



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2024 – 10:35 AM JST

PDB ID : 7YE2
EMDB ID : EMD-33762
Title : The cryo-EM structure of C. crescentus GcrA-TACdown
Authors : Wu, X.X.; Zhang, Y.
Deposited on : 2022-07-05
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

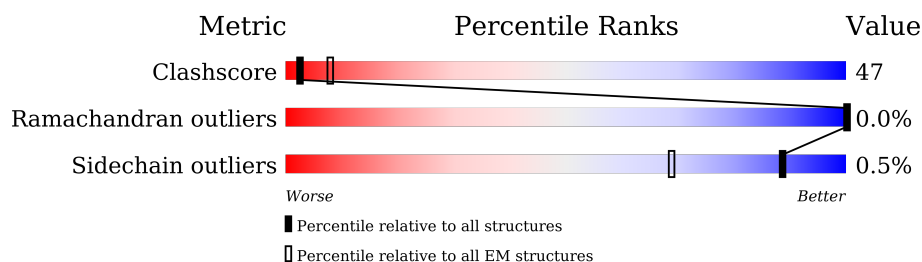
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 $\leq 5\%$. 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	338	
1	B	338	
2	C	1356	
3	D	1396	
4	E	119	
5	F	652	
6	H	90	
7	I	90	

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Mol	Chain	Length	Quality of chain	
				
8	G	173		

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28925 atoms, of which 12 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2054	1300	353	397	4		
1	B	220	Total	C	N	O	S	0	0
			1633	1044	274	311	4		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1303	Total	C	H	N	O	S	0	0
			9603	6112	12	1598	1841	40		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1140	Total	C	N	O	S	0	0
			8691	5586	1432	1630	43		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	69	Total	C	N	O	S	0	0
			510	323	85	101	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	497	Total	C	N	O	S	0	0
			3266	2049	576	631	10		

- Molecule 6 is a DNA chain called DNA (90-MER)-non template.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	68	Total	C	N	O	P	0	0
			1396	663	257	408	68		

- Molecule 7 is a DNA chain called DNA (90-MER)-template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	68	Total	C	N	O	P	0	0
			1396	663	257	408	68		

- Molecule 8 is a protein called Cell cycle regulatory protein GcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	53	Total	C	N	O	S	0	0
			372	237	61	70	4		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	
9	G	1	Total	Zn	0
			1	1	

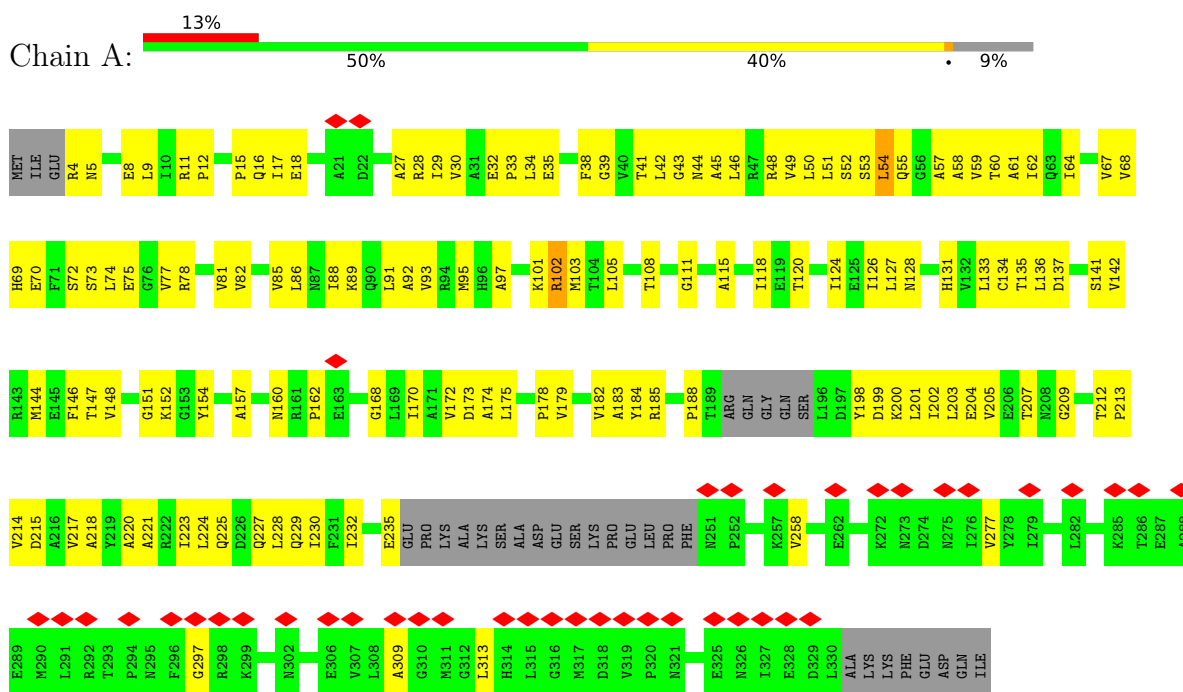
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

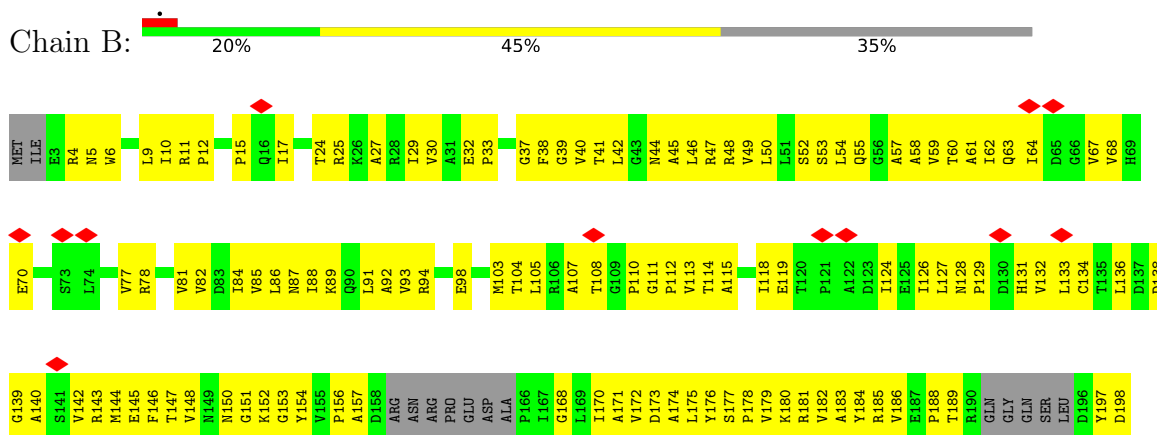
3 Residue-property plots

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-directed RNA polymerase subunit alpha



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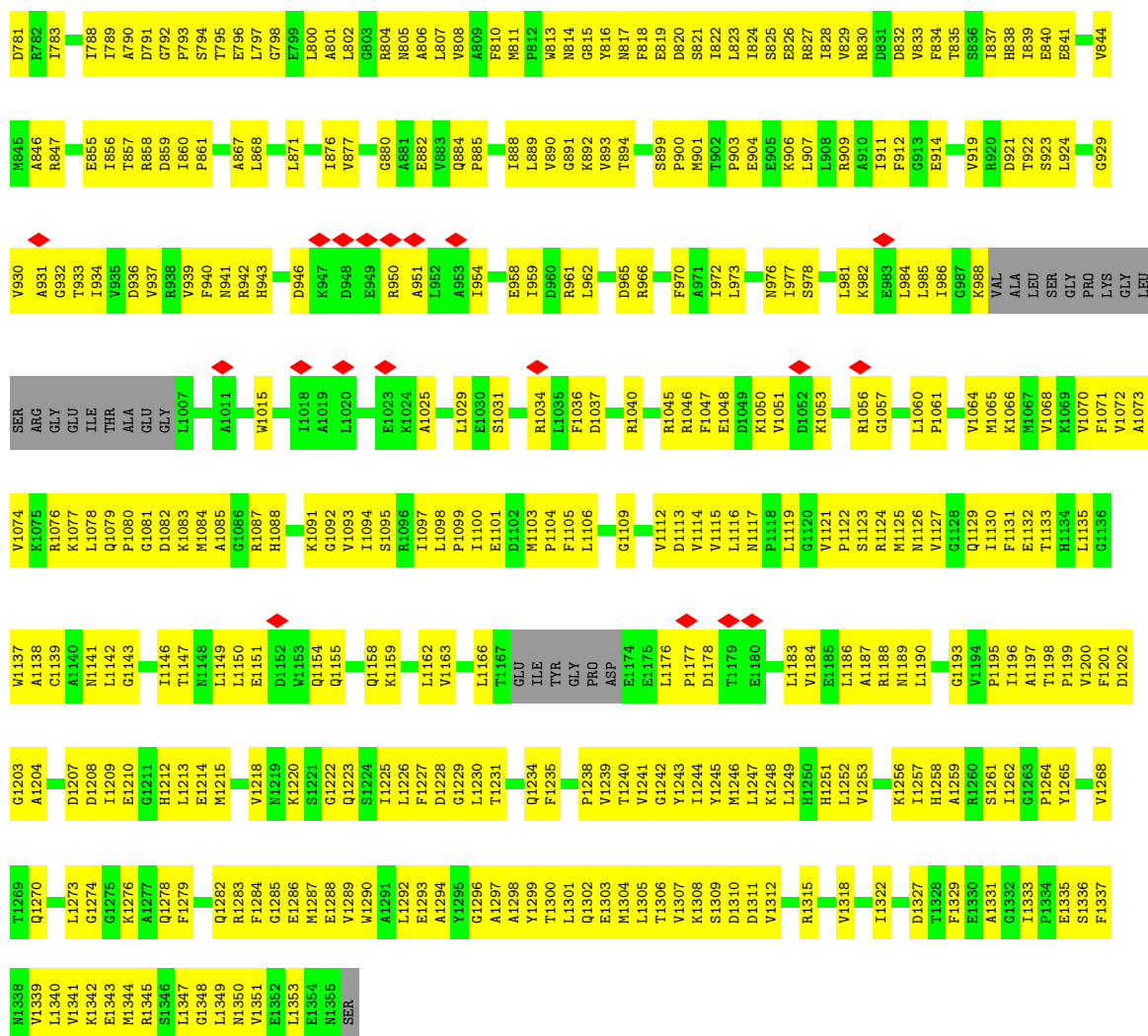


