



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 04:12 PM JST

PDB ID : 9VM2 / pdb_00009vm2
EMDB ID : EMD-65174
Title : Structure of DOCK6-Cdc42 complex protomer
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Yonemochi, M.;
Hanada, K.; Shirouzu, M.
Deposited on : 2025-06-27
Resolution : 3.94 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

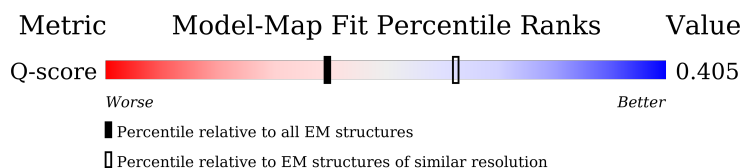
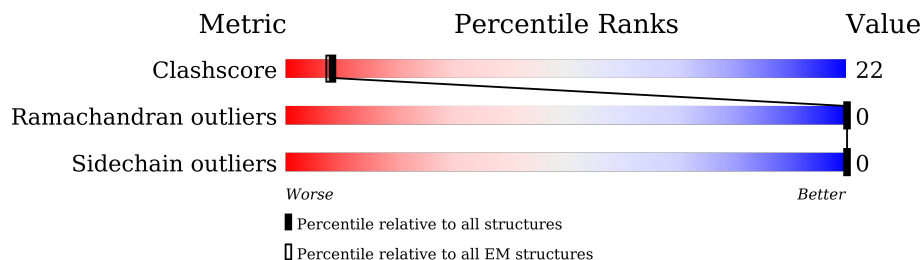
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.94 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7757 (3.44 - 4.43)

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

Mol	Chain	Length	Quality of chain
1	A	2053	
2	B	195	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14860 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 Deducator of cytokinesis protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q96HP0
A	-4	GLY	-	expression tag	UNP Q96HP0
A	-3	SER	-	expression tag	UNP Q96HP0
A	-2	GLY	-	expression tag	UNP Q96HP0
A	-1	GLY	-	expression tag	UNP Q96HP0
A	0	SER	-	expression tag	UNP Q96HP0

- Molecule 2 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	178	Total	C	N	O	S	0	0
			1389	894	221	267	7		

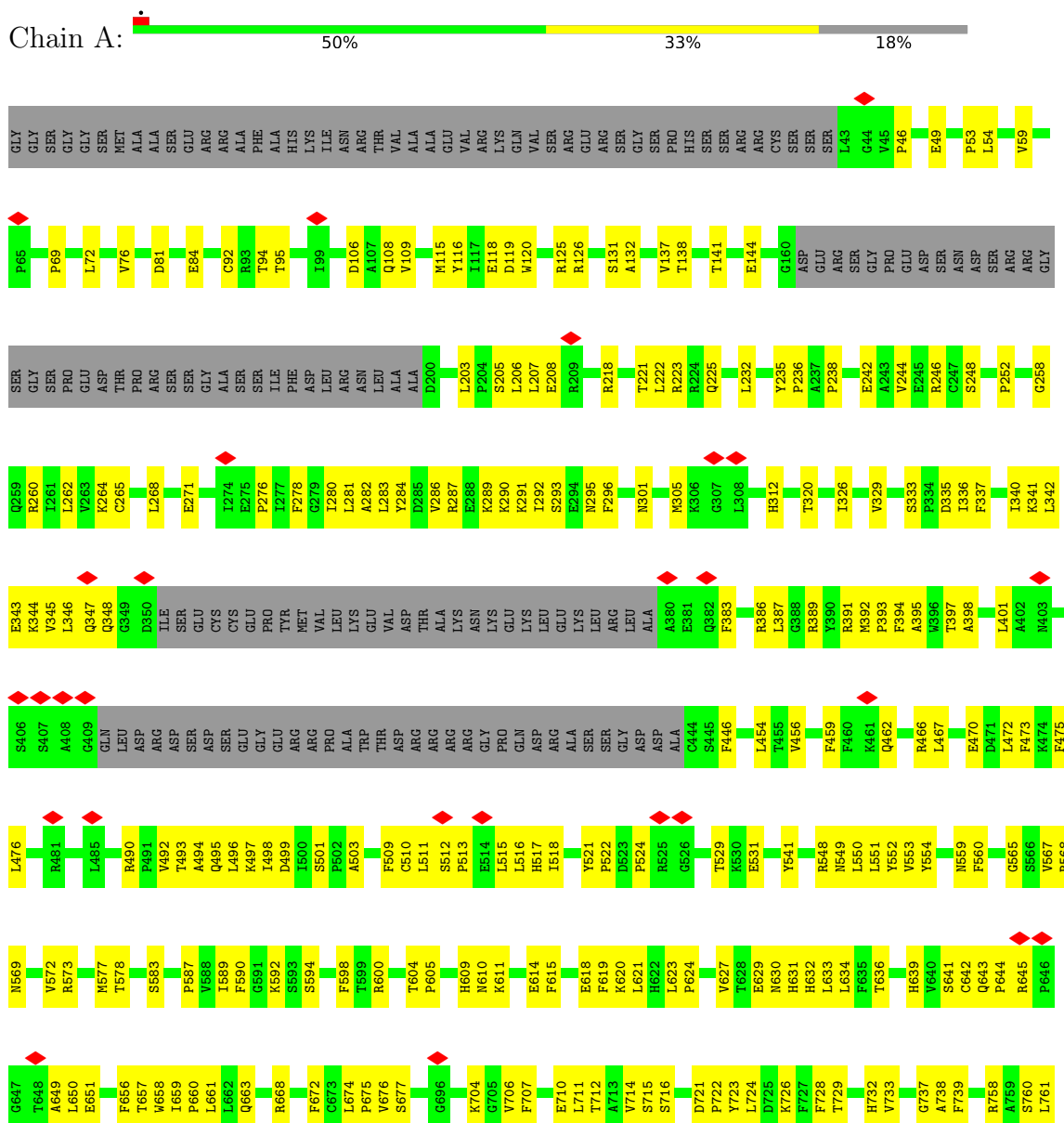
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P60953
B	-5	SER	-	expression tag	UNP P60953
B	-4	SER	-	expression tag	UNP P60953
B	-3	GLY	-	expression tag	UNP P60953
B	-2	SER	-	expression tag	UNP P60953
B	-1	SER	-	expression tag	UNP P60953
B	0	GLY	-	expression tag	UNP P60953
B	15	ALA	GLY	engineered mutation	UNP P60953
B	188	SER	-	expression tag	UNP P60953

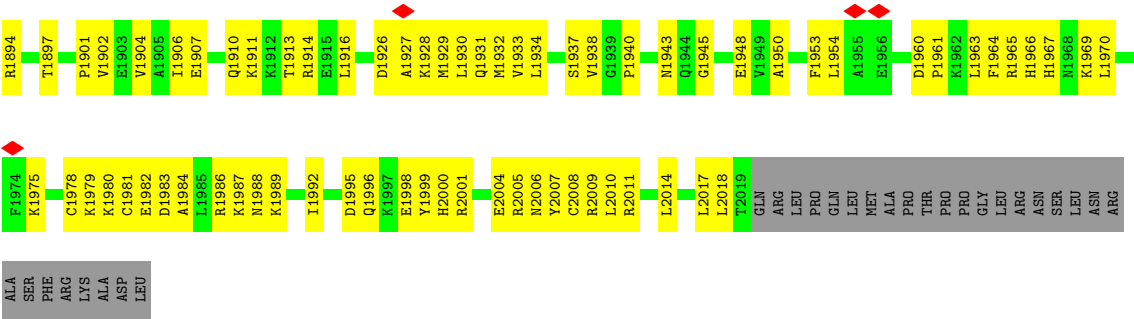
3 Residue-property plots

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.

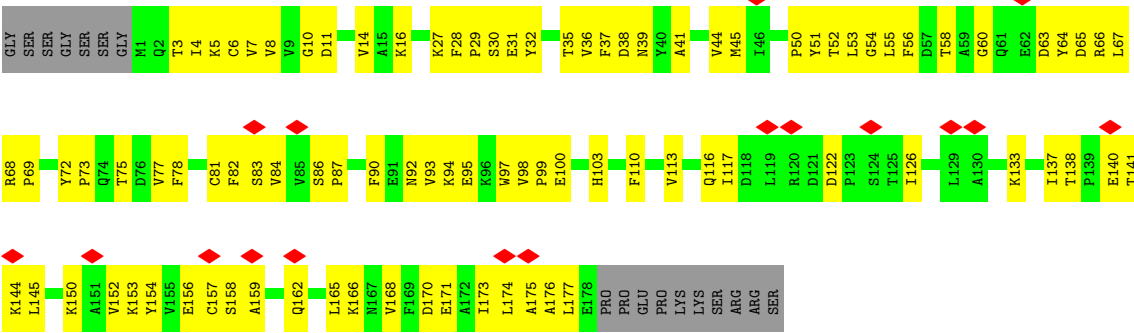
• Molecule 1: Dedicator of cytokinesis protein 6



T1823	Y1824	V1825	E1826	E1833	D1836	R1837	V1838	T1839	Y1840	F1841	R1842	R1843	Y1844	Y1845	G1846	L1847	R1848	T1849	F1850	L1851	F1852	C1853	T1854	F1855	F1856	T1857	F1858	D1859	R1860	R1861	A1862	H1863	G1864	Y1790	E1791	E1792	R1893	F1794	E1868	Q1869	H1870	K1871	R1872	K1873	L1876	S1877	T1878	D1879	H1880	K1886	T1887	R1888	I1889	V1890	C1891	H1892	H1893
Q1740	E1745	R1746	G1749	T1750	Y1751	F1752	R1753	V1754	G1755	F1756	Y1757	D1763	L1764	D1765	E1766	Q1767	F1769	V1769	F1769	L1770	Y1771	K1772	E1773	P1774	S1775	L1776	T1777	K1778	E1781	F1789	Y1790	E1791	E1792	R1793	F1794	E1800	K1803	N1806	P1807	Y1808	D1809	K1810	L1813	D1814	S1815	Q1816	Y1819	V1820	Q1821	I1822							
E1635	D1636	H1637	R1638	V1654	L1655	E1656	E1657	D1663	I1664	L1665	D1668	E1669	F1672	C1673	K1676	H1677	F1678	T1679	K1680	L1681	G1682	L1683	L1687	G1692	M1696	Y1700	E1701	A1702	V1703	H1704	E1705	L1710	I1711	P1712	L1713	L1714	H1717	R1718	Q1731	E1732	A1733	F1734	T1735	K1736	I1737	M1738	H1739										
V1551	M1555	L1558	L1561	L1562	T1563	D1564	T1565	V1566	K1567	M1568	K1569	E1570	H1571	Q1572	E1573	P1574	E1576	M1577	L1578	I1579	D1580	L1581	M1582	Y1583	R1584	I1585	A1586	R1587	G1588	Y1589	Q1590	G1591	S1592	P1593	R1596	L1597	L1600	Q1601	N1602	M1603	A1604	G1605	E1609	E1615	C1619	Y1630	L1633	L1634									
E1453	E1454	D1455	T1456	E1457	L1458	C1459	A1460	R1465	T1479	S1482	A1483	S1484	Y1485	Y1486	L1487	Q1491	I1495	G1496	H1497	N1498	R1501	V1502	K1503	A1504	Q1505	V1506	T1507	M1508	L1513	V1514	G1515	T1516	T1517	F1520	E1523	R1527	S1528	L1529	K1530	T1531	L1532	L1533	T1534	E1538	D1539	L1542											
LYS	SER	VAL	THR	HIS	TRP	LYS	GLN	THR	ASP	ARG	V1367	D1368	K1369	M1374	L1383	D1394	E1397	V1400	V1403	M1404	L1405	S1406	E1407	A1408	R1409	E1410	V1416	L1417	V1420	L1421	Y1422	S1423	L1424	G1425	S1426	A1427	Q1428	F1432	H1435	R1441	K1446	F1447	P1448	E1449	V1450	L1451	F1452										
Y1289	L1292	A1293	A1294	F1295	E1296	Y1297	K1298	G1299	I1306	N1307	SER	LEU	THR	PHE	LYS	SER	LEU	ASP	MET	LYS	ARG	ALA	ILE	SER	GLN	PRO	ALA	THR	ALA	ARG	ALA	GLY	C1243	S1246	A1247	S1250	L1253	V1257	L1258	W1259	V1260	T1264	L1268	A1273	L1276	T1277	L1278										
ALA	GLY	THR	ILE	ASN	PRO	SER	VAL	ALA	MET	SER	ILE	ALA	GLY	GLY	PRO	LEU	ALA	PRO	GLY	SER	ARG	ALA	ILE	SER	GLN	PRO	ALA	THR	ALA	ARG	ALA	GLY	C1243	S1246	A1247	S1250	L1253	V1257	L1258	W1259	V1260	T1264	L1268	A1273	L1276	T1277	L1278										
L1117	E1122	P1123	E1124	F1129	L1130	L1131	H1132	K1133	V1139	L1142	L1143	C1144	D1147	E1154	V1157	R1160	L1166	P1167	I1171	L1176	L1179	F1182	A1183	E1184	GLY	PRO	GLY	GLN	ARG	SER	ARG	LEU	ALA	SER	MET	SER	LEU	PRO	ASP	ASP	THR	GLU	GLY	GLU	GLY	ASP	ILE										
V1024	R1027	L1028	S1031	L1037	L1040	R1041	R1046	S1050	Y1054	N1058	L1059	P1060	C1061	C1062	P1063	L1064	S1065	PRO	ALA	SER	PRO	ALA	SER	PRO	PRO	VAL	SER	VAL	SER	THR	THR	SER	GLN	SER	THR	THR	PHE	SER	Q1087	F1097	F1103	H1107	G1111	T1115	E1116												
Y923	R924	I927	H930	F933	F934	L937	N938	V939	K940	S941	M942	A943	L944	H945	L946	R951	L952	D953	R956	R959	F960	L965	L971	V975	G976	V979	I980	V983	V987	E988	N994	D1003	V1008	D1009	F1012	S1015	W1016	V1017	R1018	T1021																	
L764	R765	T766	A767	L772	V773	S776	H777	ARG	H778	W779	L780	D781	L783	I788	R789	P790	I792	L800	G801	R802	F805	E806	H810	L814	R817	R826	Y835	V836	H837	A839	F840	T845	E846	P847	SER	LEU	PRO	ASP	GLY	ALA	PRO	V917	S919	S920													
GLN	ALA	ALA	THR	LEU	LEU	ARG	GLY	SER	GLY	PRO	ALA	SER	LEU	ARG	SER	SER	ILE	SER	SER	ASN	PRO	ASP	LEU	ALA	VAL	VAL	ASP	D897	E898	V899	S900	R901	L903	K906	L907	L908	E911	L912	Q915	W916	V917	V918	S919	S920													



