



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:40 PM UTC

PDB ID : 9B8L / pdb_00009b8l
EMDB ID : EMD-44349
Title : Cryo-EM structure of human dysferlin dimer
Authors : Huang, H.L.; Heissler, S.M.; Chinthalapudi, K.
Deposited on : 2024-03-30
Resolution : 4.65 Å(reported)
Based on initial model : .

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

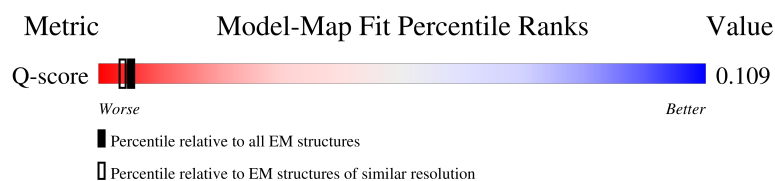
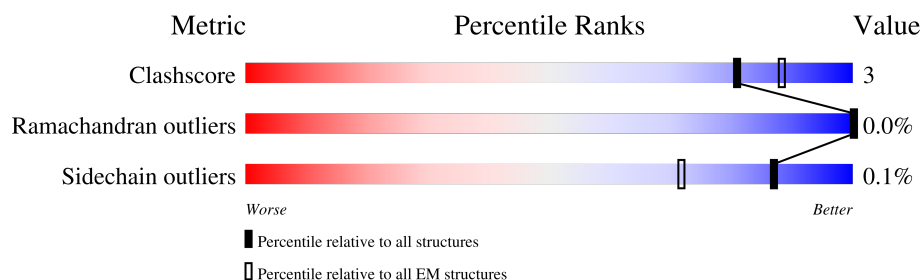
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.65 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	2043 (4.15 - 5.15)

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	2080	
1	B	2080	

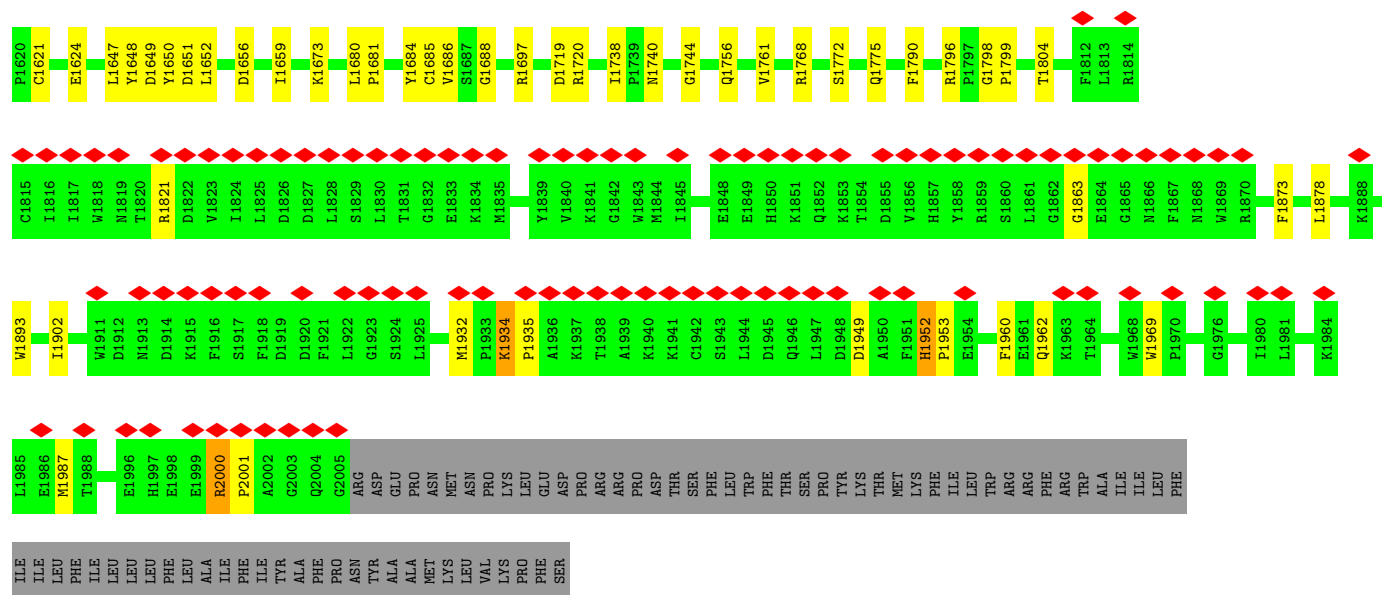
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28456 atoms, of which 0 are hydrogens and 0 are deuteriums.

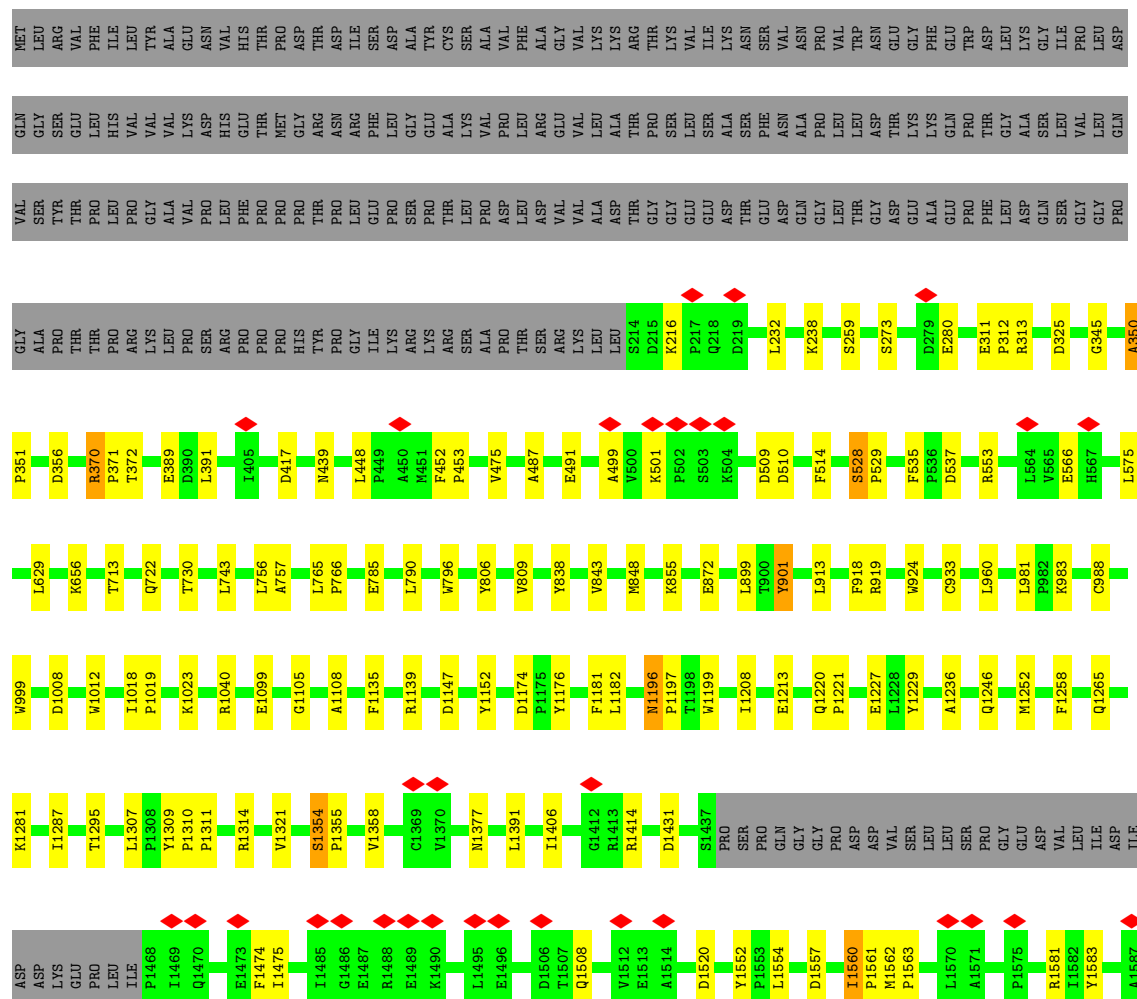
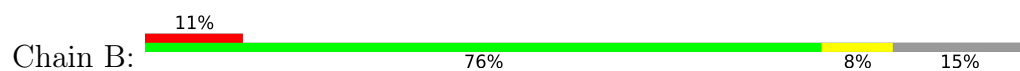
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dysferlin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1762	Total	C	N	O	S	0	0
			14228	9084	2426	2646	72		
1	B	1762	Total	C	N	O	S	0	0
			14228	9084	2426	2646	72		



• Molecule 1: Dysferlin



LEU	VAL	LYS	PRO	PHE	SER	LEU	GLU	ASP	PRO	ARG	PRO	ASP	THR	SER	PHE	LEU	TRP	PHE	THR	SER	PRO	TYR	LYS	THR	MET	LYS	PHE	ILE	LEU	TRP	ARG	PHE	ARG	TRP	ALA	ILE	ILE	PHE	LEU	LEU	PHE	LEU	ALA	ILE	ILE	PHE	LEU	LEU	PHE	ALA	ILE	ILE	PHE	ILE	TYR	ALA	PHE	PRO	PRO	ASN	TYR	ALA	ALA	ALA	MET	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
							P1953	E1954	W1955	F1956	P1957	S1958	L1959	F1960	E1961	Q1962	K1963	T1964	V1965	K1966	G1967	W1968	W1969		V1972	A1973	E1974	E1975	P1976	E1977	K1978	K1979	I1980	L1981	A1982	G1983	K1984	L1985	E1986	M1987	T1988	L1989	E1990	I1991	V1992		S1995	E1996	H1997	E1998	E1999	R2000	P2001	A2002	G2003	Q2004	G2005	ARG	ASP	GLU	PRO	ASN	MET	ASN	PRO	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
							K1888	K1889	D1890	A1891	F1892	W1893	R1894	L1895	D1896	K1897	E1898	E1899	S1900	K1901	I1902	P1903	A1904	R1905		I1910	W1911	D1912	M1913	D1914	K1915	F1916	S1917	F1918	D1919	D1920		S1924	L1925	Q1926	L1927	D1928	L1929	M1930	R1931	M1932	P1933	K1934	P1935	A1936	K1937	T1938	A1939	K1940	K1941	C1942	S1943	L1944	D1945	Q1946	L1947	D1948	D1949	A1950	F1951	H1952																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
							V1823	I1824	L1825	D1826	L1827	L1828	S1829	L1830	T1831	G1832	E1833	K1834	M1835	S1836	D1837	I1838	Y1839	V1840	K1841		G1842	W1843	M1844	I1845	G1846	F1847	E1848	E1849	H1850	K1851	Q1852	K1853	T1854	D1855	V1856	H1857	Y1858	R1859	S1860	L1861	G1862	G1863	E1864	G1865	M1866	F1867	N1868	W1869	R1870	F1871	I1872	F1873	P1874	D1875	F1876	Y1877	L1878		T1885	I1886	A1887																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
							D1719	R1720	V1721	M1722	D1725	K1726	E1727		E1731		A1735		P1739	N1740		G1744	P1745	V1746		V1761		R1768		S1772	Q1775	P1776	D1777	I1778		M1785		D1788	L1789	F1790		R1796	P1797	G1798	P1799			T1804		R1807	A1808	R1809	R1810	F1811	F1812	L1813	R1814	C1815	I1816	I1817	W1818	N1819	T1820	R1821	D1822																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74427	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.269	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	456.192, 456.192, 456.192	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.891, 0.891, 0.891	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	0.63	0/14598	1.02	214/19794 (1.1%)
1	B	0.63	0/14598	1.01	198/19794 (1.0%)
All	All	0.63	0/29196	1.02	412/39588 (1.0%)

There are no bond length outliers.