K199	ASP
L200	GLU
I201	LEU
L202	GLU
E203	LEU
V204	SER
E205	VAL
T206	ARG
N207	SER
A208	ALA
A209	ASN
V210	CYS
T211	LEU
P212	LYS
V213	ASN
D214	ASP
A215	ASN
V216	VAL
A217	ILE
Y218	TYR
A219	ILE
A220	GLY
R221	ASP
L222	LEU
L223	ILE
Q224	GLN
D225	LYS
Q226	THR
L227	GLU
Q228	ALA
I229	GLU
F230	MET
I231	LEU
T232	ARG
F233	THR
E234	PRO
GLU	ASN
PRO	PHE
LYS	GLY
ALA	ARG
LYS	LYS
SER	SER
ALA	LEU
ASP	ASN
GLU	GLU
SER	ILE
LYS	LYS
PRO	PRO
VAL	VAL
GLU	LEU
PRO	ALA
PHE	GLY
ASN	MET
PRO	GLY
ALA	LEU
LEU	HIS
LYS	LEU
LYS	GLY
MET	MET
VAL	ASP

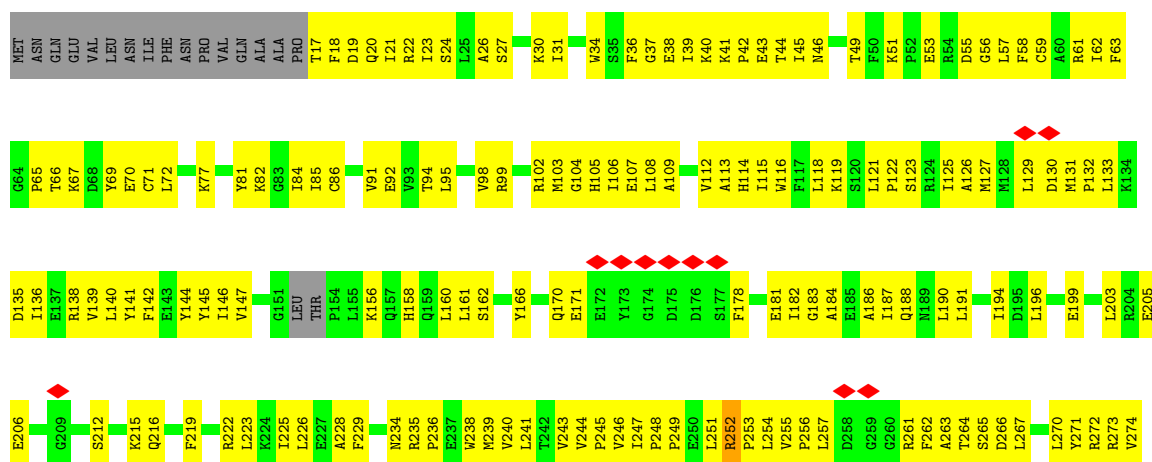
• Molecule 2: DNA-directed RNA polymerase subunit beta



D718	S719	G720	A721	V722	V723	A724	A725	K726	R727	T728	G729	V730	A731	Q732	Q733	I734	D735	R738	L739	V740	I741	D742	A743	T744	E745	E746	T747	D748	P749	A750	N751	S752	I756	Y757	R758	M759	S760	K761	F762	Q763	R764	S765	N766	Q767	S768	T769	C770	I771	N772	Q773	R774	P775	L776	V777	K778	V779	G780					
D658	H586	M660	D661	V662	S663	P664	R665	Q666	V667	V668	S669	V670	R671	A672	A673	L674	I675	P676	F677	L678	E679	N680	D681	D682	A683	N684	R685	L686	Q687	G688	S689	N690	M691	H692	Q693	R694	Q695	A696	V697	P698	L699	V700	Q701	S702	D703	A704	P705	I645	R646	L647	G647	E648	P649	T650	L651	L652	Q653	K654	S655	V656	T657	V657
T585	H586	A587	N590	K591	L592	I595	E596	S597	V598	P599	R600	R601	V602	L603	D604	P607	L546	T547	R548	E549	R550	A551	G552	E554	V555	R556	D557	V558	H559	P560	T561	H562	Y563	G564	R565	I566	C567	P568	I569	T570	G571	S571	P572	E573	G574	P575	R576	I577	G578	L579	L580	R581	S582	L583	A584							
D524	Q525	T526	N527	P528	L529	S530	E531	I532	H534	K535	R536	R537	L538	S539	R600	R601	V602	L603	D604	P607	L546	T547	R548	E549	R550	A551	G552	E554	V555	R556	D557	V558	H559	P560	T561	H562	Y563	G564	R565	I566	C567	P568	I569	T570	G571	S571	P572	E573	G574	P575	R576	I577	G578	L579	L580	R581	S582	L583	A584			
D451	D452	N455	L456	G457	N458	R469	R460	V461	R462	S463	V464	K394	S395	L396	F397	F398	D399	Y403	D404	L405	S406	S407	V408	G409	R410	V411	K412	M413	R414	M415	R416	L417	S422	V425	R426	I427	L428	R429	K430	E431	D432	V433	L434	A435	V436	L437	L440	V441	G442	L443	R444	D445	G446	R447								
D451	D452	N455	L456	G457	N458	R469	R460	V461	R462	S463	V464	K394	S395	L396	F397	F398	D399	Y403	D404	L405	S406	S407	V408	G409	R410	V411	K412	M413	R414	M415	R416	L417	S422	V425	R426	I427	L428	R429	K430	E431	D432	V433	L434	A435	V436	L437	L440	V441	G442	L443	R444	D445	G446	R447								
F372	D373	I374	V377	M378	G381	A389	R460	V461	R462	S463	V464	K394	S395	L396	F397	F398	D399	Y403	D404	L405	S406	S407	V408	G409	R410	V411	K412	M413	R414	M415	R416	L417	S422	V425	R426	I427	L428	R429	K430	E431	D432	V433	L434	A435	V436	L437	L440	V441	G442	L443	R444	D445	G446	R447								
PRO	GLU	ALA	L300	A309	VAL	ASN	MET	ALA	THR	GLY	E316	A321	G322	D323	E324	L325	D326	V327	T328	S329	D335	GLN	GLY	PHE	SER	THR	ILE	ASP	VAL	ASP	ILE	ASP	HIS	VAL	T350	A353	Y354	M355	R356	N357	T358	L359	R360	V361	D362	K363	N364	A365	I366	R367	E368	D369	A370	L371								
L216	Y217	A218	L219	D222	E225	I226	L227	Y231	P235	K238	R239	S240	G241	G242	W243	P246	Y247	W252	R253	K256	P260	L261	V262	D263	A264	I427	D265	T266	Q267	E268	E269	V270	A271	P272	T275	T278	A282	K283	K284	F285	A286	D287	Q288	L293	LEU	ALA																
Y144	T145	G146	T147	E148	L149	V150	I151	V152	S153	K154	M155	S158	P159	G160	V161	F162	D166	A172	L176	L177	F178	A179	R180	R181	V182	I183	P184	S188	L189	D191	F192	E193	F194	D195	A196	I199	V200	Y201	V202	R203	T204	D205	R206	R207	R208	R209	P211	A212	T213	T214	F215											
Y144	T145	G146	T147	E148	L149	V150	I151	V152	S153	K154	M155	S158	P159	G160	V161	F162	D166	A172	L176	L177	F178	A179	R180	R181	V182	I183	P184	S188	L189	D191	F192	E193	F194	D195	A196	I199	V200	Y201	V202	R203	T204	D205	R206	R207	R208	R209	P211	A212	T213	T214	F215											
Y74	Y77	E78	F79	Y84	D85	Y86	E87	E88	C89	I90	M94	T95	F96	A97	A98	F99	K100	K101	V102	K103	L104	R105	L106	I107	V108	T111	E112	E113	E114	T115	G116	A117	R118	S119	D122	Q126	D127	V128	Y129	M130	G131	D132	I133	F134	L135	M136	T137	D138	K139	G140	T141	F142	I143									
MET	ALA	Q3	S4	F5	K8	K9	I10	I11	R12	K13	S14	F15	G16	R17	E20	A21	V22	Q23	N24	P25	N26	L27	I28	E29	R32	Y35	E36	Q37	F38	L39	T43	R44	P45	G46	L47	R48	E54	F57	K58	S59	V60	F61	P62	I63	K64	D65	F66	A70	V71	L72	E73											

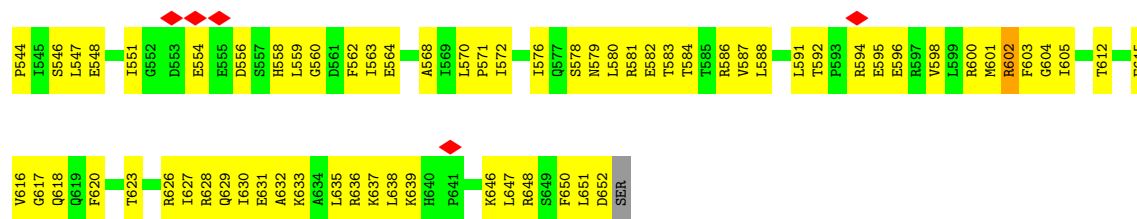


• Molecule 3: DNA-directed RNA polymerase subunit beta'

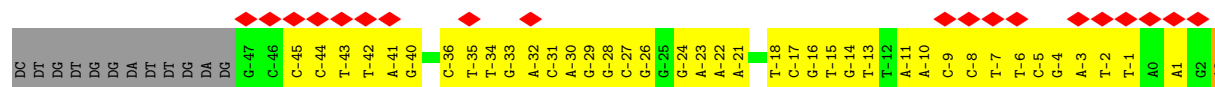
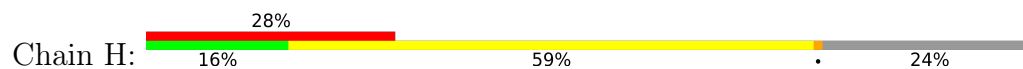


