Full wwPDB EM Validation Report (i)

Nov 8, 2022 – 09:08 AM JST

PDB ID	:	5ZAK
EMDB ID	:	EMD-6904
Title	:	Cryo-EM structure of human Dicer and its complexes with a pre-miRNA substrate
Authors	:	Liu, Z.; Wang, J.; Cheng, H.; Ke, X.; Sun, L.; Zhang, Q.C.; Wang, H.-W.
Deposited on	:	2018-02-07
Resolution	:	4.40 Å(reported)
Based on initial models	:	4GL2, 3C4T, 2KOU, 5B16

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 (i) 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 (i)) were used in the production of this report:

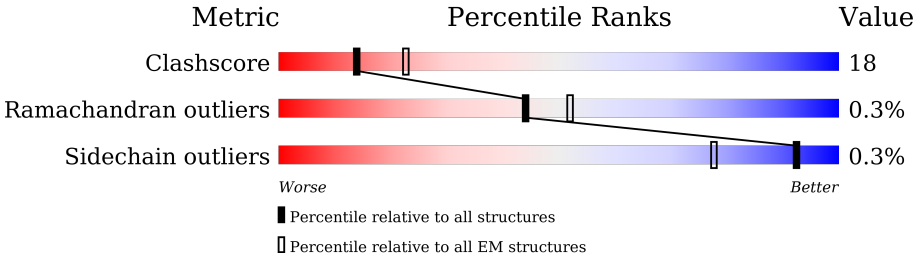
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.40 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	1922	20% 41% 27% • 32%
2	B	366	14% 13% 8% 80%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11112 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 Endoribonuclease Dicer.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1314	10552	6742	1807	1943	60	0	0

- Molecule 2 is a protein called RISC-loading complex subunit TARBP2.

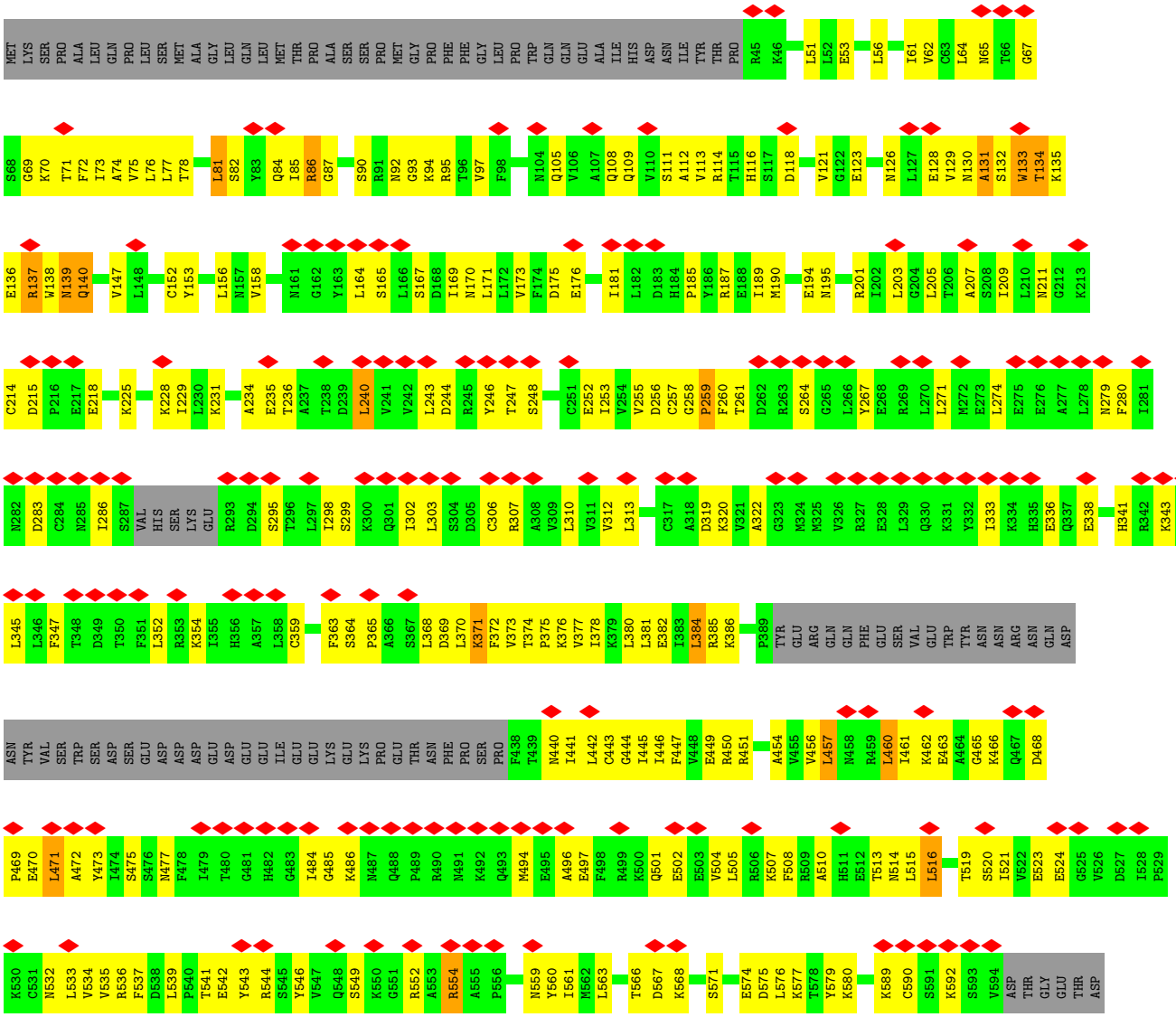
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	75	560	345	99	110	6	0	0

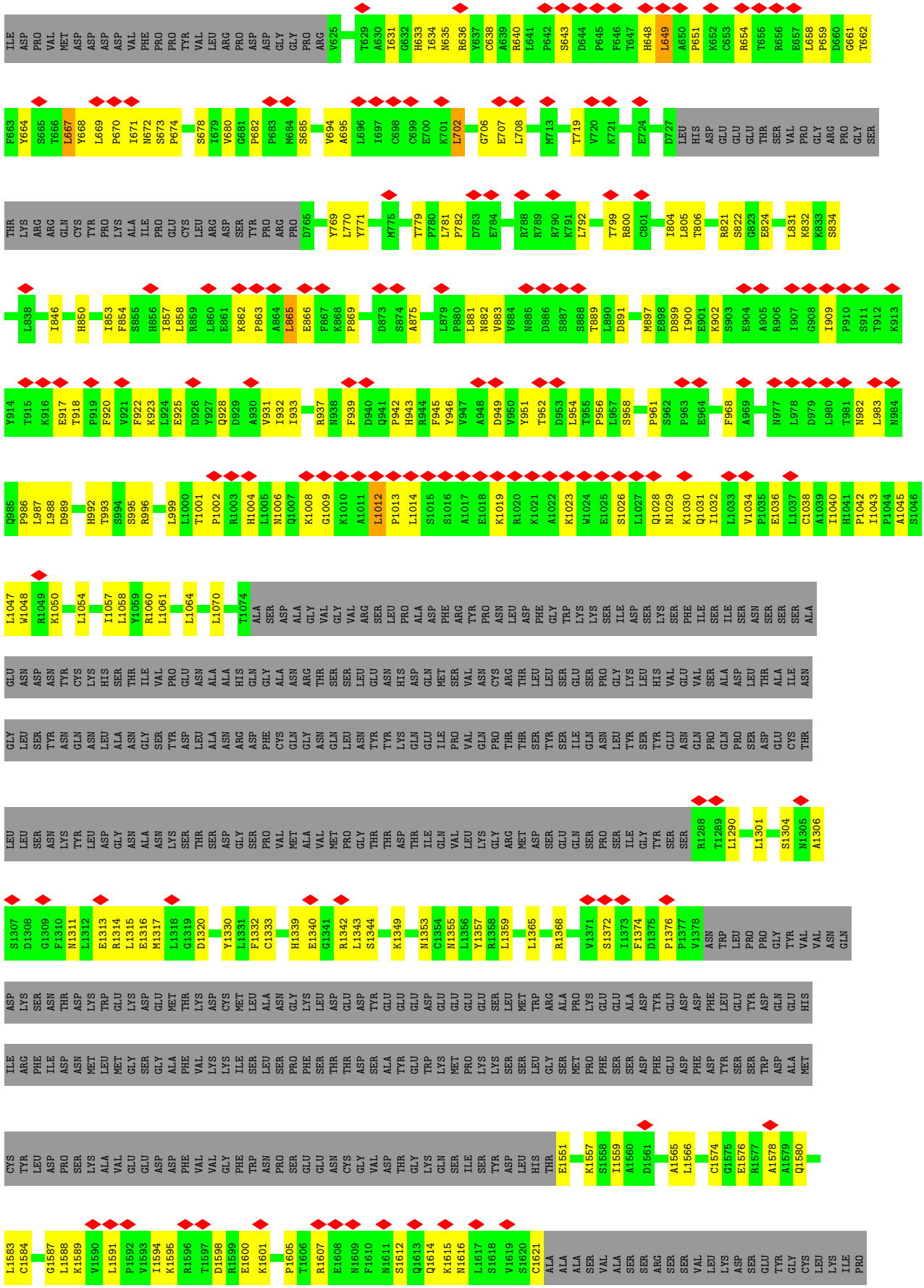
3 Residue-property plots (i)

