



Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 09:02 AM EDT

PDB ID : 8ESC
EMDB ID : EMD-28575
Title : Structure of the Yeast NuA4 Histone Acetyltransferase Complex
Authors : Patel, A.B.; Zukin, S.A.; Nogales, E.
Deposited on : 2022-10-13
Resolution : 3.10 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

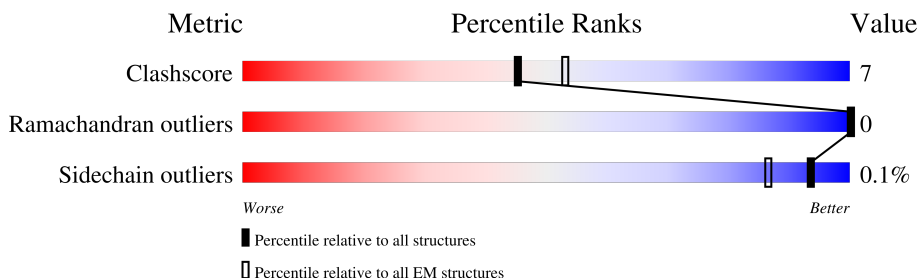
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	Z	3744	
2	R	489	
3	A	375	
4	P	832	
5	E	982	
6	S	476	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 43279 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 Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	3543	Total	C	N	O	S	0	0
			28974	18748	4827	5278	121		

- Molecule 2 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	417	Total	C	N	O	S	0	0
			3311	2110	548	642	11		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	360	Total	C	N	O	S	0	0
			2814	1787	474	536	17		

- Molecule 4 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	272	Total	C	N	O	S	0	0
			2281	1446	389	441	5		

- Molecule 5 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	440	Total	C	N	O	S	0	0
			3645	2317	655	656	17		

- Molecule 6 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	268	Total	C	N	O	S	0	0
			2221	1417	377	419	8		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
7	R	1	Total	C	N	O	P	0
			31	10	5	13	3	

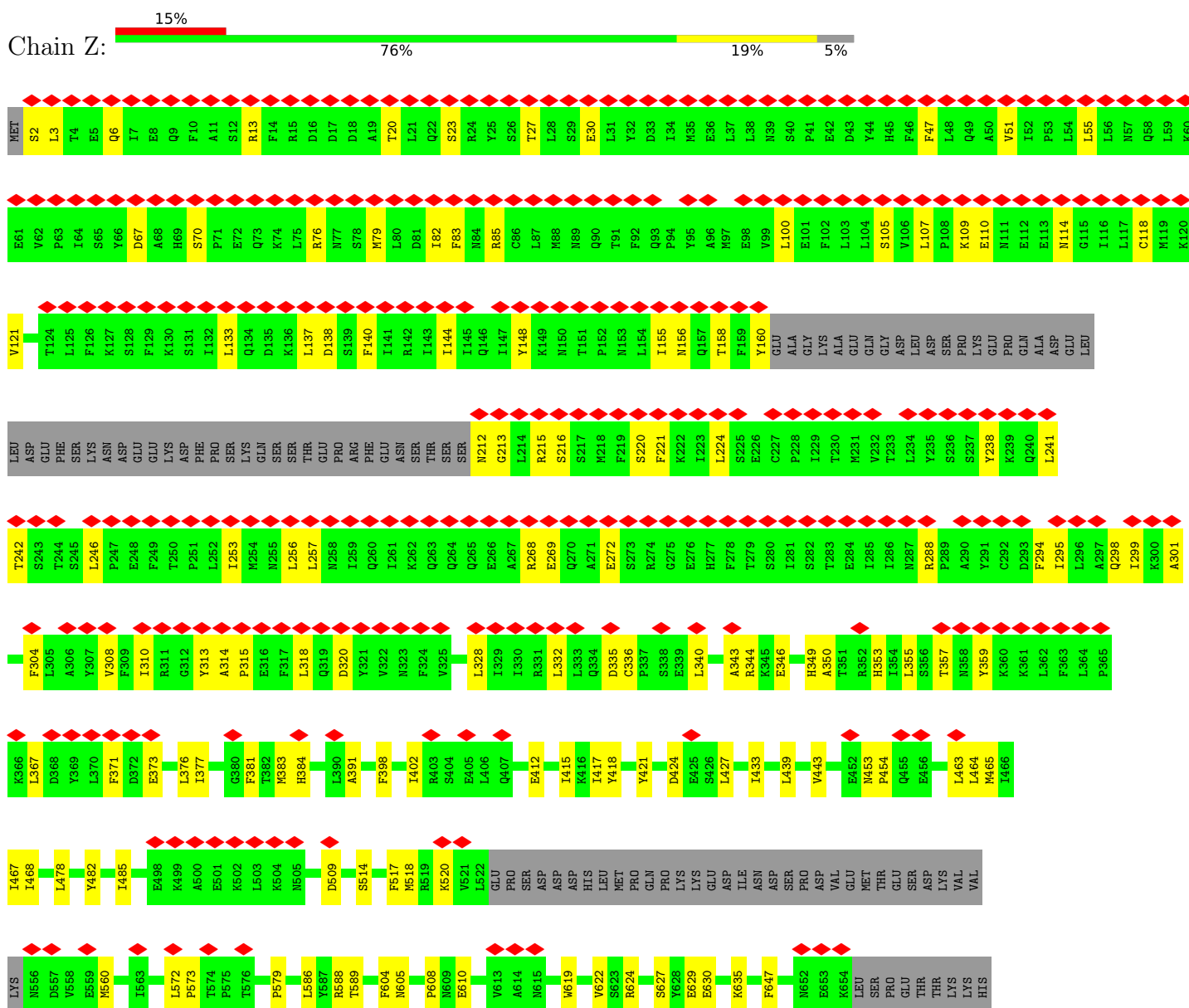
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	R	2	Total	Mg	0
			2	2	

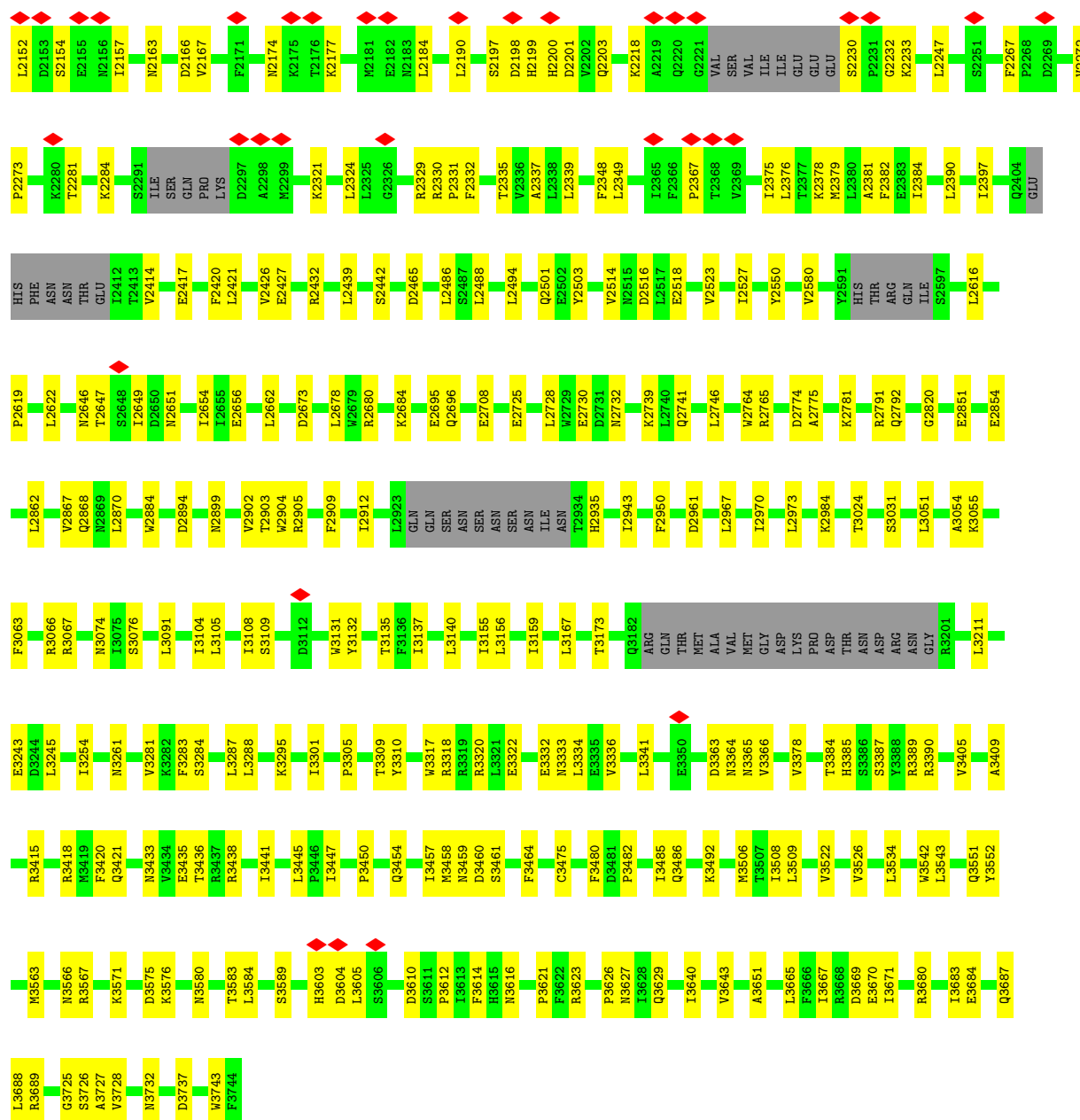
3 Residue-property plots

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: Transcription-associated protein 1

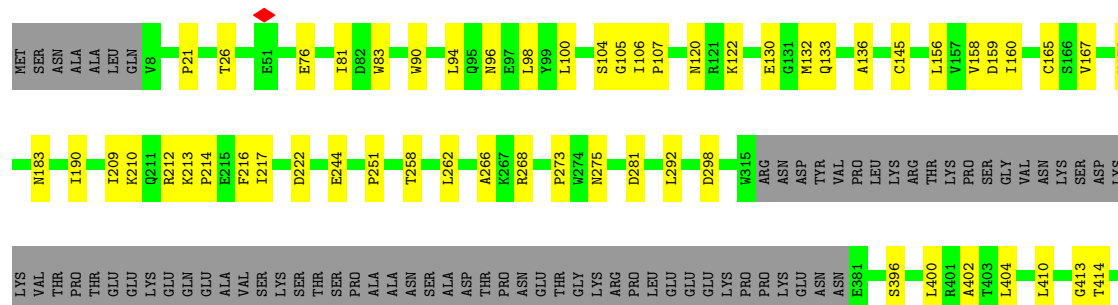


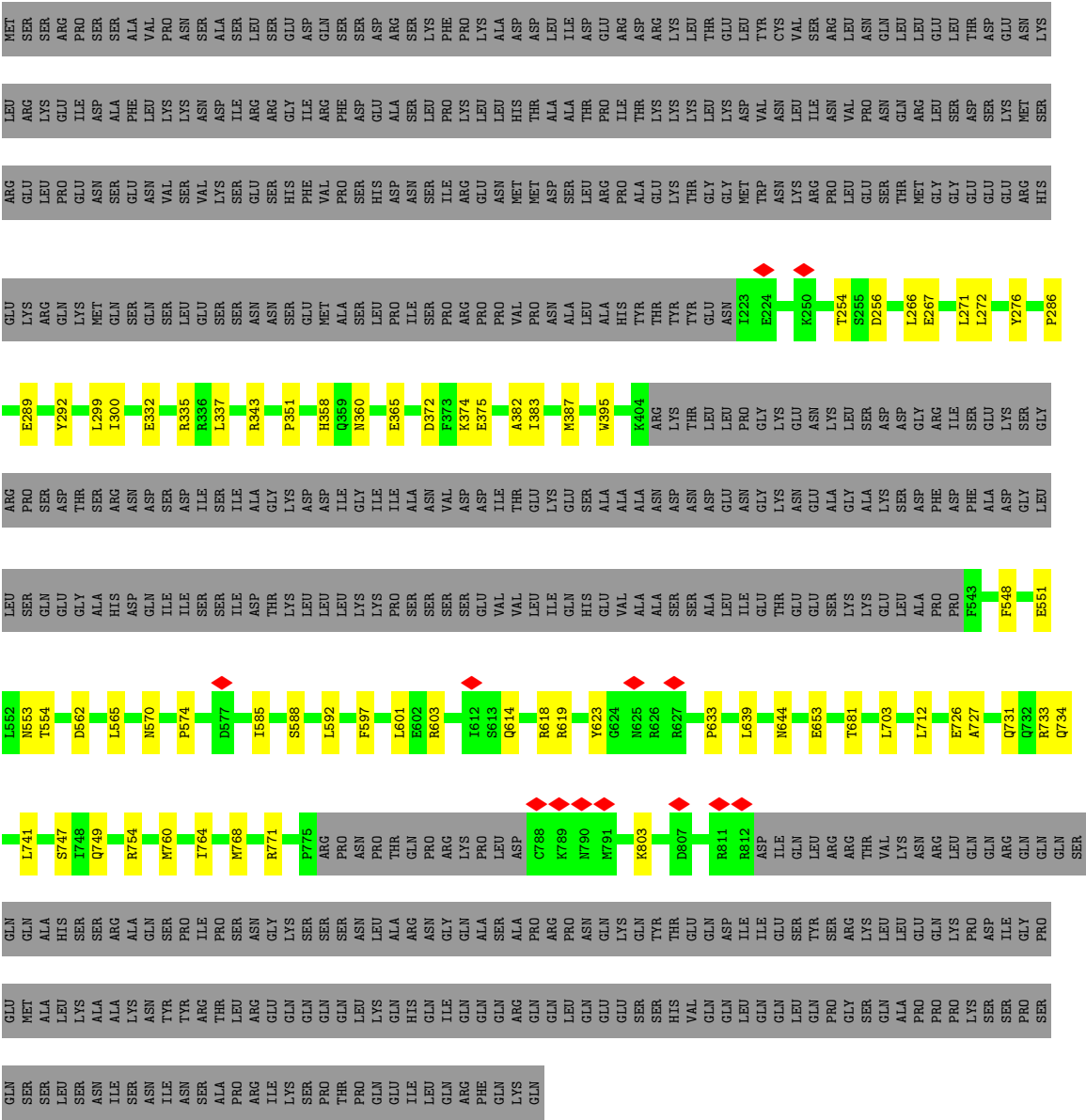
THR	ALA	ILE	ILE	VAL	ASP	ALA	ASN	ASN	ASN	SER	P2087	L2088	S2089	L2090	H2091	L2092	R2093	E2094	A2095	C2096	F2099	L2100	N2108	H2109	R2110	A2111	I2112	E2113	T2114	E2115	L2118	E2126	L2127	I2128	K2131	H2132	T2133	T2134	N2135	V2136	N2137	V2138	K2139	L2140	V2141	E2144	K2145	F2146	L2147	T2148	Z2149	D2150	D2151						
H1992	F1993	D1994	L1995	F1996	F1997	N1998	S1999	R2000	T2015	F2016	M2017	S2018	M2019	S2020	D2023	S2024	H2025	L2031	W2038	K2041	T2042	L2043	GLU	ILE	THR	ASN	VAL	ASN	ASN	ASN	THR	LYS	THR	ASP	ASP	ASP	GLY	ASP	VAL	VAL	MET	SER	ASP	SER	LYS	THR	ASP	ASP	SER	LYS	THR	ILE	ASN	PRO	VAL	GLU	ALA	ASP	THR
H1838	N1839	W1842	K1843	N1844	S1845	N1846	A1847	I1848	L1849	A1850	Y1851	D1852	V1853	L1854	D1855	H1856	H1857	D1858	L1859	E1863	Q1866	I1870	A1874	D1875	P1876	E1877	L1878	H1879	A1880	E1881	I1882	K1883	L1884	D1885	I1886	I1887	K1888	F1889	C1890	V1891	N1892	F1893	I1894	K1895	S1897	S1898	Q1899	N1901	Y1906	T1909									
F1912	I1913	S1914	K1915	F1916	D1917	F1918	P1919	I1920	K1921	V1922	T1923	T1924	Q1925	V1926	R1932	V1936	R1939	Y1940	Q1944	S1945	L1946	L1949	V1952	L1953	H1954	E1955	R1956	M1957	N1958	A1959	A1960	G1961	T1962	P1963	W1966	I1967	M1974	V1975	E1976	N1977	M1978	S1979	S1980	Q1981	N1982	M1983	Y1986	I1990	S1991										
S1773	S1774	M1775	K1776	E1777	K1778	Q1779	N1780	N1781	F1782	I1783	F1788	N1789	V1790	L1791	S1792	D1793	K1794	C1795	D1797	A1798	R1799	V1802	L1803	K1804	V1806	I1807	N1808	S1809	T1810	L1811	I1812	V1813	E1814	T1817	S1818	L1819	S1820	K1822	S1823	Y1824	L1825	V1826	E1827	D1828	K1829	K1830	P1831	W1832	W1833	L1834	E1835	L1836	L1837						
K1687	K1688	G1689	N1690	M1691	K1694	L1699	T1702	L1703	E1708	N1709	S1710	F1711	Q1712	F1713	I1714	T1715	I1716	A1717	K1718	I1719	K1720	L1721	E1722	A1723	K1724	F1725	Q1726	L1727	L1728	Y1729	L1730	R1731	E1734	L1735	S1736	E1737	R1738	D1739	Q1740	L1745	I1748	F1752	S1753	N1754	G1755	S1759	L1762	F1765	I1766	F1767	H1768	N1769	A1772						
L1579	L1580	E1581	R1582	K1583	L1584	R1585	L1586	Q1587	L1588	F1592	R1593	T1594	P1595	E1609	Y1610	F1611	M1614	M1615	T1616	L1617	R1618	M1624	C1625	N1626	E1641	N1646	I1655	V1656	E1657	N1658	Q1659	V1660	R1661	V1662	F1666	F1673	N1674	T1675	M1676	V1677	I1678	G1681	D1682	E1683	L1684	L1685	K1686												
N1488	L1489	S1490	D1491	H1492	Q1493	K1494	L1495	T1496	V1497	L1500	L1509	L1510	I1511	A1512	K1515	V1516	E1517	I1518	G1519	R1520	K1521	D1524	A1528	R1531	V1532	E1533	D1536	T1537	G1540	Q1541	D1542	L1543	A1544	E1545	V1553	I1558	F1559	L1562	Q1565	A1566	D1567	M1568	F1569	D1572	K1576														
GLN	LYS	THR	THR	GLU	Y1402	L1419	A1420	K1424	N1425	E1426	E1427	F1428	A1429	T1430	A1431	Q1432	Q1433	G1434	M1435	I1436	R1437	I1438	R1439	I1440	T1447	M1448	L1449	K1450	T1451	A1462	L1463	G1465	S1466	L1467	A1468	E1469	N1470	S1471	K1472	L1473	P1474	K1475	E1476	L1477	L1478	Q1479	N1480	G1481	L1482	K1483	P1484	L1485	L1486	M1487					
E1295	L1296	S1297	N1298	A1299	C1307	L1311	H1312	T1313	I1314	I1322	L1325	K1330	I1337	R1343	M1353	V1354	D1355	A1356	I1357	C1360	L1361	S1362	L1363	T1366	F1367	L1368	T1369	F1370	R1376	L1377	L1378	I1382	V1383	L1384	A1385	D1386	A1387	E1388	D1389	E1390	SER	LEU	SER	THR	ASN	ILE													
Q1114	V1115	I1131	P1136	L1140	L1146	P1150	S1154	Y1155	Y1156	Y1168	L1177	A1184	S1188	F1189	L1193	L1200	N1208	K1209	R1210	I1220	V1223	F1229	Q1234	I1256	I1265	T1271	F1272	K1276	D1279	M1282	K1283	V1284	L1285	L1289																									
Y875	L876	P877	M880	V884	E902	L903	C904	L908	T909	Y912	T916	V920	I921	V924	L932	I941	I948	L949	N956	P963	L972	D973	I974	K981	I982	D986	V993	I997	Q998	L1027	L1042	L1043	K1044	M1062	V1062	L1078	L1082																						
P864	S670	L671	A687	M691	D694	T697	E700	F726	I731	T732	S733	P734	L744	F756	L765	I779	N780	L793	L796	S799	Y808	I812	R817	I834	L835	Q836	L851	E854	E860	V865	P866	V867	A873	P874																									