VAL	GLU	GLY	ASP	THR	ARG	VAL	GLN	V872	V806	R740	GLY	L604	GLS33	D464	V403	R339	I275
GLU	THR	ASP	ASP	THR	THR	LYS	VAL	V873	E907	G741	LEU	I605	E534	Q467	E404	F340	R276
LEU	ALA	ALA	ALA	ALA	ALA	ASP	ALA	I673	E908	L742	ASP	D906	I535	M468	R406	R341	R277
ILE	THR	THR	THR	THR	THR	GLY	GLN	V874	E909	M743	GLN	D907	E536	A469	Q407	N342	R278
PRO	GLY	GLY	GLY	GLY	GLY	LEU	ASP	V875	C910	A744	ASP	V908	A537	V470	Q408	N343	R279
LYS	ASP	ASP	ASP	ASP	ASP	VAL	PHE	V876	T812	K745	THR	R610	A538	H471	Q409	L344	R280
GLY	THR	THR	THR	THR	THR	VAL	THR	V877	T813	P746	THR	H611	M539	H472	V410	L345	L281
ASP	ASP	ASP	ASP	ASP	ASP	PHE	THR	S747	R880	S747	ASP	V473	V543	P473	W411	G346	K282
THR	THR	THR	THR	THR	THR	ARG	THR	I751	K881	I751	THR	L474	L546	L474	R347	K347	R283
LEU	THR	THR	THR	THR	THR	ALA	THR	E752	V882	E752	THR	S475	L546	L475	R348	L284	L284
ALA	THR	THR	THR	THR	THR	ALA	THR	E753	R883	E753	THR	L476	H547	L476	V349	D350	L287
THR	THR	THR	THR	THR	THR	ALA	THR	E754	D884	E754	THR	E477	A548	E477	D351	Y351	L288
VAL	THR	THR	THR	THR	THR	ALA	THR	E755	A885	E755	THR	I619	K549	E416	E416	S352	A289
GLY	THR	THR	THR	THR	THR	ALA	THR	E756	R886	E756	THR	V618	A549	E417	R349	G353	P290
ASP	THR	THR	THR	THR	THR	ALA	THR	E757	K888	E757	THR	I619	K550	E418	R350	S354	P291
THR	THR	THR	THR	THR	THR	ALA	THR	E758	A889	E758	THR	V619	K551	E419	R351	S355	P292
LEU	THR	THR	THR	THR	THR	ALA	THR	E759	R890	E759	THR	I620	K552	E420	R352	S356	P293
ALA	THR	THR	THR	THR	THR	ALA	THR	E760	D891	E760	THR	V620	K553	E421	R353	S357	P294
THR	THR	THR	THR	THR	THR	ALA	THR	E761	R892	E761	THR	V621	K554	E422	R354	S358	P295
GLY	THR	THR	THR	THR	THR	ALA	THR	E762	V893	E762	THR	V622	K555	E423	R355	S359	P296
ASP	THR	THR	THR	THR	THR	ALA	THR	E763	R894	E763	THR	V623	K556	E424	R356	S360	P297
THR	THR	THR	THR	THR	THR	ALA	THR	E764	V895	E764	THR	V624	K557	E425	R357	S361	P298
LEU	THR	THR	THR	THR	THR	ALA	THR	E765	R896	E765	THR	V625	K558	E426	R358	S362	P299
ALA	THR	THR	THR	THR	THR	ALA	THR	E766	R897	E766	THR	V626	K559	E427	R359	S363	P300
THR	THR	THR	THR	THR	THR	ALA	THR	E767	D898	E767	THR	V627	K560	E428	R360	S364	P301
GLY	THR	THR	THR	THR	THR	ALA	THR	E768	R899	E768	THR	V628	K561	E429	R361	S365	P302
ASP	THR	THR	THR	THR	THR	ALA	THR	E769	R900	E769	THR	V629	K562	E430	R362	S366	P303
THR	THR	THR	THR	THR	THR	ALA	THR	E770	R901	E770	THR	V630	K563	E431	R363	S367	P304
LEU	THR	THR	THR	THR	THR	ALA	THR	E771	R902	E771	THR	V631	K564	E432	R364	S368	P305
ALA	THR	THR	THR	THR	THR	ALA	THR	E772	R903	E772	THR	V632	K565	E433	R365	S369	P306
THR	THR	THR	THR	THR	THR	ALA	THR	E773	R904	E773	THR	V633	K566	E434	R366	S370	P307
GLY	THR	THR	THR	THR	THR	ALA	THR	E774	R905	E774	THR	V634	K567	E435	R367	S371	P308
ASP	THR	THR	THR	THR	THR	ALA	THR	E775	R906	E775	THR	V635	K568	E436	R368	S372	P309
THR	THR	THR	THR	THR	THR	ALA	THR	E776	R907	E776	THR	V636	K569	E437	R369	S373	P310
LEU	THR	THR	THR	THR	THR	ALA	THR	E777	R908	E777	THR	V637	K570	E438	R370	S374	P311
ALA	THR	THR	THR	THR	THR	ALA	THR	E778	R909	E778	THR	V638	K571	E439	R371	S375	P312
THR	THR	THR	THR	THR	THR	ALA	THR	E779	R910	E779	THR	V639	K572	E440	R372	S376	P313
GLY	THR	THR	THR	THR	THR	ALA	THR	E780	R911	E780	THR	V640	K573	E441	R373	S377	P314
ASP	THR	THR	THR	THR	THR	ALA	THR	E781	R912	E781	THR	V641	K574	E442	R374	S378	P315
THR	THR	THR	THR	THR	THR	ALA	THR	E782	R913	E782	THR	V642	K575	E443	R375	S379	P316
LEU	THR	THR	THR	THR	THR	ALA	THR	E783	R914	E783	THR	V643	K576	E444	R376	S380	P317
ALA	THR	THR	THR	THR	THR	ALA	THR	E784	R915	E784	THR	V644	K577	E445	R377	S381	P318
THR	THR	THR	THR	THR	THR	ALA	THR	E785	R916	E785	THR	V645	K578	E446	R378	S382	P319
GLY	THR	THR	THR	THR	THR	ALA	THR	E786	R917	E786	THR	V646	K579	E447	R379	S383	P320
ASP	THR	THR	THR	THR	THR	ALA	THR	E787	R918	E787	THR	V647	K580	E448	R380	S384	P321
THR	THR	THR	THR	THR	THR	ALA	THR	E788	R919	E788	THR	V648	K581	E449	R381	S385	P322
LEU	THR	THR	THR	THR	THR	ALA	THR	E789	R920	E789	THR	V649	K582	E450	R382	S386	P323
ALA	THR	THR	THR	THR	THR	ALA	THR	E790	R921	E790	THR	V650	K583	E451	R383	S387	P324
THR	THR	THR	THR	THR	THR	ALA	THR	E791	R922	E791	THR	V651	K584	E452	R384	S388	P325
GLY	THR	THR	THR	THR	THR	ALA	THR	E792	R923	E792	THR	V652	K585	E453	R385	S389	P326
ASP	THR	THR	THR	THR	THR	ALA	THR	E793	R924	E793	THR	V653	K586	E454	R386	S390	P327
THR	THR	THR	THR	THR	THR	ALA	THR	E794	R925	E794	THR	V654	K587	E455	R387	S391	P328
LEU	THR	THR	THR	THR	THR	ALA	THR	E795	R926	E795	THR	V655	K588	E456	R388	S392	P329
ALA	THR	THR	THR	THR	THR	ALA	THR	E796	R927	E796	THR	V656	K589	E457	R389	S393	P330
THR	THR	THR	THR	THR	THR	ALA	THR	E797	R928	E797	THR	V657	K590	E458	R390	S394	P331
GLY	THR	THR	THR	THR	THR	ALA	THR	E798	R929	E798	THR	V658	K591	E459	R391	S395	P332
ASP	THR	THR	THR	THR	THR	ALA	THR	E799	R930	E799	THR	V659	K592	E460	R392	S396	P333
THR	THR	THR	THR	THR	THR	ALA	THR	E800	R931	E800	THR	V660	K593	E461	R393	S397	P334
LEU	THR	THR	THR	THR	THR	ALA	THR	E801	R932	E801	THR	V661	K594	E462	R394	S398	P335
ALA	THR	THR	THR	THR	THR	ALA	THR	E802	R933	E802	THR	V662	K595	E463	R395	S399	P336
THR	THR	THR	THR	THR	THR	ALA	THR	E803	R934	E803	THR	V663	K596	E464	R396	S400	P337
GLY	THR	THR	THR	THR	THR	ALA	THR	E804	R935	E804	THR	V664	K597	E465	R397	S401	P338
ASP	THR	THR	THR	THR	THR	ALA	THR	E805	R936	E805	THR	V665	K598	E466	R398	S402	P339
THR	THR	THR	THR	THR	THR	ALA	THR	E806	R937	E806	THR	V666	K599	E467	R399	S403	P340
LEU	THR	THR	THR	THR	THR	ALA	THR	E807	R938	E807	THR	V667	K600	E468	R400	S404	P341
ALA	THR	THR	THR	THR	THR	ALA	THR	E808	R939	E808	THR	V668	K601	E469	R401	S405	P342
THR	THR	THR	THR	THR	THR	ALA	THR	E809	R940	E809	THR	V669	K602	E470	R402	S406	P343
GLY	THR	THR	THR	THR	THR	ALA	THR	E810	R941	E810	THR	V670	K603	E471	R403	S407	P344
ASP	THR	THR	THR	THR	THR	ALA	THR	E811	R942	E811	THR	V671	K604	E472	R404	S408	P345
THR	THR	THR	THR	THR	THR	ALA	THR	E812	R943	E812	THR	V672	K605	E473	R405	S409	P346
LEU	THR	THR	THR	THR	THR	ALA	THR	E813	R944	E813	THR	V673	K606	E474	R406	S410	P347
ALA	THR	THR	THR	THR	THR	ALA	THR	E814	R945	E814	THR	V674	K607	E475	R407	S411	P348
THR	THR	THR	THR	THR	THR	ALA	THR	E815	R946	E815	THR	V675	K608	E476	R408	S412	P349
GLY	THR	THR	THR	THR	THR	ALA	THR	E816	R947	E816	THR	V676	K609	E477	R409	S413	P350
ASP	THR	THR	THR	THR	THR	ALA	THR	E817	R948	E817	THR	V677	K610	E478	R410	S414	P351
THR	THR	THR	THR	THR	THR	ALA	THR	E818	R949	E818	THR	V678	K611	E479	R411	S415	P352
LEU	THR	THR	THR	THR	THR	ALA	THR	E819	R950	E819	THR	V679	K612	E480	R412	S416	P353
ALA	THR	THR	THR	THR	THR	ALA	THR	E820	R951	E820	THR	V680	K613	E481	R413	S417	P354
THR	THR	THR	THR	THR	THR	ALA	THR	E821	R952	E821	THR	V681	K614	E482	R414	S418	P355
GLY	THR	THR	THR	THR	THR	ALA	THR	E822	R953	E822	THR	V682	K615	E483	R415	S419	P356
ASP	THR	THR	THR	THR	THR	ALA	THR	E823	R954	E823	THR	V683	K616	E484	R416	S420	P357
THR	THR	THR	THR	THR	THR	ALA	THR	E824	R955	E824	THR	V684	K617	E485	R417	S421	P358
LEU	THR	THR	THR	THR	THR	ALA	THR	E825	R956	E825	THR	V685	K618	E486	R418	S422	P359
ALA	THR	THR	THR	THR	THR	ALA	THR	E826	R957	E826	THR	V686	K619	E487	R419	S423	P360
THR	THR	THR	THR	THR	THR	ALA	THR	E827	R958	E827	THR	V687	K620	E488	R420	S424	P361
GLY	THR	THR	THR	THR	THR	ALA	THR	E828	R959	E828	THR	V688	K621	E489	R421	S425	P362
ASP	THR	THR	THR	THR	THR	ALA	THR	E829	R960	E829	THR	V689	K622	E490	R422	S426	P363
THR	THR	THR	THR	THR	THR	ALA	THR	E830	R961	E830	THR	V690	K623	E491	R423	S427	P364
LEU	THR	THR	THR	THR	THR	ALA	THR	E831	R962	E831	THR	V691	K624	E492	R424	S428	P365
ALA	THR	THR	THR	THR	THR	ALA	THR	E832	R963	E832	THR	V692	K625	E493	R425	S429	P366
THR	THR	THR	THR	THR	THR	ALA	THR	E833	R964	E833	THR	V693	K626	E494	R426	S430	P367
GLY	THR	THR	THR	THR	THR	ALA	THR	E834	R965	E834	THR	V694	K627	E495	R427	S431	P368
ASP	THR	THR	THR	THR	THR	ALA	THR	E835	R966	E835	THR	V695	K628	E496	R428	S432	P369
THR	THR	THR	THR	THR	THR	ALA	THR	E836	R967	E836	THR	V696	K629	E497			

