Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 01:57 AM JST

PDB ID	:	6KWX
EMDB ID	:	EMD-0780
Title	:	cryo-EM structure of human PA200
Authors	:	Ouyang, S.; Hongxin, G.
Deposited on	:	2019-09-09
Resolution	:	3.75 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:

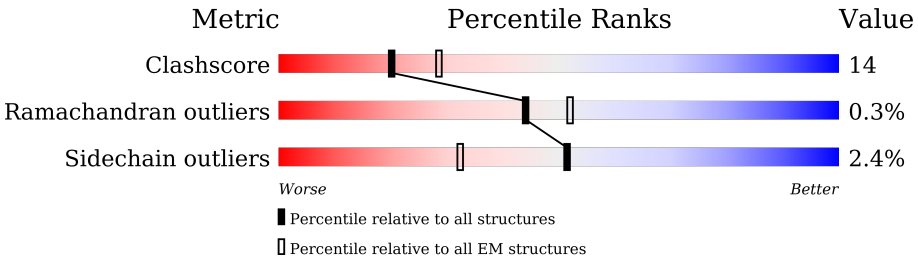
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.75 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	1878	16% 70% 22% • 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IHP	A	1902	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14227 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 Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1751	14147	9105	2414	2549	79	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q14997
A	-33	GLY	-	expression tag	UNP Q14997
A	-32	THR	-	expression tag	UNP Q14997
A	-31	THR	-	expression tag	UNP Q14997
A	-30	ARG	-	expression tag	UNP Q14997
A	-29	SER	-	expression tag	UNP Q14997
A	-28	THR	-	expression tag	UNP Q14997
A	-27	MET	-	expression tag	UNP Q14997
A	-26	SER	-	expression tag	UNP Q14997
A	-25	TYR	-	expression tag	UNP Q14997
A	-24	TYR	-	expression tag	UNP Q14997
A	-23	HIS	-	expression tag	UNP Q14997
A	-22	HIS	-	expression tag	UNP Q14997
A	-21	HIS	-	expression tag	UNP Q14997
A	-20	HIS	-	expression tag	UNP Q14997
A	-19	HIS	-	expression tag	UNP Q14997
A	-18	HIS	-	expression tag	UNP Q14997
A	-17	ASP	-	expression tag	UNP Q14997
A	-16	TYR	-	expression tag	UNP Q14997
A	-15	ASP	-	expression tag	UNP Q14997
A	-14	ILE	-	expression tag	UNP Q14997
A	-13	PRO	-	expression tag	UNP Q14997
A	-12	THR	-	expression tag	UNP Q14997
A	-11	THR	-	expression tag	UNP Q14997
A	-10	GLU	-	expression tag	UNP Q14997
A	-9	ASN	-	expression tag	UNP Q14997
A	-8	LEU	-	expression tag	UNP Q14997
A	-7	TYR	-	expression tag	UNP Q14997

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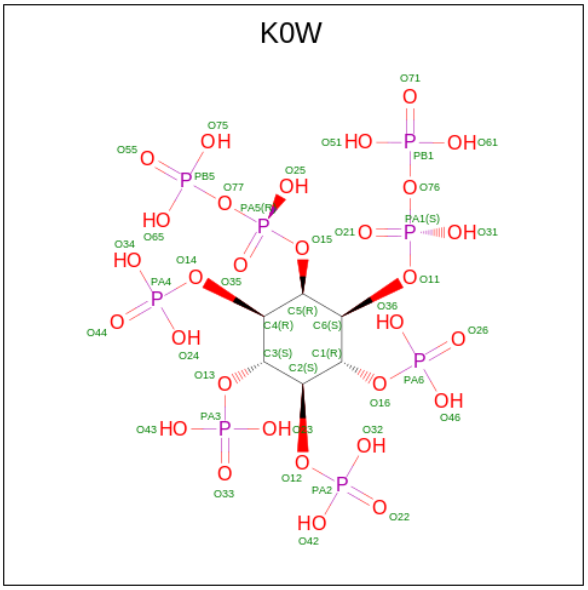
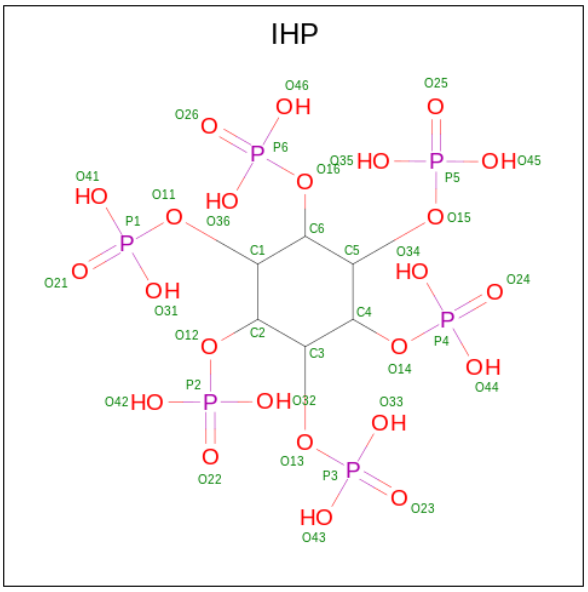
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q14997
A	-5	GLN	-	expression tag	UNP Q14997
A	-4	GLY	-	expression tag	UNP Q14997
A	-3	ALA	-	expression tag	UNP Q14997
A	-2	MET	-	expression tag	UNP Q14997
A	-1	ASP	-	expression tag	UNP Q14997
A	0	PRO	-	expression tag	UNP Q14997
A	821	ILE	LEU	conflict	UNP Q14997
A	822	LEU	ILE	conflict	UNP Q14997

- Molecule 2 is [(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[oxidanyl(phosphonooxy)phosphoryl]oxy-3,4,5,6-tetraphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (three-letter code: K0W) (formula: $C_6H_{20}O_{30}P_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	44	6	30	8	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



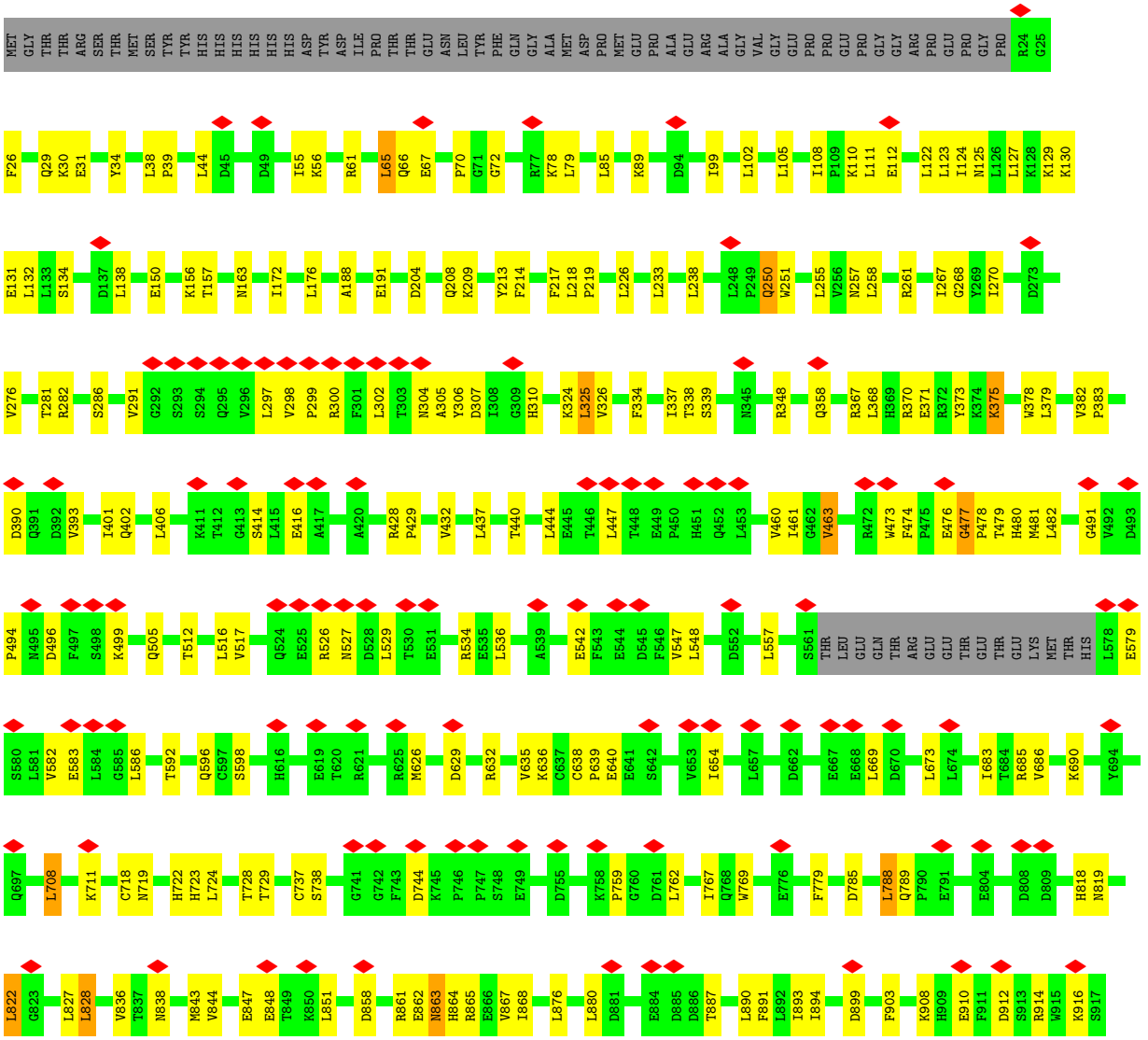
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	A	1	36	6	24	6	0

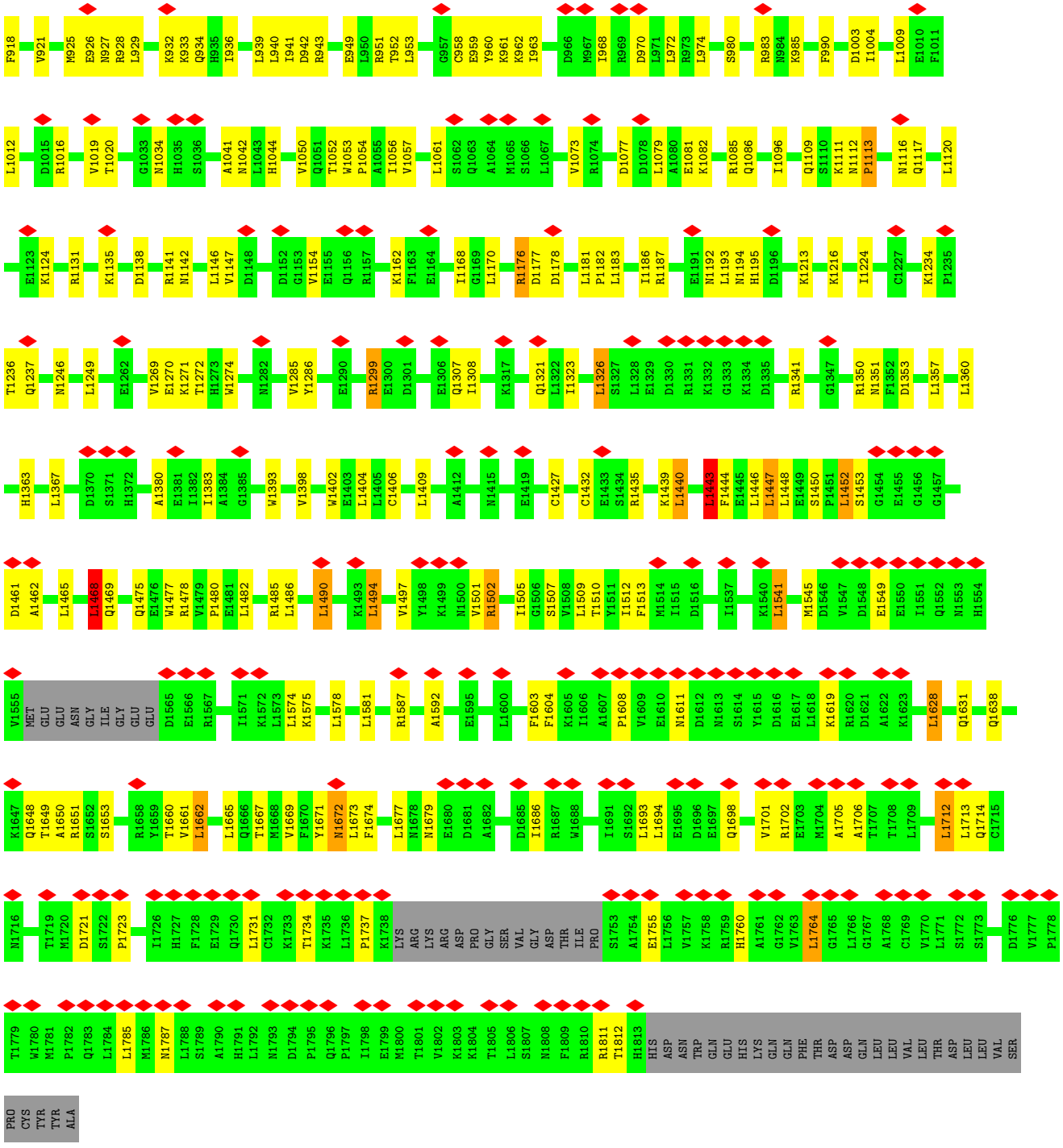
3 Residue-property plots (i)