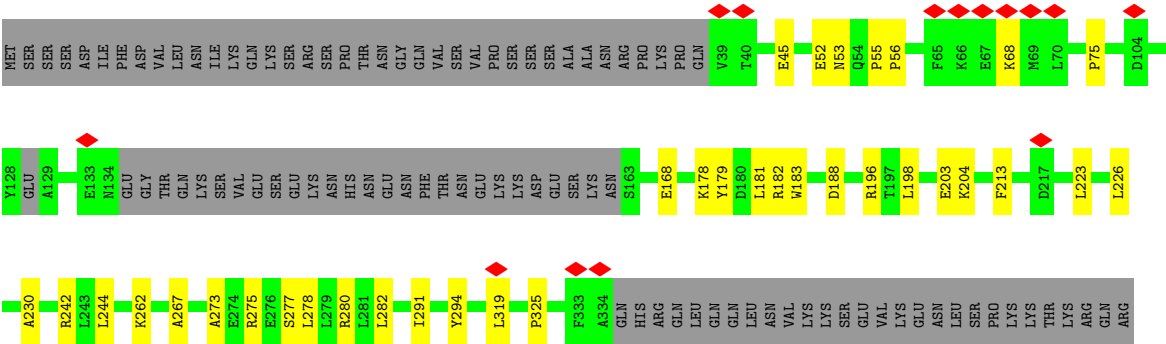
• Molecule 2: Actin-related protein 4

Chain R: 72% 14% 15%





● Molecule 6: SWR1-complex protein 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	635860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	428.92798, 428.92798, 428.92798	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3404, 1.3404, 1.3404	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: MG, ATP

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	Z	0.25	0/29612	0.46	0/40123
2	R	0.24	0/3385	0.45	0/4591
3	A	0.25	0/2876	0.46	0/3896
4	P	0.25	0/2329	0.47	0/3131
5	E	0.24	0/3730	0.47	0/5044
6	S	0.25	0/2273	0.45	0/3060
All	All	0.25	0/44205	0.46	0/59845

