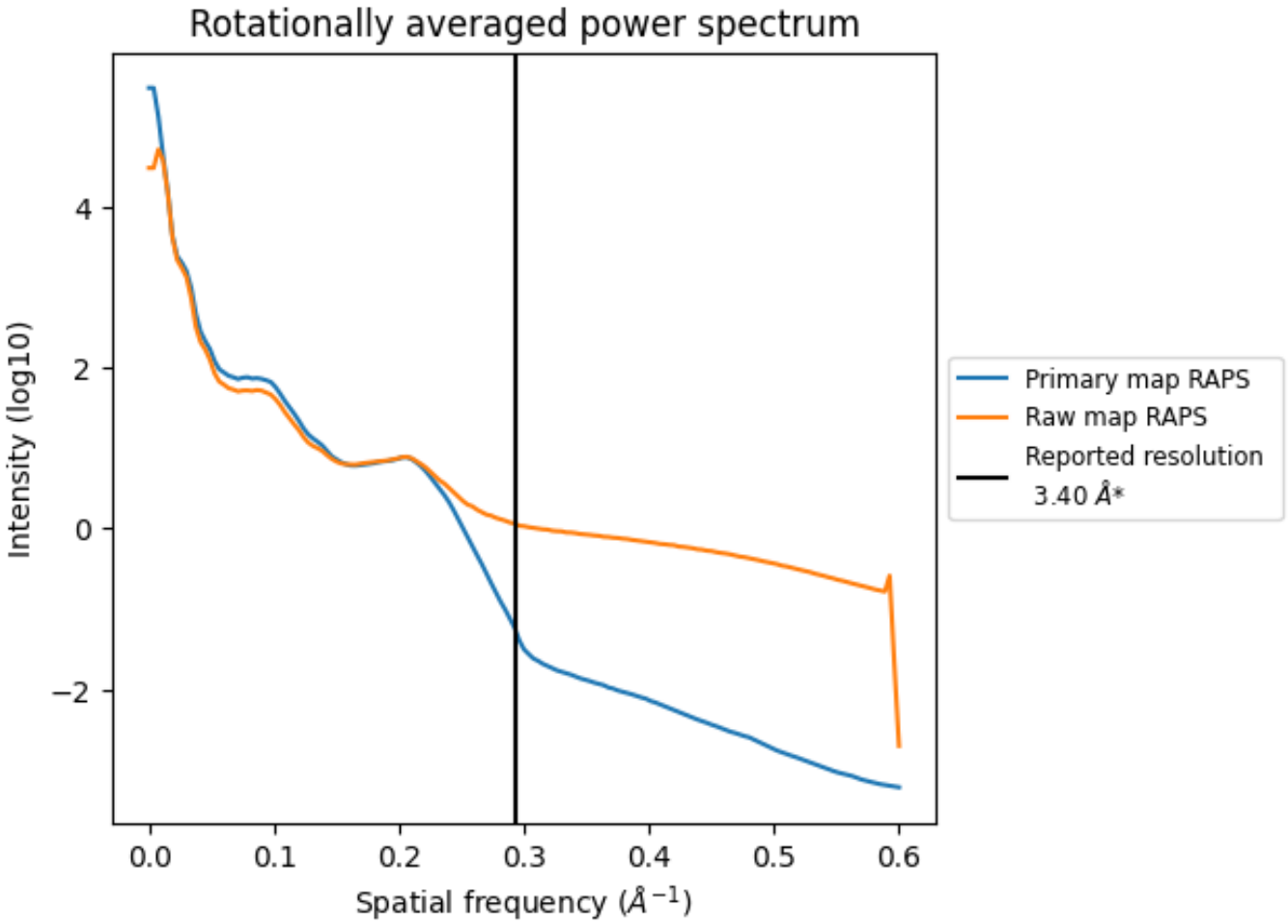
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 192 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)