● Molecule 2: Cell division control protein 42 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	259012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.099	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	319.2, 319.2, 319.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/13787	0.51	1/18706 (0.0%)
2	B	0.23	0/1419	0.51	0/1932
All	All	0.37	0/15206	0.51	1/20638 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	PRO	CA-N-CD	-5.27	104.62	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13471	0	13448	565	0
2	B	1389	0	1407	96	0
All	All	14860	0	14855	641	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 22.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:TYR:HB2	1:A:710:GLU:HB2	1.46	0.95
1:A:1054:TYR:O	1:A:1058:ASN:ND2	2.07	0.88
2:B:92:ASN:HB3	2:B:97:TRP:HZ3	1.38	0.88
1:A:633:LEU:HD23	1:A:661:LEU:HD11	1.55	0.86
1:A:569:ASN:ND2	1:A:642:CYS:SG	2.51	0.84
1:A:510:CYS:HB3	1:A:518:ILE:HB	1.61	0.82
1:A:1929:MET:HE2	2:B:3:THR:HG21	1.61	0.81
2:B:99:PRO:O	2:B:103:HIS:ND1	2.11	0.81
1:A:837:HIS:O	1:A:940:LYS:NZ	2.13	0.81
1:A:952:LEU:HA	1:A:959:ARG:HH12	1.46	0.80
1:A:1406:SER:O	1:A:1409:ARG:NH2	2.14	0.80
1:A:845:THR:HG21	1:A:945:HIS:HD1	1.46	0.80
2:B:63:ASP:O	2:B:66:ARG:NH1	2.14	0.80
1:A:911:GLU:OE2	1:A:915:GLN:NE2	2.14	0.79
1:A:553:VAL:HB	1:A:619:PHE:HB2	1.64	0.78
1:A:674:LEU:N	1:A:707:PHE:O	2.18	0.76
2:B:92:ASN:HA	2:B:95:GLU:HG2	1.66	0.76
2:B:81:CYS:HA	2:B:113:VAL:HB	1.68	0.75
1:A:242:GLU:O	1:A:1046:ARG:NH1	2.19	0.75
1:A:1945:GLY:H	2:B:36:VAL:HB	1.52	0.75
1:A:551:LEU:HD23	1:A:621:LEU:HD12	1.68	0.74
1:A:490:ARG:HH21	1:A:492:VAL:HG22	1.53	0.73
1:A:806:GLU:O	1:A:810:HIS:ND1	2.21	0.73
1:A:513:PRO:HD3	1:A:531:GLU:HB3	1.69	0.73
1:A:583:SER:O	1:A:600:ARG:NH2	2.22	0.72
1:A:1529:LEU:HB3	1:A:1555:MET:HE1	1.70	0.72
2:B:90:PHE:O	2:B:94:LYS:NZ	2.22	0.72
1:A:1937:SER:HA	2:B:37:PHE:HE2	1.55	0.72
2:B:92:ASN:ND2	2:B:95:GLU:OE2	2.23	0.72
1:A:95:THR:N	1:A:517:HIS:O	2.19	0.71
1:A:1853:CYS:O	2:B:27:LYS:NZ	2.23	0.71
1:A:223:ARG:NE	1:A:1394:ASP:OD1	2.22	0.71
1:A:467:LEU:HD11	1:A:475:PHE:HE2	1.56	0.71
1:A:1498:ASN:O	1:A:1501:ARG:NH2	2.24	0.71
1:A:1515:GLY:HA3	1:A:1602:ASN:HD21	1.54	0.71
1:A:1876:LEU:HD12	1:A:1891:VAL:HG11	1.72	0.71
1:A:660:PRO:O	1:A:668:ARG:NH2	2.20	0.70
1:A:1297:TYR:CZ	1:A:1299:GLY:HA2	2.26	0.70
1:A:554:TYR:HE2	1:A:618:GLU:HG3	1.56	0.69
1:A:1866:LEU:HB2	1:A:1867:PRO:HD3	1.73	0.69
1:A:1111:GLY:O	1:A:1115:THR:OG1	2.06	0.69
1:A:1954:LEU:HD13	1:A:2017:LEU:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:ARG:NH1	1:A:1484:SER:OG	2.26	0.69
1:A:1833:GLU:OE2	1:A:1837:ARG:NH1	2.25	0.69
2:B:117:ILE:HG12	2:B:156:GLU:HG2	1.74	0.69
2:B:35:THR:HG23	2:B:37:PHE:H	1.56	0.68
1:A:565:GLY:O	1:A:568:ARG:NH1	2.26	0.68
2:B:6:CYS:HB3	2:B:55:LEU:HD23	1.74	0.68
1:A:1803:LYS:HZ1	2:B:29:PRO:HD2	1.59	0.68
2:B:44:VAL:O	2:B:51:TYR:N	2.26	0.68
1:A:1460:ALA:HB2	1:A:1676:LYS:HD2	1.75	0.67
1:A:1913:THR:HG23	1:A:1980:LYS:HG3	1.76	0.67
1:A:1790:TYR:O	1:A:1794:PHE:HB2	1.94	0.67
2:B:16:LYS:NZ	2:B:58:THR:O	2.28	0.67
1:A:1454:GLU:N	1:A:1454:GLU:OE1	2.27	0.67
1:A:1873:LYS:HB3	1:A:1897:THR:HB	1.76	0.67
1:A:1954:LEU:HA	1:A:1967:HIS:HE1	1.61	0.66
1:A:573:ARG:HB3	1:A:636:THR:HB	1.76	0.66
1:A:1587:ARG:HH22	1:A:1590:GLN:HG2	1.59	0.66
1:A:951:ARG:NH2	1:A:959:ARG:O	2.29	0.66
1:A:1892:CYS:SG	1:A:1893:HIS:N	2.69	0.66
1:A:223:ARG:NH2	1:A:1397:GLU:OE1	2.29	0.65
1:A:1848:ARG:NH2	1:A:1879:ASP:O	2.31	0.64
1:A:221:THR:O	1:A:225:GLN:NE2	2.29	0.64
1:A:456:VAL:HB	1:A:496:LEU:HB2	1.79	0.64
1:A:663:GLN:HG2	1:A:668:ARG:HH11	1.62	0.64
1:A:1862:ALA:O	1:A:1869:GLN:NE2	2.27	0.64
1:A:92:CYS:SG	1:A:94:THR:OG1	2.55	0.64
1:A:1735:THR:O	1:A:1739:HIS:ND1	2.25	0.64
1:A:1012:PHE:O	1:A:1015:SER:OG	2.14	0.64
1:A:1906:ILE:HG23	1:A:1910:GLN:HE22	1.63	0.64
2:B:3:THR:HG23	2:B:52:THR:HG22	1.80	0.64
1:A:115:MET:HG2	1:A:778:HIS:CE1	2.33	0.63
1:A:1428:GLN:HB3	1:A:1432:PHE:HD2	1.63	0.63
1:A:120:TRP:HB3	1:A:838:TYR:HB3	1.79	0.63
1:A:264:LYS:O	1:A:499:ASP:N	2.30	0.63
1:A:1673:CYS:HB3	1:A:1678:PHE:CD1	2.33	0.63
1:A:1916:LEU:HD22	1:A:1980:LYS:HB3	1.80	0.63
1:A:1932:MET:HA	2:B:56:PHE:HE1	1.63	0.63
1:A:1943:ASN:ND2	2:B:38:ASP:OD1	2.31	0.63
1:A:1449:GLU:OE1	1:A:1449:GLU:N	2.30	0.63
1:A:1711:ILE:HA	1:A:1714:LEU:HD13	1.81	0.63
1:A:1457:GLU:N	1:A:1457:GLU:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:PHE:O	1:A:938:MET:HG3	1.99	0.62
1:A:919:SER:OG	1:A:920:SER:N	2.31	0.62
2:B:7:VAL:HA	2:B:56:PHE:HB2	1.80	0.62
1:A:548:ARG:O	1:A:716:SER:N	2.32	0.62
1:A:1916:LEU:HD21	1:A:1984:ALA:HB2	1.80	0.62
1:A:284:TYR:HB3	1:A:473:PHE:HE1	1.64	0.62
1:A:1753:ARG:HH21	1:A:1823:THR:HG21	1.64	0.62
1:A:264:LYS:NZ	1:A:501:SER:OG	2.33	0.62
1:A:938:MET:O	1:A:942:MET:HG3	2.00	0.61
1:A:1937:SER:HA	2:B:37:PHE:CE2	2.34	0.61
2:B:92:ASN:HB3	2:B:97:TRP:CZ3	2.28	0.61
1:A:393:PRO:HG2	1:A:462:GLN:HG2	1.81	0.61
1:A:733:VAL:HG23	1:A:738:ALA:HB3	1.83	0.61
1:A:1369:LYS:HB3	1:A:1374:MET:SD	2.40	0.61
1:A:467:LEU:HG	1:A:472:LEU:HD12	1.83	0.61
1:A:511:LEU:N	1:A:529:THR:O	2.33	0.61
1:A:1750:THR:N	1:A:1773:GLU:O	2.22	0.61
2:B:53:LEU:HD22	2:B:173:ILE:HD11	1.82	0.61
1:A:344:LYS:HE2	1:A:394:PHE:CD2	2.35	0.61
1:A:115:MET:HG2	1:A:778:HIS:HE1	1.66	0.61
1:A:1853:CYS:HB3	1:A:1871:LYS:HD3	1.81	0.61
1:A:1803:LYS:NZ	2:B:28:PHE:HB3	2.16	0.60
1:A:1960:ASP:HB3	1:A:1963:LEU:HG	1.83	0.60
1:A:898:GLU:HA	1:A:901:ARG:HG3	1.83	0.60
1:A:268:LEU:HD23	1:A:301:ASN:ND2	2.16	0.60
1:A:900:SER:HA	1:A:903:LEU:HB2	1.83	0.60
1:A:1441:ARG:HD2	1:A:1487:LEU:HD23	1.82	0.60
1:A:549:ASN:HA	1:A:715:SER:HA	1.83	0.60
1:A:1504:MET:O	1:A:1508:MET:HG3	2.00	0.60
2:B:90:PHE:HD2	2:B:137:ILE:HD12	1.66	0.60
2:B:174:LEU:HA	2:B:177:LEU:HD23	1.83	0.60
2:B:99:PRO:C	2:B:103:HIS:HD1	2.07	0.60
1:A:1803:LYS:NZ	2:B:30:SER:OG	2.32	0.60
2:B:6:CYS:O	2:B:56:PHE:N	2.31	0.60
1:A:345:VAL:HG22	1:A:391:ARG:HD2	1.82	0.60
1:A:1574:ASP:HB3	1:A:1577:MET:SD	2.41	0.59
1:A:1167:PRO:O	1:A:1171:ILE:HG12	2.03	0.59
1:A:1771:TYR:OH	1:A:1888:ARG:NH1	2.33	0.59
1:A:1757:TYR:HD1	1:A:1766:GLU:HG3	1.67	0.59
2:B:77:VAL:HB	2:B:176:ALA:HB2	1.85	0.59
2:B:5:LYS:NZ	2:B:73:PRO:O	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PRO:HA	2:B:32:TYR:HD1	1.68	0.59
1:A:1734:PHE:O	1:A:1738:MET:HG2	2.02	0.59
1:A:1856:PHE:N	1:A:1870:HIS:O	2.26	0.59
1:A:286:VAL:HG23	1:A:473:PHE:HB3	1.85	0.59
1:A:916:TRP:O	1:A:924:ARG:NH1	2.35	0.59
1:A:1873:LYS:N	1:A:1897:THR:O	2.36	0.58
2:B:162:GLN:HA	2:B:165:LEU:HD13	1.84	0.58
1:A:2008:CYS:SG	1:A:2011:ARG:NH2	2.76	0.58
1:A:2014:LEU:O	1:A:2018:LEU:N	2.24	0.58
1:A:559:ASN:HB2	1:A:706:VAL:HB	1.86	0.58
1:A:1876:LEU:HD13	1:A:1894:ARG:HG3	1.85	0.58
1:A:2010:LEU:HD23	1:A:2014:LEU:HD23	1.85	0.58
1:A:138:THR:O	1:A:141:THR:OG1	2.14	0.58
1:A:459:PHE:CE2	1:A:494:ALA:HB3	2.38	0.58
1:A:587:PRO:HA	1:A:600:ARG:HA	1.86	0.58
1:A:59:VAL:HG11	1:A:1059:LEU:HD21	1.84	0.58
1:A:1558:LEU:HA	1:A:1561:ILE:HD12	1.85	0.58
1:A:2001:ARG:HA	1:A:2004:GLU:HG2	1.84	0.58
1:A:2014:LEU:HB3	1:A:2018:LEU:HG	1.84	0.58
1:A:567:VAL:HG13	1:A:639:HIS:HB2	1.86	0.58
1:A:1273:ALA:HA	1:A:1276:LEU:HD12	1.85	0.58
1:A:1406:SER:OG	1:A:1407:GLU:N	2.32	0.58
1:A:1781:GLU:N	1:A:1781:GLU:OE1	2.32	0.58
2:B:69:PRO:HA	2:B:72:TYR:CE1	2.39	0.58
1:A:721:ASP:OD1	1:A:722:PRO:HD2	2.04	0.58
1:A:1757:TYR:HB2	1:A:1819:TYR:HB2	1.85	0.58
1:A:1551:VAL:O	1:A:1555:MET:HG2	2.03	0.57
1:A:1486:TYR:HB2	1:A:1532:ILE:HG23	1.85	0.57
1:A:1789:PHE:O	1:A:1792:GLU:HG2	2.03	0.57