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	Z	28974	0	29356	439	0
2	R	3311	0	3270	43	0
3	A	2814	0	2784	30	0
4	P	2281	0	2232	35	0
5	E	3645	0	3661	53	0
6	S	2221	0	2187	31	0
7	R	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	2	0	0	0	0
All	All	43279	0	43502	581	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (581) 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:Z:629:GLU:HG3	1:Z:1717:GLN:HG2	1.67	0.77
1:Z:3054:ALA:HB2	1:Z:3091:LEU:HB2	1.67	0.75
1:Z:3551:GLN:HG3	1:Z:3580:ASN:HA	1.71	0.73
5:E:299:LEU:HD23	6:S:278:LEU:HD13	1.71	0.73
1:Z:1898:ASP:HB3	1:Z:1901:ILE:HG22	1.70	0.72
1:Z:2902:VAL:HG21	1:Z:2950:PHE:HB2	1.72	0.71
1:Z:1234:GLN:HE21	1:Z:1284:VAL:HG22	1.55	0.70
1:Z:357:THR:HG23	1:Z:359:TYR:H	1.56	0.70
1:Z:3051:LEU:HD22	5:E:803:LYS:HB2	1.74	0.69
2:R:410:LEU:HB3	2:R:441:THR:HG22	1.74	0.68
1:Z:346:GLU:HA	1:Z:349:HIS:HB2	1.75	0.68
1:Z:694:ASP:HB3	1:Z:697:THR:HG22	1.75	0.68
1:Z:3318:ARG:NH1	1:Z:3322:GLU:OE2	2.27	0.68
1:Z:2680:ARG:NH2	1:Z:2696:GLN:OE1	2.28	0.67
2:R:413:GLY:HA3	7:R:501:ATP:H5'2	1.75	0.67
5:E:271:LEU:HD12	5:E:601:LEU:HD23	1.74	0.67
1:Z:624:ARG:NH1	1:Z:694:ASP:OD1	2.26	0.67
1:Z:76:ARG:HA	1:Z:79:MET:HG2	1.76	0.67
1:Z:2730:GLU:HG2	5:E:760:MET:HG3	1.75	0.67
1:Z:3:LEU:O	1:Z:6:GLN:NE2	2.28	0.67
1:Z:1838:HIS:HA	1:Z:1842:TRP:HD1	1.60	0.67
1:Z:3305:PRO:HB2	1:Z:3310:TYR:HB2	1.78	0.66
1:Z:1656:PRO:O	1:Z:1659:GLN:NE2	2.28	0.66
1:Z:1625:CYS:HB3	1:Z:1675:THR:HG21	1.76	0.66
1:Z:963:PRO:HG2	1:Z:3543:LEU:HD23	1.77	0.66
1:Z:908:LEU:HD12	1:Z:912:TYR:HB3	1.77	0.66
1:Z:2154:SER:HB3	1:Z:2157:ILE:HG12	1.76	0.65
1:Z:691:MET:HB3	1:Z:731:ILE:HD11	1.78	0.65
1:Z:1790:VAL:HG21	1:Z:1803:LEU:HB2	1.79	0.65
1:Z:85:ARG:NH2	1:Z:1976:GLU:O	2.31	0.64
1:Z:1553:VAL:HG22	1:Z:1592:PHE:HB3	1.80	0.64
1:Z:1831:PRO:HG2	1:Z:1834:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:2656:GLU:OE2	6:S:280:ARG:NH1	2.31	0.63
1:Z:3626:PRO:HA	1:Z:3629:GLN:HE21	1.64	0.63
1:Z:1150:PRO:HB3	1:Z:1200:LEU:HD11	1.81	0.62
1:Z:3364:ASN:HB3	1:Z:3366:VAL:HG22	1.79	0.62
1:Z:355:LEU:HD13	1:Z:398:PHE:HB2	1.81	0.62
1:Z:2765:ARG:HG3	1:Z:2903:THR:HG21	1.82	0.62
1:Z:478:LEU:HD22	1:Z:586:LEU:HD23	1.82	0.62
5:E:633:PRO:HG3	5:E:712:LEU:HD22	1.82	0.61
1:Z:629:GLU:OE2	1:Z:1618:ARG:NH2	2.32	0.61
1:Z:3409:ALA:HB2	1:Z:3454:GLN:HA	1.83	0.61
1:Z:3031:SER:OG	1:Z:3066:ARG:NH1	2.32	0.61
1:Z:3604:ASP:OD1	1:Z:3605:LEU:N	2.34	0.60
1:Z:3318:ARG:NH2	1:Z:3384:THR:O	2.34	0.60
1:Z:1432:GLN:HB2	1:Z:1436:ILE:HG21	1.83	0.60
1:Z:873:ALA:HA	1:Z:876:LEU:HD23	1.83	0.60
1:Z:1790:VAL:HG13	1:Z:1791:LEU:HD12	1.82	0.60
3:A:202:THR:HG23	3:A:205:GLU:H	1.67	0.59
3:A:237:GLU:HG2	3:A:251:GLY:HA2	1.84	0.59
1:Z:268:ARG:NH2	1:Z:335:ASP:OD1	2.35	0.59
1:Z:1361:LEU:HD23	1:Z:1366:THR:HG21	1.84	0.59
3:A:220:ALA:HB1	3:A:226:GLU:HG3	1.84	0.59
1:Z:2128:ILE:HB	1:Z:2174:ASN:HD22	1.66	0.59
1:Z:2741:GLN:OE1	1:Z:2899:ASN:ND2	2.35	0.59
1:Z:318:LEU:HD23	1:Z:320:ASP:H	1.67	0.59
1:Z:3159:ILE:HG22	1:Z:3167:LEU:HD22	1.85	0.59
1:Z:3283:PHE:HB2	1:Z:3287:LEU:HB2	1.84	0.59
3:A:105:LEU:HD12	3:A:132:PHE:HE1	1.67	0.59
6:S:183:TRP:HB3	6:S:198:LEU:HD11	1.83	0.59
5:E:703:LEU:HD11	6:S:325:PRO:HD2	1.84	0.59
1:Z:635:LYS:HD2	1:Z:1588:LEU:HD11	1.85	0.59
1:Z:2970:ILE:HA	1:Z:2973:LEU:HD23	1.84	0.59
1:Z:1838:HIS:HA	1:Z:1842:TRP:CD1	2.38	0.58
1:Z:67:ASP:HB3	1:Z:70:SER:HB3	1.85	0.58
1:Z:1803:LEU:HD22	1:Z:1863:GLU:HB3	1.83	0.58
1:Z:2337:ALA:HB1	1:Z:2378:LYS:HE3	1.84	0.58
1:Z:3567:ARG:NH1	1:Z:3583:THR:OG1	2.35	0.58
2:R:158:VAL:HG23	2:R:167:VAL:HG22	1.84	0.58
1:Z:3261:ASN:OD1	1:Z:3486:GLN:NE2	2.35	0.58
5:E:337:LEU:O	6:S:242:ARG:NH2	2.37	0.58
1:Z:2739:LYS:NZ	1:Z:2894:ASP:OD1	2.37	0.57
1:Z:3563:MET:HB3	1:Z:3616:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:236:ILE:O	3:A:254:ARG:NH1	2.36	0.57
1:Z:1913:ILE:HD12	1:Z:1923:VAL:HG22	1.86	0.57
1:Z:2649:ILE:HB	6:S:277:SER:HB2	1.87	0.57
1:Z:3135:THR:O	1:Z:3421:GLN:NE2	2.38	0.57
1:Z:1516:VAL:HG11	1:Z:1566:ALA:HB3	1.86	0.57
1:Z:1322:ILE:HA	1:Z:1325:LEU:HD23	1.86	0.57
1:Z:1737:GLU:HB2	1:Z:1738:ARG:HH11	1.68	0.57
1:Z:1790:VAL:HA	1:Z:1799:ARG:HG3	1.87	0.57
1:Z:3566:ASN:OD1	1:Z:3571:LYS:NZ	2.37	0.57
1:Z:3621:PRO:HD2	1:Z:3727:ALA:HB2	1.86	0.57
1:Z:2:SER:OG	1:Z:3:LEU:N	2.36	0.56
1:Z:1850:ALA:HB3	1:Z:1853:VAL:HB	1.87	0.56
1:Z:2862:LEU:HD21	1:Z:2912:ILE:HA	1.86	0.56
1:Z:242:THR:HA	1:Z:246:LEU:HD23	1.87	0.56
2:R:160:ILE:HG22	2:R:414:THR:HB	1.88	0.56
1:Z:1234:GLN:NE2	1:Z:1284:VAL:O	2.38	0.56
1:Z:1353:ASN:OD1	1:Z:1354:VAL:N	2.38	0.56
3:A:104:LEU:HD22	3:A:347:ALA:HB2	1.86	0.56
6:S:203:GLU:HB2	6:S:230:ALA:HB2	1.87	0.56
1:Z:793:LEU:HD21	1:Z:834:ILE:HD12	1.87	0.56
1:Z:1464:LYS:HA	1:Z:1509:LEU:HD11	1.87	0.56
1:Z:20:THR:HG23	1:Z:23:SER:H	1.70	0.56
1:Z:972:LEU:HD13	1:Z:998:GLN:HG3	1.87	0.56
2:R:190:ILE:HD11	2:R:292:LEU:HD11	1.86	0.56
1:Z:1062:ASP:O	1:Z:3320:ARG:NH2	2.39	0.56
3:A:35:VAL:HG11	3:A:81:ASP:HB3	1.88	0.56
5:E:747:SER:O	5:E:749:GLN:NE2	2.39	0.56
3:A:10:ILE:HG23	3:A:89:THR:HG21	1.88	0.56
1:Z:340:LEU:HD13	1:Z:343:ALA:HB3	1.86	0.55
1:Z:3418:ARG:NH1	1:Z:3669:ASP:OD2	2.38	0.55
1:Z:1284:VAL:HG13	1:Z:1285:LEU:HD12	1.88	0.55
2:R:130:GLU:O	2:R:133:GLN:NE2	2.39	0.55
1:Z:216:SER:O	1:Z:220:SER:N	2.40	0.55
1:Z:1476:GLU:O	1:Z:1480:ASN:ND2	2.39	0.55
1:Z:3420:PHE:HA	1:Z:3445:LEU:HD22	1.89	0.55
5:E:653:GLU:OE2	5:E:754:ARG:NH2	2.40	0.55
1:Z:610:GLU:O	1:Z:1583:LYS:NZ	2.39	0.55
1:Z:1289:LEU:HD11	1:Z:1325:LEU:HD12	1.88	0.55
1:Z:1967:ILE:HG21	1:Z:2000:ARG:HG3	1.89	0.55
1:Z:2662:LEU:HD23	1:Z:2678:LEU:HD11	1.88	0.55
1:Z:3104:ILE:O	1:Z:3108:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:382:ALA:HB2	6:S:55:PRO:HG3	1.88	0.55
2:R:21:PRO:HA	2:R:26:THR:HG23	1.89	0.54
1:Z:412:GLU:HG3	1:Z:463:LEU:HD21	1.90	0.54
1:Z:1447:THR:HA	1:Z:1450:LYS:HE3	1.89	0.54
1:Z:3508:ILE:HG13	4:P:747:THR:HG22	1.89	0.54
1:Z:726:PHE:O	1:Z:732:THR:OG1	2.24	0.54
1:Z:1114:GLN:HG3	1:Z:1189:PHE:HB2	1.89	0.54
1:Z:2199:HIS:CE1	1:Z:2201:ASP:HB2	2.42	0.54
1:Z:13:ARG:HE	1:Z:27:THR:HG23	1.71	0.54
1:Z:308:VAL:HG23	1:Z:313:TYR:HD2	1.71	0.54
1:Z:671:LEU:HD23	1:Z:756:PHE:HE2	1.71	0.54
1:Z:3243:GLU:OE2	1:Z:3389:ARG:NH1	2.38	0.54
1:Z:3334:LEU:HD21	1:Z:3341:LEU:HB2	1.90	0.54
1:Z:3726:SER:O	1:Z:3732:ASN:ND2	2.38	0.54
2:R:156:LEU:HB2	2:R:404:LEU:HG	1.89	0.54
1:Z:731:ILE:HG13	1:Z:732:THR:HG23	1.89	0.54
1:Z:1843:LYS:NZ	1:Z:1885:ASP:OD2	2.39	0.54
4:P:666:SER:OG	4:P:667:LEU:N	2.41	0.54
5:E:585:ILE:HD12	6:S:244:LEU:HD21	1.90	0.54
1:Z:2149:PHE:HE2	1:Z:2152:LEU:HA	1.72	0.54
2:R:462:LEU:HD22	5:E:365:GLU:HG2	1.90	0.54
1:Z:376:LEU:HG	1:Z:391:ALA:HB1	1.89	0.53
1:Z:2774:ASP:OD1	1:Z:2775:ALA:N	2.40	0.53
1:Z:1804:LYS:HA	1:Z:1808:ASN:HD22	1.74	0.53
1:Z:3610:ASP:OD2	1:Z:3680:ARG:NH2	2.41	0.53
1:Z:1737:GLU:O	1:Z:1738:ARG:HD3	2.08	0.53
1:Z:1946:LEU:HD21	1:Z:1990:ILE:HD12	1.90	0.53
1:Z:2851:GLU:OE2	1:Z:2905:ARG:NH2	2.36	0.53
3:A:102:PRO:HB3	3:A:131:ALA:HB3	1.90	0.53
3:A:153:LEU:HD11	3:A:274:ILE:HB	1.90	0.53
4:P:602:ARG:NH2	5:E:267:GLU:OE2	2.41	0.53
5:E:266:LEU:HD12	5:E:267:GLU:HB2	1.90	0.53
3:A:359:LYS:HE2	6:S:68:LYS:HE3	1.89	0.53
1:Z:2680:ARG:HH22	1:Z:3643:VAL:HG11	1.74	0.53
1:Z:3433:ASN:HD22	1:Z:3651:ALA:HB2	1.74	0.53
1:Z:3485:ILE:HG21	1:Z:3743:TRP:CZ2	2.44	0.53
1:Z:1027:LEU:HB3	1:Z:2488:LEU:HD13	1.91	0.53
1:Z:1177:LEU:HD11	1:Z:2518:GLU:HB3	1.91	0.53
3:A:244:ASP:OD1	3:A:245:GLY:N	2.42	0.53
1:Z:1337:ILE:HG21	1:Z:1357:ILE:HD11	1.91	0.53
1:Z:257:LEU:HD13	1:Z:328:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:439:LEU:HD12	1:Z:467:ILE:HG12	1.92	0.52
1:Z:3492:LYS:HD2	4:P:739:ILE:HD11	1.89	0.52
1:Z:2382:PHE:HD2	1:Z:2390:LEU:HB3	1.73	0.52
2:R:210:LYS:HB3	2:R:217:ILE:HG13	1.91	0.52
4:P:643:GLY:N	4:P:647:ILE:O	2.24	0.52
1:Z:156:ASN:HA	1:Z:160:TYR:HD2	1.74	0.52
1:Z:1518:ILE:HG13	1:Z:1521:LYS:HE3	1.91	0.52
4:P:545:PRO:O	6:S:262:LYS:NZ	2.38	0.52
1:Z:1438:ILE:HG13	1:Z:1439:ARG:HD3	1.90	0.52
1:Z:1382:ILE:HG23	1:Z:1383:VAL:HG13	1.92	0.52
1:Z:1825:LEU:HD13	1:Z:1878:ILE:HG22	1.91	0.52
1:Z:2764:TRP:HZ2	1:Z:2904:TRP:HB2	1.75	0.52
2:R:83:TRP:NE1	2:R:120:ASN:OD1	2.36	0.52
1:Z:2112:ILE:HG23	1:Z:2118:LEU:HD13	1.92	0.52
1:Z:299:ILE:HD13	1:Z:332:LEU:HD21	1.92	0.52
1:Z:2197:SER:O	1:Z:2203:GLN:NE2	2.43	0.52
6:S:168:GLU:OE2	6:S:196:ARG:NE	2.43	0.52
1:Z:221:PHE:HZ	1:Z:294:PHE:HB2	1.75	0.51
1:Z:2673:ASP:HB3	1:Z:3640:ILE:HG12	1.93	0.51
1:Z:949:LEU:O	1:Z:956:ASN:ND2	2.44	0.51
1:Z:1611:PHE:O	1:Z:1615:MET:HB3	2.11	0.51
1:Z:1979:SER:H	1:Z:1983:ASN:HB2	1.75	0.51
1:Z:877:PRO:HG3	1:Z:916:ILE:HD12	1.92	0.51
1:Z:1043:LEU:HD11	1:Z:1115:VAL:HG21	1.91	0.51
1:Z:2382:PHE:CD2	1:Z:2390:LEU:HB3	2.45	0.51
1:Z:1682:ASP:OD2	1:Z:1731:ARG:NH2	2.44	0.51
1:Z:2111:ALA:N	1:Z:2163:ASN:OD1	2.44	0.51
1:Z:2854:GLU:OE1	1:Z:2884:TRP:NE1	2.41	0.51
1:Z:2967:LEU:HD22	1:Z:2984:LYS:HG3	1.93	0.51
1:Z:865:VAL:HG12	1:Z:867:VAL:HG12	1.93	0.50
1:Z:3542:TRP:HE3	1:Z:3543:LEU:HD12	1.76	0.50
1:Z:2420:PHE:HE2	1:Z:2439:LEU:HD12	1.76	0.50
5:E:276:TYR:HA	5:E:592:LEU:HD23	1.93	0.50
2:R:396:SER:HB3	2:R:400:LEU:HD21	1.93	0.50
1:Z:630:GLU:N	1:Z:630:GLU:OE1	2.44	0.50
2:R:76:GLU:HG2	2:R:81:ILE:HG21	1.93	0.50
5:E:727:ALA:O	5:E:731:GLN:NE2	2.45	0.50
1:Z:880:MET:HB3	1:Z:920:VAL:HG21	1.94	0.50
1:Z:2272:VAL:N	1:Z:2273:PRO:HD2	2.26	0.50
1:Z:1360:CYS:HA	1:Z:1363:LEU:HD23	1.93	0.50
3:A:359:LYS:HD2	6:S:75:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:981:LYS:NZ	1:Z:982:ILE:O	2.43	0.50
3:A:322:PRO:HD2	3:A:325:MET:HG3	1.94	0.50
1:Z:13:ARG:NH2	1:Z:30:GLU:OE2	2.45	0.50
1:Z:993:VAL:HG11	1:Z:2488:LEU:HD11	1.94	0.49
2:R:258:THR:HG22	2:R:262:LEU:HG	1.92	0.49
1:Z:997:ILE:HD11	1:Z:1082:LEU:HD11	1.94	0.49
1:Z:2166:ASP:OD1	1:Z:2167:VAL:N	2.45	0.49
1:Z:3612:PRO:HG2	1:Z:3671:ILE:HD12	1.94	0.49
1:Z:2381:ALA:HA	1:Z:2384:ILE:HD13	1.95	0.49
3:A:271:SER:OG	3:A:272:ALA:N	2.45	0.49
1:Z:622:VAL:HG21	1:Z:694:ASP:H	1.77	0.49
1:Z:744:LEU:HD11	1:Z:765:LEU:HB3	1.95	0.49
1:Z:1641:GLU:HG3	1:Z:1676:MET:HE2	1.94	0.49
4:P:753:LEU:HB2	5:E:300:ILE:HD11	1.94	0.49
1:Z:1673:PHE:CE2	1:Z:1728:LEU:HD21	2.48	0.49
1:Z:3156:LEU:HB3	1:Z:3211:LEU:HD21	1.95	0.49
1:Z:3390:ARG:NH1	1:Z:3460:ASP:OD1	2.42	0.49
5:E:332:GLU:OE2	5:E:335:ARG:NH2	2.42	0.49
1:Z:1478:LEU:HG	1:Z:1482:LEU:HD23	1.94	0.49
1:Z:1737:GLU:C	1:Z:1738:ARG:HD3	2.33	0.49
1:Z:1957:MET:HG3	1:Z:1966:TRP:CD1	2.47	0.49
1:Z:2619:PRO:HG2	1:Z:2622:LEU:HB3	1.95	0.49
1:Z:560:MET:HB3	1:Z:1767:PHE:CD2	2.48	0.49
1:Z:1140:LEU:HB2	1:Z:2494:LEU:HD12	1.95	0.49
1:Z:3109:SER:OG	1:Z:3689:ARG:NH2	2.41	0.49
2:R:266:ALA:O	2:R:268:ARG:NH1	2.44	0.49
1:Z:100:LEU:HD23	1:Z:133:LEU:HD11	1.93	0.48
1:Z:3435:GLU:OE1	1:Z:3438:ARG:NH1	2.45	0.48
1:Z:3737:ASP:OD1	1:Z:3737:ASP:N	2.46	0.48
2:R:100:LEU:HD21	2:R:106:ILE:HD13	1.95	0.48
1:Z:608:PRO:HB3	1:Z:619:TRP:CG	2.48	0.48
1:Z:3074:ASN:OD1	1:Z:3076:SER:OG	2.31	0.48
2:R:443:GLY:HA3	4:P:709:TRP:CZ3	2.47	0.48
3:A:146:GLY:HA2	5:E:395:TRP:CD1	2.48	0.48
4:P:550:SER:HB2	5:E:254:THR:HG21	1.95	0.48
1:Z:443:VAL:HG13	1:Z:464:LEU:HD21	1.95	0.48
1:Z:1828:ASP:N	1:Z:1828:ASP:OD1	2.45	0.48
1:Z:3461:SER:H	1:Z:3464:PHE:HE1	1.61	0.48
4:P:593:ARG:NH1	5:E:562:ASP:OD1	2.46	0.48
1:Z:138:ASP:OD1	1:Z:138:ASP:N	2.47	0.48
1:Z:295:ILE:O	1:Z:299:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:605:ASN:ND2	1:Z:622:VAL:O	2.43	0.48
1:Z:1866:GLN:O	1:Z:1870:ILE:HD12	2.13	0.48
2:R:281:ASP:OD1	2:R:281:ASP:N	2.43	0.48
1:Z:485:ILE:HG23	1:Z:579:PRO:HB2	1.96	0.48
1:Z:734:PRO:HG3	1:Z:779:ILE:HG21	1.94	0.48
1:Z:2376:LEU:HD11	1:Z:2397:ILE:HD11	1.96	0.48
1:Z:2523:VAL:O	1:Z:2527:ILE:HG12	2.13	0.48
3:A:167:ALA:HB2	6:S:45:GLU:HG2	1.95	0.48
1:Z:1995:LEU:H	1:Z:1995:LEU:HD23	1.78	0.48
1:Z:2432:ARG:HD3	1:Z:2550:TYR:CZ	2.48	0.48
1:Z:3684:GLU:HB2	1:Z:3687:GLN:HE22	1.79	0.48
1:Z:1042:LEU:HD21	1:Z:2501:GLN:HA	1.95	0.48
1:Z:1828:ASP:OD2	1:Z:1829:LYS:NZ	2.46	0.48
1:Z:2147:LEU:HD12	1:Z:2190:LEU:HD21	1.96	0.48
1:Z:2339:LEU:HD21	1:Z:2348:PHE:HE2	1.78	0.48
1:Z:3333:ASN:HB2	1:Z:3336:VAL:HG12	1.96	0.48
1:Z:517:PHE:HA	1:Z:520:LYS:HG2	1.95	0.48
1:Z:1752:PHE:HB2	1:Z:1798:ALA:HB2	1.94	0.48
1:Z:3332:GLU:O	1:Z:3378:VAL:N	2.47	0.48
1:Z:3552:TYR:OH	1:Z:3623:ARG:O	2.24	0.48
2:R:467:GLN:HE21	5:E:358:HIS:CE1	2.31	0.48
1:Z:588:ARG:HG2	1:Z:588:ARG:HH11	1.79	0.48
1:Z:1992:HIS:HE1	1:Z:2031:LEU:HD22	1.78	0.47
1:Z:817:ARG:NH2	1:Z:860:GLU:OE2	2.37	0.47
1:Z:1420:ALA:O	1:Z:1424:LYS:NZ	2.45	0.47
3:A:240:TYR:O	3:A:248:ILE:N	2.41	0.47
1:Z:3447:ILE:HG12	1:Z:3459:ASN:ND2	2.30	0.47
6:S:291:ILE:HG23	6:S:294:TYR:HD2	1.79	0.47
1:Z:894:VAL:HG11	1:Z:941:ILE:HD12	1.96	0.47
1:Z:3475:CYS:HB2	1:Z:3482:PRO:HG3	1.96	0.47
6:S:213:PHE:HB3	6:S:223:LEU:HD21	1.95	0.47
1:Z:1980:SER:OG	1:Z:1981:GLN:N	2.48	0.47
1:Z:2684:LYS:N	1:Z:2725:GLU:OE2	2.46	0.47
2:R:145:CYS:O	2:R:455:GLY:HA3	2.15	0.47
3:A:88:HIS:NE2	3:A:93:GLU:OE2	2.44	0.47
3:A:272:ALA:HB1	3:A:276:GLN:HB3	1.97	0.47
1:Z:2110:ARG:HB3	1:Z:2113:GLU:OE1	2.14	0.47
1:Z:2870:LEU:HD23	1:Z:2935:HIS:HD2	1.80	0.47
1:Z:3629:GLN:HE22	1:Z:3728:VAL:HG23	1.79	0.47
4:P:573:ASP:OD1	4:P:721:LYS:NZ	2.39	0.47
2:R:400:LEU:HD23	2:R:400:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:351:PRO:HG2	6:S:226:LEU:HD23	1.97	0.47
1:Z:1580:LEU:HD22	1:Z:1592:PHE:CZ	2.50	0.47
1:Z:2867:VAL:O	1:Z:2868:GLN:HG3	2.15	0.47
1:Z:298:GLN:HB3	1:Z:332:LEU:HD11	1.97	0.47
1:Z:1210:ARG:HB2	1:Z:1256:ILE:HG12	1.97	0.47
1:Z:2649:ILE:HG22	6:S:273:ALA:HB1	1.95	0.47
3:A:107:GLU:HB2	3:A:111:ASN:ND2	2.29	0.47
1:Z:482:TYR:HD1	1:Z:647:PHE:HD1	1.64	0.46
1:Z:572:LEU:HD12	1:Z:573:PRO:HD2	1.97	0.46
1:Z:1666:PHE:CE2	1:Z:1699:LEU:HD13	2.50	0.46
1:Z:51:VAL:O	1:Z:55:LEU:N	2.47	0.46
1:Z:257:LEU:HD21	1:Z:301:ALA:HB3	1.96	0.46
5:E:618:ARG:NH1	5:E:623:TYR:O	2.48	0.46
1:Z:336:CYS:HB3	1:Z:344:ARG:HH21	1.78	0.46
1:Z:921:ILE:HA	1:Z:924:VAL:HG12	1.98	0.46
4:P:595:TYR:HE2	5:E:272:LEU:HB2	1.80	0.46
5:E:570:ASN:HD21	5:E:574:PRO:HG3	1.79	0.46
1:Z:2695:GLU:OE1	1:Z:2732:ASN:ND2	2.49	0.46
2:R:251:PRO:HB3	2:R:422:ASP:HB3	1.98	0.46
