wwPDB EM Validation Summary Report

Mar 7, 2026 – 01:44 AM UTC

PDB ID	:	9G08 / pdb_00009g08
EMDB ID	:	EMD-50913
Title	:	Structure of human RNF213 bound to the secreted effector IpaH1.4 from Shigella flexneri
Authors	:	Naydenova, K.; Randow, F.
Deposited on	:	2024-07-07
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Validation Summary 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:

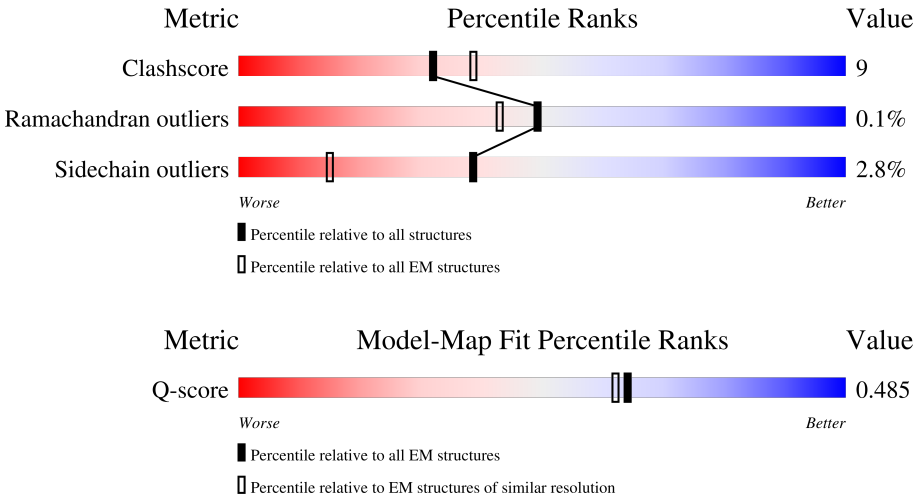
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	5247	7% 68% 17% • 14%
2	B	575	8% 27% 14% • 59%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 77075 atoms, of which 38644 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	H	N	O	S		
1	A	4529	73234	23323	36721	6289	6681	220	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP Q63HN8
A	-38	ALA	-	expression tag	UNP Q63HN8
A	-37	SER	-	expression tag	UNP Q63HN8
A	-36	TRP	-	expression tag	UNP Q63HN8
A	-35	SER	-	expression tag	UNP Q63HN8
A	-34	HIS	-	expression tag	UNP Q63HN8
A	-33	PRO	-	expression tag	UNP Q63HN8
A	-32	GLN	-	expression tag	UNP Q63HN8
A	-31	PHE	-	expression tag	UNP Q63HN8
A	-30	GLU	-	expression tag	UNP Q63HN8
A	-29	LYS	-	expression tag	UNP Q63HN8
A	-28	GLY	-	expression tag	UNP Q63HN8
A	-27	SER	-	expression tag	UNP Q63HN8
A	-26	ALA	-	expression tag	UNP Q63HN8
A	-25	GLY	-	expression tag	UNP Q63HN8
A	-24	SER	-	expression tag	UNP Q63HN8
A	-23	ALA	-	expression tag	UNP Q63HN8
A	-22	ALA	-	expression tag	UNP Q63HN8
A	-21	GLY	-	expression tag	UNP Q63HN8
A	-20	SER	-	expression tag	UNP Q63HN8
A	-19	GLY	-	expression tag	UNP Q63HN8
A	-18	ALA	-	expression tag	UNP Q63HN8
A	-17	GLY	-	expression tag	UNP Q63HN8
A	-16	TRP	-	expression tag	UNP Q63HN8
A	-15	SER	-	expression tag	UNP Q63HN8
A	-14	HIS	-	expression tag	UNP Q63HN8
A	-13	PRO	-	expression tag	UNP Q63HN8
A	-12	GLN	-	expression tag	UNP Q63HN8

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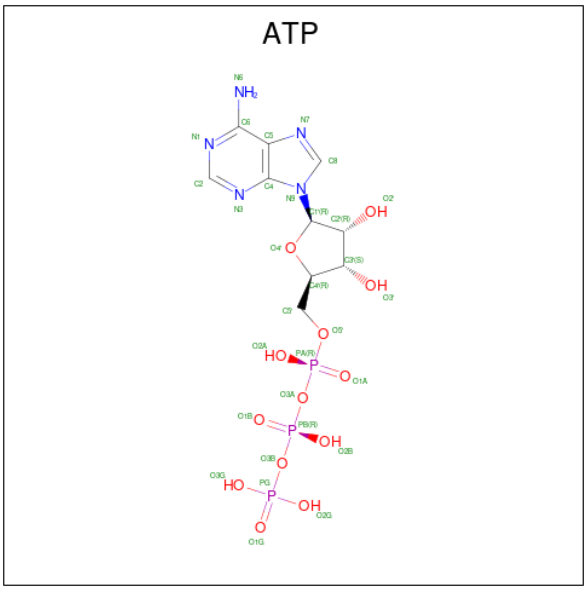
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	PHE	-	expression tag	UNP Q63HN8
A	-10	GLU	-	expression tag	UNP Q63HN8
A	-9	LYS	-	expression tag	UNP Q63HN8
A	-8	GLU	-	expression tag	UNP Q63HN8
A	-7	ASN	-	expression tag	UNP Q63HN8
A	-6	LEU	-	expression tag	UNP Q63HN8
A	-5	TYR	-	expression tag	UNP Q63HN8
A	-4	PHE	-	expression tag	UNP Q63HN8
A	-3	GLN	-	expression tag	UNP Q63HN8
A	-2	ALA	-	expression tag	UNP Q63HN8
A	-1	MET	-	expression tag	UNP Q63HN8
A	0	SER	-	expression tag	UNP Q63HN8

- Molecule 2 is a protein called E3 ubiquitin-protein ligase IpaH1.4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	237	3794	1205	1911	322	349	7	0	0

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



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	43	10	12	5	13	3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

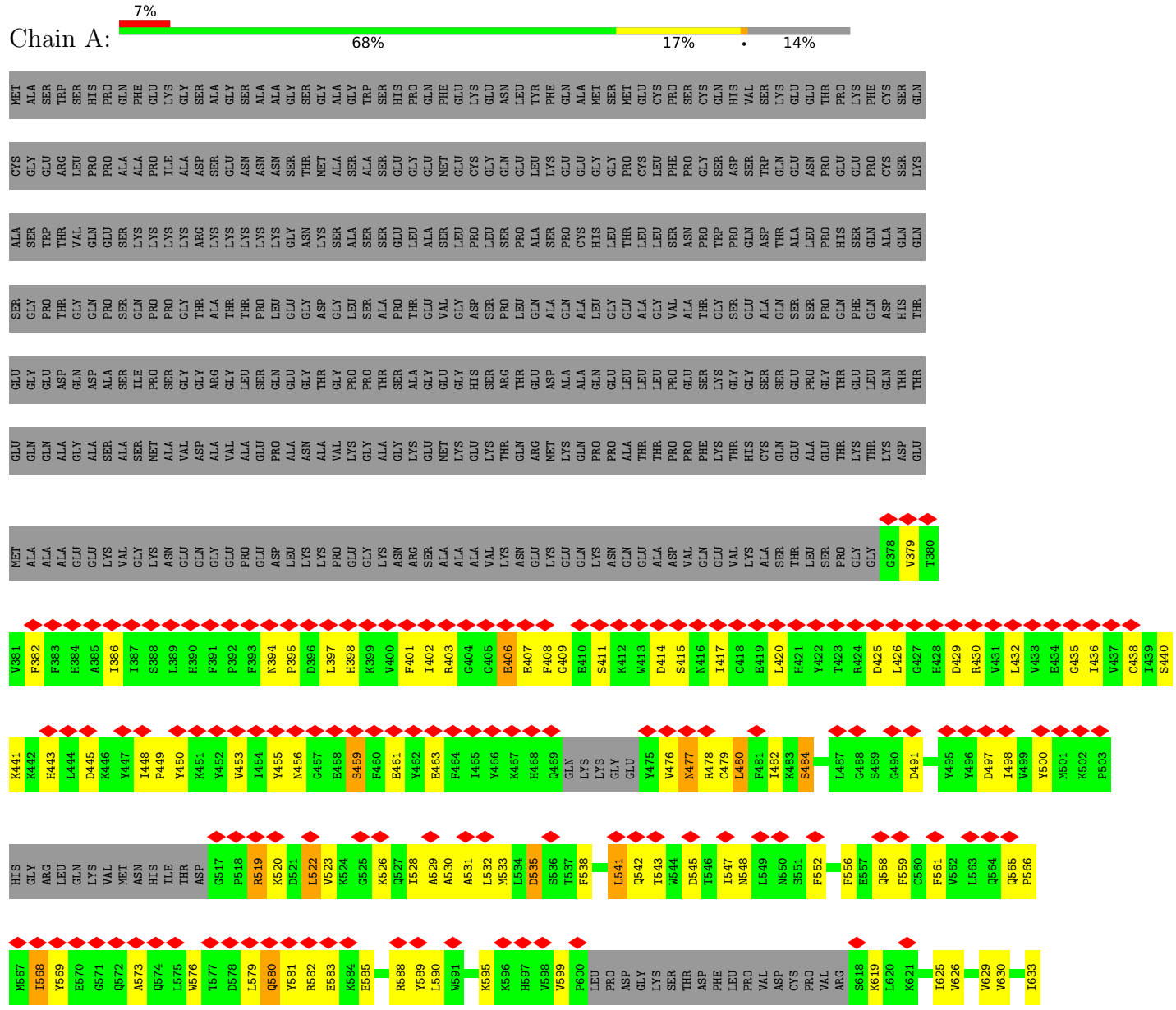
Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	Zn	0
			3	3	