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: Proteasome activator complex subunit 4

Chain A:




F918 V921 M925 E926 N927 R928 L929 K932 K933 Q934 H935 I936 L939 L940 I941 D942 R943 E949 L950 R951 T952 L953 G957 C958 E959 Y960 K961 K962 I963 D966 M967 I968 R969 D970 L971 L972 R973 L974 S980 R983 N984 K985 F990 D1003 I1004 L1009 E1010 F1011
L1012 D1015 R1016 V1019 T1020 G1033 N1034 H1035 S1036 A1041 N1042 L1043 H1044 V1050 Q1051 T1052 W1053 P1054 A1055 I1056 V1057 L1061 S1062 Q1063 A1064 M1065 S1066 L1067 V1073 R1074 D1077 D1078 L1079 A1080 E1081 K1082 R1085 Q1086 I1096 Q1109 S1110 K1111 N1112 P1113 N1116 Q1117 L1120
E1123 K1124 R1131 K1135 D1138 R1141 N1142 L1146 V1147 D1148 D1152 G1153 V1154 E1155 Q1156 R1157 K1162 F1163 E1164 I1168 G1169 L1170 R1176 D1177 D1178 L1181 P1182 L1183 I1186 R1187 E1191 N1192 L1193 N1194 H1195 D1196 K1213 K1216 I1224 C1227 K1234 P1235
T1236 Q1237 N1246 L1249 E1262 V1269 E1270 K1271 T1272 H1273 W1274 N1282 V1285 Y1286 E1290 R1299 E1300 D1301 E1306 Q1307 I1308 K1317 Q1321 L1322 I1323 L1326 S1327 L1328 E1329 D1330 R1331 K1332 G1333 K1334 D1335 R1341 G1347 R1350 N1351 F1352 D1353 L1357 L1360
H1363 L1367 D1370 S1371 H1372 A1380 E1381 I1382 I1383 A1384 G1385 W1393 V1398 W1402 E1403 L1404 L1405 C1406 L1409 A1412 N1415 E1419 C1427 C1432 E1433 S1434 R1435 K1439 L1440 L1443 F1444 E1445 L1446 L1447 L1448 E1449 S1450 P1451 L1452 S1453 G1454 E1455 G1456 G1457
D1461 A1462 L1465 L1468 Q1469 Q1475 E1476 W1477 R1478 V1479 P1480 E1481 L1482 R1485 L1486 L1490 K1493 L1494 V1497 Y1498 K1499 N1500 V1501 R1502 I1505 G1506 S1507 V1508 L1509 T1510 Y1511 I1512 F1513 M1514 I1515 D1516 I1537 K1540 L1541 M1545 D1546 V1547 D1548 E1549 E1550 I1551 Q1552 N1553 H1554
V1555 MET GLU GLU ASN GLY ILE GLY GLU D1565 E1566 R1567 I1571 K1572 L1573 L1574 K1575 L1578 L1581 R1587 A1592 E1595 L1600 F1603 F1604 K1605 I1606 A1607 P1608 V1609 E1610 N1611 D1612 N1613 S1614 Y1615 D1616 E1617 L1618 K1619 R1620 D1621 A1622 K1623 L1628 Q1631 Q1638
K1647 Q1648 T1649 A1650 R1651 S1652 S1653 R1658 Y1659 T1660 V1661 L1662 L1665 Q1666 T1667 M1668 V1669 F1670 Y1671 N1672 L1673 F1674 L1677 M1678 N1679 E1680 D1681 A1682 D1685 I1686 R1687 W1688 I1691 S1692 L1693 L1694 E1695 D1696 E1697 Q1698 V1701 R1702 E1703 M1704 A1705 A1706 T1707 T1708 L1709 L1712 L1713 Q1714 C1715
N1716 T1719 M1720 D1721 S1722 P1723 I1726 H1727 F1728 E1729 Q1730 L1731 C1732 K1733 T1734 K1735 L1736 P1737 K1738 LYS ARG LYS ARG ASP PRO GLY SER VAL GLY ASP THR ILE PRO S1753 A1754 E1755 L1756 V1757 R1758 R1759 H1760 A1761 G1762 V1763 L1764 G1765 L1766 G1767 A1768 C1769 V1770 L1771 S1772 S1773 D1776 V1777 P1778
T1779 W1780 M1781 P1782 Q1783 L1784 L1785 M1786 N1787 L1788 S1789 A1790 H1791 L1792 N1793 D1794 P1795 Q1796 P1797 I1798 E1799 M1800 T1801 V1802 K1803 K1804 T1805 L1806 S1807 N1808 F1809 R1810 R1811 T1812 H1813 HIS ASP ASN TRP GLN GLU HIS LYS GLN GLN PHE THR ASP ASP GLN LEU LEU VAL LEU THR ASP LEU LEU VAL SER
PRO CYS TYR TYR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.901	Depositor
Minimum map value	-11.801	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.005	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, K0W

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	0.47	0/14476	0.79	39/19631 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1353	ASP	CB-CG-OD1	10.33	127.60	118.30
1	A	516	LEU	CA-CB-CG	8.77	135.48	115.30
1	A	1177	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	1468	LEU	CA-CB-CG	8.20	134.15	115.30
1	A	302	LEU	CA-CB-CG	8.04	133.78	115.30
1	A	1440	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	444	LEU	CB-CG-CD2	-7.38	98.45	111.00
1	A	1465	LEU	CA-CB-CG	7.18	131.82	115.30
1	A	586	LEU	CA-CB-CG	6.95	131.28	115.30
1	A	1447	LEU	CA-CB-CG	6.80	130.94	115.30
1	A	1490	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	1764	LEU	CA-CB-CG	6.63	130.56	115.30
1	A	1662	LEU	CA-CB-CG	6.47	130.18	115.30
1	A	337	ILE	CG1-CB-CG2	-6.06	98.06	111.40
1	A	65	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	1249	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	1662	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	A	1713	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	708	LEU	CB-CG-CD2	-5.92	100.93	111.00
1	A	1061	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	1326	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	708	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	1176	ARG	C-N-CA	5.71	135.97	121.70
1	A	1694	LEU	CA-CB-CG	5.66	128.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1494	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	1628	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	444	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	1367	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	1443	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	447	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	1541	LEU	CA-CB-CG	5.38	127.66	115.30
1	A	258	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	233	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	105	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	899	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	788	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	1353	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	1404	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	1193	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14147	0	14364	393	0
2	A	44	0	0	14	0
3	A	36	0	6	11	0
All	All	14227	0	14370	393	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 14.

