Full wwPDB EM Validation Report ⓘ

Nov 23, 2025 – 06:16 PM EST

PDB ID	:	9OT6 / pdb_00009ot6
EMDB ID	:	EMD-70826
Title	:	Cryo-EM structure of the PI4KA complex bound to an EFR3 interfering nanobody (F3IN)
Authors	:	Shaw, A.L.; Suresh, S.; Yip, C.K.; Burke, J.E.
Deposited on	:	2025-05-26
Resolution	:	3.54 Å(reported)
Based on initial models	:	9BAX, .

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:

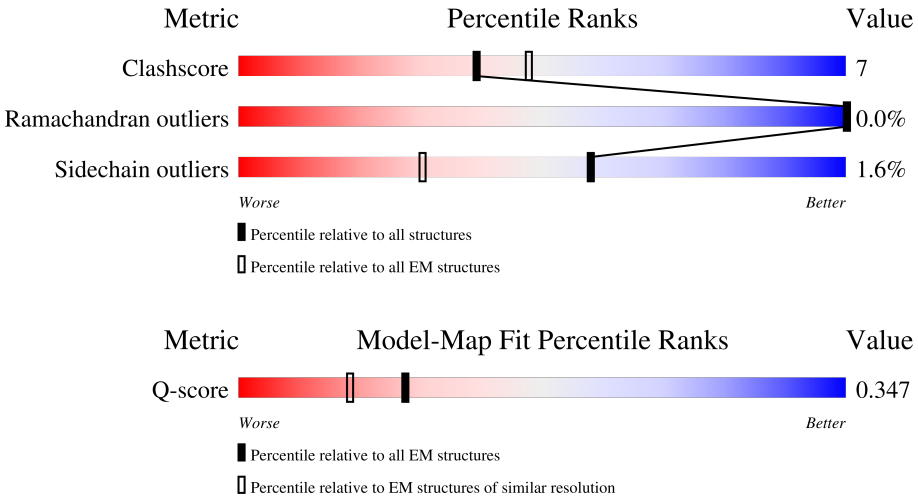
EMDB validation analysis	:	0.0.1.dev129
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 3.54 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12891 (3.04 - 4.04)

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	2104	67% 14% 18%
1	B	2104	67% 15% 18%
2	C	165	7% 48% 14% 37%
2	H	165	5% 50% 12% 37%

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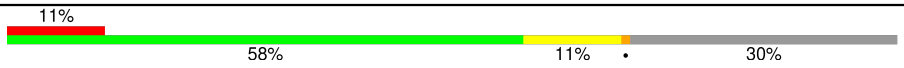
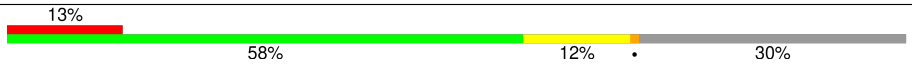
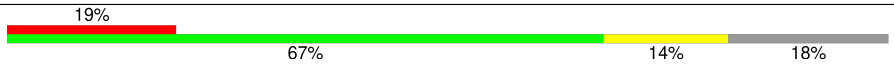
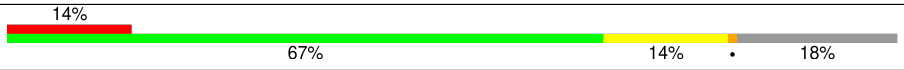
Mol	Chain	Length	Quality of chain
3	D	843	
3	F	843	
4	E	308	
4	G	308	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 42678 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 Phosphatidylinositol 4-kinase alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		
1	B	1724	Total	C	N	O	S	0	0
			13842	8951	2305	2489	97		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42356
A	0	SER	-	expression tag	UNP P42356
B	-1	GLY	-	expression tag	UNP P42356
B	0	SER	-	expression tag	UNP P42356

- Molecule 2 is a protein called EFR3 interfering Nanobody (F3IN).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	104	Total	C	N	O	S	0	0
			811	511	141	154	5		
2	H	104	Total	C	N	O	S	0	0
			811	511	141	154	5		

- Molecule 3 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		
3	F	592	Total	C	N	O	S	0	0
			4676	2983	811	855	27		

- Molecule 4 is a protein called Hyccin.

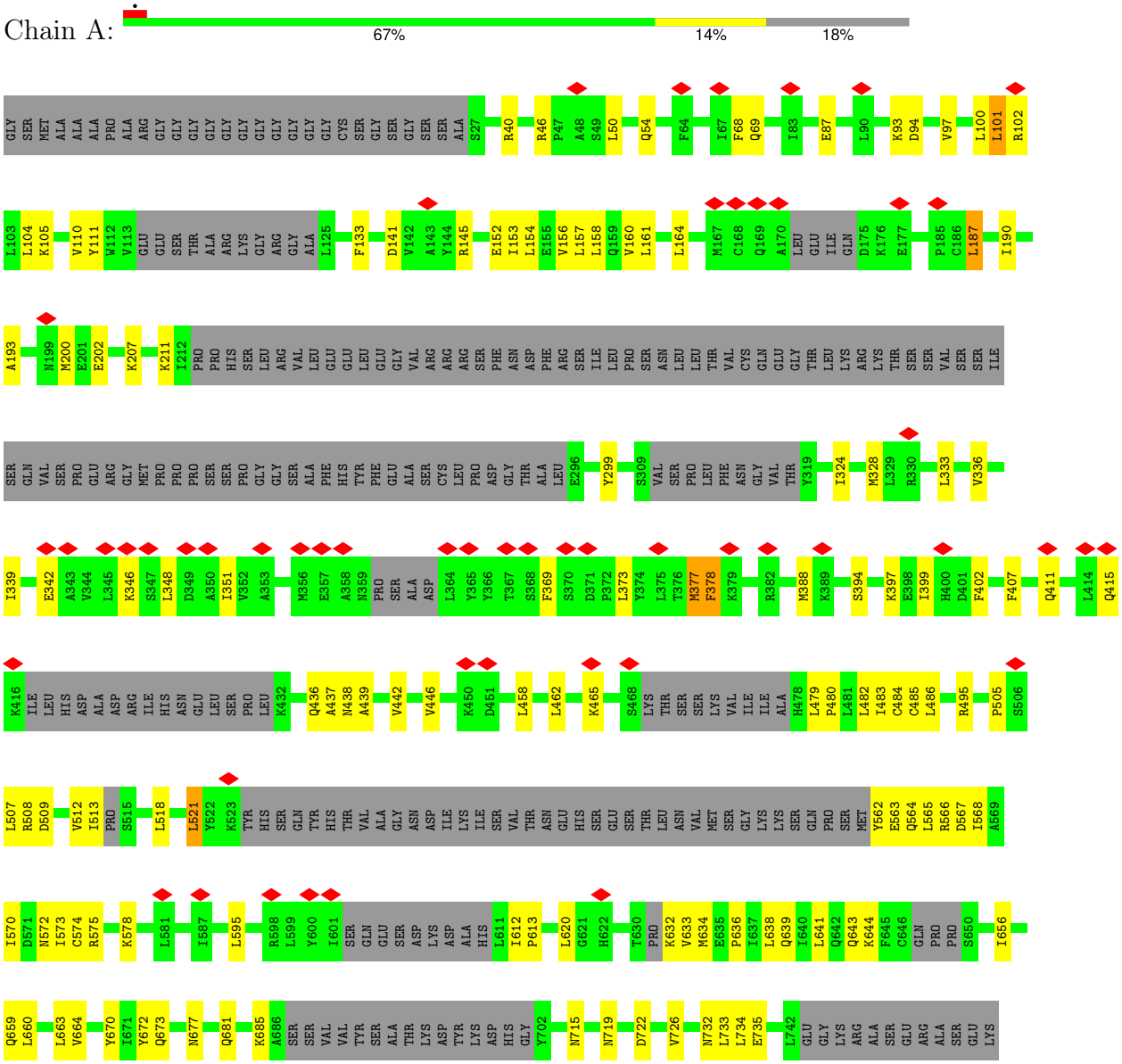
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	252	Total 2010	C 1309	N 323	O 366	S 12	0	0
4	G	252	Total 2010	C 1309	N 323	O 366	S 12	0	0

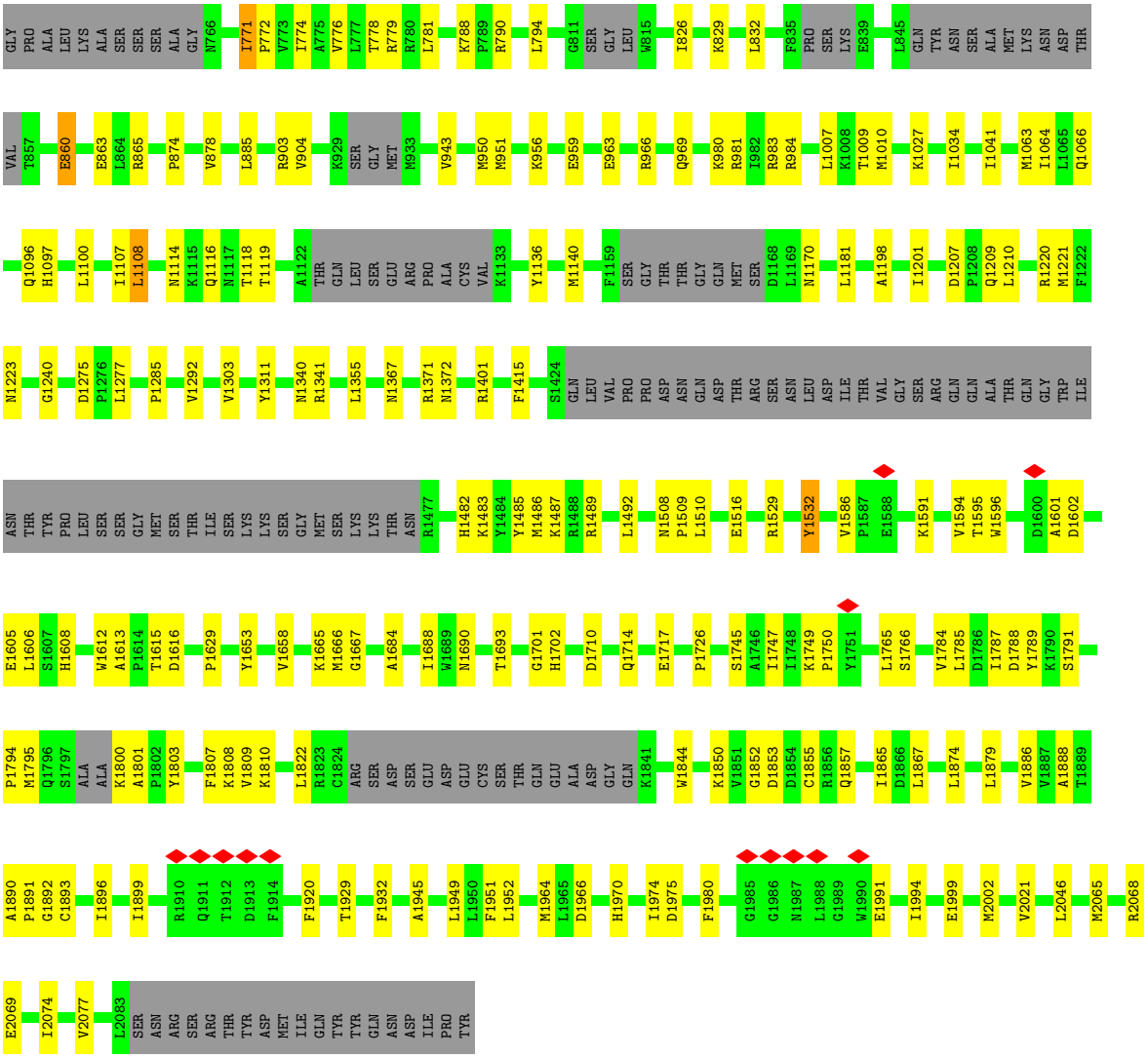
3 Residue-property plots (i)

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: Phosphatidylinositol 4-kinase alpha

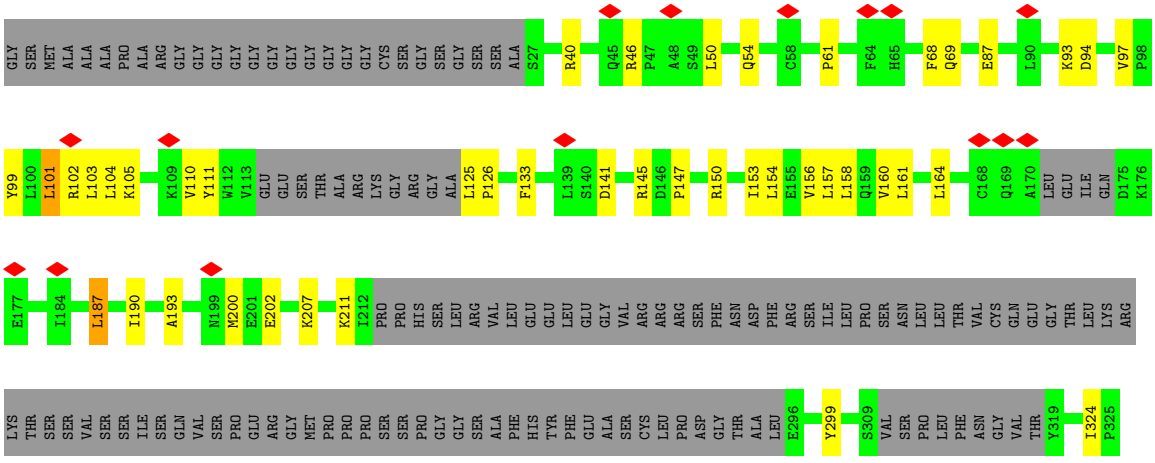
Chain A:

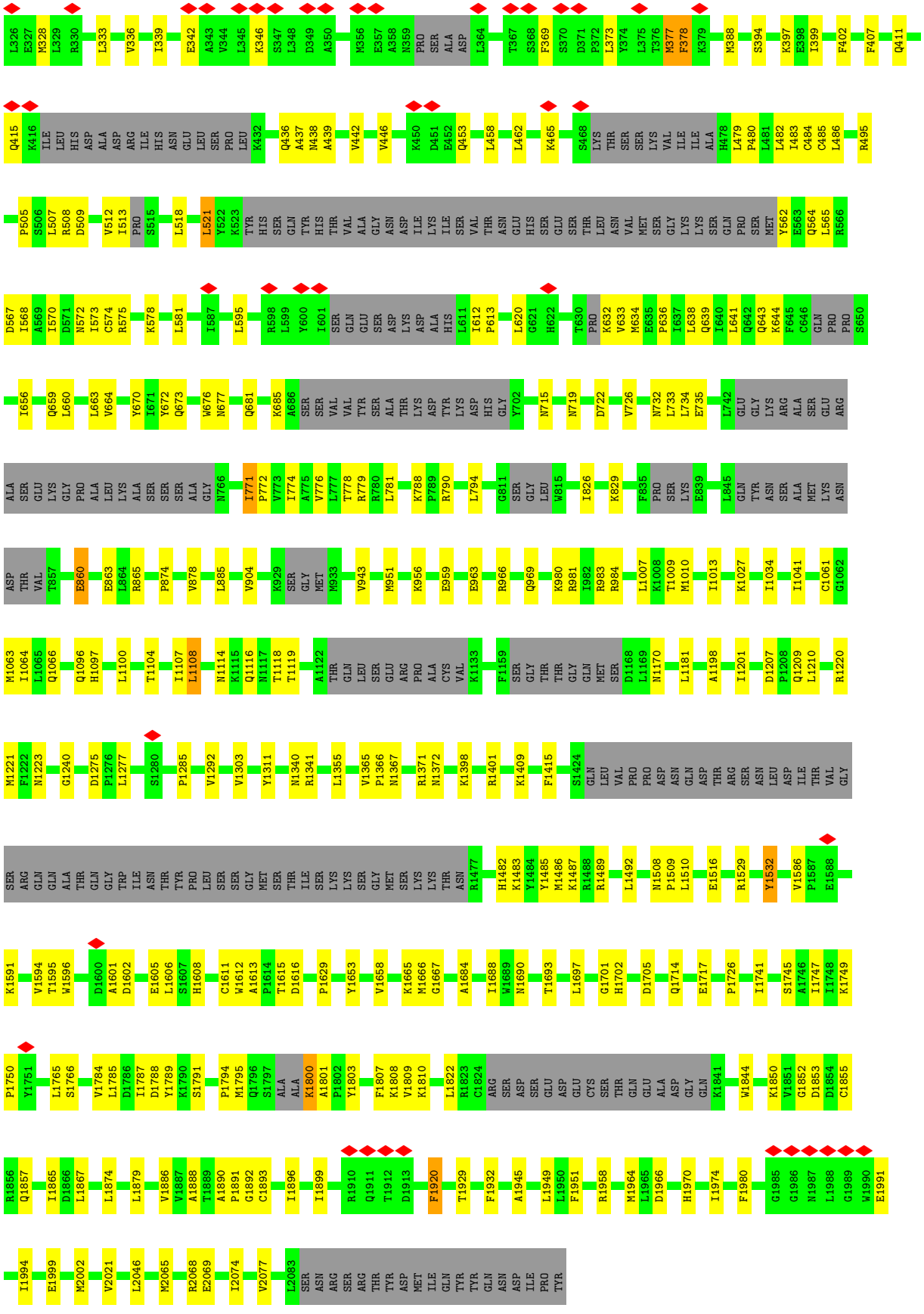




• Molecule 1: Phosphatidylinositol 4-kinase alpha

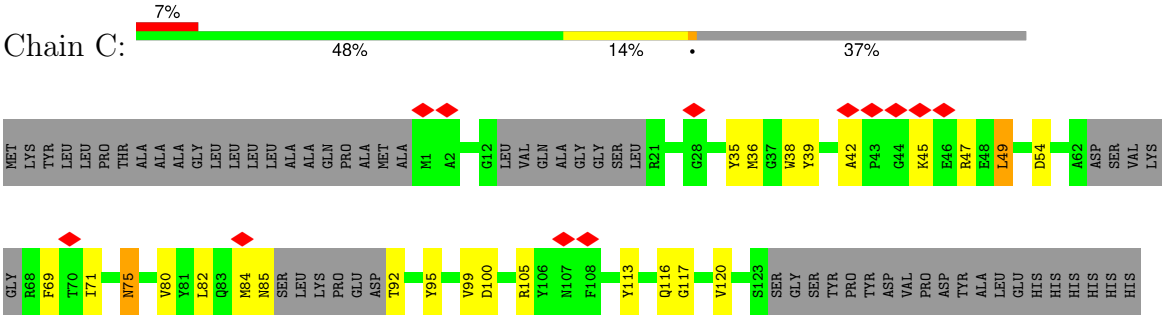
Chain B:




L326 E327 M328 L329 R330 L333 V336 I339 E342 A343 V344 L345 K346 S347 L348 D349 A350 M356 E357 A358 N359 PRO SER ALA ASP L364 T367 S368 F369 S370 D371 P372 L373 Y374 L375 T376 M377 F378 K379 M388 S394 K397 E398 I399 F402 F407 Q411
Q415 K416 ILE LEU HIS ASP ALA ASP ARG ILE HIS ASN GLU LEU SER PRO LEU K432 Q436 A437 N438 A439 V442 V446 K450 D451 E452 Q453 L458 L462 K465 S468 LYS THR SER SER LYS VAL ILE ILE ALA H478 L479 P480 L481 L482 I483 C484 C485 L486 R495
P505 S506 L507 R508 D509 V512 I513 PRO S515 L518 L521 Y522 K523 TYR HIS SER GLN TYR HIS THR VAL ALA GLY ASN ASP ILE LYS ILE SER VAL THR ASN GLU HIS SER GLU SER THR LEU ASN VAL MET SER GLY LYS LYS SER GLN PRO SER MET Y562 E563 Q564 L565 R566
D567 I568 A569 I570 D571 N572 I573 C574 R575 K578 L581 I587 L595 R598 L599 Y600 I601 SER GLN GLU SER ASP LYS ASP ALA HIS L611 I612 P613 L620 G621 H622 T630 PRO K632 V633 M634 E635 P636 I637 L638 Q639 I640 L641 Q642 Q643 K644 F645 C646 GLN PRO PRO S650
I656 Q659 L660 L663 V664 Y670 I671 Y672 Q673 W676 N677 Q681 K685 A686 SER SER VAL VAL TYR SER ALA THR LYS ASP TYR LYS ASP HIS GLY Y702 N715 N719 D722 V726 N732 L733 L734 E735 L742 GLU GLU LYS ARG ALA SER GLU ARG
ALA SER GLU LYS GLY PRO ALA LEU LYS ALA SER SER SER ALA GLY N766 I771 P772 V773 I774 A775 V776 L777 T778 R779 R780 L781 K788 P789 R790 L794 G811 SER GLY LEU W815 I826 K829 F835 PRO SER LYS E839 L845 GLN TYR ASN SER ALA MET LYS ASN
ASP THR VAL T857 E860 E863 L864 R865 P874 V878 L885 V904 K929 SER GLY MET M933 V943 M951 K956 E959 E963 R966 Q969 K980 R981 I982 R983 R984 L1007 K1008 T1009 M1010 I1013 K1027 I1034 I1041 C1061 G1062
M1063 I1064 L1065 Q1066 Q1096 H1097 L1100 T1104 I1107 L1108 N1114 K1115 Q1116 N1117 T1118 T1119 A1122 THR GLN LEU SER GLU ARG PRO ALA CYS VAL K1133 F1159 SER GLY THR THR GLY GLN MET SER D1168 L1169 N1170 L1181 A1198 I1201 D1207 P1208 Q1209 L1210 R1220
M1221 F1222 M1223 G1240 D1275 P1276 L1277 S1280 P1285 V1292 V1303 Y1311 N1340 R1341 L1355 L1365 V1365 P1366 N1367 R1371 N1372 K1398 R1401 K1409 F1415 S1424 GLN LEU VAL PRO PRO ASP ASN GLN ASP THR ARG SER ASN LEU ASP ILE THR VAL GLY
SER ARG GLN GLN ALA THR GLN GLY TRP ILE ASN THR TYR PRO LEU SER SER GLY MET SER THR ILE SER LYS LYS SER GLY MET SER LYS LYS THR ASN R1477 H1482 K1483 Y1484 Y1485 M1486 K1487 R1488 R1489 L1492 N1508 P1509 L1510 E1516 R1529 Y1532 V1586 P1587 E1588
K1591 V1594 T1595 W1596 D1600 A1601 D1602 E1605 L1606 S1607 H1608 C1611 W1612 A1613 P1614 T1615 D1616 P1629 Y1653 V1658 K1665 M1666 G1667 A1684 I1688 W1689 N1690 T1693 L1697 G1701 H1702 D1705 Q1714 E1717 P1726 I1741 S1745 A1746 I1747 I1748 K1749
P1750 Y1751 L1765 S1766 V1784 L1785 D1786 I1787 D1788 Y1789 K1790 S1791 P1794 M1795 Q1796 S1797 ALA ALA K1800 A1801 P1802 Y1803 F1807 K1808 V1809 K1810 L1822 R1823 C1824 ARG SER ASP SER GLU ASP GLU CYS SER THR GLN GLU ALA ASP GLY GLN K1841 W1844 K1850 V1851 G1852 D1853 D1854 C1855
R1856 Q1857 I1865 D1866 L1867 L1874 L1879 V1886 V1887 A1888 T1889 A1890 P1891 G1892 C1893 I1896 I1899 R1910 Q1911 T1912 D1913 F1920 T1929 F1932 A1945 L1949 L1950 F1951 R1958 M1964 L1965 D1966 H1970 I1974 F1980 G1985 G1986 N1987 L1988 G1989 W1990 E1991
I1994 E1999 M2002 V2021 L2046 M2065 R2068 E2069 I2074 V2077 L2083 SER ASN ARG SER ARG THR TYR ASP MET ILE GLN TYR TYR GLN ASN ASP ILE PRO TYR

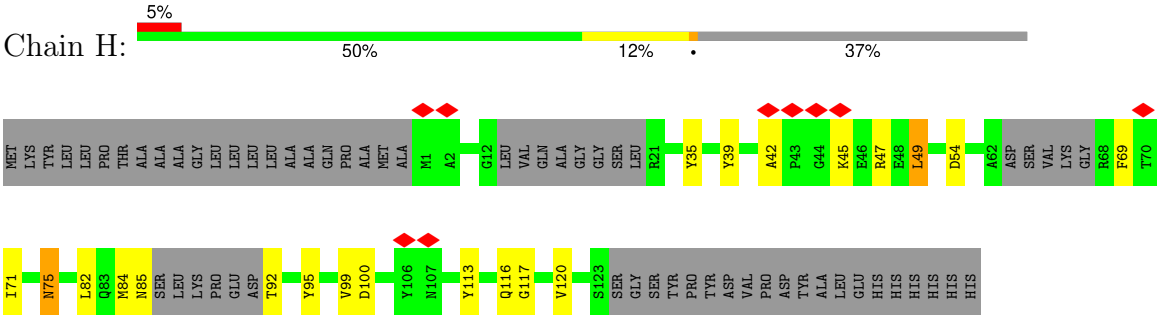
• Molecule 2: EFR3 interfering Nanobody (F3IN)

Chain C:



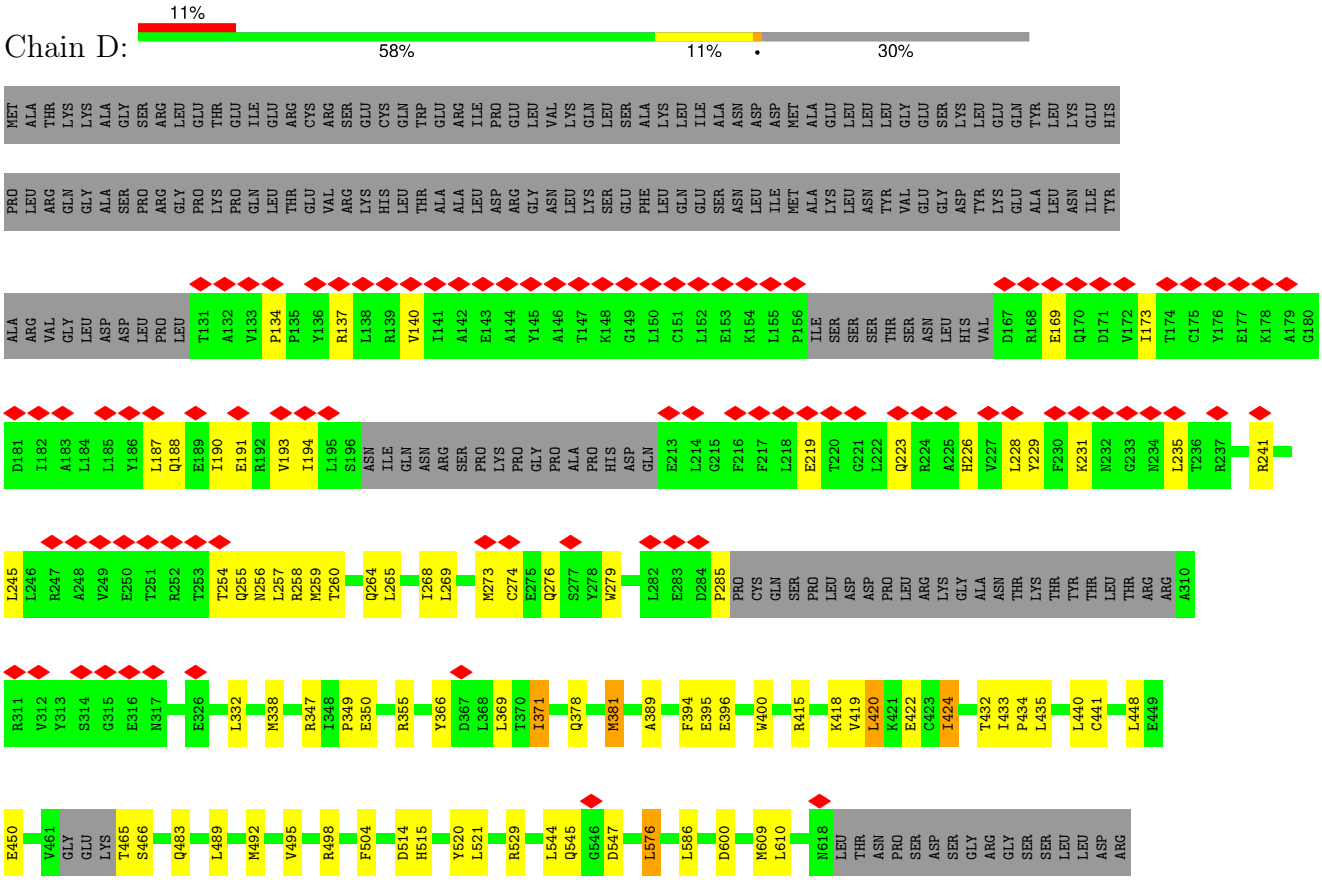
• Molecule 2: EFR3 interfering Nanobody (F3IN)

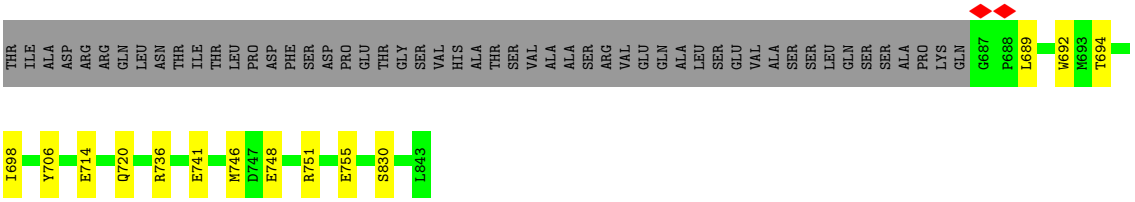
Chain H:



• Molecule 3: Tetratricopeptide repeat protein 7B

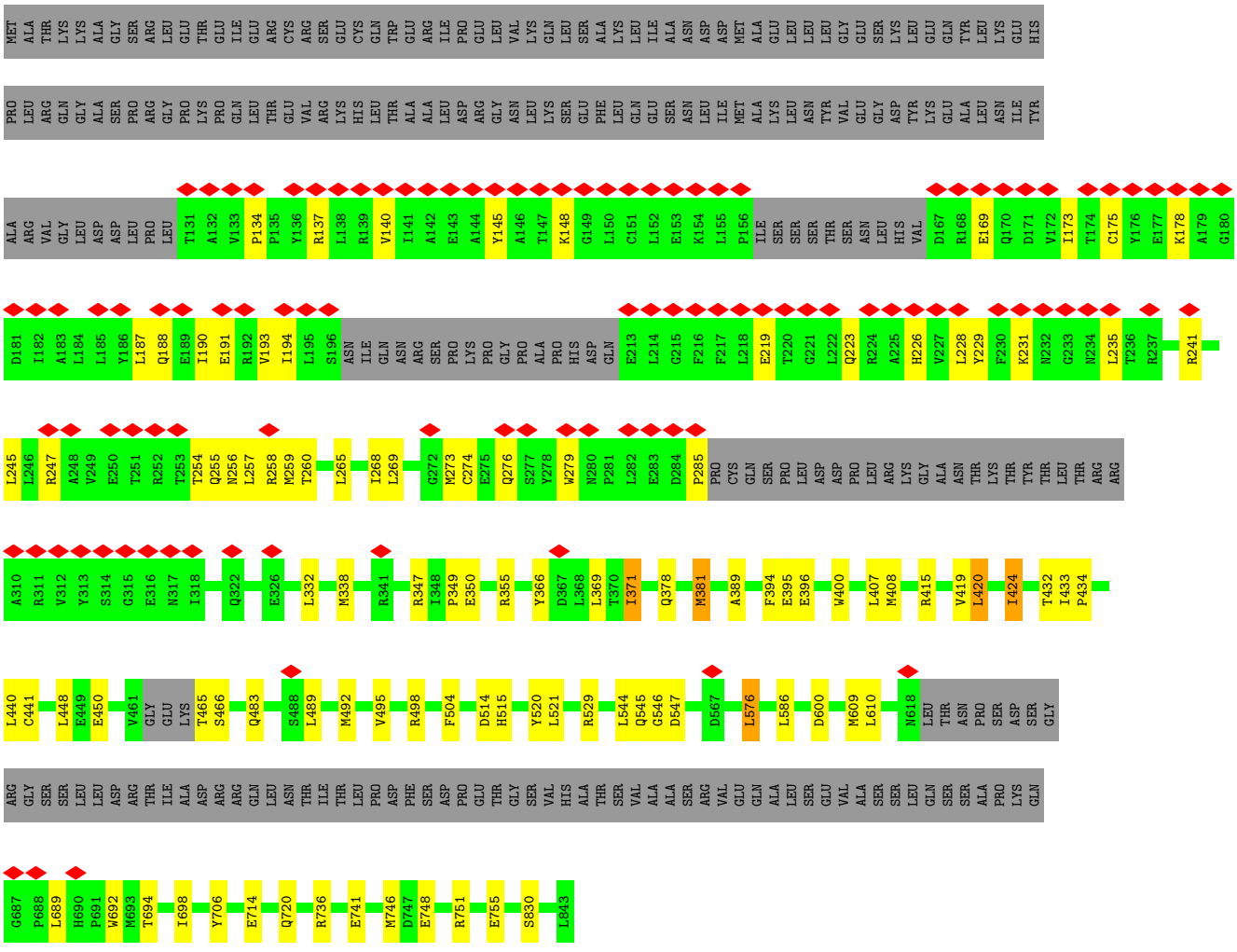
Chain D:





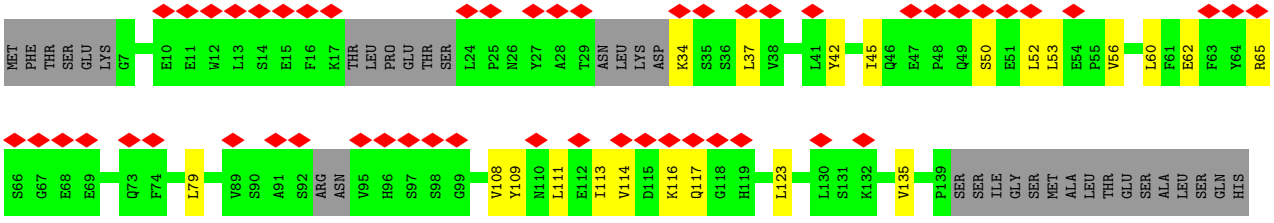
• Molecule 3: Tetratricopeptide repeat protein 7B

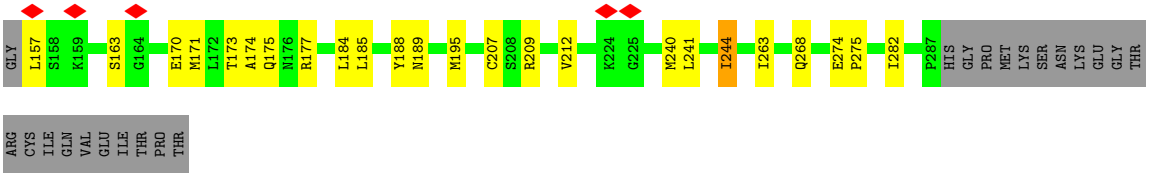
Chain F:



• Molecule 4: Hyccin

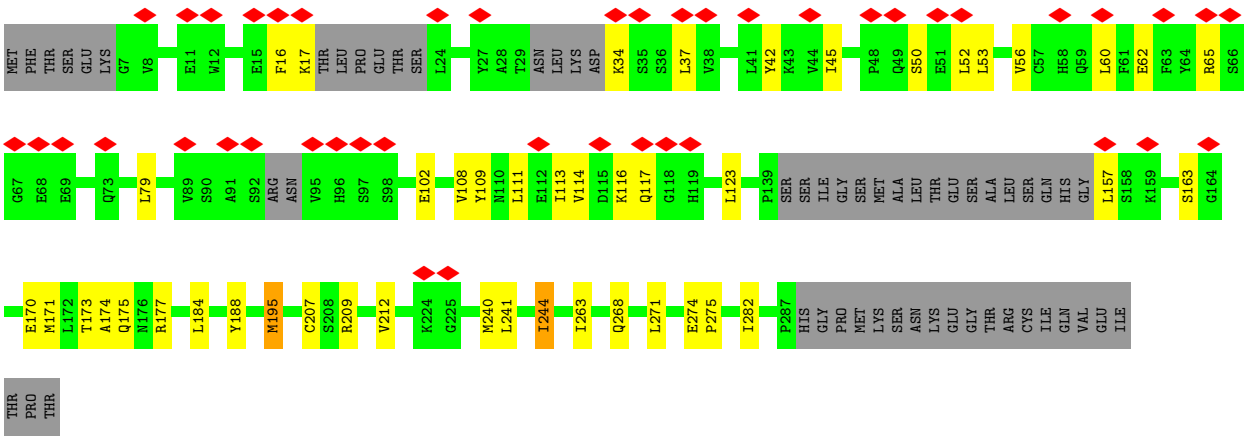
Chain E:





• Molecule 4: Hyccin

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	282982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0371	Depositor
Map size (Å)	431.19998, 431.19998, 431.19998	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.77, 0.77, 0.77	Depositor

5 Model quality

5.1 Standard geometry

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	0.10	0/14149	0.26	0/19141
1	B	0.10	0/14149	0.26	0/19141
2	C	0.11	0/826	0.33	0/1116
2	H	0.11	0/826	0.33	0/1116
3	D	0.09	0/4762	0.25	0/6443
3	F	0.09	0/4762	0.25	0/6443
4	E	0.10	0/2058	0.28	0/2793
4	G	0.10	0/2058	0.28	0/2793
All	All	0.10	0/43590	0.26	0/58986

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	13842	0	13974	193	0
1	B	13842	0	13974	197	0
2	C	811	0	771	20	0
2	H	811	0	771	15	0
3	D	4676	0	4734	66	0
3	F	4676	0	4734	68	0
4	E	2010	0	2017	27	0
4	G	2010	0	2017	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	42678	0	42992	598	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 7.

