



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:17 AM UTC

PDB ID : 8VDR / pdb_00008vdr
EMDB ID : EMD-43156
Title : Cryogenic electron microscopy model of full-length talin without R12 and FABD
Authors : Izard, T.; Rangarajan, E.S.
Deposited on : 2023-12-17
Resolution : 3.70 Å(reported)
Based on initial model : 6r9t

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 EMD 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

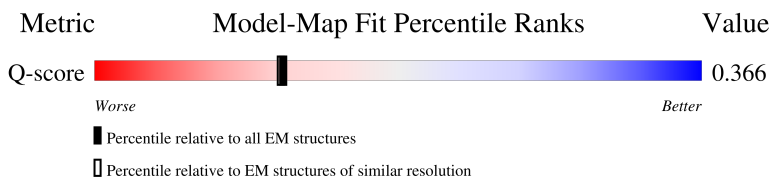
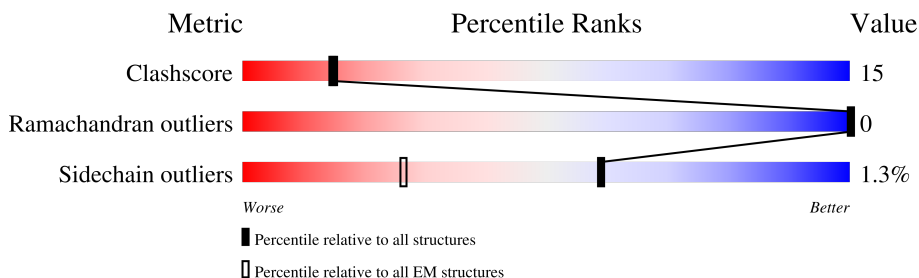
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

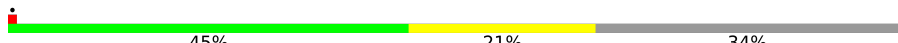
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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	2804	 45% 21% 34%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13547 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 Green fluorescent protein, Talin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1852	Total	C	N	O	S	0	0
			13547	8340	2412	2729	66		

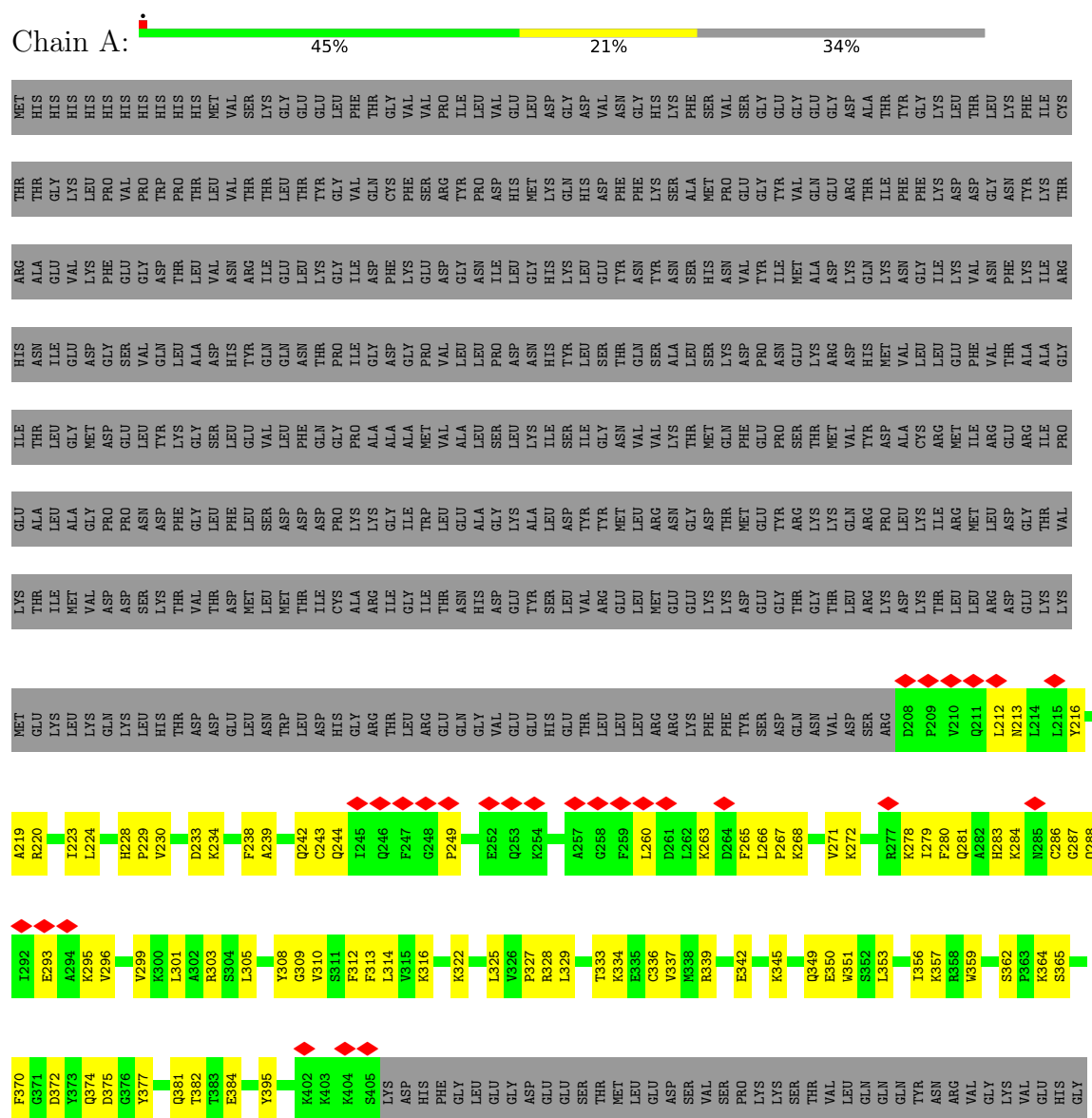
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	LEU	GLN	conflict	UNP P26039
A	673	ASN	LYS	conflict	UNP P26039
A	1227	LEU	SER	conflict	UNP P26039
A	2349	VAL	ALA	conflict	UNP P26039

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: Green fluorescent protein,Talin-1



K2024	A1900	Q1758	P1627	C1509	D1386	F1278	E1180	L1079	L917	T772	N673	I543	SER
V2025	K1901	T1778	P1628	A1512	M1387	L1282	R1184	P1080	E918	Q776	A674	I543	VAL
L2026	P1902		R1629	A1512	S1388	E1283	R1185	G1081	H919	Q777	V675	I543	ALA
	A1903		W1630	T1516	Y1389	E1283	A1186	G1082	E919	A776	A676	Q546	LEU
T2030	E1908	A1782	V1632	R1523	G1391	V1286	A1189	T1083	T929	L778	S677	V547	PRO
V2032	M1909	N1785	L1633	R1523	C1391	E1287	A1189	M1084		N779	A678	D548	ALA
L2033	H1918	Q1788	H1636	Q1527	S1395	E1287	A1189	E1085		E780	A679	A549	ILE
V2034	R1919	A1789	S1637	Q1527	V1396	M1288	A1195	E1086	I932	L781	V683	I550	MET
Q2035	R1920	A1790	R1638	V1532	E1397	A1289	A1195	C1087	A933	L782	L684	T551	ARG
N2036	V1920	A1790	V1632	V1532	E1398	Q1291	R1198	C1088	A935	H784			SER
A2037	Q1921	H1791	V1632	V1532	E1399	A1292	R1198	Q1089	Q936				GLY
	E1922	T1792	D1642	S1535	M1399	A1292	S1201	D1090		K786	K687	T554	ALA
Q2046	L1923	Q1793	S1643	T1536	E1405	S1293	G1202	S1094	A939	A787	S688	D569	SER
A2047	G1924		I1644	T1536	A1406	P1294	L1203		S940	H788	V689	Y570	GLY
A2048	M1802	M1802	K1645	T1542	M1407	Q1295	P1204		A941		A690	T571	PRO
Q2049	M1803	M1803		I1543	T1408	E1296	G1205	A1101	P942	Q800	Q691	A572	GLU
S2050	C1927		E1660	I1544	G1409	D1297	Q1206		K943	A801	R692	V573	ASN
S2051	V1931	V1807		A1545	I1410	R1298	R1207	K1104		T802	F694	G574	PHE
V2052	L1937	L1814	L1668	F1550	K1415	Q1300	D1208		P948	I805	D695	C575	GLN
A2053	T1946	E1816	D1676	T1551	N1418	V1301	V1209	E1108				A576	VAL
T2054	T1946	E1816		E1552	M1418	V1302	D1210	I1109	L951			V577	GLY
R2057	V1961	S1819	S1679	E1553	L1419	S1303	L1213	G1111	C956	F813	Q699	S581	SER
V2062	V1964	V1824	V1683	N1554	P1420	R1214	L1213	G1112		L829	Q701	L584	PRO
G2065	L1968	G1825	S1684	R1555	A1425	K1306	R1215	N1113	Q968	L836	V702	T585	ALA
A2066		G1826	Q1686	Q1557	A1425	K1306	V1216	E1114	L986		A704	E586	GLN
D2073	T1975	D1829	P1689	R1559	A1429	M1310	S1220	Y1116	Q991	I840	T707	S588	GLN
P2074	Q1976	S1830	T1562	F1436	F1437	K1314	R1221	L1128	R854	Q708	C709	L593	THR
E2075	A1977	I1831	I1693	T1437	T1437	L1316	R1222	R136	R855	A710	L597	L598	SER
T2076	C1978	V1835	L1698	A1440	A1440	L1317	L1224	G1137	Q995	S858	T712	L598	GLY
Q2077	I1979	I1835	L1698	L1446	L1446	K1332	S1225	V1138	L1020	L863	S714	E601	MET
V2078			L1566	Q1455	Q1455	S1333	L1227	A1140	K1025	Q715	V619		HIS
V2079	I1989	L1838	M1702	Q1455	Q1455	A1338	L1228	L1141	L1031	T867	V723	Q627	GLY
L2080	A1990	V1851	S1710	Q1458	Q1458	A1338	P1229	T1142	L1031	A868	T727	Q627	HIS
T2081	D1991	D1852	I1713	Q1459	Q1459	N1347	T1234	D1144	R1035	V871	I727	R634	ALA
A2083	M1997	Y1853	S1583	Q1459	Q1459	Q1348	F1235	V1147	Q1039	R889	S728	L637	LEU
V2084	F1998	Q1854	S1583	Q1472	Q1472	T1351	Q1236	Q1148	K1040	S729	L651	L652	VAL
K2085	G2002	M1857	S1725	Q1472	Q1472	M1352	E1237	V1147	Q1039	V373	I655	I655	GLY
D2086	R2006	A1863	G1728	Q1475	Q1475	C1353	R1241	D1157	A1041	R741	G856	G856	ALA
V2087	M2006	I1864	Q1733	M1476	M1476	Q1353	R1241	V1158	A1041	R741	G856	G856	LEU
A2088	E2010	A1865	M1734	A1477	A1477	C1353	R1241	L1159	Q1042	A753	S657	S657	ILE
L2091	T2011	V1866	A1735	C1478	C1478	Q1360	E1244	D1160	E1043	A753	D659	D659	VAL
G2092	F2012	V1866	Q1736	S1480	S1480	N1365	E1244	K1161	A1044	A753	T660	T660	GLY
T2095	A2013	L1882	Q1736	G1611	G1611	R1368	T1254	D1157	L1048	N807	D760	Q665	ALA
K2099	D2014	A1886	E1739	L1612	L1612	R1368	E1255	V1158	D1051	A900	C761	Q665	LEU
R2016	H2015	I1614	P1740	L1613	L1613	V1373	L1256	D1160	D1051	A900	C761	Q665	VAL
E2017	Q2016	Q1615	Q1615	Q1485	Q1485	R1374	Q1258	K1161	S1055	N807	D760	Q665	GLY
A2102	E2017	L1899	A1744	C1486	C1486	E1375	A1259	K1161	S1055	N807	D760	Q665	ALA
		T1890		T1487	T1487	V1375	A1259	K1161	S1055	N807	D760	Q665	LEU
D2108	L2020	A1748	A1748	Q1488	Q1488	V1381	R1261	A1169	K1068	A908	C761	Q665	VAL
P2109	K2021	Y1893	S1750	Q1488	Q1488	V1381	R1261	K1170	A1069	Y909	C761	Q665	GLY
A2110	T2022	Q1899		Q1490	Q1490	T1384	L1267	S1173	A1070	K911	L671	L671	ALA
V2111	A2023			Q1490	Q1490	T1384	L1267	S1173	L1076	K912	L671	L671	VAL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.273	Depositor
Minimum map value	-0.684	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.124	Depositor
Map size (Å)	368.64, 368.64, 368.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44, 1.44, 1.44	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	0.32	0/13699	0.53	3/18572 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1582	SER	N-CA-C	6.73	119.30	109.07
1	A	1583	SER	N-CA-C	6.12	122.39	113.40
1	A	1581	PHE	N-CA-C	5.60	117.38	111.28