All (412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1310	PRO	CA-C-N	9.88	126.77	119.66
1	B	1310	PRO	C-N-CA	9.88	126.77	119.66
1	B	1562	MET	CA-C-N	9.69	126.73	119.66
1	B	1562	MET	C-N-CA	9.69	126.73	119.66
1	B	1309	TYR	CA-C-N	8.93	126.09	119.66
1	B	1309	TYR	C-N-CA	8.93	126.09	119.66
1	B	1220	GLN	CA-C-N	8.55	125.82	119.66
1	B	1220	GLN	C-N-CA	8.55	125.82	119.66
1	A	1377	ASN	CA-C-N	8.52	128.17	119.82
1	A	1377	ASN	C-N-CA	8.52	128.17	119.82
1	A	1932	MET	CA-C-N	8.33	128.26	119.85
1	A	1932	MET	C-N-CA	8.33	128.26	119.85
1	A	722	GLN	CA-C-N	7.97	127.92	120.03
1	A	722	GLN	C-N-CA	7.97	127.92	120.03
1	B	1799	PRO	CA-C-N	7.89	127.84	120.03
1	B	1799	PRO	C-N-CA	7.89	127.84	120.03
1	A	1563	PRO	CA-C-N	7.78	127.73	120.03
1	A	1563	PRO	C-N-CA	7.78	127.73	120.03
1	B	1563	PRO	CA-C-N	7.77	128.22	120.52
1	B	1563	PRO	C-N-CA	7.77	128.22	120.52
1	A	1799	PRO	CA-C-N	7.75	127.67	119.85
1	A	1799	PRO	C-N-CA	7.75	127.67	119.85
1	A	1744	GLY	CA-C-N	7.73	127.79	119.90
1	A	1744	GLY	C-N-CA	7.73	127.79	119.90
1	A	448	LEU	CA-C-N	7.72	127.67	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	LEU	C-N-CA	7.72	127.67	120.03
1	A	1221	PRO	CA-C-N	7.71	127.66	120.03
1	A	1221	PRO	C-N-CA	7.71	127.66	120.03
1	B	1246	GLN	CA-C-N	7.71	127.86	120.31
1	B	1246	GLN	C-N-CA	7.71	127.86	120.31
1	A	1246	GLN	CA-C-N	7.68	127.69	119.78
1	A	1246	GLN	C-N-CA	7.68	127.69	119.78
1	B	1377	ASN	CA-C-N	7.65	127.36	119.56
1	B	1377	ASN	C-N-CA	7.65	127.36	119.56
1	B	1688	GLY	CA-C-N	7.61	127.24	119.56
1	B	1688	GLY	C-N-CA	7.61	127.24	119.56
1	B	1594	ASP	CA-C-N	7.59	127.26	119.82
1	B	1594	ASP	C-N-CA	7.59	127.26	119.82
1	A	487	ALA	CA-C-N	7.59	127.22	119.56
1	A	487	ALA	C-N-CA	7.59	127.22	119.56
1	B	1744	GLY	CA-C-N	7.58	127.56	119.76
1	B	1744	GLY	C-N-CA	7.58	127.56	119.76
1	B	1311	PRO	CA-C-N	7.56	127.51	120.03
1	B	1311	PRO	C-N-CA	7.56	127.51	120.03
1	B	1552	TYR	CA-C-N	7.55	127.48	119.85
1	B	1552	TYR	C-N-CA	7.55	127.48	119.85
1	A	933	CYS	CA-C-N	7.54	127.49	120.03
1	A	933	CYS	C-N-CA	7.54	127.49	120.03
1	B	1768	ARG	CA-C-N	7.54	127.46	119.85
1	B	1768	ARG	C-N-CA	7.54	127.46	119.85
1	B	1932	MET	CA-C-N	7.53	127.48	120.03
1	B	1932	MET	C-N-CA	7.53	127.48	120.03
1	A	1775	GLN	CA-C-N	7.52	127.23	119.56
1	A	1775	GLN	C-N-CA	7.52	127.23	119.56
1	A	232	LEU	CA-C-N	7.50	127.42	119.85
1	A	232	LEU	C-N-CA	7.50	127.42	119.85
1	B	1798	GLY	CA-C-N	7.49	128.10	120.38
1	B	1798	GLY	C-N-CA	7.49	128.10	120.38
1	B	1600	ASP	CA-C-N	7.48	127.41	119.85
1	B	1600	ASP	C-N-CA	7.48	127.41	119.85
1	A	1196	ASN	CA-C-N	7.46	127.22	119.76
1	A	1196	ASN	C-N-CA	7.46	127.22	119.76
1	A	238	LYS	CA-C-N	7.46	127.38	119.85
1	A	238	LYS	C-N-CA	7.46	127.38	119.85
1	A	350	ALA	CA-C-N	7.45	127.62	119.87
1	A	350	ALA	C-N-CA	7.45	127.62	119.87
1	A	1761	VAL	CA-C-N	7.40	127.32	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1761	VAL	C-N-CA	7.40	127.32	120.21
1	B	1680	LEU	CA-C-N	7.38	127.54	120.31
1	B	1680	LEU	C-N-CA	7.38	127.54	120.31
1	A	1552	TYR	CA-C-N	7.38	127.30	119.85
1	A	1552	TYR	C-N-CA	7.38	127.30	119.85
1	A	1220	GLN	CA-C-N	7.37	127.97	120.38
1	A	1220	GLN	C-N-CA	7.37	127.97	120.38
1	A	1391	LEU	CA-C-N	7.34	127.34	119.78
1	A	1391	LEU	C-N-CA	7.34	127.34	119.78
1	B	1878	LEU	CA-C-N	7.33	126.97	119.56
1	B	1878	LEU	C-N-CA	7.33	126.97	119.56
1	A	1624	GLU	CA-C-N	7.32	127.24	119.85
1	A	1624	GLU	C-N-CA	7.32	127.24	119.85
1	B	238	LYS	CA-C-N	7.31	127.07	119.76
1	B	238	LYS	C-N-CA	7.31	127.07	119.76
1	A	1594	ASP	CA-C-N	7.30	127.01	119.56
1	A	1594	ASP	C-N-CA	7.30	127.01	119.56
1	B	1221	PRO	CA-C-N	7.29	127.21	119.85
1	B	1221	PRO	C-N-CA	7.29	127.21	119.85
1	B	1591	GLN	CA-C-N	7.28	127.26	119.76
1	B	1591	GLN	C-N-CA	7.28	127.26	119.76
1	A	391	LEU	CA-C-N	7.28	127.24	120.03
1	A	391	LEU	C-N-CA	7.28	127.24	120.03
1	B	575	LEU	CA-C-N	7.26	127.22	120.03
1	B	575	LEU	C-N-CA	7.26	127.22	120.03
1	A	417	ASP	CA-C-N	7.24	127.20	120.03
1	A	417	ASP	C-N-CA	7.24	127.20	120.03
1	A	1969	TRP	CA-C-N	7.23	127.15	119.85
1	A	1969	TRP	C-N-CA	7.23	127.15	119.85
1	A	1934	LYS	CA-C-N	7.22	127.21	119.78
1	A	1934	LYS	C-N-CA	7.22	127.21	119.78
1	A	439	ASN	CA-C-N	7.21	127.19	119.76
1	A	439	ASN	C-N-CA	7.21	127.19	119.76
1	A	1414	ARG	CA-C-N	7.21	127.17	120.03
1	A	1414	ARG	C-N-CA	7.21	127.17	120.03
1	A	656	LYS	CA-C-N	7.19	127.23	119.90
1	A	656	LYS	C-N-CA	7.19	127.23	119.90
1	B	356	ASP	CA-C-N	7.19	127.35	119.87
1	B	356	ASP	C-N-CA	7.19	127.35	119.87
1	B	1952	HIS	CA-C-N	7.19	126.82	119.56
1	B	1952	HIS	C-N-CA	7.19	126.82	119.56
1	B	1804	THR	CA-C-N	7.18	127.10	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1804	THR	C-N-CA	7.18	127.10	119.85
1	B	232	LEU	CA-C-N	7.18	127.10	119.85
1	B	232	LEU	C-N-CA	7.18	127.10	119.85
1	A	1768	ARG	CA-C-N	7.17	126.94	119.76
1	A	1768	ARG	C-N-CA	7.17	126.94	119.76
1	B	391	LEU	CA-C-N	7.17	127.13	120.03
1	B	391	LEU	C-N-CA	7.17	127.13	120.03
1	B	1775	GLN	CA-C-N	7.17	126.80	119.56
1	B	1775	GLN	C-N-CA	7.17	126.80	119.56
1	B	809	VAL	CA-C-N	7.17	127.14	119.76
1	B	809	VAL	C-N-CA	7.17	127.14	119.76
1	B	501	LYS	CA-C-N	7.16	126.79	119.56
1	B	501	LYS	C-N-CA	7.16	126.79	119.56
1	B	1307	LEU	CA-C-N	7.13	127.09	120.03
1	B	1307	LEU	C-N-CA	7.13	127.09	120.03
1	A	575	LEU	CA-C-N	7.13	127.09	120.03
1	A	575	LEU	C-N-CA	7.13	127.09	120.03
1	A	1619	ILE	CA-C-N	7.11	127.08	119.76
1	A	1619	ILE	C-N-CA	7.11	127.08	119.76
1	B	1258	PHE	CA-C-N	7.11	127.03	119.85
1	B	1258	PHE	C-N-CA	7.11	127.03	119.85
1	A	1688	GLY	CA-C-N	7.09	126.72	119.56
1	A	1688	GLY	C-N-CA	7.09	126.72	119.56
1	A	259	SER	CA-C-N	7.09	127.06	119.76
1	A	259	SER	C-N-CA	7.09	127.06	119.76
1	B	1414	ARG	CA-C-N	7.09	127.26	120.31
1	B	1414	ARG	C-N-CA	7.09	127.26	120.31
1	A	1680	LEU	CA-C-N	7.09	127.01	119.85
1	A	1680	LEU	C-N-CA	7.09	127.01	119.85
1	A	1740	ASN	CA-C-N	7.09	126.79	119.56
1	A	1740	ASN	C-N-CA	7.09	126.79	119.56
1	B	981	LEU	CA-C-N	7.07	127.06	119.78
1	B	981	LEU	C-N-CA	7.07	127.06	119.78
1	A	1258	PHE	CA-C-N	7.06	127.03	119.76
1	A	1258	PHE	C-N-CA	7.06	127.03	119.76
1	B	439	ASN	CA-C-N	7.05	126.81	119.76
1	B	439	ASN	C-N-CA	7.05	126.81	119.76
1	A	1798	GLY	CA-C-N	7.04	127.63	120.38
1	A	1798	GLY	C-N-CA	7.04	127.63	120.38
1	A	1431	ASP	CA-C-N	7.02	126.65	119.56
1	A	1431	ASP	C-N-CA	7.02	126.65	119.56
1	A	356	ASP	CA-C-N	7.01	127.17	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	C-N-CA	7.01	127.17	119.87
1	A	790	LEU	CA-C-N	7.01	126.97	120.03
1	A	790	LEU	C-N-CA	7.01	126.97	120.03
1	B	1560	ILE	CA-C-N	7.01	127.00	119.78
1	B	1560	ILE	C-N-CA	7.01	127.00	119.78
1	B	1391	LEU	CA-C-N	7.00	126.97	119.76
1	B	1391	LEU	C-N-CA	7.00	126.97	119.76
1	B	1252	MET	CA-C-N	7.00	127.42	119.93
1	B	1252	MET	C-N-CA	7.00	127.42	119.93
1	B	1431	ASP	CA-C-N	6.99	126.62	119.56
1	B	1431	ASP	C-N-CA	6.99	126.62	119.56
1	B	259	SER	CA-C-N	6.99	126.75	119.76
1	B	259	SER	C-N-CA	6.99	126.75	119.76
1	B	1790	PHE	CA-C-N	6.99	126.98	119.78
1	B	1790	PHE	C-N-CA	6.99	126.98	119.78
1	A	1174	ASP	CA-C-N	6.96	126.72	119.76
1	A	1174	ASP	C-N-CA	6.96	126.72	119.76
1	B	1761	VAL	CA-C-N	6.95	127.40	120.52
1	B	1761	VAL	C-N-CA	6.95	127.40	120.52
1	A	988	CYS	CA-C-N	6.93	126.89	120.03
1	A	988	CYS	C-N-CA	6.93	126.89	120.03
1	B	1213	GLU	CA-C-N	6.92	126.89	119.28
1	B	1213	GLU	C-N-CA	6.92	126.89	119.28
1	A	501	LYS	CA-C-N	6.90	126.53	119.56
1	A	501	LYS	C-N-CA	6.90	126.53	119.56
1	A	280	GLU	CA-C-N	6.90	127.35	120.52
1	A	280	GLU	C-N-CA	6.90	127.35	120.52
1	B	280	GLU	CA-C-N	6.89	127.06	120.31
1	B	280	GLU	C-N-CA	6.89	127.06	120.31
1	A	1019	PRO	CA-C-N	6.88	127.45	119.47
1	A	1019	PRO	C-N-CA	6.88	127.45	119.47
1	A	528	SER	CA-C-N	6.87	126.85	119.78
1	A	528	SER	C-N-CA	6.87	126.85	119.78
1	B	1196	ASN	CA-C-N	6.81	126.78	119.76
1	B	1196	ASN	C-N-CA	6.81	126.78	119.76
1	A	1878	LEU	CA-C-N	6.81	127.37	119.47
1	A	1878	LEU	C-N-CA	6.81	127.37	119.47
1	A	495	GLU	CA-C-N	6.79	126.71	119.85
1	A	495	GLU	C-N-CA	6.79	126.71	119.85
1	A	535	PHE	CA-C-N	6.77	126.80	119.90
1	A	535	PHE	C-N-CA	6.77	126.80	119.90
1	B	1281	LYS	CA-C-N	6.77	126.94	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1281	LYS	C-N-CA	6.77	126.94	120.31
1	A	1281	LYS	CA-C-N	6.76	126.72	120.03
1	A	1281	LYS	C-N-CA	6.76	126.72	120.03
1	B	417	ASP	CA-C-N	6.75	126.67	119.85
1	B	417	ASP	C-N-CA	6.75	126.67	119.85
1	B	1713	ALA	CA-C-N	6.75	126.67	119.85
1	B	1713	ALA	C-N-CA	6.75	126.67	119.85
1	B	1557	ASP	CA-C-N	6.74	126.88	119.87
1	B	1557	ASP	C-N-CA	6.74	126.88	119.87
1	A	537	ASP	CA-C-N	6.74	126.88	119.87
1	A	537	ASP	C-N-CA	6.74	126.88	119.87
1	A	1354	SER	CA-C-N	6.74	127.28	120.14
1	A	1354	SER	C-N-CA	6.74	127.28	120.14
1	A	2000	ARG	CA-C-N	6.74	126.43	119.56