1:A:1842:ASP:HA	1:A:1845:TYR:HB3	1.86	0.57
1:A:466:ARG:CZ	1:A:615:PHE:HA	2.34	0.57
1:A:1950:ALA:O	1:A:1954:LEU:HB2	2.04	0.57
2:B:117:ILE:CG1	2:B:156:GLU:HG2	2.33	0.57
1:A:724:LEU:HD12	1:A:724:LEU:H	1.70	0.57
1:A:1954:LEU:HB3	1:A:2017:LEU:HD12	1.85	0.57
1:A:971:LEU:O	1:A:975:VAL:HG23	2.05	0.57
1:A:1837:ARG:HD3	1:A:1842:ASP:O	2.05	0.57
1:A:572:VAL:HB	1:A:604:THR:OG1	2.04	0.57
1:A:802:ARG:NH2	1:A:920:SER:OG	2.36	0.57
1:A:1673:CYS:HB3	1:A:1678:PHE:HD1	1.68	0.57
2:B:141:THR:HA	2:B:144:LYS:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:MET:HE3	1:A:577:MET:HA	1.87	0.56
1:A:723:TYR:HD2	1:A:767:ALA:HA	1.69	0.56
1:A:1692:GLY:O	1:A:1696:MET:HG3	2.05	0.56
1:A:1810:LYS:O	1:A:1813:LEU:HG	2.04	0.56
2:B:8:VAL:HG12	2:B:56:PHE:O	2.05	0.56
1:A:541:TYR:HB3	1:A:773:VAL:HG11	1.88	0.56
1:A:1916:LEU:HA	1:A:1933:VAL:HG11	1.86	0.56
1:A:1580:ASP:OD1	1:A:1584:ARG:NH2	2.39	0.56
1:A:1988:ASN:O	1:A:1992:ILE:HG23	2.05	0.56
1:A:917:VAL:O	1:A:924:ARG:NH1	2.39	0.56
1:A:1911:LYS:HA	1:A:1914:ARG:HE	1.71	0.56
1:A:118:GLU:OE2	1:A:119:ASP:N	2.39	0.56
1:A:1615:GLU:OE1	1:A:1615:GLU:N	2.31	0.55
1:A:1523:GLU:O	1:A:1527:ARG:HG3	2.05	0.55
1:A:1966:HIS:HA	1:A:1969:LYS:HE2	1.89	0.55
2:B:11:ASP:HA	2:B:60:GLY:HA3	1.87	0.55
1:A:397:THR:HB	1:A:459:PHE:HD1	1.71	0.55
1:A:633:LEU:CD2	1:A:661:LEU:HD11	2.35	0.55
1:A:1597:LEU:O	1:A:1601:GLN:HG3	2.07	0.55
2:B:157:CYS:HB2	2:B:165:LEU:HD12	1.88	0.55
1:A:554:TYR:CE2	1:A:618:GLU:HG3	2.40	0.54
1:A:1393:LEU:HD22	1:A:1432:PHE:HE1	1.72	0.54
1:A:1982:GLU:HB2	1:A:2007:TYR:OH	2.08	0.54
1:A:789:ARG:HG3	1:A:903:LEU:HD22	1.89	0.54
1:A:1515:GLY:HA3	1:A:1602:ASN:ND2	2.22	0.54
1:A:1865:GLU:CD	1:A:1867:PRO:HD2	2.32	0.54
2:B:69:PRO:HA	2:B:72:TYR:CZ	2.42	0.54
1:A:467:LEU:HD11	1:A:475:PHE:CE2	2.40	0.54
1:A:1103:PHE:CE2	1:A:1167:PRO:HG2	2.43	0.54
1:A:792:ILE:HD11	1:A:899:VAL:HG13	1.89	0.54
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.07	0.54
1:A:1755:GLY:HA2	1:A:1768:GLU:HA	1.89	0.54
2:B:45:MET:HA	2:B:50:PRO:HA	1.90	0.54
1:A:223:ARG:HH22	1:A:1397:GLU:CD	2.16	0.54
1:A:348:GLN:H	1:A:383:PHE:HE1	1.56	0.54
1:A:244:VAL:O	1:A:246:ARG:HD3	2.07	0.54
1:A:1998:GLU:HA	1:A:2001:ARG:HD2	1.90	0.54
1:A:72:LEU:HD21	1:A:1160:ARG:HH12	1.73	0.54
1:A:1564:ASP:HA	1:A:1567:LYS:HD2	1.90	0.54
1:A:1751:TYR:HE1	1:A:1772:LYS:HG3	1.73	0.54
1:A:1849:THR:HG23	1:A:1876:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1995:ASP:OD1	1:A:1996:GLN:NE2	2.41	0.54
1:A:203:LEU:HB3	1:A:206:LEU:HD23	1.91	0.53
1:A:205:SER:HA	1:A:208:GLU:HG3	1.90	0.53
1:A:630:ASN:O	1:A:632:HIS:ND1	2.41	0.53
1:A:1986:ARG:O	1:A:1989:LYS:HG3	2.09	0.53
2:B:87:PRO:HB3	2:B:137:ILE:HD11	1.91	0.53
1:A:590:PHE:CD2	1:A:620:LYS:HE2	2.43	0.53
1:A:1978:CYS:O	1:A:2007:TYR:OH	2.15	0.53
1:A:278:PHE:H	1:A:343:GLU:HB3	1.72	0.53
1:A:1572:GLN:HG3	1:A:1573:GLU:HG2	1.91	0.53
1:A:281:LEU:HD21	1:A:340:ILE:HG12	1.91	0.53
1:A:207:LEU:HD11	1:A:1486:TYR:HE2	1.74	0.53
1:A:1943:ASN:ND2	2:B:37:PHE:O	2.42	0.53
1:A:1565:THR:O	1:A:1568:MET:HB3	2.10	0.52
1:A:54:LEU:HD13	1:A:59:VAL:HG21	1.92	0.52
1:A:108:GLN:HG3	1:A:732:HIS:CE1	2.45	0.52
1:A:116:TYR:OH	1:A:778:HIS:NE2	2.42	0.52
1:A:1989:LYS:HB3	1:A:2000:HIS:CE1	2.44	0.52
2:B:83:SER:HB3	2:B:86:SER:OG	2.10	0.52
1:A:641:SER:HB2	1:A:650:LEU:HA	1.92	0.52
1:A:289:LYS:NZ	1:A:470:GLU:OE1	2.28	0.52
1:A:333:SER:O	1:A:336:ILE:HG12	2.10	0.52
1:A:1097:PHE:HE1	1:A:1268:LEU:HD11	1.74	0.52
1:A:1934:LEU:O	1:A:1938:VAL:HG12	2.10	0.52
1:A:569:ASN:H	1:A:639:HIS:CE1	2.27	0.52
1:A:728:PHE:O	1:A:732:HIS:ND1	2.43	0.52
1:A:1583:TYR:CD2	1:A:1886:LYS:HD2	2.45	0.52
1:A:1964:PHE:HB3	1:A:1965:ARG:HH21	1.74	0.52
1:A:629:GLU:OE1	1:A:629:GLU:N	2.38	0.52
1:A:1749:GLY:HA2	1:A:1774:PRO:HA	1.92	0.52
1:A:1778:LYS:H	1:A:1781:GLU:CD	2.18	0.52
1:A:1894:ARG:HB3	1:A:1894:ARG:CZ	2.40	0.52
1:A:1911:LYS:HG3	1:A:1914:ARG:HH21	1.75	0.51
1:A:1050:SER:O	1:A:1050:SER:OG	2.22	0.51
1:A:1529:LEU:HD22	1:A:1555:MET:HE1	1.91	0.51
1:A:552:TYR:CE1	1:A:620:LYS:HB2	2.45	0.51
1:A:1633:LEU:HD13	1:A:1665:LEU:HD13	1.91	0.51
2:B:75:THR:HG21	2:B:78:PHE:HD1	1.75	0.51
1:A:643:GLN:OE1	1:A:645:ARG:NE	2.33	0.51
1:A:835:TYR:CD1	1:A:839:ALA:HB3	2.45	0.51
1:A:1680:GLU:OE2	1:A:1717:HIS:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:VAL:O	1:A:1506:VAL:HG23	2.10	0.51
1:A:1700:TYR:O	1:A:1703:VAL:N	2.44	0.51
1:A:1732:GLU:O	1:A:1735:THR:OG1	2.27	0.51
1:A:125:ARG:NH2	1:A:1003:ASP:OD1	2.44	0.51
1:A:1495:ILE:O	1:A:1497:HIS:N	2.43	0.51
1:A:1865:GLU:OE2	1:A:1867:PRO:HD2	2.11	0.51
1:A:845:THR:HG21	1:A:945:HIS:ND1	2.22	0.51
1:A:1407:GLU:HA	1:A:1409:ARG:NH2	2.26	0.51
1:A:569:ASN:O	1:A:639:HIS:ND1	2.44	0.51
1:A:657:THR:HG21	1:A:707:PHE:HD2	1.75	0.51
1:A:1954:LEU:HD23	1:A:1967:HIS:CE1	2.46	0.51
1:A:258:GLY:HA3	1:A:329:VAL:O	2.11	0.51
1:A:1683:LEU:O	1:A:1687:LEU:HD23	2.11	0.51
1:A:1983:ASP:HB2	1:A:1987:LYS:NZ	2.26	0.51
1:A:137:VAL:HG11	1:A:1144:CYS:SG	2.50	0.51
1:A:326:ILE:HB	1:A:531:GLU:HA	1.93	0.51
1:A:344:LYS:HB3	1:A:394:PHE:HB2	1.92	0.51
1:A:983:VAL:HG21	1:A:1037:LEU:HD13	1.92	0.51
1:A:1929:MET:O	1:A:1933:VAL:HG23	2.10	0.51
1:A:1307:ASN:OD1	1:A:1369:LYS:NZ	2.42	0.50
1:A:1770:VAL:HG11	1:A:1850:PHE:CE2	2.46	0.50
1:A:1857:THR:OG1	1:A:1859:ASP:OD1	2.28	0.50
1:A:1487:LEU:HD11	1:A:1491:GLN:HE21	1.76	0.50
2:B:170:ASP:O	2:B:174:LEU:HG	2.11	0.50
1:A:724:LEU:HD11	1:A:767:ALA:HB1	1.93	0.50
1:A:283:LEU:HD21	1:A:336:ILE:HG23	1.94	0.50
1:A:512:SER:OG	1:A:516:LEU:N	2.32	0.50
1:A:778:HIS:O	1:A:782:LYS:HG2	2.11	0.50
1:A:1838:VAL:O	1:A:1843:ARG:NE	2.34	0.50
1:A:592:LYS:HZ1	1:A:605:PRO:HG3	1.77	0.50
1:A:814:LEU:HA	1:A:817:ARG:HD3	1.93	0.50
1:A:1929:MET:CE	2:B:3:THR:HG21	2.38	0.50
1:A:454:LEU:HD22	1:A:456:VAL:HG22	1.94	0.50
1:A:466:ARG:NE	1:A:615:PHE:HA	2.27	0.50
1:A:1732:GLU:O	1:A:1736:LYS:HG3	2.11	0.50
1:A:1840:TYR:HA	1:A:1843:ARG:HD2	1.93	0.50
2:B:68:ARG:HD2	2:B:69:PRO:CD	2.41	0.50
1:A:951:ARG:C	1:A:953:ASP:H	2.20	0.50
1:A:975:VAL:O	1:A:979:VAL:HG23	2.12	0.50
1:A:1117:LEU:HD22	1:A:1139:VAL:HG21	1.94	0.50
1:A:1927:ALA:HA	1:A:1930:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:HIS:O	1:A:389:ARG:HG3	2.12	0.49
1:A:549:ASN:C	1:A:550:LEU:HD12	2.36	0.49
1:A:551:LEU:HB2	1:A:623:LEU:HD11	1.93	0.49
1:A:578:THR:HA	1:A:631:HIS:HA	1.93	0.49
1:A:1825:VAL:HA	1:A:1852:PHE:HB3	1.94	0.49
1:A:1776:ILE:HG12	2:B:45:MET:SD	2.51	0.49
1:A:276:PRO:HA	1:A:305:MET:HE2	1.94	0.49
1:A:344:LYS:N	1:A:392:MET:O	2.44	0.49
1:A:656:PHE:N	1:A:677:SER:O	2.27	0.49
1:A:287:ARG:HH12	1:A:335:ASP:HB2	1.78	0.49
1:A:1669:GLU:HB3	1:A:1672:PHE:CE2	2.48	0.49
1:A:1926:ASP:OD2	1:A:1928:LYS:NZ	2.32	0.49
2:B:84:VAL:HG11	2:B:117:ILE:HG13	1.93	0.49
1:A:1714:LEU:O	1:A:1718:ARG:N	2.43	0.49
2:B:153:LYS:NZ	2:B:154:TYR:H	2.10	0.49
1:A:1837:ARG:HG3	1:A:1842:ASP:HB3	1.93	0.49
1:A:397:THR:HB	1:A:459:PHE:CD1	2.47	0.49
2:B:8:VAL:O	2:B:58:THR:OG1	2.28	0.49
2:B:90:PHE:CZ	2:B:145:LEU:HD23	2.47	0.49
1:A:659:ILE:HD11	1:A:668:ARG:HH21	1.78	0.48
1:A:1998:GLU:H	1:A:1998:GLU:CD	2.21	0.48
1:A:1566:VAL:HA	1:A:1569:LYS:HD3	1.95	0.48
1:A:772:LEU:HD23	1:A:814:LEU:HD23	1.95	0.48
1:A:917:VAL:C	1:A:924:ARG:HH12	2.20	0.48
1:A:1855:PRO:HA	1:A:1871:LYS:HA	1.93	0.48
1:A:252:PRO:HG3	1:A:838:TYR:CZ	2.48	0.48
1:A:552:TYR:HE1	1:A:620:LYS:HB2	1.78	0.48
1:A:1528:SER:O	1:A:1532:ILE:HG13	2.14	0.48
1:A:1733:ALA:O	1:A:1737:ILE:HG13	2.12	0.48
1:A:1877:SER:HB3	1:A:1893:HIS:HB2	1.94	0.48
1:A:2005:ARG:HB3	1:A:2009:ARG:NH2	2.29	0.48
1:A:459:PHE:HE2	1:A:494:ALA:HB3	1.79	0.48
