Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 06:11 pm BST

PDB ID	:	7OIK
EMDB ID	:	EMD-12931
Title	:	Mouse RNF213:UBE2L3 transthiolation intermediate, chemically stabilized
Authors	:	Grabarczyk, D.; Ahel, J.; Clausen, T.
Deposited on	:	2021-05-11
Resolution	:	3.50 Å(reported)
Based on initial models	:	4Q5E, 6TAX

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

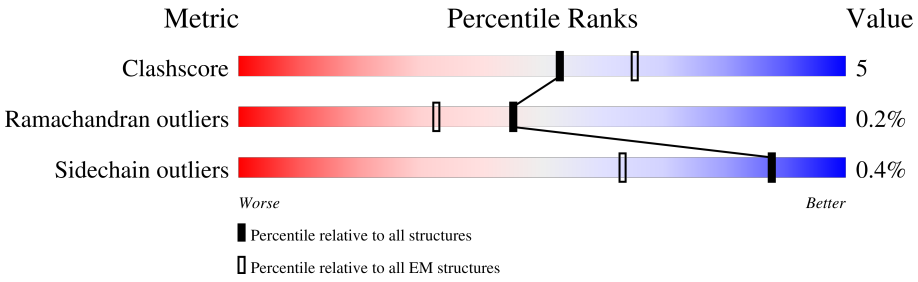
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5161	6% 72% 13% • 14%
2	B	166	8% 83% 9% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36779 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4426	35505	22641	6093	6561	210	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

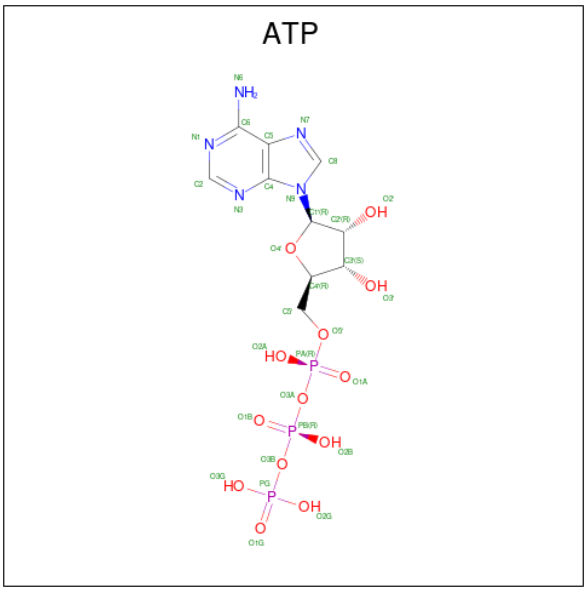
- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	153	1240	792	214	230	4	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLY	-	expression tag	UNP P68036
B	-10	TRP	-	expression tag	UNP P68036
B	-9	SER	-	expression tag	UNP P68036
B	-8	HIS	-	expression tag	UNP P68036
B	-7	PRO	-	expression tag	UNP P68036
B	-6	GLN	-	expression tag	UNP P68036
B	-5	PHE	-	expression tag	UNP P68036
B	-4	GLU	-	expression tag	UNP P68036
B	-3	LYS	-	expression tag	UNP P68036
B	-2	PRO	-	expression tag	UNP P68036
B	-1	GLY	-	expression tag	UNP P68036
B	0	SER	-	expression tag	UNP P68036
B	17	SER	CYS	conflict	UNP P68036
B	137	SER	CYS	conflict	UNP P68036

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

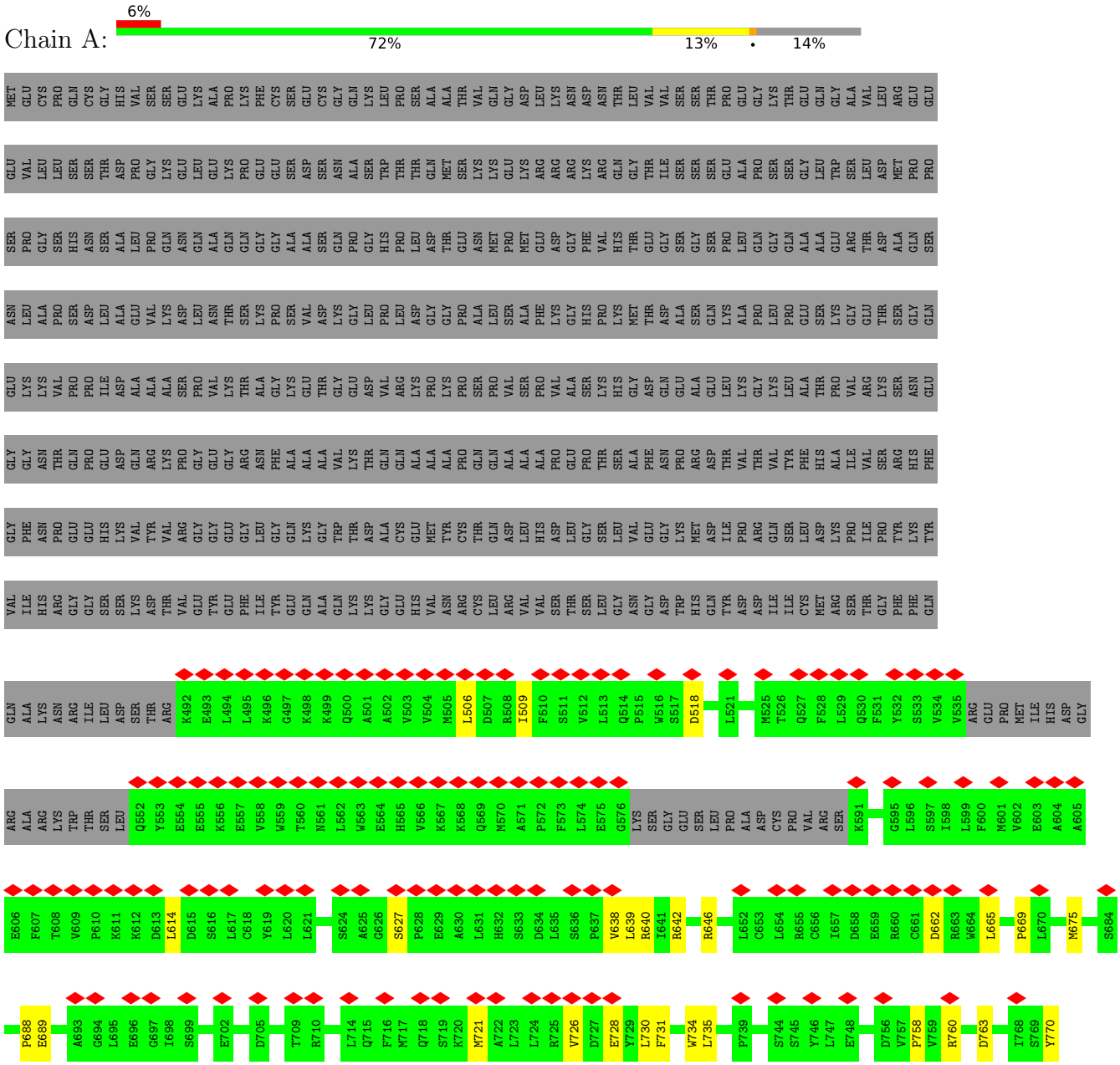
Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Zn 2 2	0

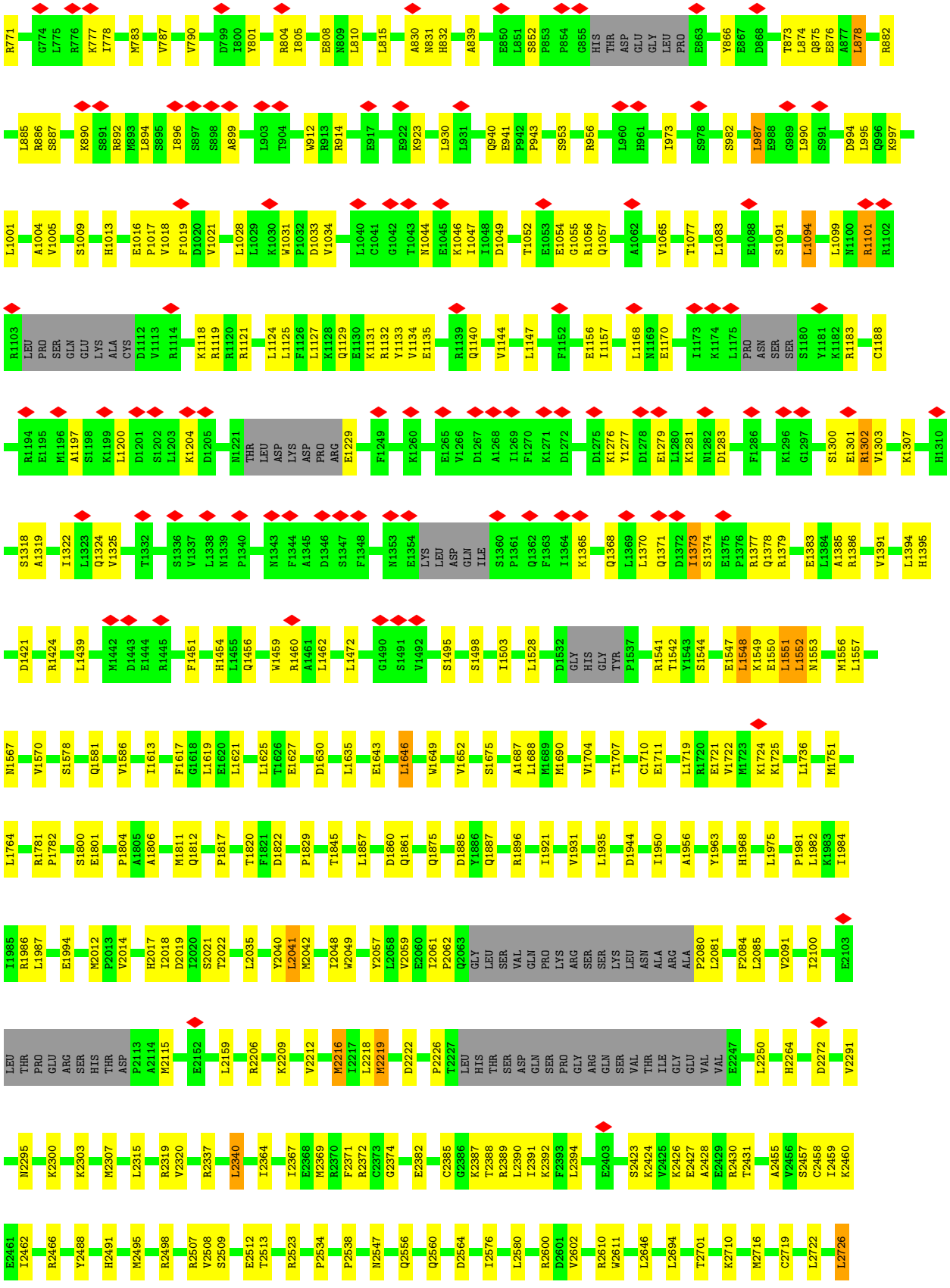
3 Residue-property plots (i)

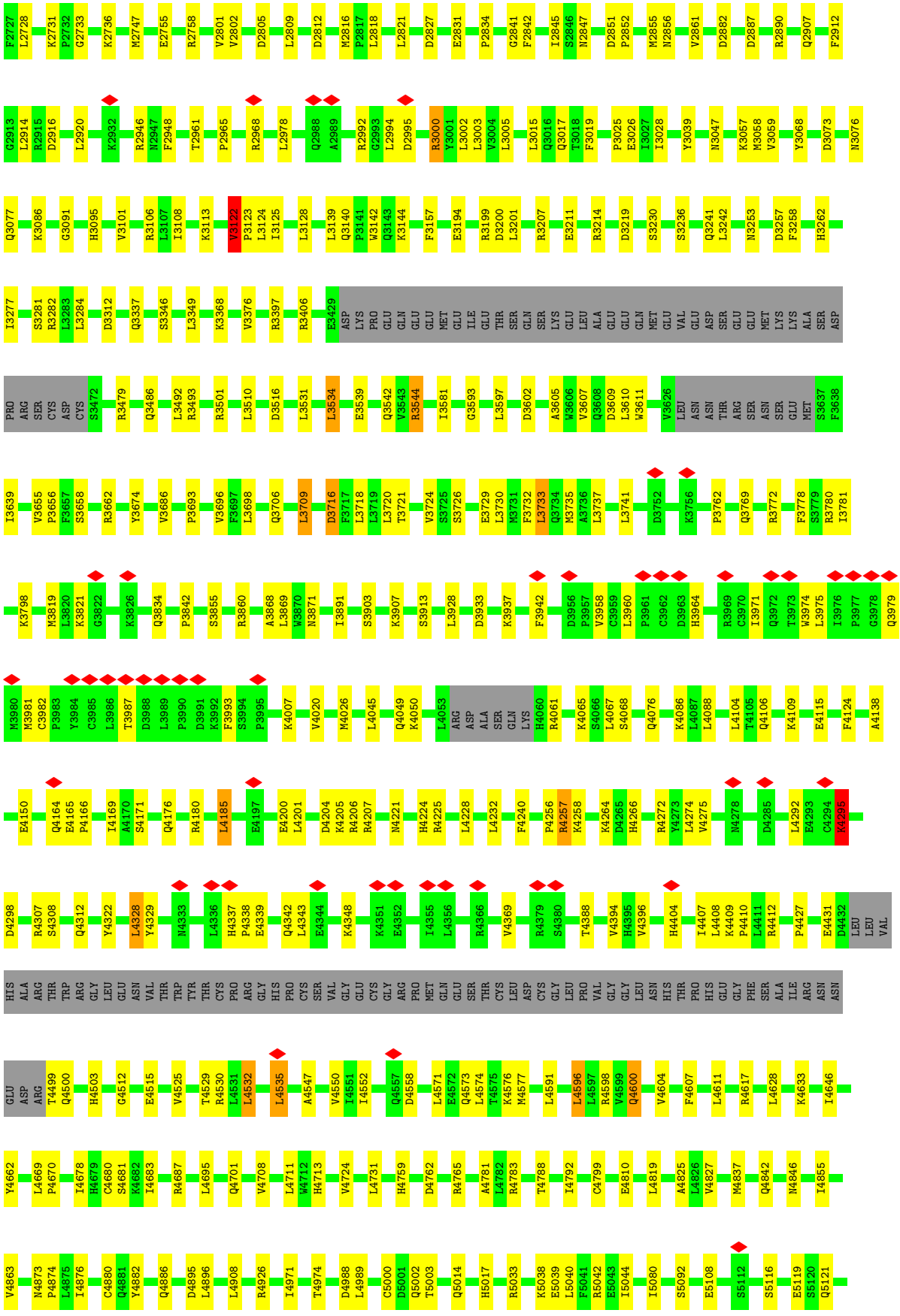
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase RNF213