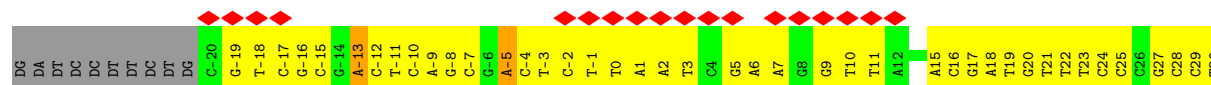
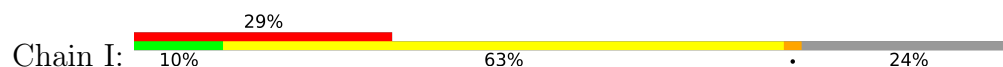




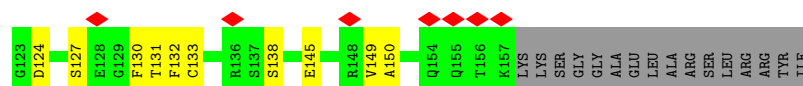
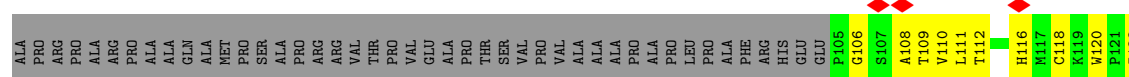
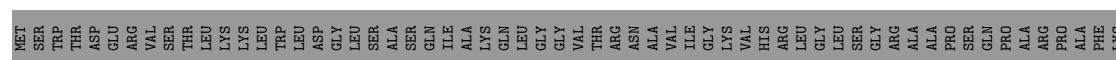
• Molecule 6: DNA (90-MER)-non template



• Molecule 7: DNA (90-MER)-template



• Molecule 8: Cell cycle regulatory protein GcrA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MA, ZN, MG

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	0.24	0/2078	0.41	0/2838
1	B	0.23	0/1657	0.42	0/2249
2	C	0.24	0/9735	0.40	0/13133
3	D	0.24	0/8829	0.39	0/11870
4	E	0.23	0/514	0.39	0/695
5	F	0.23	0/3294	0.38	0/4467
6	H	0.49	0/1513	0.88	0/2328
7	I	0.52	0/1513	0.89	0/2328
8	G	0.24	0/384	0.39	0/522
All	All	0.28	0/29517	0.48	0/40430

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2054	0	1816	216	0
1	B	1633	0	1618	203	0
2	C	9591	12	9110	1038	0
3	D	8691	0	8727	1024	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	510	0	505	57	0
5	F	3266	0	2751	248	0
6	H	1396	0	768	82	0
7	I	1396	0	768	87	0
8	G	372	0	325	14	0
9	D	2	0	0	0	0
9	G	1	0	0	0	0
10	D	1	0	0	0	0
All	All	28913	12	26388	2614	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 47.

The worst 5 of 2614 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:45:ALA:O	1:A:49:VAL:HG12	1.48	1.11
1:A:50:LEU:HB2	1:A:220:ALA:CB	1.84	1.07
5:F:123:MET:HE2	5:F:123:MET:HA	1.34	1.04
1:A:51:LEU:HD21	2:C:1100:ILE:HG13	1.40	1.04
3:D:504:PRO:HB3	3:D:508:ILE:HB	1.39	1.04

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	300/338 (89%)	280 (93%)	19 (6%)	1 (0%)	41	74
1	B	214/338 (63%)	202 (94%)	12 (6%)	0	100	100
2	C	1291/1356 (95%)	1207 (94%)	84 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1128/1396 (81%)	1072 (95%)	56 (5%)	0	100	100
4	E	67/119 (56%)	64 (96%)	3 (4%)	0	100	100
5	F	493/652 (76%)	477 (97%)	16 (3%)	0	100	100
8	G	51/173 (30%)	49 (96%)	2 (4%)	0	100	100
All	All	3544/4372 (81%)	3351 (95%)	192 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LEU

5.3.2 Protein sidechains ⓘ

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	176/285 (62%)	175 (99%)	1 (1%)	86	92
1	B	173/285 (61%)	173 (100%)	0	100	100
2	C	975/1137 (86%)	971 (100%)	4 (0%)	91	95
3	D	941/1157 (81%)	937 (100%)	4 (0%)	91	95
4	E	56/100 (56%)	56 (100%)	0	100	100
5	F	247/542 (46%)	244 (99%)	3 (1%)	71	84
8	G	37/134 (28%)	37 (100%)	0	100	100
All	All	2605/3640 (72%)	2593 (100%)	12 (0%)	89	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	776	ARG
3	D	901	ARG
5	F	602	ARG
5	F	491	ARG
2	C	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	158	HIS
3	D	801	GLN
3	D	276	ASN
3	D	491	ASN
3	D	1227	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	6MA	H	11	7,6	18,24,25	3.10	10 (55%)	15,34,37	2.02	3 (20%)
7	6MA	I	-13	7,6	18,24,25	3.12	10 (55%)	15,34,37	2.03	3 (20%)
6	6MA	H	3	6	18,24,25	3.09	10 (55%)	15,34,37	2.20	4 (26%)
7	6MA	I	-5	7	18,24,25	3.13	10 (55%)	15,34,37	2.09	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	6MA	H	11	7,6	-	5/5/23/24	0/3/3/3
7	6MA	I	-13	7,6	-	4/5/23/24	0/3/3/3
6	6MA	H	3	6	-	2/5/23/24	0/3/3/3
7	6MA	I	-5	7	-	4/5/23/24	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	-5	6MA	O4'-C4'	8.03	1.63	1.45
7	I	-13	6MA	C3'-C4'	-7.89	1.31	1.53
7	I	-13	6MA	O4'-C4'	7.89	1.62	1.45
6	H	11	6MA	O4'-C4'	7.85	1.62	1.45
6	H	11	6MA	C3'-C4'	-7.82	1.31	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	-13	6MA	N3-C2-N1	-5.62	119.89	128.68
6	H	11	6MA	N3-C2-N1	-5.62	119.90	128.68
7	I	-5	6MA	N3-C2-N1	-5.53	120.03	128.68
6	H	3	6MA	N3-C2-N1	-5.50	120.09	128.68
6	H	3	6MA	C1-N6-C6	-3.76	119.64	122.87

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	3	6MA	C5-C6-N6-C1
6	H	3	6MA	N1-C6-N6-C1
6	H	11	6MA	C5-C6-N6-C1
6	H	11	6MA	N1-C6-N6-C1
7	I	-13	6MA	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	-13	6MA	3	0
6	H	3	6MA	2	0
7	I	-5	6MA	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

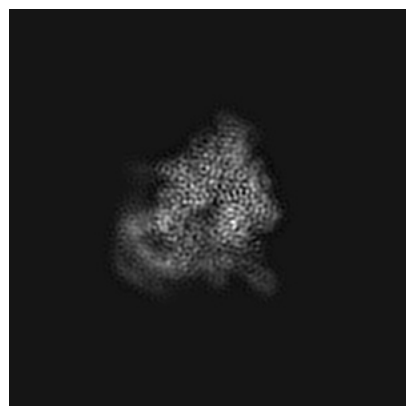
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33762. These allow visual inspection of the internal detail of the map and identification of artifacts.

