



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 5OEJ / pdb_00005oej
EMDB ID : EMD-3790
Title : Structure of Tra1 subunit within the chromatin modifying complex SAGA
Authors : Sharov, G.; Voltz, K.; Durand, A.; Kolesnikova, O.; Papai, G.; Myasnikov, A.G.; Dejaegere, A.; Ben-Shem, A.; Schultz, P.
Deposited on : 2017-07-07
Resolution : 5.70 Å(reported)
Based on initial model : 4JSN

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

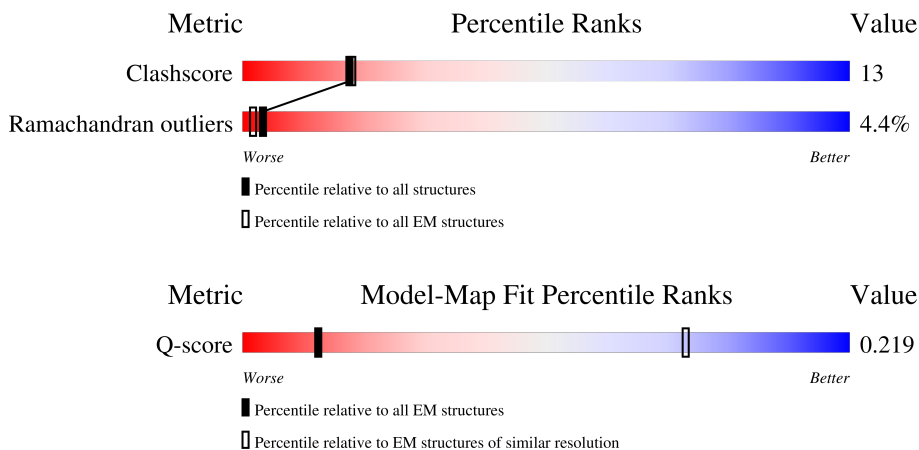
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (5.20 - 6.20)

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 $\leq 5\%$. 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	B	3825	19% 60% 14% 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14023 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.

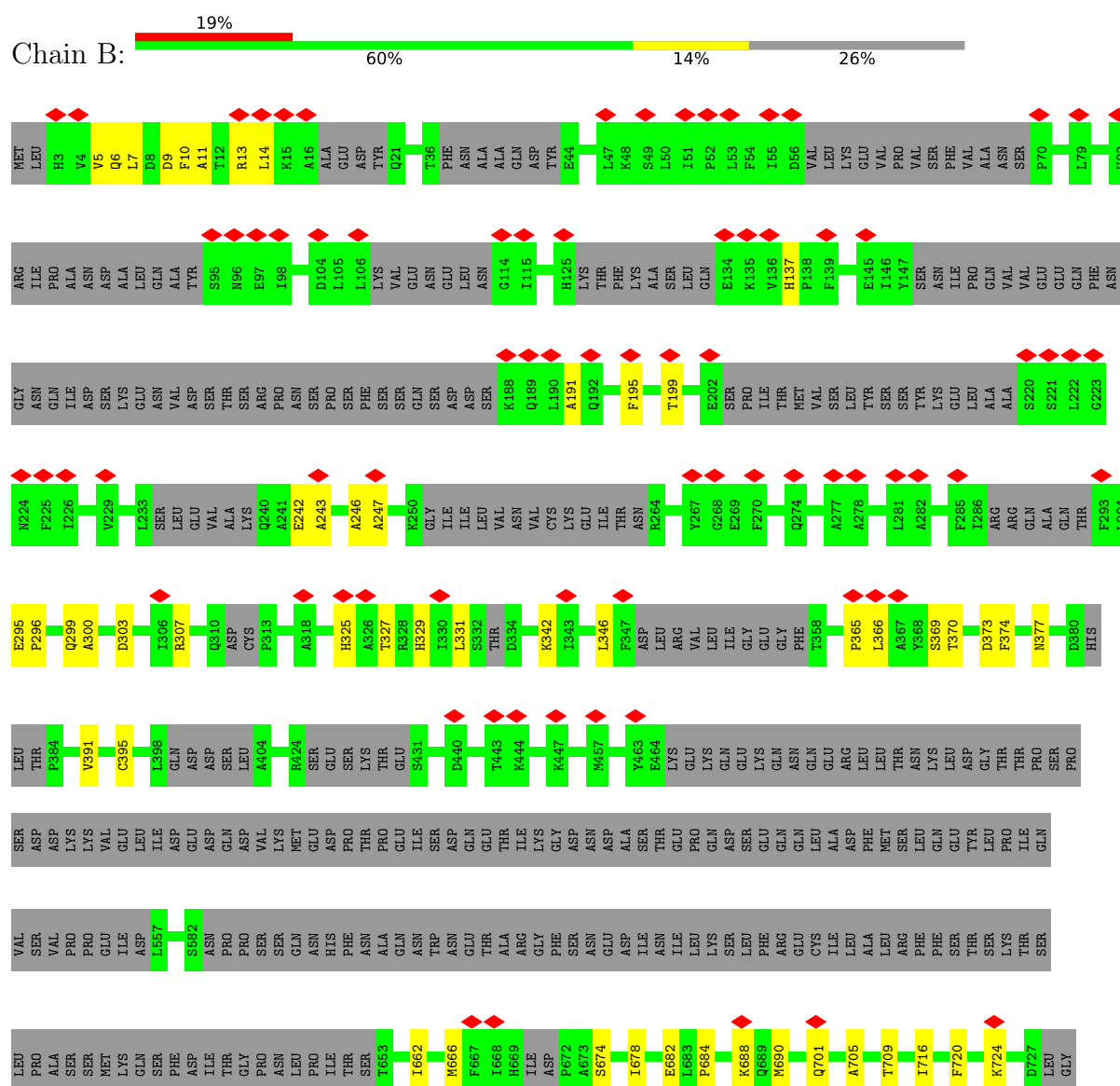
- Molecule 1 is a protein called Tra1 subunit within the chromatin modifying complex SAGA.

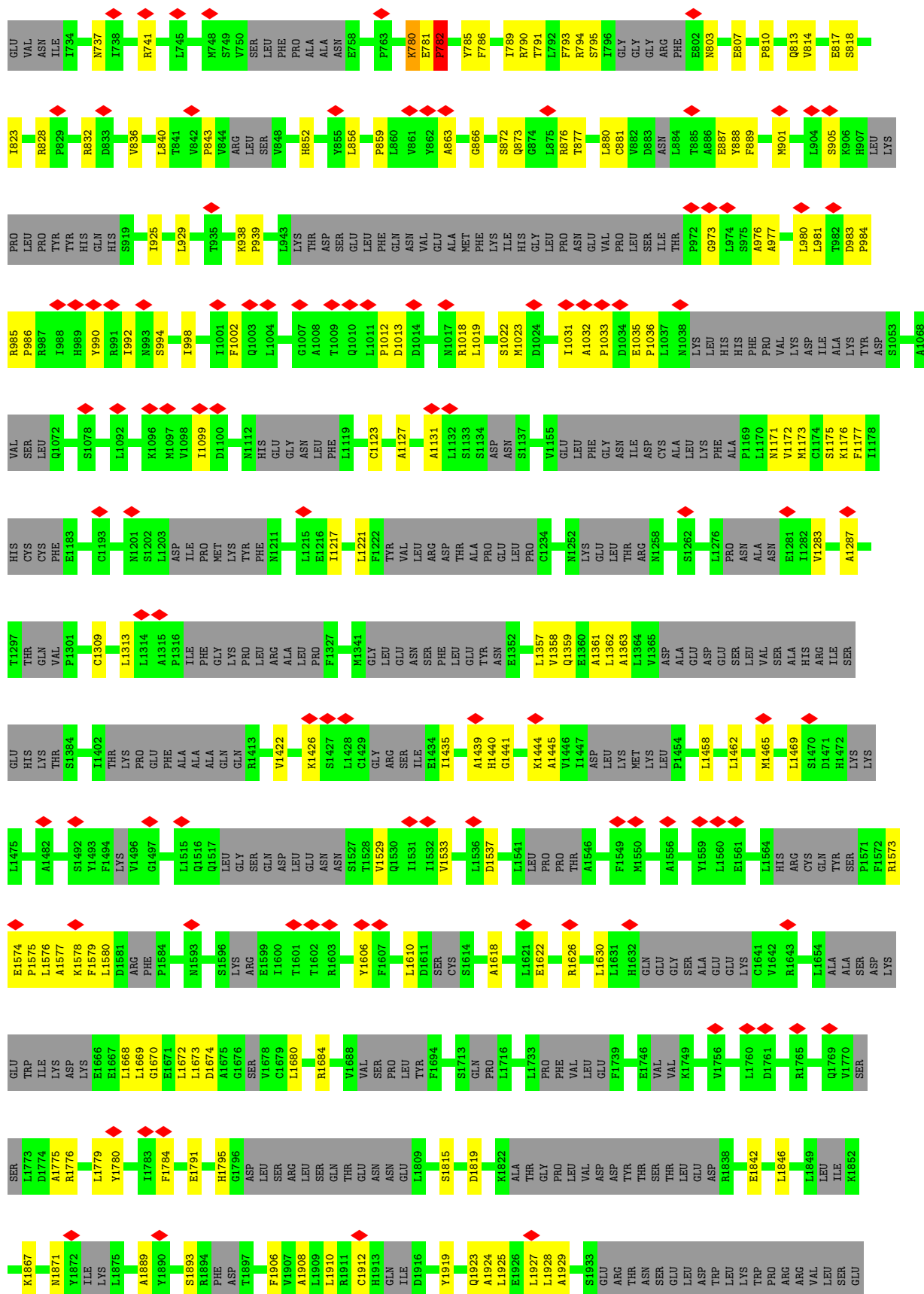
Mol	Chain	Residues	Atoms				AltConf	Trace
1	B	2825	Total	C	N	O	0	0
			14023	8373	2825	2825		

