



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 07:12 am GMT

PDB ID : 7QCD
EMDB ID : EMD-13895
Title : CryoEM structure of the Smc5/6-holo complex (composite structure)
Authors : Hallett, S.T.; Oliver, A.W.
Deposited on : 2021-11-23
Resolution : 8.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

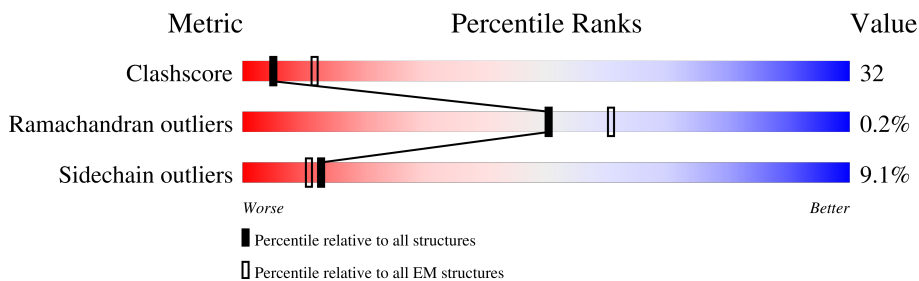
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	1093	
2	B	1114	
3	C	281	
4	D	358	
5	E	303	
6	F	715	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 25133 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 Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1028	8257	5179	1449	1598	31	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1015	GLN	GLU	engineered mutation	UNP Q08204

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	998	8028	4979	1444	1574	31	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1048	GLN	GLU	engineered mutation	UNP Q12749

- Molecule 3 is a protein called E3 SUMO-protein ligase MMS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	267	2121	1325	356	426	14	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	initiating methionine	UNP P38632
C	-12	GLY	-	expression tag	UNP P38632
C	-11	SER	-	expression tag	UNP P38632
C	-10	TYR	-	expression tag	UNP P38632

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	PRO	-	expression tag	UNP P38632
C	-8	TYR	-	expression tag	UNP P38632
C	-7	ASP	-	expression tag	UNP P38632
C	-6	VAL	-	expression tag	UNP P38632
C	-5	PRO	-	expression tag	UNP P38632
C	-4	ASP	-	expression tag	UNP P38632
C	-3	TYR	-	expression tag	UNP P38632
C	-2	ALA	-	expression tag	UNP P38632
C	-1	GLY	-	expression tag	UNP P38632
C	0	SER	-	expression tag	UNP P38632
C	1	GLY	-	expression tag	UNP P38632

- Molecule 4 is a protein called Non-structural maintenance of chromosomes element 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	326	2614	1653	446	501	14	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	initiating methionine	UNP Q07913
D	-20	GLY	-	expression tag	UNP Q07913
D	-19	SER	-	expression tag	UNP Q07913
D	-18	SER	-	expression tag	UNP Q07913
D	-17	HIS	-	expression tag	UNP Q07913
D	-16	HIS	-	expression tag	UNP Q07913
D	-15	HIS	-	expression tag	UNP Q07913
D	-14	HIS	-	expression tag	UNP Q07913
D	-13	HIS	-	expression tag	UNP Q07913
D	-12	HIS	-	expression tag	UNP Q07913
D	-11	SER	-	expression tag	UNP Q07913
D	-10	SER	-	expression tag	UNP Q07913
D	-9	GLY	-	expression tag	UNP Q07913
D	-8	ARG	-	expression tag	UNP Q07913
D	-7	GLU	-	expression tag	UNP Q07913
D	-6	ASN	-	expression tag	UNP Q07913
D	-5	LEU	-	expression tag	UNP Q07913
D	-4	TYR	-	expression tag	UNP Q07913
D	-3	PHE	-	expression tag	UNP Q07913
D	-2	GLN	-	expression tag	UNP Q07913
D	-1	GLY	-	expression tag	UNP Q07913

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q07913

- Molecule 5 is a protein called Non-structural maintenance of chromosome element 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	261	2091	1329	354	402	6	0	0

- Molecule 6 is a protein called Non-structural maintenance of chromosome element 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	257	2019	1277	359	375	8	0	0