All (393) 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:972:LEU:HD11	1:A:1004:ILE:CD1	1.30	1.60
1:A:972:LEU:CD1	1:A:1004:ILE:HD11	1.34	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:NH1	1:A:1631:GLN:HG2	1.26	1.49
1:A:298:VAL:CG2	1:A:299:PRO:HD3	1.57	1.33
1:A:324:LYS:O	1:A:326:VAL:N	1.63	1.31
1:A:972:LEU:HD21	1:A:990:PHE:CE1	1.70	1.26
1:A:307:ASP:OD2	1:A:310:HIS:HD2	1.11	1.25
1:A:933:LYS:CG	2:A:1901:K0W:O71	1.87	1.21
1:A:300:ARG:NH1	1:A:1631:GLN:CG	2.04	1.21
1:A:887:THR:O	1:A:891:PHE:CE2	1.96	1.17
1:A:300:ARG:CZ	1:A:1631:GLN:HG2	1.78	1.14
1:A:298:VAL:HG23	1:A:299:PRO:CD	1.78	1.12
1:A:933:LYS:HG2	2:A:1901:K0W:O71	0.95	1.12
1:A:960:TYR:HE2	1:A:1003:ASP:OD2	1.32	1.12
1:A:307:ASP:OD2	1:A:310:HIS:CD2	2.02	1.10
1:A:34:TYR:OH	1:A:933:LYS:CE	2.00	1.09
1:A:375:LYS:H	1:A:375:LYS:HE3	1.14	1.09
1:A:972:LEU:CD2	1:A:990:PHE:CE1	2.33	1.09
1:A:297:LEU:HD13	1:A:1631:GLN:NE2	1.68	1.08
1:A:887:THR:O	1:A:891:PHE:CD2	2.07	1.07
1:A:1112:ASN:HB2	1:A:1113:PRO:CD	1.85	1.06
1:A:1112:ASN:CB	1:A:1113:PRO:HD3	1.74	1.06
1:A:972:LEU:HD21	1:A:990:PHE:CZ	1.89	1.05
1:A:300:ARG:NH1	1:A:1631:GLN:O	1.91	1.01
1:A:34:TYR:OH	1:A:933:LYS:HE2	1.56	1.01
1:A:1271:LYS:HB2	1:A:1274:TRP:CD1	1.98	0.99
1:A:1271:LYS:O	1:A:1478:ARG:NH2	1.98	0.97
1:A:300:ARG:NH1	1:A:1631:GLN:C	2.19	0.95
1:A:300:ARG:HH12	1:A:1631:GLN:HG2	1.26	0.95
1:A:131:GLU:HG3	1:A:379:LEU:CD1	1.97	0.94
1:A:933:LYS:NZ	2:A:1901:K0W:O61	2.01	0.93
1:A:300:ARG:HH12	1:A:1631:GLN:CG	1.75	0.93
1:A:208:GLN:NE2	1:A:251:TRP:HB3	1.83	0.93
1:A:1286:TYR:OH	3:A:1902:IHP:O42	1.87	0.91
1:A:933:LYS:HG2	2:A:1901:K0W:PB1	2.11	0.91
1:A:960:TYR:CE2	1:A:1003:ASP:OD2	2.24	0.89
1:A:1112:ASN:HB2	1:A:1113:PRO:HD3	0.89	0.88
1:A:1213:LYS:NZ	3:A:1902:IHP:O33	2.07	0.87
1:A:1181:LEU:HD12	1:A:1182:PRO:CD	2.05	0.87
1:A:887:THR:O	1:A:891:PHE:HE2	1.47	0.86
1:A:300:ARG:NH1	1:A:1631:GLN:CB	2.38	0.86
1:A:1147:VAL:HG11	1:A:1182:PRO:HG2	1.58	0.85
1:A:1181:LEU:CD1	1:A:1182:PRO:HD2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:LYS:CG	2:A:1901:K0W:PB1	2.66	0.81
1:A:375:LYS:HE3	1:A:375:LYS:N	1.93	0.81
1:A:298:VAL:HG23	1:A:299:PRO:HD3	0.84	0.81
1:A:297:LEU:HD13	1:A:1631:GLN:HE21	1.44	0.80
1:A:131:GLU:HG3	1:A:379:LEU:HD11	1.62	0.80
1:A:56:LYS:NZ	1:A:1113:PRO:HD2	1.96	0.79
1:A:267:ILE:HD12	1:A:370:ARG:HH12	1.47	0.79
1:A:1181:LEU:HD12	1:A:1182:PRO:HD3	1.63	0.79
1:A:929:LEU:HD13	1:A:929:LEU:O	1.84	0.78
1:A:131:GLU:HG3	1:A:379:LEU:HD13	1.65	0.78
1:A:281:THR:OG1	1:A:1672:ASN:HA	1.84	0.77
1:A:291:VAL:CG1	1:A:1671:TYR:CE2	2.69	0.75
1:A:972:LEU:HD23	1:A:990:PHE:CE1	2.22	0.74
1:A:30:LYS:HE2	1:A:129:LYS:HD3	1.70	0.74
1:A:373:TYR:CE2	1:A:929:LEU:HD11	2.23	0.74
1:A:297:LEU:HD23	1:A:297:LEU:H	1.53	0.73
1:A:379:LEU:HD12	1:A:379:LEU:H	1.53	0.73
1:A:887:THR:O	1:A:891:PHE:HD2	1.70	0.73
1:A:914:ARG:NH1	1:A:942:ASP:OD1	2.23	0.72
1:A:1181:LEU:HG	1:A:1182:PRO:HD2	1.69	0.72
1:A:208:GLN:OE1	1:A:250:GLN:NE2	2.23	0.72
1:A:1216:LYS:HA	1:A:1351:ASN:HD21	1.52	0.72
1:A:34:TYR:CZ	1:A:933:LYS:HE2	2.25	0.71
1:A:298:VAL:CG2	1:A:299:PRO:CD	2.52	0.71
1:A:300:ARG:HH12	1:A:1631:GLN:C	1.93	0.71
1:A:130:LYS:HG2	1:A:378:TRP:HZ3	1.54	0.71
1:A:300:ARG:HH12	1:A:1631:GLN:CA	2.03	0.71
1:A:56:LYS:HZ2	1:A:1113:PRO:HD2	1.57	0.70
1:A:1181:LEU:CG	1:A:1182:PRO:HD2	2.21	0.70
1:A:933:LYS:CD	2:A:1901:K0W:PB1	2.81	0.69
1:A:297:LEU:HD13	1:A:1631:GLN:HE22	1.54	0.69
1:A:34:TYR:OH	1:A:933:LYS:HE3	1.93	0.69
1:A:1271:LYS:HB2	1:A:1274:TRP:NE1	2.07	0.69
1:A:297:LEU:HD12	1:A:300:ARG:HG2	1.75	0.68
1:A:933:LYS:NZ	2:A:1901:K0W:PB1	2.66	0.68
1:A:208:GLN:HE22	1:A:251:TRP:HB3	1.59	0.68
1:A:1181:LEU:HD12	1:A:1182:PRO:HD2	1.71	0.68
1:A:759:PRO:HB2	1:A:934:GLN:HB3	1.75	0.67
1:A:1673:LEU:C	1:A:1673:LEU:HD23	2.14	0.67
1:A:150:GLU:OE2	1:A:209:LYS:CE	2.44	0.66
1:A:371:GLU:HG2	1:A:382:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:GLU:O	1:A:914:ARG:HG3	1.94	0.66
1:A:718:CYS:SG	1:A:819:ASN:ND2	2.69	0.66
1:A:1050:VAL:HG22	1:A:1146:LEU:HB2	1.78	0.66
1:A:933:LYS:HD2	2:A:1901:K0W:PB1	2.36	0.65
1:A:390:ASP:OD1	1:A:428:ARG:NH1	2.29	0.65
1:A:865:ARG:NH2	1:A:903:PHE:O	2.29	0.65
1:A:1662:LEU:HD13	1:A:1693:LEU:HD12	1.79	0.65
1:A:218:LEU:O	1:A:261:ARG:NH1	2.30	0.65
1:A:887:THR:HG22	1:A:891:PHE:HE2	1.63	0.64
1:A:324:LYS:C	1:A:326:VAL:N	2.50	0.64
1:A:300:ARG:HH12	1:A:1631:GLN:CB	2.03	0.64
1:A:1109:GLN:O	1:A:1111:LYS:HD2	1.96	0.64
1:A:297:LEU:CD1	1:A:1631:GLN:NE2	2.56	0.64
1:A:1041:ALA:HA	1:A:1052:THR:HG21	1.80	0.64
1:A:1216:LYS:NZ	3:A:1902:IHP:O12	2.32	0.63
1:A:297:LEU:HD23	1:A:297:LEU:N	2.12	0.63
1:A:300:ARG:NH1	1:A:1631:GLN:CA	2.61	0.63
1:A:1432:CYS:O	1:A:1475:GLN:NE2	2.32	0.62
1:A:208:GLN:HA	1:A:208:GLN:HE21	1.64	0.62
1:A:478:PRO:HB2	1:A:536:LEU:HD11	1.82	0.62
1:A:1706:ALA:HB2	1:A:1764:LEU:HG	1.82	0.62
1:A:339:SER:OG	1:A:1714:GLN:NE2	2.32	0.62
1:A:1673:LEU:HD21	1:A:1677:LEU:CD1	2.29	0.62
1:A:669:LEU:HD11	1:A:708:LEU:HD21	1.81	0.62
1:A:972:LEU:CG	1:A:1004:ILE:HD11	2.23	0.62
1:A:1004:ILE:HG12	1:A:1004:ILE:O	2.00	0.61
1:A:926:GLU:HG3	1:A:928:ARG:HG2	1.80	0.61
1:A:379:LEU:HD12	1:A:379:LEU:N	2.14	0.61
1:A:1402:TRP:HH2	1:A:1443:LEU:HD22	1.66	0.61
1:A:367:ARG:NH1	1:A:371:GLU:OE2	2.34	0.61
1:A:375:LYS:H	1:A:375:LYS:CE	2.02	0.61
1:A:56:LYS:NZ	1:A:1113:PRO:CD	2.64	0.61
1:A:1216:LYS:HZ1	3:A:1902:IHP:P2	2.23	0.61
1:A:474:PHE:CE1	1:A:476:GLU:HG3	2.36	0.60
1:A:1326:LEU:O	1:A:1341:ARG:NH2	2.35	0.60
1:A:1181:LEU:CD1	1:A:1182:PRO:CD	2.73	0.59
1:A:208:GLN:HE22	1:A:251:TRP:CA	2.15	0.59
1:A:324:LYS:O	1:A:325:LEU:C	2.38	0.59
1:A:324:LYS:N	1:A:324:LYS:HD2	2.16	0.59
1:A:474:PHE:CE2	1:A:477:GLY:HA2	2.37	0.59
1:A:933:LYS:NZ	2:A:1901:K0W:O71	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HG2	1:A:1120:LEU:HD11	1.85	0.59
1:A:1271:LYS:HG3	1:A:1274:TRP:HE1	1.68	0.59
1:A:1592:ALA:O	1:A:1638:GLN:NE2	2.36	0.59
1:A:61:ARG:HH11	1:A:1117:GLN:HB2	1.67	0.58
1:A:1760:HIS:O	1:A:1764:LEU:HB2	2.03	0.58
1:A:267:ILE:CD1	1:A:370:ARG:HH12	2.15	0.58
1:A:297:LEU:HB2	1:A:300:ARG:HB3	1.85	0.58
1:A:926:GLU:CG	1:A:928:ARG:HG2	2.32	0.58
1:A:156:LYS:NZ	3:A:1902:IHP:O25	2.26	0.58
1:A:150:GLU:OE2	1:A:209:LYS:HE2	2.03	0.58
1:A:298:VAL:N	1:A:299:PRO:CD	2.66	0.58
1:A:56:LYS:HZ1	1:A:1113:PRO:CD	2.16	0.58
1:A:932:LYS:HB2	1:A:934:GLN:NE2	2.19	0.58
1:A:297:LEU:HB3	1:A:1631:GLN:HE22	1.69	0.57
1:A:1181:LEU:HB3	1:A:1186:ILE:HD11	1.86	0.57
1:A:1271:LYS:CG	1:A:1274:TRP:HE1	2.17	0.57
1:A:267:ILE:HG21	1:A:367:ARG:NH2	2.20	0.57
1:A:1448:LEU:HD12	1:A:1468:LEU:HD21	1.86	0.57
1:A:108:ILE:HB	1:A:111:LEU:HB2	1.87	0.57
1:A:1323:ILE:HD13	1:A:1363:HIS:HB3	1.87	0.57
1:A:478:PRO:O	1:A:481:MET:N	2.30	0.57
1:A:912:ASP:O	1:A:916:LYS:HG3	2.05	0.57
1:A:968:ILE:O	1:A:972:LEU:HG	2.04	0.57
1:A:876:LEU:HD11	1:A:974:LEU:HD21	1.86	0.57
1:A:767:ILE:HG12	1:A:941:ILE:HG12	1.86	0.56
1:A:876:LEU:HD13	1:A:893:ILE:HG21	1.87	0.56
1:A:1468:LEU:HD11	1:A:1486:LEU:HD11	1.86	0.56
1:A:157:THR:OG1	1:A:163:ASN:ND2	2.39	0.56
1:A:1673:LEU:CD2	1:A:1677:LEU:HD12	2.35	0.56
1:A:1224:ILE:HG12	1:A:1285:VAL:HG22	1.87	0.56
1:A:1192:ASN:HB2	1:A:1195:HIS:HB2	1.87	0.56
1:A:972:LEU:CD2	1:A:990:PHE:CZ	2.71	0.55
1:A:1216:LYS:NZ	3:A:1902:IHP:O22	2.38	0.55
1:A:1648:GLN:OE1	1:A:1651:ARG:NH2	2.40	0.55
1:A:373:TYR:HE2	1:A:929:LEU:HD11	1.69	0.55
1:A:1667:THR:HG23	1:A:1671:TYR:CE2	2.41	0.55
1:A:102:LEU:HD22	1:A:122:LEU:HD22	1.87	0.55
1:A:286:SER:HB2	1:A:306:TYR:HB2	1.89	0.55
1:A:373:TYR:CD2	1:A:929:LEU:CD1	2.90	0.55
1:A:635:VAL:HG12	1:A:686:VAL:HG21	1.89	0.55
1:A:334:PHE:O	1:A:338:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:LEU:HA	1:A:1360:LEU:HB2	1.89	0.55
1:A:379:LEU:CD1	1:A:379:LEU:H	2.17	0.54
1:A:1469:GLN:HE22	1:A:1507:SER:HG	1.55	0.54
1:A:188:ALA:HA	1:A:191:GLU:HG2	1.90	0.54
1:A:596:GLN:HE22	1:A:738:SER:H	1.54	0.54
1:A:972:LEU:HD11	1:A:1004:ILE:CG1	2.25	0.54
1:A:529:LEU:HD13	1:A:534:ARG:HB2	1.88	0.54
1:A:491:GLY:HA2	1:A:499:LYS:HE3	1.88	0.54
1:A:788:LEU:HD11	1:A:868:ILE:HD11	1.89	0.54
1:A:929:LEU:HD13	1:A:929:LEU:C	2.27	0.54
1:A:669:LEU:HD22	1:A:673:LEU:HD23	1.90	0.54
1:A:1443:LEU:O	1:A:1447:LEU:HB3	2.08	0.53
1:A:482:LEU:HD11	1:A:542:GLU:HB3	1.89	0.53
1:A:208:GLN:HE22	1:A:251:TRP:CB	2.19	0.53
1:A:1721:ASP:HB3	1:A:1723:PRO:HD2	1.91	0.53
1:A:268:GLY:HA3	1:A:383:PRO:HG2	1.89	0.53
1:A:972:LEU:HD21	1:A:990:PHE:HE1	1.56	0.53
1:A:1452:LEU:HD22	1:A:1461:ASP:HB3	1.89	0.53
1:A:267:ILE:HG22	1:A:267:ILE:O	2.09	0.53
1:A:373:TYR:CE2	1:A:929:LEU:CD1	2.90	0.53
1:A:1056:ILE:HD11	1:A:1079:LEU:HD13	1.91	0.53
1:A:863:ASN:HD22	1:A:864:HIS:N	2.07	0.53
1:A:324:LYS:C	1:A:326:VAL:H	2.05	0.52
1:A:208:GLN:NE2	1:A:208:GLN:HA	2.23	0.52
1:A:1216:LYS:NZ	3:A:1902:IHP:P2	2.82	0.52
1:A:31:GLU:HG2	1:A:89:LYS:HG2	1.92	0.52
1:A:276:VAL:HG21	1:A:326:VAL:HG22	1.91	0.52
1:A:887:THR:HG22	1:A:891:PHE:CE2	2.42	0.52
1:A:908:LYS:HA	1:A:953:LEU:HD11	1.90	0.52
1:A:208:GLN:HE21	1:A:251:TRP:HB3	1.67	0.52
1:A:1112:ASN:H	1:A:1113:PRO:CD	2.23	0.52
1:A:933:LYS:CD	2:A:1901:K0W:O71	2.56	0.52
1:A:936:ILE:HD11	1:A:939:LEU:HD23	1.92	0.51
1:A:858:ASP:OD2	1:A:861:ARG:NH1	2.43	0.51
1:A:1604:PHE:HD1	1:A:1660:THR:HG23	1.75	0.51
1:A:286:SER:HB2	1:A:306:TYR:CB	2.41	0.51
1:A:918:PHE:CE1	1:A:943:ARG:HB2	2.45	0.51