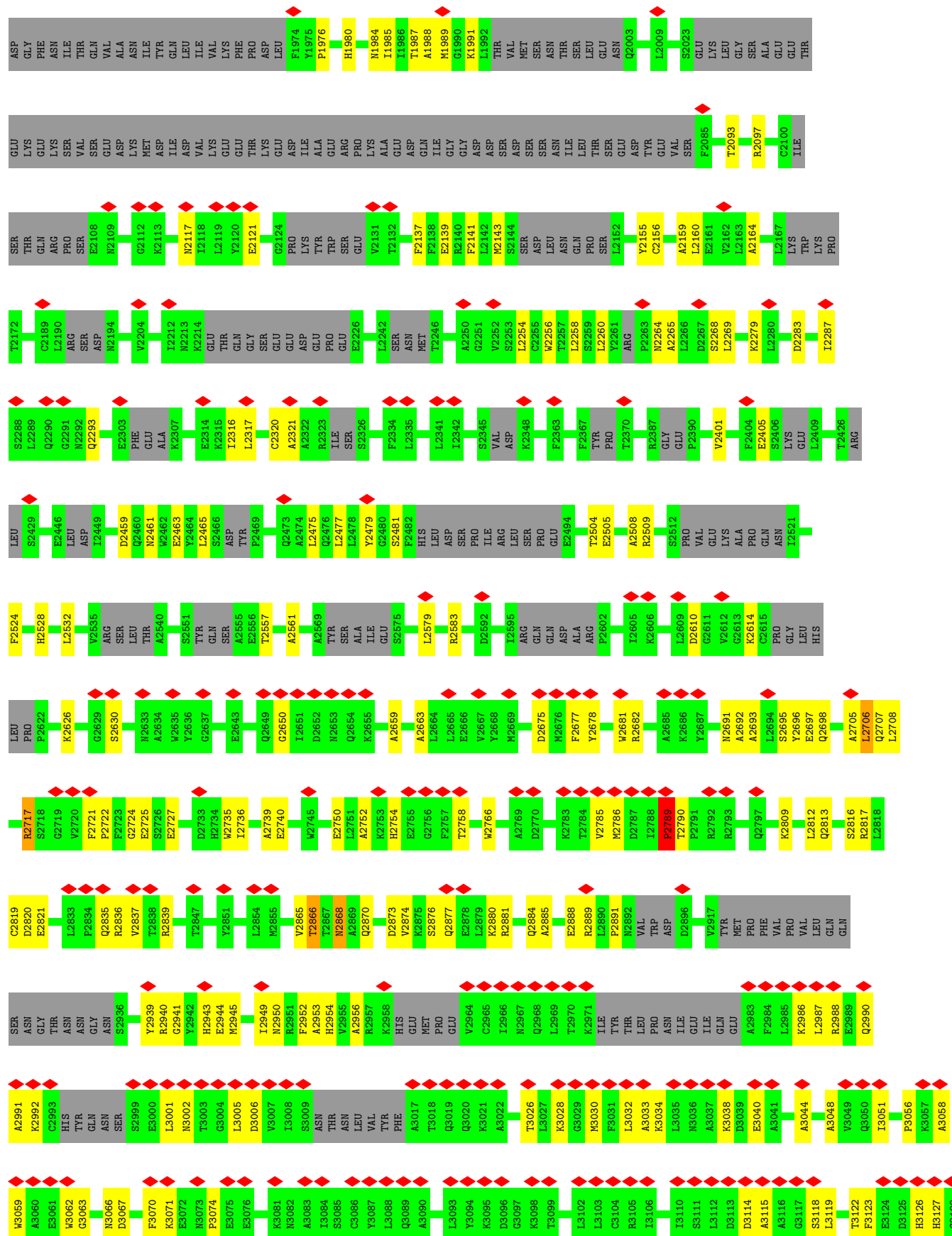
3 Residue-property plots [i](#)

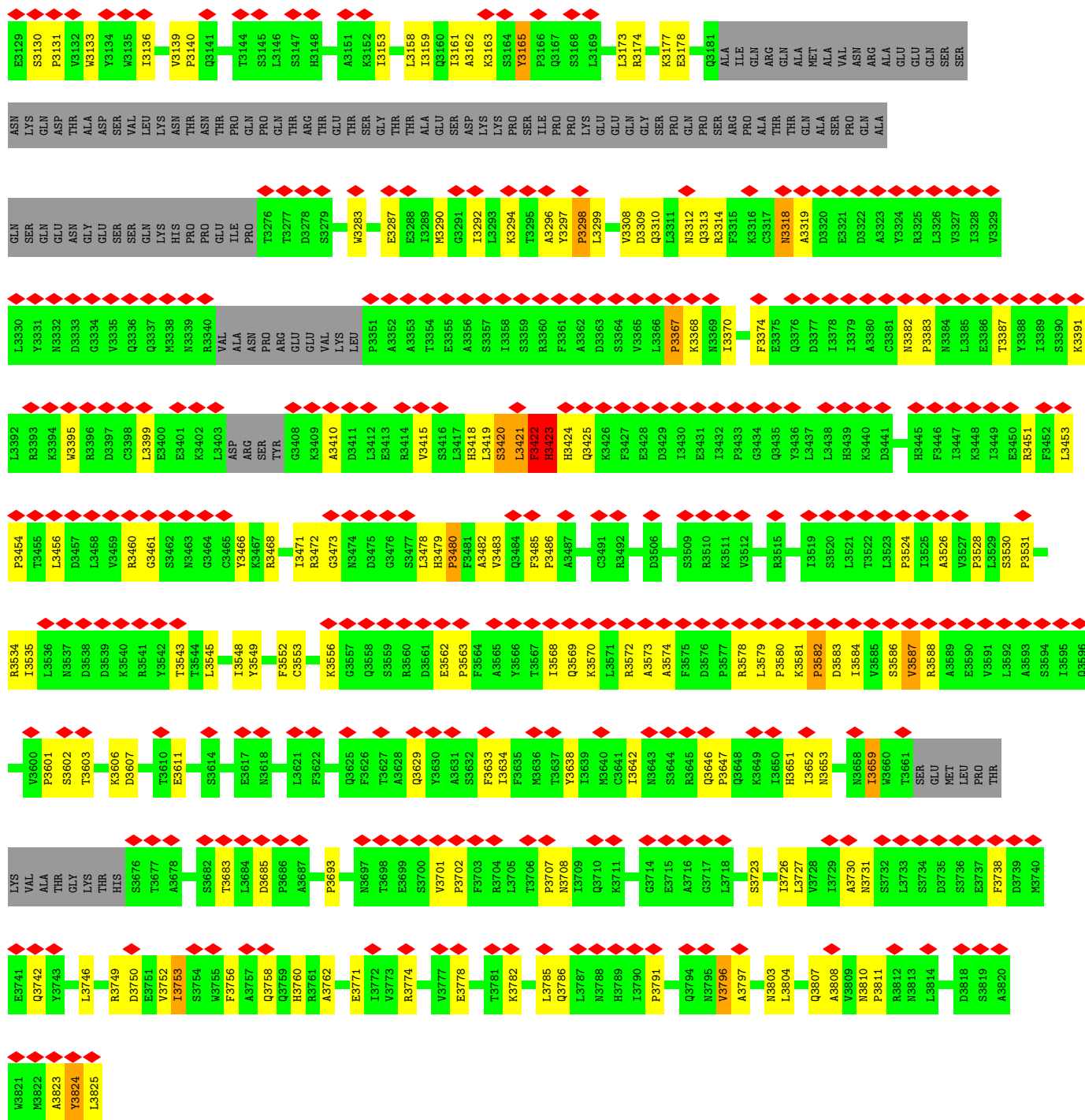
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tra1 subunit within the chromatin modifying complex SAGA









