



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 04:41 AM JST

PDB ID : 7ELB
EMDB ID : EMD-31179
Title : Structure of Machupo virus L polymerase in complex with Z protein (dimeric form)
Authors : Peng, R.; Xu, X.; Peng, Q.; Shi, Y.
Deposited on : 2021-04-09
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

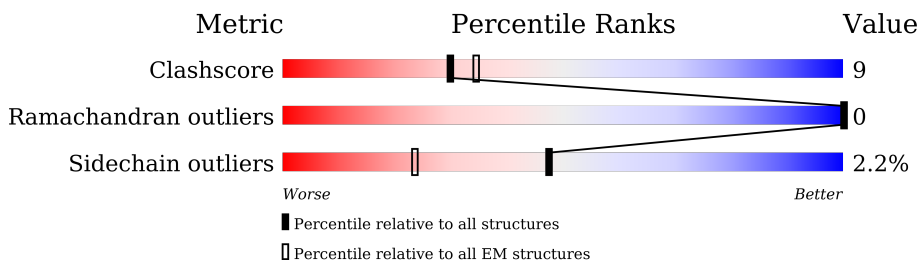
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2209	<div> <div>13%</div> <div>67%</div> <div>20%</div> <div>12%</div> </div>
1	C	2209	<div> <div>13%</div> <div>67%</div> <div>20%</div> <div>12%</div> </div>
2	B	94	<div> <div>46%</div> <div>6%</div> <div>48%</div> </div>
2	D	94	<div> <div>46%</div> <div>6%</div> <div>48%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 31012 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		
1	C	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	49	Total	C	N	O	S	0	0
			407	257	73	68	9		
2	D	49	Total	C	N	O	S	0	0
			407	257	73	68	9		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mn	0
			1	1	
3	C	1	Total	Mn	0
			1	1	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	
4	B	2	Total	Zn	0
			2	2	
4	C	2	Total	Zn	0
			2	2	

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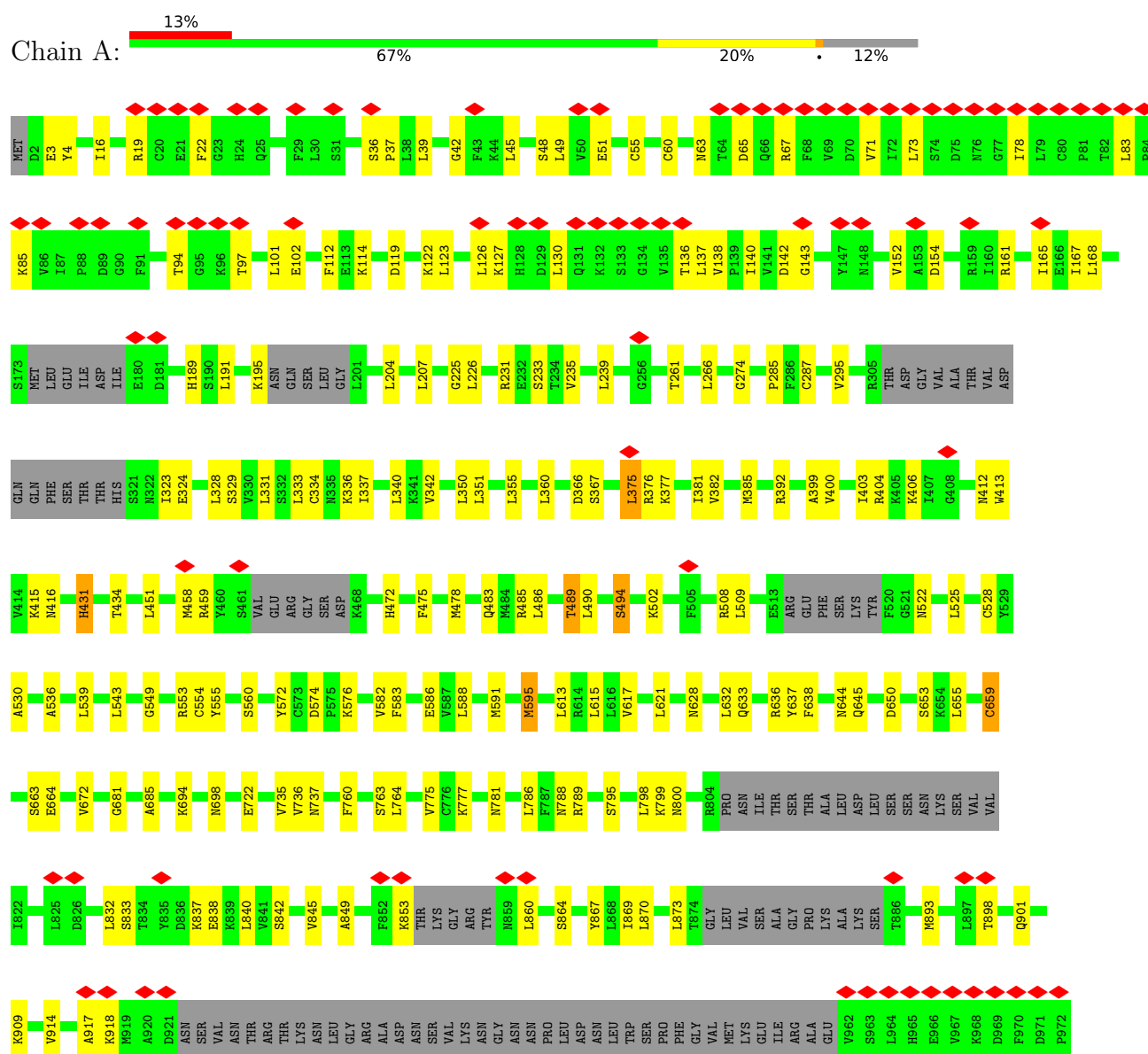
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Mol	Chain	Residues	Atoms		AltConf
4	D	2	Total	Zn	0
			2	2	

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: RNA-directed RNA polymerase L



D973	Y974	L975	P976	P977	E978	Y979	Y980	K981	E982	L983	C984	D985	A986	Y987	Y988	K989	S990	S991	E992	K993	C994	N995	F996	L998	E999	G1000	V1001	L1002	D1003	V1004	C1005	F1006	L1007	G1008	L1009	L1010	L1011	K1012	N1013	L1014	T1015	T1016	S1017	S1018	Y1019	Y1024	F1025	M1026	C1027	F1028	X1029	Y1030	L1031	L1032	L1033	Q1034	G1035
H1036	F1037	D1038	Q1039	LYS	LEU	GLY	SER	TVR	GLU	HIS	LEU	SER	ARG	ARG	GLY	THR	ASP	GLU	THR	LEU	ARG	LEU	LEU	ASP	VAL	ARG	LEU	SER	ASN	SER	GLU	ALA	ILE	ALA	ASP	LYS	LEU	ASP	LYS	SER	TYR	F1086	T1087	N1088	A1089	N1093	Y1097	D1100									
S1109	G1113	N1137	M1141	T1142	R1143	E1146	D1147	E1150	A1151	V1152	S1155	T1159	L1183	S1184	C1185	H1189	S1190	L1200	A1203	L1204	E1209	L1210	R1211	T1212	D1215	R1216	D1220	L1221	D1222	S1223	I1227	E1237	V1238	G1249	LYS	LEU	LYS	ARG	SER	LEU	GLY																
LEU	MET	GLY	CYS	GLY	S1262	S1266	S1282	M1285	L1288	G1291	I1294	D1300	L1301	Y1302	G1303	L1304	I1305	T1306	L1310	C1311	Y1312	T1326	S1327	S1328	Q1331	I1335	S1339	LEU	ASP	ILE	GLU	GLY	SER	W1351	L1352	E1353	M1354	I1355	C1356	L1361	L1365	N1366															
V1369	K1372	V1374	I1375	V1388	M1389	A1402	M1406	D1420	R1438	R1442	L1446	I1460	V1465	K1466	D1467	D1488	I1494	R1499	D1504	I1505	R1509	F1510	E1511	E1512	E1513	L1531	E1538	Q1539	M1542	L1552	S1553	S1554	F1555	L1558	L1562	R1563																					
T1564	K1565	L1566	M1567	T1568	SER	ARG	VAL	LEU	GLU	ARG	GLU	V1578	K1588	L1589	S1590	R1591	ASN	PHE	THR	LYS	GLY	VAL	LYS	LYS	ILE	LEU	ALA	GLU	SER	ILE	ASN	LYS	SER	ALA	PHE	Q1611	I1619	S1624	S1627	K1628	C1629	V1630	R1631	D1632	G1633	LYS	GLY	G1636	S1648	A1649	C1650	T1651					
I1661	I1662	S1667	L1679	L1687	T1688	C1691	W1696	S1699	T1700	Q1705	LYS	PRO	L1825	S1826	M1711	F1715	E1728	M1733	N1734	V1736	L1737	Q1738	R1741	R1742	N1743	Y1744	L1747	L1752	T1753	P1754	F1755	Q1760	T1764	M1765	R1769	I1777	A1778	L1779																			
I1788	I1789	T1795	R1796	D1797	N1798	Y1801	Q1805	S1806	A1811	S1816	T1819	L1823	G1824	P1827	Q1828	Q1829	C1831	N1833	F1834	K1835	T1836	Q1837	S1842	M1843	L1849	L1854	K1855	S1856	W1859	F1860	N1861	E1862	V1863	L1866	D1869	Q1871	S1870	I1871	E1872	L1874	A1875	E1876															
L1877	T1878	D1879	M1883	N1886	Q1887	N1888	V1895	E1896	D1897	I1898	A1899	M1900	G1901	Y1902	N1906	F1907	E1908	I1909	S1915	N1916	V1917	M1918	V1919	D1920	G1921	V1922	Q1923	L1924	P1925	P1926	Q1927	GLU	LYS	ALA	PRO	D1932	E1935	L1936	F1937	G1938	L1939	K1940	A1941	GLU	ASN	VAL	ILE	VAL	G1947	L1948	V1949	V1950	Q1951				
T1952	D1953	H1954	V1955	K1962	D1978	V1979	G1980	E1981	I1982	Q1983	N1984	K1985	E1986	V1987	I1988	L1989	V1991	V1992	A1993	V1994	D1995	Q1996	N2004	H2005	M2006	L2007	L2008	D2009	G2010	V2011	S2012	V2013	V2014	A2015	S2016	L2017	P2018	L2019	F2020	T2021	G2022	Q2023	A2024	S2025	L2028	A2029	A2030	M2031	L2032	N2036	L2037	S2040					
N2041	D2042	N2043	F2044	L2045	M2046	R2047	M2048	V2049	T2050	L2051	D2052	L2053	G2054	F2055	G2056	S2057	P2058	E2059	L2060	S2061	D2062	K2063	Y2064	S2065	Y2066	R2067	L2068	F2071	E2072	N2073	Q2074	E2075	D2076	L2080	K2081	D2082	G2083	A2084	F2085	R2091	L2092	S2093	K2096	F2099	T2100	G2101	L2108	L2111	S2116	V2117	V2118						
H2122	Q2123	L2124	A2130	T2131	S2132	Q2133	V2134	I2135	E2140	D2141	T2142	T2143	V2144	L2145	L2148	L2153	S2156	T2157	E2158	SER	PHE	GLY	GLU	TRP	ILE	GLU	PHE	THR	ASN	PHE	LYS	VAL	ALA	TYR	LYS	SER	LEU	LYS	GLU	LEU	VAL	ILE	SER	ASP	THR	GLN	GLY	PHE	ARG	LEU	LYS						

- Molecule 1: RNA-directed RNA polymerase L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36056	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/15349	0.44	0/20744
1	C	0.24	0/15349	0.44	0/20744
2	B	0.22	0/419	0.45	0/569
2	D	0.22	0/419	0.46	0/569
All	All	0.25	0/31536	0.44	0/42626

There are no bond length outliers.

There are no bond angle outliers.

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	15094	0	14961	274	0
1	C	15094	0	14961	271	0
2	B	407	0	383	5	0
2	D	407	0	383	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
All	All	31012	0	30688	550	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 9.