There are 313 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	403	GLY	-	expression tag	UNP P43124
F	404	SER	-	expression tag	UNP P43124
F	405	SER	-	expression tag	UNP P43124
F	406	GLY	-	expression tag	UNP P43124
F	407	MET	-	expression tag	UNP P43124
F	408	ALA	-	expression tag	UNP P43124
F	409	GLU	-	expression tag	UNP P43124
F	410	ILE	-	expression tag	UNP P43124
F	411	GLY	-	expression tag	UNP P43124
F	412	THR	-	expression tag	UNP P43124
F	413	GLY	-	expression tag	UNP P43124
F	414	PHE	-	expression tag	UNP P43124
F	415	PRO	-	expression tag	UNP P43124
F	416	PHE	-	expression tag	UNP P43124
F	417	ASP	-	expression tag	UNP P43124
F	418	PRO	-	expression tag	UNP P43124
F	419	HIS	-	expression tag	UNP P43124
F	420	TYR	-	expression tag	UNP P43124
F	421	VAL	-	expression tag	UNP P43124
F	422	GLU	-	expression tag	UNP P43124
F	423	VAL	-	expression tag	UNP P43124
F	424	LEU	-	expression tag	UNP P43124
F	425	GLY	-	expression tag	UNP P43124
F	426	GLU	-	expression tag	UNP P43124
F	427	ARG	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	MET	-	expression tag	UNP P43124
F	429	HIS	-	expression tag	UNP P43124
F	430	TYR	-	expression tag	UNP P43124
F	431	VAL	-	expression tag	UNP P43124
F	432	ASP	-	expression tag	UNP P43124
F	433	VAL	-	expression tag	UNP P43124
F	434	GLY	-	expression tag	UNP P43124
F	435	PRO	-	expression tag	UNP P43124
F	436	ARG	-	expression tag	UNP P43124
F	437	ASP	-	expression tag	UNP P43124
F	438	GLY	-	expression tag	UNP P43124
F	439	THR	-	expression tag	UNP P43124
F	440	PRO	-	expression tag	UNP P43124
F	441	VAL	-	expression tag	UNP P43124
F	442	LEU	-	expression tag	UNP P43124
F	443	PHE	-	expression tag	UNP P43124
F	444	LEU	-	expression tag	UNP P43124
F	445	HIS	-	expression tag	UNP P43124
F	446	GLY	-	expression tag	UNP P43124
F	447	ASN	-	expression tag	UNP P43124
F	448	PRO	-	expression tag	UNP P43124
F	449	THR	-	expression tag	UNP P43124
F	450	SER	-	expression tag	UNP P43124
F	451	SER	-	expression tag	UNP P43124
F	452	TYR	-	expression tag	UNP P43124
F	453	VAL	-	expression tag	UNP P43124
F	454	TRP	-	expression tag	UNP P43124
F	455	ARG	-	expression tag	UNP P43124
F	456	ASN	-	expression tag	UNP P43124
F	457	ILE	-	expression tag	UNP P43124
F	458	ILE	-	expression tag	UNP P43124
F	459	PRO	-	expression tag	UNP P43124
F	460	HIS	-	expression tag	UNP P43124
F	461	VAL	-	expression tag	UNP P43124
F	462	ALA	-	expression tag	UNP P43124
F	463	PRO	-	expression tag	UNP P43124
F	464	THR	-	expression tag	UNP P43124
F	465	HIS	-	expression tag	UNP P43124
F	466	ARG	-	expression tag	UNP P43124
F	467	CYS	-	expression tag	UNP P43124
F	468	ILE	-	expression tag	UNP P43124
F	469	ALA	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	470	PRO	-	expression tag	UNP P43124
F	471	ASP	-	expression tag	UNP P43124
F	472	LEU	-	expression tag	UNP P43124
F	473	ILE	-	expression tag	UNP P43124
F	474	GLY	-	expression tag	UNP P43124
F	475	MET	-	expression tag	UNP P43124
F	476	GLY	-	expression tag	UNP P43124
F	477	LYS	-	expression tag	UNP P43124
F	478	SER	-	expression tag	UNP P43124
F	479	ASP	-	expression tag	UNP P43124
F	480	LYS	-	expression tag	UNP P43124
F	481	PRO	-	expression tag	UNP P43124
F	482	ASP	-	expression tag	UNP P43124
F	483	LEU	-	expression tag	UNP P43124
F	484	GLY	-	expression tag	UNP P43124
F	485	TYR	-	expression tag	UNP P43124
F	486	PHE	-	expression tag	UNP P43124
F	487	PHE	-	expression tag	UNP P43124
F	488	ASP	-	expression tag	UNP P43124
F	489	ASP	-	expression tag	UNP P43124
F	490	HIS	-	expression tag	UNP P43124
F	491	VAL	-	expression tag	UNP P43124
F	492	ARG	-	expression tag	UNP P43124
F	493	PHE	-	expression tag	UNP P43124
F	494	MET	-	expression tag	UNP P43124
F	495	ASP	-	expression tag	UNP P43124
F	496	ALA	-	expression tag	UNP P43124
F	497	PHE	-	expression tag	UNP P43124
F	498	ILE	-	expression tag	UNP P43124
F	499	GLU	-	expression tag	UNP P43124
F	500	ALA	-	expression tag	UNP P43124
F	501	LEU	-	expression tag	UNP P43124
F	502	GLY	-	expression tag	UNP P43124
F	503	LEU	-	expression tag	UNP P43124
F	504	GLU	-	expression tag	UNP P43124
F	505	GLU	-	expression tag	UNP P43124
F	506	VAL	-	expression tag	UNP P43124
F	507	VAL	-	expression tag	UNP P43124
F	508	LEU	-	expression tag	UNP P43124
F	509	VAL	-	expression tag	UNP P43124
F	510	ILE	-	expression tag	UNP P43124
F	511	HIS	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	512	ASP	-	expression tag	UNP P43124
F	513	TRP	-	expression tag	UNP P43124
F	514	GLY	-	expression tag	UNP P43124
F	515	SER	-	expression tag	UNP P43124
F	516	ALA	-	expression tag	UNP P43124
F	517	LEU	-	expression tag	UNP P43124
F	518	GLY	-	expression tag	UNP P43124
F	519	PHE	-	expression tag	UNP P43124
F	520	HIS	-	expression tag	UNP P43124
F	521	TRP	-	expression tag	UNP P43124
F	522	ALA	-	expression tag	UNP P43124
F	523	LYS	-	expression tag	UNP P43124
F	524	ARG	-	expression tag	UNP P43124
F	525	ASN	-	expression tag	UNP P43124
F	526	PRO	-	expression tag	UNP P43124
F	527	GLU	-	expression tag	UNP P43124
F	528	ARG	-	expression tag	UNP P43124
F	529	VAL	-	expression tag	UNP P43124
F	530	LYS	-	expression tag	UNP P43124
F	531	GLY	-	expression tag	UNP P43124
F	532	ILE	-	expression tag	UNP P43124
F	533	ALA	-	expression tag	UNP P43124
F	534	PHE	-	expression tag	UNP P43124
F	535	MET	-	expression tag	UNP P43124
F	536	GLU	-	expression tag	UNP P43124
F	537	PHE	-	expression tag	UNP P43124
F	538	ILE	-	expression tag	UNP P43124
F	539	ARG	-	expression tag	UNP P43124
F	540	PRO	-	expression tag	UNP P43124
F	541	ILE	-	expression tag	UNP P43124
F	542	PRO	-	expression tag	UNP P43124
F	543	THR	-	expression tag	UNP P43124
F	544	TRP	-	expression tag	UNP P43124
F	545	ASP	-	expression tag	UNP P43124
F	546	GLU	-	expression tag	UNP P43124
F	547	TRP	-	expression tag	UNP P43124
F	548	PRO	-	expression tag	UNP P43124
F	549	GLU	-	expression tag	UNP P43124
F	550	PHE	-	expression tag	UNP P43124
F	551	ALA	-	expression tag	UNP P43124
F	552	ARG	-	expression tag	UNP P43124
F	553	GLU	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	554	THR	-	expression tag	UNP P43124
F	555	PHE	-	expression tag	UNP P43124
F	556	GLN	-	expression tag	UNP P43124
F	557	ALA	-	expression tag	UNP P43124
F	558	PHE	-	expression tag	UNP P43124
F	559	ARG	-	expression tag	UNP P43124
F	560	THR	-	expression tag	UNP P43124
F	561	THR	-	expression tag	UNP P43124
F	562	ASP	-	expression tag	UNP P43124
F	563	VAL	-	expression tag	UNP P43124
F	564	GLY	-	expression tag	UNP P43124
F	565	ARG	-	expression tag	UNP P43124
F	566	LYS	-	expression tag	UNP P43124
F	567	LEU	-	expression tag	UNP P43124
F	568	ILE	-	expression tag	UNP P43124
F	569	ILE	-	expression tag	UNP P43124
F	570	ASP	-	expression tag	UNP P43124
F	571	GLN	-	expression tag	UNP P43124
F	572	ASN	-	expression tag	UNP P43124
F	573	VAL	-	expression tag	UNP P43124
F	574	PHE	-	expression tag	UNP P43124
F	575	ILE	-	expression tag	UNP P43124
F	576	GLU	-	expression tag	UNP P43124
F	577	GLY	-	expression tag	UNP P43124
F	578	THR	-	expression tag	UNP P43124
F	579	LEU	-	expression tag	UNP P43124
F	580	PRO	-	expression tag	UNP P43124
F	581	MET	-	expression tag	UNP P43124
F	582	GLY	-	expression tag	UNP P43124
F	583	VAL	-	expression tag	UNP P43124
F	584	VAL	-	expression tag	UNP P43124
F	585	ARG	-	expression tag	UNP P43124
F	586	PRO	-	expression tag	UNP P43124
F	587	LEU	-	expression tag	UNP P43124
F	588	THR	-	expression tag	UNP P43124
F	589	GLU	-	expression tag	UNP P43124
F	590	VAL	-	expression tag	UNP P43124
F	591	GLU	-	expression tag	UNP P43124
F	592	MET	-	expression tag	UNP P43124
F	593	ASP	-	expression tag	UNP P43124
F	594	HIS	-	expression tag	UNP P43124
F	595	TYR	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	596	ARG	-	expression tag	UNP P43124
F	597	GLU	-	expression tag	UNP P43124
F	598	PRO	-	expression tag	UNP P43124
F	599	PHE	-	expression tag	UNP P43124
F	600	LEU	-	expression tag	UNP P43124
F	601	ASN	-	expression tag	UNP P43124
F	602	PRO	-	expression tag	UNP P43124
F	603	VAL	-	expression tag	UNP P43124
F	604	ASP	-	expression tag	UNP P43124
F	605	ARG	-	expression tag	UNP P43124
F	606	GLU	-	expression tag	UNP P43124
F	607	PRO	-	expression tag	UNP P43124
F	608	LEU	-	expression tag	UNP P43124
F	609	TRP	-	expression tag	UNP P43124
F	610	ARG	-	expression tag	UNP P43124
F	611	PHE	-	expression tag	UNP P43124
F	612	PRO	-	expression tag	UNP P43124
F	613	ASN	-	expression tag	UNP P43124
F	614	GLU	-	expression tag	UNP P43124
F	615	LEU	-	expression tag	UNP P43124
F	616	PRO	-	expression tag	UNP P43124
F	617	ILE	-	expression tag	UNP P43124
F	618	ALA	-	expression tag	UNP P43124
F	619	GLY	-	expression tag	UNP P43124
F	620	GLU	-	expression tag	UNP P43124
F	621	PRO	-	expression tag	UNP P43124
F	622	ALA	-	expression tag	UNP P43124
F	623	ASN	-	expression tag	UNP P43124
F	624	ILE	-	expression tag	UNP P43124
F	625	VAL	-	expression tag	UNP P43124
F	626	ALA	-	expression tag	UNP P43124
F	627	LEU	-	expression tag	UNP P43124
F	628	VAL	-	expression tag	UNP P43124
F	629	GLU	-	expression tag	UNP P43124
F	630	GLU	-	expression tag	UNP P43124
F	631	TYR	-	expression tag	UNP P43124
F	632	MET	-	expression tag	UNP P43124
F	633	ASP	-	expression tag	UNP P43124
F	634	TRP	-	expression tag	UNP P43124
F	635	LEU	-	expression tag	UNP P43124
F	636	HIS	-	expression tag	UNP P43124
F	637	GLN	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	638	SER	-	expression tag	UNP P43124
F	639	PRO	-	expression tag	UNP P43124
F	640	VAL	-	expression tag	UNP P43124
F	641	PRO	-	expression tag	UNP P43124
F	642	LYS	-	expression tag	UNP P43124
F	643	LEU	-	expression tag	UNP P43124
F	644	LEU	-	expression tag	UNP P43124
F	645	PHE	-	expression tag	UNP P43124
F	646	TRP	-	expression tag	UNP P43124
F	647	GLY	-	expression tag	UNP P43124
F	648	THR	-	expression tag	UNP P43124
F	649	PRO	-	expression tag	UNP P43124
F	650	GLY	-	expression tag	UNP P43124
F	651	VAL	-	expression tag	UNP P43124
F	652	LEU	-	expression tag	UNP P43124
F	653	ILE	-	expression tag	UNP P43124
F	654	PRO	-	expression tag	UNP P43124
F	655	PRO	-	expression tag	UNP P43124
F	656	ALA	-	expression tag	UNP P43124
F	657	GLU	-	expression tag	UNP P43124
F	658	ALA	-	expression tag	UNP P43124
F	659	ALA	-	expression tag	UNP P43124
F	660	ARG	-	expression tag	UNP P43124
F	661	LEU	-	expression tag	UNP P43124
F	662	ALA	-	expression tag	UNP P43124
F	663	LYS	-	expression tag	UNP P43124
F	664	SER	-	expression tag	UNP P43124
F	665	LEU	-	expression tag	UNP P43124
F	666	PRO	-	expression tag	UNP P43124
F	667	ASN	-	expression tag	UNP P43124
F	668	CYS	-	expression tag	UNP P43124
F	669	LYS	-	expression tag	UNP P43124
F	670	ALA	-	expression tag	UNP P43124
F	671	VAL	-	expression tag	UNP P43124
F	672	ASP	-	expression tag	UNP P43124
F	673	ILE	-	expression tag	UNP P43124
F	674	GLY	-	expression tag	UNP P43124
F	675	PRO	-	expression tag	UNP P43124
F	676	GLY	-	expression tag	UNP P43124
F	677	LEU	-	expression tag	UNP P43124
F	678	ASN	-	expression tag	UNP P43124
F	679	LEU	-	expression tag	UNP P43124

