



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 09:32 AM UTC

PDB ID : 7ZSK / pdb_00007zsk
EMDB ID : EMD-14945
Title : K3DAK4 bimodule core of BGC11 from *Brevibacillus brevis*.
Authors : Tittes, Y.U.; Herbst, D.A.; Jakob, R.P.; Maier, T.
Deposited on : 2022-05-07
Resolution : 6.80 Å (reported)
Based on initial models : 7MZF, 7MZA, 7ZM9, 7MZD, 7ZMC

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

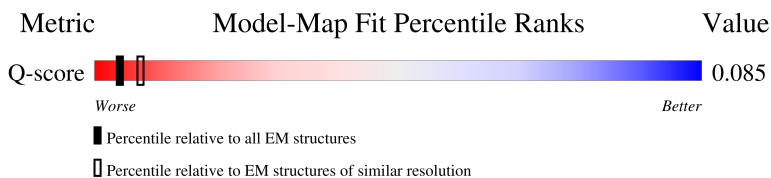
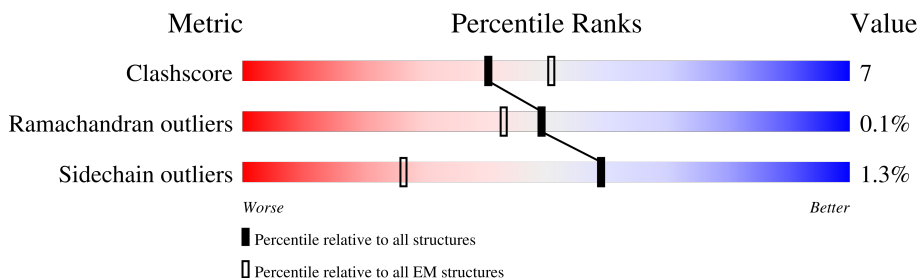
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	A	1690	14% 74% 14% 12%
1	B	1690	14% 71% 16% • 13%
1	C	1690	16% 73% 14% • 13%
1	D	1690	15% 75% 13% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 91396 atoms, of which 45268 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 Putative polyketide synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	1476	Total	C	H	N	O	S	0	0
			22811	7290	11298	1973	2201	49		
1	A	1482	Total	C	H	N	O	S	0	0
			22887	7314	11336	1979	2208	50		
1	D	1482	Total	C	H	N	O	S	0	0
			22887	7314	11336	1979	2208	50		
1	C	1476	Total	C	H	N	O	S	0	0
			22811	7290	11298	1973	2201	49		

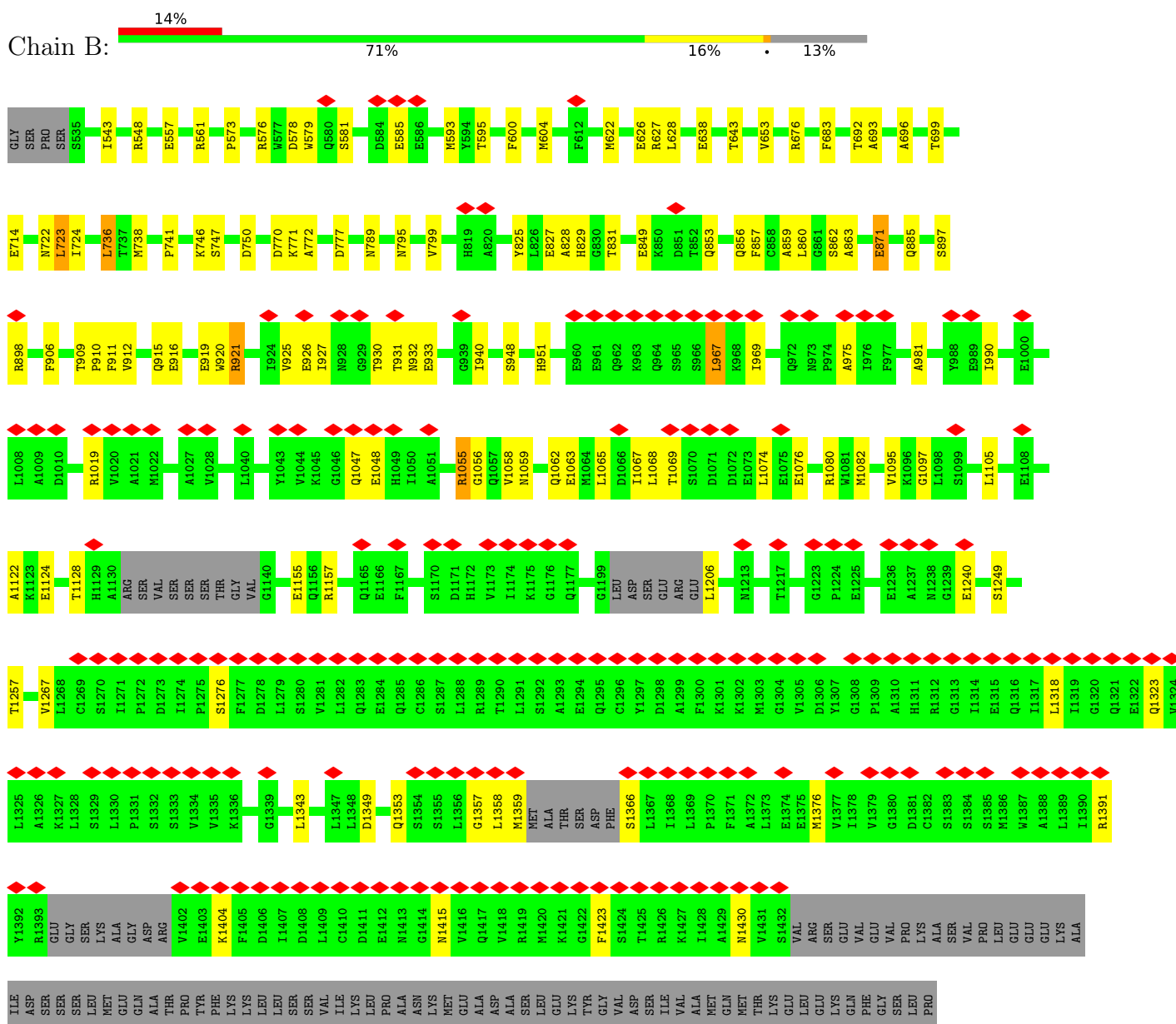
There are 4 discrepancies between the modelled and reference sequences:

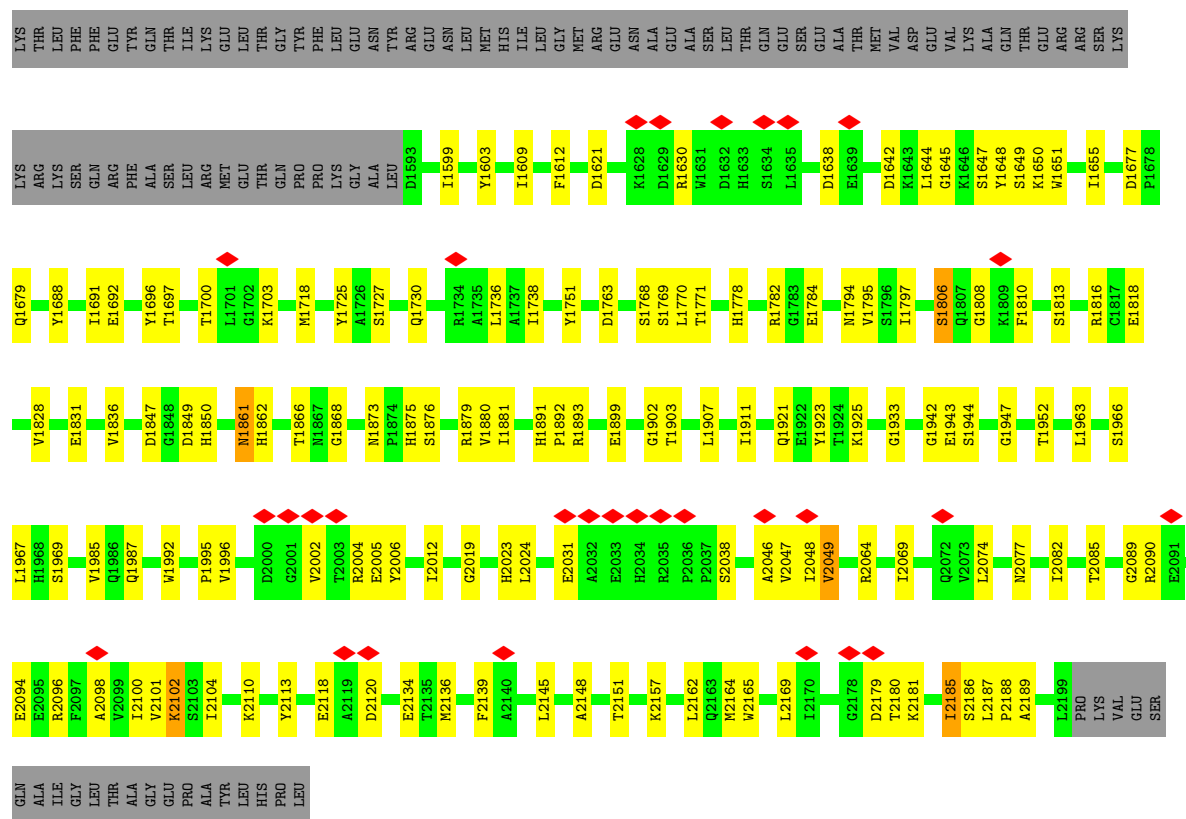
Chain	Residue	Modelled	Actual	Comment	Reference
B	531	GLY	-	expression tag	UNP C0ZGQ6
A	531	GLY	-	expression tag	UNP C0ZGQ6
D	531	GLY	-	expression tag	UNP C0ZGQ6
C	531	GLY	-	expression tag	UNP C0ZGQ6

3 Residue-property plots

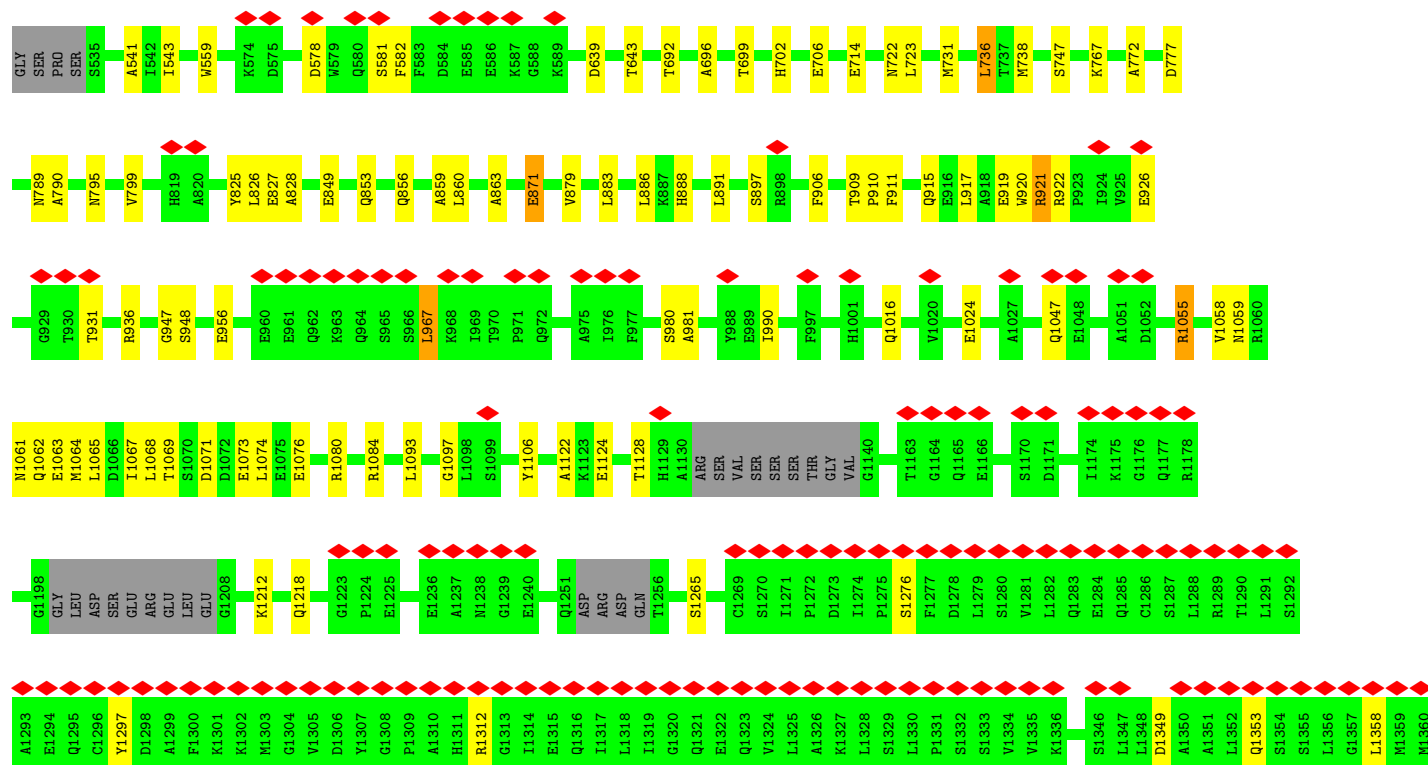
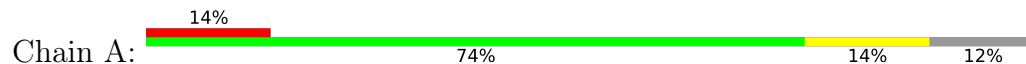
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

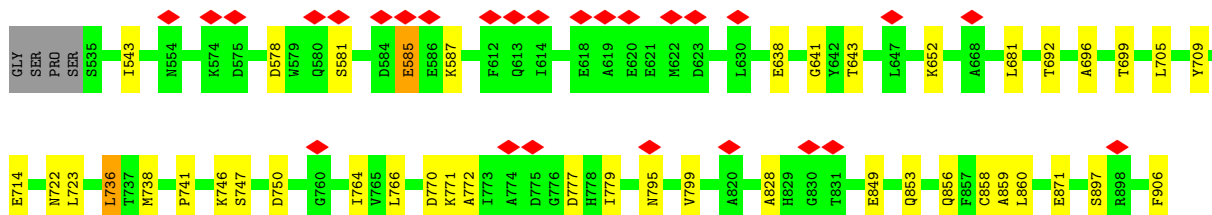
• Molecule 1: Putative polyketide synthase





