



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:30 AM UTC

PDB ID : 7ALP / pdb_00007alp
EMDB ID : EMD-0828
Title : Severe fever with thrombocytopenia syndrome virus (Phenuiviridae) L protein
Authors : Cusack, S.; Rosenthal, M.
Deposited on : 2020-10-07
Resolution : 3.40 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

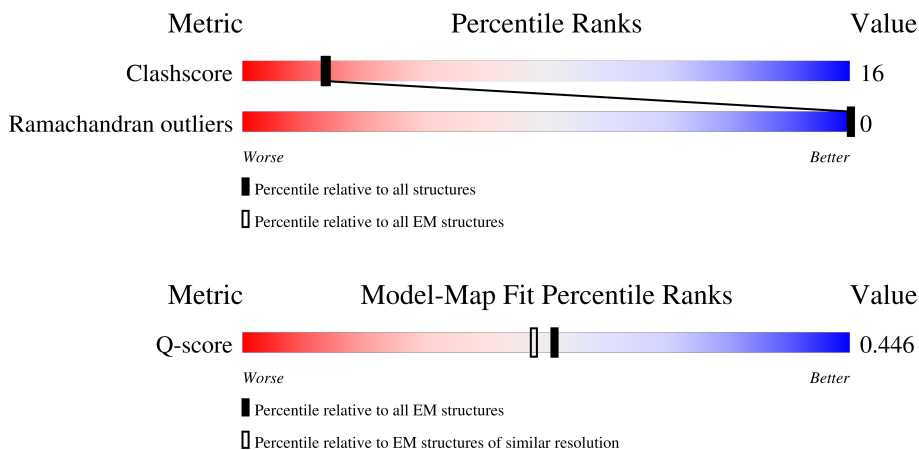
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	U	2084	 67% 26% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15398 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 Replicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	1935	Total	C	N	O	S	0	0
			15396	9759	2666	2877	94		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	U	2	Total	Mg	0
			2	2	

Q2047	Q2048	R2049	P2050	P2051	LEU	ILE	PHE	LEU	LEU	GLN	ILE	PRO	E2059	I2062	S2066	F2069	CYS	ASP	SER	SER	ARG	GLY	LEU	LEU	ASP	GLU	GLU	SER	SER	THR	ILE	MET	TRP	TRP	GLY											
S1867	N1868	R1869	L1870	L1871	F1872	S1873	F1874	GLY	LYS	LYS	GLU	P1879	I1884	C1885	L1886	K1887	THR	LEU	ASP	ASN	TRP	ALA	TRP	SER	HIS	A1897	L1900	L1901	A1902	N1903	D1904	M1915	G1916	N1917	I1918	F1919	R1920									
Q1951	L1952	L1953	D1954	D1955	I1956	L1957	I1961	D1965	V1966	V1967	A1968	I1978	F1982	E1992	G1997	E1998	G1999	V2000	VAL	ALA	VAL	SER	SER	TYR	SER	TYR	HIS	LEU	T2013	L2014	M2015	D2016	A2019	I2020	I2025	M2026	G2027	C2031	R2032	L2035	T2036	E2037	R2038	R2039	R2045	
G1773	I1774	V1778	A1779	R1783	R1789	L1790	S1791	G1792	F1793	K1794	I1795	K1796	P1797	T1801	P1805	V1806	M1809	R1816	E1823	R1829	I1832	L1833	N1834	L1835	S1836	V1837	T1838	I1839	Q1840	H1733	E1841	V1844	M1845	L1848	S1849	Y1850	R1851	P1852	R1853	D1856	T1857	A1862	L1863	Y1864	L1865	W1866
R1670	T1671	M1672	T1673	L1674	N1679	TYR	LEU	SER	SER	ARG	GLY	S1687	I1688	Q1691	G1698	K1705	P1713	G1714	G1715	G1716	V1717	G1718	Y1719	V1724	V1728	W1729	E1730	D1731	T1732	H1733	V1734	L1737	I1738	D1739	G1740	S1744	N1745	R1751	L1752	D1755	A1756	R1757	R1766	C1769		
D1508	L1509	R1510	L1516	V1517	V1520	W1521	F1522	G1523	L1524	K1525	K1528	L1533	E1537	W1538	D1539	K1540	L1541	R1542	A1543	S1544	W1547	L1548	S1549	T1550	D1551	P1552	T1555	D1558	L1562	S1563	H1564	A1572	H1573	V1574	D1575	A1576	R1579	R1582	G1585	A1586	P1587	V1588	LYS	LYS	GLY	
V1395	T1396	S1397	H1403	R1407	V1413	S1424	SER	ILE	HIS	GLY	ARG	GLY	S1432	K1435	L1438	L1441	S1445	SER	ILE	SER	ALA	MET	HIS	GLY	S1455	L1456	N1457	P1458	N1459	M1463	E1470	T1485	N1494	I1495	V1496	R1497	S1498	R1499	I1500	D1501	L1502	V1507				
L1257	I1266	F1275	D1279	R1290	R1295	F1310	I1313	Q1314	G1315	K1316	T1317	D1320	A1325	L1326	T1329	T1333	L1334	S1335	H1336	S1337	V1340	R1345	Y1348	Q1349	W1361	I1365	P1369	G1370	V1371	L1372	A1377	N1378	E1381	K1385	L1386	A1387	E1388	V1389	V1390							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147344	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 ($e^-/\text{\AA}^2$)	40	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	0.061	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0085	Depositor
Map size ($\text{\AA}$)	237.6, 237.6, 237.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: MG

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	U	0.23	0/15697	0.41	0/21173

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	U	15396	0	15401	487	0
2	U	2	0	0	0	0
All	All	15398	0	15401	487	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 16.

