



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 03:59 PM UTC

PDB ID : 7NFC / pdb_00007nfc
EMDB ID : EMD-12299
Title : Cryo-EM structure of NHEJ super-complex (dimer)
Authors : Chaplin, A.K.; Hardwick, S.W.; Kefala Stavridi, A.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2021-02-05
Resolution : 4.14 Å(reported)

This is a wwPDB EM Validation Summary 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:

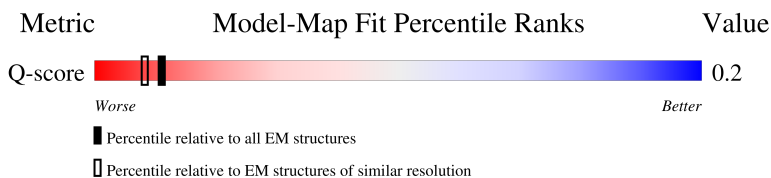
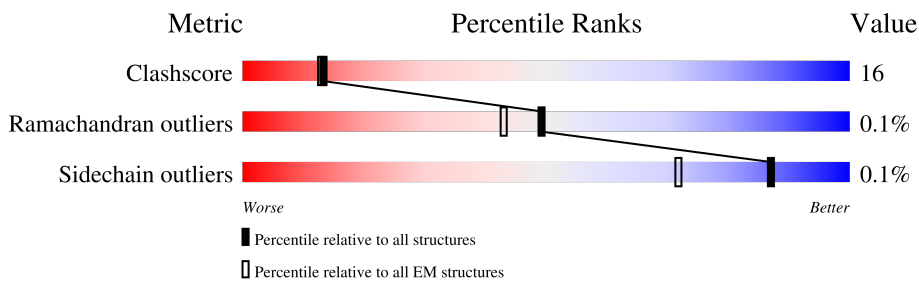
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.14 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.



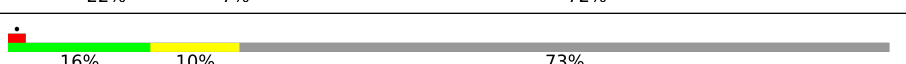
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5577 (3.64 - 4.64)

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	A	4148	
1	F	4148	
2	B	609	
2	G	609	

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Mol	Chain	Length	Quality of chain
3	C	732	
3	H	732	
4	K	336	
4	L	336	
4	N	336	
4	O	336	
5	M	911	
5	P	911	
6	Q	299	
6	R	299	
7	D	27	
8	E	28	
8	I	28	
9	J	27	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 89069 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3562	Total	C	N	O	S	0	0
			28076	18032	4728	5132	184		
1	F	3557	Total	C	N	O	S	0	0
			28060	18026	4720	5131	183		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	476	Total	C	N	O	S	0	0
			3822	2452	648	705	17		
2	G	489	Total	C	N	O	S	0	0
			3948	2529	669	732	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	477	Total	C	N	O	S	0	0
			3849	2466	646	714	23		
3	H	642	Total	C	N	O	S	0	0
			5150	3298	864	963	25		

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	201	Total	C	N	O	S	0	0
			1625	1028	278	312	7		
4	L	195	Total	C	N	O	S	0	0
			1592	1009	272	304	7		
4	N	201	Total	C	N	O	S	0	0
			1625	1028	278	312	7		
4	O	194	Total	C	N	O	S	0	0
			1579	1000	271	301	7		

- Molecule 5 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	258	Total	C	N	O	S	0	0
			2095	1333	353	396	13		
5	P	246	Total	C	N	O	S	0	0
			1965	1248	330	374	13		

- Molecule 6 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	211	Total	C	N	O	S	0	0
			1690	1084	282	310	14		
6	R	218	Total	C	N	O	S	0	0
			1728	1105	288	320	15		

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	27	Total	C	N	O	P	0	0
			556	268	95	166	27		

- Molecule 8 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	28	Total	C	N	O	P	0	0
			576	277	107	164	28		
8	I	28	Total	C	N	O	P	0	0
			576	277	107	164	28		

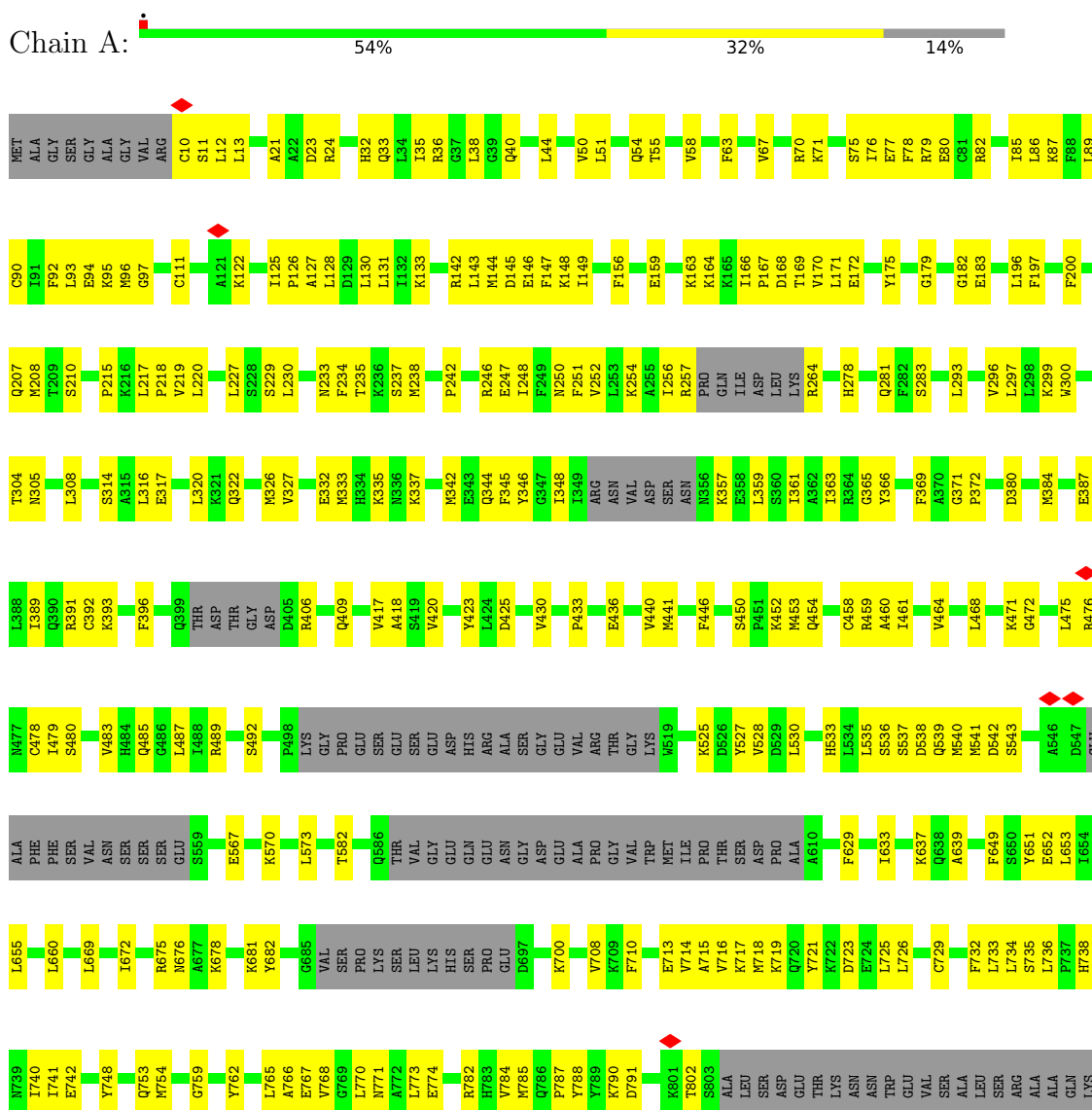
- Molecule 9 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	27	Total	C	N	O	P	0	0
			557	269	94	167	27		

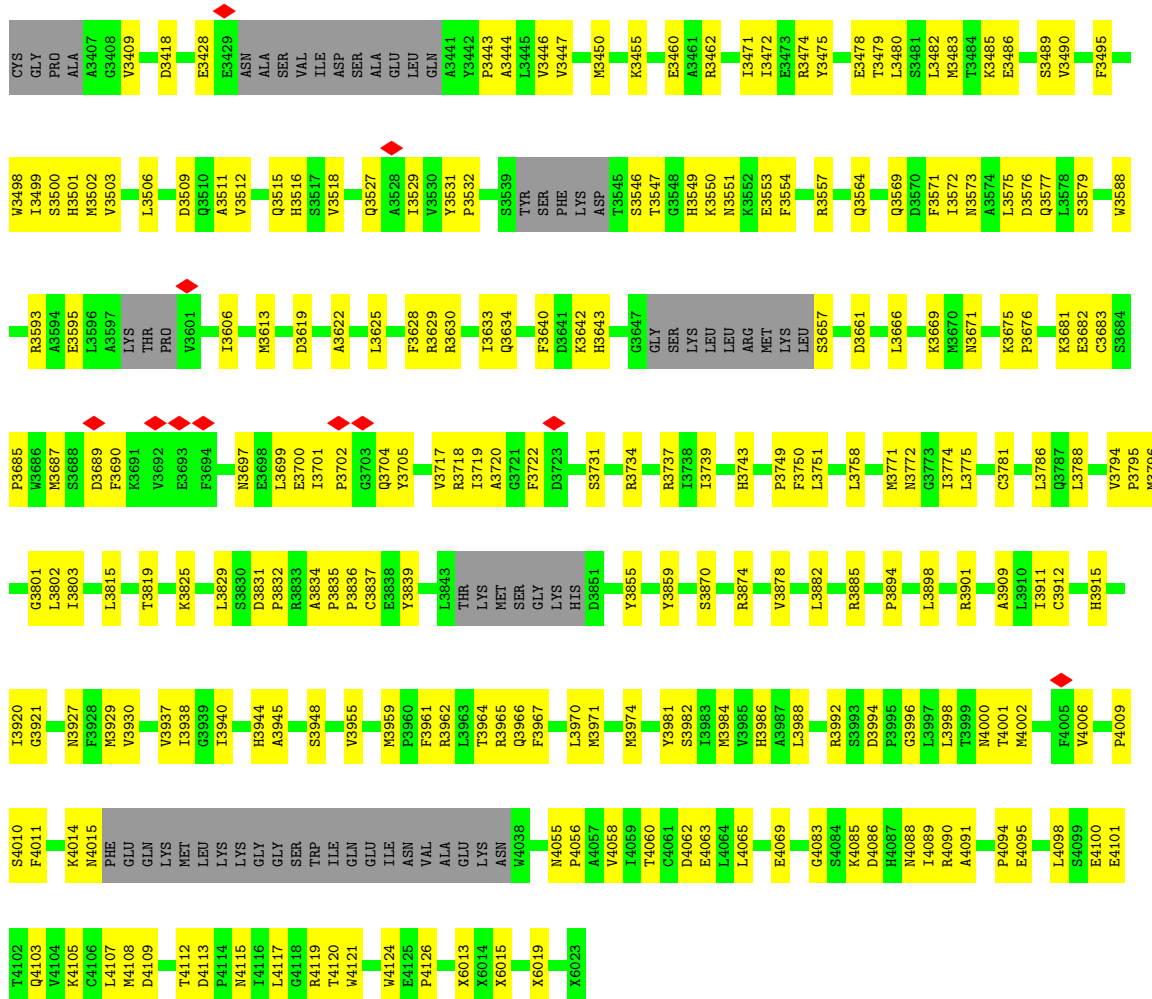
3 Residue-property plots [i](#)

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.