1:A:1077:ASP:O	1:A:1081:GLU:HB2	2.10	0.51
1:A:512:THR:HG23	1:A:592:THR:HG23	1.92	0.51
1:A:297:LEU:HB3	1:A:1631:GLN:NE2	2.26	0.51
1:A:818:HIS:O	1:A:822:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:GLU:O	1:A:953:LEU:HB2	2.10	0.51
1:A:1034:ASN:O	1:A:1082:LYS:NZ	2.40	0.51
1:A:1462:ALA:HB2	1:A:1501:VAL:HG22	1.92	0.51
1:A:1486:LEU:HD22	1:A:1512:ILE:HD11	1.93	0.51
1:A:1147:VAL:CG1	1:A:1182:PRO:HG2	2.35	0.50
1:A:1435:ARG:HH22	3:A:1902:IHP:P4	2.34	0.50
1:A:26:PHE:HB3	1:A:1112:ASN:HB3	1.94	0.50
1:A:851:LEU:HD23	1:A:951:ARG:HG3	1.93	0.50
1:A:304:ASN:O	1:A:305:ALA:HB3	2.11	0.50
1:A:1608:PRO:HD3	1:A:1619:LYS:HB3	1.94	0.50
1:A:297:LEU:N	1:A:297:LEU:CD2	2.75	0.49
1:A:1138:ASP:HA	1:A:1141:ARG:HB2	1.93	0.49
1:A:1662:LEU:HD21	1:A:1705:ALA:HB2	1.94	0.49
1:A:78:LYS:NZ	1:A:847:GLU:O	2.30	0.49
1:A:547:VAL:HG23	1:A:548:LEU:HD12	1.94	0.49
1:A:1176:ARG:HG3	1:A:1178:ASP:H	1.77	0.49
1:A:1350:ARG:O	1:A:1350:ARG:HG2	2.12	0.49
1:A:1154:VAL:HG21	1:A:1168:ILE:HG13	1.94	0.49
1:A:1009:LEU:HD21	1:A:1052:THR:HA	1.95	0.49
1:A:124:ILE:HG13	1:A:176:LEU:HD23	1.95	0.49
1:A:496:ASP:HB2	1:A:499:LYS:HG2	1.94	0.48
1:A:291:VAL:HG12	1:A:1671:TYR:CE2	2.44	0.48
1:A:1082:LYS:HG3	1:A:1085:ARG:HH21	1.78	0.48
1:A:1183:LEU:HD11	1:A:1308:ILE:HD11	1.94	0.48
1:A:1380:ALA:HB1	1:A:1427:CYS:HB2	1.96	0.48
1:A:112:GLU:OE2	1:A:1044:HIS:NE2	2.46	0.48
1:A:1667:THR:HG23	1:A:1671:TYR:HE2	1.78	0.48
1:A:1669:VAL:O	1:A:1673:LEU:HA	2.13	0.48
1:A:1737:PRO:HG3	1:A:1755:GLU:HB3	1.95	0.48
1:A:1269:VAL:HG12	1:A:1478:ARG:HH22	1.79	0.48
1:A:1406:CYS:HA	1:A:1446:LEU:HD11	1.95	0.48
1:A:1502:ARG:HH12	1:A:1575:LYS:HD3	1.79	0.48
1:A:1182:PRO:O	1:A:1186:ILE:HG12	2.14	0.47
1:A:478:PRO:O	1:A:480:HIS:N	2.47	0.47
1:A:130:LYS:HG2	1:A:378:TRP:CZ3	2.41	0.47
1:A:1181:LEU:HB3	1:A:1186:ILE:CD1	2.45	0.47
1:A:238:LEU:HG	1:A:255:LEU:HD11	1.97	0.47
1:A:267:ILE:HD12	1:A:370:ARG:NH1	2.24	0.47
1:A:478:PRO:O	1:A:479:THR:C	2.52	0.47
1:A:949:GLU:HA	1:A:952:THR:HG22	1.97	0.47
1:A:579:GLU:HA	1:A:582:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1183:LEU:HD11	1:A:1308:ILE:CD1	2.45	0.47
1:A:1541:LEU:HD11	1:A:1574:LEU:HB2	1.97	0.46
1:A:636:LYS:HA	1:A:686:VAL:HG23	1.98	0.46
1:A:299:PRO:HB2	1:A:1628:LEU:HD11	1.97	0.46
1:A:517:VAL:HG22	1:A:598:SER:HB3	1.97	0.46
1:A:1181:LEU:CG	1:A:1182:PRO:CD	2.91	0.46
1:A:1271:LYS:CB	1:A:1274:TRP:NE1	2.77	0.46
1:A:129:LYS:NZ	2:A:1901:K0W:O44	2.47	0.46
1:A:1393:TRP:HB2	1:A:1398:VAL:HG13	1.98	0.46
1:A:1435:ARG:NH1	3:A:1902:IHP:O34	2.49	0.46
1:A:933:LYS:CG	2:A:1901:K0W:O51	2.63	0.46
1:A:39:PRO:HG3	1:A:769:TRP:CG	2.51	0.46
1:A:1194:ASN:HD22	1:A:1321:GLN:HB2	1.81	0.46
1:A:1109:GLN:O	1:A:1111:LYS:CD	2.64	0.46
1:A:1574:LEU:O	1:A:1578:LEU:HB2	2.16	0.46
1:A:1702:ARG:HB3	1:A:1764:LEU:HD21	1.97	0.46
1:A:30:LYS:CE	1:A:129:LYS:HD3	2.42	0.45
1:A:891:PHE:O	1:A:894:ILE:HB	2.16	0.45
1:A:640:GLU:HG2	1:A:690:LYS:HD2	1.98	0.45
1:A:1811:ARG:HG3	1:A:1812:THR:HG23	1.98	0.45
1:A:1673:LEU:HD21	1:A:1677:LEU:HD11	1.98	0.45
1:A:324:LYS:N	1:A:324:LYS:CD	2.79	0.45
1:A:402:GLN:O	1:A:406:LEU:HB2	2.17	0.45
1:A:123:LEU:HD23	1:A:176:LEU:HD21	1.98	0.45
1:A:891:PHE:HD1	1:A:985:LYS:HD2	1.81	0.45
1:A:1236:THR:OG1	1:A:1237:GLN:N	2.47	0.45
1:A:429:PRO:HD2	1:A:473:TRP:HE1	1.82	0.45
1:A:460:VAL:HA	1:A:463:VAL:HG12	1.98	0.45
1:A:1272:THR:O	1:A:1477:TRP:NE1	2.42	0.45
1:A:980:SER:HA	1:A:983:ARG:HE	1.82	0.45
1:A:298:VAL:N	1:A:299:PRO:HD2	2.32	0.45
1:A:724:LEU:O	1:A:728:THR:OG1	2.24	0.45
1:A:862:GLU:OE2	1:A:867:VAL:HG21	2.17	0.45
1:A:1085:ARG:HE	1:A:1086:GLN:HG3	1.82	0.45
1:A:629:ASP:HA	1:A:632:ARG:HG2	1.98	0.45
1:A:891:PHE:HA	1:A:894:ILE:HD12	1.99	0.45
1:A:925:MET:SD	1:A:936:ILE:HD13	2.57	0.45
1:A:929:LEU:CD1	1:A:929:LEU:C	2.86	0.45
1:A:56:LYS:NZ	1:A:1113:PRO:HG2	2.32	0.45
1:A:85:LEU:HD11	1:A:951:ARG:HA	1.99	0.45
1:A:368:LEU:HD11	1:A:393:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ILE:CD1	1:A:939:LEU:HD23	2.47	0.45
1:A:55:ILE:HG21	1:A:79:LEU:HD13	1.98	0.44
1:A:67:GLU:O	1:A:72:GLY:N	2.51	0.44
1:A:728:THR:HG21	1:A:779:PHE:HD2	1.82	0.44
1:A:1054:PRO:HA	1:A:1057:VAL:HG12	1.99	0.44
1:A:1077:ASP:OD1	1:A:1162:LYS:NZ	2.50	0.44
1:A:99:ILE:HG23	1:A:127:LEU:HD11	2.00	0.44
1:A:959:GLU:HB3	1:A:961:LYS:HE3	1.99	0.44
1:A:1019:VAL:HG23	1:A:1020:THR:H	1.82	0.44
1:A:29:GLN:HG2	1:A:132:LEU:HD22	1.99	0.44
1:A:729:THR:HG23	1:A:827:LEU:HG	1.98	0.44
1:A:1482:LEU:HA	1:A:1485:ARG:HB2	1.98	0.44
1:A:358:GLN:HB3	1:A:416:GLU:HB3	1.98	0.44
1:A:1216:LYS:CE	3:A:1902:IHP:O22	2.65	0.44
1:A:1402:TRP:CH2	1:A:1443:LEU:HD22	2.51	0.44
1:A:685:ARG:HB3	1:A:723:HIS:HB3	2.00	0.44
1:A:990:PHE:HZ	1:A:1004:ILE:HD13	1.82	0.44
1:A:1510:THR:HG21	1:A:1587:ARG:HD2	1.98	0.44
1:A:286:SER:CB	1:A:306:TYR:CB	2.95	0.44
1:A:297:LEU:HD12	1:A:300:ARG:CG	2.44	0.44
1:A:737:CYS:SG	1:A:738:SER:N	2.91	0.44
1:A:933:LYS:HD2	2:A:1901:K0W:O51	2.17	0.44
1:A:1649:THR:HG23	1:A:1661:VAL:HG11	1.99	0.44
1:A:1490:LEU:HD21	1:A:1505:ILE:HG23	1.98	0.44
1:A:1509:LEU:HD12	1:A:1513:PHE:CE2	2.53	0.44
1:A:933:LYS:HD2	2:A:1901:K0W:O61	2.18	0.44
1:A:1673:LEU:C	1:A:1673:LEU:CD2	2.85	0.44
1:A:1698:GLN:HB3	1:A:1701:VAL:HG22	1.99	0.43
1:A:213:TYR:O	1:A:217:PHE:HB2	2.18	0.43
1:A:762:LEU:HD13	1:A:940:LEU:HD11	1.99	0.43
1:A:785:ASP:OD1	1:A:789:GLN:NE2	2.51	0.43
1:A:99:ILE:HG21	1:A:138:LEU:HD21	2.00	0.43
1:A:936:ILE:HG12	1:A:939:LEU:HD23	2.00	0.43
1:A:1112:ASN:N	1:A:1113:PRO:CD	2.74	0.43
1:A:1181:LEU:HG	1:A:1182:PRO:CD	2.44	0.43
1:A:1270:GLU:OE2	1:A:1439:LYS:CD	2.67	0.43
1:A:66:GLN:HA	1:A:1096:ILE:HD12	2.00	0.43
1:A:880:LEU:CD2	1:A:890:LEU:HD11	2.49	0.43
1:A:1016:ARG:HH11	1:A:1019:VAL:HG12	1.83	0.43
1:A:1444:PHE:HB3	1:A:1482:LEU:HD21	2.01	0.43
1:A:1383:ILE:HG21	1:A:1409:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:VAL:HG21	1:A:1142:ASN:HB3	2.00	0.42
1:A:972:LEU:CD1	1:A:1004:ILE:CD1	2.26	0.42
1:A:1650:ALA:HB1	1:A:1693:LEU:HD21	2.00	0.42
1:A:1665:LEU:HD21	1:A:1686:ILE:HG23	2.00	0.42
1:A:1673:LEU:HD23	1:A:1673:LEU:O	2.18	0.42
1:A:1731:LEU:O	1:A:1734:THR:OG1	2.37	0.42
1:A:478:PRO:C	1:A:480:HIS:N	2.72	0.42
1:A:1435:ARG:HH12	3:A:1902:IHP:P4	2.42	0.42
1:A:282:ARG:HB3	1:A:306:TYR:OH	2.20	0.42
1:A:990:PHE:CZ	1:A:1004:ILE:HD13	2.54	0.42
1:A:1712:LEU:HD13	1:A:1712:LEU:HA	1.87	0.42
1:A:34:TYR:OH	1:A:933:LYS:NZ	2.50	0.42
1:A:218:LEU:HA	1:A:219:PRO:HD3	1.85	0.42
1:A:368:LEU:HB3	1:A:929:LEU:HD21	2.02	0.42
1:A:1053:TRP:CD2	1:A:1170:LEU:HD12	2.54	0.42
1:A:1450:SER:HB3	1:A:1453:SER:HB3	2.01	0.42
1:A:437:LEU:HA	1:A:440:THR:HB	2.01	0.42
1:A:1673:LEU:CD2	1:A:1677:LEU:CD1	2.94	0.42
1:A:635:VAL:HG21	1:A:683:ILE:HG13	2.01	0.42
1:A:1440:LEU:HD12	1:A:1443:LEU:HD23	2.02	0.42
1:A:1549:GLU:OE1	1:A:1653:SER:OG	2.33	0.42
1:A:204:ASP:OD1	1:A:204:ASP:N	2.51	0.41
1:A:208:GLN:HE21	1:A:208:GLN:CA	2.26	0.41
1:A:297:LEU:HG	1:A:297:LEU:O	2.20	0.41
1:A:373:TYR:CD2	1:A:929:LEU:HD11	2.52	0.41
1:A:1581:LEU:HD22	1:A:1603:PHE:HE2	1.85	0.41
1:A:297:LEU:CD1	1:A:1631:GLN:HE22	2.28	0.41
1:A:282:ARG:HD3	1:A:306:TYR:OH	2.21	0.41
1:A:828:LEU:H	1:A:828:LEU:HG	1.51	0.41
1:A:921:VAL:HG12	1:A:939:LEU:HD22	2.02	0.41
1:A:494:PRO:HG3	1:A:557:LEU:HA	2.03	0.41
1:A:38:LEU:HD12	1:A:44:LEU:HD11	2.02	0.41
1:A:134:SER:O	1:A:134:SER:OG	2.34	0.41
1:A:638:CYS:HA	1:A:639:PRO:HD2	1.89	0.41
1:A:1073:VAL:HG23	1:A:1162:LYS:HE3	2.01	0.41
1:A:291:VAL:CG1	1:A:1671:TYR:HE2	2.30	0.41
1:A:297:LEU:HB2	1:A:300:ARG:CB	2.49	0.41
1:A:414:SER:O	1:A:414:SER:OG	2.32	0.41
1:A:719:ASN:HA	1:A:722:HIS:HB3	2.02	0.41
1:A:461:ILE:HG21	1:A:505:GLN:HE22	1.85	0.41
1:A:843:MET:HG3	1:A:1131:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:ARG:HA	1:A:1505:ILE:HB	2.03	0.41
1:A:208:GLN:HE22	1:A:251:TRP:N	2.19	0.41
1:A:836:VAL:HG11	1:A:960:TYR:HD2	1.85	0.41
1:A:848:GLU:HB3	1:A:958:CYS:HA	2.02	0.41
1:A:932:LYS:HB2	1:A:934:GLN:HE21	1.82	0.41
1:A:583:GLU:HB3	1:A:626:MET:HG2	2.03	0.41
1:A:654:ILE:HG23	1:A:673:LEU:HD11	2.02	0.41
1:A:1674:PHE:O	1:A:1677:LEU:N	2.54	0.41
1:A:961:LYS:O	1:A:963:ILE:N	2.54	0.41
1:A:1187:ARG:HG2	1:A:1308:ILE:HG12	2.02	0.41
1:A:1667:THR:O	1:A:1671:TYR:HD2	2.04	0.40
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.92	0.40
1:A:401:ILE:HD12	1:A:432:VAL:HG22	2.03	0.40
1:A:936:ILE:CG1	1:A:939:LEU:HD23	2.51	0.40
1:A:1299:ARG:HH22	1:A:1307:GLN:NE2	2.20	0.40
1:A:214:PHE:CD1	1:A:218:LEU:HD22	2.57	0.40
1:A:928:ARG:HD3	1:A:928:ARG:HA	1.86	0.40
1:A:1447:LEU:HD23	1:A:1468:LEU:HD23	2.04	0.40
1:A:1611:ASN:OD1	1:A:1611:ASN:N	2.55	0.40
1:A:70:PRO:HD3	1:A:1135:LYS:NZ	2.36	0.40
1:A:744:ASP:OD1	1:A:744:ASP:N	2.52	0.40
1:A:876:LEU:HD23	1:A:970:ASP:HB3	2.03	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	1743/1878 (93%)	1580 (91%)	157 (9%)	6 (0%)	41 74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	LEU
1	A	477	GLY
1	A	962	LYS
1	A	1113	PRO
1	A	1480	PRO
1	A	270	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	1593/1705 (93%)	1555 (98%)	38 (2%)	49 71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	110	LYS
1	A	125	ASN
1	A	172	ILE
1	A	226	LEU
1	A	250	GLN
1	A	257	ASN
1	A	348	ARG
1	A	375	LYS
1	A	463	VAL
1	A	526	ARG
1	A	527	ASN
1	A	711	LYS
1	A	822	LEU
1	A	828	LEU
1	A	838	ASN
1	A	844	VAL
1	A	863	ASN
1	A	927	ASN
1	A	1012	LEU
1	A	1042	ASN