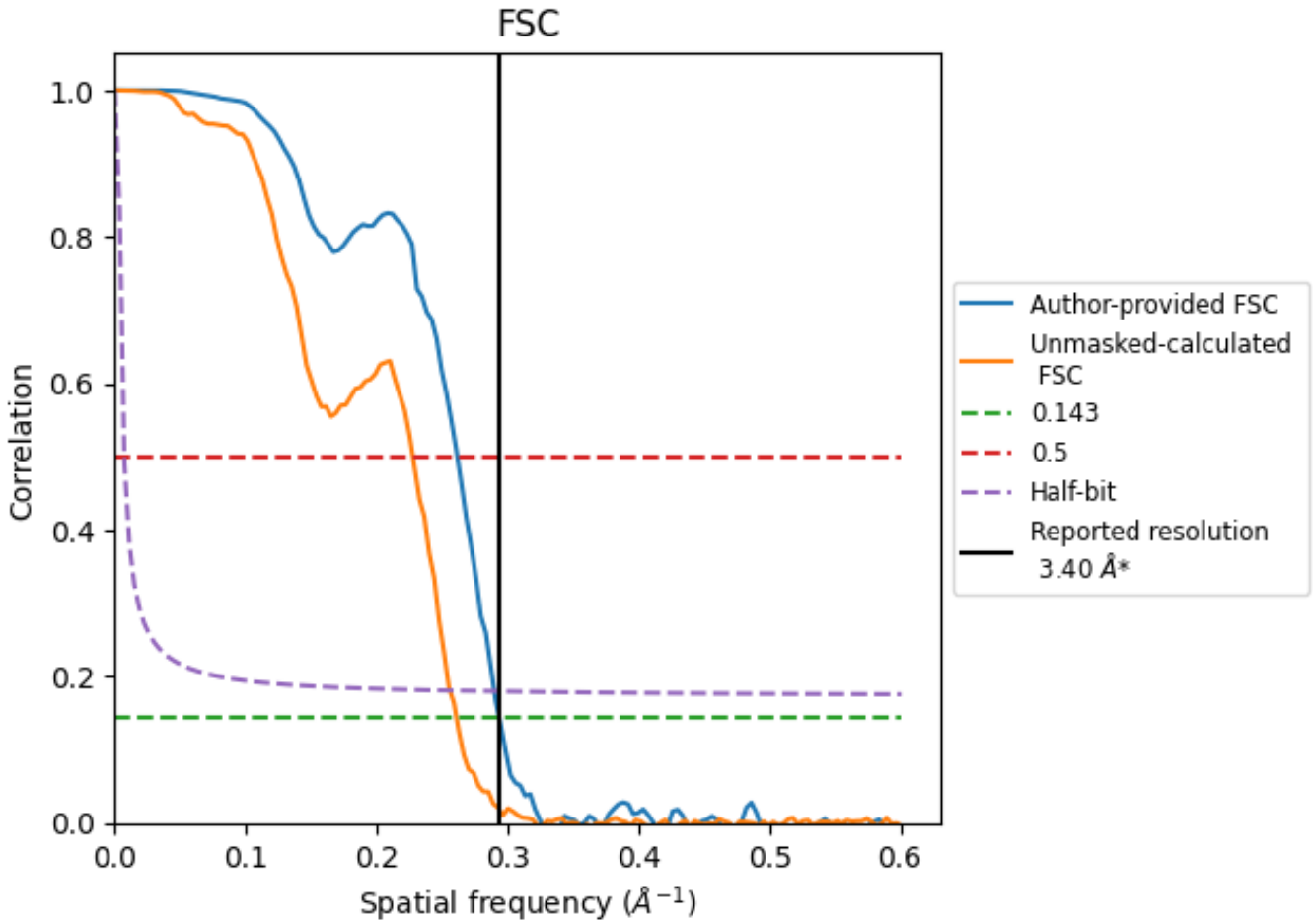


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

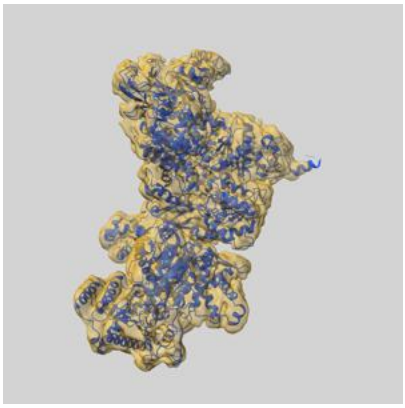
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.82	3.45
Unmasked-calculated*	3.83	4.39	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.4 by more than 10 %

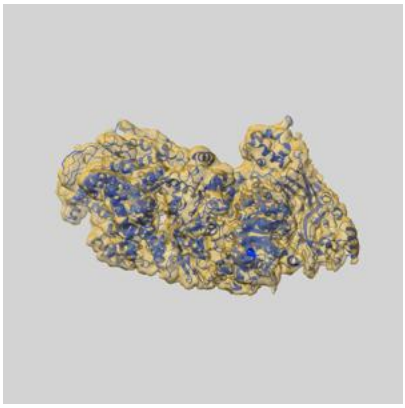
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15521 and PDB model 8ALZ. Per-residue inclusion information can be found in section 3 on page 4.

