Full wwPDB EM Validation Report ⓘ

May 8, 2023 – 08:21 AM EDT

PDB ID	:	8D4X
EMDB ID	:	EMD-27201
Title	:	Structure of the human UBR5 HECT-type E3 ubiquitin ligase in a dimeric form
Authors	:	Wang, F.; He, Q.; Lin, G.; Li, H.
Deposited on	:	2022-06-02
Resolution	:	2.80 Å(reported)

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

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

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

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

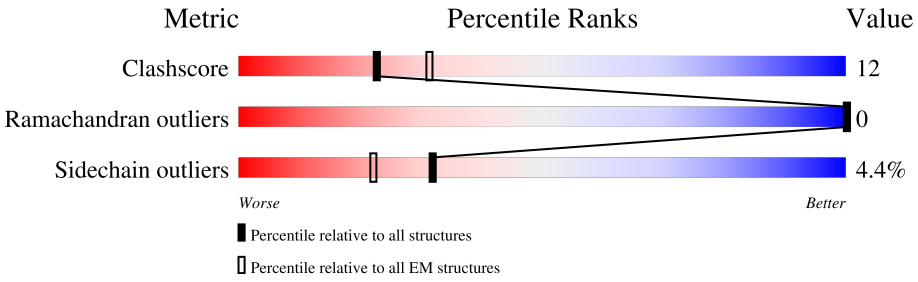
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2806	5% 43% 17% · 40%
1	B	2806	5% 42% 17% · 41%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26409 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 UBR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1684	Total 13260	C 8374	N 2321	O 2465	S 100	0	0
1	B	1669	Total 13143	C 8305	N 2300	O 2439	S 99	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP O95071
A	-5	TYR	-	expression tag	UNP O95071
A	-4	LYS	-	expression tag	UNP O95071
A	-3	ASP	-	expression tag	UNP O95071
A	-2	ASP	-	expression tag	UNP O95071
A	-1	ASP	-	expression tag	UNP O95071
A	0	LYS	-	expression tag	UNP O95071
B	-6	ASP	-	expression tag	UNP O95071
B	-5	TYR	-	expression tag	UNP O95071
B	-4	LYS	-	expression tag	UNP O95071
B	-3	ASP	-	expression tag	UNP O95071
B	-2	ASP	-	expression tag	UNP O95071
B	-1	ASP	-	expression tag	UNP O95071
B	0	LYS	-	expression tag	UNP O95071

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

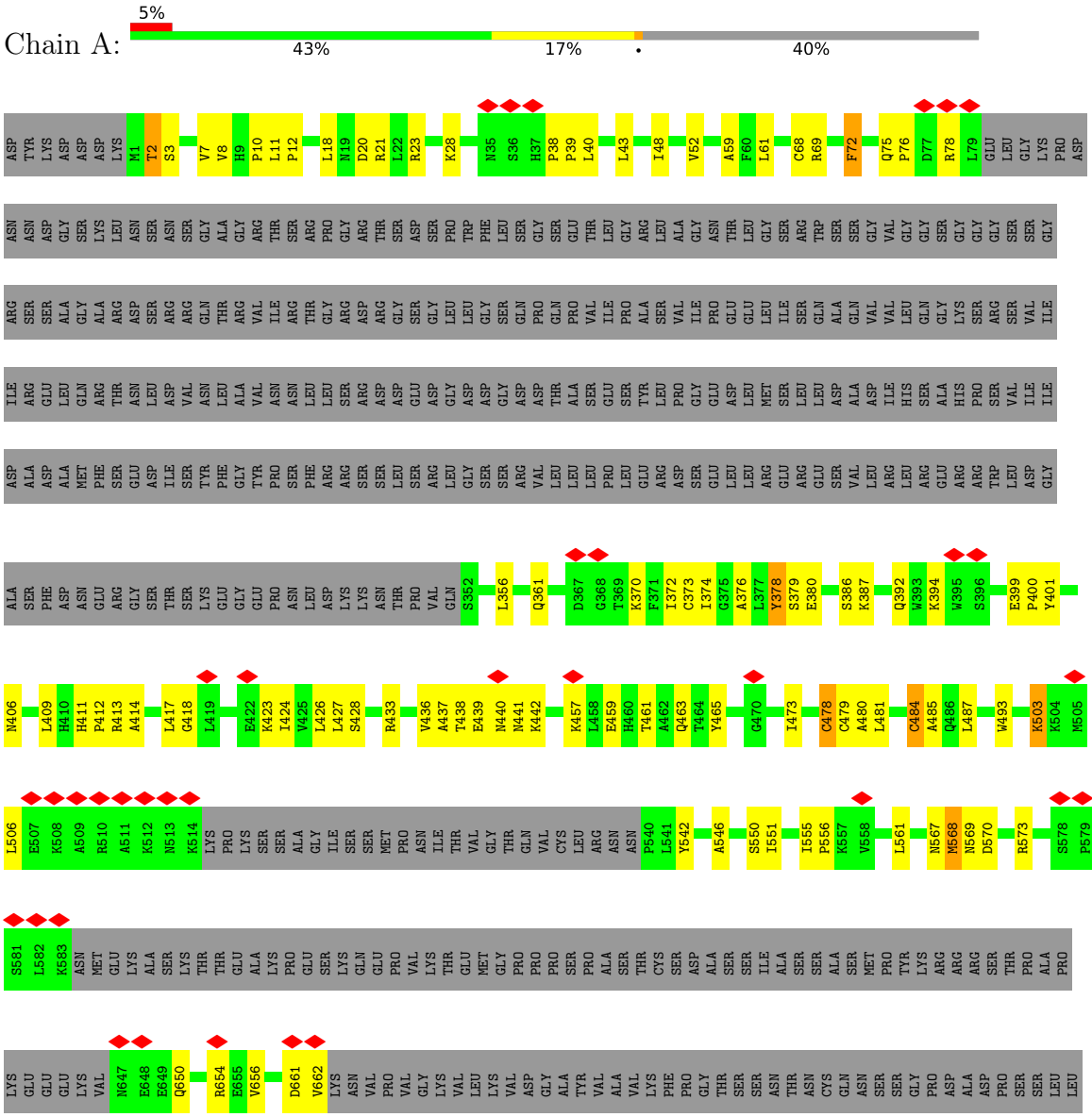
Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total 3	Zn 3	0
2	B	3	Total 3	Zn 3	0

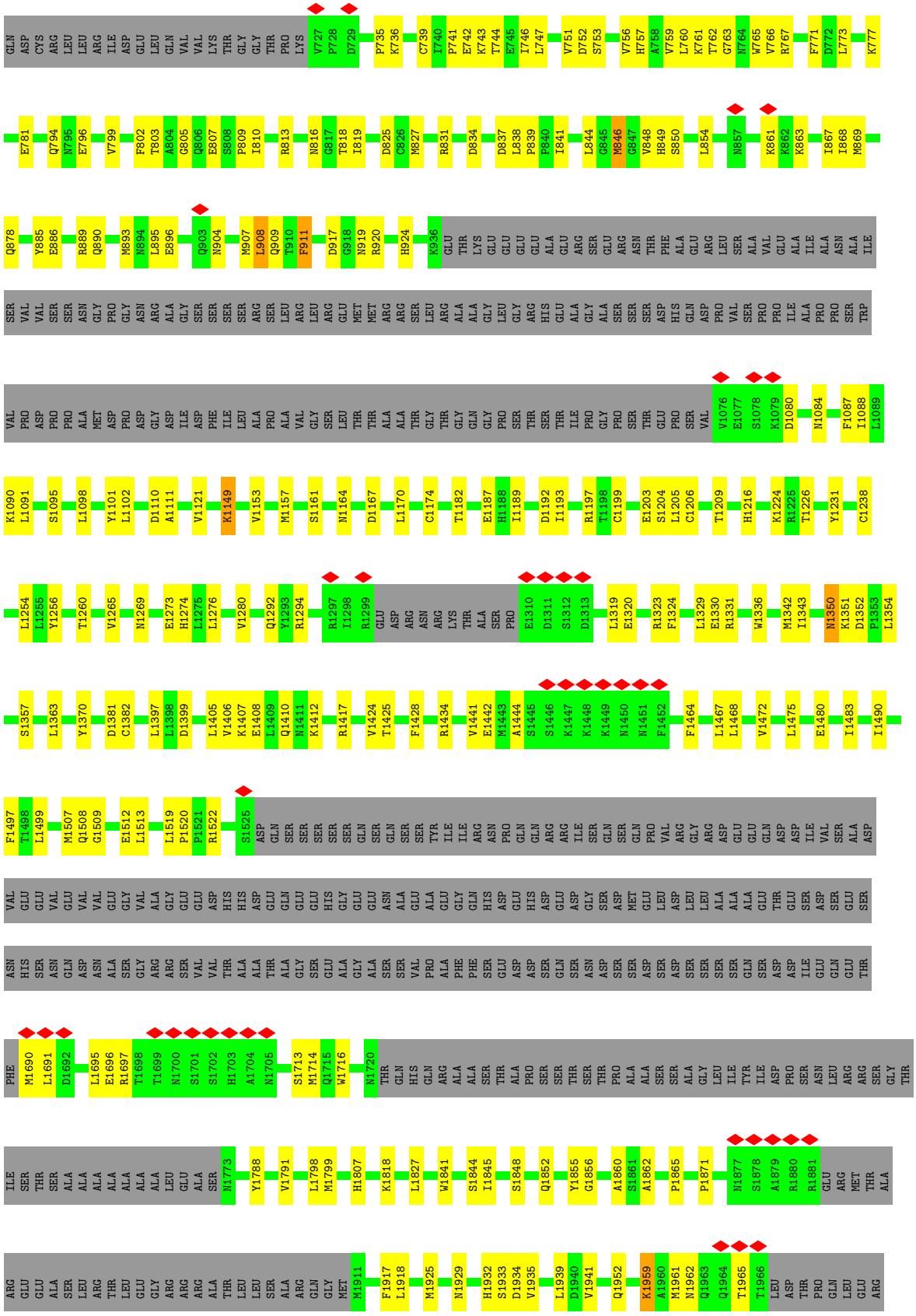
3 Residue-property plots (i)

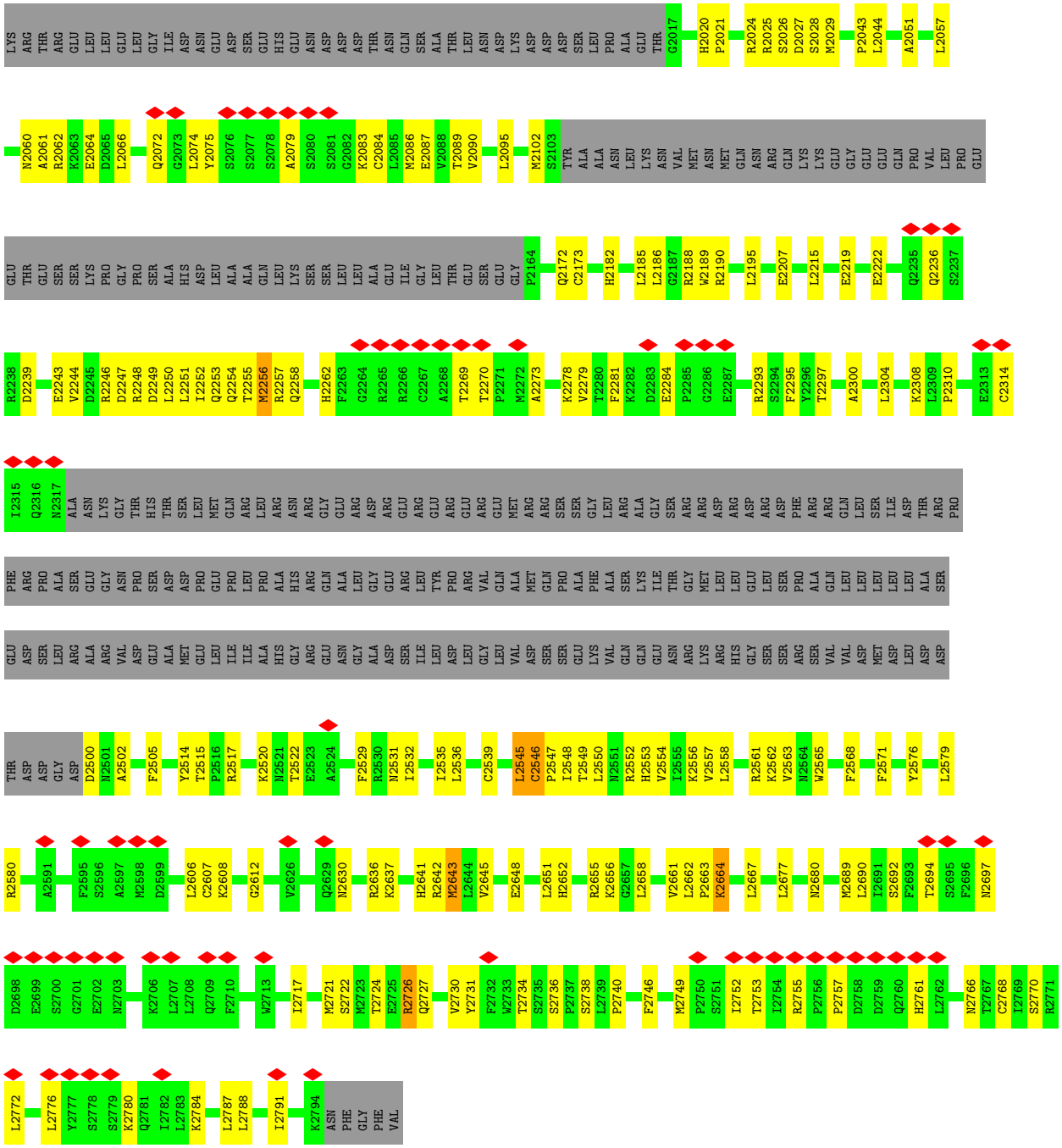
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 UBR5

Chain A:

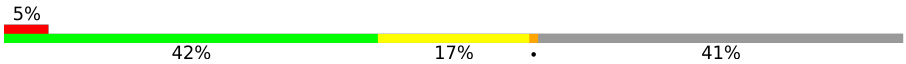


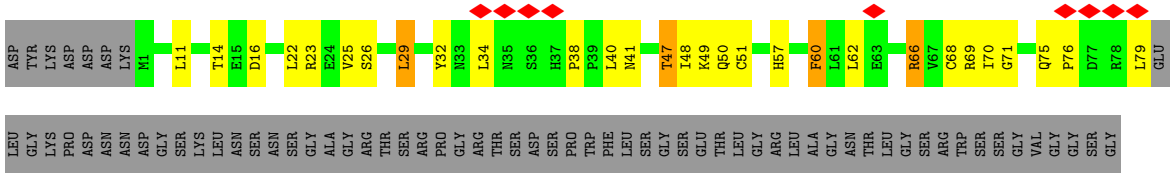


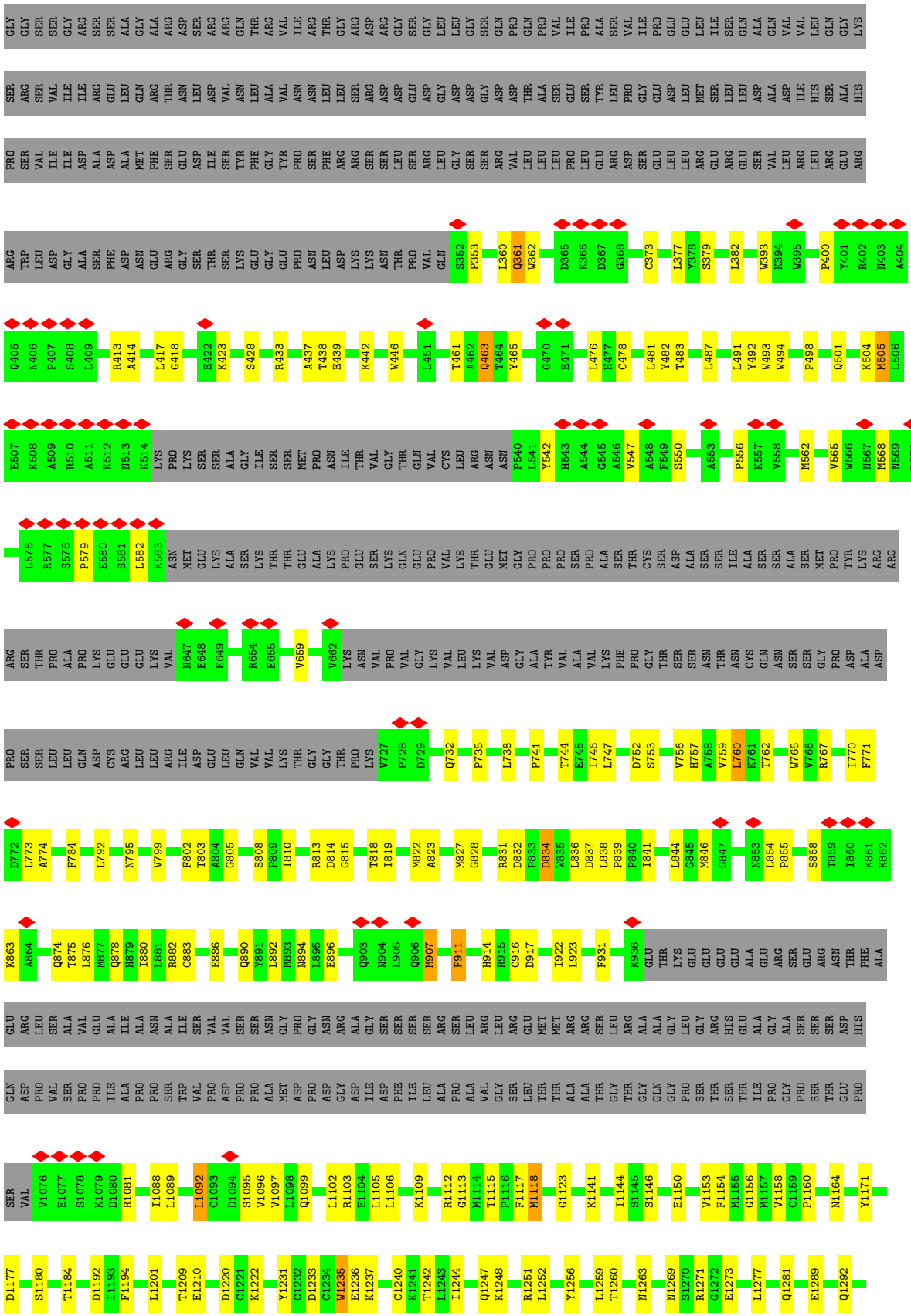


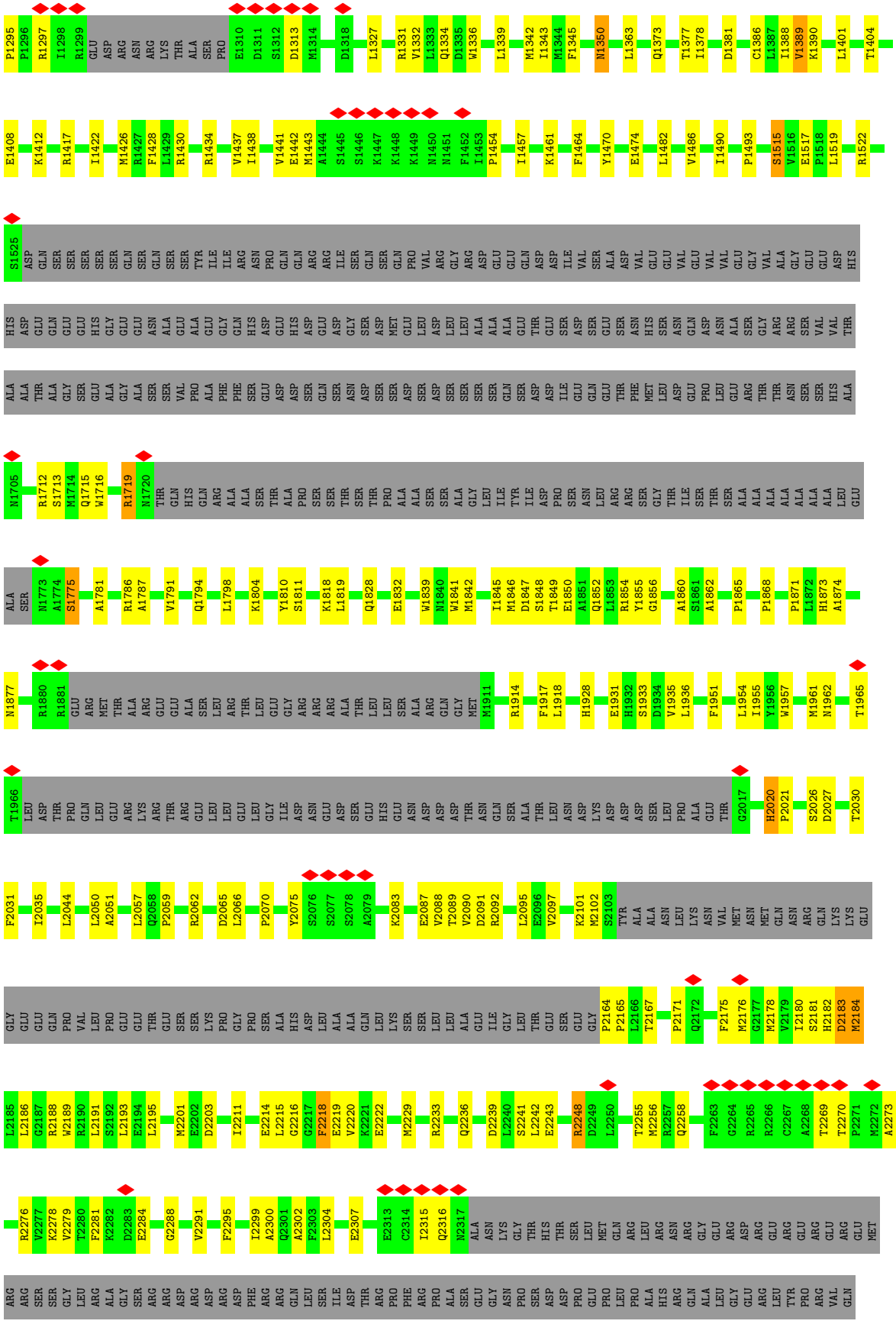
• Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain B:






GLY GLY SER SER GLY ARG SER SER ALA GLY ALA ARG ASP SER ARG ARG GLN THR ARG VAL ILE ARG THR GLY ARG ASP ARG GLY SER GLY LEU LEU GLY SER GLN PRO GLN PRO VAL ILE PRO GLU GLU LEU ILE SER GLN ALA GLN VAL VAL LEU GLN GLY LYS
SER ARG SER VAL ILE ILE ARG GLU LEU GLN ARG THR ASN LEU ASP VAL ASN LEU LEU LEU SER ARG ASP ASP GLU ASP GLY ASP ASP GLY ASP ASP THR ALA SER GLU SER TYR LEU PRO GLY GLU ASP LEU MET SER LEU LEU ASP ALA ASP ILE HIS SER ALA HIS
PRO SER VAL ILE ILE ASP ALA ASP ALA MET PHE SER GLU ASP ILE SER TYR PHE GLY TYR PRO SER PHE ARG ARG SER SER LEU SER ARG LEU GLY SER SER ARG ARG VAL LEU LEU LEU PRO LEU GLU LEU LEU ARG GLU ARG GLU SER VAL ARG LEU ARG GLU
ARG TRP LEU ASP GLY ALA SER PHE ASP ASN GLU ARG GLY SER THR SER LYS GLU GLY GLU PRO ASN LEU ASP LYS LYS ASN THR PRO VAL GLN S352 P353 L360 Q361 W362 D365 K366 D367 G368 C373 L377 Y378 S379 L382 W393 K394 W395 P400 Y401 R402 N403 A404
Q405 N406 P407 S408 L409 R413 A414 L417 G418 E422 K423 S428 R433 A437 T438 E439 K442 W446 L451 T461 A462 Q463 T464 Y465 G470 E471 L476 H477 C478 L481 Y482 T483 L487 L491 Y492 W493 W494 P498 Q501 K504 M505 L506
E507 K508 A509 R510 A511 K512 N513 K514 LYS PRO LYS SER SER ALA GLY ILE SER SER MET PRO ASN ILE THR VAL GLY THR GLN VAL CYS LEU ARG ASN ASN P540 L541 Y542 H543 A544 G545 A546 V547 A548 F549 S550 A553 P556 K557 V558 M562 V565 W566 N567 M568 N569 D570 S571
L576 R577 S578 P579 E580 S581 L582 K583 ASN MET GLU LYS ALA SER LYS THR THR GLU ALA LYS PRO GLU SER LYS GLN GLU PRO VAL LYS THR GLU MET GLY PRO PRO PRO SER PRO ALA SER THR CYS SER ASP ALA SER SER ILE ALA SER SER ALA SER MET PRO TYR LYS ARG ARG
ARG SER THR PRO ALA PRO LYS GLU GLU GLU LYS VAL N647 E648 E649 R654 E655 V659 V662 LYS ASN VAL PRO VAL GLY LYS VAL LEU LYS VAL ASP GLY ALA TYR VAL ALA VAL LYS PHE PRO GLY THR SER SER ASN THR ASN CYS GLN ASN SER SER GLY PRO ASP ALA ASP
PRO SER SER LEU LEU GLN ASP CYS ARG LEU LEU ARG ILE ASP GLU LEU GLN VAL VAL LYS THR GLY GLY THR PRO LYS V727 P728 D729 Q732 P735 L738 P741 T744 E745 T746 L747 D752 S753 V756 H757 A758 V759 L760 K761 T762 W765 V766 R767 I770 F771
D772 L773 A774 F784 L792 N795 V799 F802 T803 A804 G805 S808 P809 I810 R813 D814 G815 T818 I819 M822 A823 M827 G828 R831 D832 P833 D834 W835 L836 D837 L838 P839 P840 I841 L844 G845 M846 G847 N853 L854 P855 S858 T859 I860 K861 K862
K863 A864 Q874 T875 L876 M877 Q878 H879 I880 L881 R882 C883 E886 Q890 Y891 L892 M893 N894 L895 E896 Q903 N904 L905 Q906 M907 F911 H914 R915 C916 D917 I922 L923 F931 K936 GLU THR LYS GLU GLU GLU ALA GLU ARG SER GLU ARG ASN THR PHE ALA
GLU ARG LEU SER ALA VAL GLU ALA ILE ALA ASN ARG ALA GLY SER SER SER SER ARG SER LEU ARG GLU MET MET ARG ARG SER LEU ARG ALA HIS GLU ALA GLY ALA SER SER SER ASP HIS
GLN ASP PRO VAL SER PRO PRO ILE ALA PRO PRO SER TRP VAL PRO ASP PRO PRO ALA MET ASP PRO ASP GLY ASP ILE ASP PHE ILE LEU LEU ALA PRO PRO ALA VAL GLY SER LEU THR THR ALA ALA THR GLY THR GLY GLN GLY PRO SER THR SER THR ILE PRO GLY PRO SER THR GLU PRO
SER VAL V1076 E1077 S1078 K1079 D1080 R1081 I1088 L1089 L1092 C1093 D1094 S1095 V1096 V1097 L1098 Q1099 L1102 R1103 E1104 L1105 L1106 K1109 R1112 G1113 M1114 T1115 P1116 F1117 M1118 G1123 K1141 I1144 S1145 S1146 E1150 V1153 F1154 M1155 G1156 M1157 V1158 C1159 P1160 N1164 Y1171
D1177 S1180 T1184 D1192 I1193 F1194 L1201 T1209 E1210 D1220 C1221 K1222 Y1231 C1232 D1233 C1234 W1235 E1236 K1237 C1240 K1241 T1242 L1243 I1244 Q1247 K1248 R1251 L1252 Y1256 L1259 T1260 N1263 N1269 S1270 R1271 G1272 E1273 L1277 Q1281 E1289 Q1292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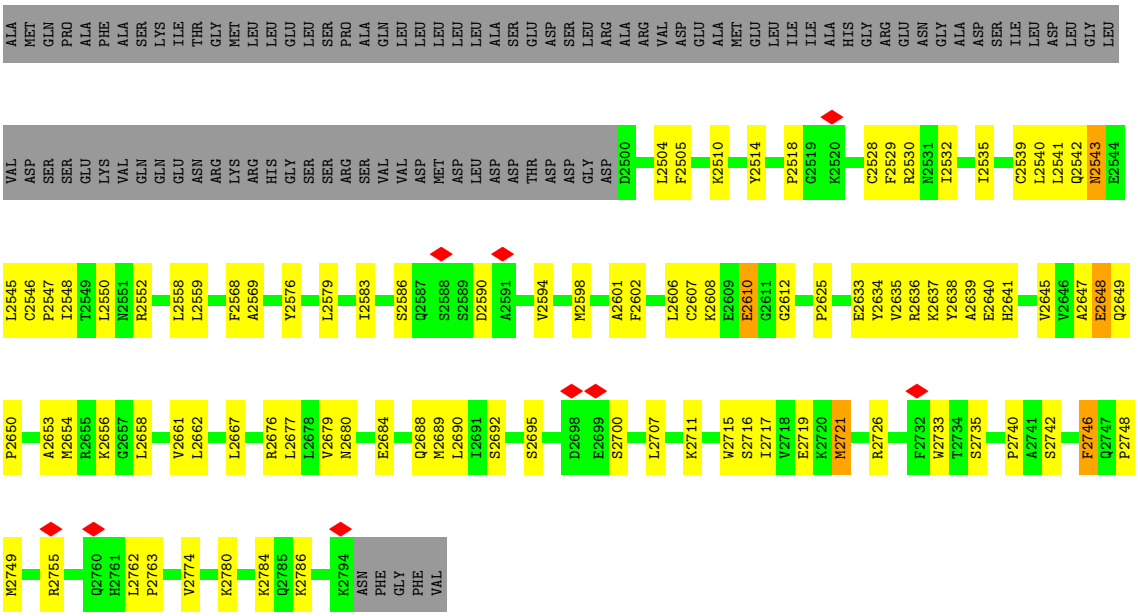
E1408 K1412 R1417 I1422 M1426 R1427 F1428 L1429 R1430 R1434 V1437 I1438 V1441 E1442 M1443 A1444 A1445 S1446 K1447 K1448 K1449 N1450 N1451 F1452 I1453 P1454 I1457 K1461 F1464 Y1470 E1474 L1482 V1486 I1490 P1493 S1515 V1516 E1517 P1518 L1519 R1522
S1525 ASP GLN SER SER SER SER GLN SER GLN SER GLN ARG ARG ILE SER GLN SER GLN PRO VAL ARG GLY ARG ASP GLU GLU GLN ASP ASP ILE VAL SER ALA ASP VAL GLU GLU VAL GLU VAL VAL GLU GLY VAL ALA GLY GLU ARG ASP
HIS ASP GLU GLN GLU GLU HIS GLY GLU GLU ASN ALA GLU ALA GLU GLY GLN HIS ASP GLU HIS ASP GLU ASP GLY GLN ASP GLU ASP SER GLY SER ASP MET GLU LEU ASP LEU ALA ALA GLU THR GLU SER ASP SER GLU SER ASN HIS SER ASN GLN ASP ASN ALA SER GLY ARG ARG SER VAL THR
ALA ALA THR ALA GLY SER GLU ALA GLY ALA SER SER VAL PRO ALA PHE PHE SER GLU ASP ASP SER GLN SER ASN ASP SER SER ASP SER SER SER SER GLN SER ASP ASP ILE GLU GLN GLU THR PHE MET LEU LEU ASP GLU PRO LEU GLU ARG THR THR ASN SER SER HIS ALA
N1705 R1712 S1713 M1714 Q1715 W1716 R1719 N1720 THR GLN HIS GLN ARG ALA ALA SER THR ALA PRO SER SER THR SER THR PRO ALA ALA SER SER ALA GLY LEU ILE TYR ILE ASP PRO SER ASN LEU ARG ARG SER GLY THR ILE SER THR SER ALA ALA ALA ALA ALA ALA ALA ALA LEU GLU
ALA SER N1773 A1774 S1775 A1781 R1786 A1787 V1791 Q1794 L1798 K1804 Y1810 S1811 K1818 L1819 Q1828 E1832 W1839 N1840 W1841 M1842 I1845 M1846 D1847 S1848 T1849 E1850 A1851 Q1852 L1853 R1854 Y1855 G1856 A1860 S1861 A1862 P1865 P1868 P1871 L1872 H1873 A1874
N1877 R1880 R1881 GLU ARG MET THR ALA ARG GLU GLU ALA SER LEU ARG THR LEU GLU GLY ARG ARG ARG ALA THR LEU LEU SER ALA ARG GLN GLY MET M1911 R1914 F1917 L1918 H1928 E1931 H1932 S1933 D1934 V1935 L1936 F1951 L1954 I1955 Y1956 W1957 M1961 N1962 T1965
T1966 LEU ASP THR PRO GLN LEU GLU ARG LYS ARG THR ARG GLU LEU LEU GLU LEU GLY ILE ASP ASN GLU ASP SER GLU HIS GLU ASN ASP ASP ASP THR ASN GLN SER ALA THR LEU LEU ASN ASP LYS ASP ASP SER LEU PRO ALA GLU THR G2017 H2020 P2021 S2026 D2027 T2030
F2031 I2035 L2044 L2050 A2051 L2057 Q2058 P2059 R2062 D2065 L2066 P2070 Y2075 S2076 S2077 S2078 A2079 K2083 E2087 V2088 T2089 V2090 D2091 R2092 L2095 E2096 V2097 K2101 M2102 S2103 TYR ALA ALA ASN LEU LYS ASN VAL MET ASN MET GLN ASN ARG GLN LYS LYS GLU
GLY GLU GLU GLN PRO VAL LEU PRO GLU GLU THR GLU SER SER LYS PRO GLY PRO SER ALA HIS ASP LEU ALA ALA GLN LEU LYS SER SER LEU LEU ALA GLU ILE GLY LEU THR GLU SER GLU GLY P2164 P2165 L2166 T2167 P2171 Q2172 F2175 M2176 G2177 M2178 V2179 I2180 S2181 H2182 D2183 M2184
L2185 L2186 G2187 R2188 W2189 R2190 L2191 S2192 L2193 E2194 L2195 M2201 E2202 D2203 I2211 E2214 L2215 G2216 G2217 F2218 E2219 V2220 K2221 E2222 M2229 R2233 Q2236 D2239 L2240 S2241 L2242 E2243 R2248 D2249 L2250 T2255 M2256 R2257 Q2258 F2263 G2264 R2265 R2266 C2267 A2268 T2269 T2270 P2271 M2272 A2273
R2276 V2277 K2278 V2279 T2280 F2281 K2282 D2283 E2284 G2288 V2291 F2295 I2299 A2300 Q2301 A2302 F2303 L2304 E2307 E2313 C2314 I2315 Q2316 N2317 ALA ASN LYS GLY THR HIS THR SER LEU MET GLN ARG LEU ARG ASN ARG GLY GLU ARG ASP ARG GLU ARG GLU ARG GLU ARG VAL ARG GLU MET
ARG ARG SER SER GLY LEU ARG ARG ALA GLY SER ARG ARG ASP ARG ASP ARG ASP PHE ARG ARG GLN LEU SER ILE ASP THR ARG PRO PHE ARG PRO ALA SER GLU GLY ASN PRO SER ASP ASP PRO GLU PRO LEU PRO LEU ALA HIS ARG GLN ALA LEU GLY GLU ARG GLU LEU ARG TYR PRO ARG VAL GLN