Chain A:

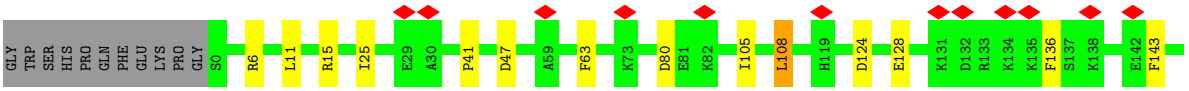


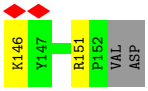

R771 G774 L775 R776 K777 I778 M783 V787 V790 D799 I800 Y801 R804 I805 E808 N809 L810 L815 A830 N831 H832 A839 E850 L851 S852 P853 P854 G855 HIS THR ASP GLU GLY LEU PRO E863 Y866 E867 D868 T873 L874 Q875 E876 A877 L878 R882
L885 R886 S887 K890 S891 R892 M893 L894 S895 I896 S897 S898 A899 L903 T904 W912 R913 R914 E917 E922 K923 L930 L931 Q940 E941 P942 P943 S953 R956 L960 H961 I973 S978 S982 L987 E988 G989 L990 S991 D994 L995 Q996 K997
L1001 A1004 V1005 S1009 H1013 E1016 P1017 V1018 F1019 D1020 V1021 L1028 L1029 K1030 W1031 P1032 D1033 V1034 L1040 C1041 G1042 T1043 N1044 E1045 K1046 I1047 I1048 D1049 T1052 E1053 E1054 G1055 R1056 Q1057 A1062 V1065 T1077 L1083 E1088 S1091 L1094 L1099 N1100 R1101 R1102
R1103 LEU PRO SER GLN GLU LYS ALA CYS D1112 V1113 R1114 K1118 R1119 R1120 R1121 L1124 L1125 F1126 L1127 K1128 Q1129 E1130 K1131 R1132 Y1133 V1134 E1135 R1139 Q1140 V1144 L1147 F1152 E1156 I1157 L1168 N1169 E1170 I1173 K1174 L1175 PRO ASN SER SER S1180 Y1181 K1182 R1183 C1188
R1194 E1195 M1196 A1197 S1198 K1199 L1200 D1201 S1202 L1203 K1204 D1205 N1221 THR LEU ASP LYS ASP PRO ARG E1229 F1249 K1260 E1265 V1266 D1267 A1268 I1269 F1270 K1271 D1272 D1275 K1276 Y1277 D1278 E1279 L1280 K1281 N1282 D1283 F1286 K1296 G1297 S1300 E1301 R1302 V1303 K1307 H1310
S1318 A1319 I1322 L1323 Q1324 V1325 T1332 S1336 V1337 L1338 N1339 P1340 N1343 F1344 A1345 D1346 S1347 F1348 N1353 E1354 LYS LEU ASP GLN ILE S1360 P1361 Q1362 F1363 I1364 K1365 Q1368 L1369 L1370 Q1371 D1372 I1373 S1374 E1375 P1376 R1377 Q1378 R1379 E1383 L1384 A1385 R1386 V1391 L1394 H1395
D1421 R1424 L1439 M1442 D1443 E1444 R1445 F1451 H1454 L1455 Q1456 W1459 R1460 A1461 L1462 L1472 G1490 S1491 V1492 S1495 S1498 I1503 L1528 D1532 GLY HIS GLY TYR P1537 R1541 T1542 Y1543 S1544 E1547 L1548 K1549 E1550 L1551 L1552 N1553 M1556 L1557
N1567 V1570 S1578 Q1581 V1586 I1613 F1617 G1618 L1619 E1620 L1621 L1625 T1626 E1627 D1630 L1635 E1643 L1646 W1649 V1652 S1675 A1687 L1688 M1689 M1690 V1704 T1707 C1710 E1711 L1719 R1720 E1721 V1722 M1723 K1724 K1725 L1736 M1751
L1764 R1781 P1782 S1800 E1801 P1804 A1805 A1806 M1811 Q1812 P1817 T1820 F1821 D1822 P1829 T1845 L1857 D1860 Q1861 Q1875 D1885 Y1886 Q1887 R1896 I1921 V1931 L1935 D1944 I1950 A1956 Y1963 H1968 L1975 P1981 L1982 K1983 I1984
I1985 R1986 L1987 E1994 M2012 P2013 V2014 H2017 I2018 D2019 I2020 S2021 T2022 L2035 Y2040 L2041 M2042 I2048 W2049 Y2057 L2058 V2059 E2060 I2061 P2062 Q2063 GLY LEU SER VAL GLN PRO LYS ARG SER SER LYS LEU ASN ALA ARG ALA P2080 L2081 F2084 L2085 V2091 I2100 E2103
LEU THR PRO GLU ARG SER HIS THR ASP P2113 A2114 M2115 E2152 L2159 R2206 K2209 V2212 M2216 I2217 L2218 M2219 D2222 P2226 T2227 LEU HIS THR SER ASP GLN SER PRO GLY ARG GLN SER VAL THR ILE GLY GLU VAL VAL E2247 L2250 H2264 D2272 V2291
N2295 K2300 K2303 M2307 L2315 R2319 V2320 R2337 L2340 I2364 I2367 E2368 M2369 R2370 F2371 R2372 C2373 G2374 E2382 C2385 G2386 K2387 T2388 R2389 L2390 I2391 K2392 F2393 L2394 E2403 S2423 K2424 V2425 K2426 E2427 A2428 E2429 R2430 T2431 A2455 V2456 S2457 C2458 I2459 K2460
E2461 I2462 R2466 Y2488 H2491 M2495 R2498 R2507 V2508 S2509 E2512 T2513 R2523 P2534 P2538 N2547 Q2556 Q2560 D2564 I2576 L2580 R2600 D2601 V2602 R2610 W2611 L2646 L2694 T2701 K2710 M2716 C2719 L2722 L2726



• Molecule 2: Ubiquitin-conjugating enzyme E2 L3

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98000	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	377.344, 377.344, 377.344	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/36242	0.75	73/49026 (0.1%)
2	B	0.30	0/1271	0.73	3/1719 (0.2%)
All	All	0.31	0/37513	0.75	76/50745 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	721	MET	CA-CB-CG	10.81	131.68	113.30
1	A	878	LEU	CA-CB-CG	9.87	138.01	115.30
1	A	2012	MET	CA-CB-CG	9.67	129.74	113.30
1	A	1028	LEU	CA-CB-CG	8.98	135.95	115.30
1	A	5127	LEU	CA-CB-CG	8.95	135.89	115.30
1	A	1944	ASP	CB-CG-OD1	8.57	126.01	118.30
1	A	1688	LEU	CA-CB-CG	8.46	134.75	115.30
1	A	1975	LEU	CA-CB-CG	8.42	134.67	115.30
1	A	675	MET	CG-SD-CE	8.25	113.39	100.20
1	A	1646	LEU	CA-CB-CG	8.18	134.11	115.30
1	A	2747	MET	CA-CB-CG	8.12	127.10	113.30
1	A	1548	LEU	CA-CB-CG	8.04	133.78	115.30
1	A	2816	MET	CA-CB-CG	7.89	126.72	113.30
2	B	11	LEU	CA-CB-CG	7.50	132.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3531	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	5121	GLN	CA-CB-CG	7.18	129.19	113.40
1	A	1551	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	4855	ILE	CG1-CB-CG2	-6.96	96.08	111.40
1	A	3709	LEU	CA-CB-CG	6.96	131.31	115.30
1	A	2340	LEU	CA-CB-CG	6.89	131.15	115.30
2	B	80	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	1135	GLU	N-CA-CB	6.70	122.67	110.60
1	A	2216	MET	CA-CB-CG	6.70	124.70	113.30
1	A	1099	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	1094	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	4185	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	1127	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	2831	GLU	CA-CB-CG	6.52	127.73	113.40
1	A	675	MET	CA-CB-CG	6.48	124.32	113.30
1	A	894	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	4596	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	1552	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	1370	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	4695	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	1557	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	3602	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	3733	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	3716	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	A	987	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	1001	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	4532	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	3933	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	4571	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	2390	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	4908	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	4989	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	4328	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	3122	VAL	CA-CB-CG1	5.50	119.14	110.90
1	A	614	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	4088	LEU	CA-CB-CG	5.47	127.87	115.30
2	B	108	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	4535	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	4274	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	1125	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	783	MET	CB-CG-SD	5.31	128.33	112.40
1	A	2216	MET	CB-CG-SD	5.31	128.32	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3000	ARG	C-N-CA	5.29	134.92	121.70
1	A	3928	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	4558	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	3716	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	2041	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	3534	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	2726	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	2219	MET	CA-CB-CG	5.17	122.09	113.30
1	A	2726	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	3819	MET	CA-CB-CG	5.14	122.04	113.30
1	A	874	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	4076	GLN	C-N-CA	5.13	134.53	121.70
1	A	2216	MET	N-CA-CB	5.11	119.80	110.60
1	A	4292	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	1101	ARG	CA-CB-CG	5.07	124.55	113.40
1	A	4295	LYS	CA-CB-CG	5.06	124.52	113.40
1	A	3741	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	1719	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	3981	MET	CB-CA-C	5.01	120.41	110.40
1	A	1302	ARG	CB-CG-CD	5.00	124.61	111.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1170	GLU	Peptide
1	A	1373	ILE	Peptide
1	A	1845	THR	Peptide
1	A	3122	VAL	Peptide
1	A	4165	GLU	Peptide
1	A	688	PRO	Peptide

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	35505	0	35641	372	0
2	B	1240	0	1240	9	0
3	A	31	0	12	1	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
All	All	36779	0	36893	379	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 5.