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Full CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	127272	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0429	Depositor
Map size ($\text{\AA}$)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	B	0.13	0/13920	0.33	10/19262 (0.1%)

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	B	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	3422	PHE	CA-C-N	7.16	135.21	121.54
1	B	3422	PHE	C-N-CA	7.16	135.21	121.54
1	B	2717	ARG	O-C-N	6.87	131.73	122.59
1	B	3298	PRO	CA-C-N	6.74	133.83	121.70
1	B	3298	PRO	C-N-CA	6.74	133.83	121.70
1	B	782	PRO	N-CA-CB	6.52	110.09	103.25
1	B	3587	VAL	CA-C-N	6.02	132.54	121.70
1	B	3587	VAL	C-N-CA	6.02	132.54	121.70
1	B	2789	PRO	CA-C-N	5.95	132.41	121.70
1	B	2789	PRO	C-N-CA	5.95	132.41	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	3421	LEU	Peptide
1	B	3423	HIS	Peptide

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	B	14023	0	6129	271	0
All	All	14023	0	6129	271	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 13.

All (271) 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:B:3651:HIS:O	1:B:3659:ILE:HA	1.02	1.20
1:B:3651:HIS:O	1:B:3659:ILE:CA	1.95	1.12
1:B:3420:SER:O	1:B:3423:HIS:CA	2.00	1.09
1:B:3420:SER:O	1:B:3423:HIS:HA	1.50	1.09
1:B:3420:SER:O	1:B:3423:HIS:N	1.95	0.99
1:B:2705:ALA:O	1:B:2707:GLN:N	2.00	0.94
1:B:3421:LEU:C	1:B:3423:HIS:H	1.79	0.91
1:B:3419:LEU:O	1:B:3422:PHE:O	1.93	0.84
1:B:3423:HIS:N	1:B:3425:GLN:H	1.85	0.74
1:B:2785:VAL:H	1:B:2786:MET:HA	1.53	0.73
1:B:3422:PHE:O	1:B:3424:HIS:N	2.20	0.73
1:B:3419:LEU:O	1:B:3422:PHE:C	2.31	0.73
1:B:3466:TYR:HA	1:B:3483:VAL:O	1.89	0.72
1:B:2750:GLU:CA	1:B:2758:THR:CB	2.68	0.72
1:B:2750:GLU:HA	1:B:2758:THR:CB	2.19	0.72
1:B:2705:ALA:O	1:B:2706:LEU:C	2.36	0.69
1:B:3587:VAL:H	1:B:3588:ARG:C	2.01	0.69
1:B:3526:ALA:HA	1:B:3535:ILE:O	1.94	0.68
1:B:3421:LEU:C	1:B:3423:HIS:N	2.42	0.68
1:B:3578:ARG:H	1:B:3579:LEU:HA	1.59	0.67
1:B:3570:LYS:O	1:B:3574:ALA:HB2	1.96	0.66
1:B:2705:ALA:O	1:B:2708:LEU:N	2.27	0.66
1:B:3569:GLN:O	1:B:3573:ALA:HB3	1.97	0.65
1:B:3422:PHE:C	1:B:3424:HIS:N	2.57	0.63
1:B:3422:PHE:C	1:B:3425:GLN:H	2.06	0.62
1:B:3582:PRO:N	1:B:3583:ASP:HA	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3410:ALA:HB3	1:B:3456:LEU:O	2.00	0.61
1:B:3804:LEU:O	1:B:3808:ALA:HB3	1.99	0.61
1:B:2987:LEU:O	1:B:2991:ALA:HB3	2.03	0.59
1:B:3726:ILE:O	1:B:3730:ALA:HB3	2.03	0.58
1:B:1441:GLY:O	1:B:1445:ALA:HB3	2.03	0.58
1:B:3543:THR:O	1:B:3652:ILE:C	2.47	0.58
1:B:3583:ASP:H	1:B:3584:ILE:HA	1.68	0.57
1:B:1573:ARG:O	1:B:1577:ALA:HB3	2.04	0.57
1:B:3418:HIS:O	1:B:3422:PHE:CB	2.53	0.56
1:B:859:PRO:O	1:B:863:ALA:HB3	2.06	0.56
1:B:3578:ARG:N	1:B:3579:LEU:HA	2.21	0.55
1:B:2750:GLU:CB	1:B:2758:THR:CB	2.84	0.54
1:B:1359:GLN:O	1:B:1363:ALA:HB3	2.08	0.54
1:B:3823:ALA:C	1:B:3825:LEU:HA	2.33	0.54
1:B:3318:ASN:HA	1:B:3319:ALA:C	2.33	0.54
1:B:3421:LEU:O	1:B:3423:HIS:N	2.29	0.53
1:B:3796:VAL:HA	1:B:3797:ALA:C	2.33	0.53
1:B:3583:ASP:N	1:B:3584:ILE:HA	2.23	0.53
1:B:2693:ALA:HB1	1:B:2706:LEU:CB	2.39	0.52
1:B:242:GLU:O	1:B:246:ALA:HB3	2.10	0.52
1:B:887:GLU:O	1:B:889:PHE:N	2.41	0.52
1:B:2866:THR:O	1:B:2868:ASN:C	2.53	0.52
1:B:2949:ILE:O	1:B:2953:ALA:HB3	2.09	0.51
1:B:3292:ILE:O	1:B:3296:ALA:HB2	2.11	0.51
1:B:243:ALA:O	1:B:247:ALA:HB3	2.11	0.51
1:B:2504:THR:O	1:B:2508:ALA:HB3	2.11	0.51
1:B:3420:SER:O	1:B:3422:PHE:C	2.54	0.50
1:B:296:PRO:O	1:B:300:ALA:HB3	2.12	0.50
1:B:2317:LEU:O	1:B:2321:ALA:HB3	2.11	0.50
1:B:2952:PHE:O	1:B:2956:ALA:HB3	2.11	0.50
1:B:7:LEU:O	1:B:11:ALA:HB3	2.11	0.50
1:B:701:GLN:O	1:B:705:ALA:HB3	2.12	0.50
1:B:2724:GLY:O	1:B:2727:GLU:N	2.45	0.49
1:B:3044:ALA:O	1:B:3048:ALA:HB3	2.13	0.49
1:B:3468:ARG:HA	1:B:3482:ALA:HA	1.92	0.49
1:B:3758:GLN:O	1:B:3762:ALA:HB3	2.12	0.49
1:B:3158:LEU:O	1:B:3162:ALA:HB3	2.12	0.49
1:B:3033:ALA:HA	1:B:3034:LYS:C	2.38	0.49
1:B:2705:ALA:C	1:B:2707:GLN:N	2.69	0.48
1:B:1984:ASN:O	1:B:1988:ALA:HB3	2.14	0.48
1:B:973:GLY:O	1:B:977:ALA:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:ALA:O	1:B:1131:ALA:HB3	2.14	0.48
1:B:2724:GLY:O	1:B:2725:GLU:C	2.57	0.47
1:B:2866:THR:O	1:B:2870:GLN:N	2.47	0.47
1:B:3059:TRP:O	1:B:3063:GLY:HA3	2.14	0.47
1:B:1357:LEU:O	1:B:1361:ALA:HB3	2.13	0.47
1:B:1435:ILE:O	1:B:1439:ALA:HB3	2.15	0.47
1:B:876:ARG:O	1:B:880:LEU:CB	2.63	0.47
1:B:2155:TYR:O	1:B:2159:ALA:HB3	2.15	0.47
1:B:2160:LEU:O	1:B:2164:ALA:HB3	2.14	0.47
1:B:2835:GLN:HA	1:B:2836:ARG:HA	1.57	0.47
1:B:2659:ALA:O	1:B:2663:ALA:HB3	2.16	0.46
1:B:3451:ARG:O	1:B:3472:ARG:CB	2.64	0.46
1:B:3471:ILE:H	1:B:3480:PRO:HA	1.80	0.46
1:B:872:SER:O	1:B:876:ARG:CB	2.63	0.46
1:B:2692:ALA:O	1:B:2696:TYR:CB	2.64	0.46
1:B:2678:TYR:O	1:B:2682:ARG:CB	2.64	0.45
1:B:3543:THR:CB	1:B:3653:ASN:O	2.64	0.45
1:B:3749:ARG:HA	1:B:3750:ASP:HA	1.56	0.45
1:B:3067:ASP:O	1:B:3071:LYS:CB	2.65	0.45
1:B:3367:PRO:HA	1:B:3368:LYS:HA	1.48	0.45
1:B:3066:ASN:O	1:B:3070:PHE:CB	2.65	0.45
1:B:2880:LYS:O	1:B:2884:GLN:CB	2.65	0.45
1:B:2881:ARG:O	1:B:2885:ALA:HB3	2.16	0.45
1:B:3473:GLY:H	1:B:3478:LEU:HA	1.81	0.45
1:B:2876:SER:O	1:B:2880:LYS:CB	2.65	0.44
1:B:877:THR:O	1:B:881:CYS:CB	2.66	0.44
1:B:1123:CYS:O	1:B:1127:ALA:HB3	2.18	0.44
1:B:2691:ASN:O	1:B:2695:SER:CB	2.65	0.44
1:B:3528:PRO:HA	1:B:3534:ARG:HA	1.99	0.44
1:B:1925:LEU:O	1:B:1929:ALA:HB2	2.17	0.44
1:B:2884:GLN:O	1:B:2888:GLU:CB	2.66	0.44
1:B:3752:VAL:HA	1:B:3753:ILE:HA	1.54	0.44
1:B:3548:ILE:O	1:B:3552:PHE:CB	2.66	0.44
1:B:3586:SER:HA	1:B:3587:VAL:HA	1.55	0.44
1:B:2877:GLN:O	1:B:2881:ARG:CB	2.66	0.43
1:B:3062:TRP:O	1:B:3066:ASN:CB	2.67	0.43
1:B:3063:GLY:O	1:B:3067:ASP:CB	2.66	0.43
1:B:3785:LEU:HA	1:B:3786:GLN:HA	1.50	0.43
1:B:1574:GLU:O	1:B:1578:LYS:CB	2.67	0.43
1:B:1780:TYR:O	1:B:1784:PHE:CB	2.67	0.43
1:B:2819:CYS:O	1:B:2821:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3058:ALA:O	1:B:3062:TRP:CB	2.67	0.43
1:B:3803:ASN:O	1:B:3807:GLN:CB	2.67	0.43
1:B:1669:LEU:O	1:B:1673:LEU:CB	2.67	0.43
1:B:3824:TYR:N	1:B:3825:LEU:HA	2.34	0.43
1:B:2785:VAL:N	1:B:2786:MET:HA	2.21	0.43
1:B:3607:ASP:O	1:B:3611:GLU:CB	2.67	0.43
1:B:790:ARG:O	1:B:794:ARG:CB	2.67	0.43
1:B:684:PRO:O	1:B:688:LYS:CB	2.66	0.43
1:B:2812:LEU:O	1:B:2816:SER:CB	2.67	0.42
1:B:3370:ILE:O	1:B:3374:PHE:CB	2.67	0.42
1:B:365:PRO:O	1:B:369:SER:CB	2.67	0.42
1:B:2677:PHE:O	1:B:2681:TRP:CB	2.67	0.42
1:B:3387:THR:O	1:B:3391:LYS:CB	2.67	0.42
1:B:3778:GLU:O	1:B:3782:LYS:CB	2.68	0.42