ALA MET GLN PRO ALA PHE ALA SER LYS ILE THR GLY MET LEU LEU GLU LEU SER PRO ALA GLN LEU LEU LEU LEU LEU ALA SER GLU ASP SER LEU ARG ALA ARG VAL ASP GLU ALA MET GLU LEU ILE ILE ALA HIS GLY ARG GLU ASN GLY ALA ASP SER ILE LEU ASP LEU GLY LEU
VAL ASP SER SER GLU LYS VAL GLN GLN GLU ASN ARG LYS ARG HIS GLY SER SER ARG SER VAL VAL ASP MET ASP LEU ASP ASP THR ASP ASP GLY ASP D2500 L2504 F2505 K2510 Y2514 P2518 G2519 K2520 C2528 F2529 R2530 N2531 I2532 I2535 C2539 L2540 L2541 Q2542 N2543 E2544
L2545 C2546 P2547 I2548 T2549 L2550 N2551 R2552 L2558 L2559 F2568 A2569 Y2576 L2579 I2583 S2586 Q2587 S2588 S2589 D2590 A2591 V2594 M2598 A2601 F2602 L2606 C2607 K2608 E2609 E2610 G2611 G2612 P2625 E2633 Y2634 V2635 R2636 K2637 Y2638 A2639 E2640 H2641 V2645 V2646 A2647 E2648 Q2649
P2650 A2653 M2654 R2655 K2656 G2657 L2658 V2661 L2662 L2667 R2676 L2677 L2678 V2679 N2680 E2684 Q2688 M2689 L2690 I2691 S2692 S2695 D2698 E2699 S2700 L2707 K2711 W2715 S2716 I2717 V2718 E2719 K2720 M2721 R2726 F2732 W2733 T2734 S2735 P2740 A2741 S2742 F2746 Q2747 P2748
M2749 R2755 Q2760 H2761 L2762 P2763 V2774 K2780 K2784 Q2785 K2786 K2794 ASN PHE GLY PHE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	844403	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.744	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/13536	0.53	0/18339
1	B	0.27	0/13417	0.52	0/18177
All	All	0.27	0/26953	0.53	0/36516

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	13260	0	13247	358	0
1	B	13143	0	13138	331	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	26409	0	26385	660	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 12.