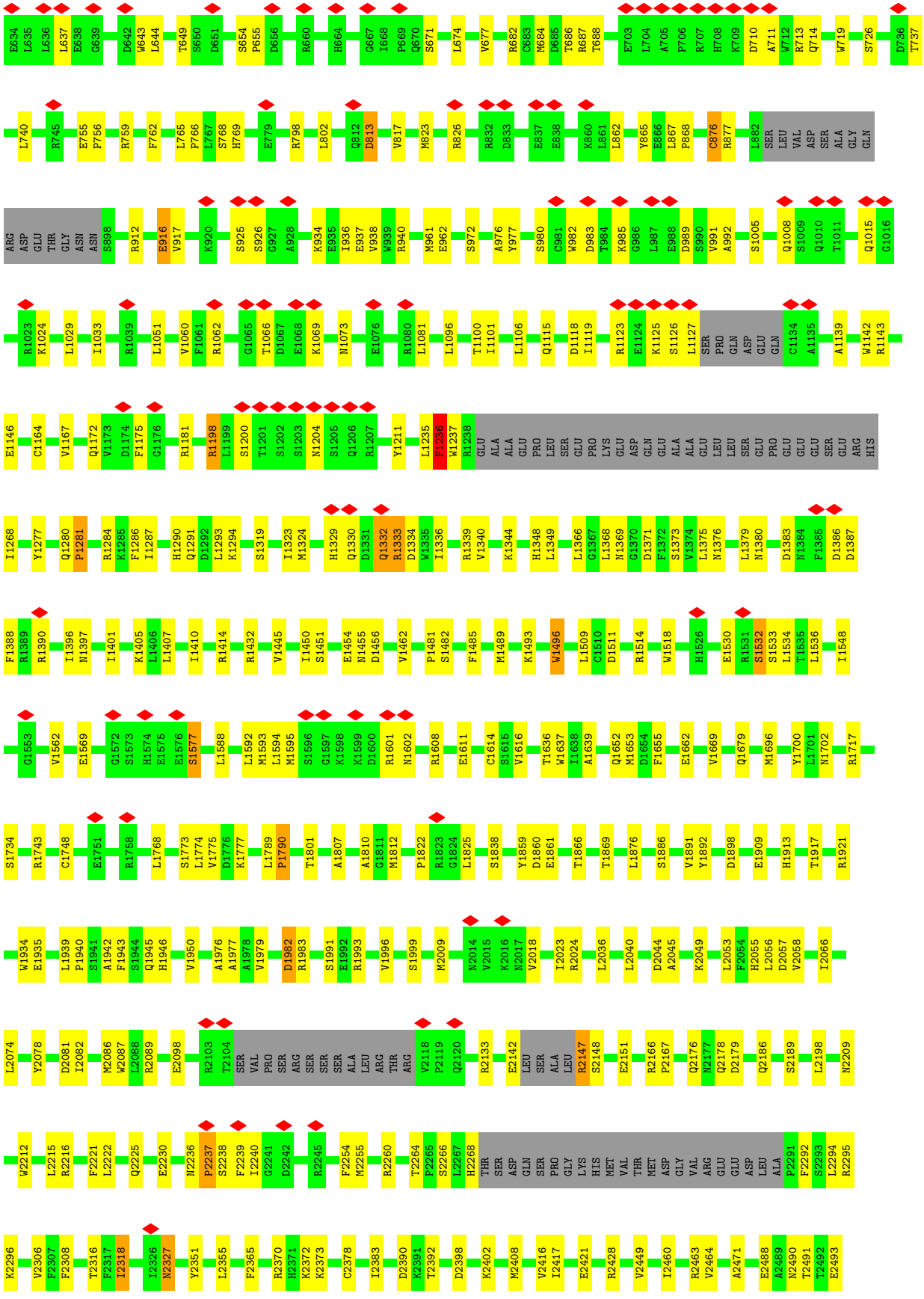
3 Residue-property plots (i)

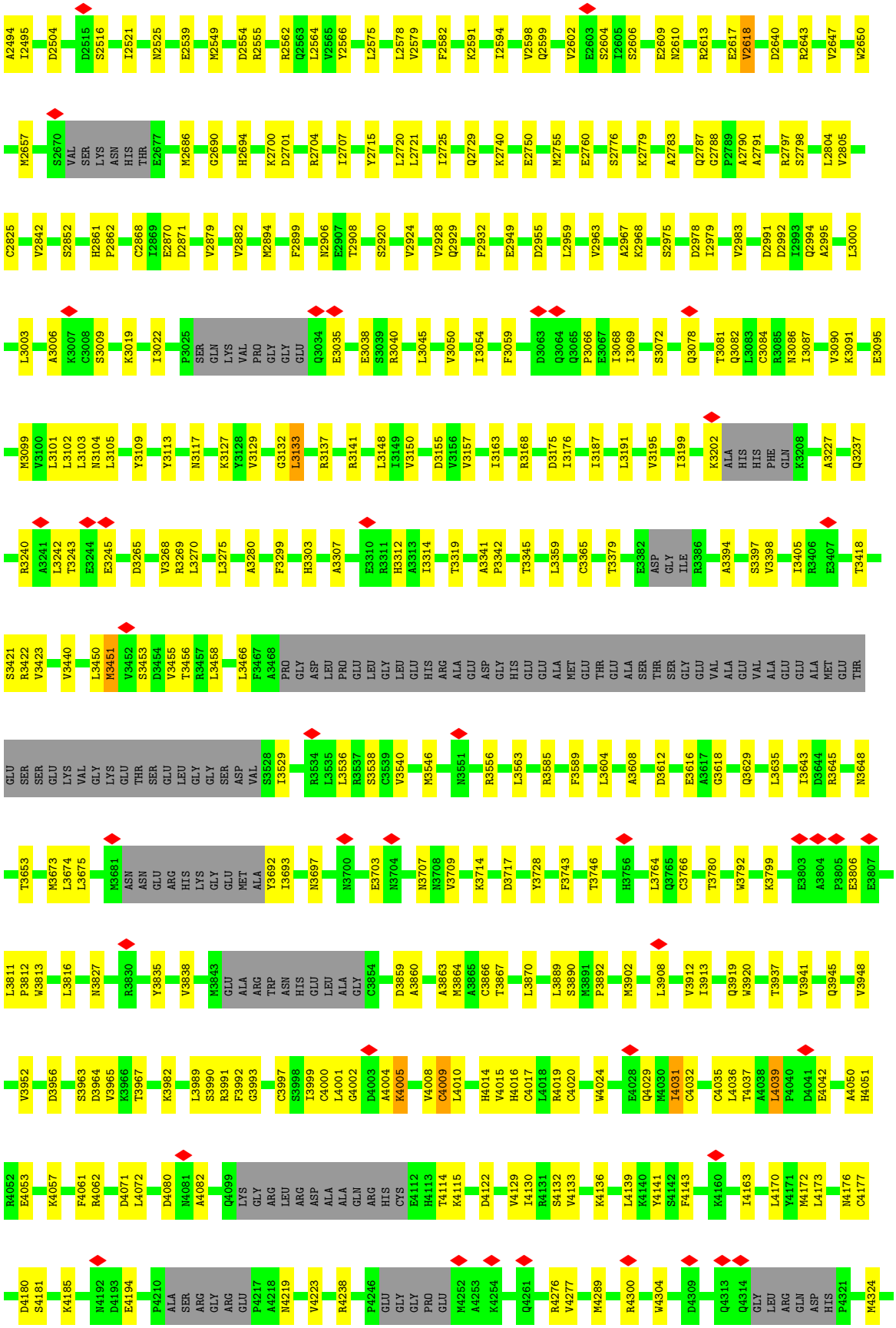
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