All (487) 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:U:1900:LEU:HD22	1:U:2032:ARG:CG	1.54	1.37
1:U:1900:LEU:CD2	1:U:2032:ARG:HG2	1.62	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1900:LEU:HD22	1:U:2032:ARG:HG3	1.34	1.07
1:U:1886:LEU:H	1:U:1886:LEU:HD12	1.18	1.05
1:U:1900:LEU:HD22	1:U:2032:ARG:HG2	1.22	0.99
1:U:1670:ARG:O	1:U:1674:LEU:HD13	1.65	0.95
1:U:1900:LEU:HD21	1:U:2032:ARG:HG2	1.44	0.95
1:U:1900:LEU:HD13	1:U:2032:ARG:HD2	1.49	0.93
1:U:950:GLU:CD	1:U:952:VAL:HG12	1.94	0.93
1:U:1900:LEU:CD2	1:U:2032:ARG:CG	2.32	0.92
1:U:128:THR:HG23	1:U:171:VAL:HG23	1.54	0.88
1:U:732:THR:HG23	1:U:746:MET:SD	2.14	0.87
1:U:1521:TRP:HH2	1:U:1555:THR:HG21	1.40	0.87
1:U:696:THR:HG22	1:U:698:LEU:H	1.38	0.86
1:U:950:GLU:OE1	1:U:952:VAL:HG12	1.75	0.86
1:U:732:THR:CG2	1:U:746:MET:SD	2.63	0.85
1:U:1521:TRP:CH2	1:U:1555:THR:HG21	2.13	0.84
1:U:1507:VAL:HG23	1:U:1508:ASP:H	1.41	0.83
1:U:1874:PHE:HE1	1:U:1884:ILE:HG12	1.43	0.83
1:U:1919:PHE:CZ	1:U:1923:LEU:HD22	2.14	0.82
1:U:1539:ASP:OD1	1:U:1796:LYS:HD3	1.79	0.81
1:U:1728:VAL:HG11	1:U:1816:ARG:HH21	1.46	0.81
1:U:1525:LYS:H	1:U:1525:LYS:HD2	1.44	0.80
1:U:1874:PHE:CE1	1:U:1884:ILE:HG12	2.16	0.80
1:U:1521:TRP:CE3	1:U:1552:PRO:HB3	2.18	0.78
1:U:1766:ARG:HA	1:U:1793:PHE:CE1	2.18	0.78
1:U:1790:LEU:HD12	1:U:1790:LEU:O	1.83	0.78
1:U:1633:LEU:HD11	1:U:1672:MET:HE1	1.68	0.76
1:U:1179:VAL:HG12	1:U:1180:GLU:N	2.01	0.75
1:U:37:ASP:OD1	1:U:48:ASP:N	2.20	0.75
1:U:98:VAL:HG21	1:U:114:ILE:CD1	2.18	0.74
1:U:33:LEU:HB2	1:U:1948:LEU:HD21	1.70	0.72
1:U:1832:ILE:CG2	1:U:1834:ASN:HD21	2.02	0.72
1:U:726:ARG:NH1	1:U:1494:ASN:O	2.24	0.71
1:U:1671:THR:HB	1:U:1848:LEU:HD21	1.71	0.71
1:U:1640:PRO:HB2	1:U:1915:MET:HG3	1.72	0.71
1:U:1539:ASP:OD1	1:U:1796:LYS:HA	1.91	0.71
1:U:848:MET:SD	1:U:1395:VAL:HG13	2.30	0.71
1:U:1143:VAL:CG1	1:U:1978:ILE:HG22	2.21	0.70
1:U:37:ASP:OD2	1:U:48:ASP:HB2	1.91	0.70
1:U:1640:PRO:HA	1:U:1918:ILE:HG21	1.72	0.70
1:U:954:ASN:N	1:U:954:ASN:OD1	2.25	0.69
1:U:3:LEU:HD11	1:U:113:VAL:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1424:SER:HG	1:U:1432:SER:N	1.91	0.68
1:U:1178:CYS:SG	1:U:1187:PHE:HD1	2.17	0.68
1:U:1832:ILE:HD11	1:U:1851:ARG:HG2	1.76	0.67
1:U:950:GLU:OE2	1:U:952:VAL:HG12	1.95	0.67
1:U:1190:HIS:CD2	1:U:1494:ASN:ND2	2.63	0.67
1:U:1191:LEU:C	1:U:1191:LEU:HD23	2.20	0.67
1:U:1189:ARG:O	1:U:1998:GLU:HG2	1.94	0.67
1:U:1290:ARG:HE	1:U:1576:ALA:HB3	1.59	0.67
1:U:1194:PRO:HG2	1:U:1197:ARG:HH21	1.60	0.66
1:U:2059:GLU:HA	1:U:2059:GLU:OE1	1.95	0.66
1:U:37:ASP:OD2	1:U:48:ASP:CB	2.43	0.66
1:U:98:VAL:HG21	1:U:114:ILE:HD11	1.76	0.66
1:U:787:PHE:CZ	1:U:793:THR:OG1	2.49	0.66
1:U:1640:PRO:HB3	1:U:1918:ILE:HG22	1.79	0.65
1:U:981:ASN:HB3	1:U:1179:VAL:HG22	1.75	0.65
1:U:1539:ASP:CG	1:U:1796:LYS:HD3	2.22	0.65
1:U:1874:PHE:CE1	1:U:1884:ILE:CG1	2.79	0.65
1:U:1829:ARG:HB2	1:U:1832:ILE:HG22	1.79	0.65
1:U:1640:PRO:HA	1:U:1918:ILE:CG2	2.27	0.65
1:U:973:LEU:O	1:U:1135:ARG:NH1	2.30	0.64
1:U:300:ASN:OD1	1:U:682:LYS:NZ	2.29	0.64
1:U:462:PHE:O	1:U:466:ASN:ND2	2.30	0.64
1:U:1857:ILE:HB	1:U:2020:ILE:HG12	1.78	0.64
1:U:1507:VAL:HG23	1:U:1508:ASP:N	2.09	0.64
1:U:987:LYS:HG2	1:U:988:LYS:HG3	1.80	0.64
1:U:1377:ALA:N	1:U:1381:GLU:OE2	2.28	0.63
1:U:742:ASN:OD1	1:U:742:ASN:N	2.18	0.63
1:U:248:SER:OG	1:U:1022:ARG:NH1	2.32	0.63
1:U:48:ASP:OD1	1:U:67:LEU:N	2.31	0.63
1:U:95:LEU:HD12	1:U:109:MET:HB2	1.78	0.63
1:U:1070:THR:HG23	1:U:1070:THR:O	1.97	0.63
1:U:1738:ILE:HD11	1:U:1774:ILE:HG21	1.81	0.62
1:U:1457:ASN:ND2	1:U:1459:ASN:HB3	2.14	0.62
1:U:1874:PHE:HE1	1:U:1884:ILE:CG1	2.10	0.62
1:U:856:LYS:HE3	1:U:907:ARG:HH22	1.65	0.62
1:U:999:ALA:HB2	1:U:1018:ILE:HG21	1.81	0.62
1:U:1844:VAL:HG12	1:U:1845:MET:N	2.14	0.62
1:U:1110:TYR:OH	1:U:1144:ARG:NH1	2.33	0.62
1:U:1740:GLY:HA3	1:U:1745:ASN:HA	1.80	0.62
1:U:732:THR:HG22	1:U:733:PHE:N	2.14	0.62
1:U:1140:MET:HE2	1:U:1144:ARG:HE	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:309:GLN:HA	1:U:309:GLN:NE2	2.15	0.61
1:U:1886:LEU:H	1:U:1886:LEU:CD1	1.97	0.61
1:U:1521:TRP:CH2	1:U:1552:PRO:HA	2.36	0.61
1:U:1928:ARG:HE	1:U:2025:ILE:HG23	1.64	0.61
1:U:1310:PHE:HA	1:U:1547:TRP:HZ3	1.66	0.61
1:U:1387:ALA:O	1:U:1390:VAL:HG12	2.01	0.61
1:U:244:THR:O	1:U:1023:ARG:NH2	2.34	0.61
1:U:608:ASN:ND2	1:U:655:ASP:OD2	2.33	0.61
1:U:1670:ARG:O	1:U:1674:LEU:CD1	2.43	0.61
1:U:1919:PHE:CE2	1:U:1923:LEU:HD22	2.35	0.61
1:U:356:MET:SD	1:U:356:MET:N	2.74	0.60
1:U:106:SER:OG	1:U:156:ARG:NH2	2.35	0.60
1:U:1966:VAL:HG23	1:U:1967:ILE:HD12	1.84	0.60
1:U:1688:ILE:O	1:U:1691:GLN:NE2	2.35	0.60
1:U:493:MET:SD	1:U:1295:ARG:NH1	2.74	0.60
1:U:1179:VAL:HG12	1:U:1180:GLU:H	1.65	0.59
1:U:815:ARG:NH1	1:U:1951:GLN:OE1	2.35	0.59
1:U:1648:GLU:O	1:U:1652:GLU:HG2	2.02	0.59
1:U:1734:VAL:HG12	1:U:1752:LEU:HG	1.85	0.59
1:U:1791:SER:O	1:U:1794:LYS:HB2	2.02	0.59
1:U:1336:HIS:CD2	1:U:1336:HIS:N	2.70	0.59
1:U:1095:GLN:HB3	1:U:1121:VAL:HG11	1.83	0.59
1:U:1930:GLN:OE1	1:U:1934:ARG:NH1	2.36	0.59
1:U:1179:VAL:CG1	1:U:1180:GLU:N	2.65	0.59
1:U:226:ARG:NH1	1:U:838:GLY:O	2.35	0.59
1:U:1249:LEU:O	1:U:1249:LEU:HG	2.03	0.59
1:U:1336:HIS:CD2	1:U:1336:HIS:H	2.18	0.58
1:U:1724:VAL:HG22	1:U:1737:LEU:HD22	1.86	0.58
1:U:128:THR:CG2	1:U:171:VAL:HG23	2.30	0.58
1:U:1751:ARG:HE	1:U:1783:ARG:HH12	1.51	0.58
1:U:841:ASN:OD1	1:U:842:ILE:N	2.37	0.58
1:U:1633:LEU:HD11	1:U:1672:MET:CE	2.32	0.58
1:U:1886:LEU:HD12	1:U:1886:LEU:N	2.03	0.58
1:U:1832:ILE:CD1	1:U:1851:ARG:HG2	2.34	0.58
1:U:1119:VAL:HG23	1:U:1132:ILE:HG12	1.87	0.57
1:U:2032:ARG:NH2	1:U:2066:SER:OG	2.34	0.57
