Full wwPDB EM Validation Report ⓘ

May 8, 2023 – 09:54 PM EDT

PDB ID	:	8E0Q
EMDB ID	:	EMD-27822
Title	:	Structure of the human UBR5 HECT-type E3 ubiquitin ligase in a C2 symmetric dimeric form
Authors	:	Wang, F.; He, Q.; Lin, G.; Li, H.
Deposited on	:	2022-08-09
Resolution	:	2.66 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:

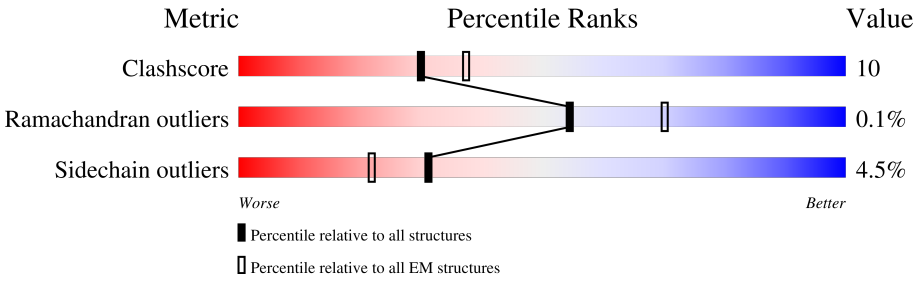
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.66 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	2807	6% 45% 14% · 40%
1	B	2807	6% 45% 15% · 40%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26604 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	1689	Total 13299	C 8398	N 2327	O 2474	S 100	0	0
1	B	1689	Total 13299	C 8398	N 2327	O 2474	S 100	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP O95071
A	-6	TYR	-	expression tag	UNP O95071
A	-5	LYS	-	expression tag	UNP O95071
A	-4	ASP	-	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	-7	ASP	-	expression tag	UNP O95071
B	-6	TYR	-	expression tag	UNP O95071
B	-5	LYS	-	expression tag	UNP O95071
B	-4	ASP	-	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).

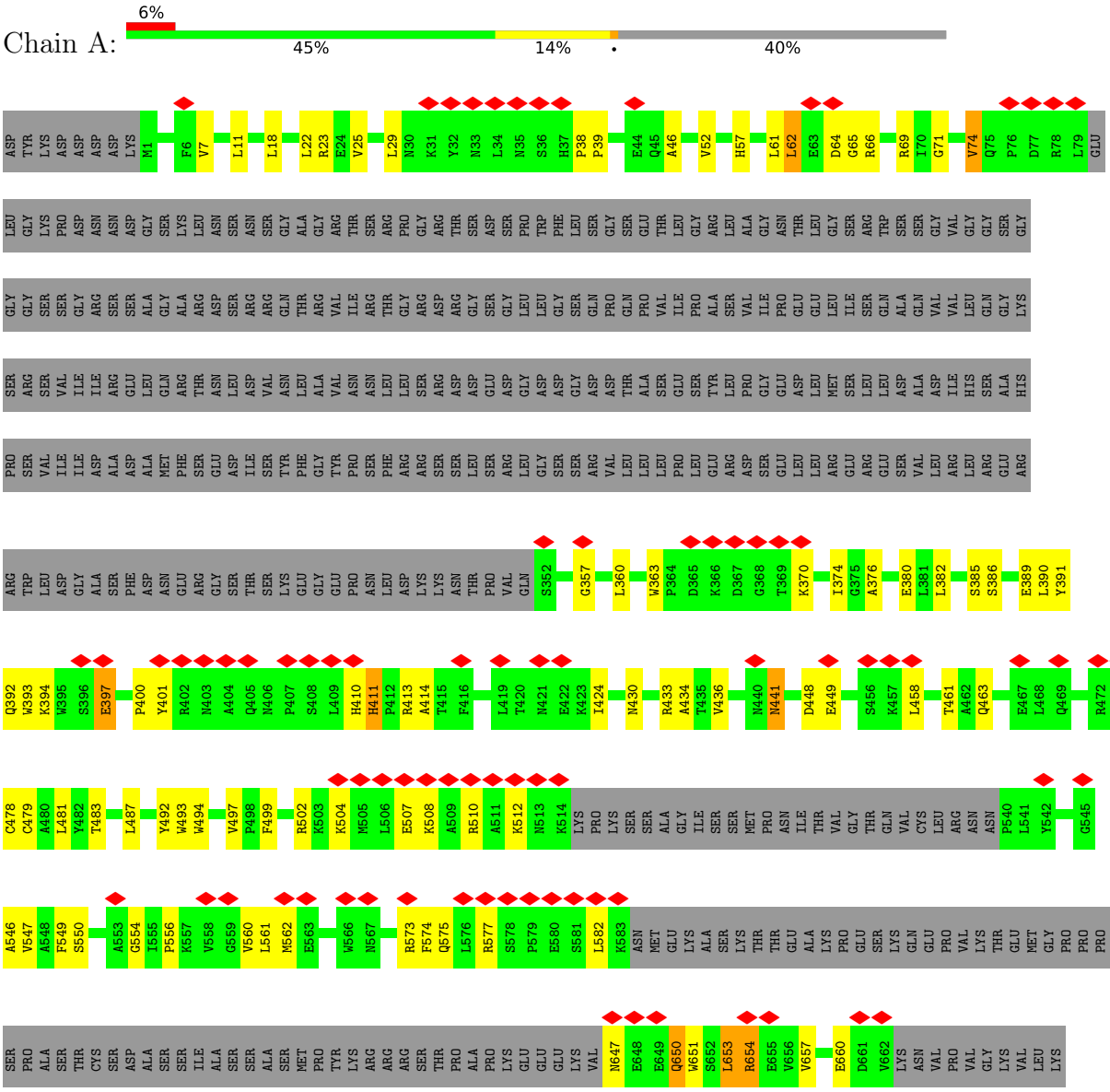
Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total 3	Zn 3	0
2	B	3	Total 3	Zn 3	0

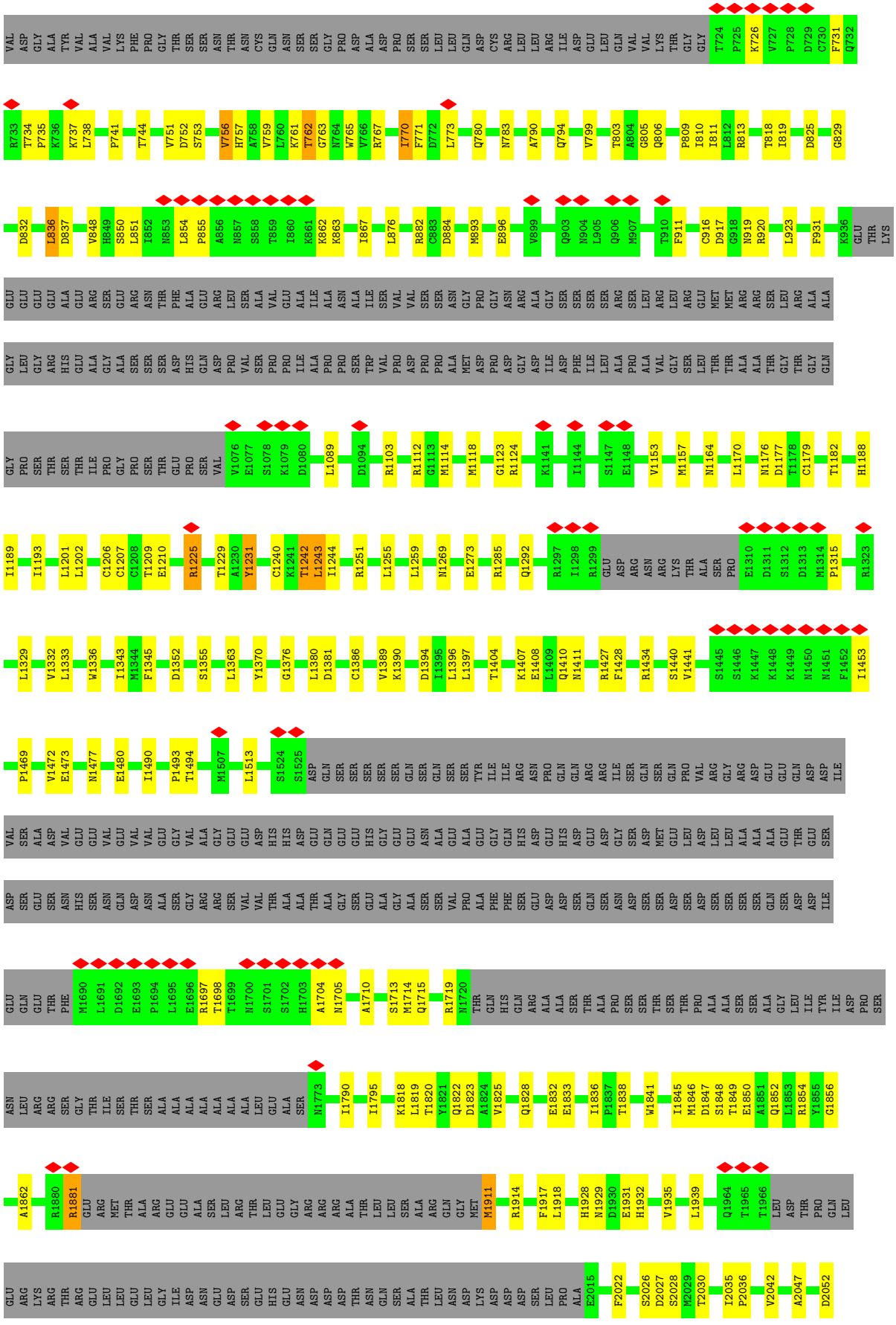
3 Residue-property plots (i)

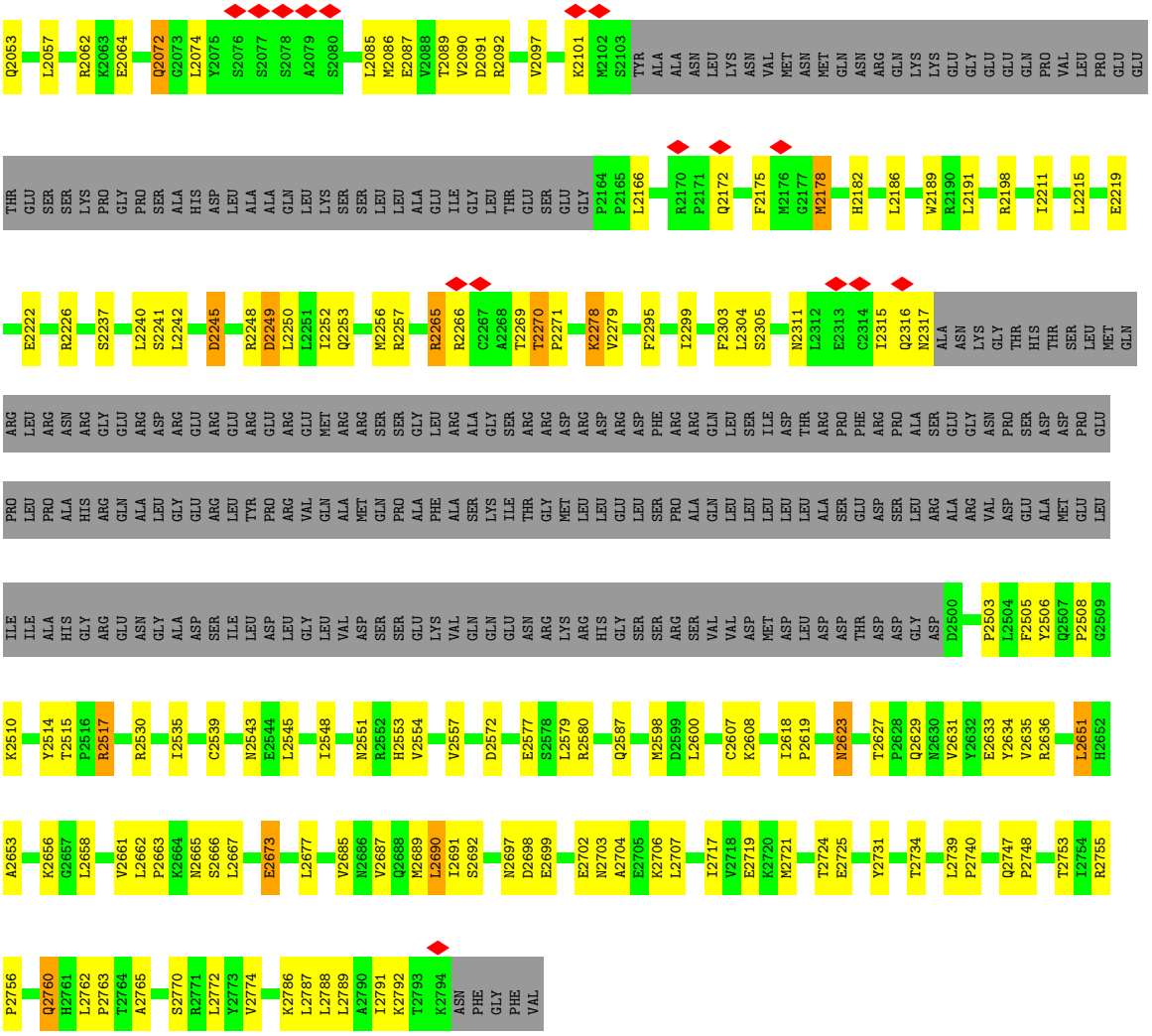
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