All (660) 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:2505:PHE:CE2	1:A:2548:ILE:HD11	1.45	1.48
1:A:2505:PHE:HE2	1:A:2548:ILE:CD1	1.53	1.22
1:A:2300:ALA:CB	1:A:2547:PRO:HG2	1.74	1.17
1:A:2304:LEU:HD21	1:A:2548:ILE:HG13	1.29	1.06
1:A:2300:ALA:HB3	1:A:2547:PRO:HG2	1.27	1.06
1:A:2300:ALA:HB2	1:A:2547:PRO:HD2	1.50	0.93
1:A:1442:GLU:OE2	1:A:1509:GLY:HA3	1.75	0.87
1:A:2553:HIS:ND1	1:A:2643:MET:SD	2.49	0.85
1:A:2606:LEU:O	1:A:2612:GLY:HA2	1.77	0.85
1:B:2606:LEU:O	1:B:2612:GLY:HA2	1.77	0.84
1:A:2300:ALA:CB	1:A:2547:PRO:CG	2.55	0.84
1:B:29:LEU:O	1:B:29:LEU:HD22	1.79	0.83
1:B:818:THR:HG21	1:B:917:ASP:HA	1.64	0.80
1:B:2579:LEU:HD22	1:B:2635:VAL:HG22	1.60	0.80
1:A:2505:PHE:CE2	1:A:2548:ILE:CD1	2.40	0.80
1:B:799:VAL:HA	1:B:813:ARG:O	1.85	0.77
1:A:2545:LEU:HD23	1:A:2545:LEU:N	2.01	0.75
1:B:2097:VAL:HG13	1:B:2101:LYS:HD2	1.68	0.74
1:A:2532:ILE:HD11	1:A:2548:ILE:HD12	1.69	0.74
1:B:2186:LEU:HD13	1:B:2215:LEU:HD11	1.70	0.74
1:A:478:CYS:SG	1:A:479:CYS:N	2.61	0.74
1:A:2539:CYS:SG	1:A:2546:CYS:HB3	2.28	0.74
1:A:747:LEU:HD21	1:A:761:LYS:HB3	1.68	0.74
1:A:2545:LEU:HD11	1:A:2740:PRO:HD3	1.71	0.73
1:B:463:GLN:HG3	1:B:465:TYR:HE1	1.51	0.72
1:B:922:ILE:HD11	1:B:1105:LEU:HD21	1.71	0.72
1:B:827:MET:SD	1:B:828:GLY:N	2.63	0.72
1:A:1343:ILE:HD13	1:A:1428:PHE:HB2	1.71	0.72
1:A:2545:LEU:HD12	1:A:2738:SER:O	1.89	0.72
1:B:1386:CYS:HA	1:B:1390:LYS:HB2	1.72	0.71
1:A:2300:ALA:HB2	1:A:2547:PRO:CD	2.21	0.71
1:A:503:LYS:HE2	1:A:506:LEU:HD23	1.73	0.70
1:A:463:GLN:HG3	1:A:465:TYR:HE1	1.54	0.70
1:A:2304:LEU:CD2	1:A:2548:ILE:HG13	2.16	0.70
1:A:1256:TYR:HE1	1:A:1331:ARG:HG3	1.56	0.70
1:A:2557:VAL:HB	1:A:2651:LEU:HD12	1.73	0.69
1:B:22:LEU:HB3	1:B:836:LEU:HD11	1.74	0.68
1:B:2044:LEU:HD11	1:B:2051:ALA:HB3	1.75	0.68
1:B:76:PRO:HG3	1:B:854:LEU:HD11	1.74	0.68
1:B:433:ARG:NH1	1:B:481:LEU:O	2.27	0.68
1:A:1269:ASN:HD21	1:A:1273:GLU:HG3	1.58	0.68
1:A:479:CYS:SG	1:A:480:ALA:N	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:HG	1:B:379:SER:H	1.58	0.67
1:B:813:ARG:NH2	1:B:841:ILE:O	2.27	0.67
1:B:2607:CYS:SG	1:B:2608:LYS:N	2.67	0.67
1:A:2637:LYS:HE2	1:A:2637:LYS:HA	1.75	0.67
1:A:23:ARG:NH2	1:A:834:ASP:OD1	2.27	0.67
1:A:760:LEU:HD12	1:A:767:ARG:HH12	1.59	0.67
1:A:1697:ARG:HH12	1:B:2695:SER:HB3	1.59	0.67
1:B:1408:GLU:OE1	1:B:1417:ARG:NH1	2.26	0.67
1:A:908:LEU:HD13	1:A:911:PHE:HE1	1.59	0.67
1:A:2505:PHE:HB3	1:A:2514:TYR:HB3	1.76	0.67
1:A:1852:GLN:HG2	1:A:2090:VAL:HG13	1.77	0.66
1:B:747:LEU:HB2	1:B:759:VAL:HG13	1.78	0.66
1:B:2050:LEU:HD13	1:B:2066:LEU:HD22	1.76	0.66
1:B:2505:PHE:HB3	1:B:2514:TYR:HB3	1.78	0.66
1:B:1810:TYR:OH	1:B:1818:LYS:NZ	2.29	0.65
1:B:837:ASP:N	1:B:917:ASP:OD2	2.24	0.65
1:B:1088:ILE:HD12	1:B:1089:LEU:N	2.12	0.65
1:A:1265:VAL:O	1:A:1274:HIS:NE2	2.28	0.65
1:A:2062:ARG:NH1	1:B:1713:SER:OG	2.28	0.65
1:A:2607:CYS:SG	1:A:2608:LYS:N	2.68	0.65
1:A:413:ARG:HH22	1:A:459:GLU:HG3	1.61	0.65
1:A:2087:GLU:OE1	1:A:2087:GLU:N	2.19	0.65
1:A:1434:ARG:NH2	1:B:1931:GLU:OE1	2.29	0.65
1:B:1331:ARG:O	1:B:1331:ARG:NH1	2.30	0.65
1:B:1850:GLU:HG3	1:B:2189:TRP:HA	1.78	0.64
1:A:361:GLN:N	1:A:361:GLN:OE1	2.31	0.64
1:A:2074:LEU:HB3	1:A:2086:MET:HB2	1.78	0.64
1:B:547:VAL:HG13	1:B:659:VAL:HB	1.80	0.64
1:A:1490:ILE:HD13	1:B:1845:ILE:HD12	1.80	0.64
1:B:2688:GLN:OE1	1:B:2688:GLN:N	2.25	0.64
1:A:2248:ARG:NH2	1:A:2308:LYS:O	2.30	0.64
1:A:1407:LYS:NZ	1:A:1408:GLU:OE2	2.31	0.63
1:A:2243:GLU:O	1:A:2258:GLN:NE2	2.31	0.63
1:A:841:ILE:HD13	1:A:869:MET:HE1	1.80	0.63
1:A:2057:LEU:HG	1:A:2677:LEU:HD13	1.81	0.63
1:A:569:ASN:OD1	1:A:654:ARG:NH2	2.32	0.63
1:B:66:ARG:HH22	1:B:68:CYS:HB2	1.64	0.63
1:A:818:THR:HG21	1:A:917:ASP:HA	1.81	0.62
1:A:2061:ALA:HB1	1:A:2066:LEU:HD11	1.81	0.62
1:B:916:CYS:SG	1:B:917:ASP:N	2.70	0.62
1:B:2637:LYS:HA	1:B:2637:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:ARG:HD3	1:A:2029:MET:HB3	1.81	0.62
1:B:1088:ILE:O	1:B:1092:LEU:HD12	2.00	0.62
1:A:2552:ARG:NH1	1:A:2556:LYS:HE3	2.15	0.62
1:A:1444:ALA:HB2	1:A:1499:LEU:HB3	1.82	0.62
1:A:747:LEU:HB2	1:A:759:VAL:HG13	1.82	0.61
1:B:2218:PHE:CE1	1:B:2222:GLU:HB3	2.35	0.61
1:A:414:ALA:O	1:A:418:GLY:N	2.33	0.61
1:B:501:GLN:O	1:B:505:MET:HG3	2.00	0.61
1:A:2548:ILE:HG23	1:A:2550:LEU:CD1	2.30	0.60
1:A:799:VAL:HA	1:A:813:ARG:O	2.00	0.60
1:B:1461:LYS:NZ	1:B:1794:GLN:OE1	2.32	0.60
1:A:18:LEU:HD22	1:A:809:PRO:HG2	1.84	0.60
1:A:1925:MET:HE1	1:B:1434:ARG:HA	1.83	0.60
1:A:2300:ALA:HB3	1:A:2547:PRO:CG	2.16	0.60
1:B:2218:PHE:CE2	1:B:2677:LEU:HD21	2.36	0.60
1:B:1343:ILE:HD13	1:B:1428:PHE:HB2	1.84	0.60
1:B:66:ARG:HG3	1:B:66:ARG:HH11	1.65	0.59
1:B:1373:GLN:O	1:B:1373:GLN:NE2	2.32	0.59
1:A:372:ILE:HG22	1:A:373:CYS:SG	2.42	0.59
1:A:2249:ASP:O	1:A:2253:GLN:HG2	2.03	0.59
1:A:2552:ARG:HH12	1:A:2556:LYS:HE3	1.67	0.59
1:A:2766:ASN:O	1:A:2770:SER:N	2.35	0.59
1:A:1149:LYS:HE2	1:A:1149:LYS:H	1.68	0.59
1:A:2186:LEU:HD13	1:A:2215:LEU:HD11	1.85	0.59
1:B:838:LEU:HD23	1:B:839:PRO:HD2	1.85	0.59
1:A:761:LYS:HB2	1:A:766:VAL:HG22	1.84	0.59
1:B:2650:PRO:O	1:B:2654:MET:HG2	2.03	0.59
1:B:428:SER:OG	1:B:478:CYS:SG	2.61	0.58
1:A:11:LEU:HD11	1:A:848:VAL:HG13	1.85	0.58
1:A:2641:HIS:HA	1:A:2645:VAL:HG12	1.85	0.58
1:B:1109:LYS:HB3	1:B:1113:GLY:HA2	1.84	0.58
1:A:2662:LEU:HD12	1:A:2663:PRO:HD2	1.85	0.58
1:B:1144:ILE:HG23	1:B:1146:SER:H	1.68	0.58
1:B:2545:LEU:HD11	1:B:2740:PRO:HA	1.86	0.58
1:A:2293:ARG:NH1	1:A:2734:THR:OG1	2.37	0.57
1:A:2247:ASP:O	1:A:2251:LEU:N	2.32	0.57
1:A:1197:ARG:HG3	1:A:1197:ARG:HH11	1.69	0.57
1:A:2539:CYS:SG	1:A:2546:CYS:CB	2.92	0.57
1:B:498:PRO:HD2	1:B:501:GLN:HE22	1.69	0.57
1:B:2558:LEU:HD23	1:B:2658:LEU:HD13	1.85	0.57
1:B:2780:LYS:O	1:B:2784:LYS:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2044:LEU:HB2	1:A:2576:TYR:HE2	1.66	0.57
1:A:742:GLU:HB2	1:A:743:LYS:NZ	2.20	0.57
1:A:1480:GLU:OE1	1:B:1928:HIS:NE2	2.37	0.57
1:A:1513:LEU:HD22	1:B:1918:LEU:HB3	1.86	0.57
1:B:2233:ARG:HB3	1:B:2541:LEU:HD11	1.87	0.57
1:A:2064:GLU:OE2	1:A:2190:ARG:NH1	2.38	0.57
1:A:2182:HIS:HA	1:A:2185:LEU:HD12	1.87	0.57
1:A:2548:ILE:HG23	1:A:2550:LEU:HD11	1.86	0.57
1:A:52:VAL:HB	1:A:376:ALA:HB2	1.87	0.56
1:A:2257:ARG:NH2	1:A:2314:CYS:SG	2.78	0.56
1:B:2020:HIS:ND1	1:B:2021:PRO:HD2	2.20	0.56
1:A:61:LEU:HD22	1:A:374:ILE:HG23	1.87	0.56
1:A:1512:GLU:HA	1:A:1512:GLU:OE2	2.05	0.56
1:A:1845:ILE:HD12	1:B:1490:ILE:HD13	1.86	0.56
1:B:1854:ARG:HG2	1:B:2191:LEU:HD12	1.87	0.56
1:B:2610:GLU:OE2	1:B:2612:GLY:N	2.38	0.56
1:B:2044:LEU:HD21	1:B:2569:ALA:HB1	1.88	0.56
1:A:2249:ASP:HA	1:A:2310:PRO:HG3	1.87	0.56
1:A:796:GLU:N	1:A:796:GLU:OE1	2.39	0.56
1:B:48:ILE:HD12	1:B:48:ILE:H	1.69	0.56
1:B:2216:GLY:HA3	1:B:2220:VAL:HG21	1.87	0.56
1:A:2083:LYS:O	1:A:2188:ARG:NH1	2.39	0.56
1:A:2548:ILE:HG23	1:A:2548:ILE:O	2.05	0.56
1:B:2679:VAL:HG12	1:B:2680:ASN:OD1	2.06	0.56
1:A:461:THR:O	1:A:463:GLN:NE2	2.36	0.56
1:A:567:ASN:HB3	1:A:570:ASP:HB2	1.87	0.56
1:A:2652:HIS:CE1	1:A:2656:LYS:HE3	2.39	0.56
1:A:2236:GLN:HG3	1:A:2273:ALA:HB3	1.88	0.56
1:A:2502:ALA:HB1	1:A:2517:ARG:HH11	1.70	0.56
1:B:1334:GLN:HA	1:B:1404:THR:HG21	1.87	0.56
1:B:2735:SER:O	1:B:2735:SER:OG	2.24	0.56
1:A:2749:MET:O	1:A:2749:MET:HG2	2.06	0.55
1:A:752:ASP:HA	1:A:805:GLY:HA2	1.87	0.55
1:A:2690:LEU:O	1:A:2694:THR:OG1	2.21	0.55
1:B:2044:LEU:HD23	1:B:2576:TYR:CE1	2.41	0.55
1:A:1224:LYS:NZ	1:A:1226:THR:O	2.39	0.55
1:B:2248:ARG:NE	1:B:2307:GLU:OE2	2.40	0.55
1:B:2636:ARG:HD2	1:B:2640:GLU:OE1	2.05	0.55
1:B:461:THR:O	1:B:463:GLN:NE2	2.39	0.55
1:B:752:ASP:HA	1:B:805:GLY:HA2	1.88	0.55
1:B:2300:ALA:CB	1:B:2547:PRO:HD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2504:LEU:HD11	1:B:2528:CYS:SG	2.46	0.55
1:B:76:PRO:HA	1:B:79:LEU:HD12	1.88	0.55
1:B:1103:ARG:HH21	1:B:1153:VAL:HG23	1.72	0.55
1:B:1177:ASP:HB2	1:B:1210:GLU:HG2	1.88	0.55
1:B:2763:PRO:HB3	1:B:2774:VAL:HA	1.89	0.55
1:A:387:LYS:HA	1:A:423:LYS:HE3	1.88	0.54
1:A:2300:ALA:CB	1:A:2547:PRO:CD	2.85	0.54
1:A:68:CYS:SG	1:A:69:ARG:N	2.81	0.54
1:B:2583:ILE:HD11	1:B:2635:VAL:HG21	1.88	0.54
1:A:1848:SER:O	1:A:1852:GLN:HG3	2.08	0.54
1:B:746:ILE:HD11	1:B:760:LEU:HD23	1.89	0.54
1:B:876:LEU:HD11	1:B:911:PHE:CE1	2.42	0.54
1:B:1381:ASP:OD1	1:B:1434:ARG:NH1	2.41	0.54
1:A:2247:ASP:HB3	1:A:2250:LEU:HB2	1.88	0.54
1:A:12:PRO:HG2	1:A:861:LYS:HD3	1.90	0.54
1:A:503:LYS:HZ3	1:A:568:MET:HB2	1.71	0.54
1:A:2074:LEU:HD23	1:A:2086:MET:HA	1.89	0.54
1:A:2664:LYS:HA	1:A:2667:LEU:HD23	1.89	0.54
1:B:1951:PHE:CZ	1:B:2193:LEU:HD11	2.42	0.54
1:A:2553:HIS:CD2	1:A:2563:VAL:HB	2.43	0.54
1:B:1295:PRO:HD2	1:B:1297:ARG:HH21	1.72	0.54
1:A:1468:LEU:HD11	1:A:1798:LEU:HB3	1.90	0.54
1:B:784:PHE:HE1	1:B:822:MET:HE1	1.72	0.54
1:A:1522:ARG:HH21	1:B:1865:PRO:HG3	1.71	0.54
1:A:2717:ILE:HG21	1:A:2787:LEU:HD23	1.90	0.54
1:B:2641:HIS:HA	1:B:2645:VAL:HB	1.90	0.54
1:A:1841:TRP:O	1:A:1845:ILE:HG12	2.07	0.54
1:B:14:THR:HG23	1:B:16:ASP:H	1.71	0.54
1:A:438:THR:HG23	1:A:440:ASN:H	1.73	0.54
1:B:2684:GLU:N	1:B:2684:GLU:OE1	2.40	0.54
1:A:803:THR:HB	1:A:810:ILE:HD13	1.90	0.53
1:A:1164:ASN:OD1	1:A:1164:ASN:N	2.40	0.53
1:B:1515:SER:O	1:B:1515:SER:OG	2.26	0.53
1:A:816:ASN:ND2	1:A:919:ASN:OD1	2.39	0.53
1:A:1865:PRO:HG3	1:B:1522:ARG:HH21	1.72	0.53
1:A:2752:ILE:HG12	1:A:2772:LEU:HB3	1.90	0.53
1:B:1464:PHE:HB3	1:B:1798:LEU:HD11	1.89	0.53
1:B:2546:CYS:SG	1:B:2548:ILE:HG22	2.48	0.53
1:A:473:ILE:HA	1:A:487:LEU:HD13	1.90	0.53
1:A:1464:PHE:HB3	1:A:1798:LEU:HD11	1.91	0.53
1:A:1472:VAL:HG11	1:A:1827:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD22	1:A:807:GLU:HB3	1.89	0.53
1:A:546:ALA:HB3	1:A:561:LEU:HB3	1.90	0.53
1:A:885:TYR:HE1	1:A:1091:LEU:HD12	1.74	0.53
1:A:479:CYS:HB2	1:A:751:VAL:HG12	1.91	0.53
1:A:2079:ALA:HB1	1:A:2084:CYS:HB2	1.91	0.53
1:A:2300:ALA:CB	1:A:2547:PRO:HD2	2.33	0.53
1:B:1156:GLY:HA2	1:B:1160:PRO:HA	1.91	0.53
1:B:2529:PHE:CE2	1:B:2650:PRO:HB3	2.44	0.53
1:A:2689:MET:O	1:A:2692:SER:OG	2.26	0.53
1:B:874:GLN:OE1	1:B:914:HIS:ND1	2.40	0.53
1:A:765:TRP:CH2	1:A:767:ARG:HD3	2.44	0.53
1:A:493:TRP:CE2	1:A:773:LEU:HD13	2.44	0.53
1:A:1405:LEU:HD23	1:A:1425:THR:HG23	1.91	0.52
1:A:40:LEU:HD21	1:A:356:LEU:HD13	1.90	0.52
1:B:1180:SER:O	1:B:1184:THR:HG23	2.09	0.52
1:B:2543:ASN:ND2	1:B:2543:ASN:O	2.42	0.52
1:A:568:MET:SD	1:A:569:ASN:N	2.82	0.52
1:A:399:GLU:HG2	1:A:400:PRO:HD2	1.91	0.52
1:A:414:ALA:HA	1:A:417:LEU:HB2	1.89	0.52
1:A:917:ASP:N	1:A:917:ASP:OD1	2.40	0.52
1:A:2664:LYS:HE2	1:A:2664:LYS:H	1.73	0.52
1:B:1962:ASN:ND2	1:B:2180:ILE:O	2.32	0.52
1:B:47:THR:O	1:B:47:THR:OG1	2.24	0.52
1:A:661:ASP:N	1:A:661:ASP:OD1	2.43	0.52
1:A:756:VAL:HG13	1:A:771:PHE:HB2	1.91	0.52
1:A:837:ASP:OD1	1:A:920:ARG:NH2	2.38	0.52
1:B:66:ARG:HH21	1:B:362:TRP:HB3	1.74	0.52
1:A:1280:VAL:HG22	1:A:1329:LEU:HD21	1.92	0.52
1:A:1475:LEU:HD22	1:A:1791:VAL:HG13	1.91	0.52
1:A:2554:VAL:HG13	1:A:2651:LEU:HD11	1.92	0.52
1:B:2542:GLN:HA	1:B:2542:GLN:OE1	2.10	0.52
1:B:2183:ASP:N	1:B:2183:ASP:OD1	2.42	0.52
1:B:2594:VAL:O	1:B:2598:MET:HG3	2.09	0.52
1:A:1343:ILE:HD12	1:A:1424:VAL:HG13	1.91	0.51
1:A:2297:THR:HA	1:A:2547:PRO:HG3	1.92	0.51
1:B:68:CYS:SG	1:B:69:ARG:N	2.83	0.51
1:A:850:SER:HA	1:A:863:LYS:HA	1.92	0.51
1:B:1493:PRO:O	1:B:1719:ARG:NH2	2.42	0.51
1:A:825:ASP:HB3	1:A:831:ARG:HG3	1.93	0.51
1:A:2697:ASN:HB2	1:A:2753:THR:HG23	1.92	0.51
1:B:1095:SER:O	1:B:1099:GLN:NE2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:MET:O	1:A:896:GLU:HG3	2.11	0.51
1:A:2545:LEU:CD1	1:A:2738:SER:O	2.58	0.51
1:B:494:TRP:HB3	1:B:735:PRO:HB3	1.92	0.51
1:A:1490:ILE:HD12	1:B:2092:ARG:HD3	1.93	0.51
1:B:501:GLN:HA	1:B:504:LYS:HB2	1.93	0.51
1:A:1713:SER:OG	1:B:2062:ARG:NH1	2.42	0.51
1:B:413:ARG:O	1:B:417:LEU:N	2.40	0.51
1:B:875:THR:OG1	1:B:876:LEU:N	2.44	0.51
1:B:1171:TYR:OH	1:B:1271:ARG:NH2	2.38	0.51
1:A:406:ASN:HB3	1:A:409:LEU:HB2	1.92	0.51
1:A:1084:ASN:O	1:A:1088:ILE:HG13	2.12	0.51
1:A:433:ARG:NH2	1:A:481:LEU:O	2.44	0.50
1:B:23:ARG:NH2	1:B:834:ASP:OD1	2.44	0.50
1:B:50:GLN:N	1:B:50:GLN:OE1	2.44	0.50
1:B:2690:LEU:HD11	1:B:2733:TRP:CZ3	2.46	0.50
1:A:427:LEU:HD23	1:A:436:VAL:HG22	1.92	0.50
1:A:744:THR:HG22	1:A:762:THR:HB	1.92	0.50
1:A:1192:ASP:OD1	1:A:1209:THR:OG1	2.29	0.50
1:B:757:HIS:HD2	1:B:810:ILE:HD11	1.75	0.50
1:A:1174:CYS:HA	1:A:1324:PHE:HE2	1.77	0.50
1:B:907:MET:CE	1:B:907:MET:H	2.24	0.50
1:A:1363:LEU:HD11	1:B:1862:ALA:HB2	1.93	0.50
1:A:2026:SER:OG	1:A:2027:ASP:N	2.42	0.50
1:A:2724:THR:O	1:A:2727:GLN:HG2	2.12	0.50
1:A:1508:GLN:HA	1:A:1508:GLN:HE21	1.77	0.50
1:B:756:VAL:HG13	1:B:771:PHE:HB2	1.93	0.50
1:B:823:ALA:HB1	1:B:831:ARG:HH21	1.76	0.50
1:B:886:GLU:O	1:B:890:GLN:HG2	2.12	0.50
1:B:1096:VAL:HA	1:B:1099:GLN:HG2	1.92	0.50
1:A:1412:LYS:HE2	1:A:1412:LYS:HA	1.92	0.50
1:A:2757:PRO:HG3	1:A:2776:LEU:HD23	1.93	0.50
1:B:1961:MET:O	1:B:1965:THR:HG23	2.11	0.50
1:A:1441:VAL:HG11	1:B:1917:PHE:HE2	1.76	0.50
1:B:22:LEU:O	1:B:25:VAL:HG12	2.12	0.50
1:A:1274:HIS:HB3	1:A:1342:MET:CE	2.42	0.49
1:A:1941:VAL:HG21	1:A:2195:LEU:HD23	1.94	0.49
1:A:1153:VAL:O	1:A:1157:MET:HG3	2.11	0.49
1:B:1955:ILE:HG21	1:B:2211:ILE:HD13	1.94	0.49
1:A:746:ILE:HG13	1:A:760:LEU:HD22	1.93	0.49
1:B:836:LEU:HD22	1:B:838:LEU:HD12	1.94	0.49
1:B:1233:ASP:HB2	1:B:1236:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2186:LEU:HD22	1:B:2193:LEU:HD21	1.94	0.49
1:A:802:PHE:CG	1:A:844:LEU:HD12	2.47	0.49
1:B:1871:PRO:HG3	1:B:1936:LEU:HD11	1.94	0.49
1:A:741:PRO:HB2	1:A:744:THR:HG21	1.94	0.49
1:A:392:GLN:OE1	1:A:411:HIS:ND1	2.45	0.49
1:A:1256:TYR:CE1	1:A:1331:ARG:HG3	2.43	0.49
1:B:2568:PHE:HE2	1:B:2639:ALA:HA	1.77	0.49
1:A:2500:ASP:OD2	1:A:2522:THR:OG1	2.21	0.49
1:B:757:HIS:ND1	1:B:770:ILE:HG12	2.27	0.49
1:B:922:ILE:HG13	1:B:923:LEU:HD22	1.93	0.49
1:A:568:MET:HE3	1:A:568:MET:H	1.77	0.49
1:A:886:GLU:O	1:A:890:GLN:NE2	2.44	0.49
1:B:414:ALA:O	1:B:418:GLY:N	2.44	0.49
1:B:2176:MET:HB2	1:B:2180:ILE:HD11	1.95	0.49
1:A:1918:LEU:HD22	1:B:1438:ILE:HD12	1.95	0.49
1:A:2630:ASN:OD1	1:A:2630:ASN:N	2.45	0.49
1:B:493:TRP:CE2	1:B:773:LEU:HD13	2.48	0.49
1:B:2721:MET:SD	1:B:2721:MET:N	2.86	0.49
1:A:839:PRO:HG3	1:A:878:GLN:HE21	1.77	0.49
1:B:32:TYR:HB3	1:B:34:LEU:HD23	1.94	0.49
1:B:2281:PHE:HB3	1:B:2284:GLU:HB2	1.93	0.49
1:B:832:ASP:OD1	1:B:1112:ARG:NH2	2.40	0.48
1:B:1828:GLN:HE22	1:B:2171:PRO:HB3	1.78	0.48
1:B:1852:GLN:HG2	1:B:2090:VAL:CG1	2.43	0.48
1:A:1381:ASP:OD1	1:A:1434:ARG:NH1	2.47	0.48
1:A:2565:TRP:O	1:A:2568:PHE:HB3	2.13	0.48
1:B:1269:ASN:HD21	1:B:1273:GLU:HG3	1.78	0.48
1:B:1712:ARG:HA	1:B:1715:GLN:HG2	1.96	0.48
1:A:895:LEU:HD11	1:A:907:MET:HG2	1.94	0.48
1:A:1199:CYS:SG	1:A:1216:HIS:HE1	2.35	0.48
1:A:1442:GLU:OE2	1:A:1509:GLY:CA	2.56	0.48
1:B:836:LEU:N	1:B:917:ASP:OD2	2.47	0.48
1:B:1259:LEU:HD11	1:B:1332:VAL:HG22	1.95	0.48
1:A:75:GLN:OE1	1:A:78:ARG:N	2.46	0.48
1:A:438:THR:OG1	1:A:439:GLU:OE1	2.32	0.48
1:A:1799:MET:HE2	1:A:1799:MET:HA	1.96	0.48
1:A:2087:GLU:H	1:A:2087:GLU:CD	2.13	0.48
1:A:2549:THR:HA	1:A:2680:ASN:ND2	2.28	0.48
1:B:437:ALA:HB2	1:B:476:LEU:HD11	1.96	0.48
1:B:433:ARG:NE	1:B:483:THR:OG1	2.46	0.48
1:A:818:THR:OG1	1:A:819:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2269:THR:OG1	1:A:2270:THR:N	2.47	0.48
1:B:1848:SER:O	1:B:1852:GLN:HG3	2.14	0.48
1:A:38:PRO:N	1:A:39:PRO:HD2	2.29	0.48
1:A:378:TYR:CD2	1:A:556:PRO:HD2	2.48	0.48