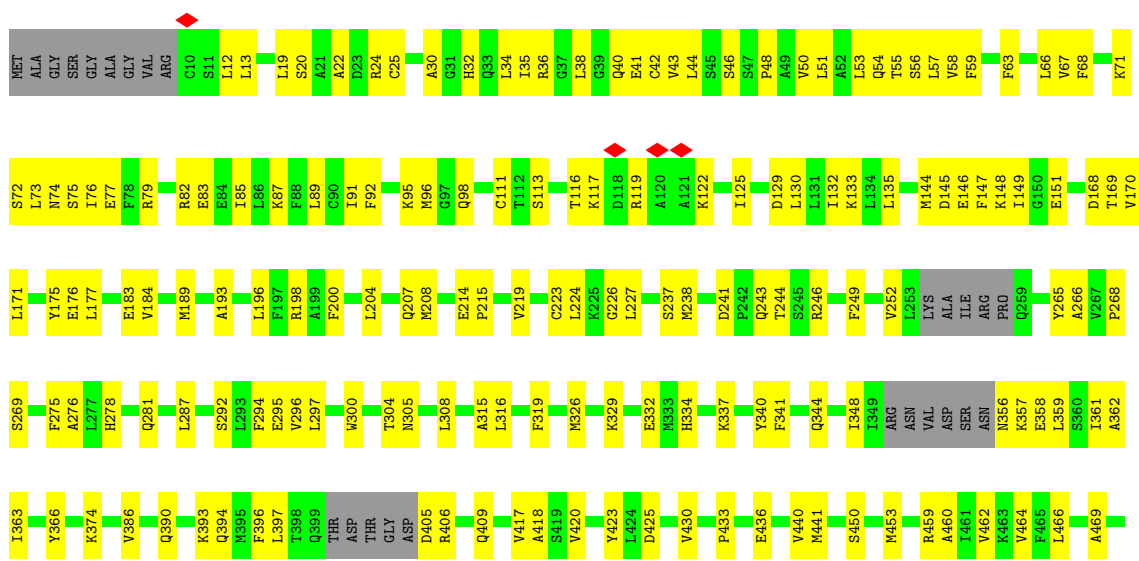
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs

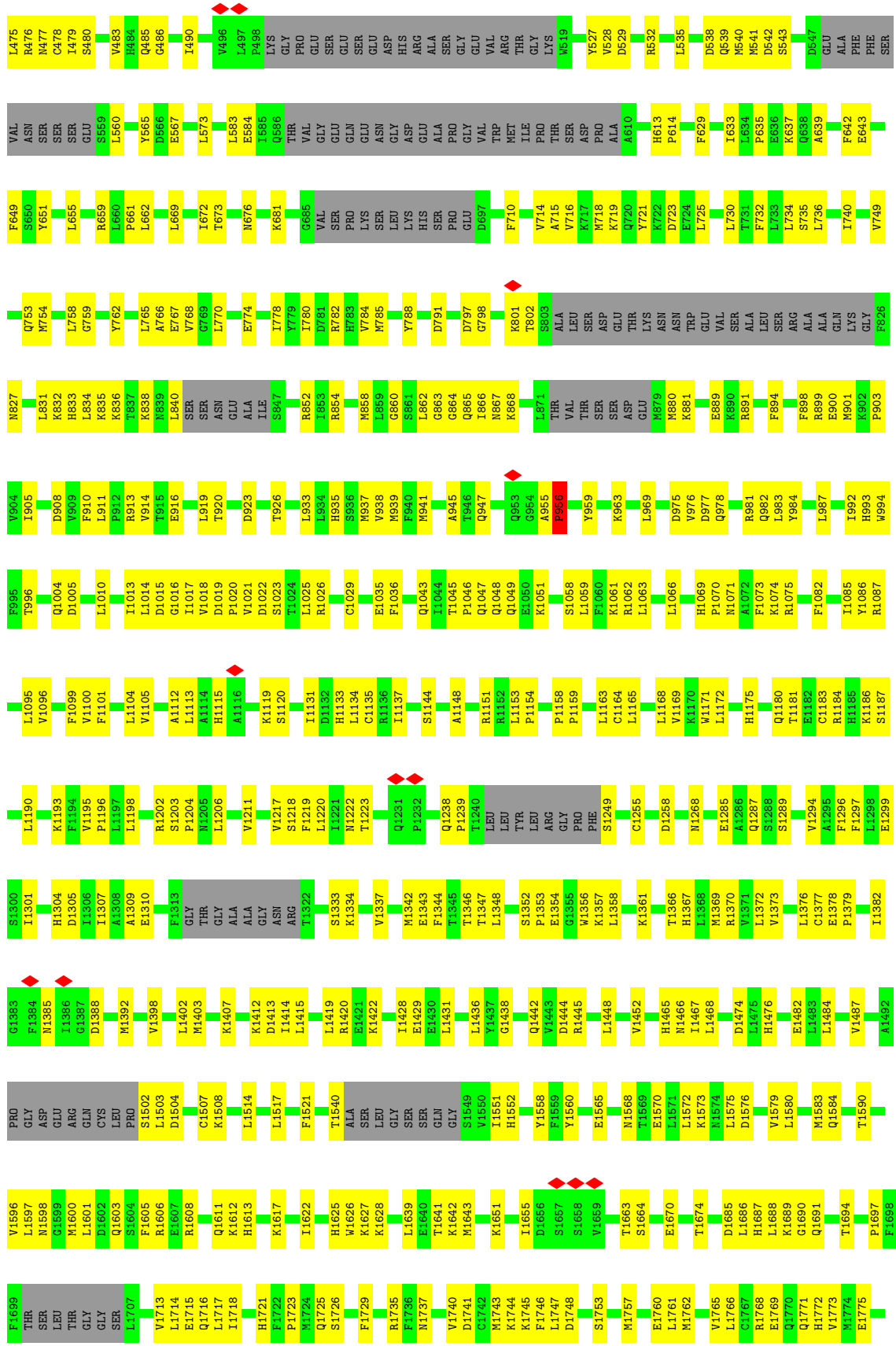


LEU	ASN	V1820	F1729	L1575	L1402	ASN	L1250	F1073	E985	P903	GLY
LYS	GLN	P1730	P1731	D1576	L1406	ARG	Q1251	K1074	P986	V904	F826
ARG	VAL	L1824	L1652	A1577	K1407	THR	A1252	L1075	L987	R1075	M827
THR	HIS	V1736	V1579	V1578	M1408	GLN	L1253	L1076	V988	F906	K828
PHE	ASN	S1658	M1583	V1579	S1409	ARG	L1254	D907	M989	L907	V829
PRD	CYS	V1659	M1583	M1583	M1412	GLN	M1255	D908	M909	D908	D908
VAL	PRO	T1663	S1586	S1586	K1412	CYS	K1170	F910	L834	L834	L834
GLU	THR	S1664	D1587	D1587	H1418	PRO	V1337	L919	K835	K835	K835
VAL	GLU	S1664	D1588	D1588	L1419	S1502	L1419	T920	T837	T837	T837
GLU	GLY	G1665	M1589	M1589	L1420	L1503	L1419	A921	S841	S841	S841
VAL	GLY	S1666	T1590	T1590	D1504	D1504	L1259	R922	L848	L848	L848
PRD	VAL	S1667	K1591	K1591	E1421	S1506	L1261	D923	E849	E849	E849
MET	PRD	P1669	M1592	M1592	K1422	C1507	L1264	R924	E850	E850	E850
GLU	ARG	V1670	V1593	V1593	I1423	F1344	M1268	R925	R851	R851	R851
ARG	ARG	E1671	V1596	V1596	A1425	T1345	I1271	R926	I852	I852	I852
LYS	LYS	T1672	L1597	L1597	S1427	T1347	R1274	K927	R853	R853	R853
LYS	ALA	T1673	M1598	M1598	I1428	L1348	R1274	V928	R854	R854	R854
TYR	ALA	T1674	G1599	G1599	L1431	T1351	A1278	L933	M858	M858	M858
ILE	GLU	V1675	M1600	M1600	L1431	S1352	L1278	L934	L859	L859	L859
GLU	ASN	I1676	L1601	L1601	M1435	P1353	L1279	L935	G850	G850	G850
ILE	THR	S1677	D1602	D1602	F1521	E1354	Q1280	S936	S861	S861	S861
ARG	LEU	L1678	S1604	S1604	P1439	G1355	L1282	M941	G863	G863	G863
LYS	LEU	D1685	F1605	F1605	D1440	M1356	G1283	M941	G864	G864	G864
GLU	ASN	H1686	R1606	R1606	L1444	K1357	L1282	M941	G865	G865	G865
ALA	GLU	H1687	L1607	L1607	Q1442	E1358	Q1287	T946	I866	I866	I866
GLU	ARG	H1688	E1607	E1607	L1443	L1359	Q1287	T946	I867	I867	I867
ARG	THR	K1689	R1608	R1608	L1444	L1360	P1204	T946	M867	M867	M867
LYS	THR	K1689	A1609	A1609	R1445	K1361	S1288	P949	K868	K868	K868
LYS	LEU	A1692	S1630	S1630	R1445	L1361	L1290	P949	M869	M869	M869
ASN	ASN	E1692	M1610	M1610	L1446	L1366	L1290	P949	K869	K869	K869
GLY	ASN	P1697	Q1611	Q1611	R1447	H1367	L1294	Q953	L870	L870	L870
ASP	ASP	F1698	K1612	K1612	V1452	L1368	V1294	Q953	L871	L871	L871
SER	SER	F1699	H1613	H1613	V1452	L1369	L1294	P956	VAL	VAL	VAL
ASP	ASP	F1699	Q1614	Q1614	A1461	M1370	F1297	P957	THR	THR	THR
GLY	THR	S1781	Q1617	Q1617	H1465	R1370	L1298	M958	SER	SER	SER
PRD	THR	R1788	K1617	K1617	H1466	L1372	L1298	Y959	SER	SER	SER
TYR	LEU	Q1794	L1623	L1623	N1466	L1375	E1299	Y962	GLU	GLU	GLU
MET	LEU	E1799	Q1624	Q1624	I1467	T1375	S1300	Y962	GLU	GLU	GLU
SER	GLY	S1800	H1625	H1625	I1468	L1376	I1301	K963	M879	M879	M879
SER	GLY	V1800	W1626	W1626	P1469	C1377	A1302	K963	M880	M880	M880
LEU	SER	V1801	K1627	K1627	M1469	E1378	M1303	K964	K851	K851	K851
SER	THR	Y1802	K1628	K1628	D1474	L1382	H1304	T965	W856	W856	W856
GLU	LYS	E1803	C1629	C1629	L1475	I1382	D1305	P966	D857	D857	D857
LYS	LYS	R1883	W1633	W1633	V1479	G1383	I1307	L969	R858	R858	R858
LEU	LEU	L1884	A1634	A1634	E1482	F1384	I1307	L969	R858	R858	R858
ALA	GLU	P1885	K1635	K1635	E1482	F1384	A1308	L972	R891	R891	R891
ASP	LYS	LYS	L1639	L1639	L1483	V1389	A1309	D975	L892	L892	L892
SER	ASN	ASP	E1640	E1640	L1484	V1390	I1310	D975	L892	L892	L892
THR	THR	ASP	T1641	T1641	L1484	V1391	F1313	D976	F894	F894	F894
LEU	LEU	VAL	M1642	M1642	V1487	M1392	GLY	D977	F894	F894	F894
SER	THR	VAL	K1643	K1643	Y1488	M1392	THR	T980	F898	F898	F898
GLU	GLU	ALA	A1644	A1644	Y1488	D1397	ARG	T980	F898	F898	F898
GLU	GLU	LYS	M1645	M1645	K1489	V1397	GLY	R899	R899	R899	R899
ASN	ASN	LEU	L1646	L1646	M1568	V1399	ALA	E900	E900	E900	E900
LEU	LEU	PHE	L1646	L1646	M1568	C1399	ALA	L983	L983	L983	L983
ILE	LYS	T1815	L1647	L1647	M1574	V1400	GLY	M901	M901	M901	M901
ASP	ASP	E1728	A1647	A1647	A1492	M1401	GLY	K902	K902	K902	K902