1:B:998:ILE:O	1:B:1002:PHE:CB	2.67	0.42
1:B:3002:ASN:O	1:B:3006:ASP:CB	2.67	0.42
1:B:2885:ALA:O	1:B:2889:ARG:CB	2.67	0.42
1:B:295:GLU:O	1:B:299:GLN:CB	2.67	0.42
1:B:786:PHE:O	1:B:790:ARG:CB	2.67	0.42
1:B:813:GLN:O	1:B:817:GLU:CB	2.68	0.42
1:B:814:VAL:O	1:B:818:SER:CB	2.67	0.42
1:B:1985:ILE:O	1:B:1989:MET:CB	2.68	0.42
1:B:3391:LYS:O	1:B:3395:TRP:CB	2.67	0.42
1:B:3603:THR:O	1:B:3607:ASP:CB	2.67	0.42
1:B:3774:ARG:O	1:B:3778:GLU:CB	2.68	0.42
1:B:1458:LEU:O	1:B:1462:LEU:CB	2.68	0.42
1:B:191:ALA:O	1:B:195:PHE:CB	2.68	0.42
1:B:789:ILE:O	1:B:793:PHE:CB	2.68	0.42
1:B:2459:ASP:O	1:B:2463:GLU:CB	2.68	0.42
1:B:2610:ASP:O	1:B:2614:LYS:CB	2.68	0.42
1:B:791:THR:O	1:B:795:SER:CB	2.68	0.42
1:B:3602:SER:O	1:B:3606:LYS:CB	2.68	0.42
1:B:662:ILE:O	1:B:666:MET:CB	2.68	0.42
1:B:1976:PRO:O	1:B:1980:HIS:CB	2.68	0.42
1:B:2986:LYS:O	1:B:2990:GLN:CB	2.68	0.42
1:B:3549:TYR:O	1:B:3553:CYS:CB	2.68	0.42
1:B:678:ILE:O	1:B:682:GLU:CB	2.68	0.42
1:B:1776:ARG:O	1:B:1780:TYR:CB	2.68	0.42
1:B:9:ASP:O	1:B:13:ARG:CB	2.68	0.41
1:B:1775:ALA:O	1:B:1779:LEU:CB	2.68	0.41
1:B:2477:LEU:O	1:B:2481:SER:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2557:THR:O	1:B:2561:ALA:HB3	2.19	0.41
1:B:3395:TRP:O	1:B:3399:LEU:CB	2.68	0.41
1:B:3634:ILE:O	1:B:3638:TYR:CB	2.68	0.41
1:B:873:GLN:O	1:B:877:THR:CB	2.69	0.41
1:B:1923:GLN:O	1:B:1927:LEU:CB	2.69	0.41
1:B:1987:THR:O	1:B:1991:LYS:CB	2.68	0.41
1:B:2940:ARG:O	1:B:2944:GLU:CB	2.69	0.41
1:B:3026:THR:O	1:B:3030:MET:CB	2.68	0.41
1:B:3161:ILE:O	1:B:3165:TYR:CB	2.69	0.41
1:B:3283:TRP:O	1:B:3287:GLU:CB	2.69	0.41
1:B:1309:CYS:O	1:B:1313:LEU:CB	2.68	0.41
1:B:1670:GLY:O	1:B:1674:ASP:CB	2.68	0.41
1:B:3123:PHE:O	1:B:3127:HIS:CB	2.68	0.41
1:B:303:ASP:O	1:B:307:ARG:CB	2.69	0.41
1:B:1533:VAL:O	1:B:1537:ASP:CB	2.68	0.41
1:B:1618:ALA:O	1:B:1622:GLU:CB	2.68	0.41
1:B:1908:ALA:O	1:B:1912:CYS:CB	2.69	0.41
1:B:2256:TRP:O	1:B:2260:LEU:CB	2.69	0.41
1:B:2789:PRO:N	1:B:2790:THR:C	2.79	0.41
1:B:3159:ILE:O	1:B:3163:LYS:CB	2.68	0.41
1:B:780:LYS:O	1:B:782:PRO:N	2.52	0.41
1:B:1283:VAL:O	1:B:1287:ALA:HB3	2.21	0.41
1:B:1465:MET:O	1:B:1469:LEU:CB	2.68	0.41
1:B:1668:LEU:O	1:B:1672:LEU:CB	2.69	0.41
1:B:195:PHE:O	1:B:199:THR:CB	2.69	0.41
1:B:720:PHE:O	1:B:724:LYS:CB	2.69	0.41
1:B:977:ALA:O	1:B:981:LEU:CB	2.68	0.41
1:B:1529:VAL:O	1:B:1533:VAL:CB	2.69	0.41
1:B:1573:ARG:O	1:B:1577:ALA:CB	2.69	0.41
1:B:2137:PHE:O	1:B:2141:PHE:CB	2.68	0.41
1:B:2254:LEU:O	1:B:2258:LEU:CB	2.68	0.41
1:B:3119:LEU:O	1:B:3123:PHE:CB	2.68	0.41
1:B:3310:GLN:O	1:B:3314:ARG:CB	2.69	0.41
1:B:5:VAL:O	1:B:9:ASP:CB	2.68	0.41
1:B:366:LEU:O	1:B:370:THR:CB	2.69	0.41
1:B:369:SER:O	1:B:373:ASP:CB	2.69	0.41
1:B:674:SER:O	1:B:678:ILE:CB	2.69	0.41
1:B:810:PRO:O	1:B:814:VAL:CB	2.69	0.41
1:B:1171:ASN:O	1:B:1175:SER:CB	2.68	0.41
1:B:2988:ARG:O	1:B:2992:LYS:CB	2.69	0.41
1:B:3308:VAL:O	1:B:3312:ASN:CB	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3629:GLN:O	1:B:3633:PHE:CB	2.68	0.41
1:B:370:THR:O	1:B:374:PHE:CB	2.69	0.41
1:B:373:ASP:O	1:B:377:ASN:CB	2.69	0.41
1:B:1919:TYR:O	1:B:1923:GLN:CB	2.69	0.41
1:B:2156:CYS:O	1:B:2160:LEU:CB	2.69	0.41
1:B:2265:ALA:O	1:B:2269:LEU:CB	2.68	0.41
1:B:2279:LYS:O	1:B:2283:ASP:CB	2.69	0.41
1:B:3309:ASP:O	1:B:3313:GLN:CB	2.68	0.41
1:B:3723:SER:O	1:B:3727:LEU:CB	2.69	0.41
1:B:10:PHE:O	1:B:14:LEU:CB	2.69	0.41
1:B:325:HIS:O	1:B:329:HIS:CB	2.69	0.41
1:B:716:ILE:O	1:B:720:PHE:CB	2.69	0.41
1:B:803:ASN:O	1:B:807:GLU:CB	2.69	0.41
1:B:828:ARG:O	1:B:832:ARG:CB	2.69	0.41
1:B:1217:ILE:O	1:B:1221:LEU:CB	2.68	0.41
1:B:1576:LEU:O	1:B:1580:LEU:CB	2.69	0.41
1:B:1842:GLU:O	1:B:1846:LEU:CB	2.68	0.41
1:B:2264:ASN:O	1:B:2268:SER:CB	2.69	0.41
1:B:2316:ILE:O	1:B:2320:CYS:CB	2.69	0.41
1:B:2461:ASN:O	1:B:2465:LEU:CB	2.69	0.41
1:B:2524:PHE:O	1:B:2528:HIS:CB	2.69	0.41
1:B:2528:HIS:O	1:B:2532:LEU:CB	2.69	0.41
1:B:2579:LEU:O	1:B:2583:ARG:CB	2.69	0.41
1:B:2735:TRP:O	1:B:2739:ALA:N	2.54	0.41
1:B:2881:ARG:O	1:B:2885:ALA:CB	2.68	0.41
1:B:3568:ILE:O	1:B:3572:ARG:CB	2.68	0.41
1:B:342:LYS:O	1:B:346:LEU:CB	2.69	0.41
1:B:1019:LEU:O	1:B:1023:MET:CB	2.68	0.41
1:B:1791:GLU:O	1:B:1795:HIS:CB	2.69	0.41
1:B:2160:LEU:O	1:B:2164:ALA:CB	2.69	0.41
1:B:2401:VAL:O	1:B:2405:GLU:CB	2.69	0.41
1:B:2813:GLN:O	1:B:2817:ARG:CB	2.69	0.41
1:B:2939:TYR:O	1:B:2943:HIS:CB	2.69	0.41
1:B:3173:LEU:O	1:B:3177:LYS:CB	2.69	0.41
1:B:3545:LEU:O	1:B:3549:TYR:CB	2.69	0.41
1:B:327:THR:O	1:B:331:LEU:CB	2.69	0.40
1:B:391:VAL:O	1:B:395:CYS:CB	2.69	0.40
1:B:785:TYR:O	1:B:789:ILE:CB	2.69	0.40
1:B:836:VAL:O	1:B:840:LEU:CB	2.70	0.40
1:B:976:ALA:O	1:B:980:LEU:CB	2.69	0.40
1:B:1018:ARG:O	1:B:1022:SER:CB	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1358:VAL:O	1:B:1362:LEU:CB	2.68	0.40
1:B:2093:THR:O	1:B:2097:ARG:CB	2.69	0.40
1:B:2505:GLU:O	1:B:2509:ARG:CB	2.69	0.40
1:B:852:HIS:O	1:B:856:LEU:CB	2.69	0.40
1:B:1172:VAL:O	1:B:1176:LYS:CB	2.69	0.40
1:B:1575:PRO:O	1:B:1579:PHE:CB	2.68	0.40
1:B:1984:ASN:O	1:B:1988:ALA:CB	2.69	0.40
1:B:3001:LEU:O	1:B:3005:LEU:CB	2.69	0.40
1:B:3174:ARG:O	1:B:3178:GLU:CB	2.70	0.40
1:B:901:MET:O	1:B:905:SER:CB	2.69	0.40
1:B:1440:HIS:O	1:B:1444:LYS:CB	2.69	0.40
1:B:1606:TYR:O	1:B:1610:LEU:CB	2.69	0.40
1:B:1815:SER:O	1:B:1819:ASP:CB	2.70	0.40
1:B:1889:ALA:O	1:B:1893:SER:CB	2.69	0.40
1:B:1906:PHE:O	1:B:1910:LEU:CB	2.70	0.40
1:B:1924:ALA:O	1:B:1928:LEU:CB	2.69	0.40
1:B:2475:LEU:O	1:B:2479:TYR:CB	2.69	0.40
1:B:3028:LYS:O	1:B:3032:LEU:CB	2.69	0.40
1:B:3727:LEU:O	1:B:3731:ASN:CB	2.69	0.40
1:B:3742:GLN:O	1:B:3746:LEU:CB	2.69	0.40
1:B:296:PRO:O	1:B:300:ALA:CB	2.69	0.40
1:B:737:ASN:O	1:B:741:ARG:CB	2.70	0.40
1:B:1422:VAL:O	1:B:1426:LYS:CB	2.70	0.40
1:B:1867:LYS:O	1:B:1871:ASN:CB	2.69	0.40
1:B:2139:GLU:O	1:B:2143:MET:CB	2.69	0.40
1:B:2736:ILE:O	1:B:2739:ALA:CB	2.70	0.40
1:B:2950:ASN:O	1:B:2954:HIS:CB	2.69	0.40
1:B:3756:PHE:O	1:B:3760:HIS:CB	2.70	0.40
1:B:6:GLN:O	1:B:10:PHE:CB	2.69	0.40
1:B:925:ILE:O	1:B:929:LEU:CB	2.70	0.40
1:B:994:SER:O	1:B:998:ILE:CB	2.69	0.40
1:B:1173:MET:O	1:B:1177:PHE:CB	2.69	0.40
1:B:1626:ARG:O	1:B:1630:LEU:CB	2.69	0.40
1:B:1680:LEU:O	1:B:1684:ARG:CB	2.70	0.40
1:B:2117:ASN:O	1:B:2121:GLU:CB	2.70	0.40
1:B:2626:LYS:O	1:B:2630:SER:CB	2.69	0.40
1:B:2941:GLY:O	1:B:2945:MET:CB	2.69	0.40
1:B:3122:THR:O	1:B:3126:HIS:CB	2.69	0.40
1:B:3290:MET:O	1:B:3294:LYS:CB	2.70	0.40
1:B:3543:THR:O	1:B:3652:ILE:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	2619/3825 (68%)	2264 (86%)	240 (9%)	115 (4%)	2	16