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Chain	Residue	Modelled	Actual	Comment	Reference
F	680	LEU	-	expression tag	UNP P43124
F	681	GLN	-	expression tag	UNP P43124
F	682	GLU	-	expression tag	UNP P43124
F	683	ASP	-	expression tag	UNP P43124
F	684	ASN	-	expression tag	UNP P43124
F	685	PRO	-	expression tag	UNP P43124
F	686	ASP	-	expression tag	UNP P43124
F	687	LEU	-	expression tag	UNP P43124
F	688	ILE	-	expression tag	UNP P43124
F	689	GLY	-	expression tag	UNP P43124
F	690	SER	-	expression tag	UNP P43124
F	691	GLU	-	expression tag	UNP P43124
F	692	ILE	-	expression tag	UNP P43124
F	693	ALA	-	expression tag	UNP P43124
F	694	ARG	-	expression tag	UNP P43124
F	695	TRP	-	expression tag	UNP P43124
F	696	LEU	-	expression tag	UNP P43124
F	697	SER	-	expression tag	UNP P43124
F	698	THR	-	expression tag	UNP P43124
F	699	LEU	-	expression tag	UNP P43124
F	700	GLU	-	expression tag	UNP P43124
F	701	ILE	-	expression tag	UNP P43124
F	702	SER	-	expression tag	UNP P43124
F	703	GLY	-	expression tag	UNP P43124
F	704	GLY	-	expression tag	UNP P43124
F	705	SER	-	expression tag	UNP P43124
F	706	GLU	-	expression tag	UNP P43124
F	707	GLN	-	expression tag	UNP P43124
F	708	LYS	-	expression tag	UNP P43124
F	709	LEU	-	expression tag	UNP P43124
F	710	ILE	-	expression tag	UNP P43124
F	711	SER	-	expression tag	UNP P43124
F	712	GLU	-	expression tag	UNP P43124
F	713	GLU	-	expression tag	UNP P43124
F	714	ASP	-	expression tag	UNP P43124
F	715	LEU	-	expression tag	UNP P43124

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
7	C	1	Total Zn 1 1	0

Continued on next page...