- Molecule 1: DNA-dependent protein kinase catalytic subunit, DNA-dependent protein kinase catalytic subunit, DNA-PKcs



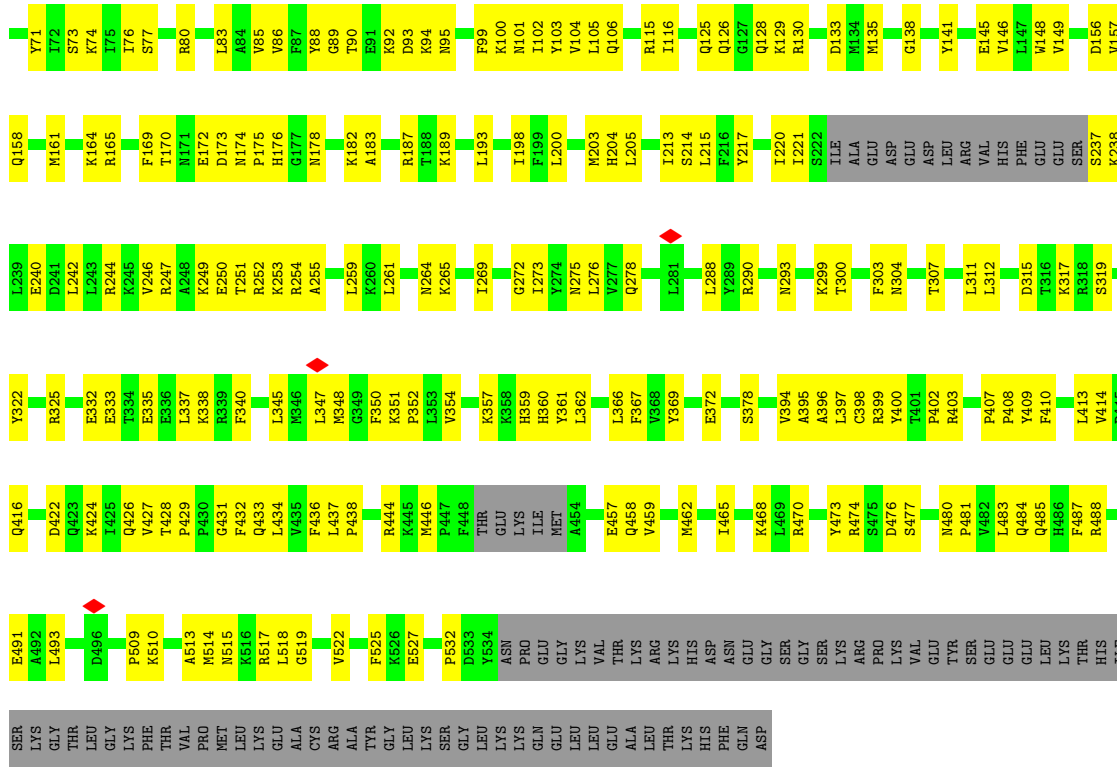


Q3037	E3038	E3039	Y3040	S3047	K3048	L3049	K3050	L3051	L3052	E3056	L3061	L3062	L3065	K3069	L3080	L3088	L3089	D3097	R3098	K3100	L3103	F3110	K3111	Q3112	S3115	D3118	V3119	L3120	L3121	K3122	Q3123	L3126	K3127	L3129	Q3130	Q3133	A3134	L3135	T3136	E3137	L3138	F3141											
I3143	S3144	F3144	T3039	S3146	K3147	Q3148	Q3149	N3150	L3151	L3052	V3155	K3158	R3159	L3160	L3161	N3162	T3165	N3166	R3167	Y3168	P3169	D3170	A3171	D3174	A3099	P3175	K3100	K3176	N3177	L3178	W3179	D3180	L3183	R3186	F3189	L3190	M3256	L3121	E3194	L3197	THR	PRO	LEU	PRO	GLU	ASP	ASN	SER	MET	ASN	VAL	ASP	GLN
ASP	GLY	ASP	PRD	SER	ASP	ARG	LEU	VAL	GLN	GLU	GLU	D3226	S3229	L3230	I3231	R3232	C3234	K3238	K3239	M3240	K3241	K3242	I3243	I3244	R3247	K3248	Q3249	N3250	N3251	F3252	S3253	L3254	A3255	M3256	K3257	L3258	L3262	S3266	K3267	T3268	R3269	W3272	Q3278	C3281	R3282	L3283	S3284	C3281	R3282	L3283	S3284		
H3285	G3286	R3287	S3288	G3292	C3293	S3294	V3297	L3298	V3304	S3305	D3308	L3321	R3324	D3325	Q3326	L3329	T3333	D3354	R3358	G3364	SER	SER	SER	SER	D3368	E3369	S3370	E3371	K3372	V3373	R3380	Q3383	H3384	L3385	E3387	A3388	V3389	A3391	A3392	E3395	ALA	GLN	PRO	PRO	ALA	GLN	PRO	PRO	ALA	GLN	PRO	PRO	
SER	TRP	CYS	GLY	PRO	ALA	K3407	G3408	V3409	Y3413	K3414	T3415	L3416	F3419	G3420	D3421	Q3422	Q3423	E3428	E3429	ALA	SER	VAL	ILE	ASP	SER	ALA	A3441	V3442	P3443	A3444	L3445	V3446	V3447	E3448	K3455	R3462	L3463	K3464	R3467	I3471	L3472	E3473	R3474	E3478	L3479	L3480							
S3481	L3482	M3483	P3491	C3492	M3493	W3498	I3499	S3500	H3501	M3502	V3503	A3504	L3505	L3506	D3507	K3508	D3509	Q3510	V3511	V3512	A3513	V3514	Q3515	I3521	Q3527	A3528	I3529	V3530	Y3531	P3532	F3533	I3534	S3537	E3538	S3539	TYR	SER	PHE	LYS	ASP	T3545	F3554	R3557	I3558	L3562	D3563	Q3564	G3565	G3566	Q3569			
D3570	F3571	L3572	D3576	L3577	L3578	L3583	K3586	D3587	M3588	R3593	A3597	LYS	THR	V3601	K3609	D3619	P3620	K3621	Q3629	R3630	I3633	Q3634	Y3631	F3633	I3634	E3639	H3643	G3647	GLY	SER	LYS	LEU	LEU	ARG	MET	LYS	LEU	D3658	F3659	R3660	D3661	I3662	H3665	L3666	L3667	L3668							
K3669	M3670	P3677	N3679	L3680	K3681	E3682	S3683	S3684	W3686	M3687	D3688	S3689	F3690	F3694	L3695	E3700	I3701	P3702	G3703	Y3705	E3714	Y3715	H3716	V3717	R3718	I3719	A3720	D3723	E3724	R3725	V3726	M3729	A3730	S3731	R3732	R3733	R3734	K3736	R3737	I3738	I3739	I3740	H3743	P3749	F3750	L3751	L3752						
G3755	L3758	M3771	N3772	G3773	L3774	L3775	G3781	A3785	L3786	Q3787	L3788	R3789	S3792	V3793	V3794	P3795	N3796	G3801	L3802	I3803	E3804	N3808	V3810	T3811	D3814	K3820	E3823	E3824	K3825	A3827	Y3828	L3829	S3830	D3831	P3832	P3835	Y3839	L3843	THR	LYS	MET	SER	GLY										
LYS	HIS	D3851	M3855	K3856	S3870	R3874	K3875	S3876	L3882	R3885	A3886	F3887	R3888	R3889	M3890	S3891	P3894	A3899	L3910	I3911	C3912	H3915	G3919	I3920	G3921	D3922	R3923	F3928	M3929	V3930	E3933	V3937	I3938	H3944	G3947	V3955	I3958	M3959	R3962	I3968	N3969												
L3970	K3971	L3972	P3973	K3974	E3976	L3979	K3980	V3981	S3982	L3983	K3984	V3985	H3986	R3992	S3993	D3994	L3997	L3998	L4010	L4011	L4012	L4013	L4014	L4015	PHE	GLU	GLN	LYS	MET	LEU	LYS	GLY	TRP	ILE	GLN	GLU	ILE	ASN	VAL	ALA	ASN	Y4038	A4054	P4055	A4057								
V4058	L4065	E4069	R4082	D4086	H4087	N4088	I4089	R4090	A4091	P4094	E4095	S4096	G4097	Q4103	C4106	L4107	A4111	T4112	D4113	P4114	N4115	I4116	L4117	G4118	R4119	T4120	W4121	W4124	E4125	W4127	X6018	X6023																					