1:U:1290:ARG:NH2	1:U:1574:VAL:O	2.37	0.57
1:U:1629:LEU:O	1:U:1633:LEU:HG	2.03	0.57
1:U:1717:VAL:HG23	1:U:1717:VAL:O	2.04	0.57
1:U:1864:TYR:O	1:U:1868:ASN:ND2	2.38	0.57
1:U:129:THR:HG22	1:U:172:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:309:GLN:HA	1:U:309:GLN:HE21	1.69	0.56
1:U:1325:ALA:HB2	1:U:1336:HIS:ND1	2.20	0.56
1:U:1558:ASP:N	1:U:1558:ASP:OD1	2.35	0.56
1:U:1766:ARG:HA	1:U:1793:PHE:HE1	1.68	0.56
1:U:1369:PRO:HB3	1:U:1564:HIS:CD2	2.40	0.56
1:U:1533:LEU:O	1:U:1537:GLU:HG2	2.05	0.56
1:U:84:PHE:HD2	1:U:87:LEU:HD12	1.69	0.56
1:U:1755:ASP:N	1:U:1755:ASP:OD1	2.39	0.56
1:U:1143:VAL:HG12	1:U:1978:ILE:HG22	1.86	0.56
1:U:2046:GLU:HG3	1:U:2049:ARG:H	1.71	0.56
1:U:93:ARG:HB2	1:U:114:ILE:HG21	1.88	0.56
1:U:855:SER:OG	1:U:856:LYS:N	2.39	0.56
1:U:1916:GLY:O	1:U:1920:ARG:NH1	2.38	0.56
1:U:1066:ASP:OD1	1:U:1067:LYS:N	2.39	0.56
1:U:981:ASN:CB	1:U:1179:VAL:HG22	2.36	0.55
1:U:1189:ARG:HG3	1:U:1997:GLY:O	2.06	0.55
1:U:1257:LEU:HD23	1:U:1257:LEU:H	1.72	0.55
1:U:1730:GLU:OE1	1:U:1757:ARG:NH1	2.39	0.55
1:U:865:GLN:HG3	1:U:866:THR:HG23	1.87	0.55
1:U:745:ASN:N	1:U:745:ASN:HD22	2.04	0.55
1:U:464:THR:O	1:U:642:ARG:NH1	2.40	0.55
1:U:1900:LEU:CD1	1:U:2032:ARG:HD2	2.29	0.55
1:U:1326:LEU:CD1	1:U:1562:LEU:HD23	2.37	0.55
1:U:1143:VAL:HG12	1:U:1978:ILE:CG2	2.36	0.55
1:U:1521:TRP:CZ3	1:U:1552:PRO:HA	2.42	0.55
1:U:1179:VAL:CG1	1:U:1180:GLU:H	2.19	0.55
1:U:1934:ARG:HA	1:U:2045:ARG:HG2	1.87	0.55
1:U:1992:GLU:H	1:U:1992:GLU:CD	2.14	0.55
1:U:729:TRP:CZ2	1:U:1178:CYS:SG	3.00	0.55
1:U:168:GLY:HA2	1:U:180:ASN:HD21	1.72	0.54
1:U:1789:ARG:HA	1:U:1805:PRO:HA	1.89	0.54
1:U:1841:GLU:N	1:U:1841:GLU:OE1	2.40	0.54
1:U:792:ASP:OD1	1:U:792:ASP:N	2.41	0.54
1:U:143:ARG:NH2	1:U:1508:ASP:OD1	2.40	0.54
1:U:1177:TYR:O	1:U:1178:CYS:SG	2.64	0.54
1:U:1856:ASP:OD1	1:U:1856:ASP:N	2.39	0.54
1:U:1766:ARG:HG2	1:U:1793:PHE:CZ	2.43	0.54
1:U:674:PHE:O	1:U:1175:THR:HG23	2.08	0.54
1:U:1222:LEU:HD11	1:U:1235:THR:HG23	1.89	0.54
1:U:583:VAL:HG23	1:U:583:VAL:O	2.08	0.53
1:U:1455:SER:OG	1:U:1456:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1470:GLU:N	1:U:1470:GLU:OE1	2.40	0.53
1:U:1602:ARG:HE	1:U:1612:GLU:HG2	1.72	0.53
1:U:1838:THR:O	1:U:1838:THR:HG23	2.08	0.53
1:U:576:THR:HG22	1:U:577:ARG:HG3	1.90	0.53
1:U:1326:LEU:HD13	1:U:1562:LEU:HD23	1.90	0.53
1:U:217:SER:OG	1:U:218:GLU:N	2.40	0.53
1:U:760:GLU:OE1	1:U:871:ARG:NH2	2.33	0.53
1:U:134:ASN:HD22	1:U:134:ASN:C	2.17	0.53
1:U:723:ARG:HG3	1:U:724:GLU:H	1.74	0.53
1:U:1806:VAL:HG13	1:U:1806:VAL:O	2.08	0.53
1:U:663:ILE:O	1:U:666:THR:HG22	2.09	0.53
1:U:1215:GLN:NE2	1:U:1275:PHE:O	2.34	0.53
1:U:1095:GLN:HG3	1:U:1123:GLU:HG2	1.91	0.53
1:U:1539:ASP:CG	1:U:1796:LYS:CD	2.82	0.53
1:U:114:ILE:HG23	1:U:114:ILE:O	2.09	0.52
1:U:786:GLU:O	1:U:790:TRP:HB2	2.09	0.52
1:U:1688:ILE:HB	1:U:1691:GLN:HE21	1.73	0.52
1:U:969:SER:O	1:U:973:LEU:HB2	2.09	0.52
1:U:367:LYS:NZ	1:U:414:ALA:O	2.35	0.52
1:U:830:GLU:HB2	1:U:1007:PRO:HG2	1.91	0.52
1:U:1385:LYS:O	1:U:1388:GLU:HG3	2.10	0.52
1:U:1596:THR:OG1	1:U:1597:ILE:N	2.43	0.52
1:U:68:ILE:HD11	1:U:1941:VAL:HG11	1.91	0.52
1:U:79:ASN:O	1:U:83:THR:OG1	2.24	0.52
1:U:98:VAL:HG21	1:U:114:ILE:HD13	1.92	0.52
1:U:2031:CYS:O	1:U:2035:LEU:HG	2.09	0.52
1:U:1507:VAL:CG2	1:U:1508:ASP:H	2.19	0.52
1:U:102:THR:OG1	1:U:104:ASP:OD1	2.27	0.51
1:U:355:LEU:HB3	1:U:366:ALA:HB2	1.92	0.51
1:U:1189:ARG:HD3	1:U:1496:VAL:HG21	1.92	0.51
1:U:1766:ARG:CA	1:U:1793:PHE:CE1	2.92	0.51
1:U:1325:ALA:HB1	1:U:1336:HIS:CG	2.45	0.51
1:U:1020:MET:HE3	1:U:1021:PHE:HE1	1.75	0.51
1:U:1542:ARG:NH1	1:U:1548:LEU:O	2.44	0.51
1:U:1728:VAL:HG21	1:U:1816:ARG:HE	1.75	0.51
1:U:1520:VAL:HG21	1:U:1538:TRP:CD2	2.46	0.51
1:U:1435:LYS:HB2	1:U:1438:LEU:HG	1.93	0.51
1:U:13:GLU:OE1	1:U:1853:ARG:NH2	2.44	0.51
1:U:1326:LEU:HB2	1:U:1337:SER:HB3	1.93	0.51
1:U:1325:ALA:CB	1:U:1336:HIS:ND1	2.73	0.51
1:U:1525:LYS:HD2	1:U:1525:LYS:N	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1562:LEU:HD12	1:U:1562:LEU:C	2.36	0.50
1:U:1524:LEU:HD12	1:U:1524:LEU:N	2.26	0.50
1:U:1832:ILE:HG23	1:U:1834:ASN:HD21	1.75	0.50
1:U:1844:VAL:CG1	1:U:1845:MET:N	2.74	0.50
1:U:1606:PHE:CD1	1:U:1607:PRO:HD2	2.46	0.50
1:U:365:TRP:CD1	1:U:595:LEU:HD13	2.46	0.50
1:U:661:GLU:HA	1:U:664:THR:HG22	1.94	0.50
1:U:1751:ARG:HH11	1:U:1783:ARG:NH2	2.09	0.50
1:U:1778:VAL:HG12	1:U:1779:ALA:N	2.26	0.50
1:U:919:LEU:HD22	1:U:1080:GLN:HE22	1.77	0.49
1:U:1239:GLN:NE2	1:U:1279:ASP:OD1	2.44	0.49
1:U:1732:THR:HB	1:U:1752:LEU:HD23	1.94	0.49
1:U:1744:SER:OG	1:U:1745:ASN:N	2.41	0.49
1:U:1829:ARG:NH2	1:U:1834:ASN:OD1	2.45	0.49
1:U:1867:SER:HA	1:U:1869:ARG:HH21	1.76	0.49
1:U:35:ASP:N	1:U:35:ASP:OD1	2.45	0.49
1:U:220:GLU:OE2	1:U:835:ARG:NH1	2.45	0.49
1:U:371:ASP:OD2	1:U:376:ASN:ND2	2.41	0.49
1:U:1115:ILE:H	1:U:1115:ILE:HD12	1.76	0.49
1:U:84:PHE:CD2	1:U:87:LEU:HD12	2.47	0.49
1:U:122:ILE:HB	1:U:165:VAL:HG22	1.93	0.49
1:U:996:THR:HG22	1:U:1022:ARG:HH21	1.77	0.49
1:U:1463:MET:HG3	1:U:1544:SER:OG	2.12	0.49
1:U:37:ASP:OD2	1:U:48:ASP:HB3	2.13	0.49
1:U:382:SER:O	1:U:406:ILE:HG22	2.11	0.49
1:U:787:PHE:CE1	1:U:793:THR:OG1	2.65	0.49
1:U:1203:HIS:O	1:U:1203:HIS:ND1	2.41	0.49
1:U:1751:ARG:HD3	1:U:1809:MET:CE	2.43	0.49
1:U:280:ASP:O	1:U:284:SER:OG	2.29	0.49
1:U:636:LYS:HE2	1:U:637:PRO:HD2	1.95	0.49
1:U:1340:VAL:HG12	1:U:1340:VAL:O	2.12	0.49
1:U:1953:LEU:CD1	1:U:1961:ILE:HD13	2.42	0.49
1:U:25:ASP:OD1	1:U:25:ASP:N	2.43	0.49
1:U:113:VAL:CG1	1:U:125:VAL:HB	2.43	0.49
1:U:1497:ARG:NH1	1:U:1604:ASN:OD1	2.46	0.49
1:U:1336:HIS:H	1:U:1336:HIS:HD2	1.60	0.49