1:Z:424:ASP:HB3	1:Z:427:LEU:HD13	1.97	0.46
4:P:639:ARG:HB2	5:E:597:PHE:HA	1.97	0.46
1:Z:465:MET:HA	1:Z:468:ILE:HD12	1.98	0.46
1:Z:670:SER:HA	1:Z:756:PHE:HZ	1.79	0.46
1:Z:1184:ALA:O	1:Z:1188:SER:HB3	2.15	0.46
1:Z:1330:LYS:NZ	1:Z:1367:PHE:HB2	2.31	0.46
1:Z:1662:VAL:HG22	1:Z:1702:THR:HG23	1.98	0.46
2:R:213:LYS:HG2	2:R:275:ASN:ND2	2.31	0.46
3:A:80:ASP:OD1	3:A:81:ASP:N	2.48	0.46
5:E:614:GLN:O	5:E:619:ARG:NH2	2.36	0.46
1:Z:1543:LEU:HD11	1:Z:1586:LEU:HD21	1.97	0.46
1:Z:1730:LEU:O	1:Z:1734:GLU:N	2.49	0.46
1:Z:2486:LEU:HD23	1:Z:2486:LEU:H	1.81	0.46
3:A:107:GLU:HB2	3:A:111:ASN:HD21	1.81	0.46
1:Z:310:ILE:HD11	1:Z:353:HIS:HB3	1.98	0.46
1:Z:398:PHE:O	1:Z:402:ILE:HG12	2.16	0.46
5:E:733:ARG:HG3	5:E:734:GLN:NE2	2.31	0.46
1:Z:1673:PHE:HE2	1:Z:1728:LEU:HD21	1.81	0.46
1:Z:1674:ASN:ND2	1:Z:1724:LYS:HD2	2.31	0.46
4:P:531:ASP:HB3	4:P:535:PHE:HB2	1.98	0.46
1:Z:1806:VAL:O	1:Z:1810:THR:OG1	2.25	0.46
1:Z:1940:TYR:O	1:Z:1944:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:256:ASP:N	5:E:256:ASP:OD1	2.48	0.46
1:Z:1745:LEU:HD13	1:Z:1748:ILE:HD11	1.98	0.45
1:Z:3415:ARG:NH1	1:Z:3670:GLU:OE1	2.49	0.45
1:Z:3667:ILE:O	1:Z:3671:ILE:HG12	2.16	0.45
4:P:592:ILE:HG21	4:P:615:LYS:HB3	1.99	0.45
1:Z:1762:LEU:HD23	1:Z:1762:LEU:H	1.80	0.45
2:R:402:ALA:HA	2:R:435:LEU:HD22	1.98	0.45
1:Z:1783:ILE:HD11	1:Z:1810:THR:HG21	1.98	0.45
1:Z:2127:LEU:O	1:Z:2133:TRP:HB2	2.17	0.45
2:R:94:LEU:HD23	2:R:98:LEU:HD22	1.98	0.45
4:P:544:ASN:HB3	4:P:545:PRO:HD3	1.99	0.45
1:Z:514:SER:O	1:Z:518:MET:HG2	2.15	0.45
1:Z:1796:LEU:HD13	1:Z:1799:ARG:NH2	2.32	0.45
1:Z:2149:PHE:CE2	1:Z:2152:LEU:HA	2.50	0.45
1:Z:2961:ASP:OD1	1:Z:2961:ASP:N	2.48	0.45
1:Z:3063:PHE:CZ	1:Z:3067:ARG:HD2	2.51	0.45
4:P:494:SER:HB3	5:E:747:SER:HA	1.99	0.45
1:Z:464:LEU:HD12	1:Z:604:PHE:HE2	1.82	0.45
1:Z:1542:ASP:OD1	1:Z:1542:ASP:N	2.49	0.45
1:Z:1703:LEU:HG	1:Z:1754:ASN:HB3	1.98	0.45
1:Z:1906:TYR:HA	1:Z:1909:THR:HG22	1.97	0.45
1:Z:2421:LEU:HD23	1:Z:2421:LEU:HA	1.85	0.45
5:E:299:LEU:HD11	6:S:275:ARG:HG3	1.99	0.45
1:Z:836:GLN:HG2	1:Z:875:TYR:HE1	1.81	0.45
1:Z:997:ILE:HD13	1:Z:1078:LEU:HD11	1.99	0.45
1:Z:1311:LEU:HD23	1:Z:1314:ILE:HD11	1.98	0.45
1:Z:1957:MET:HB3	1:Z:1963:PRO:HA	1.98	0.45
1:Z:3131:TRP:CZ3	1:Z:3365:ASN:HB2	2.51	0.45
1:Z:3683:ILE:HG23	1:Z:3688:LEU:HB2	1.98	0.45
1:Z:3684:GLU:HB2	1:Z:3687:GLN:NE2	2.32	0.45
2:R:107:PRO:HB3	2:R:136:ALA:HB3	1.99	0.45
2:R:212:ARG:NE	2:R:273:PRO:O	2.47	0.45
2:R:486:ASP:O	6:S:178:LYS:NZ	2.49	0.45
1:Z:988:ASP:OD1	1:Z:988:ASP:N	2.48	0.45
1:Z:2090:LEU:HD23	1:Z:2090:LEU:H	1.81	0.45
1:Z:2230:SER:HB2	1:Z:2233:LYS:HB2	1.99	0.45
1:Z:2580:VAL:HG22	1:Z:2616:LEU:HG	1.99	0.45
4:P:561:PRO:HG2	6:S:267:ALA:HB2	1.99	0.45
1:Z:241:LEU:HD23	1:Z:241:LEU:H	1.81	0.45
1:Z:1849:LEU:HD21	1:Z:1893:PHE:CE2	2.51	0.45
1:Z:1974:MET:O	1:Z:1978:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:3167:LEU:HD23	1:Z:3167:LEU:H	1.82	0.45
4:P:722:PHE:CZ	5:E:588:SER:HB3	2.51	0.45
1:Z:850:ARG:HD2	1:Z:1156:TYR:HB3	1.99	0.45
1:Z:3589:SER:O	1:Z:3614:PHE:HA	2.17	0.45
2:R:122:LYS:HG3	2:R:480:VAL:HG11	1.99	0.45
1:Z:1519:GLY:HA3	1:Z:1569:PHE:HE1	1.82	0.45
1:Z:1655:ILE:HG22	1:Z:1656:PRO:HD3	1.99	0.45
1:Z:2093:ARG:HB2	1:Z:2133:TRP:CZ3	2.52	0.45
1:Z:3173:THR:HG21	1:Z:3450:PRO:HB2	1.99	0.45
2:R:96:ASN:O	3:A:177:ARG:NH2	2.50	0.45
2:R:178:LYS:HB2	6:S:188:ASP:HB2	1.98	0.45
1:Z:1718:LEU:O	1:Z:1722:ILE:HG12	2.16	0.44
1:Z:417:ILE:HG13	1:Z:418:TYR:N	2.32	0.44
1:Z:1500:LEU:HD21	1:Z:1558:ILE:HD13	1.98	0.44
1:Z:1655:ILE:HD11	1:Z:1662:VAL:HG23	1.98	0.44
2:R:159:ASP:O	2:R:165:CYS:HA	2.17	0.44
2:R:213:LYS:HA	2:R:214:PRO:HA	1.78	0.44
1:Z:876:LEU:HD11	1:Z:904:CYS:SG	2.57	0.44
1:Z:2851:GLU:HB3	1:Z:2904:TRP:CH2	2.53	0.44
1:Z:509:ASP:OD1	1:Z:509:ASP:N	2.49	0.44
1:Z:733:SER:OG	1:Z:780:ASN:OD1	2.35	0.44
1:Z:1168:TYR:CD1	1:Z:1193:LEU:HD23	2.52	0.44
1:Z:1361:LEU:HA	1:Z:1366:THR:HG21	1.99	0.44
1:Z:1489:LEU:HD22	1:Z:1521:LYS:NZ	2.33	0.44
1:Z:2015:THR:HG21	1:Z:2099:PHE:HE1	1.82	0.44
1:Z:2329:ARG:HH12	1:Z:2367:PRO:HD2	1.82	0.44
1:Z:2375:ILE:O	1:Z:2379:MET:N	2.50	0.44
1:Z:2792:GLN:HG2	1:Z:2820:GLY:HA2	2.00	0.44
1:Z:2781:LYS:HD3	5:E:644:ASN:HD21	1.83	0.44
2:R:165:CYS:HB3	2:R:183:ASN:OD1	2.18	0.44
1:Z:1820:SER:HB2	1:Z:1875:ASP:H	1.82	0.44
1:Z:107:LEU:HD13	1:Z:118:CYS:SG	2.57	0.44
5:E:383:ILE:O	5:E:387:MET:HG3	2.17	0.44
1:Z:1298:ASN:OD1	1:Z:1299:ALA:N	2.48	0.44
1:Z:1709:ASN:HB3	1:Z:1711:PHE:HD1	1.82	0.44
1:Z:1859:LEU:O	1:Z:1863:GLU:N	2.33	0.44
1:Z:2139:LYS:HB2	1:Z:2141:VAL:HG22	1.99	0.44
1:Z:1265:ILE:HG23	1:Z:1313:THR:HG21	2.00	0.44
2:R:475:TYR:HA	2:R:483:LEU:HD11	2.00	0.44
4:P:653:MET:HG2	4:P:654:PRO:HD2	2.00	0.44
1:Z:1783:ILE:HG22	1:Z:1833:TRP:NE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:1936:VAL:O	1:Z:1939:ARG:NH1	2.51	0.43
1:Z:1223:VAL:HG21	1:Z:1229:PHE:HB3	2.00	0.43
1:Z:1883:LYS:O	1:Z:1887:ILE:HG12	2.17	0.43
1:Z:2332:PHE:O	1:Z:2335:THR:OG1	2.31	0.43
1:Z:1594:THR:N	1:Z:1595:PRO:HD2	2.33	0.43
2:R:104:SER:OG	2:R:105:GLY:N	2.51	0.43
1:Z:381:PHE:HB2	1:Z:1858:ASP:HB2	2.01	0.43
1:Z:1343:ARG:O	1:Z:1343:ARG:HG2	2.17	0.43
1:Z:1559:PHE:HD2	1:Z:1562:LEU:HD11	1.83	0.43
1:Z:1611:PHE:CE1	1:Z:1624:MET:HG3	2.54	0.43
1:Z:1825:LEU:HD23	1:Z:1825:LEU:H	1.84	0.43
1:Z:1887:ILE:HD12	1:Z:1918:PHE:HZ	1.83	0.43
1:Z:2514:VAL:HG12	1:Z:2516:ASP:H	1.83	0.43
3:A:113:LYS:HB3	3:A:113:LYS:HE2	1.73	0.43
4:P:631:SER:HB2	5:E:601:LEU:HD11	1.99	0.43
6:S:319:LEU:H	6:S:319:LEU:HD23	1.84	0.43
1:Z:1726:GLN:OE1	1:Z:1759:SER:OG	2.26	0.43
1:Z:3137:ILE:HD11	1:Z:3159:ILE:HG21	2.00	0.43
2:R:94:LEU:HA	2:R:98:LEU:HB2	2.01	0.43
4:P:527:ARG:NH2	5:E:292:TYR:OH	2.51	0.43
1:Z:851:LEU:O	1:Z:854:GLU:HG2	2.18	0.43
1:Z:876:LEU:HB3	1:Z:916:ILE:HG21	2.01	0.43
1:Z:1295:GLU:OE2	1:Z:1307:CYS:HB2	2.18	0.43
1:Z:3436:THR:HG23	1:Z:3441:ILE:HG13	2.00	0.43
1:Z:1762:LEU:HA	1:Z:1765:PHE:HB3	2.01	0.43
1:Z:1997:PHE:HB2	1:Z:2038:TRP:CD1	2.53	0.43
1:Z:2708:GLU:OE2	5:E:771:ARG:NH2	2.47	0.43
1:Z:2728:LEU:HA	5:E:681:THR:HG21	2.01	0.43
5:E:360:ASN:OD1	6:S:182:ARG:NH2	2.51	0.43
1:Z:212:ASN:HB3	1:Z:213:GLY:H	1.64	0.43
1:Z:1146:LEU:HD12	1:Z:1193:LEU:HD13	2.01	0.43
1:Z:1154:SER:HB2	1:Z:1208:ASN:HA	2.01	0.43
1:Z:1271:THR:HG23	1:Z:1272:PHE:HD1	1.82	0.43
1:Z:1495:LEU:HD12	1:Z:1495:LEU:H	1.83	0.43
1:Z:1887:ILE:HA	1:Z:1912:PHE:CE2	2.53	0.43
1:Z:2330:ARG:HB2	1:Z:2331:PRO:HD3	2.01	0.43
2:R:90:TRP:HB2	2:R:132:MET:HE1	2.00	0.43
2:R:178:LYS:HD3	6:S:188:ASP:HA	2.00	0.43
4:P:640:LYS:HE3	5:E:565:LEU:HD13	2.01	0.43
1:Z:288:ARG:NH1	1:Z:1851:TYR:OH	2.48	0.43
1:Z:1297:SER:HB2	1:Z:1353:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:2093:ARG:HB2	1:Z:2133:TRP:CH2	2.54	0.43
1:Z:2651:ASN:O	1:Z:2654:ILE:N	2.50	0.43
4:P:715:GLN:NE2	6:S:52:GLU:OE1	2.52	0.43
6:S:278:LEU:HD21	6:S:282:LEU:HD12	2.01	0.43
1:Z:105:SER:O	1:Z:109:LYS:NZ	2.52	0.43
1:Z:155:ILE:HA	1:Z:158:THR:HG22	2.00	0.43
1:Z:1789:PHE:HD2	1:Z:1802:VAL:HG11	1.84	0.43
5:E:375:GLU:HB3	6:S:56:PRO:HG3	2.01	0.43
1:Z:485:ILE:HG21	1:Z:647:PHE:HZ	1.84	0.42
1:Z:3105:LEU:HD23	1:Z:3665:LEU:HD21	2.01	0.42
4:P:672:ASP:O	4:P:676:ILE:HG12	2.19	0.42
1:Z:47:PHE:O	1:Z:51:VAL:HG12	2.20	0.42
1:Z:1220:ILE:HA	1:Z:1223:VAL:HG12	2.01	0.42
1:Z:1936:VAL:O	1:Z:1939:ARG:HG3	2.19	0.42
1:Z:1997:PHE:CD2	1:Z:2041:LYS:HD2	2.54	0.42
1:Z:2247:LEU:HD22	1:Z:2281:THR:HG21	2.01	0.42
1:Z:2426:VAL:O	1:Z:2427:GLU:HG3	2.19	0.42
1:Z:3534:LEU:HD21	1:Z:3576:LYS:HD2	2.01	0.42
1:Z:3725:GLY:HA2	1:Z:3728:VAL:HG12	2.00	0.42
3:A:94:LEU:HB3	3:A:96:VAL:HG22	2.00	0.42
5:E:553:ASN:OD1	5:E:554:THR:N	2.52	0.42
5:E:764:ILE:O	5:E:768:MET:HG3	2.19	0.42
1:Z:453:ASN:HA	1:Z:454:PRO:HD3	1.90	0.42
1:Z:485:ILE:HG21	1:Z:647:PHE:CZ	2.54	0.42
1:Z:1808:ASN:O	1:Z:1812:ILE:HG12	2.18	0.42
6:S:204:LYS:HA	6:S:204:LYS:HD3	1.84	0.42
1:Z:1297:SER:HB3	1:Z:1356:ALA:HB2	2.01	0.42
1:Z:1658:ASN:HD21	1:Z:1665:PHE:HE2	1.66	0.42
1:Z:1572:ASP:OD1	1:Z:1576:LYS:NZ	2.42	0.42
1:Z:3243:GLU:OE1	1:Z:3387:SER:OG	2.36	0.42
1:Z:110:GLU:OE2	1:Z:114:ASN:HB2	2.20	0.42
1:Z:3245:LEU:HD21	1:Z:3317:TRP:HZ3	1.85	0.42
1:Z:83:PHE:HB3	1:Z:121:VAL:HG21	2.01	0.42
1:Z:148:TYR:CE1	1:Z:224:LEU:HB2	2.54	0.42
1:Z:215:ARG:HG3	1:Z:220:SER:HA	2.02	0.42
1:Z:253:ILE:HG21	1:Z:304:PHE:HE2	1.84	0.42
1:Z:1378:LEU:HD11	1:Z:1419:LEU:HD21	2.02	0.42
1:Z:1579:LEU:HD21	1:Z:1583:LYS:HE2	2.01	0.42
1:Z:3458:MET:SD	1:Z:3584:LEU:HD11	2.59	0.42
1:Z:796:LEU:O	1:Z:799:SER:OG	2.31	0.42
1:Z:1773:SER:OG	1:Z:1774:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:1876:PRO:O	1:Z:1880:ALA:N	2.52	0.42
1:Z:2646:ASN:OD1	1:Z:2647:THR:N	2.53	0.42
1:Z:2909:PHE:HB2	1:Z:2943:ILE:HD11	2.00	0.42
1:Z:3024:THR:HG21	1:Z:3055:LYS:HG2	2.01	0.42
4:P:490:VAL:HG21	5:E:741:LEU:HD11	2.02	0.42
5:E:286:PRO:HG2	5:E:289:GLU:HG3	2.01	0.42
1:Z:622:VAL:O	1:Z:624:ARG:HG3	2.19	0.42
1:Z:1437:ARG:HA	1:Z:1440:ILE:HD13	2.01	0.42
4:P:618:GLU:HB2	5:E:603:ARG:HH12	1.84	0.42
1:Z:373:GLU:OE1	1:Z:421:TYR:OH	2.33	0.42
1:Z:2284:LYS:HE3	1:Z:2284:LYS:HB2	1.86	0.42
1:Z:3132:TYR:OH	1:Z:3363:ASP:OD1	2.29	0.42
1:Z:3405:VAL:HG22	1:Z:3457:ILE:HG22	2.02	0.42
3:A:219:VAL:HG22	3:A:258:PRO:HB2	2.01	0.42
1:Z:377:ILE:HD12	1:Z:384:HIS:HB3	2.02	0.41
1:Z:1932:ARG:NH1	1:Z:1977:ASN:OD1	2.42	0.41
1:Z:148:TYR:CE1	1:Z:256:LEU:HD22	2.55	0.41
1:Z:3305:PRO:HB3	1:Z:3309:THR:OG1	2.20	0.41
1:Z:3480:PHE:HZ	1:Z:3522:VAL:HG23	1.85	0.41
1:Z:687:ALA:O	1:Z:691:MET:HG3	2.20	0.41
1:Z:2099:PHE:CD2	1:Z:2100:LEU:HD22	2.55	0.41
4:P:568:SER:HB3	4:P:738:VAL:HG11	2.02	0.41
1:Z:269:GLU:HA	1:Z:272:GLU:HG3	2.03	0.41
1:Z:367:LEU:HD23	1:Z:367:LEU:HA	1.90	0.41
1:Z:433:ILE:HG23	1:Z:589:THR:HG21	2.03	0.41
1:Z:627:SER:HB3	1:Z:630:GLU:OE1	2.20	0.41
4:P:596:ASP:OD1	4:P:602:ARG:NE	2.36	0.41
1:Z:1994:ASP:HB2	1:Z:2038:TRP:HE1	1.86	0.41
1:Z:2093:ARG:NH2	1:Z:2135:ASN:HD21	2.18	0.41
1:Z:2198:ASP:OD1	1:Z:2198:ASP:N	2.53	0.41
4:P:537:ASN:OD1	5:E:343:ARG:HG3	2.20	0.41
5:E:548:PHE:HB2	5:E:551:GLU:HG2	2.03	0.41
1:Z:835:LEU:HD12	1:Z:835:LEU:HA	1.86	0.41
1:Z:865:VAL:HA	1:Z:866:PRO:HD3	1.97	0.41
1:Z:932:LEU:O	1:Z:932:LEU:HD12	2.21	0.41
1:Z:2184:LEU:HD13	1:Z:2232:GLY:HA2	2.02	0.41
1:Z:2414:VAL:O	1:Z:2417:GLU:HG2	2.21	0.41
1:Z:2746:LEU:HD23	1:Z:2746:LEU:HA	1.92	0.41
3:A:131:ALA:HB1	3:A:356:TRP:CD1	2.55	0.41
4:P:644:ARG:HB2	5:E:372:ASP:OD2	2.20	0.41
1:Z:1684:TRP:CD1	1:Z:1687:LYS:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:2439:LEU:O	1:Z:2442:SER:OG	2.35	0.41
1:Z:3254:ILE:HD11	1:Z:3385:HIS:CE1	2.55	0.41
1:Z:3526:VAL:HG22	1:Z:3627:ASN:ND2	2.36	0.41
6:S:179:TYR:O	6:S:181:LEU:N	2.53	0.41
1:Z:140:PHE:CZ	1:Z:144:ILE:HD11	2.55	0.41
1:Z:1814:GLU:OE1	1:Z:1821:LEU:HD23	2.21	0.41
1:Z:2015:THR:HG21	1:Z:2099:PHE:CE1	2.55	0.41
1:Z:367:LEU:HD22	1:Z:371:PHE:CZ	2.56	0.41
1:Z:700:GLU:HG3	1:Z:1588:LEU:HB3	2.02	0.41
1:Z:808:TYR:O	1:Z:812:ILE:HG13	2.21	0.41
1:Z:1188:SER:OG	1:Z:1189:PHE:N	2.54	0.41
1:Z:1584:LEU:HD23	1:Z:1584:LEU:HA	1.89	0.41
1:Z:1691:MET:O	1:Z:1694:LYS:HG2	2.21	0.41
1:Z:1894:ILE:HD12	1:Z:1906:TYR:CE1	2.55	0.41
1:Z:2200:HIS:O	1:Z:2200:HIS:CG	2.74	0.41
1:Z:2465:ASP:OD1	1:Z:2465:ASP:N	2.54	0.41
2:R:298:ASP:OD1	2:R:298:ASP:N	2.53	0.41
5:E:565:LEU:HD12	5:E:565:LEU:HA	1.93	0.41
1:Z:314:ALA:N	1:Z:315:PRO:HD2	2.36	0.41
1:Z:1279:ASP:OD1	1:Z:1279:ASP:N	2.53	0.41
1:Z:1440:ILE:HD12	1:Z:1440:ILE:H	1.86	0.41
2:R:222:ASP:N	2:R:222:ASP:OD1	2.53	0.41
5:E:374:LYS:HD3	5:E:374:LYS:HA	1.87	0.41
1:Z:137:LEU:HD22	1:Z:238:TYR:HE2	1.87	0.40
1:Z:346:GLU:O	1:Z:350:ALA:N	2.47	0.40
1:Z:377:ILE:O	1:Z:383:MET:HB3	2.21	0.40
1:Z:1044:LYS:HA	1:Z:1044:LYS:HD2	1.92	0.40
1:Z:1463:LEU:HB3	1:Z:1509:LEU:HG	2.02	0.40
1:Z:1796:LEU:HD23	1:Z:1856:HIS:H	1.85	0.40
1:Z:1881:GLU:HG2	1:Z:1882:ILE:HG23	2.03	0.40
1:Z:3284:SER:HA	1:Z:3288:LEU:HD23	2.03	0.40
1:Z:3464:PHE:HB3	1:Z:3575:ASP:HA	2.03	0.40
1:Z:3603:HIS:CD2	1:Z:3603:HIS:H	2.38	0.40
2:R:209:ILE:HG12	2:R:216:PHE:HE1	1.87	0.40
2:R:244:GLU:OE1	3:A:290:ARG:NH2	2.53	0.40
4:P:714:PRO:HD3	6:S:53:ASN:OD1	2.21	0.40
1:Z:2218:LYS:HB3	1:Z:2267:PHE:HE2	1.86	0.40
1:Z:2321:LYS:HD2	1:Z:2324:LEU:HD21	2.03	0.40
4:P:544:ASN:HA	4:P:581:LEU:HD23	2.03	0.40
5:E:639:LEU:HD21	5:E:726:GLU:HG3	2.02	0.40
1:Z:82:ILE:H	1:Z:82:ILE:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:212:ASN:O	1:Z:215:ARG:NH2	2.55	0.40
1:Z:3140:LEU:HD21	1:Z:3155:ILE:HB	2.04	0.40
1:Z:3281:VAL:HG22	1:Z:3301:ILE:HD12	2.02	0.40
1:Z:3506:MET:SD	1:Z:3509:LEU:HD23	2.62	0.40
3:A:32:PRO:HB2	3:A:34:ILE:HG12	2.03	0.40
1:Z:415:ILE:HD12	1:Z:463:LEU:HD22	2.02	0.40
1:Z:902:GLU:HB2	1:Z:948:ILE:HD11	2.04	0.40
1:Z:1436:ILE:HA	1:Z:1439:ARG:HH22	1.87	0.40
1:Z:3211:LEU:HD12	1:Z:3211:LEU:HA	1.94	0.40
4:P:560:VAL:O	4:P:567:SER:HB2	2.21	0.40
4:P:740:ARG:HA	4:P:740:ARG:HD2	1.80	0.40
1:Z:974:ILE:HD11	1:Z:1078:LEU:HD22	2.04	0.40
1:Z:1131:ILE:HB	1:Z:3295:LYS:HE2	2.04	0.40
1:Z:1136:PRO:HD3	1:Z:2503:TYR:CE2	2.56	0.40
1:Z:1282:ASN:ND2	1:Z:1285:LEU:HD13	2.36	0.40
1:Z:2349:LEU:HD23	1:Z:2349:LEU:H	1.86	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	Z	3519/3744 (94%)	3335 (95%)	184 (5%)	0	100	100
2	R	413/489 (84%)	390 (94%)	23 (6%)	0	100	100
3	A	356/375 (95%)	349 (98%)	7 (2%)	0	100	100
4	P	266/832 (32%)	253 (95%)	13 (5%)	0	100	100
5	E	434/982 (44%)	411 (95%)	23 (5%)	0	100	100
6	S	264/476 (56%)	253 (96%)	11 (4%)	0	100	100
All	All	5252/6898 (76%)	4991 (95%)	261 (5%)	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	Z	3261/3452 (94%)	3254 (100%)	7 (0%)	93	97
2	R	370/434 (85%)	370 (100%)	0	100	100
3	A	308/320 (96%)	308 (100%)	0	100	100
4	P	259/769 (34%)	259 (100%)	0	100	100
5	E	402/892 (45%)	402 (100%)	0	100	100
6	S	247/441 (56%)	247 (100%)	0	100	100
All	All	4847/6308 (77%)	4840 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	1521	LYS
1	Z	1626	ASN
1	Z	1687	LYS
1	Z	1709	ASN
1	Z	1738	ARG
1	Z	2177	LYS
1	Z	2791	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	6	GLN
1	Z	1234	GLN
1	Z	1808	ASN
1	Z	1838	HIS
1	Z	1839	ASN
1	Z	2899	ASN
1	Z	3087	GLN