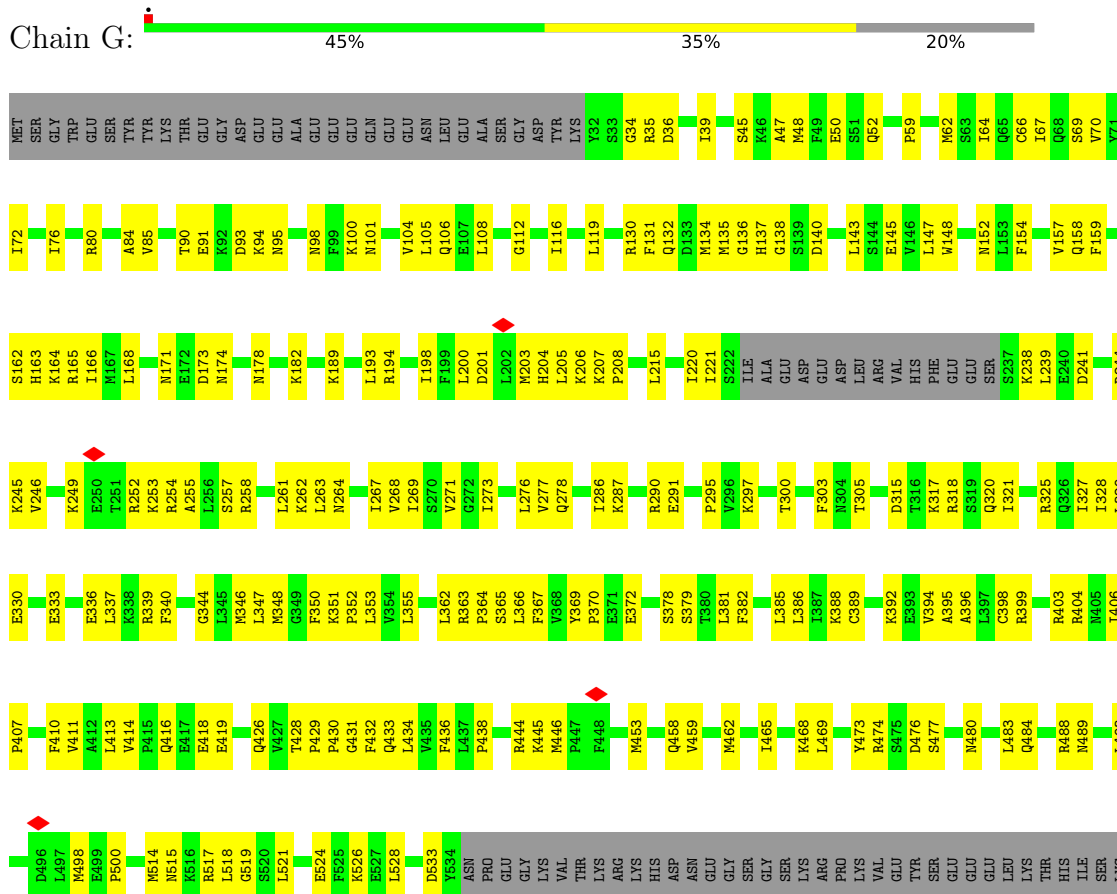
• Molecule 2: X-ray repair cross-complementing protein 6

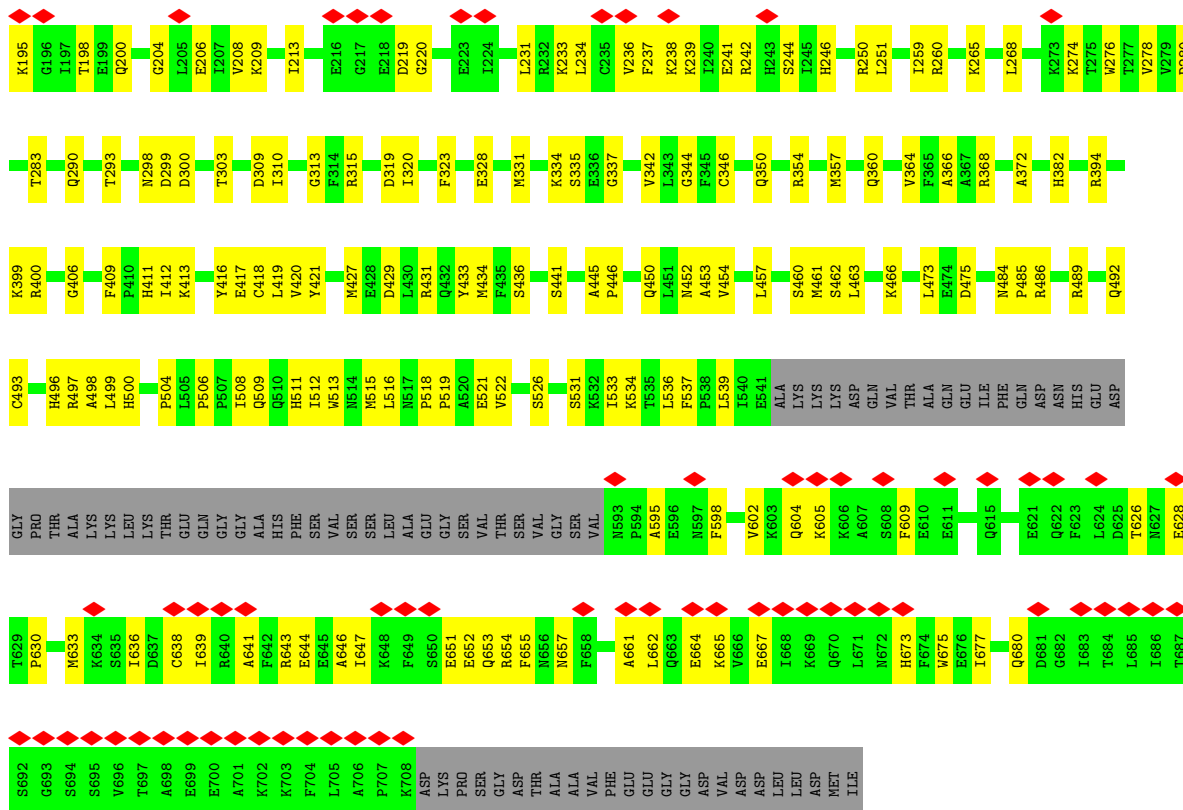


MET	SER	GLY	TRP	GLU	SER	TYR	LYS	THR	GLU	GLY	ASP	GLU	GLN	GLN	GLU	ASN	LEU	LEU	ALA	SER	GLY	ASP	TYR	LYS	Y32	R35	L38	I41	F40	V42	S45	W48	F49	GLU	SER	GLN	SER	GLU	ASP	GLU	LEU	T58	P59	F60	S63	C66
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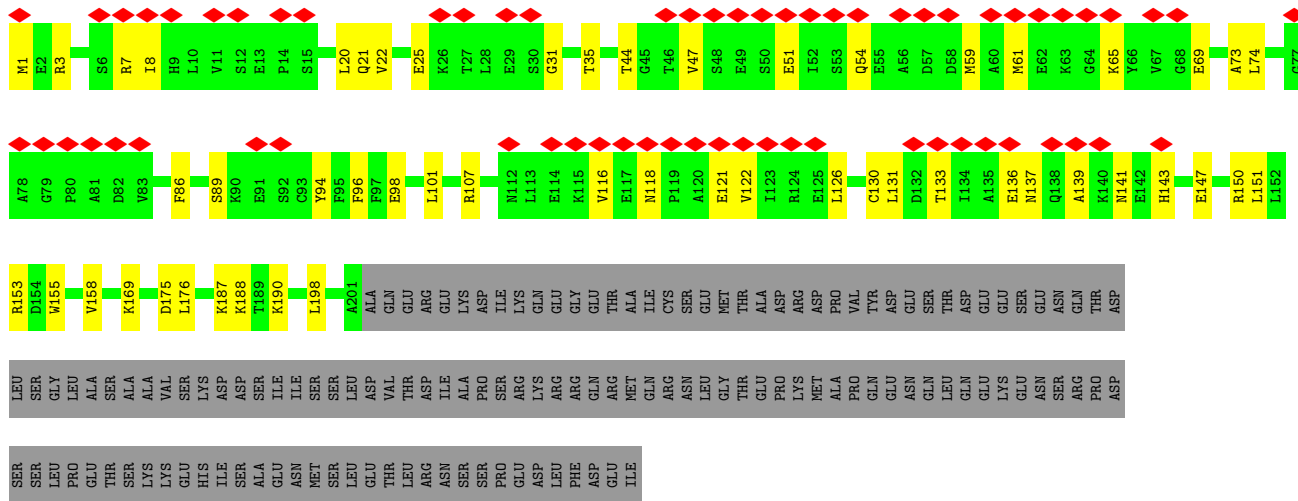


• Molecule 2: X-ray repair cross-complementing protein 6

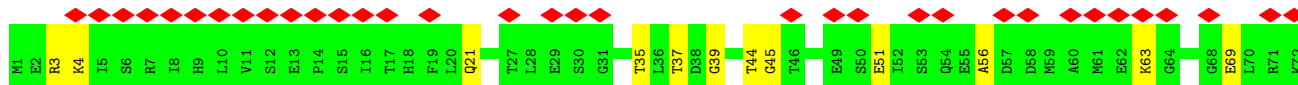
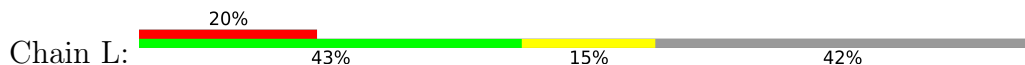


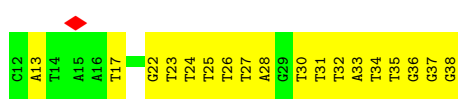


• Molecule 4: DNA repair protein XRCC4



• Molecule 4: DNA repair protein XRCC4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23421	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 ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.695	Depositor
Minimum map value	-0.275	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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	0.17	0/28527	0.36	0/38582
1	F	0.16	0/28510	0.35	2/38552 (0.0%)
2	B	0.13	0/3896	0.33	0/5248
2	G	0.13	0/4025	0.30	0/5421
3	C	0.11	0/3921	0.26	0/5282
3	H	0.13	0/5254	0.34	1/7085 (0.0%)
4	K	0.11	0/1654	0.27	0/2224
4	L	0.13	0/1619	0.35	0/2174
4	N	0.11	0/1654	0.31	0/2224
4	O	0.11	0/1605	0.29	0/2155
5	M	0.10	0/2144	0.24	0/2895
5	P	0.23	0/2008	0.36	0/2712
6	Q	0.13	0/1722	0.41	2/2332 (0.1%)
6	R	0.14	0/1762	0.39	0/2389
7	D	0.22	0/622	0.39	0/959
8	E	0.23	0/647	0.42	0/996
8	I	0.23	0/647	0.40	0/996
9	J	0.24	0/623	0.47	0/961
All	All	0.16	0/90840	0.35	5/123187 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	956	PRO	N-CA-CB	7.92	110.77	103.08
3	H	16	VAL	N-CA-C	-6.85	105.81	111.91
6	Q	132	SER	CA-C-N	-5.86	111.91	122.46
6	Q	132	SER	C-N-CA	-5.86	111.91	122.46
1	F	1540	THR	CA-C-O	5.73	127.93	121.51

There are no chirality outliers.