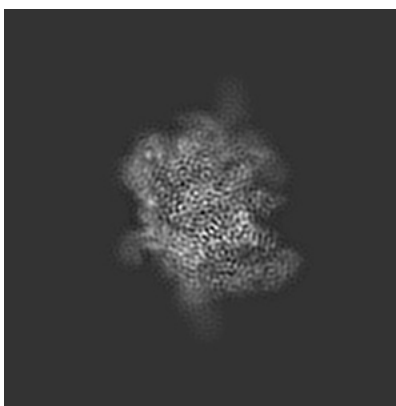
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

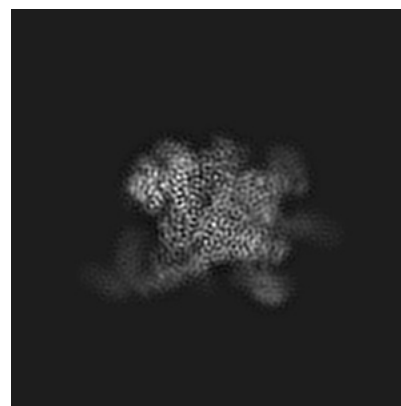
6.1.1 Primary map



X

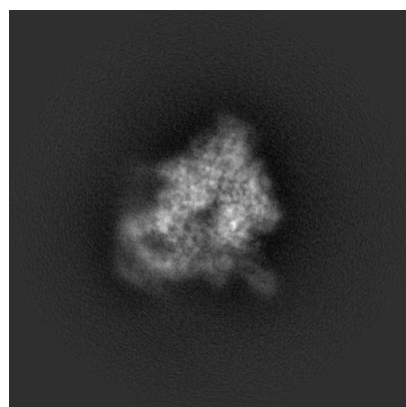


Y

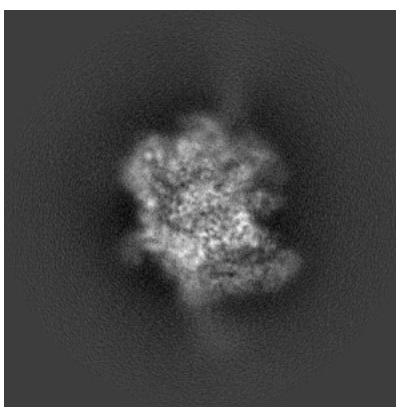


Z

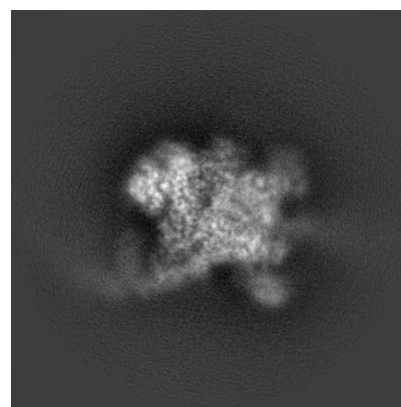
6.1.2 Raw map



X



Y

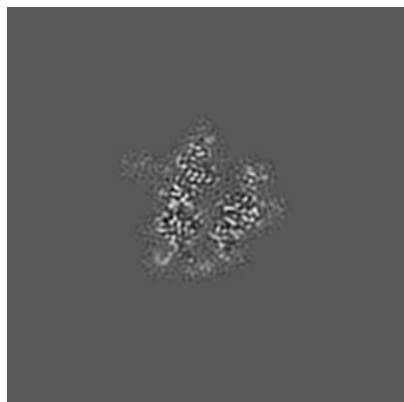


Z

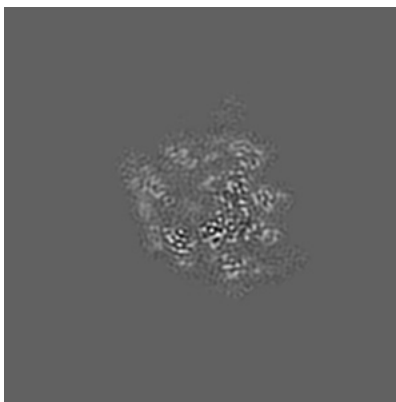
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

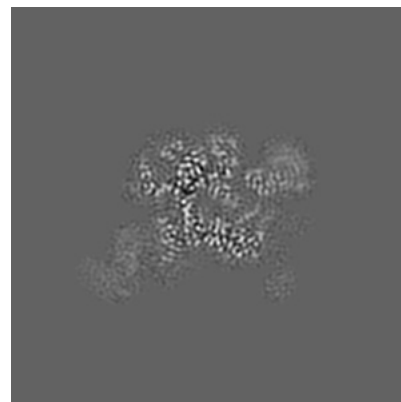
6.2.1 Primary map



X Index: 150

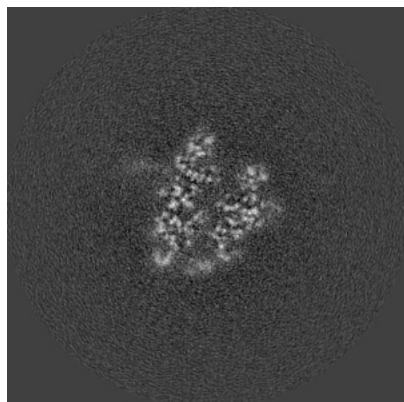


Y Index: 150

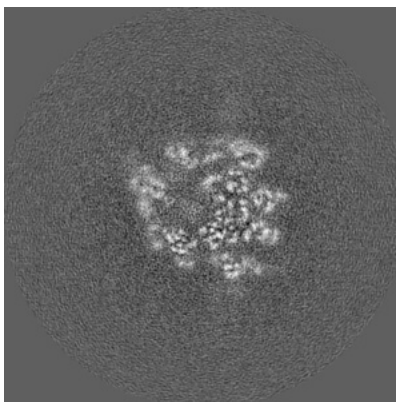


Z Index: 150

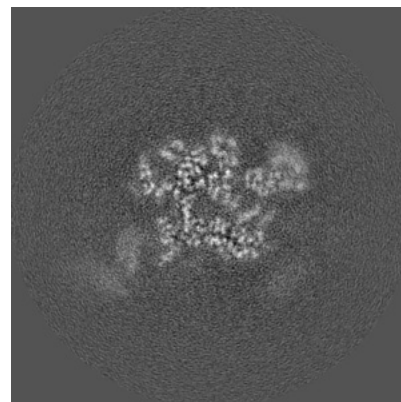
6.2.2 Raw map



X Index: 150



Y Index: 150

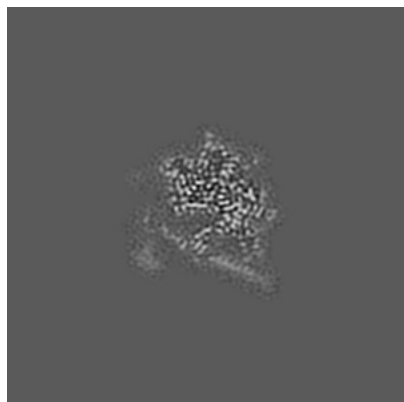


Z Index: 150

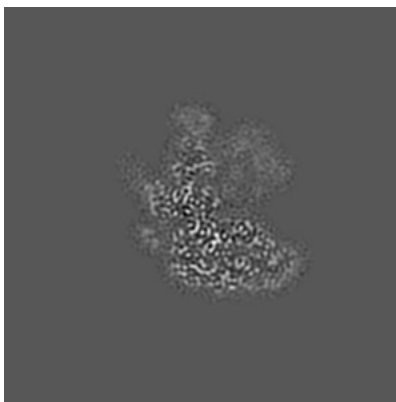
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

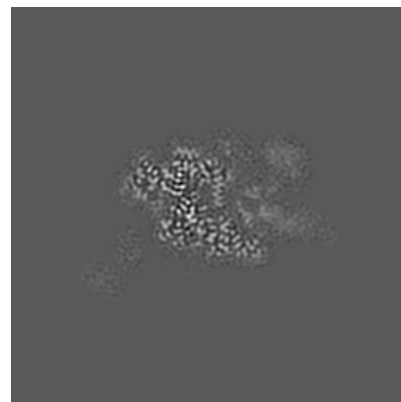
6.3.1 Primary map



X Index: 131

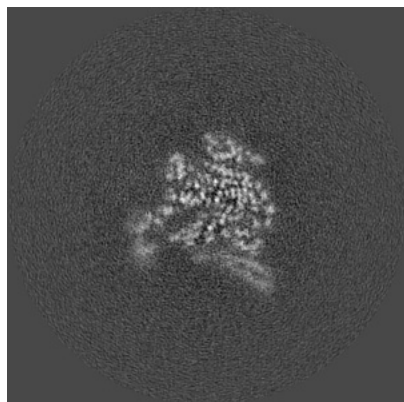


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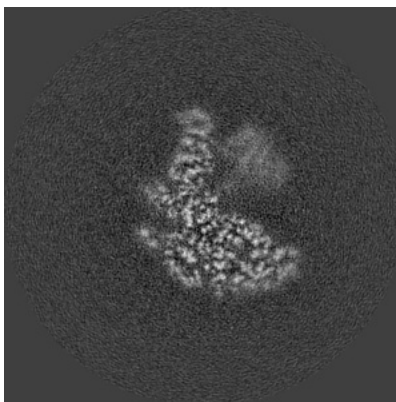


Z Index: 159

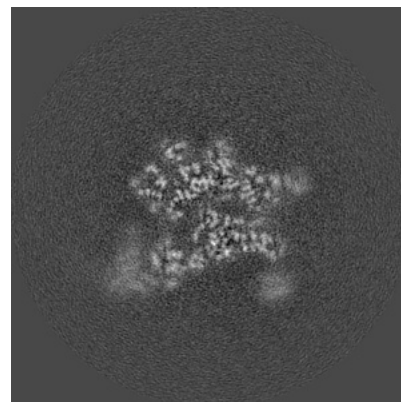
6.3.2 Raw map



X Index: 125



Y Index: 168

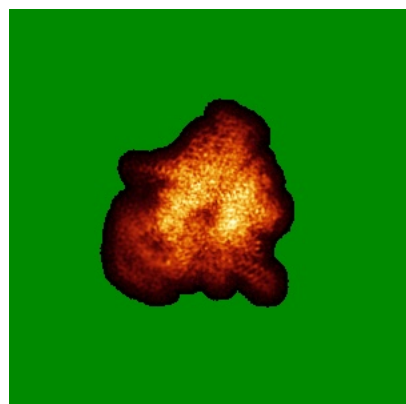


Z Index: 138

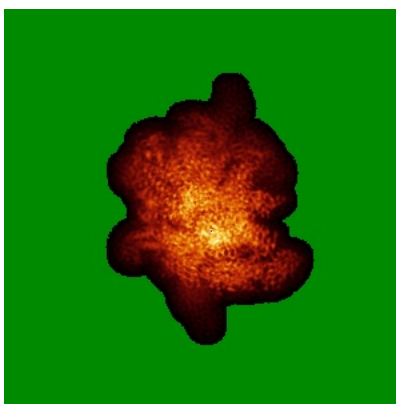
The images above show the largest variance slices of the map in three orthogonal directions.