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Mol	Chain	Res	Type
1	Z	3459	ASN
1	Z	3629	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ATP	R	501	8	26,33,33	0.62	0	31,52,52	0.73	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	R	501	8	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	501	ATP	C5-C6-N6	2.26	123.79	120.35
7	R	501	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

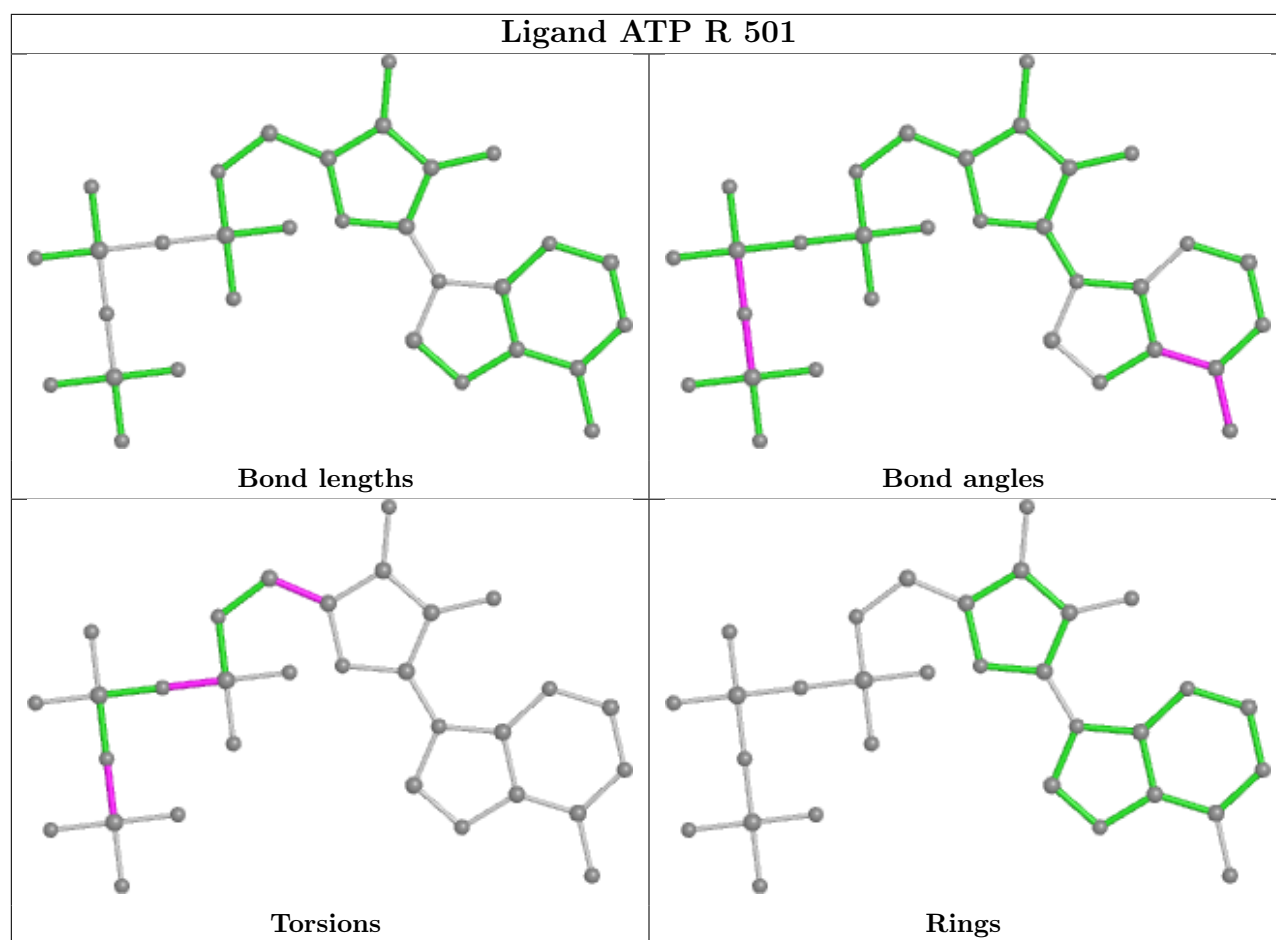
Mol	Chain	Res	Type	Atoms
7	R	501	ATP	PB-O3B-PG-O2G
7	R	501	ATP	PB-O3B-PG-O3G
7	R	501	ATP	O4'-C4'-C5'-O5'
7	R	501	ATP	C3'-C4'-C5'-O5'
7	R	501	ATP	PB-O3A-PA-O2A
7	R	501	ATP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	501	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