All (379) 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:731:PHE:HB3	1:A:760:ARG:HH21	1.49	0.77
1:A:4328:LEU:HD21	1:A:4337:HIS:H	1.55	0.72
1:A:4783:ARG:HB2	1:A:4799:CYS:HB2	1.79	0.64
1:A:2218:LEU:HD21	1:A:2303:LYS:HE2	1.79	0.64
1:A:2385:CYS:SG	1:A:2387:LYS:NZ	2.71	0.63
1:A:2801:VAL:HG12	1:A:2841:GLY:HA3	1.80	0.63
1:A:2291:VAL:HB	1:A:2307:MET:HB3	1.81	0.63
1:A:1318:SER:HB2	1:A:1378:GLN:HE21	1.64	0.62
2:B:15:ARG:NH2	2:B:25:ILE:O	2.33	0.62
1:A:1567:ASN:HA	1:A:1570:VAL:HG12	1.81	0.61
1:A:728:GLU:O	1:A:760:ARG:NH2	2.34	0.61
1:A:1721:GLU:HA	1:A:1724:LYS:HE2	1.81	0.61
1:A:3639:ILE:HA	1:A:4926:ARG:HH21	1.66	0.61
1:A:5108:GLU:OE2	2:B:6:ARG:NH1	2.34	0.61
1:A:943:PRO:HD3	1:A:3207:ARG:HH21	1.65	0.61
1:A:3501:ARG:HH12	1:A:3593:GLY:HA2	1.65	0.61
1:A:994:ASP:HB3	1:A:997:LYS:HE2	1.82	0.61
1:A:5040:LEU:HD21	1:A:5136:LYS:HE2	1.83	0.61
1:A:4065:LYS:NZ	1:A:4068:SER:O	2.33	0.60
1:A:4396:VAL:HG11	1:A:4535:LEU:HD13	1.83	0.60
1:A:3605:ALA:O	1:A:3609:ASP:HB2	2.00	0.59
1:A:4185:LEU:HD21	1:A:4228:LEU:HA	1.84	0.59
1:A:2216:MET:HA	1:A:2219:MET:HG2	1.84	0.59
1:A:3122:VAL:HG23	1:A:3125:ILE:HB	1.83	0.59
1:A:3258:PHE:O	1:A:3262:HIS:HB2	2.02	0.59
1:A:4512:GLY:HA2	1:A:4781:ALA:HA	1.85	0.59
1:A:4086:LYS:NZ	1:A:4880:CYS:SG	2.76	0.59
2:B:41:PRO:O	2:B:151:ARG:NH2	2.35	0.59
1:A:1829:PRO:HD3	1:A:1861:GLN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LYS:NZ	1:A:778:ILE:O	2.33	0.59
1:A:4272:ARG:HH12	1:A:4388:THR:HG22	1.67	0.58
1:A:758:PRO:HB2	1:A:805:ILE:HA	1.85	0.58
1:A:2731:LYS:O	1:A:2736:LYS:NZ	2.34	0.58
1:A:3937:LYS:HG3	1:A:3942:PHE:HA	1.86	0.58
1:A:1956:ALA:HB3	1:A:2534:PRO:HB2	1.86	0.58
1:A:2716:MET:HA	1:A:2726:LEU:HD21	1.86	0.58
1:A:4200:GLU:HA	1:A:4206:ARG:HH21	1.67	0.58
1:A:4328:LEU:HD11	1:A:4337:HIS:HB3	1.85	0.58
1:A:2042:MET:HG2	1:A:2048:ILE:HG12	1.86	0.58
1:A:787:VAL:HA	1:A:790:VAL:HG22	1.86	0.58
1:A:2382:GLU:O	1:A:2387:LYS:NZ	2.38	0.57
1:A:2040:TYR:HA	1:A:2049:TRP:O	2.04	0.57
1:A:3610:LEU:HD23	1:A:3656:PRO:HD2	1.87	0.57
1:A:3718:LEU:HD21	1:A:3737:LEU:HD22	1.87	0.57
1:A:3534:LEU:HD22	1:A:3581:ILE:HG23	1.86	0.57
1:A:4339:GLU:HA	1:A:4343:LEU:HD22	1.87	0.57
1:A:2887:ASP:OD1	1:A:2890:ARG:NH1	2.38	0.57
1:A:1140:GLN:HG3	1:A:1204:LYS:HZ2	1.69	0.57
1:A:1183:ARG:NH1	1:A:1188:CYS:SG	2.78	0.57
1:A:3003:LEU:HB2	1:A:3128:LEU:HB3	1.86	0.57
1:A:887:SER:O	1:A:890:LYS:NZ	2.36	0.56
1:A:953:SER:O	1:A:956:ARG:NH2	2.37	0.56
1:A:3891:ILE:HD13	1:A:4007:LYS:HD2	1.87	0.56
1:A:4525:VAL:HG13	1:A:4628:LEU:HD12	1.86	0.56
1:A:1300:SER:HA	1:A:1303:VAL:HG12	1.88	0.56
1:A:1077:THR:HA	1:A:1168:LEU:HD22	1.88	0.56
1:A:2364:ILE:HG23	1:A:2394:LEU:HD13	1.87	0.56
1:A:2992:ARG:NH2	1:A:2995:ASP:OD1	2.39	0.56
1:A:4045:LEU:O	1:A:4065:LYS:NZ	2.39	0.55
1:A:4515:GLU:HG2	1:A:4530:ARG:HH12	1.70	0.55
1:A:3139:LEU:O	1:A:3144:LYS:NZ	2.38	0.55
1:A:735:LEU:O	1:A:771:ARG:NH2	2.39	0.55
1:A:3479:ARG:NH2	1:A:5000:CYS:SG	2.80	0.55
1:A:4842:GLN:HA	1:A:4846:ASN:HB2	1.88	0.55
1:A:1049:ASP:O	1:A:1056:ARG:NH2	2.39	0.55
1:A:1548:LEU:HA	1:A:1551:LEU:HG	1.89	0.55
1:A:1675:SER:HB3	1:A:1764:LEU:HD11	1.89	0.55
1:A:3000:ARG:O	1:A:3077:GLN:NE2	2.40	0.55
1:A:1133:TYR:HB3	1:A:1197:ALA:HB1	1.87	0.55
1:A:1547:GLU:HA	1:A:1550:GLU:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2965:PRO:HA	1:A:2968:ARG:HH11	1.72	0.55
1:A:2523:ARG:HG3	1:A:2851:ASP:HB3	1.87	0.55
1:A:2847:ASN:HD22	1:A:3123:PRO:HG3	1.71	0.55
1:A:2115:MET:HA	3:A:5201:ATP:HN62	1.71	0.54
1:A:940:GLN:NE2	1:A:3241:GLN:OE1	2.40	0.54
1:A:2374:GLY:O	1:A:2466:ARG:NH2	2.40	0.54
1:A:2852:PRO:HA	1:A:2855:MET:HG2	1.88	0.54
1:A:5033:ARG:NH2	1:A:5039:GLU:O	2.40	0.54
1:A:1617:PHE:HB3	1:A:1619:LEU:HD13	1.89	0.54
1:A:2733:GLY:HA3	1:A:2914:LEU:HB2	1.89	0.54
1:A:2916:ASP:OD1	1:A:3000:ARG:NH1	2.33	0.54
1:A:3015:LEU:HD23	1:A:3019:PHE:HD2	1.72	0.54
1:A:831:ASN:O	1:A:832:HIS:ND1	2.41	0.54
1:A:1541:ARG:NH1	1:A:1542:THR:O	2.41	0.54
1:A:3277:ILE:HB	1:A:3376:VAL:HG12	1.90	0.54
1:A:4503:HIS:HB3	1:A:4552:ILE:HG23	1.89	0.54
1:A:1129:GLN:HA	1:A:1132:ARG:HG2	1.88	0.53
1:A:4204:ASP:OD1	1:A:4207:ARG:NH2	2.41	0.53
1:A:3778:PHE:HA	1:A:3781:ILE:HG12	1.90	0.53
1:A:4873:ASN:HA	1:A:4876:ILE:HG12	1.90	0.53
1:A:882:ARG:NH2	1:A:3230:SER:O	2.42	0.53
1:A:3724:VAL:HG21	1:A:3730:LEU:HD13	1.91	0.53
1:A:3693:PRO:HA	1:A:3696:VAL:HG22	1.89	0.53
1:A:4687:ARG:NH2	1:A:4882:TYR:OH	2.42	0.53
1:A:995:LEU:HD11	1:A:1047:ILE:HG13	1.91	0.53
1:A:4050:LYS:HD2	1:A:4061:ARG:HH11	1.73	0.53
1:A:4713:HIS:ND1	1:A:4837:MET:SD	2.81	0.53
1:A:5116:SER:HA	1:A:5119:GLU:HG3	1.90	0.53
1:A:1984:ILE:HD13	1:A:2017:HIS:HB3	1.90	0.52
1:A:4338:PRO:HA	1:A:4342:GLN:HB2	1.89	0.52
1:A:4708:VAL:HB	1:A:4896:LEU:HD13	1.91	0.52
1:A:4138:ALA:HB2	1:A:4874:PRO:HG3	1.90	0.52
1:A:1544:SER:N	1:A:1547:GLU:OE2	2.39	0.52
1:A:2337:ARG:HA	1:A:2340:LEU:HG	1.91	0.52
1:A:1613:ILE:HD11	1:A:1635:LEU:HD22	1.92	0.52
1:A:3211:GLU:OE2	1:A:3214:ARG:NH1	2.43	0.52
1:A:4221:ASN:O	1:A:4224:HIS:ND1	2.38	0.52
1:A:2035:LEU:HD11	1:A:2057:TYR:HE2	1.75	0.52
1:A:1322:ILE:HA	1:A:1325:VAL:HG12	1.92	0.52
1:A:1383:GLU:OE2	1:A:1386:ARG:NH2	2.43	0.52
1:A:4971:ILE:HA	1:A:4974:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2507:ARG:NH1	1:A:2809:LEU:O	2.43	0.52
1:A:1391:VAL:HA	1:A:1394:LEU:HG	1.91	0.52
1:A:4762:ASP:N	1:A:4762:ASP:OD1	2.42	0.52
1:A:3658:SER:HB3	1:A:3720:LEU:HD11	1.93	0.51
1:A:1503:ILE:HD12	1:A:1528:LEU:HD21	1.93	0.51
1:A:2061:ILE:HD12	1:A:2062:PRO:HD2	1.93	0.51
1:A:665:LEU:HB3	1:A:734:TRP:HE1	1.75	0.51
1:A:1021:VAL:HG12	1:A:1065:VAL:HG22	1.92	0.51
1:A:3718:LEU:HD13	1:A:3733:LEU:HD23	1.93	0.51
1:A:1147:LEU:O	1:A:1229:GLU:N	2.44	0.51
1:A:2513:THR:OG1	1:A:2812:ASP:OD2	2.28	0.51
1:A:2556:GLN:O	1:A:2560:GLN:NE2	2.43	0.51
1:A:896:ILE:HD11	1:A:899:ALA:HA	1.92	0.51
1:A:2250:LEU:HD22	1:A:2488:TYR:HB3	1.93	0.51
1:A:4338:PRO:O	1:A:4343:LEU:N	2.43	0.51
1:A:1549:LYS:HA	1:A:1552:LEU:HG	1.93	0.50
1:A:4407:ILE:HB	1:A:4604:VAL:HG11	1.93	0.50
1:A:4678:ILE:HD12	1:A:4683:ILE:HD13	1.94	0.50
1:A:4104:LEU:HD13	1:A:4124:PHE:HE2	1.76	0.50
1:A:1379:ARG:HH12	1:A:1383:GLU:HG2	1.76	0.50
1:A:1578:SER:HA	1:A:1581:GLN:HG2	1.94	0.50
1:A:3284:LEU:HB2	1:A:3337:GLN:HE22	1.76	0.50
1:A:3855:SER:O	1:A:3860:ARG:NH1	2.44	0.50
1:A:4164:GLN:HG3	1:A:4169:ILE:HG22	1.93	0.50
1:A:1820:THR:OG1	1:A:1822:ASP:OD1	2.24	0.50
1:A:2369:MET:SD	1:A:2372:ARG:NH2	2.85	0.49
1:A:3662:ARG:HH21	1:A:3721:THR:HG22	1.75	0.49
1:A:1031:TRP:HE1	1:A:1033:ASP:HB2	1.77	0.49
1:A:2459:ILE:HA	1:A:2462:ILE:HD12	1.93	0.49
1:A:638:VAL:HG23	1:A:639:LEU:HG	1.93	0.49
1:A:3982:CYS:HB3	1:A:3987:THR:H	1.76	0.49
1:A:5033:ARG:HH12	1:A:5042:ARG:HH21	1.59	0.49
1:A:3868:ALA:HB1	1:A:3913:SER:HB3	1.95	0.49
1:A:1994:GLU:HB3	1:A:2041:LEU:HD12	1.95	0.49
1:A:1649:TRP:HA	1:A:1652:VAL:HG12	1.95	0.49
1:A:1811:MET:HE3	1:A:1921:ILE:HG12	1.94	0.49
1:A:3091:GLY:HA2	1:A:3095:HIS:O	2.12	0.49
1:A:3732:PHE:HA	1:A:3735:MET:HG2	1.95	0.49
1:A:1005:VAL:O	1:A:1009:SER:HB3	2.13	0.49
1:A:2226:PRO:HG2	1:A:2538:PRO:HA	1.95	0.49
1:A:758:PRO:HG3	1:A:804:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:GLU:HG2	1:A:1157:ILE:HG12	1.94	0.49
1:A:760:ARG:NH1	1:A:763:ASP:OD2	2.46	0.48
1:A:875:GLN:HA	1:A:878:LEU:HD23	1.94	0.48
1:A:1625:LEU:HB3	1:A:1736:LEU:HD11	1.95	0.48
1:A:4329:TYR:OH	1:A:4369:VAL:O	2.31	0.48
1:A:4810:GLU:HB2	1:A:4819:LEU:HD23	1.94	0.48
1:A:1931:VAL:HG13	1:A:1935:LEU:HD23	1.95	0.48
1:A:3017:GLN:HB3	1:A:3194:GLU:HG3	1.95	0.48
1:A:4312:GLN:NE2	1:A:4600:GLN:OE1	2.47	0.48
1:A:1782:PRO:HG2	1:A:1812:GLN:HB3	1.94	0.48
1:A:3086:LYS:HG3	1:A:3101:VAL:HB	1.96	0.48
2:B:128:GLU:HG2	2:B:136:PHE:HB2	1.94	0.48
1:A:1981:PRO:HB2	1:A:2014:VAL:HG13	1.95	0.48
1:A:3610:LEU:HD13	1:A:3698:LEU:HD21	1.95	0.48
1:A:4427:PRO:HA	1:A:4617:ARG:HD2	1.96	0.48
1:A:2920:LEU:HD22	1:A:2948:PHE:HE2	1.79	0.48
1:A:3834:GLN:HE22	1:A:4846:ASN:HB3	1.79	0.48
1:A:2961:THR:O	1:A:2968:ARG:NH1	2.47	0.48
1:A:3257:ASP:OD1	1:A:3406:ARG:NH2	2.47	0.48
1:A:4574:LEU:HA	1:A:4577:MET:HG2	1.96	0.48
1:A:1704:VAL:HA	1:A:1707:THR:HG22	1.96	0.47
1:A:1751:MET:SD	1:A:1751:MET:N	2.87	0.47
1:A:2728:LEU:HD23	1:A:2861:VAL:HB	1.95	0.47
1:A:3492:LEU:O	1:A:3493:ARG:NH1	2.39	0.47
1:A:1031:TRP:NE1	1:A:1033:ASP:HB2	2.30	0.47
1:A:1301:GLU:OE2	1:A:1302:ARG:NH1	2.46	0.47
1:A:2600:ARG:NH2	1:A:2856:ASN:O	2.47	0.47
1:A:4499:THR:OG1	1:A:4500:GLN:N	2.46	0.47
1:A:912:TRP:HZ3	1:A:930:LEU:HD22	1.79	0.47
1:A:1722:VAL:HA	1:A:1725:LYS:HG2	1.96	0.47
1:A:2701:THR:HG22	1:A:2994:LEU:HD22	1.97	0.47
1:A:1885:ASP:O	1:A:1887:GLN:NE2	2.47	0.47
1:A:1804:PRO:HD3	1:A:2084:PHE:HE1	1.78	0.47
1:A:3253:ASN:ND2	1:A:3257:ASP:OD2	2.48	0.47
1:A:4164:GLN:HG2	1:A:4171:SER:H	1.78	0.47
1:A:1200:LEU:HB3	1:A:1204:LYS:HE3	1.97	0.47
1:A:4759:HIS:HB2	1:A:4765:ARG:HG2	1.96	0.47
1:A:777:LYS:HE2	1:A:830:ALA:H	1.79	0.47
1:A:2564:ASP:HB3	1:A:2610:ARG:HH12	1.80	0.47
1:A:2495:MET:HA	1:A:2498:ARG:HG2	1.96	0.47