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	13547	0	13649	409	0
All	All	13547	0	13649	409	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 15.

All (409) 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:1373:VAL:HB	1:A:1437:THR:HG21	1.55	0.85
1:A:1147:VAL:HG13	1:A:1204:PRO:HG2	1.59	0.84
1:A:783:GLN:HE22	1:A:786:LYS:HE2	1.44	0.82
1:A:522:LEU:HD11	1:A:1080:PRO:HD3	1.63	0.79
1:A:1304:ASN:ND2	1:A:1353:CYS:SG	2.55	0.79
1:A:1613:LEU:HD13	1:A:1636:HIS:HB2	1.68	0.75
1:A:244:GLN:NE2	1:A:287:GLY:O	2.20	0.74
1:A:1306:LYS:HB3	1:A:1310:MET:HE1	1.71	0.72
1:A:534:ASN:ND2	1:A:968:GLN:OE1	2.23	0.71
1:A:760:ASP:HB3	1:A:762:GLN:HG2	1.73	0.70
1:A:1086:LYS:O	1:A:1089:GLN:NE2	2.24	0.70
1:A:333:THR:HB	1:A:336:CYS:H	1.56	0.69
1:A:322:LYS:HD3	1:A:1802:MET:HG2	1.74	0.69
1:A:932:ILE:HG13	1:A:956:CYS:SG	2.33	0.69
1:A:1713:ILE:HG12	1:A:1803:MET:HE3	1.72	0.69
1:A:1084:MET:HE1	1:A:1138:VAL:HG13	1.75	0.68
1:A:1484:PRO:HA	1:A:1559:ARG:HH21	1.58	0.68
1:A:1207:ARG:HE	1:A:1208:ASP:H	1.39	0.68
1:A:1113:ASN:ND2	1:A:1173:SER:O	2.26	0.68
1:A:281:GLN:HA	1:A:284:LYS:HE2	1.76	0.67
1:A:1261:ARG:NH2	1:A:1375:GLU:OE1	2.27	0.67
1:A:2017:GLU:HG3	1:A:2021:LYS:HZ3	1.58	0.66
1:A:1485:GLY:O	1:A:1490:GLN:NE2	2.28	0.66
1:A:357:LYS:NZ	1:A:370:PHE:O	2.21	0.66
1:A:2006:ARG:NH2	1:A:2010:GLU:O	2.28	0.66
1:A:2046:GLN:O	1:A:2050:SER:N	2.25	0.65
1:A:365:SER:HA	1:A:381:GLN:HA	1.78	0.64
1:A:2108:ASP:HB3	1:A:2111:VAL:HG13	1.79	0.64
1:A:1886:ALA:HB1	1:A:1931:VAL:HG13	1.78	0.64
1:A:279:ILE:O	1:A:283:HIS:ND1	2.31	0.63
1:A:760:ASP:OD1	1:A:761:GLY:N	2.30	0.63
1:A:1562:THR:HG22	1:A:1566:LEU:HD23	1.80	0.63
1:A:1826:GLY:HA2	1:A:1829:ASP:HB3	1.79	0.63
1:A:1550:PHE:O	1:A:1555:ARG:NH1	2.31	0.63
1:A:1180:GLU:OE1	1:A:1184:ARG:NE	2.29	0.63
1:A:1857:MET:HE1	1:A:1900:ALA:HA	1.81	0.63
1:A:1486:CYS:HA	1:A:1490:GLN:HE21	1.64	0.63
1:A:1259:ALA:HB1	1:A:1267:LEU:HA	1.80	0.63
1:A:279:ILE:HG22	1:A:283:HIS:CE1	2.33	0.62
1:A:1223:LEU:HD12	1:A:1227:LEU:HD11	1.81	0.62
1:A:1235:PHE:HD2	1:A:1291:GLN:HG3	1.64	0.62
1:A:1975:THR:HG22	1:A:1977:ALA:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1613:LEU:HD11	1:A:1633:LEU:HD12	1.81	0.62
1:A:329:LEU:HD13	1:A:342:GLU:HA	1.80	0.62
1:A:543:ILE:HD11	1:A:587:MET:HG3	1.81	0.62
1:A:299:VAL:O	1:A:303:ARG:HG2	2.00	0.61
1:A:547:VAL:HG21	1:A:652:LEU:HD21	1.81	0.61
1:A:929:THR:HA	1:A:932:ILE:HG22	1.81	0.61
1:A:889:ARG:NH1	1:A:892:GLU:OE2	2.32	0.61
1:A:1488:GLN:HG2	1:A:1550:PHE:HZ	1.66	0.61
1:A:1542:THR:HG23	1:A:1557:GLN:HG3	1.83	0.61
1:A:220:ARG:NH1	1:A:242:GLN:HG2	2.16	0.61
1:A:377:TYR:N	1:A:1676:ASP:OD2	2.32	0.60
1:A:2066:ALA:O	1:A:2077:GLN:NE2	2.29	0.60
1:A:1070:ALA:HB1	1:A:1076:LEU:HD21	1.83	0.59
1:A:802:THR:HG21	1:A:908:ALA:HB3	1.85	0.59
1:A:671:LEU:HB3	1:A:780:GLU:HG2	1.84	0.59
1:A:673:ASN:O	1:A:677:SER:N	2.32	0.59
1:A:1090:ASP:O	1:A:1094:SER:N	2.34	0.59
1:A:2032:VAL:HA	1:A:2035:GLN:HG2	1.85	0.58
1:A:310:VAL:HG23	1:A:312:PHE:CE2	2.38	0.58
1:A:729:SER:OG	1:A:732:CYS:SG	2.53	0.58
1:A:1486:CYS:HB2	1:A:1555:ARG:HD2	1.84	0.58
1:A:1390:PHE:HD2	1:A:1785:ASN:HA	1.69	0.58
1:A:1475:GLN:HE22	1:A:1476:MET:HE3	1.67	0.58
1:A:574:GLY:HA2	1:A:577:VAL:HG22	1.86	0.58
1:A:1458:GLN:O	1:A:1459:GLN:HG2	2.04	0.58
1:A:1472:GLN:HA	1:A:1475:GLN:HE21	1.69	0.57
1:A:517:GLU:OE1	1:A:518:THR:OG1	2.18	0.57
1:A:584:LEU:HD22	1:A:619:VAL:HG11	1.84	0.57
1:A:723:VAL:HG13	1:A:732:CYS:HB3	1.87	0.57
1:A:1620:LEU:HD11	1:A:1629:ARG:HB3	1.86	0.57
1:A:1710:SER:HB2	1:A:1807:VAL:HG11	1.85	0.57
1:A:1977:ALA:HB1	1:A:2048:ALA:HB3	1.87	0.56
1:A:2034:VAL:HB	1:A:2114:LEU:HD21	1.86	0.56
1:A:733:GLN:OE1	1:A:788:HIS:ND1	2.38	0.56
1:A:863:LEU:O	1:A:867:THR:N	2.30	0.56
1:A:1509:CYS:SG	1:A:1572:LEU:HD11	2.45	0.56
1:A:1304:ASN:OD1	1:A:1348:GLN:NE2	2.32	0.56
1:A:1387:MET:HE1	1:A:1391:GLY:C	2.31	0.56
1:A:1082:GLU:OE1	1:A:1082:GLU:N	2.38	0.56
1:A:2054:THR:HA	1:A:2057:ARG:HH11	1.70	0.56
1:A:1347:ASN:O	1:A:1351:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:VAL:O	1:A:741:ARG:N	2.33	0.55
1:A:829:LEU:HD21	1:A:897:LEU:HD21	1.87	0.55
1:A:1488:GLN:HG2	1:A:1550:PHE:CZ	2.41	0.55
1:A:1554:ASN:OD1	1:A:1557:GLN:NE2	2.40	0.55
1:A:1302:VAL:O	1:A:1306:LYS:N	2.35	0.55
1:A:1365:ASN:OD1	1:A:1368:ARG:NH1	2.39	0.55
1:A:336:CYS:SG	1:A:350:GLU:HG2	2.46	0.55
1:A:1606:MET:HE2	1:A:1644:ILE:HD11	1.89	0.55
1:A:2017:GLU:HG3	1:A:2021:LYS:NZ	2.20	0.55
1:A:1201:SER:HA	1:A:1206:GLN:HE22	1.72	0.55
1:A:991:GLN:NE2	1:A:1042:GLN:OE1	2.39	0.55
1:A:249:PRO:HB3	1:A:288:GLN:HB3	1.89	0.54
1:A:1816:GLU:O	1:A:1819:SER:OG	2.24	0.54
1:A:308:TYR:CD1	1:A:309:GLY:N	2.76	0.54
1:A:729:SER:HG	1:A:732:CYS:HG	1.47	0.54
1:A:1260:SER:HA	1:A:1267:LEU:HD12	1.89	0.54
1:A:506:VAL:HG22	1:A:584:LEU:HD23	1.90	0.54
1:A:2062:VAL:HG11	1:A:2084:VAL:HG11	1.88	0.54
1:A:293:GLU:HA	1:A:296:VAL:HG12	1.90	0.54
1:A:1088:THR:HG22	1:A:1203:LEU:HD11	1.90	0.54
1:A:1835:ILE:HD11	1:A:1924:GLY:HA3	1.89	0.54
1:A:855:LYS:HA	1:A:858:SER:HB3	1.89	0.53
1:A:242:GLN:NE2	1:A:265:PHE:O	2.41	0.53
1:A:543:ILE:CD1	1:A:587:MET:HG3	2.38	0.53
1:A:2108:ASP:O	1:A:2111:VAL:HG22	2.09	0.53
1:A:1476:MET:HE2	1:A:1476:MET:HA	1.90	0.53
1:A:296:VAL:HA	1:A:299:VAL:HG12	1.90	0.53
1:A:1660:GLU:OE2	1:A:1728:GLY:HA2	2.09	0.53
1:A:1216:VAL:HG22	1:A:1278:PHE:CD2	2.43	0.53
1:A:781:LEU:O	1:A:784:HIS:HB3	2.08	0.53
1:A:1989:ILE:HD11	1:A:2088:ALA:HB3	1.90	0.53
1:A:1293:PRO:O	1:A:1295:GLN:NE2	2.39	0.53
1:A:325:LEU:HD22	1:A:381:GLN:HE22	1.74	0.53
1:A:1223:LEU:HA	1:A:1227:LEU:HD21	1.91	0.53
1:A:1111:GLN:OE1	1:A:1523:ARG:NH1	2.42	0.52
1:A:1396:VAL:HG13	1:A:1436:PHE:CE1	2.44	0.52
1:A:729:SER:O	1:A:733:GLN:NE2	2.43	0.52
1:A:1111:GLN:HG3	1:A:1527:GLN:HG3	1.90	0.52
1:A:1405:GLU:O	1:A:1408:THR:OG1	2.21	0.52
1:A:1144:ASP:HB3	1:A:1147:VAL:HB	1.91	0.52
1:A:1300:GLN:HG3	1:A:1304:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:GLU:OE2	1:A:601:GLU:N	2.43	0.52
1:A:690:ALA:O	1:A:693:THR:OG1	2.26	0.52
1:A:1254:THR:O	1:A:1258:GLN:NE2	2.40	0.52
1:A:502:SER:HB2	1:A:581:SER:HB3	1.92	0.51
1:A:1142:THR:HG23	1:A:1148:GLN:HG2	1.92	0.51
1:A:1186:ALA:HA	1:A:1189:ALA:HB3	1.91	0.51
1:A:2011:THR:O	1:A:2015:HIS:NE2	2.43	0.51
1:A:1301:VAL:HA	1:A:1304:ASN:HD22	1.74	0.51
1:A:896:GLY:O	1:A:900:ALA:N	2.41	0.51
1:A:2014:ASP:OD1	1:A:2015:HIS:N	2.44	0.51