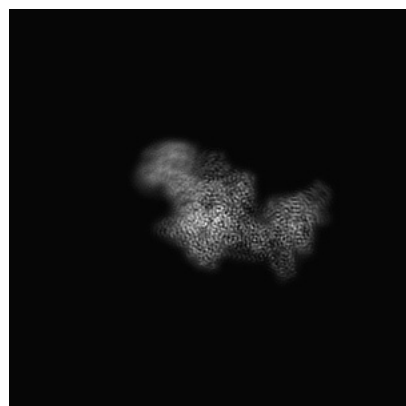
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28575. These allow visual inspection of the internal detail of the map and identification of artifacts.

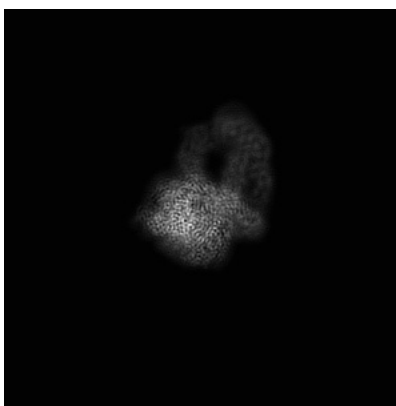
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

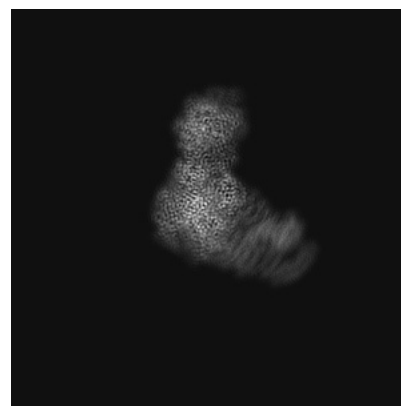
6.1.1 Primary map



X

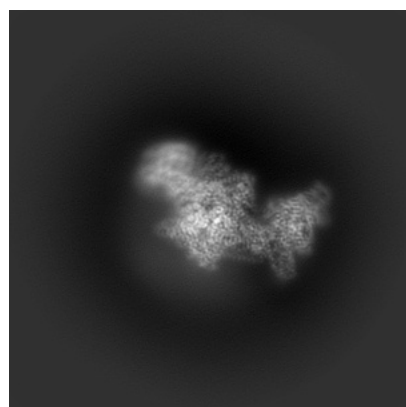


Y

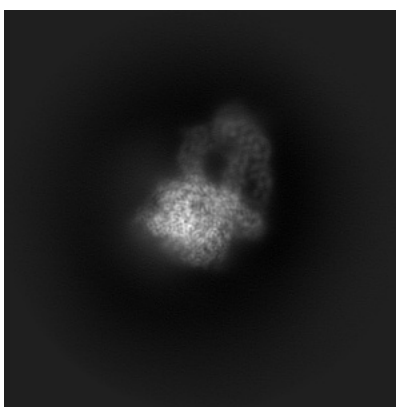


Z

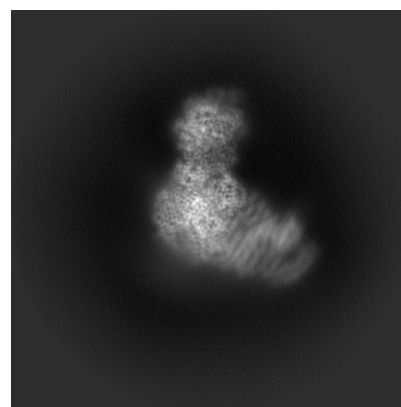
6.1.2 Raw map



X



Y

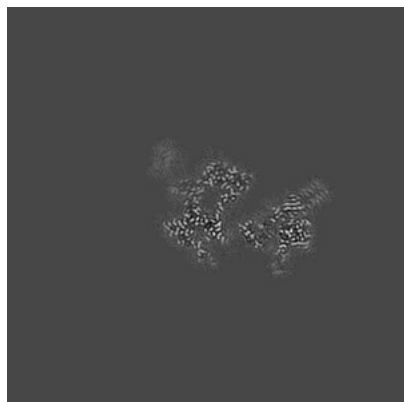


Z

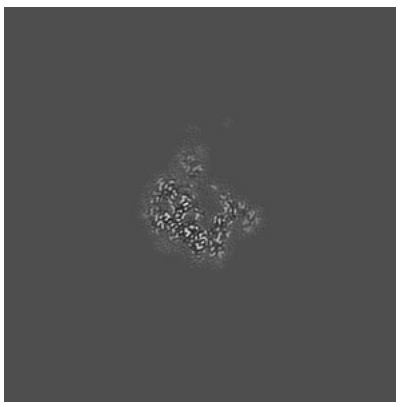
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

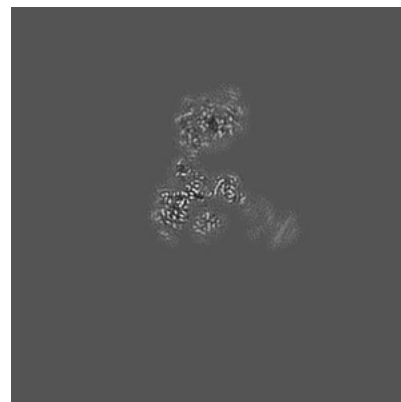
6.2.1 Primary map



X Index: 160

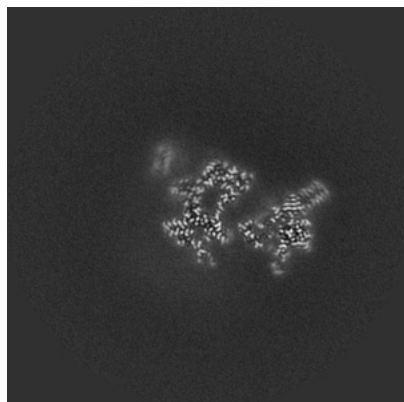


Y Index: 160

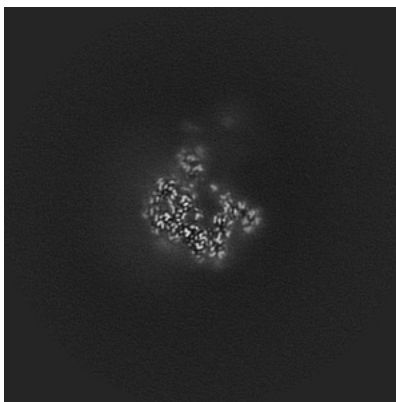


Z Index: 160

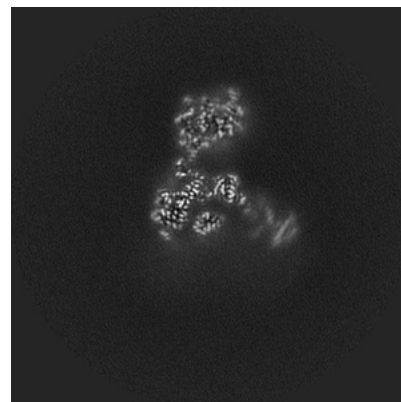
6.2.2 Raw map



X Index: 160



Y Index: 160

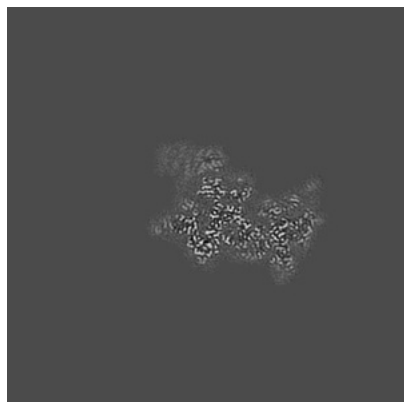


Z Index: 160

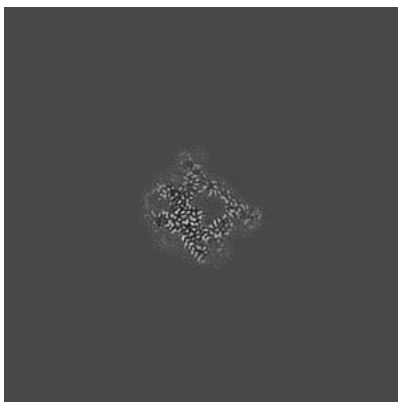
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

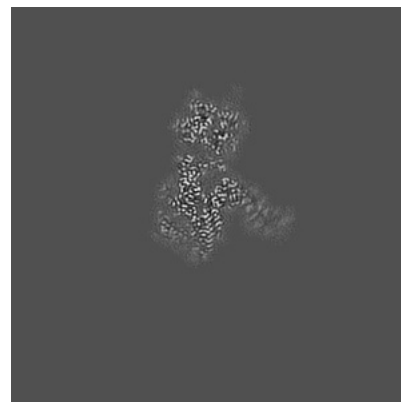
6.3.1 Primary map



X Index: 149

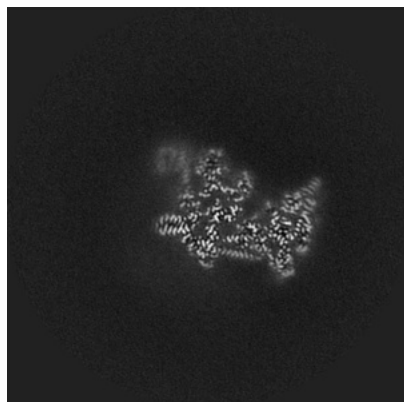


Y Index: 164

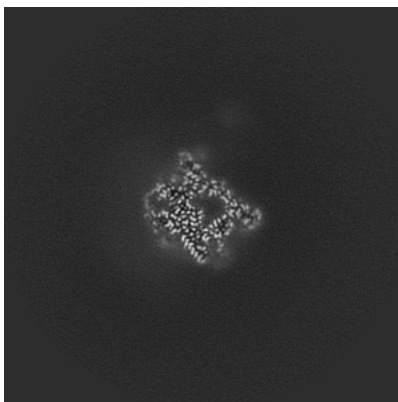


Z Index: 147

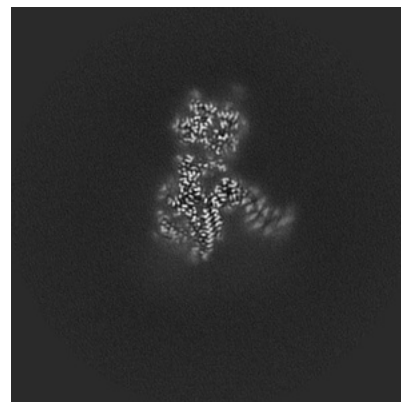
6.3.2 Raw map



X Index: 152



Y Index: 164

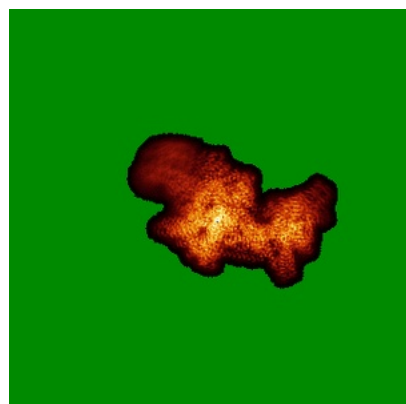


Z Index: 147

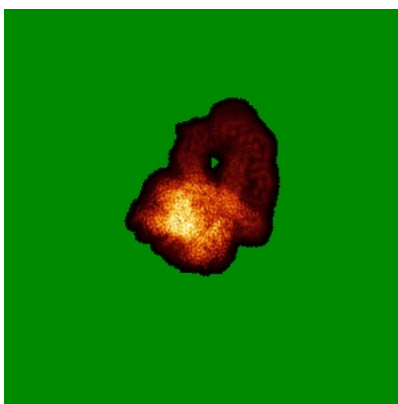
The images above show the largest variance slices of the map in three orthogonal directions.