1:A:1627:GLU:HB2	1:A:1736:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3960:LEU:HB2	1:A:3964:HIS:HB2	1.98	0.46
1:A:4322:TYR:CE2	1:A:4394:VAL:HG21	2.50	0.46
1:A:4573:GLN:HA	1:A:4576:LYS:HG2	1.96	0.46
1:A:815:LEU:HB3	1:A:873:THR:HG21	1.97	0.46
1:A:1083:LEU:HD23	1:A:1124:LEU:HD13	1.97	0.46
1:A:627:SER:HA	1:A:726:VAL:HG12	1.98	0.46
1:A:1118:LYS:HG2	1:A:1121:ARG:HH22	1.79	0.46
1:A:1279:GLU:O	1:A:1283:ASP:HB2	2.15	0.46
1:A:4404:HIS:O	1:A:4404:HIS:ND1	2.48	0.46
1:A:1368:GLN:HA	1:A:1371:GLN:HG2	1.96	0.46
1:A:4201:LEU:HB3	1:A:4205:LYS:HB2	1.96	0.46
1:A:4257:ARG:HH11	1:A:4258:LYS:HB2	1.80	0.46
1:A:1277:TYR:CE2	1:A:1307:LYS:HG2	2.50	0.46
1:A:1553:ASN:ND2	1:A:3039:TYR:OH	2.35	0.46
1:A:1800:SER:OG	1:A:1801:GLU:OE1	2.30	0.46
1:A:2818:LEU:HD22	1:A:2821:LEU:HD22	1.98	0.46
1:A:3975:LEU:HD23	1:A:3993:PHE:HD2	1.81	0.46
1:A:3140:GLN:OE1	1:A:3142:TRP:NE1	2.46	0.46
1:A:3958:VAL:HG11	1:A:3971:ILE:HG21	1.97	0.46
1:A:4257:ARG:HH22	1:A:4670:PRO:HG2	1.81	0.46
1:A:4275:VAL:HG11	1:A:4591:LEU:HA	1.98	0.46
1:A:1091:SER:HA	1:A:1094:LEU:HG	1.98	0.46
1:A:1619:LEU:HD23	1:A:1621:LEU:HD21	1.98	0.46
1:A:2611:TRP:HB2	1:A:2722:LEU:HD21	1.97	0.46
1:A:3486:GLN:HE21	1:A:3510:LEU:HD11	1.81	0.46
1:A:4532:LEU:HA	1:A:4535:LEU:HG	1.97	0.46
1:A:4708:VAL:HG22	1:A:4711:LEU:HB2	1.97	0.46
1:A:1630:ASP:OD1	1:A:1630:ASP:N	2.49	0.46
1:A:4020:VAL:HG12	1:A:4067:LEU:HD23	1.98	0.46
1:A:518:ASP:OD2	1:A:640:ARG:NE	2.49	0.45
1:A:4680:CYS:SG	1:A:4681:SER:N	2.90	0.45
1:A:1052:THR:HG1	1:A:1055:GLY:H	1.61	0.45
1:A:2491:HIS:ND1	1:A:2495:MET:SD	2.90	0.45
1:A:4115:GLU:HG2	1:A:4886:GLN:HE22	1.82	0.45
1:A:886:ARG:HD3	1:A:3236:SER:HB3	1.98	0.45
1:A:1495:SER:HG	1:A:1498:SER:H	1.58	0.45
1:A:2209:LYS:HA	1:A:2212:VAL:HB	1.98	0.45
1:A:3005:LEU:HD23	1:A:3113:LYS:HA	1.98	0.45
1:A:4431:GLU:O	1:A:4788:THR:OG1	2.33	0.45
1:A:987:LEU:HA	1:A:990:LEU:HD13	1.98	0.45
1:A:1811:MET:HE1	1:A:1921:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:GLU:HG3	1:A:3544:ARG:HD2	1.98	0.45
1:A:1968:HIS:CE1	1:A:1982:LEU:HB2	2.52	0.45
1:A:2576:ILE:HG12	1:A:2646:LEU:HD13	1.98	0.45
1:A:3068:TYR:HE2	1:A:3124:LEU:HB2	1.81	0.45
1:A:3903:SER:OG	1:A:3907:LYS:NZ	2.50	0.45
1:A:4408:LEU:HD21	1:A:4596:LEU:HD21	1.98	0.45
1:A:5002:GLN:HG2	1:A:5003:THR:H	1.82	0.45
1:A:1200:LEU:O	1:A:1204:LYS:HG2	2.16	0.45
1:A:3655:VAL:HG12	1:A:3716:ASP:OD1	2.17	0.45
1:A:3974:TRP:O	1:A:3979:GLN:NE2	2.47	0.45
1:A:1981:PRO:HD2	1:A:2014:VAL:HG22	1.98	0.44
1:A:2080:PRO:HB2	1:A:2081:LEU:H	1.66	0.44
1:A:5080:ILE:HD13	1:A:5132:ILE:HG22	1.99	0.44
1:A:1421:ASP:HA	1:A:1424:ARG:HE	1.82	0.44
1:A:3026:GLU:HB2	1:A:3057:LYS:HE2	1.99	0.44
1:A:646:ARG:HD2	1:A:646:ARG:HA	1.80	0.44
1:A:982:SER:HA	1:A:3201:LEU:HD21	2.00	0.44
1:A:2100:ILE:HD13	1:A:2159:LEU:HD23	2.00	0.44
1:A:506:LEU:HD23	1:A:509:ILE:HD11	1.98	0.44
1:A:852:SER:OG	1:A:866:TYR:OH	2.35	0.44
1:A:1987:LEU:HD13	1:A:2018:ILE:HG23	1.99	0.44
1:A:3686:VAL:HG22	1:A:3762:PRO:HG2	1.99	0.44
1:A:1687:ALA:HA	1:A:1690:MET:HG2	1.99	0.44
1:A:2580:LEU:HD13	1:A:2602:VAL:HG13	2.00	0.44
1:A:3073:ASP:HA	1:A:3076:ASN:HD22	1.82	0.44
1:A:4150:GLU:OE2	1:A:4180:ARG:NH1	2.51	0.44
1:A:4257:ARG:NH1	1:A:4258:LYS:HB2	2.31	0.44
1:A:1377:ARG:HG3	1:A:1459:TRP:CZ3	2.52	0.44
1:A:2719:CYS:HB2	1:A:2726:LEU:HD23	2.00	0.44
1:A:1986:ARG:HD3	1:A:2019:ASP:HB2	1.99	0.44
1:A:2272:ASP:OD1	1:A:2272:ASP:N	2.49	0.44
1:A:2389:ARG:HA	1:A:2392:LYS:HG2	1.99	0.44
1:A:2509:SER:HB3	1:A:2512:GLU:HG3	1.99	0.44
1:A:2907:GLN:HE22	1:A:2912:PHE:H	1.66	0.44
1:A:5014:GLN:H	1:A:5017:HIS:HD2	1.66	0.44
1:A:1875:GLN:HB2	1:A:5148:ARG:HH22	1.83	0.44
1:A:4529:THR:HA	1:A:4532:LEU:HG	2.00	0.44
1:A:839:ALA:HB1	1:A:914:ARG:HH21	1.83	0.43
1:A:1044:ASN:HB3	1:A:1046:LYS:HG2	2.00	0.43
1:A:1456:GLN:OE1	1:A:1460:ARG:NH1	2.50	0.43
1:A:1781:ARG:NH2	1:A:1817:PRO:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2424:LYS:HA	1:A:2427:GLU:HG2	2.00	0.43
1:A:3281:SER:OG	1:A:3282:ARG:N	2.51	0.43
1:A:1394:LEU:HD13	1:A:1439:LEU:HD13	1.99	0.43
1:A:2802:VAL:HG23	1:A:2842:PHE:HD1	1.83	0.43
1:A:3028:ILE:HD13	1:A:3059:VAL:HG13	2.00	0.43
1:A:3662:ARG:HD2	1:A:3720:LEU:HD13	2.00	0.43
1:A:4646:ILE:HG22	1:A:4662:TYR:HE2	1.83	0.43
1:A:1031:TRP:HD1	1:A:1034:VAL:HG23	1.84	0.43
1:A:1621:LEU:HD23	1:A:1621:LEU:H	1.82	0.43
1:A:2455:ALA:O	1:A:2458:CYS:HB2	2.17	0.43
1:A:3706:GLN:HA	1:A:3709:LEU:HG	2.00	0.43
1:A:892:ARG:NH2	1:A:941:GLU:OE1	2.52	0.43
1:A:1556:MET:HG3	1:A:3047:ASN:HB2	2.01	0.43
1:A:3346:SER:HA	1:A:3349:LEU:HD23	2.01	0.43
2:B:124:ASP:N	2:B:124:ASP:OD1	2.52	0.43
1:A:2423:SER:HA	1:A:2426:LYS:HE2	1.99	0.43
1:A:3200:ASP:N	1:A:3200:ASP:OD1	2.51	0.43
1:A:1451:PHE:HA	1:A:1454:HIS:CD2	2.53	0.43
1:A:2457:SER:O	1:A:2460:LYS:HB3	2.19	0.43
1:A:3219:ASP:OD2	1:A:3397:ARG:NH2	2.52	0.43
2:B:143:PHE:HA	2:B:146:LYS:HG2	2.01	0.43
1:A:1013:HIS:HB3	1:A:1017:PRO:HG2	2.00	0.43
1:A:4604:VAL:HG12	1:A:4607:PHE:HE1	1.84	0.43
1:A:1319:ALA:HA	1:A:1322:ILE:HG22	2.00	0.42
1:A:1860:ASP:O	1:A:1896:ARG:NH1	2.50	0.42
1:A:3312:ASP:OD1	1:A:3312:ASP:N	2.50	0.42
1:A:1054:GLU:OE2	1:A:1057:GLN:NE2	2.49	0.42
1:A:1276:LYS:NZ	1:A:2882:ASP:OD1	2.52	0.42
1:A:882:ARG:HA	1:A:885:LEU:HG	2.01	0.42
1:A:3025:PRO:HB3	1:A:3058:MET:HB2	2.02	0.42
1:A:4225:ARG:HH11	1:A:4256:PRO:HA	1.83	0.42
2:B:47:ASP:O	2:B:151:ARG:NE	2.52	0.42
2:B:105:ILE:HA	2:B:108:LEU:HG	2.01	0.42
1:A:1643:GLU:HA	1:A:1646:LEU:HG	2.02	0.42
1:A:2295:ASN:HD21	1:A:2300:LYS:HD3	1.84	0.42
1:A:2430:ARG:HA	1:A:2430:ARG:NH1	2.33	0.42
1:A:3002:LEU:HB2	1:A:3108:ILE:HG12	2.02	0.42
1:A:4264:LYS:HG3	1:A:4266:HIS:H	1.85	0.42
1:A:4792:ILE:HD12	1:A:4825:ALA:HA	2.00	0.42
1:A:4258:LYS:HE3	1:A:4669:LEU:HD23	2.02	0.42
1:A:4724:VAL:HG12	1:A:4863:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1963:TYR:CZ	1:A:2091:VAL:HG11	2.54	0.42
1:A:2222:ASP:OD2	1:A:2264:HIS:ND1	2.43	0.42
1:A:4295:LYS:NZ	1:A:4298:ASP:HB3	2.34	0.42
1:A:3516:ASP:OD1	1:A:3516:ASP:N	2.53	0.42
1:A:3539:GLU:HA	1:A:3542:GLN:HG2	2.02	0.42
1:A:3597:LEU:HD23	1:A:3607:VAL:HG13	2.02	0.42
1:A:4547:ALA:HA	1:A:4550:VAL:HG22	2.02	0.42
1:A:689:GLU:HG2	1:A:770:TYR:CD1	2.55	0.42
1:A:1456:GLN:HA	1:A:1459:TRP:HD1	1.83	0.42
1:A:2315:LEU:HD23	1:A:2320:VAL:HG11	2.01	0.42
1:A:2827:ASP:HB2	1:A:2834:PRO:HB3	2.01	0.42
1:A:640:ARG:NH1	1:A:3674:TYR:OH	2.51	0.42
1:A:3726:SER:HB3	1:A:3729:GLU:HB3	2.02	0.42
1:A:5044:ILE:HD11	1:A:5132:ILE:HD13	2.02	0.42
1:A:642:ARG:HD2	1:A:4765:ARG:HH12	1.85	0.41
1:A:808:GLU:HG2	1:A:810:LEU:HD23	2.02	0.41
1:A:3958:VAL:HG21	1:A:3993:PHE:HB2	2.02	0.41
1:A:3821:LYS:HG3	1:A:3869:LEU:HD11	2.02	0.41
1:A:4988:ASP:HA	1:A:5014:GLN:HG3	2.02	0.41
1:A:1054:GLU:O	1:A:1057:GLN:HG3	2.20	0.41
1:A:1395:HIS:NE2	1:A:1439:LEU:O	2.51	0.41
1:A:1586:VAL:HG13	1:A:1646:LEU:HD23	2.01	0.41
1:A:2018:ILE:O	1:A:2059:VAL:HA	2.20	0.41
1:A:2755:GLU:OE1	1:A:2758:ARG:NH1	2.48	0.41
1:A:3058:MET:HG2	1:A:3106:ARG:HB2	2.02	0.41
1:A:3157:PHE:HE2	1:A:3242:LEU:HD13	1.85	0.41
1:A:4731:LEU:HD21	1:A:4827:VAL:HG11	2.03	0.41
1:A:662:ASP:OD1	1:A:662:ASP:N	2.54	0.41
1:A:1131:LYS:HA	1:A:1134:VAL:HG12	2.01	0.41
1:A:1710:CYS:SG	1:A:1711:GLU:N	2.93	0.41
1:A:2388:THR:HA	1:A:2391:ILE:HG12	2.03	0.41
1:A:4307:ARG:HG3	1:A:4308:SER:H	1.86	0.41
1:A:5033:ARG:HE	1:A:5038:LYS:HB2	1.86	0.41
1:A:5144:ASP:O	1:A:5148:ARG:HB3	2.21	0.41
1:A:2507:ARG:HE	1:A:2508:VAL:HG13	1.85	0.41
1:A:2694:LEU:HD22	1:A:2710:LYS:HG2	2.01	0.41
1:A:5092:SER:OG	2:B:63:PHE:O	2.35	0.41
1:A:801:TYR:HD2	1:A:805:ILE:HD11	1.85	0.41
1:A:1018:VAL:HG23	1:A:1019:PHE:H	1.86	0.41
1:A:1324:GLN:HG3	1:A:1385:ALA:HB1	2.01	0.41
1:A:973:ILE:HG12	1:A:1004:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:VAL:HG22	1:A:1147:LEU:HB2	2.03	0.41
1:A:3769:GLN:OE1	1:A:3772:ARG:NH2	2.53	0.41
1:A:2428:ALA:HA	1:A:2431:THR:HG22	2.03	0.41
1:A:669:PRO:HG3	1:A:730:LEU:HD22	2.02	0.40
1:A:1806:ALA:HB2	1:A:1857:LEU:HD21	2.03	0.40
1:A:2805:ASP:HA	1:A:2845:ILE:HG23	2.01	0.40
1:A:4410:PRO:HB3	1:A:4611:LEU:HG	2.04	0.40
1:A:4895:ASP:OD1	1:A:4895:ASP:N	2.54	0.40
1:A:1365:LYS:HA	1:A:1365:LYS:HD3	1.84	0.40
1:A:2021:SER:OG	1:A:2022:THR:N	2.54	0.40
1:A:2722:LEU:HD23	1:A:2722:LEU:HA	1.86	0.40
1:A:3780:ARG:HH21	1:A:3842:PRO:HB3	1.85	0.40
1:A:3871:ASN:HA	1:A:4026:MET:HE1	2.03	0.40
1:A:2946:ARG:HG3	1:A:2978:LEU:HD22	2.03	0.40
1:A:3611:TRP:HD1	1:A:3656:PRO:HB3	1.87	0.40
1:A:1377:ARG:HD3	1:A:1462:LEU:HD22	2.03	0.40
1:A:1383:GLU:HB3	1:A:1472:LEU:HD23	2.04	0.40
1:A:1950:ILE:HG21	1:A:2085:LEU:HD12	2.03	0.40
1:A:2367:ILE:HG22	1:A:2371:PHE:HE1	1.86	0.40
1:A:4106:GLN:HA	1:A:4109:LYS:HG2	2.02	0.40
1:A:4232:LEU:HD22	1:A:4240:PHE:HE2	1.86	0.40
1:A:4409:LYS:HG2	1:A:4412:ARG:HH22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4394/5161 (85%)	3983 (91%)	404 (9%)	7 (0%)	44 75
2	B	151/166 (91%)	150 (99%)	1 (1%)	0	100 100
All	All	4545/5327 (85%)	4133 (91%)	405 (9%)	7 (0%)	45 75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4600	GLN
1	A	1374	SER
1	A	4049	GLN
1	A	4166	PRO
1	A	5128	MET
1	A	2547	ASN
1	A	1373	ILE