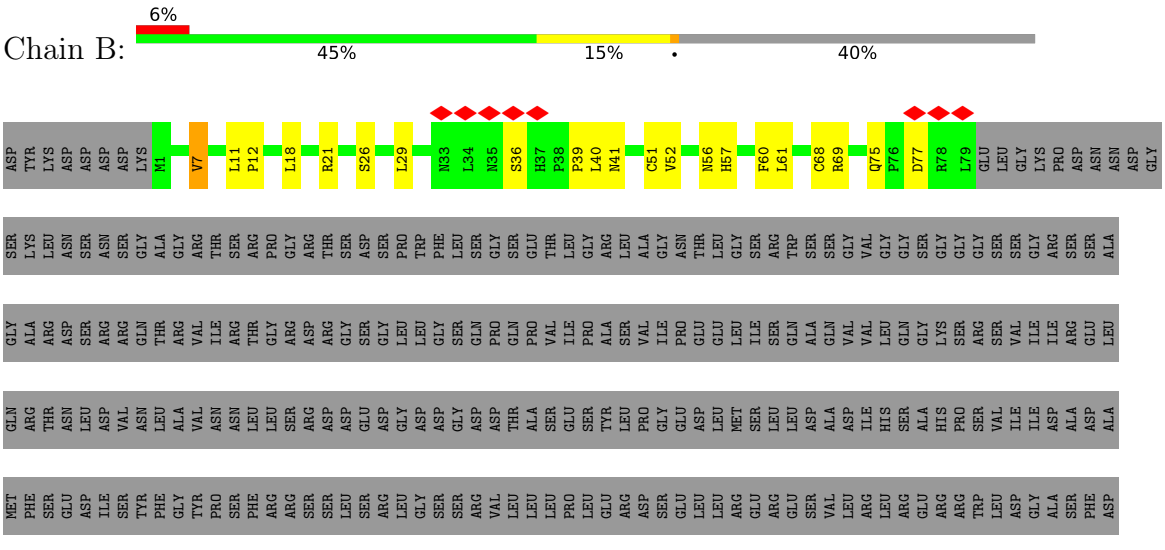
Chain A:

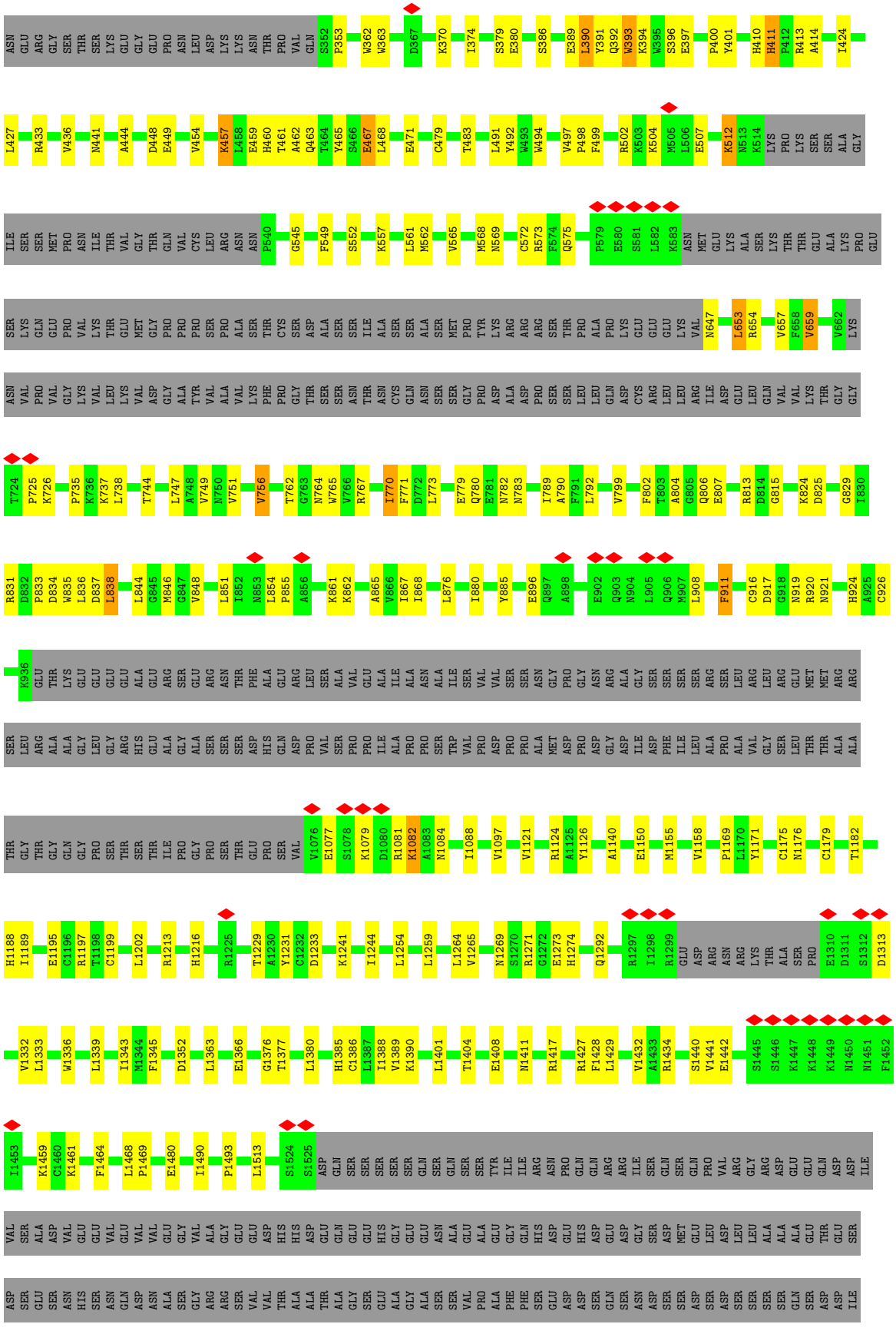


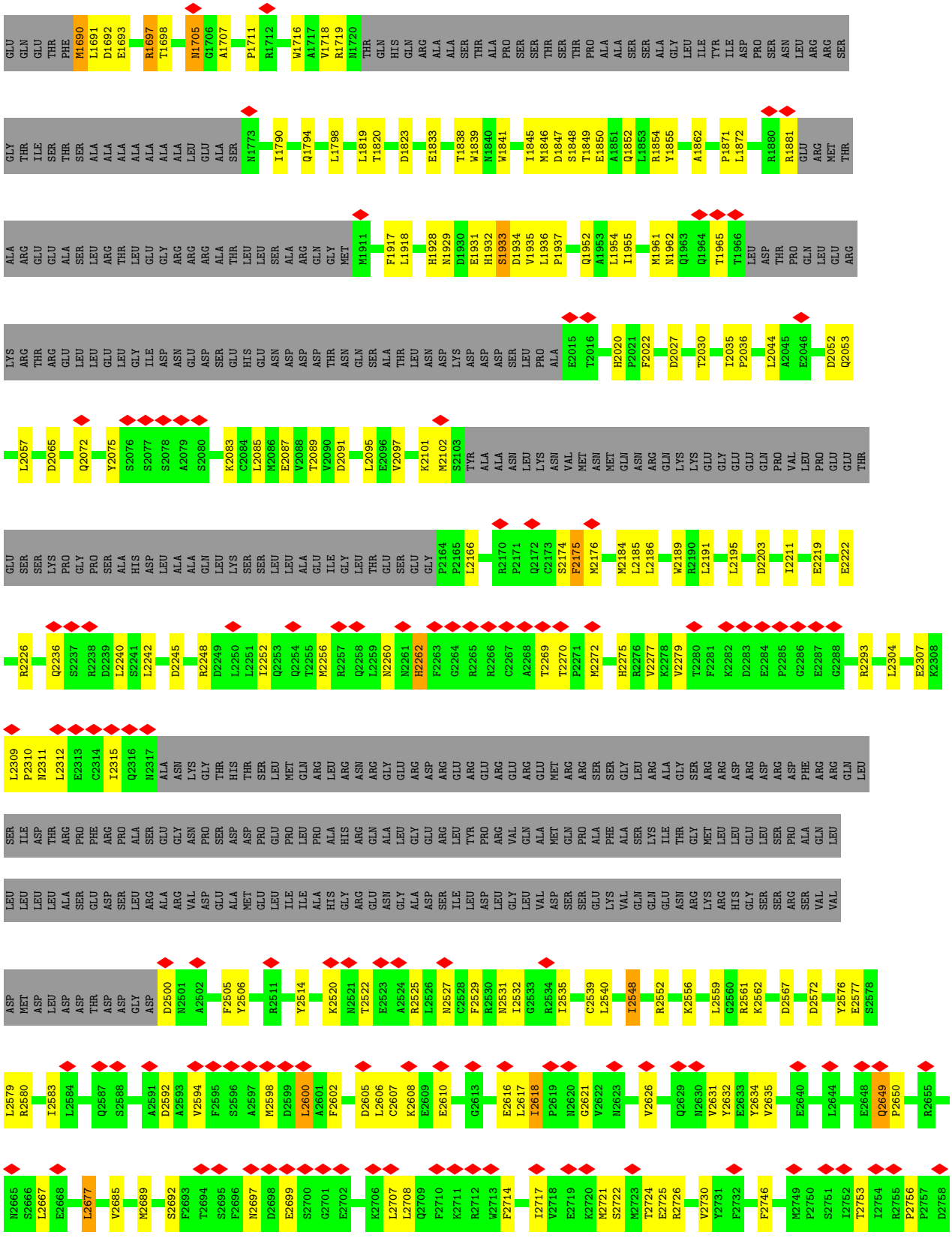


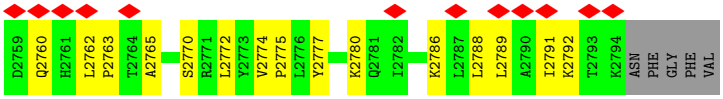


• Molecule 1: E3 ubiquitin-protein ligase UBR5








D2759
Q2760
H2761
L2762
P2763
T2764
A2765
S2770
R2771
L2772
Y2773
V2774
P2775
L2776
Y2777
K2780
Q2781
I2782
K2786
L2787
L2788
L2789
A2790
I2791
K2792
T2793
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	2.273	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.1	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	0.27	0/13576	0.49	0/18394
1	B	0.28	0/13576	0.48	0/18394
All	All	0.28	0/27152	0.48	0/36788

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	13299	0	13287	283	0
1	B	13299	0	13287	274	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	26604	0	26574	530	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 10.