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Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1124	LYS
1	A	1234	LYS
1	A	1246	ASN
1	A	1299	ARG
1	A	1443	LEU
1	A	1452	LEU
1	A	1468	LEU
1	A	1494	LEU
1	A	1497	VAL
1	A	1502	ARG
1	A	1545	MET
1	A	1672	ASN
1	A	1679	ASN
1	A	1712	LEU
1	A	1785	LEU
1	A	1787	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	125	ASN
1	A	163	ASN
1	A	208	GLN
1	A	250	GLN
1	A	257	ASN
1	A	310	HIS
1	A	527	ASN
1	A	596	GLN
1	A	607	GLN
1	A	611	ASN
1	A	703	GLN
1	A	789	GLN
1	A	818	HIS
1	A	819	ASN
1	A	838	ASN
1	A	863	ASN
1	A	882	ASN
1	A	907	HIS
1	A	927	ASN
1	A	1021	GLN

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Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1132	GLN
1	A	1246	ASN
1	A	1307	GLN
1	A	1351	ASN
1	A	1363	HIS
1	A	1469	GLN
1	A	1474	GLN
1	A	1613	ASN
1	A	1631	GLN
1	A	1679	ASN
1	A	1714	GLN
1	A	1725	GLN
1	A	1760	HIS
1	A	1787	ASN
1	A	1813	HIS

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	$\#\|Z\|>2$
2	K0W	A	1901	-	40,44,44	1.27	4 (10%)	66,74,74	1.25	8 (12%)
3	IHP	A	1902	-	36,36,36	0.72	0	54,60,60	0.94	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
2	K0W	A	1901	-	-	8/42/66/66	0/1/1/1
3	IHP	A	1902	-	-	2/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	K0W	PA3-O13	3.41	1.65	1.59
2	A	1901	K0W	PA6-O16	2.92	1.64	1.59
2	A	1901	K0W	PA4-O14	2.77	1.64	1.59
2	A	1901	K0W	PA2-O12	2.75	1.64	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1901	K0W	O77-PA5-O15	3.39	109.32	102.48
2	A	1901	K0W	C5-C6-C1	3.37	117.78	110.41
2	A	1901	K0W	C5-C4-C3	2.79	116.52	110.41
2	A	1901	K0W	PA1-O76-PB1	-2.69	123.58	132.83
2	A	1901	K0W	C4-C3-C2	2.61	116.12	110.41
2	A	1901	K0W	O76-PA1-O11	2.56	107.66	102.48
2	A	1901	K0W	C6-C1-C2	2.37	115.61	110.41
2	A	1901	K0W	O51-PB1-O76	2.00	111.36	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1901	K0W	C4-C3-O13-PA3
2	A	1901	K0W	C2-O12-PA2-O22
3	A	1902	IHP	C3-O13-P3-O43
2	A	1901	K0W	C6-O11-PA1-O76

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Mol	Chain	Res	Type	Atoms
2	A	1901	K0W	C3-O13-PA3-O23
2	A	1901	K0W	C2-C3-O13-PA3
2	A	1901	K0W	C4-O14-PA4-O44
2	A	1901	K0W	C2-O12-PA2-O32
2	A	1901	K0W	C3-O13-PA3-O43
3	A	1902	IHP	C5-O15-P5-O35

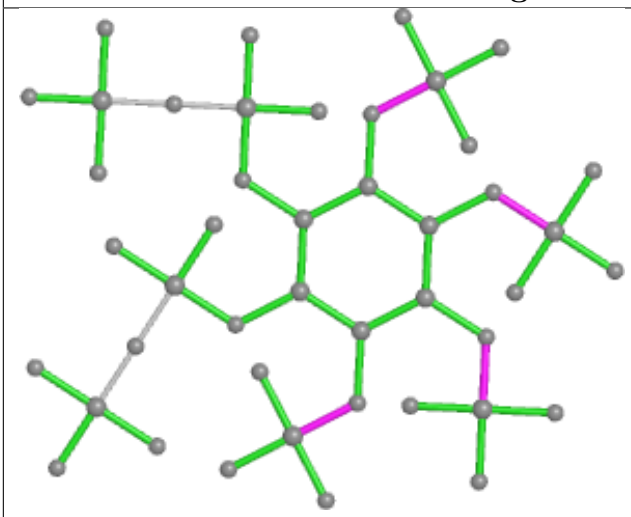
There are no ring outliers.

2 monomers are involved in 25 short contacts:

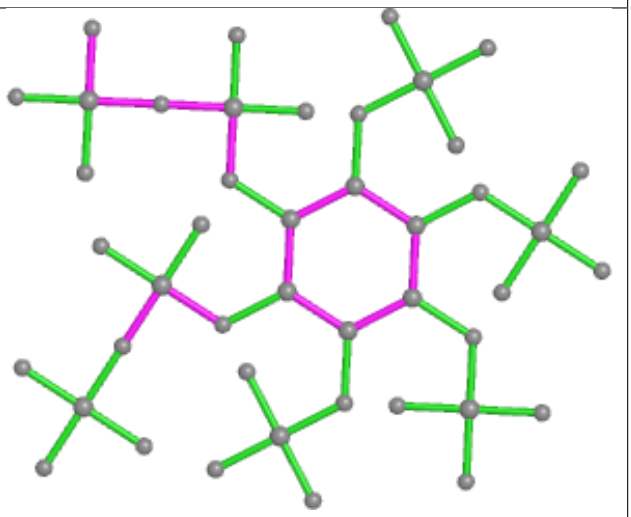
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	K0W	14	0
3	A	1902	IHP	11	0

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.