All (550) 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:C:1011:LEU:HD12	1:C:1034:GLN:HG2	1.60	0.83
1:A:1011:LEU:HD12	1:A:1034:GLN:HG2	1.60	0.81
1:A:1835:LYS:HD3	1:A:1872:ILE:HD12	1.67	0.76
1:C:287:CYS:HB3	1:C:472:HIS:HE1	1.51	0.75
1:A:287:CYS:HB3	1:A:472:HIS:HE1	1.51	0.74
1:C:1835:LYS:HD3	1:C:1872:ILE:HD12	1.67	0.74
1:C:1002:LEU:HD21	1:C:1006:PRO:HD2	1.71	0.73
1:A:412:ASN:O	1:A:416:ASN:ND2	2.23	0.72
1:A:1002:LEU:HD21	1:A:1006:PRO:HD2	1.71	0.72
1:C:412:ASN:O	1:C:416:ASN:ND2	2.23	0.71
1:C:873:LEU:HD22	1:C:1566:LEU:HD11	1.72	0.71
1:C:1886:ASN:HD22	1:C:1888:ASN:H	1.39	0.71
1:A:1886:ASN:HD22	1:A:1888:ASN:H	1.39	0.70
1:A:136:THR:HG21	1:A:918:LYS:HE3	1.74	0.70
1:A:873:LEU:HD22	1:A:1566:LEU:HD11	1.72	0.70
1:C:1552:LEU:HD12	1:C:1630:VAL:HG11	1.75	0.69
1:A:1552:LEU:HD12	1:A:1630:VAL:HG11	1.75	0.68
1:C:136:THR:HG21	1:C:918:LYS:HE3	1.74	0.68
1:C:638:PHE:HB2	1:C:655:LEU:HD21	1.76	0.68
1:A:832:LEU:HG	1:A:837:LYS:HE2	1.76	0.67
1:C:502:LYS:HG2	1:C:1619:ILE:HD12	1.76	0.67
1:A:638:PHE:HB2	1:A:655:LEU:HD21	1.76	0.67
1:C:1738:GLN:NE2	1:C:1765:MET:SD	2.68	0.67
1:A:1004:VAL:HG23	1:A:1006:PRO:HD3	1.77	0.67
1:A:2122:HIS:HB2	1:A:2153:LEU:HD22	1.77	0.67
1:C:832:LEU:HG	1:C:837:LYS:HE2	1.76	0.66
1:C:2111:LEU:HD12	1:C:2117:VAL:HG22	1.77	0.66
1:A:1738:GLN:NE2	1:A:1765:MET:SD	2.68	0.66
1:C:1420:ASP:HB2	1:C:1460:ILE:HD11	1.77	0.66
1:A:2111:LEU:HD12	1:A:2117:VAL:HG22	1.76	0.66
1:C:2084:ALA:HB1	1:C:2091:ARG:HG3	1.78	0.66
1:C:2122:HIS:HB2	1:C:2153:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:HB2	1:A:1460:ILE:HD11	1.77	0.66
1:C:901:GLN:HE22	1:C:1566:LEU:HD13	1.61	0.66
1:A:502:LYS:HG2	1:A:1619:ILE:HD12	1.76	0.65
1:C:323:ILE:HD13	1:C:375:LEU:HD13	1.78	0.65
1:A:2084:ALA:HB1	1:A:2091:ARG:HG3	1.78	0.65
1:C:1979:VAL:HG22	1:C:1994:VAL:HG23	1.79	0.65
1:A:323:ILE:HD13	1:A:375:LEU:HD13	1.78	0.65
1:C:1004:VAL:HG23	1:C:1006:PRO:HD3	1.77	0.65
1:C:1994:VAL:HB	1:C:2053:LEU:HD11	1.78	0.64
1:A:901:GLN:HE22	1:A:1566:LEU:HD13	1.62	0.64
1:C:860:LEU:HA	1:C:1006:PRO:HA	1.79	0.64
1:A:1979:VAL:HG22	1:A:1994:VAL:HG23	1.79	0.64
1:A:231:ARG:HD2	1:A:789:ARG:HH12	1.63	0.64
1:A:1948:LEU:HG	1:A:1950:VAL:HG22	1.80	0.64
1:A:287:CYS:HB3	1:A:472:HIS:CE1	2.32	0.64
1:A:694:LYS:O	1:A:698:ASN:ND2	2.30	0.63
1:C:1948:LEU:HG	1:C:1950:VAL:HG22	1.80	0.63
1:A:1994:VAL:HB	1:A:2053:LEU:HD11	1.78	0.63
1:C:138:VAL:HG11	1:C:845:VAL:HG11	1.79	0.63
1:A:351:LEU:HD13	1:A:406:LYS:HD3	1.80	0.63
1:A:860:LEU:HA	1:A:1006:PRO:HA	1.79	0.63
1:A:138:VAL:HG11	1:A:845:VAL:HG11	1.79	0.63
1:C:1553:SER:O	1:C:1553:SER:OG	2.17	0.63
1:A:65:ASP:HB3	1:A:67:ARG:HD3	1.81	0.63
1:A:998:LEU:HD22	1:A:1012:LYS:HB3	1.80	0.63
1:C:231:ARG:HD2	1:C:789:ARG:HH12	1.63	0.63
1:C:287:CYS:HB3	1:C:472:HIS:CE1	2.32	0.63
1:C:998:LEU:HD22	1:C:1012:LYS:HB3	1.80	0.63
1:C:788:ASN:ND2	1:C:1209:GLU:OE1	2.32	0.62
1:C:1200:LEU:HD22	1:C:1366:ASN:HD22	1.63	0.62
1:C:549:GLY:O	1:C:553:ARG:NH2	2.33	0.62
1:A:788:ASN:ND2	1:A:1209:GLU:OE1	2.32	0.62
1:A:1200:LEU:HD22	1:A:1366:ASN:HD22	1.63	0.61
1:A:1711:ASN:N	1:A:1806:SER:HG	1.98	0.61
1:C:351:LEU:HD13	1:C:406:LYS:HD3	1.80	0.61
1:C:1711:ASN:N	1:C:1806:SER:HG	1.99	0.61
1:A:1936:LEU:HD13	1:A:2037:LEU:HD13	1.82	0.61
1:C:65:ASP:HB3	1:C:67:ARG:HD3	1.81	0.61
1:C:737:ASN:HD21	1:C:1282:SER:H	1.48	0.61
1:A:1465:VAL:HG22	1:A:1466:LYS:H	1.66	0.61
1:A:549:GLY:O	1:A:553:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1553:SER:O	1:A:1553:SER:OG	2.17	0.60
1:C:1936:LEU:HD13	1:C:2037:LEU:HD13	1.82	0.60
1:A:1538:GLU:O	1:A:1542:ASN:ND2	2.35	0.60
1:A:832:LEU:HD12	1:A:837:LYS:HG2	1.84	0.60
1:C:1538:GLU:O	1:C:1542:ASN:ND2	2.35	0.60
1:C:1465:VAL:HG22	1:C:1466:LYS:H	1.66	0.60
1:A:1825:LEU:HG	1:A:1830:ILE:HD11	1.84	0.59
1:A:737:ASN:HD21	1:A:1282:SER:H	1.48	0.59
1:C:694:LYS:O	1:C:698:ASN:ND2	2.30	0.59
1:C:1494:ILE:HG13	1:C:1679:LEU:HD12	1.85	0.59
1:A:114:LYS:HZ3	1:A:1137:ASN:HB2	1.68	0.59
1:C:1825:LEU:HG	1:C:1830:ILE:HD11	1.84	0.59
1:A:1512:GLU:HB3	1:C:1769:ARG:HD3	1.84	0.58
1:C:485:ARG:O	1:C:489:THR:OG1	2.22	0.58
1:A:1923:GLN:NE2	1:A:2036:ASN:O	2.36	0.58
1:C:83:LEU:HD21	1:C:126:LEU:HD21	1.85	0.58
1:A:1494:ILE:HG13	1:A:1679:LEU:HD12	1.85	0.58
1:A:1764:THR:O	1:C:1517:ASN:ND2	2.36	0.58
1:C:274:GLY:HA3	1:C:672:VAL:HG21	1.86	0.58
1:A:1159:THR:HB	1:A:1304:LEU:HD22	1.85	0.58
1:C:2051:LEU:HD21	1:C:2053:LEU:HD13	1.86	0.58
1:A:539:LEU:HA	1:A:560:SER:O	2.04	0.58
1:A:1210:LEU:HG	1:A:1221:LEU:HD11	1.85	0.58
1:C:1923:GLN:NE2	1:C:2036:ASN:O	2.36	0.57
1:A:1984:ASN:HB3	1:A:1989:LEU:HA	1.87	0.57
1:C:1210:LEU:HG	1:C:1221:LEU:HD11	1.85	0.57
1:A:83:LEU:HD21	1:A:126:LEU:HD21	1.85	0.57
1:A:225:GLY:O	1:A:781:ASN:ND2	2.37	0.57
1:A:274:GLY:HA3	1:A:672:VAL:HG21	1.86	0.57
1:C:539:LEU:HA	1:C:560:SER:O	2.04	0.57
1:C:832:LEU:HD12	1:C:837:LYS:HG2	1.84	0.57
1:C:1159:THR:HB	1:C:1304:LEU:HD22	1.85	0.57
1:A:485:ARG:O	1:A:489:THR:OG1	2.21	0.57
1:A:1769:ARG:HD3	1:C:1512:GLU:HB3	1.87	0.57
1:C:1984:ASN:HB3	1:C:1989:LEU:HA	1.87	0.57
1:A:1505:ILE:HG13	1:A:1511:PHE:HB2	1.86	0.57
1:A:1994:VAL:HG21	1:A:2053:LEU:HD21	1.87	0.57
1:A:2141:ASP:O	1:A:2145:VAL:HG23	2.05	0.57
1:A:840:LEU:HD22	1:A:873:LEU:HD21	1.86	0.56
1:C:840:LEU:HD22	1:C:873:LEU:HD21	1.86	0.56
1:A:1465:VAL:HG21	1:A:1811:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1872:ILE:HG13	1:A:1873:GLU:H	1.70	0.56
1:C:1994:VAL:HG21	1:C:2053:LEU:HD21	1.87	0.56
1:A:2051:LEU:HD21	1:A:2053:LEU:HD13	1.86	0.56
1:C:1505:ILE:HG13	1:C:1511:PHE:HB2	1.86	0.56
1:C:2141:ASP:O	1:C:2145:VAL:HG23	2.05	0.56
1:A:508:ARG:HE	1:A:509:LEU:H	1.54	0.56
1:C:225:GLY:O	1:C:781:ASN:ND2	2.37	0.56
1:C:1465:VAL:HG21	1:C:1811:ALA:HA	1.87	0.56
1:C:1152:VAL:O	1:C:1155:SER:OG	2.22	0.56
1:A:1856:SER:O	1:A:1856:SER:OG	2.23	0.55
1:A:1849:LEU:HD11	1:A:2080:LEU:HB2	1.87	0.55
1:A:1402:ALA:O	1:A:1406:ASN:ND2	2.39	0.55
1:A:1650:CYS:SG	1:A:1667:SER:OG	2.65	0.55
1:C:633:GLN:HG2	1:C:636:ARG:HH12	1.71	0.55
1:C:917:ALA:HB2	1:C:1010:LEU:HD22	1.89	0.55
2:D:55:HIS:HE1	2:D:75:CYS:HB3	1.72	0.55
1:A:633:GLN:HG2	1:A:636:ARG:HH12	1.71	0.55
1:A:1555:PHE:HD2	1:A:1632:ASP:HA	1.72	0.55
1:C:508:ARG:HE	1:C:509:LEU:H	1.54	0.55
1:C:650:ASP:OD1	1:C:653:SER:OG	2.21	0.55
1:C:736:VAL:HG22	1:C:737:ASN:H	1.71	0.55
1:C:1650:CYS:SG	1:C:1667:SER:OG	2.65	0.54
1:C:1849:LEU:HD11	1:C:2080:LEU:HB2	1.87	0.54
1:C:1872:ILE:HG13	1:C:1873:GLU:H	1.70	0.54
1:A:644:ASN:HD22	1:A:1374:VAL:HG12	1.72	0.54
1:C:101:LEU:HD11	1:C:142:ASP:HB2	1.90	0.54
1:C:140:ILE:HG12	1:C:842:SER:HB2	1.88	0.54
1:C:1555:PHE:HD2	1:C:1632:ASP:HA	1.72	0.54
1:A:595:MET:HE3	1:A:613:LEU:HD21	1.89	0.54
2:B:55:HIS:HE1	2:B:75:CYS:HB3	1.72	0.54
1:A:736:VAL:HG22	1:A:737:ASN:H	1.71	0.54
1:A:1093:ASN:HA	1:A:1097:TYR:HB3	1.90	0.54
1:A:1661:ILE:HG22	1:A:1662:ILE:HG12	1.90	0.54
1:A:1211:ARG:HD3	1:A:1216:ARG:HD2	1.90	0.54
1:C:664:GLU:N	1:C:664:GLU:OE1	2.41	0.54
1:A:152:VAL:HG13	1:A:154:ASP:H	1.73	0.54
1:C:152:VAL:HG13	1:C:154:ASP:H	1.73	0.54
1:A:628:ASN:O	1:A:632:LEU:HG	2.08	0.54
1:A:917:ALA:HB2	1:A:1010:LEU:HD22	1.89	0.54
1:A:650:ASP:OD1	1:A:653:SER:OG	2.21	0.53
1:A:1829:GLN:HA	1:A:1832:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HG12	1:A:842:SER:HB2	1.88	0.53
1:C:595:MET:HE3	1:C:613:LEU:HD21	1.91	0.53
1:C:1211:ARG:HD3	1:C:1216:ARG:HD2	1.90	0.53
1:A:664:GLU:N	1:A:664:GLU:OE1	2.41	0.53
1:C:588:LEU:HA	1:C:591:MET:HG2	1.91	0.53
1:C:1777:ILE:HG13	1:C:1789:ILE:HG13	1.89	0.53
1:A:101:LEU:HD11	1:A:142:ASP:HB2	1.90	0.53
1:A:1777:ILE:HG13	1:A:1789:ILE:HG13	1.89	0.53
1:C:1402:ALA:O	1:C:1406:ASN:ND2	2.39	0.53
1:A:588:LEU:HA	1:A:591:MET:HG2	1.91	0.53
1:C:628:ASN:O	1:C:632:LEU:HG	2.09	0.53
1:C:1465:VAL:HG13	1:C:1467:ASP:H	1.74	0.53
1:C:644:ASN:HD22	1:C:1374:VAL:HG12	1.72	0.53
1:A:849:ALA:O	1:A:853:LYS:NZ	2.42	0.53
1:C:849:ALA:O	1:C:853:LYS:NZ	2.42	0.53
1:A:1388:VAL:HG12	1:A:1389:MET:H	1.73	0.53
1:A:1465:VAL:HG13	1:A:1467:ASP:H	1.74	0.52
1:C:1661:ILE:HG22	1:C:1662:ILE:HG12	1.90	0.52
1:C:1093:ASN:HA	1:C:1097:TYR:HB3	1.90	0.52
1:A:1223:SER:O	1:A:1227:ILE:HG12	2.10	0.52
1:C:681:GLY:HA3	1:C:685:ALA:HB2	1.92	0.52
1:C:1011:LEU:O	1:C:1015:THR:HG23	2.10	0.52
1:C:2062:ASP:O	1:C:2063:LYS:HD3	2.10	0.52
1:A:1011:LEU:O	1:A:1015:THR:HG23	2.10	0.52
1:C:1738:GLN:HG3	1:C:1741:ARG:HH21	1.75	0.52
1:C:1829:GLN:HA	1:C:1832:THR:HG22	1.90	0.52
1:A:2062:ASP:O	1:A:2063:LYS:HD3	2.10	0.52
1:C:1030:TYR:HD1	1:C:1033:ILE:HD11	1.75	0.52
1:A:1738:GLN:HG3	1:A:1741:ARG:HH21	1.75	0.52
1:C:1388:VAL:HG12	1:C:1389:MET:H	1.74	0.51