There are no planarity outliers.

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	28076	0	28047	959	0
1	F	28060	0	28056	913	0
2	B	3822	0	3899	173	0
2	G	3948	0	4036	186	0
3	C	3849	0	3892	123	0
3	H	5150	0	5176	185	0
4	K	1625	0	1611	42	0
4	L	1592	0	1583	45	0
4	N	1625	0	1611	35	0
4	O	1579	0	1571	39	0
5	M	2095	0	2046	44	0
5	P	1965	0	1904	77	0
6	Q	1690	0	1699	54	0
6	R	1728	0	1728	66	0
7	D	556	0	310	35	0
8	E	576	0	318	28	0
8	I	576	0	318	35	0
9	J	557	0	311	29	0
All	All	89069	0	88116	2871	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 16.

The worst 5 of 2871 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:1549:SER:O	1:A:1550:VAL:HG22	1.17	1.29
1:A:1549:SER:O	1:A:1550:VAL:CG2	2.04	1.05
3:H:56:LEU:H	3:H:81:ARG:HB2	1.39	0.88
1:A:327:VAL:HG13	1:A:333:MET:HB2	1.58	0.85
5:P:811:SER:HB2	5:P:849:GLY:HA3	1.57	0.84

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	A	3474/4148 (84%)	3222 (93%)	248 (7%)	4 (0%)	48	81
1	F	3467/4148 (84%)	3198 (92%)	265 (8%)	4 (0%)	48	81
2	B	468/609 (77%)	430 (92%)	37 (8%)	1 (0%)	43	76
2	G	485/609 (80%)	460 (95%)	25 (5%)	0	100	100
3	C	465/732 (64%)	445 (96%)	20 (4%)	0	100	100
3	H	636/732 (87%)	597 (94%)	39 (6%)	0	100	100
4	K	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
4	L	191/336 (57%)	184 (96%)	7 (4%)	0	100	100
4	N	199/336 (59%)	191 (96%)	8 (4%)	0	100	100
4	O	190/336 (56%)	182 (96%)	8 (4%)	0	100	100
5	M	256/911 (28%)	239 (93%)	17 (7%)	0	100	100
5	P	242/911 (27%)	225 (93%)	16 (7%)	1 (0%)	30	65
6	Q	205/299 (69%)	185 (90%)	20 (10%)	0	100	100
6	R	214/299 (72%)	200 (94%)	14 (6%)	0	100	100
All	All	10691/14742 (72%)	9953 (93%)	728 (7%)	10 (0%)	49	81

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2291	GLN
1	F	955	ALA
1	F	956	PRO
1	F	2291	GLN
1	A	1550	VAL

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	3054/3671 (83%)	3049 (100%)	5 (0%)	87	86
1	F	3058/3671 (83%)	3058 (100%)	0	100	100
2	B	427/548 (78%)	427 (100%)	0	100	100
2	G	444/548 (81%)	444 (100%)	0	100	100
3	C	434/649 (67%)	434 (100%)	0	100	100
3	H	575/649 (89%)	575 (100%)	0	100	100
4	K	179/303 (59%)	179 (100%)	0	100	100
4	L	177/303 (58%)	177 (100%)	0	100	100
4	N	179/303 (59%)	179 (100%)	0	100	100
4	O	175/303 (58%)	175 (100%)	0	100	100
5	M	234/808 (29%)	234 (100%)	0	100	100
5	P	217/808 (27%)	216 (100%)	1 (0%)	81	81
6	Q	187/262 (71%)	187 (100%)	0	100	100
6	R	191/262 (73%)	191 (100%)	0	100	100
All	All	9531/13088 (73%)	9525 (100%)	6 (0%)	87	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1539	SER
1	A	1549	SER
5	P	817	THR
1	A	946	THR
1	A	802	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1231	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	143	HIS
1	F	2353	GLN
5	M	680	ASN
3	H	290	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	4128:MET	C	6004:UNK	N	90.10
1	A	4128:MET	C	6004:UNK	N	89.52

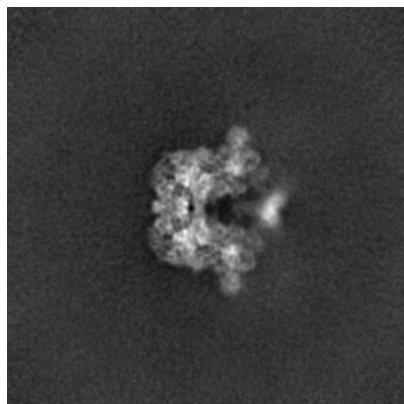
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12299. These allow visual inspection of the internal detail of the map and identification of artifacts.

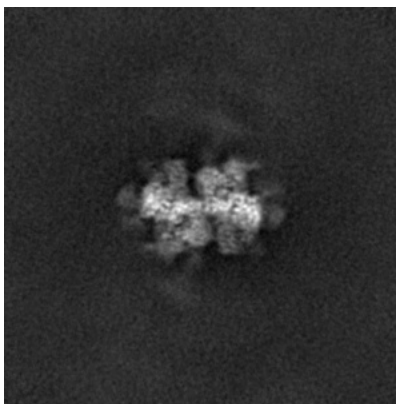
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

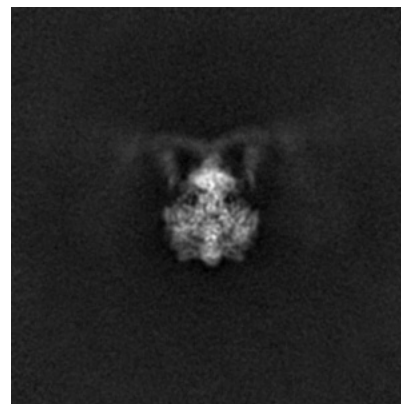
6.1.1 Primary map



X

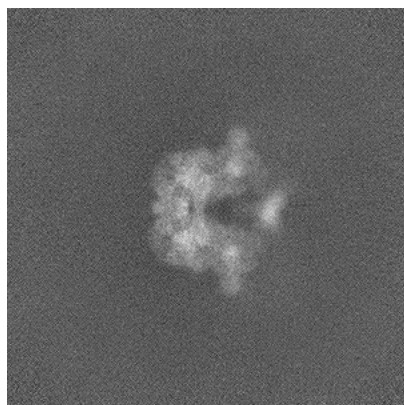


Y

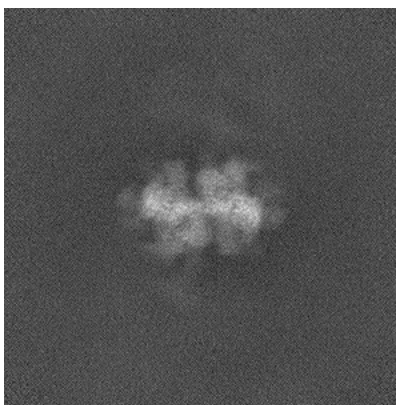


Z

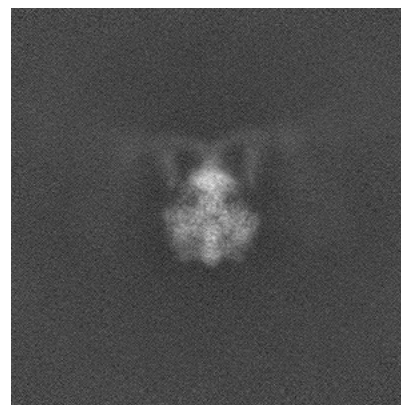
6.1.2 Raw map



X



Y

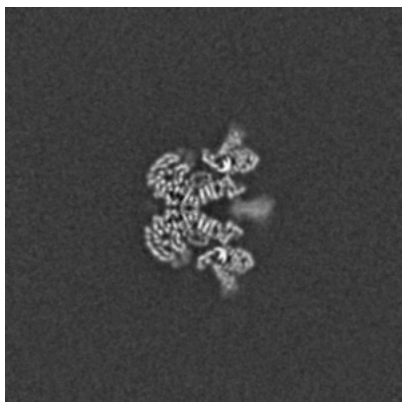


Z

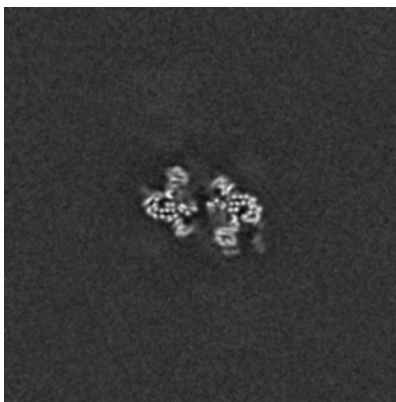
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

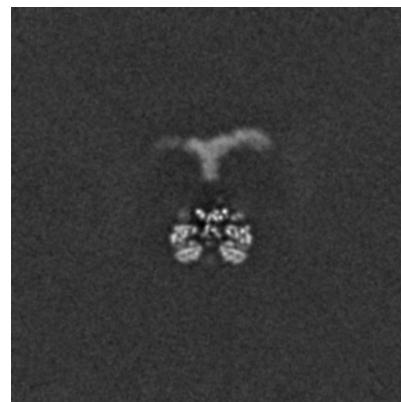
6.2.1 Primary map



X Index: 270

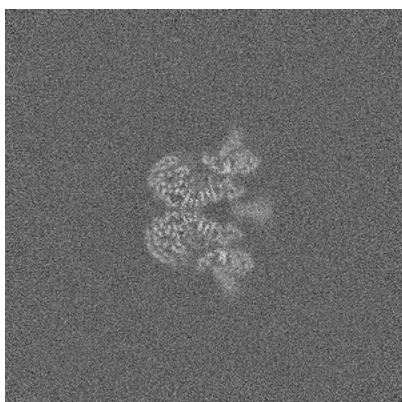


Y Index: 270



Z Index: 270

6.2.2 Raw map



X Index: 270



Y Index: 270

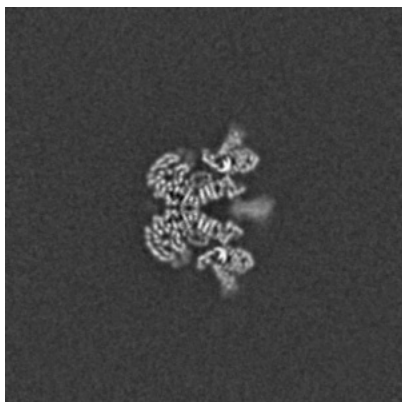


Z Index: 270

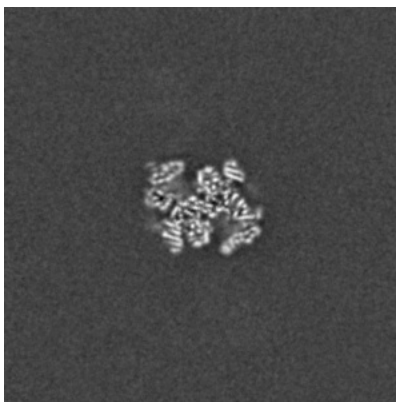
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 270