All (598) 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)
2:H:92:THR:HA	2:H:120:VAL:O	1.73	0.88
2:C:92:THR:HA	2:C:120:VAL:O	1.73	0.88
3:F:378:GLN:HB3	3:F:381:MET:HE1	1.56	0.88
3:D:378:GLN:HB3	3:D:381:MET:HE1	1.56	0.87
3:D:347:ARG:HG3	3:D:349:PRO:HD3	1.66	0.76
3:F:347:ARG:HG3	3:F:349:PRO:HD3	1.66	0.75
1:A:1666:MET:HE3	1:A:1667:GLY:H	1.53	0.74
1:B:1666:MET:HE3	1:B:1667:GLY:H	1.53	0.73
3:D:424:ILE:HD11	3:D:434:PRO:HD3	1.72	0.72
3:F:424:ILE:HD11	3:F:434:PRO:HD3	1.72	0.70
3:D:371:ILE:HG13	4:G:282:ILE:HD11	1.70	0.70
4:E:113:ILE:HG23	4:E:114:VAL:HG23	1.74	0.70
4:G:113:ILE:HG23	4:G:114:VAL:HG23	1.74	0.69
1:B:1201:ILE:HD11	1:B:1240:GLY:HA3	1.75	0.69
1:B:1865:ILE:HG12	1:B:1949:LEU:HD11	1.76	0.68
1:A:46:ARG:NH2	1:A:87:GLU:O	2.27	0.67
1:B:46:ARG:NH2	1:B:87:GLU:O	2.27	0.67
1:A:1201:ILE:HD11	1:A:1240:GLY:HA3	1.75	0.67
1:A:1865:ILE:HG12	1:A:1949:LEU:HD11	1.76	0.67
1:B:1596:TRP:HE1	1:B:1602:ASP:H	1.43	0.66
1:A:339:ILE:HD12	1:A:377:MET:HG3	1.78	0.65
1:B:980:LYS:HD2	1:B:983:ARG:HH21	1.62	0.65
4:E:135:VAL:O	3:F:247:ARG:NH2	2.29	0.65
1:A:1596:TRP:HE1	1:A:1602:ASP:H	1.43	0.65
1:B:1034:ILE:HD11	1:B:1041:ILE:HG12	1.79	0.65
3:F:274:CYS:SG	3:F:276:GLN:NE2	2.70	0.65
1:A:568:ILE:O	1:A:572:ASN:ND2	2.30	0.65
1:A:771:ILE:HG13	1:A:772:PRO:HD3	1.78	0.65
2:H:95:TYR:O	2:H:117:GLY:HA2	1.97	0.65
1:A:980:LYS:HD2	1:A:983:ARG:HH21	1.62	0.65
3:D:274:CYS:SG	3:D:276:GLN:NE2	2.70	0.65
1:B:339:ILE:HD12	1:B:377:MET:HG3	1.78	0.64
1:A:507:LEU:HD13	1:A:573:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:ILE:HD11	1:A:1041:ILE:HG12	1.79	0.64
1:A:1221:MET:O	1:A:1223:ASN:ND2	2.30	0.64
1:B:507:LEU:HD13	1:B:573:ILE:HG12	1.79	0.64
1:B:1221:MET:O	1:B:1223:ASN:ND2	2.30	0.64
2:C:95:TYR:O	2:C:117:GLY:HA2	1.97	0.64
1:B:771:ILE:HG13	1:B:772:PRO:HD3	1.79	0.63
1:B:568:ILE:O	1:B:572:ASN:ND2	2.30	0.63
1:B:378:PHE:HD2	1:B:437:ALA:HB1	1.63	0.63
1:A:378:PHE:HD2	1:A:437:ALA:HB1	1.64	0.63
1:A:735:GLU:OE2	1:A:790:ARG:NH2	2.30	0.63
4:E:79:LEU:HD21	4:E:188:TYR:HB2	1.81	0.62
1:A:673:GLN:O	1:A:677:ASN:ND2	2.28	0.62
3:D:259:MET:HG2	3:D:338:MET:HE1	1.82	0.62
2:C:42:ALA:H	2:C:45:LYS:HG2	1.65	0.62
3:F:259:MET:HG2	3:F:338:MET:HE1	1.82	0.62
1:B:1850:LYS:NZ	1:B:1855:CYS:SG	2.65	0.62
1:B:865:ARG:NH2	1:B:885:LEU:O	2.32	0.61
2:H:42:ALA:H	2:H:45:LYS:HG2	1.64	0.61
1:A:164:LEU:HD22	1:A:187:LEU:HD11	1.82	0.61
1:A:1207:ASP:OD1	1:A:1209:GLN:NE2	2.34	0.61
1:A:1114:ASN:OD1	1:B:1096:GLN:NE2	2.34	0.60
1:A:1890:ALA:HB3	1:A:1893:CYS:HB2	1.83	0.60
1:B:164:LEU:HD22	1:B:187:LEU:HD11	1.82	0.60
1:B:1749:LYS:HE2	1:B:1801:ALA:HB2	1.83	0.60
4:G:79:LEU:HD21	4:G:188:TYR:HB2	1.81	0.60
1:B:673:GLN:O	1:B:677:ASN:ND2	2.28	0.60
1:B:1207:ASP:OD1	1:B:1209:GLN:NE2	2.34	0.60
1:B:480:PRO:HA	1:B:483:ILE:HG12	1.83	0.60
1:B:1890:ALA:HB3	1:B:1893:CYS:HB2	1.83	0.60
1:A:1749:LYS:HE2	1:A:1801:ALA:HB2	1.83	0.60
1:A:865:ARG:NH2	1:A:885:LEU:O	2.32	0.59
1:A:1277:LEU:HD23	1:A:1867:LEU:HD11	1.84	0.59
1:B:1665:LYS:O	3:D:347:ARG:NH1	2.26	0.59
4:E:62:GLU:O	4:E:65:ARG:NE	2.34	0.59
3:D:576:LEU:HD21	3:D:586:LEU:HD12	1.85	0.58
1:A:480:PRO:HA	1:A:483:ILE:HG12	1.83	0.58
1:A:634:MET:SD	1:A:634:MET:N	2.76	0.58
1:A:595:LEU:HD13	1:A:620:LEU:HD21	1.84	0.58
1:B:634:MET:SD	1:B:634:MET:N	2.76	0.58
1:A:512:VAL:HG23	1:A:513:ILE:HG13	1.85	0.58
1:A:788:LYS:HG3	1:A:790:ARG:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:LEU:HD13	1:B:620:LEU:HD21	1.84	0.58
1:A:1850:LYS:NZ	1:A:1855:CYS:SG	2.65	0.58
3:F:257:LEU:O	3:F:260:THR:OG1	2.18	0.58
3:F:586:LEU:HB3	3:F:609:MET:HE2	1.86	0.58
3:D:545:GLN:HE21	3:D:547:ASP:HB2	1.68	0.58
1:A:572:ASN:OD1	1:A:575:ARG:NH2	2.37	0.58
3:F:576:LEU:HD21	3:F:586:LEU:HD12	1.84	0.58
4:G:62:GLU:O	4:G:65:ARG:NE	2.34	0.58
1:A:1852:GLY:N	1:A:1892:GLY:O	2.37	0.58
1:B:788:LYS:HG3	1:B:790:ARG:H	1.67	0.58
1:B:1277:LEU:HD23	1:B:1867:LEU:HD11	1.84	0.58
1:A:446:VAL:HG12	1:A:458:LEU:HD11	1.86	0.57
1:B:512:VAL:HG23	1:B:513:ILE:HG13	1.85	0.57
3:F:545:GLN:HE21	3:F:547:ASP:HB2	1.68	0.57
1:B:735:GLU:OE2	1:B:790:ARG:NH2	2.30	0.57
1:B:1372:ASN:OD1	1:B:1485:TYR:OH	2.22	0.57
1:B:1852:GLY:N	1:B:1892:GLY:O	2.37	0.57
3:D:586:LEU:HB3	3:D:609:MET:HE2	1.85	0.57
2:H:39:TYR:CZ	2:H:49:LEU:HD13	2.40	0.57
1:B:446:VAL:HG12	1:B:458:LEU:HD11	1.87	0.57
1:A:1372:ASN:OD1	1:A:1485:TYR:OH	2.22	0.57
1:B:1303:VAL:HG22	1:B:1355:LEU:HD13	1.87	0.57
2:C:39:TYR:CZ	2:C:49:LEU:HD13	2.40	0.57
3:D:515:HIS:HB3	3:D:544:LEU:HD22	1.85	0.57
1:B:1483:LYS:HG2	1:B:1487:LYS:HE2	1.87	0.57
1:B:1596:TRP:NE1	1:B:1602:ASP:O	2.38	0.57
1:A:154:LEU:O	1:A:157:LEU:HB2	2.05	0.57
1:A:981:ARG:HG2	1:A:984:ARG:HH21	1.70	0.57
1:B:572:ASN:OD1	1:B:575:ARG:NH2	2.37	0.57
1:A:1483:LYS:HG2	1:A:1487:LYS:HE2	1.87	0.56
1:A:1303:VAL:HG22	1:A:1355:LEU:HD13	1.87	0.56
1:A:1787:ILE:HG22	1:A:1807:PHE:HD2	1.70	0.56
1:B:154:LEU:O	1:B:157:LEU:HB2	2.05	0.56
1:B:1787:ILE:HG22	1:B:1807:PHE:HD2	1.70	0.56
3:F:235:LEU:HD11	3:F:268:ILE:HD11	1.87	0.56
3:F:515:HIS:HB3	3:F:544:LEU:HD22	1.85	0.56
4:G:116:LYS:HG3	4:G:117:GLN:H	1.70	0.56
1:B:1726:PRO:HB2	1:B:1822:LEU:HD12	1.87	0.56
3:D:235:LEU:HD11	3:D:268:ILE:HD11	1.86	0.56
3:D:741:GLU:HG2	3:D:746:MET:HE1	1.88	0.56
3:F:741:GLU:HG2	3:F:746:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1285:PRO:HB2	1:A:1874:LEU:HD13	1.88	0.56
1:B:981:ARG:HG2	1:B:984:ARG:HH21	1.70	0.56
1:B:369:PHE:O	1:B:373:LEU:HB2	2.06	0.56
1:B:963:GLU:OE1	1:B:966:ARG:NH1	2.30	0.56
1:A:1596:TRP:NE1	1:A:1602:ASP:O	2.38	0.56
1:B:521:LEU:HD21	1:B:562:TYR:HA	1.87	0.56
1:B:1285:PRO:HB2	1:B:1874:LEU:HD13	1.88	0.56
1:A:521:LEU:HD21	1:A:562:TYR:HA	1.87	0.56
1:B:565:LEU:HD23	1:B:565:LEU:H	1.71	0.56
4:E:116:LYS:HG3	4:E:117:GLN:H	1.70	0.55
1:B:1784:VAL:HA	1:B:1809:VAL:HG23	1.89	0.55
1:A:369:PHE:O	1:A:373:LEU:HB2	2.05	0.55
4:E:50:SER:HB2	4:E:53:LEU:HG	1.88	0.55
3:F:720:GLN:HG2	3:F:736:ARG:HH22	1.72	0.55
1:A:1784:VAL:HA	1:A:1809:VAL:HG23	1.89	0.55
1:A:565:LEU:HD23	1:A:565:LEU:H	1.71	0.55
1:B:505:PRO:HA	1:B:508:ARG:HG2	1.89	0.55
1:B:1586:VAL:HG12	1:B:1612:TRP:HE3	1.72	0.55
4:G:50:SER:HB2	4:G:53:LEU:HG	1.88	0.55
1:B:2065:MET:HE2	1:B:2069:GLU:HB3	1.89	0.54
1:B:161:LEU:HD13	1:B:164:LEU:HD12	1.89	0.54
1:A:161:LEU:HD13	1:A:164:LEU:HD12	1.89	0.54
1:A:1726:PRO:HB2	1:A:1822:LEU:HD12	1.87	0.54
1:A:505:PRO:HA	1:A:508:ARG:HG2	1.89	0.54
1:A:1586:VAL:HG12	1:A:1612:TRP:HE3	1.72	0.54
1:A:1794:PRO:HA	1:A:1803:TYR:HA	1.89	0.54
1:A:2065:MET:HE2	1:A:2069:GLU:HB3	1.89	0.54
1:A:436:GLN:N	1:A:436:GLN:OE1	2.40	0.54
1:A:101:LEU:HD13	1:A:104:LEU:HD21	1.90	0.54
1:A:1608:HIS:O	1:A:1608:HIS:ND1	2.41	0.54
1:B:101:LEU:HD13	1:B:104:LEU:HD21	1.90	0.54
3:D:720:GLN:HG2	3:D:736:ARG:HH22	1.72	0.54
3:F:169:GLU:O	3:F:173:ILE:HG12	2.08	0.54
1:B:639:GLN:O	1:B:643:GLN:NE2	2.41	0.53
1:B:1794:PRO:HA	1:B:1803:TYR:HA	1.89	0.53
1:B:1899:ILE:HD11	1:B:1964:MET:HG2	1.89	0.53
1:A:438:ASN:O	1:A:442:VAL:HG23	2.09	0.53
1:B:388:MET:SD	1:B:388:MET:N	2.80	0.53
1:B:438:ASN:O	1:B:442:VAL:HG23	2.09	0.53
1:B:1529:ARG:HA	1:B:1532:TYR:HD1	1.73	0.53
3:D:257:LEU:O	3:D:260:THR:OG1	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLN:O	1:A:643:GLN:NE2	2.41	0.53
3:D:256:ASN:HA	3:D:259:MET:HE3	1.91	0.53
1:B:1608:HIS:O	1:B:1608:HIS:ND1	2.41	0.53
1:A:715:ASN:O	1:A:719:ASN:ND2	2.38	0.53
1:A:963:GLU:OE1	1:A:966:ARG:NH1	2.30	0.53
1:A:1899:ILE:HD11	1:A:1964:MET:HG2	1.89	0.53
3:F:256:ASN:HA	3:F:259:MET:HE3	1.91	0.53
1:A:388:MET:SD	1:A:388:MET:N	2.80	0.53
1:B:612:ILE:N	1:B:613:PRO:HD2	2.24	0.53
1:A:1529:ARG:HA	1:A:1532:TYR:HD1	1.73	0.52
1:B:1951:PHE:HB2	1:B:1994:ILE:HD11	1.92	0.52
1:B:202:GLU:OE2	1:B:207:LYS:NZ	2.32	0.52
1:B:1401:ARG:NH2	1:B:1516:GLU:O	2.43	0.52
3:D:169:GLU:O	3:D:173:ILE:HG12	2.08	0.52
3:F:600:ASP:OD1	3:F:600:ASP:N	2.41	0.52
2:H:95:TYR:O	2:H:117:GLY:CA	2.57	0.52
1:A:612:ILE:N	1:A:613:PRO:HD2	2.24	0.52
1:A:1401:ARG:NH2	1:A:1516:GLU:O	2.43	0.52
1:B:68:PHE:HB2	1:B:110:VAL:HG22	1.91	0.52
1:B:1929:THR:HG23	1:B:1932:PHE:H	1.75	0.52
1:B:715:ASN:O	1:B:719:ASN:ND2	2.38	0.52
3:D:273:MET:SD	3:D:273:MET:N	2.83	0.52
2:C:95:TYR:O	2:C:117:GLY:CA	2.57	0.52
3:D:255:GLN:O	3:D:258:ARG:HB2	2.10	0.52
3:D:751:ARG:NH1	3:D:755:GLU:OE2	2.43	0.52
1:A:1951:PHE:HB2	1:A:1994:ILE:HD11	1.92	0.51
1:A:1701:GLY:O	1:A:1702:HIS:ND1	2.44	0.51
3:F:273:MET:SD	3:F:273:MET:N	2.83	0.51
1:B:436:GLN:OE1	1:B:436:GLN:N	2.40	0.51
1:A:160:VAL:O	1:A:164:LEU:HG	2.11	0.51
4:E:268:GLN:NE2	3:F:432:THR:OG1	2.36	0.51
1:A:68:PHE:HB2	1:A:110:VAL:HG22	1.91	0.51
1:A:1136:TYR:HB2	1:B:1104:THR:HG21	1.93	0.51
1:B:61:PRO:O	1:B:99:TYR:OH	2.25	0.51
1:B:160:VAL:O	1:B:164:LEU:HG	2.11	0.51
1:B:1701:GLY:O	1:B:1702:HIS:ND1	2.44	0.51
3:D:366:TYR:CZ	3:D:389:ALA:HB2	2.46	0.51
3:F:366:TYR:CZ	3:F:389:ALA:HB2	2.46	0.51
3:F:751:ARG:NH1	3:F:755:GLU:OE2	2.43	0.51
1:A:1170:ASN:HD22	1:A:1210:LEU:HD11	1.75	0.51
1:A:1929:THR:HG23	1:A:1932:PHE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:255:GLN:O	3:F:258:ARG:HB2	2.11	0.51
1:B:1785:LEU:HD11	1:B:1810:LYS:HB2	1.93	0.51
3:D:492:MET:SD	3:D:492:MET:N	2.84	0.51
2:H:69:PHE:CD1	2:H:84:MET:HG2	2.46	0.51
1:A:1785:LEU:HD11	1:A:1810:LYS:HB2	1.93	0.51
1:B:1170:ASN:HD22	1:B:1210:LEU:HD11	1.75	0.50
1:A:672:TYR:OH	1:A:732:ASN:OD1	2.28	0.50
1:A:781:LEU:O	1:A:829:LYS:NZ	2.37	0.50
1:B:1509:PRO:O	1:B:2068:ARG:NH1	2.44	0.50
1:B:1063:MET:O	1:B:1066:GLN:HG3	2.11	0.50
1:B:1367:ASN:O	1:B:1371:ARG:NH1	2.44	0.50
1:B:904:VAL:HG11	1:B:943:VAL:HG23	1.93	0.50
1:B:1482:HIS:O	1:B:1486:MET:HG2	2.12	0.50
3:D:432:THR:OG1	4:G:268:GLN:NE2	2.34	0.50
2:H:71:ILE:HG22	2:H:82:LEU:HG	1.93	0.50
4:E:282:ILE:HD11	3:F:371:ILE:HG13	1.94	0.50
1:A:904:VAL:HG11	1:A:943:VAL:HG23	1.93	0.50
1:A:1850:LYS:HZ3	1:A:1853:ASP:HB3	1.77	0.50
1:A:1063:MET:O	1:A:1066:GLN:HG3	2.11	0.49
2:C:105:ARG:NH2	3:F:546:GLY:H	2.10	0.49
1:A:1665:LYS:O	3:F:347:ARG:NH1	2.33	0.49
1:B:781:LEU:O	1:B:829:LYS:NZ	2.37	0.49
2:C:69:PHE:CD1	2:C:84:MET:HG2	2.46	0.49
3:D:187:LEU:HA	3:D:190:ILE:HG12	1.95	0.49
1:A:1367:ASN:O	1:A:1371:ARG:NH1	2.44	0.49
1:B:956:LYS:NZ	1:B:1311:TYR:O	2.46	0.49
3:F:254:THR:O	3:F:257:LEU:HG	2.13	0.49
2:C:71:ILE:HG22	2:C:82:LEU:HG	1.93	0.49
1:A:1509:PRO:O	1:A:2068:ARG:NH1	2.44	0.49
3:D:254:THR:O	3:D:257:LEU:HG	2.13	0.49
4:E:135:VAL:HG22	3:F:247:ARG:NH2	2.27	0.49
1:A:1482:HIS:O	1:A:1486:MET:HG2	2.12	0.49
1:B:672:TYR:OH	1:B:732:ASN:OD1	2.28	0.49
1:A:202:GLU:OE2	1:A:207:LYS:NZ	2.32	0.49
1:B:153:ILE:O	1:B:156:VAL:HG22	2.12	0.48
1:A:153:ILE:O	1:A:156:VAL:HG22	2.12	0.48
1:A:377:MET:SD	1:A:377:MET:N	2.85	0.48
2:H:39:TYR:CE1	2:H:49:LEU:HD13	2.48	0.48
1:A:518:LEU:HD12	1:A:521:LEU:HD22	1.95	0.48
1:A:1596:TRP:HE1	1:A:1602:ASP:N	2.11	0.48
4:E:241:LEU:HA	4:E:244:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HD11	1:A:328:MET:HB2	1.96	0.48
1:B:479:LEU:HD12	1:B:479:LEU:H	1.78	0.48
1:B:1415:PHE:O	1:B:1489:ARG:NH2	2.43	0.48
2:C:39:TYR:CE1	2:C:49:LEU:HD13	2.48	0.48
3:F:504:PHE:CE2	3:F:520:TYR:HB3	2.48	0.48
3:D:495:VAL:HG22	3:D:498:ARG:HH21	1.78	0.48
4:E:56:VAL:O	4:E:60:LEU:HG	2.13	0.48
3:F:495:VAL:HG22	3:F:498:ARG:HH21	1.78	0.48
2:H:75:ASN:OD1	2:H:75:ASN:N	2.47	0.48
1:A:1096:GLN:NE2	1:B:1114:ASN:OD1	2.47	0.48
1:A:956:LYS:NZ	1:A:1311:TYR:O	2.46	0.48
1:B:377:MET:SD	1:B:377:MET:N	2.85	0.48
3:F:492:MET:SD	3:F:492:MET:N	2.84	0.48
1:A:483:ILE:HG13	1:A:484:CYS:N	2.29	0.48
1:B:483:ILE:HG13	1:B:484:CYS:N	2.29	0.48
3:D:529:ARG:NH1	3:D:830:SER:O	2.47	0.48
3:F:187:LEU:HA	3:F:190:ILE:HG12	1.94	0.48
1:A:394:SER:HA	1:A:397:LYS:HZ2	1.78	0.47
1:A:479:LEU:HD12	1:A:479:LEU:H	1.78	0.47
1:B:1601:ALA:HB2	1:B:1629:PRO:HG2	1.96	0.47
3:D:600:ASP:OD1	3:D:600:ASP:N	2.41	0.47
1:B:1658:VAL:HG21	1:B:1690:ASN:ND2	2.29	0.47
3:D:504:PHE:CE2	3:D:520:TYR:HB3	2.48	0.47
3:F:529:ARG:NH1	3:F:830:SER:O	2.47	0.47
4:G:56:VAL:O	4:G:60:LEU:HG	2.13	0.47
1:A:1658:VAL:HG21	1:A:1690:ASN:ND2	2.30	0.47
4:G:123:LEU:HD12	4:G:163:SER:HB3	1.97	0.47
1:A:638:LEU:HD21	1:A:670:TYR:HE2	1.79	0.47
1:B:93:LYS:HE2	1:B:97:VAL:HG21	1.97	0.47
1:B:638:LEU:HD21	1:B:670:TYR:HE2	1.79	0.47
3:F:420:LEU:HD13	3:F:433:ILE:HG23	1.96	0.47
1:A:399:ILE:HA	1:A:402:PHE:CD2	2.50	0.47
1:B:1596:TRP:HE1	1:B:1602:ASP:N	2.11	0.47
3:D:256:ASN:OD1	3:D:257:LEU:N	2.47	0.47
1:A:1857:GLN:HG3	1:A:2046:LEU:HD13	1.97	0.47
1:B:324:ILE:HD11	1:B:328:MET:HB2	1.96	0.47
1:B:518:LEU:HD12	1:B:521:LEU:HD22	1.95	0.47
1:B:1966:ASP:OD1	1:B:1970:HIS:N	2.47	0.47
3:D:279:TRP:CE2	3:D:285:PRO:HG3	2.50	0.47
3:F:332:LEU:HD13	3:F:369:LEU:HA	1.97	0.47
1:A:93:LYS:HE2	1:A:97:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1601:ALA:HB2	1:A:1629:PRO:HG2	1.96	0.47
1:B:1107:ILE:HG23	1:B:1108:LEU:HG	1.97	0.47
1:B:1958:ARG:NH1	1:B:1974:ILE:O	2.39	0.47
3:D:420:LEU:HD13	3:D:433:ILE:HG23	1.96	0.47
4:E:116:LYS:HG3	4:E:117:GLN:N	2.30	0.47
1:B:1857:GLN:HG3	1:B:2046:LEU:HD13	1.97	0.47
3:F:689:LEU:HA	3:F:692:TRP:HD1	1.80	0.47
1:A:1107:ILE:HG23	1:A:1108:LEU:HG	1.97	0.47
1:A:1966:ASP:OD1	1:A:1970:HIS:N	2.47	0.47
2:C:47:ARG:HA	2:C:47:ARG:HH11	1.80	0.47
3:D:190:ILE:HA	3:D:193:VAL:HG22	1.97	0.47
2:H:47:ARG:HA	2:H:47:ARG:HH11	1.80	0.47
2:H:99:VAL:HB	2:H:113:TYR:HB2	1.97	0.46
1:A:1415:PHE:O	1:A:1489:ARG:NH2	2.43	0.46
1:B:399:ILE:HA	1:B:402:PHE:CD2	2.50	0.46
4:G:116:LYS:HG3	4:G:117:GLN:N	2.30	0.46
4:G:171:MET:HE2	4:G:171:MET:HB2	1.84	0.46
1:A:1596:TRP:HZ2	1:A:1601:ALA:HA	1.81	0.46
3:D:226:HIS:HA	3:D:229:TYR:CD2	2.50	0.46
4:G:241:LEU:HA	4:G:244:ILE:HG22	1.95	0.46
2:H:84:MET:SD	2:H:85:ASN:N	2.88	0.46
2:C:75:ASN:OD1	2:C:75:ASN:N	2.47	0.46
2:C:84:MET:SD	2:C:85:ASN:N	2.88	0.46
3:D:332:LEU:HD13	3:D:369:LEU:HA	1.97	0.46
1:A:154:LEU:HA	1:A:157:LEU:HD12	1.98	0.46
1:A:659:GLN:O	1:A:663:LEU:HG	2.16	0.46
1:A:1027:LYS:HB3	1:A:1027:LYS:HE3	1.78	0.46
1:A:1795:MET:SD	1:A:1795:MET:N	2.87	0.46
1:B:411:GLN:O	1:B:415:GLN:NE2	2.39	0.46
3:D:748:GLU:H	3:D:748:GLU:CD	2.23	0.46