2:D:46:ASP:HA	2:D:49:LEU:HD11	1.91	0.51
1:A:681:GLY:HA3	1:A:685:ALA:HB2	1.92	0.51
1:C:1856:SER:O	1:C:1856:SER:OG	2.23	0.51
1:C:1925:PRO:HG2	1:C:1926:PRO:HD3	1.93	0.51
1:C:2099:PHE:HD2	1:C:2101:GLY:H	1.58	0.51
1:A:1030:TYR:HD1	1:A:1033:ILE:HD11	1.75	0.51
1:A:2099:PHE:HD2	1:A:2101:GLY:H	1.59	0.51
2:B:46:ASP:HA	2:B:49:LEU:HD11	1.91	0.51
1:C:36:SER:OG	1:C:37:PRO:HD3	2.11	0.51
1:C:165:ILE:HG23	1:C:191:LEU:HD23	1.93	0.51
1:A:360:LEU:HD13	1:A:434:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2028:LEU:HD12	1:A:2032:LEU:HD21	1.92	0.51
1:C:39:LEU:HD13	1:C:168:LEU:HD11	1.93	0.51
1:C:799:LYS:HG3	1:C:800:ASN:ND2	2.26	0.51
1:C:898:THR:H	1:C:901:GLN:HB2	1.76	0.51
1:C:2028:LEU:HD12	1:C:2032:LEU:HD21	1.92	0.51
1:A:36:SER:OG	1:A:37:PRO:HD3	2.11	0.51
1:A:39:LEU:HD13	1:A:168:LEU:HD11	1.93	0.51
1:A:617:VAL:O	1:A:621:LEU:HG	2.11	0.51
1:C:864:SER:O	1:C:867:TYR:HB3	2.11	0.51
1:C:1855:LYS:HA	1:C:1860:PHE:HD1	1.76	0.51
1:A:400:VAL:O	1:A:404:ARG:HG2	2.11	0.50
1:C:400:VAL:O	1:C:404:ARG:HG2	2.11	0.50
1:A:1925:PRO:HG2	1:A:1926:PRO:HD3	1.93	0.50
1:C:360:LEU:HD13	1:C:434:THR:HG21	1.93	0.50
1:A:864:SER:O	1:A:867:TYR:HB3	2.11	0.50
1:A:340:LEU:HB3	1:A:342:VAL:HG13	1.93	0.50
1:C:1699:SER:OG	1:C:1700:THR:N	2.45	0.50
1:A:204:LEU:HD23	1:A:204:LEU:H	1.77	0.50
1:C:1223:SER:O	1:C:1227:ILE:HG12	2.10	0.50
1:A:1855:LYS:HA	1:A:1860:PHE:HD1	1.76	0.50
1:C:617:VAL:O	1:C:621:LEU:HG	2.11	0.50
1:A:334:CYS:HA	1:A:337:ILE:HG22	1.94	0.50
1:A:554:CYS:HB3	1:A:572:TYR:HD1	1.76	0.50
1:A:914:VAL:O	1:A:918:LYS:HE2	2.12	0.50
1:A:1924:LEU:N	1:A:1925:PRO:HD2	2.27	0.50
1:A:1991:VAL:HG21	1:A:2053:LEU:HD12	1.94	0.50
1:A:799:LYS:HG3	1:A:800:ASN:ND2	2.26	0.50
1:A:898:THR:H	1:A:901:GLN:HB2	1.76	0.50
1:A:1699:SER:OG	1:A:1700:THR:N	2.45	0.50
1:C:1991:VAL:HG21	1:C:2053:LEU:HD12	1.94	0.50
1:A:165:ILE:HG23	1:A:191:LEU:HD23	1.93	0.49
1:C:1924:LEU:N	1:C:1925:PRO:HD2	2.27	0.49
1:A:1826:SER:O	1:A:1829:GLN:N	2.42	0.49
1:C:554:CYS:HB3	1:C:572:TYR:HD1	1.76	0.49
1:C:340:LEU:HB3	1:C:342:VAL:HG13	1.93	0.49
1:A:1152:VAL:O	1:A:1155:SER:OG	2.23	0.49
1:C:914:VAL:O	1:C:918:LYS:HE2	2.12	0.49
1:C:1650:CYS:SG	1:C:1651:THR:N	2.86	0.49
1:C:334:CYS:HA	1:C:337:ILE:HG22	1.94	0.49
1:A:285:PRO:HG2	1:A:615:LEU:HD21	1.95	0.48
1:A:1014:LEU:HD13	1:A:1030:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1715:PHE:HD2	1:C:1805:GLN:HB2	1.78	0.48
1:C:1915:SER:HB2	1:C:1954:HIS:CG	2.48	0.48
1:A:659:CYS:HB2	1:A:664:GLU:HB2	1.96	0.48
1:C:48:SER:HA	1:C:51:GLU:HG2	1.96	0.48
1:C:659:CYS:HB2	1:C:664:GLU:HB2	1.96	0.48
1:C:1014:LEU:HD13	1:C:1030:TYR:CZ	2.48	0.48
1:C:2096:LYS:NZ	1:C:2130:ALA:O	2.38	0.48
1:C:204:LEU:HD23	1:C:204:LEU:H	1.77	0.48
1:A:1627:SER:OG	1:A:1628:LYS:N	2.47	0.48
1:C:1627:SER:OG	1:C:1628:LYS:N	2.47	0.48
1:A:102:GLU:HG3	1:A:123:LEU:HD21	1.95	0.48
1:A:1650:CYS:SG	1:A:1651:THR:N	2.86	0.48
1:A:1915:SER:HB2	1:A:1954:HIS:CG	2.48	0.48
1:A:1948:LEU:HD11	1:A:1950:VAL:HG13	1.94	0.48
1:C:1948:LEU:HD11	1:C:1950:VAL:HG13	1.94	0.48
1:A:2017:LEU:HG	1:A:2018:PRO:HD2	1.96	0.48
1:A:860:LEU:HD11	1:A:1004:VAL:HB	1.96	0.48
1:A:127:LYS:NZ	1:A:137:LEU:O	2.47	0.48
1:A:737:ASN:ND2	1:A:1282:SER:OG	2.47	0.48
1:C:127:LYS:NZ	1:C:137:LEU:O	2.47	0.48
2:D:46:ASP:OD1	2:D:46:ASP:N	2.46	0.48
1:A:1855:LYS:HA	1:A:1860:PHE:CD1	2.49	0.47
1:C:1855:LYS:HA	1:C:1860:PHE:CD1	2.49	0.47
1:A:329:SER:O	1:A:333:LEU:HG	2.14	0.47
1:A:336:LYS:O	1:A:336:LYS:NZ	2.43	0.47
1:A:1915:SER:H	1:A:1954:HIS:HB2	1.79	0.47
1:C:1711:ASN:N	1:C:1806:SER:OG	2.46	0.47
1:A:1711:ASN:N	1:A:1806:SER:OG	2.46	0.47
2:B:46:ASP:OD1	2:B:46:ASP:N	2.46	0.47
1:C:1915:SER:H	1:C:1954:HIS:HB2	1.79	0.47
1:A:786:LEU:HD21	1:A:1312:TYR:CD2	2.50	0.47
1:C:329:SER:O	1:C:333:LEU:HG	2.14	0.47
1:C:285:PRO:HG2	1:C:615:LEU:HD21	1.95	0.47
1:C:737:ASN:ND2	1:C:1282:SER:OG	2.47	0.47
1:C:2017:LEU:HG	1:C:2018:PRO:HD2	1.96	0.47
1:A:48:SER:HA	1:A:51:GLU:HG2	1.96	0.47
1:A:1204:LEU:HD22	1:A:1302:TYR:HD1	1.79	0.47
1:A:1512:GLU:HG3	1:A:1513:GLU:HG3	1.97	0.47
1:A:1871:GLN:HA	1:A:1871:GLN:OE1	2.15	0.47
1:C:860:LEU:HD11	1:C:1004:VAL:HB	1.96	0.47
1:C:1109:SER:OG	1:C:1113:GLY:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1189:HIS:NE2	1:C:1331:GLN:OE1	2.48	0.47
1:C:1204:LEU:HD22	1:C:1302:TYR:HD1	1.79	0.47
1:A:490:LEU:O	1:A:494:SER:OG	2.33	0.47
1:A:1220:ASP:OD1	1:A:1220:ASP:N	2.44	0.47
1:A:1715:PHE:HD2	1:A:1805:GLN:HB2	1.78	0.47
1:A:1688:THR:HA	1:A:1691:CYS:SG	2.55	0.47
1:C:483:GLN:HA	1:C:486:LEU:HD12	1.97	0.47
1:C:833:SER:O	1:C:837:LYS:HG3	2.16	0.47
1:C:1211:ARG:HG3	1:C:1216:ARG:HA	1.97	0.47
1:C:1512:GLU:HG3	1:C:1513:GLU:HG3	1.97	0.47
1:C:1688:THR:HA	1:C:1691:CYS:SG	2.55	0.47
1:C:102:GLU:HG3	1:C:123:LEU:HD21	1.95	0.46
1:C:490:LEU:O	1:C:494:SER:OG	2.33	0.46
1:A:1189:HIS:NE2	1:A:1331:GLN:OE1	2.48	0.46
1:C:350:LEU:HD22	1:C:392:ARG:HH12	1.80	0.46
1:C:1752:LEU:HG	1:C:1753:THR:HG23	1.97	0.46
1:A:350:LEU:HD22	1:A:392:ARG:HH12	1.80	0.46
1:C:189:HIS:CD2	1:C:195:LYS:HD3	2.51	0.46
1:A:189:HIS:CD2	1:A:195:LYS:HD3	2.51	0.46
1:A:226:LEU:HD21	1:A:1203:ALA:HB1	1.98	0.46
1:C:1310:LEU:HD11	1:C:1361:LEU:HB3	1.97	0.46
1:A:833:SER:O	1:A:837:LYS:HG3	2.16	0.46
1:C:324:GLU:O	1:C:328:LEU:HG	2.15	0.46
1:C:355:LEU:HD13	1:C:413:TRP:HZ3	1.81	0.46
1:A:235:VAL:O	1:A:239:LEU:HG	2.15	0.46
1:A:355:LEU:HD13	1:A:413:TRP:HZ3	1.81	0.46
1:A:2073:ASN:O	1:A:2074:GLN:HG3	2.16	0.46
1:C:235:VAL:O	1:C:239:LEU:HG	2.15	0.46
1:A:1752:LEU:HG	1:A:1753:THR:HG23	1.97	0.46
1:C:722:GLU:CD	1:C:1266:SER:HB3	2.36	0.46
1:A:582:VAL:HG22	1:A:583:PHE:CD2	2.51	0.46
1:A:1310:LEU:HD11	1:A:1361:LEU:HB3	1.98	0.46
1:A:1499:ARG:HD3	1:A:1819:THR:HB	1.98	0.46
1:C:114:LYS:HZ3	1:C:1137:ASN:HB2	1.80	0.46
1:C:582:VAL:HG22	1:C:583:PHE:CD2	2.51	0.46
1:C:684:ASP:OD1	1:C:684:ASP:N	2.44	0.46
1:C:786:LEU:HD21	1:C:1312:TYR:CD2	2.50	0.46
1:A:586:GLU:HG3	1:A:1438:ARG:HD3	1.98	0.45
1:A:1211:ARG:HG3	1:A:1216:ARG:HA	1.97	0.45
1:A:1872:ILE:HD11	1:A:1875:ALA:HB3	1.98	0.45
1:C:543:LEU:HD11	1:C:555:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1664:CYS:SG	1:C:1667:SER:OG	2.64	0.45
1:C:1871:GLN:HA	1:C:1871:GLN:OE1	2.15	0.45
1:A:458:MET:HB2	1:A:525:LEU:HD13	1.98	0.45
1:C:586:GLU:HG3	1:C:1438:ARG:HD3	1.98	0.45
1:C:1872:ILE:HD11	1:C:1875:ALA:HB3	1.98	0.45
1:A:323:ILE:HD12	1:A:323:ILE:H	1.80	0.45
1:A:415:LYS:H	1:A:415:LYS:HD2	1.82	0.45
1:A:459:ARG:HD3	1:A:522:ASN:HD21	1.82	0.45
1:A:1109:SER:OG	1:A:1113:GLY:O	2.28	0.45
1:C:458:MET:HB2	1:C:525:LEU:HD13	1.99	0.45
1:C:585:ASP:OD1	1:C:585:ASP:N	2.45	0.45
1:A:324:GLU:O	1:A:328:LEU:HG	2.15	0.45
1:A:722:GLU:CD	1:A:1266:SER:HB3	2.36	0.45
1:A:775:VAL:HG23	1:A:1365:LEU:HA	1.97	0.45
1:C:459:ARG:HD3	1:C:522:ASN:HD21	1.82	0.45
1:C:1558:LEU:HD12	1:C:1629:CYS:HB2	1.98	0.45
1:C:2073:ASN:O	1:C:2074:GLN:HG3	2.16	0.45
1:A:483:GLN:HA	1:A:486:LEU:HD12	1.97	0.45
1:C:525:LEU:HD23	1:C:528:CYS:SG	2.56	0.45
1:A:663:SER:OG	1:A:664:GLU:OE1	2.34	0.45
1:C:1499:ARG:HD3	1:C:1819:THR:HB	1.98	0.45
2:B:55:HIS:CE1	2:B:75:CYS:HB3	2.52	0.45
1:C:1488:ASP:OD1	1:C:1488:ASP:N	2.50	0.45
1:A:543:LEU:HD11	1:A:555:TYR:HB3	1.98	0.45
1:A:63:ASN:OD1	1:A:67:ARG:NH1	2.50	0.45
1:A:1566:LEU:HG	1:A:1567:MET:HG3	1.99	0.45
1:A:1742:ARG:HH22	1:A:1769:ARG:H	1.64	0.45
1:A:2096:LYS:NZ	1:A:2130:ALA:O	2.38	0.45
1:C:1742:ARG:HH22	1:C:1769:ARG:H	1.64	0.45
1:C:1826:SER:O	1:C:1829:GLN:N	2.42	0.45
1:C:415:LYS:H	1:C:415:LYS:HD2	1.82	0.44
2:D:55:HIS:CE1	2:D:75:CYS:HB3	2.52	0.44
1:A:2118:VAL:HA	1:A:2153:LEU:HD11	1.99	0.44
1:C:204:LEU:HB2	1:C:207:LEU:HD23	1.99	0.44
1:C:226:LEU:HD21	1:C:1203:ALA:HB1	1.98	0.44
1:C:2060:LEU:HD23	1:C:2060:LEU:H	1.82	0.44
1:C:2108:LEU:HD22	1:C:2117:VAL:HG13	1.99	0.44
1:C:2118:VAL:HA	1:C:2153:LEU:HD11	1.99	0.44
1:A:2060:LEU:H	1:A:2060:LEU:HD23	1.82	0.44
1:C:63:ASN:OD1	1:C:67:ARG:NH1	2.50	0.44
1:C:323:ILE:HD12	1:C:323:ILE:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1955:VAL:HB	1:C:1979:VAL:HB	2.00	0.44
1:A:377:LYS:HE2	1:A:451:LEU:HD22	1.99	0.44
1:A:525:LEU:HD23	1:A:528:CYS:SG	2.56	0.44
1:C:586:GLU:O	1:C:1438:ARG:NH2	2.43	0.44
1:C:775:VAL:HG23	1:C:1365:LEU:HA	1.97	0.44
1:C:1353:GLU:HA	1:C:1356:CYS:SG	2.58	0.44
1:C:1842:SER:HB2	1:C:2080:LEU:HG	1.99	0.44
1:C:42:GLY:O	1:C:45:LEU:HG	2.18	0.44
1:C:475:PHE:HA	1:C:478:MET:HG3	1.99	0.44
1:C:1291:GLY:HA3	1:C:1294:ILE:HD12	2.00	0.44
1:A:1488:ASP:OD1	1:A:1488:ASP:N	2.50	0.44
1:A:1842:SER:HB2	1:A:2080:LEU:HG	1.99	0.44
1:C:1843:MET:HG2	1:C:2082:ASP:HA	2.00	0.44
1:C:2140:GLU:O	1:C:2143:THR:OG1	2.30	0.44