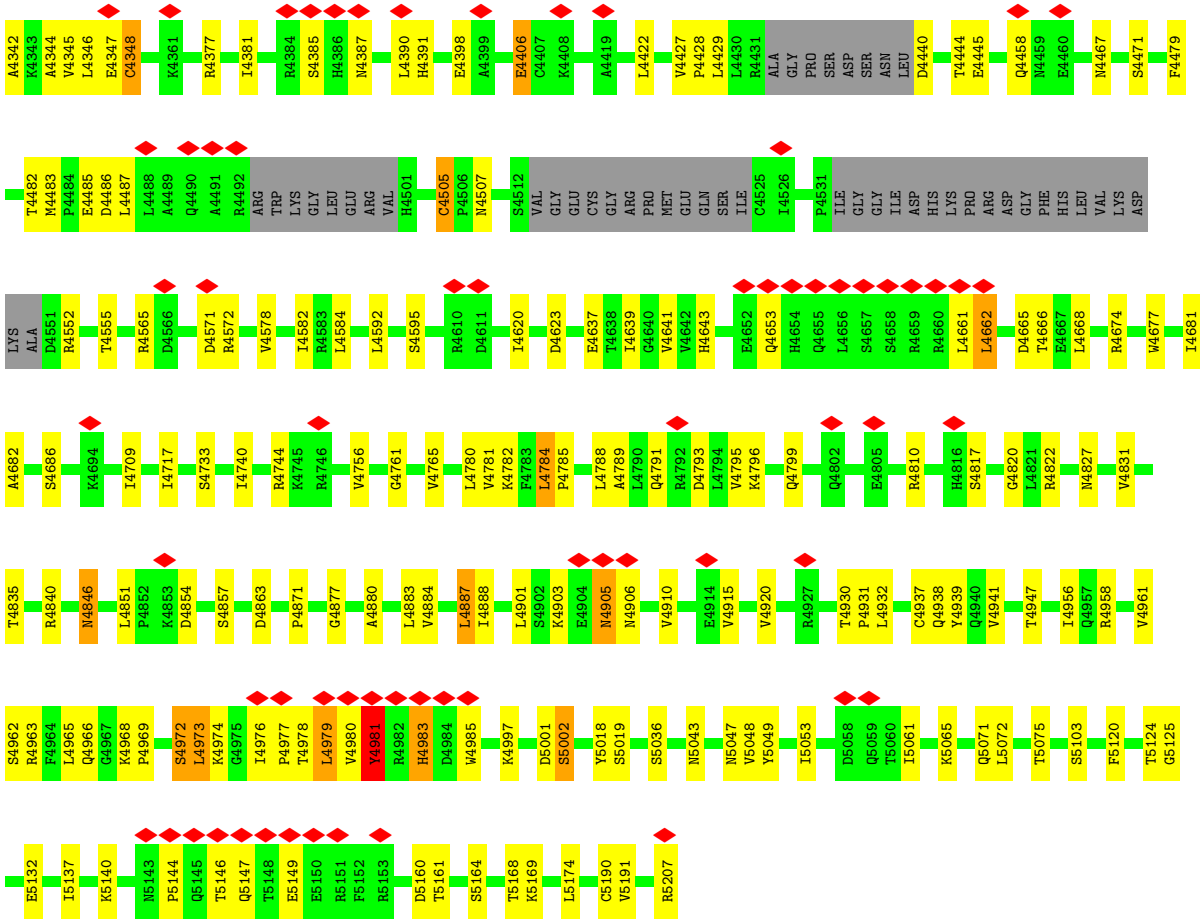
- Molecule 1: E3 ubiquitin-protein ligase RNF213

Chain A:




E634 L635 L636 L637 E638 G639 D642 W643 L644 T649 S650 D651 S654 P655 D656 R660 H664 G667 I668 P669 Q670 S671 L674 V677 R682 C683 M684 D685 T686 R687 T688 E703 L704 A705 P706 R707 H708 K709 D710 A711 W712 R713 Q714 W719 S726 D736 T737
L740 R745 E755 P756 R759 F762 L765 P766 L767 S768 H769 E779 R798 L802 Q812 D813 V817 M823 R826 R832 D833 E837 E838 K860 L861 L862 Y865 E866 L867 P868 C876 R877 L882 SER LEU VAL ASP SER ALA GLY GLN
ARG ASP GLU THR GLY ASN ASN S898 R912 E916 V917 K920 S925 S926 G927 A928 K934 E935 I936 E937 V938 W939 R940 M961 E962 S972 A976 Y977 S980 C981 W982 D983 T984 K985 G986 L987 E988 D989 S990 V991 A992 S1005 Q1008 S1009 Q1010 T1011 Q1015 G1016
R1023 K1024 L1029 I1033 R1039 L1051 V1060 F1061 R1062 G1065 T1066 D1067 E1068 K1069 N1073 E1076 R1080 L1081 L1096 T1100 I1101 L1106 Q1115 D1118 I1119 R1123 E1124 K1125 S1126 L1127 SER PRO GLN ASP GLU GLN C1134 A1135 A1139 W1142 R1143
E1146 C1164 V1167 Q1172 V1173 D1174 F1175 G1176 R1181 R1198 L1199 S1200 T1201 S1202 S1203 N1204 S1205 Q1206 R1207 Y1211 L1235 F1236 W1237 R1238 GLU ALA ALA GLU PRO LEU SER GLU PRO LYS GLU ASP GLN GLU ALA ALA GLU LEU LEU SER GLU PRO GLU GLU GLU SER GLU ARG HIS
I1268 Y1277 Q1280 P1281 R1284 K1285 F1286 I1287 H1290 Q1291 D1292 L1293 K1294 S1319 I1323 M1324 H1329 Q1330 D1331 Q1332 R1333 D1334 W1335 I1336 R1339 V1340 K1344 H1348 L1349 L1366 G1367 L1368 N1369 G1370 D1371 F1372 S1373 V1374 L1375 N1376 L1379 N1380 D1383 N1384 F1385 D1386 D1387
F1388 R1389 R1390 I1396 N1397 I1401 K1405 K1406 L1407 I1410 R1414 R1432 V1445 I1450 S1451 E1454 N1455 D1456 V1462 P1481 S1482 F1485 M1489 K1493 W1496 L1509 C1510 D1511 R1514 W1518 H1526 E1530 R1531 S1532 S1533 L1534 T1535 L1536 I1548
G1553 V1562 E1569 G1572 S1573 H1574 E1575 E1576 S1577 L1588 L1592 M1593 L1594 M1595 S1596 G1597 K1598 K1599 D1600 R1601 N1602 R1608 E1611 C1614 S1615 V1616 T1636 W1637 I1638 A1639 Q1652 M1653 D1654 F1655 E1662 V1669 Q1679 M1696 Y1700 L1701 N1702 R1717
S1734 R1743 C1748 E1751 R1758 L1768 S1773 L1774 V1775 D1776 K1777 L1789 P1790 T1801 A1807 A1810 G1811 M1812 P1822 R1823 G1824 L1825 S1838 Y1859 D1860 E1861 T1866 T1869 L1876 S1886 V1891 Y1892 D1898 E1909 H1913 T1917 R1921
W1934 E1935 L1939 P1940 S1941 A1942 F1943 S1944 Q1945 H1946 V1950 A1976 A1977 A1978 V1979 D1982 R1983 S1991 E1992 R1993 V1996 S1999 M2009 N2014 V2015 K2016 N2017 V2018 I2023 R2024 L2036 L2040 D2044 A2045 K2049 L2053 F2054 H2055 L2056 D2057 V2058 I2066
L2074 Y2078 D2081 I2082 M2086 W2087 L2088 R2089 E2098 R2103 T2104 SER VAL PRO SER ARG SER SER SER ALA LEU ARG THR ARG V2118 P2119 Q2120 R2133 E2142 LEU SER ALA LEU R2147 S2148 E2151 R2166 P2167 Q2176 N2177 Q2178 D2179 Q2186 S2189 L2198 N2209
W2212 L2215 R2216 F2221 L2222 Q2225 E2230 N2236 P2237 S2238 F2239 I2240 G2241 D2242 R2245 F2254 M2255 R2260 T2264 P2265 S2266 L2267 H2268 THR SER ASP GLN SER PRO GLY LYS HIS MET VAL THR MET ASP GLY VAL ARG GLU GLU ASP LEU ALA P2291 F2292 S2293 L2294 R2295
K2296 V2306 F2307 F2308 T2316 F2317 I2318 T2326 N2327 Y2351 L2355 F2365 R2370 H2371 K2372 K2373 C2378 I2383 D2390 K2391 T2392 D2398 K2402 M2408 V2416 I2417 E2421 R2428 V2449 I2460 R2463 V2464 A2471 E2488 A2489 N2490 T2491 T2492 E2493