1:A:908:LEU:HD12	1:A:1101:TYR:CE2	2.49	0.48
1:B:1839:TRP:HE1	1:B:2176:MET:CE	2.27	0.48
1:A:413:ARG:O	1:A:417:LEU:N	2.42	0.48
1:B:2279:VAL:HB	1:B:2291:VAL:HG13	1.96	0.48
1:B:2530:ARG:HD2	1:B:2656:LYS:HE3	1.96	0.48
1:B:1240:CYS:SG	1:B:1242:THR:OG1	2.72	0.47
1:B:1854:ARG:NH1	1:B:2087:GLU:OE2	2.47	0.47
1:B:2218:PHE:HE1	1:B:2222:GLU:HB3	1.79	0.47
1:A:503:LYS:HE3	1:A:503:LYS:HA	1.95	0.47
1:A:2500:ASP:OD1	1:A:2520:LYS:N	2.41	0.47
1:A:742:GLU:HB2	1:A:743:LYS:HZ3	1.77	0.47
1:B:66:ARG:HH12	1:B:68:CYS:HB2	1.79	0.47
1:B:482:TYR:CE2	1:B:773:LEU:HD11	2.49	0.47
1:A:1962:ASN:O	1:A:1965:THR:OG1	2.20	0.47
1:A:2571:PHE:HE2	1:A:2642:ARG:HE	1.62	0.47
1:B:2532:ILE:HA	1:B:2535:ILE:HD12	1.96	0.47
1:B:2762:LEU:HD23	1:B:2786:LYS:HD3	1.96	0.47
1:A:427:LEU:HD22	1:A:428:SER:N	2.29	0.47
1:A:2637:LYS:O	1:A:2641:HIS:HB2	2.14	0.47
1:B:1117:PHE:CD2	1:B:1158:VAL:HG23	2.50	0.47
1:B:1256:TYR:CE1	1:B:1331:ARG:HG3	2.50	0.47
1:B:1928:HIS:HA	1:B:2091:ASP:HB3	1.96	0.47
1:A:43:LEU:HD11	1:A:48:ILE:HD11	1.97	0.47
1:A:846:MET:HB3	1:A:867:ILE:HD13	1.96	0.47
1:A:1256:TYR:O	1:A:1260:THR:HG23	2.15	0.47
1:A:1351:LYS:HE3	1:A:1357:SER:HB2	1.97	0.47
1:A:2044:LEU:HD11	1:A:2051:ALA:HB3	1.97	0.47
1:A:2529:PHE:O	1:A:2532:ILE:HG22	2.15	0.47
1:A:2740:PRO:HD2	1:A:2746:PHE:CE2	2.50	0.47
1:A:1871:PRO:HB3	1:B:1716:TRP:CD1	2.49	0.47
1:B:498:PRO:HD2	1:B:501:GLN:NE2	2.29	0.47
1:B:2031:PHE:CD2	1:B:2070:PRO:HG3	2.49	0.47
1:A:2766:ASN:O	1:A:2770:SER:CA	2.63	0.47
1:B:2269:THR:OG1	1:B:2270:THR:N	2.45	0.47
1:B:2653:ALA:HA	1:B:2656:LYS:HE2	1.96	0.47
1:A:417:LEU:O	1:A:461:THR:OG1	2.33	0.46
1:A:908:LEU:HD12	1:A:1101:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:NE2	1:B:69:ARG:HB2	2.30	0.46
1:B:501:GLN:HB3	1:B:774:ALA:HB2	1.96	0.46
1:B:1164:ASN:N	1:B:1164:ASN:OD1	2.41	0.46
1:B:1868:PRO:HA	1:B:1873:HIS:ND1	2.30	0.46
1:B:2700:SER:OG	1:B:2755:ARG:O	2.33	0.46
1:A:2546:CYS:SG	1:A:2547:PRO:N	2.88	0.46
1:B:48:ILE:HD12	1:B:48:ILE:N	2.31	0.46
1:B:417:LEU:HD21	1:B:446:TRP:HB3	1.96	0.46
1:B:931:PHE:CE1	1:B:1123:GLY:HA3	2.50	0.46
1:B:2035:ILE:HD12	1:B:2035:ILE:O	2.14	0.46
1:B:2583:ILE:O	1:B:2586:SER:OG	2.30	0.46
1:A:2207:GLU:H	1:A:2207:GLU:CD	2.14	0.46
1:A:2281:PHE:HB3	1:A:2284:GLU:HB2	1.96	0.46
1:A:2558:LEU:O	1:A:2655:ARG:NH1	2.49	0.46
1:B:57:HIS:CE1	1:B:69:ARG:HB2	2.50	0.46
1:B:550:SER:O	1:B:556:PRO:HA	2.14	0.46
1:A:837:ASP:N	1:A:917:ASP:OD2	2.43	0.46
1:A:1274:HIS:HB3	1:A:1342:MET:HE2	1.98	0.46
1:A:2553:HIS:O	1:A:2557:VAL:HG23	2.15	0.46
1:A:1370:TYR:HE1	1:B:2088:VAL:HA	1.80	0.46
1:A:1695:LEU:HD12	1:A:1696:GLU:HG2	1.97	0.46
1:A:2239:ASP:OD2	1:A:2278:LYS:NZ	2.48	0.46
1:B:29:LEU:HD22	1:B:29:LEU:C	2.36	0.46
1:B:438:THR:HG22	1:B:442:LYS:HB2	1.97	0.46
1:A:573:ARG:HA	1:A:650:GLN:HA	1.98	0.46
1:A:753:SER:N	1:A:805:GLY:O	2.49	0.46
1:A:2545:LEU:HD11	1:A:2740:PRO:CD	2.44	0.46
1:A:2656:LYS:H	1:A:2656:LYS:HD2	1.80	0.46
1:B:1855:TYR:OH	1:B:1933:SER:HA	2.15	0.46
1:B:1962:ASN:ND2	1:B:2181:SER:HA	2.31	0.46
1:B:2315:ILE:HG23	1:B:2316:GLN:HG3	1.96	0.46
1:A:1329:LEU:HD23	1:A:1397:LEU:HD13	1.97	0.46
1:B:66:ARG:HG3	1:B:66:ARG:NH1	2.29	0.46
1:B:393:TRP:CZ2	1:B:400:PRO:HG3	2.51	0.46
1:B:2300:ALA:HB3	1:B:2547:PRO:HD2	1.96	0.46
1:A:1513:LEU:CD2	1:B:1918:LEU:HB3	2.46	0.46
1:A:2244:VAL:HG13	1:A:2251:LEU:HD23	1.98	0.46
1:A:2532:ILE:CD1	1:A:2548:ILE:HD12	2.41	0.46
1:B:1313:ASP:OD1	1:B:1313:ASP:N	2.38	0.46
1:B:2057:LEU:HG	1:B:2677:LEU:HD12	1.97	0.46
1:A:767:ARG:NH1	1:A:781:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HD13	1:B:360:LEU:HB3	1.98	0.45
1:B:1443:MET:HE1	1:B:1454:PRO:HG2	1.98	0.45
1:B:2648:GLU:OE2	1:B:2649:GLN:NE2	2.49	0.45
1:A:76:PRO:HG3	1:A:854:LEU:HD11	1.98	0.45
1:A:920:ARG:HG2	1:A:924:HIS:HB3	1.98	0.45
1:A:1508:GLN:HA	1:A:1508:GLN:NE2	2.31	0.45
1:A:2652:HIS:O	1:A:2656:LYS:HD2	2.16	0.45
1:A:378:TYR:HE2	1:A:555:ILE:HG23	1.81	0.45
1:A:1932:HIS:ND1	1:A:1935:VAL:HG23	2.31	0.45
1:A:2730:VAL:HG12	1:A:2736:SER:O	2.17	0.45
1:B:1847:ASP:OD2	1:B:2188:ARG:NH2	2.34	0.45
1:B:1852:GLN:HG2	1:B:2090:VAL:HG12	1.98	0.45
1:B:1860:ALA:HB2	1:B:1871:PRO:HG2	1.98	0.45
1:A:752:ASP:OD1	1:A:757:HIS:NE2	2.50	0.45
1:B:579:PRO:HA	1:B:582:LEU:HD12	1.98	0.45
1:B:1201:LEU:HG	1:B:1237:LYS:HZ2	1.81	0.45
1:B:1350:ASN:N	1:B:1350:ASN:OD1	2.49	0.45
1:B:1437:VAL:HG11	1:B:1482:LEU:HD11	1.97	0.45
1:B:2218:PHE:HB3	1:B:2219:GLU:OE1	2.17	0.45
1:B:2288:GLY:O	1:B:2291:VAL:HG12	2.16	0.45
1:A:1408:GLU:OE1	1:A:1417:ARG:HD3	2.16	0.45
1:A:2021:PRO:HA	1:A:2024:ARG:HG3	1.99	0.45
1:B:2083:LYS:HB2	1:B:2083:LYS:NZ	2.31	0.45
1:A:1406:VAL:O	1:A:1410:GLN:HG2	2.16	0.45
1:A:2244:VAL:HG21	1:A:2295:PHE:CD1	2.51	0.45
1:B:1775:SER:O	1:B:1775:SER:OG	2.32	0.45
1:A:392:GLN:HE22	1:A:411:HIS:HB2	1.82	0.45
1:A:2780:LYS:O	1:A:2784:LYS:HG2	2.16	0.45
1:B:491:LEU:HB2	1:B:738:LEU:HD12	1.99	0.45
1:B:542:TYR:HB2	1:B:565:VAL:HB	1.98	0.45
1:A:2089:THR:O	1:A:2095:LEU:HD21	2.16	0.45
1:A:2182:HIS:O	1:A:2186:LEU:HG	2.17	0.45
1:B:911:PHE:HA	1:B:914:HIS:CD2	2.52	0.45
1:B:1517:GLU:OE1	1:B:1517:GLU:N	2.44	0.45
1:B:1787:ALA:O	1:B:1791:VAL:HG23	2.16	0.45
1:B:2091:ASP:O	1:B:2095:LEU:HD23	2.17	0.45
1:B:2633:GLU:O	1:B:2637:LYS:HG2	2.17	0.45
1:A:904:ASN:HB3	1:A:907:MET:HB3	1.98	0.45
1:B:1289:GLU:O	1:B:1292:GLN:NE2	2.47	0.45
1:B:2087:GLU:HG2	1:B:2087:GLU:O	2.17	0.45
1:A:380:GLU:HB2	1:A:394:LYS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TRP:CZ3	1:A:736:LYS:HD3	2.51	0.44
1:B:75:GLN:NE2	1:B:353:PRO:O	2.51	0.44
1:B:855:PRO:O	1:B:858:SER:OG	2.35	0.44
1:B:1327:LEU:HD12	1:B:1327:LEU:H	1.81	0.44
1:B:2579:LEU:CD2	1:B:2635:VAL:HG22	2.39	0.44
1:A:1121:VAL:HG22	1:A:1254:LEU:HD21	1.99	0.44
1:A:1276:LEU:HD12	1:A:1342:MET:HB2	1.99	0.44
1:A:2072:GLN:HG2	1:A:2074:LEU:HD13	1.99	0.44
1:A:2755:ARG:HH12	1:A:2761:HIS:CG	2.34	0.44
1:B:1443:MET:O	1:B:1786:ARG:NH2	2.39	0.44
1:A:1320:GLU:OE2	1:A:1320:GLU:HA	2.17	0.44
1:A:1917:PHE:HE2	1:B:1441:VAL:HG11	1.83	0.44
1:A:2248:ARG:HG3	1:A:2249:ASP:N	2.32	0.44
1:B:1222:LYS:HB3	1:B:1222:LYS:HZ3	1.83	0.44
1:B:1842:MET:HG3	1:B:1951:PHE:HB2	1.99	0.44
1:A:2:THR:OG1	1:A:3:SER:N	2.50	0.44
1:A:1204:SER:OG	1:A:1205:LEU:N	2.51	0.44
1:A:2252:ILE:O	1:A:2256:MET:HG3	2.18	0.44
1:B:762:THR:HG23	1:B:767:ARG:NH2	2.32	0.44
1:B:814:ASP:OD1	1:B:814:ASP:N	2.35	0.44
1:B:2182:HIS:O	1:B:2186:LEU:HG	2.17	0.44
1:B:2203:ASP:OD1	1:B:2203:ASP:N	2.50	0.44
1:A:1845:ILE:HD12	1:B:1490:ILE:HG21	2.00	0.44
1:B:1248:LYS:H	1:B:1248:LYS:HG2	1.58	0.44
1:A:1193:ILE:HG23	1:A:1206:CYS:HB3	1.99	0.44
1:B:29:LEU:O	1:B:878:GLN:NE2	2.51	0.44
1:B:2518:PRO:HG3	1:B:2647:ALA:HB2	1.99	0.44
1:B:2689:MET:O	1:B:2692:SER:OG	2.32	0.44
1:A:2219:GLU:O	1:A:2222:GLU:HG3	2.18	0.44
1:A:2556:LYS:HD2	1:A:2561:ARG:HB2	1.99	0.44
1:B:361:GLN:HE22	1:B:393:TRP:HZ3	1.66	0.44
1:B:2201:MET:O	1:B:2201:MET:HG3	2.18	0.44
1:A:1934:ASP:HB3	1:B:1519:LEU:H	1.82	0.44
1:A:1935:VAL:HG13	1:B:1378:ILE:HD11	2.00	0.44
1:A:2075:TYR:HA	1:A:2086:MET:H	1.82	0.44
1:B:438:THR:CG2	1:B:442:LYS:HB2	2.48	0.44
1:B:741:PRO:HB2	1:B:744:THR:HG21	1.98	0.44
1:B:1454:PRO:HD2	1:B:1457:ILE:HB	2.00	0.44
1:B:2027:ASP:HA	1:B:2030:THR:HG22	1.99	0.44
1:B:2164:PRO:HA	1:B:2165:PRO:HD3	1.92	0.44
1:B:2229:MET:O	1:B:2233:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2559:LEU:HD22	1:B:2667:LEU:HG	1.98	0.44
1:A:378:TYR:HD2	1:A:556:PRO:HD2	1.83	0.44
1:A:1860:ALA:HB2	1:A:1871:PRO:HG2	2.00	0.44
1:A:1959:LYS:HB2	1:A:1959:LYS:NZ	2.33	0.44
1:B:26:SER:HB3	1:B:838:LEU:HG	2.00	0.44
1:B:802:PHE:CD2	1:B:844:LEU:HD22	2.52	0.44
1:B:2707:LEU:O	1:B:2711:LYS:HG3	2.18	0.44
1:B:2716:SER:O	1:B:2719:GLU:HG2	2.17	0.44
1:A:438:THR:HG22	1:A:442:LYS:HB2	2.00	0.43
1:A:2020:HIS:CD2	1:A:2636:ARG:HD2	2.53	0.43
1:B:49:LYS:HB3	1:B:50:GLN:OE1	2.17	0.43
1:B:1874:ALA:O	1:B:1877:ASN:HB2	2.18	0.43
1:B:2181:SER:HB3	1:B:2184:MET:CE	2.48	0.43
1:A:2788:LEU:HA	1:A:2791:ILE:HG12	2.00	0.43
1:B:923:LEU:HD22	1:B:923:LEU:H	1.83	0.43
1:B:2097:VAL:HG22	1:B:2101:LYS:NZ	2.33	0.43
1:A:72:PHE:C	1:A:72:PHE:CD1	2.90	0.43
1:A:1690:MET:HB3	1:A:1691:LEU:H	1.55	0.43
1:A:2549:THR:HA	1:A:2680:ASN:HD21	1.83	0.43
1:A:2648:GLU:O	1:A:2652:HIS:HB3	2.18	0.43
1:A:550:SER:HB2	1:A:656:VAL:HG12	2.00	0.43
1:A:1102:LEU:HD23	1:A:1102:LEU:HA	1.78	0.43
1:A:1714:MET:HE3	1:B:2195:LEU:HD13	2.01	0.43
1:B:1336:TRP:CE3	1:B:1408:GLU:HG3	2.52	0.43
1:B:1474:GLU:OE2	1:B:1474:GLU:HA	2.18	0.43
1:A:1351:LYS:HD3	1:A:1351:LYS:HA	1.82	0.43
1:A:2766:ASN:O	1:A:2770:SER:HA	2.18	0.43
1:B:1256:TYR:O	1:B:1260:THR:HG23	2.18	0.43
1:B:1412:LYS:HD3	1:B:1412:LYS:HA	1.92	0.43
1:B:2255:THR:HG21	1:B:2299:ILE:CD1	2.49	0.43
1:B:2601:ALA:HA	1:B:2625:PRO:HA	2.00	0.43
1:A:28:LYS:HB2	1:A:28:LYS:HE2	1.84	0.43
1:A:426:LEU:HB2	1:A:437:ALA:HB3	2.00	0.43
1:A:2020:HIS:HE2	1:A:2636:ARG:CZ	2.31	0.43
1:A:2250:LEU:O	1:A:2254:GLN:HG2	2.19	0.43
1:B:1841:TRP:O	1:B:1845:ILE:HG12	2.18	0.43
1:A:2279:VAL:HG11	1:A:2295:PHE:HB2	2.00	0.43
1:A:2558:LEU:HG	1:A:2658:LEU:HD13	2.00	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.71	0.43
1:B:487:LEU:HD23	1:B:492:TYR:HD1	1.84	0.43
1:B:1339:LEU:HD21	1:B:1401:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2726:ARG:O	1:A:2730:VAL:HG23	2.19	0.43
1:B:819:ILE:HG21	1:B:836:LEU:HD13	2.01	0.43
1:B:2304:LEU:HD23	1:B:2304:LEU:HA	1.84	0.43
1:B:2550:LEU:O	1:B:2676:ARG:NH2	2.42	0.43
1:A:7:VAL:CG2	1:A:867:ILE:HB	2.49	0.43
1:A:10:PRO:HB3	1:A:861:LYS:HD2	2.00	0.43
1:A:457:LYS:NZ	1:A:662:VAL:O	2.52	0.43
1:A:1294:ARG:H	1:A:1294:ARG:HG2	1.62	0.43
1:A:2207:GLU:OE2	1:A:2207:GLU:N	2.32	0.43
1:B:1422:ILE:O	1:B:1426:MET:HG2	2.19	0.43
1:A:838:LEU:HD23	1:A:839:PRO:HD2	2.01	0.42
1:A:1862:ALA:HB2	1:B:1363:LEU:HD11	2.01	0.42
1:A:1918:LEU:HD11	1:B:1442:GLU:HG3	2.00	0.42
1:A:2645:VAL:HA	1:A:2648:GLU:OE2	2.19	0.42
1:B:1846:MET:HA	1:B:1849:THR:HG22	2.01	0.42
1:B:2059:PRO:HB3	1:B:2218:PHE:HE2	1.84	0.42
1:A:52:VAL:HG23	1:A:59:ALA:HB3	2.01	0.42
1:A:886:GLU:HA	1:A:889:ARG:HH12	1.84	0.42
1:A:2083:LYS:HZ3	1:A:2189:TRP:HH2	1.65	0.42
1:B:1106:LEU:HD23	1:B:1106:LEU:HA	1.92	0.42
1:B:1115:THR:HG23	1:B:1118:MET:HE2	2.02	0.42
1:A:378:TYR:CE2	1:A:555:ILE:HG23	2.55	0.42
1:A:1170:LEU:HD12	1:A:1170:LEU:HA	1.83	0.42
1:A:1468:LEU:HD13	1:A:1798:LEU:HD22	2.00	0.42
1:A:2546:CYS:SG	1:A:2548:ILE:HG22	2.59	0.42
1:B:57:HIS:HD1	1:B:71:GLY:HA2	1.84	0.42
1:A:1352:ASP:OD1	1:A:1352:ASP:N	2.35	0.42
1:A:1519:LEU:HA	1:A:1520:PRO:HD3	1.93	0.42
1:A:2579:LEU:HD12	1:A:2579:LEU:HA	1.84	0.42
1:B:1486:VAL:HG22	1:B:1781:ALA:HA	2.01	0.42
1:B:2236:GLN:HG3	1:B:2273:ALA:HB3	2.01	0.42
1:B:2243:GLU:O	1:B:2258:GLN:NE2	2.52	0.42
1:A:739:CYS:HB2	1:A:777:LYS:HD2	2.01	0.42
1:A:1472:VAL:HG13	1:A:1827:LEU:HD11	2.02	0.42
1:A:2060:ASN:OD1	1:A:2060:ASN:N	2.49	0.42
1:A:2256:MET:SD	1:A:2257:ARG:N	2.93	0.42
1:B:423:LYS:C	1:B:438:THR:HG1	2.22	0.42
1:A:378:TYR:HD1	1:A:378:TYR:O	2.03	0.42
1:A:1961:MET:O	1:A:1965:THR:HG23	2.19	0.42
1:A:2535:ILE:HD12	1:A:2536:LEU:N	2.34	0.42
1:A:2766:ASN:ND2	1:A:2768:CYS:SG	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD12	1:B:863:LYS:HD2	2.02	0.42
1:A:868:ILE:O	1:A:868:ILE:HD12	2.20	0.42
1:A:1189:ILE:HD11	1:A:1292:GLN:HB2	2.00	0.42
1:A:1336:TRP:CD2	1:A:1408:GLU:HG3	2.55	0.42
1:B:2552:ARG:N	1:B:2676:ARG:HH22	2.17	0.42
1:B:753:SER:N	1:B:805:GLY:O	2.52	0.42
1:B:756:VAL:CG1	1:B:771:PHE:HB2	2.50	0.42
1:B:1954:LEU:HD23	1:B:1954:LEU:HA	1.85	0.42
1:A:1110:ASP:OD1	1:A:1111:ALA:N	2.49	0.42
1:B:1342:MET:O	1:B:1345:PHE:HB2	2.20	0.42
1:B:2540:LEU:HD23	1:B:2540:LEU:HA	1.83	0.42
1:A:370:LYS:HB2	1:A:386:SER:OG	2.19	0.41
1:A:761:LYS:NZ	1:A:763:GLY:O	2.53	0.41
1:A:1350:ASN:OD1	1:A:1350:ASN:N	2.53	0.41
1:A:2043:PRO:HA	1:A:2580:ARG:CZ	2.50	0.41
1:B:2746:PHE:HB3	1:B:2748:PRO:O	2.20	0.41
1:A:568:MET:H	1:A:568:MET:CE	2.32	0.41
1:A:1084:ASN:HA	1:A:1087:PHE:HD2	1.84	0.41
1:B:38:PRO:O	1:B:40:LEU:N	2.53	0.41
1:B:2667:LEU:HD12	1:B:2667:LEU:HA	1.92	0.41
1:A:484:CYS:SG	1:A:485:ALA:N	2.93	0.41
1:A:1203:GLU:O	1:A:1204:SER:HB3	2.21	0.41
1:A:1497:PHE:CD2	1:B:1914:ARG:HG3	2.56	0.41
1:B:51:CYS:SG	1:B:60:PHE:HB3	2.60	0.41
1:B:1256:TYR:HE1	1:B:1331:ARG:HG3	1.84	0.41
1:B:2248:ARG:NH2	1:B:2302:ALA:HA	2.35	0.41
1:B:803:THR:HB	1:B:810:ILE:HD13	2.02	0.41
1:B:66:ARG:NH2	1:B:68:CYS:HB2	2.34	0.41
1:B:892:LEU:HD13	1:B:892:LEU:HA	1.86	0.41
1:B:1150:GLU:OE1	1:B:1150:GLU:HA	2.20	0.41
1:B:2089:THR:O	1:B:2095:LEU:HD21	2.19	0.41
1:B:2717:ILE:HD11	1:B:2784:LYS:HZ2	1.86	0.41
1:A:401:TYR:CZ	1:A:412:PRO:HD3	2.55	0.41
1:A:401:TYR:CE2	1:A:412:PRO:HD3	2.55	0.41
1:A:2548:ILE:O	1:A:2550:LEU:CD1	2.69	0.41
1:B:438:THR:OG1	1:B:439:GLU:N	2.52	0.41
1:B:2083:LYS:HB2	1:B:2083:LYS:HZ3	1.86	0.41
1:A:480:ALA:HB1	1:A:551:ILE:HD12	2.03	0.41
1:A:493:TRP:O	1:A:735:PRO:HA	2.21	0.41
1:A:1695:LEU:HB2	1:B:2715:TRP:HE1	1.84	0.41
1:A:1855:TYR:OH	1:A:1933:SER:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2532:ILE:O	1:A:2535:ILE:HD12	2.21	0.41
1:B:2241:SER:HB2	1:B:2278:LYS:H	1.85	0.41
1:A:439:GLU:HG2	1:A:440:ASN:N	2.35	0.41
1:B:802:PHE:HB3	1:B:846:MET:CE	2.51	0.41
1:B:1426:MET:HB3	1:B:1430:ARG:HH12	1.86	0.41
1:A:424:ILE:HG23	1:A:436:VAL:HG13	2.02	0.41
1:A:1182:THR:HG22	1:A:1319:LEU:HB3	2.03	0.41
1:A:1716:TRP:CZ2	1:B:1856:GLY:HA3	2.55	0.41
1:B:874:GLN:O	1:B:878:GLN:HB2	2.21	0.41
1:B:882:ARG:C	1:B:1081:ARG:HH22	2.24	0.41
1:B:1233:ASP:HA	1:B:1235:TRP:CZ3	2.56	0.41
1:B:1277:LEU:O	1:B:1281:GLN:HG3	2.20	0.41
1:B:1951:PHE:CE1	1:B:1955:ILE:HG13	2.56	0.41
1:B:2661:VAL:HG13	1:B:2662:LEU:HD13	2.03	0.41
1:A:1187:GLU:H	1:A:1187:GLU:HG2	1.73	0.41
1:B:2602:PHE:CE1	1:B:2634:TYR:HB2	2.56	0.41
1:A:1483:ILE:HB	1:A:1788:TYR:CD1	2.56	0.40
1:A:1856:GLY:HA3	1:B:1716:TRP:CZ2	2.56	0.40
1:A:2062:ARG:HE	1:A:2062:ARG:HB3	1.69	0.40
1:A:2562:LYS:HD3	1:A:2563:VAL:N	2.36	0.40
1:B:792:LEU:O	1:B:815:GLY:HA3	2.20	0.40
1:B:2529:PHE:O	1:B:2532:ILE:HG22	2.21	0.40
1:A:794:GLN:H	1:A:794:GLN:HG2	1.61	0.40
1:A:2531:ASN:O	1:A:2535:ILE:HG13	2.21	0.40
1:B:1154:PHE:O	1:B:1158:VAL:HG12	2.21	0.40
1:B:1828:GLN:O	1:B:1832:GLU:HG3	2.21	0.40
1:B:2241:SER:OG	1:B:2242:LEU:N	2.54	0.40
1:A:1468:LEU:O	1:A:1472:VAL:HG12	2.21	0.40
1:B:414:ALA:HA	1:B:417:LEU:HB2	2.03	0.40
1:B:883:CYS:HB2	1:B:1081:ARG:NH2	2.36	0.40
1:B:1102:LEU:HD23	1:B:1102:LEU:HA	1.86	0.40
1:B:1252:LEU:HD11	1:B:1327:LEU:HD22	2.03	0.40
1:B:2784:LYS:HD2	1:B:2784:LYS:H	1.87	0.40
1:A:757:HIS:N	1:A:757:HIS:CD2	2.87	0.40
1:A:777:LYS:HE2	1:A:777:LYS:HB3	1.89	0.40
1:A:2717:ILE:HD11	1:A:2784:LYS:HZ3	1.86	0.40
1:B:482:TYR:CZ	1:B:773:LEU:HD11	2.57	0.40
1:B:1388:ILE:HG22	1:B:1389:VAL:HG12	2.03	0.40
1:B:2239:ASP:OD1	1:B:2276:ARG:N	2.54	0.40
1:A:1080:ASP:O	1:A:1084:ASN:ND2	2.36	0.40
1:A:1149:LYS:HE2	1:A:1149:LYS:N	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:LEU:O	1:B:880:ILE:HG23	2.20	0.40
1:B:1194:PHE:HE2	1:B:1209:THR:HG23	1.85	0.40
1:B:1247:GLN:O	1:B:1251:ARG:HG3	2.22	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	1658/2806 (59%)	1589 (96%)	69 (4%)	0	100	100
1	B	1643/2806 (59%)	1568 (95%)	75 (5%)	0	100	100
All	All	3301/5612 (59%)	3157 (96%)	144 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1482/2426 (61%)	1422 (96%)	60 (4%)	31	65
1	B	1468/2426 (60%)	1397 (95%)	71 (5%)	25	58
All	All	2950/4852 (61%)	2819 (96%)	131 (4%)	32	61