All (530) 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:1370:TYR:CZ	1:B:1854:ARG:HD2	1.91	1.05
1:A:1370:TYR:OH	1:B:1854:ARG:HD2	1.76	0.84
1:A:1114:MET:HA	1:A:1118:MET:HE3	1.66	0.76
1:A:1854:ARG:HG3	1:A:1854:ARG:HH11	1.52	0.73
1:B:1468:LEU:HD11	1:B:1798:LEU:HB3	1.70	0.73
1:A:2186:LEU:HD13	1:A:2215:LEU:HD11	1.71	0.73
1:A:46:ALA:HB1	1:A:62:LEU:HD11	1.72	0.72
1:B:454:VAL:HG13	1:B:659:VAL:HG21	1.72	0.71
1:B:1690:MET:SD	1:B:1690:MET:N	2.63	0.71
1:B:393:TRP:HB3	1:B:400:PRO:HA	1.72	0.71
1:B:2649:GLN:HG2	1:B:2650:PRO:HD3	1.71	0.71
1:A:546:ALA:HB1	1:A:660:GLU:HG3	1.72	0.70
1:B:804:ALA:HB2	1:B:846:MET:HG2	1.73	0.70
1:A:2226:ARG:HE	1:A:2543:ASN:HD21	1.40	0.69
1:B:885:TYR:HA	1:B:1088:ILE:HD11	1.74	0.69
1:A:2598:MET:HG3	1:A:2600:LEU:HD13	1.75	0.69
1:A:547:VAL:HG12	1:A:560:VAL:HG12	1.75	0.69
1:B:744:THR:HG22	1:B:762:THR:HB	1.76	0.68
1:B:1852:GLN:HE21	1:B:1937:PRO:CB	2.07	0.68
1:B:799:VAL:HA	1:B:813:ARG:O	1.93	0.67
1:B:1155:MET:HA	1:B:1158:VAL:HG12	1.77	0.67
1:A:1103:ARG:HH21	1:A:1153:VAL:HG23	1.59	0.67
1:A:2248:ARG:NH1	1:A:2305:SER:OG	2.28	0.67
1:A:2765:ALA:HB2	1:A:2772:LEU:HD23	1.77	0.66
1:B:468:LEU:HD23	1:B:492:TYR:HD2	1.61	0.66
1:A:380:GLU:HB3	1:A:394:LYS:HD3	1.78	0.66
1:A:433:ARG:NH1	1:A:481:LEU:O	2.29	0.66
1:A:2690:LEU:HG	1:A:2739:LEU:HD11	1.78	0.66
1:B:1169:PRO:HD2	1:B:1264:LEU:HD21	1.79	0.65
1:B:454:VAL:HG22	1:B:659:VAL:HG11	1.78	0.65
1:A:2178:MET:SD	1:A:2178:MET:N	2.70	0.65
1:B:433:ARG:NH1	1:B:483:THR:OG1	2.30	0.65
1:A:1850:GLU:HA	1:A:1850:GLU:OE1	1.97	0.65
1:B:1854:ARG:HH11	1:B:1854:ARG:HG2	1.62	0.64
1:A:1854:ARG:HE	1:A:2191:LEU:HD13	1.61	0.64
1:B:2505:PHE:HB3	1:B:2514:TYR:HB3	1.80	0.64
1:A:74:VAL:HG13	1:A:851:LEU:HD21	1.79	0.64
1:B:497:VAL:O	1:B:502:ARG:NH1	2.31	0.64
1:A:1854:ARG:HG3	1:A:1854:ARG:NH1	2.10	0.64
1:B:1124:ARG:NH1	1:B:1244:ILE:O	2.31	0.64
1:A:2072:GLN:HG3	1:A:2074:LEU:HB2	1.80	0.63
1:B:7:VAL:HG13	1:B:867:ILE:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HG2	1:B:40:LEU:HD12	1.80	0.63
1:B:1852:GLN:HE21	1:B:1937:PRO:HB2	1.63	0.63
1:A:1852:GLN:HG2	1:A:2090:VAL:HG13	1.80	0.63
1:B:2248:ARG:NH1	1:B:2307:GLU:OE2	2.32	0.63
1:A:2265:ARG:HD3	1:A:2266:ARG:H	1.63	0.63
1:A:799:VAL:HA	1:A:813:ARG:O	1.98	0.63
1:B:575:GLN:NE2	1:B:647:ASN:OD1	2.32	0.63
1:A:1848:SER:O	1:A:1852:GLN:HG3	1.98	0.63
1:B:2222:GLU:OE1	1:B:2226:ARG:NH1	2.29	0.63
1:A:2579:LEU:HD23	1:A:2635:VAL:HG13	1.81	0.62
1:B:1461:LYS:NZ	1:B:1794:GLN:OE1	2.32	0.62
1:B:1850:GLU:OE1	1:B:1850:GLU:HA	1.99	0.62
1:A:458:LEU:HD23	1:A:731:PHE:HE2	1.65	0.62
1:B:1871:PRO:HG3	1:B:1936:LEU:HD21	1.80	0.62
1:A:2035:ILE:HD12	1:A:2036:PRO:HD2	1.81	0.62
1:A:1124:ARG:NH1	1:A:1244:ILE:O	2.32	0.62
1:B:2260:ASN:HD21	1:B:2527:ASN:HD21	1.47	0.62
1:A:2279:VAL:HG11	1:A:2295:PHE:HB2	1.81	0.62
1:B:448:ASP:OD1	1:B:449:GLU:N	2.33	0.62
1:A:2699:GLU:HG3	1:A:2756:PRO:HD3	1.82	0.62
1:B:1469:PRO:HG3	1:B:1819:LEU:HD13	1.82	0.61
1:A:2618:ILE:HG13	1:A:2619:PRO:HD2	1.82	0.61
1:B:1847:ASP:HB3	1:B:2095:LEU:HD23	1.80	0.61
1:B:2186:LEU:HD21	1:B:2211:ILE:HD11	1.82	0.61
1:B:2607:CYS:SG	1:B:2608:LYS:N	2.74	0.61
1:A:2505:PHE:HB3	1:A:2514:TYR:HB3	1.81	0.61
1:A:1269:ASN:HD21	1:A:1273:GLU:HG3	1.65	0.61
1:A:2557:VAL:HG11	1:A:2651:LEU:HB3	1.81	0.61
1:A:1381:ASP:OD1	1:A:1434:ARG:NH1	2.33	0.61
1:B:1269:ASN:HD21	1:B:1273:GLU:HG3	1.66	0.61
1:A:1513:LEU:HD22	1:B:1918:LEU:HB3	1.82	0.61
1:B:2616:GLU:OE2	1:B:2621:GLY:N	2.33	0.60
1:A:393:TRP:HB3	1:A:400:PRO:HA	1.82	0.60
1:A:2760:GLN:O	1:A:2760:GLN:NE2	2.34	0.60
1:A:18:LEU:HD22	1:A:809:PRO:HB2	1.83	0.60
1:A:1928:HIS:NE2	1:B:1480:GLU:OE1	2.32	0.60
1:B:1171:TYR:OH	1:B:1271:ARG:NH2	2.30	0.60
1:A:882:ARG:NH1	1:A:884:ASP:OD2	2.35	0.60
1:A:2699:GLU:OE2	1:A:2755:ARG:NE	2.28	0.60
1:B:2786:LYS:HD3	1:B:2789:LEU:HD21	1.82	0.60
1:A:1704:ALA:O	1:A:1705:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:HH12	1:A:657:VAL:HA	1.67	0.60
1:A:2691:ILE:HG23	1:B:1697:ARG:HA	1.84	0.60
1:A:2702:GLU:HG2	1:A:2706:LYS:HD2	1.84	0.60
1:B:756:VAL:HG23	1:B:771:PHE:HB2	1.84	0.60
1:A:2242:LEU:HD11	1:A:2279:VAL:HG22	1.82	0.60
1:B:1692:ASP:OD1	1:B:1693:GLU:N	2.34	0.60
1:A:1343:ILE:HD13	1:A:1428:PHE:HB2	1.83	0.59
1:A:2658:LEU:HD22	1:A:2667:LEU:HD11	1.83	0.59
1:B:880:ILE:HD11	1:B:926:CYS:HB2	1.85	0.59
1:B:1848:SER:O	1:B:1852:GLN:HG3	2.03	0.59
1:A:1336:TRP:CE3	1:A:1408:GLU:HG3	2.38	0.59
1:A:1469:PRO:HG3	1:A:1819:LEU:HD13	1.83	0.59
1:A:2503:PRO:HD2	1:A:2517:ARG:HH21	1.67	0.59
1:B:390:LEU:O	1:B:411:HIS:HB2	2.01	0.59
1:B:2035:ILE:HD12	1:B:2036:PRO:HD2	1.84	0.59
1:A:2697:ASN:ND2	1:A:2753:THR:OG1	2.36	0.59
1:A:825:ASP:OD1	1:A:829:GLY:N	2.28	0.59
1:A:1881:ARG:HH22	1:B:1693:GLU:HB3	1.68	0.59
1:A:2027:ASP:HA	1:A:2030:THR:HG22	1.83	0.59
1:A:2721:MET:HB3	1:A:2725:GLU:HG3	1.84	0.59
1:A:818:THR:HG21	1:A:917:ASP:HA	1.85	0.59
1:A:744:THR:HG22	1:A:762:THR:HB	1.85	0.58
1:A:430:ASN:ND2	1:A:478:CYS:O	2.34	0.58
1:B:1343:ILE:HD13	1:B:1428:PHE:HB2	1.84	0.58
1:A:2587:GLN:O	1:A:2587:GLN:NE2	2.36	0.58
1:B:2256:MET:SD	1:B:2531:ASN:ND2	2.74	0.58
1:B:545:GLY:N	1:B:561:LEU:O	2.35	0.58
1:A:832:ASP:OD1	1:A:1112:ARG:NH1	2.36	0.58
1:B:2579:LEU:HD23	1:B:2635:VAL:HG13	1.85	0.58
1:A:837:ASP:OD1	1:A:920:ARG:NH2	2.36	0.58
1:A:1225:ARG:H	1:A:1225:ARG:HD3	1.69	0.58
1:B:2075:TYR:HA	1:B:2085:LEU:HD12	1.86	0.57
1:A:1911:MET:SD	1:A:1911:MET:N	2.77	0.57
1:A:2607:CYS:SG	1:A:2608:LYS:N	2.77	0.57
1:A:370:LYS:O	1:A:386:SER:OG	2.22	0.57
1:A:2788:LEU:HD13	1:A:2791:ILE:HD11	1.85	0.57
1:B:2765:ALA:HB2	1:B:2772:LEU:HD23	1.87	0.57
1:B:2089:THR:HB	1:B:2095:LEU:HD11	1.87	0.57
1:A:1493:PRO:O	1:A:1719:ARG:NH2	2.38	0.56
1:B:825:ASP:OD1	1:B:829:GLY:N	2.38	0.56
1:A:499:PHE:HD1	1:A:502:ARG:HH21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1854:ARG:NE	1:A:2191:LEU:HD13	2.20	0.56
1:B:770:ILE:HG23	1:B:780:GLN:HB3	1.87	0.56
1:A:7:VAL:HG12	1:A:867:ILE:HB	1.87	0.56
1:A:2633:GLU:HG2	1:A:2636:ARG:HH12	1.69	0.56
1:A:753:SER:N	1:A:805:GLY:O	2.39	0.56
1:B:2631:VAL:O	1:B:2634:TYR:HB3	2.06	0.56
1:B:565:VAL:HG11	1:B:653:LEU:HD22	1.88	0.56
1:A:2747:GLN:HB3	1:A:2748:PRO:HD3	1.86	0.56
1:A:1494:THR:HG21	1:B:1917:PHE:HB2	1.87	0.56
1:B:370:LYS:O	1:B:386:SER:OG	2.24	0.56
1:A:790:ALA:HA	1:A:919:ASN:HD22	1.71	0.55
1:A:2249:ASP:OD1	1:A:2249:ASP:N	2.38	0.55
1:A:803:THR:HB	1:A:810:ILE:HD13	1.89	0.55
1:A:1124:ARG:NH2	1:A:1176:ASN:O	2.38	0.55
1:B:1854:ARG:NH1	1:B:2191:LEU:HD13	2.20	0.55
1:B:36:SER:OG	1:B:41:ASN:ND2	2.39	0.55
1:A:2241:SER:HA	1:A:2278:LYS:HG3	1.89	0.55
1:B:61:LEU:HB2	1:B:374:ILE:HG12	1.87	0.55
1:B:880:ILE:HG13	1:B:1088:ILE:HG21	1.88	0.55
1:B:1343:ILE:O	1:B:1427:ARG:NH1	2.40	0.55
1:B:2027:ASP:HA	1:B:2030:THR:HG22	1.86	0.55
1:B:12:PRO:HG2	1:B:861:LYS:HG2	1.89	0.55
1:B:2500:ASP:HB2	1:B:2520:LYS:HD2	1.87	0.55
1:B:1855:TYR:OH	1:B:1933:SER:HA	2.06	0.55
1:B:2240:LEU:HG	1:B:2262:HIS:HD2	1.71	0.55
1:A:577:ARG:HD3	1:A:582:LEU:HD21	1.88	0.55
1:A:2623:ASN:OD1	1:A:2623:ASN:N	2.38	0.55
1:B:396:SER:OG	1:B:397:GLU:OE1	2.24	0.55
1:A:504:LYS:HD2	1:A:508:LYS:HE3	1.89	0.54
1:B:75:GLN:NE2	1:B:353:PRO:O	2.40	0.54
1:B:1429:LEU:HA	1:B:1432:VAL:HG12	1.89	0.54
1:A:1370:TYR:CZ	1:B:1854:ARG:CD	2.80	0.54
1:A:1480:GLU:OE1	1:B:1928:HIS:NE2	2.37	0.54
1:A:2270:THR:HB	1:A:2271:PRO:HD2	1.89	0.54
1:A:2763:PRO:HB3	1:A:2774:VAL:HG12	1.89	0.54
1:B:441:ASN:ND2	1:B:471:GLU:O	2.28	0.54
1:A:2222:GLU:OE1	1:A:2226:ARG:NH1	2.37	0.54
1:B:512:LYS:HE2	1:B:725:PRO:HG2	1.88	0.54
1:B:2600:LEU:HB2	1:B:2626:VAL:HB	1.89	0.54
1:B:1376:GLY:O	1:B:1427:ARG:NH2	2.33	0.54
1:A:1269:ASN:ND2	1:A:1273:GLU:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:HB3	1:B:838:LEU:HD22	1.88	0.54
1:B:1820:THR:OG1	1:B:1823:ASP:OD1	2.26	0.54
1:A:1820:THR:OG1	1:A:1823:ASP:OD1	2.26	0.54
1:A:1928:HIS:HA	1:A:2091:ASP:HB3	1.90	0.54
1:B:1852:GLN:NE2	1:B:1937:PRO:HB3	2.23	0.54
1:B:2272:MET:SD	1:B:2272:MET:N	2.72	0.54
1:A:575:GLN:NE2	1:A:647:ASN:OD1	2.36	0.54
1:B:1179:CYS:O	1:B:1182:THR:OG1	2.24	0.54
1:B:2293:ARG:NH2	1:B:2770:SER:OG	2.41	0.54
1:B:2699:GLU:HG3	1:B:2756:PRO:HD3	1.90	0.54
1:A:497:VAL:HG23	1:A:502:ARG:HG2	1.90	0.53
1:B:1377:THR:HB	1:B:1434:ARG:HH12	1.74	0.53