1	A	2000	ARG	C-N-CA	6.74	126.43	119.56
1	A	1600	ASP	CA-C-N	6.73	126.49	119.76
1	A	1600	ASP	C-N-CA	6.73	126.49	119.76
1	B	487	ALA	CA-C-N	6.73	126.36	119.56
1	B	487	ALA	C-N-CA	6.73	126.36	119.56
1	A	809	VAL	CA-C-N	6.72	126.90	120.31
1	A	809	VAL	C-N-CA	6.72	126.90	120.31
1	B	843	VAL	CA-C-N	6.71	126.40	119.56
1	B	843	VAL	C-N-CA	6.71	126.40	119.56
1	B	216	LYS	CA-C-N	6.71	126.67	119.76
1	B	216	LYS	C-N-CA	6.71	126.67	119.76
1	B	345	GLY	CA-C-N	6.68	126.37	119.56
1	B	345	GLY	C-N-CA	6.68	126.37	119.56
1	A	1557	ASP	CA-C-N	6.67	126.81	119.87
1	A	1557	ASP	C-N-CA	6.67	126.81	119.87
1	B	1287	ILE	CA-C-N	6.66	126.69	119.90
1	B	1287	ILE	C-N-CA	6.66	126.69	119.90
1	A	1311	PRO	CA-C-N	6.66	126.64	119.78
1	A	1311	PRO	C-N-CA	6.66	126.64	119.78
1	B	1619	ILE	CA-C-N	6.65	126.61	119.76
1	B	1619	ILE	C-N-CA	6.65	126.61	119.76
1	A	1287	ILE	CA-C-N	6.63	126.59	119.76
1	A	1287	ILE	C-N-CA	6.63	126.59	119.76
1	B	1174	ASP	CA-C-N	6.63	126.39	119.76
1	B	1174	ASP	C-N-CA	6.63	126.39	119.76
1	A	1252	MET	CA-C-N	6.62	126.38	119.76
1	A	1252	MET	C-N-CA	6.62	126.38	119.76
1	A	1018	ILE	CA-C-N	6.61	127.19	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1018	ILE	C-N-CA	6.61	127.19	120.38
1	A	1772	SER	CA-C-N	6.60	126.23	119.56
1	A	1772	SER	C-N-CA	6.60	126.23	119.56
1	B	350	ALA	CA-C-N	6.60	127.17	120.04
1	B	350	ALA	C-N-CA	6.60	127.17	120.04
1	A	1804	THR	CA-C-N	6.60	126.57	119.78
1	A	1804	THR	C-N-CA	6.60	126.57	119.78
1	B	1018	ILE	CA-C-N	6.59	127.17	120.38
1	B	1018	ILE	C-N-CA	6.59	127.17	120.38
1	A	1591	GLN	CA-C-N	6.57	126.53	119.76
1	A	1591	GLN	C-N-CA	6.57	126.53	119.76
1	B	730	THR	CA-C-N	6.57	126.26	119.56
1	B	730	THR	C-N-CA	6.57	126.26	119.56
1	A	1902	ILE	CA-C-N	6.56	126.54	119.78
1	A	1902	ILE	C-N-CA	6.56	126.54	119.78
1	A	1790	PHE	CA-C-N	6.55	126.51	119.76
1	A	1790	PHE	C-N-CA	6.55	126.51	119.76
1	B	901	TYR	CA-C-N	6.54	126.49	119.76
1	B	901	TYR	C-N-CA	6.54	126.49	119.76
1	B	325	ASP	CA-C-N	6.52	127.03	119.47
1	B	325	ASP	C-N-CA	6.52	127.03	119.47
1	B	535	PHE	CA-C-N	6.51	126.54	119.90
1	B	535	PHE	C-N-CA	6.51	126.54	119.90
1	B	1934	LYS	CA-C-N	6.46	126.42	119.76
1	B	1934	LYS	C-N-CA	6.46	126.42	119.76
1	B	528	SER	CA-C-N	6.46	126.43	119.78
1	B	528	SER	C-N-CA	6.46	126.43	119.78
1	B	1796	ARG	CA-C-N	6.45	126.42	120.03
1	B	1796	ARG	C-N-CA	6.45	126.42	120.03
1	A	981	LEU	CA-C-N	6.45	126.47	119.89
1	A	981	LEU	C-N-CA	6.45	126.47	119.89
1	A	1560	ILE	CA-C-N	6.45	126.36	119.85
1	A	1560	ILE	C-N-CA	6.45	126.36	119.85
1	B	790	LEU	CA-C-N	6.44	126.41	119.78
1	B	790	LEU	C-N-CA	6.44	126.41	119.78
1	A	843	VAL	CA-C-N	6.43	126.01	119.19
1	A	843	VAL	C-N-CA	6.43	126.01	119.19
1	B	656	LYS	CA-C-N	6.43	126.46	119.90
1	B	656	LYS	C-N-CA	6.43	126.46	119.90
1	B	988	CYS	CA-C-N	6.42	126.39	120.03
1	B	988	CYS	C-N-CA	6.42	126.39	120.03
1	A	325	ASP	CA-C-N	6.42	126.92	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	C-N-CA	6.42	126.92	119.47
1	B	1624	GLU	CA-C-N	6.41	126.17	119.76
1	B	1624	GLU	C-N-CA	6.41	126.17	119.76
1	A	1562	MET	CA-C-N	6.39	126.96	120.38
1	A	1562	MET	C-N-CA	6.39	126.96	120.38
1	B	933	CYS	CA-C-N	6.38	126.35	119.78
1	B	933	CYS	C-N-CA	6.38	126.35	119.78
1	A	1697	ARG	CA-C-N	6.36	126.28	119.28
1	A	1697	ARG	C-N-CA	6.36	126.28	119.28
1	B	913	LEU	CA-C-N	6.35	126.31	119.76
1	B	913	LEU	C-N-CA	6.35	126.31	119.76
1	B	1354	SER	CA-C-N	6.34	126.29	119.76
1	B	1354	SER	C-N-CA	6.34	126.29	119.76
1	B	629	LEU	CA-C-N	6.33	126.24	119.28
1	B	629	LEU	C-N-CA	6.33	126.24	119.28
1	A	1028	VAL	CA-C-N	6.32	126.01	119.56
1	A	1028	VAL	C-N-CA	6.32	126.01	119.56
1	B	1740	ASN	CA-C-N	6.32	126.44	119.87
1	B	1740	ASN	C-N-CA	6.32	126.44	119.87
1	A	1309	TYR	CA-C-N	6.30	126.87	120.38
1	A	1309	TYR	C-N-CA	6.30	126.87	120.38
1	A	730	THR	CA-C-N	6.30	125.99	119.56
1	A	730	THR	C-N-CA	6.30	125.99	119.56
1	B	722	GLN	CA-C-N	6.30	126.22	119.85
1	B	722	GLN	C-N-CA	6.30	126.22	119.85
1	B	1554	LEU	CA-C-N	6.30	126.25	119.76
1	B	1554	LEU	C-N-CA	6.30	126.25	119.76
1	A	1326	LYS	CA-C-N	6.29	126.24	119.76
1	A	1326	LYS	C-N-CA	6.29	126.24	119.76
1	A	345	GLY	CA-C-N	6.27	126.17	119.28
1	A	345	GLY	C-N-CA	6.27	126.17	119.28
1	B	1265	GLN	CA-C-N	6.26	126.63	119.93
1	B	1265	GLN	C-N-CA	6.26	126.63	119.93
1	A	785	GLU	CA-C-N	6.25	125.87	119.56
1	A	785	GLU	C-N-CA	6.25	125.87	119.56
1	B	2000	ARG	CA-C-N	6.24	125.92	119.56
1	B	2000	ARG	C-N-CA	6.24	125.92	119.56
1	B	1772	SER	CA-C-N	6.23	125.85	119.56
1	B	1772	SER	C-N-CA	6.23	125.85	119.56
1	B	785	GLU	CA-C-N	6.22	125.84	119.56
1	B	785	GLU	C-N-CA	6.22	125.84	119.56
1	A	1307	LEU	CA-C-N	6.22	126.24	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1307	LEU	C-N-CA	6.22	126.24	119.90
1	A	515	LEU	CA-C-N	6.19	126.52	119.83
1	A	515	LEU	C-N-CA	6.19	126.52	119.83
1	B	1902	ILE	CA-C-N	6.15	126.10	119.76
1	B	1902	ILE	C-N-CA	6.15	126.10	119.76
1	A	1796	ARG	CA-C-N	6.14	126.15	119.89
1	A	1796	ARG	C-N-CA	6.14	126.15	119.89
1	B	1099	GLU	CA-C-N	6.14	125.90	119.76
1	B	1099	GLU	C-N-CA	6.14	125.90	119.76
1	B	311	GLU	CA-C-N	6.13	126.16	119.90
1	B	311	GLU	C-N-CA	6.13	126.16	119.90
1	A	311	GLU	CA-C-N	6.13	126.16	119.90
1	A	311	GLU	C-N-CA	6.13	126.16	119.90
1	B	448	LEU	CA-C-N	6.11	125.87	119.76
1	B	448	LEU	C-N-CA	6.11	125.87	119.76
1	A	1105	GLY	CA-C-N	6.10	127.46	119.84
1	A	1105	GLY	C-N-CA	6.10	127.46	119.84
1	B	1321	VAL	CA-C-N	6.07	126.02	119.76
1	B	1321	VAL	C-N-CA	6.07	126.02	119.76
1	B	537	ASP	CA-C-N	6.02	126.13	119.87
1	B	537	ASP	C-N-CA	6.02	126.13	119.87
1	A	1265	GLN	CA-C-N	5.99	125.93	119.76
1	A	1265	GLN	C-N-CA	5.99	125.93	119.76
1	A	370	ARG	CA-C-N	5.97	125.88	119.85
1	A	370	ARG	C-N-CA	5.97	125.88	119.85
1	A	1399	PRO	CA-C-N	5.93	125.84	119.85
1	A	1399	PRO	C-N-CA	5.93	125.84	119.85
1	A	1554	LEU	CA-C-N	5.91	125.87	119.78
1	A	1554	LEU	C-N-CA	5.91	125.87	119.78
1	A	1139	ARG	CA-C-N	5.85	126.04	119.90
1	A	1139	ARG	C-N-CA	5.85	126.04	119.90
1	B	1105	GLY	CA-C-N	5.85	127.15	119.84
1	B	1105	GLY	C-N-CA	5.85	127.15	119.84
1	A	901	TYR	CA-C-N	5.84	125.86	119.90
1	A	901	TYR	C-N-CA	5.84	125.86	119.90
1	A	913	LEU	CA-C-N	5.83	125.77	119.76
1	A	913	LEU	C-N-CA	5.83	125.77	119.76
1	A	848	MET	CA-C-N	5.82	127.11	119.84
1	A	848	MET	C-N-CA	5.82	127.11	119.84
1	A	919	ARG	CA-C-N	5.82	126.11	119.83
1	A	919	ARG	C-N-CA	5.82	126.11	119.83
1	A	273	SER	CA-C-N	5.81	126.21	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	SER	C-N-CA	5.81	126.21	119.47
1	A	629	LEU	CA-C-N	5.80	125.93	119.32
1	A	629	LEU	C-N-CA	5.80	125.93	119.32
1	B	1969	TRP	CA-C-N	5.79	126.08	119.83
1	B	1969	TRP	C-N-CA	5.79	126.08	119.83
1	A	1023	LYS	CA-C-N	5.76	125.70	119.76
1	A	1023	LYS	C-N-CA	5.76	125.70	119.76
1	B	1019	PRO	CA-C-N	5.75	127.03	119.84
1	B	1019	PRO	C-N-CA	5.75	127.03	119.84
1	B	1139	ARG	CA-C-N	5.75	125.94	119.90
1	B	1139	ARG	C-N-CA	5.75	125.94	119.90
1	A	1310	PRO	CA-C-N	5.75	126.30	120.38
1	A	1310	PRO	C-N-CA	5.75	126.30	120.38
1	A	960	LEU	CA-C-N	5.74	125.42	119.56
1	A	960	LEU	C-N-CA	5.74	125.42	119.56
1	A	1398	CYS	CA-C-N	5.74	126.30	120.38
1	A	1398	CYS	C-N-CA	5.74	126.30	120.38
1	B	919	ARG	CA-C-N	5.72	125.66	119.76
1	B	919	ARG	C-N-CA	5.72	125.66	119.76
1	A	216	LYS	CA-C-N	5.67	125.96	119.83
1	A	216	LYS	C-N-CA	5.67	125.96	119.83
1	A	1213	GLU	CA-C-N	5.67	126.05	119.47
1	A	1213	GLU	C-N-CA	5.67	126.05	119.47
1	A	1873	PHE	CA-C-N	5.67	126.92	119.84
1	A	1873	PHE	C-N-CA	5.67	126.92	119.84
1	A	1952	HIS	CA-C-N	5.66	127.74	120.89
1	A	1952	HIS	C-N-CA	5.66	127.74	120.89
1	B	273	SER	CA-C-N	5.66	126.03	119.47
1	B	273	SER	C-N-CA	5.66	126.03	119.47
1	B	370	ARG	CA-C-N	5.64	125.54	119.85
1	B	370	ARG	C-N-CA	5.64	125.54	119.85
1	A	1099	GLU	CA-C-N	5.63	125.54	119.85
1	A	1099	GLU	C-N-CA	5.63	125.54	119.85
1	A	1321	VAL	CA-C-N	5.62	125.63	119.90
1	A	1321	VAL	C-N-CA	5.62	125.63	119.90
1	B	1697	ARG	CA-C-N	5.59	125.95	119.47
1	B	1697	ARG	C-N-CA	5.59	125.95	119.47
1	B	960	LEU	CA-C-N	5.49	125.84	119.47
1	B	960	LEU	C-N-CA	5.49	125.84	119.47
1	A	838	TYR	CA-C-N	5.48	125.42	119.78
1	A	838	TYR	C-N-CA	5.48	125.42	119.78
1	A	519	GLY	CA-C-N	5.45	125.72	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	GLY	C-N-CA	5.45	125.72	119.83
1	A	1738	ILE	CA-C-N	5.22	125.22	119.90
1	A	1738	ILE	C-N-CA	5.22	125.22	119.90
1	B	848	MET	CA-C-N	5.19	126.33	119.84
1	B	848	MET	C-N-CA	5.19	126.33	119.84
1	B	1023	LYS	CA-C-N	5.17	125.42	119.83
1	B	1023	LYS	C-N-CA	5.17	125.42	119.83
1	B	838	TYR	CA-C-N	5.02	125.30	119.93
1	B	838	TYR	C-N-CA	5.02	125.30	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14228	0	13963	86	0
1	B	14228	0	13963	61	0
All	All	28456	0	27926	146	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 3.