1:A:204:LEU:HB2	1:A:207:LEU:HD23	1.98	0.44
1:A:1742:ARG:NH2	1:A:1769:ARG:H	2.16	0.44
1:A:2028:LEU:HD22	1:A:2049:VAL:HG22	1.99	0.44
1:C:663:SER:OG	1:C:664:GLU:OE1	2.34	0.44
1:C:1862:GLU:HG2	1:C:1871:GLN:HE22	1.83	0.44
1:A:1291:GLY:HA3	1:A:1294:ILE:HD12	2.00	0.44
1:C:114:LYS:NZ	1:C:1135:ASP:OD2	2.51	0.44
1:C:119:ASP:HA	1:C:122:LYS:HE3	2.00	0.44
1:C:377:LYS:HE2	1:C:451:LEU:HD22	1.99	0.44
1:C:536:ALA:HB3	1:C:539:LEU:HG	1.99	0.44
1:C:1326:THR:HA	1:C:1331:GLN:HG3	1.99	0.44
1:C:1742:ARG:NH2	1:C:1769:ARG:H	2.16	0.44
1:A:1212:THR:OG1	1:A:1216:ARG:N	2.50	0.44
1:A:2108:LEU:HD22	1:A:2117:VAL:HG13	1.99	0.44
1:A:2117:VAL:HG11	1:A:2148:LEU:HD13	2.00	0.44
1:C:1948:LEU:HD12	1:C:1949:VAL:H	1.83	0.44
1:C:2011:VAL:HA	1:C:2014:VAL:HG12	2.00	0.44
1:A:1843:MET:HG2	1:A:2082:ASP:HA	2.00	0.43
1:A:1955:VAL:HB	1:A:1979:VAL:HB	2.00	0.43
1:C:4:TYR:HB2	1:C:167:ILE:HD11	1.99	0.43
1:A:4:TYR:HB2	1:A:167:ILE:HD11	1.99	0.43
1:A:1288:LEU:H	1:A:1288:LEU:HD23	1.83	0.43
1:A:1305:ILE:HG13	1:A:1306:THR:N	2.33	0.43
1:A:2011:VAL:HA	1:A:2014:VAL:HG12	2.00	0.43
1:A:2017:LEU:HB3	1:A:2019:LEU:HG	2.01	0.43
1:A:42:GLY:O	1:A:45:LEU:HG	2.18	0.43
1:A:536:ALA:HB3	1:A:539:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1558:LEU:HD12	1:A:1629:CYS:HB2	1.99	0.43
1:A:1906:ASN:HD21	1:A:1962:LYS:HB2	1.83	0.43
1:C:1212:THR:OG1	1:C:1216:ARG:N	2.51	0.43
1:C:1505:ILE:O	1:C:1509:ARG:NH1	2.51	0.43
1:A:295:VAL:HG23	1:A:489:THR:HB	2.00	0.43
1:A:1143:ARG:O	1:A:1146:GLU:HG2	2.19	0.43
1:A:1826:SER:O	1:A:1828:GLN:N	2.51	0.43
1:A:1862:GLU:HG2	1:A:1871:GLN:HE22	1.83	0.43
1:C:295:VAL:HG23	1:C:489:THR:HB	2.00	0.43
1:C:1566:LEU:HG	1:C:1567:MET:HG3	1.99	0.43
1:A:870:LEU:HB3	1:A:893:MET:HE3	2.01	0.43
1:C:67:ARG:HB2	1:C:71:VAL:HG11	2.01	0.43
1:C:1826:SER:O	1:C:1828:GLN:N	2.51	0.43
1:C:2028:LEU:HD22	1:C:2049:VAL:HG22	1.99	0.43
1:A:1238:VAL:HG22	1:A:1282:SER:HA	2.01	0.43
1:A:1326:THR:HA	1:A:1331:GLN:HG3	1.99	0.43
1:A:1835:LYS:HA	1:A:1835:LYS:HD2	1.81	0.43
1:C:1143:ARG:O	1:C:1146:GLU:HG2	2.19	0.43
1:A:266:LEU:HD12	1:A:638:PHE:CE1	2.54	0.43
1:A:475:PHE:HA	1:A:478:MET:HG3	2.00	0.43
1:A:1505:ILE:O	1:A:1509:ARG:NH1	2.51	0.43
1:C:1300:ASP:OD1	1:C:1328:SER:HB3	2.19	0.43
1:C:1566:LEU:HG	1:C:1567:MET:N	2.34	0.43
1:A:119:ASP:HA	1:A:122:LYS:HE3	2.00	0.43
1:A:1353:GLU:HA	1:A:1356:CYS:SG	2.58	0.43
1:A:1879:ASP:O	1:A:1883:MET:HG2	2.19	0.43
1:C:336:LYS:O	1:C:336:LYS:NZ	2.43	0.43
1:C:530:ALA:HA	1:C:543:LEU:O	2.19	0.43
1:C:366:ASP:OD1	1:C:367:SER:N	2.52	0.42
1:C:982:GLU:HG2	1:C:983:LEU:HD22	2.00	0.42
1:C:1185:CYS:HB3	1:C:1375:ILE:HG13	2.01	0.42
1:C:1305:ILE:HG13	1:C:1306:THR:N	2.33	0.42
1:C:2017:LEU:HB3	1:C:2019:LEU:HG	2.01	0.42
1:A:735:VAL:HG22	1:A:1285:MET:O	2.18	0.42
1:C:2117:VAL:HG11	1:C:2148:LEU:HD13	2.00	0.42
1:A:530:ALA:HA	1:A:543:LEU:O	2.19	0.42
1:A:1300:ASP:OD1	1:A:1328:SER:HB3	2.19	0.42
1:A:2140:GLU:O	1:A:2143:THR:OG1	2.30	0.42
1:C:735:VAL:HG22	1:C:1285:MET:O	2.18	0.42
1:C:1183:LEU:HB3	1:C:1335:ILE:HB	2.01	0.42
1:C:1733:MET:HG3	1:C:1734:ASN:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1835:LYS:HA	1:C:1835:LYS:HD2	1.81	0.42
1:A:982:GLU:HG2	1:A:983:LEU:HD22	2.00	0.42
1:A:1147:ASP:O	1:A:1150:GLU:HG2	2.20	0.42
1:A:1798:ASN:ND2	1:A:1801:TYR:OH	2.44	0.42
1:A:1834:PHE:HZ	1:A:1854:LEU:HD12	1.84	0.42
2:B:72:CYS:SG	2:B:74:ILE:HG22	2.60	0.42
1:C:1237:GLU:N	1:C:1237:GLU:OE1	2.52	0.42
1:C:1906:ASN:HD21	1:C:1962:LYS:HB2	1.83	0.42
1:C:2019:LEU:C	1:C:2024:ALA:HA	2.39	0.42
2:D:72:CYS:SG	2:D:74:ILE:HG22	2.60	0.42
1:A:366:ASP:OD1	1:A:367:SER:N	2.52	0.42
1:A:406:LYS:HE2	1:A:406:LYS:HB2	1.90	0.42
1:A:1100:ASP:OD1	1:A:1100:ASP:N	2.50	0.42
1:A:1948:LEU:HD12	1:A:1949:VAL:H	1.83	0.42
1:C:83:LEU:HD22	1:C:130:LEU:HD13	2.02	0.42
1:C:870:LEU:HB3	1:C:893:MET:HE3	2.02	0.42
1:C:1879:ASP:O	1:C:1883:MET:HG2	2.19	0.42
1:C:1978:ASP:OD2	1:C:1995:ASP:HB3	2.20	0.42
1:A:67:ARG:HB2	1:A:71:VAL:HG11	2.01	0.42
1:A:637:TYR:CZ	1:A:1372:LYS:HD2	2.55	0.42
1:A:1442:ARG:O	1:A:1446:LEU:HD23	2.19	0.42
1:A:1566:LEU:HG	1:A:1567:MET:N	2.34	0.42
1:A:1237:GLU:N	1:A:1237:GLU:OE1	2.52	0.42
1:C:161:ARG:O	1:C:165:ILE:HG12	2.20	0.42
1:A:1795:THR:HG22	1:A:1796:ARG:H	1.85	0.42
1:A:2032:LEU:HD23	1:A:2032:LEU:H	1.85	0.42
1:C:266:LEU:HD12	1:C:638:PHE:CE1	2.54	0.42
1:C:1139:LYS:HE3	1:C:1139:LYS:HB2	1.90	0.42
1:C:1238:VAL:HG22	1:C:1282:SER:HA	2.01	0.42
1:C:1834:PHE:HZ	1:C:1854:LEU:HD12	1.84	0.42
1:A:1183:LEU:HB3	1:A:1335:ILE:HB	2.01	0.42
1:A:1539:GLN:HA	1:A:1542:ASN:HD21	1.85	0.42
1:C:376:ARG:O	1:C:381:ILE:HG22	2.20	0.42
1:C:1011:LEU:HG	1:C:1034:GLN:HE21	1.85	0.42
1:C:1288:LEU:HD23	1:C:1288:LEU:H	1.83	0.42
1:C:1539:GLN:HA	1:C:1542:ASN:HD21	1.85	0.42
1:C:1795:THR:HG22	1:C:1796:ARG:H	1.85	0.42
1:A:1200:LEU:HD21	1:A:1302:TYR:CZ	2.55	0.42
1:C:574:ASP:OD2	1:C:576:LYS:HG2	2.20	0.42
1:C:1147:ASP:O	1:C:1150:GLU:HG2	2.20	0.42
1:A:119:ASP:HA	1:A:122:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:O	1:A:381:ILE:HG22	2.20	0.41
1:A:2019:LEU:C	1:A:2024:ALA:HA	2.39	0.41
1:C:1200:LEU:HD21	1:C:1302:TYR:CZ	2.55	0.41
1:C:1442:ARG:O	1:C:1446:LEU:HD23	2.19	0.41
1:C:2032:LEU:HD23	1:C:2032:LEU:H	1.84	0.41
1:A:1978:ASP:OD2	1:A:1995:ASP:HB3	2.20	0.41
1:C:112:PHE:HE1	1:C:143:GLY:HA3	1.85	0.41
1:C:382:VAL:HG23	1:C:385:MET:HB2	2.01	0.41
1:A:382:VAL:HG23	1:A:385:MET:HB2	2.01	0.41
1:A:1011:LEU:HG	1:A:1034:GLN:HE21	1.85	0.41
1:A:1185:CYS:HB3	1:A:1375:ILE:HG13	2.01	0.41
1:A:1588:LYS:HE3	1:A:1588:LYS:HB3	1.96	0.41
1:C:1420:ASP:CB	1:C:1460:ILE:HD11	2.49	0.41
1:C:637:TYR:CZ	1:C:1372:LYS:HD2	2.55	0.41
1:C:1410:LYS:HD2	1:C:1562:LEU:HD12	2.03	0.41
1:A:83:LEU:HD22	1:A:130:LEU:HD13	2.02	0.41
1:C:1738:GLN:NE2	1:C:1765:MET:HA	2.36	0.41
1:C:1744:TYR:HB3	1:C:1747:LEU:HB3	2.02	0.41
1:A:161:ARG:O	1:A:165:ILE:HG12	2.20	0.41
1:A:1744:TYR:HB3	1:A:1747:LEU:HB3	2.02	0.41
1:A:1823:LEU:HD21	1:C:2107:ALA:HB2	2.03	0.41
1:A:2041:ASN:OD1	1:A:2042:ASP:N	2.53	0.41
1:C:760:PHE:HB3	1:C:777:LYS:HE3	2.03	0.41
1:C:2017:LEU:HD23	1:C:2019:LEU:HD23	2.02	0.41
1:A:112:PHE:HE1	1:A:143:GLY:HA3	1.85	0.41
1:A:1837:GLN:NE2	1:A:1859:TRP:HB2	2.36	0.41
1:C:73:LEU:HD12	1:C:78:ILE:HG21	2.03	0.41
1:C:899:GLU:O	1:C:902:VAL:HG12	2.21	0.41
1:C:1696:TRP:HA	1:C:1816:SER:OG	2.21	0.41
1:A:19:ARG:H	1:A:22:PHE:HD2	1.68	0.41
1:A:2007:LEU:HD21	1:A:2063:LYS:O	2.21	0.41
1:C:2041:ASN:OD1	1:C:2042:ASP:N	2.53	0.41
1:C:2139:GLN:O	1:C:2142:PHE:N	2.49	0.41
1:A:94:THR:O	1:A:97:THR:OG1	2.36	0.41
1:A:261:THR:HG23	1:A:645:GLN:O	2.21	0.41
1:A:431:HIS:ND1	1:A:431:HIS:N	2.69	0.41
1:A:760:PHE:HB3	1:A:777:LYS:HE3	2.03	0.41
1:A:1137:ASN:O	1:A:1141:MET:HG2	2.21	0.41
1:A:1733:MET:HG3	1:A:1734:ASN:H	1.86	0.41
1:C:1589:LEU:HB2	1:C:1755:PHE:HE2	1.85	0.41
1:A:1420:ASP:CB	1:A:1460:ILE:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1696:TRP:HA	1:A:1816:SER:OG	2.21	0.41
1:C:1860:PHE:CE2	1:C:1862:GLU:HB2	2.56	0.41
1:A:1388:VAL:HG12	1:A:1389:MET:N	2.36	0.40
1:A:1589:LEU:HB2	1:A:1755:PHE:HE2	1.86	0.40
1:A:1753:THR:N	1:A:1754:PRO:HD3	2.36	0.40
1:A:55:CYS:C	1:A:60:CYS:HB2	2.42	0.40
1:A:574:ASP:OD2	1:A:576:LYS:HG2	2.20	0.40
1:A:586:GLU:O	1:A:1438:ARG:NH2	2.43	0.40
1:A:763:SER:OG	1:A:764:LEU:N	2.54	0.40
1:A:1823:LEU:HA	1:C:2106:LYS:HG2	2.03	0.40
1:C:19:ARG:H	1:C:22:PHE:HD2	1.68	0.40
1:A:73:LEU:HD12	1:A:78:ILE:HG21	2.03	0.40
1:A:1688:THR:HG22	1:A:1788:ILE:HD12	2.04	0.40
1:C:119:ASP:HA	1:C:122:LYS:HG2	2.02	0.40
1:C:1871:GLN:NE2	1:C:1872:ILE:HG12	2.36	0.40
1:C:2007:LEU:HD21	1:C:2063:LYS:O	2.21	0.40
1:A:399:ALA:O	1:A:403:ILE:HG12	2.21	0.40
1:A:1351:TRP:HB3	1:A:1354:MET:HE2	2.02	0.40
1:C:533:PHE:CZ	1:C:541:GLY:HA3	2.57	0.40
1:C:1351:TRP:HB3	1:C:1354:MET:HE2	2.02	0.40
1:C:1770:LEU:HB2	1:C:1773:LEU:HB3	2.04	0.40
1:A:16:ILE:O	1:A:16:ILE:HG13	2.21	0.40
1:A:1687:LEU:HD23	1:A:1779:LEU:HD11	2.03	0.40
1:A:2021:THR:O	1:A:2021:THR:OG1	2.37	0.40
1:C:55:CYS:C	1:C:60:CYS:HB2	2.42	0.40
1:C:1137:ASN:O	1:C:1141:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
1	C	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
2	B	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
2	D	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
All	All	3892/4606 (84%)	3556 (91%)	336 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	1690/2007 (84%)	1651 (98%)	39 (2%)	45	64
1	C	1690/2007 (84%)	1651 (98%)	39 (2%)	45	64
2	B	47/88 (53%)	47 (100%)	0	100	100
2	D	47/88 (53%)	47 (100%)	0	100	100
All	All	3474/4190 (83%)	3396 (98%)	78 (2%)	47	65