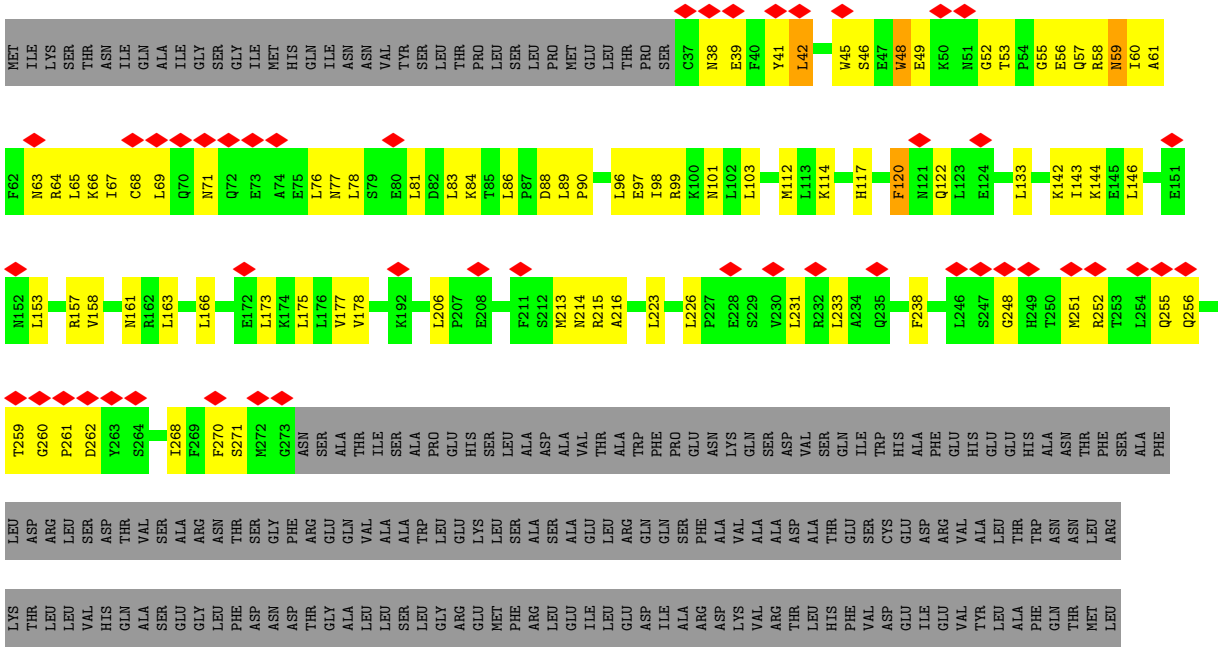

A2494 I2495 D2504 D2515 S2516 I2521 N2525 E2539 M2549 D2554 R2555 R2562 Q2563 L2564 V2565 Y2566 L2575 L2578 V2579 F2582 K2591 I2594 V2598 Q2599 V2602 E2603 S2604 I2605 S2606 E2609 N2610 R2613 E2617 V2618 D2640 R2643 V2647 W2650
M2657 S2670 VAL SER LYS ASN HIS THR E2677 M2686 G2690 H2694 K2700 D2701 R2704 I2707 Y2715 L2720 L2721 I2725 Q2729 K2740 E2750 M2755 E2760 S2776 K2779 A2783 Q2787 G2788 P2789 A2790 A2791 R2797 S2798 L2804 V2805
C2825 V2842 S2852 H2861 P2862 C2868 I2869 E2870 D2871 V2879 V2882 M2894 F2899 N2906 E2907 T2908 S2920 V2924 V2928 Q2929 F2932 E2949 D2955 L2959 V2963 A2967 K2968 S2975 D2978 I2979 V2983 D2991 D2992 I2993 Q2994 A2995 L3000
L3003 A3006 K3007 C3008 S3009 K3019 I3022 P3025 SER GLN LYS VAL PRO GLY GLY GLU Q3034 E3035 E3038 S3039 R3040 L3045 V3050 I3054 F3059 D3063 Q3064 Q3065 P3066 E3067 I3068 I3069 S3072 Q3078 T3081 Q3082 L3083 C3084 R3085 N3086 I3087 V3090 K3091 E3095
M3099 V3100 L3101 L3102 L3103 N3104 L3105 Y3109 Y3113 N3117 K3127 Y3128 V3129 G3132 L3133 R3137 R3141 L3148 I3149 V3150 D3155 V3156 V3157 I3163 R3168 D3175 I3176 I3187 L3191 V3195 I3199 K3202 ALA HIS HIS PHE GLN K3208 A3227 Q3237
R3240 A3241 L3242 T3243 E3244 E3245 D3265 V3268 R3269 L3270 L3275 A3280 F3299 H3303 A3307 E3310 R3311 H3312 A3313 I3314 T3319 A3341 P3342 T3345 L3359 C3365 T3379 E3382 ASP GLY ILE R3386 A3394 S3397 V3398 I3405 R3406 E3407 T3418
S3421 R3422 V3423 V3440 L3450 M3451 V3452 S3453 D3454 V3455 T3456 R3457 L3458 L3466 F3467 A3468 PRO GLY ASP LEU PRO GLU LEU GLY LEU GLU HIS ARG ALA GLU ASP GLY HIS GLU GLU ALA MET GLU THR GLU ALA SER THR SER GLY GLU VAL ALA GLU VAL ALA GLU GLU ALA MET GLU THR
GLU SER SER GLU LYS VAL GLY LYS GLU THR SER GLU LEU GLY GLY SER ASP VAL S3528 I3529 R3534 L3535 L3536 R3537 S3538 C3539 V3540 M3546 N3551 R3556 L3563 R3585 F3589 L3604 A3608 D3612 E3616 A3617 G3618 Q3629 L3635 I3643 D3644 R3645 N3648
T3653 M3673 L3674 L3675 M3681 ASN ASN GLU ARG HIS LYS GLY GLU MET ALA Y3692 I3693 N3697 N3700 E3703 N3704 N3707 N3708 V3709 K3714 D3717 Y3728 F3743 T3746 H3756 L3764 Q3765 C3766 T3780 W3792 K3799 E3803 A3804 P3805 E3806 E3807
L3811 P3812 W3813 L3816 N3827 R3830 Y3835 V3838 M3843 GLU ALA ARG TRP ASN HIS GLU LEU ALA GLY C3854 D3859 A3860 A3863 M3864 A3865 C3866 T3867 L3870 L3889 S3890 M3891 P3892 M3902 L3908 V3912 I3913 Q3919 W3920 T3937 V3941 Q3945 V3948
V3952 D3956 S3963 D3964 V3965 K3966 T3967 K3982 L3989 S3990 R3991 F3992 G3993 C3997 S3998 I3999 C4000 L4001 G4002 D4003 A4004 K4005 V4008 C4009 L4010 H4014 V4015 H4016 C4017 L4018 R4019 C4020 W4024 E4028 Q4029 M4030 I4031 C4032 C4035 L4036 T4037 A4038 L4039 P4040 D4041 E4042 A4050 H4051
R4052 E4053 K4057 F4061 R4062 D4071 L4072 D4080 N4081 A4082 Q4099 LYS GLY ARG LEU ARG ASP ALA ALA GLN ARG HIS CYS E4112 H4113 T4114 K4115 D4122 V4129 I4130 R4131 S4132 V4133 K4136 L4139 K4140 Y4141 S4142 F4143 K4160 I4163 L4170 Y4171 M4172 L4173 N4176 C4177
D4180 S4181 K4185 N4192 D4193 E4194 P4210 ALA SER ARG GLY ARG GLU P4217 A4218 N4219 V4223 R4238 P4246 GLU GLY GLY PRO GLU M4252 A4253 K4254 Q4261 R4276 V4277 M4289 R4300 W4304 D4309 Q4313 Q4314 GLY LEU ARG GLN ASP HIS P4321 M4324



• Molecule 2: E3 ubiquitin-protein ligase IpaH1.4

Chain B:





ALA GLU LYS LEU GLN LEU SER THR ALA VAL LYS GLU MET ARG PHE TYR GLY VAL SER GLY VAL THR ALA ASN ASP LEU ARG THR ALA GLU ALA MET VAL ARG SER ARG GLU GLU ASN GLU PHE THR ASP TRP PHE SER LEU TRP GLY PRO TRP HIS ALA VAL LEU LYS ARG THR GLU ALA