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

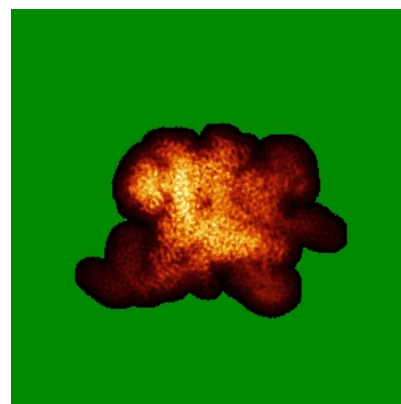
6.4.1 Primary map



X

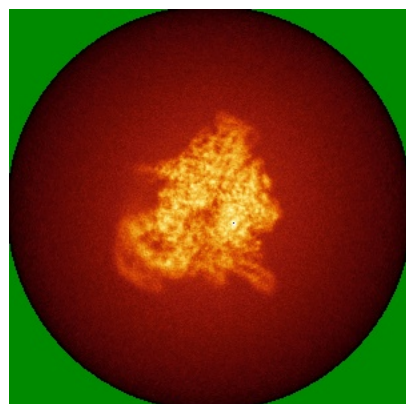


Y

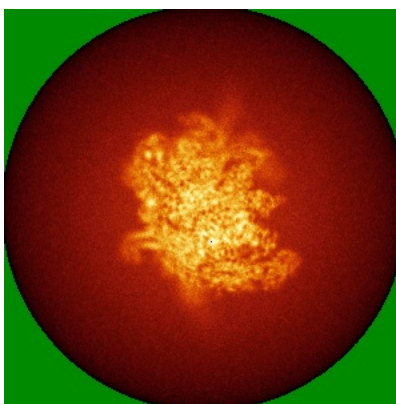


Z

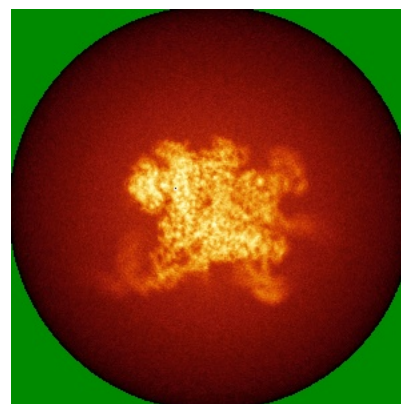
6.4.2 Raw map



X



Y

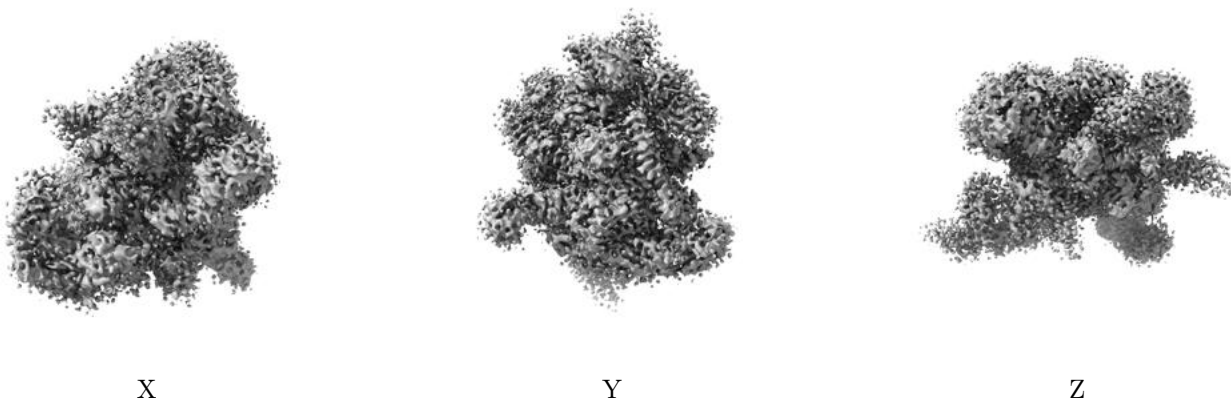


Z

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.

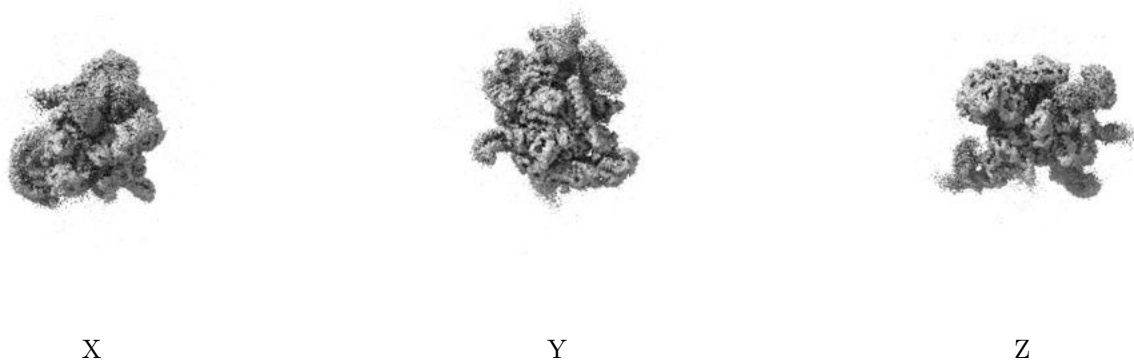
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

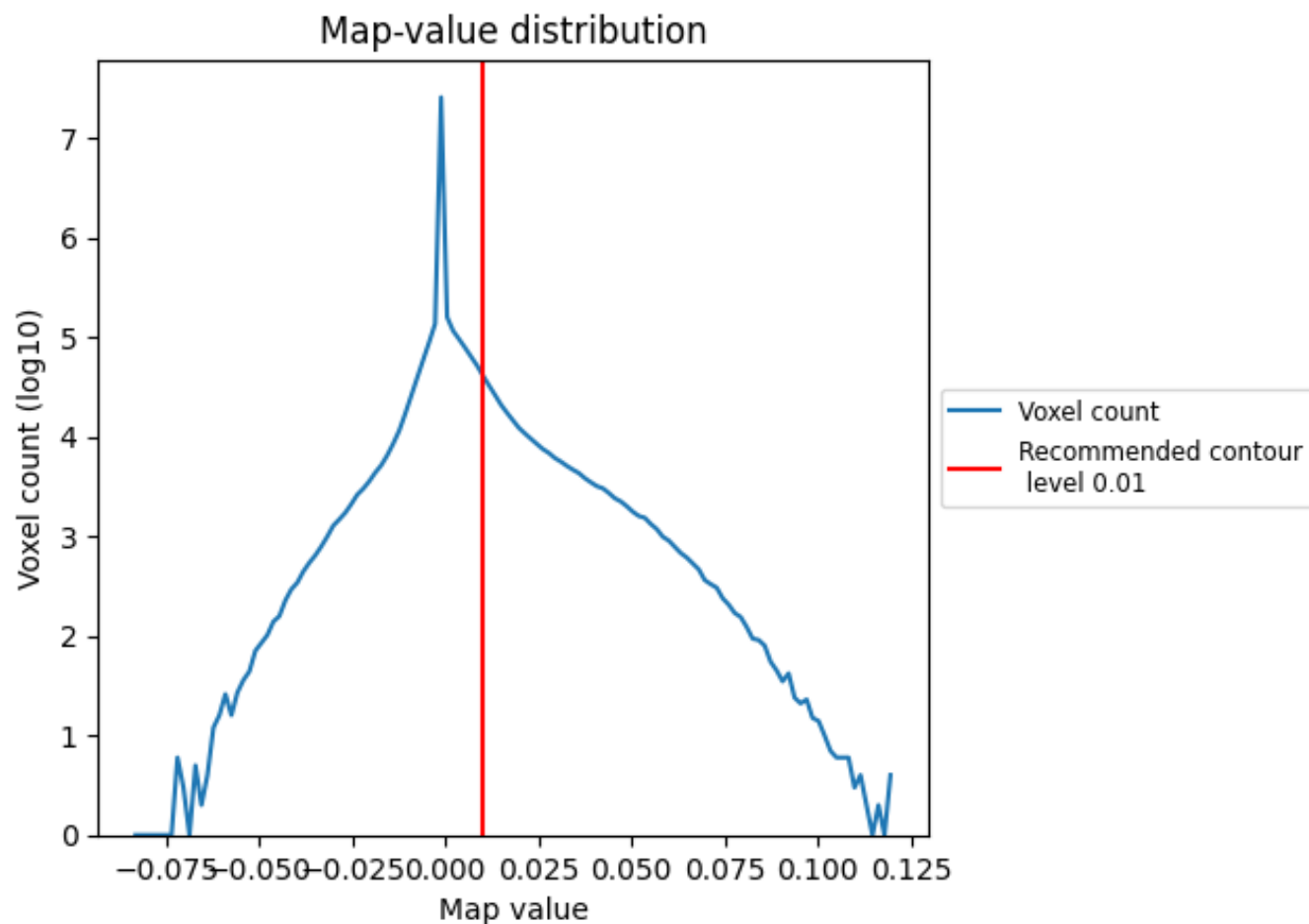
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