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	HIS
1	B	781	GLU
1	B	782	PRO
1	B	939	PRO
1	B	983	ASP
1	B	984	PRO
1	B	985	ARG
1	B	986	PRO
1	B	1012	PRO
1	B	1033	PRO
1	B	1036	PRO
1	B	2697	GLU
1	B	2706	LEU
1	B	2722	PRO
1	B	2754	HIS
1	B	2789	PRO
1	B	2865	VAL
1	B	2868	ASN
1	B	2891	PRO
1	B	3056	PRO
1	B	3074	PRO
1	B	3139	VAL
1	B	3140	PRO
1	B	3165	TYR
1	B	3298	PRO
1	B	3367	PRO
1	B	3382	ASN
1	B	3383	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3420	SER
1	B	3422	PHE
1	B	3423	HIS
1	B	3453	LEU
1	B	3454	PRO
1	B	3480	PRO
1	B	3485	PHE
1	B	3486	PRO
1	B	3524	PRO
1	B	3530	SER
1	B	3562	GLU
1	B	3563	PRO
1	B	3580	PRO
1	B	3582	PRO
1	B	3601	PRO
1	B	3685	ASP
1	B	3701	VAL
1	B	3702	PRO
1	B	3707	PRO
1	B	3810	ASN
1	B	3811	PRO
1	B	3824	TYR
1	B	866	GLY
1	B	2287	ILE
1	B	2740	GLU
1	B	2820	ASP
1	B	2837	VAL
1	B	2874	VAL
1	B	3153	ILE
1	B	3297	TYR
1	B	690	MET
1	B	780	LYS
1	B	888	TYR
1	B	990	TYR
1	B	1031	ILE
1	B	1032	ALA
1	B	2675	ASP
1	B	2698	GLN
1	B	2717	ARG
1	B	2766	TRP
1	B	2809	LYS
1	B	2839	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2866	THR
1	B	3040	GLU
1	B	3051	ILE
1	B	3118	SER
1	B	3130	SER
1	B	3299	LEU
1	B	3738	PHE
1	B	3771	GLU
1	B	823	ILE
1	B	938	LYS
1	B	1035	GLU
1	B	2752	ALA
1	B	2873	ASP
1	B	3038	LYS
1	B	3114	ASP
1	B	3133	TRP
1	B	3461	GLY
1	B	3479	HIS
1	B	3556	LYS
1	B	3581	LYS
1	B	3646	GLN
1	B	3659	ILE
1	B	3683	THR
1	B	3708	ASN
1	B	709	THR
1	B	843	PRO
1	B	1013	ASP
1	B	2721	PHE
1	B	3115	ALA
1	B	3460	ARG
1	B	3531	PRO
1	B	3693	PRO
1	B	3753	ILE
1	B	3791	PRO
1	B	3796	VAL
1	B	2650	GLY
1	B	3131	PRO
1	B	3318	ASN
1	B	2293	GLN
1	B	992	ILE
1	B	3415	VAL
1	B	3642	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1099	ILE
1	B	3647	PRO
1	B	3136	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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-3790. 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: 160