1:B:1269:ASN:ND2	1:B:1273:GLU:O	2.41	0.53
1:A:1189:ILE:HD12	1:A:1292:GLN:HB3	1.89	0.53
1:A:1355:SER:HB3	1:B:1934:ASP:OD2	2.09	0.53
1:A:2508:PRO:HD3	1:A:2515:THR:HG22	1.91	0.53
1:B:380:GLU:HA	1:B:394:LYS:HA	1.90	0.53
1:B:379:SER:OG	1:B:380:GLU:OE1	2.21	0.53
1:B:2532:ILE:O	1:B:2535:ILE:HG13	2.08	0.53
1:A:654:ARG:H	1:A:654:ARG:HD3	1.74	0.53
1:A:1376:GLY:O	1:A:1427:ARG:NH2	2.33	0.53
1:A:2702:GLU:N	1:A:2702:GLU:OE1	2.42	0.53
1:B:1852:GLN:NE2	1:B:1937:PRO:CB	2.71	0.53
1:B:459:GLU:O	1:B:460:HIS:ND1	2.42	0.53
1:B:411:HIS:O	1:B:414:ALA:N	2.38	0.52
1:A:394:LYS:N	1:A:397:GLU:OE2	2.42	0.52
1:A:2042:VAL:HG23	1:A:2047:ALA:HB2	1.90	0.52
1:A:2687:VAL:HG11	1:A:2719:GLU:HA	1.90	0.52
1:A:550:SER:O	1:A:556:PRO:HA	2.10	0.52
1:B:549:PHE:CE2	1:B:657:VAL:HG21	2.43	0.52
1:A:554:GLY:HA3	1:A:850:SER:HB3	1.92	0.52
1:A:893:MET:O	1:A:896:GLU:HG3	2.09	0.52
1:A:2689:MET:O	1:A:2692:SER:OG	2.25	0.52
1:A:837:ASP:N	1:A:917:ASP:OD2	2.37	0.52
1:B:1199:CYS:SG	1:B:1216:HIS:HE1	2.30	0.52
1:A:2663:PRO:HG2	1:A:2666:SER:HB3	1.91	0.52
1:B:1493:PRO:O	1:B:1719:ARG:NH2	2.42	0.52
1:A:2577:GLU:OE1	1:A:2580:ARG:NH1	2.43	0.52
1:B:2087:GLU:O	1:B:2089:THR:N	2.43	0.52
1:A:1854:ARG:HE	1:A:2191:LEU:CD1	2.23	0.51
1:B:1962:ASN:O	1:B:1965:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2627:THR:OG1	1:A:2629:GLN:OE1	2.29	0.51
1:B:572:CYS:SG	1:B:573:ARG:N	2.84	0.51
1:B:1841:TRP:O	1:B:1845:ILE:HG12	2.09	0.51
1:B:491:LEU:HD21	1:B:749:VAL:HG11	1.92	0.51
1:A:1193:ILE:HG23	1:A:1206:CYS:HB3	1.91	0.51
1:A:2665:ASN:OD1	1:A:2665:ASN:N	2.42	0.51
1:B:562:MET:N	1:B:562:MET:SD	2.83	0.51
1:B:834:ASP:N	1:B:834:ASP:OD1	2.44	0.51
1:A:1396:LEU:HD23	1:A:1396:LEU:H	1.74	0.51
1:A:2530:ARG:HG3	1:A:2653:ALA:HB1	1.92	0.51
1:A:64:ASP:HB2	1:A:66:ARG:HD3	1.93	0.51
1:A:765:TRP:NE1	1:A:783:ASN:OD1	2.39	0.51
1:A:2256:MET:HB2	1:A:2315:ILE:HD11	1.93	0.51
1:B:765:TRP:NE1	1:B:783:ASN:OD1	2.44	0.51
1:A:1828:GLN:HE22	1:A:2172:GLN:H	1.59	0.51
1:A:57:HIS:HD2	1:A:69:ARG:HH21	1.57	0.51
1:A:2245:ASP:N	1:A:2245:ASP:OD1	2.44	0.51
1:A:1841:TRP:O	1:A:1845:ILE:HG12	2.11	0.50
1:A:2271:PRO:HG3	1:A:2663:PRO:HA	1.94	0.50
1:B:379:SER:OG	1:B:448:ASP:OD1	2.29	0.50
1:B:790:ALA:HA	1:B:919:ASN:HD22	1.75	0.50
1:A:433:ARG:NE	1:A:483:THR:OG1	2.44	0.50
1:A:573:ARG:HA	1:A:650:GLN:HA	1.93	0.50
1:A:492:TYR:HD1	1:A:737:LYS:HA	1.75	0.50
1:A:2697:ASN:O	1:A:2753:THR:HA	2.12	0.50
1:B:854:LEU:HD12	1:B:855:PRO:HD2	1.93	0.50
1:A:411:HIS:O	1:A:414:ALA:N	2.38	0.50
1:A:770:ILE:HG23	1:A:780:GLN:HB3	1.94	0.50
1:B:57:HIS:HD2	1:B:69:ARG:HH11	1.60	0.50
1:A:1490:ILE:HD13	1:B:1845:ILE:HD12	1.92	0.50
1:A:1918:LEU:HB3	1:B:1513:LEU:HD22	1.93	0.50
1:B:2174:SER:O	1:B:2176:MET:N	2.45	0.50
1:B:2583:ILE:HD11	1:B:2632:TYR:CZ	2.47	0.50
1:A:2074:LEU:HB3	1:A:2086:MET:HE2	1.94	0.50
1:A:2182:HIS:O	1:A:2186:LEU:HG	2.12	0.50
1:B:1440:SER:HB3	1:B:1790:ILE:HD13	1.94	0.50
1:B:1126:TYR:OH	1:B:1176:ASN:ND2	2.37	0.49
1:A:390:LEU:O	1:A:411:HIS:HB2	2.12	0.49
1:B:1339:LEU:HD21	1:B:1401:LEU:HD12	1.95	0.49
1:B:1854:ARG:HG2	1:B:1854:ARG:NH1	2.26	0.49
1:B:2552:ARG:NH1	1:B:2567:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:SER:HB3	1:A:1790:ILE:HD13	1.94	0.49
1:A:2506:TYR:HB3	1:A:2517:ARG:HD3	1.94	0.49
1:B:764:ASN:HD21	1:B:789:ILE:HD11	1.77	0.49
1:A:1370:TYR:OH	1:B:1854:ARG:CD	2.54	0.49
1:A:1914:ARG:HD2	1:B:1442:GLU:HG2	1.94	0.49
1:B:1929:ASN:O	1:B:1931:GLU:HG3	2.13	0.49
1:B:2522:THR:HG23	1:B:2525:ARG:H	1.78	0.49
1:B:2529:PHE:O	1:B:2532:ILE:HG22	2.12	0.49
1:A:461:THR:O	1:A:463:GLN:NE2	2.45	0.49
1:A:854:LEU:HD12	1:A:855:PRO:HD2	1.93	0.49
1:A:1164:ASN:OD1	1:A:1164:ASN:N	2.45	0.49
1:A:1845:ILE:HD12	1:B:1490:ILE:HD13	1.95	0.49
1:A:2097:VAL:HG22	1:A:2101:LYS:HB2	1.94	0.49
1:B:2714:PHE:O	1:B:2717:ILE:HG13	2.13	0.49
1:A:2087:GLU:O	1:A:2089:THR:N	2.43	0.49
1:A:2545:LEU:HD21	1:A:2740:PRO:HB3	1.95	0.49
1:A:2703:ASN:OD1	1:A:2704:ALA:N	2.46	0.49
1:A:1103:ARG:HG2	1:A:1157:MET:HE1	1.93	0.49
1:B:2020:HIS:HD2	1:B:2022:PHE:H	1.59	0.49
1:B:60:PHE:HE1	1:B:868:ILE:HD13	1.77	0.48
1:B:392:GLN:HG2	1:B:411:HIS:ND1	2.28	0.48
1:A:549:PHE:CE2	1:A:657:VAL:HG11	2.48	0.48
1:A:818:THR:OG1	1:A:819:ILE:N	2.46	0.48
1:A:2629:GLN:OE1	1:A:2629:GLN:N	2.40	0.48
1:B:1336:TRP:CE3	1:B:1408:GLU:HG3	2.49	0.48
1:B:68:CYS:HB2	1:B:362:TRP:CE3	2.48	0.48
1:A:394:LYS:HB2	1:A:397:GLU:HG3	1.96	0.48
1:B:454:VAL:HG21	1:B:549:PHE:CD2	2.48	0.48
1:A:2052:ASP:OD2	1:A:2053:GLN:NE2	2.46	0.48
1:B:57:HIS:CD2	1:B:69:ARG:HH11	2.31	0.48
1:B:1140:ALA:HB1	1:B:1150:GLU:HG2	1.94	0.48
1:B:2689:MET:O	1:B:2692:SER:OG	2.28	0.48
1:A:1410:GLN:OE1	1:A:1818:LYS:NZ	2.46	0.48
1:B:2315:ILE:HD13	1:B:2527:ASN:HD22	1.79	0.48
1:A:479:CYS:HB3	1:A:751:VAL:HG12	1.95	0.48
1:A:1862:ALA:HB2	1:B:1363:LEU:HD11	1.95	0.48
1:A:2734:THR:HG22	1:A:2770:SER:HB2	1.95	0.48
1:B:916:CYS:SG	1:B:920:ARG:HB2	2.54	0.48
1:B:2091:ASP:O	1:B:2095:LEU:HD13	2.14	0.48
1:B:837:ASP:N	1:B:917:ASP:OD2	2.39	0.48
1:B:1847:ASP:OD1	1:B:2189:TRP:NE1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1917:PHE:HE2	1:B:1441:VAL:HG11	1.79	0.48
1:B:851:LEU:N	1:B:862:LYS:O	2.43	0.47
1:B:2572:ASP:OD1	1:B:2572:ASP:N	2.46	0.47
1:A:2506:TYR:HD1	1:A:2517:ARG:HB2	1.79	0.47
1:A:38:PRO:N	1:A:39:PRO:HD2	2.29	0.47
1:B:1385:HIS:O	1:B:1389:VAL:HG12	2.14	0.47
1:B:2775:PRO:HD2	1:B:2777:TYR:HE2	1.79	0.47
1:A:448:ASP:OD1	1:A:449:GLU:N	2.40	0.47
1:A:756:VAL:HG13	1:A:771:PHE:HB2	1.96	0.47
1:A:916:CYS:SG	1:A:920:ARG:HB2	2.54	0.47
1:A:2762:LEU:H	1:A:2786:LYS:NZ	2.12	0.47
1:B:444:ALA:HB2	1:B:462:ALA:HA	1.97	0.47
1:B:1854:ARG:NH1	1:B:1854:ARG:CG	2.75	0.47
1:A:2219:GLU:O	1:A:2222:GLU:HG3	2.14	0.47
1:B:1259:LEU:HD11	1:B:1332:VAL:HG22	1.97	0.47
1:B:2559:LEU:HA	1:B:2667:LEU:HD11	1.96	0.47
1:A:1243:LEU:HG	1:A:1315:PRO:HB3	1.97	0.47
1:A:1259:LEU:HD11	1:A:1332:VAL:HG22	1.96	0.47
1:B:2506:TYR:OH	1:B:2610:GLU:OE2	2.25	0.47
1:B:424:ILE:HG23	1:B:436:VAL:HG13	1.97	0.47
1:B:762:THR:HG22	1:B:767:ARG:NH1	2.29	0.47
1:A:1209:THR:HG21	1:A:1285:ARG:NE	2.30	0.47
1:B:411:HIS:O	1:B:413:ARG:N	2.48	0.47
1:B:2219:GLU:O	1:B:2222:GLU:HG3	2.15	0.47
1:A:1370:TYR:CE2	1:B:1854:ARG:HD2	2.44	0.46
1:B:2606:LEU:HD22	1:B:2610:GLU:HG2	1.97	0.46
1:A:1854:ARG:NH1	1:A:1854:ARG:CG	2.72	0.46
1:B:1171:TYR:O	1:B:1175:CYS:HB2	2.14	0.46
1:A:836:LEU:N	1:A:917:ASP:OD2	2.49	0.46
1:A:573:ARG:HG2	1:A:650:GLN:HG2	1.97	0.46
1:B:2245:ASP:OD1	1:B:2245:ASP:N	2.47	0.46
1:B:2602:PHE:HB3	1:B:2617:LEU:HB2	1.98	0.46
1:B:2072:GLN:OE1	1:B:2072:GLN:N	2.49	0.46
1:A:1231:TYR:HD1	1:A:1231:TYR:H	1.64	0.46
1:A:1847:ASP:OD1	1:A:2189:TRP:NE1	2.41	0.46
1:A:1881:ARG:HH11	1:A:1881:ARG:HB3	1.81	0.46
1:B:479:CYS:HB3	1:B:751:VAL:HG12	1.98	0.46
1:A:401:TYR:HD2	1:A:410:HIS:HA	1.81	0.46
1:A:1193:ILE:HD12	1:A:1206:CYS:HB3	1.97	0.46
1:A:1343:ILE:O	1:A:1427:ARG:NH1	2.46	0.46
1:A:1386:CYS:HA	1:A:1390:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1197:ARG:HD3	1:B:1202:LEU:HD21	1.98	0.46
1:A:2092:ARG:HH11	1:B:1490:ILE:HD12	1.81	0.45
1:B:2594:VAL:O	1:B:2598:MET:HG2	2.16	0.45
1:A:546:ALA:HB3	1:A:561:LEU:HD21	1.98	0.45
1:A:1343:ILE:HA	1:A:1380:LEU:HD13	1.98	0.45
1:B:2763:PRO:HB3	1:B:2774:VAL:HA	1.98	0.45
1:B:2052:ASP:OD2	1:B:2053:GLN:NE2	2.50	0.45
1:A:411:HIS:O	1:A:413:ARG:N	2.49	0.45
1:A:773:LEU:HD22	1:A:773:LEU:H	1.80	0.45
1:B:2618:ILE:HD12	1:B:2621:GLY:HA3	1.98	0.45
1:A:52:VAL:HB	1:A:376:ALA:HB2	1.99	0.45
1:A:2304:LEU:HD11	1:A:2548:ILE:HG13	1.98	0.45
1:B:1343:ILE:HA	1:B:1380:LEU:HD13	1.97	0.45
1:B:1386:CYS:HA	1:B:1390:LYS:HB2	1.98	0.45
1:B:1839:TRP:HE3	1:B:1954:LEU:HD13	1.81	0.45
1:B:2256:MET:HG3	1:B:2312:LEU:HD21	1.99	0.45
1:A:71:GLY:O	1:A:357:GLY:N	2.48	0.45
1:A:2311:ASN:OD1	1:A:2311:ASN:N	2.44	0.45
1:B:401:TYR:HD2	1:B:410:HIS:HA	1.81	0.45
1:B:457:LYS:HG3	1:B:659:VAL:HG22	1.98	0.45
1:B:1189:ILE:HD12	1:B:1292:GLN:HB3	1.99	0.45
1:B:1928:HIS:HA	1:B:2091:ASP:HB3	1.99	0.45
1:A:1177:ASP:OD1	1:A:1210:GLU:HB3	2.17	0.45
1:A:1345:PHE:CZ	1:A:1352:ASP:HB3	2.52	0.45
1:A:2515:THR:HB	1:A:2551:ASN:HD22	1.81	0.45
1:B:2592:ASP:OD1	1:B:2592:ASP:N	2.50	0.45
1:A:494:TRP:HB3	1:A:735:PRO:HA	1.99	0.45
1:A:757:HIS:CE1	1:A:770:ILE:HD13	2.52	0.45