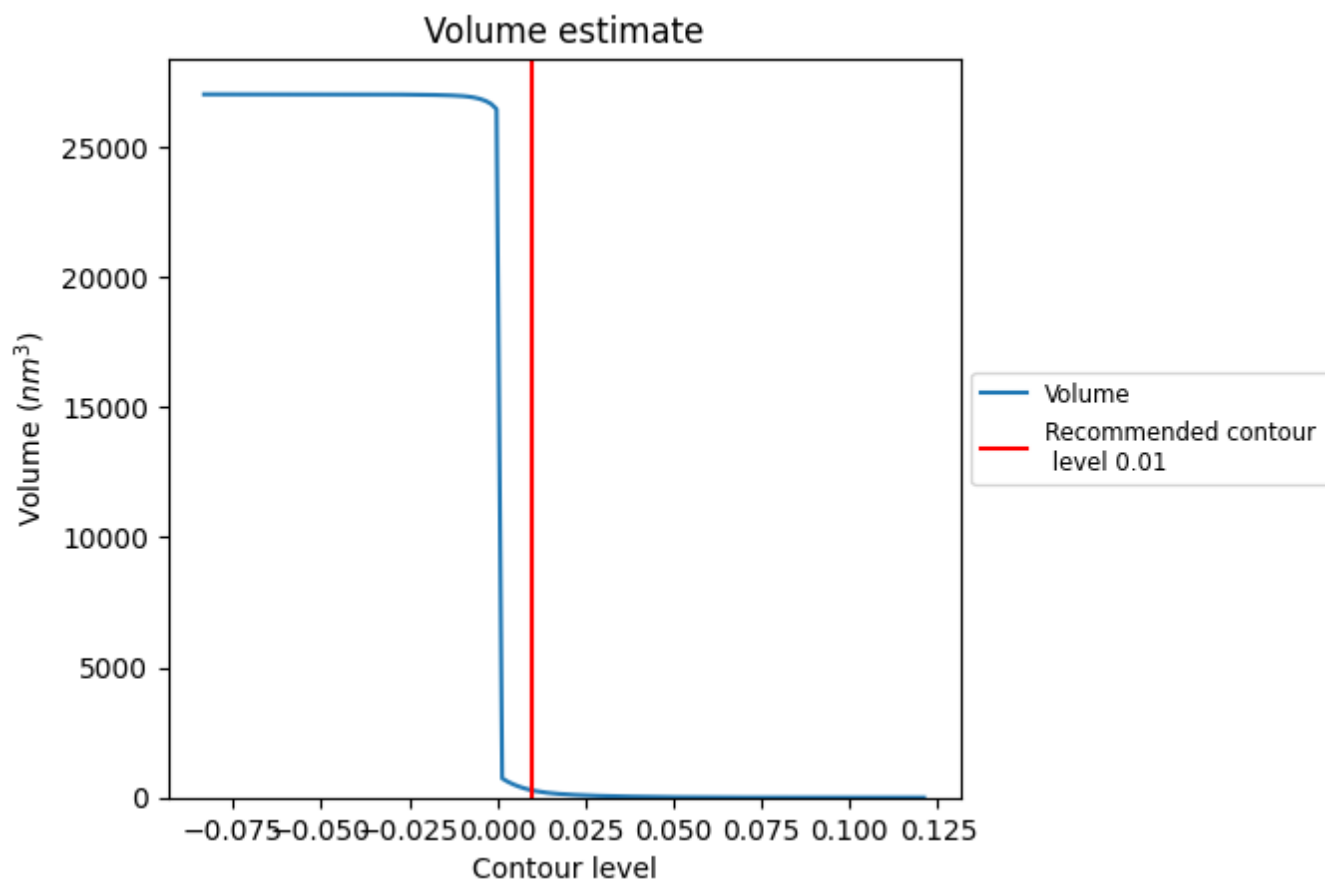
This section contains the results of statistical analysis of the map.

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.

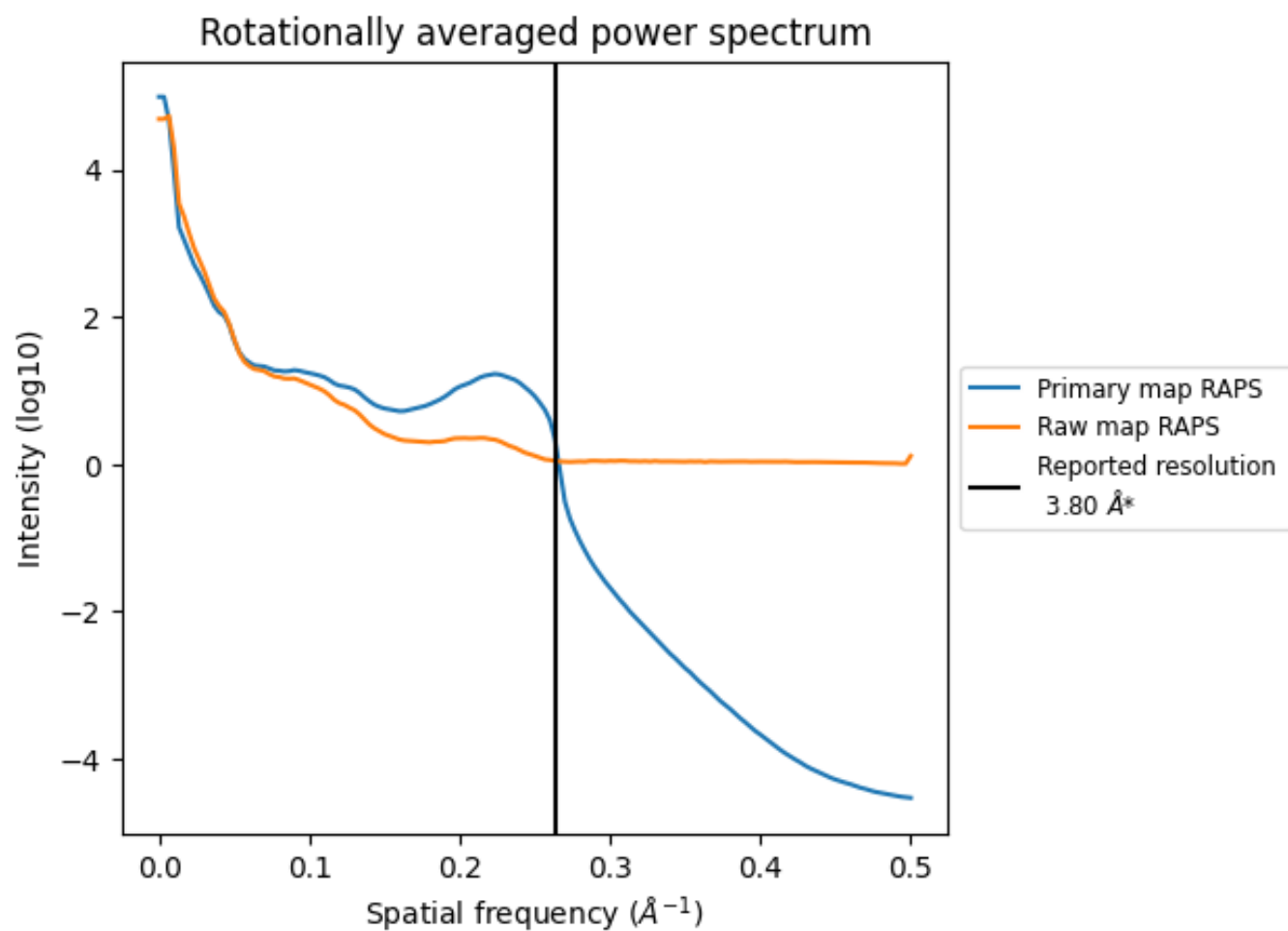
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm^3 ; this corresponds to an approximate mass of 250 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 ⓘ

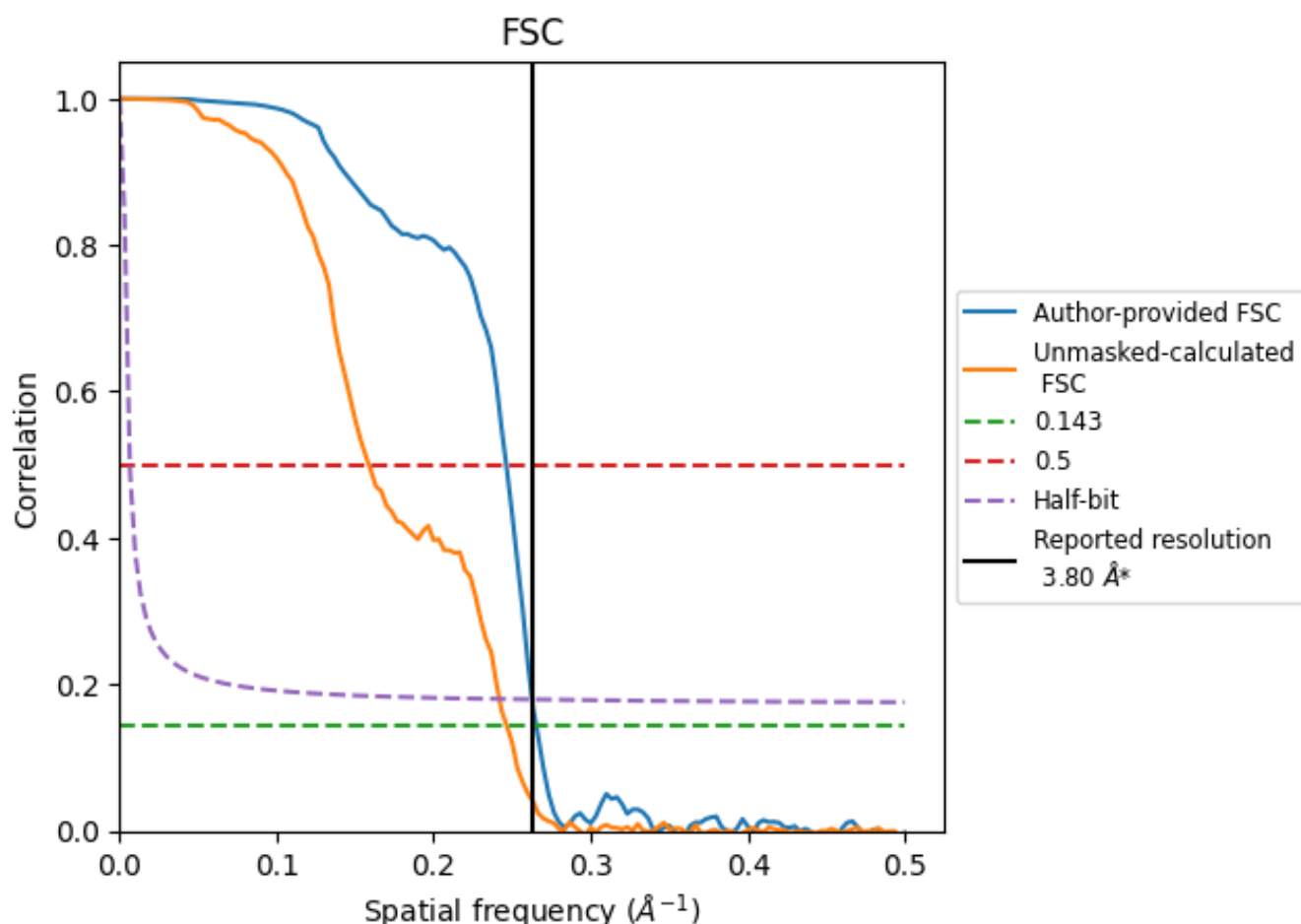


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

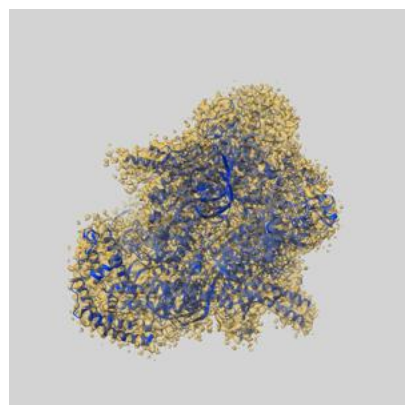
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.06	3.81
Unmasked-calculated*	4.06	6.30	4.13