Y Index: 160



Z Index: 160

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: 161



Y Index: 138

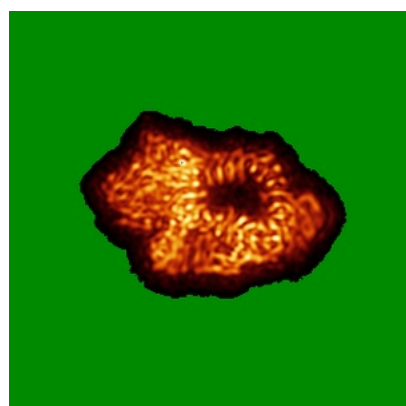


Z Index: 148

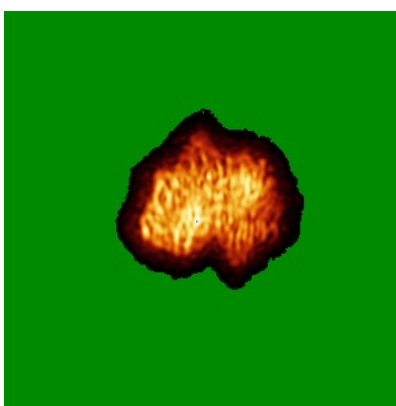
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

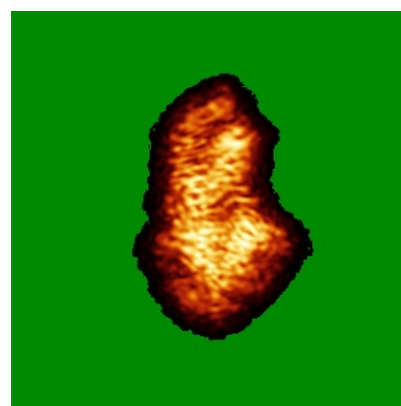
6.4.1 Primary map



X



Y

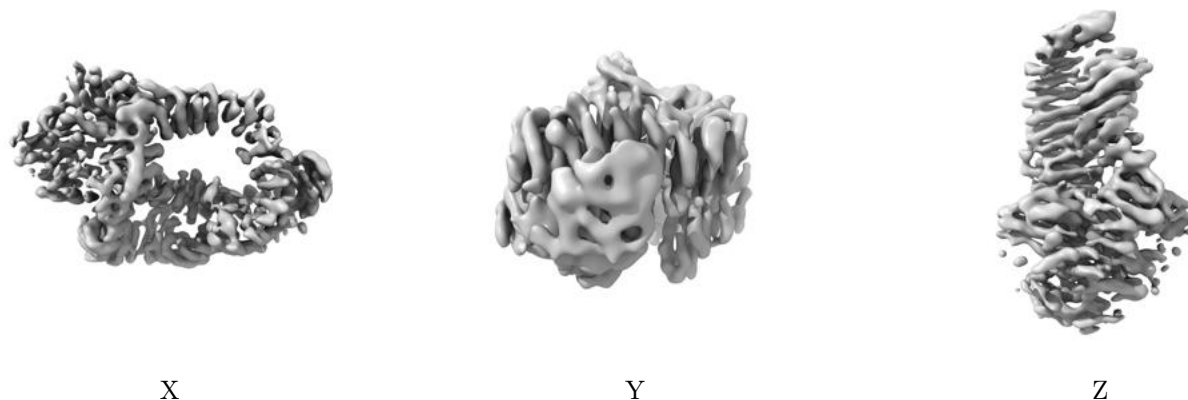


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0429. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

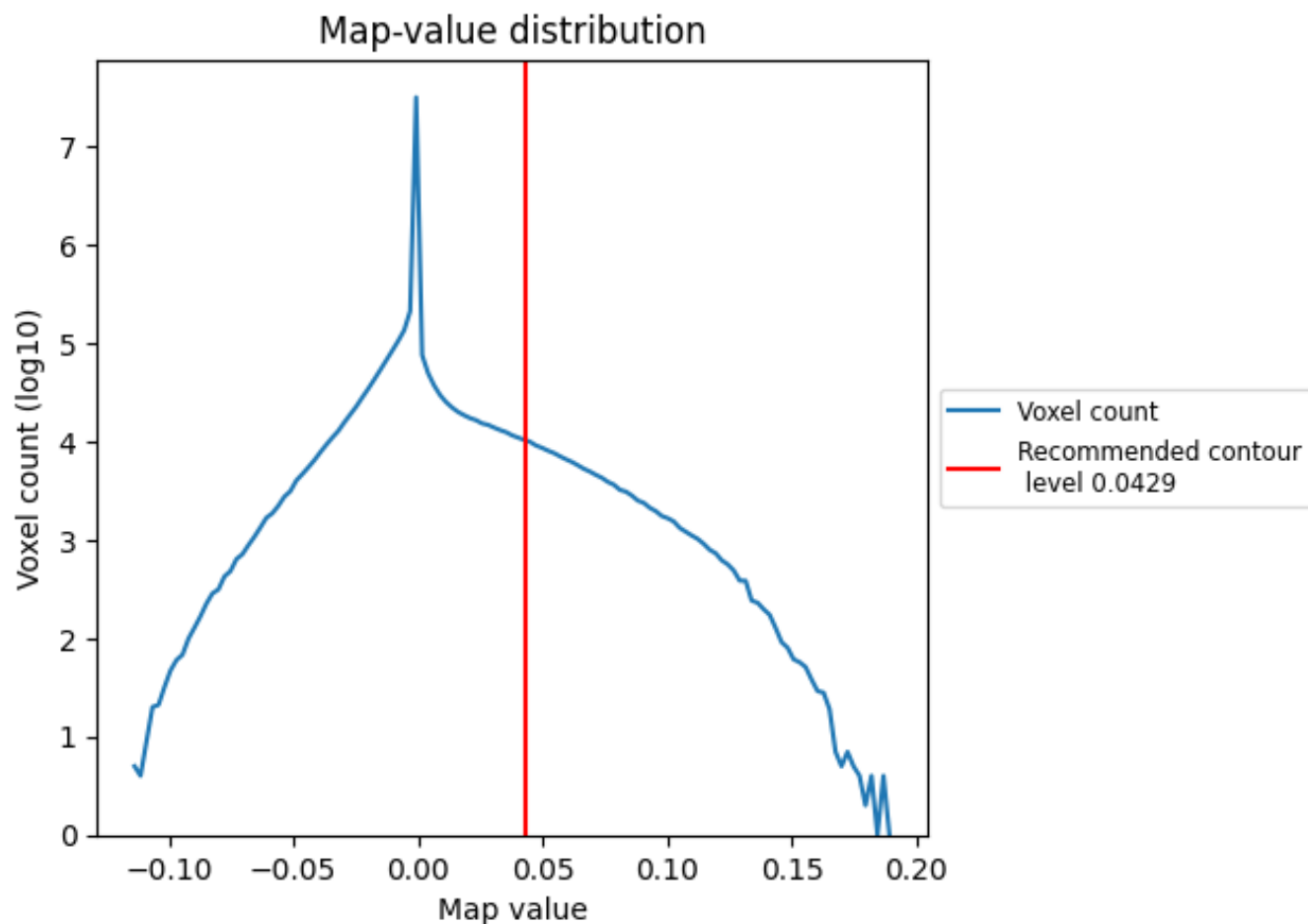
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