• Molecule 1: Putative polyketide synthase





SER	A2098	A2099	I2100	I2101	K2102	K2110	K2111	E2118	E2119	D2000	G2001	V2002	T2003	Y2006	A2007	R2008	I2012	F2015	A2022	H2023	I2026	A2032	E2033	H2034	R2035	P2036	P2037	S2038	S2039	I2040	A2046	V2047	I2048	V2049	R2064	E2071	Q2072	V2073	L2074	I2082	R2090	E2091	E2094	E2095	R2096	F2097												
	Q1986	Q1987	E1988	V1992	P1995	T1996	E1997	E1998	I1999	D2000	G2001	V2002	T2003	Y2006	A2007	R2008	I2012	F2015	A2022	H2023	I2026	A2032	E2033	H2034	R2035	P2036	P2037	S2038	S2039	I2040	A2046	V2047	I2048	V2049	R2064	E2071	Q2072	V2073	L2074	I2082	R2090	E2091	E2094	E2095	R2096	F2097												
	D1849	H1850	I1860	N1861	H1862	G1863	G1864	K1865	Y1869	T1870	N1873	P1874	H1875	S1876	Q1877	S1878	R1879	V1880	I1881	P1892	H1901	G1902	T1903	G1904	T1905	S1906	L1907	I1911	E1912	I1913	T1917	S1917	F1920	Y1923	H1941	G1942	E1943	S1944	G1947	L1951	V1964	P1965	S1969	R1970	V1984	V1985												
THR	Y1648		I1655	I1691	E1692	Y1696	T1697	R1698	Y1869	T1700	L1701	G1706	Y1725	Y1751	V1762	S1768	S1769	L1770	T1771	L1775	H1778	R1782	G1783	E1784	N1794	V1795	S1796	I1797	A1811	S1812	S1813	K1814	G1815	R1816	C1817	E1818	G1826	Y1827	G1830	V1836	A1844	D1847	G1848															
THR	MET	MET	VAL	ASP	GLU	VAL	LYS	ALA	GLN	THR	ARG	SER	LYS	ARG	LYS	THR	SER	GLN	ARG	PHE	ALA	GLN	THR	GLY	THR	PRO	GLY	PRO	LYS	GLY	ALA	LEU	D1593	I1596	Y1603	F1612	L1616	I1623	I1626	D1632	H1633	S1634	D1638	E1639	L1644	S1647												
	VAL	GLU	M1376	V1377	V1378	V1379	S1383	S1384	S1385	M1386	W1387	A1388	L1389	I1390	R1391	Y1392	R1393	GLU	GLY	SER	GLN	THR	ILE	LYS	THR	PRO	GLY	THR	PHE	LEU	LEU	ASN	SER	ILE	GLU	MET	ALA	ASP	V1416	Q1417	V1418	R1419	M1420	K1421	G1422	F1423	S1424	T1425	R1426	K1427	I1428	N1430	V1431	S1432	VAL	ARG	SER	GLU
	D1306	Y1307	G1308	P1309	A1310	H1311	R1312	G1313	I1314	E1315	Q1316	I1317	L1318	I1319	G1320	Q1321	E1322	Q1323	V1324	L1325	A1326	K1327	L1328	S1329	L1330	P1331	S1332	S1333	V1334	V1335	K1336	F1341	G1342	L1343	D1349	Q1353	S1354	S1355	L1356	G1357	L1358	M1359	MET	ALA	THR	SER	ASP	PHE	S1366	L1367	I1368	L1369	P1370	F1371	A1372	L1373	E1374	
	P1224	E1225	P1226	E1236	A1237	N1238	G1239	E1240	S1249	D1252	R1253	T1257	H1261	S1265	A1266	V1267	L1268	C1269	S1270	I1271	P1272	D1273	I1274	P1275	S1276	F1277	D1278	L1279	S1280	V1281	L1282	Q1283	E1284	Q1285	C1286	S1287	L1288	R1289	T1290	L1291	S1292	A1293	E1294	Q1295	C1296	Y1297	D1298	A1299	K1301	K1302	M1303	G1304	W1305					
	A1130	ARG	SER	VAL	SER	SER	THR	GLY	VAL	G1140	E1155	Q1156	R1157	T1163	G1164	Q1165	E1166	F1167	F1168	L1169	S1170	D1171	H1172	V1173	I1174	K1175	G1176	Q1177	R1178	S1182	G1199	LEU	ASP	SER	GLU	ARG	GLU	L1206	E1207	G1208	L1209	R1210	F1211	K1212	M1213	V1214	T1215	W1216	T1217	Q1218	P1219	L1220	A1221	V1222	G1223			
	E1024	R1025	I1026	A1027	Q1047	E1048	H1049	I1050	A1051	D1052	R1055	V1058	N1059	N1061	Q1062	E1063	M1064	L1065	D1066	I1067	L1068	T1069	E1073	L1074	E1075	E1076	R1080	K1086	K1089	W1094	G1097	L1098	S1099	I1100	Q1107	E1108	E1109	R1113	T1118	A1122	K1123	E1124	T1128	H1129														
	T909	F910	F911	V912	E919	A920	R921	E926	T924	W925	G929	T930	T931	E933	A938	Y957	E960	E961	Q962	K963	Q964	S965	S966	L967	K968	P969	T970	P971	Q972	A975	L1088	Y976	F977	S980	A981	Y988	E989	I990	Y991	F997	E1000	H1001	D1005	L1008	V1020													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293391	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.213	Depositor
Minimum map value	-0.559	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.256	Depositor
Map size ($\text{\AA}$)	541.696, 541.696, 541.696	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.116, 2.116, 2.116	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.21	0/11798	0.42	1/15969 (0.0%)
1	B	0.22	0/11758	0.44	2/15915 (0.0%)
1	C	0.21	0/11758	0.42	0/15915
1	D	0.20	0/11798	0.41	1/15969 (0.0%)
All	All	0.21	0/47112	0.42	4/63768 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	871	GLU	CB-CA-C	-5.35	109.96	117.23
1	D	693	ALA	CB-CA-C	-5.18	110.62	116.63
1	B	871	GLU	CB-CA-C	-5.14	110.23	117.23
1	B	693	ALA	CB-CA-C	-5.08	110.73	116.63

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	11551	11336	11357	157	0
1	B	11513	11298	11319	179	0
1	C	11513	11298	11319	171	0
1	D	11551	11336	11357	146	0
All	All	46128	45268	45352	636	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 7.