1:A:1529:LEU:HA	1:A:1532:ILE:HD12	1.95	0.48
1:A:1863:HIS:HE1	2:B:32:TYR:CE2	2.31	0.48
2:B:122:ASP:O	2:B:126:ILE:HG12	2.13	0.48
1:A:1763:ASP:OD1	1:A:1764:LEU:N	2.46	0.48
1:A:641:SER:OG	1:A:649:ALA:O	2.25	0.48
1:A:788:ILE:O	1:A:906:LYS:HB2	2.14	0.48
1:A:1097:PHE:CE1	1:A:1268:LEU:HD11	2.49	0.48
1:A:283:LEU:C	1:A:284:TYR:HD1	2.22	0.48
1:A:567:VAL:O	1:A:611:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:GLN:OE1	1:A:1816:GLN:N	2.46	0.48
1:A:1856:PHE:CE1	1:A:1872:ARG:HG3	2.49	0.48
2:B:66:ARG:HG2	2:B:67:LEU:HD12	1.94	0.48
1:A:291:LYS:HE2	1:A:293:SER:O	2.15	0.47
1:A:1058:ASN:O	1:A:1107:HIS:HD2	1.97	0.47
1:A:1530:LYS:HA	1:A:1533:LEU:HD12	1.96	0.47
1:A:1757:TYR:CD1	1:A:1766:GLU:HG3	2.48	0.47
1:A:495:GLN:HE21	1:A:497:LYS:HE3	1.79	0.47
1:A:1571:HIS:C	1:A:1577:MET:HE1	2.39	0.47
1:A:235:TYR:CD1	1:A:236:PRO:HD2	2.48	0.47
1:A:141:THR:O	1:A:144:GLU:HG3	2.15	0.47
1:A:636:THR:HG23	1:A:656:PHE:HE1	1.79	0.47
1:A:1012:PHE:CE2	1:A:1016:LEU:HD11	2.50	0.47
1:A:2001:ARG:HA	1:A:2004:GLU:OE2	2.13	0.47
1:A:333:SER:HB3	1:A:336:ILE:HD11	1.97	0.47
1:A:714:VAL:HG23	1:A:714:VAL:O	2.15	0.47
1:A:1751:TYR:HA	1:A:1771:TYR:O	2.15	0.47
1:A:1929:MET:HE1	2:B:54:GLY:HA3	1.97	0.47
1:A:1953:PHE:HB3	1:A:1970:LEU:HD11	1.96	0.47
1:A:1983:ASP:HB2	1:A:1987:LYS:HZ3	1.80	0.47
1:A:1800:GLU:O	1:A:1819:TYR:HA	2.15	0.47
1:A:1938:VAL:HG23	1:A:2010:LEU:HD12	1.96	0.47
1:A:232:LEU:HB2	1:A:1147:ASP:OD2	2.14	0.47
1:A:312:HIS:HB3	1:A:389:ARG:HG3	1.95	0.47
1:A:467:LEU:HG	1:A:472:LEU:CD1	2.45	0.47
1:A:956:ARG:HA	1:A:959:ARG:HG3	1.97	0.47
1:A:1253:LEU:O	1:A:1257:VAL:HG23	2.15	0.47
1:A:1260:VAL:O	1:A:1264:THR:OG1	2.28	0.47
1:A:1568:MET:O	1:A:1572:GLN:HB3	2.14	0.47
1:A:1814:ASP:N	1:A:1814:ASP:OD1	2.43	0.47
1:A:1451:LEU:HD12	1:A:1458:LEU:HB3	1.97	0.47
1:A:137:VAL:HG13	1:A:238:PRO:HD2	1.96	0.46
1:A:260:ARG:NH2	1:A:531:GLU:OE2	2.48	0.46
1:A:1420:VAL:O	1:A:1423:SER:OG	2.23	0.46
1:A:1529:LEU:HD23	1:A:1532:ILE:HD12	1.97	0.46
1:A:1859:ASP:OD1	1:A:1860:GLY:N	2.48	0.46
1:A:1061:CYS:O	1:A:1063:PRO:HD3	2.16	0.46
1:A:946:LEU:HD23	1:A:951:ARG:HB2	1.97	0.46
2:B:10:GLY:HA3	2:B:81:CYS:HB2	1.98	0.46
1:A:592:LYS:NZ	1:A:605:PRO:HG3	2.30	0.46
1:A:1751:TYR:CE1	1:A:1772:LYS:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:CYS:HA	1:A:498:ILE:HG23	1.97	0.46
1:A:919:SER:HG	1:A:920:SER:H	1.61	0.46
1:A:1417:LEU:O	1:A:1421:LEU:HG	2.15	0.46
1:A:1496:GLY:C	1:A:1498:ASN:H	2.24	0.46
2:B:68:ARG:HD2	2:B:69:PRO:HD3	1.98	0.46
1:A:980:ILE:O	1:A:983:VAL:HG23	2.16	0.46
1:A:1400:VAL:O	1:A:1404:MET:HG3	2.16	0.46
1:A:1393:LEU:HD12	1:A:1393:LEU:HA	1.67	0.46
1:A:1425:GLY:HA3	1:A:1465:ARG:NH1	2.30	0.46
1:A:1904:VAL:HA	1:A:1907:GLU:OE2	2.16	0.46
2:B:93:VAL:O	2:B:98:VAL:HG23	2.15	0.46
1:A:131:SER:OG	1:A:132:ALA:N	2.47	0.46
1:A:262:LEU:HB2	1:A:503:ALA:HB2	1.97	0.46
1:A:1446:LYS:HG3	1:A:1447:PHE:CE1	2.51	0.46
1:A:1605:GLY:O	1:A:1609:GLU:HG2	2.15	0.46
1:A:1931:GLN:HG3	1:A:1999:TYR:CE2	2.51	0.46
1:A:1983:ASP:OD1	1:A:1984:ALA:N	2.49	0.46
1:A:933:PHE:CE1	1:A:937:LEU:HD22	2.51	0.46
2:B:153:LYS:HZ3	2:B:154:TYR:H	1.63	0.46
1:A:589:ILE:HG12	1:A:621:LEU:HD23	1.96	0.45
1:A:761:LEU:HA	1:A:761:LEU:HD23	1.70	0.45
1:A:1514:VAL:HG11	1:A:1565:THR:HG21	1.97	0.45
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.72	0.45
1:A:1857:THR:OG1	1:A:1861:ARG:O	2.25	0.45
1:A:634:LEU:HA	1:A:658:TRP:HA	1.98	0.45
1:A:1021:TYR:CD2	1:A:1041:ARG:HD2	2.52	0.45
1:A:1059:LEU:HA	1:A:1059:LEU:HD12	1.75	0.45
1:A:946:LEU:HD11	1:A:960:PHE:CE1	2.52	0.45
1:A:337:PHE:CD1	1:A:476:LEU:HD22	2.51	0.45
1:A:560:PHE:HB3	1:A:611:LYS:NZ	2.32	0.45
1:A:994:ASN:HD22	1:A:1040:LEU:HD22	1.82	0.45
1:A:1008:VAL:HG22	1:A:1009:ASP:H	1.82	0.45
1:A:1246:SER:O	1:A:1250:SER:OG	2.29	0.45
1:A:281:LEU:O	1:A:296:PHE:N	2.47	0.45
1:A:729:THR:O	1:A:733:VAL:HG12	2.17	0.45
1:A:806:GLU:HG2	1:A:923:VAL:HG21	1.99	0.45
1:A:1731:GLN:O	1:A:1735:THR:HG23	2.16	0.45
1:A:1734:PHE:HA	1:A:1737:ILE:HD12	1.98	0.45
1:A:401:LEU:HB3	1:A:446:PHE:CE1	2.52	0.45
1:A:569:ASN:OD1	1:A:609:HIS:N	2.30	0.45
1:A:1142:LEU:HD23	1:A:1142:LEU:HA	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:ALA:HB1	1:A:2014:LEU:HD11	1.98	0.45
2:B:82:PHE:HE2	2:B:84:VAL:HA	1.82	0.45
1:A:805:PHE:CE1	1:A:912:LEU:HD23	2.51	0.45
1:A:1515:GLY:CA	1:A:1602:ASN:HD21	2.25	0.45
1:A:1555:MET:HB3	1:A:1555:MET:HE3	1.67	0.45
1:A:387:LEU:O	1:A:391:ARG:NH1	2.49	0.44
1:A:466:ARG:HD3	1:A:614:GLU:O	2.17	0.44
1:A:553:VAL:HG22	1:A:711:LEU:CD2	2.47	0.44
1:A:1129:PHE:CE1	1:A:1133:LYS:HE3	2.52	0.44
1:A:1529:LEU:CB	1:A:1555:MET:HE1	2.43	0.44
1:A:1701:GLU:H	1:A:1701:GLU:CD	2.21	0.44
1:A:1711:ILE:O	1:A:1714:LEU:N	2.49	0.44
1:A:1754:VAL:O	1:A:1769:PHE:N	2.49	0.44
1:A:218:ARG:HG2	1:A:222:LEU:HD13	1.98	0.44
1:A:1154:GLU:O	1:A:1157:VAL:HG22	2.17	0.44
1:A:1966:HIS:O	1:A:1969:LYS:HG2	2.18	0.44
1:A:84:GLU:OE1	1:A:126:ARG:HD3	2.17	0.44
1:A:248:SER:OG	1:A:826:ARG:NH2	2.47	0.44
1:A:1597:LEU:HA	1:A:1600:LEU:HD12	1.98	0.44
1:A:1746:ARG:HH22	1:A:1841:PHE:N	2.15	0.44
1:A:264:LYS:HB2	1:A:499:ASP:HB2	2.00	0.44
1:A:549:ASN:OD1	1:A:549:ASN:N	2.51	0.44
1:A:634:LEU:HD12	1:A:657:THR:O	2.18	0.44
1:A:938:MET:O	1:A:941:SER:OG	2.31	0.44
1:A:1432:PHE:O	1:A:1435:HIS:N	2.51	0.44
1:A:1803:LYS:HE2	2:B:28:PHE:CD1	2.51	0.44
1:A:1877:SER:CB	1:A:1893:HIS:HB2	2.46	0.44
1:A:1938:VAL:O	1:A:2006:ASN:ND2	2.50	0.44
2:B:64:TYR:O	2:B:68:ARG:HG3	2.18	0.44
1:A:567:VAL:HA	1:A:639:HIS:CE1	2.52	0.44
1:A:1292:LEU:HD23	1:A:1292:LEU:HA	1.71	0.44
1:A:1453:GLU:HB3	1:A:1454:GLU:OE1	2.17	0.44
1:A:1904:VAL:O	1:A:1907:GLU:HG2	2.17	0.44
1:A:81:ASP:OD1	1:A:81:ASP:N	2.49	0.44
1:A:915:GLN:O	1:A:919:SER:HB2	2.17	0.44
1:A:980:ILE:HG22	1:A:1027:ARG:HD3	2.00	0.44
1:A:1533:LEU:HD21	1:A:1555:MET:HG3	1.99	0.44
1:A:1576:GLU:H	1:A:1576:GLU:CD	2.25	0.44
1:A:1656:GLU:OE1	1:A:1656:GLU:N	2.36	0.44
1:A:1916:LEU:HD11	1:A:1981:CYS:HA	2.00	0.44
1:A:511:LEU:HD22	1:A:515:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PRO:HG3	1:A:531:GLU:O	2.17	0.44
1:A:551:LEU:HB3	1:A:621:LEU:HB2	2.00	0.44
1:A:1143:LEU:HD22	1:A:1259:TRP:CE3	2.53	0.44
1:A:1454:GLU:HG2	1:A:1455:ASP:N	2.32	0.44
1:A:1856:PHE:HB3	1:A:1872:ARG:HH21	1.82	0.44
1:A:1530:LYS:O	1:A:1533:LEU:HB2	2.17	0.44
1:A:53:PRO:HD3	1:A:1018:ARG:HD3	2.00	0.44
1:A:290:LYS:O	1:A:292:ILE:HG23	2.18	0.44
1:A:976:GLY:O	1:A:980:ILE:HG13	2.18	0.44
1:A:641:SER:HB2	1:A:650:LEU:HD12	1.99	0.43
2:B:133:LYS:HA	2:B:133:LYS:HD3	1.80	0.43
1:A:633:LEU:O	1:A:659:ILE:N	2.50	0.43
1:A:737:GLY:HA2	1:A:739:PHE:CE2	2.53	0.43
1:A:1932:MET:HE1	2:B:41:ALA:HB2	2.00	0.43
1:A:1961:PRO:O	1:A:1965:ARG:HG2	2.18	0.43
2:B:68:ARG:NH1	2:B:72:TYR:OH	2.51	0.43
1:A:271:GLU:H	1:A:271:GLU:HG3	1.68	0.43
1:A:956:ARG:HG2	1:A:959:ARG:HE	1.83	0.43
1:A:46:PRO:HD2	1:A:49:GLU:HB3	2.00	0.43
1:A:624:PRO:O	1:A:627:VAL:HG23	2.19	0.43
1:A:1523:GLU:CD	1:A:1523:GLU:H	2.26	0.43
1:A:1565:THR:O	1:A:1569:LYS:HD3	2.19	0.43
2:B:97:TRP:HA	2:B:100:GLU:OE2	2.19	0.43
1:A:726:LYS:HE3	1:A:726:LYS:HB2	1.75	0.43
1:A:1166:LEU:HD23	1:A:1166:LEU:HA	1.77	0.43
1:A:1278:LEU:HD11	1:A:1408:ALA:HB3	2.00	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD12	1.84	0.43
1:A:1873:LYS:O	1:A:1897:THR:N	2.50	0.43
2:B:152:VAL:HG11	2:B:175:ALA:HB2	2.00	0.43
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.68	0.43
1:A:1576:GLU:HG2	1:A:1577:MET:N	2.34	0.43
1:A:1579:ILE:HD13	1:A:1579:ILE:HA	1.91	0.43
1:A:1753:ARG:HB3	1:A:1823:THR:OG1	2.19	0.43
1:A:1861:ARG:NH2	1:A:1863:HIS:HB2	2.33	0.43
2:B:116:GLN:O	2:B:116:GLN:HG3	2.19	0.43