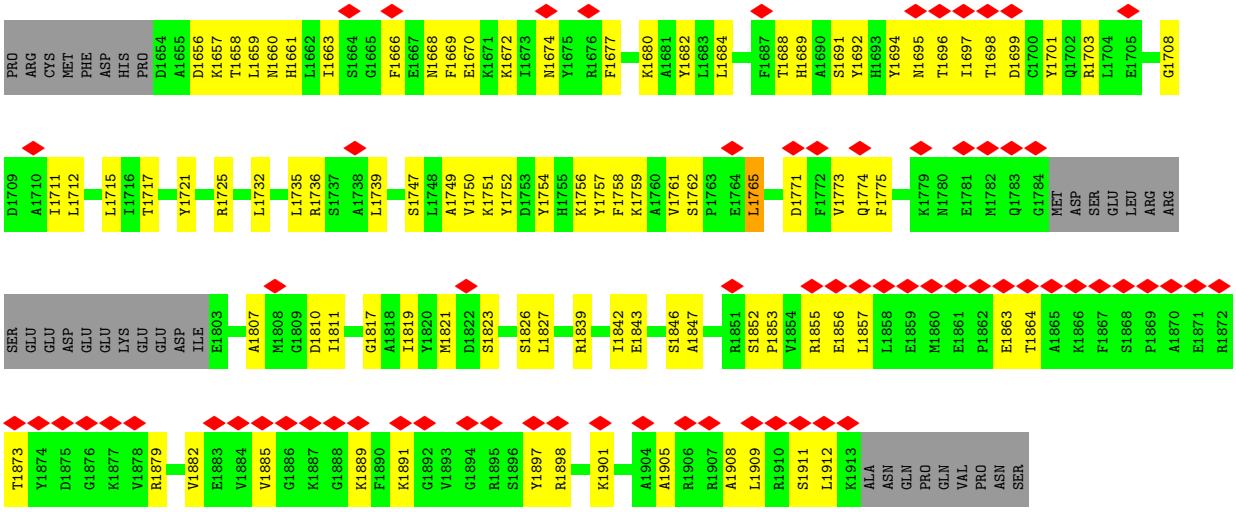
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A: 20% 41% 27% • 32%

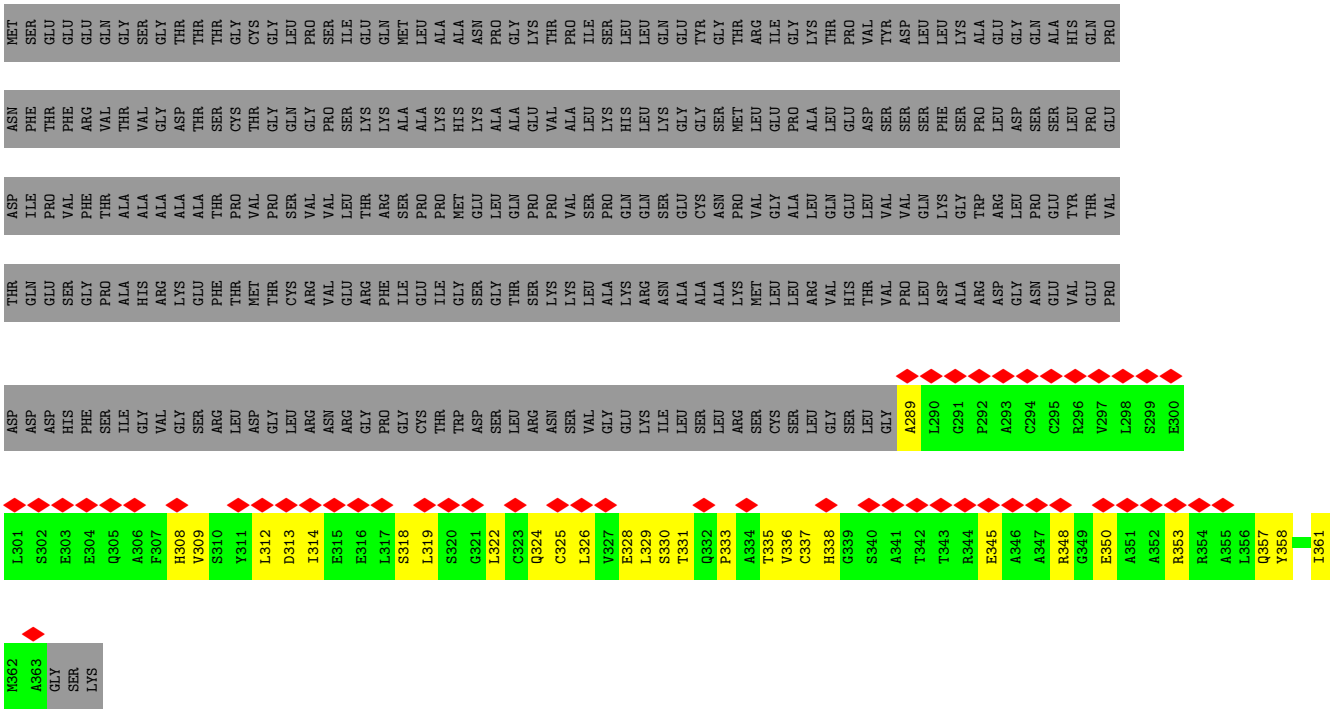



ILE ASP PRO VAL MET ASP ASP ASP VAL PHE PRO PRO TYR VAL LEU ARG PRO ASP ASP GLY GLY PRO ARG V625 T629 A630 I631 G632 H633 I634 N635 R636 Y637 C638 A639 R640 L641 P642 S643 D644 P645 F646 T647 H648 L649 A650 P651 K652 C653 R654 T655 R656 E657 L658 P659 D660 G661 T662
F663 Y664 S665 T666 L667 Y668 L669 P670 I671 N672 S673 P674 S678 I679 V680 G681 P682 P683 M684 S685 V694 A695 L696 I697 G698 G699 E700 K701 L702 G706 E707 L708 M713 T719 V720 K721 E724 D727 LEU HIS ASP GLU GLU GLU THR SER VAL PRO GLY ARG PRO GLY SER
THR LYS ARG ARG GLN CYS TYR PRO LYS ALA ILE PRO GLU CYS LEU ARG ASP SER TYR PRO ARG PRO D765 Y769 L770 Y771 M775 T779 P780 L781 P782 D783 E784 R788 R789 R790 K791 L792 T799 R800 C801 I804 L805 T806 R821 S822 G823 E824 L831 K832 K833 S834
L838 I846 H850 I853 F854 S855 H856 I857 L858 R859 L860 E861 K862 P863 A864 L865 E866 F867 K868 P869 D873 S874 A875 L879 P880 L881 N882 V883 V884 N885 D886 S887 S888 T889 L890 D891 M897 E898 D899 I900 E901 K902 S903 E904 A905 R906 I907 G908 I909 P910 S911 T912 K913
Y914 T915 K916 E917 T918 P919 F920 V921 F922 K923 L924 E925 D926 Y927 Q928 D929 A930 V931 I932 I933 R937 N938 F939 D940 Q941 P942 H943 R944 F945 Y946 V947 A948 D949 V950 Y951 T952 D953 L954 T955 P956 L957 S958 P961 S962 P963 E964 F968 A969 N977 L978 D979 L980 T981 N982 L983 N984
Q985 P986 L987 L988 D989 H992 T993 S994 S995 R996 L999 L1000 T1001 P1002 R1003 H1004 L1005 N1006 Q1007 K1008 G1009 K1010 A1011 L1012 P1013 L1014 S1015 S1016 A1017 E1018 K1019 R1020 K1021 A1022 K1023 W1024 E1025 S1026 L1027 Q1028 N1029 K1030 Q1031 I1032 L1033 V1034 P1035 E1036 L1037 C1038 A1039 I1040 H1041 P1042 I1043 P1044 A1045 S1046
L1047 W1048 R1049 K1050 L1054 I1057 L1058 Y1059 R1060 L1061 L1064 L1070 T1074 ALA SER ASP ALA GLY VAL GLY VAL ARG SER LEU PRO ALA ASP PHE ARG TYR PRO ASN LEU ASP PHE GLY TRP LYS LYS SER ILE ASP SER LYS SER PHE ILE SER ILE SER ASN ASN SER SER SER ALA
GLU ASN ASP ASN TYR CYS LYS HIS SER THR ILE VAL PRO GLU ASN ALA ALA HIS GLN GLY ALA ASN ARG THR SER SER LEU GLU ASN HIS ASP GLN MET SER VAL ASN CYS ARG THR LEU LEU SER GLU SER PRO GLY LYS LEU HIS VAL GLU VAL SER ALA ASP LEU THR ALA ILE ASN
GLY LEU SER TYR ASN GLN ASN LEU ALA ASN GLY SER TYR ASP LEU ALA ASN ARG ASP PHE CYS GLN GLY ASN GLN LEU ASN TYR TYR LYS GLN GLU ILE PRO VAL GLN PRO THR THR SER TYR SER ILE GLN ASN LEU TYR SER TYR GLU ASN GLN PRO GLN PRO SER ASP GLU CYS THR
LEU LEU SER ASN LYS TYR LEU ASP GLY ASN ALA ASN LYS SER THR SER ASP GLY SER PRO VAL MET ALA VAL MET PRO GLY THR THR ASP THR ILE GLN SER VAL LEU LYS GLY ARG MET ASP SER GLU GLN SER PRO SER ILE GLY TYR SER SER R1288 T1289 L1290 L1301 S1304 N1305 A1306
S1307 D1308 G1309 F1310 N1311 L1312 E1313 R1314 L1315 D1316 M1317 L1318 G1319 D1320 Y1330 L1331 F1332 C1333 H1339 E1340 G1341 R1342 L1343 S1344 K1349 N1353 C1354 N1355 L1356 Y1357 R1358 L1359 L1365 R1368 V1371 S1372 I1373 F1374 D1375 P1376 P1377 V1378 ASN TRP LEU PRO PRO GLY TYR VAL VAL ASN GLN
ASP LYS SER ASN THR ASP LYS TRP GLU LYS ASP GLU MET THR LYS ASP CYS MET LEU ALA ASN GLY LYS LEU GLU GLU GLU ASP GLU GLU GLU GLU SER LEU MET TRP ARG ALA PRO LYS GLU GLU ASP TYR GLU ASP ASP PHE LEU GLU TYR ASP GLN GLU HIS
ILE ARG PHE ILE ASP ASN MET LEU MET GLY SER GLY ALA PHE VAL LYS LYS ILE SER LEU SER PRO PHE SER THR THR ASP SER ALA TYR GLU TRP LYS MET PRO LYS LYS SER SER LEU GLY SER MET PRO PHE SER SER ASP PHE GLU ASP PHE ASP TYR SER SER SER TRP ASP ASP ALA MET
CYS TYR LEU ASP PRO SER LYS ALA VAL GLU GLU ASN CYS GLY VAL ASP THR GLY LYS GLN SER ILE THR HIS THR E1551 K1557 S1558 I1559 A1560 D1561 A1565 L1566 C1574 G1575 E1576 R1577 A1578 A1579 Q1580
L1583 C1584 G1587 L1588 K1589 V1590 L1591 P1592 V1593 I1594 K1595 R1596 T1597 D1598 R1599 E1600 K1601 P1605 T1606 R1607 E1608 N1609 F1610 N1611 S1612 Q1613 Q1614 K1615 N1616 L1617 S1618 V1619 S1620 C1621 ALA ALA ALA SER VAL ALA SER SER ARG SER SER VAL LEU LEU LYS ASP SER GLU TYR GLY CYS LEU LYS ILE PRO