1:U:1390:VAL:HG22	1:U:1390:VAL:O	2.12	0.49
1:U:659:THR:HG23	1:U:660:GLU:N	2.28	0.49
1:U:371:ASP:HB3	1:U:376:ASN:HB3	1.94	0.48
1:U:696:THR:HG22	1:U:697:LYS:N	2.28	0.48
1:U:724:GLU:HG2	1:U:726:ARG:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:765:ASN:O	1:U:769:GLU:HG2	2.13	0.48
1:U:1345:ARG:C	1:U:1349:GLN:HE21	2.21	0.48
1:U:139:GLU:HG3	1:U:1507:VAL:HG21	1.95	0.48
1:U:479:VAL:O	1:U:483:VAL:HG23	2.13	0.48
1:U:543:ILE:HD11	1:U:552:TYR:HB3	1.94	0.48
1:U:676:SER:OG	1:U:678:PRO:HD2	2.13	0.48
1:U:732:THR:CG2	1:U:733:PHE:N	2.76	0.48
1:U:1539:ASP:OD2	1:U:1796:LYS:HD2	2.13	0.48
1:U:471:ASP:OD2	1:U:511:SER:OG	2.22	0.48
1:U:745:ASN:HD22	1:U:745:ASN:H	1.62	0.48
1:U:875:LEU:O	1:U:878:MET:HG2	2.14	0.48
1:U:1790:LEU:HD12	1:U:1790:LEU:C	2.39	0.48
1:U:1191:LEU:HD21	1:U:1193:ARG:HG3	1.95	0.48
1:U:1837:VAL:HG13	1:U:1845:MET:HE3	1.96	0.48
1:U:955:PRO:O	1:U:958:LYS:HB2	2.13	0.47
1:U:305:ILE:O	1:U:309:GLN:HG2	2.14	0.47
1:U:1326:LEU:HD13	1:U:1562:LEU:CD2	2.43	0.47
1:U:1687:SER:OG	1:U:1688:ILE:N	2.47	0.47
1:U:1829:ARG:HB2	1:U:1832:ILE:CG2	2.43	0.47
1:U:84:PHE:HB3	1:U:87:LEU:HD12	1.96	0.47
1:U:476:ASP:OD1	1:U:476:ASP:N	2.46	0.47
1:U:764:LEU:HD12	1:U:764:LEU:H	1.79	0.47
1:U:1594:VAL:HG13	1:U:1595:THR:HG23	1.96	0.47
1:U:1178:CYS:SG	1:U:1187:PHE:CD1	3.05	0.47
1:U:743:LEU:O	1:U:747:VAL:HG23	2.14	0.47
1:U:1139:ASP:OD1	1:U:1140:MET:N	2.47	0.47
1:U:1525:LYS:H	1:U:1525:LYS:CD	2.10	0.47
1:U:1562:LEU:HD12	1:U:1563:SER:HB3	1.96	0.47
1:U:1836:SER:OG	1:U:1844:VAL:CG1	2.62	0.47
1:U:858:TRP:HA	1:U:864:VAL:HG11	1.96	0.47
1:U:294:GLN:OE1	1:U:294:GLN:N	2.44	0.47
1:U:914:ASN:OD1	1:U:914:ASN:N	2.47	0.47
1:U:1498:SER:OG	1:U:1595:THR:HG21	2.15	0.47
1:U:1540:LYS:HE3	1:U:1795:ILE:HG13	1.97	0.47
1:U:1737:LEU:HD11	1:U:1751:ARG:NH1	2.30	0.47
1:U:84:PHE:HD2	1:U:87:LEU:CD1	2.28	0.47
1:U:1239:GLN:NE2	1:U:1279:ASP:H	2.13	0.47
1:U:770:MET:O	1:U:774:ILE:HG12	2.15	0.46
1:U:1520:VAL:HG21	1:U:1538:TRP:CE3	2.50	0.46
1:U:966:GLY:O	1:U:969:SER:OG	2.21	0.46
1:U:1516:LEU:HD12	1:U:1516:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1832:ILE:HD13	1:U:1850:TYR:O	2.15	0.46
1:U:1949:THR:OG1	1:U:1950:THR:N	2.48	0.46
1:U:265:PHE:CZ	1:U:792:ASP:HB3	2.50	0.46
1:U:1370:GLY:HA2	1:U:1522:PHE:CE2	2.50	0.46
1:U:2014:LEU:H	1:U:2014:LEU:HD23	1.80	0.46
1:U:71:GLN:OE1	1:U:74:GLU:N	2.43	0.46
1:U:671:MET:HG3	1:U:1172:THR:HG21	1.97	0.46
1:U:1071:TYR:HE1	1:U:1073:LYS:HG3	1.79	0.46
1:U:921:GLU:OE2	1:U:921:GLU:N	2.49	0.46
1:U:1361:TRP:O	1:U:1365:ILE:N	2.49	0.46
1:U:1632:VAL:O	1:U:1636:VAL:HG23	2.16	0.46
1:U:1652:GLU:O	1:U:1656:THR:HG23	2.16	0.46
1:U:37:ASP:OD1	1:U:37:ASP:O	2.34	0.46
1:U:358:HIS:CE1	1:U:360:ALA:HB3	2.51	0.46
1:U:829:LEU:HD21	1:U:943:VAL:HG22	1.98	0.46
1:U:857:ASP:OD1	1:U:857:ASP:N	2.49	0.46
1:U:1596:THR:HG23	1:U:1599:GLN:H	1.81	0.46
1:U:1866:TRP:O	1:U:1869:ARG:NH2	2.49	0.46
1:U:614:CYS:SG	1:U:1245:HIS:HB2	2.56	0.46
1:U:770:MET:SD	1:U:912:LYS:HB2	2.55	0.46
1:U:1751:ARG:HE	1:U:1783:ARG:NH1	2.13	0.46
1:U:1836:SER:OG	1:U:1837:VAL:N	2.49	0.46
1:U:93:ARG:HB2	1:U:114:ILE:CG2	2.45	0.46
1:U:1517:VAL:O	1:U:1521:TRP:HB2	2.15	0.46
1:U:1572:ALA:O	1:U:1573:HIS:ND1	2.49	0.46
1:U:309:GLN:HE21	1:U:309:GLN:CA	2.26	0.46
1:U:1438:LEU:O	1:U:1441:LEU:HG	2.16	0.46
1:U:1705:LYS:HB2	1:U:1724:VAL:H	1.80	0.46
1:U:1789:ARG:NE	1:U:1801:THR:HA	2.31	0.46
1:U:37:ASP:OD1	1:U:47:VAL:C	2.59	0.45
1:U:479:VAL:HG13	1:U:480:GLN:N	2.31	0.45
1:U:37:ASP:OD1	1:U:47:VAL:HA	2.17	0.45
1:U:739:ARG:HD3	1:U:739:ARG:HA	1.68	0.45
1:U:1369:PRO:HG2	1:U:1522:PHE:HZ	1.81	0.45
1:U:1485:THR:OG1	1:U:1612:GLU:O	2.31	0.45
1:U:262:ASP:OD1	1:U:263:VAL:N	2.49	0.45
1:U:1022:ARG:O	1:U:1075:GLU:HG2	2.16	0.45
1:U:1901:LEU:HD23	1:U:1902:ALA:H	1.81	0.45
1:U:875:LEU:HA	1:U:878:MET:HE3	1.99	0.45
1:U:1018:ILE:HD13	1:U:1018:ILE:HA	1.82	0.45
1:U:1333:THR:OG1	1:U:1334:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1550:THR:O	1:U:1550:THR:OG1	2.33	0.45
1:U:472:SER:OG	1:U:511:SER:O	2.28	0.45
1:U:1314:GLN:N	1:U:1558:ASP:O	2.45	0.45
1:U:1626:ILE:CG2	1:U:1630:LYS:HE3	2.47	0.45
1:U:1789:ARG:HG2	1:U:1805:PRO:HB3	1.99	0.45
1:U:665:LEU:HD11	1:U:686:MET:HE2	1.99	0.45
1:U:1378:ASN:N	1:U:1381:GLU:OE2	2.32	0.45
1:U:498:LEU:HD11	1:U:1605:PHE:CZ	2.52	0.45
1:U:806:LEU:HD23	1:U:806:LEU:HA	1.83	0.45
1:U:139:GLU:OE1	1:U:1507:VAL:HG11	2.17	0.44
1:U:1719:TYR:OH	1:U:1841:GLU:O	2.27	0.44
1:U:267:THR:HG22	1:U:1961:ILE:HG23	2.00	0.44
1:U:383:ASP:HB3	1:U:405:LYS:HD2	1.98	0.44
1:U:1101:TYR:HA	1:U:1953:LEU:HD23	1.99	0.44
1:U:1140:MET:O	1:U:1144:ARG:HG2	2.17	0.44
1:U:1769:CYS:O	1:U:1773:GLY:N	2.51	0.44
1:U:1865:LEU:HB3	1:U:1885:CYS:SG	2.57	0.44
1:U:835:ARG:O	1:U:839:THR:HG23	2.18	0.44
1:U:1191:LEU:C	1:U:1191:LEU:CD2	2.89	0.44
1:U:1633:LEU:CD1	1:U:1672:MET:HE1	2.41	0.44
1:U:554:ILE:O	1:U:566:TYR:HA	2.18	0.44
1:U:663:ILE:HD11	1:U:702:LEU:HD13	1.99	0.44
1:U:1329:THR:HG22	1:U:1334:LEU:HB3	2.00	0.44
1:U:1403:HIS:O	1:U:1407:ARG:NH1	2.51	0.44
1:U:1666:ILE:O	1:U:1667:ARG:NH1	2.50	0.44
1:U:1751:ARG:HH11	1:U:1783:ARG:HH22	1.65	0.44
1:U:1766:ARG:CB	1:U:1793:PHE:CE1	3.01	0.44
1:U:747:VAL:HG21	1:U:1192:VAL:HG11	1.99	0.44
1:U:877:LYS:HG2	1:U:927:ALA:HB1	1.99	0.44
1:U:1348:TYR:HB3	1:U:1390:VAL:HG21	2.00	0.44
1:U:1840:GLN:NE2	1:U:1841:GLU:OE1	2.51	0.44
1:U:128:THR:HB	1:U:145:LYS:HE3	2.00	0.43
1:U:677:PRO:N	1:U:678:PRO:HD2	2.33	0.43
1:U:1143:VAL:HG11	1:U:1978:ILE:HG22	1.99	0.43
1:U:713:ILE:HG13	1:U:733:PHE:HZ	1.83	0.43
1:U:815:ARG:NH2	1:U:1955:ASP:OD2	2.51	0.43
1:U:1766:ARG:HG2	1:U:1793:PHE:CE1	2.53	0.43