1:A:1453:ILE:HD12	1:A:1453:ILE:HA	1.89	0.45
1:A:473:ILE:HA	1:A:487:LEU:HD13	2.00	0.44
1:A:761:LYS:NZ	1:A:763:GLY:O	2.33	0.44
1:A:2057:LEU:HD11	1:A:2673:GLU:HB2	1.99	0.44
1:B:77:ASP:OD1	1:B:77:ASP:N	2.49	0.44
1:B:837:ASP:OD1	1:B:920:ARG:NH2	2.43	0.44
1:B:51:CYS:SG	1:B:52:VAL:N	2.90	0.44
1:B:1871:PRO:HG3	1:B:1936:LEU:HD11	1.99	0.44
1:A:363:TRP:HZ2	1:A:391:TYR:HB3	1.82	0.44
1:A:574:PHE:CD1	1:A:651:TRP:HB2	2.52	0.44
1:A:2252:ILE:O	1:A:2256:MET:HG2	2.18	0.44
1:A:2717:ILE:HD11	1:A:2787:LEU:HD23	1.99	0.44
1:B:792:LEU:O	1:B:815:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB2	1:A:374:ILE:HD13	1.99	0.44
1:B:11:LEU:HD21	1:B:865:ALA:HB2	1.99	0.44
1:B:1124:ARG:NH2	1:B:1176:ASN:O	2.51	0.44
1:B:2312:LEU:HD23	1:B:2315:ILE:HD11	1.99	0.44
1:A:2530:ARG:HD3	1:A:2656:LYS:NZ	2.33	0.44
1:B:876:LEU:HD23	1:B:911:PHE:CE1	2.52	0.44
1:B:1464:PHE:HB3	1:B:1798:LEU:HD11	1.99	0.44
1:B:2248:ARG:HE	1:B:2252:ILE:HD11	1.83	0.44
1:A:1188:HIS:HB3	1:A:1229:THR:OG1	2.17	0.44
1:A:1441:VAL:HG11	1:B:1917:PHE:HE2	1.82	0.44
1:A:2704:ALA:HA	1:A:2707:LEU:HG	2.00	0.44
1:B:1961:MET:O	1:B:1965:THR:HG23	2.17	0.44
1:A:1177:ASP:H	1:A:1251:ARG:HH22	1.63	0.44
1:A:1363:LEU:HD11	1:B:1862:ALA:HB2	2.00	0.44
1:B:1705:ASN:HD22	1:B:1705:ASN:H	1.65	0.44
1:A:2698:ASP:OD1	1:A:2698:ASP:N	2.48	0.44
1:B:861:LYS:H	1:B:861:LYS:HD2	1.83	0.44
1:A:1333:LEU:O	1:A:1404:THR:HG21	2.18	0.44
1:A:1472:VAL:HG23	1:A:1795:ILE:HG23	2.00	0.44
1:B:363:TRP:CZ2	1:B:391:TYR:HB3	2.53	0.44
1:B:1121:VAL:HG22	1:B:1254:LEU:HD21	2.00	0.44
1:A:2299:ILE:HG21	1:A:2535:ILE:HD13	1.99	0.43
1:B:1084:ASN:O	1:B:1088:ILE:HG12	2.19	0.43
1:B:1388:ILE:HG23	1:B:1459:LYS:HB2	2.00	0.43
1:A:2299:ILE:HG13	1:A:2303:PHE:CE2	2.53	0.43
1:B:2252:ILE:O	1:B:2256:MET:HG2	2.18	0.43
1:A:2651:LEU:HD13	1:A:2651:LEU:HA	1.82	0.43
1:B:2311:ASN:OD1	1:B:2312:LEU:N	2.51	0.43
1:A:2554:VAL:HG13	1:A:2651:LEU:HD11	2.01	0.43
1:A:22:LEU:O	1:A:25:VAL:HG12	2.18	0.43
1:A:806:GLN:N	1:A:806:GLN:OE1	2.50	0.43
1:A:1240:CYS:HB3	1:A:1243:LEU:HD22	2.00	0.43
1:A:2057:LEU:HG	1:A:2677:LEU:HD13	2.01	0.43
1:B:1265:VAL:O	1:B:1274:HIS:NE2	2.52	0.43
1:B:2242:LEU:HD11	1:B:2279:VAL:HG22	1.99	0.43
1:A:1370:TYR:CE2	1:B:1854:ARG:CD	3.01	0.43
1:A:1713:SER:HA	1:B:1872:LEU:HD21	2.01	0.43
1:B:380:GLU:OE1	1:B:380:GLU:N	2.50	0.43
1:B:1079:LYS:O	1:B:1082:LYS:HG3	2.18	0.43
1:A:424:ILE:HG23	1:A:436:VAL:HG13	2.00	0.43
1:A:752:ASP:HA	1:A:805:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:LEU:N	1:A:862:LYS:O	2.46	0.43
1:B:1345:PHE:CZ	1:B:1352:ASP:HB3	2.54	0.43
1:A:2661:VAL:HG23	1:A:2662:LEU:HG	2.01	0.43
1:B:2304:LEU:HD21	1:B:2548:ILE:HG13	1.99	0.43
1:A:1124:ARG:HH22	1:A:1242:THR:HG23	1.84	0.43
1:B:780:GLN:NE2	1:B:782:ASN:OD1	2.51	0.43
1:B:2269:THR:OG1	1:B:2270:THR:N	2.52	0.43
1:B:2726:ARG:O	1:B:2730:VAL:HG23	2.19	0.43
1:A:18:LEU:HD21	1:A:811:ILE:HG12	2.00	0.42
1:A:385:SER:OG	1:A:389:GLU:OE1	2.28	0.42
1:A:1407:LYS:HE2	1:A:1407:LYS:HB3	1.84	0.42
1:A:2717:ILE:O	1:A:2721:MET:HG3	2.19	0.42
1:B:1313:ASP:OD1	1:B:1313:ASP:N	2.49	0.42
1:B:1691:LEU:HD12	1:B:1691:LEU:HA	1.89	0.42
1:B:2097:VAL:HG22	1:B:2101:LYS:HG3	2.01	0.42
1:B:2556:LYS:HG2	1:B:2561:ARG:HB2	2.01	0.42
1:A:1193:ILE:HD13	1:A:1193:ILE:HA	1.84	0.42
1:B:2577:GLU:OE1	1:B:2580:ARG:NH1	2.52	0.42
1:A:397:GLU:HG3	1:A:397:GLU:H	1.70	0.42
1:A:2026:SER:OG	1:A:2027:ASP:N	2.53	0.42
1:A:2572:ASP:OD1	1:A:2572:ASP:N	2.51	0.42
1:B:492:TYR:HD1	1:B:737:LYS:HA	1.85	0.42
1:B:552:SER:HB3	1:B:557:LYS:NZ	2.34	0.42
1:B:738:LEU:HD13	1:B:756:VAL:HG21	2.02	0.42
1:A:546:ALA:H	1:A:561:LEU:HG	1.85	0.42
1:A:653:LEU:HD22	1:A:654:ARG:N	2.34	0.42
1:A:1881:ARG:HB3	1:A:1881:ARG:NH1	2.35	0.42
1:B:825:ASP:HB3	1:B:831:ARG:HG2	2.01	0.42
1:B:463:GLN:HG3	1:B:465:TYR:CE1	2.55	0.42
1:A:2198:ARG:HG3	1:B:1711:PRO:HD3	2.02	0.42
1:A:741:PRO:HB2	1:A:744:THR:HG21	2.00	0.42
1:A:1822:GLN:HA	1:A:1825:VAL:HG22	2.01	0.42
1:B:747:LEU:HB3	1:B:799:VAL:HG11	2.00	0.42
1:B:908:LEU:HD12	1:B:911:PHE:HD2	1.84	0.42
1:A:360:LEU:HD23	1:A:360:LEU:H	1.84	0.42
1:B:568:MET:SD	1:B:653:LEU:HD23	2.59	0.42
1:B:1955:ILE:HD13	1:B:1955:ILE:HA	1.95	0.42
1:B:2236:GLN:HB2	1:B:2275:HIS:HB2	2.01	0.42
1:B:2697:ASN:O	1:B:2753:THR:HA	2.19	0.42
1:A:392:GLN:HG2	1:A:411:HIS:CG	2.53	0.42
1:A:1932:HIS:CE1	1:A:1935:VAL:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2062:ARG:NH1	1:A:2064:GLU:OE1	2.53	0.42
1:A:2762:LEU:H	1:A:2786:LYS:HZ3	1.66	0.42
1:B:1175:CYS:SG	1:B:1213:ARG:HB3	2.60	0.42
1:B:1852:GLN:NE2	1:B:1937:PRO:HB2	2.34	0.42
1:A:2697:ASN:OD1	1:A:2697:ASN:N	2.53	0.42
1:B:392:GLN:HG2	1:B:411:HIS:CG	2.55	0.42
1:B:2057:LEU:HG	1:B:2677:LEU:HD13	2.02	0.42
1:B:2788:LEU:HD13	1:B:2791:ILE:HD11	2.02	0.42
1:A:794:GLN:H	1:A:794:GLN:HG2	1.69	0.41
1:A:1170:LEU:HD11	1:A:1255:LEU:HD12	2.01	0.41
1:A:2633:GLU:HG2	1:A:2636:ARG:NH1	2.35	0.41
1:B:11:LEU:HD22	1:B:807:GLU:O	2.20	0.41
1:B:75:GLN:HB2	1:B:77:ASP:OD1	2.20	0.41
1:B:498:PRO:HG2	1:B:773:LEU:HB2	2.01	0.41
1:B:549:PHE:CD2	1:B:657:VAL:HG21	2.55	0.41
1:B:921:ASN:ND2	1:B:924:HIS:HD2	2.18	0.41
1:B:2020:HIS:CD2	1:B:2022:PHE:H	2.36	0.41
1:B:2677:LEU:HD12	1:B:2677:LEU:HA	1.86	0.41
1:A:1710:ALA:O	1:A:1715:GLN:NE2	2.53	0.41
1:B:499:PHE:CE1	1:B:654:ARG:HA	2.54	0.41
1:B:802:PHE:CD1	1:B:844:LEU:HD23	2.55	0.41
1:B:1352:ASP:OD1	1:B:1352:ASP:N	2.53	0.41
1:A:2257:ARG:HH21	1:A:2315:ILE:HA	1.85	0.41
1:A:2631:VAL:O	1:A:2634:TYR:HB3	2.20	0.41
1:B:56:ASN:C	1:B:57:HIS:HD1	2.23	0.41
1:B:467:GLU:CD	1:B:467:GLU:H	2.23	0.41
1:B:2721:MET:HB3	1:B:2725:GLU:HG3	2.02	0.41
1:A:493:TRP:CZ2	1:A:773:LEU:HB3	2.55	0.41
1:B:569:ASN:OD1	1:B:569:ASN:N	2.53	0.41
1:B:1846:MET:HA	1:B:1849:THR:HG22	2.01	0.41
1:A:69:ARG:HD3	1:A:393:TRP:CZ2	2.55	0.41
1:A:1929:ASN:O	1:A:1931:GLU:HG3	2.20	0.41
1:A:2022:PHE:CD2	1:A:2636:ARG:HG3	2.55	0.41
1:A:2250:LEU:HA	1:A:2253:GLN:HG2	2.03	0.41
1:B:824:LYS:HE2	1:B:824:LYS:HB2	1.89	0.41
1:A:1179:CYS:HB3	1:A:1182:THR:HG23	2.03	0.41
1:A:1473:GLU:O	1:A:1477:ASN:ND2	2.46	0.41
1:B:836:LEU:N	1:B:917:ASP:OD2	2.54	0.41
1:B:2788:LEU:O	1:B:2792:LYS:HG2	2.20	0.41
1:A:738:LEU:HD13	1:A:756:VAL:HG11	2.03	0.41
1:A:876:LEU:HD23	1:A:911:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HA	1:B:21:ARG:HD3	1.91	0.41
1:B:1188:HIS:HB3	1:B:1229:THR:OG1	2.20	0.41
1:B:11:LEU:HA	1:B:11:LEU:HD23	1.76	0.41
1:B:751:VAL:HG22	1:B:756:VAL:HG12	2.03	0.41
1:B:2605:ASP:OD1	1:B:2605:ASP:N	2.45	0.41
1:A:382:LEU:HD23	1:A:392:GLN:HB3	2.03	0.41
1:A:1329:LEU:HD23	1:A:1397:LEU:HD13	2.03	0.41
1:A:1714:MET:HE2	1:B:2195:LEU:HD22	2.03	0.41
1:A:1847:ASP:HA	1:A:2087:GLU:HG2	2.03	0.41
1:A:2092:ARG:NH1	1:B:1490:ILE:HD12	2.35	0.41
1:B:454:VAL:O	1:B:457:LYS:HG2	2.20	0.41
1:B:1077:GLU:O	1:B:1081:ARG:N	2.48	0.41
1:B:2044:LEU:HB2	1:B:2576:TYR:CE2	2.56	0.41
1:B:2242:LEU:HD11	1:B:2279:VAL:HG13	2.02	0.41
1:B:2309:LEU:HD12	1:B:2310:PRO:HD2	2.03	0.41
1:A:931:PHE:CE1	1:A:1123:GLY:HA3	2.56	0.41
1:A:2052:ASP:O	1:A:2510:LYS:HE3	2.20	0.41
1:B:2260:ASN:ND2	1:B:2527:ASN:HD21	2.16	0.41
1:A:441:ASN:N	1:A:441:ASN:OD1	2.54	0.40
1:A:1394:ASP:HB3	1:A:1396:LEU:HD23	2.03	0.40
1:B:1333:LEU:O	1:B:1404:THR:HG21	2.21	0.40
1:A:1832:GLU:O	1:A:1836:ILE:HG12	2.21	0.40
1:A:1856:GLY:HA3	1:B:1716:TRP:CZ2	2.57	0.40
1:B:833:PRO:HG2	1:B:835:TRP:CH2	2.56	0.40
1:B:2240:LEU:HD22	1:B:2277:VAL:HG13	2.02	0.40
1:A:433:ARG:HG2	1:A:434:ALA:N	2.36	0.40
1:A:876:LEU:HD23	1:A:911:PHE:CZ	2.56	0.40
1:B:2184:MET:HG3	1:B:2185:LEU:HD22	2.04	0.40
1:A:65:GLY:HA3	1:A:370:LYS:HA	2.03	0.40
1:A:923:LEU:HD13	1:A:923:LEU:HA	1.96	0.40
1:A:1846:MET:HA	1:A:1849:THR:HG22	2.02	0.40
1:B:494:TRP:HB3	1:B:735:PRO:HA	2.02	0.40
1:B:1707:ALA:HB1	1:B:1718:VAL:HG13	2.03	0.40
1:A:11:LEU:HD12	1:A:863:LYS:HD2	2.02	0.40
1:A:494:TRP:CD1	1:A:735:PRO:HG3	2.57	0.40
1:A:1201:LEU:HD22	1:A:1207:CYS:HB3	2.03	0.40
1:A:2316:GLN:HG2	1:A:2317:ASN:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1663/2807 (59%)	1595 (96%)	67 (4%)	1 (0%)	51 69
1	B	1663/2807 (59%)	1589 (96%)	73 (4%)	1 (0%)	51 69
All	All	3326/5614 (59%)	3184 (96%)	140 (4%)	2 (0%)	54 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2270	THR
1	B	2175	PHE