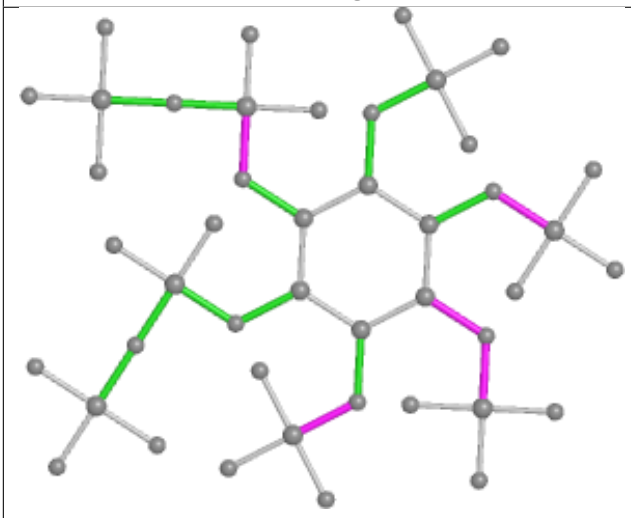
Ligand K0W A 1901



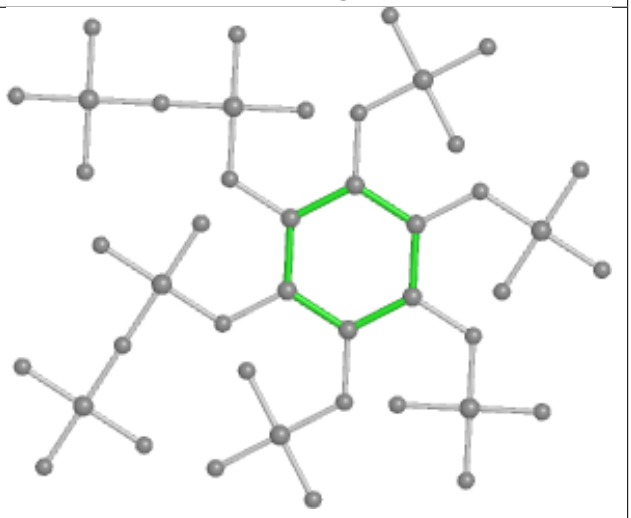
Bond lengths



Bond angles

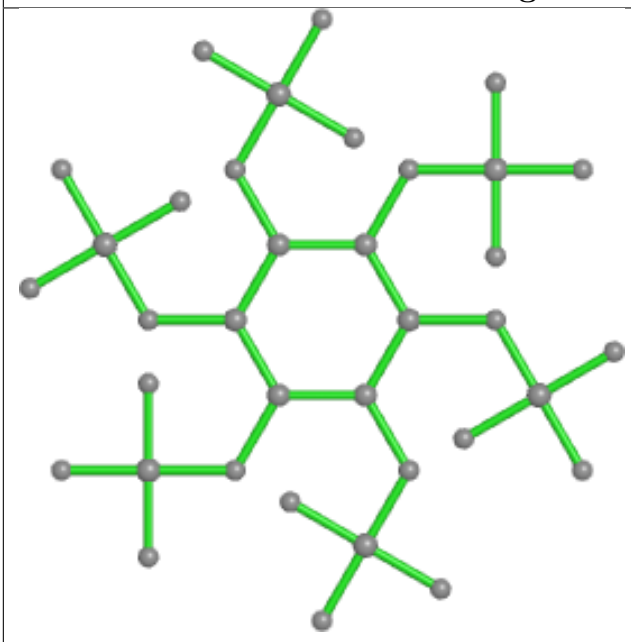


Torsions

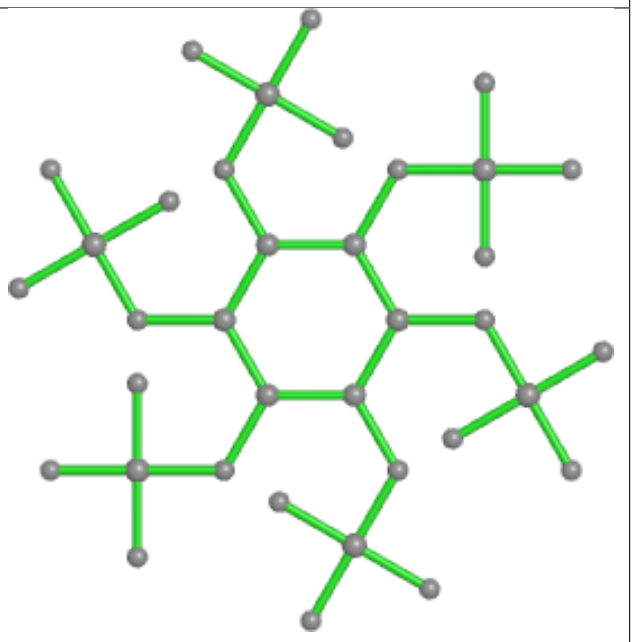


Rings

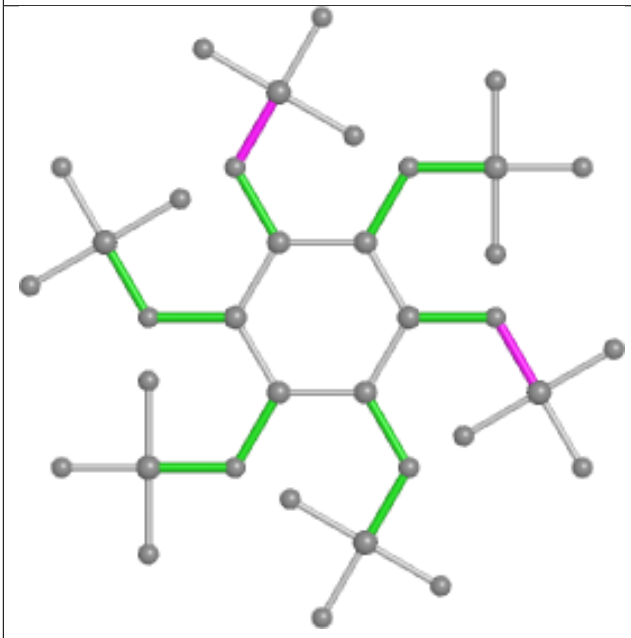
Ligand IHP A 1902



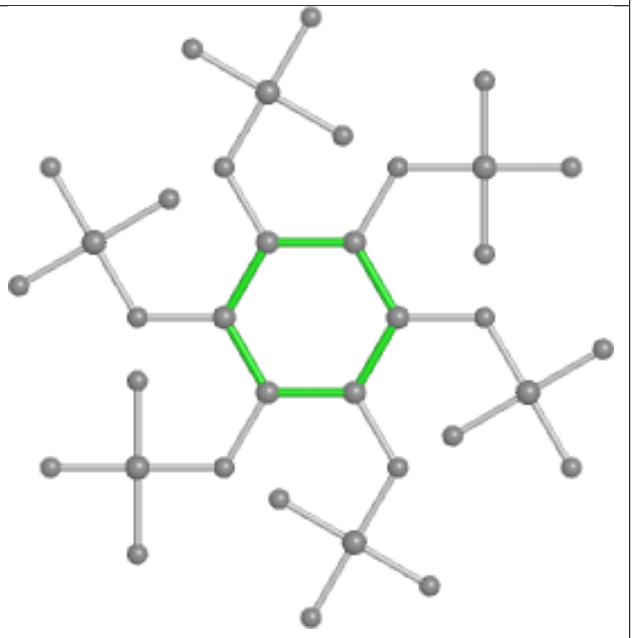
Bond lengths



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.

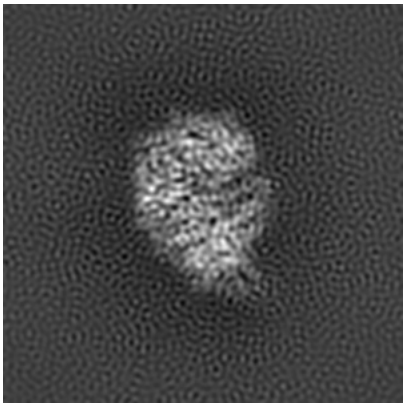
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0780. These allow visual inspection of the internal detail of the map and identification of artifacts.

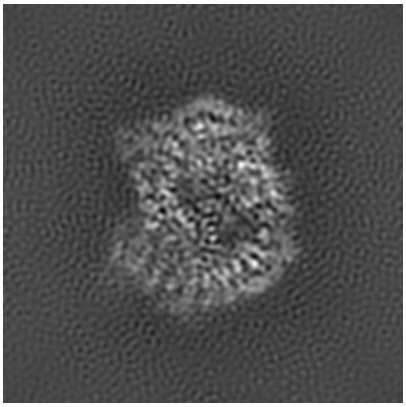
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

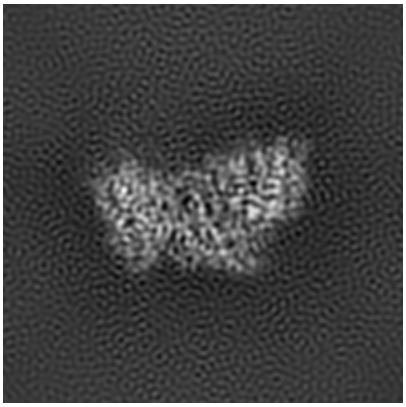
6.1.1 Primary map



X



Y

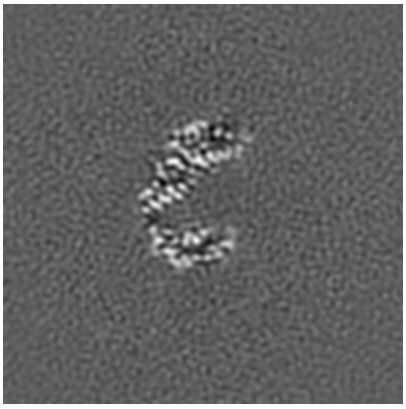


Z

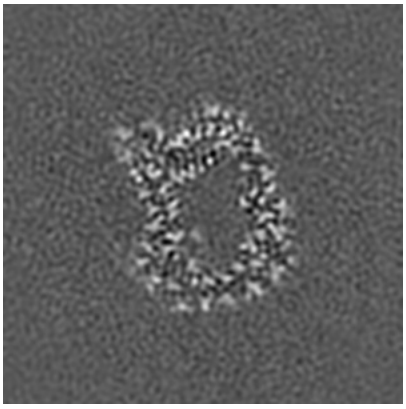
The images above show the map projected in three orthogonal directions.

6.2 Central slices

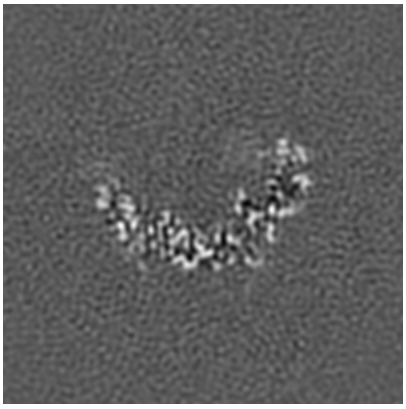
6.2.1 Primary map



X Index: 100



Y Index: 100

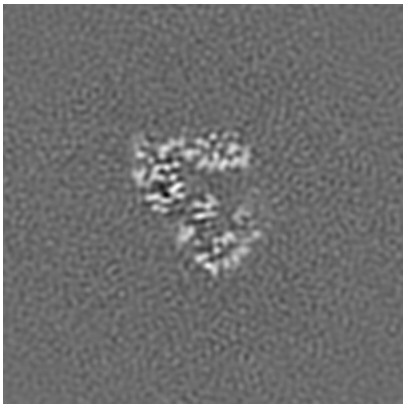


Z Index: 100

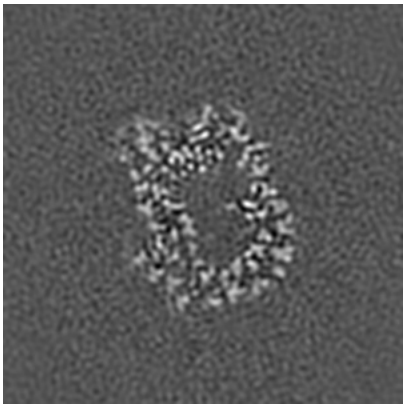
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

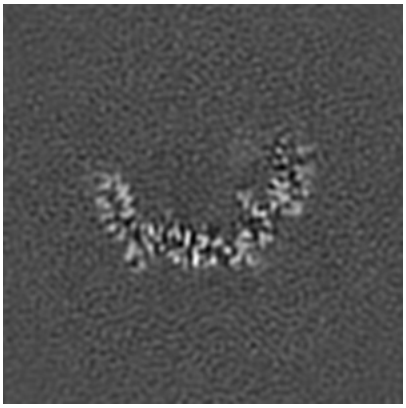
6.3.1 Primary map



X Index: 118



Y Index: 97

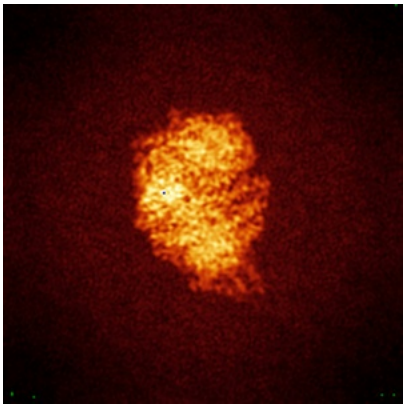


Z Index: 102

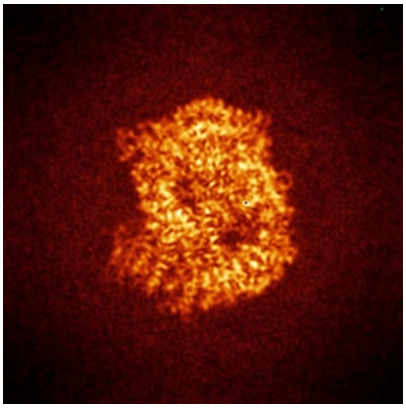
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