All (636) 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:1064:MET:HG3	1:C:1061:ASN:OD1	1.60	1.01
1:B:856:GLN:NE2	1:B:911:PHE:O	1.96	0.99
1:B:2100:ILE:O	1:B:2110:LYS:NZ	2.04	0.91
1:A:722:ASN:ND2	1:A:871:GLU:OE1	2.04	0.90
1:D:722:ASN:ND2	1:D:871:GLU:OE1	2.05	0.90
1:C:856:GLN:NE2	1:C:906:PHE:O	2.05	0.90
1:B:1769:SER:OG	1:B:1944:SER:O	1.90	0.89
1:A:856:GLN:NE2	1:A:911:PHE:O	2.05	0.89
1:A:2094:GLU:OE1	1:A:2094:GLU:N	2.05	0.89
1:C:1725:TYR:OH	1:C:1797:ILE:O	1.91	0.88
1:D:1794:ASN:ND2	1:D:1942:GLY:O	2.08	0.86
1:D:2094:GLU:N	1:D:2094:GLU:OE1	2.08	0.86
1:B:2094:GLU:N	1:B:2094:GLU:OE1	2.09	0.86
1:C:722:ASN:ND2	1:C:871:GLU:OE1	2.09	0.85
1:C:1769:SER:OG	1:C:1944:SER:O	1.92	0.85
1:C:2100:ILE:O	1:C:2110:LYS:NZ	2.09	0.85
1:A:1794:ASN:ND2	1:A:1942:GLY:O	2.11	0.84
1:A:1769:SER:OG	1:A:1944:SER:O	1.97	0.83
1:D:856:GLN:NE2	1:D:906:PHE:O	2.13	0.82
1:C:849:GLU:OE1	1:C:853:GLN:NE2	2.12	0.81
1:A:2179:ASP:OD1	1:A:2180:THR:N	2.14	0.81
1:A:1047:GLN:O	1:A:1055:ARG:NH2	2.12	0.81
1:B:1847:ASP:O	1:B:2181:LYS:NZ	2.13	0.81
1:B:849:GLU:OE1	1:B:853:GLN:NE2	2.14	0.81
1:D:1998:GLU:OE2	1:D:2002:VAL:N	2.14	0.81
1:B:714:GLU:OE1	1:B:714:GLU:N	2.14	0.80
1:B:856:GLN:NE2	1:B:906:PHE:O	2.15	0.80
1:C:856:GLN:NE2	1:C:911:PHE:O	2.14	0.80
1:D:849:GLU:OE1	1:D:853:GLN:NE2	2.15	0.79
1:B:2064:ARG:NH1	1:B:2189:ALA:O	2.16	0.79
1:D:1769:SER:OG	1:D:1944:SER:O	2.01	0.79
1:B:2012:ILE:O	1:B:2023:HIS:ND1	2.17	0.77
1:B:1794:ASN:ND2	1:B:1942:GLY:O	2.18	0.77
1:A:849:GLU:OE1	1:A:853:GLN:NE2	2.17	0.77
1:A:1818:GLU:OE1	1:A:1818:GLU:N	2.16	0.77
1:D:2179:ASP:OD1	1:D:2180:THR:N	2.18	0.76
1:A:856:GLN:NE2	1:A:906:PHE:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2148:ALA:O	1:B:2151:THR:OG1	2.04	0.76
1:C:1638:ASP:OD1	1:C:1647:SER:OG	2.05	0.75
1:C:1794:ASN:ND2	1:C:1942:GLY:O	2.19	0.75
1:D:1725:TYR:OH	1:D:1797:ILE:O	2.05	0.74
1:B:2090:ARG:NH2	1:B:2188:PRO:O	2.19	0.74
1:A:2012:ILE:O	1:A:2023:HIS:ND1	2.21	0.73
1:D:702:HIS:NE2	1:D:706:GLU:OE2	2.21	0.73
1:C:2094:GLU:OE1	1:C:2094:GLU:N	2.20	0.73
1:D:1907:LEU:O	1:D:1911:ILE:HD13	1.89	0.73
1:C:1782:ARG:NH2	1:C:1784:GLU:OE1	2.21	0.73
1:B:1621:ASP:OD2	1:B:1816:ARG:NH2	2.20	0.73
1:C:2037:PRO:O	1:C:2038:SER:OG	2.05	0.73
1:D:1818:GLU:N	1:D:1818:GLU:OE1	2.21	0.73
1:C:2148:ALA:O	1:C:2151:THR:OG1	2.05	0.72
1:C:1323:GLN:OE1	1:C:1391:ARG:NH1	2.21	0.72
1:C:1901:HIS:N	1:C:1912:GLU:OE2	2.22	0.72
1:B:1323:GLN:OE1	1:B:1391:ARG:NH1	2.21	0.72
1:B:1725:TYR:OH	1:B:1797:ILE:O	2.07	0.71
1:A:1725:TYR:OH	1:A:1797:ILE:O	2.07	0.71
1:D:856:GLN:NE2	1:D:911:PHE:O	2.25	0.70
1:A:578:ASP:OD1	1:A:581:SER:OG	2.05	0.69
1:C:714:GLU:N	1:C:714:GLU:OE1	2.25	0.69
1:B:1155:GLU:OE1	1:B:1157:ARG:NH2	2.26	0.68
1:C:2064:ARG:NH1	1:C:2189:ALA:O	2.26	0.68
1:B:1818:GLU:N	1:B:1818:GLU:OE1	2.27	0.68
1:A:1064:MET:CG	1:C:1061:ASN:OD1	2.39	0.68
1:B:1996:VAL:HG23	1:B:2004:ARG:O	1.94	0.68
1:C:1155:GLU:OE1	1:C:1157:ARG:NH2	2.26	0.67
1:C:2012:ILE:O	1:C:2023:HIS:ND1	2.28	0.67
1:B:1677:ASP:OD1	1:B:1679:GLN:N	2.27	0.66
1:B:1850:HIS:NE2	1:B:2186:SER:OG	2.28	0.66
1:C:1047:GLN:O	1:C:1055:ARG:NH2	2.28	0.66
1:A:1782:ARG:NH2	1:A:1784:GLU:OE1	2.28	0.66
1:A:1016:GLN:OE1	1:A:1106:TYR:OH	2.07	0.66
1:D:1756:HIS:ND1	1:C:1863:GLY:O	2.29	0.65
1:B:1603:TYR:C	1:B:1655:ILE:HG22	2.21	0.65
1:B:1638:ASP:OD1	1:B:1647:SER:OG	2.15	0.65
1:A:1084:ARG:NH1	1:C:1073:GLU:OE2	2.30	0.65
1:D:932:ASN:OD1	1:D:933:GLU:N	2.30	0.65
1:B:2069:ILE:HG23	1:B:2104:ILE:HD11	1.78	0.64
1:A:747:SER:O	1:A:897:SER:OG	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:GLN:O	1:B:1055:ARG:NH2	2.30	0.64
1:B:1907:LEU:O	1:B:1907:LEU:HD23	1.97	0.64
1:B:722:ASN:ND2	1:B:871:GLU:OE1	2.30	0.64
1:A:2172:ASP:OD1	1:A:2174:ASN:N	2.28	0.64
1:D:1692:GLU:OE1	1:D:2190:TYR:N	2.30	0.64
1:D:1276:SER:OG	1:D:1415:ASN:OD1	2.16	0.64
1:D:2000:ASP:OD1	1:D:2000:ASP:N	2.28	0.64
1:A:1638:ASP:HB3	1:A:1644:LEU:HD12	1.80	0.63
1:D:1638:ASP:OD1	1:D:1647:SER:OG	2.16	0.63
1:B:557:GLU:OE1	1:B:561:ARG:NH2	2.31	0.63
1:B:1730:GLN:NE2	1:B:1736:LEU:O	2.27	0.63
1:B:1907:LEU:O	1:B:1911:ILE:HD13	2.00	0.62
1:A:1998:GLU:OE2	1:A:2001:GLY:N	2.33	0.62
1:C:1902:GLY:O	1:C:1903:THR:OG1	2.14	0.62
1:B:2179:ASP:OD1	1:B:2180:THR:N	2.33	0.62
1:B:2074:LEU:HD13	1:B:2082:ILE:HD11	1.82	0.62
1:B:1697:THR:HB	1:B:1700:THR:HG22	1.82	0.61
1:C:578:ASP:OD1	1:C:581:SER:OG	2.06	0.61
1:C:1907:LEU:HD23	1:C:1907:LEU:O	2.00	0.61
1:A:1907:LEU:HD23	1:A:1907:LEU:O	2.01	0.61
1:B:1911:ILE:HD12	1:B:1911:ILE:H	1.66	0.61
1:A:1276:SER:OG	1:A:1415:ASN:OD1	2.16	0.61
1:D:2172:ASP:OD1	1:D:2174:ASN:N	2.33	0.61
1:C:1818:GLU:OE1	1:C:1818:GLU:N	2.32	0.61
1:B:1751:TYR:OH	1:A:1865:LYS:NZ	2.33	0.60
1:B:2096:ARG:NH1	1:B:2165:TRP:O	2.34	0.60
1:A:1697:THR:HB	1:A:1700:THR:HG22	1.84	0.60
1:B:1782:ARG:NH2	1:B:1784:GLU:OE1	2.33	0.60
1:C:2074:LEU:HD13	1:C:2082:ILE:HD11	1.82	0.60
1:D:714:GLU:N	1:D:714:GLU:OE1	2.35	0.60
1:C:2064:ARG:HH22	1:C:2189:ALA:H	1.49	0.60
1:B:1366:SER:N	1:B:1430:ASN:OD1	2.34	0.59
1:B:1849:ASP:OD1	1:B:1850:HIS:ND1	2.35	0.59
1:D:1645:GLY:O	1:D:1806:SER:OG	2.13	0.59
1:C:2096:ARG:NH1	1:C:2165:TRP:O	2.35	0.59
1:D:1969:SER:CB	1:D:1985:VAL:HG11	2.33	0.59
1:C:1366:SER:N	1:C:1430:ASN:OD1	2.34	0.59
1:B:1692:GLU:O	1:B:2090:ARG:NH1	2.36	0.59
1:A:2031:GLU:OE1	1:A:2031:GLU:N	2.34	0.59
1:A:1642:ASP:N	1:A:1642:ASP:OD1	2.35	0.59
1:C:1059:ASN:OD1	1:C:1062:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:827:GLU:OE2	1:D:863:ALA:N	2.26	0.58
1:D:2031:GLU:OE1	1:D:2031:GLU:N	2.31	0.58
1:B:1996:VAL:HG23	1:B:2004:ARG:C	2.28	0.58
1:A:1911:ILE:H	1:A:1911:ILE:HD12	1.69	0.58
1:D:736:LEU:HD13	1:D:738:MET:SD	2.43	0.58
1:C:2179:ASP:OD1	1:C:2180:THR:N	2.37	0.58
1:B:1969:SER:O	1:B:1987:GLN:NE2	2.32	0.58
1:A:1692:GLU:OE1	1:A:2190:TYR:N	2.36	0.58
1:C:1638:ASP:HB3	1:C:1644:LEU:HD12	1.86	0.57
1:D:2008:ARG:N	1:D:2028:GLU:OE2	2.35	0.57
1:A:1603:TYR:C	1:A:1655:ILE:HG22	2.29	0.57
1:C:1999:ILE:O	1:C:2002:VAL:N	2.27	0.57
1:A:696:ALA:O	1:A:699:THR:OG1	2.18	0.57
1:A:1621:ASP:OD1	1:A:1968:HIS:NE2	2.38	0.57
1:C:1697:THR:HB	1:C:1700:THR:HG22	1.87	0.57
1:B:1645:GLY:O	1:B:1806:SER:OG	2.17	0.57
1:C:1357:GLY:O	1:C:1359:MET:N	2.37	0.57
1:B:578:ASP:OD1	1:B:581:SER:OG	2.14	0.56
1:B:1861:ASN:C	1:B:1861:ASN:OD1	2.47	0.56
1:D:622:MET:O	1:D:627:ARG:NH2	2.32	0.56
1:C:1861:ASN:OD1	1:C:1861:ASN:C	2.49	0.56
1:A:1998:GLU:HA	1:A:2002:VAL:O	2.06	0.56
1:D:1998:GLU:OE2	1:D:2001:GLY:N	2.39	0.56
1:D:1986:GLN:NE2	1:D:1988:GLU:O	2.38	0.56
1:D:652:LYS:NZ	1:D:714:GLU:OE2	2.30	0.55
1:C:1691:ILE:HG22	1:C:1696:TYR:O	2.06	0.55
1:A:1093:LEU:CD2	1:C:1064:MET:HE3	2.37	0.55
1:B:1357:GLY:O	1:B:1359:MET:N	2.37	0.55
1:D:1818:GLU:OE2	1:D:1828:VAL:N	2.34	0.55
1:B:1995:PRO:O	1:B:2006:TYR:N	2.39	0.55
1:B:2064:ARG:HH22	1:B:2189:ALA:H	1.55	0.55
1:A:1911:ILE:HD12	1:A:1911:ILE:N	2.22	0.55
1:D:1642:ASP:OD1	1:D:1642:ASP:N	2.39	0.55
1:D:2120:ASP:OD1	1:D:2121:SER:N	2.40	0.55
1:B:736:LEU:HD13	1:B:738:MET:SD	2.47	0.55
1:C:1847:ASP:O	1:C:2181:LYS:NZ	2.40	0.55
1:D:1865:LYS:NZ	1:C:1751:TYR:OH	2.40	0.55
1:D:2012:ILE:O	1:D:2023:HIS:ND1	2.40	0.55
1:C:747:SER:O	1:C:897:SER:OG	2.25	0.55
1:D:1756:HIS:CE1	1:C:1863:GLY:O	2.60	0.54
1:C:1794:ASN:OD1	1:C:1795:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:LEU:HD13	1:A:738:MET:SD	2.47	0.54
1:B:747:SER:O	1:B:897:SER:OG	2.25	0.54
1:B:932:ASN:OD1	1:B:933:GLU:N	2.40	0.54
1:C:1623:ILE:O	1:C:1816:ARG:NH2	2.40	0.54
1:D:967:LEU:N	1:D:967:LEU:HD22	2.23	0.54
1:C:1343:LEU:CD1	1:C:1376:MET:HE1	2.37	0.54
1:C:1998:GLU:OE2	1:C:2001:GLY:N	2.40	0.54
1:B:926:GLU:HB2	1:B:931:THR:HG22	1.89	0.54
1:B:1343:LEU:CD1	1:B:1376:MET:HE1	2.37	0.54
1:A:702:HIS:NE2	1:A:706:GLU:OE2	2.41	0.54
1:A:1623:ILE:O	1:A:1816:ARG:NH2	2.41	0.54
1:D:576:ARG:NH1	1:D:724:ILE:O	2.41	0.54
1:B:1343:LEU:HD11	1:B:1376:MET:HE1	1.90	0.54
1:A:1769:SER:HB2	1:A:1947:GLY:HA3	1.90	0.54
1:A:772:ALA:HB1	1:A:777:ASP:OD2	2.08	0.53
1:A:1093:LEU:HD23	1:C:1064:MET:HE3	1.90	0.53
1:A:1093:LEU:CD2	1:C:1064:MET:CE	2.86	0.53
1:C:1692:GLU:OE1	1:C:2190:TYR:N	2.41	0.53
1:B:1630:ARG:NH2	1:B:1831:GLU:OE2	2.41	0.53
1:D:1998:GLU:OE2	1:D:2001:GLY:C	2.52	0.53
1:B:1599:ILE:HD11	1:B:1952:THR:OG1	2.09	0.53
1:B:1969:SER:HB3	1:B:1985:VAL:HG11	1.91	0.53
1:D:1691:ILE:HG22	1:D:1696:TYR:O	2.08	0.53
1:C:1343:LEU:HD11	1:C:1376:MET:HE1	1.90	0.53
1:A:1677:ASP:OD1	1:A:1679:GLN:N	2.35	0.53
1:C:1997:ILE:HD11	1:C:2006:TYR:CE1	2.43	0.53
1:D:1992:TRP:O	1:D:2008:ARG:CZ	2.57	0.53
1:C:1901:HIS:NE2	1:C:2015:PHE:O	2.42	0.53
1:B:926:GLU:HA	1:B:930:THR:O	2.09	0.52
1:A:1901:HIS:NE2	1:A:2015:PHE:O	2.42	0.52
1:B:1065:LEU:HD11	1:B:1097:GLY:HA3	1.90	0.52
1:C:1869:TYR:O	1:C:1870:THR:OG1	2.20	0.52
1:A:1638:ASP:N	1:A:1638:ASP:OD1	2.43	0.52
1:D:1911:ILE:HD12	1:D:1911:ILE:N	2.25	0.52
1:C:1769:SER:HB2	1:C:1947:GLY:HA3	1.92	0.52
1:B:2049:VAL:HG13	1:B:2098:ALA:HB2	1.92	0.52
1:A:826:LEU:N	1:A:859:ALA:O	2.41	0.52
1:A:1651:TRP:O	1:A:1828:VAL:HG13	2.09	0.52
1:D:1911:ILE:HD12	1:D:1911:ILE:H	1.74	0.51
1:C:641:GLY:O	1:C:1113:ARG:NE	2.35	0.51
1:A:1928:GLN:H	1:A:1982:PRO:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:GLU:N	1:A:714:GLU:OE1	2.43	0.51
1:A:1686:CYS:O	1:A:1690:THR:N	2.34	0.51
1:A:2142:ASP:OD1	1:A:2144:ASP:N	2.42	0.51
1:B:967:LEU:N	1:B:967:LEU:HD22	2.26	0.51
1:C:764:ILE:HD12	1:C:766:LEU:HD21	1.93	0.51
1:A:967:LEU:N	1:A:967:LEU:HD22	2.25	0.51
1:A:1645:GLY:O	1:A:1806:SER:OG	2.23	0.51
1:C:736:LEU:HD13	1:C:738:MET:SD	2.50	0.51
1:B:1638:ASP:HB3	1:B:1644:LEU:HD12	1.93	0.51
1:B:1876:SER:O	1:B:1879:ARG:N	2.43	0.51
1:A:1998:GLU:HA	1:A:2003:THR:HA	1.91	0.51
1:A:1076:GLU:O	1:A:1080:ARG:HG3	2.11	0.51
1:D:1679:GLN:HG2	1:D:1795:VAL:HG22	1.93	0.51
1:C:1076:GLU:O	1:C:1080:ARG:HG3	2.10	0.51
1:C:1877:GLN:NE2	1:C:2015:PHE:CD2	2.79	0.51
1:A:790:ALA:HA	1:A:947:GLY:O	2.11	0.50
1:B:2085:THR:O	1:B:2089:GLY:N	2.44	0.50
1:C:2185:ILE:HD12	1:C:2185:ILE:O	2.11	0.50
1:B:828:ALA:HB2	1:B:860:LEU:HD11	1.92	0.50
1:B:1911:ILE:HD12	1:B:1911:ILE:N	2.26	0.50
1:A:921:ARG:HD2	1:A:921:ARG:N	2.26	0.50
1:C:2139:PHE:HA	1:C:2145:LEU:HD13	1.93	0.50
1:A:1691:ILE:HG22	1:A:1696:TYR:O	2.11	0.50
1:B:825:TYR:OH	1:B:827:GLU:OE1	2.29	0.50
1:A:919:GLU:HB3	1:A:921:ARG:CZ	2.41	0.50
1:D:1849:ASP:OD1	1:D:1850:HIS:N	2.44	0.50
1:C:1697:THR:HG23	1:C:2091:GLU:HB2	1.93	0.50
1:C:967:LEU:N	1:C:967:LEU:HD22	2.27	0.50
1:A:2164:MET:HE3	1:A:2169:LEU:HD22	1.93	0.50
1:D:1076:GLU:O	1:D:1080:ARG:HG3	2.11	0.50
1:C:795:ASN:OD1	1:C:799:VAL:HG11	2.12	0.50
1:C:1762:VAL:HG11	1:C:1775:LEU:HD12	1.94	0.50
1:A:827:GLU:OE2	1:A:863:ALA:N	2.32	0.50
1:D:1609:ILE:O	1:D:1613:TRP:N	2.43	0.50
1:B:1074:LEU:HD23	1:B:1074:LEU:O	2.12	0.49
1:D:1928:GLN:H	1:D:1982:PRO:HA	1.76	0.49
1:D:2132:ASN:ND2	1:D:2167:GLN:OE1	2.45	0.49
1:B:770:ASP:OD1	1:B:771:LYS:N	2.45	0.49
1:A:1999:ILE:HD11	1:A:2006:TYR:OH	2.10	0.49
1:B:2002:VAL:HG11	1:B:2004:ARG:HE	1.77	0.49
1:A:2161:ILE:O	1:A:2165:TRP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1905:THR:HG22	1:D:1907:LEU:H	1.77	0.49
1:A:886:LEU:HD22	1:A:956:GLU:HB3	1.95	0.49
1:A:1059:ASN:OD1	1:A:1062:GLN:NE2	2.45	0.49
1:C:1850:HIS:NE2	1:C:2186:SER:OG	2.45	0.49
1:B:1873:ASN:OD1	1:B:1873:ASN:C	2.55	0.49
1:B:2038:SER:HA	1:B:2077:ASN:HA	1.94	0.49
1:A:1902:GLY:O	1:A:1903:THR:OG1	2.20	0.49
1:D:664:TYR:HD2	1:D:666:THR:HG1	1.60	0.49
1:C:859:ALA:HA	1:C:912:VAL:O	2.12	0.49
1:A:1873:ASN:OD1	1:A:1875:HIS:N	2.46	0.49
1:D:795:ASN:OD1	1:D:799:VAL:HG11	2.12	0.49
1:D:1892:PRO:CD	1:D:1923:TYR:HD2	2.26	0.49
1:D:1899:GLU:OE2	1:D:1935:ALA:N	2.33	0.49
1:C:772:ALA:HB1	1:C:777:ASP:OD2	2.12	0.49
1:B:1691:ILE:HG22	1:B:1696:TYR:O	2.12	0.49
1:A:1093:LEU:HD22	1:C:1064:MET:CE	2.43	0.49
1:A:2007:ALA:O	1:A:2009:ILE:HD12	2.12	0.49
1:D:1782:ARG:CD	1:C:1778:HIS:CE1	2.96	0.49
1:C:921:ARG:HD2	1:C:921:ARG:N	2.28	0.49
1:C:1830:GLY:N	1:C:1941:HIS:O	2.45	0.49
1:C:2118:GLU:OE1	1:C:2120:ASP:N	2.46	0.48
1:D:1751:TYR:OH	1:C:1865:LYS:NZ	2.43	0.48
1:D:1998:GLU:HA	1:D:2003:THR:HA	1.93	0.48
1:B:795:ASN:OD1	1:B:799:VAL:HG11	2.13	0.48
1:C:1911:ILE:HD12	1:C:1911:ILE:H	1.79	0.48
1:D:1873:ASN:OD1	1:D:1873:ASN:C	2.56	0.48
1:C:1986:GLN:NE2	1:C:1988:GLU:O	2.42	0.48
1:B:2134:GLU:OE1	1:B:2134:GLU:N	2.38	0.48
1:A:1065:LEU:HD11	1:A:1097:GLY:HA3	1.96	0.48
1:A:1596:ILE:HG12	1:A:1838:LEU:HD23	1.94	0.48
1:A:1766:CYS:HA	1:A:1943:GLU:O	2.14	0.48
1:D:1902:GLY:O	1:D:1903:THR:OG1	2.20	0.48
1:D:1969:SER:HB3	1:D:1985:VAL:HG11	1.96	0.48
1:B:1651:TRP:O	1:B:1828:VAL:HG13	2.14	0.48
1:B:1969:SER:CB	1:B:1985:VAL:HG11	2.43	0.48
1:D:1638:ASP:HB3	1:D:1644:LEU:HD12	1.96	0.48
1:D:1907:LEU:O	1:D:1907:LEU:HD23	2.13	0.48
1:A:825:TYR:HA	1:A:859:ALA:O	2.12	0.48
1:D:1074:LEU:O	1:D:1074:LEU:HD23	2.14	0.48
1:D:1794:ASN:OD1	1:D:1795:VAL:N	2.47	0.48
1:C:1861:ASN:OD1	1:C:1862:HIS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1638:ASP:OD1	1:B:1638:ASP:N	2.47	0.47
1:B:1891:HIS:ND1	1:B:1893:ARG:HB3	2.29	0.47
1:A:1998:GLU:C	1:A:1998:GLU:CD	2.83	0.47
1:D:1376:MET:HE2	1:D:1418:VAL:HG11	1.96	0.47
1:C:1969:SER:O	1:C:1987:GLN:NE2	2.47	0.47
1:A:1061:ASN:O	1:A:1065:LEU:HG	2.15	0.47
1:A:909:THR:CG2	1:A:910:PRO:HD2	2.44	0.47
1:D:1789:ILE:O	1:D:1789:ILE:HG22	2.14	0.47
1:D:2164:MET:HE3	1:D:2169:LEU:HD22	1.96	0.47
1:A:926:GLU:HB2	1:A:931:THR:HG22	1.97	0.47
1:B:1642:ASP:OD1	1:B:1642:ASP:N	2.47	0.47
1:B:1873:ASN:OD1	1:B:1875:HIS:N	2.47	0.47
1:B:2136:MET:SD	1:B:2169:LEU:N	2.88	0.47
1:A:2120:ASP:OD1	1:A:2121:SER:N	2.47	0.47
1:C:652:LYS:NZ	1:C:714:GLU:OE2	2.41	0.47
1:C:1094:TRP:HB2	1:C:1100:ILE:HD12	1.95	0.47
1:C:1992:TRP:CZ2	1:C:2008:ARG:HB3	2.50	0.47
1:A:541:ALA:N	1:A:767:LYS:O	2.43	0.47
1:A:1074:LEU:O	1:A:1074:LEU:HD23	2.14	0.47
1:D:772:ALA:HB1	1:D:777:ASP:OD2	2.14	0.47
1:C:585:GLU:N	1:C:585:GLU:OE1	2.48	0.47
1:C:1892:PRO:CD	1:C:1923:TYR:HD2	2.28	0.47
1:C:2035:ARG:O	1:C:2036:PRO:C	2.57	0.47
1:B:2012:ILE:C	1:B:2023:HIS:ND1	2.73	0.47
1:B:772:ALA:O	1:B:777:ASP:OD1	2.33	0.47
1:B:1778:HIS:CE1	1:A:1782:ARG:CD	2.98	0.47
1:C:1849:ASP:OD1	1:C:1850:HIS:ND1	2.48	0.47
1:B:827:GLU:OE2	1:B:863:ALA:N	2.33	0.46
1:B:885:GLN:HB3	1:B:920:TRP:CZ3	2.50	0.46
1:A:922:ARG:HE	1:A:936:ARG:NH2	2.14	0.46
1:A:1966:SER:OG	1:A:1967:LEU:N	2.48	0.46
1:B:653:VAL:HB	1:B:683:PHE:CD1	2.50	0.46
1:B:746:LYS:HE3	1:B:750:ASP:O	2.16	0.46
1:B:1059:ASN:OD1	1:B:1062:GLN:NE2	2.48	0.46
1:D:1626:ILE:HD12	1:D:1633:HIS:CE1	2.51	0.46
1:D:1836:VAL:HG13	1:D:1836:VAL:O	2.16	0.46
1:D:2100:ILE:O	1:D:2110:LYS:NZ	2.40	0.46
1:B:1966:SER:OG	1:B:1967:LEU:N	2.47	0.46
1:A:1905:THR:HG22	1:A:1907:LEU:H	1.80	0.46
1:B:909:THR:CG2	1:B:910:PRO:HD2	2.45	0.46
1:B:1056:GLY:HA3	1:B:1095:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1849:ASP:OD1	1:B:1850:HIS:N	2.48	0.46
1:B:2139:PHE:HA	1:B:2145:LEU:HD13	1.98	0.46