All (146) 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:B:491:GLU:OE2	1:B:514:PHE:CD2	2.29	0.85
1:B:491:GLU:OE2	1:B:514:PHE:CE2	2.36	0.77
1:B:1520:ASP:OD2	1:B:1673:LYS:NZ	2.33	0.60
1:B:1942:CYS:HG	1:B:1968:TRP:CG	2.21	0.57
1:A:993:LYS:NZ	1:A:1049:ASP:OD1	2.38	0.57
1:A:2000:ARG:N	1:A:2001:PRO:CD	2.68	0.57
1:B:491:GLU:OE1	1:B:743:LEU:HD21	2.06	0.56
1:B:2000:ARG:N	1:B:2001:PRO:CD	2.68	0.56
1:A:509:ASP:OD1	1:A:510:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1520:ASP:OD2	1:A:1673:LYS:NZ	2.39	0.56
1:A:1600:ASP:OD1	1:A:1621:CYS:N	2.39	0.55
1:B:509:ASP:OD1	1:B:510:ASP:N	2.40	0.54
1:B:1897:LYS:NZ	1:B:1899:GLU:OE1	2.41	0.54
1:B:1508:GLN:OE1	1:B:1662:THR:OG1	2.26	0.54
1:A:813:GLN:N	1:A:813:GLN:OE1	2.41	0.54
1:A:1602:TYR:CD2	1:A:1650:TYR:HB2	2.43	0.53
1:B:1841:LYS:NZ	1:B:1912:ASP:OD1	2.37	0.53
1:B:1594:ASP:OD1	1:B:1594:ASP:C	2.53	0.52
1:A:608:ASP:OD2	1:A:1025:LYS:NZ	2.42	0.51
1:A:1952:HIS:N	1:A:1953:PRO:CD	2.73	0.51
1:A:665:TRP:CG	1:A:666:GLU:H	2.29	0.51
1:A:1016:ILE:O	1:A:1017:THR:C	2.54	0.51
1:B:370:ARG:HB3	1:B:371:PRO:CD	2.41	0.51
1:A:983:LYS:O	1:A:999:TRP:NE1	2.44	0.50
1:A:1602:TYR:CE2	1:A:1648:TYR:HB2	2.46	0.50
1:B:1594:ASP:HB2	1:B:1595:PRO:CD	2.40	0.50
1:A:1032:LYS:NZ	1:B:389:GLU:OE2	2.45	0.50
1:A:1012:TRP:CE3	1:A:1040:ARG:HG3	2.47	0.49
1:A:1338:ALA:N	1:A:1383:CYS:O	2.43	0.49
1:A:370:ARG:HB3	1:A:371:PRO:CD	2.43	0.49
1:B:1181:PHE:CG	1:B:1182:LEU:N	2.79	0.49
1:A:796:TRP:CD2	1:A:806:TYR:HB3	2.47	0.48
1:A:1960:PHE:CD2	1:A:1960:PHE:N	2.78	0.48
1:A:452:PHE:N	1:A:453:PRO:HD2	2.27	0.48
1:B:499:ALA:H	1:B:757:ALA:HB1	1.79	0.48
1:B:1199:TRP:O	1:B:1314:ARG:NH2	2.47	0.48
1:A:665:TRP:CG	1:A:666:GLU:N	2.81	0.47
1:B:1147:ASP:OD2	1:B:1295:THR:N	2.45	0.47
1:B:765:LEU:N	1:B:766:PRO:CD	2.77	0.47
1:B:1684:TYR:CD2	1:B:1684:TYR:C	2.92	0.47
1:A:658:VAL:N	1:A:1142:ILE:O	2.42	0.47
1:A:1685:CYS:SG	1:A:1686:VAL:N	2.87	0.47
1:A:1531:LYS:HG2	1:A:1533:GLN:H	1.80	0.46
1:A:1121:ASP:OD1	1:A:1123:LYS:NZ	2.39	0.46
1:A:1651:ASP:OD1	1:A:1652:LEU:N	2.45	0.46
1:B:855:LYS:NZ	1:B:872:GLU:OE1	2.42	0.46
1:A:1097:ARG:NE	1:A:1288:PRO:O	2.49	0.46
1:B:350:ALA:N	1:B:351:PRO:CD	2.77	0.46
1:A:816:PHE:CD2	1:A:816:PHE:C	2.93	0.46
1:A:639:ARG:O	1:A:651:PRO:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1354:SER:N	1:B:1355:PRO:CD	2.79	0.46
1:A:312:PRO:O	1:A:313:ARG:HB3	2.16	0.46
1:B:1876:ASP:O	1:B:1885:THR:OG1	2.32	0.45
1:A:608:ASP:OD1	1:A:609:ASP:N	2.46	0.45
1:A:765:LEU:N	1:A:766:PRO:HD2	2.31	0.45
1:A:1952:HIS:N	1:A:1953:PRO:HD3	2.31	0.45
1:B:1152:TYR:N	1:B:1208:ILE:O	2.49	0.45
1:B:1874:PRO:O	1:B:1887:ALA:CB	2.64	0.45
1:B:475:VAL:O	1:B:553:ARG:NE	2.49	0.45
1:A:713:THR:HB	1:A:756:LEU:H	1.82	0.45
1:B:1690:ASN:OD1	1:B:1690:ASN:N	2.49	0.45
1:A:1237:ASP:OD1	1:A:1237:ASP:N	2.50	0.45
1:A:1949:ASP:OD1	1:A:1949:ASP:N	2.50	0.45
1:A:380:HIS:CD2	1:A:565:VAL:HG21	2.52	0.45
1:B:1594:ASP:CB	1:B:1595:PRO:CD	2.95	0.44
1:A:924:TRP:HE1	1:A:1108:ALA:C	2.25	0.44
1:A:942:MET:O	1:A:946:HIS:CE1	2.70	0.44
1:B:918:PHE:CE2	1:B:1135:PHE:CD1	3.05	0.44
1:B:1196:ASN:N	1:B:1197:PRO:CD	2.81	0.44
1:A:1189:VAL:O	1:A:1199:TRP:NE1	2.50	0.44
1:B:528:SER:HB2	1:B:529:PRO:CD	2.48	0.44
1:B:370:ARG:CB	1:B:371:PRO:CD	2.95	0.44
1:A:598:PHE:CD2	1:A:598:PHE:C	2.95	0.44
1:A:1684:TYR:CD2	1:A:1684:TYR:C	2.96	0.43
1:A:941:ASP:OD2	1:A:1057:LYS:NZ	2.38	0.43
1:B:371:PRO:O	1:B:372:THR:C	2.60	0.43
1:A:2000:ARG:HB3	1:A:2001:PRO:HD3	1.99	0.43
1:B:899:LEU:HG	1:B:901:TYR:H	1.83	0.43
1:B:1176:TYR:C	1:B:1176:TYR:CD1	2.96	0.43
1:A:370:ARG:CB	1:A:371:PRO:CD	2.97	0.43
1:A:452:PHE:HB2	1:A:453:PRO:HD3	2.01	0.43
1:B:528:SER:HB2	1:B:529:PRO:HD2	2.00	0.43
1:A:465:ASP:N	1:A:473:ASP:O	2.49	0.43
1:A:601:ALA:HA	1:A:851:GLN:O	2.19	0.43
1:B:312:PRO:O	1:B:313:ARG:HB3	2.19	0.43
1:A:320:TRP:O	1:A:368:LEU:N	2.41	0.42
1:A:662:SER:CB	1:A:1113:GLU:HG3	2.49	0.42
1:B:924:TRP:HE1	1:B:1108:ALA:C	2.26	0.42
1:B:452:PHE:HB3	1:B:453:PRO:CD	2.49	0.42
1:A:1199:TRP:O	1:A:1200:ASP:C	2.61	0.42
1:A:1649:ASP:O	1:A:1656:ASP:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:PHE:CE2	1:B:1135:PHE:CG	3.08	0.42
1:B:1890:ASP:OD1	1:B:1890:ASP:N	2.52	0.42
1:A:999:TRP:CE3	1:A:1044:ARG:HB2	2.54	0.42
1:A:1647:LEU:O	1:A:1659:ILE:N	2.44	0.42
1:B:499:ALA:H	1:B:757:ALA:CB	2.33	0.42
1:A:1719:ASP:OD1	1:A:1720:ARG:N	2.53	0.42
1:B:1560:ILE:HA	1:B:1561:PRO:HD3	1.89	0.42
1:A:1008:ASP:OD1	1:A:1008:ASP:C	2.63	0.42
1:B:350:ALA:N	1:B:351:PRO:HD3	2.35	0.42
1:A:662:SER:HB2	1:A:1113:GLU:HG3	2.02	0.42
1:A:1310:PRO:HA	1:A:1311:PRO:HD3	1.83	0.42
1:B:983:LYS:O	1:B:999:TRP:NE1	2.53	0.42
1:A:420:VAL:HG23	1:A:442:TRP:CG	2.55	0.42
1:A:1012:TRP:CE3	1:A:1038:ARG:HG2	2.54	0.42
1:A:1681:PRO:O	1:A:1756:GLN:NE2	2.53	0.42
1:A:1934:LYS:HA	1:A:1935:PRO:HD3	1.82	0.42
1:B:1227:GLU:OE1	1:B:1229:TYR:OH	2.30	0.41
1:A:884:ASN:HD21	1:A:901:TYR:HB2	1.85	0.41
1:B:1008:ASP:OD1	1:B:1008:ASP:C	2.63	0.41
1:A:734:THR:HG23	1:A:736:LEU:H	1.85	0.41
1:A:1053:MET:SD	1:A:1206:TYR:HB2	2.61	0.41
1:B:452:PHE:CB	1:B:453:PRO:CD	2.98	0.41
1:B:1358:VAL:HB	1:B:1406:ILE:H	1.85	0.41
1:B:1594:ASP:HB2	1:B:1595:PRO:HD2	2.01	0.41
1:A:1962:GLN:O	1:A:2000:ARG:NH1	2.53	0.41
1:B:796:TRP:CD2	1:B:806:TYR:HB3	2.55	0.41
1:B:1583:TYR:O	1:B:1785:MET:HB2	2.20	0.41
1:A:997:GLU:O	1:A:1044:ARG:NH2	2.54	0.41
1:B:595:PHE:CD2	1:B:595:PHE:C	2.99	0.41
1:A:755:ALA:O	1:A:756:LEU:HB2	2.21	0.41
1:A:491:GLU:HB3	1:A:509:ASP:OD2	2.21	0.41
1:A:613:PHE:CD1	1:A:613:PHE:C	2.99	0.41
1:A:1014:TYR:CD2	1:A:1014:TYR:N	2.89	0.41
1:A:1213:GLU:HA	1:A:1214:PRO:HD3	1.96	0.41
1:A:1239:PHE:O	1:A:1262:ARG:HD3	2.21	0.41
1:B:1581:ARG:HG3	1:B:1790:PHE:CE1	2.56	0.41
1:A:1158:MET:N	1:A:1158:MET:SD	2.94	0.41
1:B:713:THR:HG23	1:B:756:LEU:H	1.86	0.41
1:B:2000:ARG:HB3	1:B:2001:PRO:HD3	2.03	0.41
1:B:566:GLU:OE1	1:B:566:GLU:N	2.54	0.40
1:A:286:VAL:HG12	1:A:298:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:TYR:CE1	1:A:1038:ARG:CD	3.04	0.40
1:A:1621:CYS:O	1:A:1893:TRP:HB2	2.20	0.40
1:B:1229:TYR:HB3	1:B:1236:ALA:HB1	2.02	0.40
1:A:371:PRO:O	1:A:372:THR:C	2.63	0.40
1:A:974:ASP:OD1	1:A:974:ASP:C	2.61	0.40
1:A:1302:SER:CB	1:A:1305:THR:OG1	2.70	0.40
1:B:1012:TRP:CD2	1:B:1040:ARG:HB2	2.56	0.40
1:A:423:SER:HA	1:A:427:LYS:O	2.21	0.40
1:A:1429:LEU:HA	1:A:1551:ILE:O	2.22	0.40
1:A:1821:ARG:NH1	1:A:1863:GLY:O	2.55	0.40
1:B:1474:PHE:CD1	1:B:1475:ILE:HG13	2.57	0.40
1:A:492:ILE:O	1:A:492:ILE:HG23	2.22	0.40
1:A:598:PHE:CE2	1:A:652:TRP:CD1	3.10	0.40
1:A:632:ALA:HA	1:A:1139:ARG:HB3	2.04	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	1758/2080 (84%)	1713 (97%)	44 (2%)	1 (0%)	48	83
1	B	1758/2080 (84%)	1720 (98%)	38 (2%)	0	100	100
All	All	3516/4160 (84%)	3433 (98%)	82 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	849	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1551/1833 (85%)	1548 (100%)	3 (0%)	87	86
1	B	1551/1833 (85%)	1551 (100%)	0	100	100
All	All	3102/3666 (85%)	3099 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	942	MET
1	A	1216	THR
1	A	1987	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	GLN
1	A	722	GLN
1	A	940	HIS
1	A	1150	ASN
1	A	1278	GLN
1	A	1566	GLN
1	A	1568	HIS
1	A	1569	GLN
1	A	1707	GLN
1	A	1724	GLN
1	A	1753	HIS
1	A	1758	GLN
1	A	1857	HIS
1	A	1930	ASN
1	A	1962	GLN
1	B	314	HIS
1	B	443	ASN
1	B	693	HIS
1	B	711	GLN