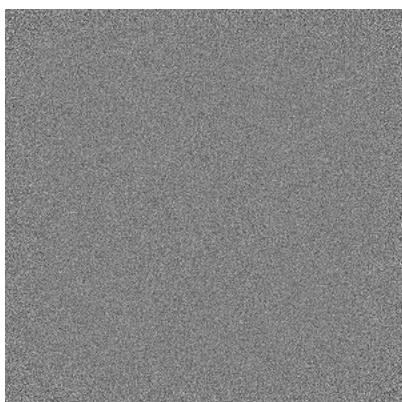


Y Index: 241

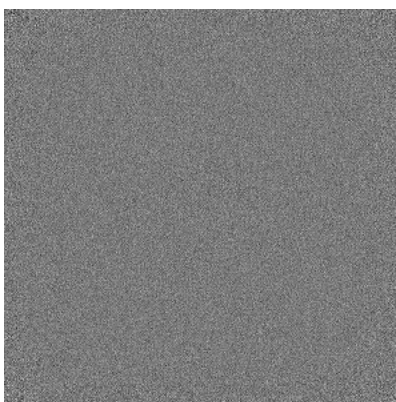


Z Index: 313

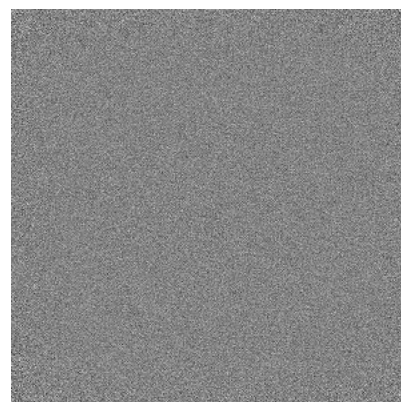
6.3.2 Raw map



X Index: 0



Y Index: 0

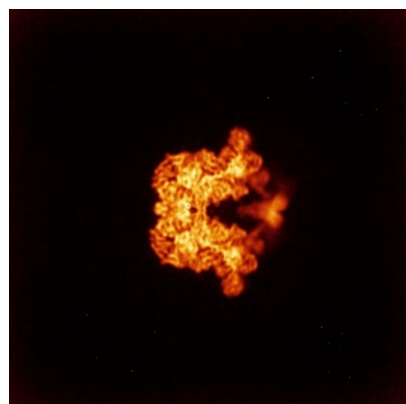


Z Index: 0

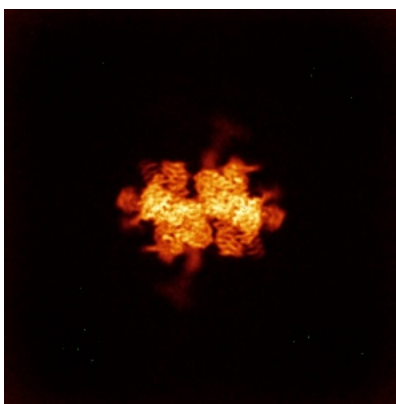
The images above show the largest variance slices of the map in three orthogonal directions.

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

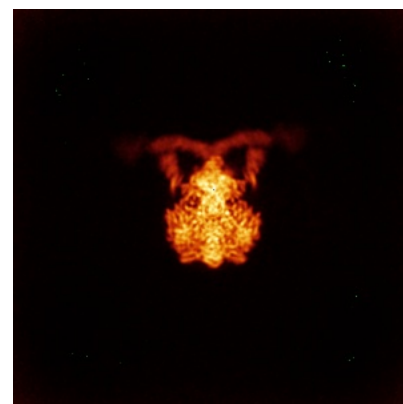
6.4.1 Primary map



X

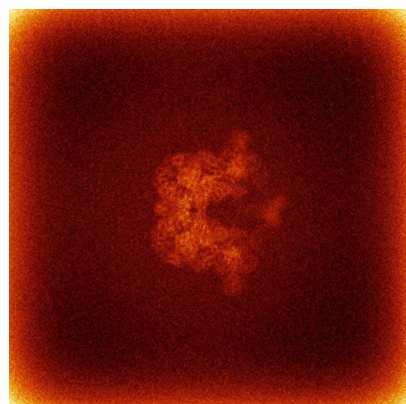


Y

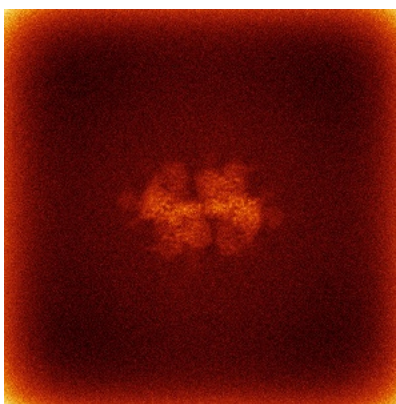


Z

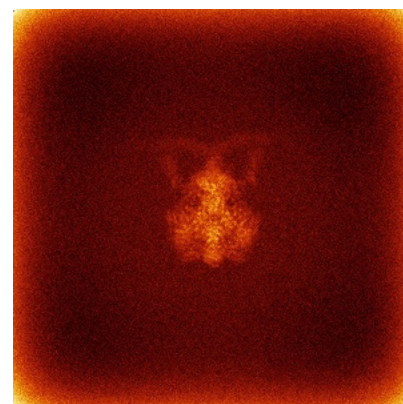
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



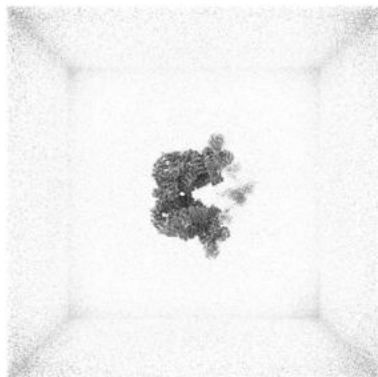
Y



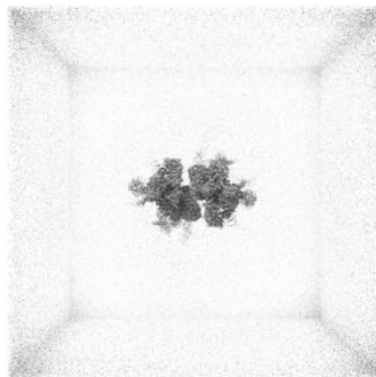
Z

The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

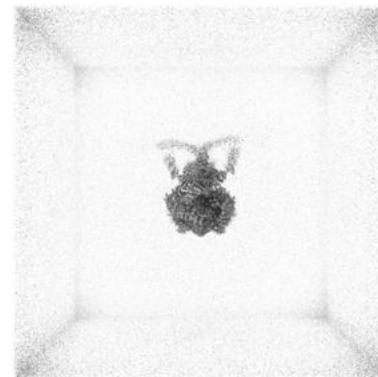
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

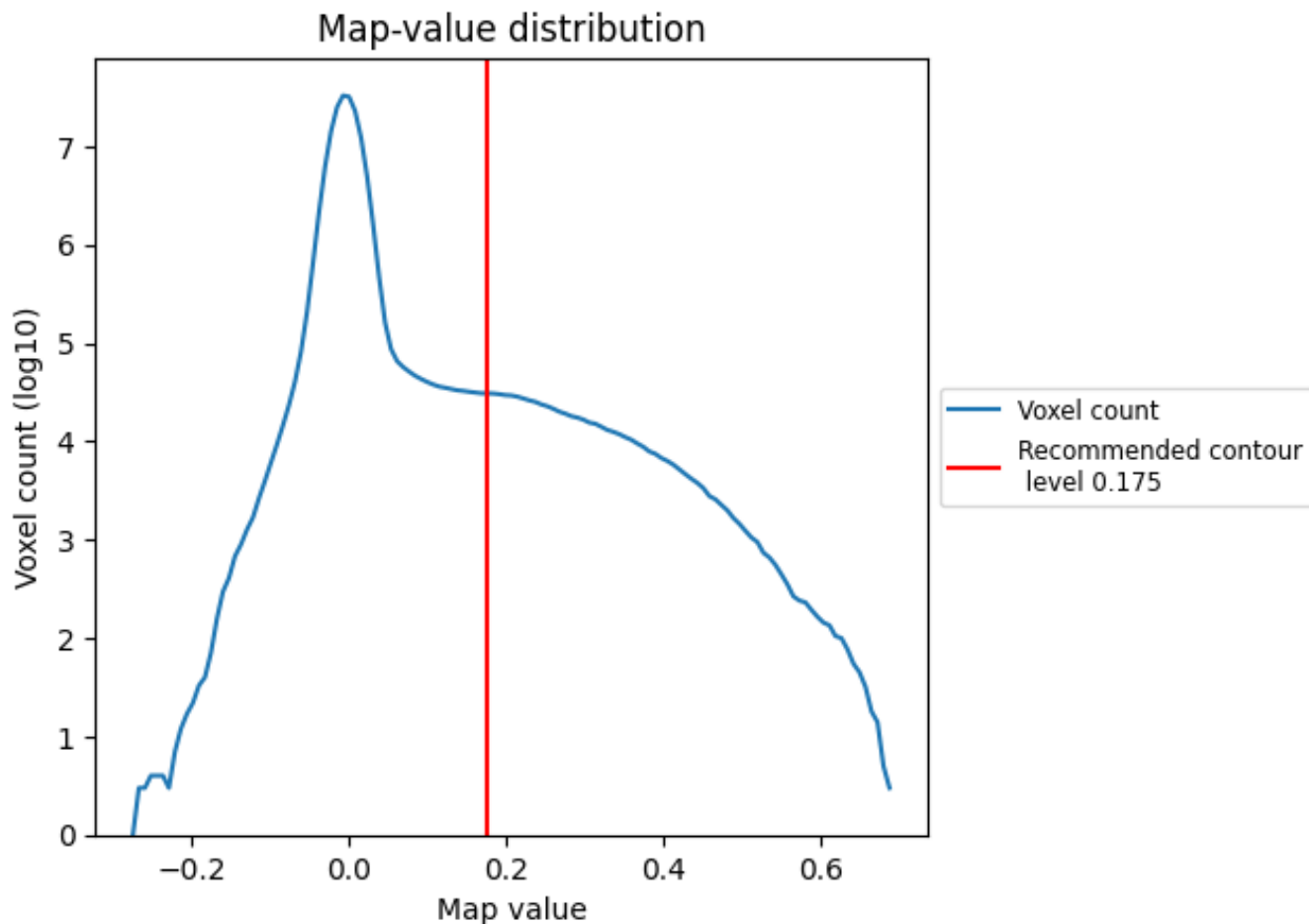
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