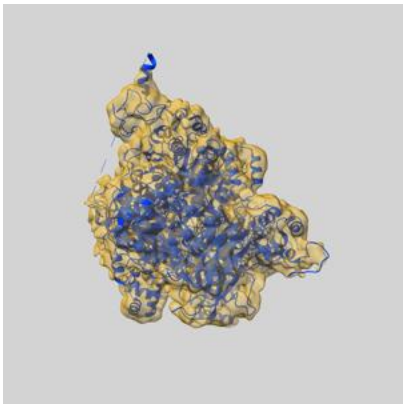
9.1 Map-model overlay



X



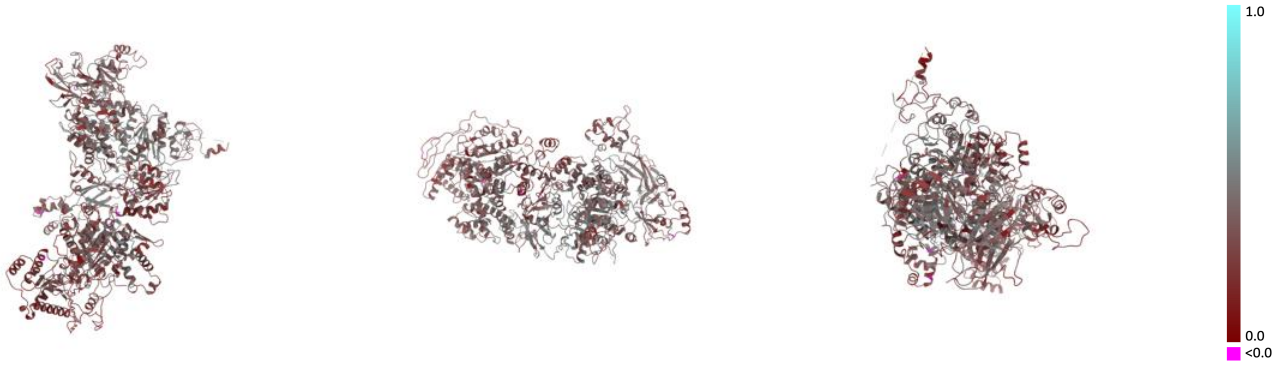
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.157 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.

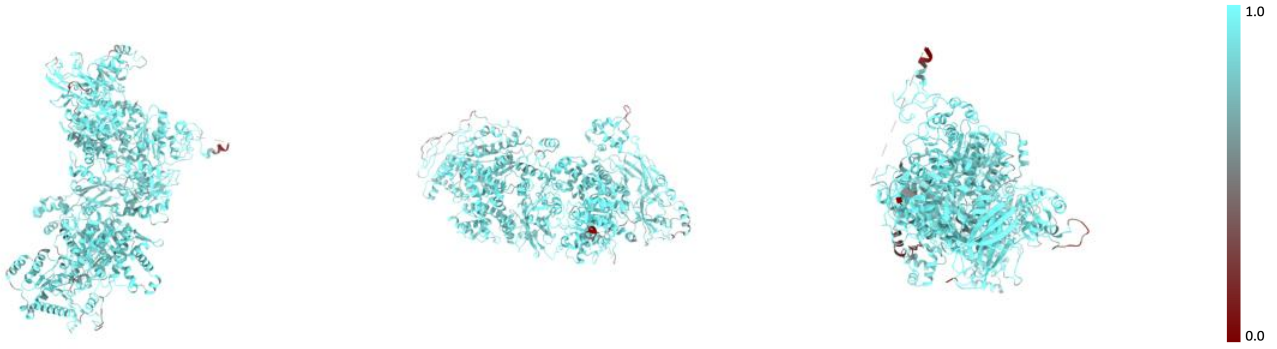
9.2 Q-score mapped to coordinate model



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.