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

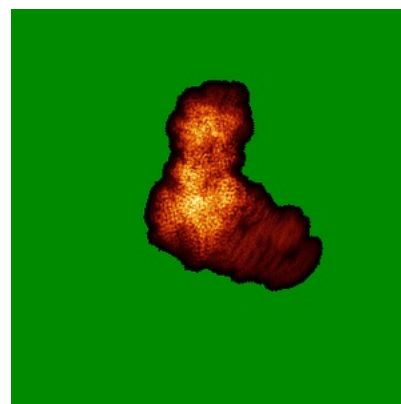
6.4.1 Primary map



X

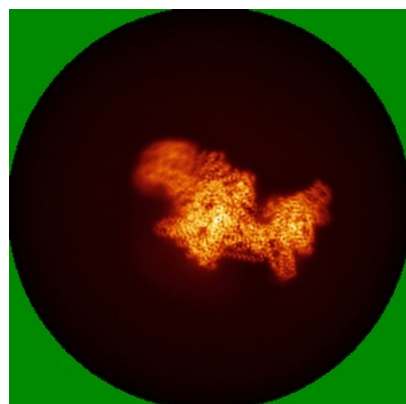


Y

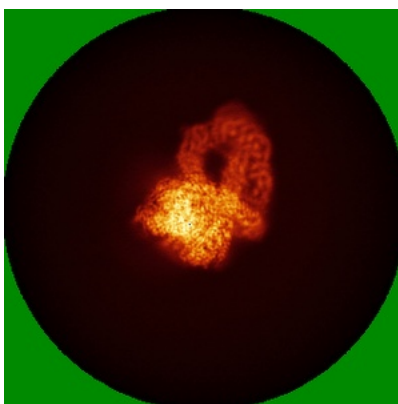


Z

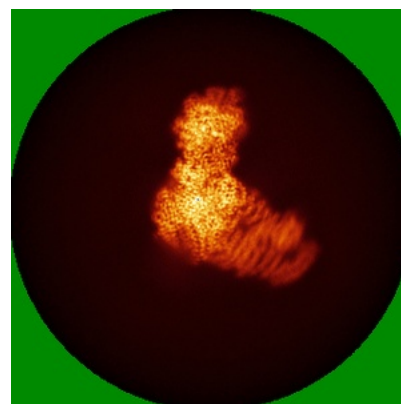
6.4.2 Raw map



X



Y

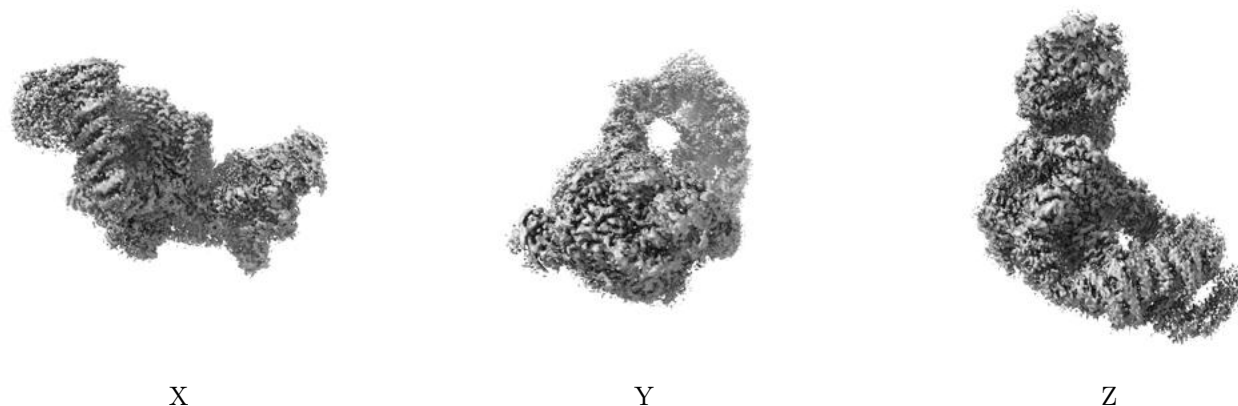


Z

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.

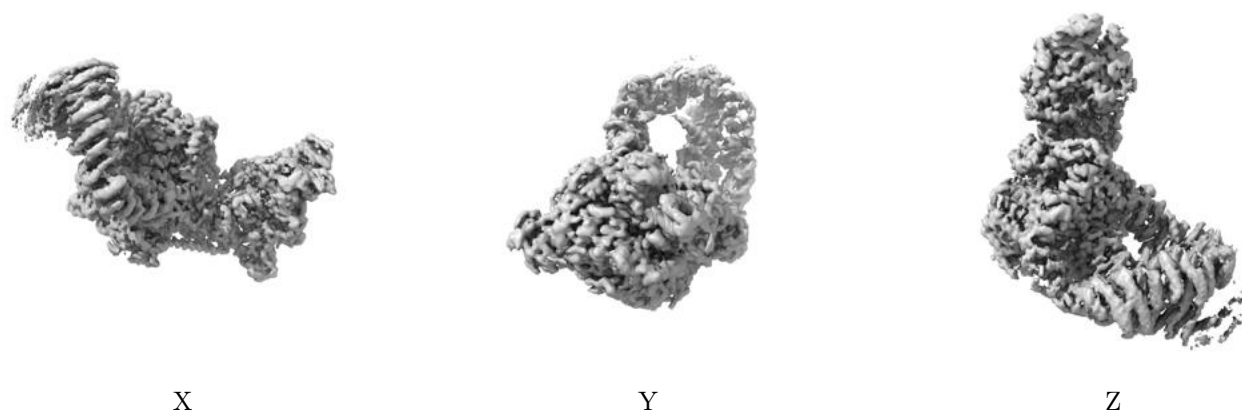
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

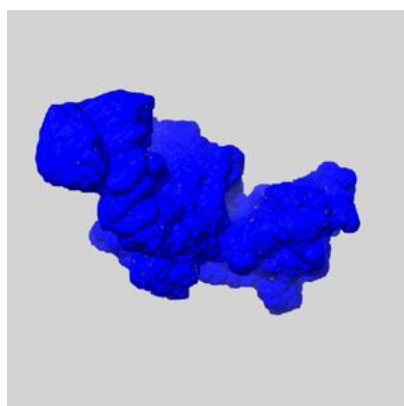
6.6 Mask visualisation [i](#)

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

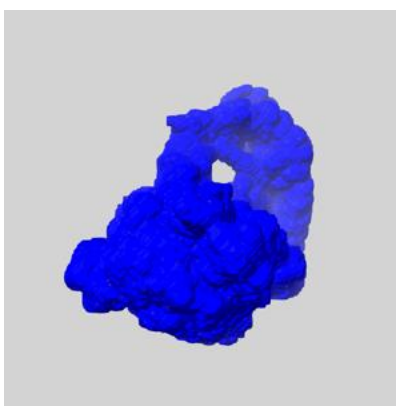
A mask typically either:

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

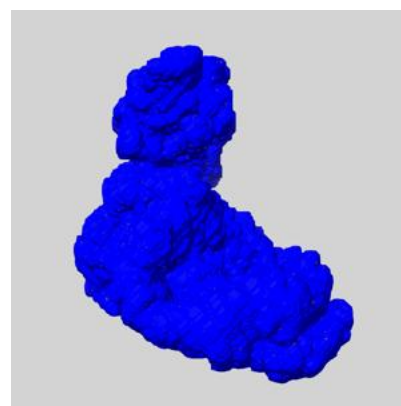
6.6.1 emd_28575_msk_1.map [i](#)



X



Y

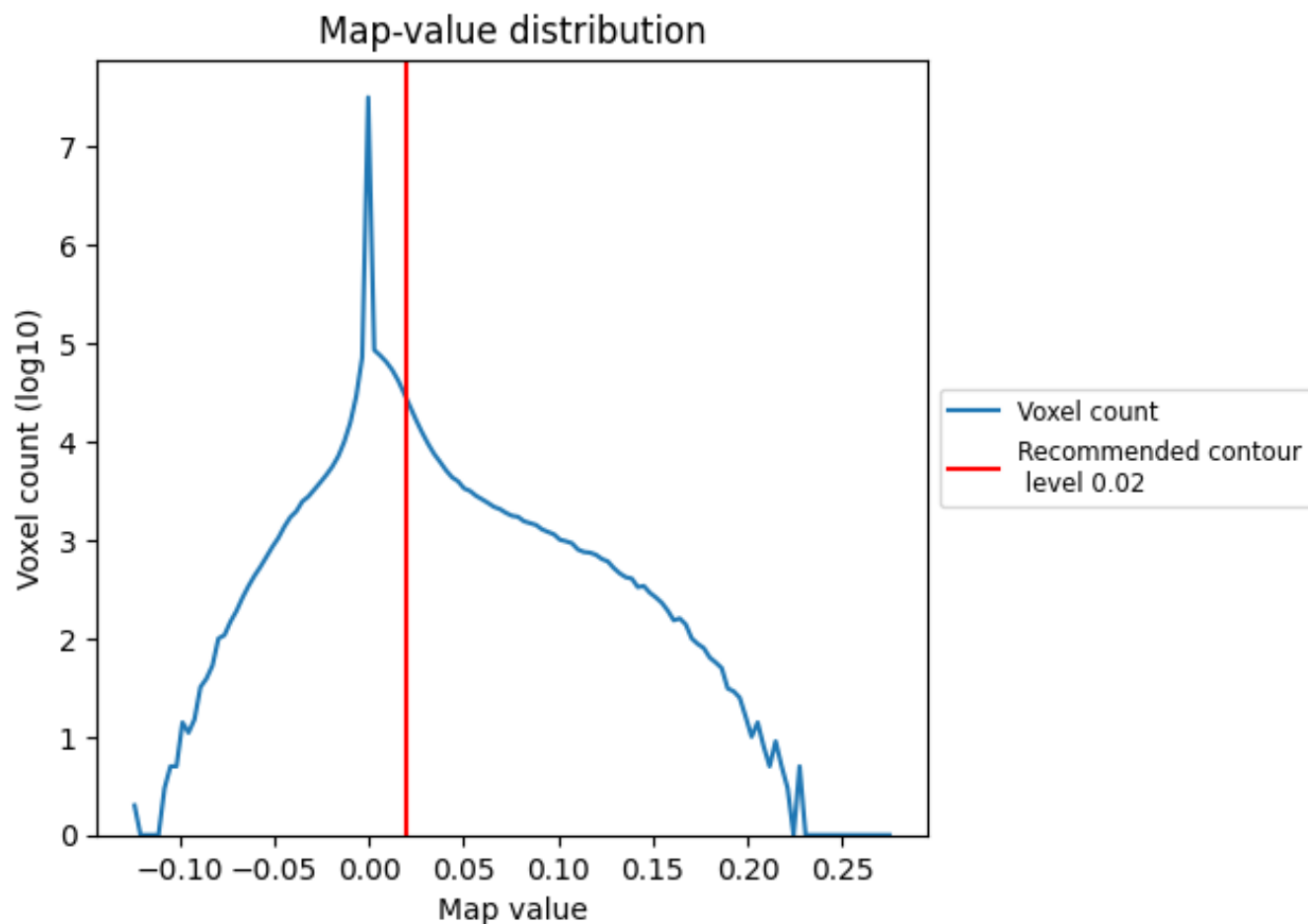


Z

7 Map analysis [i](#)

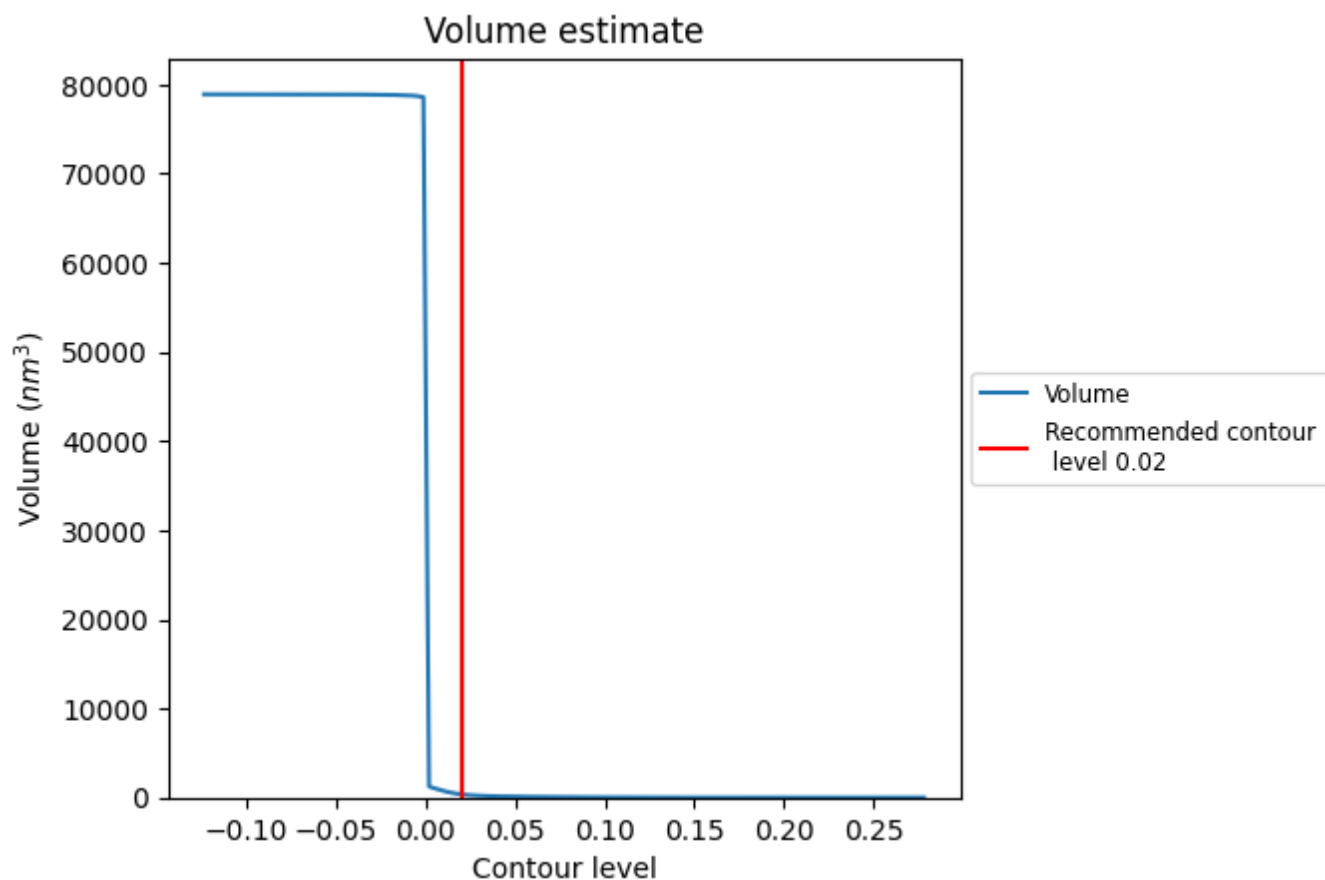
This section contains the results of statistical analysis of the map.

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.