ASP ARG TRP ALA GLN ALA GLU GLU GLN LYS TYR GLU MET LEU GLU ASN GLU TYR SER GLN ARG VAL ALA ASP ARG LEU LYS ALA SER GLY LEU SER GLY ASP ALA ASP ALA GLU ARG GLU ALA GLY ALA GLN VAL MET ARG GLU THR GLU GLN GLN ILE TYR ARG GLN LEU THR ASP GLU

VAL LEU ALA LEU ARG LEU SER GLU ASN GLY SER ASN HIS ILE ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334921	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 ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.673	Depositor
Minimum map value	0.000	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	471.552, 471.552, 471.552	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.228, 1.228, 1.228	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, ATP, ZN

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	0.25	0/37285	0.43	0/50439
2	B	0.19	0/1927	0.44	0/2629
All	All	0.25	0/39212	0.43	0/53068

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	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2237	PRO	Peptide
1	A	4981	TYR	Peptide
1	A	580	GLN	Peptide
2	B	120	PHE	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	36513	36721	36694	603	0
2	B	1883	1911	1910	64	0
3	A	31	12	12	1	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	38431	38644	38616	662	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 9.

The worst 5 of 662 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:1511:ASP:OD1	1:A:1514:ARG:NH1	1.93	1.02
1:A:5061:ILE:O	1:A:5065:LYS:NZ	2.05	0.89
1:A:1198:ARG:NH1	1:A:1200:SER:OG	2.06	0.89
1:A:386:ILE:HD11	1:A:529:ALA:HB2	1.55	0.88
1:A:4817:SER:O	1:A:4822:ARG:NH2	2.05	0.88

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	4479/5247 (85%)	4245 (95%)	228 (5%)	6 (0%)	48 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	235/575 (41%)	203 (86%)	32 (14%)	0	100 100
All	All	4714/5822 (81%)	4448 (94%)	260 (6%)	6 (0%)	49 75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	PHE
1	A	1333	ARG
1	A	3104	ASN
1	A	4981	TYR
1	A	1602	ASN

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	4076/4653 (88%)	3960 (97%)	116 (3%)	38 62
2	B	216/501 (43%)	211 (98%)	5 (2%)	44 66
All	All	4292/5154 (83%)	4171 (97%)	121 (3%)	38 62

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2327	ASN
1	A	4979	LEU
1	A	3133	LEU
1	A	4973	LEU
2	B	48	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4655	GLN
1	A	5051	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4663	ASN
1	A	4826	HIS
2	B	57	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 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	5301	-	32,33,33	1.27	5 (15%)	48,52,52	1.74	10 (20%)

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	5301	-	-	5/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5301	ATP	C5-C4	4.08	1.46	1.39
3	A	5301	ATP	C4-N9	-2.50	1.32	1.37
3	A	5301	ATP	C8-N7	2.46	1.36	1.31
3	A	5301	ATP	C5-N7	-2.38	1.34	1.39
3	A	5301	ATP	C5-C6	2.27	1.47	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5301	ATP	C5-C4-N3	-4.97	119.87	126.72
3	A	5301	ATP	N3-C4-N9	3.96	133.90	127.17
3	A	5301	ATP	C2-N3-C4	3.42	120.19	111.83
3	A	5301	ATP	C4-N9-C8	3.39	109.30	105.74
3	A	5301	ATP	C4-C5-N7	-3.18	106.94	110.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	O4'-C1'-N9-C8
3	A	5301	ATP	O4'-C1'-N9-C4
3	A	5301	ATP	PG-O3B-PB-O2B
3	A	5301	ATP	PG-O3B-PB-O1B

There are no ring outliers.

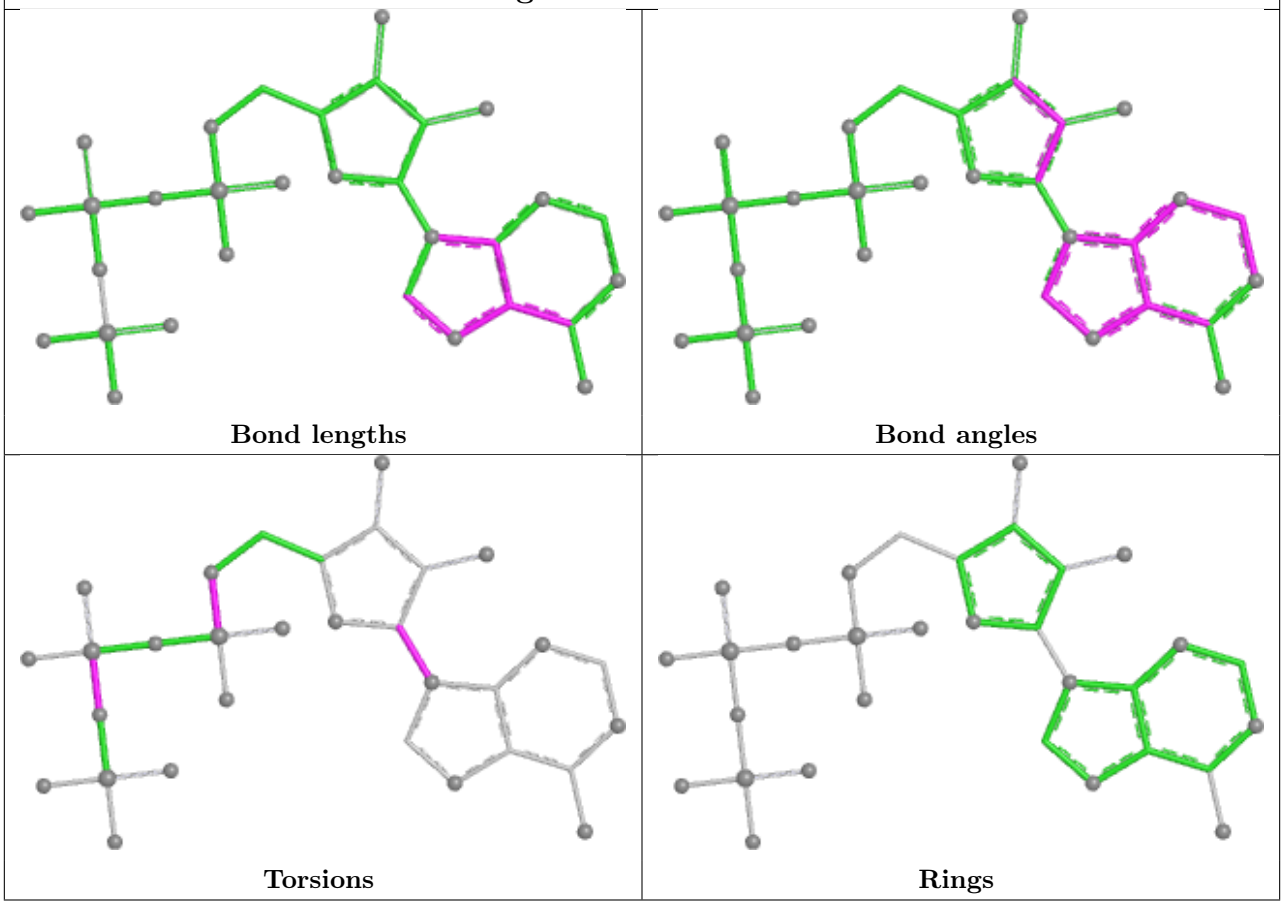
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	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 5301



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.

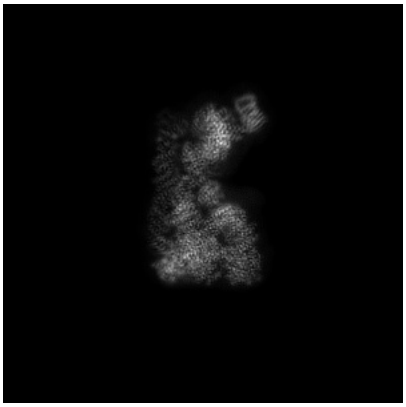
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50913. These allow visual inspection of the internal detail of the map and identification of artifacts.