3:F:256:ASN:OD1	3:F:257:LEU:N	2.47	0.46
3:F:279:TRP:CE2	3:F:285:PRO:HG3	2.50	0.46
1:B:133:PHE:CE2	1:B:193:ALA:HB2	2.51	0.46
3:F:226:HIS:HA	3:F:229:TYR:CD2	2.51	0.46
1:A:1010:MET:HE3	1:A:1010:MET:HB2	1.71	0.46
1:B:187:LEU:HD12	1:B:190:ILE:HD11	1.98	0.46
1:B:1795:MET:SD	1:B:1795:MET:N	2.87	0.46
3:D:689:LEU:HA	3:D:692:TRP:HD1	1.80	0.46
4:E:123:LEU:HD12	4:E:163:SER:HB3	1.97	0.46
1:B:659:GLN:O	1:B:663:LEU:HG	2.16	0.45
2:C:99:VAL:HB	2:C:113:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD12	1:A:190:ILE:HD11	1.98	0.45
1:A:1615:THR:OG1	1:A:1616:ASP:N	2.49	0.45
1:A:1999:GLU:O	1:A:2002:MET:HG3	2.17	0.45
1:A:681:GLN:O	1:A:685:LYS:HG2	2.16	0.45
1:B:333:LEU:HA	1:B:336:VAL:HG22	1.99	0.45
3:F:190:ILE:HA	3:F:193:VAL:HG22	1.97	0.45
3:F:338:MET:HE3	3:F:338:MET:HB3	1.68	0.45
2:H:116:GLN:OE1	2:H:116:GLN:N	2.46	0.45
1:A:1508:ASN:ND2	1:A:1510:LEU:O	2.48	0.45
1:B:154:LEU:HA	1:B:157:LEU:HD12	1.98	0.45
1:B:1275:ASP:N	1:B:1275:ASP:OD1	2.48	0.45
1:B:1850:LYS:HZ3	1:B:1853:ASP:HB3	1.82	0.45
1:B:1999:GLU:O	1:B:2002:MET:HG3	2.16	0.45
2:C:116:GLN:OE1	2:C:116:GLN:N	2.46	0.45
1:A:567:ASP:HA	1:A:570:ILE:HG12	1.98	0.45
3:D:714:GLU:OE1	3:D:714:GLU:N	2.44	0.45
4:E:42:TYR:HA	4:E:45:ILE:HG22	1.99	0.45
3:F:514:ASP:OD1	3:F:514:ASP:N	2.50	0.45
4:G:42:TYR:HA	4:G:45:ILE:HG22	1.99	0.45
1:A:342:GLU:O	1:A:346:LYS:HG2	2.17	0.45
1:B:508:ARG:HG3	1:B:509:ASP:N	2.32	0.45
1:B:1714:GLN:O	1:B:1717:GLU:HG2	2.17	0.45
4:G:207:CYS:HB3	4:G:240:MET:HE3	1.99	0.45
1:A:133:PHE:CE2	1:A:193:ALA:HB2	2.51	0.45
1:B:969:GLN:NE2	1:B:1009:THR:OG1	2.50	0.45
1:B:1596:TRP:HZ2	1:B:1601:ALA:HA	1.81	0.45
4:G:102:GLU:OE1	4:G:102:GLU:N	2.44	0.45
1:A:1693:THR:HG23	1:A:1891:PRO:HA	1.99	0.45
1:B:681:GLN:O	1:B:685:LYS:HG2	2.17	0.45
2:C:39:TYR:OH	2:C:100:ASP:OD2	2.33	0.45
1:A:333:LEU:HA	1:A:336:VAL:HG22	1.99	0.44
1:A:1591:LYS:HA	1:A:1594:VAL:HG12	1.99	0.44
1:B:1277:LEU:O	1:B:1653:TYR:OH	2.33	0.44
4:E:171:MET:HE2	4:E:171:MET:HB2	1.84	0.44
4:E:174:ALA:HA	4:E:177:ARG:HD2	2.00	0.44
4:E:185:LEU:O	4:E:189:ASN:ND2	2.30	0.44
3:F:714:GLU:OE1	3:F:714:GLU:N	2.44	0.44
3:D:448:LEU:HD13	3:D:483:GLN:HG2	1.99	0.44
3:F:441:CYS:SG	3:F:450:GLU:HB2	2.57	0.44
4:G:109:TYR:HB2	4:G:184:LEU:HD21	2.00	0.44
1:A:660:LEU:O	1:A:664:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LEU:HA	1:B:465:LYS:HG2	2.00	0.44
1:B:660:LEU:O	1:B:664:VAL:HG23	2.17	0.44
4:E:109:TYR:HB2	4:E:184:LEU:HD21	2.00	0.44
1:A:1114:ASN:ND2	1:A:1116:GLN:H	2.14	0.44
3:F:145:TYR:HA	3:F:148:LYS:HZ3	1.82	0.44
4:G:174:ALA:HA	4:G:177:ARG:HD2	2.00	0.44
1:A:462:LEU:HA	1:A:465:LYS:HG2	2.00	0.44
1:B:93:LYS:HG2	1:B:97:VAL:HG21	2.00	0.44
1:B:342:GLU:O	1:B:346:LYS:HG2	2.17	0.44
1:B:394:SER:HA	1:B:397:LYS:HZ2	1.82	0.44
1:B:1114:ASN:ND2	1:B:1116:GLN:H	2.14	0.44
1:A:508:ARG:HG3	1:A:509:ASP:N	2.32	0.44
3:D:441:CYS:SG	3:D:450:GLU:HB2	2.57	0.44
3:D:504:PHE:HE2	3:D:520:TYR:HB3	1.83	0.44
4:E:207:CYS:HB3	4:E:240:MET:HE3	1.99	0.44
4:E:240:MET:HE2	4:E:263:ILE:HD11	2.00	0.44
4:G:195:MET:HE2	4:G:195:MET:HB2	1.91	0.44
1:A:632:LYS:HG3	1:A:633:VAL:HG23	2.00	0.44
1:A:1007:LEU:HA	1:A:1010:MET:HG2	2.00	0.44
1:B:1508:ASN:ND2	1:B:1510:LEU:O	2.48	0.44
1:B:1787:ILE:HG22	1:B:1807:PHE:CD2	2.51	0.44
1:B:567:ASP:HA	1:B:570:ILE:HG12	1.98	0.44
1:B:633:VAL:C	1:B:636:PRO:HD2	2.43	0.44
1:B:1010:MET:SD	1:B:1064:ILE:HD11	2.58	0.44
1:B:1693:THR:HG23	1:B:1891:PRO:HA	1.99	0.44
4:E:170:GLU:HG2	4:E:171:MET:SD	2.58	0.44
3:F:748:GLU:H	3:F:748:GLU:CD	2.23	0.44
4:G:240:MET:HE2	4:G:263:ILE:HD11	2.00	0.44
1:A:93:LYS:HG2	1:A:97:VAL:HG21	2.00	0.44
1:A:1714:GLN:O	1:A:1717:GLU:HG2	2.17	0.44
1:B:1529:ARG:HA	1:B:1532:TYR:CD1	2.52	0.44
1:A:141:ASP:O	1:A:145:ARG:HG2	2.19	0.43
1:B:860:GLU:O	1:B:863:GLU:HG3	2.18	0.43
1:B:1027:LYS:HB3	1:B:1027:LYS:HE3	1.78	0.43
1:B:1684:ALA:O	1:B:1688:ILE:HG22	2.18	0.43
4:E:209:ARG:HA	4:E:212:VAL:HG12	2.00	0.43
1:A:969:GLN:NE2	1:A:1009:THR:OG1	2.50	0.43
1:A:1787:ILE:HG22	1:A:1807:PHE:CD2	2.51	0.43
1:B:495:ARG:O	1:B:495:ARG:NE	2.51	0.43
1:B:632:LYS:HG3	1:B:633:VAL:HG23	2.00	0.43
1:B:1118:THR:HG23	1:B:1119:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1591:LYS:HA	1:B:1594:VAL:HG12	1.99	0.43
1:B:1596:TRP:CZ2	1:B:1601:ALA:HA	2.53	0.43
1:B:1615:THR:OG1	1:B:1616:ASP:N	2.49	0.43
1:A:633:VAL:C	1:A:636:PRO:HD2	2.43	0.43
1:A:638:LEU:O	1:A:641:LEU:HG	2.18	0.43
1:A:1181:LEU:HD13	1:A:1220:ARG:HD2	2.00	0.43
1:A:1529:ARG:HA	1:A:1532:TYR:CD1	2.52	0.43
3:D:514:ASP:N	3:D:514:ASP:OD1	2.50	0.43
4:G:108:VAL:HA	4:G:111:LEU:HG	2.00	0.43
1:A:94:ASP:OD1	1:A:94:ASP:N	2.52	0.43
1:A:1010:MET:SD	1:A:1064:ILE:HD11	2.58	0.43
3:D:137:ARG:HA	3:D:140:VAL:HG22	2.01	0.43
1:A:874:PRO:HB2	1:A:878:VAL:HB	2.01	0.43
1:A:111:TYR:HD1	2:C:116:GLN:HG3	1.83	0.43
1:B:102:ARG:HA	1:B:105:LYS:HG2	2.00	0.43
1:B:1007:LEU:HA	1:B:1010:MET:HG2	2.00	0.43
2:C:36:MET:HE3	2:C:36:MET:HB2	1.94	0.43
3:D:424:ILE:HA	3:D:424:ILE:HD13	1.86	0.43
3:D:489:LEU:HB2	3:D:492:MET:SD	2.58	0.43
3:D:504:PHE:HD2	3:D:521:LEU:HA	1.83	0.43
1:A:495:ARG:O	1:A:495:ARG:NE	2.51	0.43
1:A:1684:ALA:O	1:A:1688:ILE:HG22	2.18	0.43
1:B:1788:ASP:OD2	1:B:1791:SER:OG	2.37	0.43
3:D:258:ARG:O	3:D:259:MET:C	2.62	0.43
1:A:564:GLN:H	1:A:564:GLN:CD	2.27	0.43
1:A:1596:TRP:CZ2	1:A:1601:ALA:HA	2.53	0.43
3:F:381:MET:HE2	3:F:381:MET:HB2	1.75	0.43
3:F:504:PHE:HD2	3:F:521:LEU:HA	1.83	0.43
4:G:209:ARG:HA	4:G:212:VAL:HG12	2.00	0.43
1:B:1181:LEU:HD13	1:B:1220:ARG:HD2	2.00	0.43
1:B:1586:VAL:HG11	1:B:1613:ALA:O	2.19	0.43
1:B:1800:LYS:HE2	1:B:1800:LYS:HB2	1.85	0.43
3:F:448:LEU:HD13	3:F:483:GLN:HG2	1.99	0.43
3:F:489:LEU:HB2	3:F:492:MET:SD	2.58	0.43
1:B:575:ARG:HA	1:B:578:LYS:HG2	2.01	0.43
1:B:874:PRO:HB2	1:B:878:VAL:HB	2.01	0.43
1:B:1010:MET:HE3	1:B:1010:MET:HB2	1.71	0.43
1:A:102:ARG:HA	1:A:105:LYS:HG2	2.00	0.42
1:A:1991:GLU:CD	1:A:1991:GLU:H	2.27	0.42
1:B:141:ASP:O	1:B:145:ARG:HG2	2.19	0.42
3:F:223:GLN:HA	3:F:226:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:ASP:OD1	1:A:1275:ASP:N	2.48	0.42
1:B:776:VAL:O	1:B:779:ARG:HG2	2.20	0.42
1:B:1850:LYS:NZ	1:B:1853:ASP:HB3	2.33	0.42
3:D:435:LEU:HG	4:G:271:LEU:HD21	2.00	0.42
3:F:694:THR:O	3:F:698:ILE:HG13	2.19	0.42
1:A:950:MET:HE3	1:A:950:MET:HB3	1.94	0.42
1:A:1277:LEU:O	1:A:1653:TYR:OH	2.33	0.42
1:A:1766:SER:HA	1:A:1789:TYR:CD1	2.55	0.42
1:B:94:ASP:N	1:B:94:ASP:OD1	2.52	0.42
1:B:1879:LEU:HD12	1:B:1945:ALA:HB2	2.01	0.42
3:D:223:GLN:HA	3:D:226:HIS:NE2	2.34	0.42
4:E:108:VAL:HA	4:E:111:LEU:HG	2.00	0.42
1:B:1097:HIS:HD2	1:B:1100:LEU:HD22	1.84	0.42
4:G:170:GLU:HG2	4:G:171:MET:SD	2.58	0.42
1:A:439:ALA:HB1	1:A:484:CYS:SG	2.60	0.42
1:A:734:LEU:HD23	1:A:794:LEU:HB3	2.01	0.42
1:A:860:GLU:O	1:A:863:GLU:HG3	2.18	0.42
1:A:1118:THR:HG23	1:A:1119:THR:HG23	2.00	0.42
1:B:734:LEU:HD23	1:B:794:LEU:HB3	2.00	0.42
3:D:134:PRO:HG2	3:D:137:ARG:HG3	2.02	0.42
4:E:34:LYS:HB3	4:E:37:LEU:HB2	2.02	0.42
3:F:188:GLN:O	3:F:191:GLU:HG3	2.19	0.42
1:B:638:LEU:O	1:B:641:LEU:HG	2.18	0.42
1:B:778:THR:HG21	1:B:826:ILE:HD13	2.01	0.42
1:B:1611:CYS:HB3	3:D:418:LYS:HD3	2.01	0.42
3:D:241:ARG:O	3:D:245:LEU:HG	2.19	0.42
3:F:134:PRO:HG2	3:F:137:ARG:HG3	2.02	0.42
3:F:137:ARG:HA	3:F:140:VAL:HG22	2.01	0.42
3:F:415:ARG:O	3:F:419:VAL:HG23	2.20	0.42
1:A:776:VAL:O	1:A:779:ARG:HG2	2.20	0.42
1:B:1766:SER:HA	1:B:1789:TYR:CD1	2.55	0.42
3:F:241:ARG:O	3:F:245:LEU:HG	2.19	0.42
3:F:265:LEU:HD12	3:F:265:LEU:HA	1.82	0.42
3:F:394:PHE:CD2	3:F:395:GLU:HG2	2.55	0.42
3:F:407:LEU:HD23	3:F:407:LEU:HA	1.90	0.42
1:A:1586:VAL:HG11	1:A:1613:ALA:O	2.19	0.42
1:A:1850:LYS:NZ	1:A:1853:ASP:HB3	2.33	0.42
1:B:564:GLN:CD	1:B:564:GLN:H	2.27	0.42
4:E:52:LEU:HD23	4:E:52:LEU:H	1.84	0.42
3:F:228:LEU:HD13	3:F:231:LYS:HD2	2.01	0.42
3:F:396:GLU:O	3:F:400:TRP:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HA	1:A:644:LYS:HG2	2.01	0.42
1:A:959:GLU:O	1:A:963:GLU:HG2	2.20	0.42
1:B:439:ALA:HB1	1:B:484:CYS:SG	2.60	0.42
1:B:641:LEU:HA	1:B:644:LYS:HG2	2.02	0.42
1:B:1991:GLU:CD	1:B:1991:GLU:H	2.27	0.42
2:C:35:TYR:CZ	2:C:54:ASP:HB3	2.55	0.42
3:D:228:LEU:HD13	3:D:231:LYS:HD2	2.01	0.42
3:D:415:ARG:O	3:D:419:VAL:HG23	2.20	0.42
4:G:52:LEU:HD23	4:G:52:LEU:H	1.84	0.42
1:A:2074:ILE:HA	1:A:2077:VAL:HG12	2.02	0.42
1:B:40:ARG:HG2	1:B:211:LYS:NZ	2.35	0.42
1:B:407:PHE:CE2	1:B:442:VAL:HG22	2.55	0.42
1:B:959:GLU:O	1:B:963:GLU:HG2	2.20	0.42
3:D:396:GLU:O	3:D:400:TRP:HD1	2.02	0.42
3:D:694:THR:O	3:D:698:ILE:HG13	2.19	0.42
1:A:407:PHE:CE2	1:A:442:VAL:HG22	2.55	0.41
1:A:575:ARG:HA	1:A:578:LYS:HG2	2.01	0.41
1:A:1097:HIS:HD2	1:A:1100:LEU:HD22	1.84	0.41
1:B:1765:LEU:HD22	1:B:1789:TYR:HA	2.02	0.41
1:A:101:LEU:HD13	1:A:101:LEU:HA	1.89	0.41
1:B:636:PRO:O	1:B:639:GLN:HG2	2.20	0.41
1:B:1605:GLU:O	1:B:1606:LEU:HG	2.20	0.41
1:B:1886:VAL:HG23	1:B:1896:ILE:HG12	2.02	0.41
3:D:188:GLN:O	3:D:191:GLU:HG3	2.19	0.41
3:D:191:GLU:HA	3:D:194:ILE:HG12	2.03	0.41
4:E:274:GLU:HB2	4:E:275:PRO:HD3	2.02	0.41
2:H:35:TYR:CZ	2:H:54:ASP:HB3	2.55	0.41
1:A:778:THR:HG21	1:A:826:ILE:HD13	2.01	0.41
1:A:1710:ASP:OD1	1:A:1710:ASP:N	2.52	0.41
1:A:564:GLN:HA	1:A:567:ASP:OD2	2.21	0.41
1:A:1788:ASP:OD2	1:A:1791:SER:OG	2.37	0.41
1:B:1010:MET:HA	1:B:1013:ILE:HG12	2.02	0.41
1:B:1745:SER:OG	1:B:1801:ALA:O	2.27	0.41
1:A:1879:LEU:HD12	1:A:1945:ALA:HB2	2.01	0.41
1:B:157:LEU:O	1:B:158:LEU:C	2.63	0.41
1:B:2074:ILE:HA	1:B:2077:VAL:HG12	2.02	0.41
3:F:355:ARG:HB3	3:F:355:ARG:NH1	2.36	0.41
4:G:173:THR:HG23	4:G:175:GLN:H	1.86	0.41
1:A:1340:ASN:OD1	1:A:1341:ARG:N	2.54	0.41
1:A:1509:PRO:HB3	1:A:2021:VAL:HG11	2.03	0.41
1:B:722:ASP:O	1:B:726:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:LYS:HB2	1:B:1409:LYS:HE3	1.88	0.41
3:D:338:MET:HE3	3:D:338:MET:HB3	1.68	0.41
3:F:465:THR:OG1	3:F:466:SER:N	2.53	0.41
4:G:274:GLU:HB2	4:G:275:PRO:HD3	2.02	0.41
2:H:39:TYR:OH	2:H:100:ASP:OD2	2.33	0.41
1:A:40:ARG:HG2	1:A:211:LYS:NZ	2.35	0.41
1:A:152:GLU:O	1:A:156:VAL:HG13	2.21	0.41
1:A:348:LEU:HA	1:A:351:ILE:HG12	2.03	0.41
1:B:50:LEU:O	1:B:54:GLN:HG2	2.21	0.41
1:B:564:GLN:HA	1:B:567:ASP:OD2	2.21	0.41
1:B:1198:ALA:O	1:B:1201:ILE:HG22	2.21	0.41
1:B:1340:ASN:OD1	1:B:1341:ARG:N	2.54	0.41
1:A:69:GLN:OE1	1:A:111:TYR:HB2	2.21	0.41
1:A:157:LEU:O	1:A:158:LEU:C	2.64	0.41
1:A:1605:GLU:O	1:A:1606:LEU:HG	2.20	0.41
1:B:99:TYR:O	1:B:103:LEU:HG	2.21	0.41
1:B:1697:LEU:HD21	1:B:1705:ASP:HB3	2.03	0.41
1:B:1741:ILE:HD12	1:B:1741:ILE:HA	1.96	0.41
3:D:355:ARG:HB3	3:D:355:ARG:NH1	2.36	0.41
1:A:111:TYR:CD1	2:C:116:GLN:HG3	2.56	0.41
1:A:636:PRO:O	1:A:639:GLN:HG2	2.20	0.41
1:A:656:ILE:O	1:A:660:LEU:HG	2.21	0.41
1:A:832:LEU:HD23	1:A:903:ARG:HH22	1.86	0.41
1:A:1747:ILE:O	1:A:1750:PRO:HD2	2.21	0.41
1:A:1952:LEU:HD12	1:A:1952:LEU:HA	1.93	0.41
1:B:1747:ILE:O	1:B:1750:PRO:HD2	2.21	0.41
1:B:1808:LYS:HB2	1:B:1844:TRP:CZ3	2.56	0.41
3:D:219:GLU:OE1	3:D:219:GLU:N	2.48	0.41
3:D:265:LEU:HD12	3:D:265:LEU:HA	1.82	0.41
3:D:394:PHE:CD2	3:D:395:GLU:HG2	2.55	0.41
1:A:733:LEU:HD13	1:A:774:ILE:HG12	2.02	0.41
1:A:1855:CYS:HB2	1:A:1888:ALA:HB2	2.03	0.41
1:A:1886:VAL:HG23	1:A:1896:ILE:HG12	2.02	0.41
1:B:578:LYS:HA	1:B:581:LEU:HG	2.03	0.41
1:B:733:LEU:HD13	1:B:774:ILE:HG12	2.02	0.41
1:B:1010:MET:HE1	1:B:1061:CYS:HA	2.02	0.41
1:B:1509:PRO:HB3	1:B:2021:VAL:HG11	2.03	0.41
3:D:465:THR:OG1	3:D:466:SER:N	2.53	0.41
4:G:34:LYS:HB3	4:G:37:LEU:HB2	2.02	0.41
1:A:411:GLN:O	1:A:415:GLN:NE2	2.39	0.40
1:A:722:ASP:O	1:A:726:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:SER:HA	1:A:397:LYS:HG2	2.03	0.40
1:A:1745:SER:OG	1:A:1801:ALA:O	2.27	0.40
1:A:1765:LEU:HD22	1:A:1789:TYR:HA	2.02	0.40
1:B:69:GLN:OE1	1:B:111:TYR:HB2	2.21	0.40
1:B:1398:LYS:HD3	1:B:1398:LYS:HA	1.95	0.40
1:B:1920:PHE:HD2	1:B:1920:PHE:HA	1.72	0.40
3:D:260:THR:O	3:D:264:GLN:HG2	2.22	0.40
3:F:175:CYS:HA	3:F:178:LYS:HE3	2.03	0.40
3:F:258:ARG:O	3:F:259:MET:C	2.62	0.40
3:F:408:MET:HE2	3:F:408:MET:HB3	1.87	0.40
4:G:16:PHE:CD1	4:G:17:LYS:HG2	2.56	0.40
1:A:378:PHE:HD1	1:A:378:PHE:HA	1.72	0.40
1:A:1198:ALA:O	1:A:1201:ILE:HG22	2.21	0.40
1:B:125:LEU:HA	1:B:126:PRO:HD3	1.98	0.40
1:B:656:ILE:O	1:B:660:LEU:HG	2.21	0.40
1:B:676:TRP:CE2	1:B:732:ASN:HB3	2.57	0.40
2:C:38:TRP:HH2	2:C:80:VAL:HB	1.87	0.40
3:D:400:TRP:CZ3	3:D:422:GLU:HG2	2.57	0.40
3:F:191:GLU:HA	3:F:194:ILE:HG12	2.03	0.40
1:A:50:LEU:O	1:A:54:GLN:HG2	2.21	0.40
1:A:563:GLU:HB3	1:A:566:ARG:HH21	1.86	0.40
1:A:1140:MET:N	1:A:1140:MET:SD	2.95	0.40
1:A:1483:LYS:HE3	1:A:1483:LYS:HB2	1.90	0.40
1:A:1808:LYS:HB2	1:A:1844:TRP:CZ3	2.56	0.40
1:A:1974:ILE:HG12	1:A:1975:ASP:H	1.86	0.40
1:B:378:PHE:HD1	1:B:378:PHE:HA	1.72	0.40
3:F:219:GLU:OE1	3:F:219:GLU:N	2.48	0.40
1:B:147:PRO:HA	1:B:150:ARG:HG3	2.03	0.40
1:B:453:GLN:H	1:B:453:GLN:CD	2.29	0.40
1:B:1365:VAL:HA	1:B:1366:PRO:HD3	1.97	0.40
1:B:1855:CYS:HB2	1:B:1888:ALA:HB2	2.03	0.40
4:E:173:THR:HG23	4:E:175:GLN:H	1.86	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	1676/2104 (80%)	1605 (96%)	70 (4%)	1 (0%)	48 79
1	B	1676/2104 (80%)	1605 (96%)	70 (4%)	1 (0%)	48 79
2	C	96/165 (58%)	91 (95%)	5 (5%)	0	100 100
2	H	96/165 (58%)	91 (95%)	5 (5%)	0	100 100
3	D	580/843 (69%)	571 (98%)	9 (2%)	0	100 100
3	F	580/843 (69%)	571 (98%)	9 (2%)	0	100 100
4	E	242/308 (79%)	232 (96%)	10 (4%)	0	100 100
4	G	242/308 (79%)	233 (96%)	9 (4%)	0	100 100
All	All	5188/6840 (76%)	4999 (96%)	187 (4%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1980	PHE
1	B	1980	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	1527/1842 (83%)	1505 (99%)	22 (1%)	62 80
1	B	1527/1842 (83%)	1506 (99%)	21 (1%)	62 80
2	C	82/129 (64%)	80 (98%)	2 (2%)	44 68
2	H	82/129 (64%)	80 (98%)	2 (2%)	44 68
3	D	494/712 (69%)	484 (98%)	10 (2%)	50 72
3	F	494/712 (69%)	484 (98%)	10 (2%)	50 72
4	E	227/277 (82%)	224 (99%)	3 (1%)	65 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	227/277 (82%)	224 (99%)	3 (1%)	65 81
All	All	4660/5920 (79%)	4587 (98%)	73 (2%)	58 76