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	VAL
1	A	20	ASP
1	A	21	ARG
1	A	72	PHE
1	A	378	TYR
1	A	379	SER
1	A	441	ASN
1	A	478	CYS
1	A	484	CYS
1	A	503	LYS
1	A	542	TYR
1	A	568	MET
1	A	827	MET
1	A	846	MET
1	A	849	HIS
1	A	908	LEU
1	A	909	GLN
1	A	911	PHE
1	A	1090	LYS
1	A	1095	SER
1	A	1098	LEU
1	A	1149	LYS
1	A	1161	SER
1	A	1167	ASP
1	A	1231	TYR
1	A	1238	CYS
1	A	1323	ARG
1	A	1330	GLU
1	A	1350	ASN
1	A	1354	LEU
1	A	1382	CYS
1	A	1399	ASP
1	A	1467	LEU
1	A	1507	MET
1	A	1807	HIS
1	A	1818	LYS
1	A	1844	SER
1	A	1929	ASN
1	A	1939	LEU
1	A	1952	GLN
1	A	1959	LYS
1	A	2028	SER

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Mol	Chain	Res	Type
1	A	2102	MET
1	A	2172	GLN
1	A	2173	CYS
1	A	2246	ARG
1	A	2255	THR
1	A	2256	MET
1	A	2262	HIS
1	A	2515	THR
1	A	2545	LEU
1	A	2546	CYS
1	A	2643	MET
1	A	2661	VAL
1	A	2664	LYS
1	A	2721	MET
1	A	2722	SER
1	A	2726	ARG
1	A	2731	TYR
1	B	29	LEU
1	B	41	ASN
1	B	47	THR
1	B	60	PHE
1	B	66	ARG
1	B	361	GLN
1	B	373	CYS
1	B	382	LEU
1	B	463	GLN
1	B	505	MET
1	B	562	MET
1	B	568	MET
1	B	732	GLN
1	B	760	LEU
1	B	765	TRP
1	B	795	ASN
1	B	808	SER
1	B	834	ASP
1	B	894	ASN
1	B	896	GLU
1	B	907	MET
1	B	911	PHE
1	B	1092	LEU
1	B	1097	VAL
1	B	1118	MET

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Mol	Chain	Res	Type
1	B	1141	LYS
1	B	1192	ASP
1	B	1220	ASP
1	B	1231	TYR
1	B	1235	TRP
1	B	1244	ILE
1	B	1263	ASN
1	B	1350	ASN
1	B	1377	THR
1	B	1389	VAL
1	B	1470	TYR
1	B	1515	SER
1	B	1719	ARG
1	B	1775	SER
1	B	1804	LYS
1	B	1811	SER
1	B	1819	LEU
1	B	1935	VAL
1	B	1957	TRP
1	B	2020	HIS
1	B	2026	SER
1	B	2065	ASP
1	B	2075	TYR
1	B	2102	MET
1	B	2167	THR
1	B	2175	PHE
1	B	2178	MET
1	B	2183	ASP
1	B	2184	MET
1	B	2214	GLU
1	B	2218	PHE
1	B	2248	ARG
1	B	2256	MET
1	B	2295	PHE
1	B	2510	LYS
1	B	2539	CYS
1	B	2543	ASN
1	B	2590	ASP
1	B	2610	GLU
1	B	2638	TYR
1	B	2648	GLU
1	B	2721	MET

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Mol	Chain	Res	Type
1	B	2726	ARG
1	B	2742	SER
1	B	2746	PHE
1	B	2749	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	GLN
1	A	924	HIS
1	A	1508	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

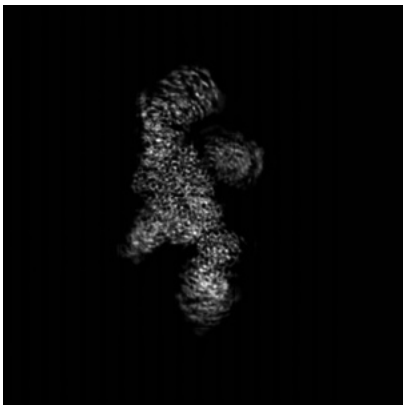
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27201. These allow visual inspection of the internal detail of the map and identification of artifacts.