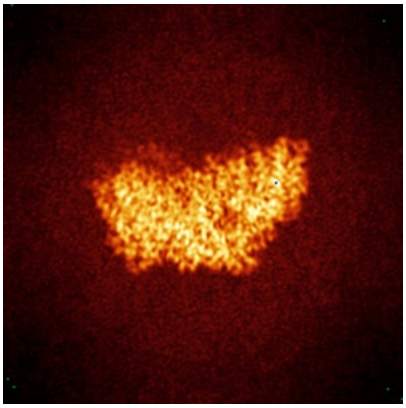
6.4.1 Primary map



X



Y

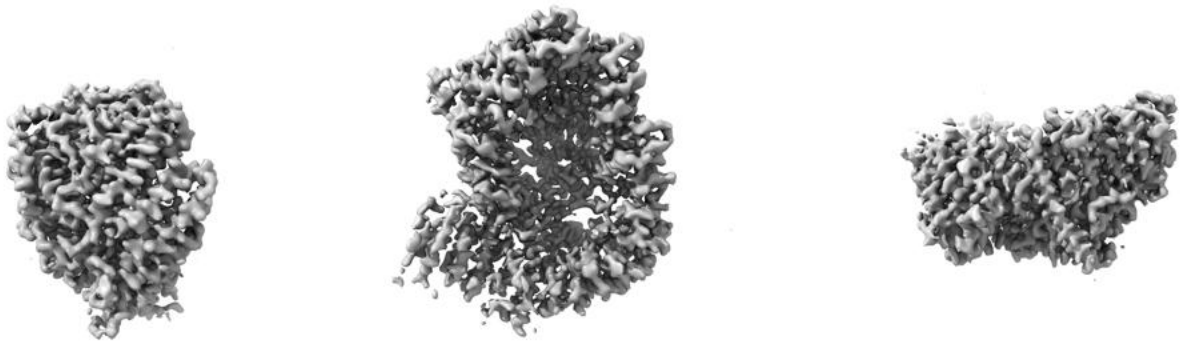


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

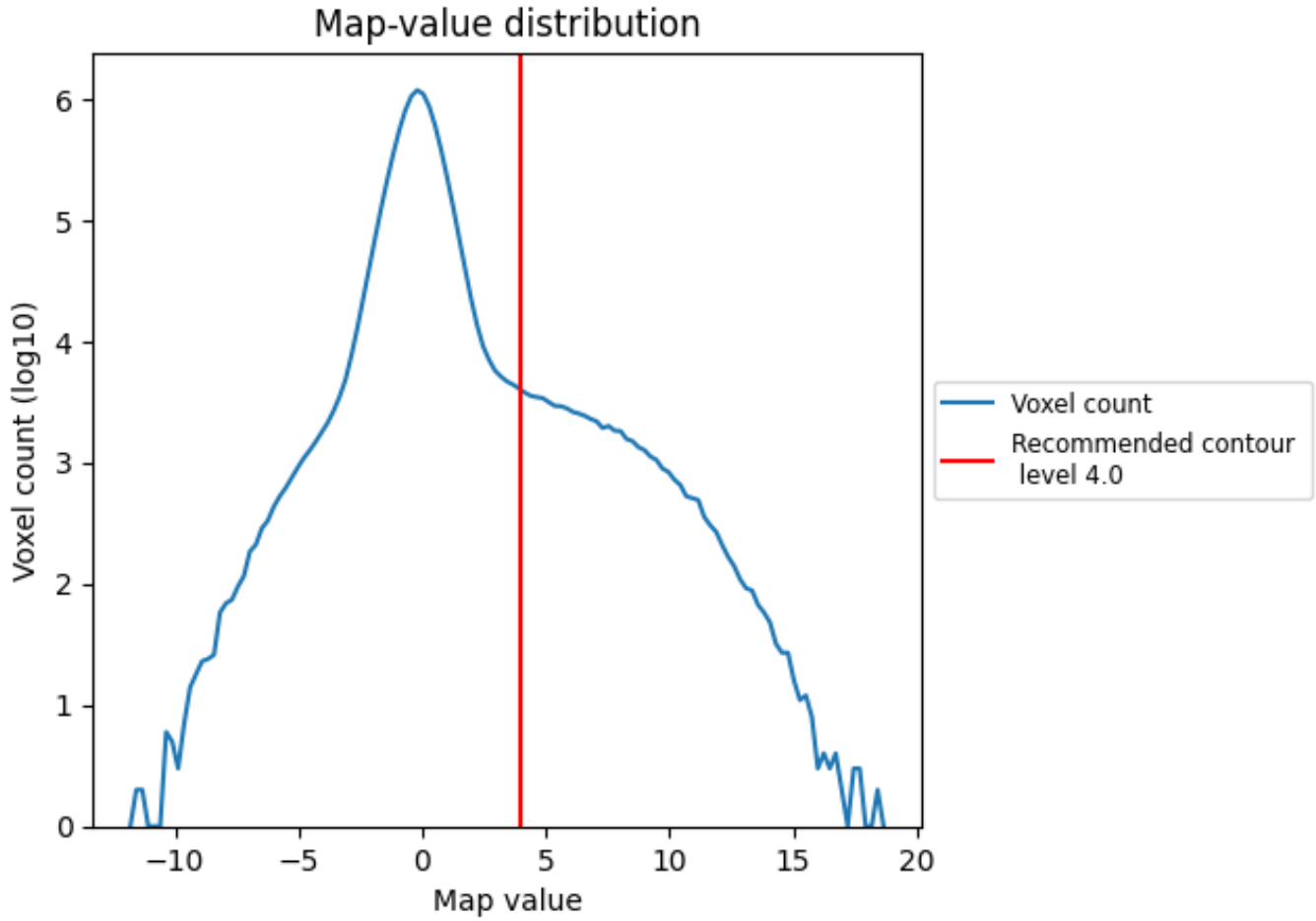
6.6 Mask visualisation (i)

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

7 Map analysis

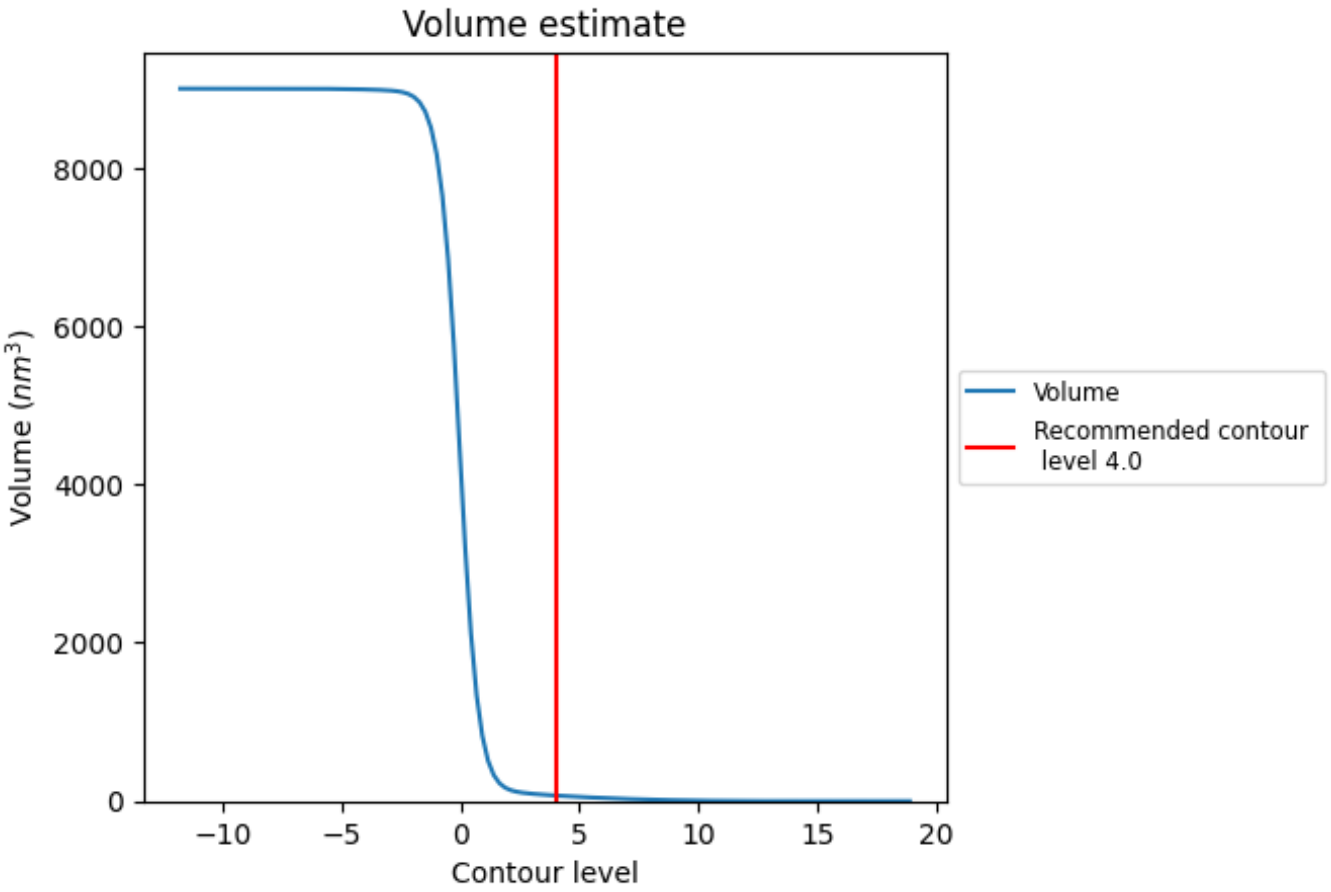
This section contains the results of statistical analysis of the map.

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.

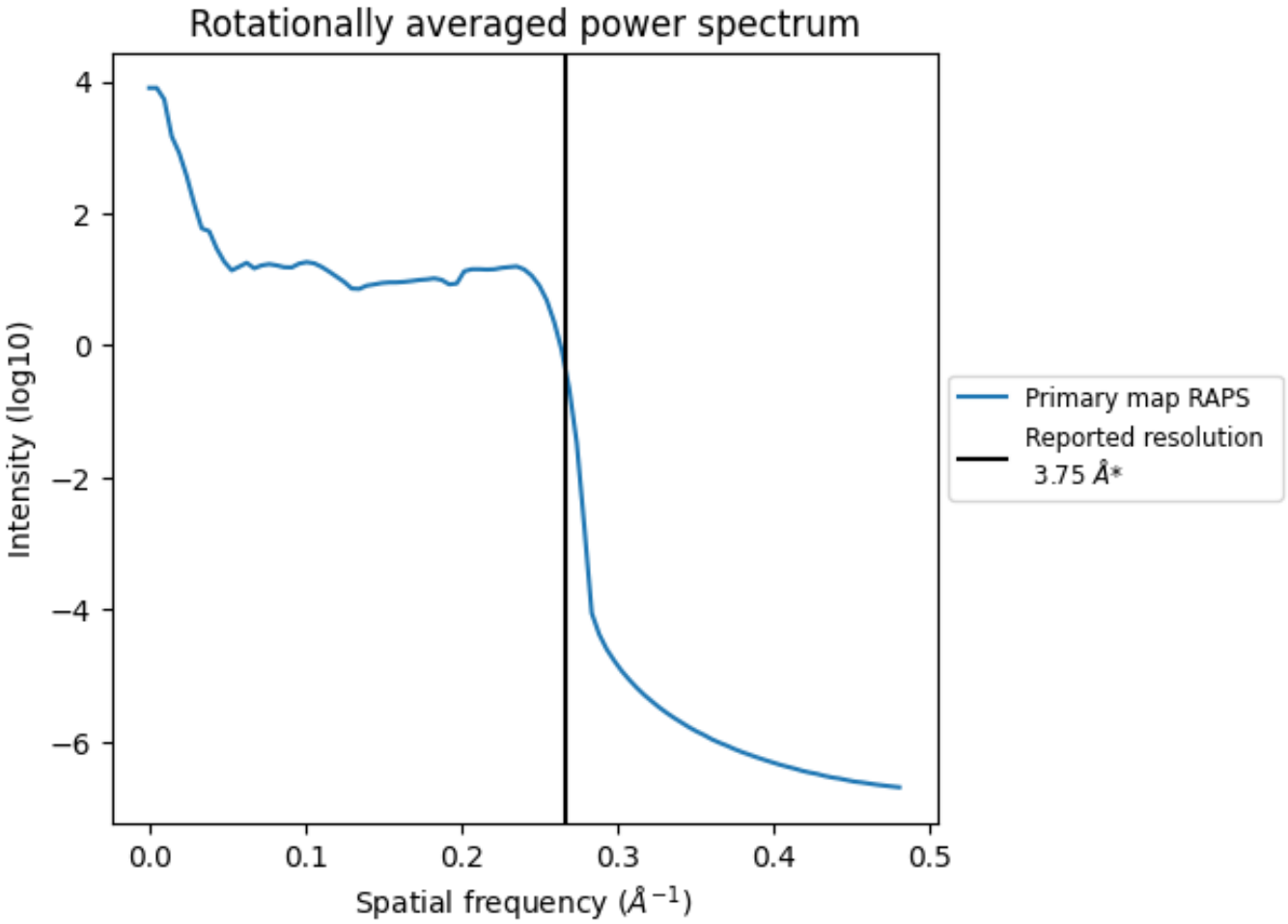
7.2 Volume estimate



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 64 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)