1:U:1191:LEU:CD2	1:U:1193:ARG:HG3	2.49	0.43
1:U:1640:PRO:CB	1:U:1918:ILE:HG22	2.47	0.43
1:U:1778:VAL:CG1	1:U:1779:ALA:N	2.81	0.43
1:U:1844:VAL:CG1	1:U:1845:MET:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:311:LEU:HD22	1:U:687:LEU:HD22	2.00	0.43
1:U:344:ILE:O	1:U:344:ILE:HG23	2.18	0.43
1:U:864:VAL:HG13	1:U:864:VAL:O	2.19	0.43
1:U:950:GLU:OE2	1:U:952:VAL:N	2.32	0.43
1:U:1049:ARG:O	1:U:1053:THR:HG22	2.18	0.43
1:U:1191:LEU:HD23	1:U:1192:VAL:N	2.34	0.43
1:U:1666:ILE:HG22	1:U:1670:ARG:HB3	2.00	0.43
1:U:1666:ILE:HB	1:U:1670:ARG:HD3	1.99	0.43
1:U:2039:ARG:CZ	1:U:2059:GLU:HB3	2.49	0.43
1:U:592:GLU:HG3	1:U:593:TRP:CD1	2.53	0.43
1:U:1562:LEU:HD12	1:U:1563:SER:N	2.34	0.43
1:U:1862:ALA:HB1	1:U:1886:LEU:CD1	2.48	0.43
1:U:1915:MET:SD	1:U:1915:MET:N	2.92	0.43
1:U:151:ASP:CG	1:U:152:PRO:HD3	2.43	0.43
1:U:377:VAL:HB	1:U:409:ARG:HB3	2.01	0.43
1:U:1106:LEU:HD23	1:U:1106:LEU:HA	1.87	0.43
1:U:1190:HIS:CD2	1:U:1494:ASN:HD22	2.37	0.43
1:U:100:PRO:HG2	1:U:159:ILE:HG13	2.00	0.43
1:U:381:VAL:O	1:U:386:LYS:NZ	2.51	0.43
1:U:678:PRO:HD3	1:U:1982:PHE:CE2	2.52	0.43
1:U:1549:SER:OG	1:U:1550:THR:N	2.51	0.43
1:U:1904:ASP:HB3	1:U:2062:ILE:HG21	2.01	0.43
1:U:141:ALA:HA	1:U:144:THR:HG22	2.00	0.43
1:U:653:LEU:HD23	1:U:653:LEU:HA	1.77	0.43
1:U:1184:GLU:OE2	1:U:1184:GLU:N	2.47	0.43
1:U:606:LEU:HD23	1:U:606:LEU:HA	1.87	0.42
1:U:700:VAL:O	1:U:704:ARG:HG2	2.18	0.42
1:U:1659:ILE:HD12	1:U:1659:ILE:HA	1.88	0.42
1:U:1871:LEU:C	1:U:1873:SER:N	2.77	0.42
1:U:199:ASN:O	1:U:203:THR:HG22	2.19	0.42
1:U:868:GLU:N	1:U:868:GLU:OE2	2.53	0.42
1:U:1369:PRO:HB3	1:U:1564:HIS:HD2	1.84	0.42
1:U:2046:GLU:OE1	1:U:2047:GLN:N	2.51	0.42
1:U:1626:ILE:HG22	1:U:1630:LYS:HE3	2.01	0.42
1:U:1871:LEU:C	1:U:1873:SER:H	2.27	0.42
1:U:154:SER:O	1:U:157:VAL:HG12	2.20	0.42
1:U:1313:ILE:HG23	1:U:1558:ASP:HB2	2.02	0.42
1:U:1372:LEU:HD23	1:U:1372:LEU:HA	1.83	0.42
1:U:1585:GLY:HA3	1:U:1600:VAL:HG22	2.00	0.42
1:U:1836:SER:HG	1:U:1845:MET:C	2.25	0.42
1:U:71:GLN:HB3	1:U:74:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:288:LYS:HA	1:U:289:PRO:HA	1.67	0.42
1:U:514:VAL:HG13	1:U:515:VAL:N	2.35	0.42
1:U:609:LEU:HD13	1:U:609:LEU:HA	1.94	0.42
1:U:781:LYS:HE2	1:U:781:LYS:HB3	1.90	0.42
1:U:1349:GLN:H	1:U:1349:GLN:HG2	1.71	0.42
1:U:1457:ASN:HD21	1:U:1459:ASN:HB3	1.81	0.42
1:U:1953:LEU:HD13	1:U:1957:LEU:HD12	2.01	0.42
1:U:771:TYR:HE1	1:U:910:LEU:HD12	1.85	0.42
1:U:958:LYS:HE3	1:U:958:LYS:HB3	1.81	0.42
1:U:965:HIS:HD1	1:U:1120:ASP:CG	2.28	0.42
1:U:1059:ASN:OD1	1:U:1059:ASN:N	2.52	0.42
1:U:1266:ILE:HD13	1:U:1266:ILE:HA	1.93	0.42
1:U:1628:ILE:HG13	1:U:1629:LEU:N	2.34	0.42
1:U:1956:ILE:HD12	1:U:1956:ILE:H	1.85	0.42
1:U:1587:PRO:HA	1:U:1595:THR:HG22	2.01	0.42
1:U:411:PHE:HB2	1:U:541:PHE:O	2.19	0.42
1:U:657:SER:OG	1:U:658:LYS:N	2.52	0.42
1:U:923:TYR:HD2	1:U:1079:MET:HB3	1.84	0.42
1:U:732:THR:CG2	1:U:733:PHE:H	2.33	0.42
1:U:890:ILE:HA	1:U:890:ILE:HD12	1.80	0.42
1:U:994:TYR:OH	1:U:1075:GLU:OE2	2.38	0.42
1:U:1633:LEU:CD1	1:U:1672:MET:CE	2.98	0.42
1:U:1646:LYS:O	1:U:1650:ILE:HG12	2.19	0.42
1:U:1666:ILE:O	1:U:1666:ILE:HG13	2.19	0.42
1:U:334:PRO:HD3	1:U:584:PHE:HB3	2.02	0.41
1:U:381:VAL:HG23	1:U:386:LYS:NZ	2.35	0.41
1:U:403:GLU:H	1:U:403:GLU:CD	2.28	0.41
1:U:737:SER:OG	1:U:739:ARG:HG2	2.19	0.41
1:U:815:ARG:HB3	1:U:1951:GLN:HE22	1.85	0.41
1:U:1502:LEU:HD23	1:U:1502:LEU:HA	1.91	0.41
1:U:1874:PHE:CD1	1:U:1884:ILE:HD13	2.55	0.41
1:U:732:THR:HG22	1:U:733:PHE:H	1.81	0.41
1:U:1667:ARG:HA	1:U:1667:ARG:HD3	1.93	0.41
1:U:361:TYR:CE2	1:U:597:GLU:HA	2.56	0.41
1:U:1524:LEU:N	1:U:1524:LEU:CD1	2.84	0.41
1:U:1925:GLY:HA3	1:U:1928:ARG:CZ	2.50	0.41
1:U:197:ILE:O	1:U:201:ILE:HG22	2.20	0.41
1:U:406:ILE:HG12	1:U:408:TYR:CE1	2.55	0.41
1:U:638:CYS:C	1:U:640:GLU:H	2.29	0.41
1:U:1064:TRP:CE3	1:U:1065:MET:HB2	2.55	0.41
1:U:1543:ALA:HA	1:U:1797:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1965:ASP:HB2	1:U:1968:ALA:HB3	2.02	0.41
1:U:608:ASN:OD1	1:U:608:ASN:N	2.53	0.41
1:U:737:SER:OG	1:U:738:GLY:N	2.53	0.41
1:U:1644:GLU:H	1:U:1644:GLU:CD	2.26	0.41
1:U:1934:ARG:HH22	1:U:2037:GLU:HG3	1.85	0.41
1:U:271:LYS:O	1:U:275:VAL:HG12	2.21	0.41
1:U:1521:TRP:HH2	1:U:1555:THR:CG2	2.21	0.41
1:U:1872:PHE:O	1:U:1872:PHE:CG	2.72	0.41
1:U:973:LEU:HD23	1:U:973:LEU:HA	1.84	0.41
1:U:1348:TYR:CE2	1:U:1397:SER:HB2	2.56	0.41
1:U:1528:LYS:HE2	1:U:1528:LYS:HB2	1.88	0.41
1:U:1925:GLY:HA3	1:U:1928:ARG:NH1	2.36	0.41
1:U:70:ILE:HD11	1:U:1938:THR:HG21	2.02	0.41
1:U:368:CYS:HA	1:U:411:PHE:CZ	2.56	0.41
1:U:745:ASN:N	1:U:745:ASN:ND2	2.69	0.41
1:U:939:MET:HB3	1:U:1006:MET:HE2	2.03	0.41
1:U:954:ASN:HB2	1:U:957:LEU:HG	2.02	0.41
1:U:1255:HIS:CE1	1:U:1413:VAL:HG11	2.55	0.41
1:U:1823:GLU:O	1:U:1837:VAL:HG23	2.21	0.41
1:U:1919:PHE:CZ	1:U:1923:LEU:CD2	2.96	0.41
1:U:335:TRP:NE1	1:U:594:GLU:OE2	2.48	0.41
1:U:1628:ILE:HD11	1:U:1657:LEU:HD21	2.02	0.41
1:U:1211:LEU:C	1:U:1213:SER:H	2.29	0.40
1:U:1766:ARG:CG	1:U:1793:PHE:CE1	3.05	0.40
1:U:258:SER:OG	1:U:259:THR:N	2.54	0.40
1:U:357:ASP:N	1:U:357:ASP:OD1	2.54	0.40
1:U:1329:THR:HA	1:U:1334:LEU:HA	2.03	0.40
1:U:919:LEU:HD22	1:U:1080:GLN:NE2	2.36	0.40
1:U:1279:ASP:OD1	1:U:1279:ASP:N	2.54	0.40
1:U:1521:TRP:CH2	1:U:1555:THR:CG2	2.95	0.40
1:U:411:PHE:HD1	1:U:411:PHE:HA	1.64	0.40
1:U:758:LYS:HE2	1:U:758:LYS:HB2	1.92	0.40
1:U:458:ASP:OD2	1:U:582:ARG:HB2	2.22	0.40
1:U:767:LEU:HG	1:U:771:TYR:CE2	2.56	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	U	1905/2084 (91%)	1753 (92%)	152 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