1:A:1794:ASN:OD1	1:A:1794:ASN:C	2.58	0.46
1:D:921:ARG:N	1:D:921:ARG:HD2	2.30	0.46
1:C:858:CYS:O	1:C:911:PHE:HA	2.16	0.46
1:C:1068:LEU:HD12	1:C:1069:THR:N	2.31	0.46
1:C:1074:LEU:HD23	1:C:1074:LEU:O	2.15	0.46
1:C:1913:ILE:O	1:C:1917:THR:OG1	2.30	0.46
1:D:1813:SER:OG	1:D:1814:LYS:N	2.46	0.46
1:D:891:LEU:O	1:D:917:LEU:HD12	2.16	0.46
1:D:919:GLU:HB3	1:D:921:ARG:CZ	2.46	0.46
1:C:909:THR:CG2	1:C:910:PRO:HD2	2.46	0.46
1:C:1122:ALA:HB1	1:C:1124:GLU:OE2	2.15	0.46
1:B:638:GLU:O	1:B:1019:ARG:NH1	2.49	0.46
1:B:859:ALA:HA	1:B:912:VAL:O	2.16	0.46
1:B:2185:ILE:HD12	1:B:2185:ILE:O	2.16	0.46
1:C:1862:HIS:CD2	1:C:1863:GLY:N	2.84	0.46
1:A:1058:VAL:HG22	1:A:1097:GLY:HA2	1.98	0.46
1:A:1376:MET:HE2	1:A:1418:VAL:HG11	1.96	0.46
1:A:2048:ILE:HD12	1:A:2048:ILE:N	2.30	0.46
1:D:984:ALA:HA	1:D:1024:GLU:HG2	1.98	0.46
1:D:1404:LYS:HA	1:D:1423:PHE:O	2.16	0.46
1:C:828:ALA:HB2	1:C:860:LEU:HD11	1.98	0.46
1:B:2002:VAL:CG1	1:B:2004:ARG:HE	2.29	0.45
1:A:1638:ASP:CB	1:A:1644:LEU:HD12	2.45	0.45
1:D:909:THR:CG2	1:D:910:PRO:HD2	2.46	0.45
1:C:543:ILE:CG2	1:C:777:ASP:OD2	2.65	0.45
1:B:925:VAL:HG12	1:B:927:ILE:HG13	1.99	0.45
1:B:1862:HIS:NE2	1:B:2019:GLY:HA3	2.31	0.45
1:A:980:SER:HA	1:A:1024:GLU:O	2.16	0.45
1:A:1404:LYS:HA	1:A:1423:PHE:O	2.17	0.45
1:C:1995:PRO:CG	1:C:2007:ALA:O	2.65	0.45
1:B:1996:VAL:HA	1:B:2005:GLU:HA	1.99	0.45
1:B:2048:ILE:N	1:B:2048:ILE:HD12	2.31	0.45
1:A:1613:TRP:CE3	1:A:1956:LEU:HB3	2.50	0.45
1:A:1817:CYS:SG	1:A:1968:HIS:NE2	2.90	0.45
1:D:2048:ILE:HD12	1:D:2048:ILE:N	2.31	0.45
1:C:909:THR:HG22	1:C:910:PRO:HD2	1.97	0.45
1:A:543:ILE:CG2	1:A:777:ASP:OD2	2.65	0.45
1:D:1885:PHE:O	1:D:1889:GLY:N	2.49	0.45
1:C:1999:ILE:O	1:C:1999:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:ALA:HB2	1:B:990:ILE:HD12	1.99	0.45
1:B:1899:GLU:HG3	1:B:1933:GLY:O	2.17	0.45
1:B:2047:VAL:HG13	1:B:2162:LEU:HD11	1.99	0.45
1:D:827:GLU:OE2	1:D:862:SER:HA	2.16	0.45
1:C:2048:ILE:N	1:C:2048:ILE:HD12	2.31	0.45
1:B:1794:ASN:OD1	1:B:1795:VAL:N	2.49	0.45
1:A:1753:CYS:HB3	1:A:1755:PHE:CE1	2.52	0.45
1:C:1596:ILE:HG23	1:C:1836:VAL:CG2	2.47	0.45
1:A:2101:VAL:HG12	1:A:2102:LYS:N	2.32	0.45
1:D:722:ASN:C	1:D:723:LEU:HD23	2.42	0.45
1:D:1603:TYR:C	1:D:1655:ILE:HG22	2.42	0.45
1:D:1720:GLU:OE1	1:D:1740:GLY:HA2	2.15	0.45
1:A:1068:LEU:HD12	1:A:1069:THR:N	2.32	0.45
1:A:1073:GLU:OE2	1:C:1086:LYS:NZ	2.44	0.45
1:C:692:THR:HG21	1:C:699:THR:HG21	1.99	0.45
1:D:1055:ARG:C	1:D:1095:VAL:HG11	2.42	0.45
1:D:1721:GLU:OE2	1:D:1797:ILE:N	2.35	0.45
1:D:1899:GLU:HG3	1:D:1934:SER:HA	1.98	0.45
1:B:857:PHE:CE2	1:B:910:PRO:HB3	2.52	0.44
1:B:898:ARG:NH2	1:B:915:GLN:O	2.51	0.44
1:B:1770:LEU:HG	1:B:2024:LEU:HD11	1.99	0.44
1:B:2101:VAL:HG12	1:B:2102:LYS:N	2.32	0.44
1:A:1860:ILE:HG22	1:A:2022:ALA:CB	2.47	0.44
1:C:1997:ILE:HD12	1:C:1999:ILE:CG2	2.46	0.44
1:C:2134:GLU:OE1	1:C:2134:GLU:N	2.41	0.44
1:A:2132:ASN:N	1:A:2132:ASN:OD1	2.50	0.44
1:D:858:CYS:O	1:D:911:PHE:HA	2.17	0.44
1:C:696:ALA:O	1:C:699:THR:OG1	2.30	0.44
1:C:1061:ASN:O	1:C:1065:LEU:HG	2.16	0.44
1:D:980:SER:HA	1:D:1024:GLU:O	2.17	0.44
1:C:1058:VAL:HG22	1:C:1097:GLY:HA2	2.00	0.44
1:A:1297:TYR:CZ	1:A:1312:ARG:HA	2.53	0.44
1:D:1063:GLU:OE1	1:D:1063:GLU:HA	2.18	0.44
1:C:932:ASN:OD1	1:C:933:GLU:N	2.50	0.44
1:B:1063:GLU:OE1	1:B:1063:GLU:HA	2.18	0.44
1:D:772:ALA:O	1:D:777:ASP:OD1	2.35	0.44
1:D:1128:THR:HG22	1:D:1129:HIS:H	1.82	0.44
1:D:1998:GLU:CG	1:D:2003:THR:OG1	2.66	0.44
1:D:2102:LYS:N	1:D:2106:GLU:OE1	2.41	0.44
1:C:1768:SER:O	1:C:1771:THR:OG1	2.30	0.44
1:A:1873:ASN:OD1	1:A:1873:ASN:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:ILE:HD12	1:D:766:LEU:HD21	1.98	0.44
1:D:1082:MET:HE2	1:D:1105:LEU:HD13	2.00	0.44
1:D:1638:ASP:OD1	1:D:1638:ASP:N	2.51	0.44
1:B:919:GLU:HG3	1:B:921:ARG:HD2	1.99	0.44
1:B:1076:GLU:O	1:B:1080:ARG:HG3	2.18	0.44
1:B:1404:LYS:HA	1:B:1423:PHE:O	2.17	0.44
1:B:2046:ALA:N	1:B:2101:VAL:O	2.46	0.44
1:B:2164:MET:HE3	1:B:2169:LEU:HD22	1.99	0.44
1:A:2059:ARG:CZ	1:A:2115:LEU:HD23	2.47	0.44
1:D:747:SER:O	1:D:897:SER:OG	2.35	0.44
1:D:1610:HIS:O	1:D:1613:TRP:HB3	2.18	0.44
1:D:1769:SER:HB2	1:D:1947:GLY:HA3	2.00	0.44
1:C:1404:LYS:HA	1:C:1423:PHE:O	2.17	0.44
1:C:1873:ASN:OD1	1:C:1873:ASN:C	2.60	0.44
1:B:626:GLU:OE2	1:B:676:ARG:HB2	2.17	0.44
1:A:1212:LYS:HG3	1:A:1265:SER:HB2	2.00	0.44
1:A:1626:ILE:HD12	1:A:1633:HIS:CE1	2.53	0.44
1:D:2097:PHE:CZ	1:D:2099:VAL:HG13	2.53	0.44
1:C:1964:VAL:CG2	1:C:1965:PRO:HD2	2.48	0.44
1:C:2164:MET:HE3	1:C:2169:LEU:HD22	1.99	0.44
1:A:2179:ASP:OD1	1:A:2180:THR:HG23	2.18	0.44
1:A:1063:GLU:OE1	1:A:1063:GLU:HA	2.17	0.43
1:C:1849:ASP:OD1	1:C:1850:HIS:N	2.51	0.43
1:B:1068:LEU:HD12	1:B:1069:THR:N	2.32	0.43
1:B:1122:ALA:HB1	1:B:1124:GLU:OE2	2.18	0.43
1:D:770:ASP:OD1	1:D:771:LYS:N	2.50	0.43
1:C:1603:TYR:C	1:C:1655:ILE:HG22	2.43	0.43
1:C:2101:VAL:HG12	1:C:2102:LYS:N	2.33	0.43
1:C:2142:ASP:OD1	1:C:2144:ASP:N	2.51	0.43
1:C:981:ALA:HB2	1:C:990:ILE:HD12	2.00	0.43
1:C:1063:GLU:HA	1:C:1063:GLU:OE1	2.18	0.43
1:B:696:ALA:O	1:B:699:THR:OG1	2.35	0.43
1:C:1638:ASP:CG	1:C:1644:LEU:HD12	2.43	0.43
1:B:1240:GLU:HG2	1:B:1267:VAL:HG12	2.01	0.43
1:D:543:ILE:CG2	1:D:777:ASP:OD2	2.66	0.43
1:C:980:SER:HA	1:C:1024:GLU:O	2.19	0.43
1:C:1240:GLU:HG2	1:C:1267:VAL:HG12	2.00	0.43
1:D:1768:SER:HA	1:D:1771:THR:OG1	2.18	0.43
1:B:543:ILE:CG2	1:B:777:ASP:OD2	2.67	0.43
1:B:576:ARG:NH1	1:B:724:ILE:O	2.51	0.43
1:A:1656:ASP:OD1	1:A:1656:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2129:VAL:HG12	1:A:2129:VAL:O	2.18	0.43
1:D:1297:TYR:CZ	1:D:1312:ARG:HA	2.53	0.43
1:C:1984:VAL:O	1:C:1984:VAL:HG13	2.18	0.43
1:C:1997:ILE:HD11	1:C:2006:TYR:HE1	1.84	0.43
1:B:557:GLU:O	1:B:561:ARG:HG2	2.18	0.43
1:A:1638:ASP:CG	1:A:1644:LEU:HD12	2.44	0.43
1:D:1999:ILE:HD11	1:D:2006:TYR:OH	2.19	0.43
1:C:1892:PRO:HD3	1:C:1923:TYR:HD2	1.83	0.43
1:B:827:GLU:OE2	1:B:862:SER:HA	2.18	0.43
1:B:1921:GLN:O	1:B:1925:LYS:NZ	2.37	0.43
1:A:2074:LEU:HD13	1:A:2082:ILE:HD11	2.01	0.43
1:D:1059:ASN:OD1	1:D:1062:GLN:NE2	2.51	0.43
1:B:1068:LEU:HD13	1:B:1074:LEU:HD13	2.01	0.43
1:A:2101:VAL:CG1	1:A:2102:LYS:N	2.81	0.43
1:D:604:MET:HG3	1:D:723:LEU:CD1	2.48	0.43
1:D:789:ASN:OD1	1:D:789:ASN:C	2.62	0.43
1:C:1632:ASP:OD2	1:C:1634:SER:N	2.43	0.43
1:B:548:ARG:NH1	1:B:628:LEU:HD22	2.33	0.42
1:B:1677:ASP:OD1	1:B:1677:ASP:C	2.61	0.42
1:B:1778:HIS:CE1	1:A:1782:ARG:HD2	2.53	0.42
1:D:541:ALA:N	1:D:767:LYS:O	2.47	0.42
1:D:1651:TRP:O	1:D:1828:VAL:HG13	2.18	0.42
1:C:1612:PHE:CZ	1:C:1616:LEU:HD11	2.53	0.42
1:B:1048:GLU:O	1:B:1055:ARG:NH1	2.52	0.42
1:A:981:ALA:HB2	1:A:990:ILE:HD12	2.01	0.42
1:A:1358:LEU:HD11	1:A:1390:ILE:HG22	2.01	0.42
1:A:1892:PRO:CD	1:A:1923:TYR:HD2	2.32	0.42
1:D:1068:LEU:HD12	1:D:1069:THR:N	2.34	0.42
1:D:1907:LEU:C	1:D:1911:ILE:HD13	2.44	0.42
1:D:2139:PHE:HA	1:D:2145:LEU:HD13	2.00	0.42
1:C:1249:SER:OG	1:C:1257:THR:HG22	2.19	0.42
1:C:2185:ILE:HD13	1:C:2187:LEU:HD21	2.00	0.42
1:B:1276:SER:OG	1:B:1415:ASN:OD1	2.31	0.42
1:A:1071:ASP:HB2	1:C:1089:LYS:NZ	2.34	0.42
1:A:1677:ASP:OD1	1:A:1677:ASP:C	2.61	0.42
1:A:1812:SER:O	1:A:1813:SER:C	2.62	0.42
1:C:1880:VAL:HG13	1:C:1881:ILE:N	2.34	0.42
1:A:2099:VAL:HG12	1:A:2124:LEU:HG	2.02	0.42
1:D:1893:ARG:NH2	1:D:1926:GLU:OE1	2.52	0.42
1:C:1860:ILE:HG22	1:C:2022:ALA:CB	2.49	0.42
1:A:1860:ILE:HG22	1:A:2022:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1890:ILE:HG13	1:A:2025:VAL:HG11	2.02	0.42
1:A:1996:VAL:HG13	1:A:1996:VAL:O	2.18	0.42
1:D:1370:PRO:HA	1:D:1425:THR:HG22	2.02	0.42
1:C:779:ILE:HB	1:C:957:TYR:CD2	2.55	0.42
1:C:1794:ASN:OD1	1:C:1794:ASN:C	2.62	0.42
1:C:1875:HIS:O	1:C:1878:SER:HB2	2.19	0.42
1:C:1951:LEU:CD1	1:C:2026:ILE:HD11	2.50	0.42
1:C:2037:PRO:O	1:C:2038:SER:CB	2.67	0.42
1:B:622:MET:O	1:B:627:ARG:NH2	2.42	0.42
1:A:789:ASN:OD1	1:A:789:ASN:C	2.61	0.42
1:D:879:VAL:O	1:D:883:LEU:HG	2.19	0.42
1:D:1935:ALA:HB2	1:D:1953:LYS:CD	2.49	0.42
1:C:1873:ASN:OD1	1:C:1875:HIS:N	2.51	0.42
1:B:573:PRO:HD3	1:B:600:PHE:CD2	2.53	0.42
1:B:1609:ILE:O	1:B:1612:PHE:HB3	2.20	0.42
1:B:1648:TYR:CE1	1:B:1813:SER:HA	2.54	0.42
1:A:639:ASP:OD1	1:A:639:ASP:C	2.63	0.42
1:A:891:LEU:O	1:A:917:LEU:HD12	2.19	0.42
1:A:2113:TYR:CE1	1:A:2121:SER:OG	2.70	0.42
1:D:1212:LYS:HG3	1:D:1265:SER:HB2	2.00	0.42
1:D:2135:THR:O	1:D:2138:VAL:HG12	2.20	0.42
1:C:1892:PRO:HB3	1:C:1920:PHE:CZ	2.54	0.42
1:B:1866:THR:O	1:B:1868:GLY:N	2.51	0.42
1:B:1963:LEU:HD21	1:B:1992:TRP:CG	2.55	0.42
1:A:1067:ILE:O	1:A:1067:ILE:HG22	2.20	0.42
1:C:2136:MET:HE1	1:C:2164:MET:HB3	2.02	0.42
1:B:1649:SER:OG	1:B:1650:LYS:N	2.52	0.42
1:B:1880:VAL:HG13	1:B:1881:ILE:N	2.34	0.42
1:A:582:PHE:CD1	1:A:731:MET:CE	3.03	0.42
1:A:1762:VAL:HG11	1:A:1775:LEU:HD12	2.02	0.42
1:A:1986:GLN:NE2	1:A:1988:GLU:O	2.40	0.42
1:C:1638:ASP:CB	1:C:1644:LEU:HD12	2.50	0.42
1:B:1718:MET:SD	1:B:1943:GLU:HB3	2.60	0.42
1:A:559:TRP:CZ2	1:A:888:HIS:CG	3.08	0.42
1:D:1358:LEU:HD11	1:D:1390:ILE:HG22	2.02	0.42
1:C:1892:PRO:HB3	1:C:1920:PHE:CE2	2.55	0.42
1:C:2132:ASN:OD1	1:C:2132:ASN:N	2.53	0.42
1:C:2157:LYS:CE	1:C:2157:LYS:HA	2.50	0.42
1:B:789:ASN:OD1	1:B:789:ASN:C	2.63	0.41
1:B:1808:GLY:HA3	1:B:1810:PHE:CE2	2.56	0.41
1:B:2002:VAL:HG11	1:B:2004:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2064:ARG:NH1	1:A:2189:ALA:O	2.49	0.41
1:D:1849:ASP:OD1	1:D:1849:ASP:C	2.63	0.41
1:C:770:ASP:OD1	1:C:771:LYS:N	2.52	0.41
1:C:1626:ILE:HD12	1:C:1633:HIS:CE1	2.55	0.41
1:C:1992:TRP:O	1:C:2008:ARG:CZ	2.67	0.41
1:B:692:THR:HG22	1:B:948:SER:CB	2.50	0.41
1:B:940:ILE:O	1:B:951:HIS:ND1	2.53	0.41
1:B:1763:ASP:OD1	1:B:1763:ASP:C	2.63	0.41
1:B:1850:HIS:CE1	1:B:2186:SER:HG	2.36	0.41
1:B:2118:GLU:OE1	1:B:2120:ASP:N	2.52	0.41
1:C:1067:ILE:O	1:C:1067:ILE:HG22	2.20	0.41
1:C:1692:GLU:O	1:C:2090:ARG:NH1	2.52	0.41
1:C:1697:THR:HG22	1:C:1698:ARG:N	2.35	0.41
1:C:1813:SER:OG	1:C:1814:LYS:N	2.53	0.41
1:B:595:THR:HG22	1:B:741:PRO:HA	2.02	0.41
1:B:969:ILE:HD12	1:B:975:ALA:HB2	2.02	0.41
1:B:1249:SER:OG	1:B:1257:THR:HG22	2.19	0.41
1:B:1655:ILE:N	1:B:1831:GLU:OE1	2.45	0.41
1:B:1703:LYS:O	1:B:1703:LYS:HG2	2.21	0.41
1:A:879:VAL:O	1:A:883:LEU:HG	2.19	0.41
1:A:1893:ARG:NH1	1:A:1929:PHE:CG	2.88	0.41
1:D:2101:VAL:CG1	1:D:2102:LYS:N	2.83	0.41
1:B:1769:SER:HB2	1:B:1947:GLY:HA3	2.03	0.41
1:B:1892:PRO:CD	1:B:1923:TYR:HD2	2.33	0.41
1:B:2157:LYS:HA	1:B:2157:LYS:CE	2.50	0.41
1:C:1844:ALA:O	1:C:1848:GLY:N	2.53	0.41
1:C:1875:HIS:HB3	1:C:1879:ARG:NH1	2.35	0.41
1:B:1768:SER:O	1:B:1771:THR:OG1	2.34	0.41
1:D:1638:ASP:CG	1:D:1644:LEU:HD12	2.45	0.41
1:D:1677:ASP:OD2	1:D:1722:TYR:HB3	2.19	0.41
1:D:2133:LYS:O	1:D:2137:ASP:HB2	2.20	0.41
1:C:587:LYS:HE3	1:C:741:PRO:HG3	2.02	0.41
1:C:1349:ASP:O	1:C:1353:GLN:HG3	2.21	0.41
1:B:604:MET:HG3	1:B:723:LEU:CD1	2.51	0.41
1:B:1688:TYR:CE2	1:B:1692:GLU:OE2	2.74	0.41
1:A:909:THR:HG22	1:A:910:PRO:HD2	2.01	0.41
1:A:1349:ASP:O	1:A:1353:GLN:HG3	2.21	0.41
1:D:1067:ILE:O	1:D:1067:ILE:HG22	2.21	0.41
1:D:2101:VAL:HG12	1:D:2102:LYS:N	2.35	0.41
1:C:1648:TYR:CE1	1:C:1813:SER:HA	2.56	0.41
1:C:1905:THR:HG22	1:C:1907:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:TRP:HB2	1:B:593:MET:CE	2.51	0.41
1:B:1349:ASP:O	1:B:1353:GLN:HG3	2.21	0.41
1:A:772:ALA:O	1:A:777:ASP:OD1	2.38	0.41
1:A:1921:GLN:HA	1:A:1924:THR:O	2.21	0.41
1:D:1410:CYS:HA	1:D:1415:ASN:O	2.21	0.41
1:A:915:GLN:HA	1:A:915:GLN:OE1	2.20	0.41
1:A:1370:PRO:HA	1:A:1425:THR:HG22	2.02	0.41
1:A:1604:PRO:N	1:A:1655:ILE:HG22	2.35	0.41
1:A:1830:GLY:N	1:A:1941:HIS:O	2.43	0.41
1:A:1862:HIS:CD2	1:A:1863:GLY:N	2.88	0.41
1:C:795:ASN:OD1	1:C:795:ASN:N	2.53	0.41
1:C:2151:THR:O	1:C:2155:LYS:HG3	2.20	0.41
1:B:1645:GLY:O	1:B:1806:SER:CB	2.69	0.41
1:B:1996:VAL:HA	1:B:2004:ARG:O	2.20	0.41
1:A:692:THR:HG22	1:A:948:SER:CB	2.50	0.41
1:A:795:ASN:OD1	1:A:799:VAL:HG11	2.20	0.41
1:A:828:ALA:HB2	1:A:860:LEU:HD11	2.02	0.41
1:A:2026:ILE:HG22	1:A:2027:GLU:N	2.36	0.41
1:D:987:LEU:HD21	1:D:1026:ILE:HG23	2.03	0.41
1:D:1405:PHE:CE2	1:D:1425:THR:HG21	2.56	0.41
1:D:1645:GLY:O	1:D:1806:SER:CB	2.68	0.41
1:C:705:LEU:HB3	1:C:709:TYR:CZ	2.56	0.41
1:C:919:GLU:HB3	1:C:921:ARG:CZ	2.51	0.41
1:D:1074:LEU:HD23	1:D:1078:ILE:HD13	2.02	0.41
1:D:1721:GLU:OE2	1:D:1796:SER:HA	2.21	0.41
1:C:1811:ALA:O	1:C:1826:GLY:HA3	2.20	0.41
1:B:1058:VAL:HG22	1:B:1097:GLY:HA2	2.02	0.40
1:B:1082:MET:HE2	1:B:1105:LEU:HD13	2.03	0.40
1:B:1902:GLY:O	1:B:1903:THR:OG1	2.26	0.40
1:B:2110:LYS:O	1:B:2113:TYR:HB3	2.21	0.40
1:B:2136:MET:HE1	1:B:2164:MET:HB3	2.03	0.40
1:B:2185:ILE:HD13	1:B:2187:LEU:HD21	2.03	0.40
1:A:921:ARG:N	1:A:921:ARG:CD	2.84	0.40
1:A:1122:ALA:HB1	1:A:1124:GLU:OE2	2.20	0.40
1:D:886:LEU:HD22	1:D:956:GLU:HB3	2.02	0.40
1:D:1349:ASP:O	1:D:1353:GLN:HG3	2.21	0.40
1:B:1055:ARG:C	1:B:1095:VAL:HG11	2.45	0.40
1:B:1648:TYR:CD1	1:B:1813:SER:HA	2.56	0.40
1:B:1836:VAL:O	1:B:1836:VAL:HG13	2.21	0.40
1:A:920:TRP:CZ2	1:A:936:ARG:HB3	2.57	0.40
1:A:1369:LEU:HD12	1:A:1428:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:CYS:HA	1:A:1415:ASN:O	2.21	0.40
1:A:1907:LEU:O	1:A:1911:ILE:HD13	2.21	0.40
1:C:638:GLU:OE1	1:C:1118:THR:HB	2.21	0.40
1:C:1410:CYS:HA	1:C:1415:ASN:O	2.21	0.40
1:C:1827:TYR:HB3	1:C:1903:THR:O	2.21	0.40
1:C:1901:HIS:O	1:C:1903:THR:HG23	2.21	0.40
1:B:921:ARG:HD2	1:B:921:ARG:N	2.37	0.40
1:B:1067:ILE:O	1:B:1067:ILE:HG22	2.21	0.40
1:B:1206:LEU:N	1:B:1206:LEU:HD12	2.37	0.40
1:B:1727:SER:HA	1:B:1730:GLN:OE1	2.21	0.40
1:D:1369:LEU:HD12	1:D:1428:ILE:HD13	2.03	0.40
1:D:1729:GLU:O	1:D:1733:GLY:N	2.52	0.40
1:D:1767:SER:HA	1:D:2014:SER:OG	2.22	0.40
1:D:1935:ALA:HB2	1:D:1953:LYS:HD2	2.03	0.40
1:B:829:HIS:CD2	1:B:831:THR:HG23	2.56	0.40
1:A:1789:ILE:O	1:A:1789:ILE:HG22	2.22	0.40
1:D:696:ALA:O	1:D:699:THR:OG1	2.37	0.40
1:D:746:LYS:HE3	1:D:750:ASP:O	2.22	0.40
1:D:1880:VAL:HG13	1:D:1881:ILE:N	2.36	0.40
1:C:746:LYS:HE3	1:C:750:ASP:O	2.21	0.40
1:C:1768:SER:HA	1:C:1771:THR:OG1	2.21	0.40
1:C:2064:ARG:NH1	1:C:2188:PRO:HB2	2.37	0.40
1:A:1405:PHE:CE2	1:A:1425:THR:HG21	2.56	0.40
1:D:1863:GLY:HA2	1:D:1876:SER:HB3	2.04	0.40
1:D:1966:SER:OG	1:D:1967:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1472/1690 (87%)	1402 (95%)	70 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1464/1690 (87%)	1386 (95%)	77 (5%)	1 (0%)	48	83
1	C	1464/1690 (87%)	1392 (95%)	70 (5%)	2 (0%)	48	83
1	D	1472/1690 (87%)	1407 (96%)	65 (4%)	0	100	100
All	All	5872/6760 (87%)	5587 (95%)	282 (5%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1358	LEU
1	C	1358	LEU
1	C	2038	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1231/1413 (87%)	1217 (99%)	14 (1%)	65	76
1	B	1228/1413 (87%)	1211 (99%)	17 (1%)	59	72
1	C	1228/1413 (87%)	1209 (98%)	19 (2%)	57	72
1	D	1231/1413 (87%)	1216 (99%)	15 (1%)	63	75
All	All	4918/5652 (87%)	4853 (99%)	65 (1%)	59	74