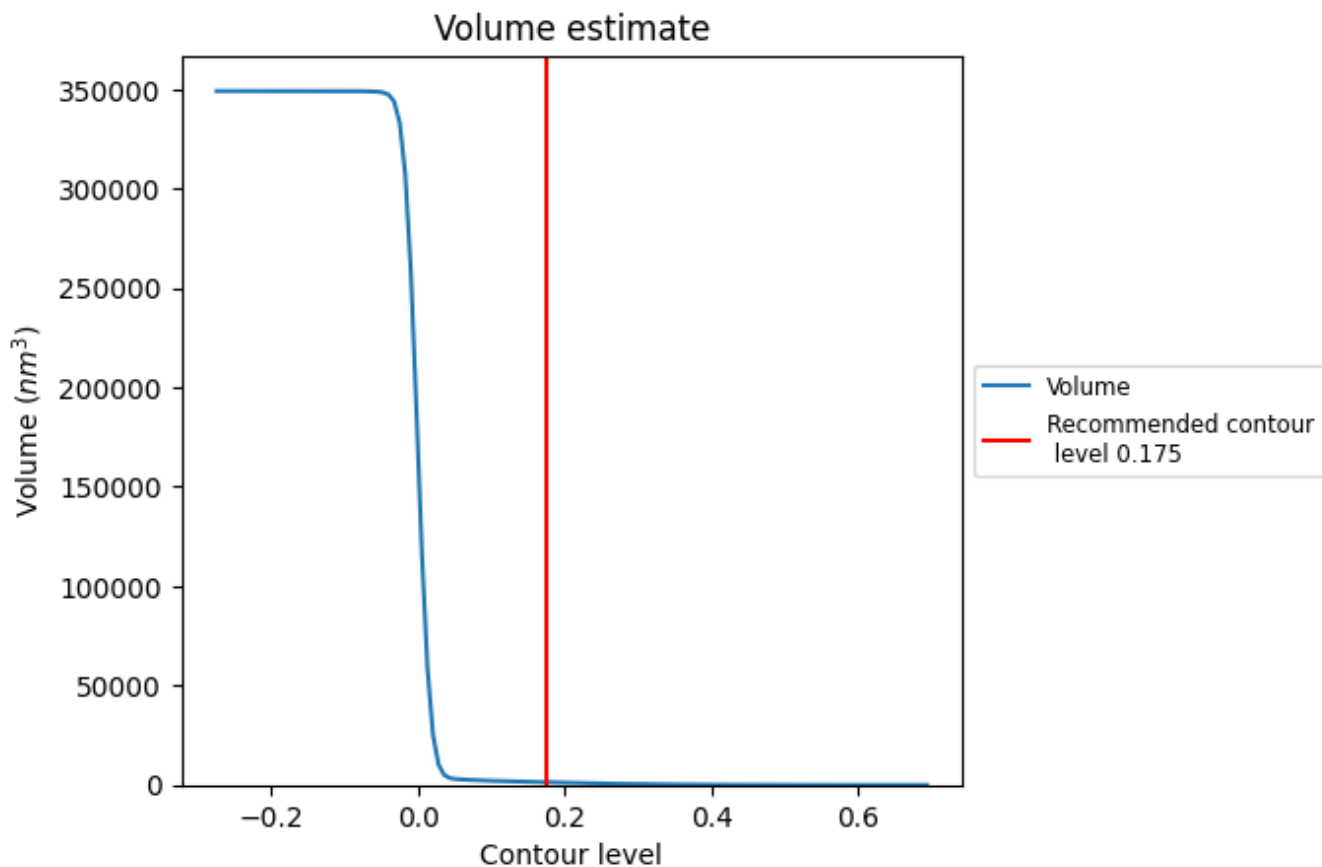
This section contains the results of statistical analysis of the map.

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.

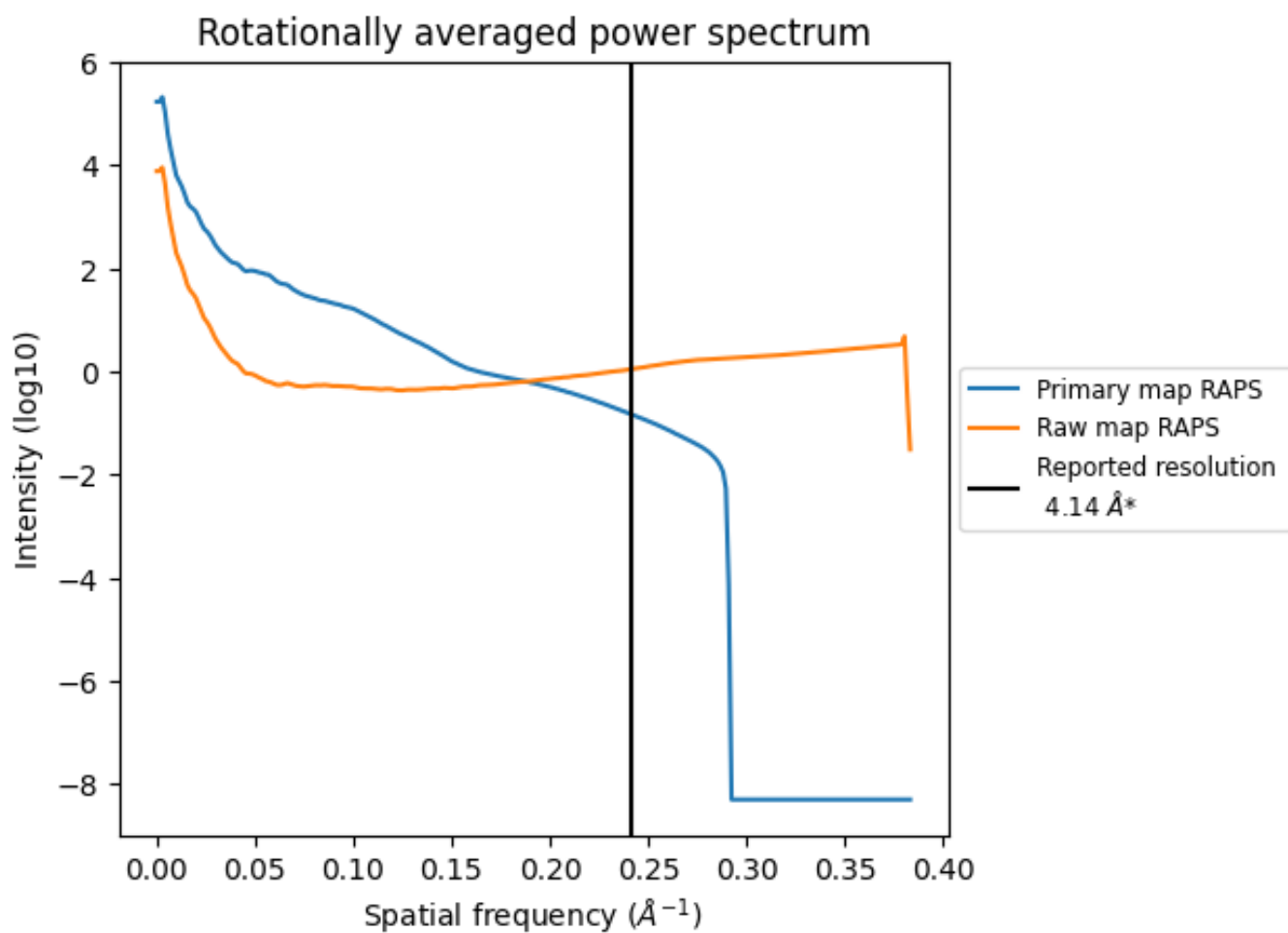
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1371 nm³; this corresponds to an approximate mass of 1239 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