1:A:76:VAL:CG2	1:A:1061:CYS:HB3	2.49	0.43
1:A:643:GLN:HB2	1:A:645:ARG:HG3	1.99	0.43
1:A:1926:ASP:OD1	1:A:1928:LYS:HG2	2.18	0.43
2:B:7:VAL:HB	2:B:78:PHE:CE1	2.53	0.43
2:B:28:PHE:HB2	2:B:31:GLU:OE2	2.19	0.43
1:A:960:PHE:HB3	1:A:965:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LEU:HA	1:A:1031:SER:HB3	1.99	0.43
1:A:1604:ALA:HB2	1:A:1619:CYS:HB2	1.99	0.43
1:A:397:THR:OG1	1:A:398:ALA:N	2.51	0.42
1:A:1246:SER:OG	1:A:1247:ALA:N	2.52	0.42
2:B:157:CYS:HB3	2:B:168:VAL:HG21	2.00	0.42
2:B:159:ALA:O	2:B:162:GLN:NE2	2.50	0.42
1:A:790:PRO:HD2	1:A:903:LEU:HD23	2.00	0.42
1:A:1446:LYS:HE3	1:A:1446:LYS:HB2	1.83	0.42
1:A:1458:LEU:HD23	1:A:1458:LEU:HA	1.91	0.42
1:A:1681:LEU:HD23	1:A:1681:LEU:HA	1.79	0.42
1:A:1826:GLU:N	1:A:1851:LEU:O	2.34	0.42
1:A:1932:MET:HE1	2:B:41:ALA:CB	2.49	0.42
2:B:6:CYS:N	2:B:54:GLY:O	2.50	0.42
1:A:552:TYR:HB2	1:A:712:THR:OG1	2.18	0.42
1:A:960:PHE:CB	1:A:965:LEU:HD11	2.49	0.42
1:A:1179:LEU:HD21	1:A:1253:LEU:HD23	2.01	0.42
1:A:1806:ASN:O	1:A:1808:VAL:HG23	2.20	0.42
1:A:1938:VAL:C	1:A:1940:PRO:HD3	2.44	0.42
2:B:68:ARG:NH1	2:B:69:PRO:HG3	2.34	0.42
2:B:150:LYS:HA	2:B:150:LYS:HD3	1.92	0.42
2:B:157:CYS:SG	2:B:165:LEU:HG	2.59	0.42
1:A:1176:LEU:HD12	1:A:1179:LEU:HD12	2.00	0.42
1:A:1529:LEU:HB3	1:A:1555:MET:CE	2.44	0.42
1:A:1926:ASP:HB3	1:A:1929:MET:HG2	2.00	0.42
2:B:90:PHE:CE1	2:B:145:LEU:HD23	2.54	0.42
1:A:395:ALA:HA	1:A:462:GLN:HB2	2.01	0.42
1:A:1296:GLU:OE2	1:A:1426:SER:HB2	2.20	0.42
1:A:1597:LEU:HD22	1:A:1678:PHE:HE2	1.85	0.42
1:A:1701:GLU:O	1:A:1705:GLU:HG2	2.19	0.42
1:A:1983:ASP:O	1:A:1987:LYS:HE2	2.19	0.42
1:A:116:TYR:CZ	1:A:778:HIS:NE2	2.87	0.42
1:A:393:PRO:CG	1:A:462:GLN:HG2	2.46	0.42
1:A:840:PHE:CD1	1:A:937:LEU:HD11	2.55	0.42
1:A:1630:TYR:CE2	1:A:1634:LEU:HD11	2.55	0.42
1:A:1866:LEU:O	1:A:1901:PRO:HB3	2.19	0.42
1:A:1878:THR:OG1	1:A:1880:HIS:O	2.35	0.42
1:A:280:ILE:HB	1:A:341:LYS:HB2	2.02	0.42
1:A:287:ARG:HH11	1:A:287:ARG:HB2	1.84	0.42
1:A:512:SER:HG	1:A:516:LEU:H	1.58	0.42
1:A:760:SER:O	1:A:764:LEU:HD12	2.20	0.42
1:A:959:ARG:C	1:A:960:PHE:HD1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:GLN:O	1:A:1495:ILE:HG22	2.19	0.42
1:A:1654:VAL:O	1:A:1657:GLU:HG2	2.20	0.42
1:A:1757:TYR:O	1:A:1819:TYR:N	2.49	0.42
2:B:138:THR:HG22	2:B:140:GLU:HG2	2.01	0.42
1:A:283:LEU:O	1:A:284:TYR:HD1	2.01	0.42
1:A:1037:LEU:HD12	1:A:1037:LEU:HA	1.65	0.42
1:A:1416:VAL:O	1:A:1420:VAL:HG23	2.20	0.42
1:A:1813:LEU:HD13	1:A:1819:TYR:CE1	2.54	0.42
1:A:1948:GLU:OE1	1:A:1948:GLU:N	2.43	0.42
1:A:268:LEU:HD23	1:A:301:ASN:HD22	1.85	0.42
1:A:386:ARG:NH2	1:A:641:SER:O	2.50	0.42
1:A:587:PRO:O	1:A:598:PHE:HB3	2.20	0.42
1:A:675:PRO:HB3	1:A:704:LYS:C	2.44	0.42
1:A:758:ARG:HG2	1:A:800:LEU:HD11	2.02	0.42
1:A:790:PRO:O	1:A:903:LEU:HD21	2.20	0.42
1:A:1711:ILE:O	1:A:1712:PRO:C	2.62	0.42
1:A:1814:ASP:HB2	1:A:1816:GLN:CD	2.45	0.42
1:A:1932:MET:HE3	2:B:39:ASN:O	2.20	0.42
2:B:29:PRO:HA	2:B:32:TYR:CD1	2.52	0.42
2:B:78:PHE:HB3	2:B:110:PHE:CB	2.50	0.42
1:A:1122:GLU:OE1	1:A:1124:GLU:HB2	2.20	0.41
1:A:1902:VAL:HG23	1:A:1970:LEU:HD12	2.02	0.41
1:A:1906:ILE:O	1:A:1910:GLN:NE2	2.53	0.41
1:A:1926:ASP:CG	1:A:1928:LYS:HG2	2.45	0.41
2:B:44:VAL:HG23	2:B:166:LYS:NZ	2.35	0.41
2:B:65:ASP:HA	2:B:68:ARG:NE	2.35	0.41
1:A:344:LYS:HE3	1:A:394:PHE:HA	2.03	0.41
1:A:776:SER:O	1:A:780:LEU:HG	2.20	0.41
1:A:1131:LEU:O	1:A:1132:HIS:C	2.63	0.41
1:A:1701:GLU:OE1	1:A:1701:GLU:N	2.34	0.41
1:A:320:THR:HB	1:A:594:SER:H	1.85	0.41
1:A:509:PHE:CZ	1:A:522:PRO:HG2	2.55	0.41
1:A:783:LEU:HD23	1:A:783:LEU:HA	1.86	0.41
1:A:927:ILE:O	1:A:930:HIS:N	2.49	0.41
1:A:1103:PHE:CZ	1:A:1167:PRO:HG2	2.55	0.41
1:A:1975:LYS:O	1:A:1979:LYS:HG2	2.20	0.41
1:A:106:ASP:H	1:A:109:VAL:HB	1.86	0.41
1:A:1677:HIS:C	1:A:1679:THR:H	2.28	0.41
1:A:1740:GLN:HG2	1:A:1746:ARG:HG2	2.02	0.41
1:A:1810:LYS:O	1:A:1810:LYS:HG2	2.20	0.41
1:A:1961:PRO:HA	1:A:1964:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:CD2	1:A:524:PRO:HB3	2.56	0.41
1:A:589:ILE:HG12	1:A:621:LEU:CD2	2.49	0.41
1:A:1021:TYR:HA	1:A:1024:VAL:HG12	2.02	0.41
1:A:282:ALA:HB2	1:A:295:ASN:HA	2.02	0.41
1:A:341:LYS:HE3	1:A:472:LEU:HD21	2.02	0.41
1:A:1040:LEU:HD23	1:A:1040:LEU:HA	1.77	0.41
1:A:1710:LEU:HG	1:A:1714:LEU:CD1	2.51	0.41
1:A:1926:ASP:OD2	1:A:1929:MET:HG2	2.21	0.41
1:A:76:VAL:HG21	1:A:1061:CYS:HB3	2.01	0.41
1:A:346:LEU:HG	1:A:347:GLN:N	2.36	0.41
1:A:1182:PHE:CE1	1:A:1294:ALA:HB2	2.56	0.41
1:A:1400:VAL:HA	1:A:1403:VAL:HG12	2.03	0.41
1:A:1740:GLN:HE21	1:A:1745:GLU:HB2	1.85	0.41
2:B:14:VAL:HB	2:B:83:SER:HB2	2.02	0.41
2:B:90:PHE:O	2:B:93:VAL:HB	2.21	0.41
1:A:386:ARG:CZ	1:A:644:PRO:HA	2.51	0.41
1:A:568:ARG:O	1:A:610:ASN:N	2.34	0.41
1:A:639:HIS:O	1:A:651:GLU:HA	2.20	0.41
1:A:1596:ARG:HH12	1:A:1600:LEU:HD21	1.86	0.41
1:A:1906:ILE:HG23	1:A:1910:GLN:NE2	2.33	0.41
1:A:1910:GLN:O	1:A:1914:ARG:HG3	2.21	0.41
2:B:117:ILE:HB	2:B:158:SER:OG	2.21	0.41
1:A:548:ARG:HG2	1:A:550:LEU:HD13	2.03	0.41
1:A:1059:LEU:HG	1:A:1062:CYS:HB2	2.01	0.41
1:A:1517:THR:HG23	1:A:1520:PHE:HB2	2.03	0.41
1:A:1593:PRO:O	1:A:1596:ARG:HB3	2.20	0.41
2:B:82:PHE:N	2:B:113:VAL:O	2.53	0.41
2:B:157:CYS:HB2	2:B:165:LEU:CD1	2.50	0.41
1:A:271:GLU:OE1	1:A:493:THR:OG1	2.33	0.41
1:A:1513:LEU:O	1:A:1517:THR:HG22	2.20	0.41
1:A:1967:HIS:O	1:A:1970:LEU:HB3	2.21	0.41
1:A:342:LEU:HB2	1:A:395:ALA:O	2.21	0.40
1:A:676:VAL:HG23	1:A:706:VAL:HG23	2.02	0.40
1:A:912:LEU:HD13	1:A:938:MET:HG2	2.02	0.40
1:A:938:MET:HE2	1:A:938:MET:HB3	1.83	0.40
1:A:987:VAL:HG13	1:A:988:GLU:N	2.36	0.40
1:A:1008:VAL:HG22	1:A:1009:ASP:N	2.36	0.40
1:A:1530:LYS:HD2	1:A:1533:LEU:HD12	2.03	0.40
1:A:1590:GLN:O	1:A:1590:GLN:HG3	2.21	0.40
1:A:1932:MET:HA	2:B:56:PHE:CE1	2.50	0.40
2:B:171:GLU:HA	2:B:174:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HA	1:A:393:PRO:HA	2.03	0.40
1:A:661:LEU:HD12	1:A:661:LEU:N	2.36	0.40
1:A:1533:LEU:CD2	1:A:1555:MET:HG3	2.51	0.40
1:A:1770:VAL:HG11	1:A:1850:PHE:HE2	1.84	0.40
1:A:1889:ILE:HG22	1:A:1890:ARG:O	2.21	0.40
1:A:554:TYR:HE2	1:A:618:GLU:CG	2.30	0.40
1:A:765:ARG:HG2	1:A:765:ARG:O	2.21	0.40
1:A:1097:PHE:HZ	1:A:1268:LEU:HG	1.87	0.40
1:A:1534:THR:O	1:A:1538:GLU:HB2	2.21	0.40
1:A:1539:ASP:OD2	1:A:1542:LEU:N	2.37	0.40
1:A:1576:GLU:HG2	1:A:1577:MET:H	1.87	0.40
1:A:1736:LYS:HA	1:A:1739:HIS:ND1	2.36	0.40
1:A:1820:ILE:O	1:A:1822:ILE:HD12	2.21	0.40
2:B:65:ASP:HA	2:B:68:ARG:HE	1.85	0.40
1:A:577:MET:O	1:A:632:HIS:N	2.43	0.40
1:A:672:PHE:HB3	1:A:674:LEU:CD2	2.52	0.40
1:A:1289:TYR:HE1	1:A:1422:TYR:CG	2.39	0.40
1:A:1479:THR:O	1:A:1482:SER:OG	2.28	0.40
1:A:1845:TYR:H	1:A:1847:LEU:HD21	1.86	0.40
1:A:1931:GLN:HG3	1:A:1999:TYR:HE2	1.86	0.40
2:B:4:ILE:O	2:B:54:GLY:N	2.49	0.40
1:A:287:ARG:HB2	1:A:287:ARG:NH1	2.36	0.40
1:A:513:PRO:HG3	1:A:531:GLU:C	2.47	0.40
1:A:912:LEU:O	1:A:916:TRP:HB2	2.20	0.40
1:A:1589:TYR:C	1:A:1591:GLY:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1672/2053 (81%)	1514 (91%)	158 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	176/195 (90%)	155 (88%)	21 (12%)	0	100	100
All	All	1848/2248 (82%)	1669 (90%)	179 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1476/1773 (83%)	1476 (100%)	0	100	100
2	B	158/172 (92%)	158 (100%)	0	100	100
All	All	1634/1945 (84%)	1634 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1383	ASN
1	A	1492	ASN
1	A	1602	ASN
1	A	1607	HIS
1	A	1648	GLN
1	A	1767	GLN
1	A	1863	HIS
1	A	1910	GLN
1	A	1943	ASN
1	A	1967	HIS
1	A	1996	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