1:A:1749:ALA:HB1	1:A:1758:GLN:HB2	1.93	0.51
1:A:313:PHE:HB3	1:A:384:GLU:OE2	2.10	0.51
1:A:522:LEU:HD21	1:A:1080:PRO:HG3	1.91	0.51
1:A:1288:MET:HA	1:A:1291:GLN:HB2	1.93	0.51
1:A:1415:LYS:HG3	1:A:1630:TRP:CH2	2.46	0.51
1:A:1388:SER:OG	1:A:1389:TYR:N	2.44	0.50
1:A:228:HIS:HE1	1:A:305:LEU:HD23	1.77	0.50
1:A:569:ASP:OD1	1:A:571:THR:OG1	2.22	0.50
1:A:1532:VAL:O	1:A:1536:THR:N	2.37	0.50
1:A:1610:ALA:O	1:A:1614:ILE:HG12	2.11	0.50
1:A:1170:LYS:O	1:A:1173:SER:OG	2.26	0.50
1:A:2080:LEU:HD11	1:A:2135:VAL:HG11	1.93	0.50
1:A:233:ASP:HA	1:A:278:LYS:NZ	2.26	0.50
1:A:800:GLN:N	1:A:800:GLN:OE1	2.39	0.50
1:A:1702:MET:HG2	1:A:1814:LEU:HD21	1.94	0.50
1:A:593:LEU:O	1:A:597:LEU:HD23	2.11	0.50
1:A:1039:GLN:HE22	1:A:1918:HIS:HB3	1.76	0.50
1:A:1079:LEU:HG	1:A:1136:ARG:NH1	2.26	0.50
1:A:1975:THR:O	1:A:1979:ILE:HD12	2.12	0.50
1:A:1128:LEU:HD22	1:A:1159:LEU:HD13	1.93	0.50
1:A:670:GLN:O	1:A:674:ALA:N	2.35	0.49
1:A:1315:LEU:HA	1:A:1338:ALA:HB1	1.94	0.49
1:A:364:LYS:O	1:A:382:THR:N	2.43	0.49
1:A:531:TRP:CZ2	1:A:1080:PRO:HG2	2.48	0.49
1:A:337:VAL:O	1:A:351:TRP:N	2.43	0.49
1:A:762:GLN:HA	1:A:765:ARG:HG2	1.93	0.49
1:A:727:ILE:HD11	1:A:784:HIS:CE1	2.48	0.49
1:A:2073:ASP:OD2	1:A:2073:ASP:N	2.46	0.49
1:A:278:LYS:HA	1:A:281:GLN:CD	2.38	0.49
1:A:263:LYS:HA	1:A:271:VAL:HG11	1.94	0.49
1:A:571:THR:O	1:A:575:CYS:N	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1396:VAL:HG13	1:A:1436:PHE:HE1	1.78	0.49
1:A:684:LEU:O	1:A:688:SER:N	2.41	0.49
1:A:2087:VAL:HG22	1:A:2124:ASN:HB3	1.95	0.49
1:A:2084:VAL:HG12	1:A:2128:LEU:HD11	1.94	0.48
1:A:700:THR:HA	1:A:703:ILE:HB	1.95	0.48
1:A:1216:VAL:HG13	1:A:1278:PHE:CE2	2.48	0.48
1:A:1679:SER:O	1:A:1683:VAL:HG23	2.12	0.48
1:A:675:VAL:HG22	1:A:776:GLN:HB3	1.95	0.48
1:A:1201:SER:HA	1:A:1206:GLN:NE2	2.29	0.48
1:A:995:GLN:HA	1:A:995:GLN:OE1	2.14	0.48
1:A:1035:ARG:HD2	1:A:1921:GLN:OE1	2.13	0.48
1:A:1824:VAL:HG21	1:A:1931:VAL:HG12	1.95	0.48
1:A:1961:VAL:HA	1:A:1964:VAL:HG12	1.96	0.48
1:A:2021:LYS:HA	1:A:2024:LYS:HZ3	1.79	0.48
1:A:1838:LEU:HD11	1:A:1900:ALA:HB3	1.95	0.48
1:A:2073:ASP:O	1:A:2076:THR:OG1	2.27	0.48
1:A:268:LYS:O	1:A:272:LYS:NZ	2.47	0.47
1:A:1851:VAL:O	1:A:1854:GLN:N	2.47	0.47
1:A:233:ASP:HA	1:A:278:LYS:HZ1	1.78	0.47
1:A:1778:THR:O	1:A:1782:ALA:N	2.40	0.47
1:A:2074:PRO:O	1:A:2078:VAL:HG23	2.14	0.47
1:A:216:TYR:OH	1:A:220:ARG:NH2	2.47	0.47
1:A:1410:ILE:HG23	1:A:1425:ALA:HB3	1.96	0.47
1:A:1863:ALA:HA	1:A:1866:VAL:HG12	1.96	0.47
1:A:1899:GLN:C	1:A:1902:PRO:HD2	2.39	0.47
1:A:687:LYS:HZ2	1:A:703:ILE:HG23	1.80	0.47
1:A:1079:LEU:N	1:A:1082:GLU:OE2	2.48	0.47
1:A:1360:GLN:HB2	1:A:1618:ARG:HH11	1.79	0.47
1:A:280:PHE:HA	1:A:283:HIS:ND1	2.30	0.47
1:A:375:ASP:OD1	1:A:375:ASP:N	2.46	0.47
1:A:1139:ALA:HB2	1:A:1152:LEU:HD11	1.97	0.47
1:A:1139:ALA:HA	1:A:1142:THR:HG22	1.96	0.47
1:A:1976:GLN:N	1:A:1976:GLN:OE1	2.47	0.47
1:A:286:CYS:O	1:A:289:MET:HG3	2.15	0.47
1:A:499:ILE:HG13	1:A:500:ASN:N	2.28	0.47
1:A:1101:ALA:O	1:A:1104:LYS:HB2	2.14	0.47
1:A:1512:ALA:O	1:A:1516:THR:HG23	2.15	0.47
1:A:1626:ASP:OD2	1:A:1629:ARG:HG3	2.15	0.47
1:A:1733:GLN:HA	1:A:1736:GLN:HE21	1.80	0.47
1:A:1789:ALA:HB3	1:A:1791:HIS:CE1	2.50	0.47
1:A:2021:LYS:HG3	1:A:2024:LYS:HZ3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:O	1:A:356:ILE:HG22	2.15	0.47
1:A:546:GLN:O	1:A:550:ILE:HG12	2.13	0.47
1:A:1483:GLU:OE2	1:A:1490:GLN:NE2	2.43	0.47
1:A:1203:LEU:HD23	1:A:1205:GLY:H	1.80	0.47
1:A:1919:ARG:HH21	1:A:1922:GLU:CD	2.23	0.47
1:A:1160:ASP:OD1	1:A:1161:LYS:N	2.48	0.47
1:A:1921:GLN:O	1:A:1924:GLY:N	2.47	0.47
1:A:2016:ARG:O	1:A:2020:LEU:HG	2.15	0.47
1:A:2031:LYS:HA	1:A:2034:VAL:HG22	1.97	0.47
1:A:2091:LEU:O	1:A:2095:ILE:HG13	2.15	0.47
1:A:1551:THR:HB	1:A:1554:ASN:HB2	1.97	0.46
1:A:333:THR:HB	1:A:336:CYS:N	2.27	0.46
1:A:1302:VAL:O	1:A:1306:LYS:HG2	2.15	0.46
1:A:702:VAL:HG22	1:A:753:ALA:HB1	1.98	0.46
1:A:260:LEU:HD11	1:A:265:PHE:CG	2.50	0.46
1:A:279:ILE:HG22	1:A:283:HIS:HE1	1.79	0.46
1:A:1927:CYS:O	1:A:1931:VAL:HG23	2.16	0.46
1:A:2047:ALA:O	1:A:2050:SER:OG	2.24	0.46
1:A:219:ALA:O	1:A:223:ILE:HG12	2.16	0.46
1:A:709:CYS:O	1:A:713:THR:HG23	2.14	0.46
1:A:836:LEU:O	1:A:840:ILE:HG22	2.15	0.46
1:A:1108:GLU:OE2	1:A:1114:GLU:HB2	2.15	0.46
1:A:1478:CYS:HB2	1:A:1562:THR:HG23	1.98	0.46
1:A:2049:GLN:HA	1:A:2052:VAL:HG22	1.97	0.46
1:A:2084:VAL:HA	1:A:2087:VAL:HB	1.97	0.46
1:A:213:ASN:HB2	1:A:295:LYS:NZ	2.31	0.46
1:A:234:LYS:NZ	1:A:301:LEU:HB3	2.30	0.46
1:A:585:THR:O	1:A:588:SER:OG	2.27	0.46
1:A:863:LEU:HD22	1:A:900:ALA:HB1	1.96	0.46
1:A:1086:LYS:HG2	1:A:1089:GLN:NE2	2.30	0.46
1:A:1418:ASN:OD1	1:A:1420:PRO:HD2	2.16	0.46
1:A:2012:PHE:HA	1:A:2015:HIS:CD2	2.50	0.46
1:A:802:THR:O	1:A:805:ILE:HG12	2.15	0.46
1:A:913:LEU:HD12	1:A:1044:ALA:HB2	1.98	0.46
1:A:1398:GLU:OE2	1:A:1399:ASN:ND2	2.48	0.46
1:A:2132:VAL:HA	1:A:2135:VAL:HG12	1.97	0.46
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.79	0.45
1:A:948:PRO:O	1:A:951:LEU:HG	2.17	0.45
1:A:1314:LYS:HA	1:A:1317:LEU:HB2	1.98	0.45
1:A:1689:PRO:HA	1:A:1750:SER:OG	2.17	0.45
1:A:243:CYS:HB3	1:A:283:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:LEU:HD23	1:A:1141:LEU:HA	1.72	0.45
1:A:1824:VAL:HG13	1:A:1824:VAL:O	2.15	0.45
1:A:2017:GLU:HA	1:A:2020:LEU:HD12	1.98	0.45
1:A:349:GLN:OE1	1:A:350:GLU:N	2.50	0.45
1:A:1220:SER:O	1:A:1224:LEU:N	2.49	0.45
1:A:1390:PHE:CD2	1:A:1785:ASN:HA	2.51	0.45
1:A:689:VAL:O	1:A:693:THR:HG23	2.17	0.45
1:A:337:VAL:HG23	1:A:353:LEU:HD23	1.98	0.45
1:A:551:THR:O	1:A:554:THR:OG1	2.31	0.45
1:A:1040:LYS:HA	1:A:1040:LYS:HD3	1.70	0.45
1:A:1222:ARG:NH1	1:A:1283:GLU:OE2	2.49	0.45
1:A:1713:ILE:HG12	1:A:1803:MET:CE	2.42	0.45
1:A:267:PRO:O	1:A:271:VAL:HG13	2.16	0.45
1:A:651:LEU:O	1:A:655:ILE:HG12	2.17	0.45
1:A:868:ALA:HA	1:A:871:VAL:HB	1.99	0.45
1:A:700:THR:O	1:A:704:ALA:N	2.40	0.45
1:A:854:ARG:O	1:A:858:SER:N	2.32	0.45
1:A:2022:THR:O	1:A:2026:LEU:N	2.42	0.44
1:A:2054:THR:HA	1:A:2057:ARG:NH1	2.31	0.44
1:A:239:ALA:HB1	1:A:265:PHE:CE1	2.52	0.44
1:A:1234:THR:HB	1:A:1237:GLU:HB3	2.00	0.44
1:A:783:GLN:NE2	1:A:786:LYS:HE2	2.24	0.44
1:A:1153:ASP:O	1:A:1157:ASP:N	2.43	0.44
1:A:1739:GLU:N	1:A:1740:PRO:HD2	2.32	0.44
1:A:1051:ASP:O	1:A:1055:SER:N	2.42	0.44
1:A:2092:GLY:HA2	1:A:2095:ILE:HD12	1.99	0.44