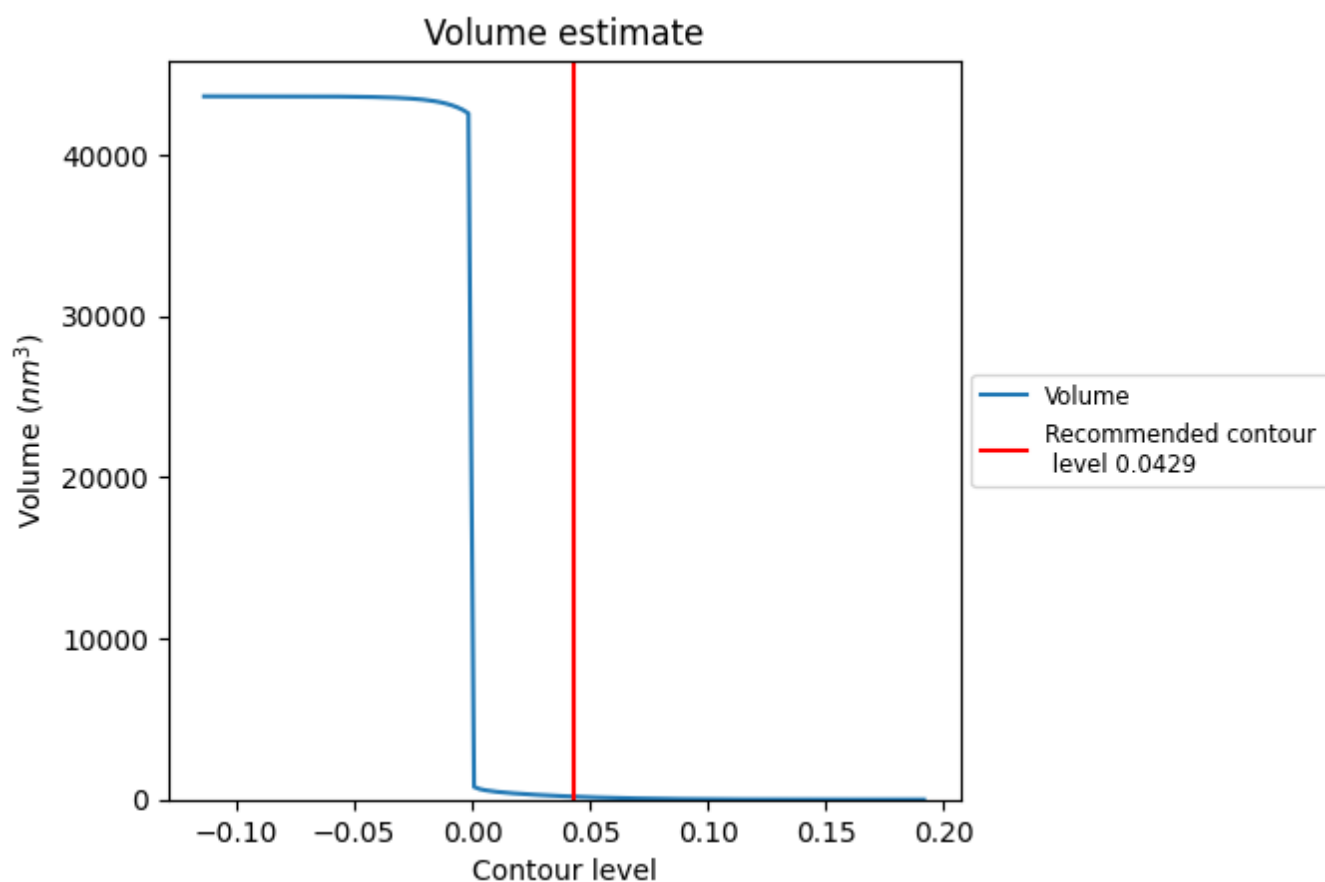
This section contains the results of statistical analysis of the map.

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.

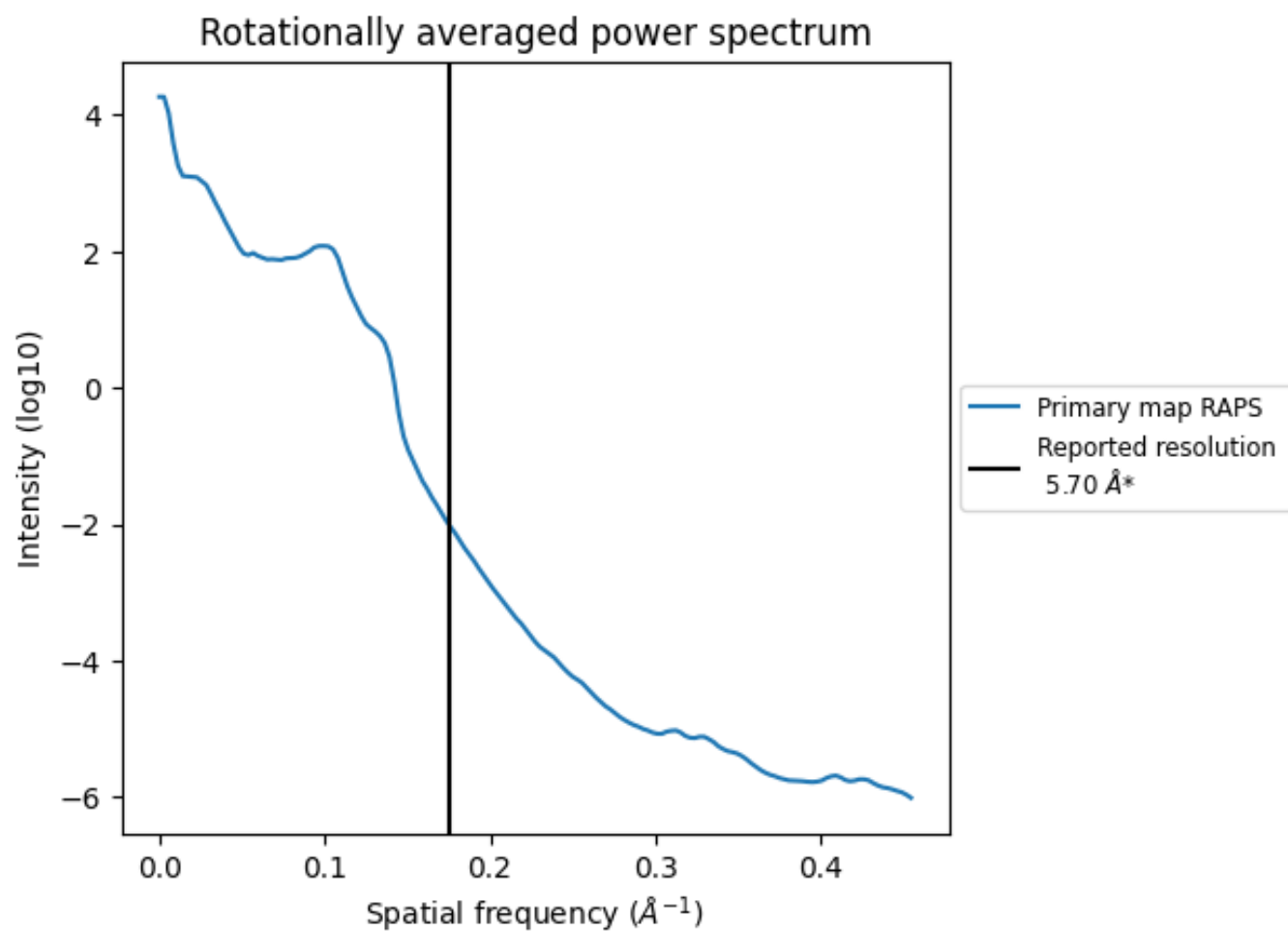
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