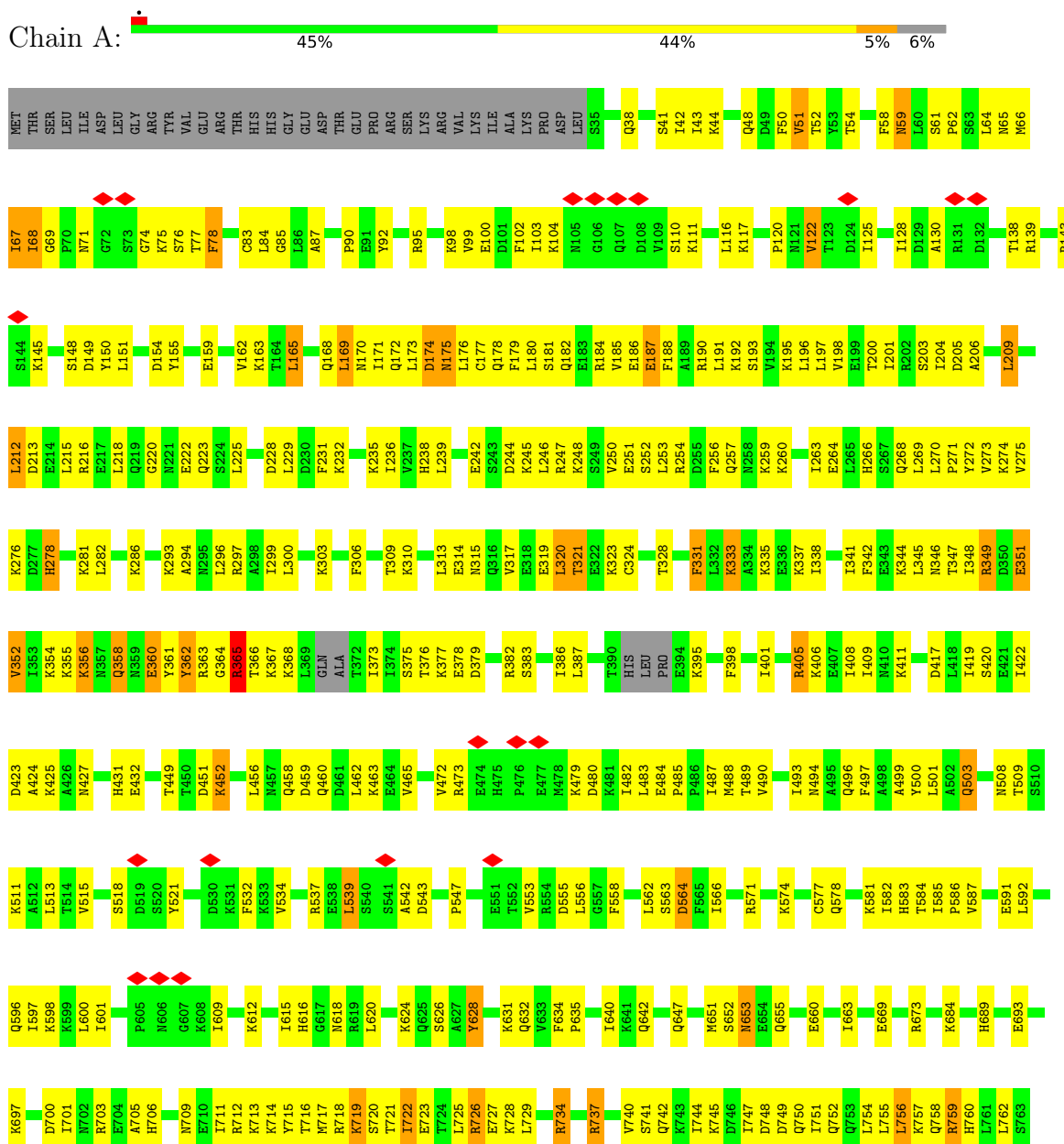
Continued from previous page...

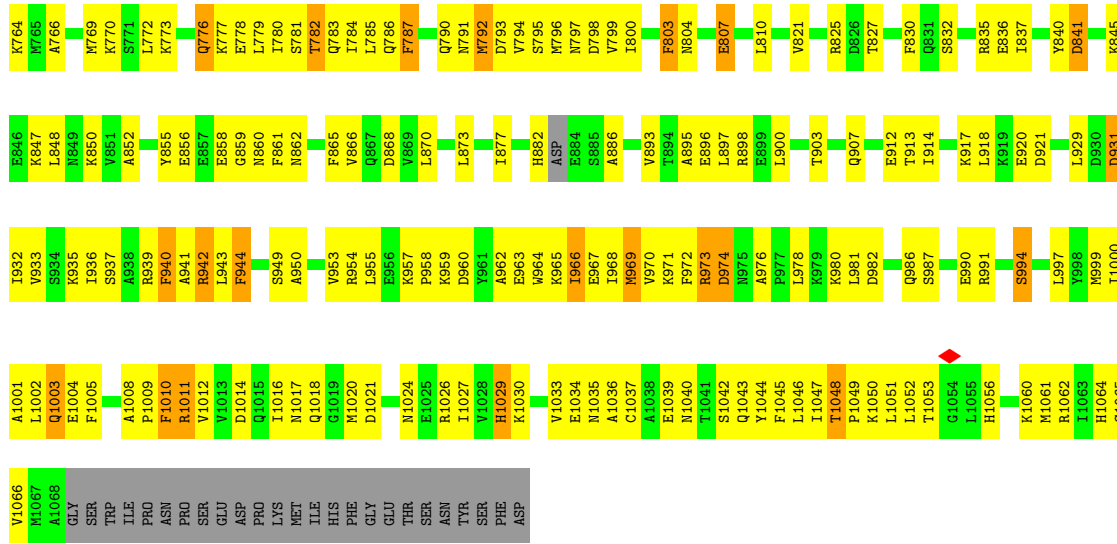
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	D	2	2	2	0