1:A:223:ILE:HG13	1:A:224:LEU:N	2.32	0.44
1:A:502:SER:O	1:A:506:VAL:HG23	2.17	0.44
1:A:634:ARG:HE	1:A:637:LEU:HD23	1.81	0.44
1:A:1627:PRO:O	1:A:1631:SER:N	2.50	0.44
1:A:908:ALA:O	1:A:909:ILE:C	2.61	0.44
1:A:1295:GLN:O	1:A:1298:ARG:HB3	2.17	0.44
1:A:316:LYS:NZ	1:A:327:PRO:HG3	2.33	0.44
1:A:1213:LEU:HD12	1:A:1214:ARG:N	2.33	0.44
1:A:1220:SER:HA	1:A:1223:LEU:HB3	2.00	0.44
1:A:1882:LEU:HD11	1:A:1937:LEU:HD23	2.00	0.44
1:A:517:GLU:CD	1:A:518:THR:H	2.26	0.43
1:A:1446:LEU:HD13	1:A:1725:SER:HB3	2.00	0.43
1:A:1455:GLN:HG2	1:A:1587:GLN:HB3	1.99	0.43
1:A:2021:LYS:HA	1:A:2024:LYS:NZ	2.33	0.43
1:A:2037:ALA:O	1:A:2102:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1865:ALA:HB2	1:A:1961:VAL:HG11	2.00	0.43
1:A:1901:LYS:CG	1:A:1902:PRO:HD3	2.48	0.43
1:A:1638:ARG:O	1:A:1642:ASP:N	2.38	0.43
1:A:1733:GLN:HA	1:A:1736:GLN:NE2	2.33	0.43
1:A:2026:LEU:O	1:A:2030:THR:N	2.46	0.43
1:A:1219:ALA:HB1	1:A:1282:LEU:HD23	2.01	0.43
1:A:1300:GLN:HG3	1:A:1304:ASN:ND2	2.33	0.43
1:A:939:ALA:O	1:A:942:PRO:HD2	2.18	0.43
1:A:1195:ALA:HA	1:A:1198:ARG:HH12	1.83	0.43
1:A:777:ALA:O	1:A:781:LEU:HG	2.19	0.43
1:A:1237:GLU:O	1:A:1241:ARG:N	2.43	0.43
1:A:502:SER:HB2	1:A:581:SER:CB	2.48	0.43
1:A:1436:PHE:O	1:A:1440:ALA:N	2.49	0.43
1:A:486:PRO:N	1:A:487:PRO:HD2	2.34	0.43
1:A:704:ALA:O	1:A:707:THR:OG1	2.34	0.43
1:A:1553:GLU:HA	1:A:1556:ALA:HB3	1.99	0.43
1:A:1620:LEU:HD11	1:A:1629:ARG:CB	2.49	0.43
1:A:229:PRO:HB2	1:A:345:LYS:HB3	2.01	0.43
1:A:1207:ARG:NH2	1:A:1210:ASP:HB2	2.33	0.43
1:A:1256:LEU:HD23	1:A:1256:LEU:HA	1.90	0.43
1:A:1978:CYS:HB3	1:A:2099:LYS:HB2	2.01	0.43
1:A:310:VAL:HG12	1:A:333:THR:HA	2.00	0.43
1:A:1207:ARG:HG3	1:A:1208:ASP:CG	2.43	0.43
1:A:2112:TRP:HA	1:A:2115:LYS:HE2	2.01	0.43
1:A:356:ILE:HD11	1:A:359:TRP:HB3	2.01	0.42
1:A:679:ALA:O	1:A:683:VAL:HG23	2.19	0.42
1:A:712:SER:O	1:A:715:GLN:HB3	2.19	0.42
1:A:1607:LEU:O	1:A:1611:GLY:N	2.44	0.42
1:A:2082:ASN:HA	1:A:2085:LYS:HB3	2.01	0.42
1:A:328:ARG:HE	1:A:339:ARG:HD2	1.84	0.42
1:A:1395:SER:O	1:A:1399:ASN:ND2	2.47	0.42
1:A:917:LEU:HD23	1:A:986:LEU:HG	2.02	0.42
1:A:1051:ASP:OD1	1:A:1051:ASP:N	2.52	0.42
1:A:1144:ASP:O	1:A:1148:GLN:HG3	2.19	0.42
1:A:1406:ALA:HB1	1:A:1429:ALA:HB2	2.01	0.42
1:A:1068:LYS:HG3	1:A:1152:LEU:HD23	2.00	0.42
1:A:1207:ARG:HE	1:A:1208:ASP:N	2.14	0.42
1:A:1480:SER:O	1:A:1483:GLU:HG3	2.19	0.42
1:A:1668:LEU:HA	1:A:1668:LEU:HD12	1.71	0.42
1:A:278:LYS:HA	1:A:281:GLN:NE2	2.34	0.42
1:A:692:ARG:HG2	1:A:762:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:LEU:HD23	1:A:1031:LEU:HA	1.82	0.42
1:A:1360:GLN:CB	1:A:1618:ARG:HE	2.33	0.42
1:A:1853:TYR:HD2	1:A:1903:ALA:HA	1.83	0.42
1:A:1908:GLU:HG2	1:A:1909:ASN:N	2.33	0.42
1:A:2015:HIS:CD2	1:A:2065:GLY:HA2	2.54	0.42
1:A:1195:ALA:HA	1:A:1198:ARG:NH1	2.34	0.42
1:A:1937:LEU:HD13	1:A:1946:THR:HG22	2.01	0.42
1:A:896:GLY:HA2	1:A:899:MET:HB3	2.01	0.42
1:A:940:SER:O	1:A:943:LYS:HG3	2.19	0.42
1:A:1203:LEU:HD23	1:A:1205:GLY:N	2.34	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.42
1:A:1734:MET:O	1:A:1734:MET:HG2	2.20	0.42
1:A:229:PRO:HB3	1:A:329:LEU:HD22	2.01	0.42
1:A:1788:GLN:HE22	1:A:1793:GLN:HB2	1.85	0.42
1:A:2130:LYS:HD2	1:A:2130:LYS:C	2.45	0.42
1:A:337:VAL:HB	1:A:351:TRP:HB2	2.02	0.41
1:A:673:ASN:HA	1:A:676:ALA:HB3	2.01	0.41
1:A:1298:ARG:HA	1:A:1301:VAL:HG22	2.02	0.41
1:A:1475:GLN:NE2	1:A:1476:MET:HE3	2.34	0.41
1:A:687:LYS:HD3	1:A:687:LYS:HA	1.75	0.41
1:A:1241:ARG:HE	1:A:1241:ARG:HB3	1.73	0.41
1:A:1535:SER:OG	1:A:1564:PRO:HB2	2.20	0.41
1:A:932:ILE:O	1:A:936:GLN:HG2	2.20	0.41
1:A:1108:GLU:OE2	1:A:1116:TYR:HB2	2.20	0.41
1:A:2087:VAL:O	1:A:2121:MET:HE1	2.20	0.41
1:A:813:PHE:HZ	1:A:895:GLU:HA	1.85	0.41
1:A:1241:ARG:HA	1:A:1244:GLU:CD	2.46	0.41
1:A:1998:PHE:O	1:A:2002:GLY:N	2.54	0.41
1:A:2079:VAL:O	1:A:2083:ALA:N	2.52	0.41
1:A:517:GLU:O	1:A:518:THR:HG23	2.20	0.41
1:A:546:GLN:O	1:A:549:ALA:N	2.54	0.41
1:A:1151:VAL:HG23	1:A:1152:LEU:HD12	2.03	0.41
1:A:1975:THR:O	1:A:1978:CYS:N	2.54	0.41
1:A:889:ARG:O	1:A:892:GLU:HG2	2.21	0.41
1:A:1684:SER:HB2	1:A:1686:GLN:HE22	1.85	0.41
1:A:1744:ALA:O	1:A:1748:ALA:N	2.44	0.41
1:A:2127:SER:O	1:A:2131:THR:OG1	2.32	0.41
1:A:266:LEU:HA	1:A:266:LEU:HD23	1.82	0.41
1:A:362:SER:HB3	1:A:365:SER:HB2	2.03	0.41
1:A:506:VAL:HG13	1:A:584:LEU:HD21	2.03	0.41
1:A:1207:ARG:HH21	1:A:1210:ASP:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HD11	1:A:627:GLN:HG3	2.01	0.41
1:A:522:LEU:HD12	1:A:528:SER:OG	2.21	0.41
1:A:572:ALA:O	1:A:576:ALA:N	2.53	0.41
1:A:1407:MET:SD	1:A:1408:THR:HG23	2.61	0.41
1:A:1642:ASP:HA	1:A:1645:LYS:HG2	2.03	0.41
1:A:1227:LEU:HD22	1:A:1286:VAL:HB	2.03	0.41
1:A:2110:ALA:O	1:A:2113:GLN:HB3	2.21	0.41
1:A:334:LYS:HA	1:A:395:TYR:CE1	2.56	0.40
1:A:372:ASP:OD1	1:A:372:ASP:N	2.54	0.40
1:A:374:GLN:NE2	1:A:375:ASP:O	2.55	0.40
1:A:913:LEU:HD23	1:A:913:LEU:HA	1.79	0.40
1:A:1543:ILE:HD12	1:A:1543:ILE:HA	1.98	0.40
1:A:1039:GLN:HE22	1:A:1918:HIS:CB	2.34	0.40
1:A:1545:ALA:O	1:A:1554:ASN:ND2	2.28	0.40
1:A:1612:GLY:O	1:A:1615:GLN:HG3	2.22	0.40
1:A:1627:PRO:HB2	1:A:1628:PRO:HD3	2.03	0.40
1:A:1831:ILE:HG12	1:A:1893:TYR:HD2	1.86	0.40
1:A:711:LEU:HD12	1:A:712:SER:N	2.36	0.40
1:A:934:ALA:O	1:A:1020:LEU:HD13	2.21	0.40
1:A:1203:LEU:HA	1:A:1204:PRO:HD3	1.94	0.40
1:A:1486:CYS:HA	1:A:1490:GLN:NE2	2.32	0.40
1:A:230:VAL:C	1:A:345:LYS:HG3	2.47	0.40
1:A:695:ASP:HB3	1:A:698:LEU:HB3	2.02	0.40
1:A:994:LEU:HD23	1:A:994:LEU:HA	1.79	0.40
1:A:1086:LYS:HG2	1:A:1089:GLN:HE21	1.85	0.40
1:A:1109:ILE:HD11	1:A:1169:ALA:HB1	2.02	0.40
1:A:1229:PRO:HD3	1:A:1290:GLY:HA3	2.04	0.40
1:A:1314:LYS:HA	1:A:1317:LEU:HD12	2.04	0.40
1:A:1693:ILE:HG21	1:A:1698:LEU:HD21	2.04	0.40
1:A:1857:MET:SD	1:A:1968:LEU:HD21	2.61	0.40
1:A:1889:LEU:HD11	1:A:1927:CYS:SG	2.61	0.40
1:A:2120:VAL:HA	1:A:2123:THR:HG22	2.04	0.40
1:A:212:LEU:HD23	1:A:295:LYS:HE2	2.03	0.40
1:A:230:VAL:HG21	1:A:238:PHE:HE2	1.85	0.40
1:A:357:LYS:HE3	1:A:357:LYS:HB3	1.93	0.40
1:A:727:ILE:O	1:A:733:GLN:NE2	2.54	0.40
1:A:919:HIS:O	1:A:919:HIS:CG	2.74	0.40
1:A:1831:ILE:HG13	1:A:1890:THR:OG1	2.22	0.40
1:A:2133:LYS:HA	1:A:2133:LYS:HD2	1.76	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	1848/2804 (66%)	1797 (97%)	51 (3%)	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	1417/2215 (64%)	1398 (99%)	19 (1%)	61	71