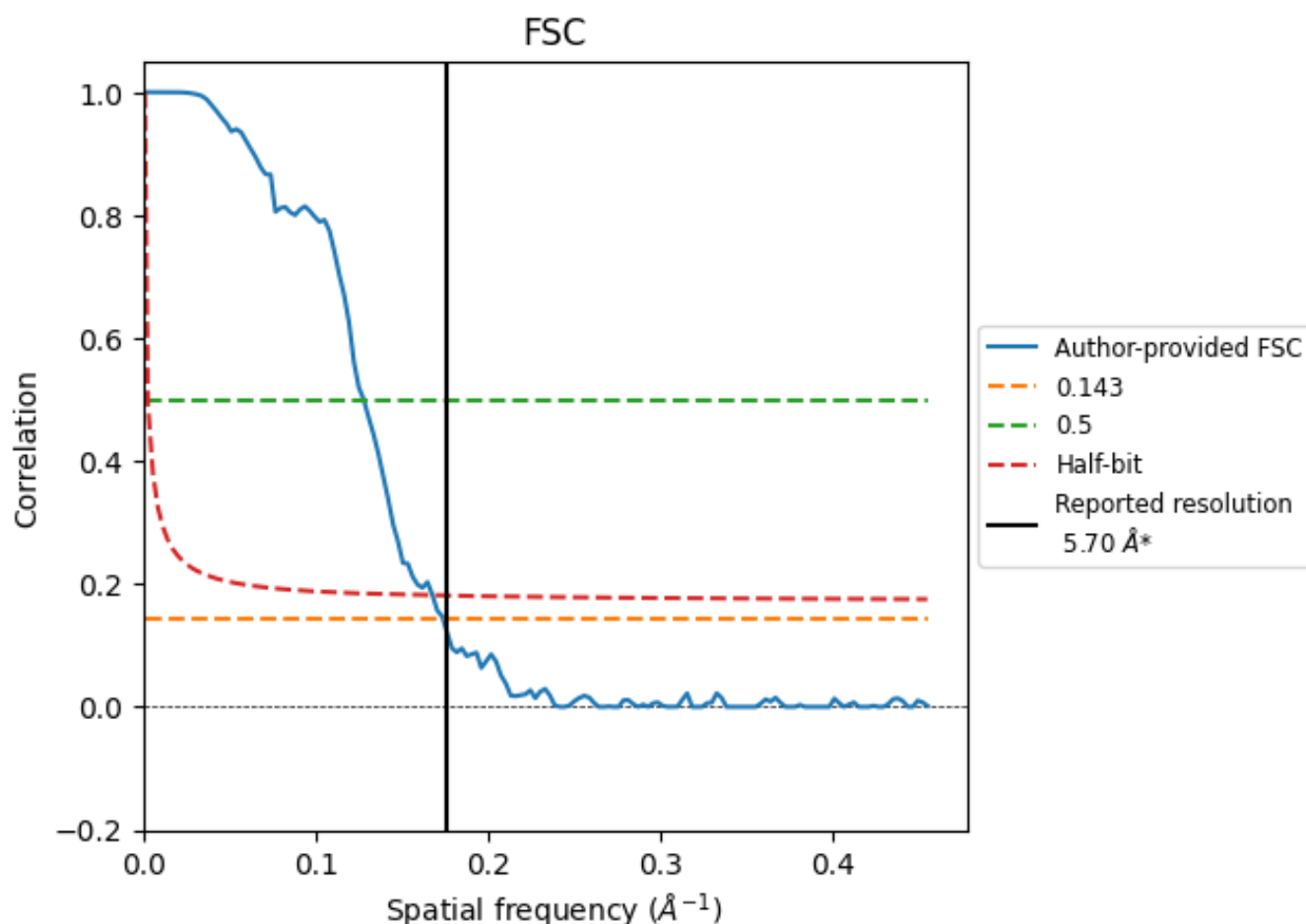


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.175 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.75	7.82	5.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

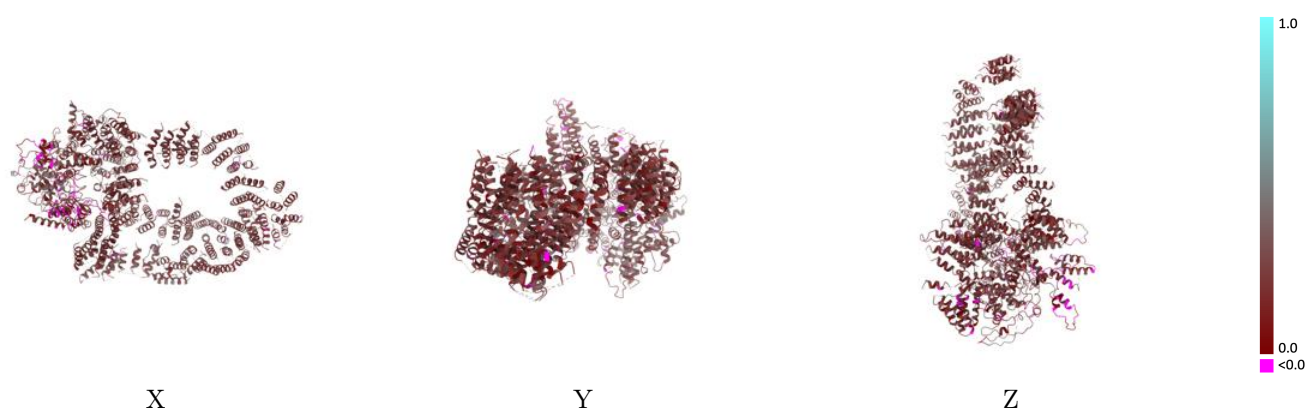
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3790 and PDB model 5OEJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

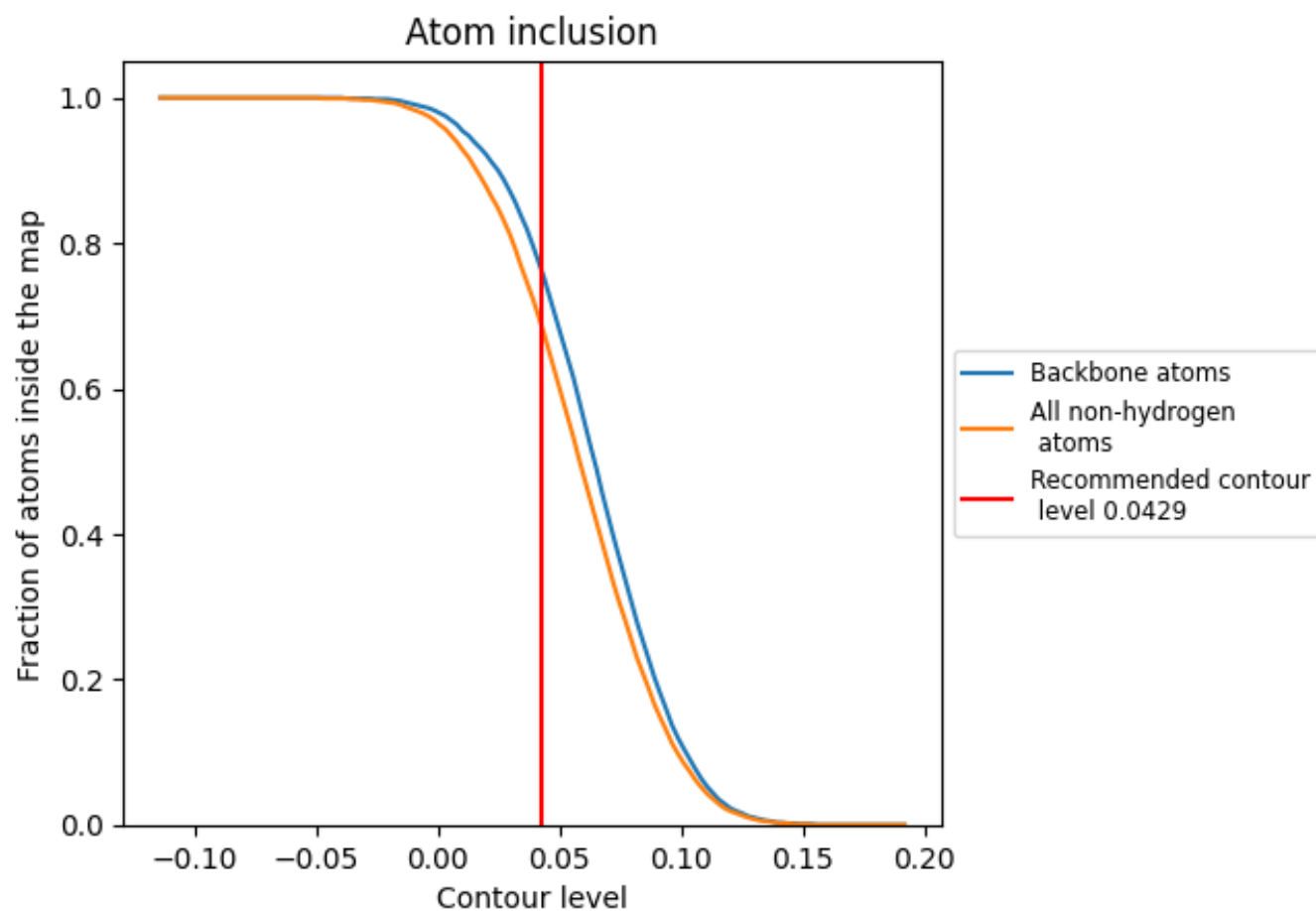


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.0429) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.2190
B	0.6830	0.2190