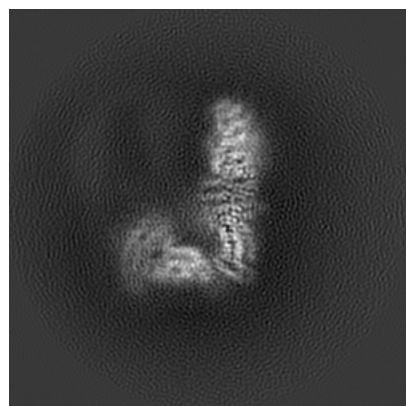
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65174. These allow visual inspection of the internal detail of the map and identification of artifacts.

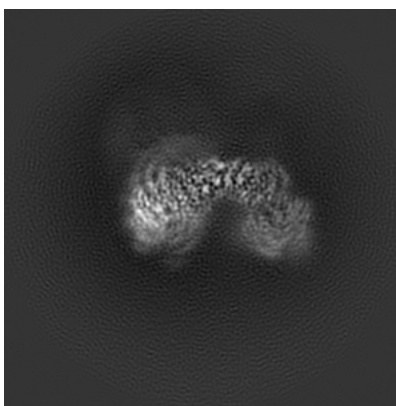
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

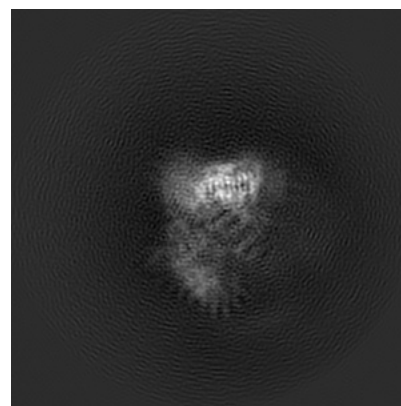
6.1.1 Primary map



X



Y

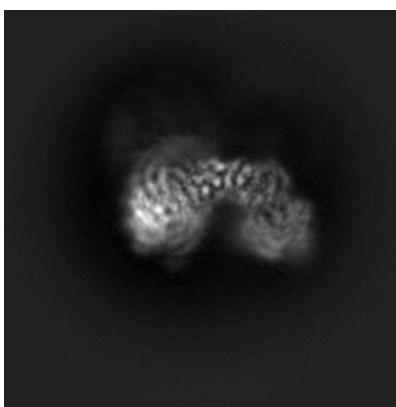


Z

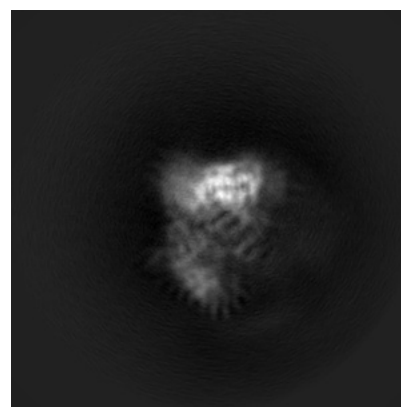
6.1.2 Raw map



X



Y

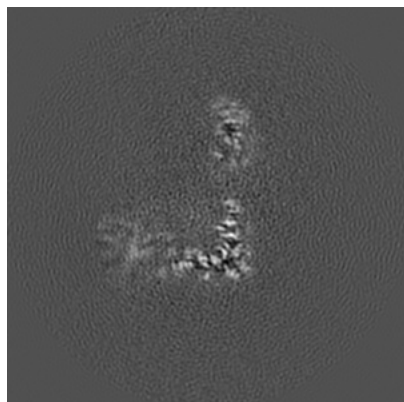


Z

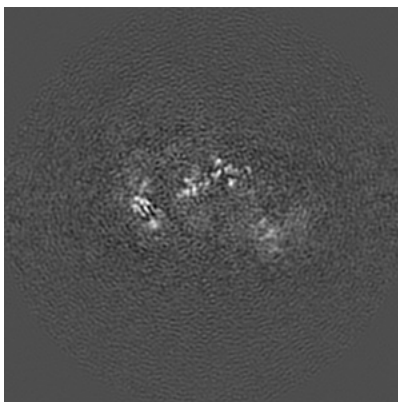
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

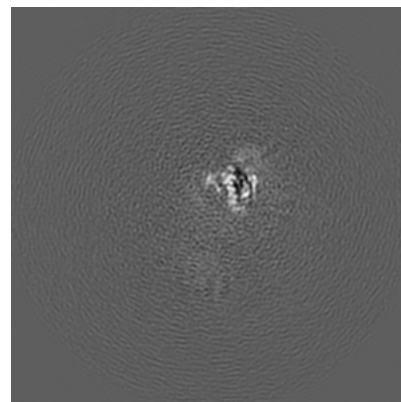
6.2.1 Primary map



X Index: 120

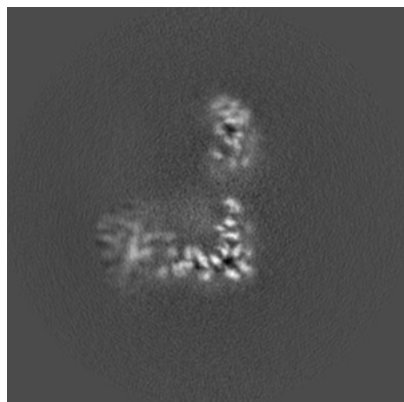


Y Index: 120

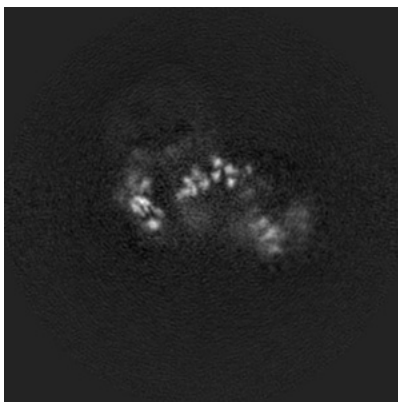


Z Index: 120

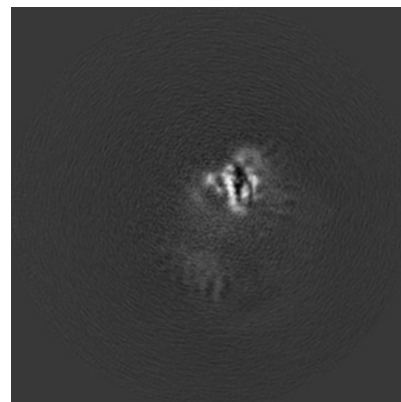
6.2.2 Raw map



X Index: 120



Y Index: 120

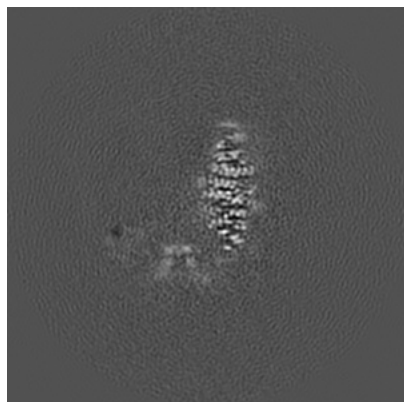


Z Index: 120

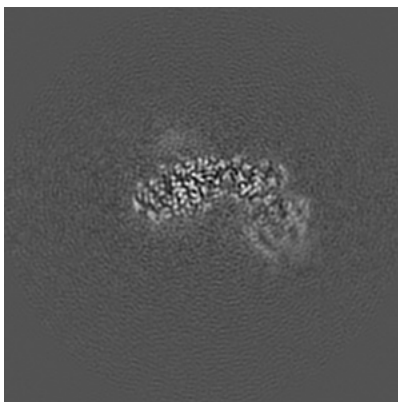
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

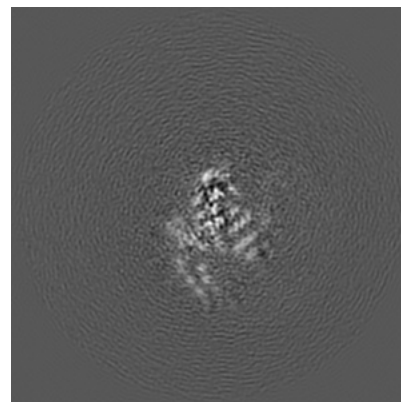
6.3.1 Primary map



X Index: 137

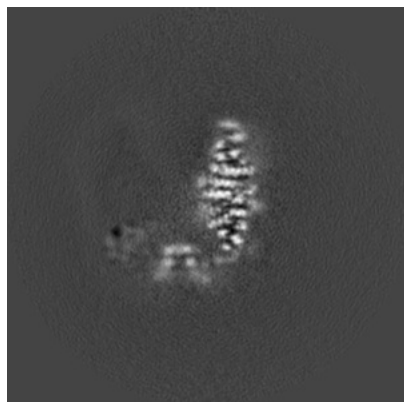


Y Index: 135

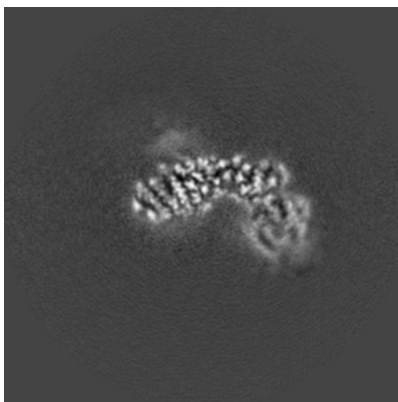


Z Index: 86

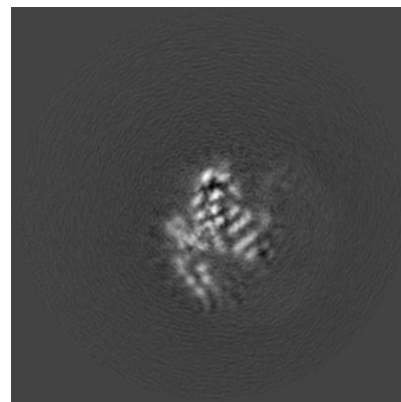
6.3.2 Raw map



X Index: 137



Y Index: 135

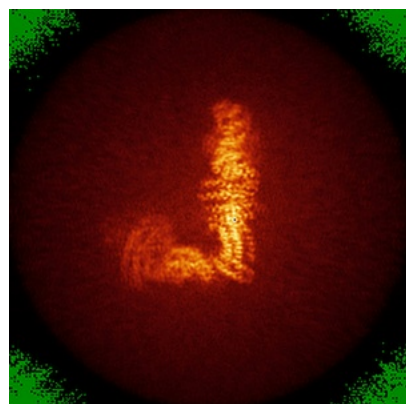


Z Index: 86

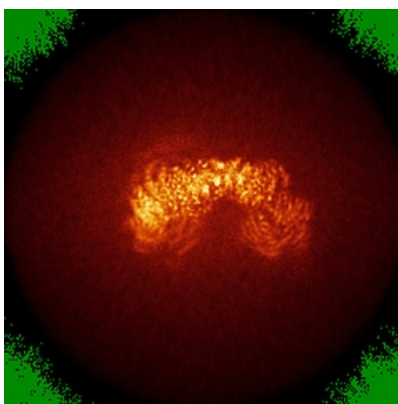
The images above show the largest variance slices of the map in three orthogonal directions.

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

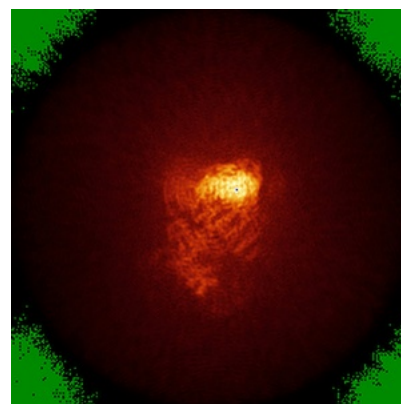
6.4.1 Primary map



X



Y

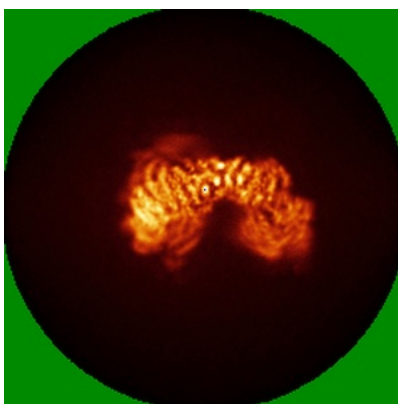


Z

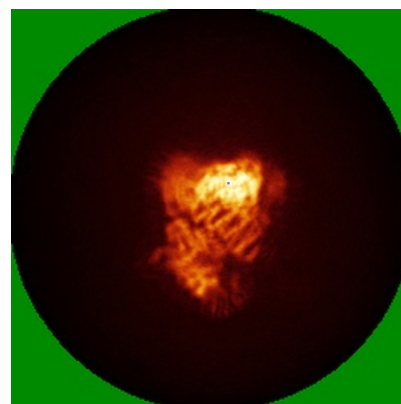
6.4.2 Raw map



X



Y

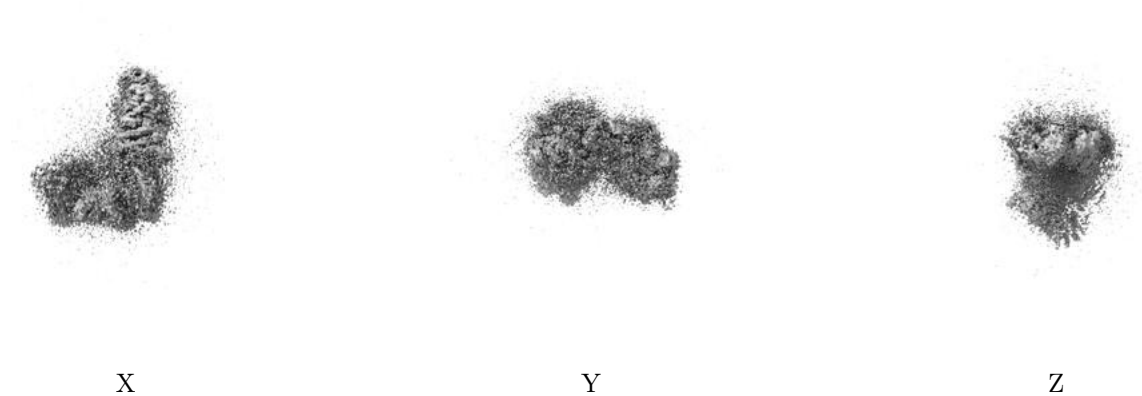


Z

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.