5.3.2 Protein sidechains (i)

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	3970/4604 (86%)	3953 (100%)	17 (0%)	89 95
2	B	135/148 (91%)	135 (100%)	0	100 100
All	All	4105/4752 (86%)	4088 (100%)	17 (0%)	88 95

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	923	LYS
1	A	1101	ARG
1	A	1119	ARG
1	A	1281	LYS
1	A	2206	ARG
1	A	2319	ARG
1	A	3199	ARG
1	A	3368	LYS
1	A	3544	ARG
1	A	3798	LYS
1	A	4176	GLN
1	A	4257	ARG
1	A	4295	LYS
1	A	4348	LYS
1	A	4598	ARG
1	A	4633	LYS

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Mol	Chain	Res	Type
1	A	4701	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1210	GLN
1	A	1314	GLN
1	A	2981	GLN
1	A	4276	HIS
1	A	4534	HIS
1	A	4590	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	5201	4	26,33,33	0.60	0	31,52,52	0.74	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	5201	4	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5201	ATP	C5-C6-N6	2.27	123.81	120.35
3	A	5201	ATP	PB-O3B-PG	2.00	139.69	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5201	ATP	O4'-C4'-C5'-O5'
3	A	5201	ATP	C3'-C4'-C5'-O5'
3	A	5201	ATP	PA-O3A-PB-O2B

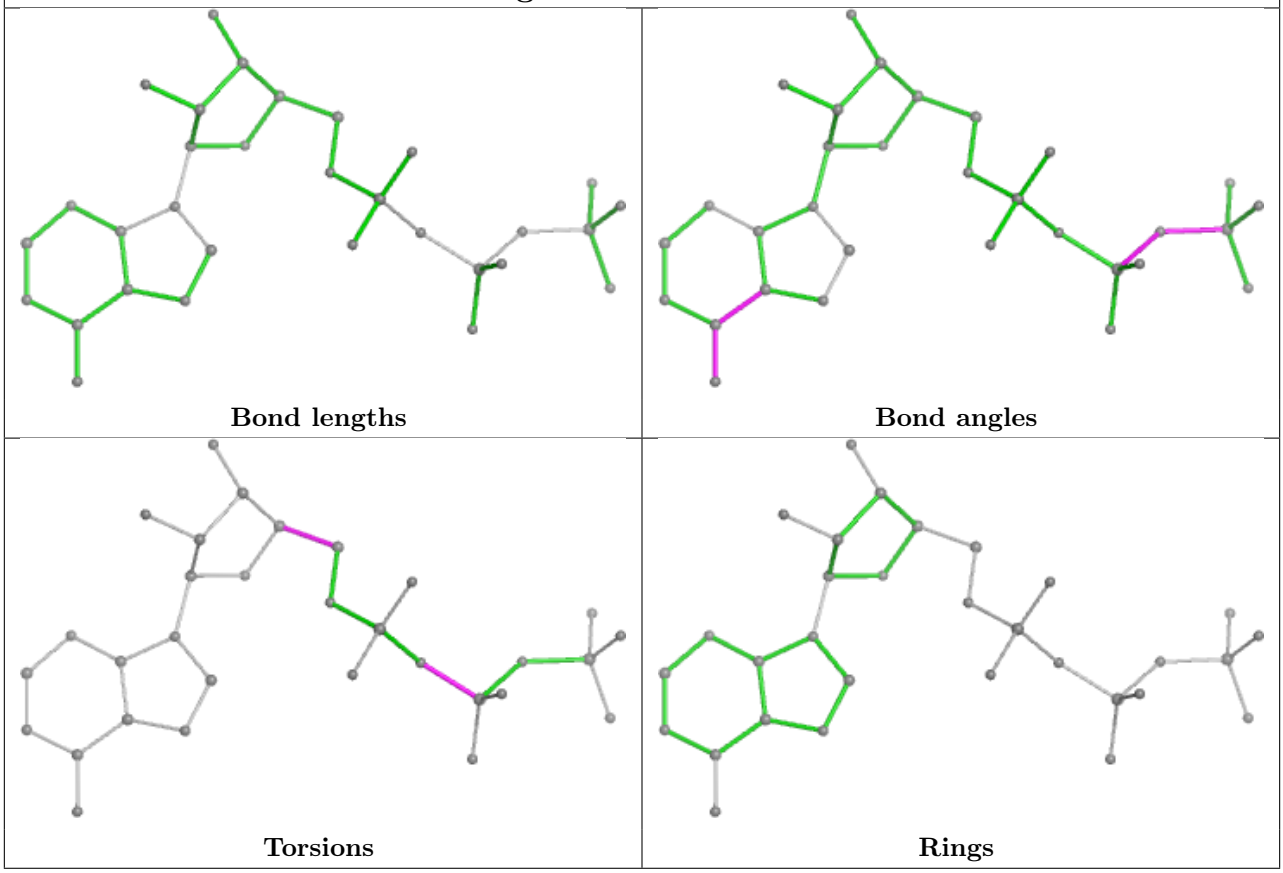
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5201	ATP	1	0

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

Ligand ATP A 5201



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.

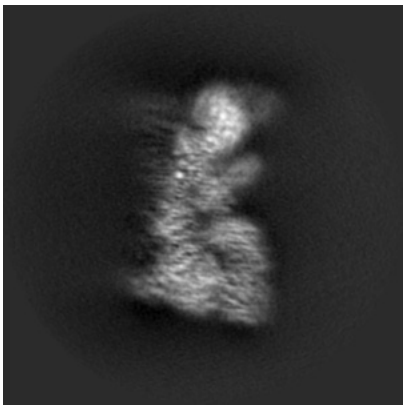
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12931. These allow visual inspection of the internal detail of the map and identification of artifacts.