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Mol	Chain	Res	Type
1	B	742	GLN
1	B	851	GLN
1	B	884	ASN
1	B	1246	GLN
1	B	1569	GLN
1	B	1682	GLN
1	B	1757	GLN
1	B	1850	HIS
1	B	1946	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

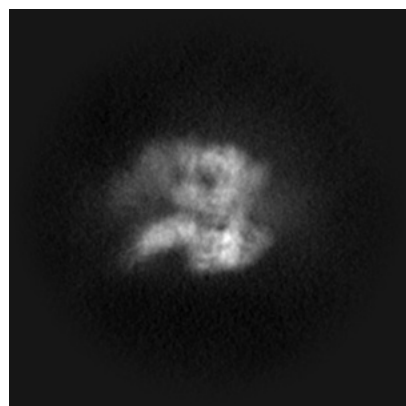
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44349. These allow visual inspection of the internal detail of the map and identification of artifacts.

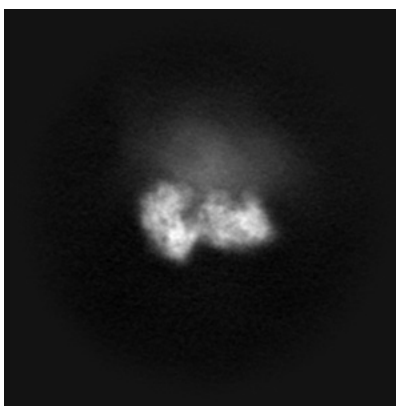
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

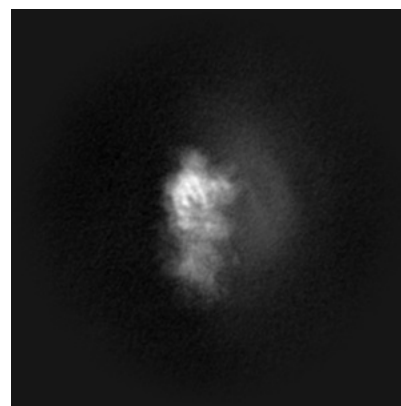
6.1.1 Primary map



X

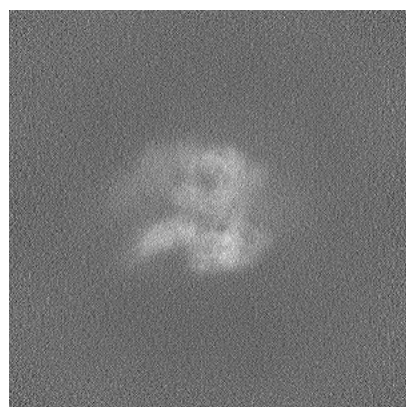


Y

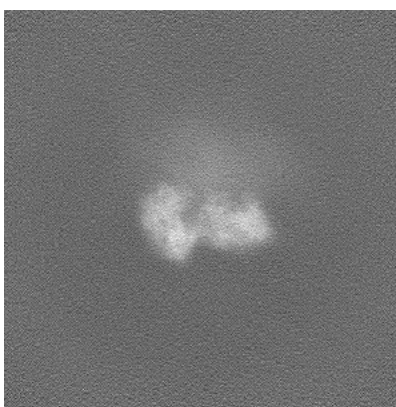


Z

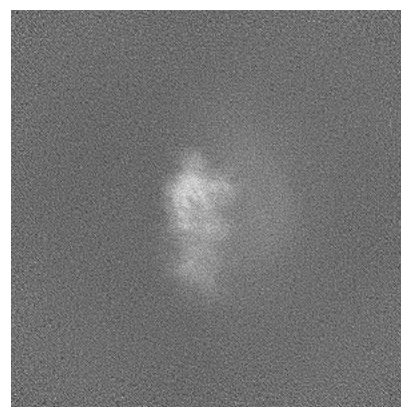
6.1.2 Raw map



X



Y

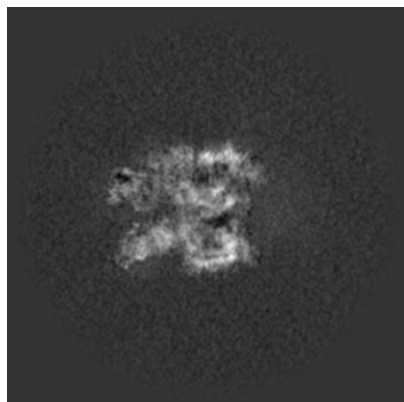


Z

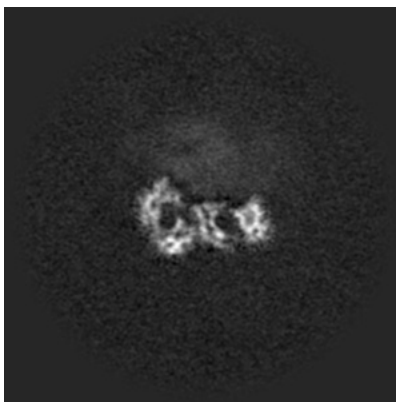
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

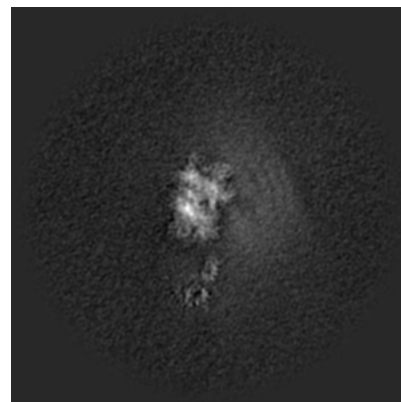
6.2.1 Primary map



X Index: 256

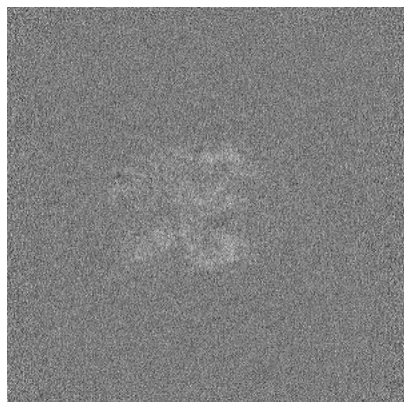


Y Index: 256

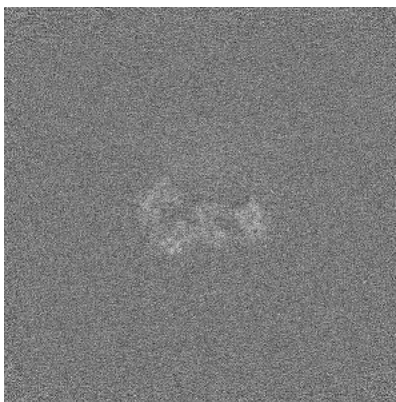


Z Index: 256

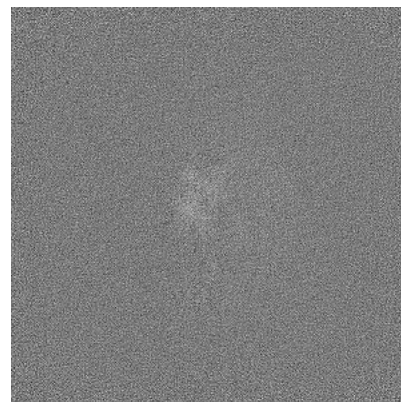
6.2.2 Raw map



X Index: 256



Y Index: 256

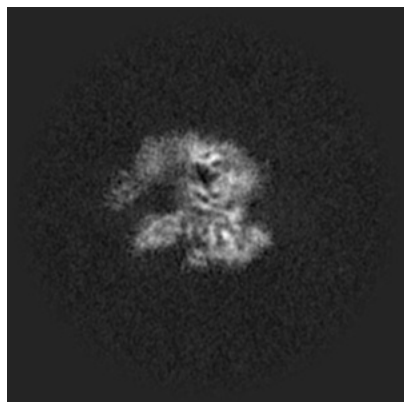


Z Index: 256

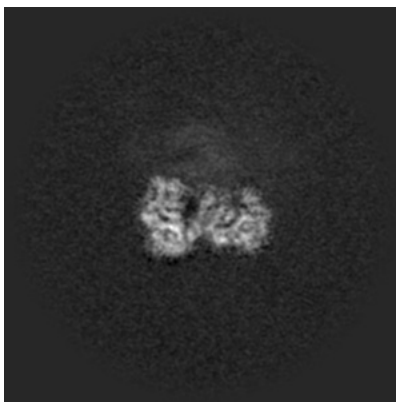
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