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	1487/2427 (61%)	1422 (96%)	65 (4%)	28 43
1	B	1487/2427 (61%)	1418 (95%)	69 (5%)	27 41
All	All	2974/4854 (61%)	2840 (96%)	134 (4%)	31 42

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	29	LEU
1	A	62	LEU
1	A	74	VAL

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Mol	Chain	Res	Type
1	A	397	GLU
1	A	411	HIS
1	A	441	ASN
1	A	507	GLU
1	A	510	ARG
1	A	512	LYS
1	A	562	MET
1	A	650	GLN
1	A	653	LEU
1	A	654	ARG
1	A	726	LYS
1	A	734	THR
1	A	756	VAL
1	A	759	VAL
1	A	762	THR
1	A	767	ARG
1	A	770	ILE
1	A	836	LEU
1	A	848	VAL
1	A	1089	LEU
1	A	1202	LEU
1	A	1225	ARG
1	A	1231	TYR
1	A	1242	THR
1	A	1243	LEU
1	A	1389	VAL
1	A	1411	ASN
1	A	1697	ARG
1	A	1698	THR
1	A	1833	GLU
1	A	1838	THR
1	A	1881	ARG
1	A	1911	MET
1	A	1939	LEU
1	A	2028	SER
1	A	2072	GLN
1	A	2085	LEU
1	A	2166	LEU
1	A	2175	PHE
1	A	2178	MET
1	A	2211	ILE
1	A	2237	SER

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Mol	Chain	Res	Type
1	A	2240	LEU
1	A	2245	ASP
1	A	2249	ASP
1	A	2265	ARG
1	A	2269	THR
1	A	2278	LYS
1	A	2517	ARG
1	A	2539	CYS
1	A	2553	HIS
1	A	2623	ASN
1	A	2651	LEU
1	A	2673	GLU
1	A	2685	VAL
1	A	2690	LEU
1	A	2724	THR
1	A	2731	TYR
1	A	2760	GLN
1	A	2789	LEU
1	A	2792	LYS
1	B	7	VAL
1	B	18	LEU
1	B	29	LEU
1	B	389	GLU
1	B	390	LEU
1	B	393	TRP
1	B	411	HIS
1	B	427	LEU
1	B	457	LYS
1	B	461	THR
1	B	467	GLU
1	B	504	LYS
1	B	507	GLU
1	B	512	LYS
1	B	653	LEU
1	B	659	VAL
1	B	726	LYS
1	B	756	VAL
1	B	770	ILE
1	B	779	GLU
1	B	806	GLN
1	B	838	LEU
1	B	848	VAL

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Mol	Chain	Res	Type
1	B	896	GLU
1	B	911	PHE
1	B	1082	LYS
1	B	1097	VAL
1	B	1195	GLU
1	B	1231	TYR
1	B	1233	ASP
1	B	1241	LYS
1	B	1366	GLU
1	B	1411	ASN
1	B	1417	ARG
1	B	1690	MET
1	B	1697	ARG
1	B	1698	THR
1	B	1705	ASN
1	B	1833	GLU
1	B	1838	THR
1	B	1881	ARG
1	B	1932	HIS
1	B	1933	SER
1	B	1935	VAL
1	B	1952	GLN
1	B	2065	ASP
1	B	2083	LYS
1	B	2102	MET
1	B	2166	LEU
1	B	2175	PHE
1	B	2203	ASP
1	B	2262	HIS
1	B	2539	CYS
1	B	2540	LEU
1	B	2548	ILE
1	B	2562	LYS
1	B	2600	LEU
1	B	2618	ILE
1	B	2649	GLN
1	B	2677	LEU
1	B	2685	VAL
1	B	2707	LEU
1	B	2708	LEU
1	B	2722	SER
1	B	2724	THR

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Mol	Chain	Res	Type
1	B	2746	PHE
1	B	2760	GLN
1	B	2762	LEU
1	B	2780	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	780	GLN
1	A	782	ASN
1	A	924	HIS
1	A	1269	ASN
1	A	1455	GLN
1	A	1508	GLN
1	A	1828	GLN
1	A	2072	GLN
1	A	2182	HIS
1	A	2253	GLN
1	A	2262	HIS
1	A	2542	GLN
1	A	2543	ASN
1	A	2614	GLN
1	A	2709	GLN
1	A	2727	GLN
1	B	41	ASN
1	B	75	GLN
1	B	469	GLN
1	B	650	GLN
1	B	780	GLN
1	B	782	ASN
1	B	806	GLN
1	B	914	HIS
1	B	924	HIS
1	B	1334	GLN
1	B	1411	ASN
1	B	1705	ASN
1	B	1852	GLN
1	B	1952	GLN
1	B	2020	HIS
1	B	2182	HIS
1	B	2236	GLN
1	B	2262	HIS

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Mol	Chain	Res	Type
1	B	2527	ASN
1	B	2542	GLN
1	B	2614	GLN
1	B	2680	ASN
1	B	2727	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.

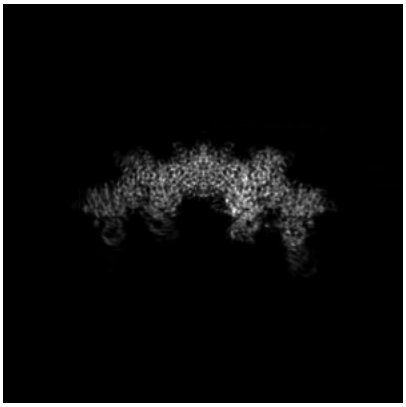
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27822. These allow visual inspection of the internal detail of the map and identification of artifacts.

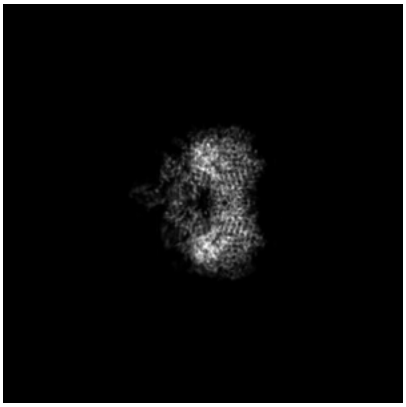
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



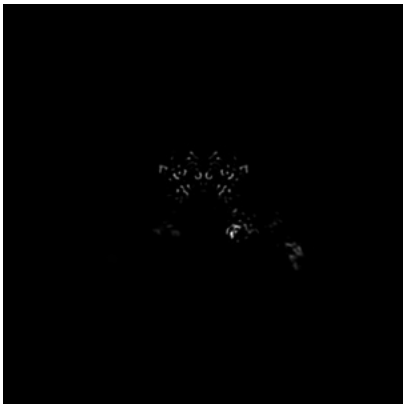
Y

Z

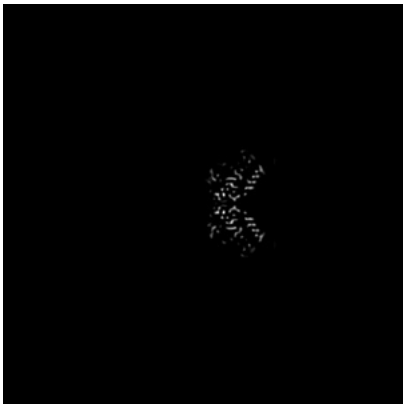
The images above show the map projected in three orthogonal directions.