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	101	LEU
1	A	187	LEU
1	A	200	MET
1	A	299	TYR
1	A	377	MET
1	A	378	PHE
1	A	482	LEU
1	A	485	CYS
1	A	486	LEU
1	A	521	LEU
1	A	574	CYS
1	A	771	ILE
1	A	860	GLU
1	A	951	MET
1	A	1108	LEU
1	A	1292	VAL
1	A	1492	LEU
1	A	1532	TYR
1	A	1595	THR
1	A	1800	LYS
1	A	1920	PHE
1	B	101	LEU
1	B	187	LEU
1	B	200	MET
1	B	299	TYR
1	B	377	MET
1	B	378	PHE
1	B	482	LEU
1	B	485	CYS
1	B	486	LEU
1	B	521	LEU
1	B	574	CYS
1	B	771	ILE
1	B	860	GLU
1	B	951	MET

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Mol	Chain	Res	Type
1	B	1108	LEU
1	B	1292	VAL
1	B	1492	LEU
1	B	1532	TYR
1	B	1595	THR
1	B	1800	LYS
1	B	1920	PHE
2	C	49	LEU
2	C	75	ASN
3	D	269	LEU
3	D	350	GLU
3	D	371	ILE
3	D	381	MET
3	D	420	LEU
3	D	424	ILE
3	D	440	LEU
3	D	576	LEU
3	D	610	LEU
3	D	706	TYR
4	E	157	LEU
4	E	195	MET
4	E	244	ILE
3	F	269	LEU
3	F	350	GLU
3	F	371	ILE
3	F	381	MET
3	F	420	LEU
3	F	424	ILE
3	F	440	LEU
3	F	576	LEU
3	F	610	LEU
3	F	706	TYR
4	G	157	LEU
4	G	195	MET
4	G	244	ILE
2	H	49	LEU
2	H	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	438	ASN
1	A	457	ASN
1	A	501	HIS
1	A	643	GLN
1	A	766	ASN
1	A	969	GLN
1	A	976	ASN
1	A	1015	GLN
1	A	1029	GLN
1	A	1096	GLN
1	A	1097	HIS
1	A	1114	ASN
1	A	1170	ASN
1	A	1262	GLN
1	A	1304	GLN
1	A	1519	GLN
1	A	1539	GLN
1	A	1557	GLN
1	A	1570	ASN
1	A	1690	ASN
1	A	1694	ASN
1	A	2064	ASN
1	B	91	GLN
1	B	438	ASN
1	B	457	ASN
1	B	501	HIS
1	B	597	ASN
1	B	643	GLN
1	B	969	GLN
1	B	976	ASN
1	B	1015	GLN
1	B	1026	HIS
1	B	1029	GLN
1	B	1096	GLN
1	B	1097	HIS
1	B	1170	ASN
1	B	1304	GLN
1	B	1519	GLN
1	B	1539	GLN
1	B	1557	GLN
1	B	1690	ASN
1	B	1694	ASN

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Mol	Chain	Res	Type
2	C	83	GLN
2	C	119	GLN
3	D	170	GLN
3	D	188	GLN
3	D	232	ASN
3	D	276	GLN
3	D	545	GLN
3	D	763	HIS
3	D	811	GLN
4	E	26	ASN
4	E	49	GLN
4	E	268	GLN
3	F	170	GLN
3	F	188	GLN
3	F	276	GLN
3	F	545	GLN
3	F	763	HIS
3	F	811	GLN
4	G	26	ASN
4	G	49	GLN
4	G	70	GLN
2	H	83	GLN
2	H	119	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

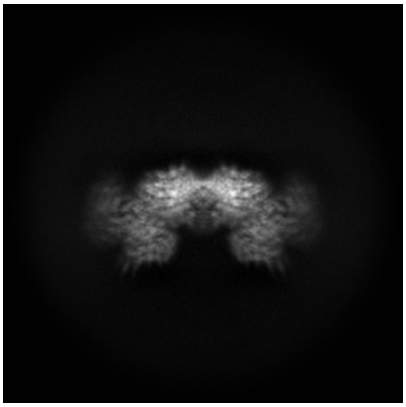
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70826. These allow visual inspection of the internal detail of the map and identification of artifacts.