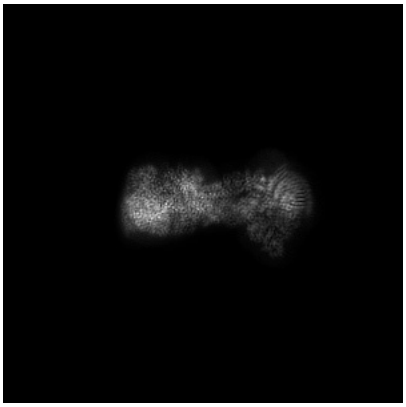
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

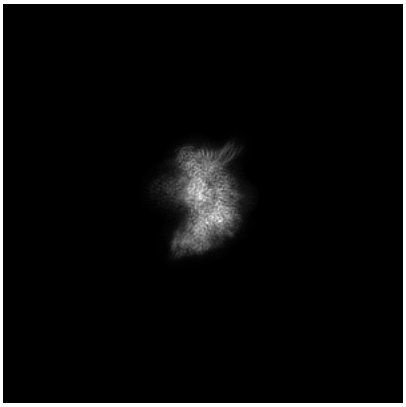
6.1.1 Primary map



X



Y

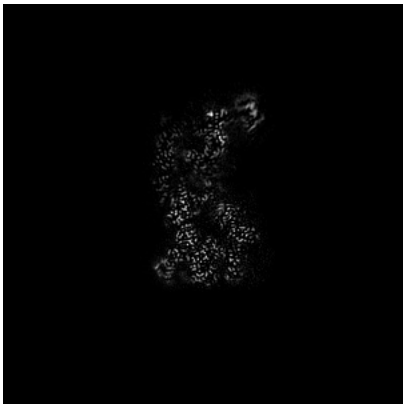


Z

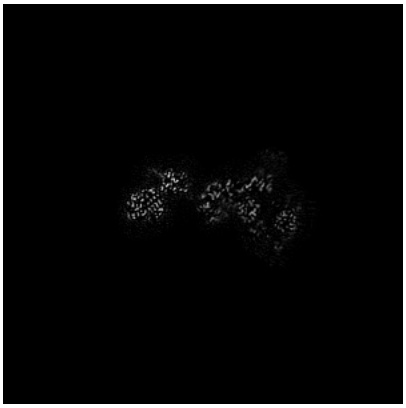
The images above show the map projected in three orthogonal directions.

6.2 Central slices

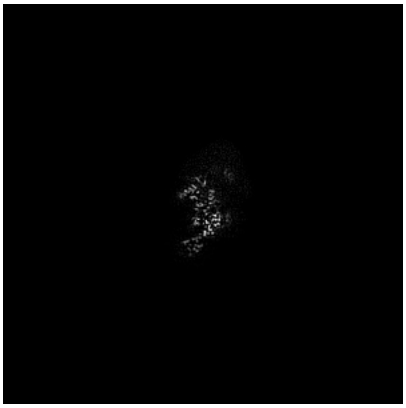
6.2.1 Primary map



X Index: 192



Y Index: 192

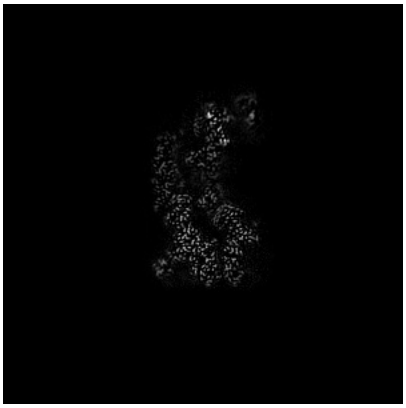


Z Index: 192

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

6.3 Largest variance slices (i)

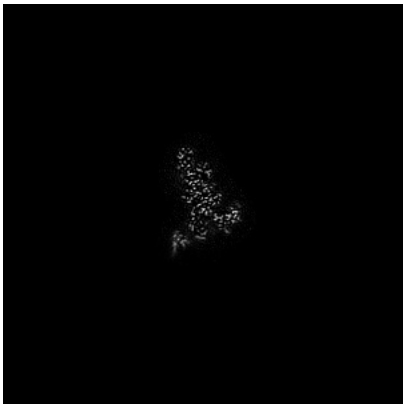
6.3.1 Primary map



X Index: 189



Y Index: 205

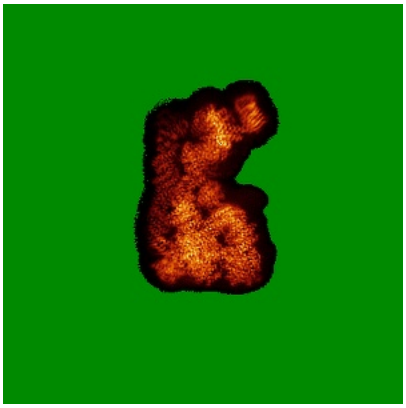


Z Index: 144

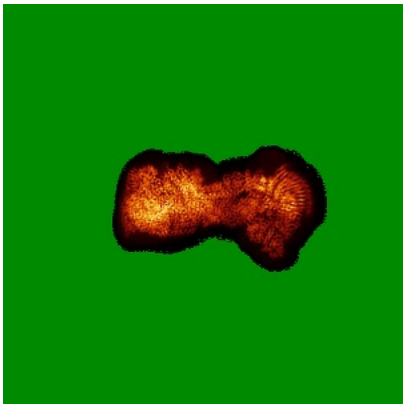
The images above show the largest variance slices of the map in three orthogonal directions.

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

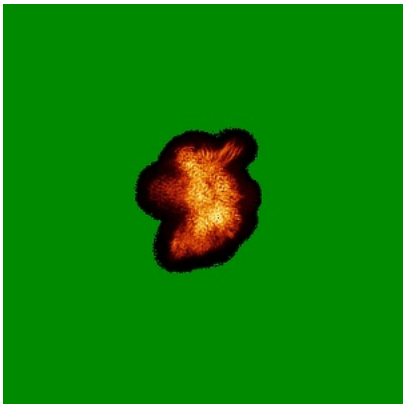
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (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 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

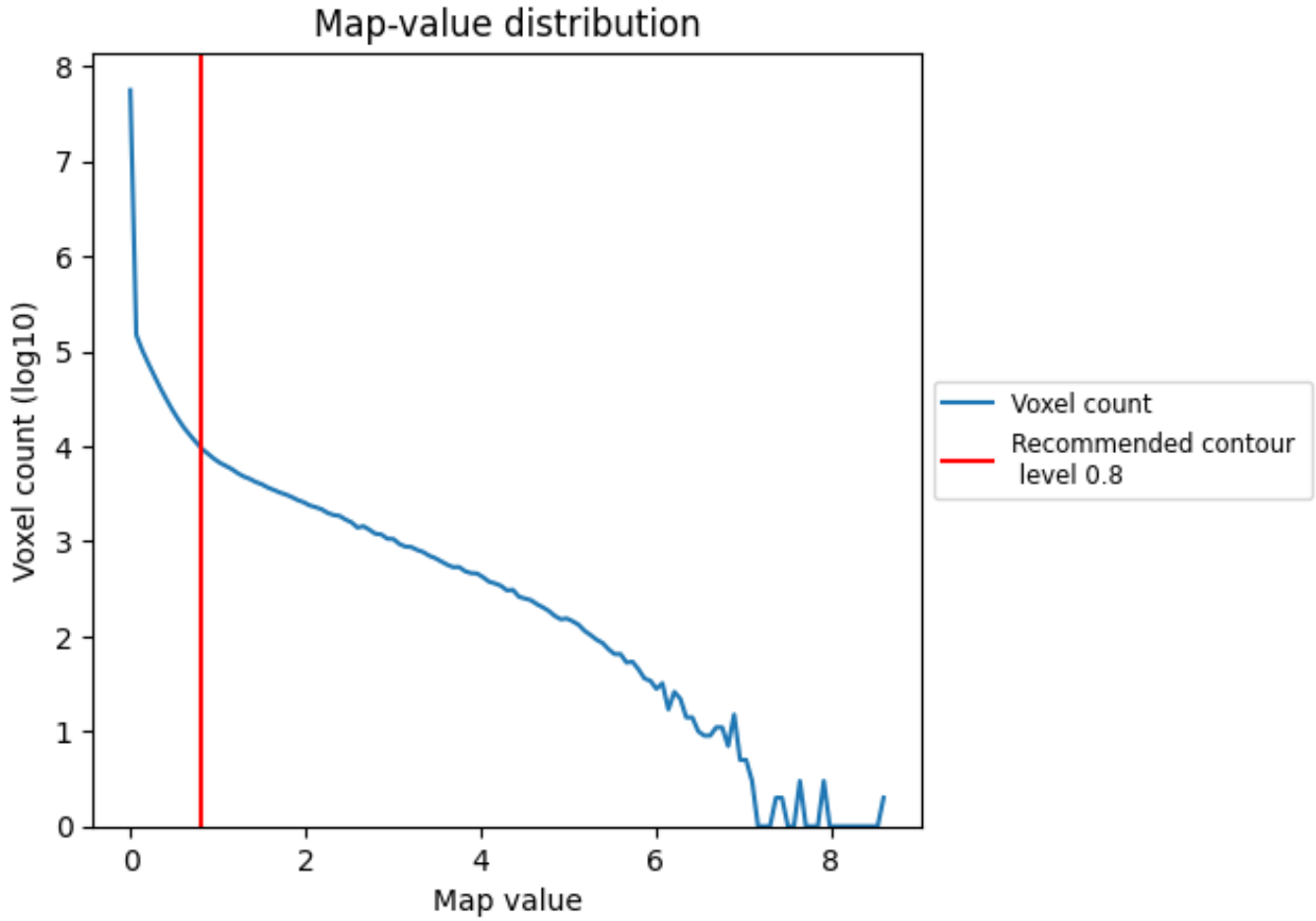
6.6 Mask visualisation (i)