6.2 Central slices

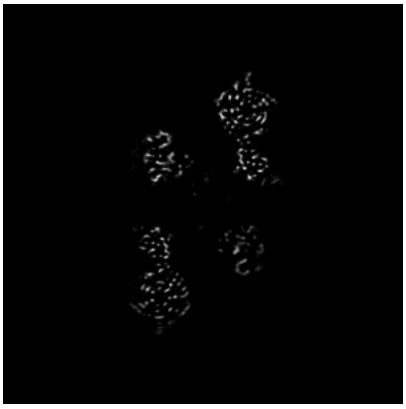
6.2.1 Primary map



X Index: 200



Y Index: 200



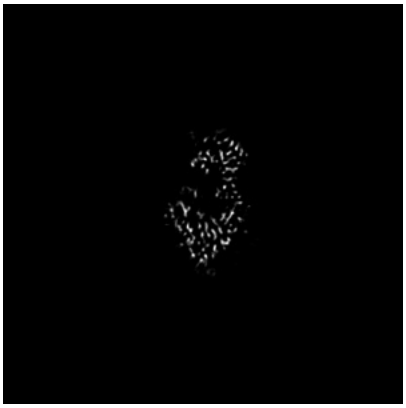
Z Index: 200

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

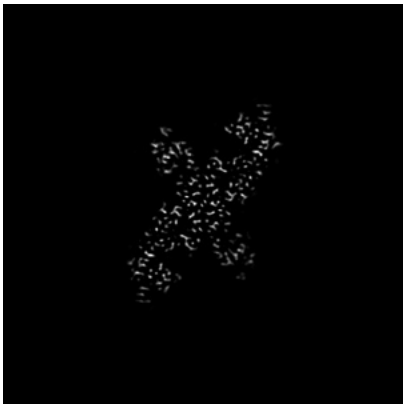
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 160



Y Index: 242

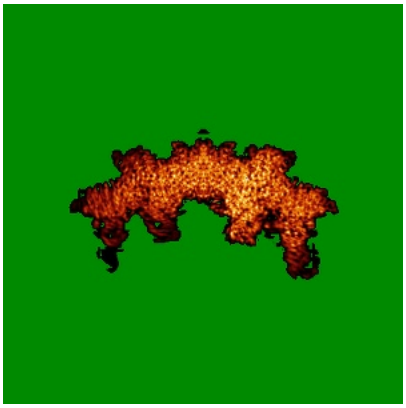


Z Index: 220

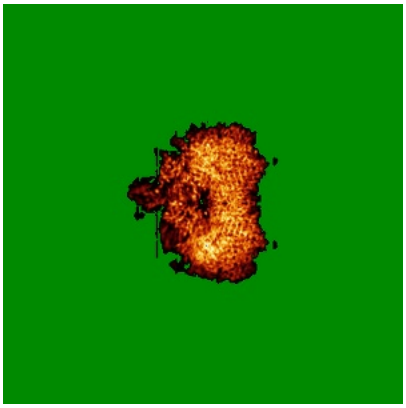
The images above show the largest variance slices of the map in three orthogonal directions.

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

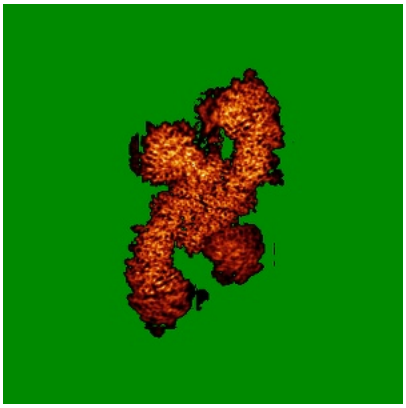
6.4.1 Primary map



X



Y

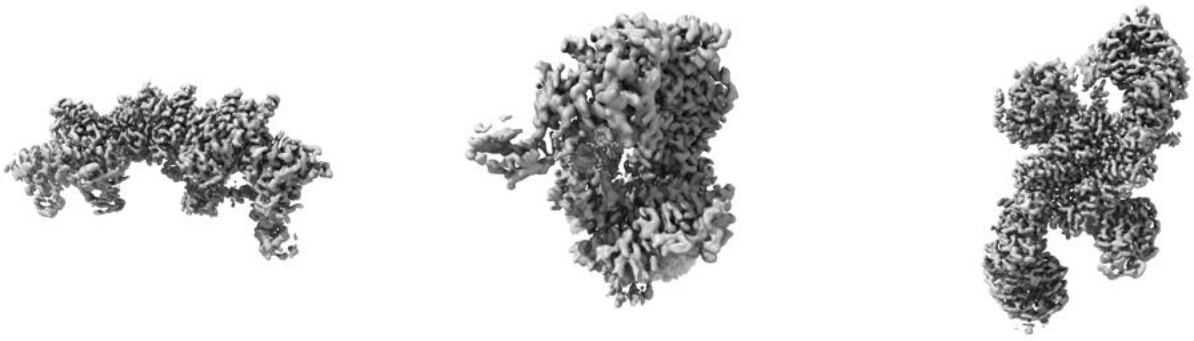


Z

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

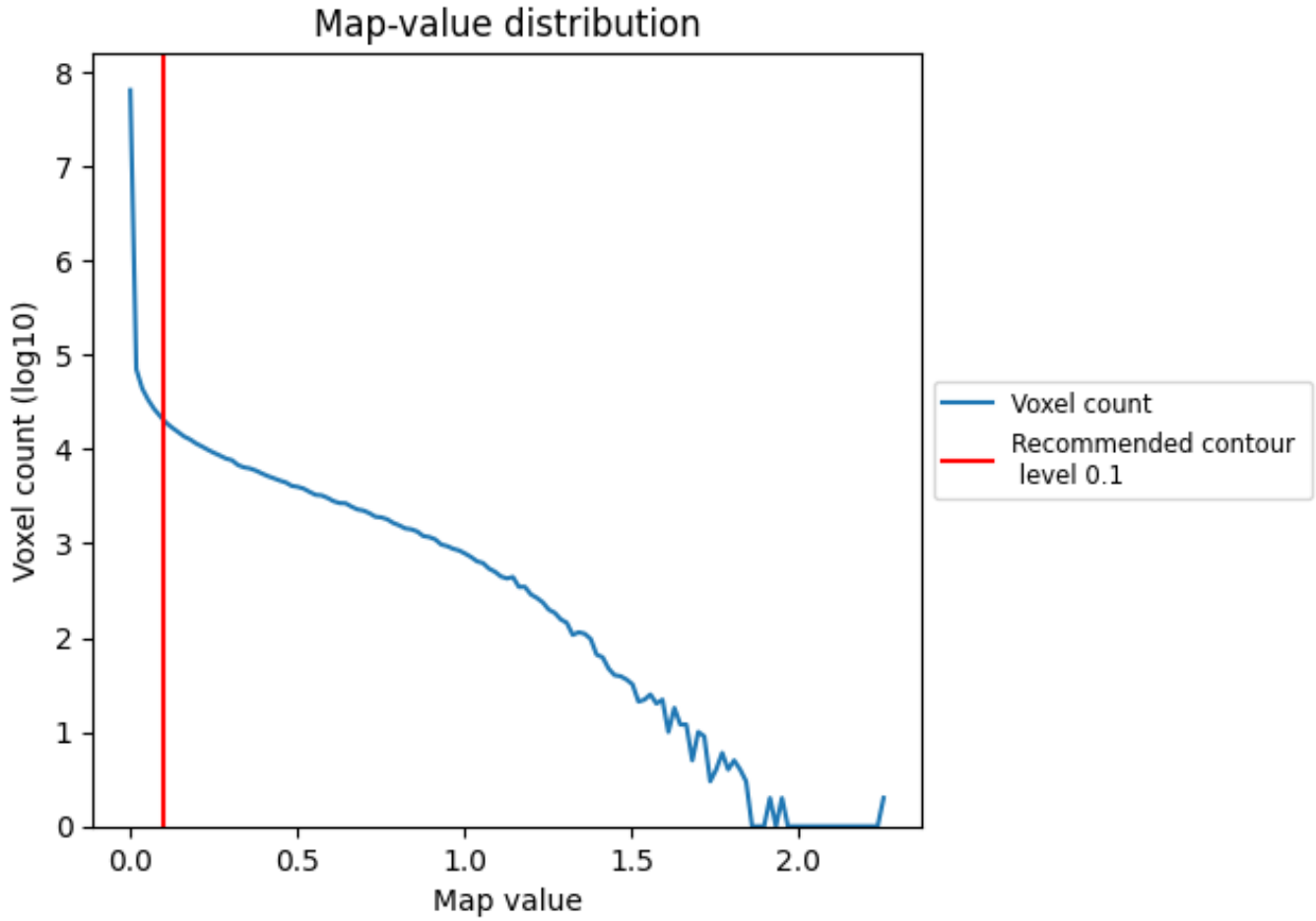
6.6 Mask visualisation (i)

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

7 Map analysis

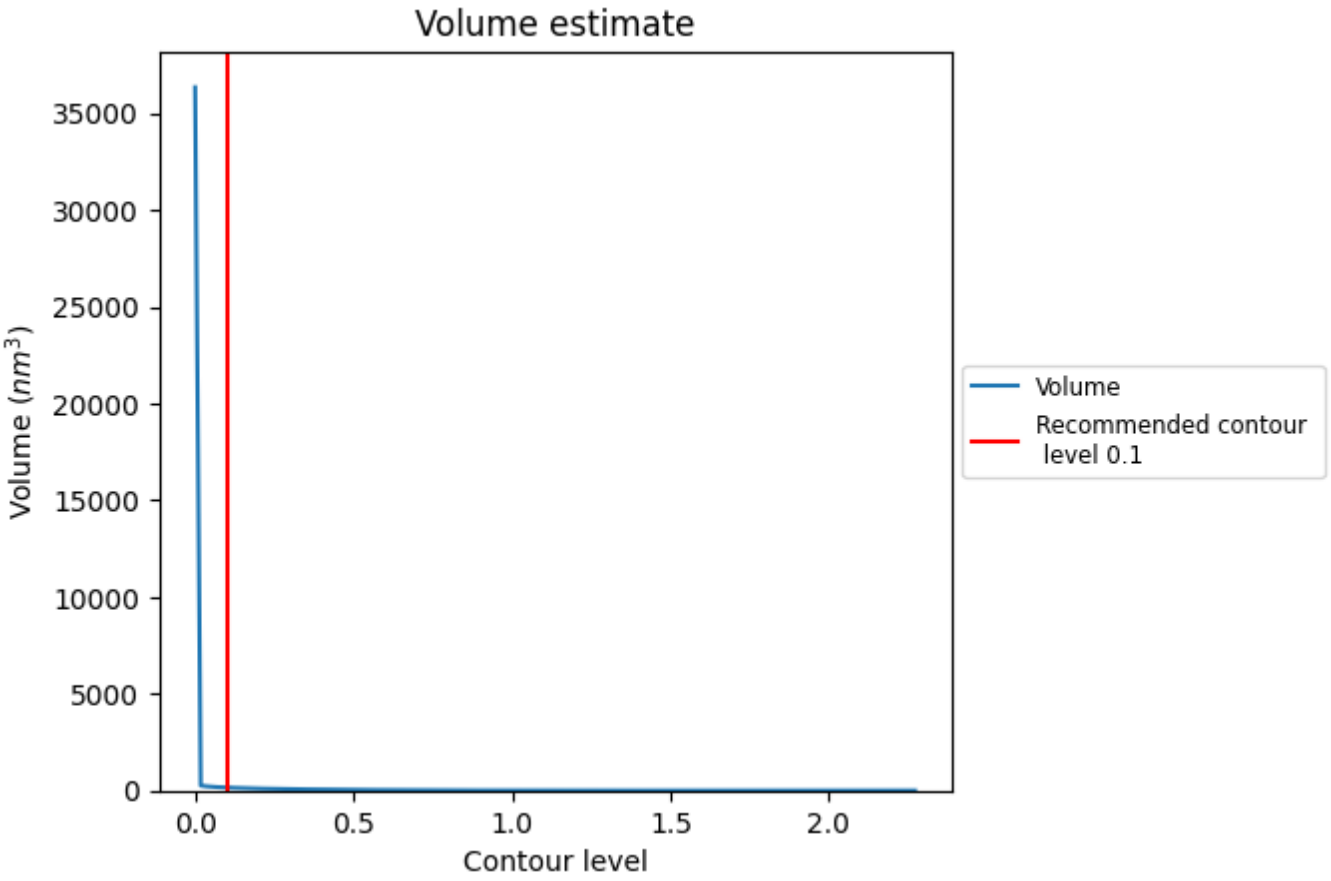
This section contains the results of statistical analysis of the map.