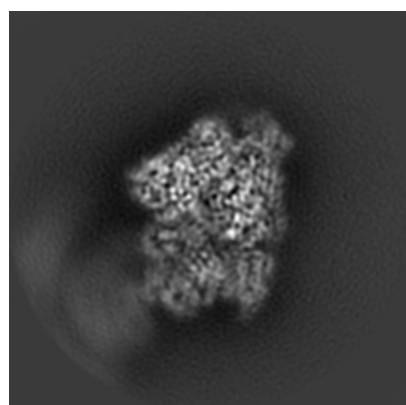
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0828. These allow visual inspection of the internal detail of the map and identification of artifacts.

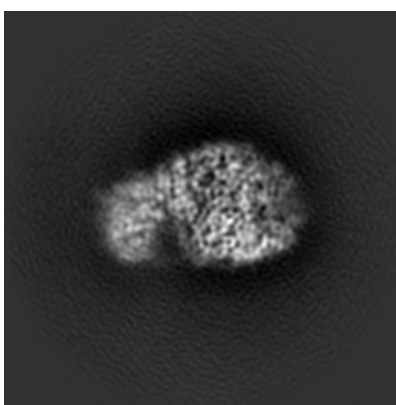
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

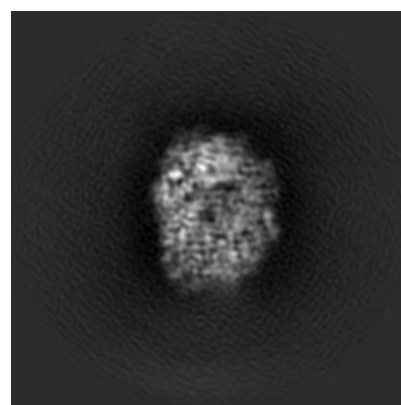
6.1.1 Primary map



X



Y

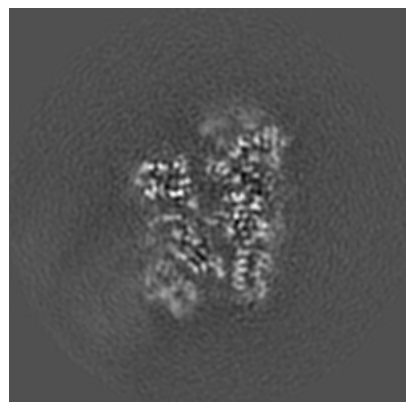


Z

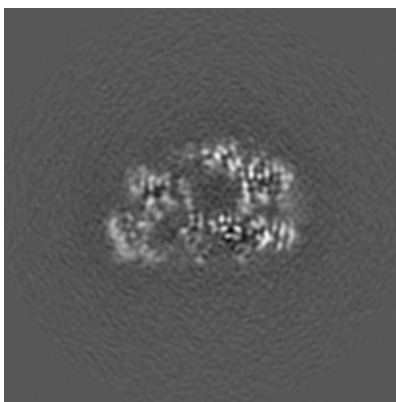
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

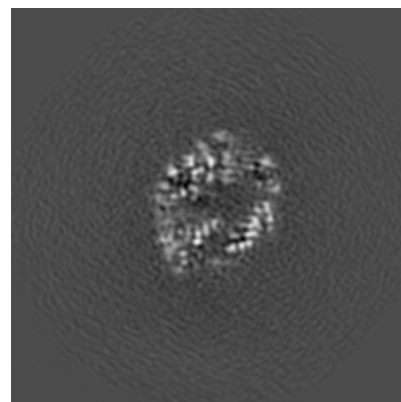
6.2.1 Primary map



X Index: 110



Y Index: 110

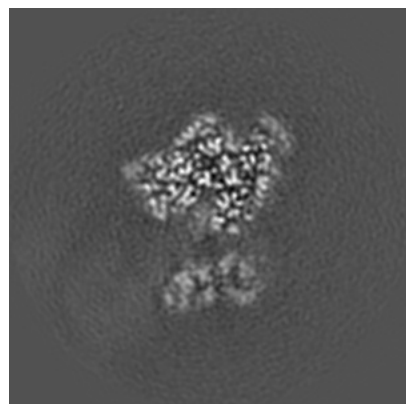


Z Index: 110

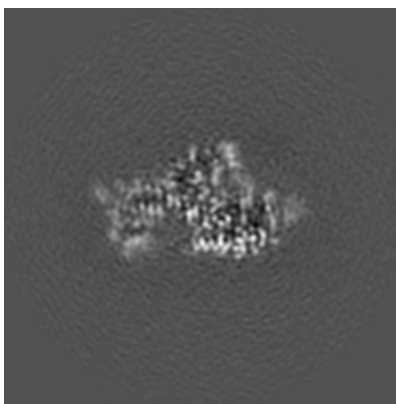
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

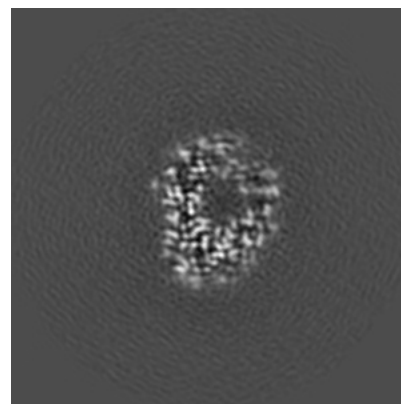
6.3.1 Primary map



X Index: 94



Y Index: 129

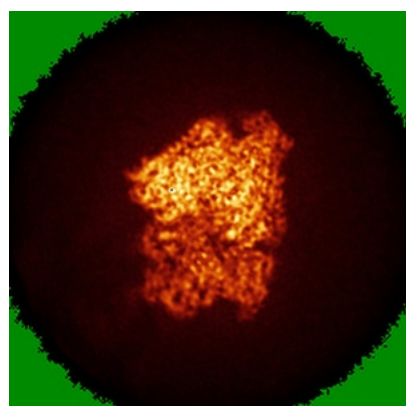


Z Index: 121

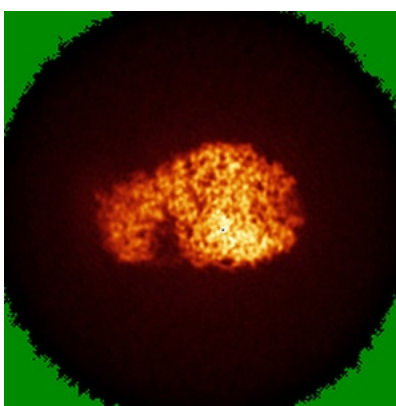
The images above show the largest variance slices of the map in three orthogonal directions.

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

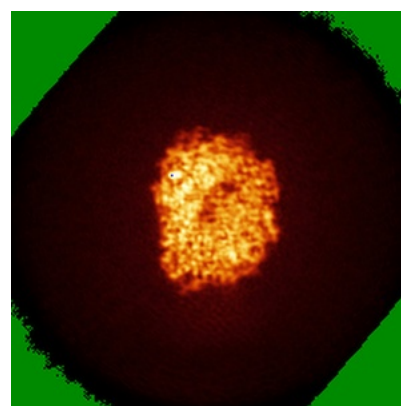
6.4.1 Primary map



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

This section was not generated.