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

7 Map analysis

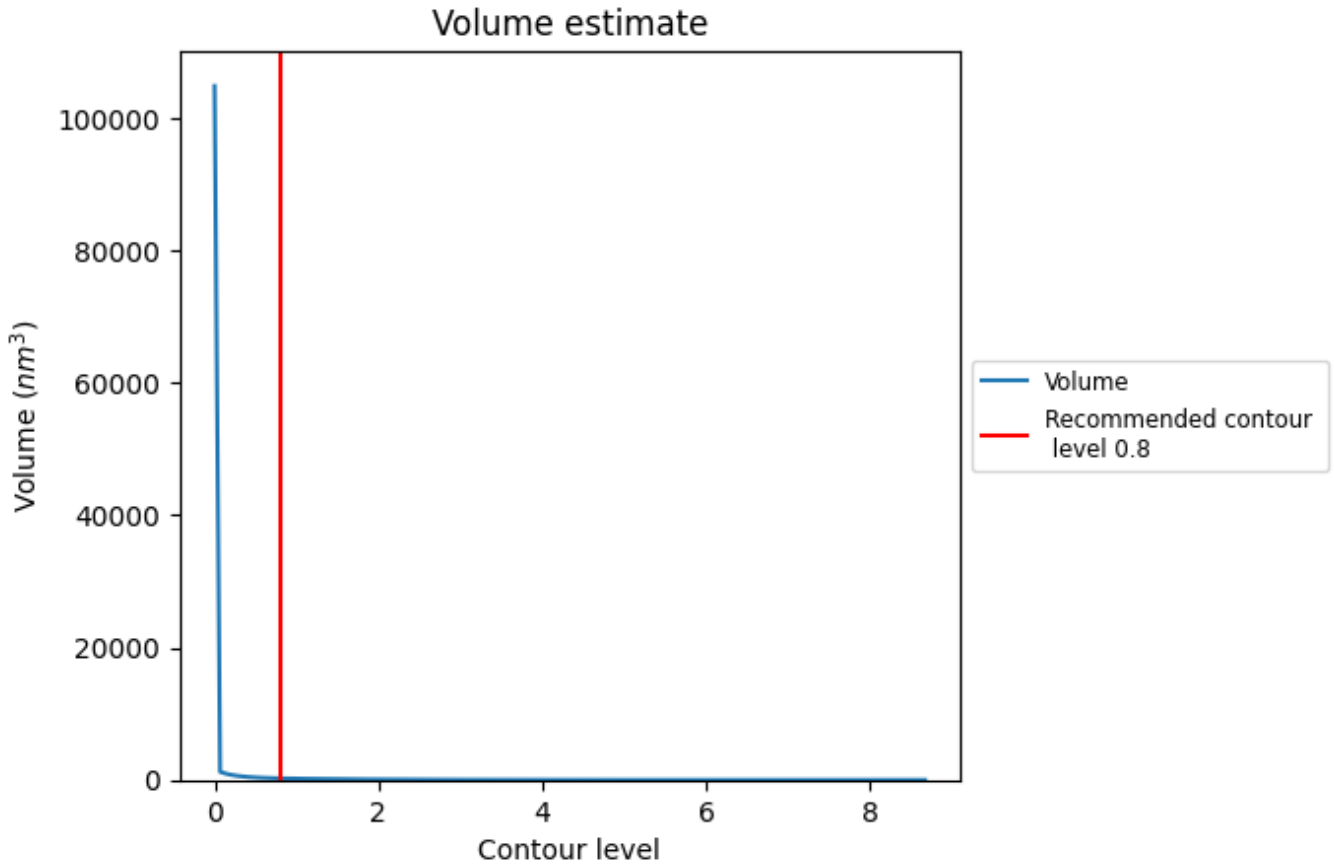
This section contains the results of statistical analysis of the map.

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.

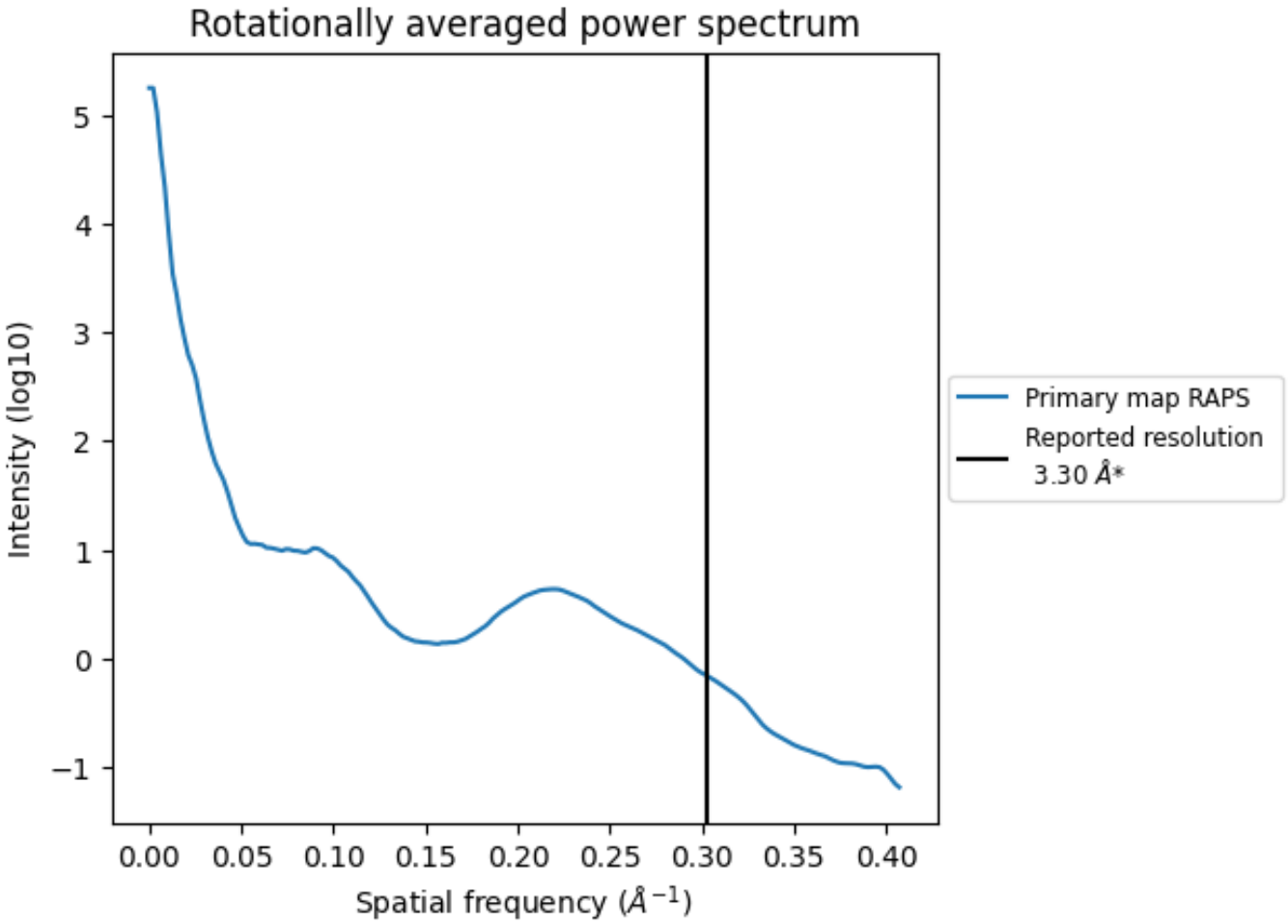
7.2 Volume estimate



The volume at the recommended contour level is 241 nm^3; this corresponds to an approximate mass of 218 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 0.303 Å^{-1}

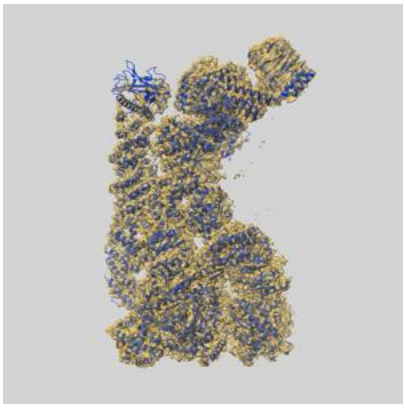
8 Fourier-Shell correlation (i)

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

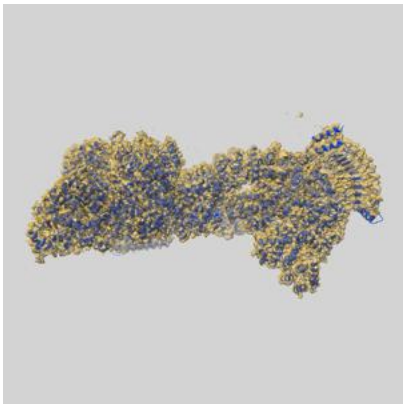
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50913 and PDB model 9G08. Per-residue inclusion information can be found in section 3 on page 6.