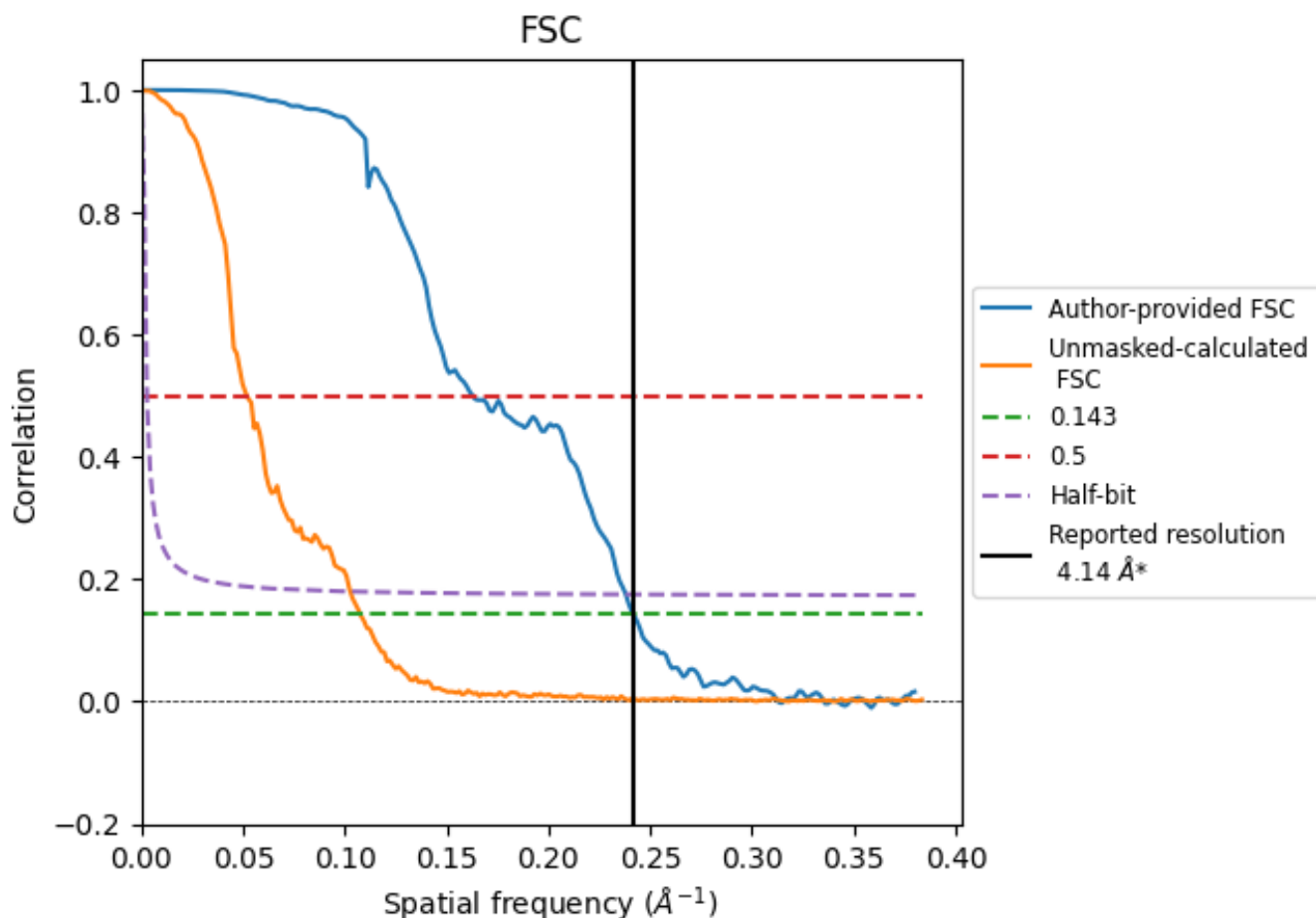


*Reported resolution corresponds to spatial frequency of 0.242 \AA^{-1}

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 0.242 Å⁻¹

8.2 Resolution estimates [i](#)

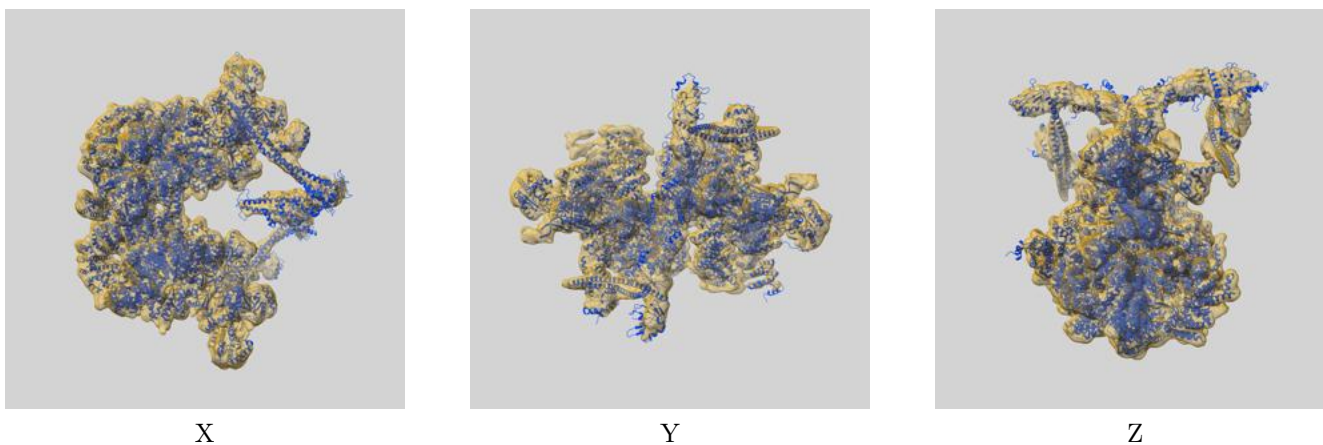
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.14	6.14	4.20
Unmasked-calculated*	9.30	19.27	9.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.30 differs from the reported value 4.14 by more than 10 %

9 Map-model fit [i](#)

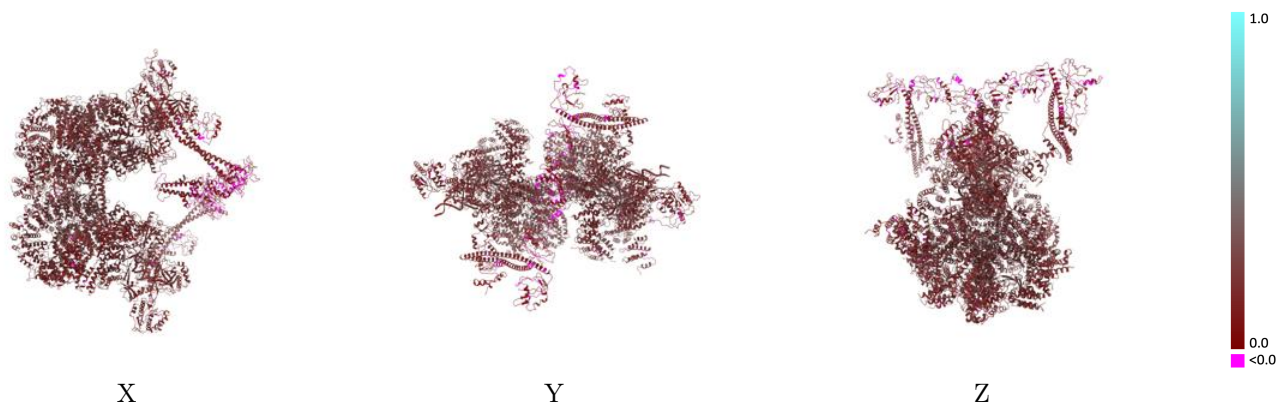
This section contains information regarding the fit between EMDB map EMD-12299 and PDB model 7NFC. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



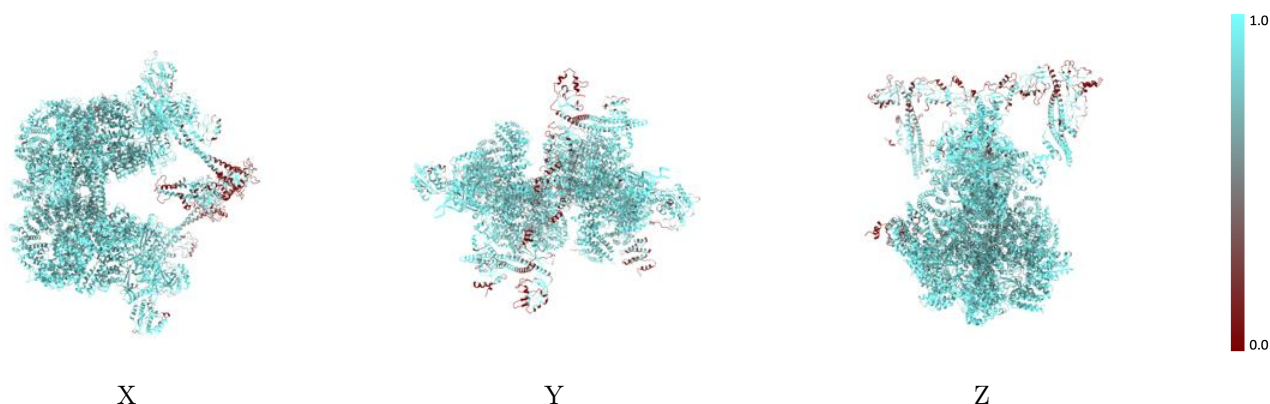
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



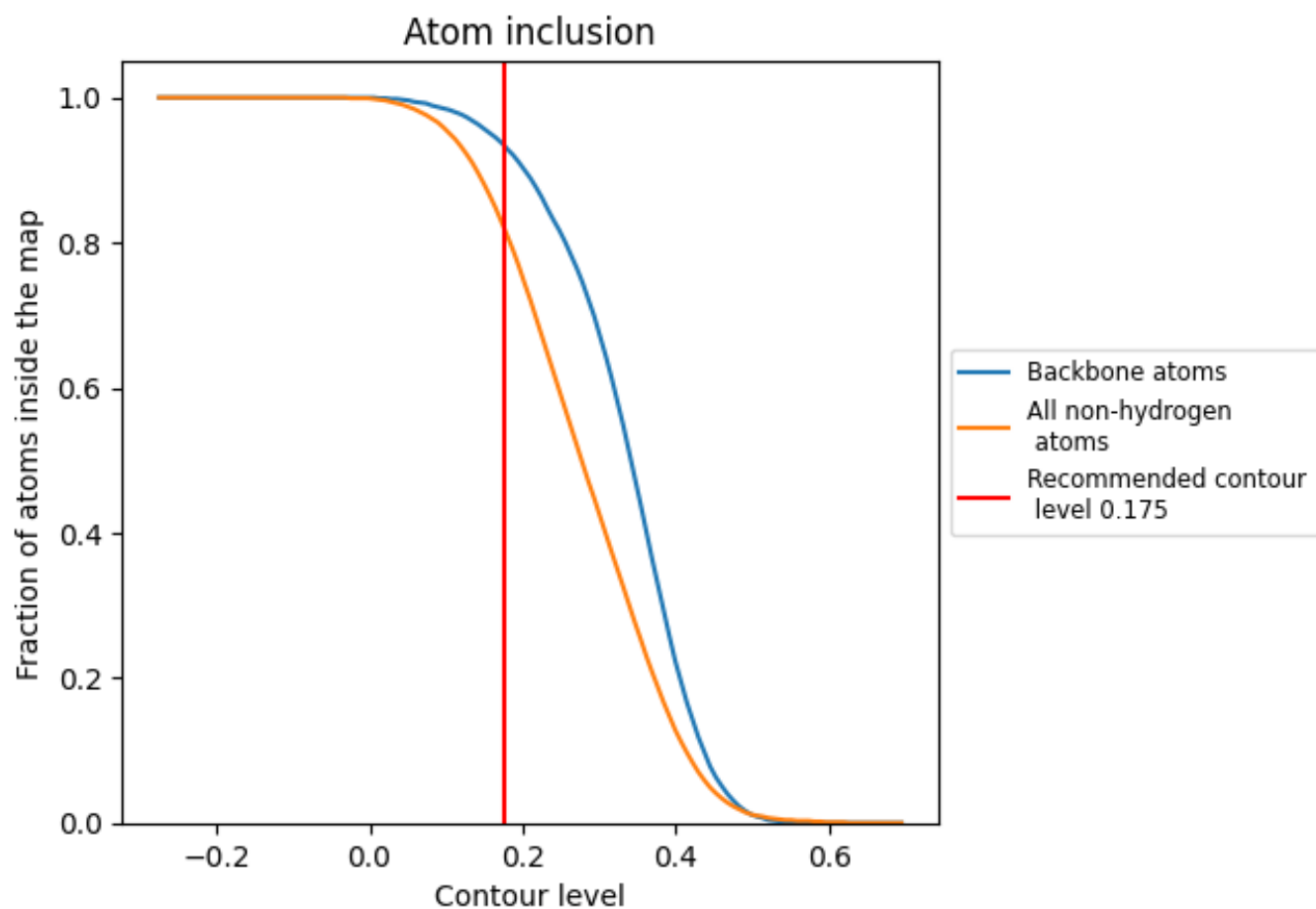
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.175).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.2000
A	 0.8610	 0.2150
B	 0.8780	 0.2140
C	 0.8580	 0.2000
D	 0.9190	 0.2360
E	 0.9290	 0.2190
F	 0.8630	 0.2170
G	 0.8790	 0.2170
H	 0.7590	 0.1840
I	 0.9290	 0.2420
J	 0.9320	 0.2470
K	 0.6290	 0.1220
L	 0.5850	 0.1210
M	 0.7290	 0.1570
N	 0.5900	 0.1080
O	 0.5000	 0.1150
P	 0.8410	 0.1680
Q	 0.5410	 0.1000
R	 0.5340	 0.0830