3 Residue-property plots i

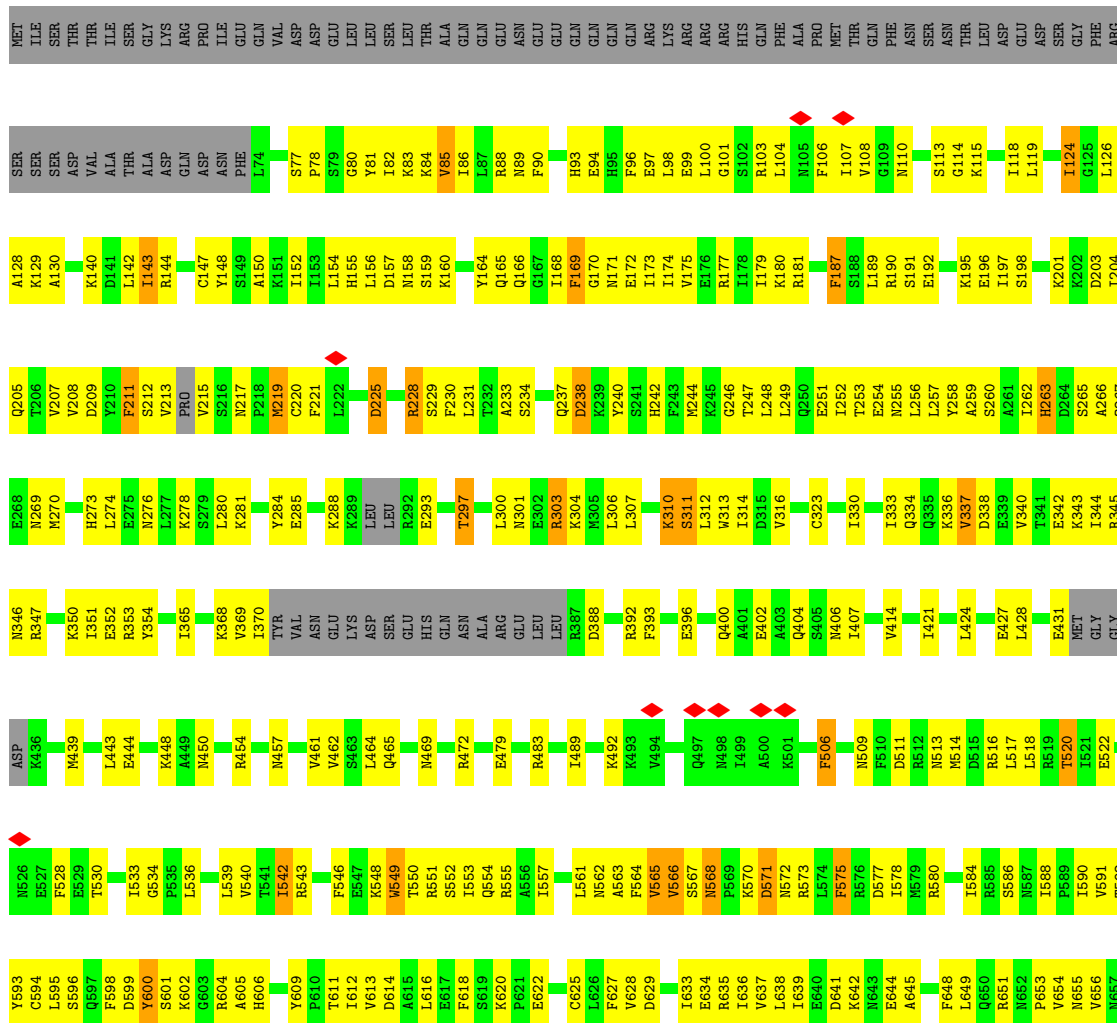
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

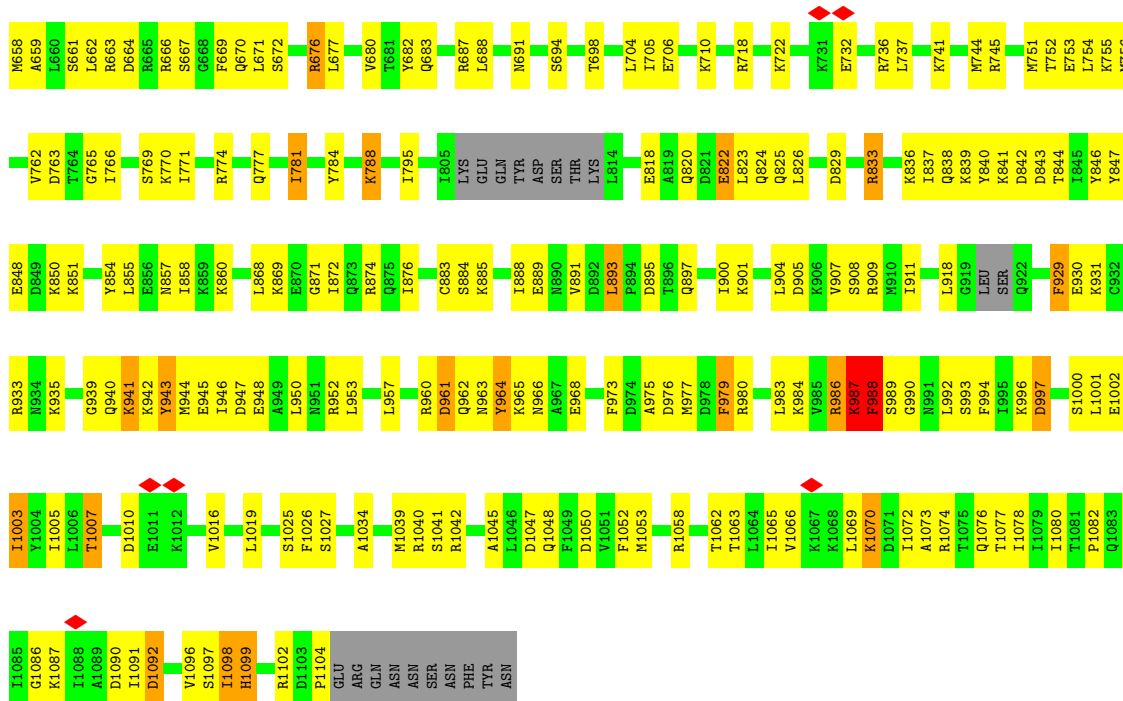
- Molecule 1: Structural maintenance of chromosomes protein 5