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	657	GLU
1	A	660	THR
1	A	665	GLN
1	A	772	THR
1	A	778	LEU
1	A	780	GLU
1	A	907	ASN
1	A	909	ILE
1	A	911	LYS
1	A	1025	LYS
1	A	1043	GLU
1	A	1048	LEU
1	A	1332	LYS

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Mol	Chain	Res	Type
1	A	1333	SER
1	A	1381	VAL
1	A	1384	ILE
1	A	1385	ASN
1	A	1991	ASP
1	A	1997	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	500	ASN
1	A	733	GLN
1	A	776	GLN
1	A	779	ASN
1	A	783	GLN
1	A	923	GLN
1	A	962	GLN
1	A	1012	GLN
1	A	1300	GLN
1	A	1382	GLN
1	A	1413	ASN
1	A	1471	ASN
1	A	1475	GLN
1	A	1479	GLN
1	A	1488	GLN
1	A	1538	ASN
1	A	1587	GLN
1	A	1685	GLN
1	A	1695	GLN
1	A	1701	GLN
1	A	1736	GLN
1	A	1918	HIS
1	A	2124	ASN

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.

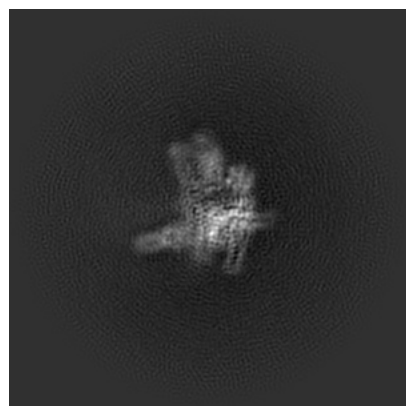
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43156. These allow visual inspection of the internal detail of the map and identification of artifacts.

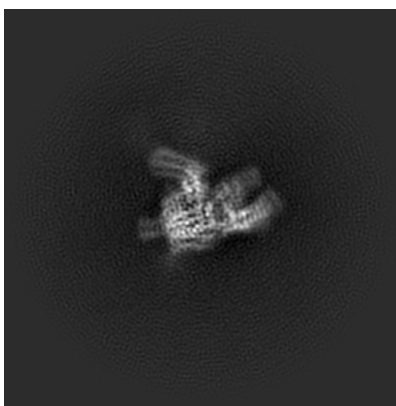
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

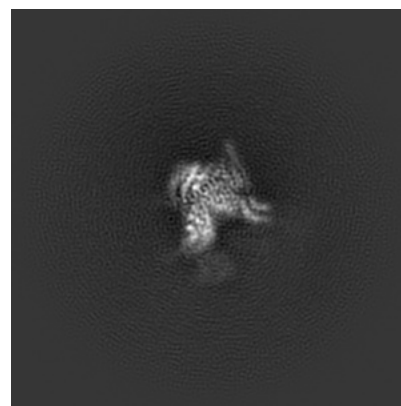
6.1.1 Primary map



X



Y

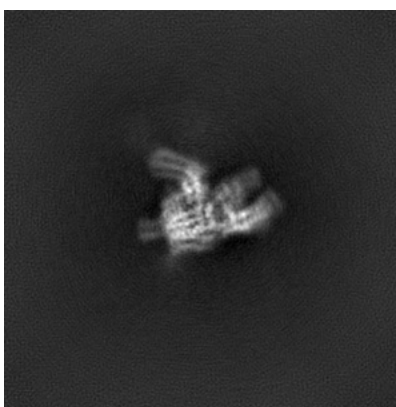


Z

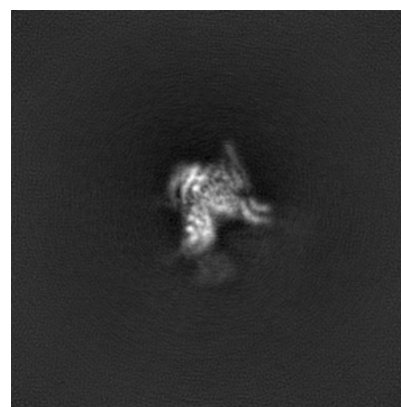
6.1.2 Raw map



X



Y

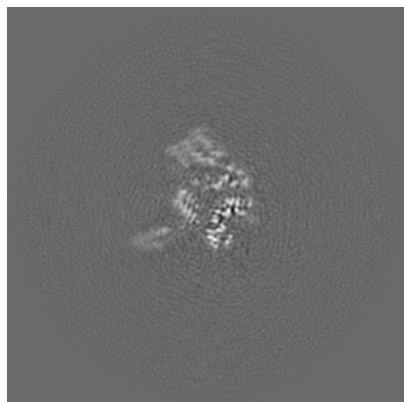


Z

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

6.2 Central slices [i](#)

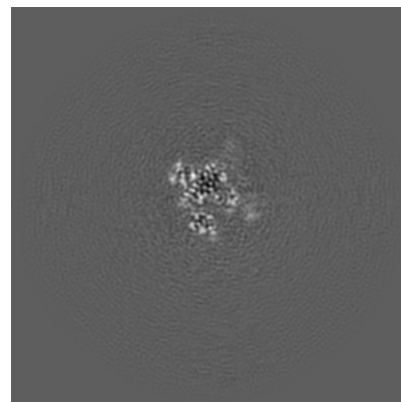
6.2.1 Primary map



X Index: 128

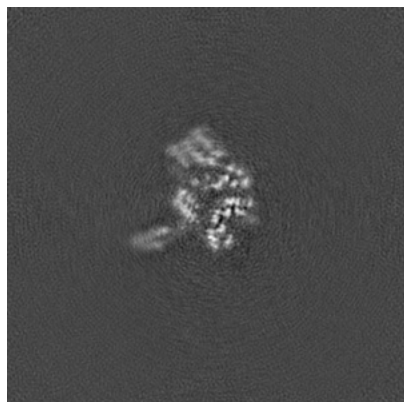


Y Index: 128



Z Index: 128

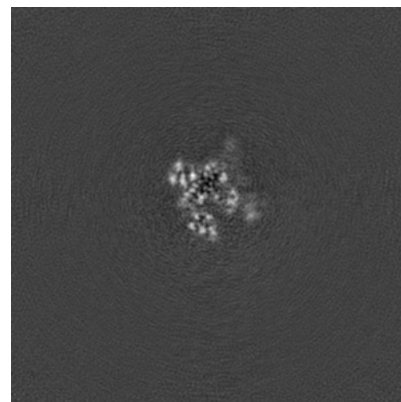
6.2.2 Raw map



X Index: 128



Y Index: 128

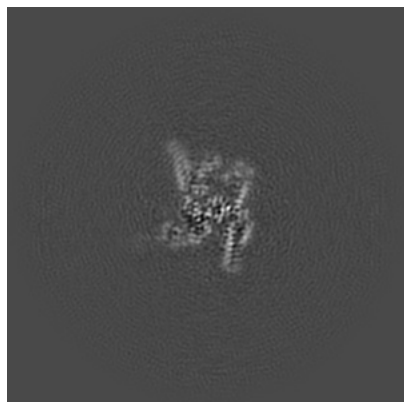


Z Index: 128

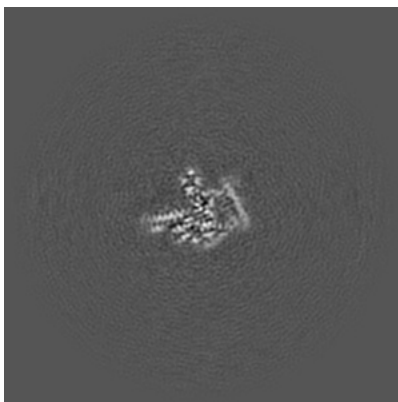
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