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	585	GLU
1	B	643	THR
1	B	723	LEU
1	B	736	LEU
1	B	916	GLU
1	B	921	ARG
1	B	967	LEU
1	B	1055	ARG

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Mol	Chain	Res	Type
1	B	1128	THR
1	B	1318	LEU
1	B	1738	ILE
1	B	1806	SER
1	B	1861	ASN
1	B	2031	GLU
1	B	2049	VAL
1	B	2102	LYS
1	B	2185	ILE
1	A	643	THR
1	A	723	LEU
1	A	736	LEU
1	A	921	ARG
1	A	967	LEU
1	A	1055	ARG
1	A	1128	THR
1	A	1218	GLN
1	A	1649	SER
1	A	1786	GLU
1	A	2066	LEU
1	A	2130	LYS
1	A	2132	ASN
1	A	2177	TYR
1	D	585	GLU
1	D	643	THR
1	D	681	LEU
1	D	723	LEU
1	D	736	LEU
1	D	921	ARG
1	D	967	LEU
1	D	1055	ARG
1	D	1128	THR
1	D	1218	GLN
1	D	2000	ASP
1	D	2066	LEU
1	D	2102	LYS
1	D	2130	LYS
1	D	2177	TYR
1	C	585	GLU
1	C	643	THR
1	C	681	LEU
1	C	723	LEU