- Molecule 2: RISC-loading complex subunit TARBP2

Chain B: 14% 13% 8% 80%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	337566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	38462	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	219.49872, 219.49872, 219.49872	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.44	0/10766	0.80	25/14558 (0.2%)
2	B	0.41	0/566	0.60	0/765
All	All	0.44	0/11332	0.80	25/15323 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	LEU	CA-CB-CG	7.82	133.29	115.30
1	A	471	LEU	CA-CB-CG	7.77	133.17	115.30
1	A	1857	LEU	CA-CB-CG	7.41	132.34	115.30
1	A	460	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	702	LEU	CA-CB-CG	6.68	130.65	115.30
1	A	134	THR	C-N-CA	6.50	137.95	121.70
1	A	1909	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	1566	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	116	HIS	C-N-CA	6.02	136.76	121.70
1	A	81	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	1566	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	1591	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	1712	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	457	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	1765	LEU	CA-CB-CG	5.53	128.03	115.30
1	A	240	LEU	CA-CB-CG	5.49	127.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1857	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	A	649	LEU	C-N-CA	5.33	135.01	121.70
1	A	516	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	865	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	1290	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	667	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	137	ARG	C-N-CA	5.08	134.41	121.70
1	A	1551	GLU	C-N-CA	5.05	134.32	121.70
1	A	209	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1012	LEU	Peptide
1	A	131	ALA	Peptide
1	A	133	TRP	Peptide
1	A	1333	CYS	Peptide
1	A	1376	PRO	Peptide
1	A	140	GLN	Peptide
1	A	164	LEU	Peptide
1	A	165	SER	Peptide
1	A	1752	TYR	Peptide
1	A	207	ALA	Peptide
1	A	661	GLY	Peptide
1	A	707	GLU	Peptide
1	A	961	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10552	0	10709	381	0
2	B	560	0	559	22	0
All	All	11112	0	11268	394	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 18.