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	49	LEU
1	A	85	LYS
1	A	233	SER
1	A	331	LEU
1	A	375	LEU
1	A	431	HIS
1	A	489	THR
1	A	494	SER
1	A	595	MET
1	A	659	CYS
1	A	795	SER
1	A	798	LEU

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Mol	Chain	Res	Type
1	A	838	GLU
1	A	869	ILE
1	A	909	LYS
1	A	992	GLU
1	A	1002	LEU
1	A	1031	LEU
1	A	1032	LEU
1	A	1036	HIS
1	A	1190	SER
1	A	1210	LEU
1	A	1215	ASP
1	A	1222	ASP
1	A	1301	LEU
1	A	1369	VAL
1	A	1466	LYS
1	A	1531	LEU
1	A	1553	SER
1	A	1624	SER
1	A	1648	SER
1	A	1736	VAL
1	A	1788	ILE
1	A	1856	SER
1	A	2016	SER
1	A	2052	ASP
1	A	2124	LEU
1	A	2156	SER
1	C	3	GLU
1	C	49	LEU
1	C	85	LYS
1	C	233	SER
1	C	331	LEU
1	C	375	LEU
1	C	431	HIS
1	C	489	THR
1	C	494	SER
1	C	595	MET
1	C	659	CYS
1	C	795	SER
1	C	798	LEU
1	C	838	GLU
1	C	869	ILE
1	C	909	LYS