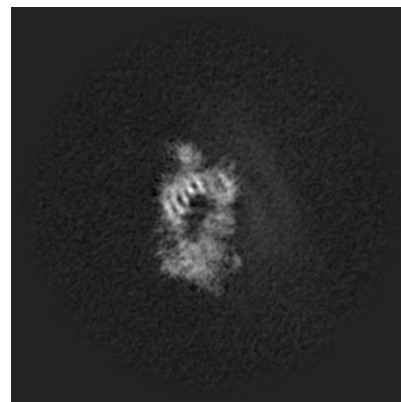
6.3.1 Primary map



X Index: 225

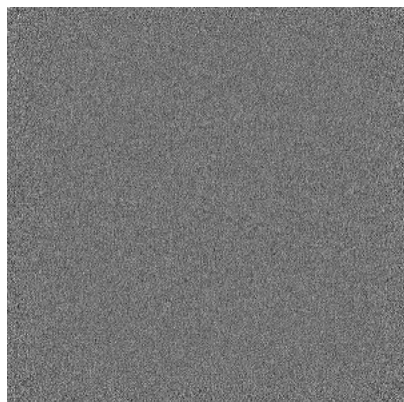


Y Index: 277

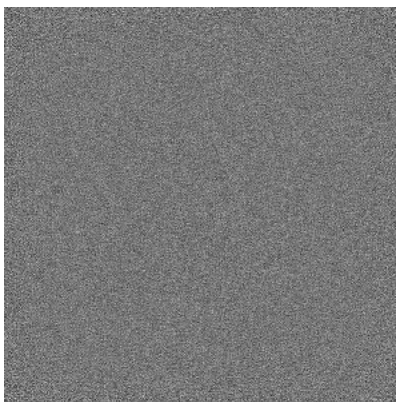


Z Index: 214

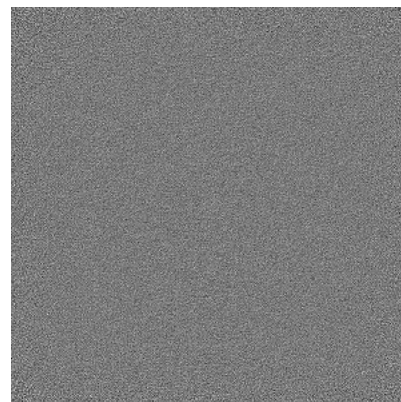
6.3.2 Raw map



X Index: 0



Y Index: 0

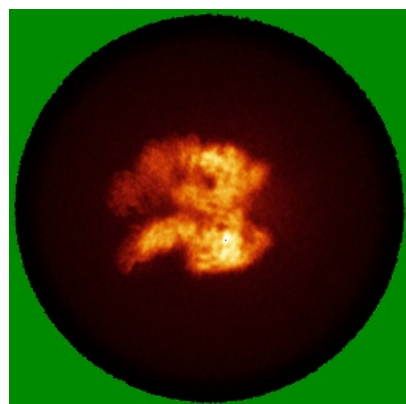


Z Index: 0

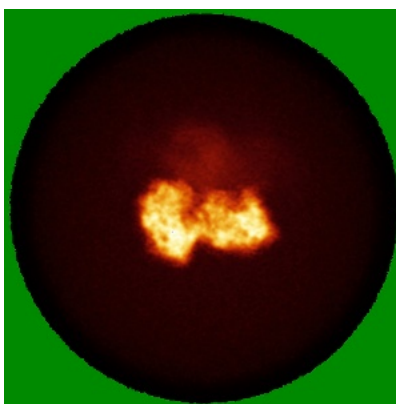
The images above show the largest variance slices of the map in three orthogonal directions.

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

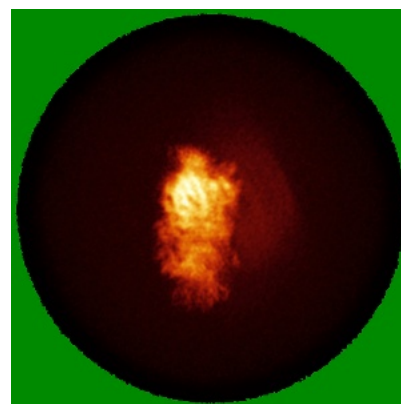
6.4.1 Primary map



X

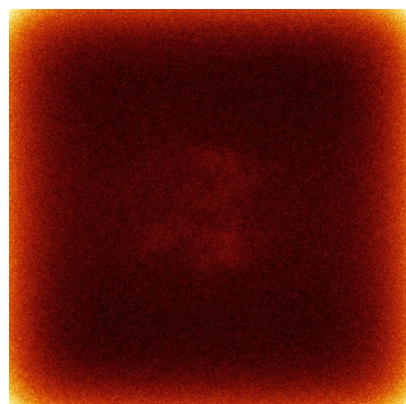


Y

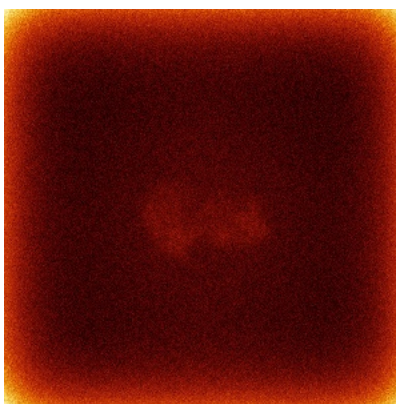


Z

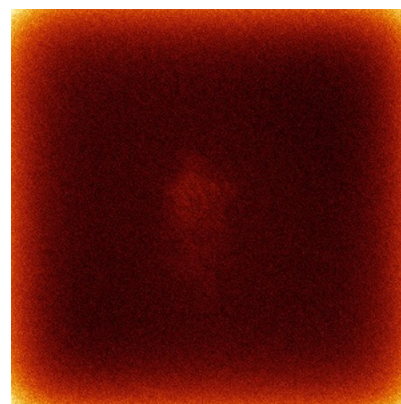
6.4.2 Raw map



X



Y

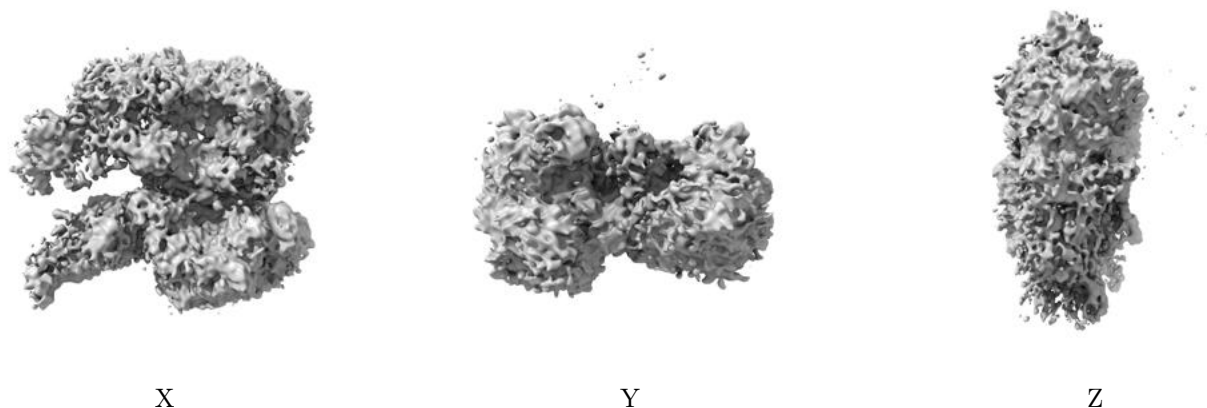


Z

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.

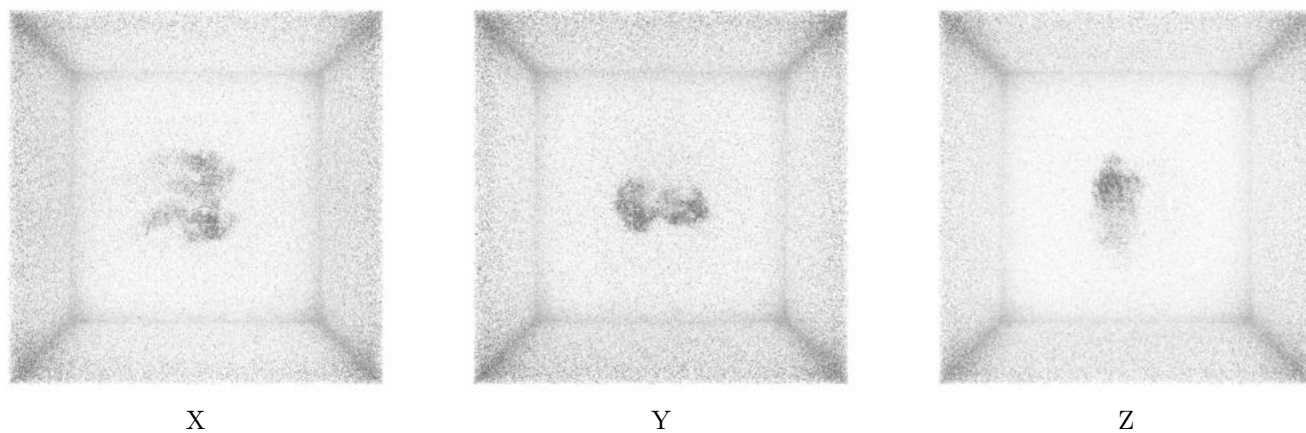
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

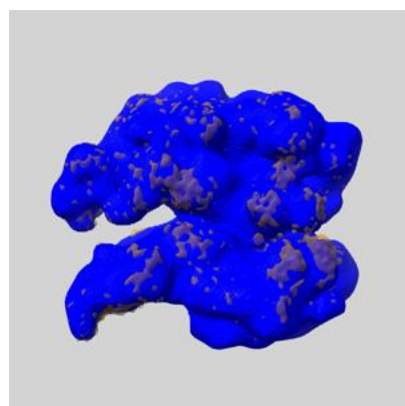
6.6 Mask visualisation [i](#)

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

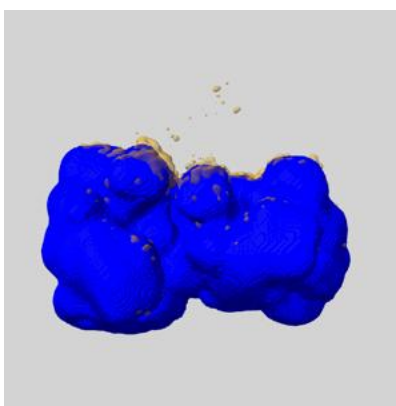
A mask typically either:

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

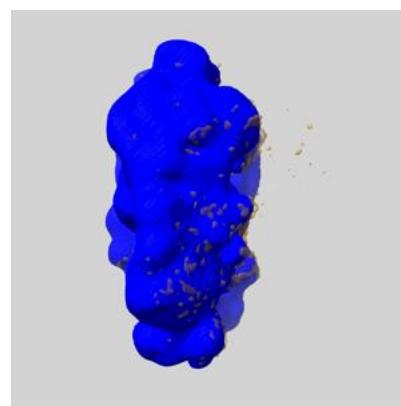
6.6.1 emd_44349_msk_1.map [i](#)