All (394) 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:1882:VAL:O	1:A:1889:LYS:HA	1.65	0.96
1:A:769:TYR:O	1:A:805:LEU:HA	1.69	0.93
1:A:279:ASN:O	1:A:283:ASP:HB2	1.69	0.93
1:A:1313:GLU:O	1:A:1317:MET:HB2	1.74	0.88
1:A:1656:ASP:O	1:A:1659:LEU:HB2	1.80	0.82
1:A:543:TYR:HA	1:A:546:TYR:HB3	1.66	0.78
1:A:883:VAL:HA	1:A:889:THR:O	1.85	0.77
1:A:1908:ALA:O	1:A:1912:LEU:HB2	1.86	0.75
2:B:318:SER:HB3	2:B:322:LEU:H	1.52	0.74
1:A:1897:TYR:O	1:A:1901:LYS:HB2	1.87	0.74
1:A:543:TYR:HB3	1:A:579:TYR:HB3	1.68	0.74
1:A:1574:CYS:HB2	1:A:1578:ALA:HB2	1.70	0.73
1:A:443:CYS:SG	1:A:444:GLY:N	2.62	0.72
1:A:1771:ASP:O	1:A:1775:PHE:HB2	1.90	0.71
1:A:306:CYS:O	1:A:310:LEU:HB2	1.90	0.70
1:A:298:ILE:O	1:A:302:ILE:HB	1.92	0.69
1:A:654:ARG:H	1:A:667:LEU:HD23	1.59	0.67
1:A:336:GLU:HG3	1:A:338:GLU:H	1.60	0.67
1:A:271:LEU:HD13	1:A:310:LEU:HD23	1.76	0.66
1:A:384:LEU:HD11	1:A:561:ILE:HG21	1.77	0.66
1:A:1306:ALA:HB1	1:A:1372:SER:HB2	1.76	0.66
1:A:475:SER:HB2	1:A:497:GLU:H	1.60	0.66
1:A:1657:LYS:O	1:A:1661:HIS:N	2.28	0.66
1:A:372:PHE:H	1:A:373:VAL:HA	1.61	0.65
1:A:1353:ASN:O	1:A:1357:TYR:HB2	1.96	0.65
1:A:86:ARG:HA	1:A:94:LYS:HD3	1.77	0.65
1:A:449:GLU:HG2	1:A:450:ARG:HG3	1.79	0.65
1:A:67:GLY:HA3	1:A:70:LYS:HG2	1.79	0.64
1:A:640:ARG:O	1:A:672:ASN:ND2	2.30	0.64
1:A:460:LEU:HG	1:A:463:GLU:HB2	1.79	0.64
1:A:84:GLN:HG2	1:A:85:ILE:HD12	1.80	0.62
1:A:109:GLN:O	1:A:113:VAL:HB	1.98	0.62
1:A:382:GLU:O	1:A:386:LYS:N	2.31	0.62
1:A:470:GLU:HG3	1:A:516:LEU:HB3	1.82	0.62
1:A:635:ASN:HA	1:A:638:CYS:HB3	1.80	0.62
1:A:799:THR:HB	1:A:883:VAL:HB	1.82	0.62
1:A:1747:SER:O	1:A:1751:LYS:HB2	1.99	0.62
1:A:1757:TYR:O	1:A:1759:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:THR:HA	1:A:516:LEU:HB2	1.81	0.61
1:A:821:ARG:HH21	1:A:995:SER:HB2	1.64	0.61
1:A:257:CYS:HB3	1:A:567:ASP:HB3	1.83	0.61
1:A:1304:SER:HB2	1:A:1311:ASN:HD22	1.65	0.61
1:A:1839:ARG:HA	1:A:1842:ILE:HB	1.82	0.61
1:A:952:THR:HA	1:A:986:PRO:HB3	1.83	0.61
1:A:993:THR:HB	1:A:1048:TRP:HE1	1.66	0.61
1:A:651:PRO:HD2	1:A:670:PRO:HB3	1.80	0.61
1:A:633:HIS:O	1:A:636:ARG:HB3	2.01	0.61
1:A:71:THR:O	1:A:75:VAL:N	2.31	0.60
1:A:1588:LEU:HG	1:A:1589:LYS:HG3	1.81	0.60
1:A:920:PHE:HB3	1:A:982:ASN:HB2	1.82	0.60
1:A:114:ARG:HH21	1:A:123:GLU:H	1.49	0.60
1:A:1002:PRO:O	1:A:1006:ASN:N	2.27	0.60
1:A:831:LEU:HD11	1:A:834:SER:HB3	1.83	0.60
1:A:1004:HIS:O	1:A:1008:LYS:HB2	2.02	0.59
1:A:769:TYR:HB2	1:A:806:THR:O	2.02	0.59
1:A:640:ARG:HB2	1:A:670:PRO:HD2	1.84	0.59
1:A:279:ASN:O	1:A:283:ASP:CB	2.49	0.59
1:A:243:LEU:O	1:A:554:ARG:NH1	2.36	0.59
1:A:244:ASP:O	1:A:248:SER:N	2.35	0.59
1:A:51:LEU:HD22	1:A:62:VAL:HG22	1.84	0.59
1:A:134:THR:HB	1:A:135:LYS:HB2	1.84	0.59
1:A:1034:VAL:HG12	1:A:1036:GLU:H	1.68	0.58
1:A:1669:PHE:HZ	1:A:1757:TYR:H	1.50	0.58
1:A:473:TYR:HB3	1:A:501:GLN:HA	1.85	0.58
1:A:255:VAL:HG11	1:A:563:LEU:HD12	1.85	0.58
1:A:1026:SER:HA	1:A:1029:ASN:HB2	1.86	0.58
1:A:173:VAL:HG13	1:A:203:LEU:HB3	1.85	0.58
1:A:1621:CYS:SG	1:A:1694:TYR:N	2.72	0.58
1:A:1725:ARG:NH1	1:A:1846:SER:O	2.37	0.58
1:A:1332:PHE:HE1	1:A:1703:ARG:HB3	1.69	0.57
1:A:135:LYS:HA	1:A:138:TRP:HA	1.85	0.57
1:A:1583:LEU:O	1:A:1587:GLY:N	2.34	0.57
1:A:932:ILE:HB	1:A:1038:CYS:HB3	1.87	0.57
1:A:770:LEU:O	1:A:832:LYS:N	2.37	0.57
1:A:322:ALA:HA	1:A:352:LEU:HD22	1.86	0.57
1:A:1715:LEU:HD21	1:A:1827:LEU:HB3	1.87	0.57
1:A:1014:LEU:O	1:A:1019:LYS:NZ	2.38	0.56
1:A:246:TYR:OH	1:A:635:ASN:ND2	2.39	0.56
1:A:477:ASN:ND2	1:A:496:ALA:O	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ILE:HG23	1:A:1042:PRO:HG2	1.87	0.56
2:B:325:CYS:SG	2:B:326:LEU:N	2.77	0.56
1:A:338:GLU:OE1	1:A:341:HIS:ND1	2.36	0.56
1:A:137:ARG:H	1:A:139:ASN:N	2.02	0.56
1:A:1692:TYR:HA	1:A:1761:VAL:HG23	1.88	0.56
1:A:863:PRO:HD2	1:A:869:PRO:HA	1.87	0.56
1:A:253:ILE:HD12	1:A:561:ILE:HG23	1.86	0.55
1:A:1732:LEU:HD23	1:A:1735:LEU:HD12	1.88	0.55
1:A:510:ALA:O	1:A:514:ASN:ND2	2.40	0.55
1:A:86:ARG:NH2	1:A:87:GLY:O	2.40	0.55
1:A:365:PRO:HB3	1:A:368:LEU:HD13	1.87	0.55
1:A:380:LEU:O	1:A:384:LEU:HB2	2.07	0.55
1:A:1908:ALA:HA	1:A:1911:SER:HB3	1.89	0.55
1:A:283:ASP:OD2	2:B:324:GLN:NE2	2.40	0.54
1:A:702:LEU:O	1:A:706:GLY:N	2.40	0.54
1:A:1349:LYS:O	1:A:1355:ASN:ND2	2.34	0.54
1:A:1607:ARG:NH2	1:A:1682:TYR:OH	2.40	0.54
1:A:1614:GLN:NE2	1:A:1699:ASP:O	2.39	0.54
1:A:1019:LYS:O	1:A:1023:LYS:HB3	2.07	0.54
1:A:1359:LEU:HD11	1:A:1587:GLY:HA2	1.90	0.54
1:A:235:GLU:HA	1:A:590:CYS:HB3	1.89	0.54
1:A:771:TYR:HA	1:A:831:LEU:HA	1.90	0.54
1:A:1669:PHE:O	1:A:1672:LYS:HB3	2.08	0.54
1:A:175:ASP:HA	1:A:205:LEU:HB2	1.89	0.54
1:A:996:ARG:NH2	1:A:1001:THR:OG1	2.33	0.54
1:A:368:LEU:HD23	1:A:369:ASP:H	1.72	0.54
1:A:457:LEU:O	1:A:461:ILE:HB	2.07	0.54
1:A:800:ARG:HE	1:A:882:ASN:HB2	1.72	0.54
1:A:306:CYS:O	1:A:310:LEU:CB	2.56	0.54
1:A:1028:GLN:HA	1:A:1031:GLN:HE21	1.73	0.54
1:A:1043:ILE:HG23	1:A:1047:LEU:HD23	1.90	0.54
1:A:92:ASN:H	1:A:95:ARG:HH22	1.56	0.53
1:A:770:LEU:HA	1:A:804:ILE:O	2.07	0.53
1:A:1708:GLY:HA2	1:A:1711:ILE:HD12	1.90	0.53
1:A:211:ASN:ND2	1:A:215:ASP:OD1	2.41	0.53
1:A:664:TYR:HA	1:A:680:VAL:HG11	1.90	0.53
1:A:1688:THR:HA	1:A:1759:LYS:HB2	1.90	0.53
1:A:354:LYS:HG3	2:B:361:ILE:HG21	1.89	0.53
1:A:931:VAL:HA	1:A:945:PHE:O	2.08	0.53
1:A:1353:ASN:O	1:A:1357:TYR:CB	2.57	0.53
1:A:1879:ARG:HD2	1:A:1891:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PHE:N	1:A:373:VAL:HA	2.24	0.53
1:A:933:ILE:HD12	1:A:942:PRO:HG2	1.91	0.53
1:A:662:THR:HG22	1:A:685:SER:HB3	1.91	0.52
1:A:374:THR:HG21	1:A:378:ILE:H	1.74	0.52
1:A:680:VAL:HG12	1:A:682:PRO:HD3	1.92	0.52
1:A:70:LYS:O	1:A:73:ILE:HB	2.09	0.52
1:A:133:TRP:HB3	1:A:158:VAL:HG12	1.91	0.52
1:A:152:CYS:SG	1:A:153:TYR:N	2.83	0.52
1:A:190:MET:O	1:A:194:GLU:N	2.43	0.52
1:A:1688:THR:O	1:A:1695:ASN:ND2	2.42	0.52
1:A:1735:LEU:O	1:A:1739:LEU:HB2	2.10	0.52
1:A:132:SER:HB2	1:A:136:GLU:HG2	1.92	0.52
1:A:770:LEU:HD11	1:A:881:LEU:HD21	1.92	0.52
1:A:523:GLU:O	1:A:552:ARG:NH2	2.43	0.52
1:A:97:VAL:HA	1:A:147:VAL:HG13	1.91	0.52
1:A:375:PRO:HG3	1:A:440:ASN:HA	1.91	0.52
1:A:649:LEU:HB3	1:A:651:PRO:HD3	1.92	0.52
1:A:937:ARG:HH22	1:A:943:HIS:HB2	1.75	0.52
1:A:77:LEU:O	1:A:81:LEU:N	2.43	0.51
1:A:114:ARG:HG2	1:A:121:VAL:HG23	1.92	0.51
1:A:171:LEU:HD11	1:A:201:ARG:HB2	1.92	0.51
1:A:502:GLU:HA	1:A:505:LEU:HD12	1.92	0.51
1:A:1725:ARG:HH12	1:A:1847:ALA:HA	1.74	0.51
1:A:384:LEU:HD23	1:A:563:LEU:HD13	1.92	0.51
1:A:371:LYS:H	1:A:465:GLY:HA3	1.75	0.51
1:A:932:ILE:HG22	1:A:1040:ILE:HA	1.92	0.51
1:A:61:ILE:HB	1:A:234:ALA:HB2	1.93	0.51
1:A:236:THR:OG1	1:A:590:CYS:SG	2.67	0.51
1:A:769:TYR:HA	1:A:834:SER:HA	1.91	0.51
1:A:949:ASP:H	1:A:989:ASP:HB3	1.76	0.51
1:A:1070:LEU:HD13	1:A:1301:LEU:HD11	1.92	0.51
1:A:1656:ASP:HA	1:A:1659:LEU:HD13	1.93	0.50
1:A:299:SER:O	1:A:303:LEU:HB2	2.10	0.50
1:A:946:TYR:HD1	1:A:1045:ALA:HB1	1.76	0.50
1:A:1901:LYS:O	1:A:1905:ALA:CB	2.59	0.50
2:B:314:ILE:HD11	2:B:326:LEU:HG	1.92	0.50
1:A:113:VAL:HG12	1:A:121:VAL:HG21	1.92	0.50
1:A:225:LYS:HA	1:A:228:LYS:HE3	1.93	0.50
1:A:376:LYS:HG3	1:A:377:VAL:HG23	1.92	0.50
2:B:331:THR:OG1	2:B:333:PRO:O	2.21	0.50
1:A:75:VAL:O	1:A:78:THR:OG1	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HG3	1:A:385:ARG:HD2	1.94	0.50
1:A:343:LYS:HE2	2:B:312:LEU:HD22	1.93	0.50
1:A:1656:ASP:HB3	1:A:1659:LEU:HD22	1.94	0.50
1:A:881:LEU:HA	1:A:891:ASP:O	2.12	0.50
1:A:1771:ASP:O	1:A:1775:PHE:CB	2.59	0.50
1:A:381:LEU:HA	1:A:384:LEU:HD13	1.94	0.49
1:A:1584:CYS:HA	1:A:1588:LEU:HB3	1.93	0.49
1:A:87:GLY:H	1:A:94:LYS:HB2	1.77	0.49
1:A:854:PHE:HA	1:A:858:LEU:HD12	1.95	0.49
1:A:466:LYS:HG2	1:A:468:ASP:H	1.77	0.49
1:A:246:TYR:HB3	1:A:554:ARG:HH22	1.77	0.49
2:B:329:LEU:N	2:B:335:THR:O	2.43	0.49
1:A:260:PHE:H	1:A:261:THR:HA	1.77	0.49
1:A:1009:GLY:HA2	1:A:1013:PRO:HG2	1.94	0.49
1:A:1697:ILE:HG22	1:A:1698:THR:HG23	1.95	0.49
1:A:90:SER:O	1:A:92:ASN:ND2	2.45	0.49
1:A:136:GLU:HB3	1:A:139:ASN:HA	1.95	0.49
1:A:451:ARG:HD3	1:A:484:ILE:HB	1.93	0.49
1:A:541:THR:OG1	1:A:542:GLU:N	2.46	0.49
2:B:350:GLU:OE1	2:B:353:ARG:NH2	2.39	0.49
1:A:447:PHE:N	1:A:535:VAL:O	2.46	0.49
1:A:442:LEU:HA	1:A:515:LEU:HD13	1.94	0.48
1:A:524:GLU:HA	1:A:552:ARG:HH22	1.78	0.48
1:A:73:ILE:O	1:A:76:LEU:HB2	2.13	0.48
1:A:194:GLU:HA	1:A:195:ASN:HA	1.63	0.48
1:A:92:ASN:O	1:A:95:ARG:NH1	2.46	0.48
1:A:128:GLU:HB3	1:A:130:ASN:H	1.76	0.48
1:A:1660:ASN:HA	1:A:1663:ILE:HG12	1.96	0.48
2:B:289:ALA:HB3	2:B:357:GLN:HG3	1.96	0.48
1:A:702:LEU:HD23	1:A:706:GLY:HA2	1.96	0.48
1:A:176:GLU:N	1:A:205:LEU:O	2.46	0.48
1:A:445:ILE:HG23	1:A:520:SER:H	1.78	0.48
1:A:457:LEU:HD11	1:A:519:THR:HG23	1.95	0.48
1:A:532:ASN:HB2	1:A:559:ASN:HD22	1.78	0.48
1:A:917:GLU:HG2	1:A:918:THR:HG23	1.96	0.48
1:A:1897:TYR:O	1:A:1901:LYS:CB	2.60	0.48
1:A:1807:ALA:HA	1:A:1810:ASP:HB2	1.96	0.48
1:A:667:LEU:N	1:A:678:SER:OG	2.47	0.48
1:A:65:ASN:OD1	1:A:544:ARG:NE	2.44	0.48
1:A:376:LYS:HA	1:A:380:LEU:HD22	1.96	0.48