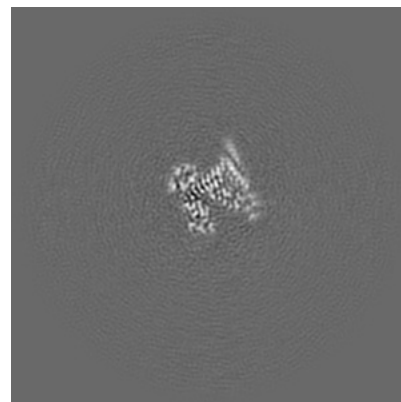
6.3.1 Primary map



X Index: 117



Y Index: 148



Z Index: 124

6.3.2 Raw map



X Index: 117



Y Index: 148

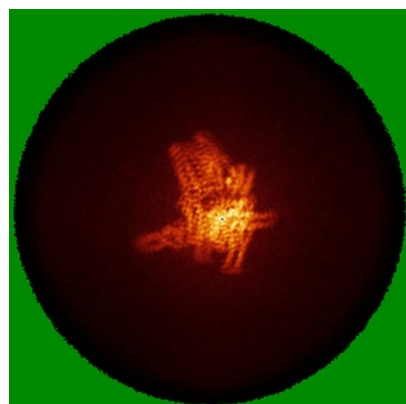


Z Index: 124

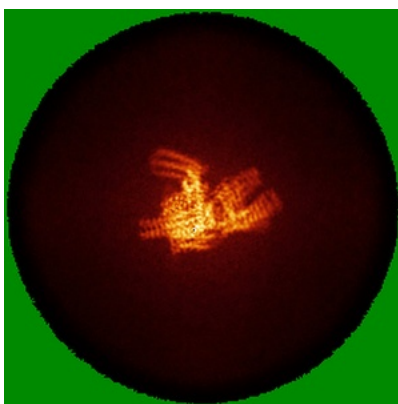
The images above show the largest variance slices of the map in three orthogonal directions.

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

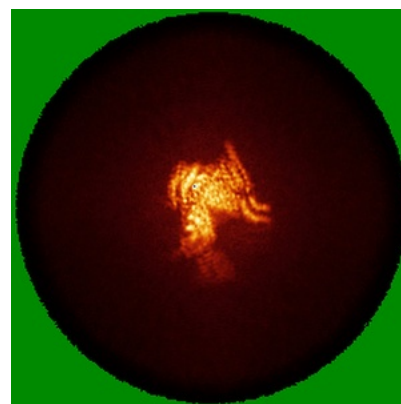
6.4.1 Primary map



X

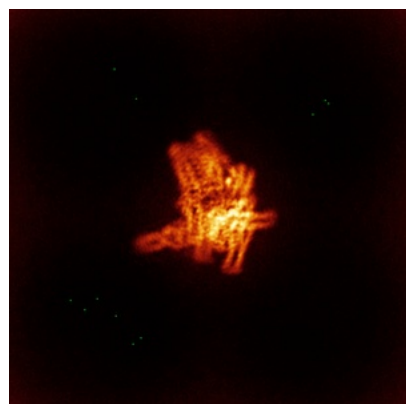


Y



Z

6.4.2 Raw map



X



Y

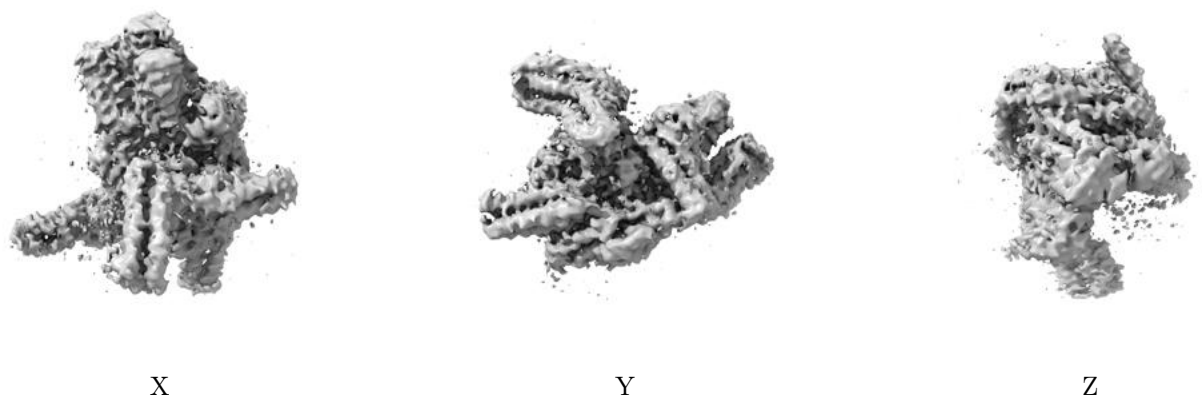


Z

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 0.124. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

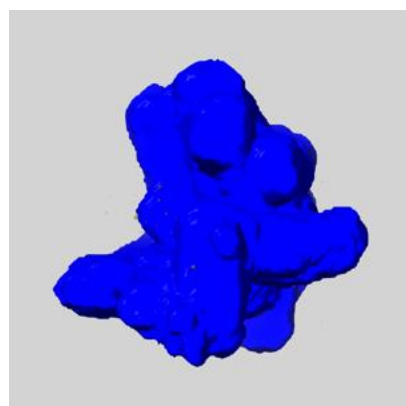
6.6 Mask visualisation [i](#)

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

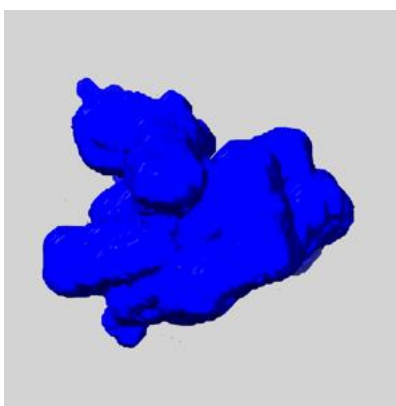
A mask typically either:

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

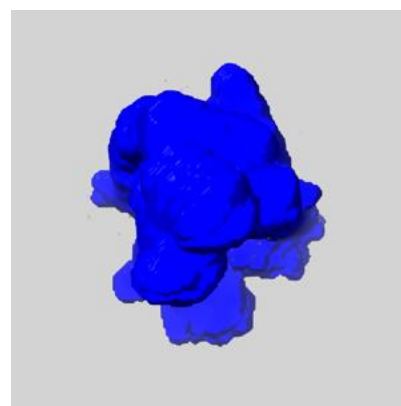
6.6.1 emd_43156_msk_1.map [i](#)