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Mol	Chain	Res	Type
1	C	736	LEU
1	C	921	ARG
1	C	967	LEU
1	C	1055	ARG
1	C	1128	THR
1	C	1318	LEU
1	C	1632	ASP
1	C	1861	ASN
1	C	1998	GLU
1	C	2000	ASP
1	C	2049	VAL
1	C	2102	LYS
1	C	2132	ASN
1	C	2145	LEU
1	C	2185	ILE

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

Mol	Chain	Res	Type
1	B	663	ASN
1	B	675	ASN
1	B	682	ASN
1	B	729	HIS
1	B	807	GLN
1	B	853	GLN
1	B	856	GLN
1	B	866	ASN
1	B	888	HIS
1	B	896	HIS
1	B	1610	HIS
1	A	661	ASN
1	A	729	HIS
1	A	789	ASN
1	A	807	GLN
1	A	853	GLN
1	A	856	GLN
1	A	866	ASN
1	A	888	HIS
1	A	896	HIS
1	A	903	ASN
1	A	1417	GLN
1	A	1800	ASN

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Mol	Chain	Res	Type
1	A	2061	GLN
1	A	2167	GLN
1	D	729	HIS
1	D	807	GLN
1	D	853	GLN
1	D	856	GLN
1	D	866	ASN
1	D	896	HIS
1	D	1037	GLN
1	D	1417	GLN
1	D	2063	GLN
1	C	661	ASN
1	C	722	ASN
1	C	729	HIS
1	C	807	GLN
1	C	856	GLN
1	C	866	ASN
1	C	888	HIS
1	C	903	ASN
1	C	1778	HIS
1	C	1941	HIS
1	C	1968	HIS
1	C	1987	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

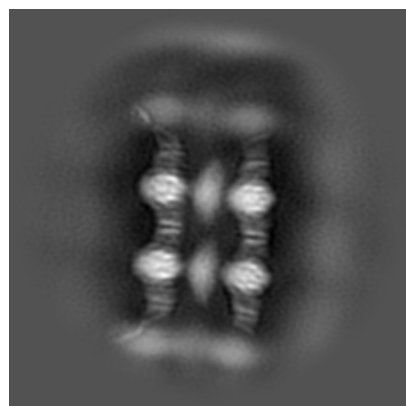
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14945. These allow visual inspection of the internal detail of the map and identification of artifacts.

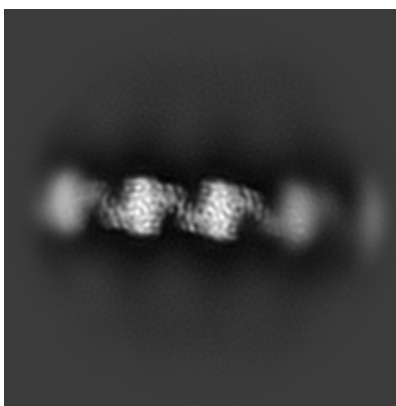
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

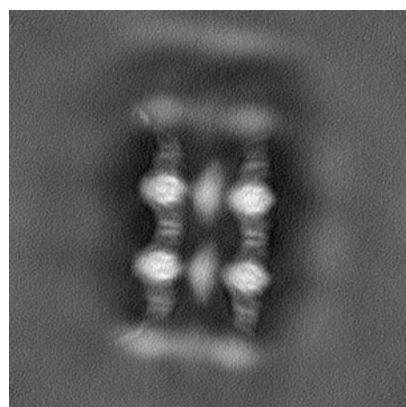


Y

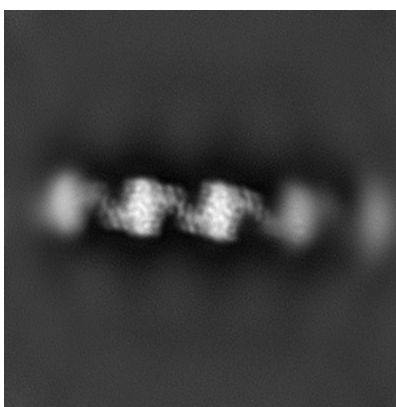


Z

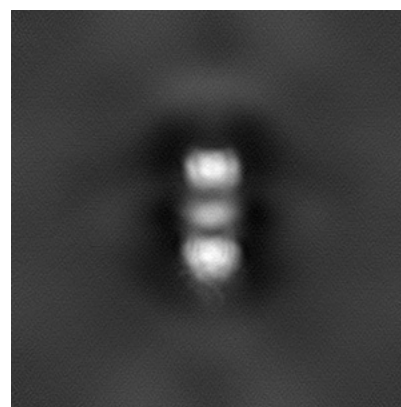
6.1.2 Raw map



X



Y

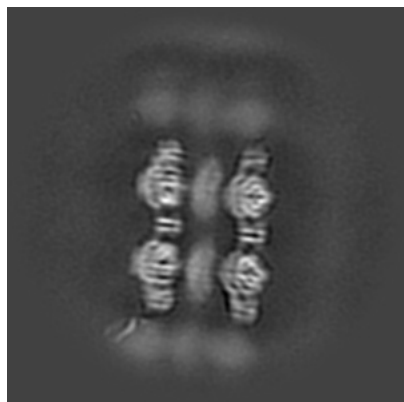


Z

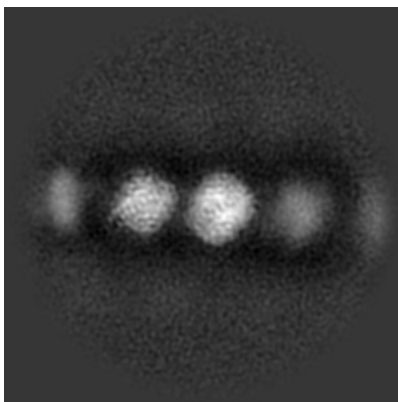
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

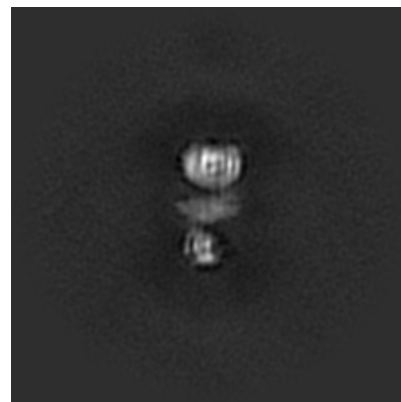
6.2.1 Primary map



X Index: 128

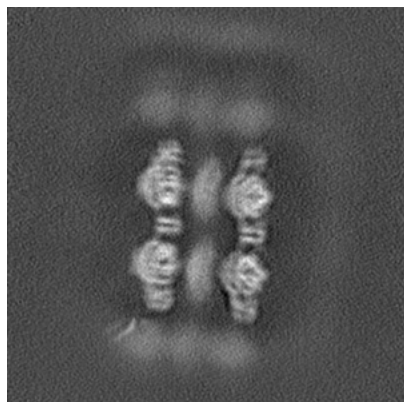


Y Index: 128

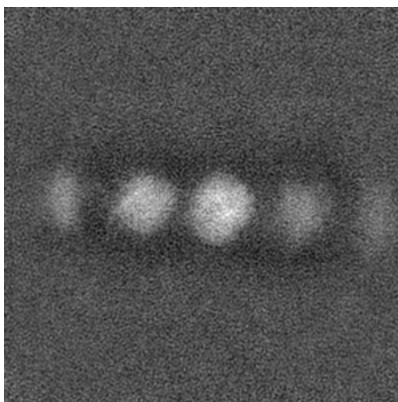


Z Index: 128

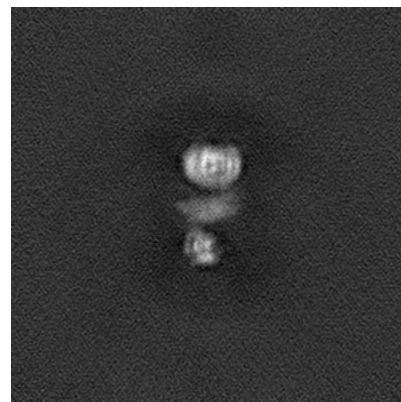
6.2.2 Raw map



X Index: 128



Y Index: 128

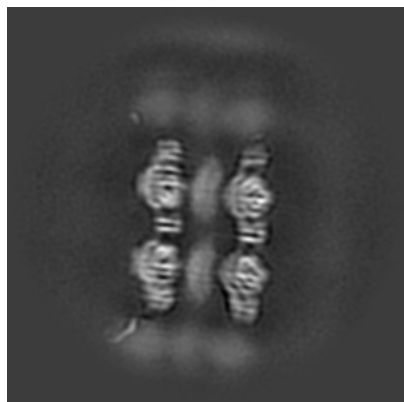


Z Index: 128

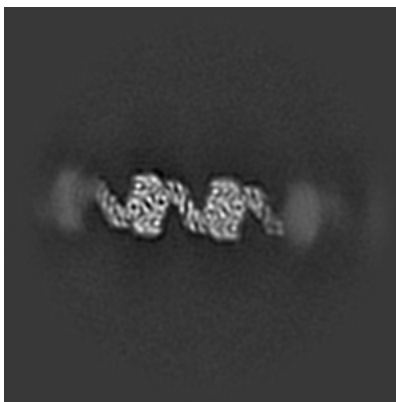
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

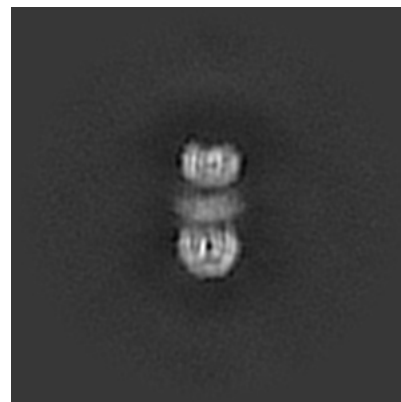
6.3.1 Primary map



X Index: 127

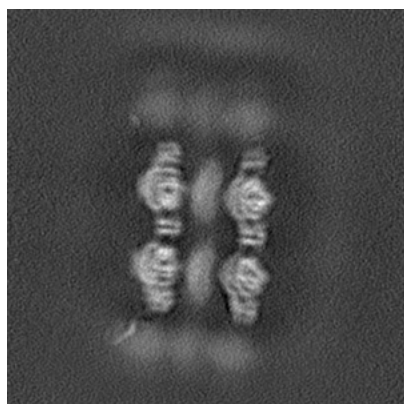


Y Index: 100

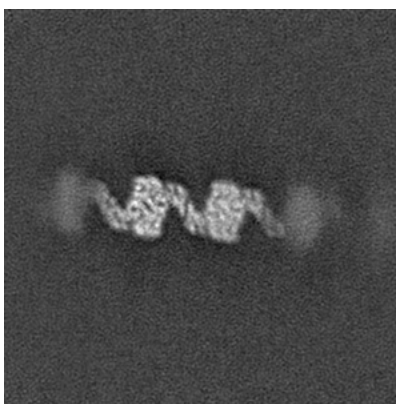


Z Index: 140

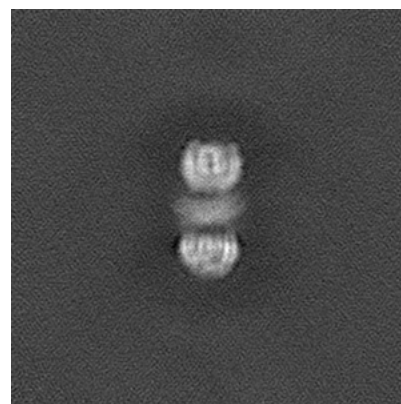
6.3.2 Raw map



X Index: 127



Y Index: 99

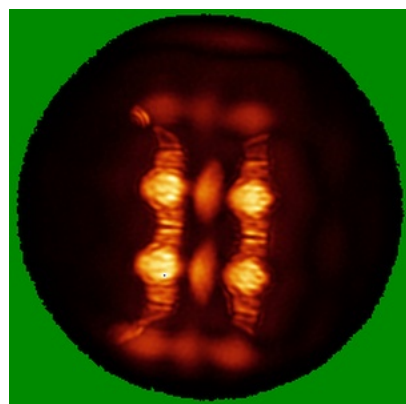


Z Index: 135

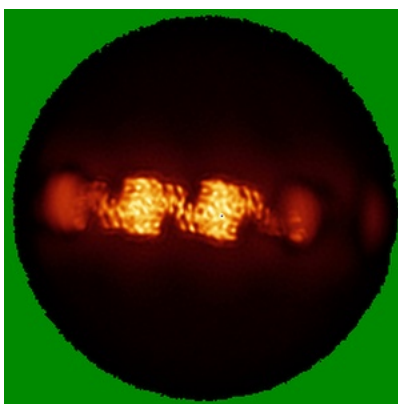
The images above show the largest variance slices of the map in three orthogonal directions.