1:A:454:ALA:HB1	1:A:471:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1908:ALA:O	1:A:1912:LEU:CB	2.59	0.47
1:A:312:VAL:HG12	1:A:313:LEU:HG	1.96	0.47
1:A:534:VAL:HG13	1:A:560:TYR:HA	1.96	0.47
1:A:862:LYS:HZ1	1:A:1374:PHE:HE1	1.60	0.47
1:A:252:GLU:HG3	1:A:560:TYR:HD2	1.79	0.47
1:A:449:GLU:OE2	1:A:450:ARG:NH1	2.48	0.47
1:A:181:ILE:O	1:A:187:ARG:NH2	2.42	0.47
1:A:1314:ARG:HB3	1:A:1721:TYR:HE1	1.80	0.47
1:A:214:CYS:SG	1:A:218:GLU:HG3	2.55	0.47
1:A:126:ASN:OD1	1:A:131:ALA:N	2.33	0.47
1:A:1340:GLU:O	1:A:1344:SER:CB	2.62	0.47
2:B:328:GLU:HG3	2:B:336:VAL:HG12	1.97	0.47
1:A:343:LYS:HD2	2:B:336:VAL:HG11	1.96	0.47
1:A:577:LYS:HA	1:A:580:LYS:HE2	1.96	0.47
1:A:671:ILE:HG22	1:A:674:PRO:HB3	1.96	0.47
1:A:680:VAL:HG13	1:A:694:VAL:HG11	1.96	0.47
1:A:1061:LEU:HD23	1:A:1064:LEU:HD12	1.96	0.47
1:A:1330:TYR:CZ	1:A:1588:LEU:HD22	2.49	0.47
2:B:313:ASP:OD2	2:B:348:ARG:NH2	2.48	0.47
1:A:320:LYS:HB2	1:A:456:VAL:HG22	1.96	0.47
1:A:1670:GLU:O	1:A:1674:ASN:N	2.45	0.47
1:A:508:PHE:HD1	1:A:513:THR:HG22	1.80	0.47
1:A:954:LEU:HB3	1:A:987:LEU:HD12	1.97	0.47
1:A:1864:THR:O	1:A:1885:VAL:N	2.44	0.47
1:A:82:SER:O	1:A:86:ARG:N	2.48	0.46
1:A:441:ILE:HG21	1:A:532:ASN:HD21	1.80	0.46
1:A:673:SER:HB2	1:A:708:LEU:HD22	1.96	0.46
1:A:1717:THR:HG21	1:A:1736:ARG:HD2	1.97	0.46
1:A:536:ARG:HB3	1:A:539:LEU:HB3	1.95	0.46
1:A:1758:PHE:HD1	1:A:1811:ILE:HD13	1.81	0.46
1:A:53:GLU:HA	1:A:56:LEU:HD13	1.97	0.46
1:A:1365:LEU:HA	1:A:1368:ARG:HD3	1.96	0.46
1:A:1669:PHE:CZ	1:A:1756:LYS:HB2	2.51	0.46
1:A:258:GLY:O	1:A:260:PHE:HA	2.15	0.46
1:A:371:LYS:HA	1:A:371:LYS:HD3	1.70	0.46
1:A:643:SER:O	1:A:672:ASN:N	2.47	0.46
1:A:897:MET:HA	1:A:900:ILE:HG12	1.98	0.46
1:A:468:ASP:HB2	1:A:515:LEU:HG	1.98	0.46
1:A:496:ALA:HB1	1:A:501:GLN:HE22	1.79	0.46
1:A:571:SER:O	1:A:575:ASP:HB2	2.15	0.46
1:A:70:LYS:HD2	1:A:205:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:LYS:NZ	1:A:866:GLU:H	2.13	0.46
1:A:996:ARG:HE	1:A:999:LEU:HD23	1.81	0.46
1:A:1600:GLU:HA	1:A:1601:LYS:HA	1.62	0.46
1:A:118:ASP:OD2	1:A:1756:LYS:NZ	2.36	0.46
1:A:244:ASP:OD1	1:A:247:THR:OG1	2.33	0.46
1:A:1677:PHE:O	1:A:1680:LYS:NZ	2.45	0.46
1:A:137:ARG:HB3	1:A:140:GLN:H	1.80	0.46
1:A:923:LYS:HB3	1:A:925:GLU:HG2	1.96	0.46
1:A:128:GLU:HB3	1:A:130:ASN:N	2.31	0.46
1:A:1058:LEU:HD23	1:A:1061:LEU:HD12	1.98	0.46
1:A:137:ARG:HD3	1:A:140:GLN:HB2	1.99	0.45
1:A:257:CYS:HB2	1:A:568:LYS:HG3	1.98	0.45
1:A:779:THR:HB	1:A:824:GLU:HB3	1.98	0.45
1:A:271:LEU:HD11	1:A:307:ARG:HG3	1.97	0.45
1:A:446:ILE:H	1:A:519:THR:HG22	1.81	0.45
1:A:1601:LYS:HD3	1:A:1605:PRO:HG3	1.97	0.45
1:A:1684:LEU:O	1:A:1688:THR:OG1	2.18	0.45
1:A:1762:SER:HB3	1:A:1765:LEU:HD23	1.99	0.45
1:A:1823:SER:HB2	1:A:1826:SER:HB3	1.98	0.45
2:B:345:GLU:OE2	2:B:348:ARG:NH1	2.49	0.45
1:A:134:THR:H	1:A:135:LYS:C	2.20	0.45
1:A:640:ARG:HG3	1:A:669:LEU:HB3	1.97	0.45
1:A:1852:SER:OG	1:A:1856:GLU:N	2.49	0.45
1:A:1340:GLU:O	1:A:1344:SER:HB3	2.16	0.45
1:A:1669:PHE:CE2	1:A:1757:TYR:HB2	2.52	0.45
1:A:1669:PHE:HE2	1:A:1757:TYR:HB2	1.82	0.45
1:A:1008:LYS:O	1:A:1012:LEU:N	2.42	0.45
1:A:1701:TYR:HE2	1:A:1810:ASP:HB3	1.82	0.45
2:B:308:HIS:N	2:B:330:SER:OG	2.47	0.45
1:A:121:VAL:HG12	1:A:147:VAL:HB	1.99	0.45
1:A:167:SER:HA	1:A:169:ILE:HG12	1.98	0.45
1:A:118:ASP:HB3	1:A:1668:ASN:HD21	1.82	0.45
1:A:128:GLU:H	1:A:129:VAL:HA	1.82	0.45
1:A:633:HIS:O	1:A:636:ARG:CB	2.65	0.45
1:A:1747:SER:O	1:A:1751:LYS:CB	2.63	0.45
1:A:295:SER:HB3	1:A:341:HIS:HD2	1.82	0.44
1:A:376:LYS:HB3	1:A:441:ILE:HG13	1.98	0.44
1:A:634:ILE:HD12	1:A:695:ALA:HB3	1.99	0.44
1:A:636:ARG:NH2	1:A:719:THR:OG1	2.50	0.44
1:A:900:ILE:HD12	1:A:1042:PRO:HG2	1.98	0.44
1:A:958:SER:O	1:A:968:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1658:THR:HA	1:A:1661:HIS:HD2	1.81	0.44
1:A:347:PHE:CD1	2:B:337:CYS:HA	2.52	0.44
1:A:354:LYS:HD3	2:B:358:TYR:HD1	1.82	0.44
1:A:1315:LEU:HB2	1:A:1565:ALA:HB1	1.98	0.44
1:A:1612:SER:HB2	1:A:1615:LYS:HB2	1.99	0.44
1:A:256:ASP:HA	1:A:566:THR:HB	2.00	0.44
1:A:298:ILE:HG23	1:A:302:ILE:HD12	2.00	0.44
1:A:375:PRO:HB2	1:A:441:ILE:HB	1.99	0.44
1:A:1853:PRO:HB2	1:A:1905:ALA:HB3	1.98	0.44
1:A:319:ASP:HB2	1:A:359:CYS:HB2	1.98	0.44
1:A:229:ILE:O	1:A:231:LYS:NZ	2.49	0.44
1:A:931:VAL:HG21	1:A:1048:TRP:CG	2.53	0.44
1:A:1612:SER:OG	1:A:1616:ASN:OD1	2.36	0.44
1:A:111:SER:OG	1:A:112:ALA:N	2.51	0.44
1:A:853:ILE:HA	1:A:857:ILE:HD12	1.99	0.43
1:A:74:ALA:O	1:A:78:THR:N	2.52	0.43
1:A:359:CYS:HA	1:A:363:PHE:HD2	1.83	0.43
1:A:589:LYS:HA	1:A:592:LYS:HB2	1.99	0.43
1:A:956:PRO:HG2	1:A:983:LEU:HA	2.00	0.43
1:A:1557:LYS:HG3	1:A:1559:ILE:HG12	2.00	0.43
1:A:1855:ARG:HG2	1:A:1898:ARG:HH12	1.83	0.43
1:A:280:PHE:CE2	2:B:338:HIS:HB2	2.53	0.43
1:A:576:LEU:HA	1:A:579:TYR:HD2	1.83	0.43
1:A:932:ILE:HG13	1:A:945:PHE:HB2	2.01	0.43
1:A:369:ASP:HA	1:A:370:LEU:HA	1.81	0.43
1:A:240:LEU:HB2	1:A:244:ASP:HB2	2.00	0.43
1:A:462:LYS:N	1:A:469:PRO:HG3	2.33	0.43
1:A:53:GLU:HG2	1:A:654:ARG:HH22	1.83	0.43
1:A:486:LYS:HG3	1:A:521:ILE:HG13	1.99	0.43
1:A:899:ASP:HA	1:A:902:LYS:HD2	2.01	0.43
1:A:922:PHE:HE1	1:A:988:LEU:HD11	1.84	0.43
1:A:447:PHE:CD1	1:A:523:GLU:HG2	2.54	0.43
1:A:651:PRO:HG3	1:A:668:TYR:HD2	1.84	0.43
1:A:667:LEU:HB2	1:A:678:SER:HB3	2.01	0.43
1:A:909:ILE:HD12	1:A:939:PHE:HA	2.01	0.43
1:A:286:ILE:HD13	2:B:314:ILE:HG23	2.01	0.42
1:A:536:ARG:NH2	1:A:539:LEU:O	2.52	0.42
1:A:1058:LEU:HA	1:A:1061:LEU:HB2	2.00	0.42
1:A:451:ARG:HD3	1:A:485:GLY:H	1.84	0.42
1:A:1688:THR:HG23	1:A:1759:LYS:HB2	2.00	0.42
1:A:1689:HIS:CD2	1:A:1691:SER:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:NH1	1:A:992:HIS:O	2.46	0.42
1:A:996:ARG:NH2	1:A:1006:ASN:OD1	2.52	0.42
1:A:1026:SER:O	1:A:1030:LYS:N	2.44	0.42
1:A:1339:HIS:H	1:A:1343:LEU:HD13	1.84	0.42
1:A:1594:ILE:H	1:A:1594:ILE:HG13	1.61	0.42
1:A:93:GLY:O	1:A:170:ASN:ND2	2.46	0.42
1:A:185:PRO:O	1:A:189:ILE:HG12	2.19	0.42
1:A:468:ASP:HB3	1:A:516:LEU:HA	2.01	0.42
1:A:153:TYR:HD1	1:A:156:LEU:HD21	1.84	0.42
1:A:989:ASP:HA	1:A:1032:ILE:HG23	2.00	0.42
1:A:992:HIS:HB3	1:A:1029:ASN:HD21	1.84	0.42
1:A:1047:LEU:HA	1:A:1050:LYS:HE2	2.02	0.42
1:A:333:ILE:HA	1:A:345:LEU:HD13	2.01	0.42
1:A:376:LYS:HD2	1:A:441:ILE:HG13	2.02	0.42
1:A:1692:TYR:O	1:A:1696:THR:OG1	2.38	0.42
1:A:259:PRO:HA	1:A:260:PHE:CG	2.55	0.42
1:A:240:LEU:O	1:A:244:ASP:CB	2.68	0.42
1:A:846:ILE:O	1:A:850:HIS:HB2	2.20	0.42
1:A:1819:ILE:O	1:A:1823:SER:N	2.51	0.42
1:A:225:LYS:HA	1:A:228:LYS:HG2	2.02	0.42
1:A:535:VAL:HG12	1:A:537:PHE:HB2	2.01	0.42
1:A:111:SER:O	1:A:1774:GLN:NE2	2.53	0.41
1:A:451:ARG:NH1	1:A:494:MET:O	2.41	0.41
1:A:925:GLU:HA	1:A:928:GLN:HG2	2.02	0.41
1:A:1873:THR:HG21	1:A:1879:ARG:HB3	2.01	0.41
1:A:631:ILE:HA	1:A:634:ILE:HB	2.02	0.41
1:A:1750:VAL:HG12	1:A:1773:VAL:HG22	2.01	0.41
1:A:536:ARG:HG2	1:A:539:LEU:HD23	2.02	0.41
1:A:951:TYR:HD2	1:A:1032:ILE:HG21	1.84	0.41
1:A:373:VAL:HG23	1:A:466:LYS:HB2	2.02	0.41
1:A:631:ILE:O	1:A:635:ASN:N	2.40	0.41
1:A:1576:GLU:HG2	1:A:1580:GLN:HE21	1.85	0.41
1:A:1595:LYS:HA	1:A:1598:ASP:HB2	2.03	0.41
1:A:69:GLY:O	1:A:72:PHE:HB3	2.20	0.41
1:A:256:ASP:N	1:A:256:ASP:OD1	2.51	0.41
1:A:536:ARG:HD2	1:A:549:SER:HB2	2.03	0.41
1:A:1054:LEU:HD23	1:A:1057:ILE:HD12	2.02	0.41
1:A:1339:HIS:HB2	1:A:1342:ARG:HB3	2.02	0.41
1:A:77:LEU:HA	1:A:77:LEU:HD23	1.89	0.41
1:A:264:SER:HB3	1:A:267:TYR:HB3	2.02	0.41
1:A:364:SER:HA	1:A:365:PRO:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:VAL:HA	1:A:507:LYS:HB2	2.03	0.41
1:A:792:LEU:HD22	1:A:822:SER:HA	2.02	0.41
1:A:865:LEU:HD22	1:A:1374:PHE:CD1	2.56	0.41
1:A:1316:GLU:O	1:A:1320:ASP:HB2	2.21	0.41
1:A:1817:GLY:O	1:A:1821:MET:HG2	2.21	0.41
1:A:64:LEU:HB3	1:A:67:GLY:HA2	2.03	0.41
1:A:73:ILE:HA	1:A:76:LEU:HD12	2.02	0.41
1:A:1863:GLU:HG2	1:A:1864:THR:HG23	2.02	0.41
1:A:1749:ALA:O	1:A:1754:TYR:N	2.46	0.41
2:B:318:SER:OG	2:B:319:LEU:N	2.54	0.41
1:A:283:ASP:HB3	2:B:324:GLN:HE22	1.85	0.41
2:B:309:VAL:HA	2:B:329:LEU:HD23	2.03	0.41
1:A:65:ASN:ND2	1:A:544:ARG:HG2	2.36	0.41
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.91	0.41
1:A:1658:THR:O	1:A:1661:HIS:HB2	2.21	0.41
1:A:105:GLN:HA	1:A:108:GLN:HB2	2.03	0.40
1:A:274:LEU:HG	1:A:303:LEU:HD22	2.03	0.40
1:A:471:LEU:HD12	1:A:472:ALA:H	1.86	0.40
1:A:574:GLU:HA	1:A:577:LYS:HE2	2.01	0.40
1:A:781:LEU:HD12	1:A:782:PRO:HD2	2.03	0.40
1:A:1663:ILE:HA	1:A:1666:PHE:CD2	2.56	0.40
1:A:1839:ARG:O	1:A:1843:GLU:HB2	2.21	0.40
1:A:1758:PHE:CD1	1:A:1811:ILE:HD13	2.55	0.40
1:A:444:GLY:HA3	1:A:533:LEU:HB3	2.02	0.40
1:A:137:ARG:H	1:A:139:ASN:H	1.70	0.40
1:A:648:HIS:HA	1:A:649:LEU:HA	1.86	0.40
1:A:640:ARG:HH11	1:A:673:SER:HB3	1.86	0.40
1:A:1735:LEU:HD23	1:A:1735:LEU:HA	1.95	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	1296/1922 (67%)	1059 (82%)	233 (18%)	4 (0%)	41	76
2	B	73/366 (20%)	69 (94%)	4 (6%)	0	100	100
All	All	1369/2288 (60%)	1128 (82%)	237 (17%)	4 (0%)	44	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	875	ALA
1	A	139	ASN
1	A	659	PRO
1	A	259	PRO