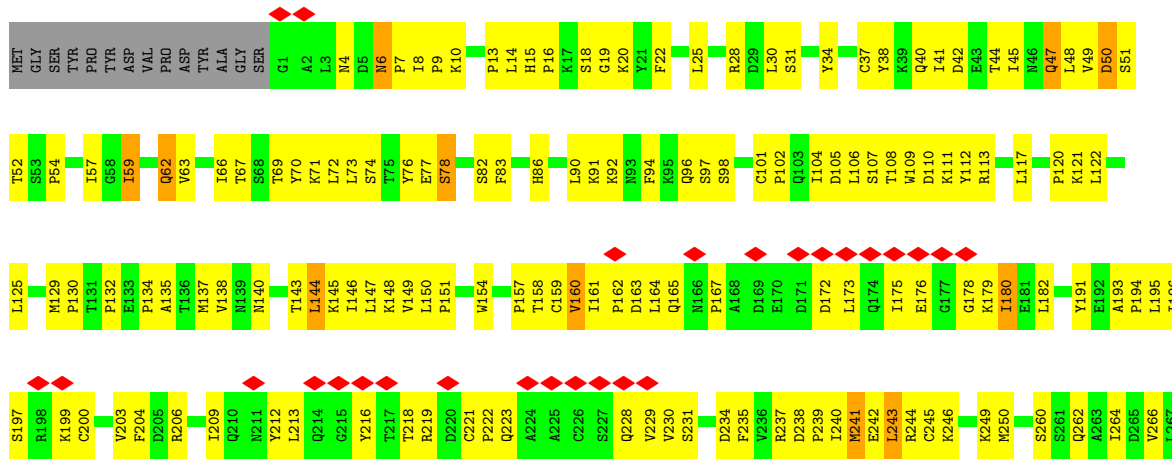


• Molecule 2: Structural maintenance of chromosomes protein 6

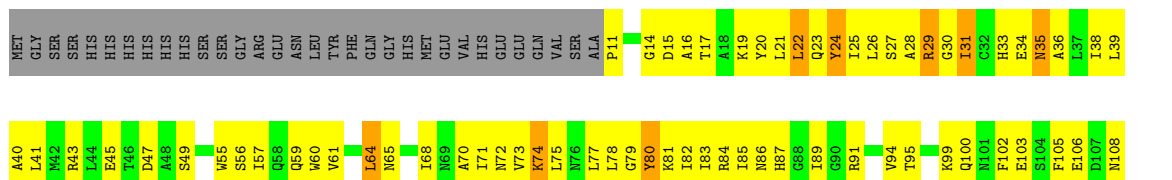


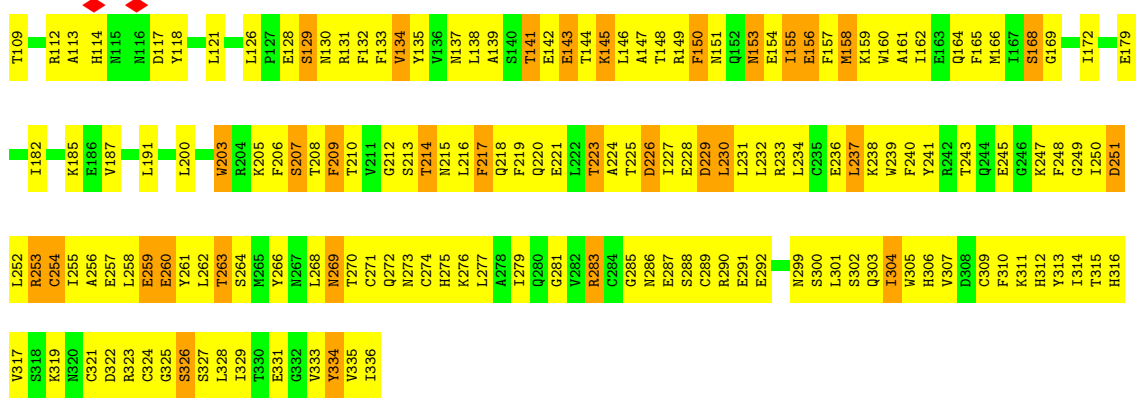


• Molecule 3: E3 SUMO-protein ligase MMS21

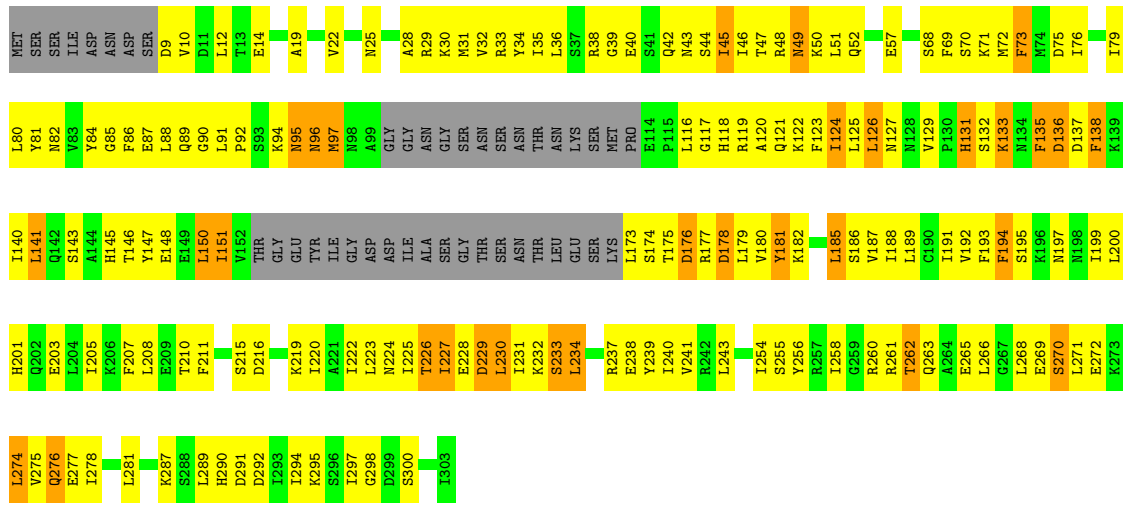
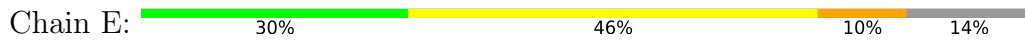