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

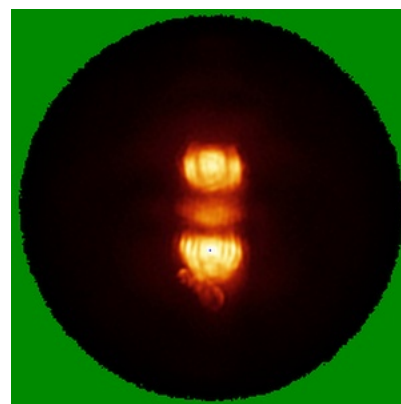
6.4.1 Primary map



X

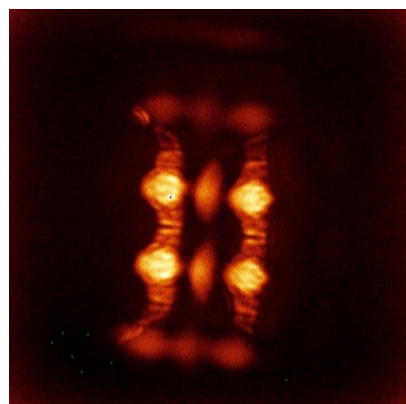


Y

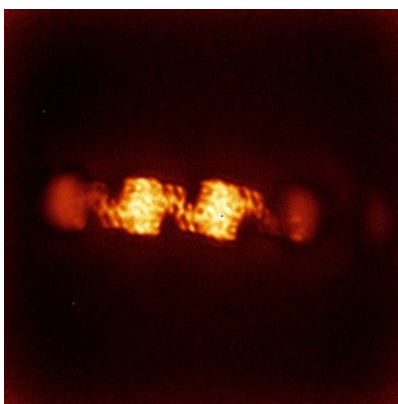


Z

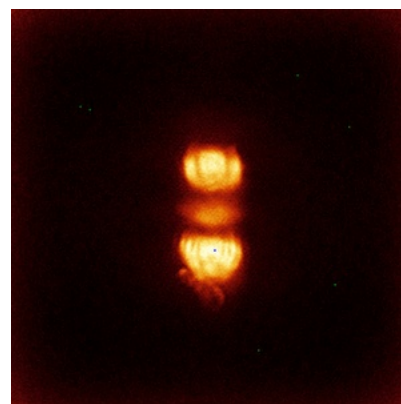
6.4.2 Raw map



X



Y

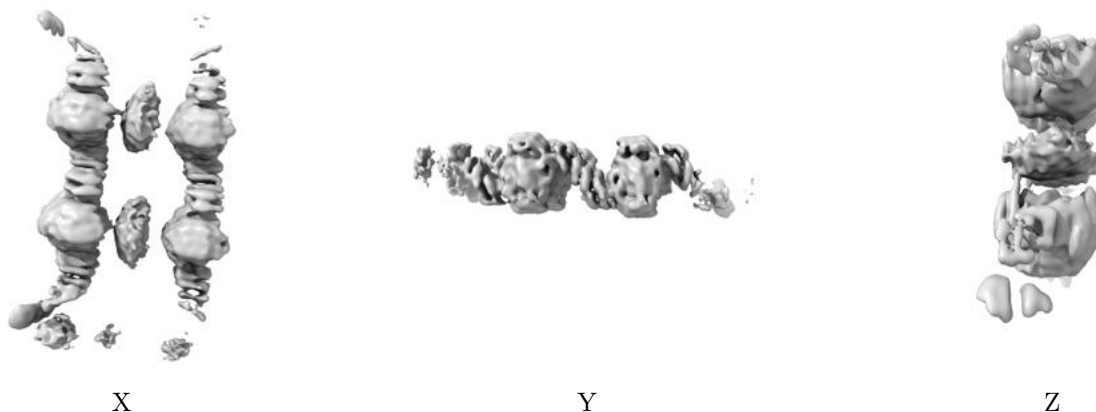


Z

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

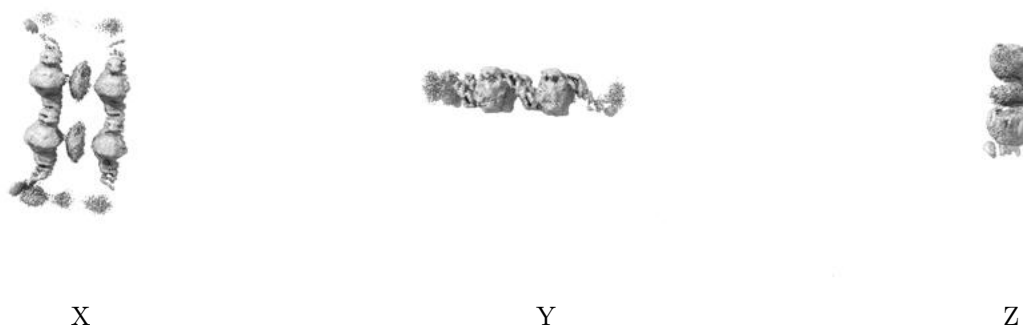
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

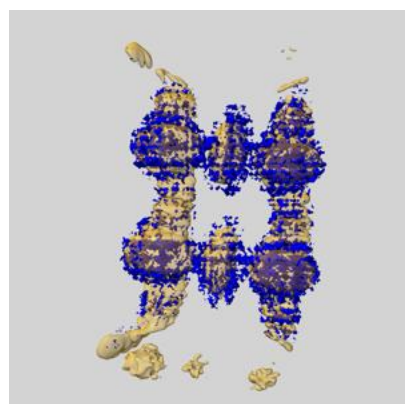
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

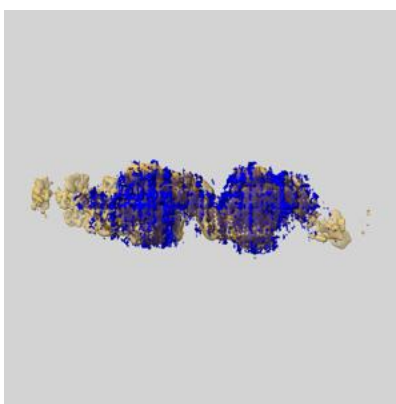
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

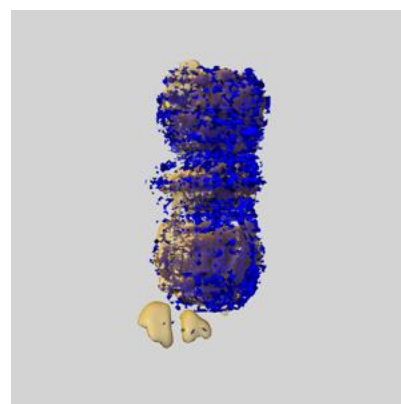
6.6.1 emd_14945_msk_1.map [i](#)



X



Y

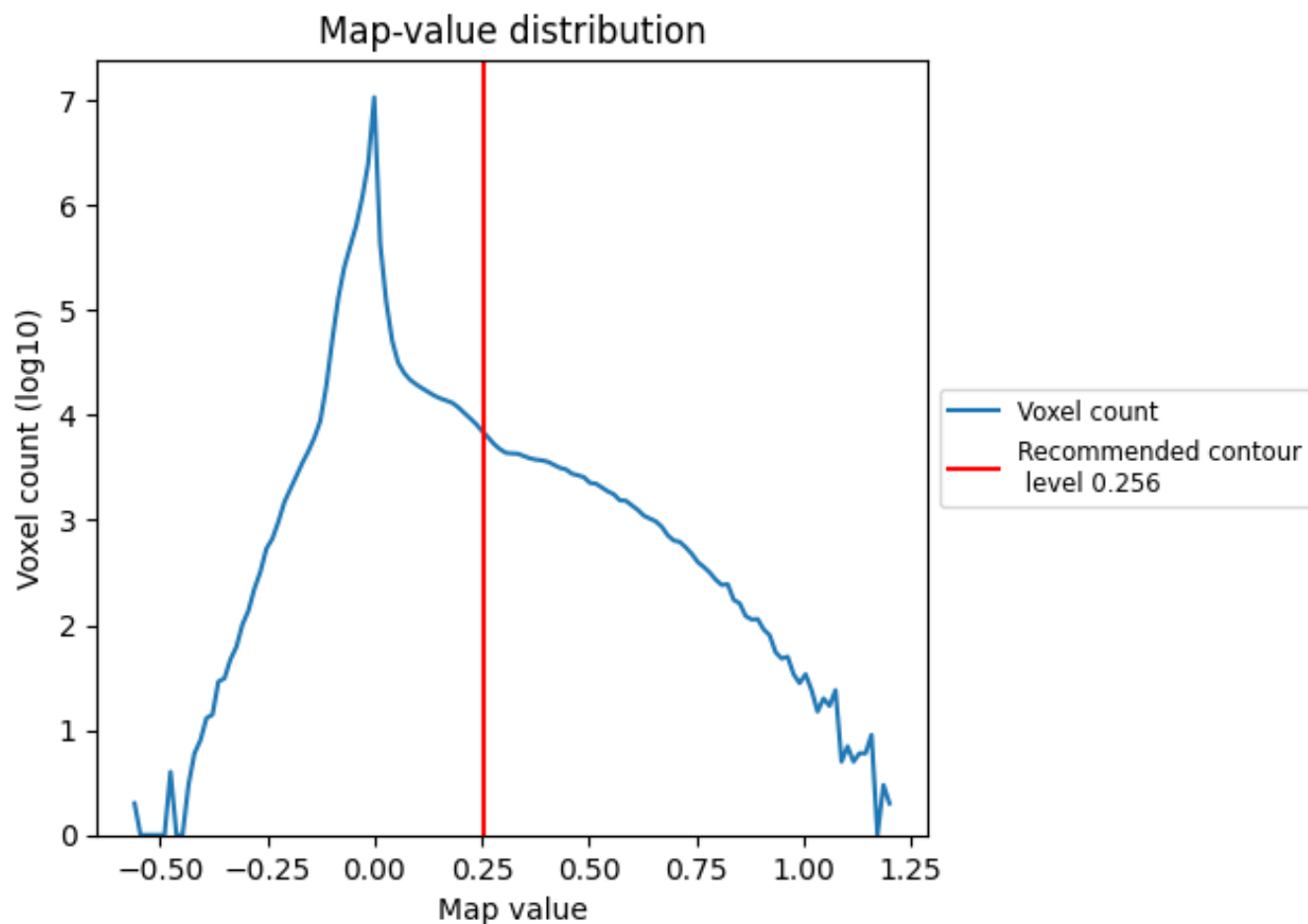


Z

7 Map analysis [i](#)

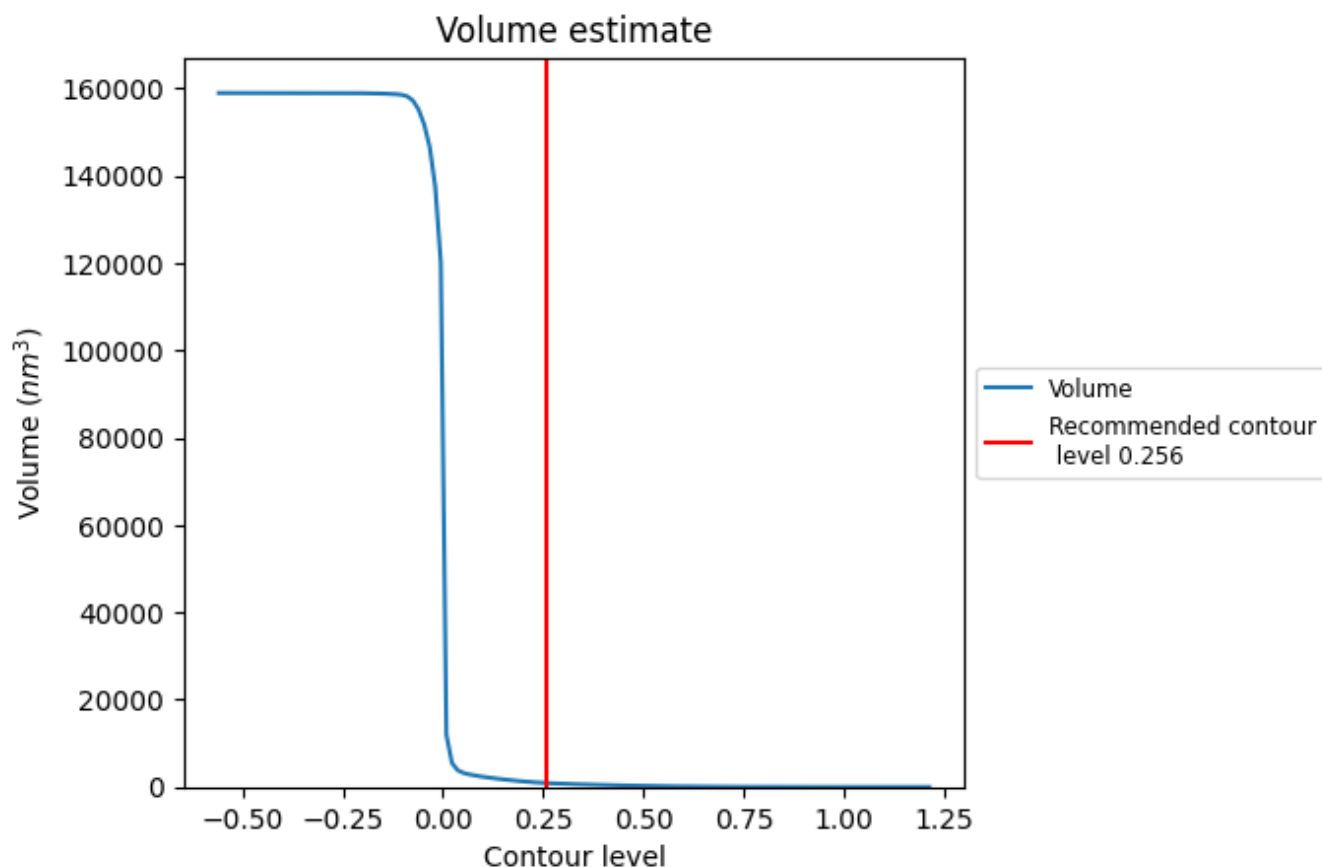
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