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	1182/1730 (68%)	1178 (100%)	4 (0%)	92	95
2	B	60/301 (20%)	60 (100%)	0	100	100
All	All	1242/2031 (61%)	1238 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	371	LYS
1	A	554	ARG
1	A	1060	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	146	GLN
1	A	532	ASN

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Mol	Chain	Res	Type
1	A	559	ASN
1	A	635	ASN
1	A	928	GLN
1	A	1029	ASN
1	A	1311	ASN
1	A	1614	GLN
1	A	1660	ASN
1	A	1661	HIS
1	A	1774	GLN
2	B	324	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)

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 (i)

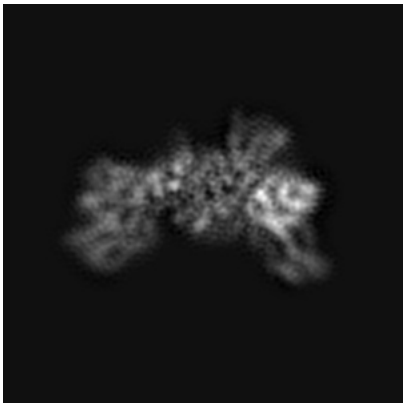
This section contains visualisations of the EMDB entry EMD-6904. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

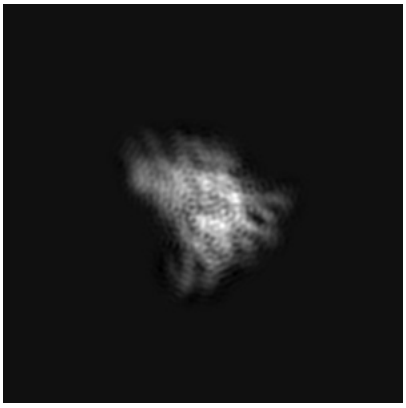
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

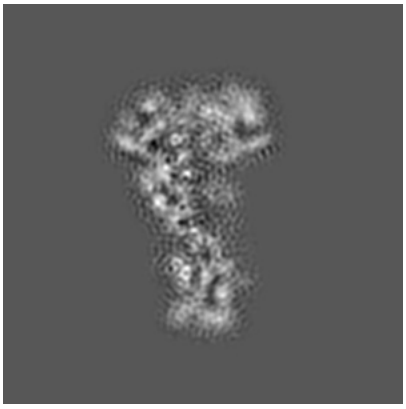


Z

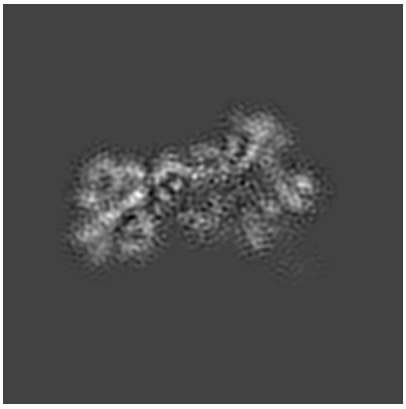
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 84



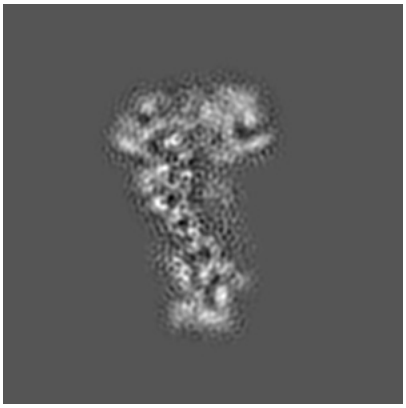
Y Index: 84

Z Index: 84

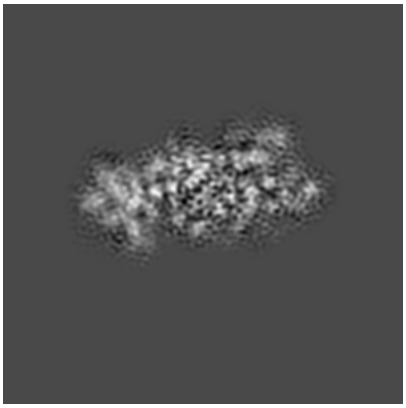
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