X



Y

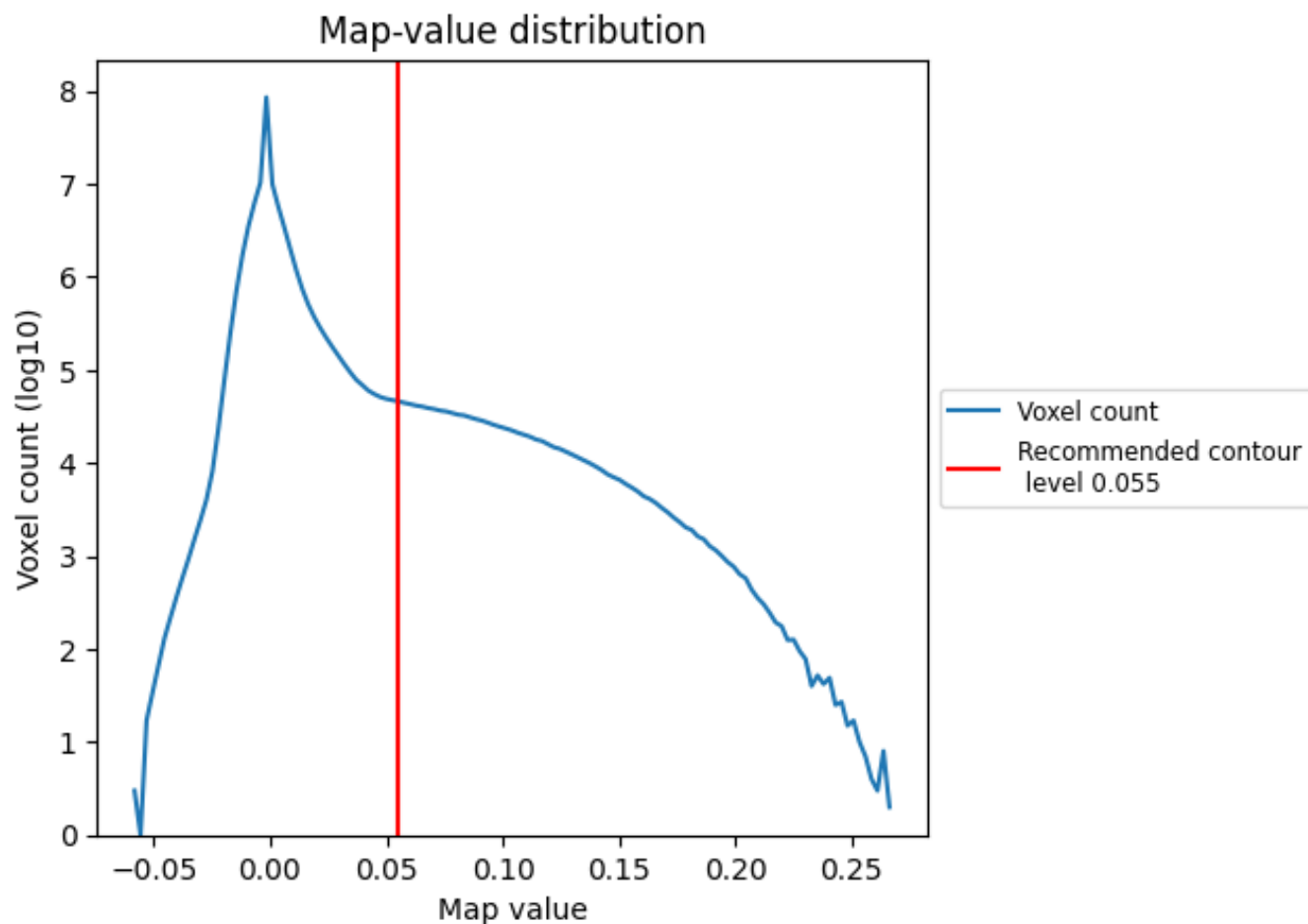


Z

7 Map analysis [i](#)

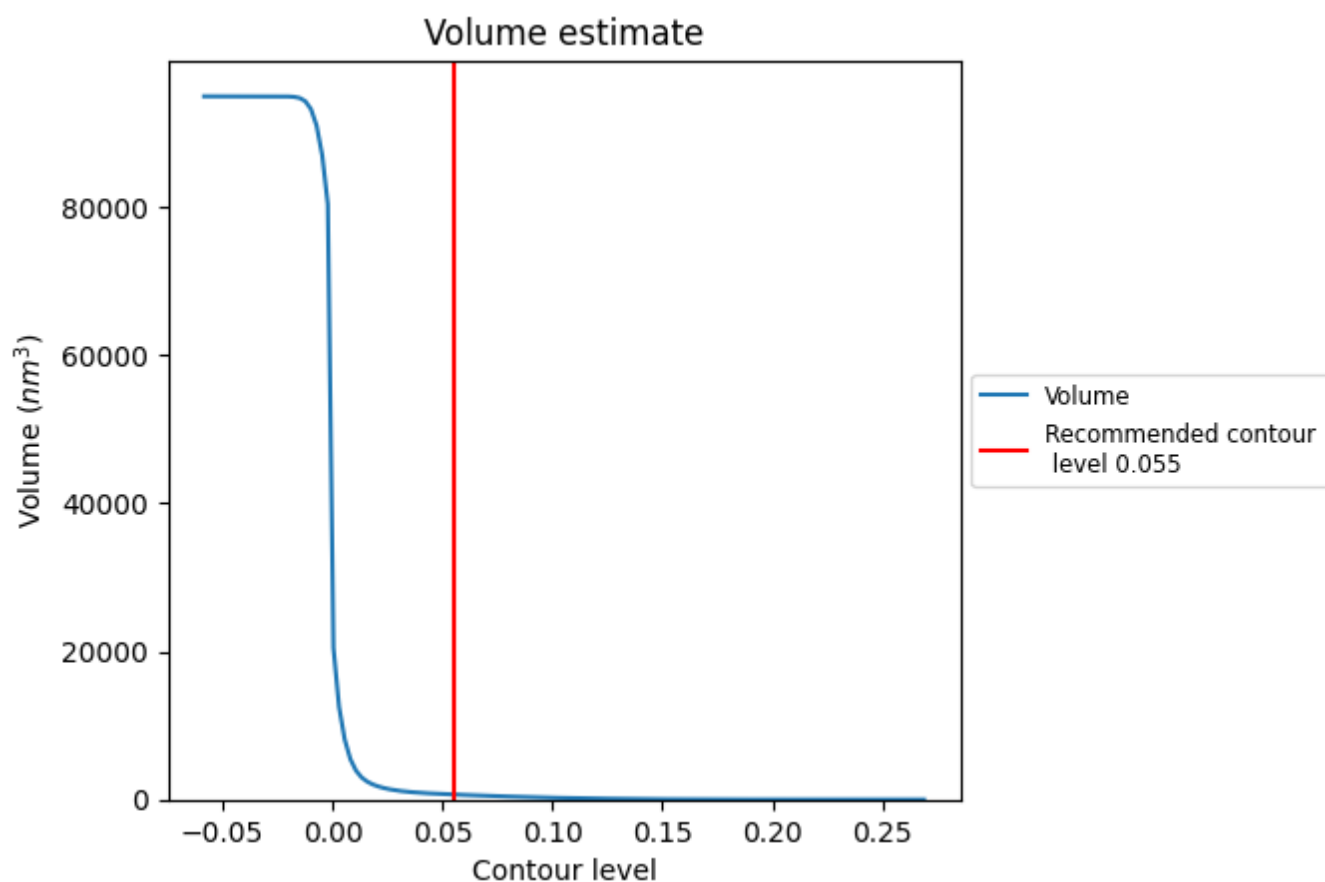
This section contains the results of statistical analysis of the map.

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.

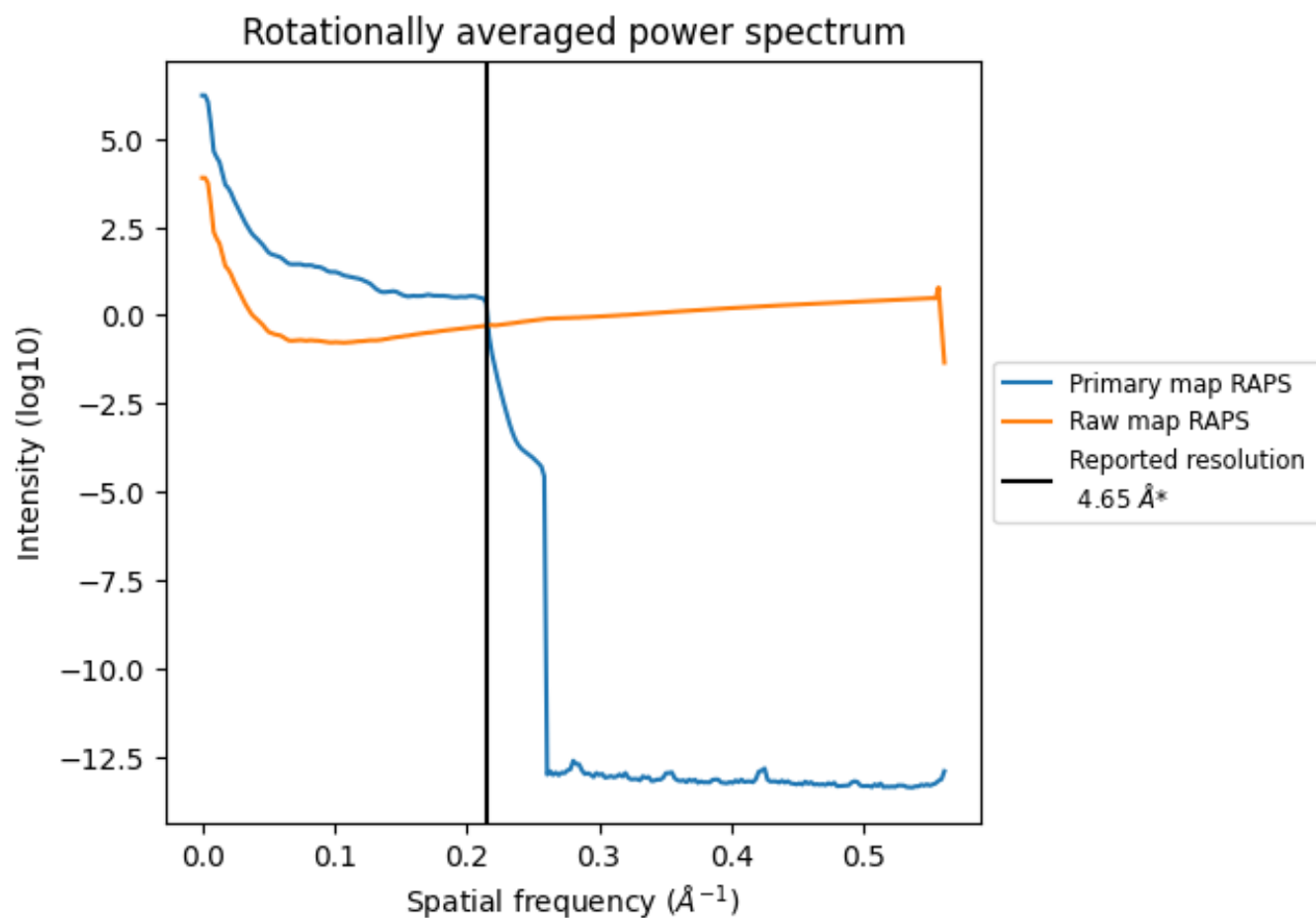
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 686 nm³; this corresponds to an approximate mass of 619 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 ⓘ