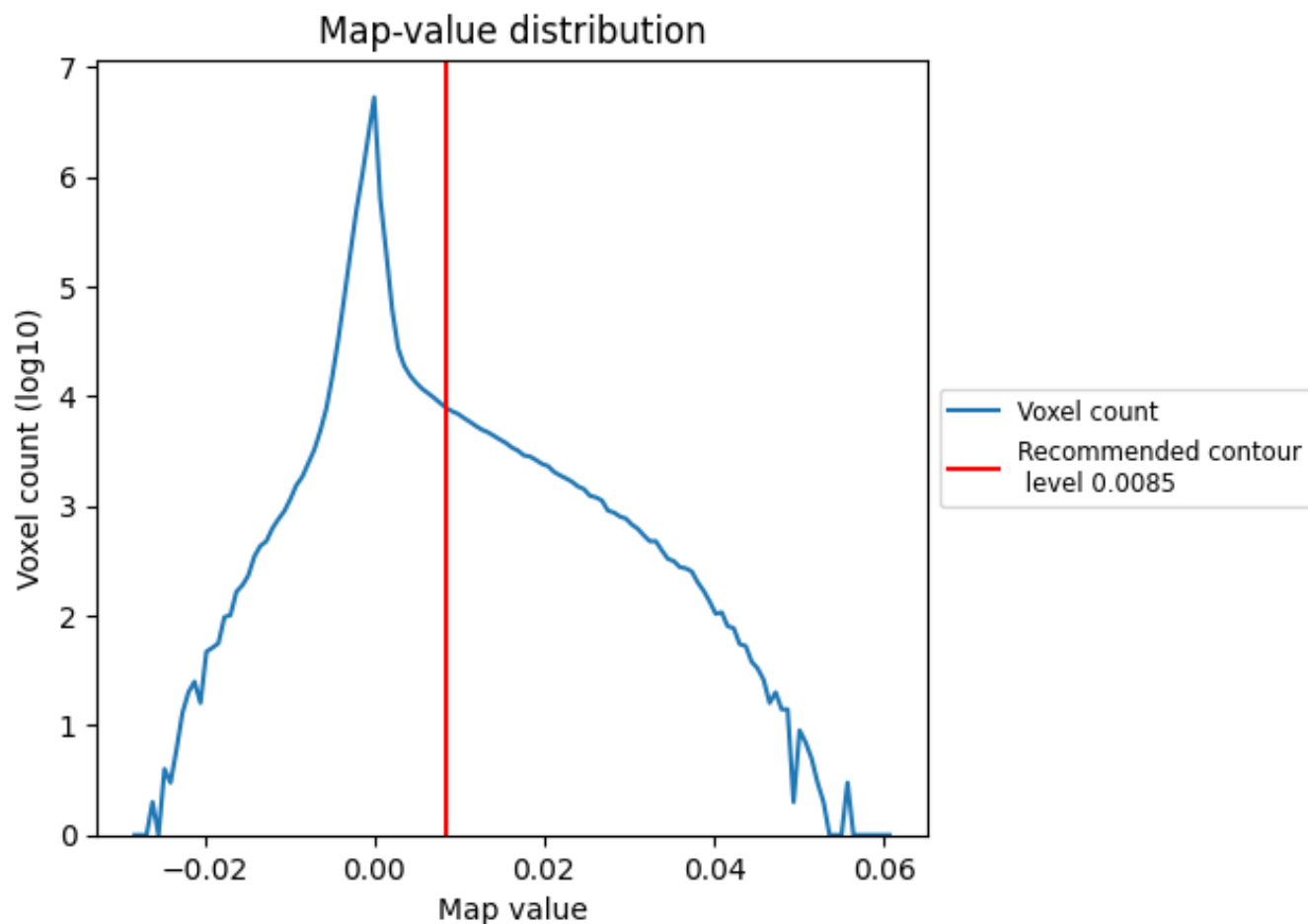
6.6 Mask visualisation

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

7 Map analysis [i](#)

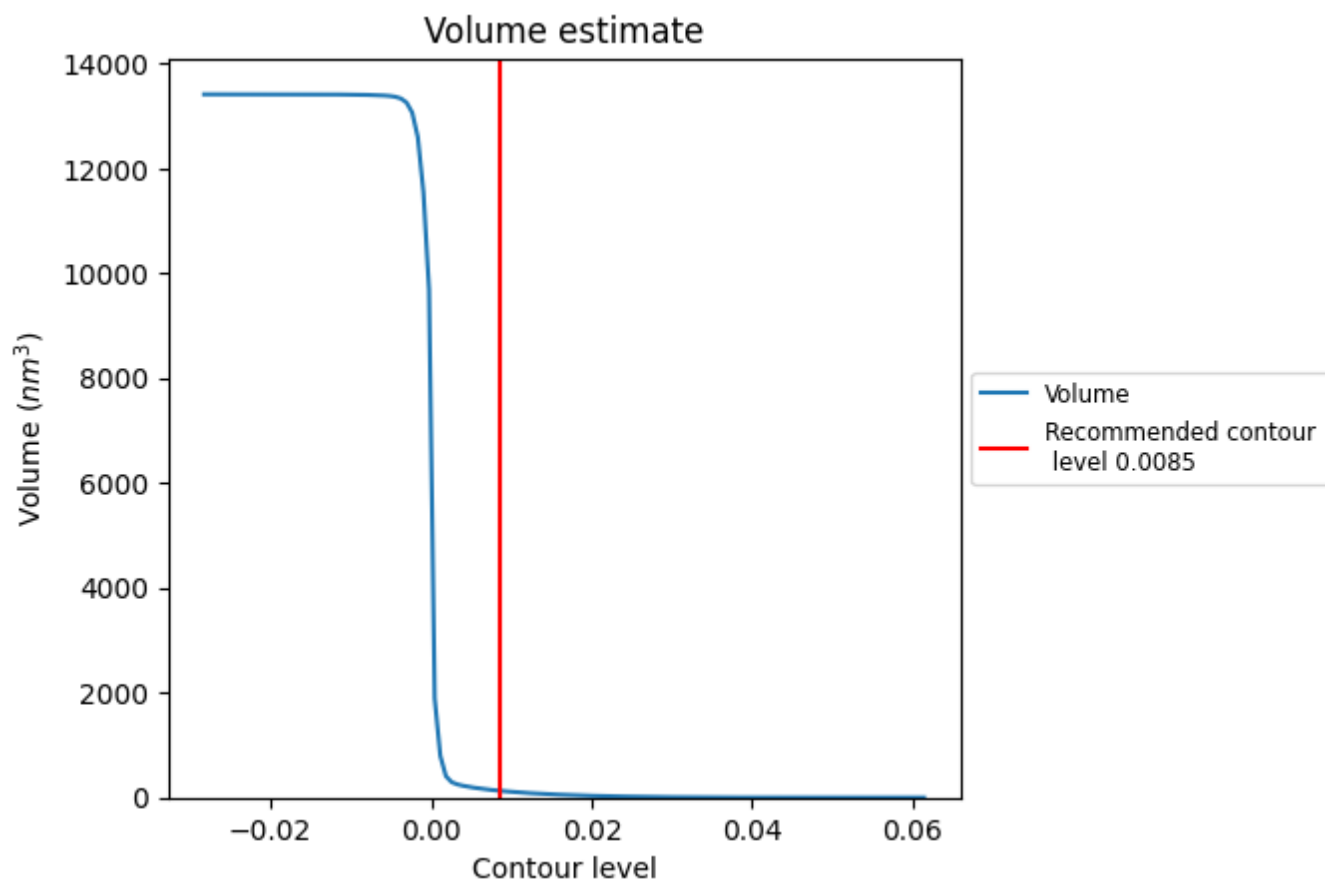
This section contains the results of statistical analysis of the map.

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.

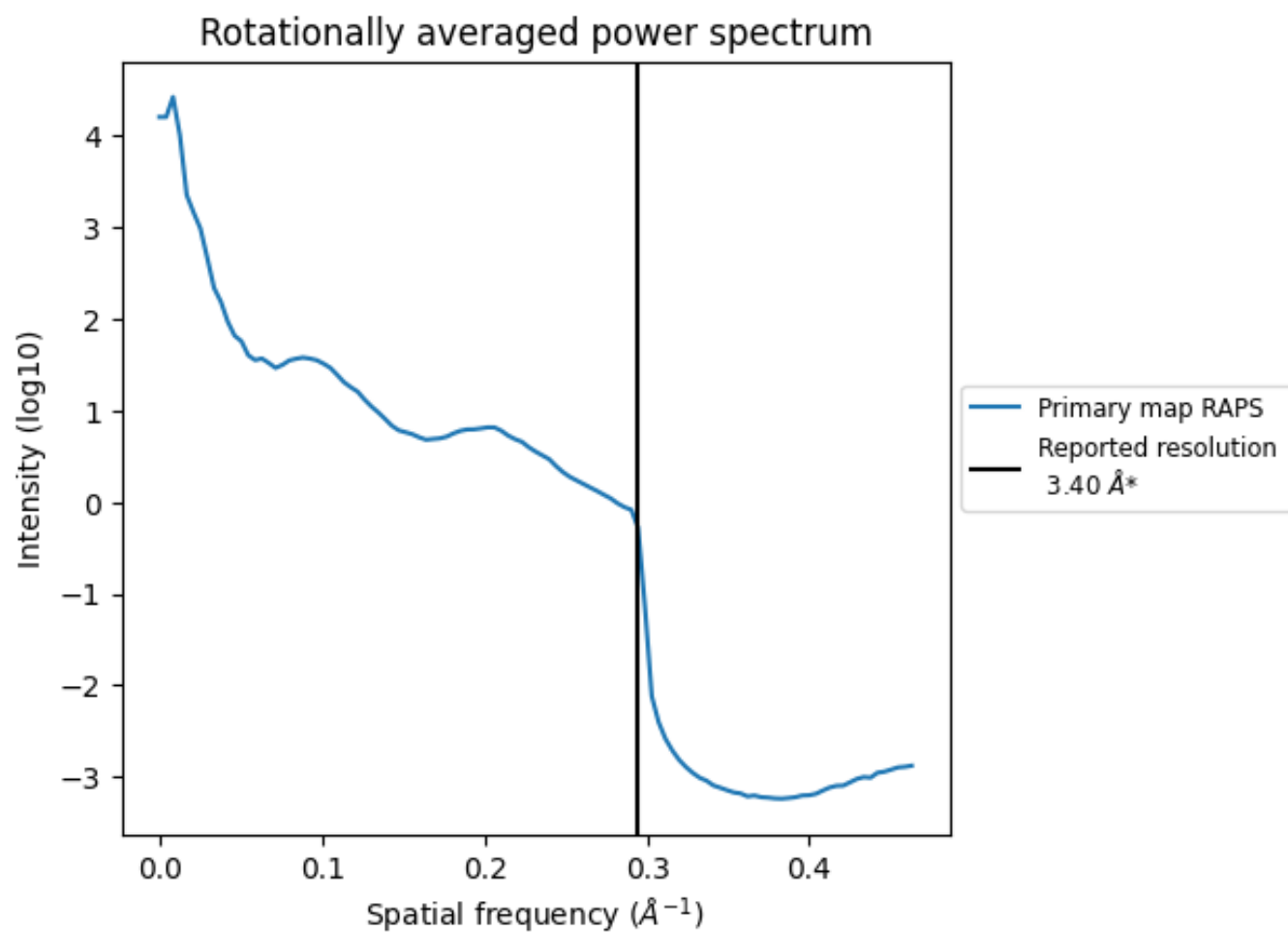
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 118 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 0.294 Å⁻¹