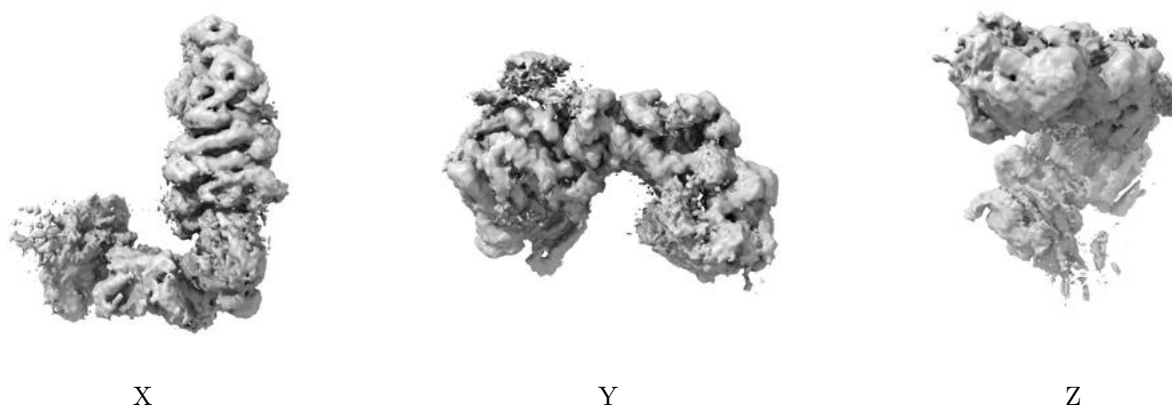
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

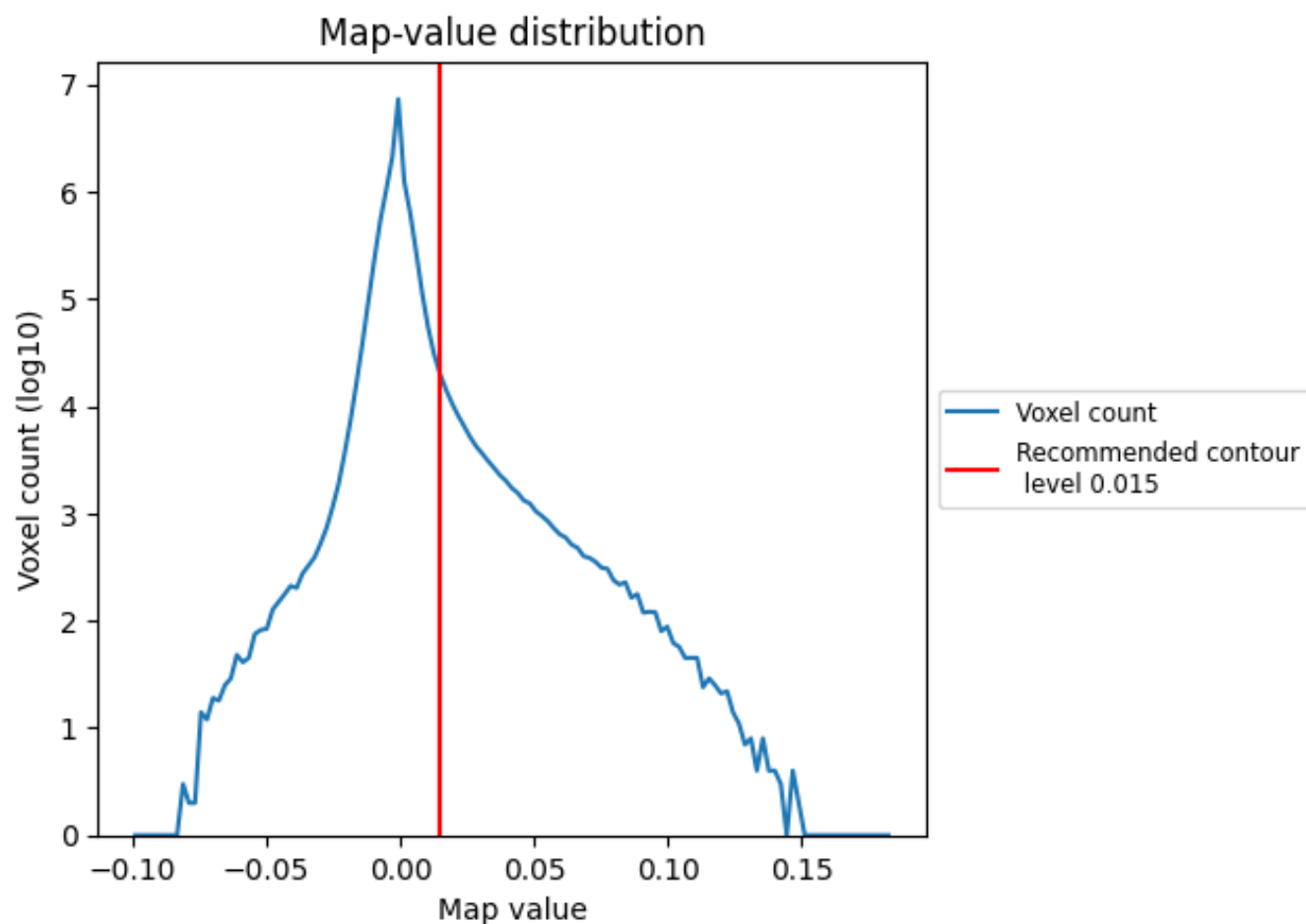
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

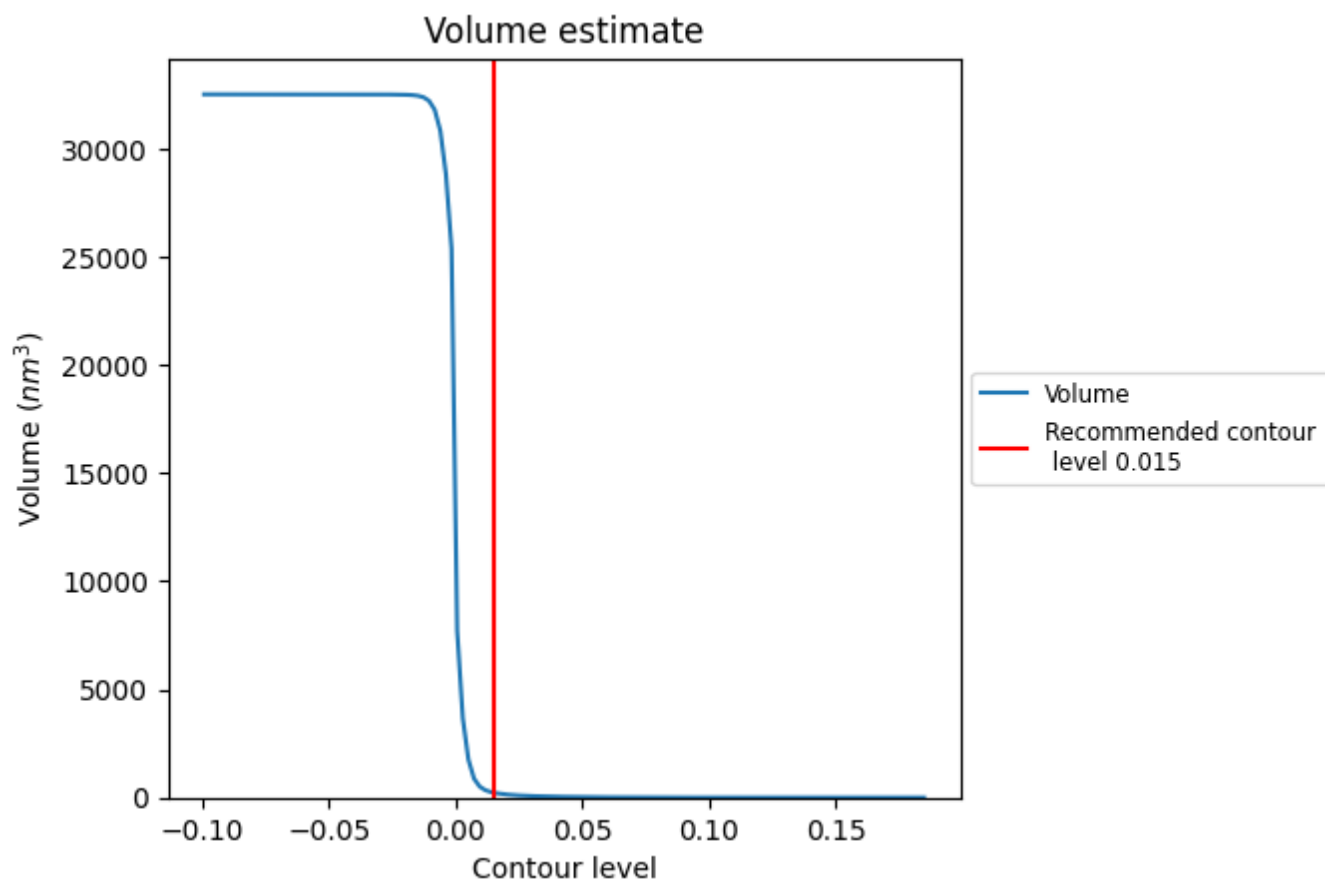
This section contains the results of statistical analysis of the map.

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.

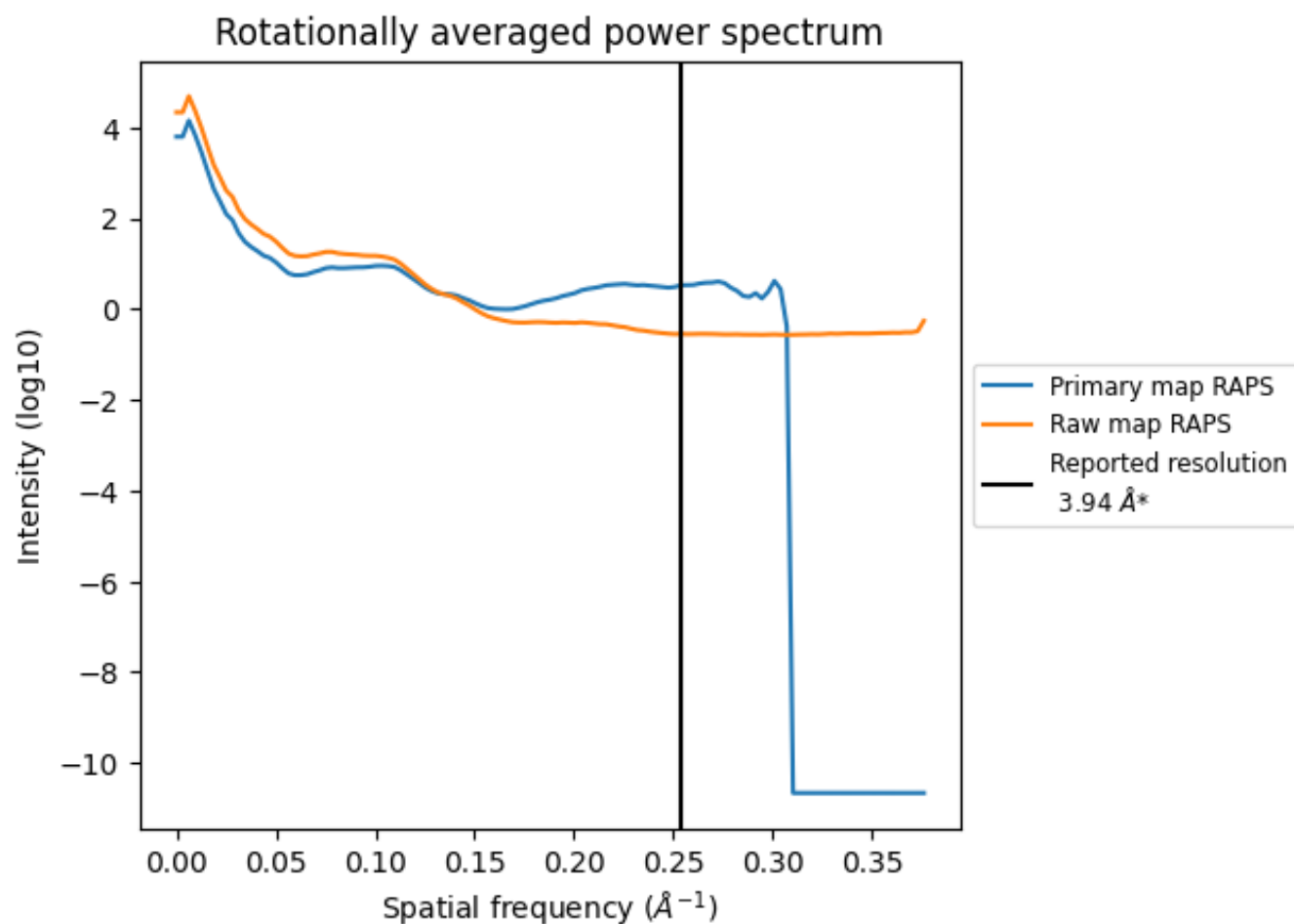
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm³; this corresponds to an approximate mass of 209 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 ⓘ