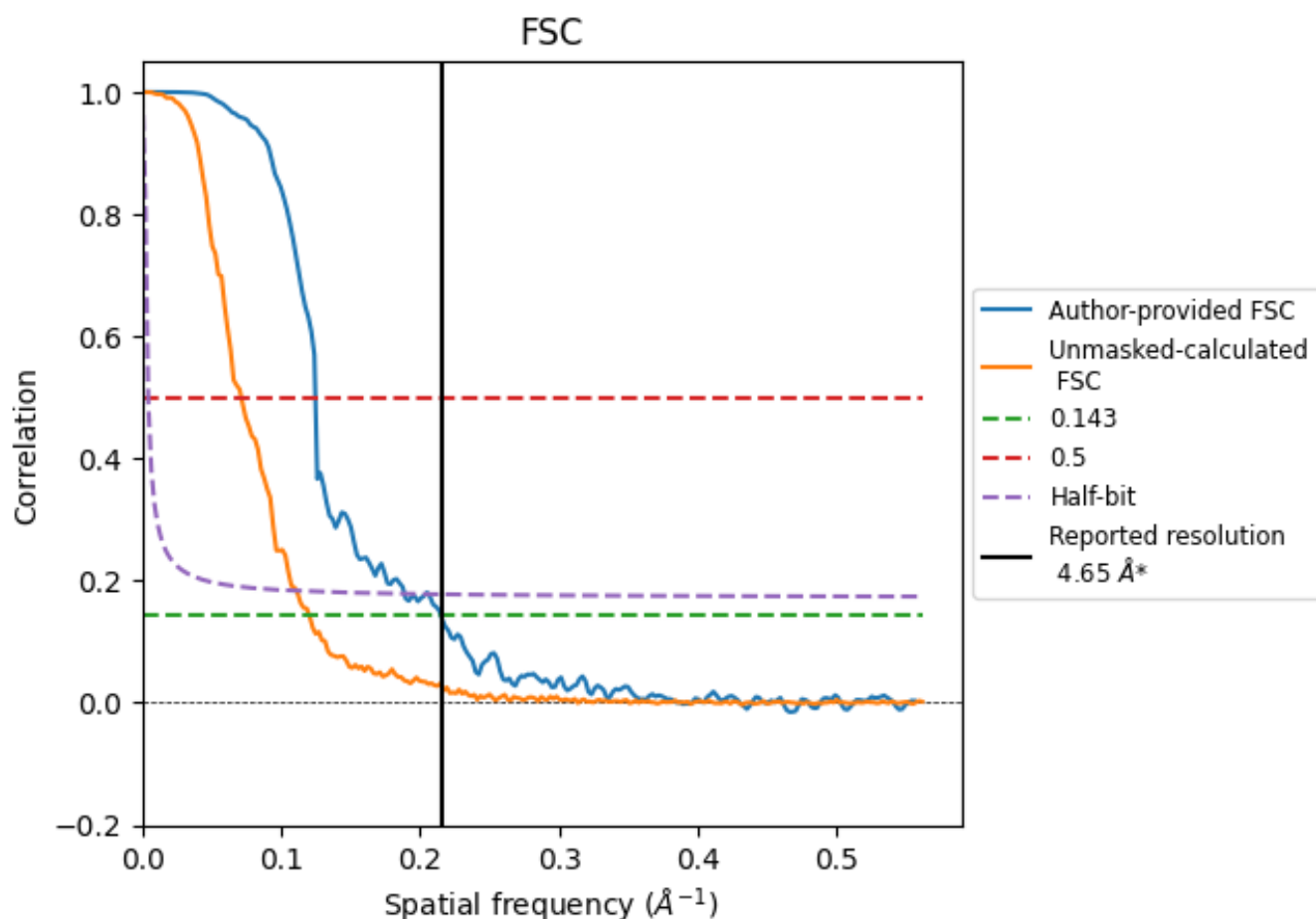


*Reported resolution corresponds to spatial frequency of 0.215 Å⁻¹

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 $0.215 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

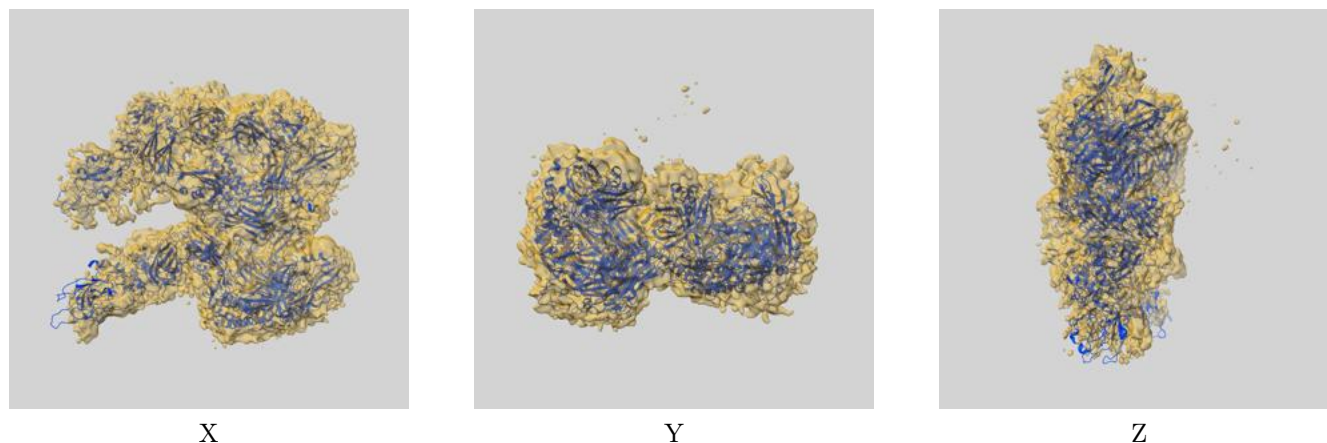
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.65	-	-
Author-provided FSC curve	4.65	8.03	5.30
Unmasked-calculated*	8.32	14.03	9.03

*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 8.32 differs from the reported value 4.65 by more than 10 %

9 Map-model fit [i](#)

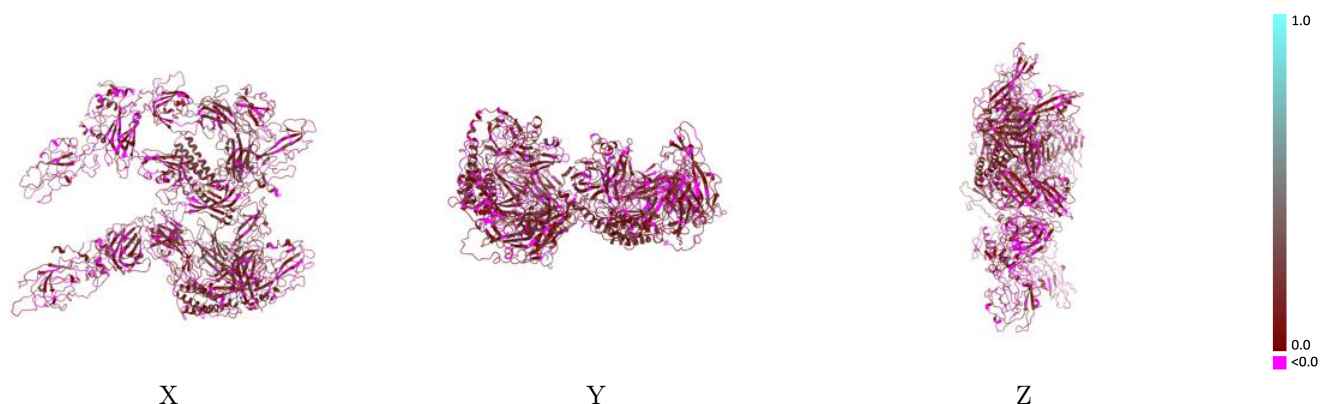
This section contains information regarding the fit between EMDB map EMD-44349 and PDB model 9B8L. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



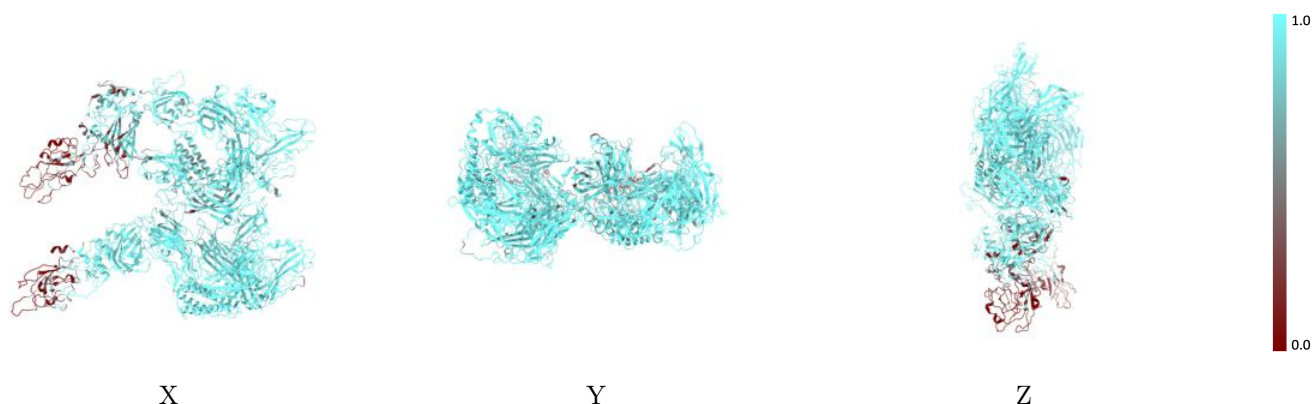
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



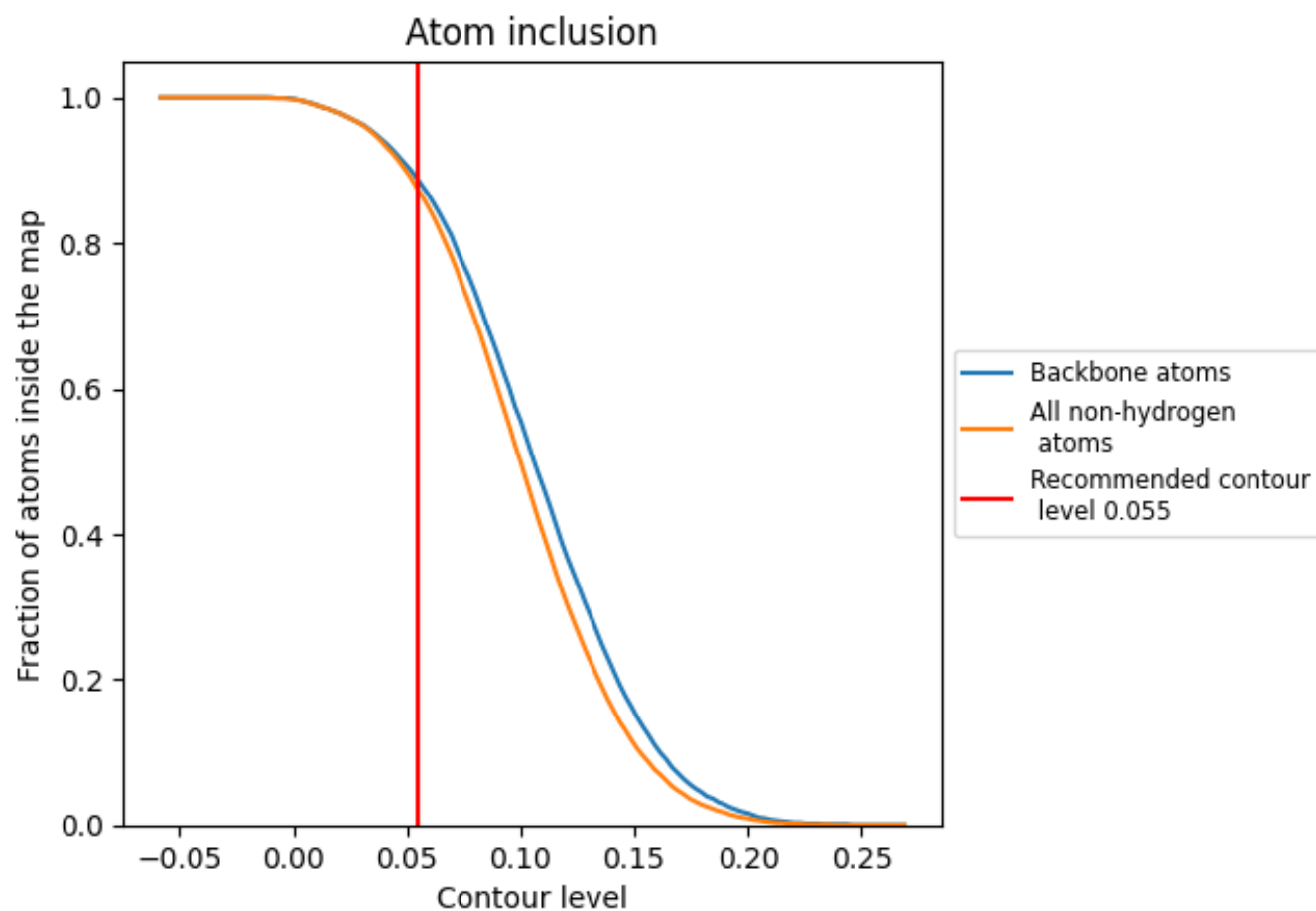
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.1090
A	0.9150	0.1140
B	0.8320	0.1030