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Mol	Chain	Res	Type
1	C	992	GLU
1	C	1002	LEU
1	C	1031	LEU
1	C	1032	LEU
1	C	1036	HIS
1	C	1190	SER
1	C	1210	LEU
1	C	1215	ASP
1	C	1222	ASP
1	C	1301	LEU
1	C	1369	VAL
1	C	1466	LYS
1	C	1531	LEU
1	C	1553	SER
1	C	1624	SER
1	C	1648	SER
1	C	1736	VAL
1	C	1788	ILE
1	C	1856	SER
1	C	2016	SER
1	C	2052	ASP
1	C	2124	LEU
1	C	2156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	522	ASN
1	A	568	GLN
1	A	628	ASN
1	A	647	HIS
1	A	737	ASN
1	A	788	ASN
1	A	800	ASN
1	A	901	GLN
1	A	1128	ASN
1	A	1206	GLN
1	A	1308	GLN
1	A	1414	GLN
1	A	1429	ASN
1	A	1539	GLN

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Mol	Chain	Res	Type
1	A	1542	ASN
1	A	1611	GLN
1	A	1669	ASN
1	A	1738	GLN
1	A	1798	ASN
1	A	1829	GLN
1	A	1837	GLN
1	A	1871	GLN
1	A	1888	ASN
1	A	1916	ASN
1	A	2043	ASN
1	A	2146	HIS
1	C	335	ASN
1	C	522	ASN
1	C	568	GLN
1	C	628	ASN
1	C	647	HIS
1	C	737	ASN
1	C	788	ASN
1	C	800	ASN
1	C	901	GLN
1	C	1128	ASN
1	C	1206	GLN
1	C	1308	GLN
1	C	1414	GLN
1	C	1429	ASN
1	C	1542	ASN
1	C	1611	GLN
1	C	1669	ASN
1	C	1798	ASN
1	C	1829	GLN
1	C	1837	GLN
1	C	1871	GLN
1	C	1888	ASN
1	C	1916	ASN
1	C	2043	ASN
1	C	2146	HIS

5.3.3 RNA ⓘ

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](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

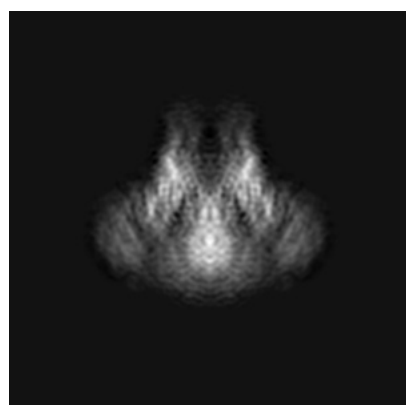
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31179. These allow visual inspection of the internal detail of the map and identification of artifacts.

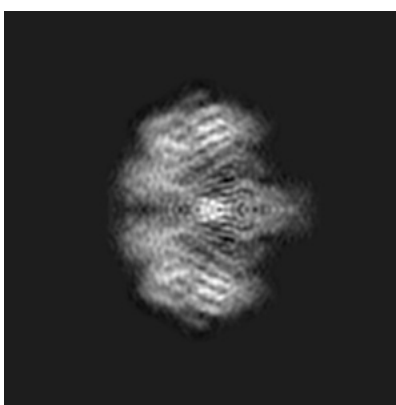
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

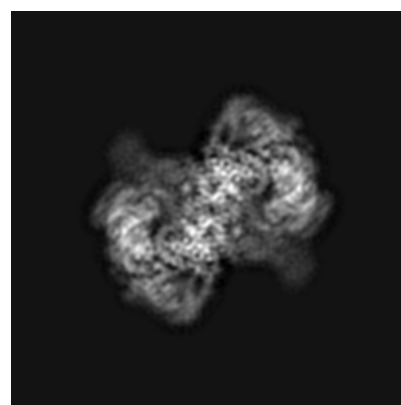
6.1.1 Primary map



X



Y



Z

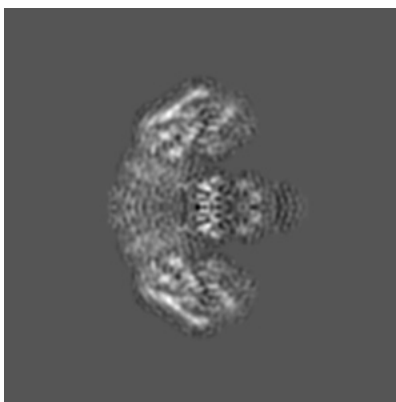
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

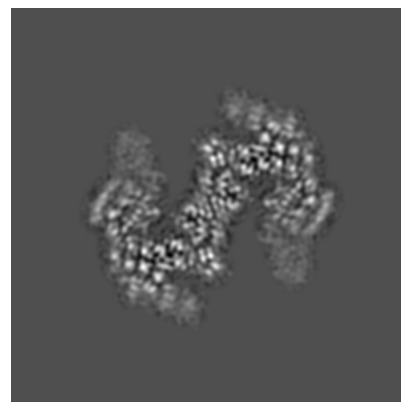
6.2.1 Primary map



X Index: 128



Y Index: 128

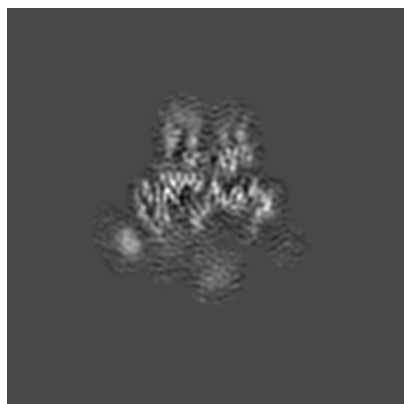


Z Index: 128

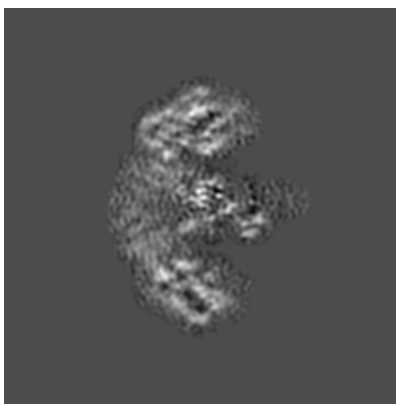
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

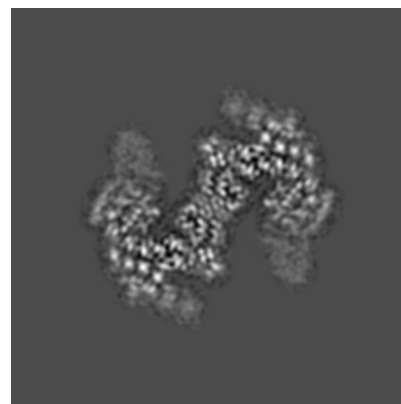
6.3.1 Primary map



X Index: 125



Y Index: 131

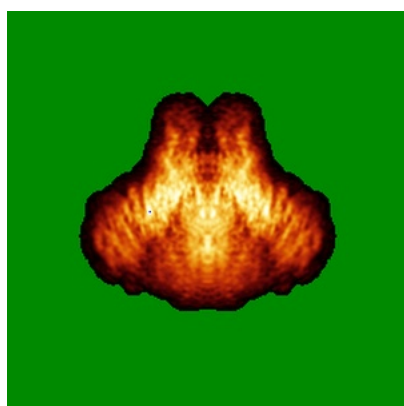


Z Index: 129

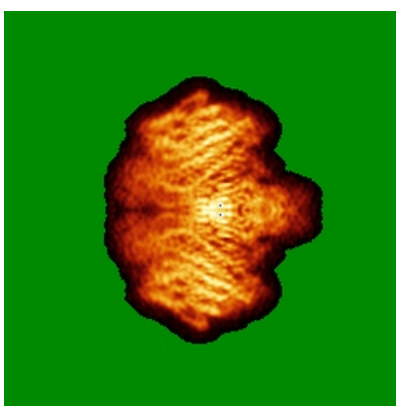
The images above show the largest variance slices of the map in three orthogonal directions.