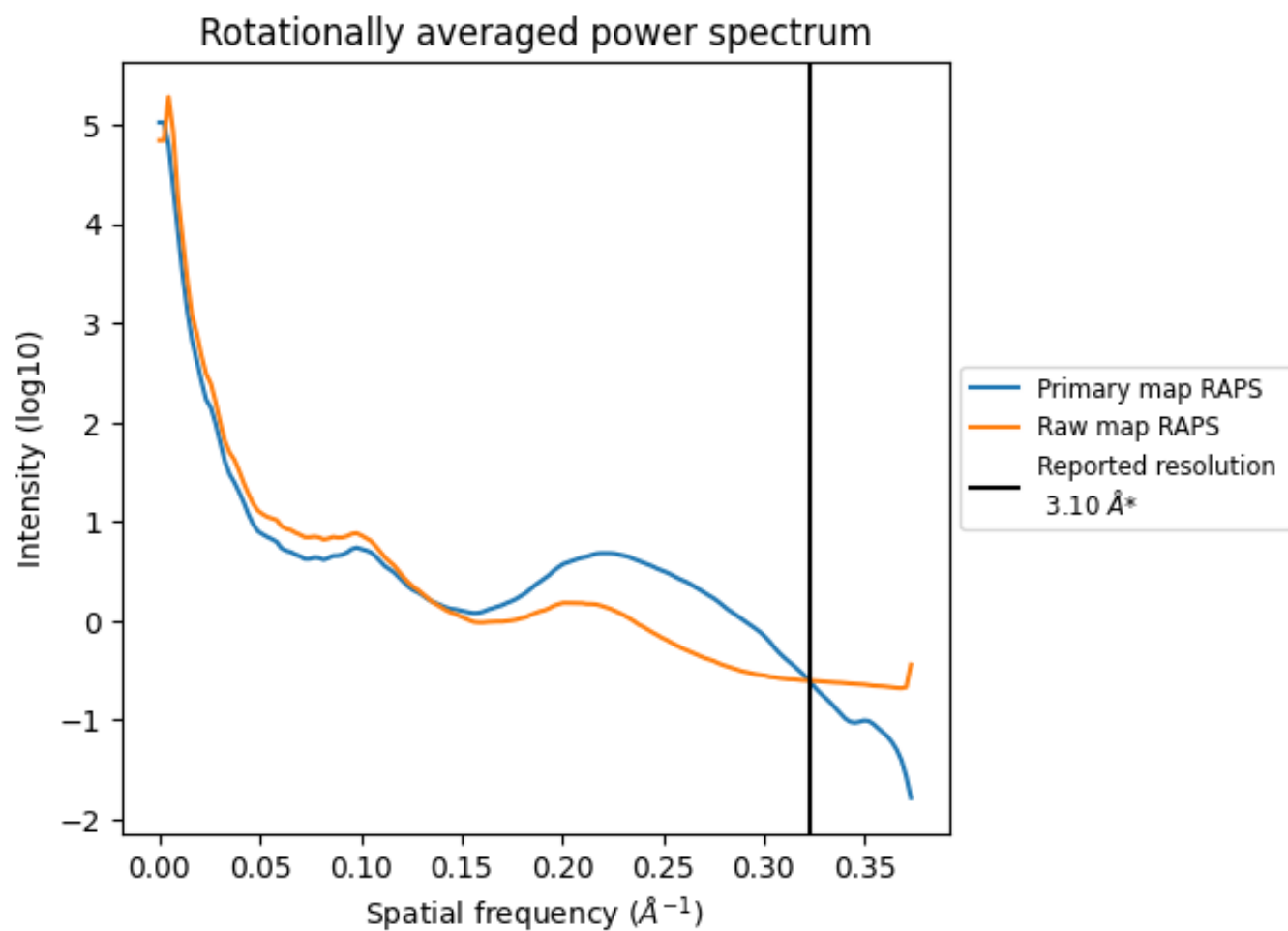
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 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 ⓘ

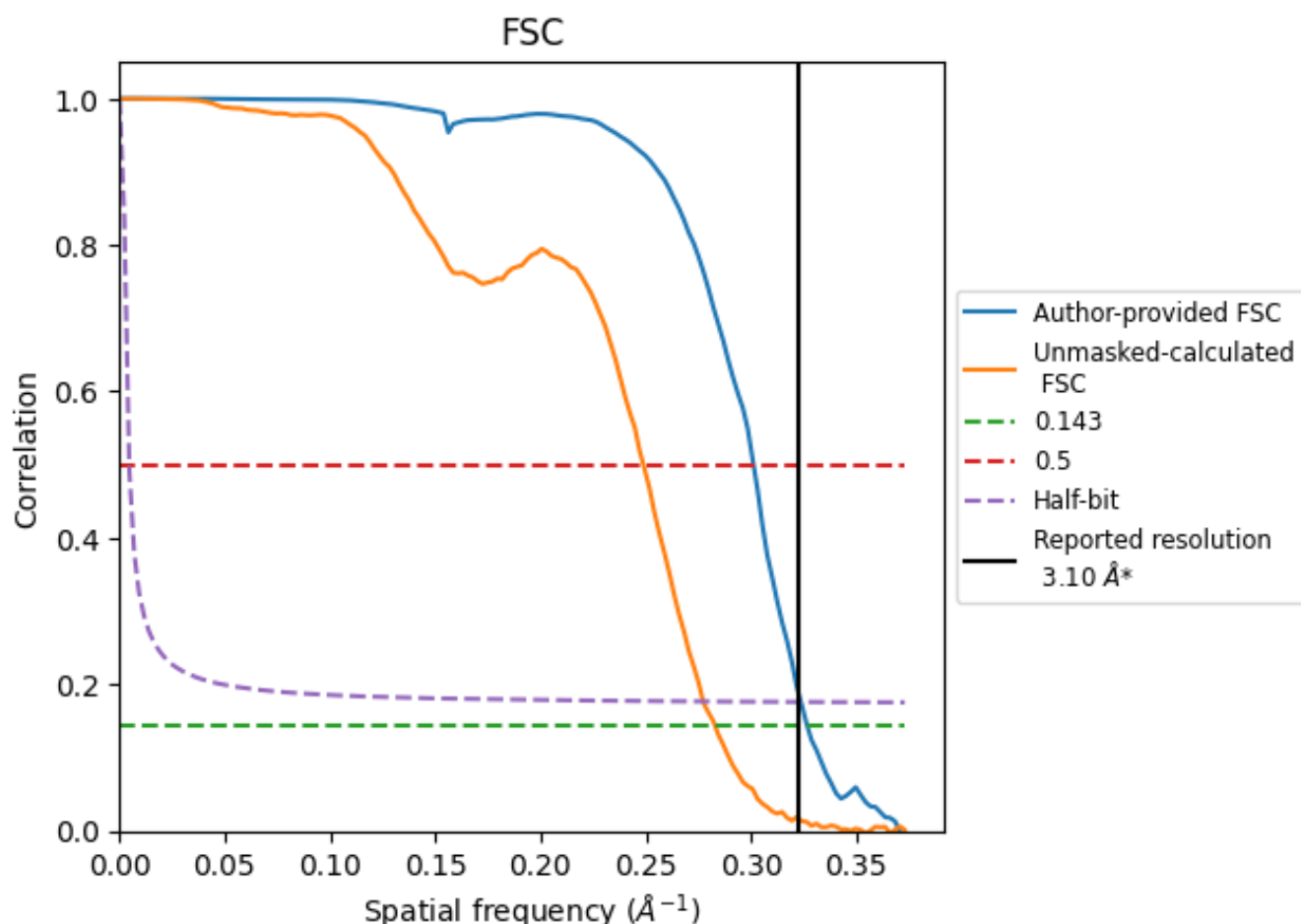


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

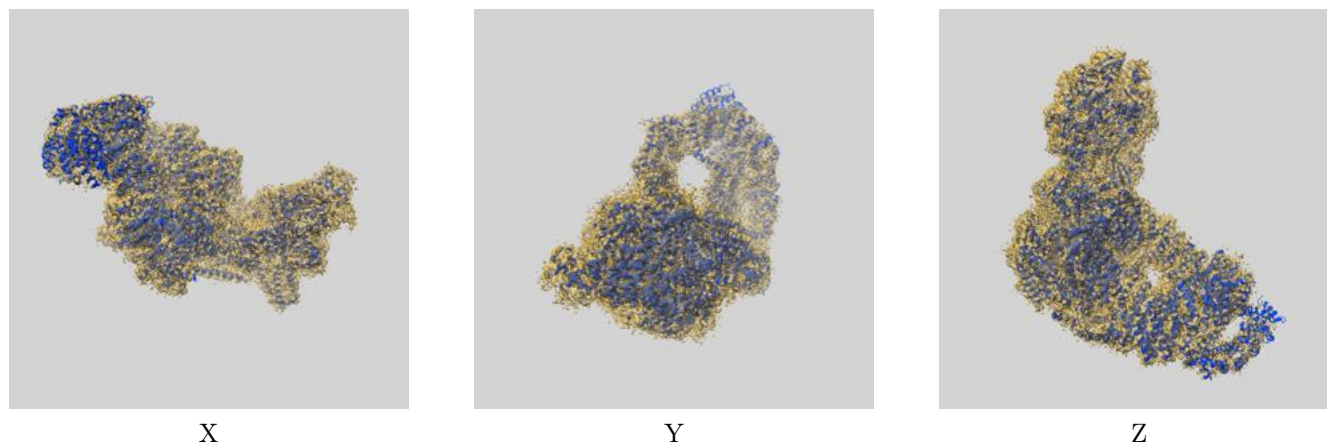
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.32	3.09
Unmasked-calculated*	3.53	4.02	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

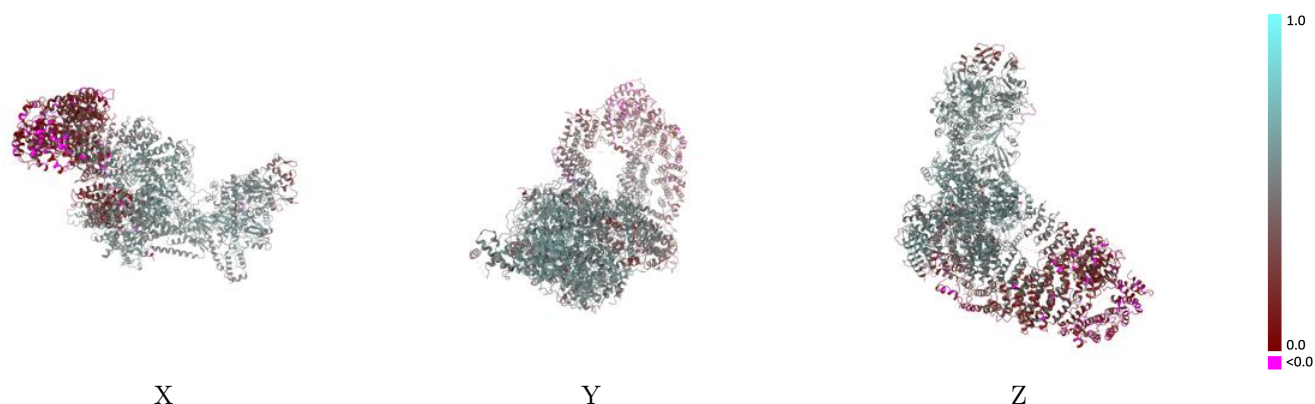
This section contains information regarding the fit between EMDB map EMD-28575 and PDB model 8ESC. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



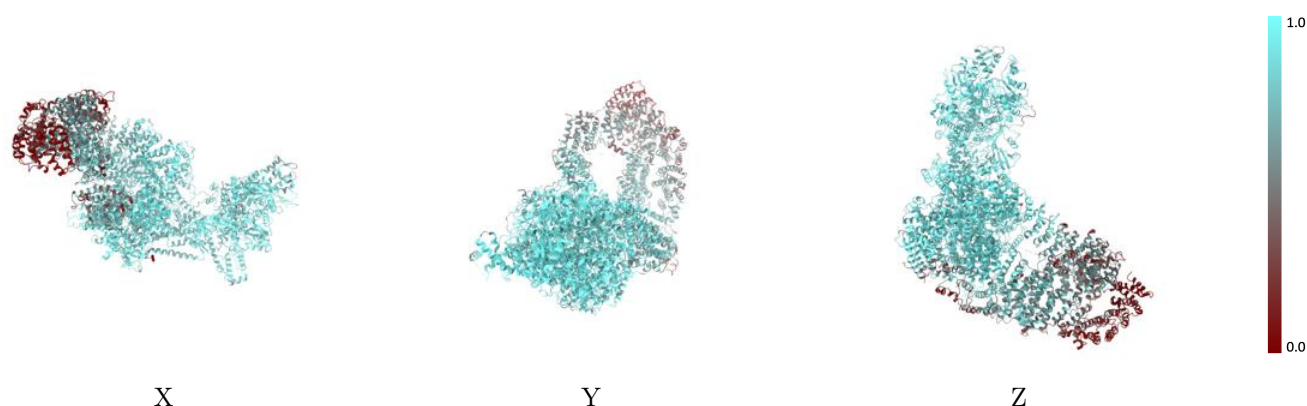
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



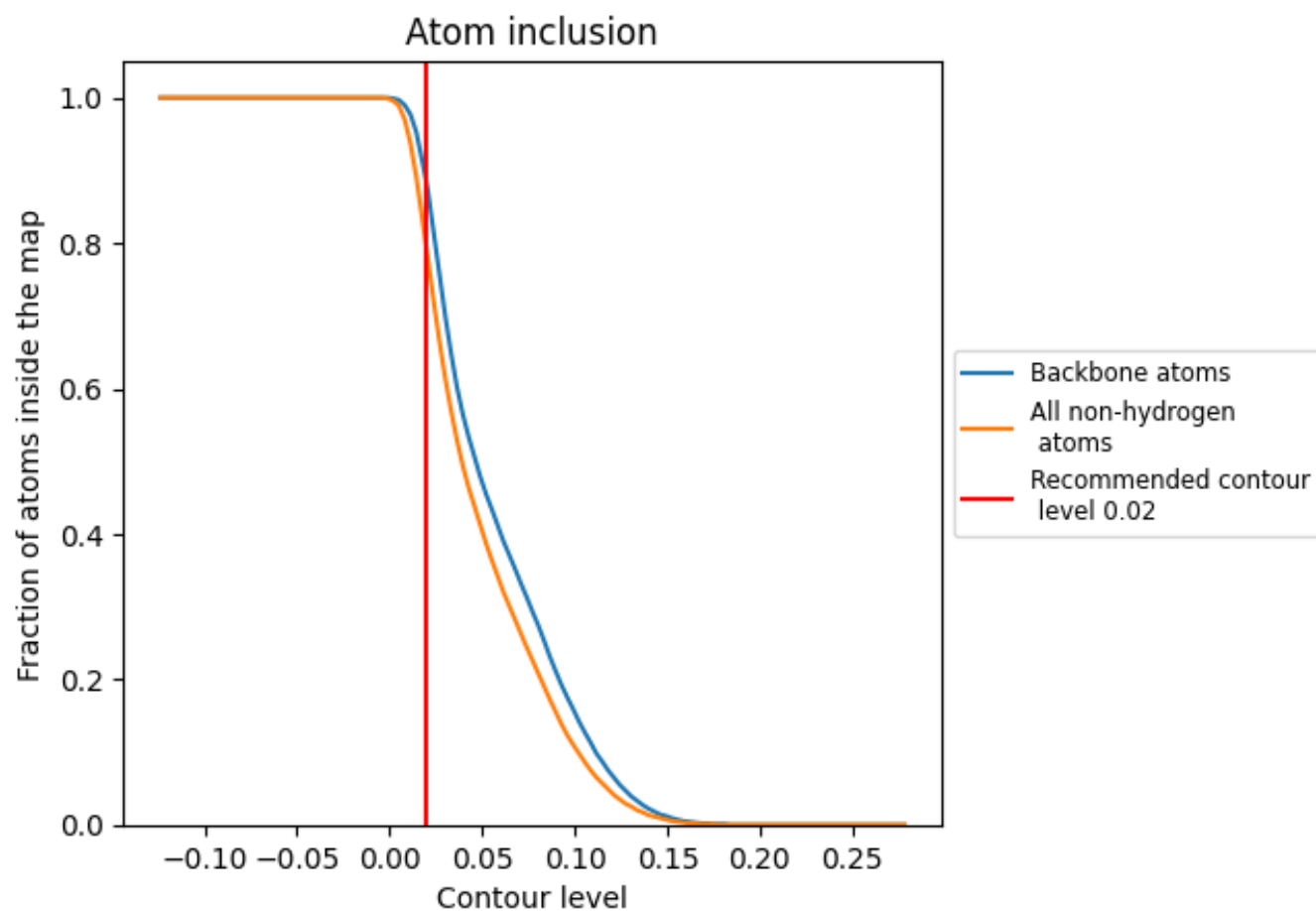
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7920	<div><div></div></div> 0.4380
A	<div><div></div></div> 0.8710	<div><div></div></div> 0.4740
E	<div><div></div></div> 0.9060	<div><div></div></div> 0.5270
P	<div><div></div></div> 0.9050	<div><div></div></div> 0.5240
R	<div><div></div></div> 0.9370	<div><div></div></div> 0.5450
S	<div><div></div></div> 0.8680	<div><div></div></div> 0.4990
Z	<div><div></div></div> 0.7390	<div><div></div></div> 0.3990

1.0

0.0

<0.0