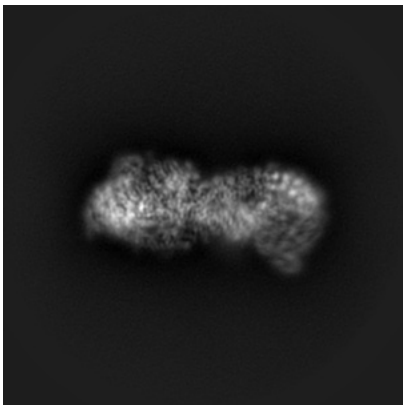
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

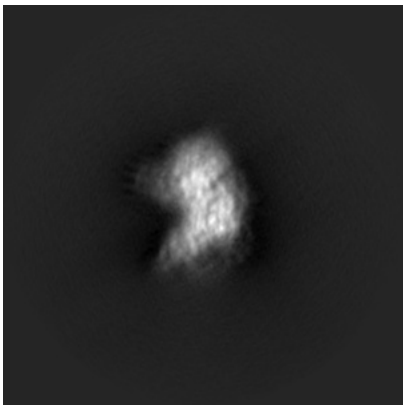
6.1.1 Primary map



X

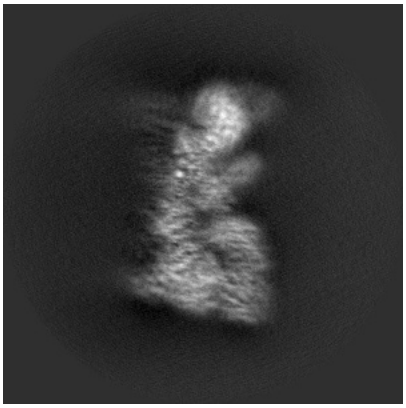


Y

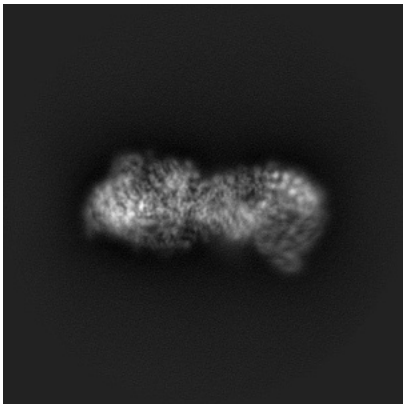


Z

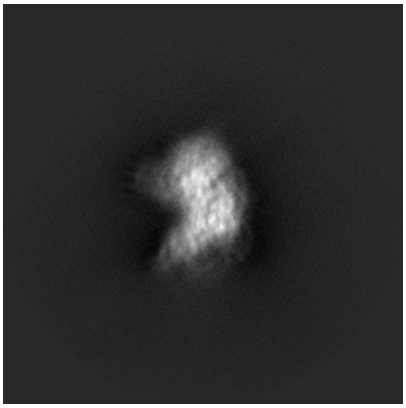
6.1.2 Raw map



X



Y

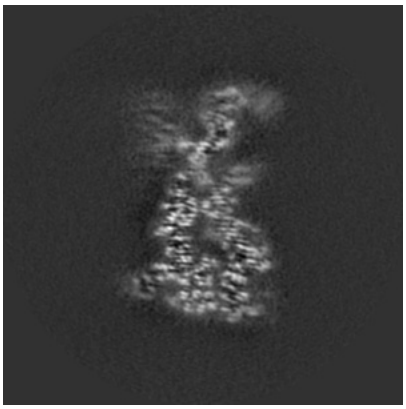


Z

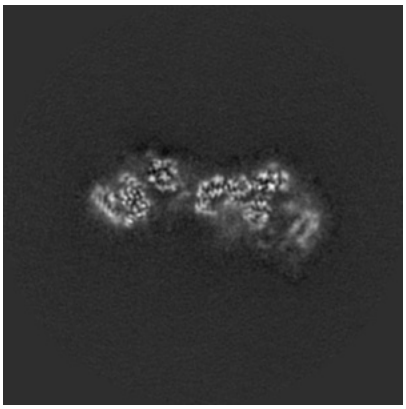
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

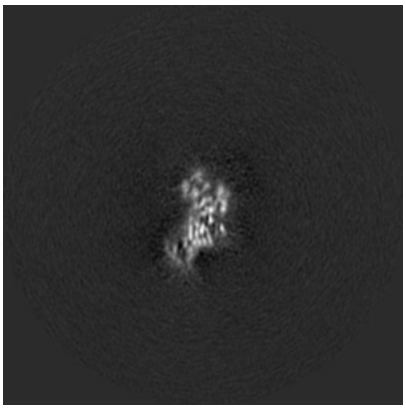
6.2.1 Primary map



X Index: 176

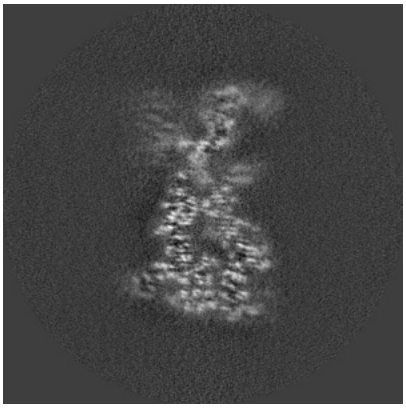


Y Index: 176

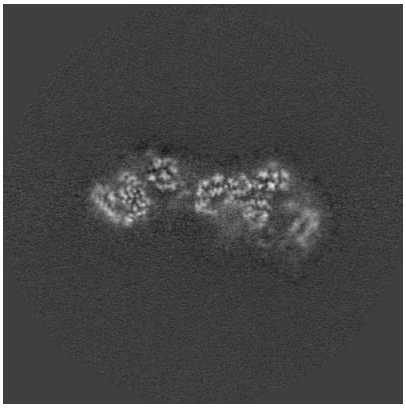


Z Index: 176

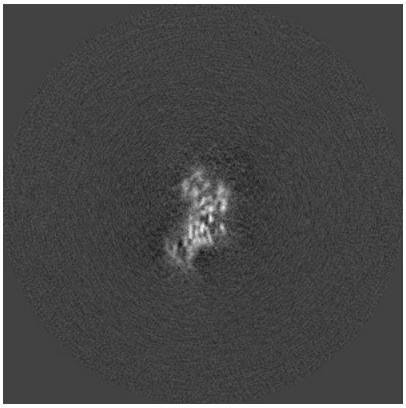
6.2.2 Raw map



X Index: 176



Y Index: 176

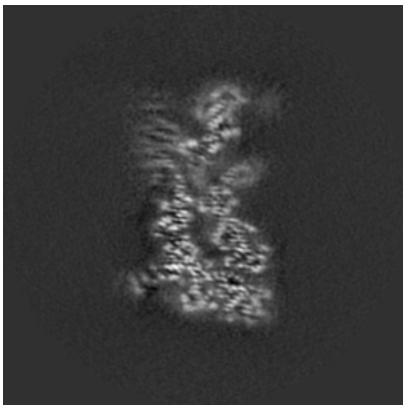


Z Index: 176

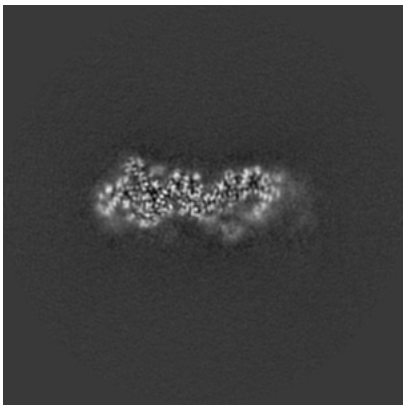
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

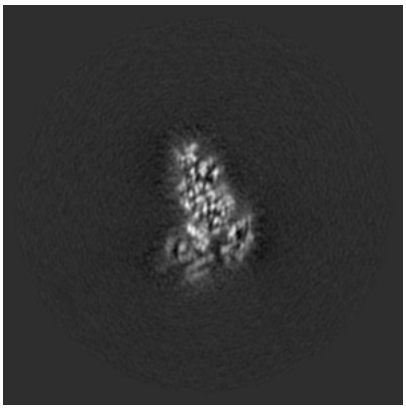
6.3.1 Primary map



X Index: 172

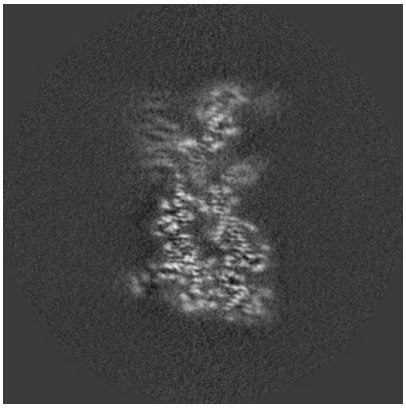


Y Index: 159

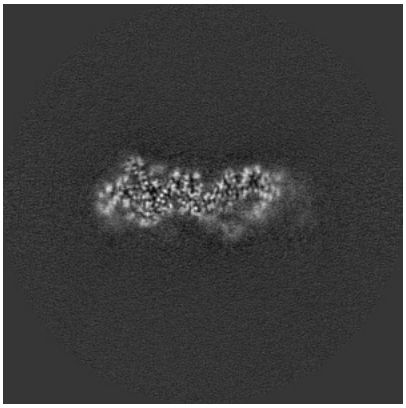


Z Index: 111

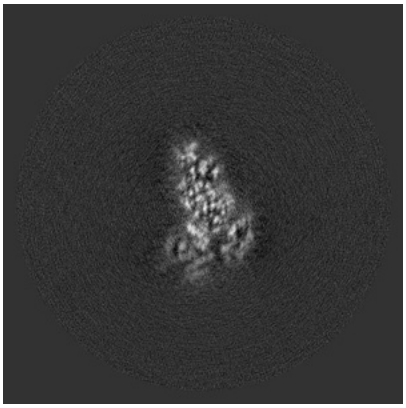
6.3.2 Raw map



X Index: 173



Y Index: 159

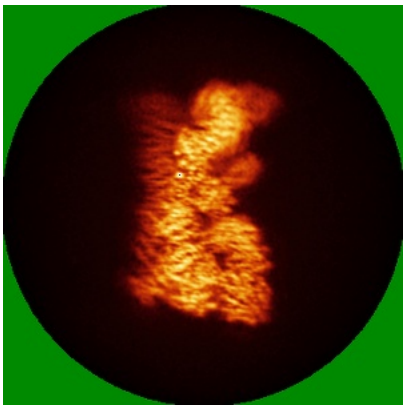


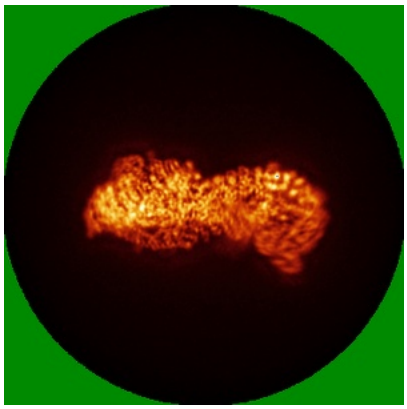
Z Index: 111

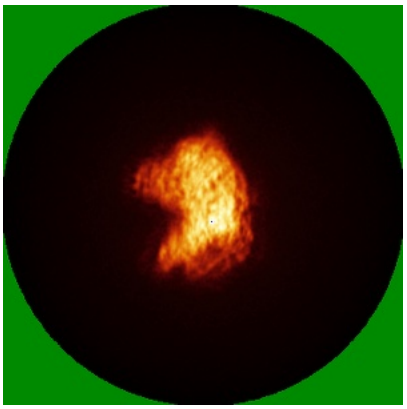
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

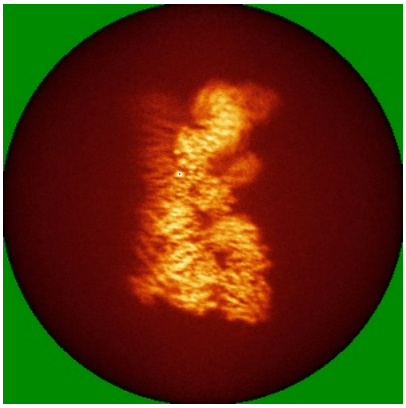
6.4.1 Primary map

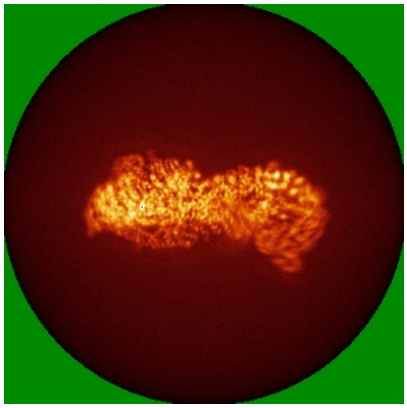

X

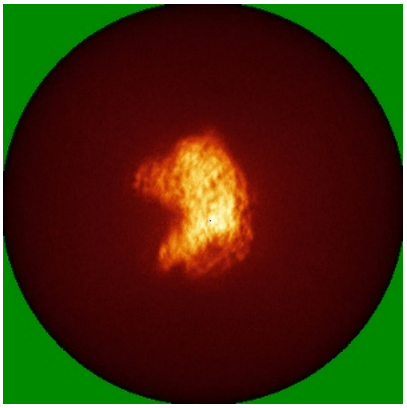

Y


Z

6.4.2 Raw map


X

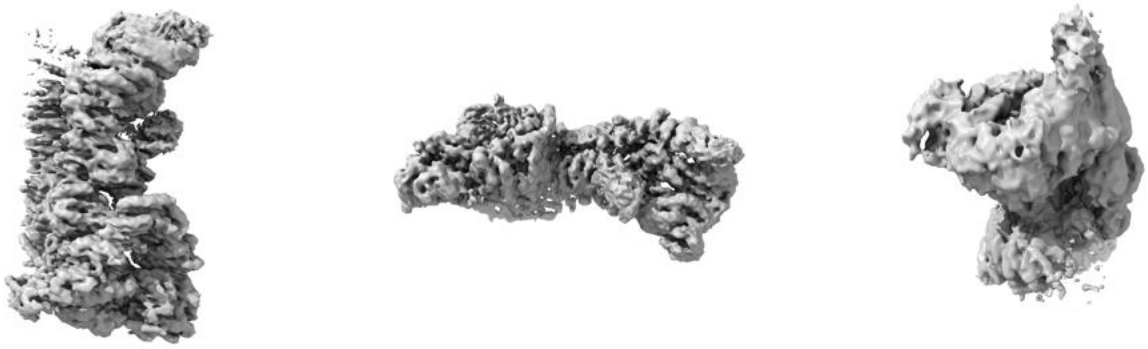

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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

X Y Z

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.