• Molecule 4: Non-structural maintenance of chromosomes element 1

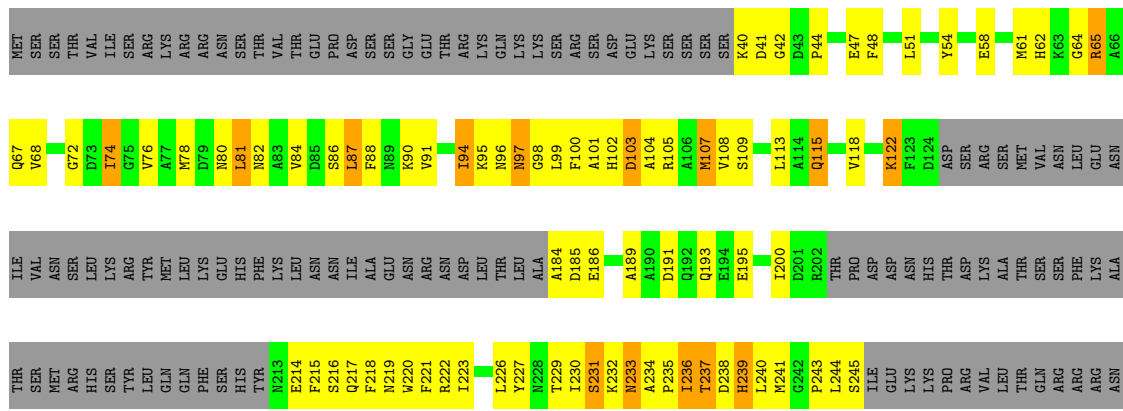


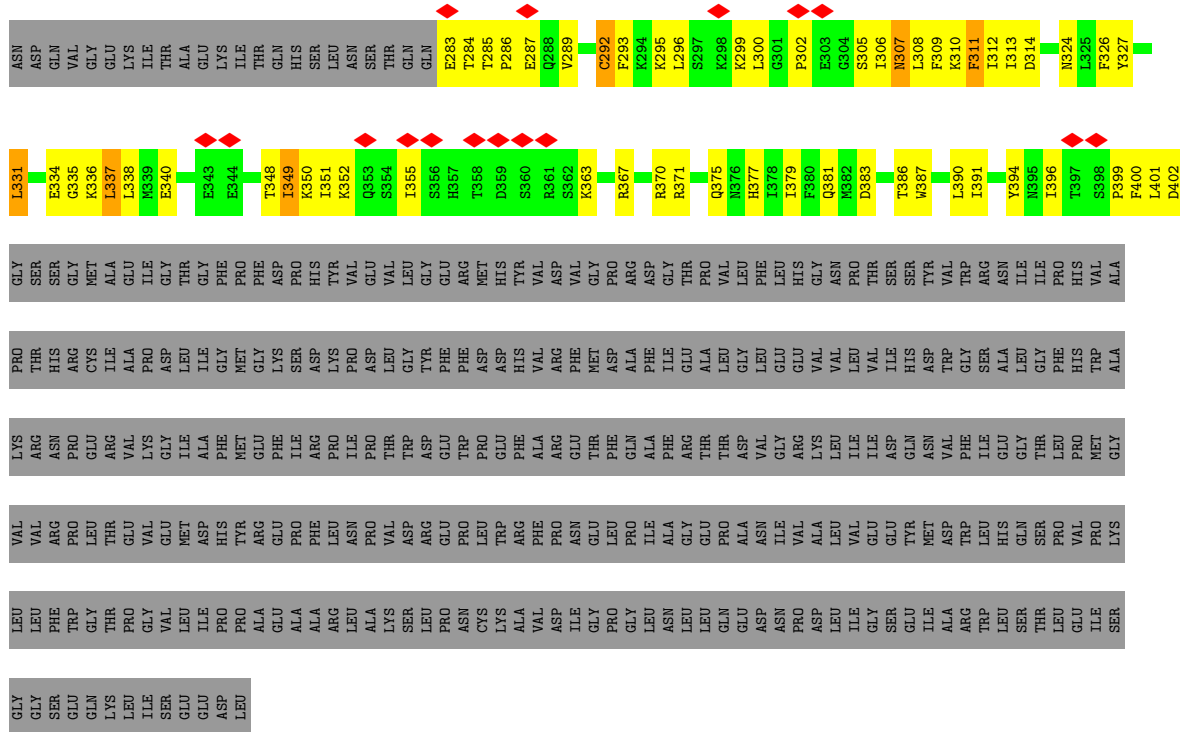


• Molecule 5: Non-structural maintenance of chromosome element 3



• Molecule 6: Non-structural maintenance of chromosome element 4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	132.478	Depositor
Minimum map value	-65.911	Depositor
Average map value	-0.023	Depositor
Map value standard deviation	0.949	Depositor
Recommended contour level	11.0	Depositor
Map size (Å)	704.0, 704.0, 704.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2, 2.2, 2.2	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:
ZN

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	0.28	0/8359	0.48	1/11228 (0.0%)
2	B	0.32	5/8109 (0.1%)	0.50	5/10859 (0.0%)
3	C	0.32	0/2164	0.62	2/2938 (0.1%)
4	D	0.40	0/2660	0.61	0/3602
5	E	0.36	0/2118	0.55	0/2848
6	F	0.32	0/2054	0.56	0/2758
All	All	0.32	5/25464 (0.0%)	0.53	8/34233 (0.0%)

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
2	B	0	1
4	D	0	1
5	E	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	989	SER	C-N	7.21	1.46	1.33
2	B	988	PHE	N-CA	6.37	1.59	1.46
2	B	989	SER	N-CA	6.19	1.58	1.46
2	B	987	LYS	N-CA	5.81	1.57	1.46
2	B	987	LYS	C-N	5.09	1.45	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	986	ARG	O-C-N	-8.93	108.42	122.70
2	B	987	LYS	CA-C-N	6.32	131.09	117.20
2	B	989	SER	CA-C-N	6.13	128.47	116.20
2	B	988	PHE	C-N-CA	5.61	135.72	121.70
2	B	988	PHE	N-CA-C	5.50	125.85	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	986	ARG	Mainchain
4	D	100	GLN	Mainchain
5	E	131	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8257	0	8408	521	0
2	B	8028	0	8137	408	0
3	C	2121	0	2086	183	0
4	D	2614	0	2575	297	0
5	E	2091	0	2139	210	0
6	F	2019	0	1989	165	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
All	All	25133	0	25334	1640	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 32.

The worst 5 of 1640 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:282:LEU:HD11	1:A:286:LYS:HE3	1.32	1.11
4:D:82:ILE:HA	4:D:134:VAL:O	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:CD1	1:A:286:LYS:HE3	1.85	1.07
2:B:215:VAL:N	2:B:220:CYS:HG	1.54	1.04
1:A:458:GLN:HE21	1:A:652:SER:HB3	1.23	1.01

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	1020/1093 (93%)	972 (95%)	45 (4%)	3 (0%)	41	77
2	B	984/1114 (88%)	931 (95%)	51 (5%)	2 (0%)	47	81
3	C	265/281 (94%)	260 (98%)	5 (2%)	0	100	100
4	D	324/358 (90%)	305 (94%)	19 (6%)	0	100	100
5	E	255/303 (84%)	229 (90%)	26 (10%)	0	100	100
6	F	249/715 (35%)	235 (94%)	13 (5%)	1 (0%)	34	72
All	All	3097/3864 (80%)	2932 (95%)	159 (5%)	6 (0%)	50	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ASN
2	B	987	LYS
6	F	200	ILE
1	A	741	SER
2	B	988	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	926/1003 (92%)	852 (92%)	74 (8%)	12	35
2	B	894/1003 (89%)	832 (93%)	62 (7%)	15	40
3	C	247/258 (96%)	237 (96%)	10 (4%)	31	55
4	D	288/316 (91%)	240 (83%)	48 (17%)	2	12
5	E	237/272 (87%)	203 (86%)	34 (14%)	3	16
6	F	215/635 (34%)	188 (87%)	27 (13%)	4	19
All	All	2807/3487 (80%)	2552 (91%)	255 (9%)	13	29

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	833	ARG
5	E	230	LEU
3	C	144	LEU
5	E	227	ILE
6	F	103	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	269	ASN
2	B	966	ASN
2	B	962	GLN
3	C	47	GLN
1	A	783	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

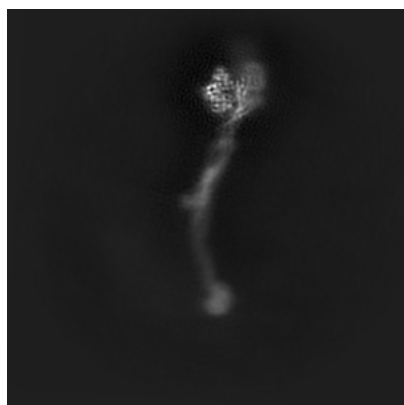
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13895. These allow visual inspection of the internal detail of the map and identification of artifacts.