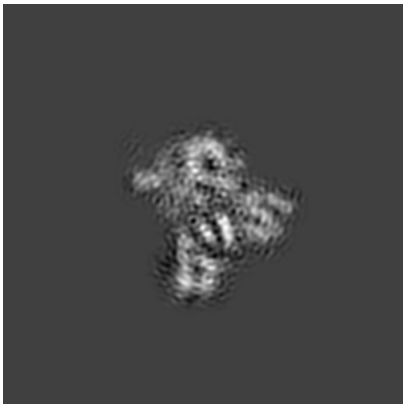
6.3.1 Primary map



X Index: 85



Y Index: 75



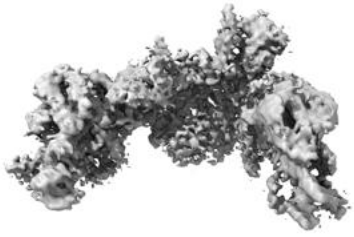
Z Index: 111

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

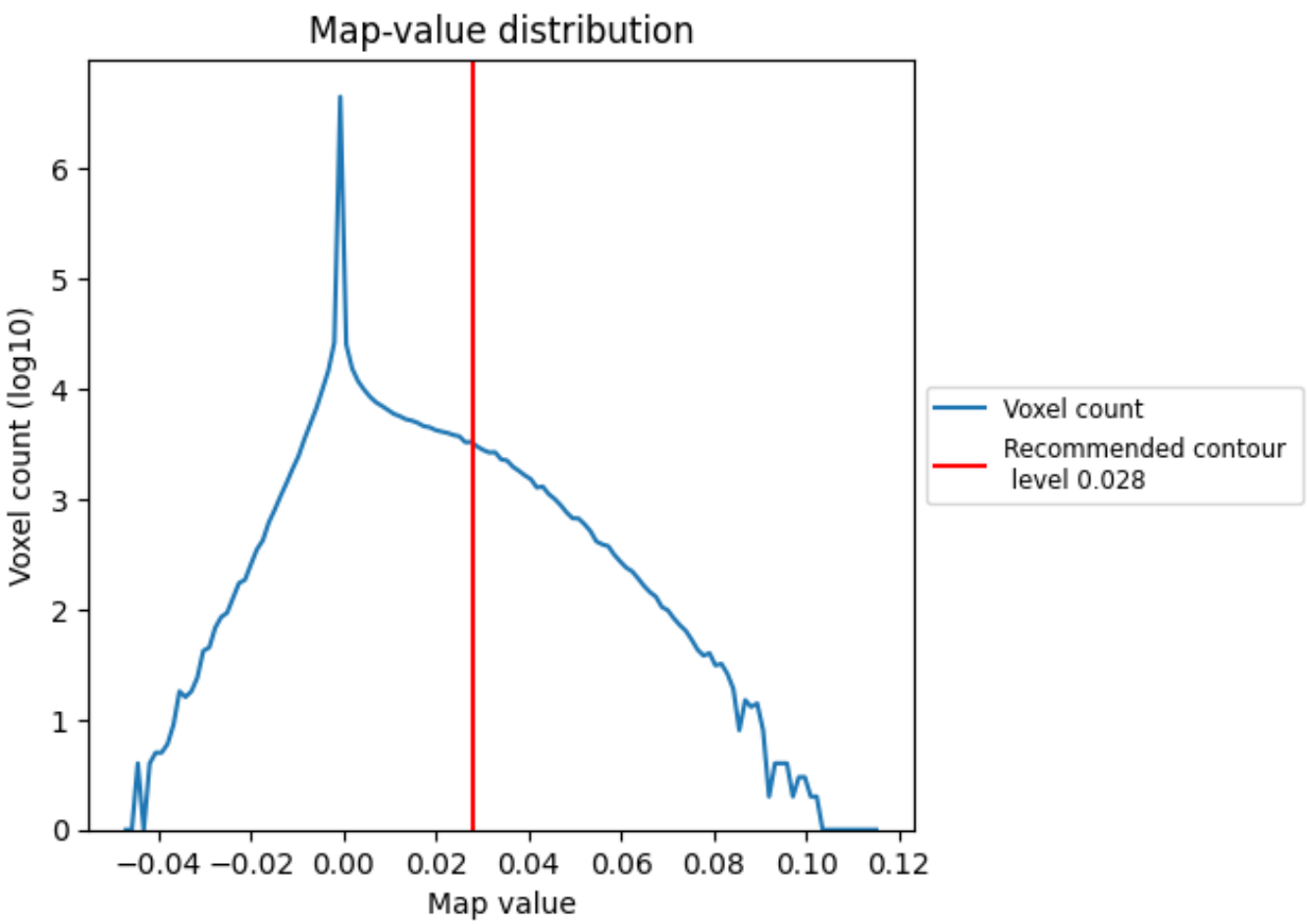
6.5 Mask visualisation (i)

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

7 Map analysis (i)

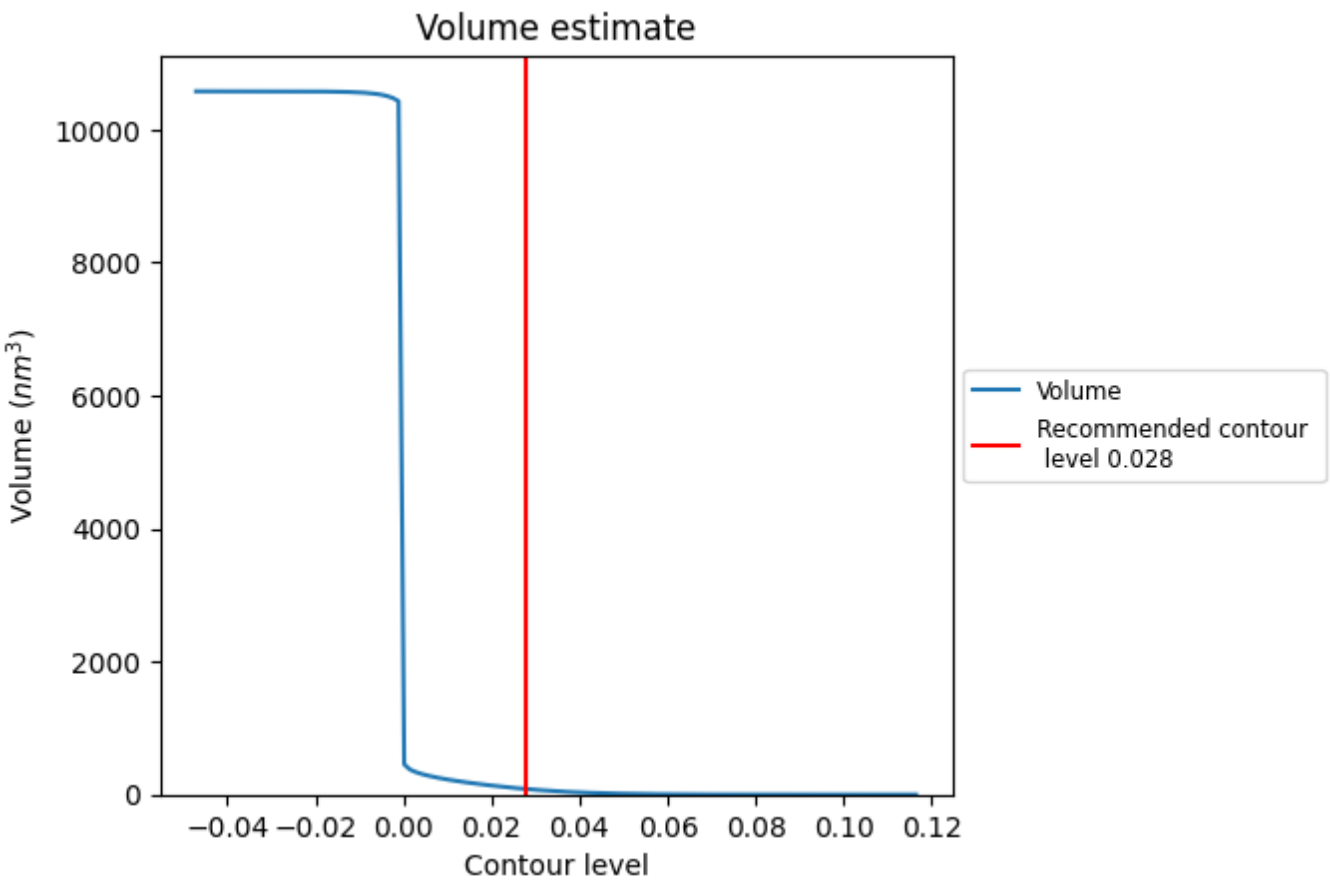
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

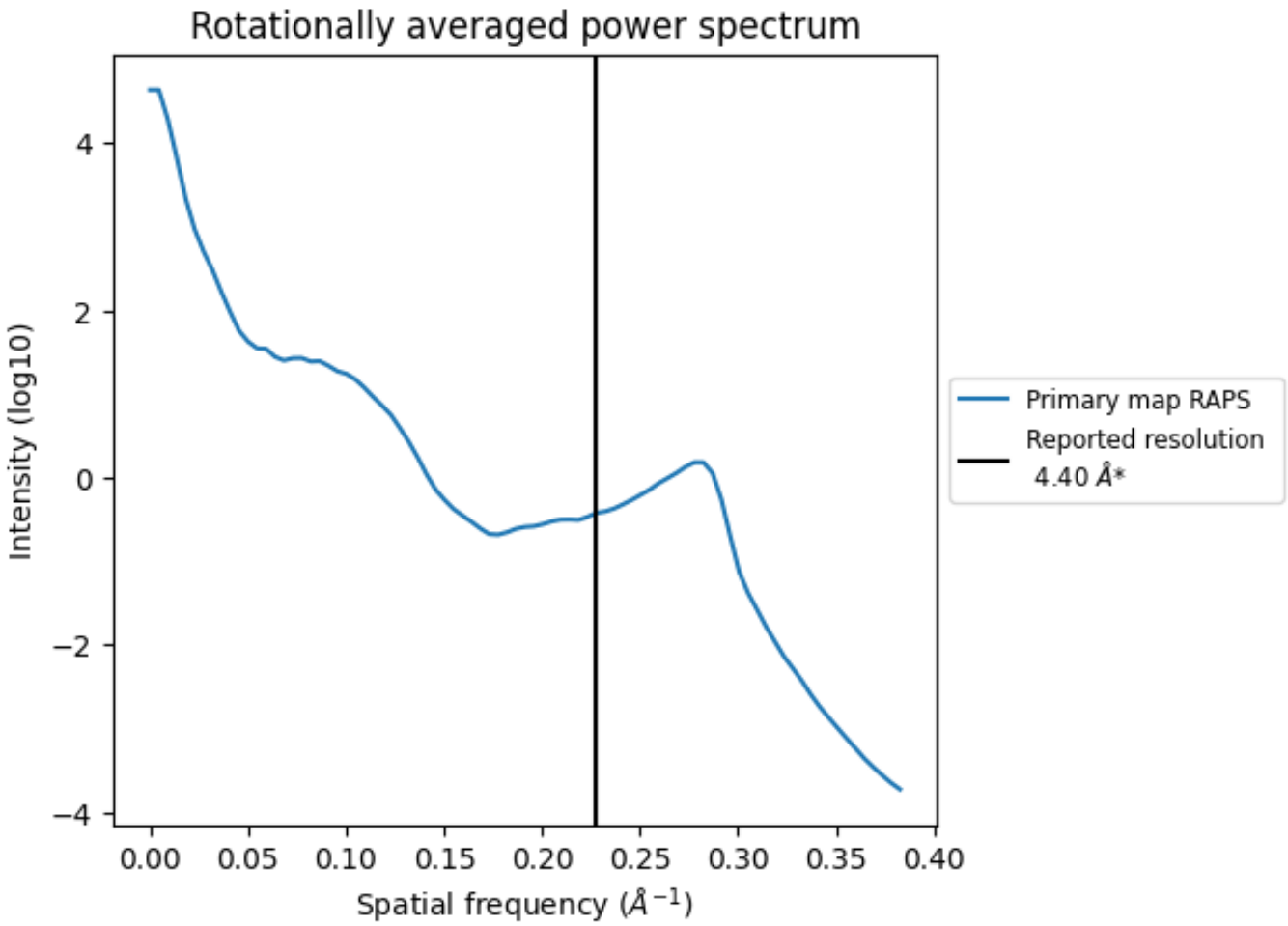
7.2 Volume estimate (i)