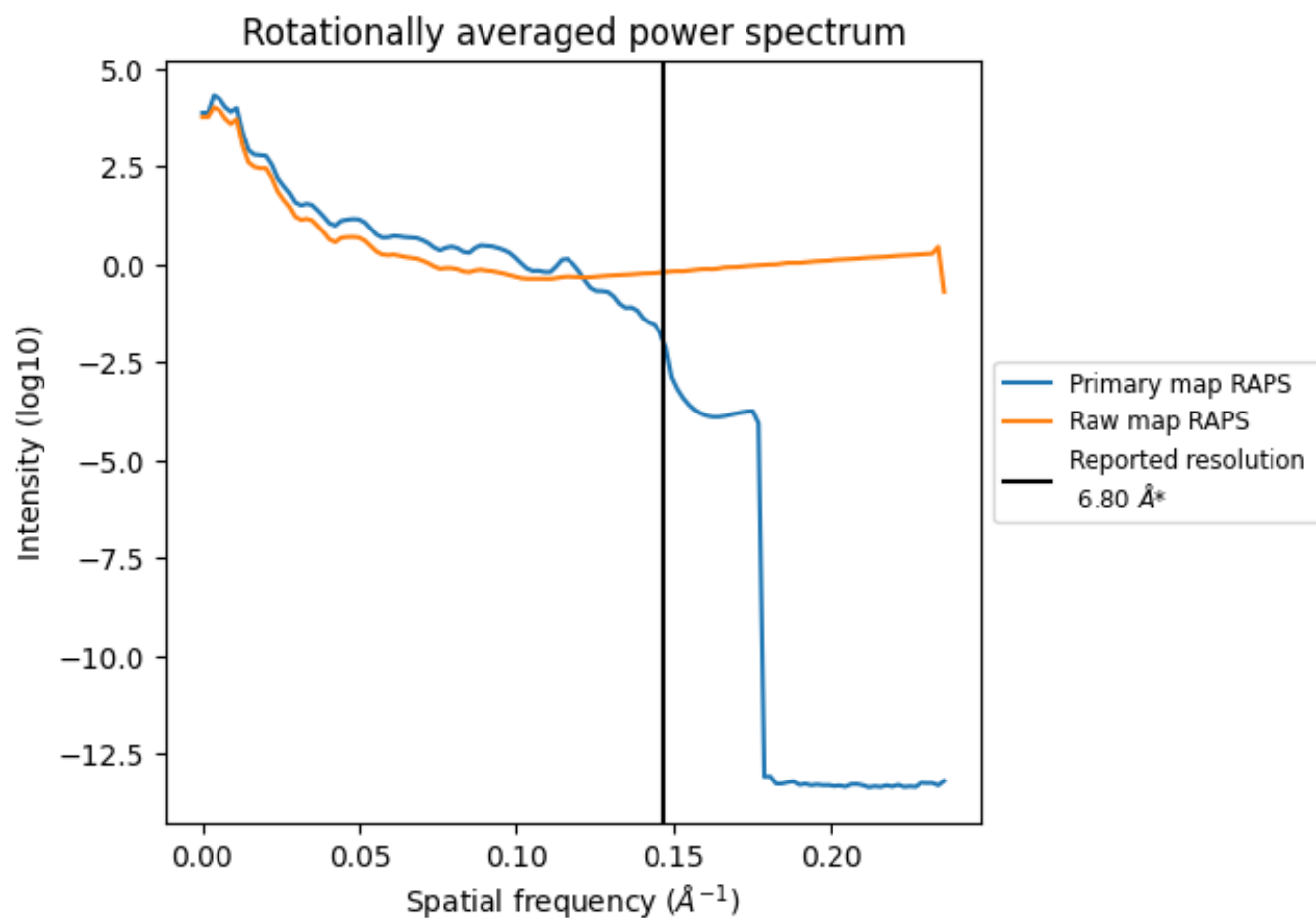
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 908 nm^3 ; this corresponds to an approximate mass of 820 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

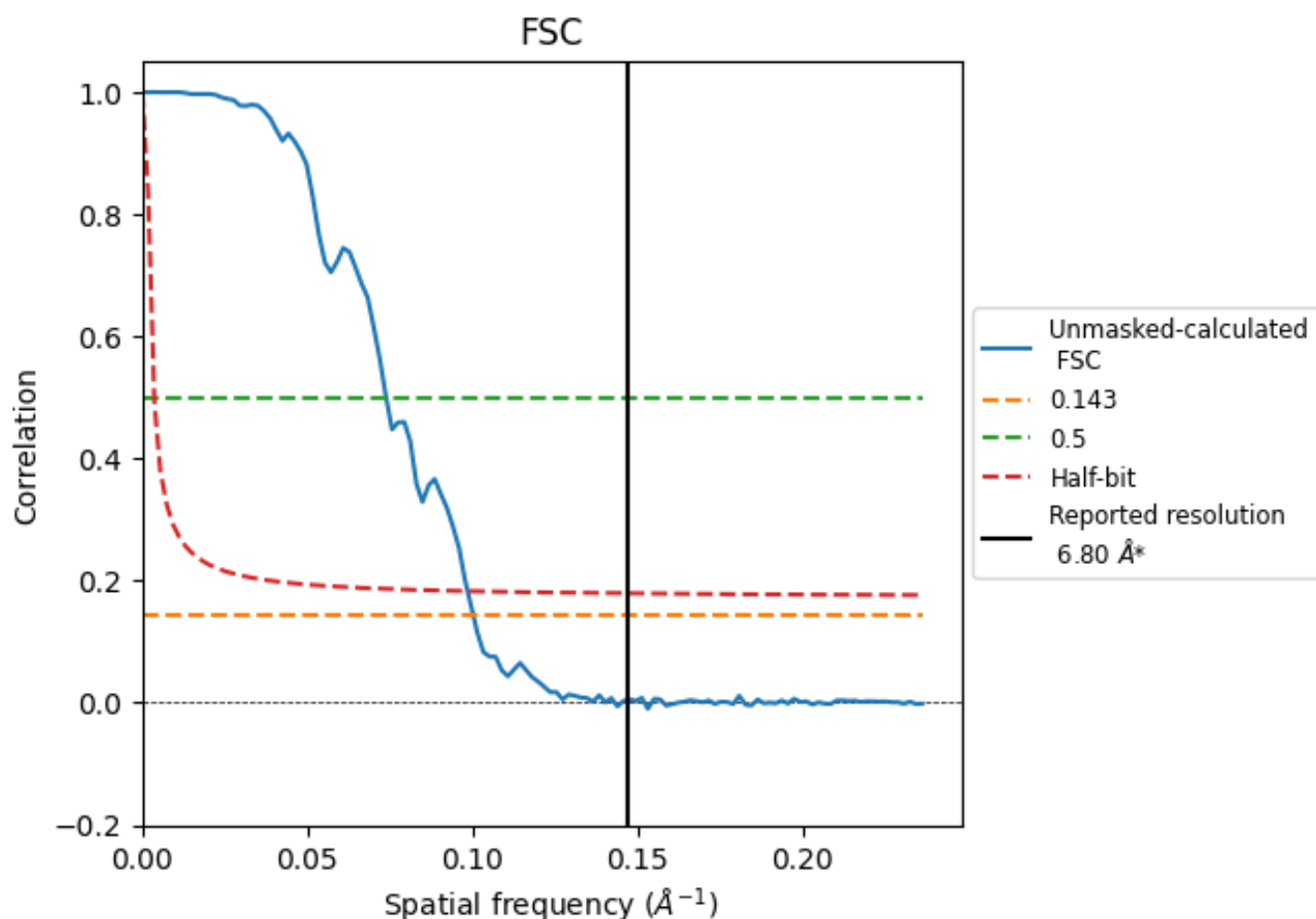


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

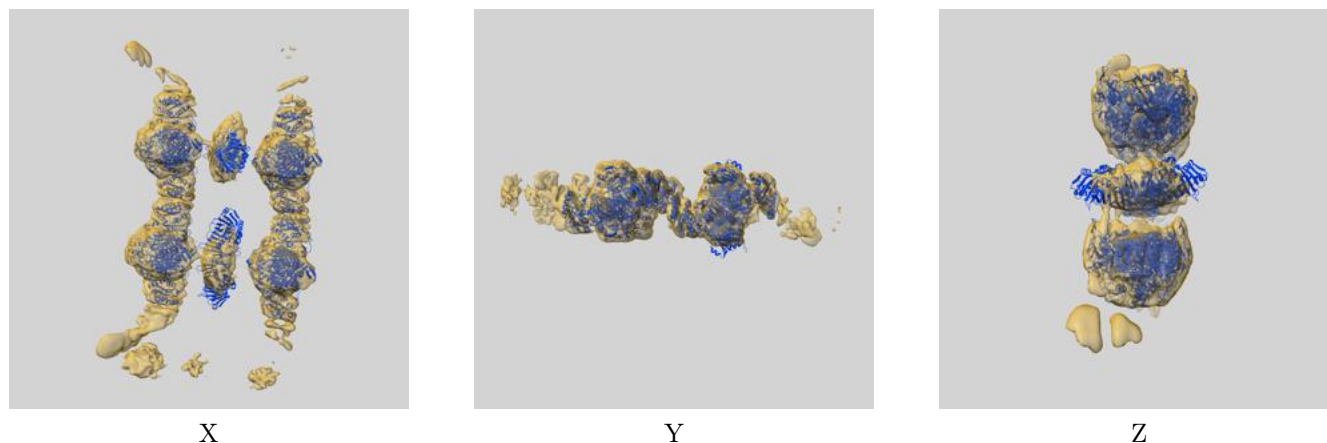
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.97	13.53	10.14

*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 9.97 differs from the reported value 6.8 by more than 10 %

9 Map-model fit [i](#)

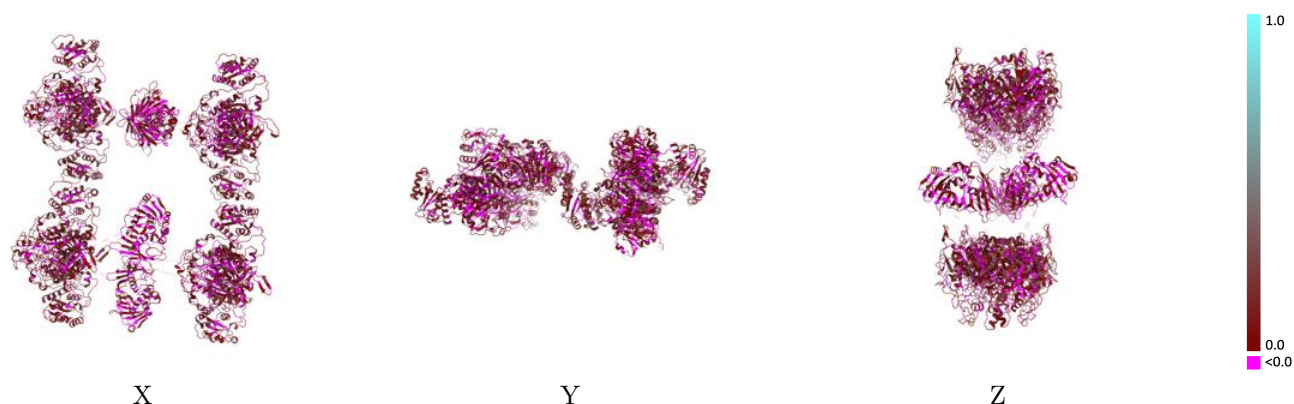
This section contains information regarding the fit between EMDB map EMD-14945 and PDB model 7ZSK. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



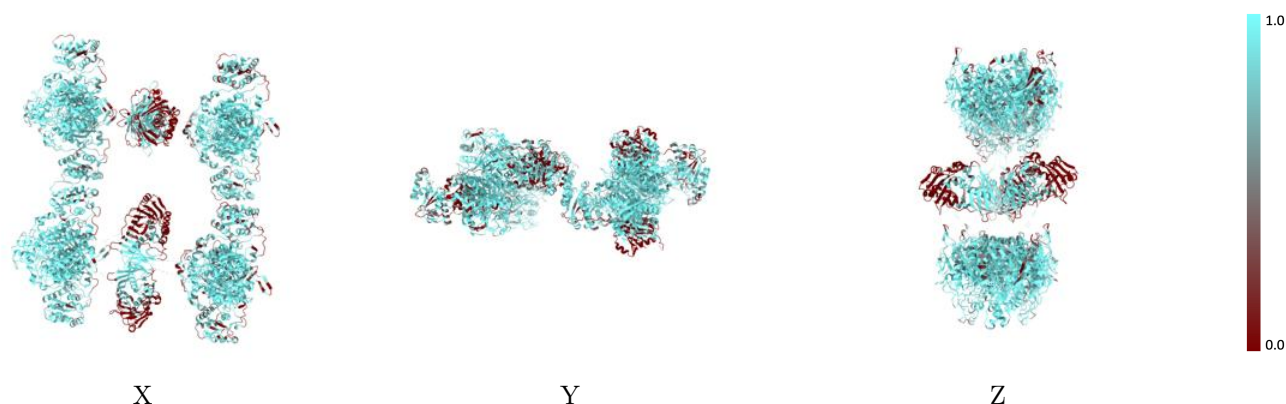
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



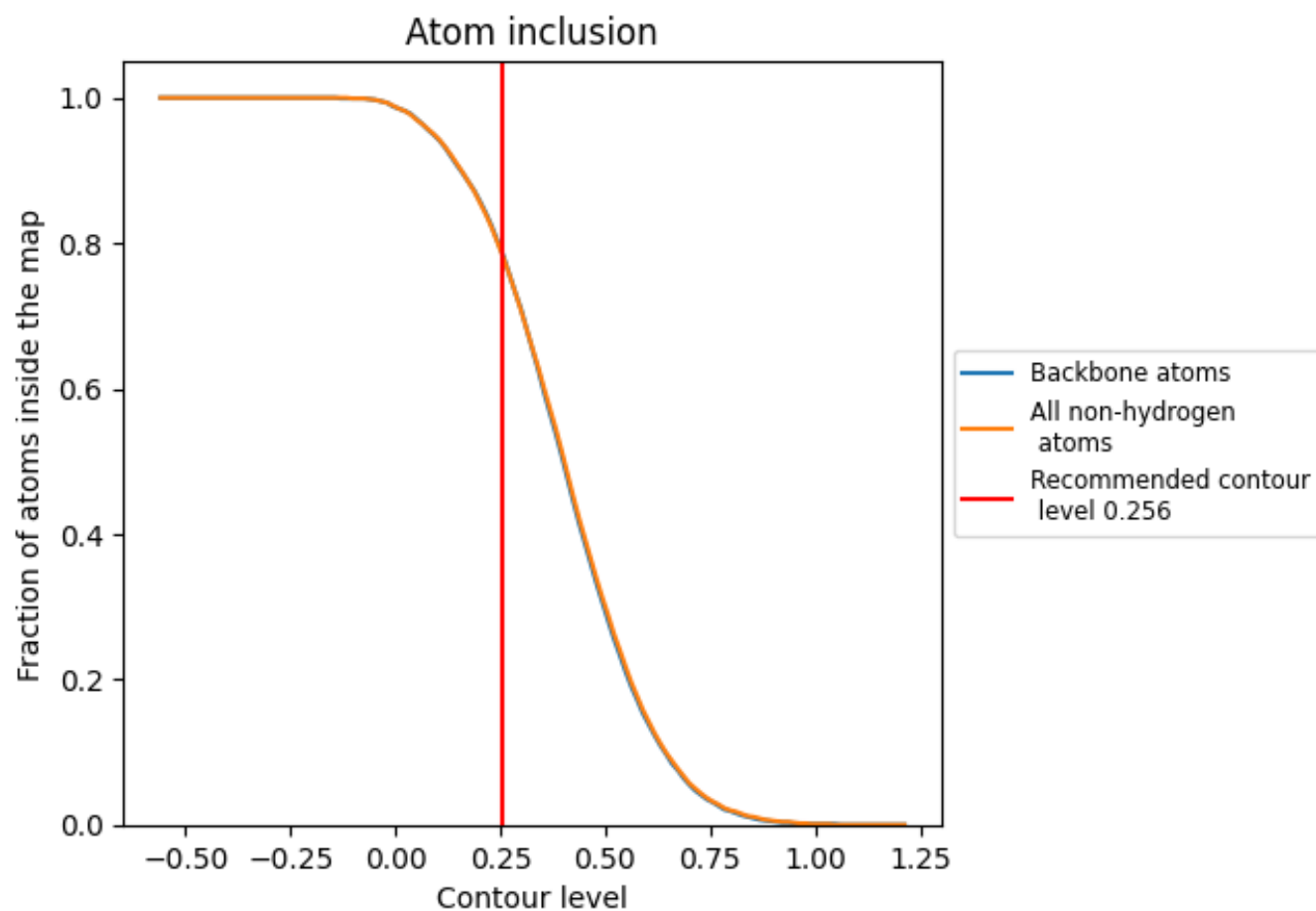
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.256).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.0850
A	0.7950	0.0880
B	0.7820	0.0840
C	0.7640	0.0860
D	0.7830	0.0830