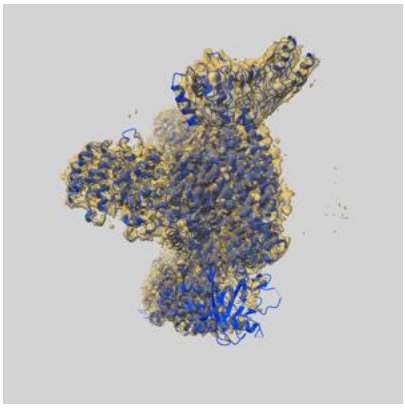
9.1 Map-model overlay



X



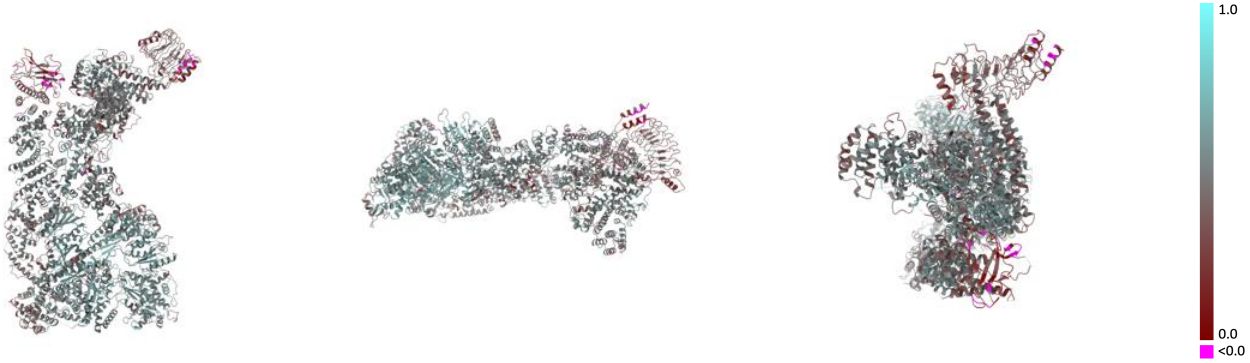
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

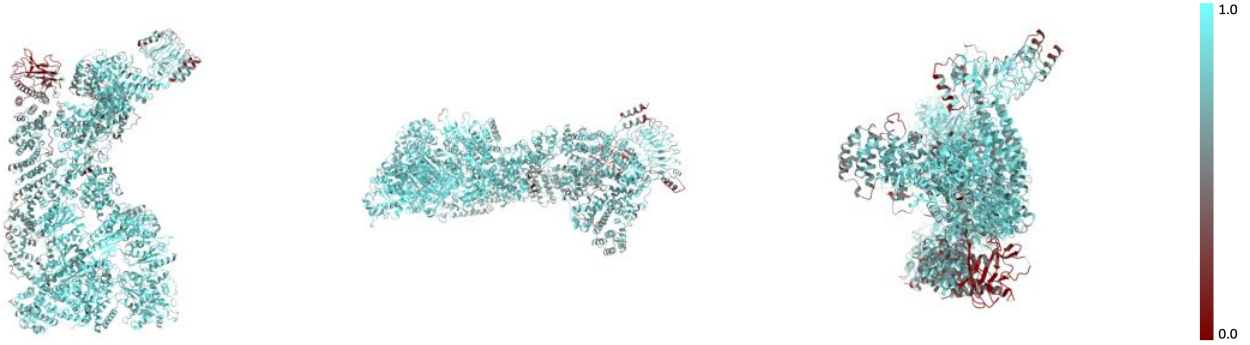
9.2 Q-score mapped to coordinate model (i)



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.

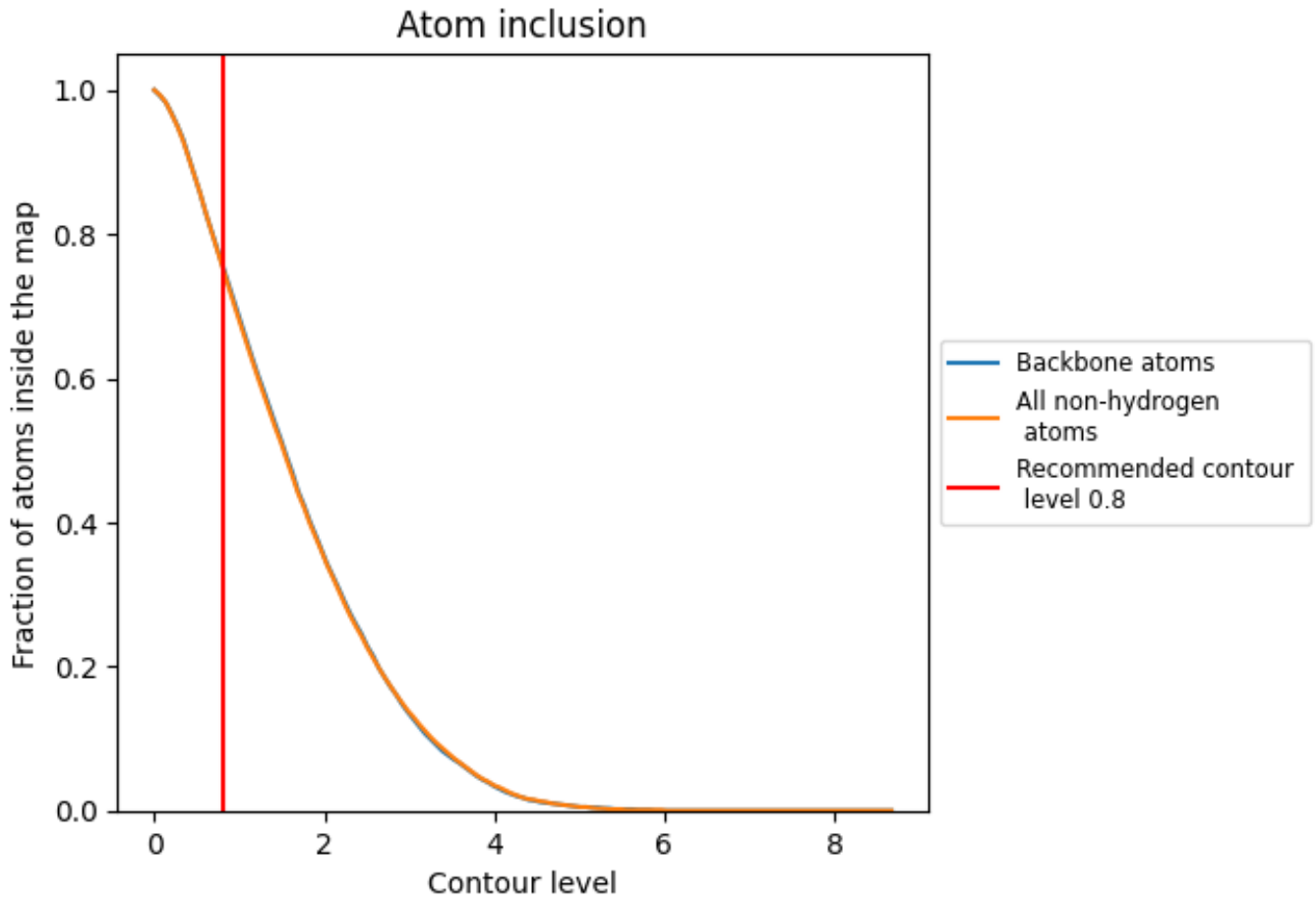
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7550	0.4850
A	0.7710	0.4940
B	0.6110	0.3240