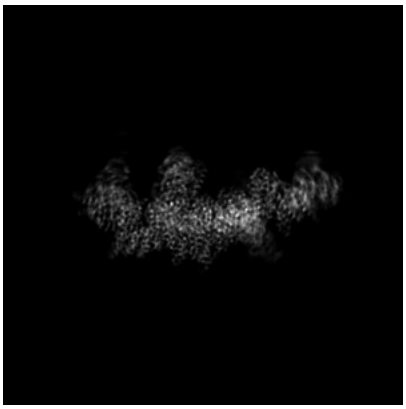
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

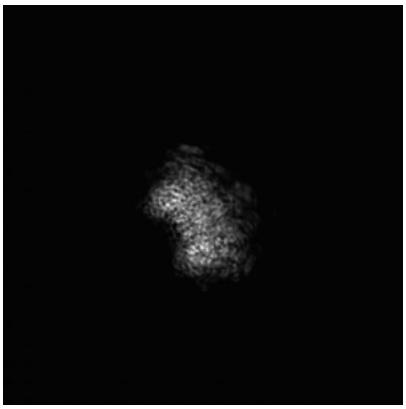
6.1.1 Primary map



X

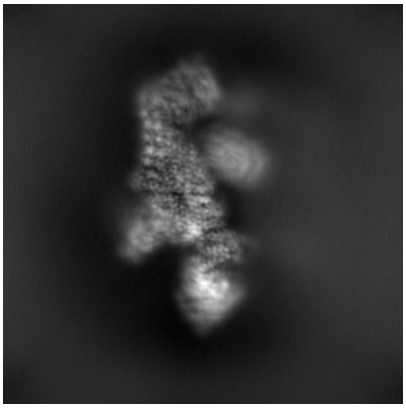


Y

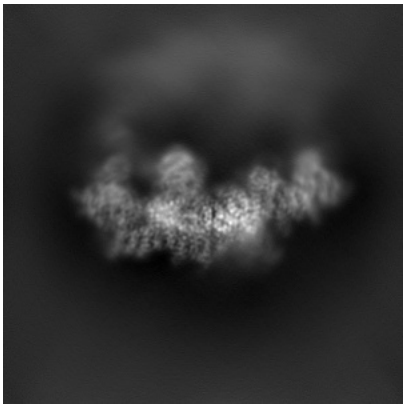


Z

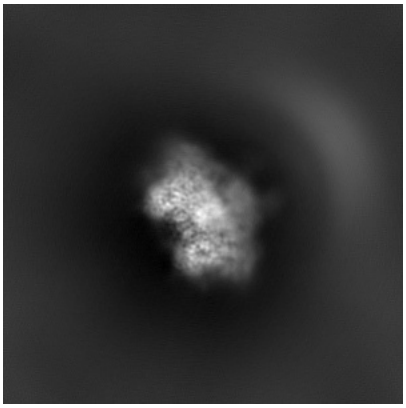
6.1.2 Raw map



X



Y



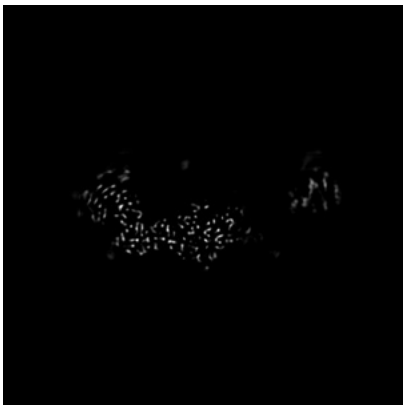
Z

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

6.2 Central slices (i)

6.2.1 Primary map

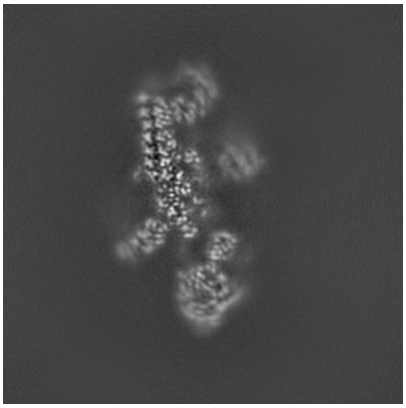
X Index: 200



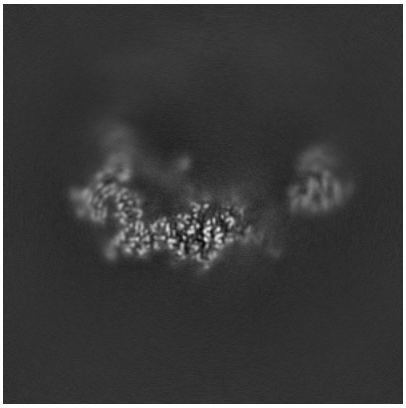
Y Index: 200

Z Index: 200

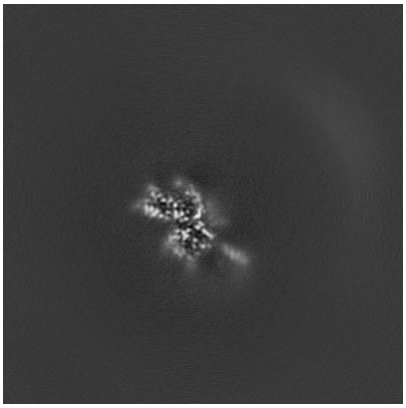
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

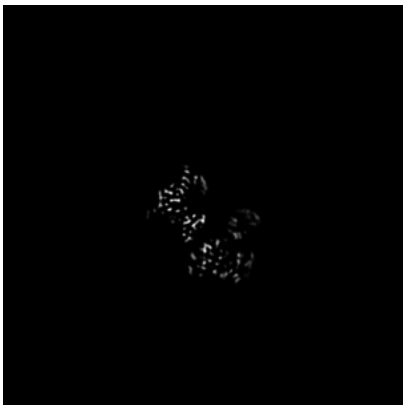
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

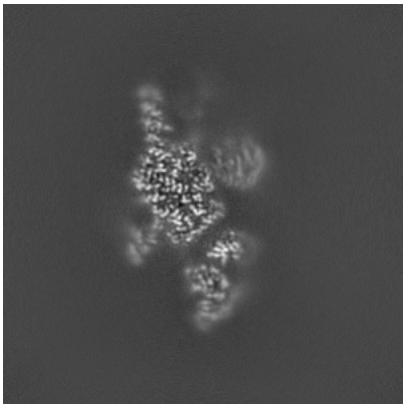
X Index: 187

Y Index: 197

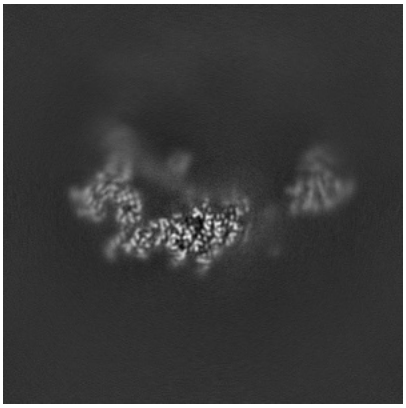


Z Index: 168

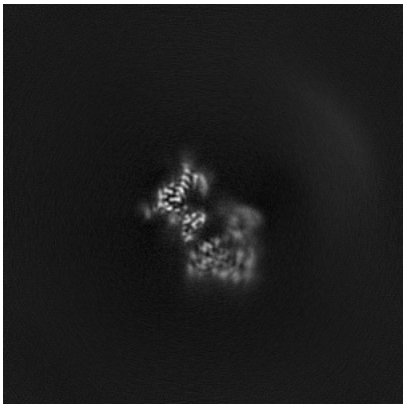
6.3.2 Raw map



X Index: 188



Y Index: 197

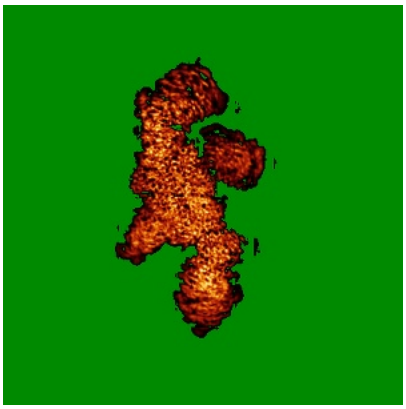


Z Index: 168

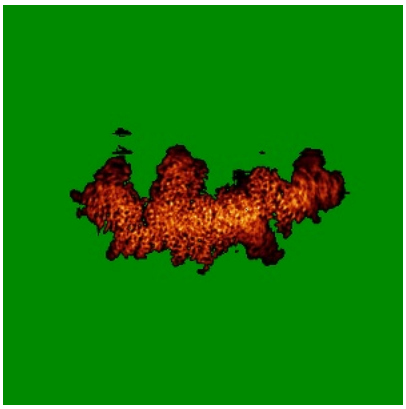
The images above show the largest variance slices of the map in three orthogonal directions.

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

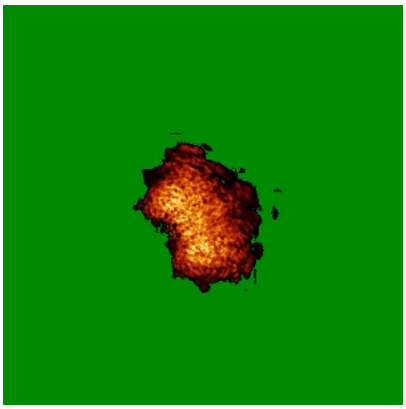
6.4.1 Primary map



X

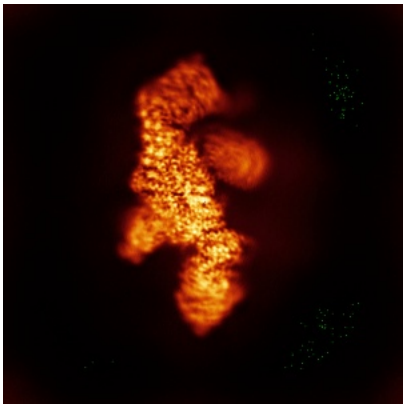


Y

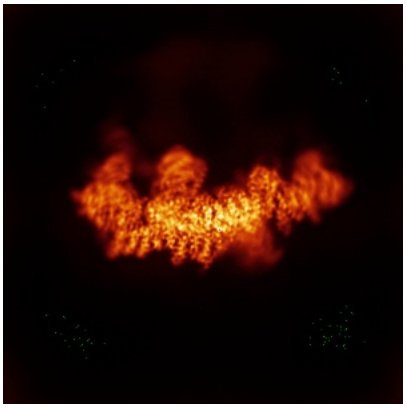


Z

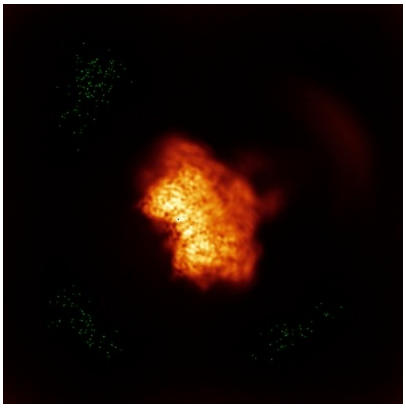
6.4.2 Raw map



X



Y

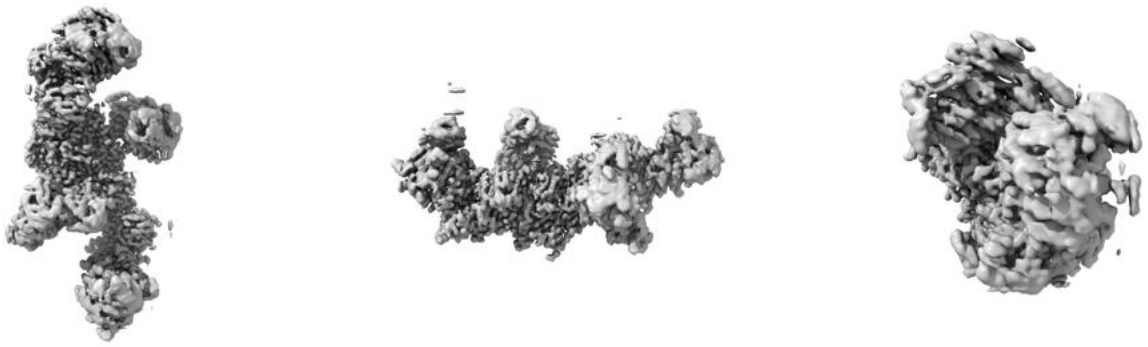


Z

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 0.02. 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.

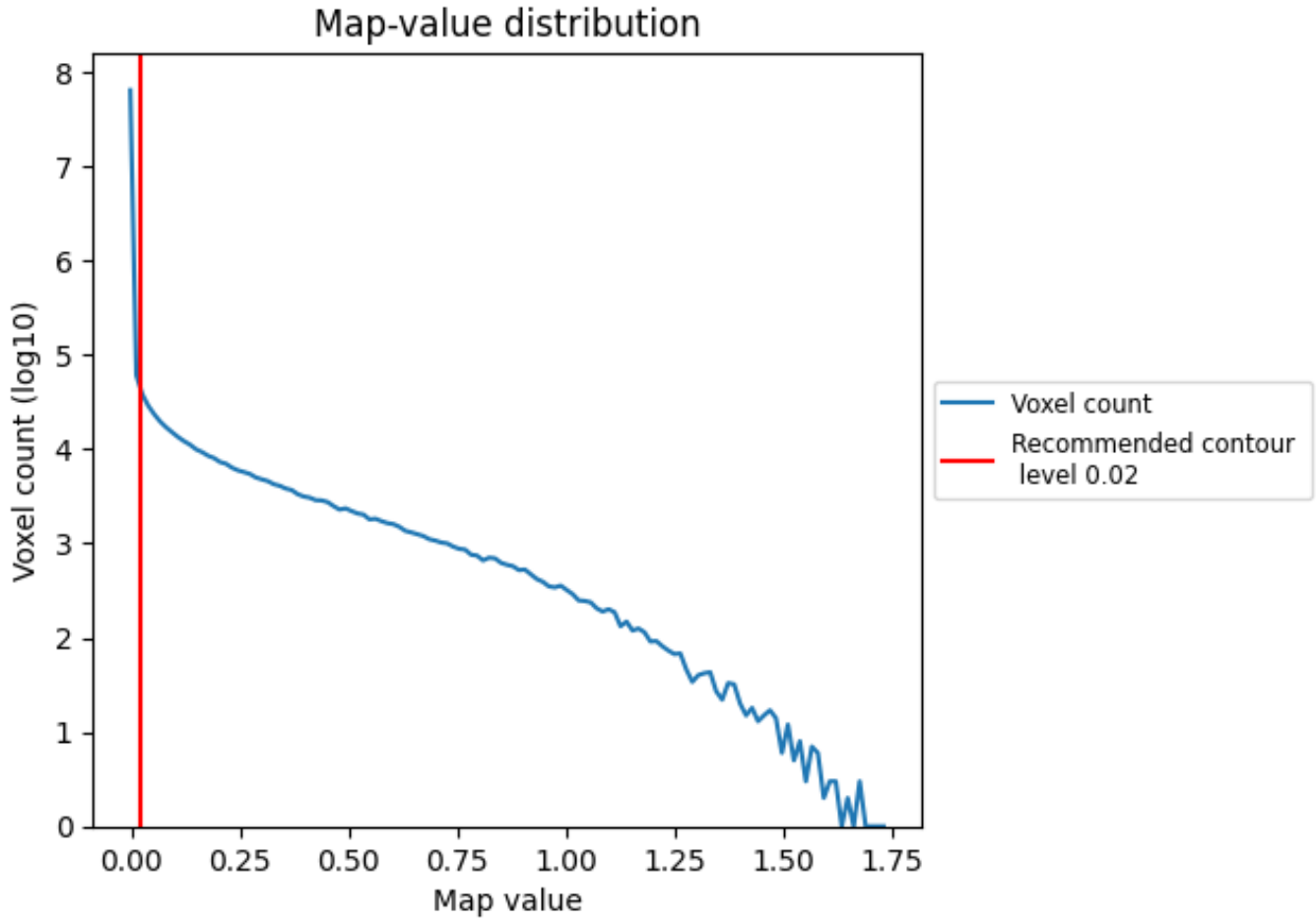
6.6 Mask visualisation (i)

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

7 Map analysis

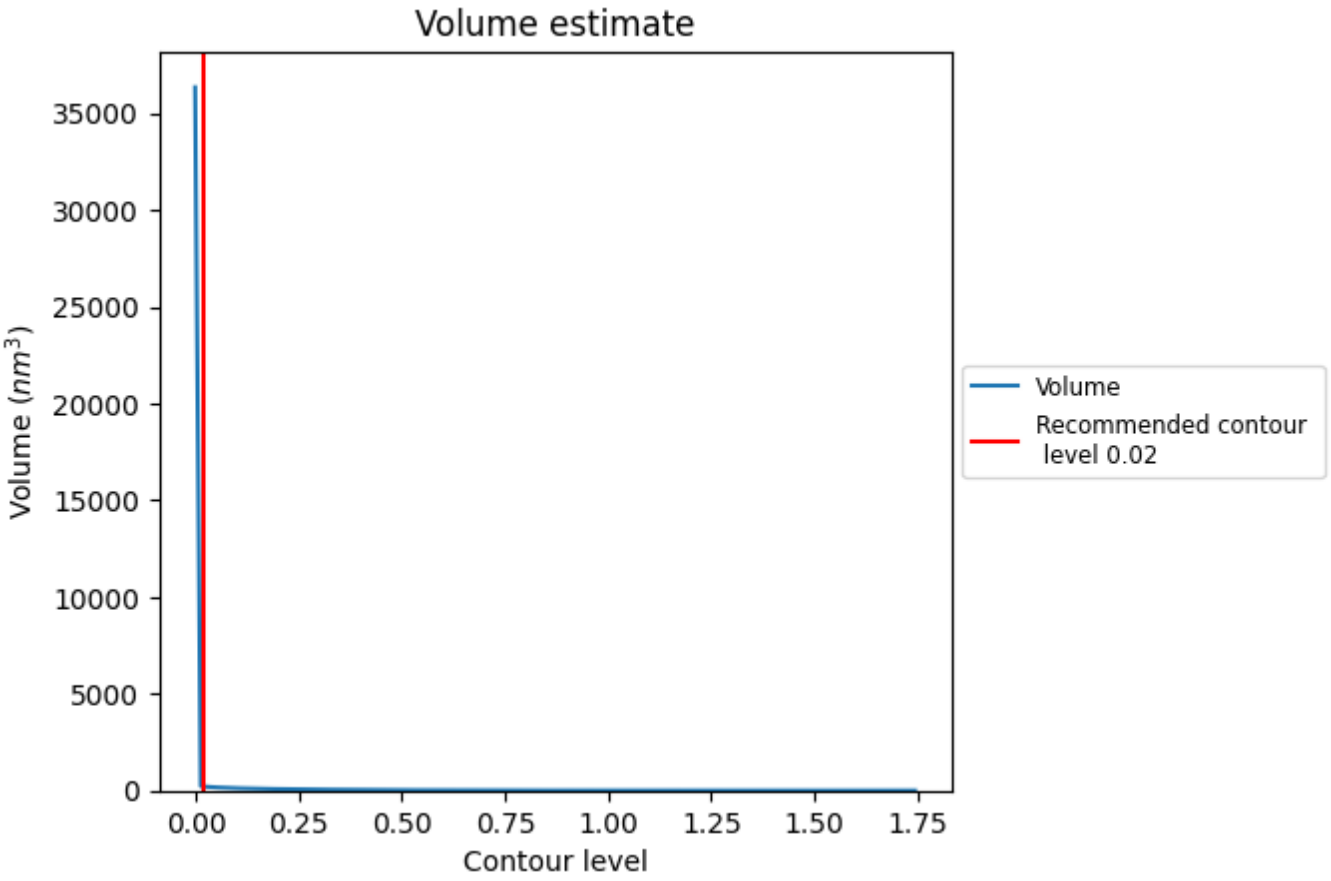
This section contains the results of statistical analysis of the map.