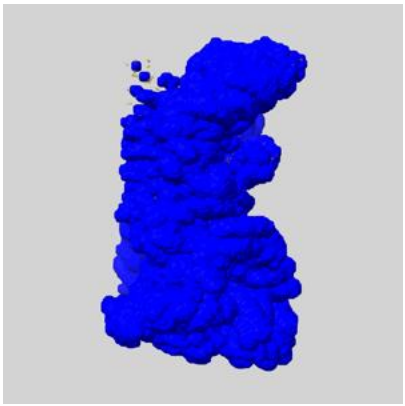
6.6 Mask visualisation

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

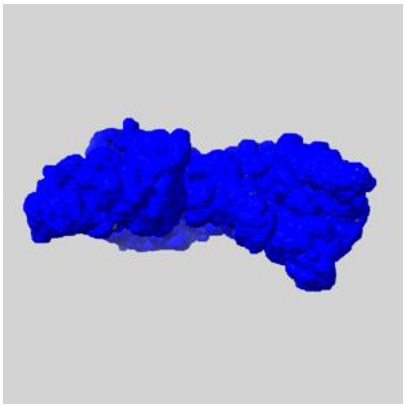
A mask typically either:

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

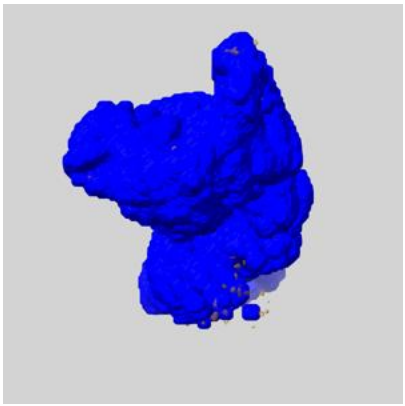
6.6.1 emd_12931_msk_1.map



X



Y

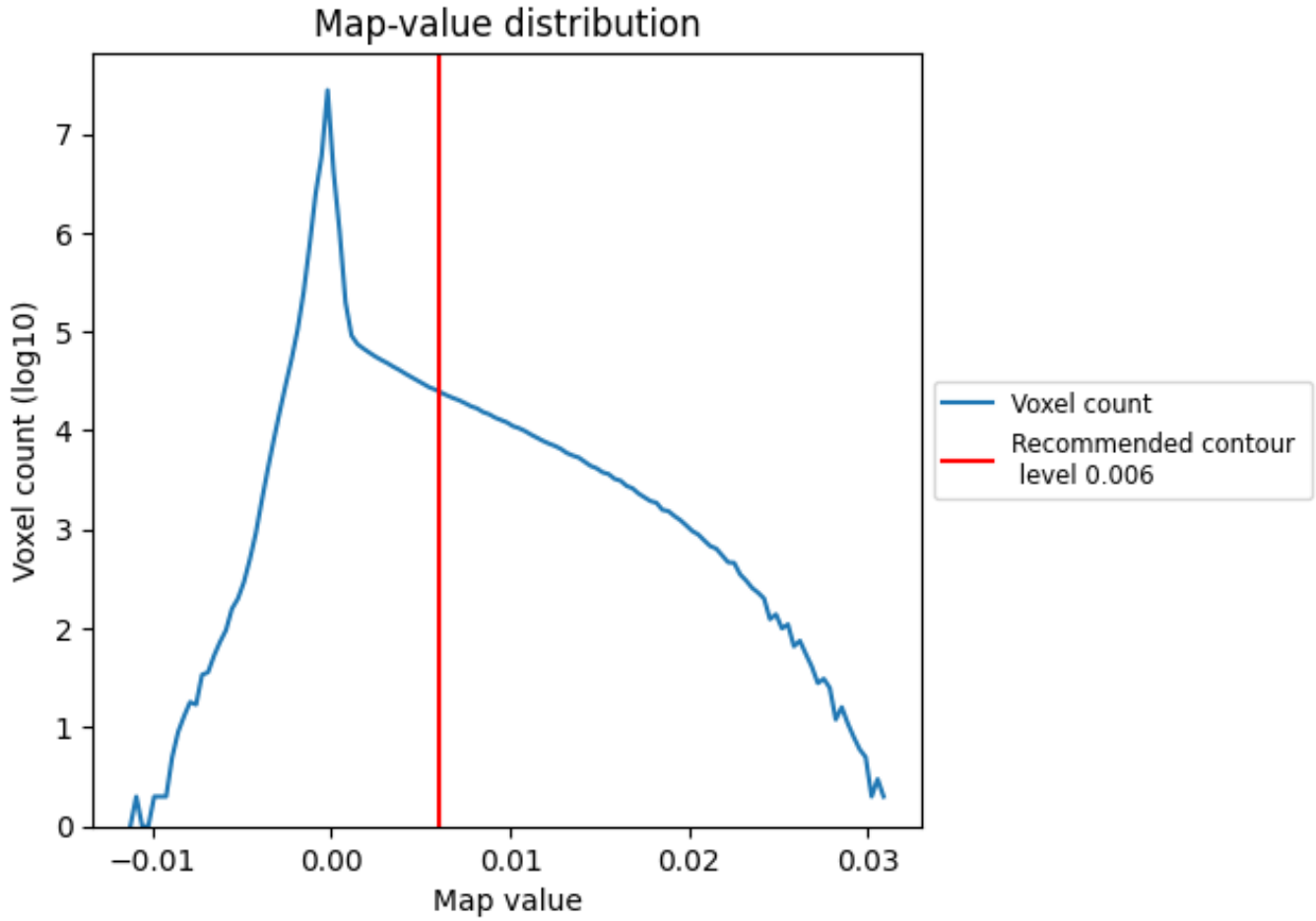


Z

7 Map analysis

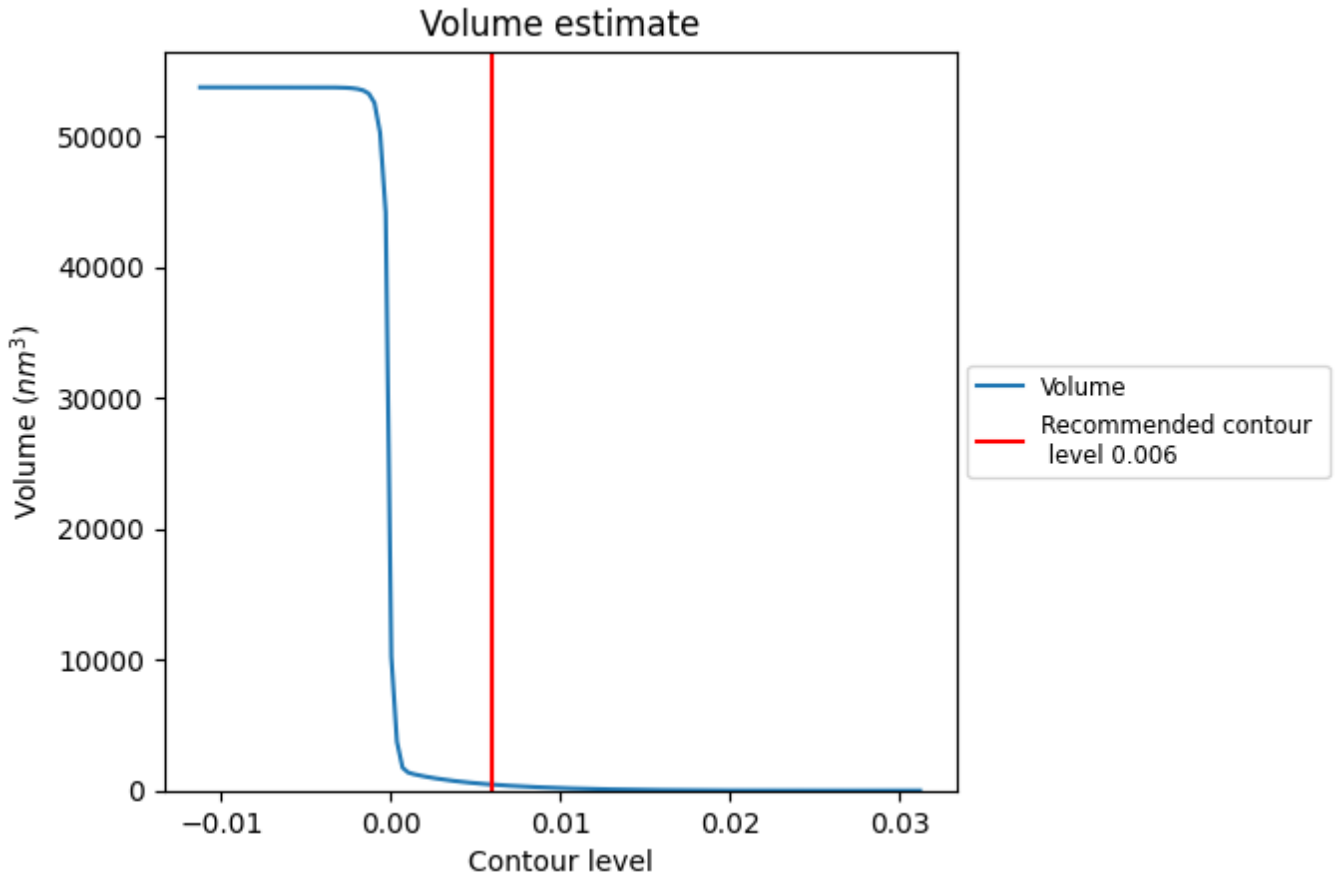
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

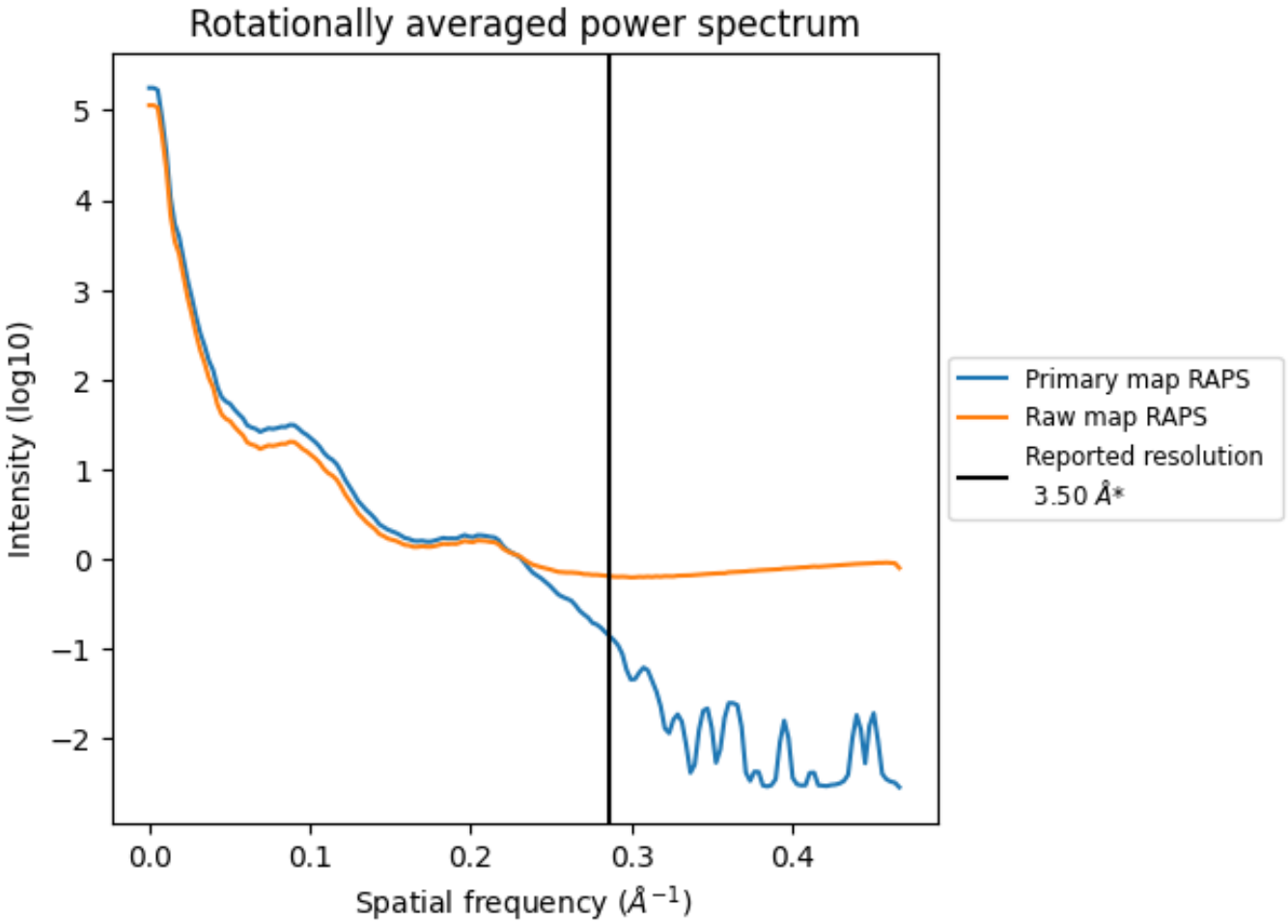
7.2 Volume estimate



The volume at the recommended contour level is 457 nm^3; this corresponds to an approximate mass of 412 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 (i)