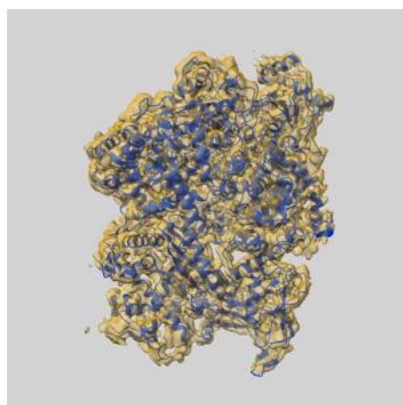
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

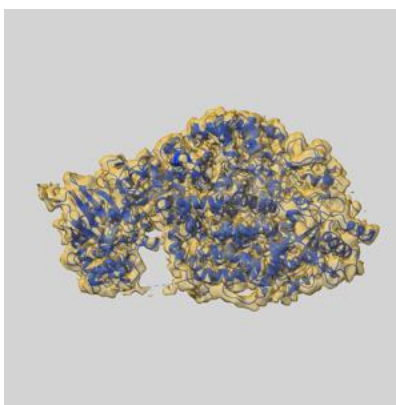
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0828 and PDB model 7ALP. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

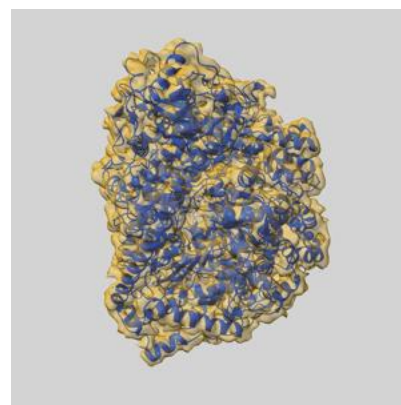
9.1 Map-model overlay [i](#)



X



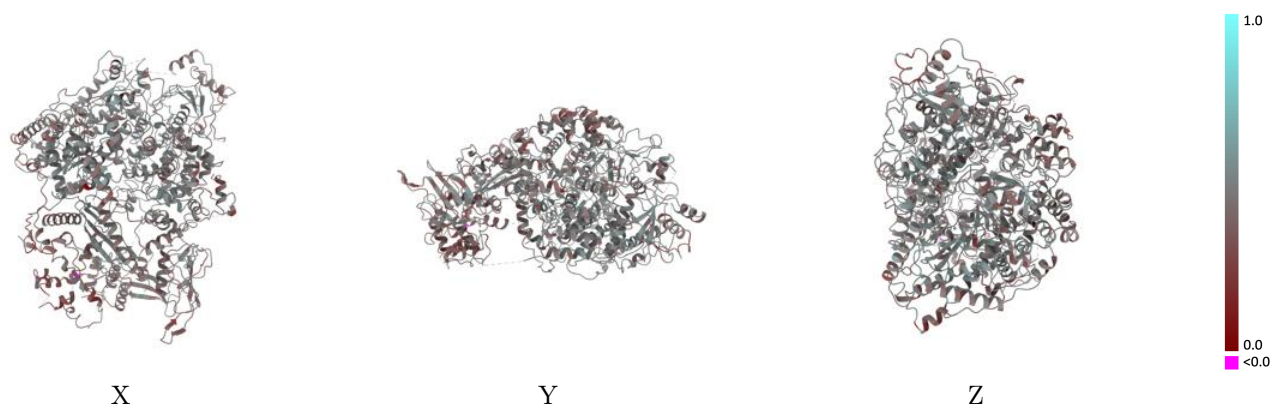
Y



Z

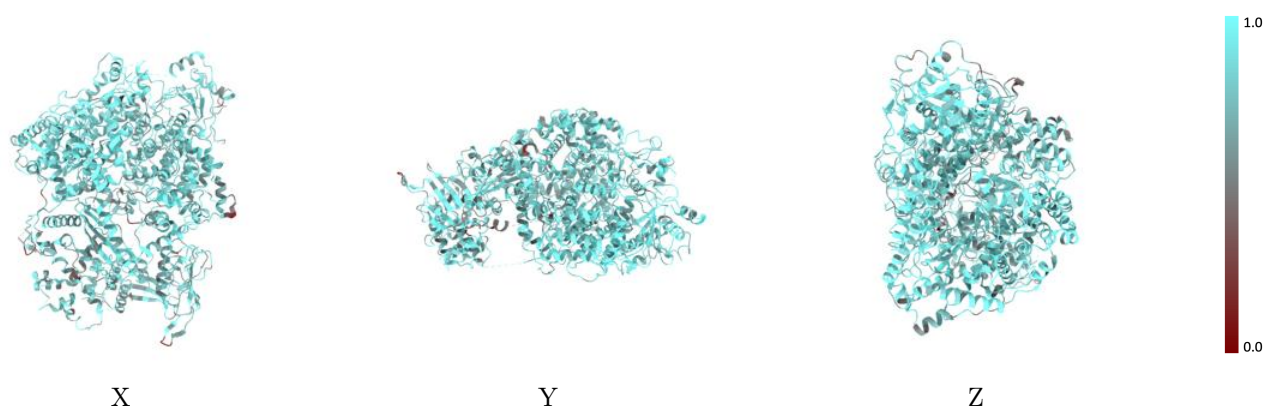
The images above show the 3D surface view of the map at the recommended contour level 0.0085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



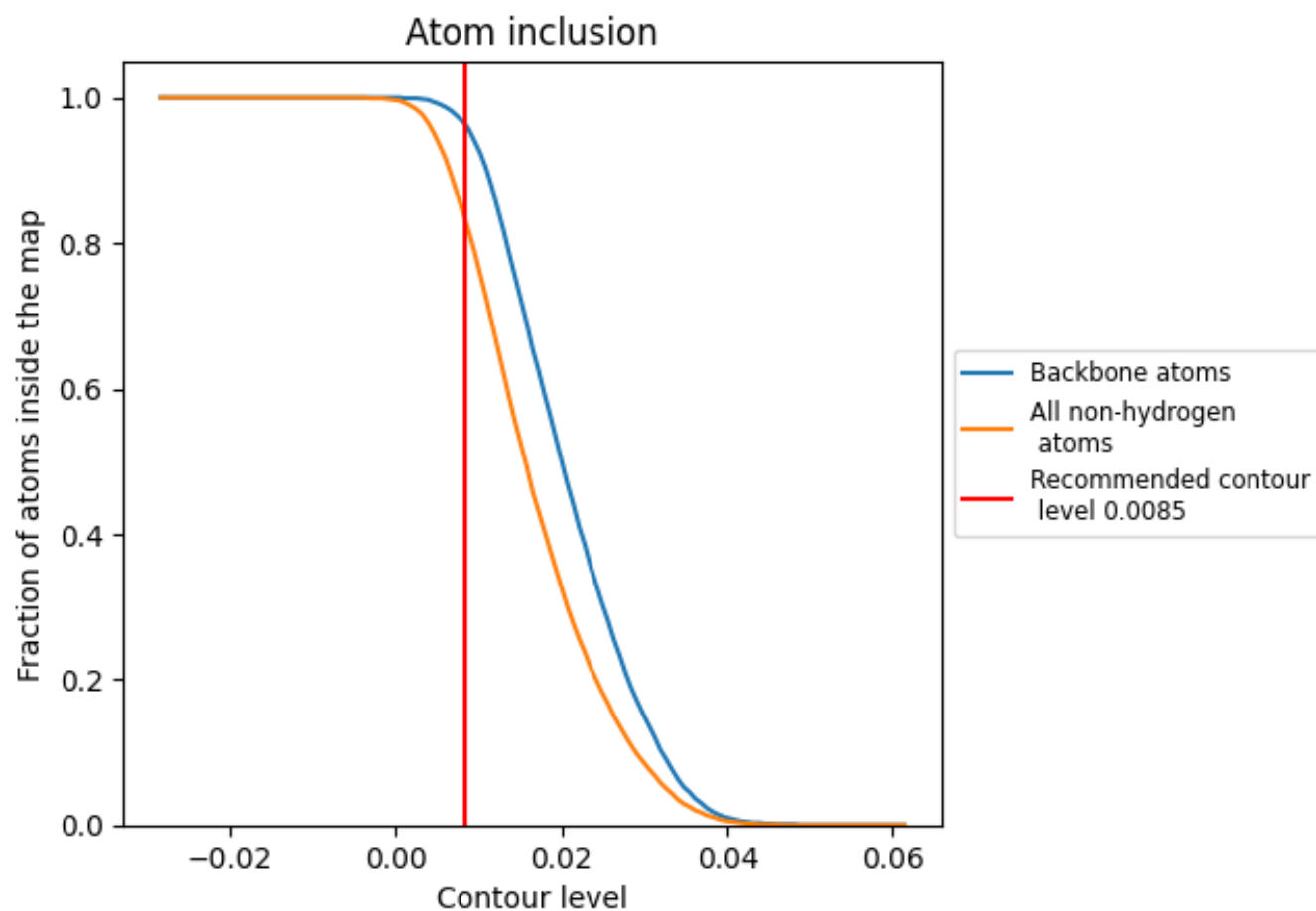
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4460
U	0.8300	0.4460