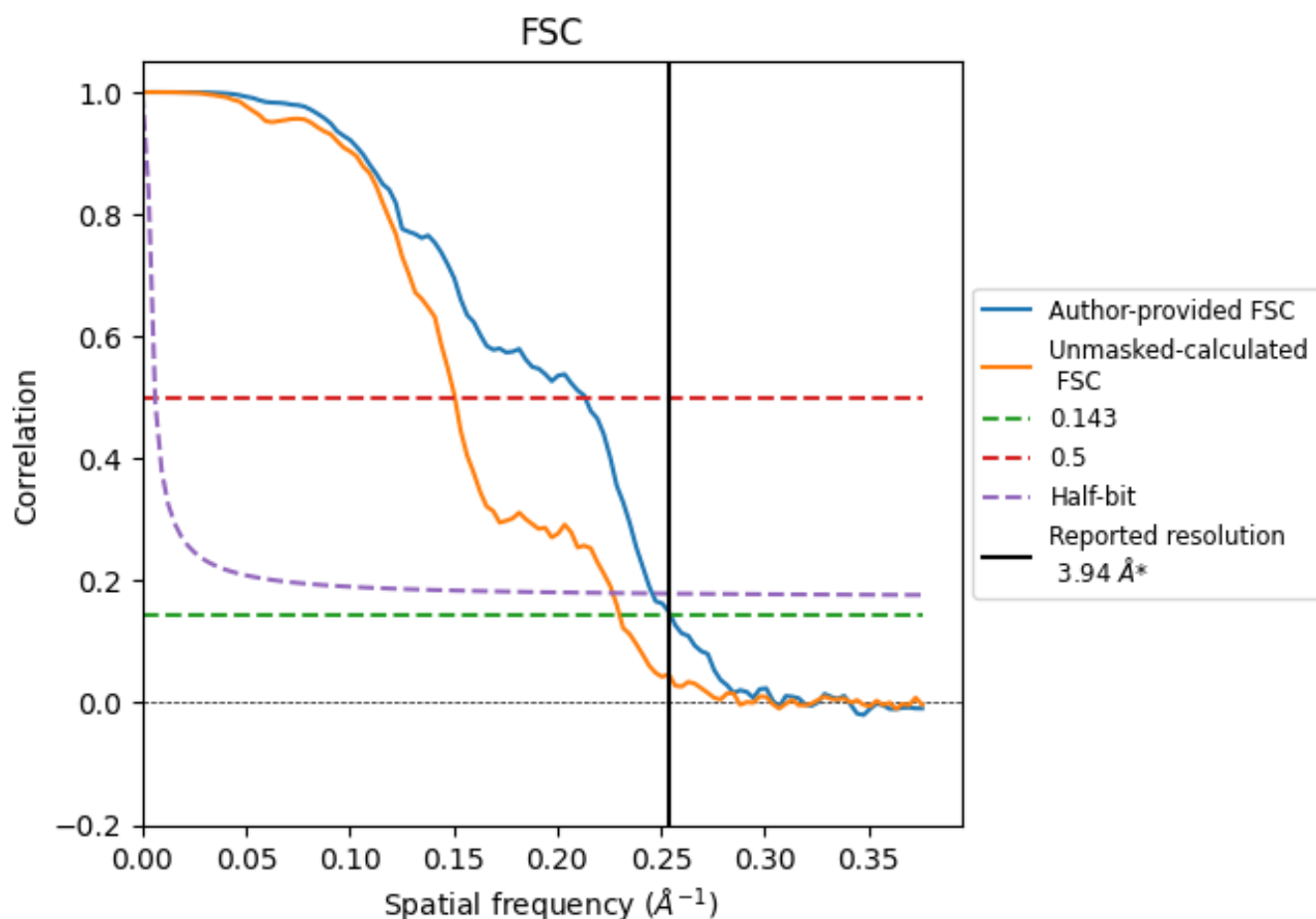


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

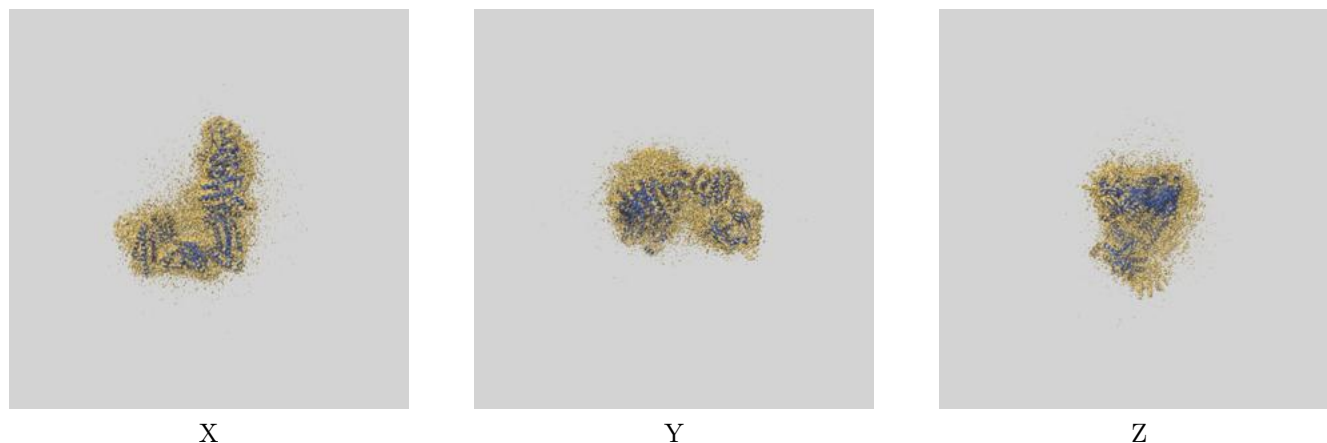
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	3.93	4.69	4.07
Unmasked-calculated*	4.35	6.64	4.41

*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 4.35 differs from the reported value 3.94 by more than 10 %

9 Map-model fit [i](#)

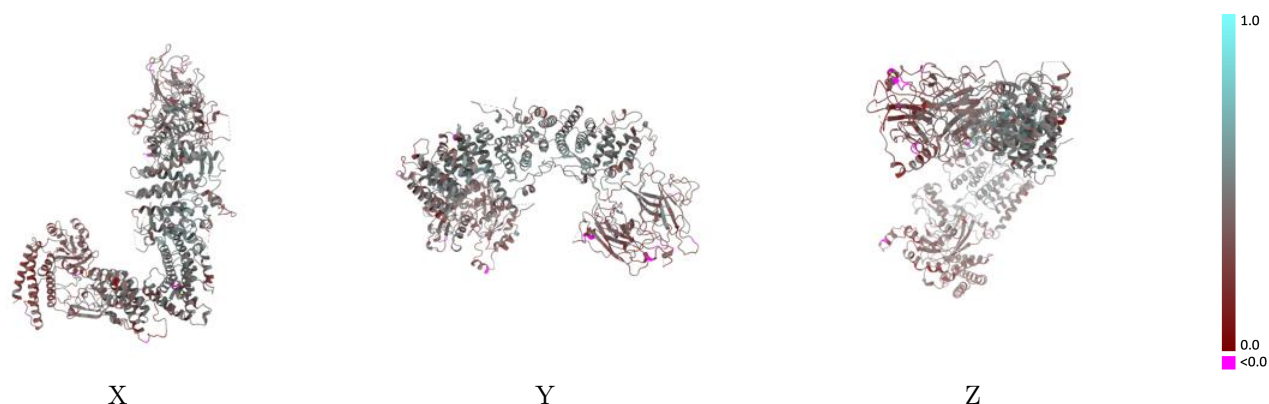
This section contains information regarding the fit between EMDB map EMD-65174 and PDB model 9VM2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



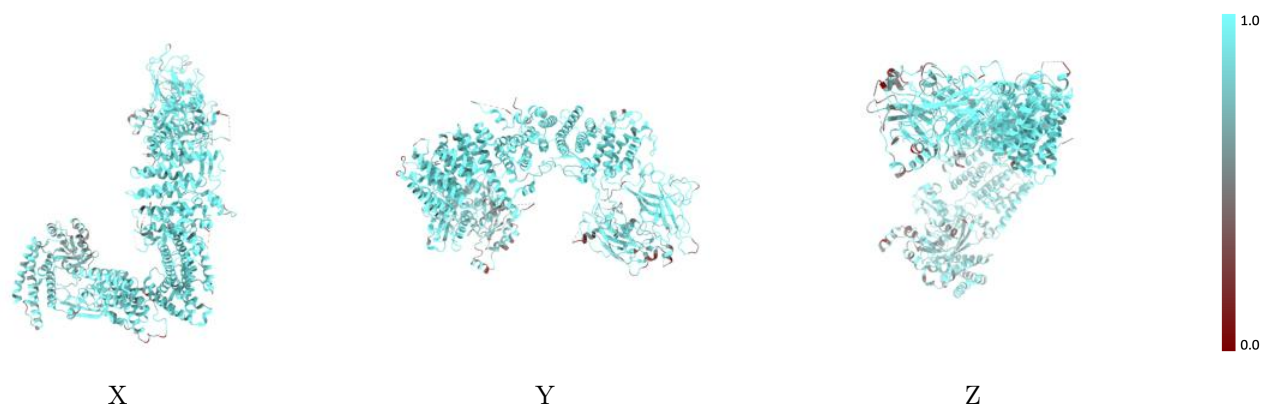
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



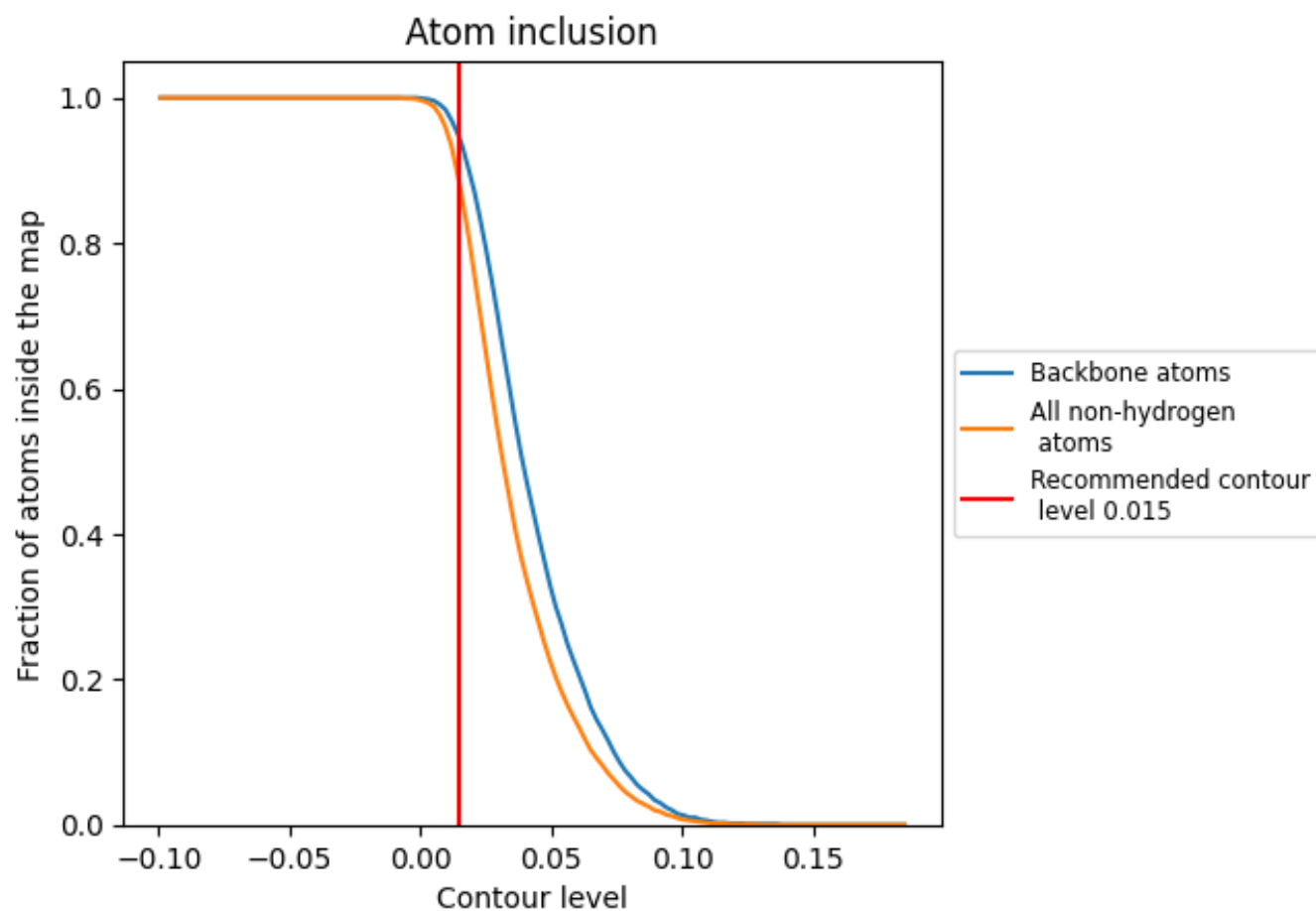
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8820	<div></div> 0.4050
A	<div></div> 0.8980	<div></div> 0.4140
B	<div></div> 0.7230	<div></div> 0.3180