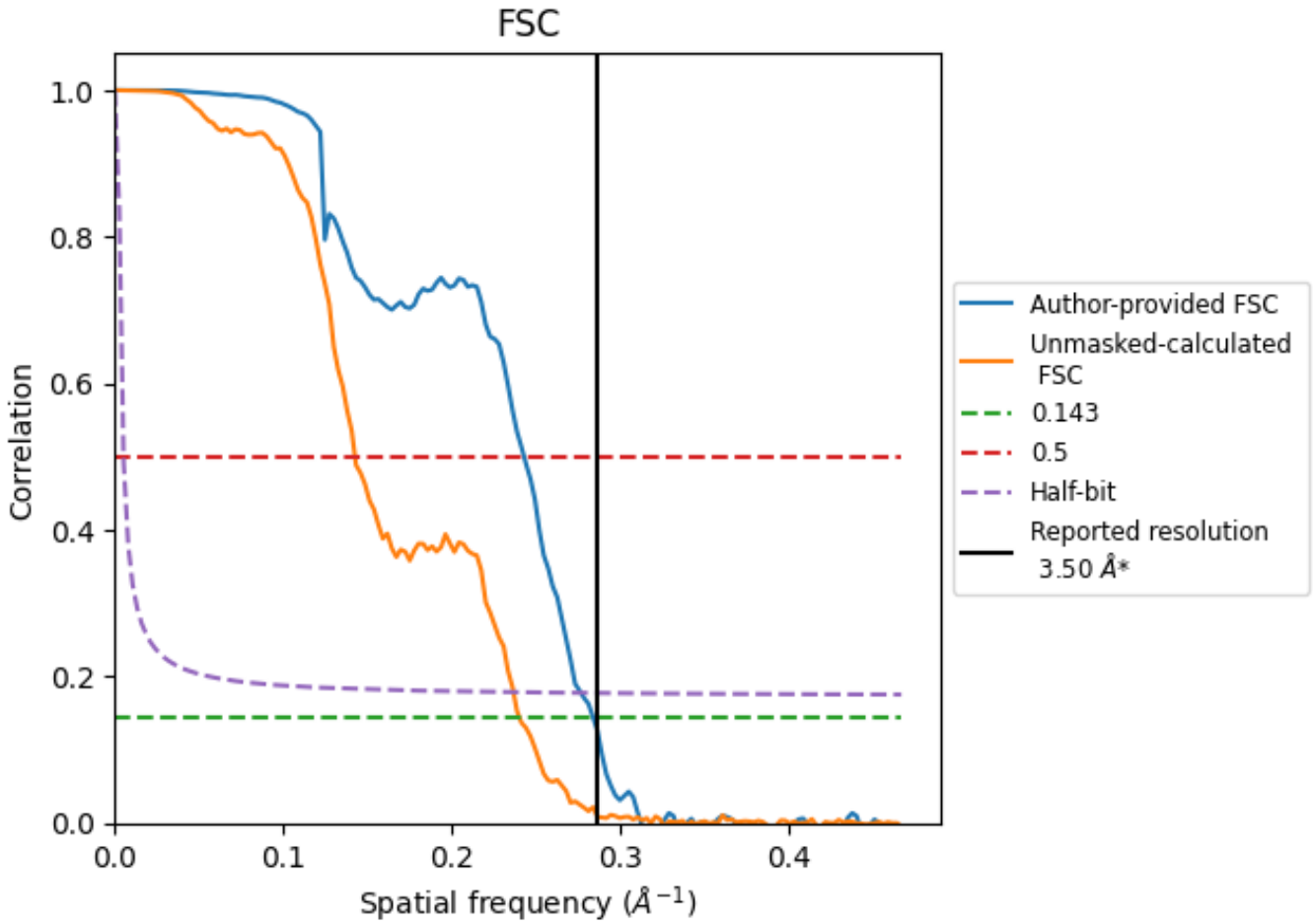


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

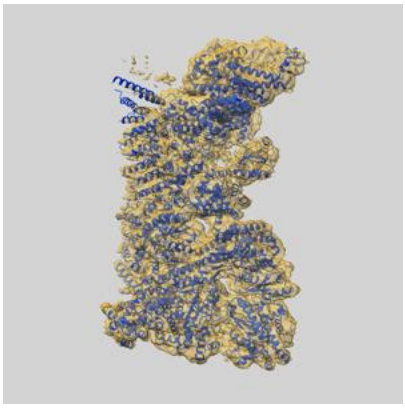
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.12	3.62
Unmasked-calculated*	4.16	7.02	4.23

*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 4.16 differs from the reported value 3.5 by more than 10 %

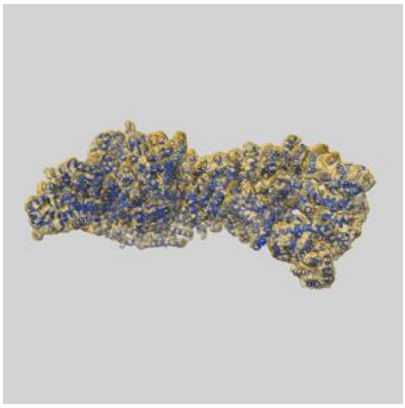
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12931 and PDB model 7OIK. Per-residue inclusion information can be found in section 3 on page 6.

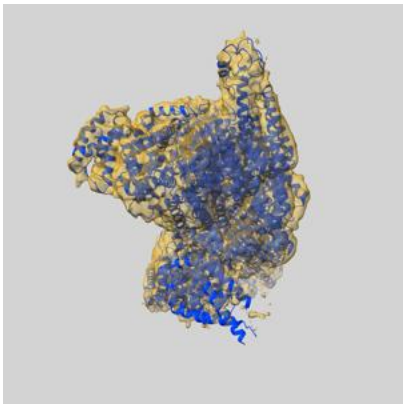
9.1 Map-model overlay



X



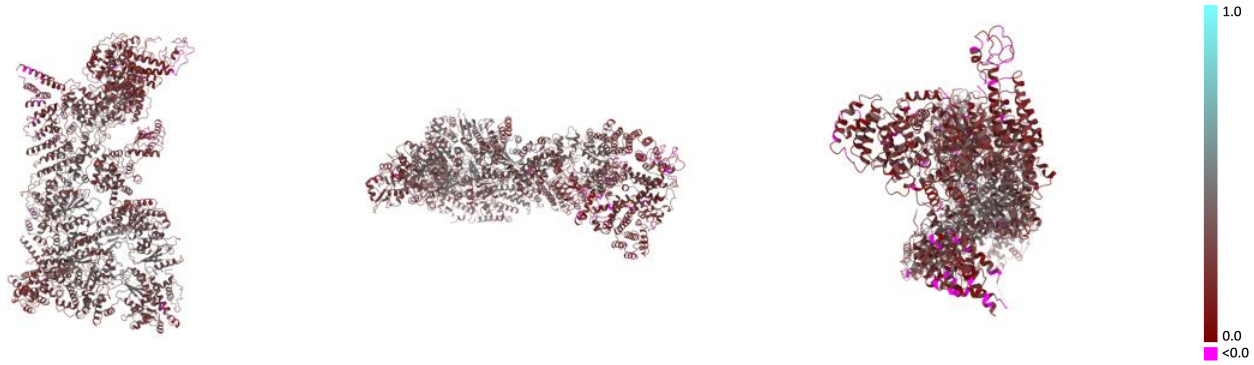
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

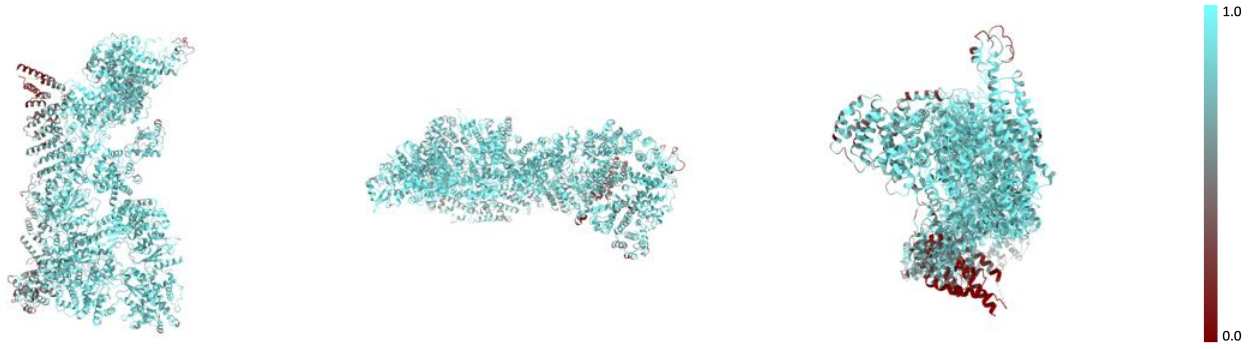
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

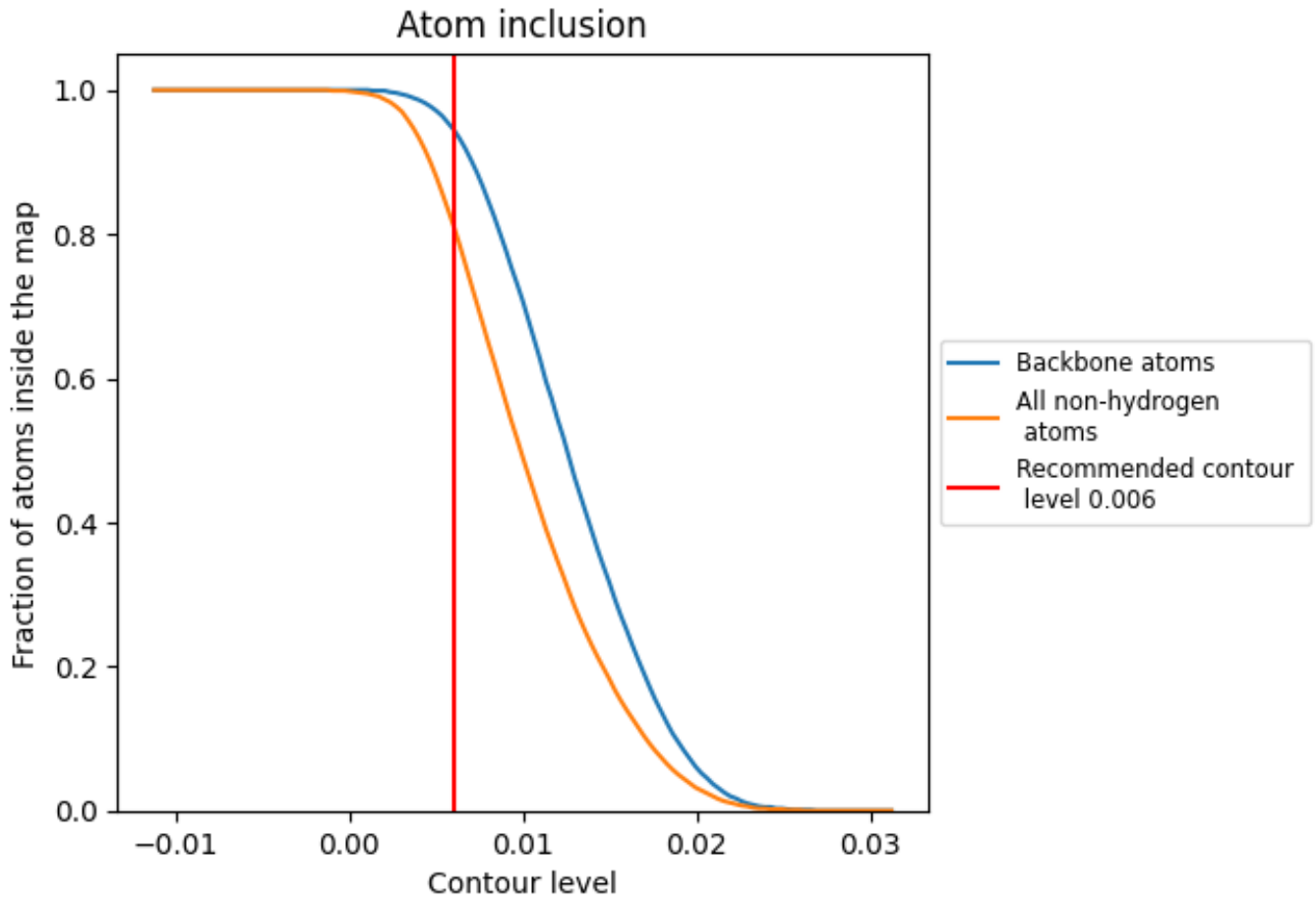
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.2940
A	0.8130	0.2970
B	0.7660	0.1960