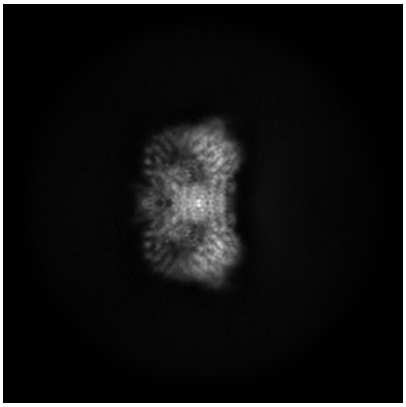
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

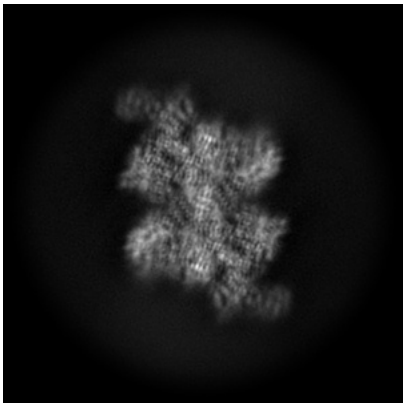
6.1.1 Primary map



X



Y

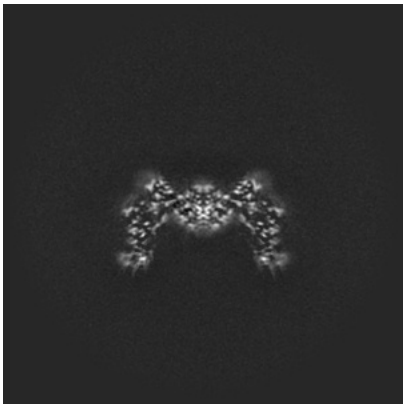


Z

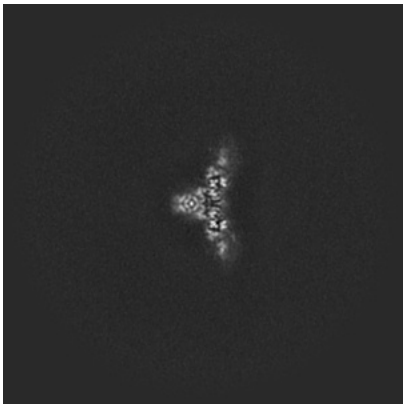
The images above show the map projected in three orthogonal directions.

6.2 Central slices

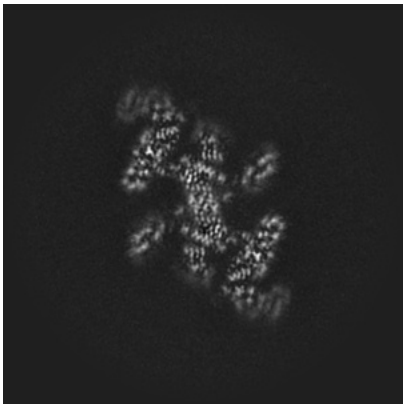
6.2.1 Primary map



X Index: 280



Y Index: 280

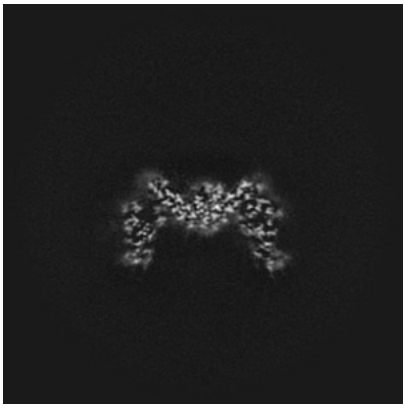


Z Index: 280

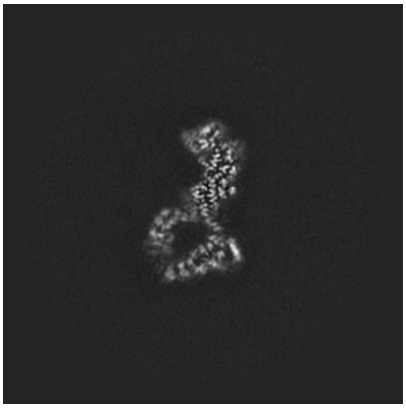
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

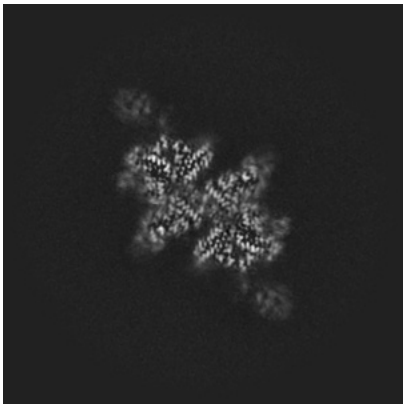
6.3.1 Primary map



X Index: 284



Y Index: 236

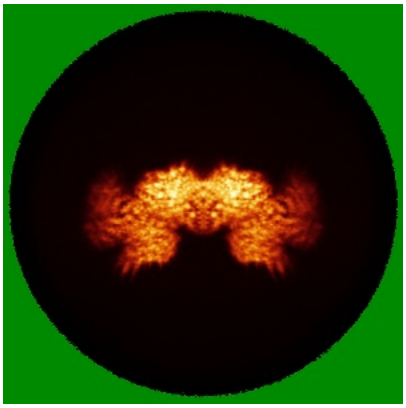


Z Index: 305

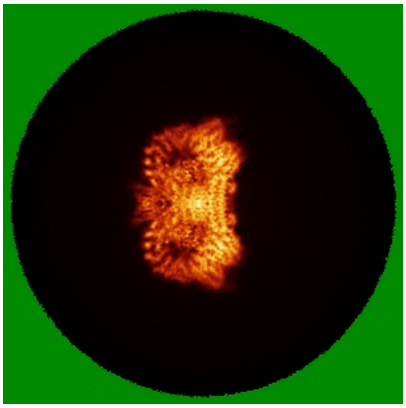
The images above show the largest variance slices of the map in three orthogonal directions.

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

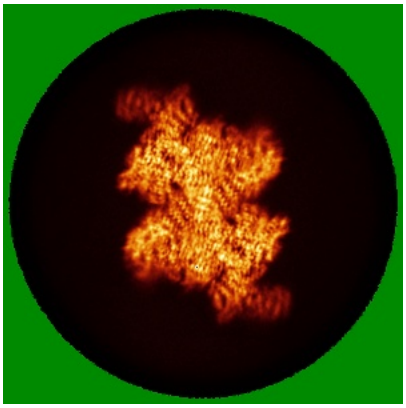
6.4.1 Primary map



X



Y

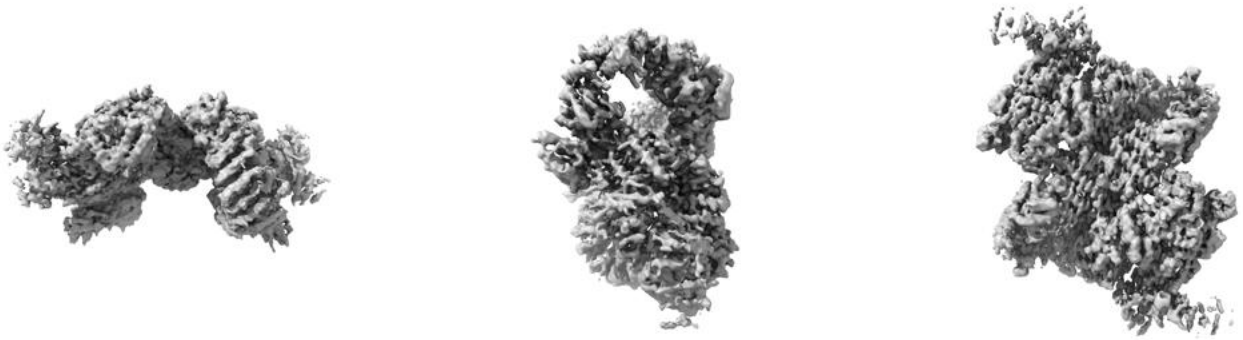


Z

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 0.0371. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

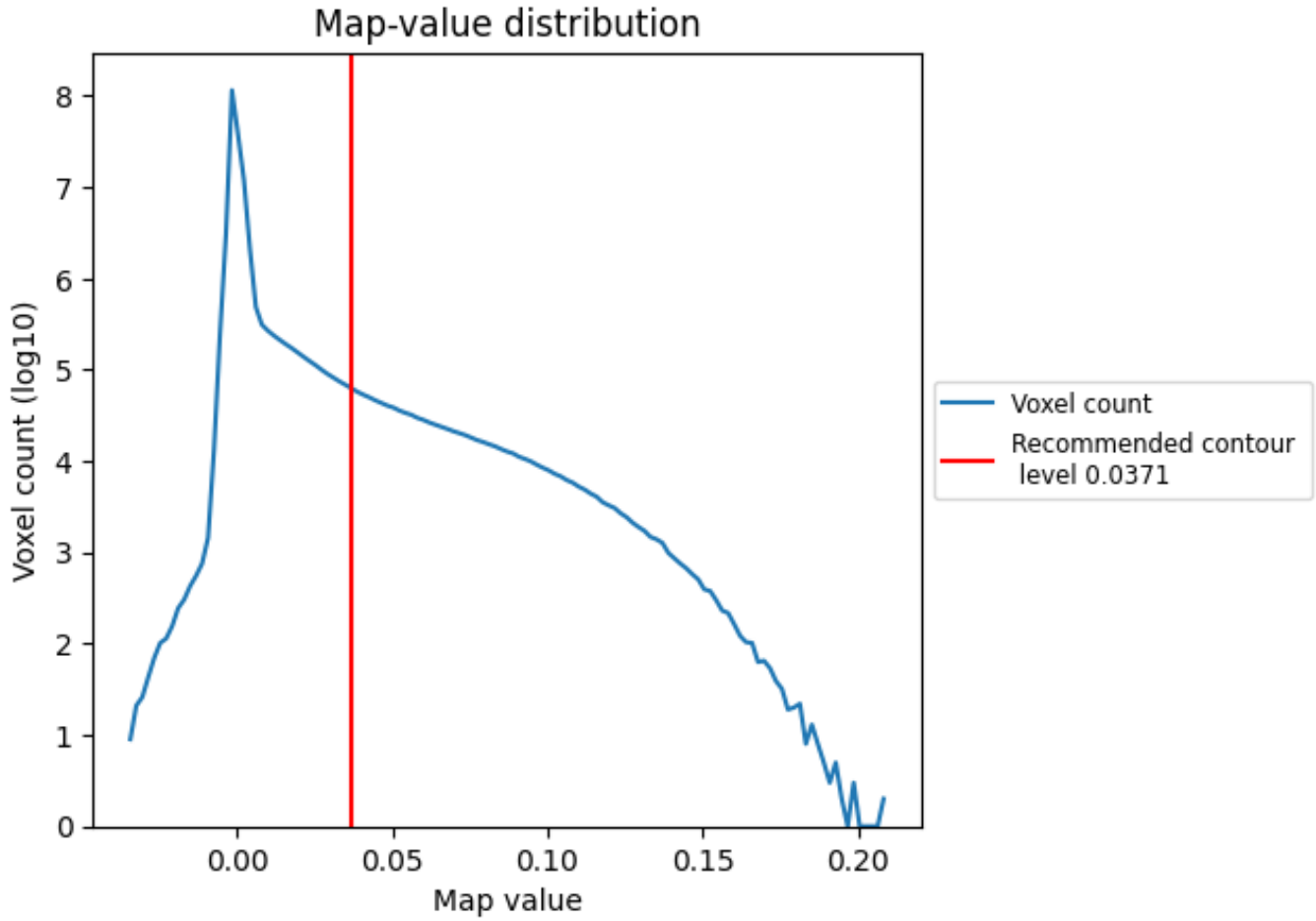
6.6 Mask visualisation (i)