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

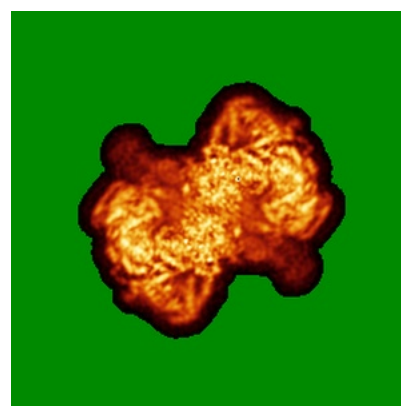
6.4.1 Primary map



X



Y

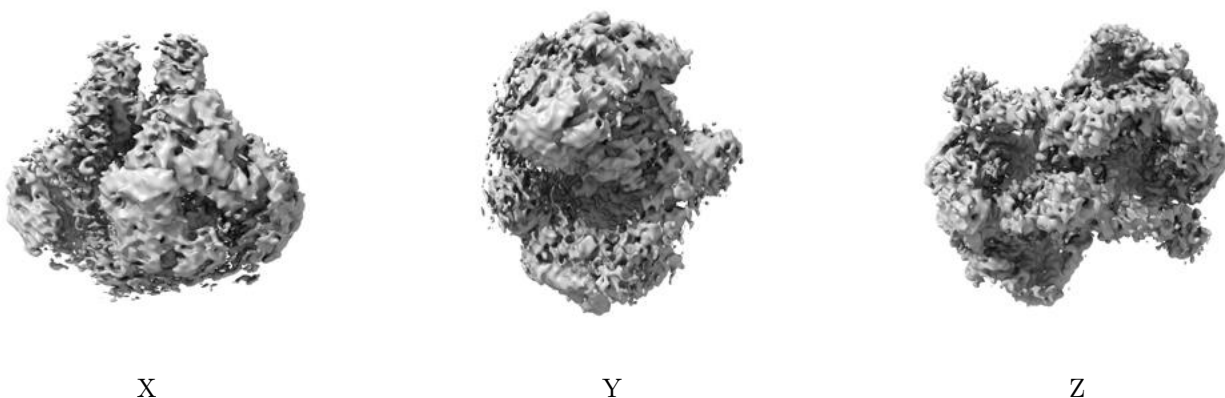


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

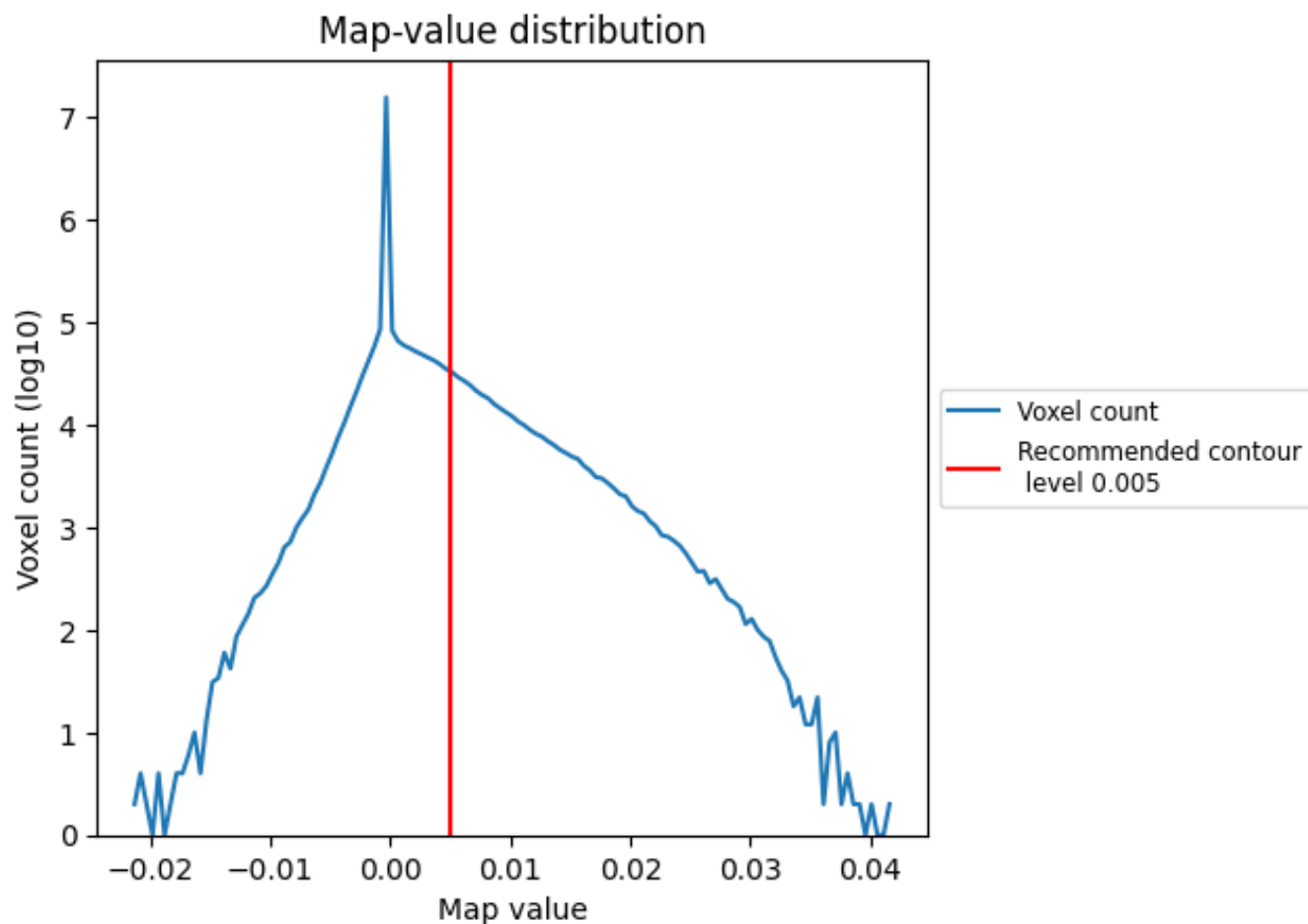
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

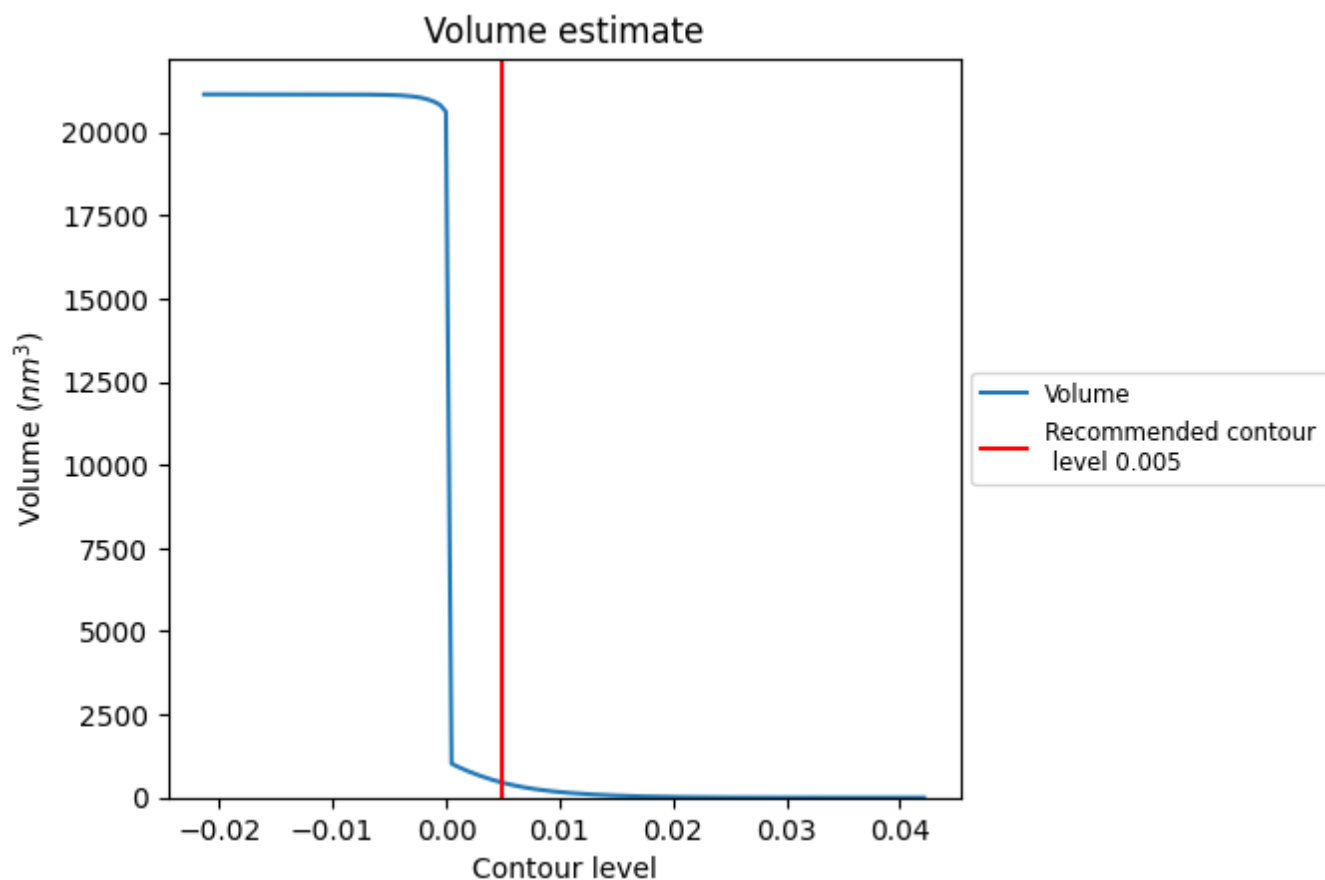
This section contains the results of statistical analysis of the map.

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.

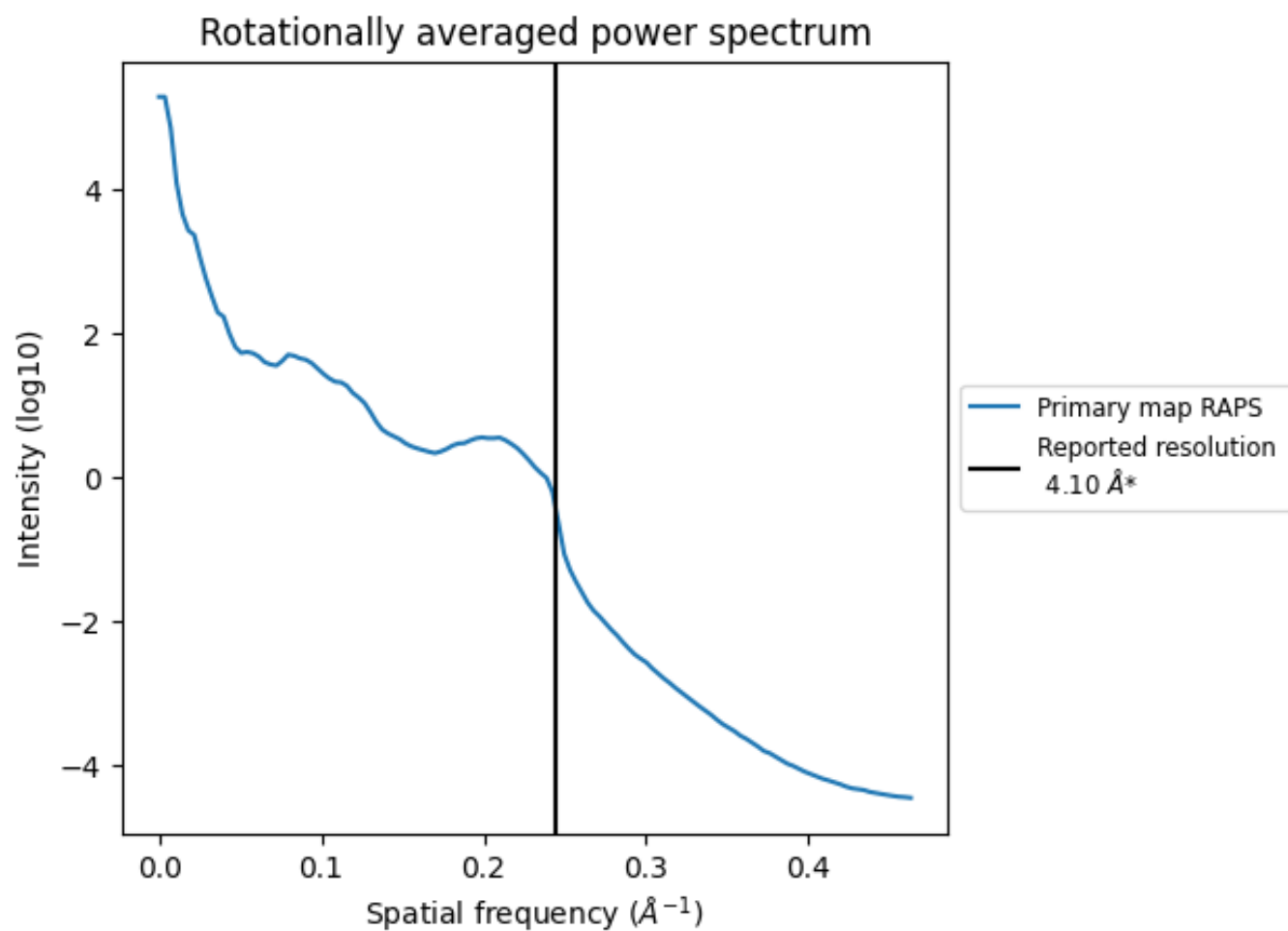
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 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 ⓘ