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.

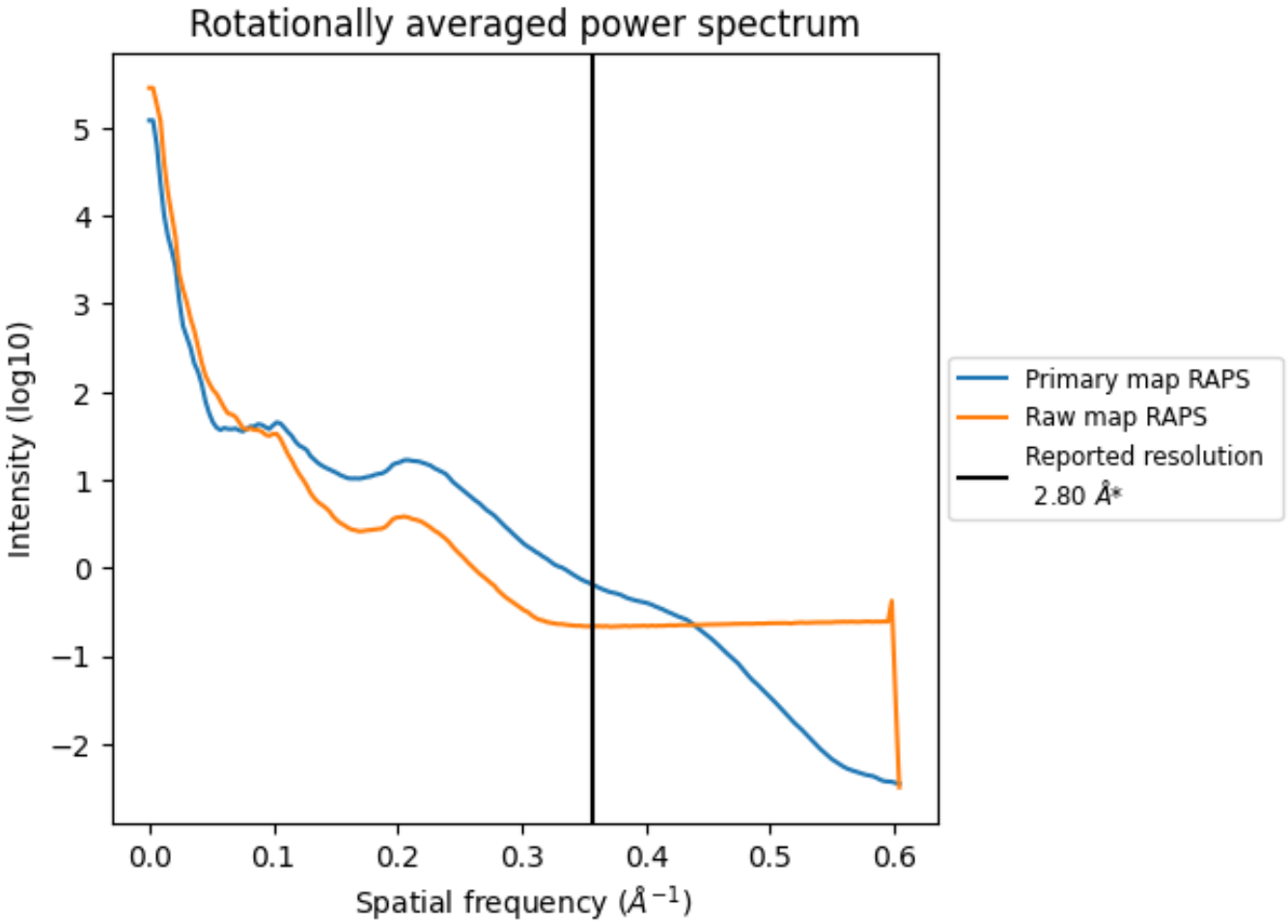
7.2 Volume estimate



The volume at the recommended contour level is 211 nm^3; this corresponds to an approximate mass of 191 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)

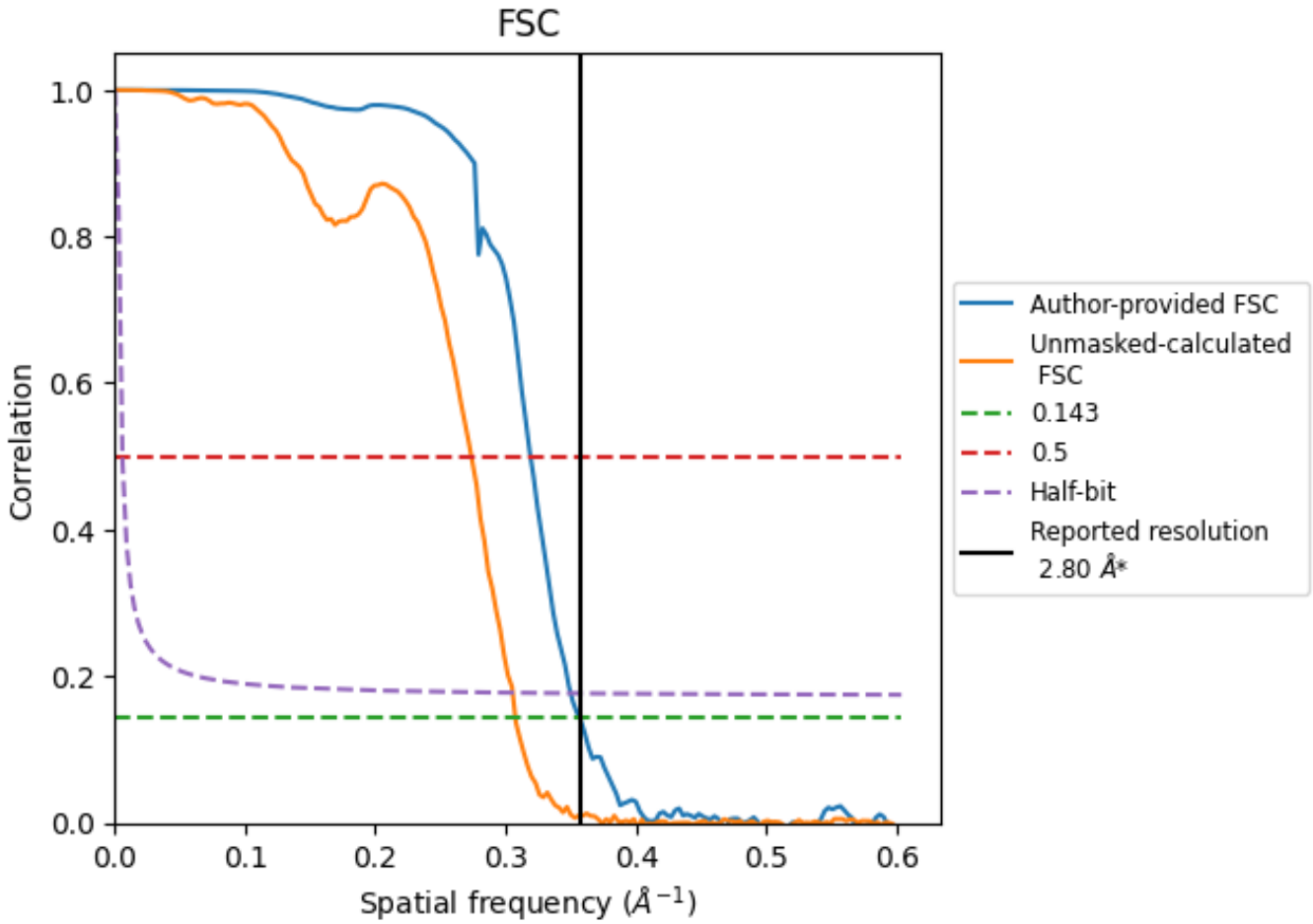


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

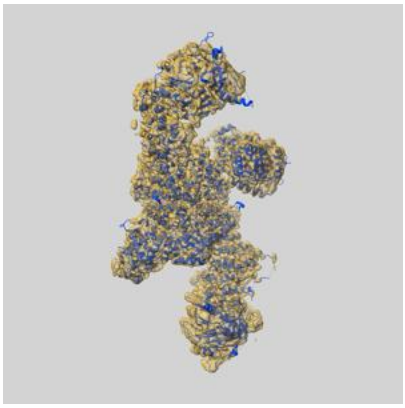
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.13	2.86
Unmasked-calculated*	3.25	3.65	3.27

*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 3.25 differs from the reported value 2.8 by more than 10 %

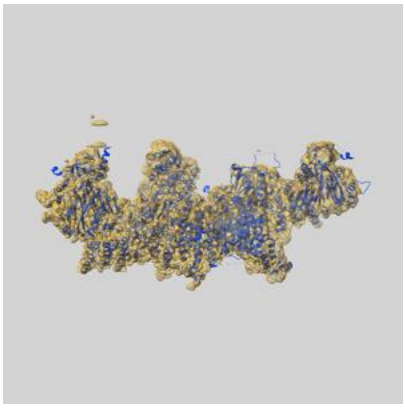
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27201 and PDB model 8D4X. Per-residue inclusion information can be found in section 3 on page 4.

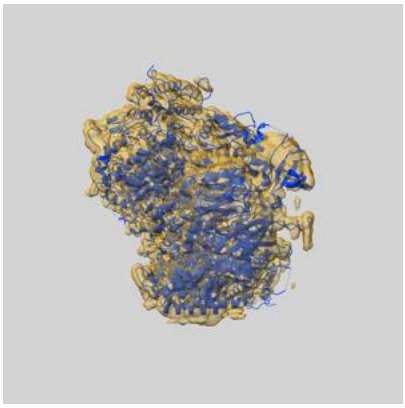
9.1 Map-model overlay



X



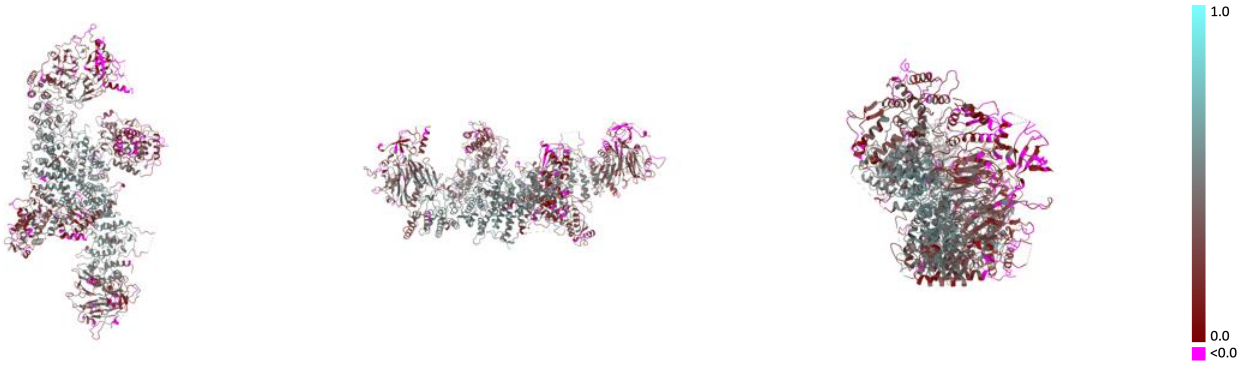
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

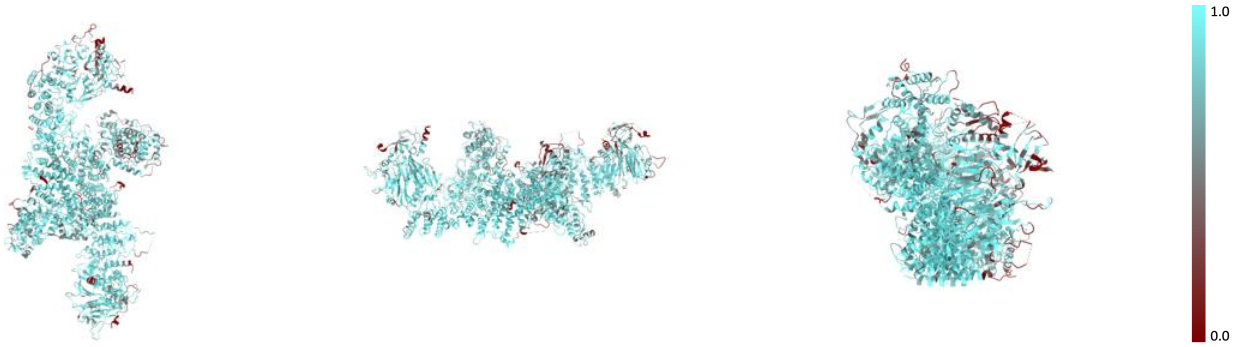
9.2 Q-score mapped to coordinate model (i)



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.

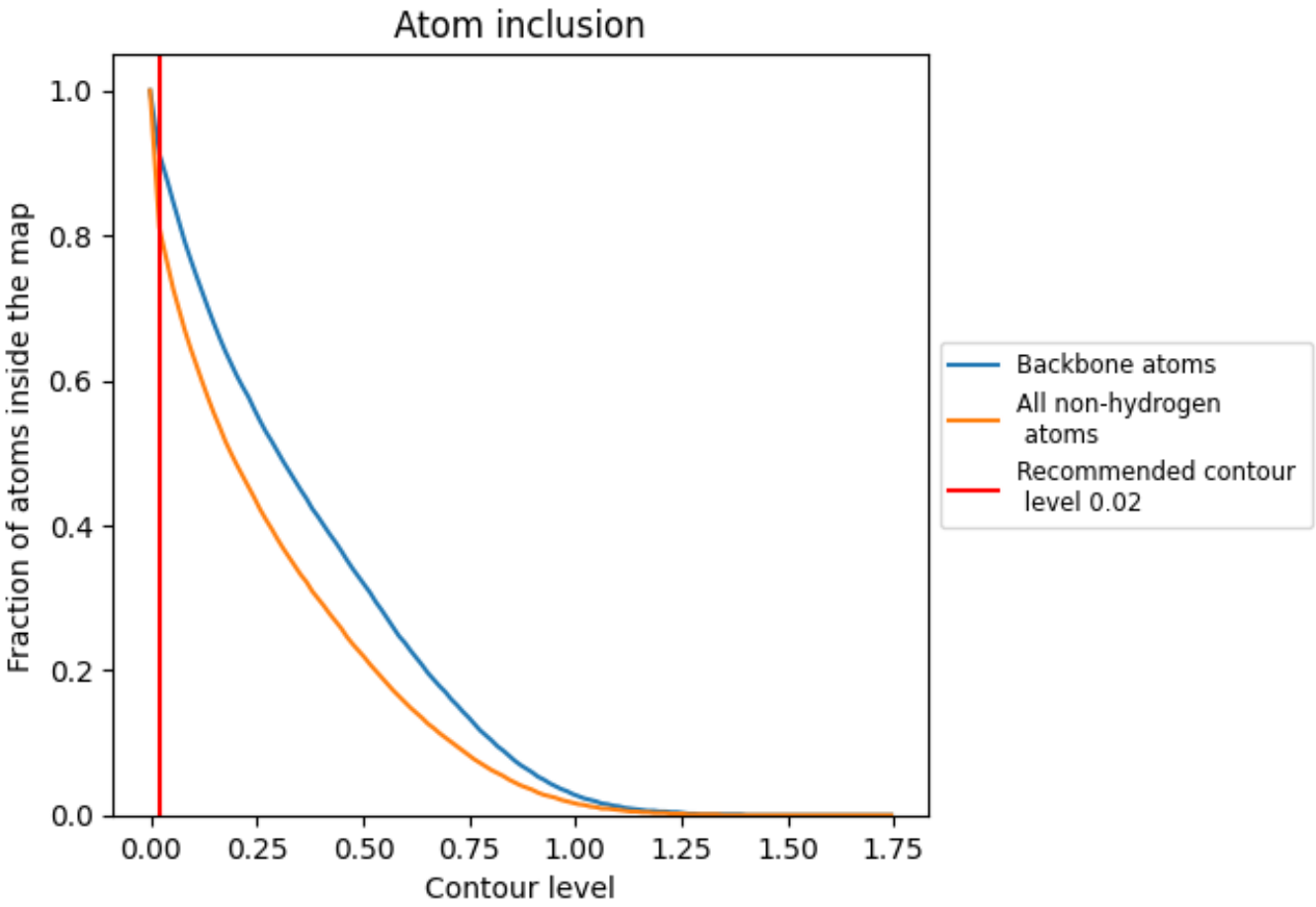
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 91% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.3580
A	0.8090	0.3680
B	0.8130	0.3490