X



Y

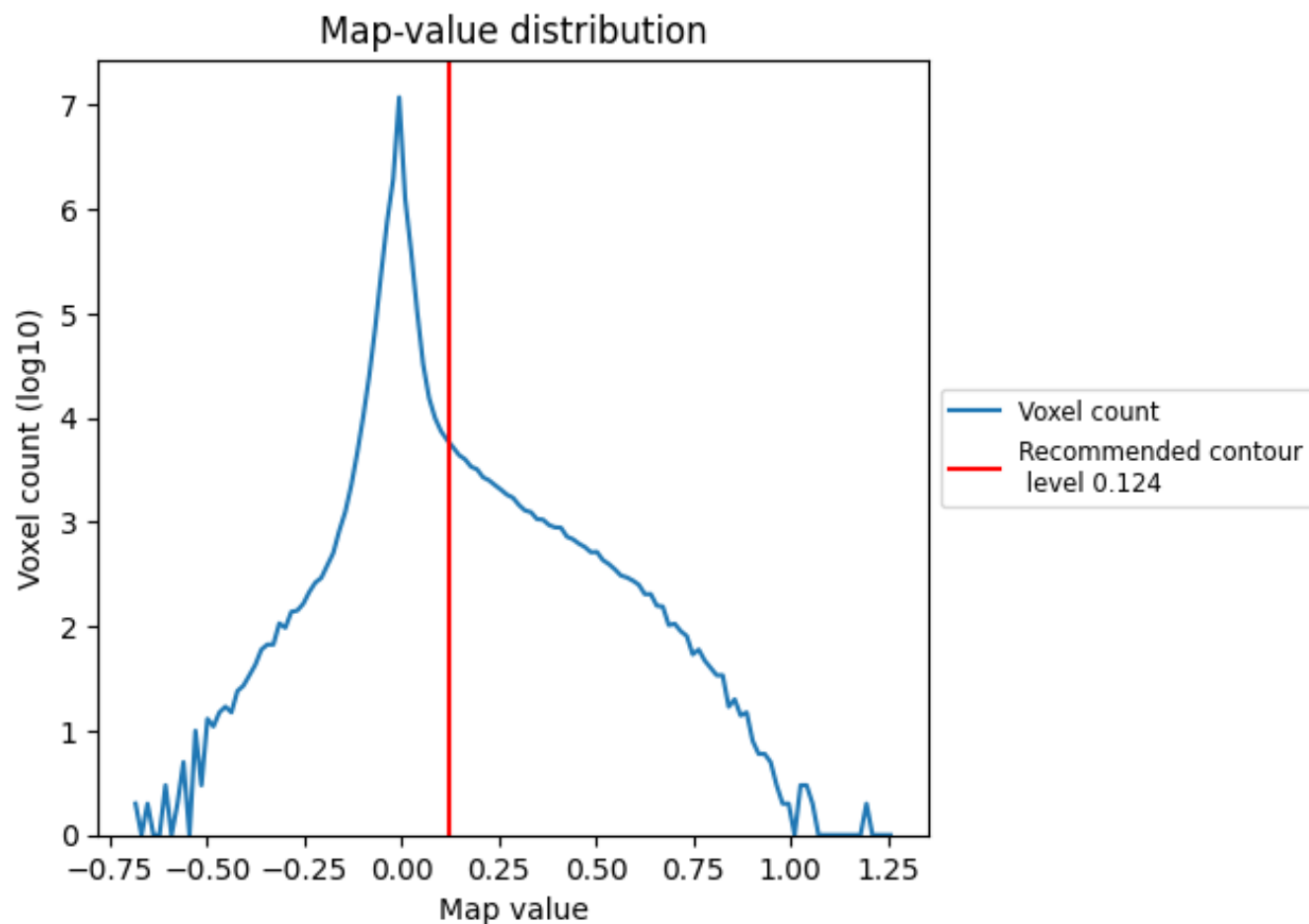


Z

7 Map analysis [i](#)

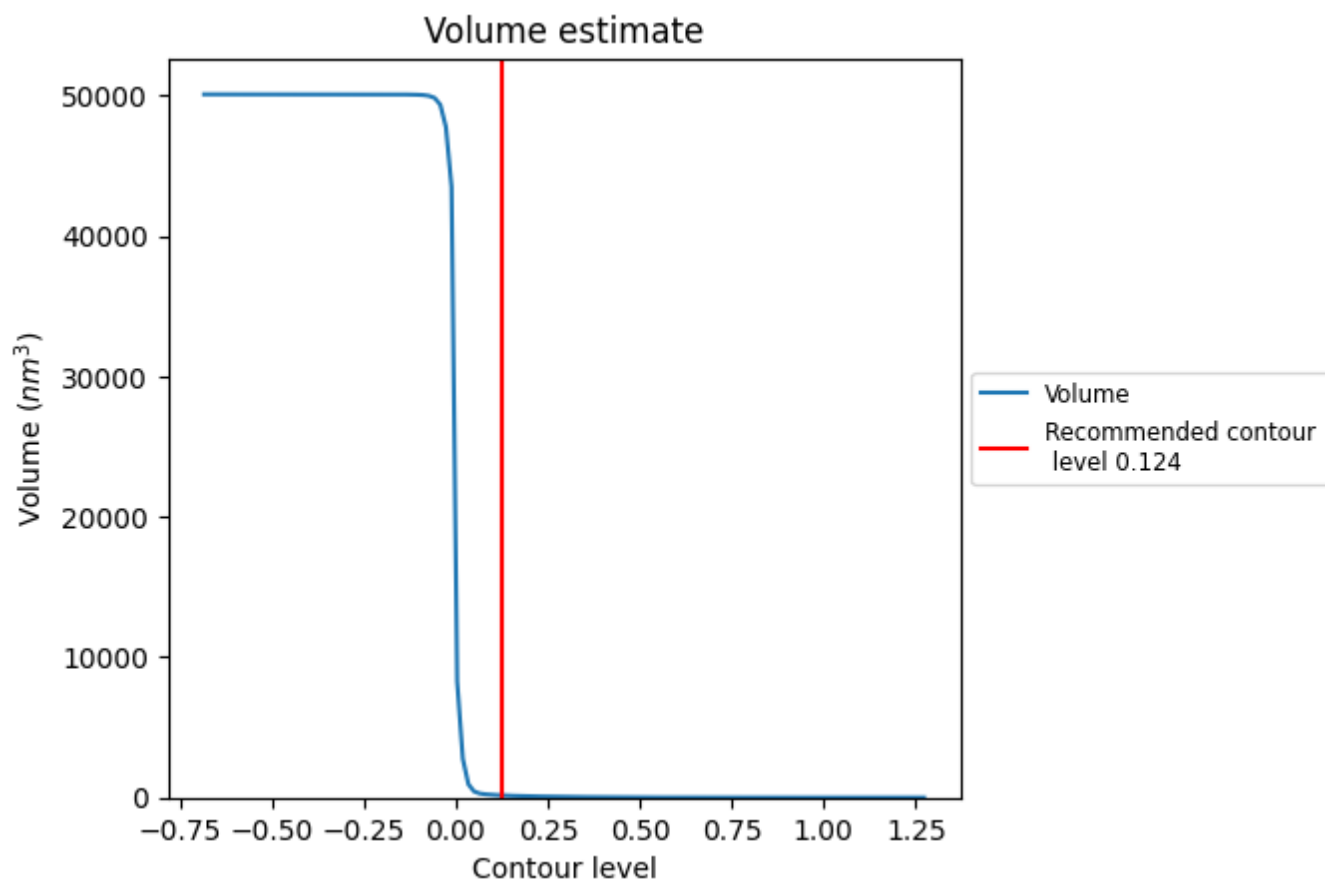
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

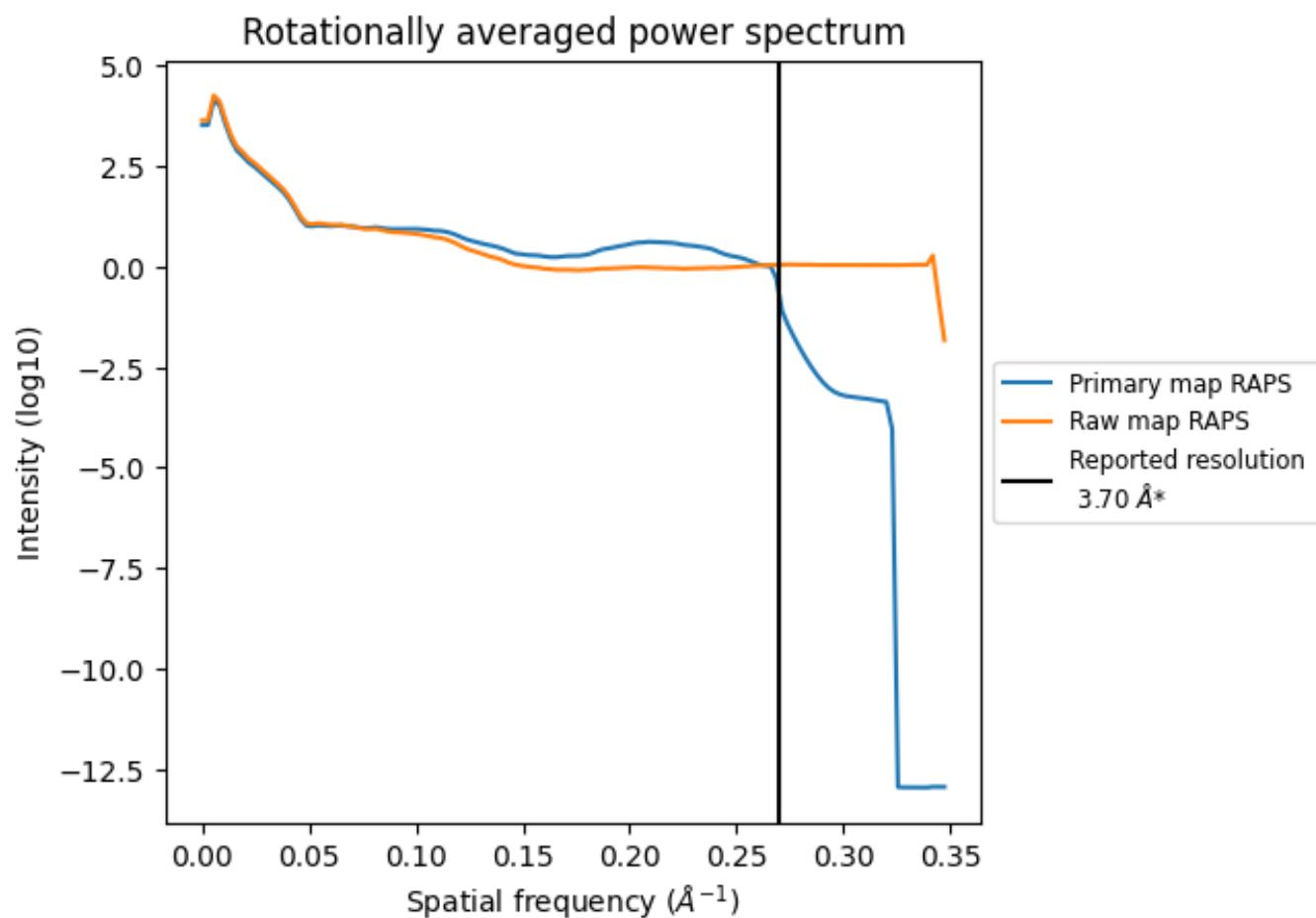
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm^3 ; this corresponds to an approximate mass of 143 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 ⓘ