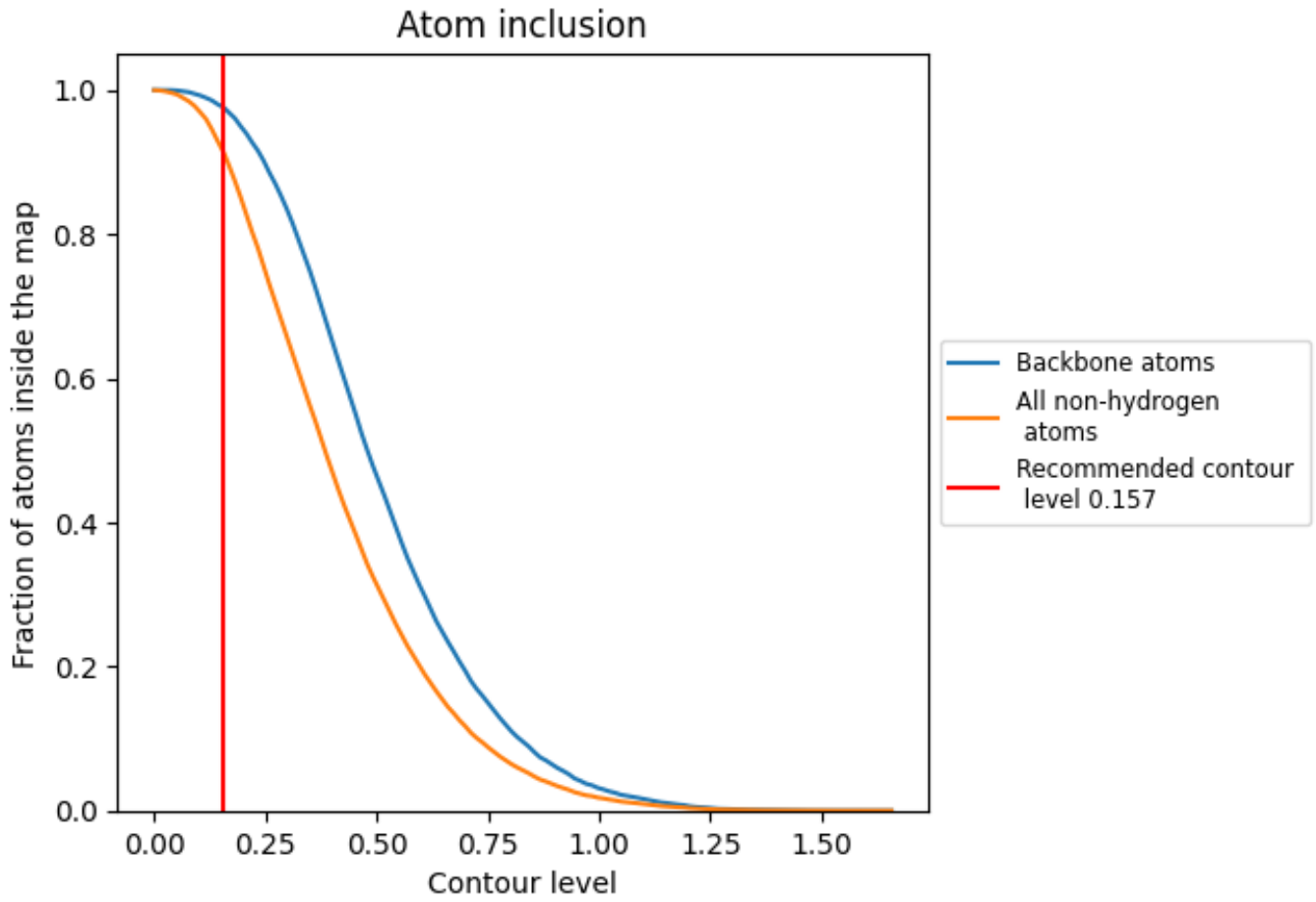
9.3 Atom inclusion mapped to coordinate model



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 (0.157).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9122	0.3430
A	0.8292	0.3300
B	0.9241	0.3450