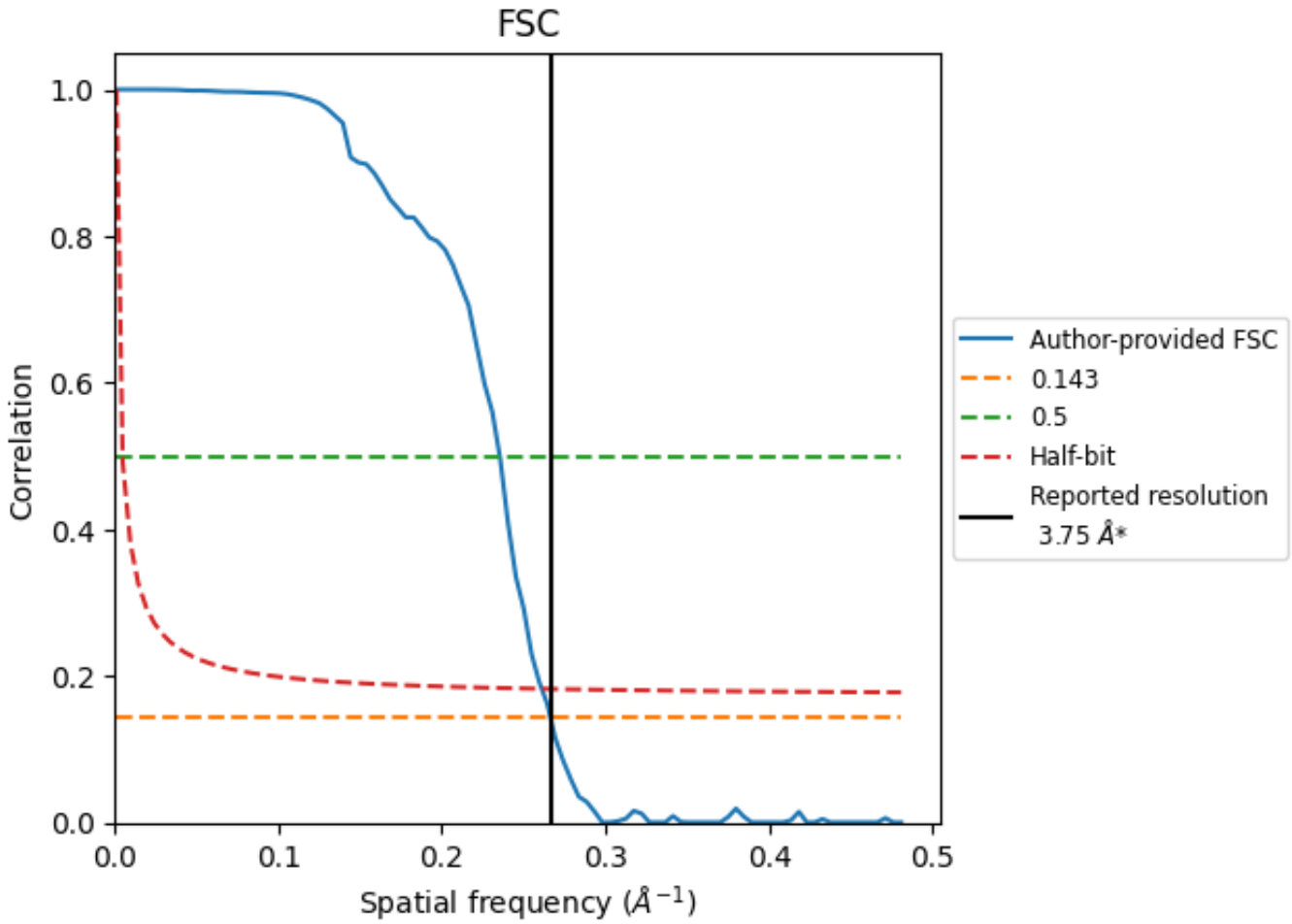


*Reported resolution corresponds to spatial frequency of 0.267 Å^{-1}

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 0.267 Å^{-1}

8.2 Resolution estimates (i)

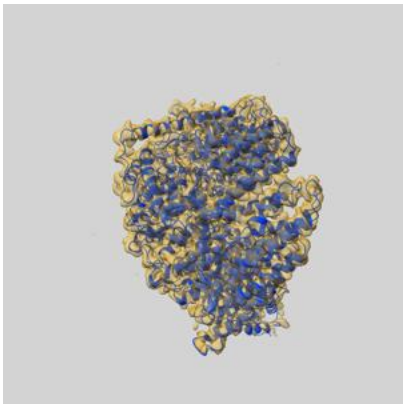
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.25	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

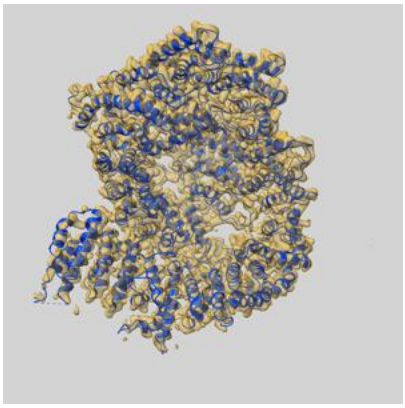
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0780 and PDB model 6KWX. Per-residue inclusion information can be found in section 3 on page 6.

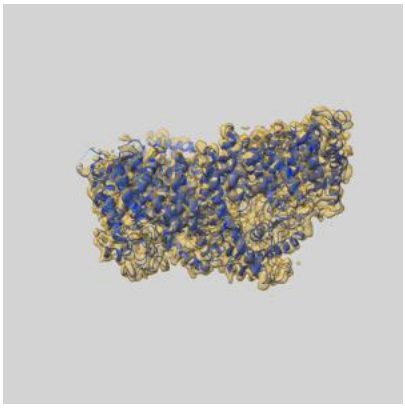
9.1 Map-model overlay



X



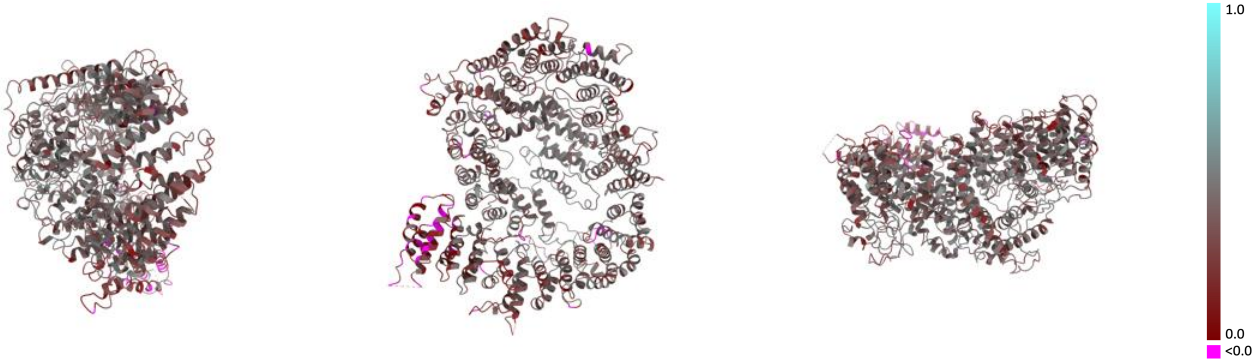
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

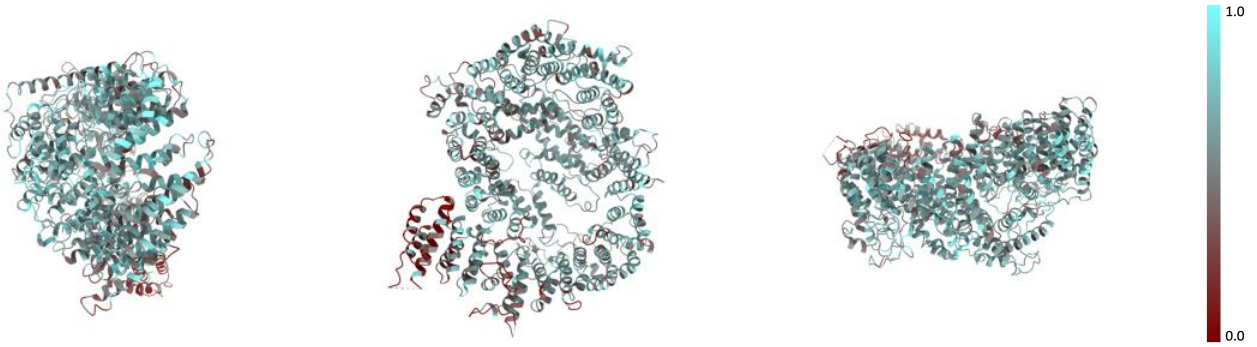
9.2 Q-score mapped to coordinate model



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.

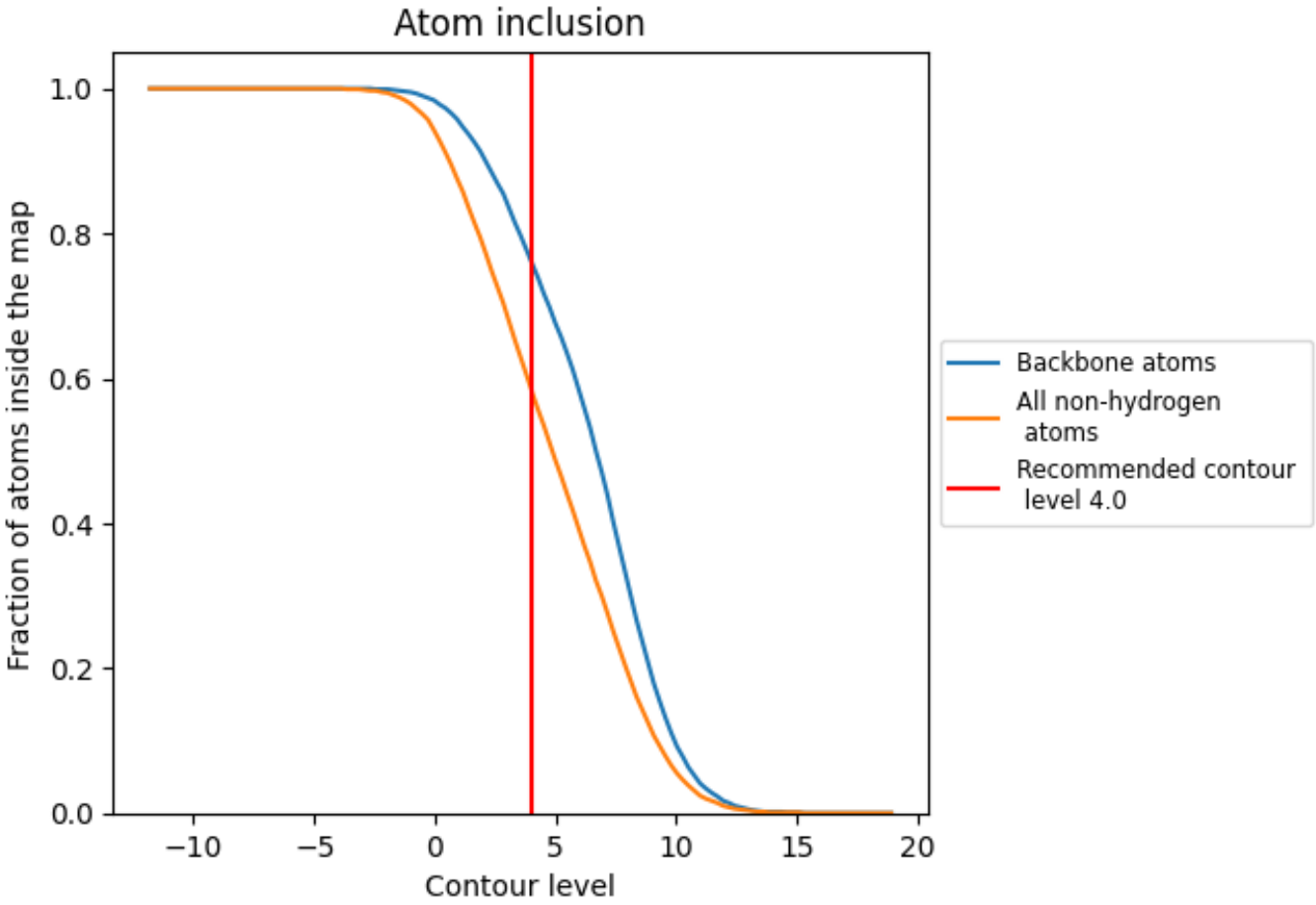
9.3 Atom inclusion mapped to coordinate model



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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 58% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5840	0.3570
A	0.5840	0.3570