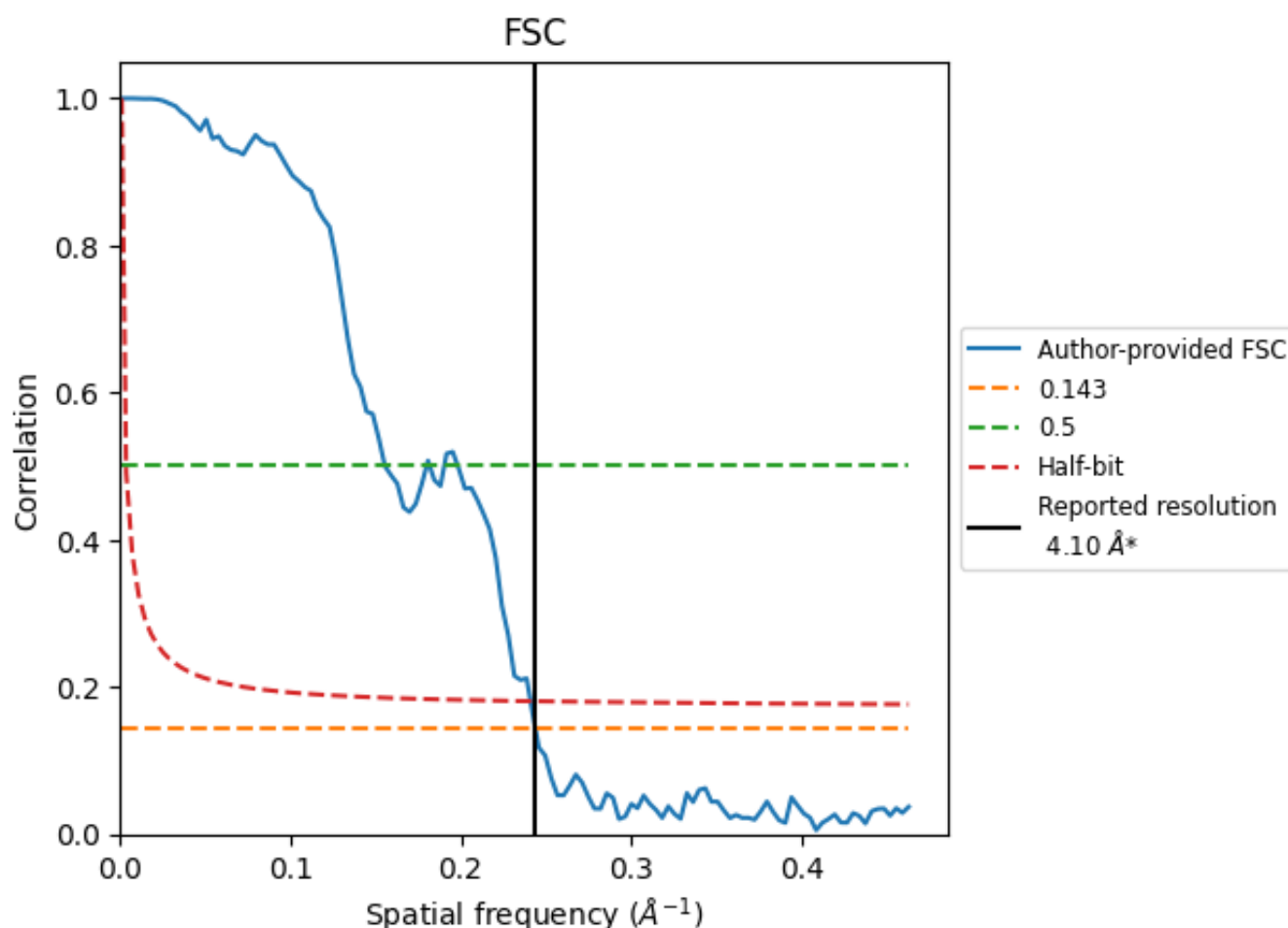


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

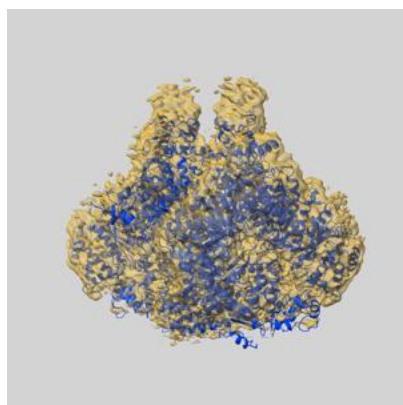
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	6.43	4.15
Unmasked-calculated*	-	-	-

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

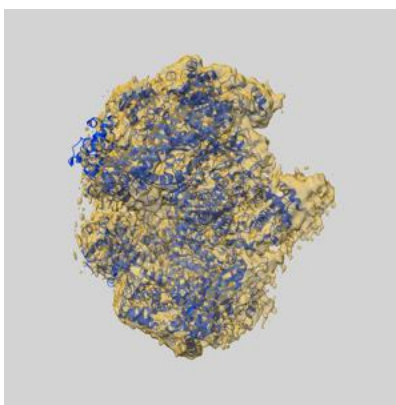
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31179 and PDB model 7ELB. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

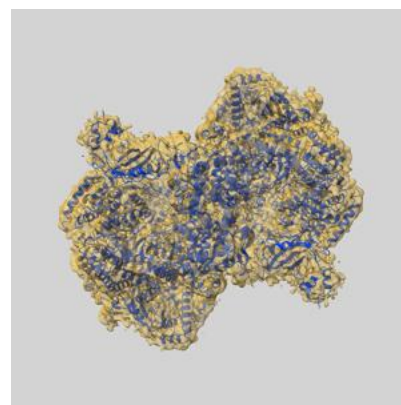
9.1 Map-model overlay [i](#)



X



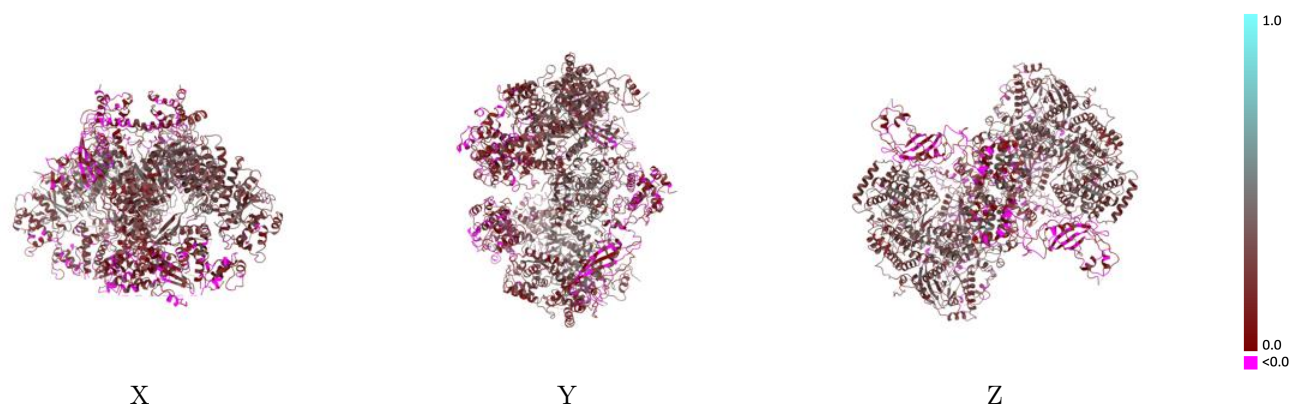
Y



Z

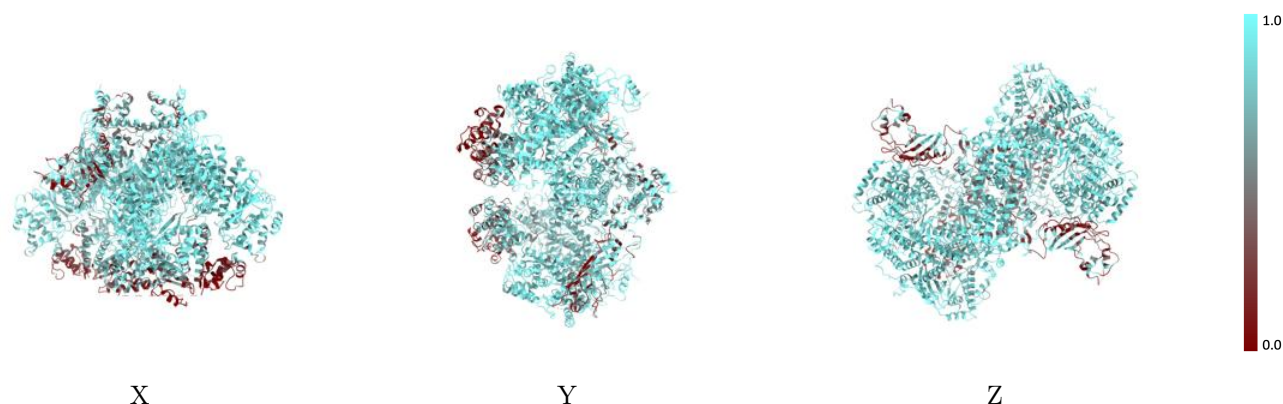
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



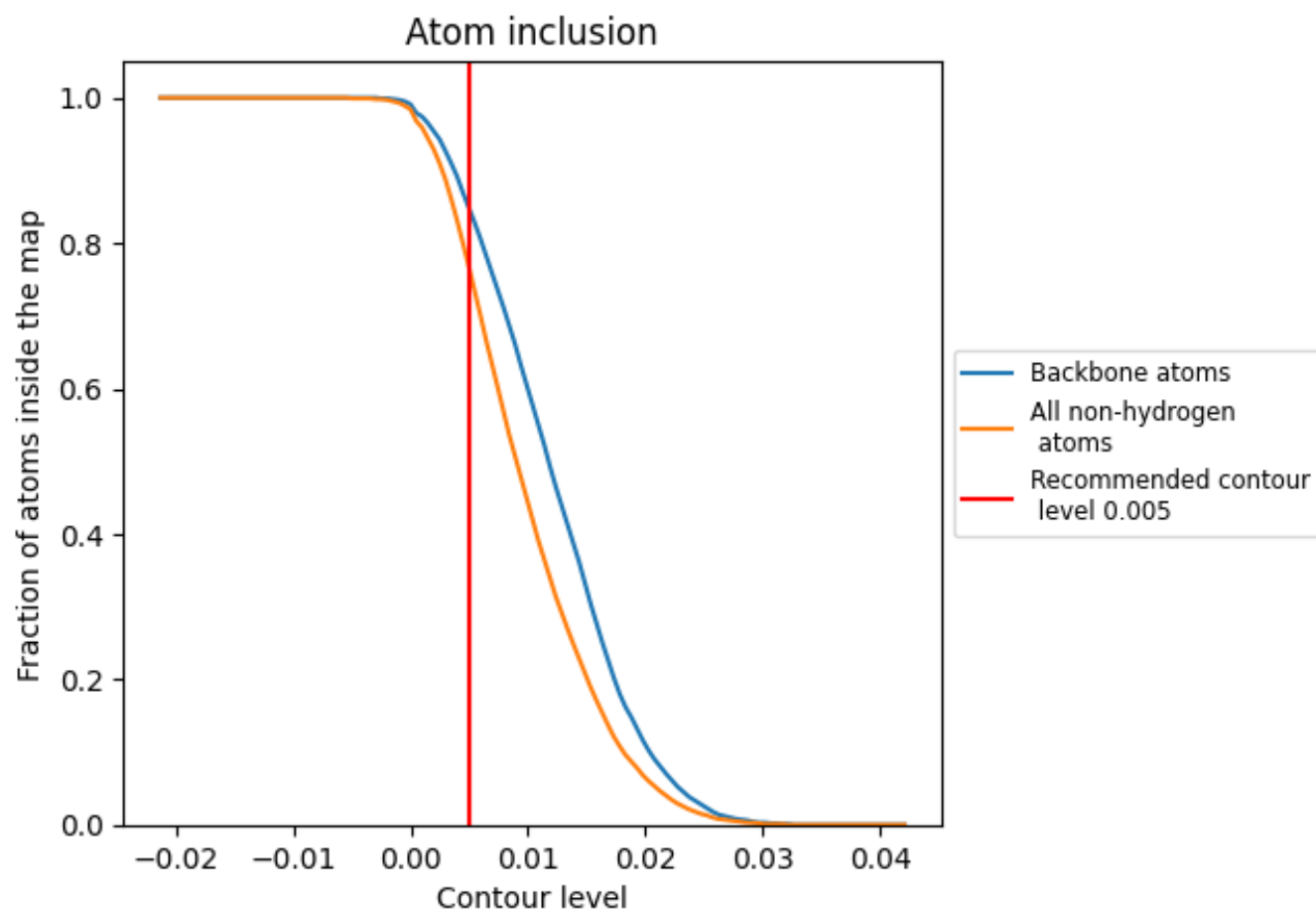
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7660	<div></div> 0.2290
A	<div></div> 0.7620	<div></div> 0.2290
B	<div></div> 0.9200	<div></div> 0.2180
C	<div></div> 0.7600	<div></div> 0.2300
D	<div></div> 0.9220	<div></div> 0.2270