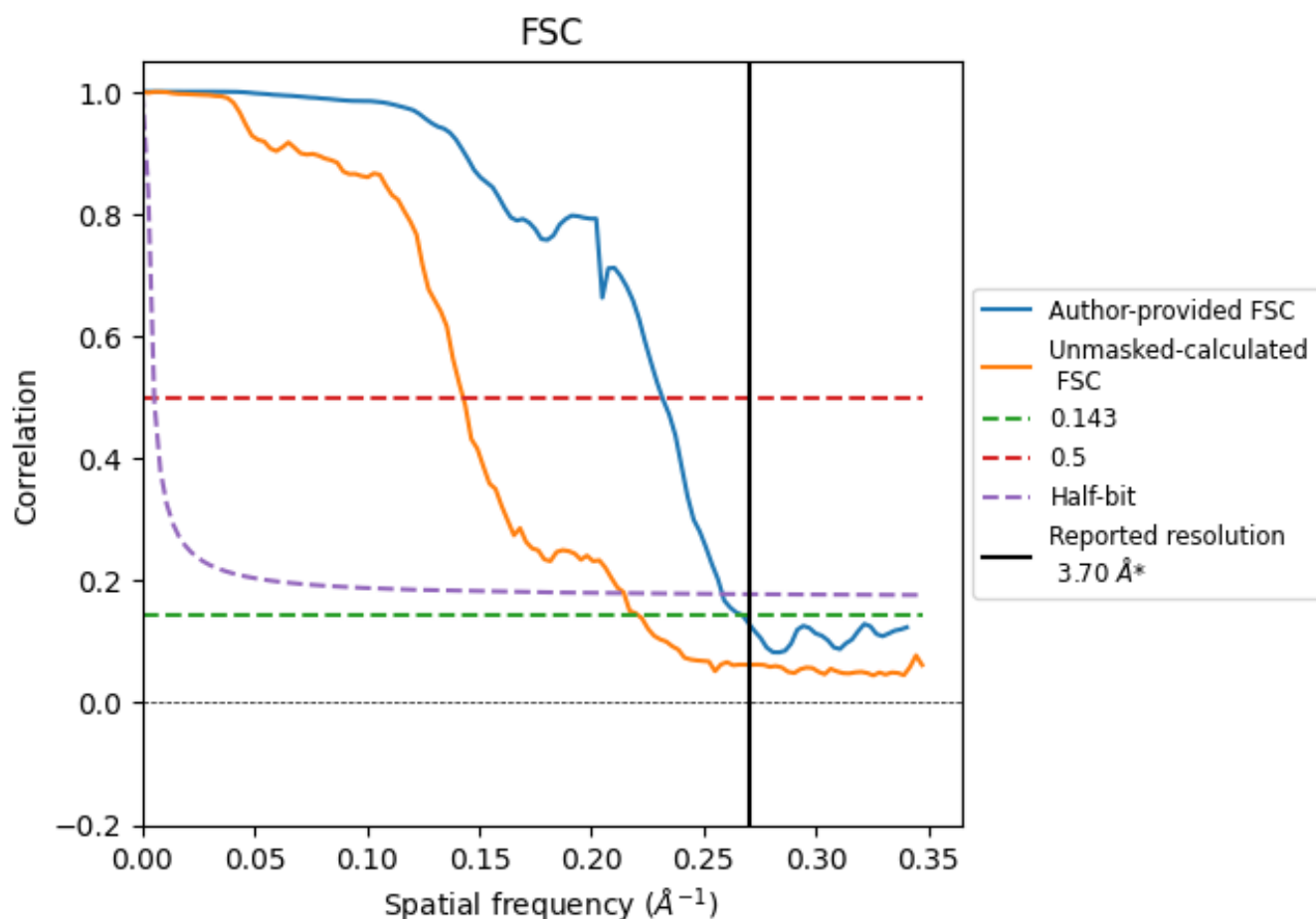


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

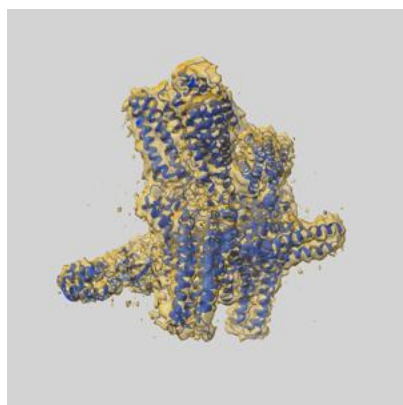
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.32	3.87
Unmasked-calculated*	4.53	7.00	4.66

*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 4.53 differs from the reported value 3.7 by more than 10 %

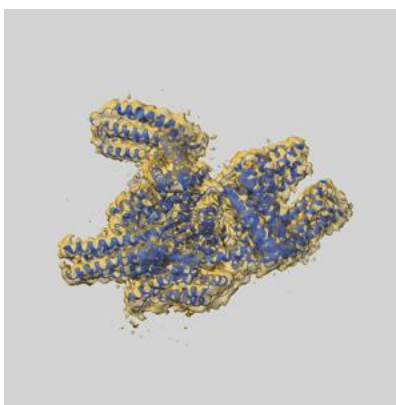
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43156 and PDB model 8VDR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

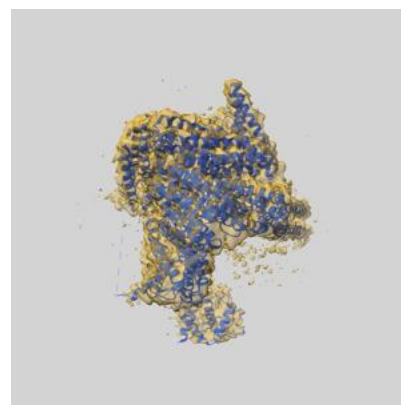
9.1 Map-model overlay [i](#)



X



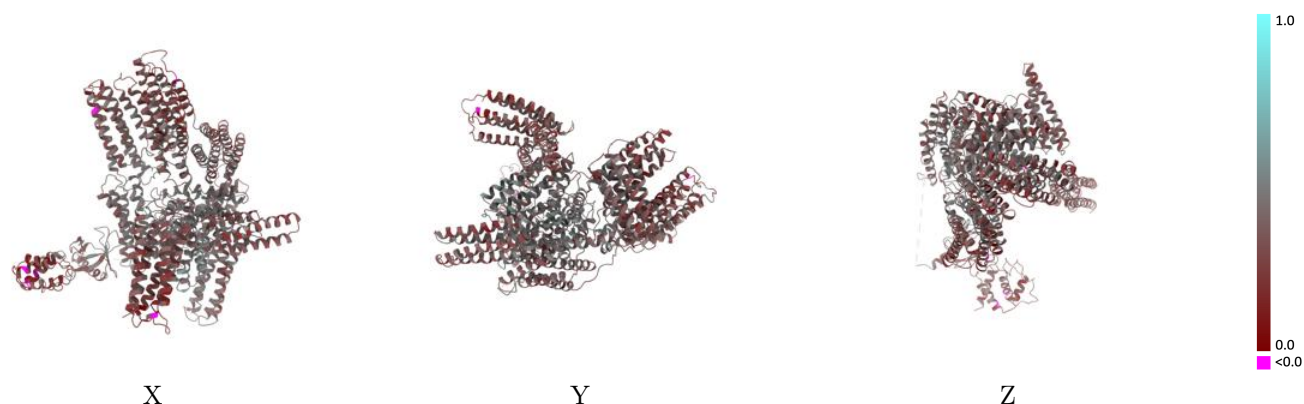
Y



Z

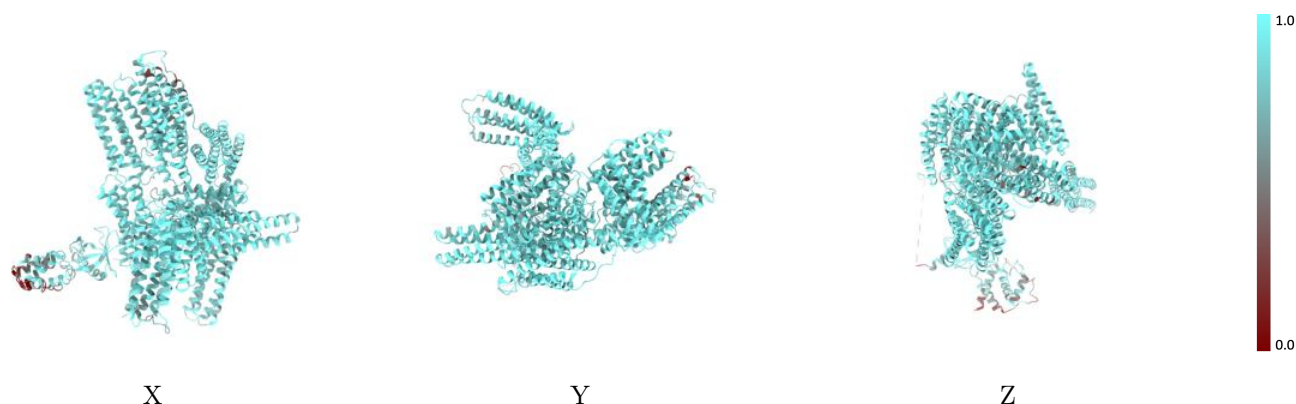
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



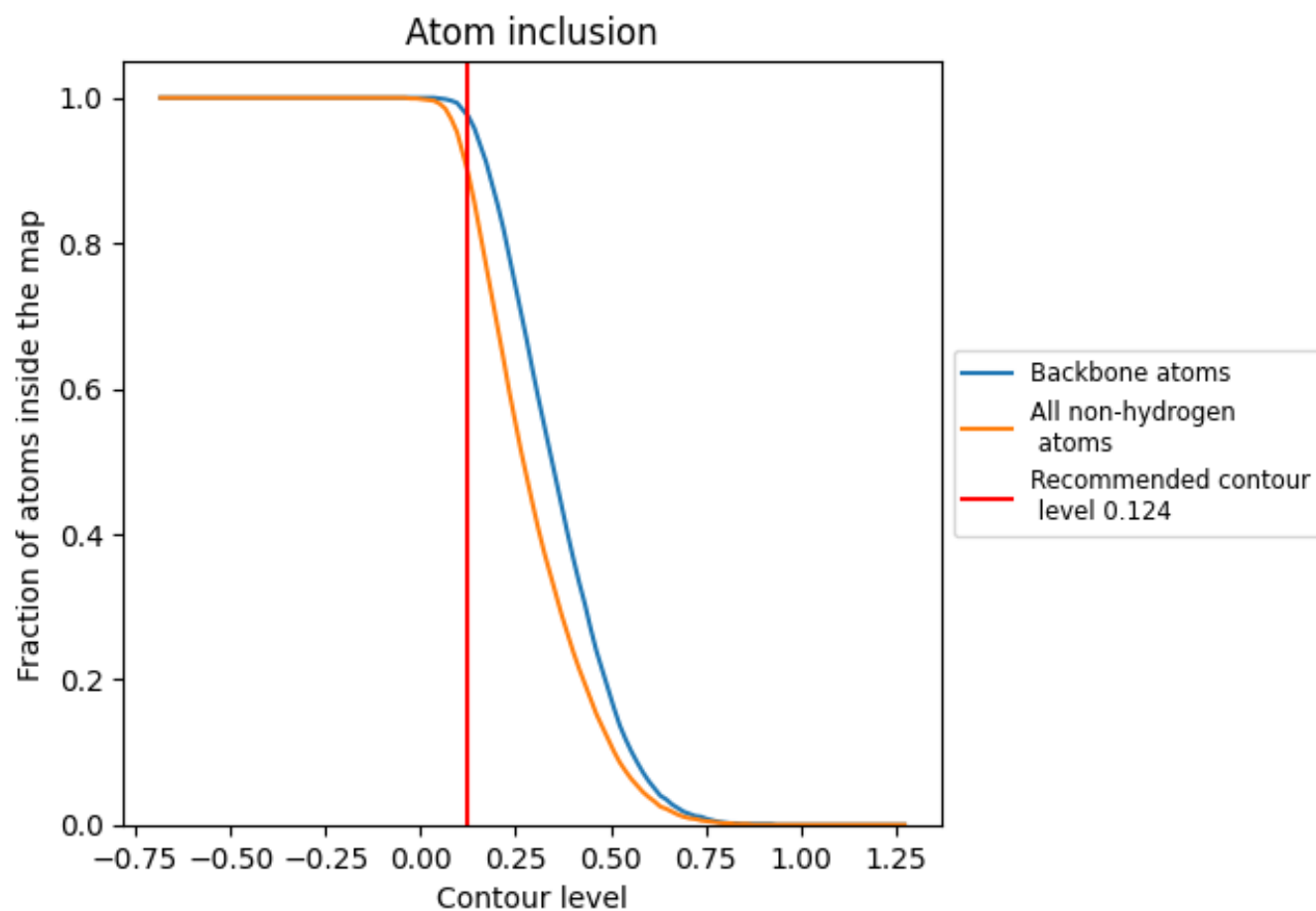
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.124).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.3660
A	0.8980	0.3660