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

7 Map analysis

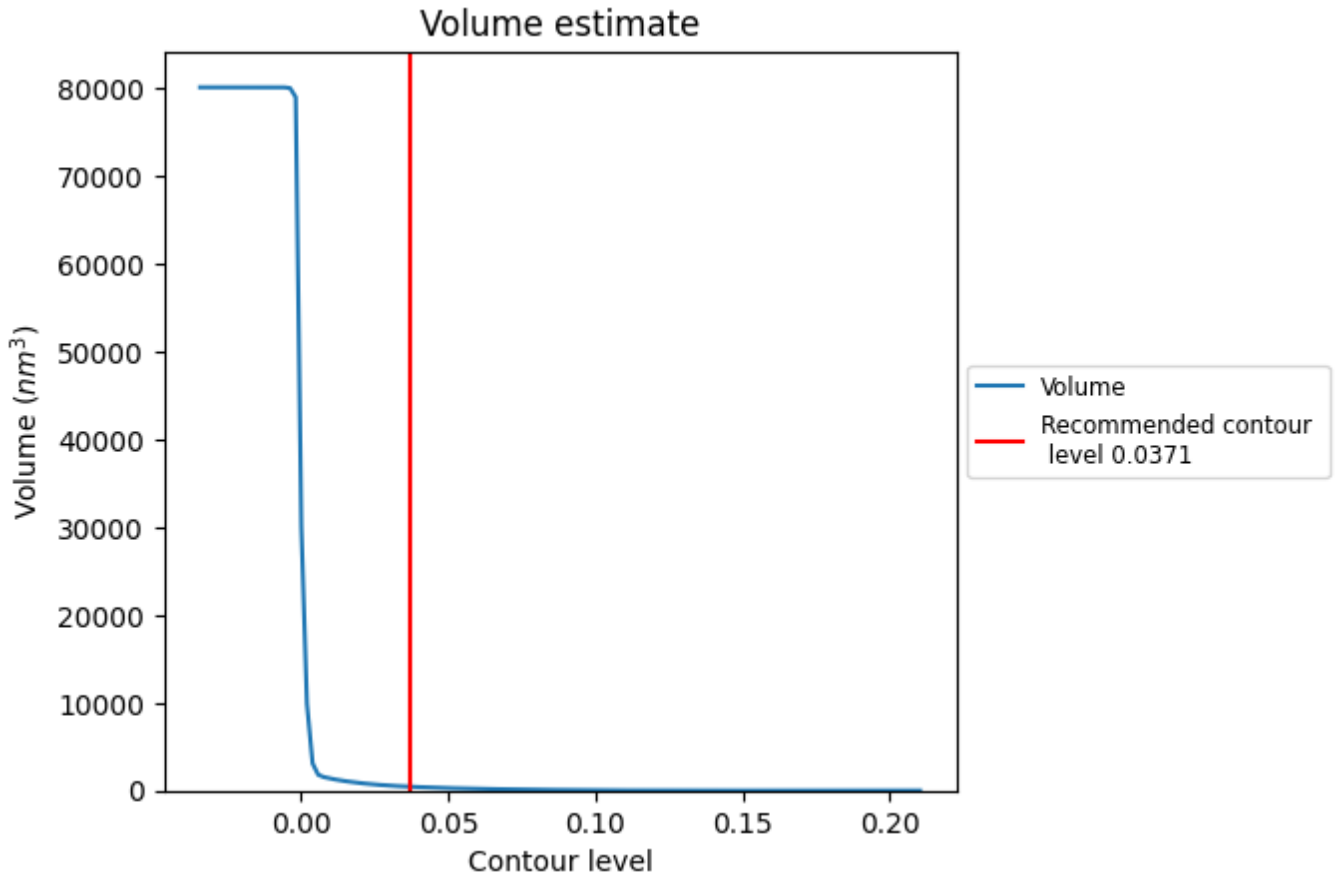
This section contains the results of statistical analysis of the map.

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.

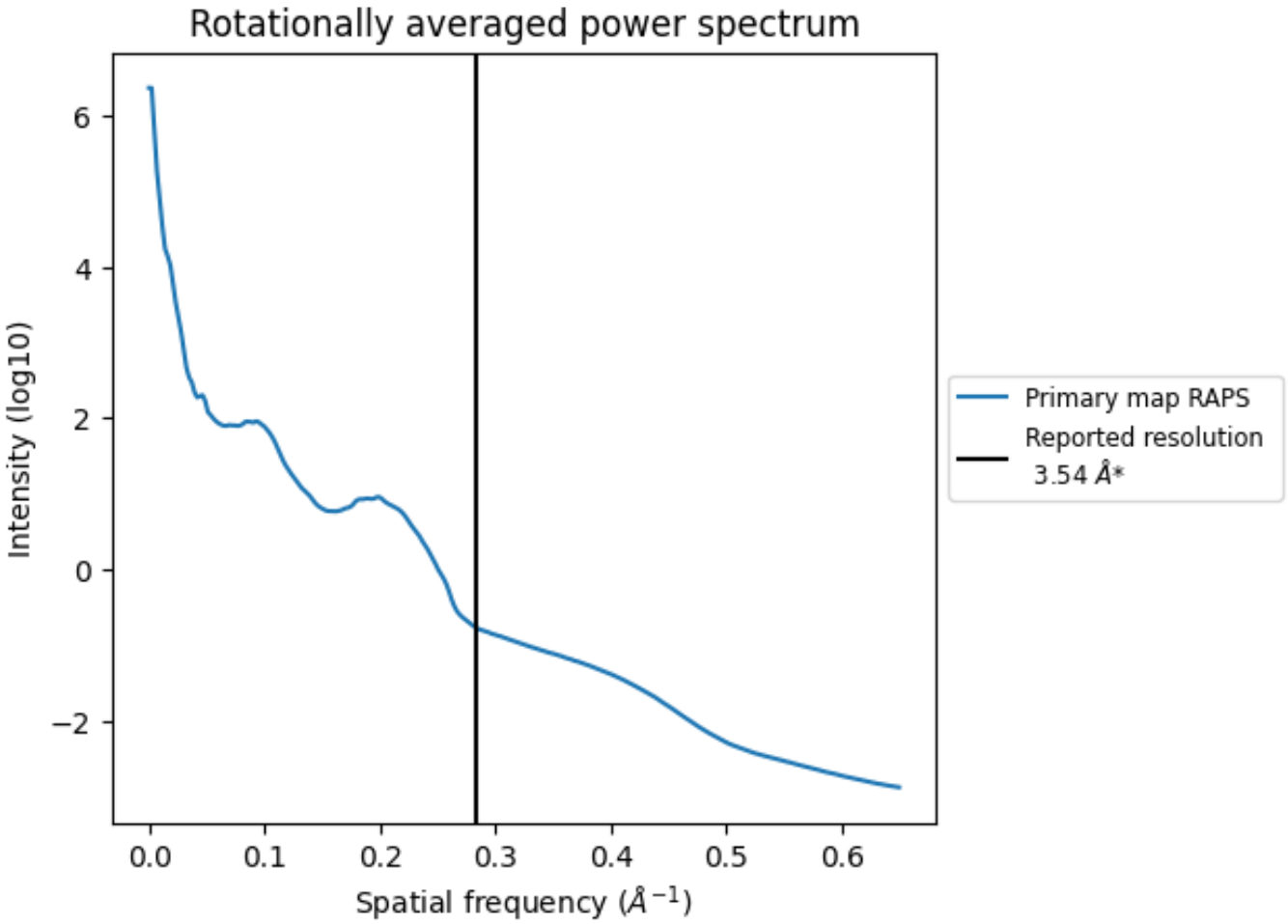
7.2 Volume estimate



The volume at the recommended contour level is 438 nm^3; this corresponds to an approximate mass of 396 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 0.282 Å^{-1}

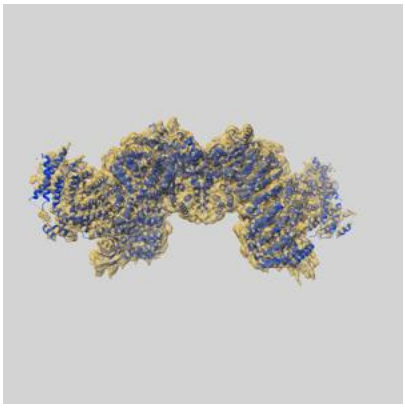
8 Fourier-Shell correlation

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

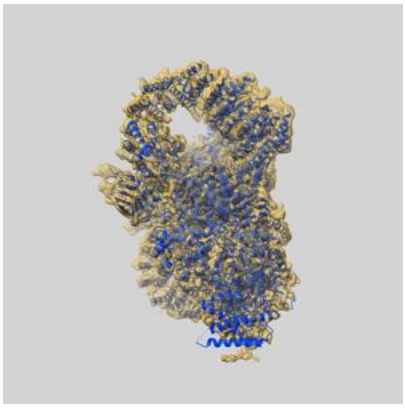
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70826 and PDB model 9OT6. Per-residue inclusion information can be found in section 3 on page 6.

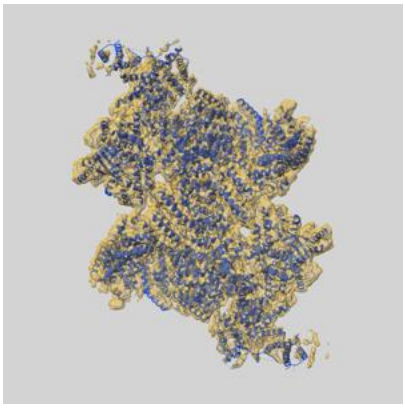
9.1 Map-model overlay



X



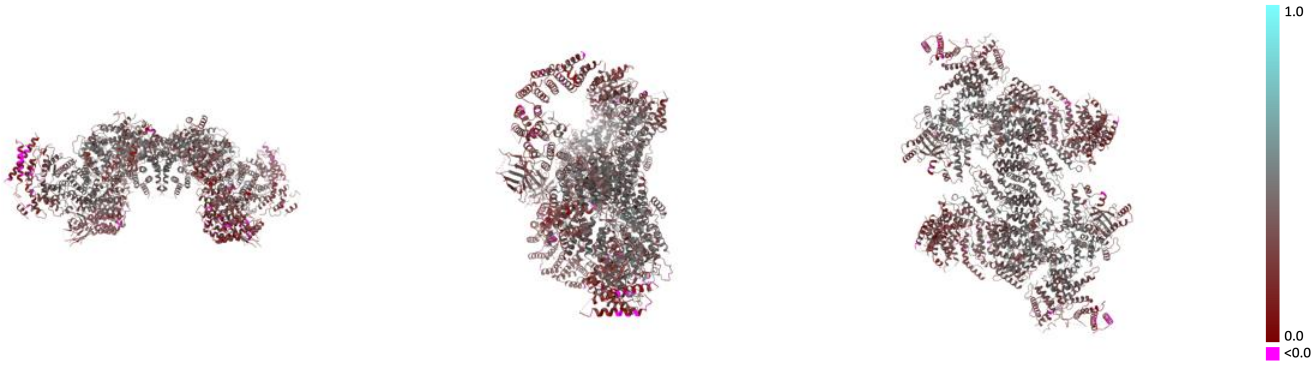
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0371 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.

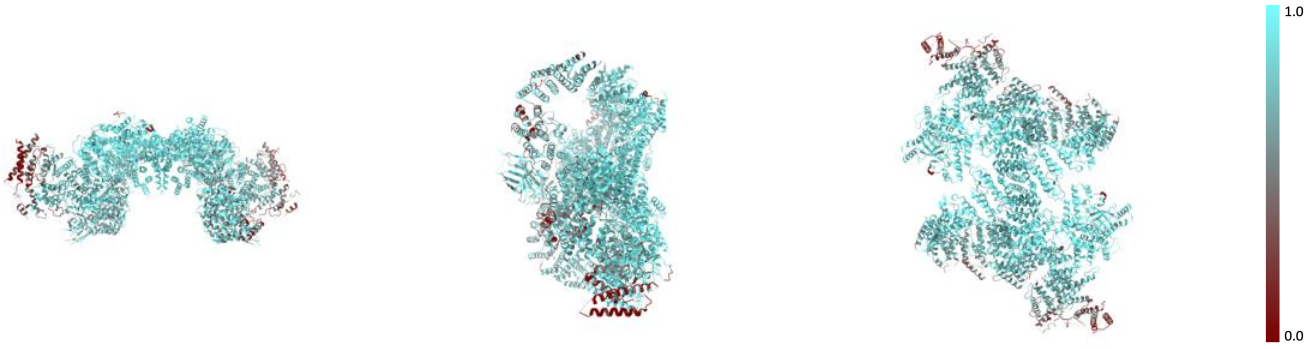
9.2 Q-score mapped to coordinate model (i)



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.

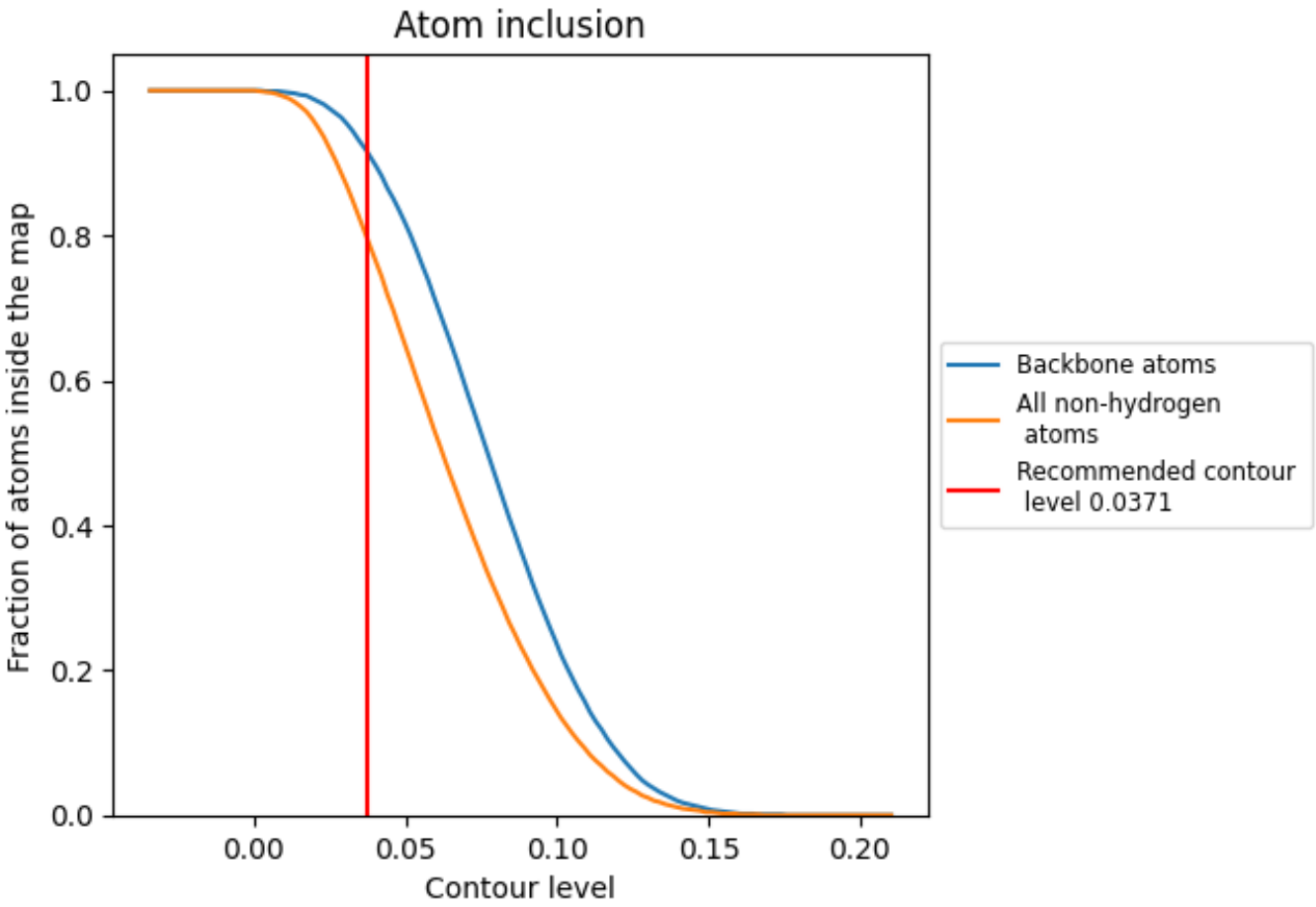
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0371).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 80% 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 (0.0371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.3470
A	0.8570	0.3560
B	0.8620	0.3520
C	0.7180	0.3140
D	0.7060	0.3440
E	0.6120	0.3240
F	0.6940	0.3410
G	0.6550	0.3170
H	0.7420	0.3050