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.

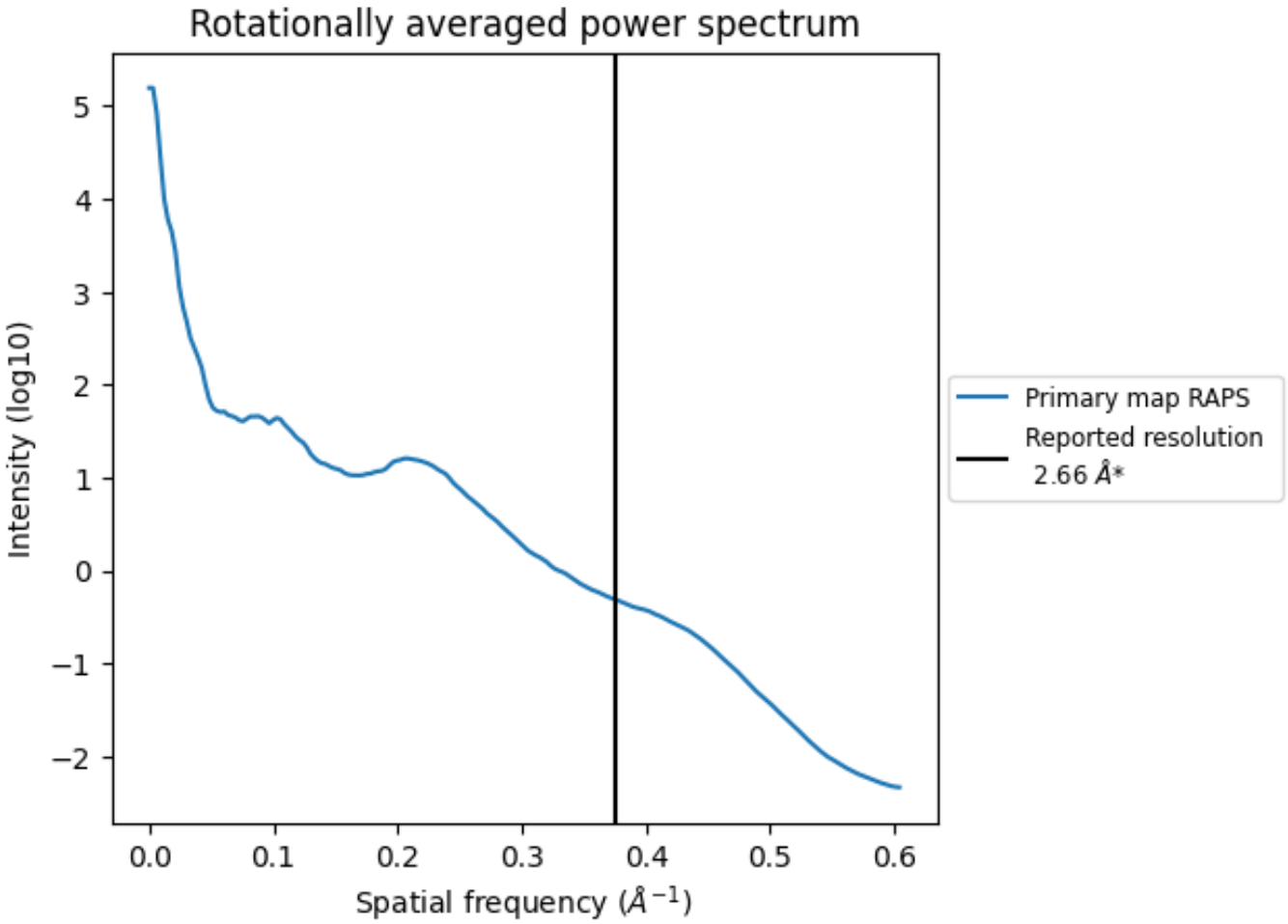
7.2 Volume estimate



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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 0.376 Å^{-1}

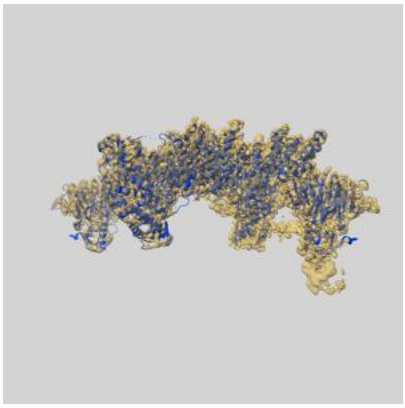
8 Fourier-Shell correlation

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

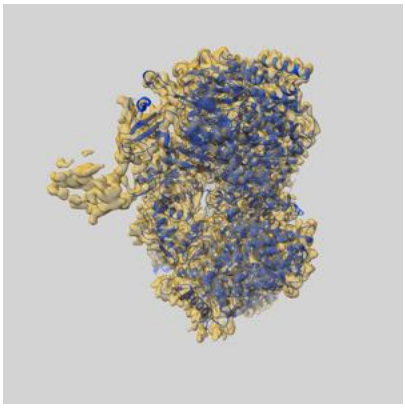
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27822 and PDB model 8E0Q. Per-residue inclusion information can be found in section 3 on page 4.

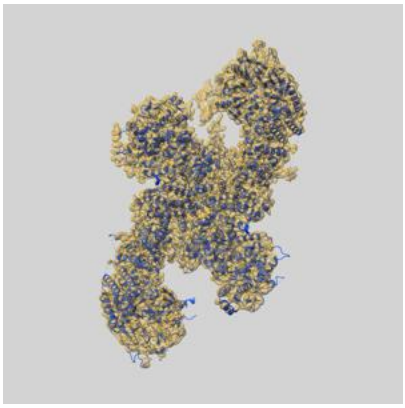
9.1 Map-model overlay



X



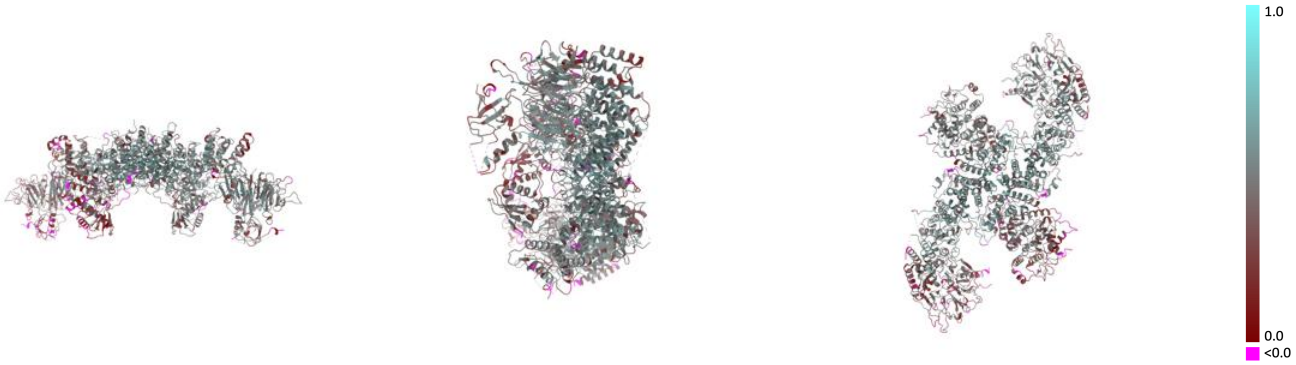
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

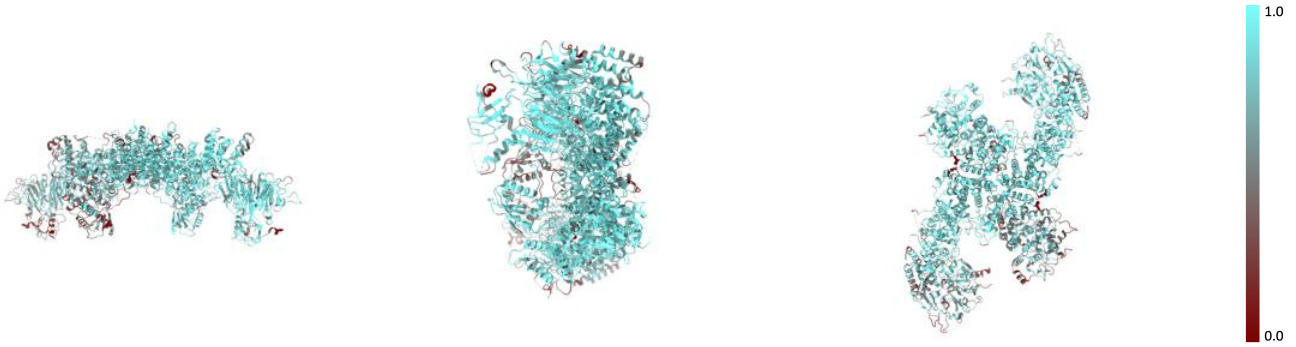
9.2 Q-score mapped to coordinate model (i)



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.

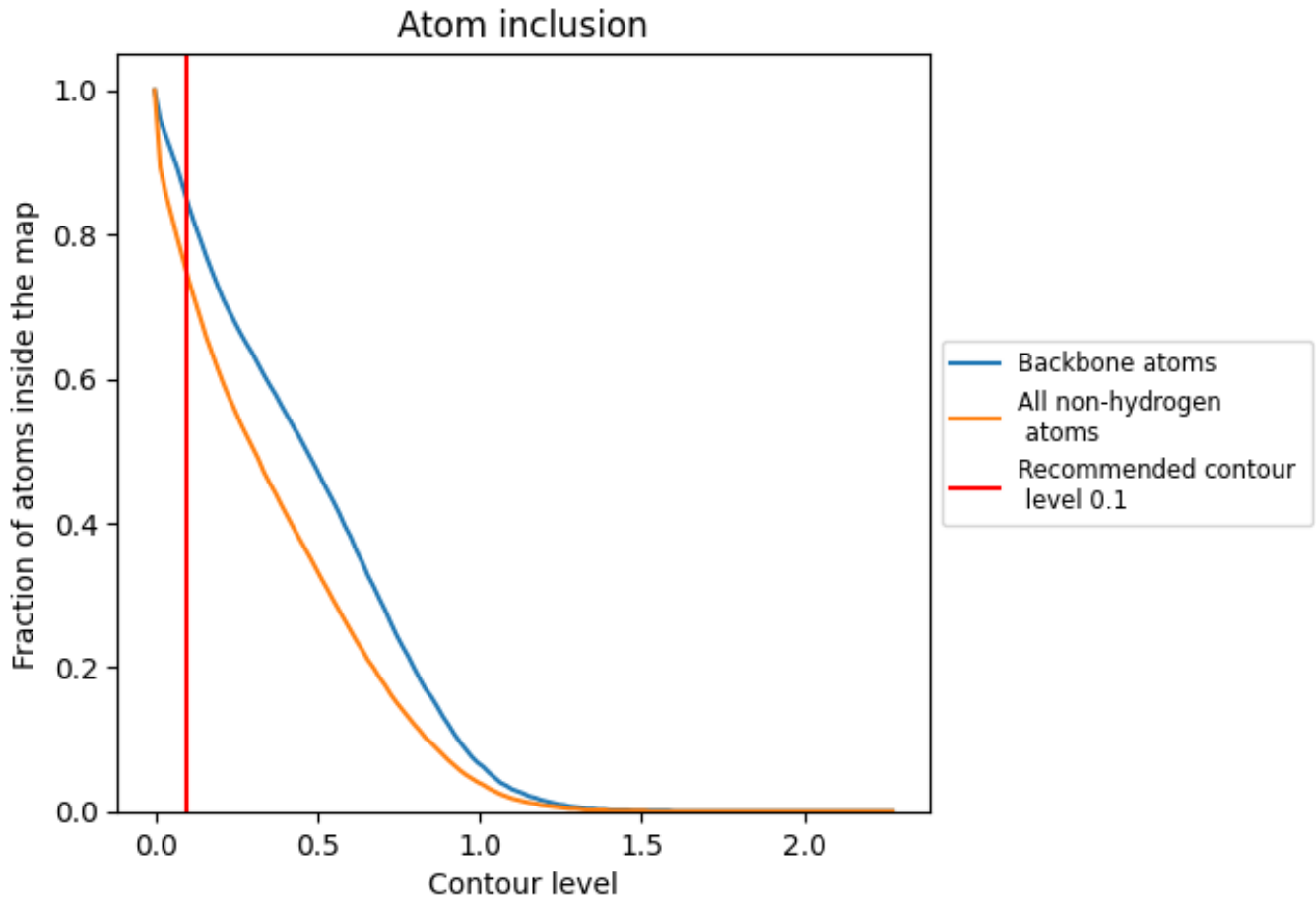
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4250
A	0.7410	0.4230
B	0.7450	0.4270