The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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 0.227 Å^{-1}

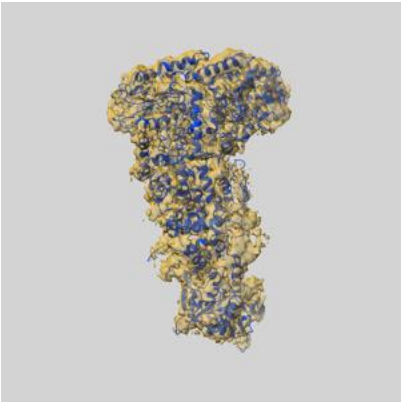
8 Fourier-Shell correlation (i)

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

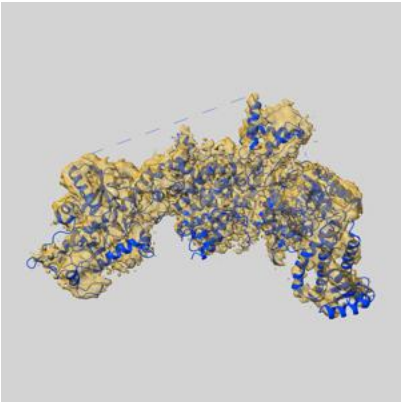
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6904 and PDB model 5ZAK. Per-residue inclusion information can be found in section 3 on page 4.

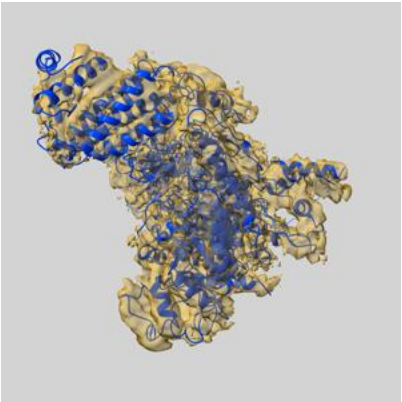
9.1 Map-model overlay (i)



X



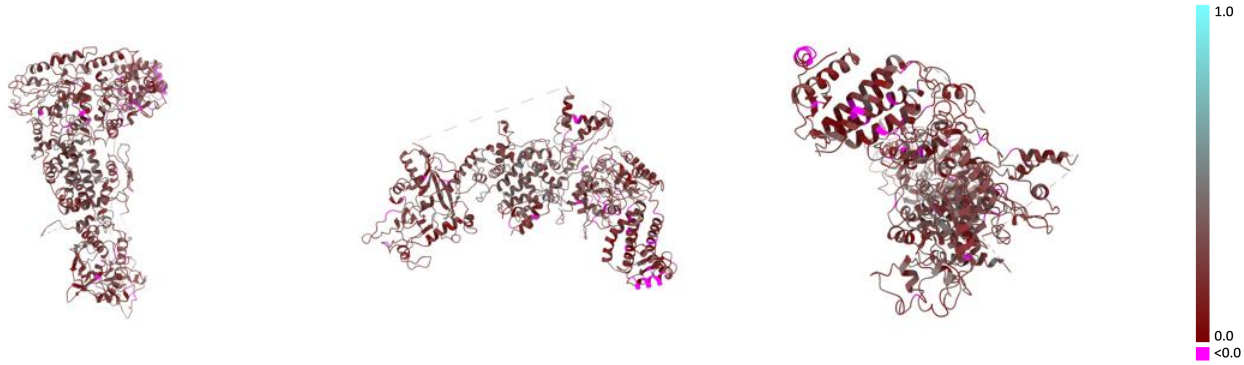
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

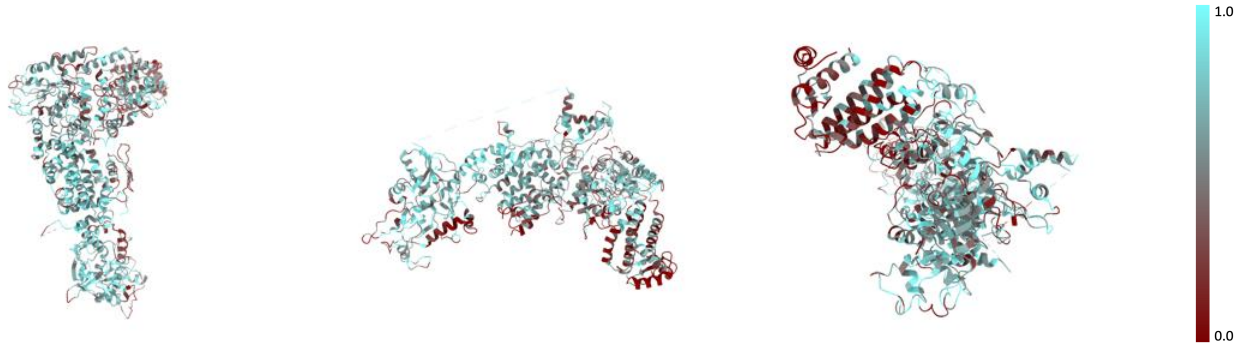
9.2 Q-score mapped to coordinate model (i)



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.

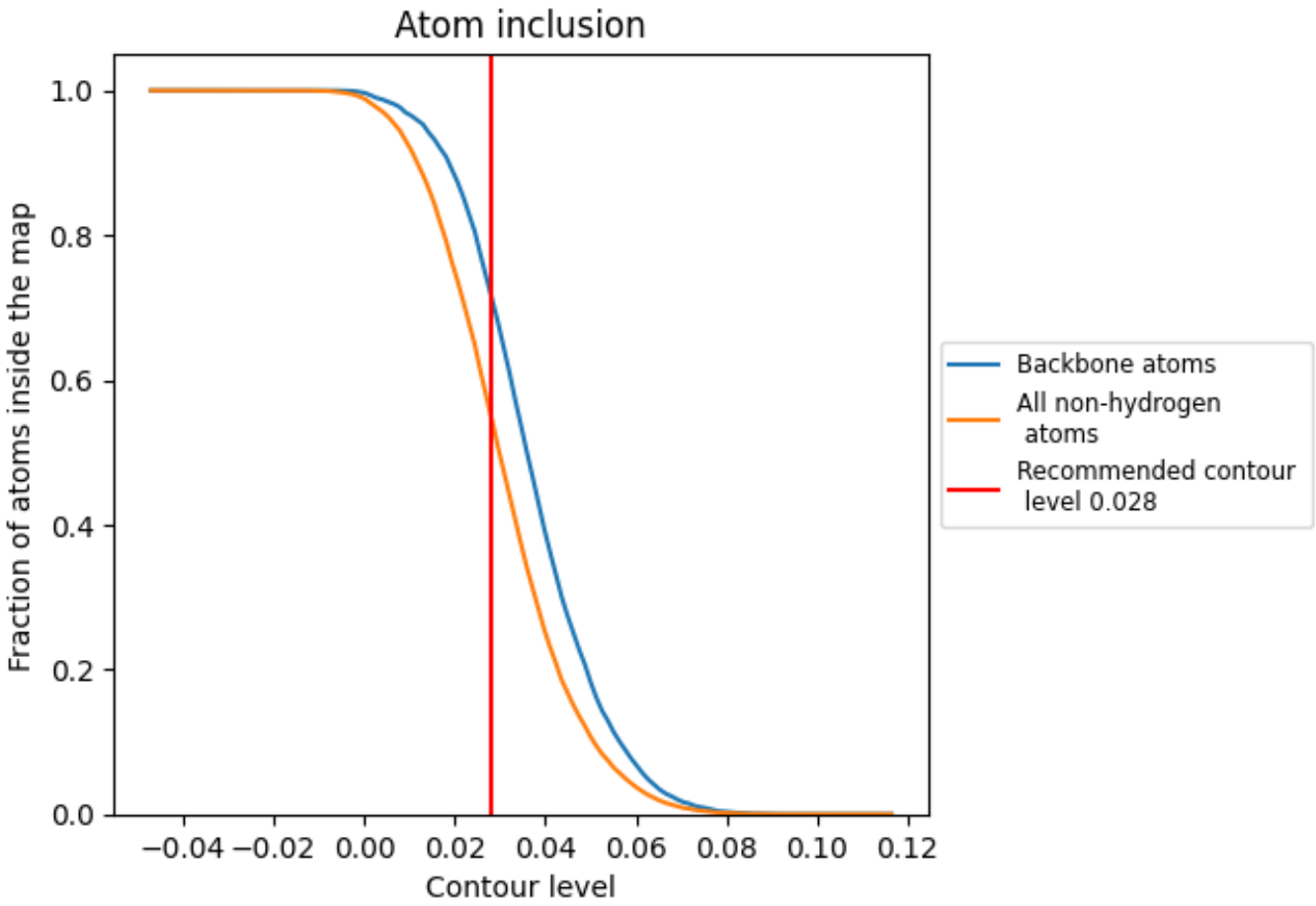
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 55% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5488	0.2500
A	0.5634	0.2540
B	0.2737	0.1680