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

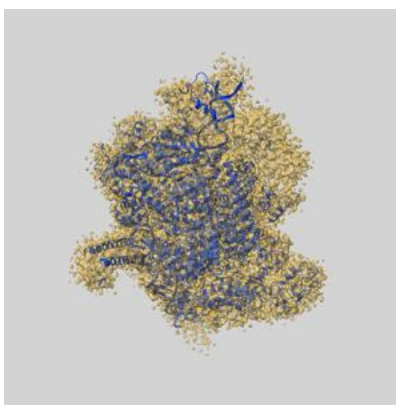
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33762 and PDB model 7YE2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

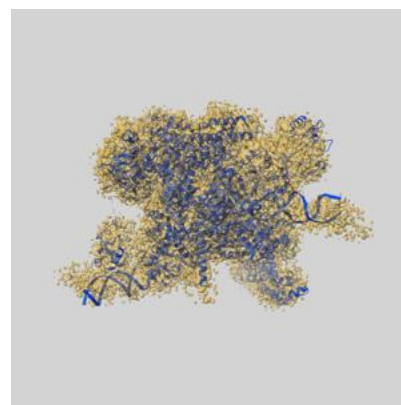
9.1 Map-model overlay [i](#)



X



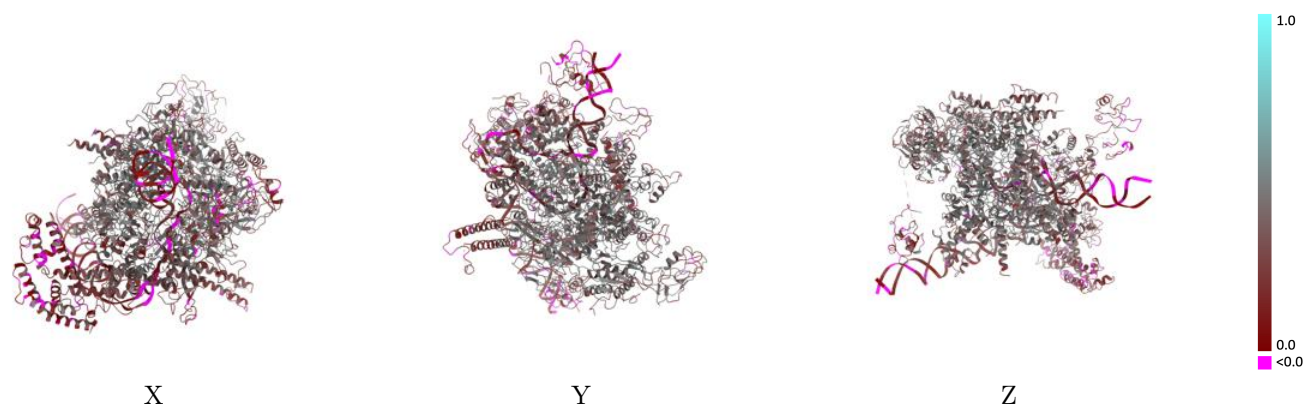
Y



Z

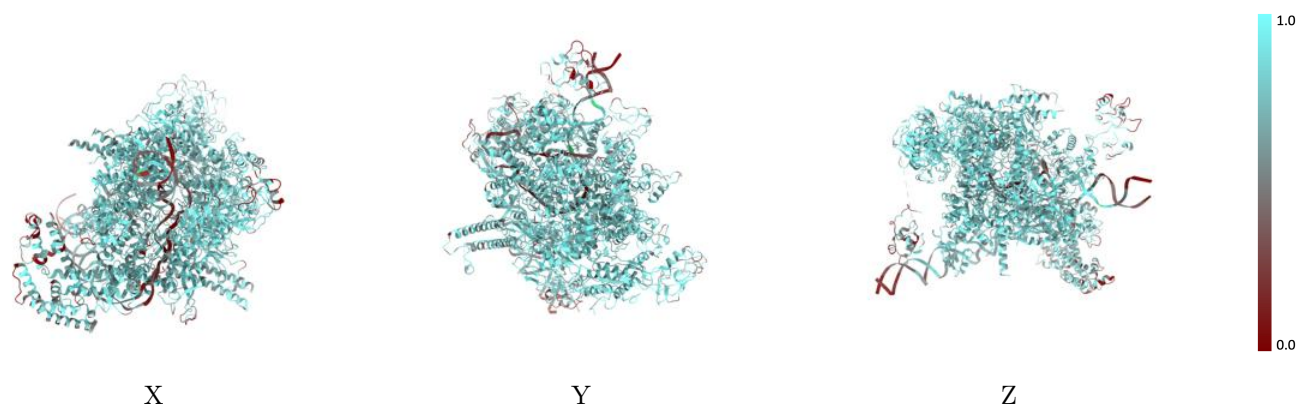
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



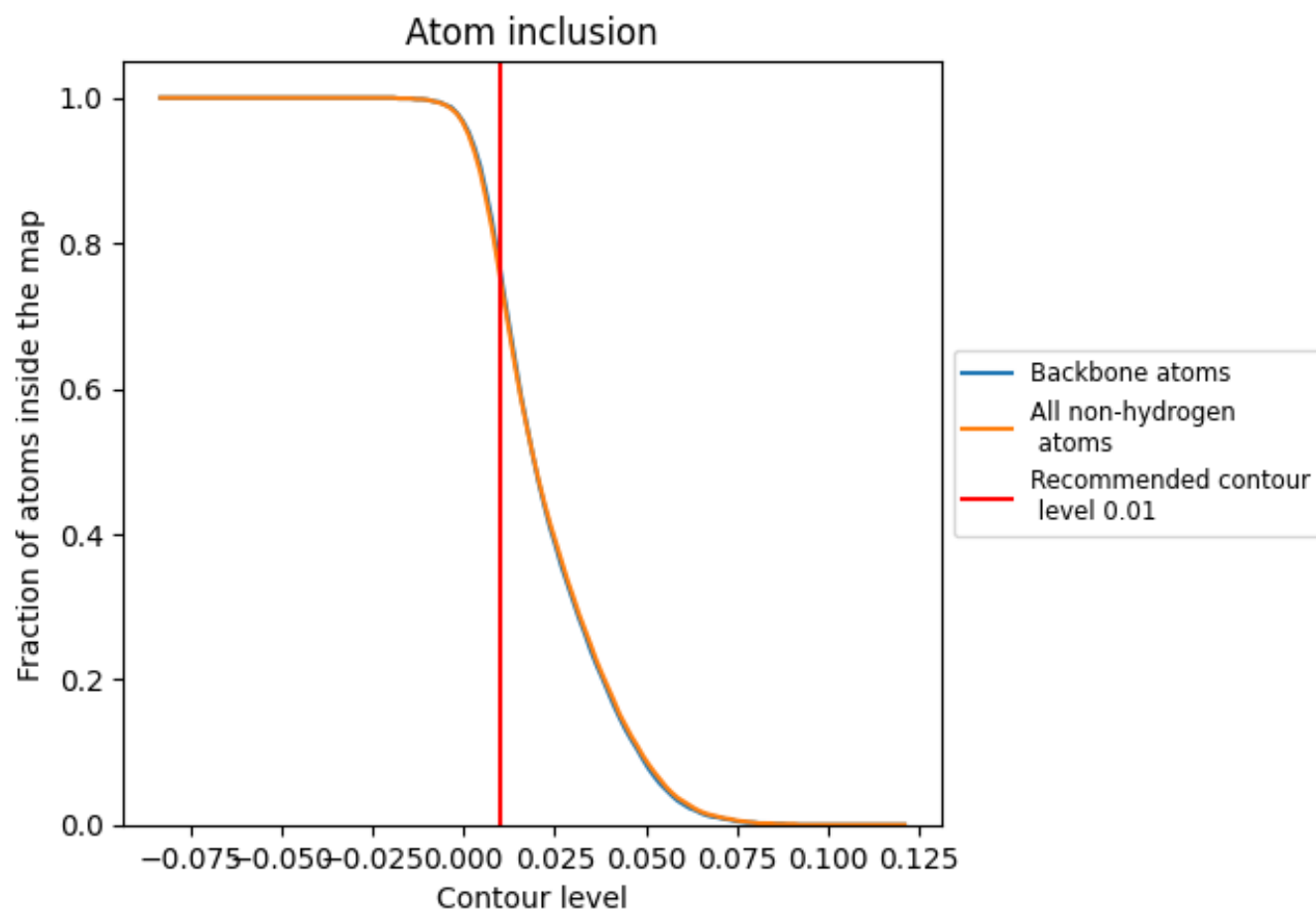
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7550	<div></div> 0.3540
A	<div></div> 0.7690	<div></div> 0.3850
B	<div></div> 0.8060	<div></div> 0.3890
C	<div></div> 0.7850	<div></div> 0.3840
D	<div></div> 0.8030	<div></div> 0.4060
E	<div></div> 0.8140	<div></div> 0.4120
F	<div></div> 0.7330	<div></div> 0.3080
G	<div></div> 0.6820	<div></div> 0.2680
H	<div></div> 0.4960	<div></div> 0.0990
I	<div></div> 0.4880	<div></div> 0.0920

1.0

0.0

<0.0