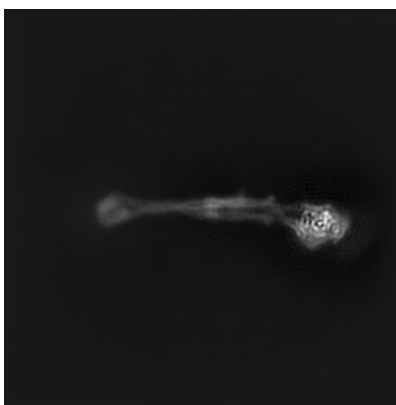
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

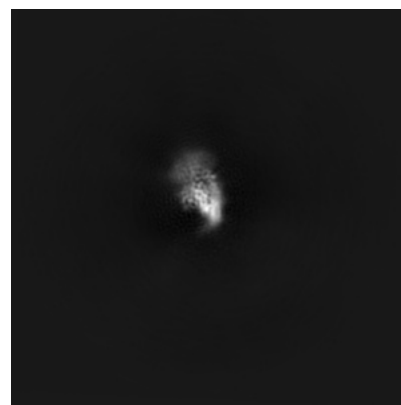
6.1.1 Primary map



X



Y

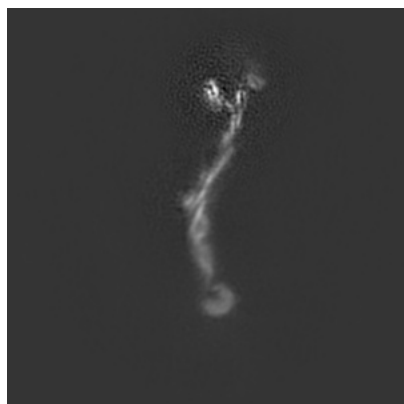


Z

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

6.2 Central slices [i](#)

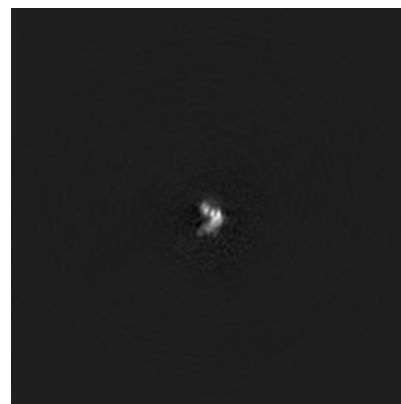
6.2.1 Primary map



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](#)

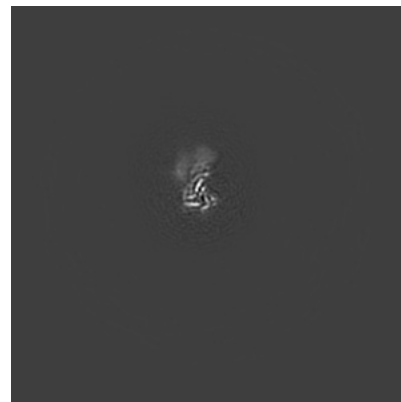
6.3.1 Primary map



X Index: 148



Y Index: 166



Z Index: 256

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 11.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

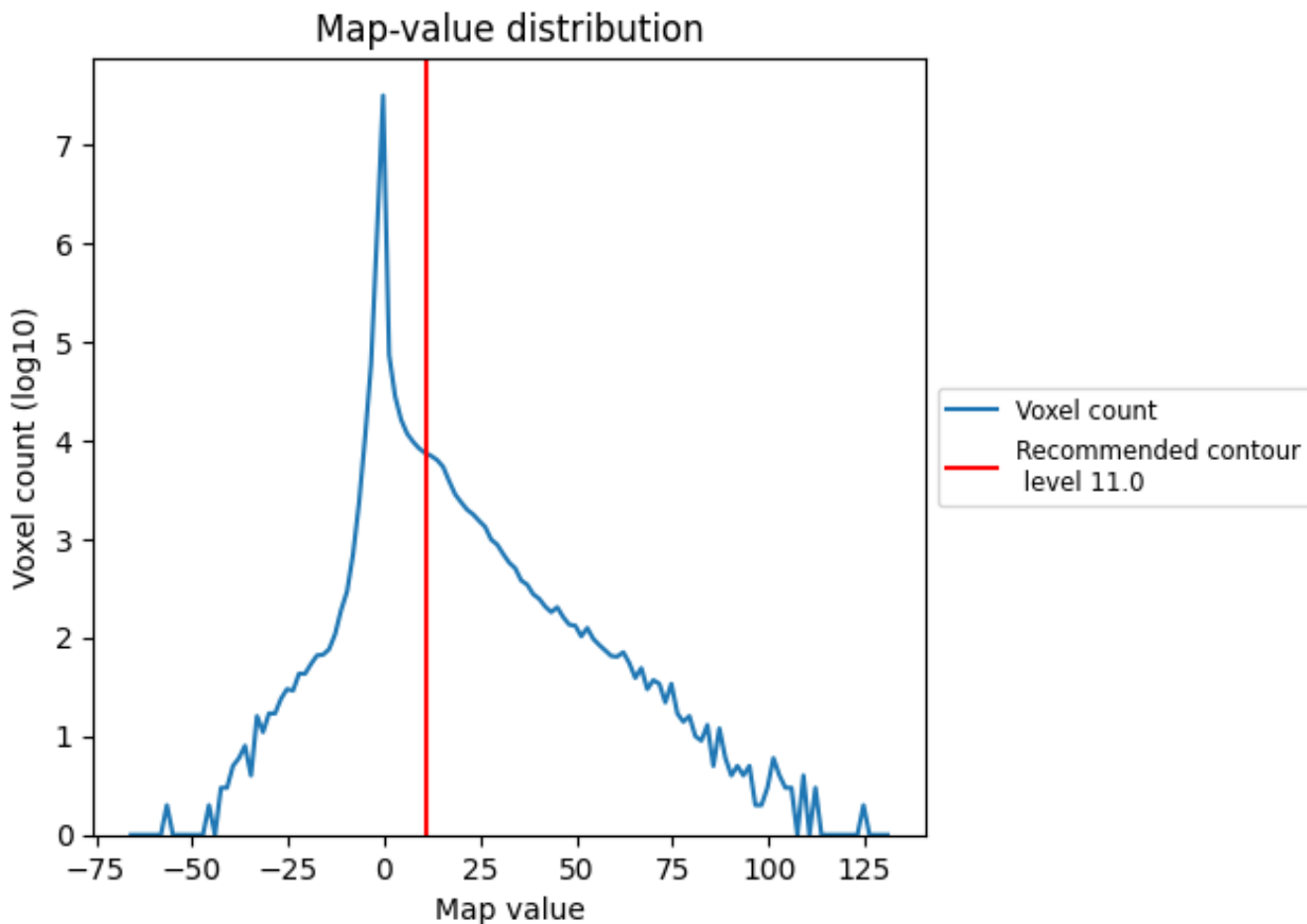
6.5 Mask visualisation

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

7 Map analysis [i](#)

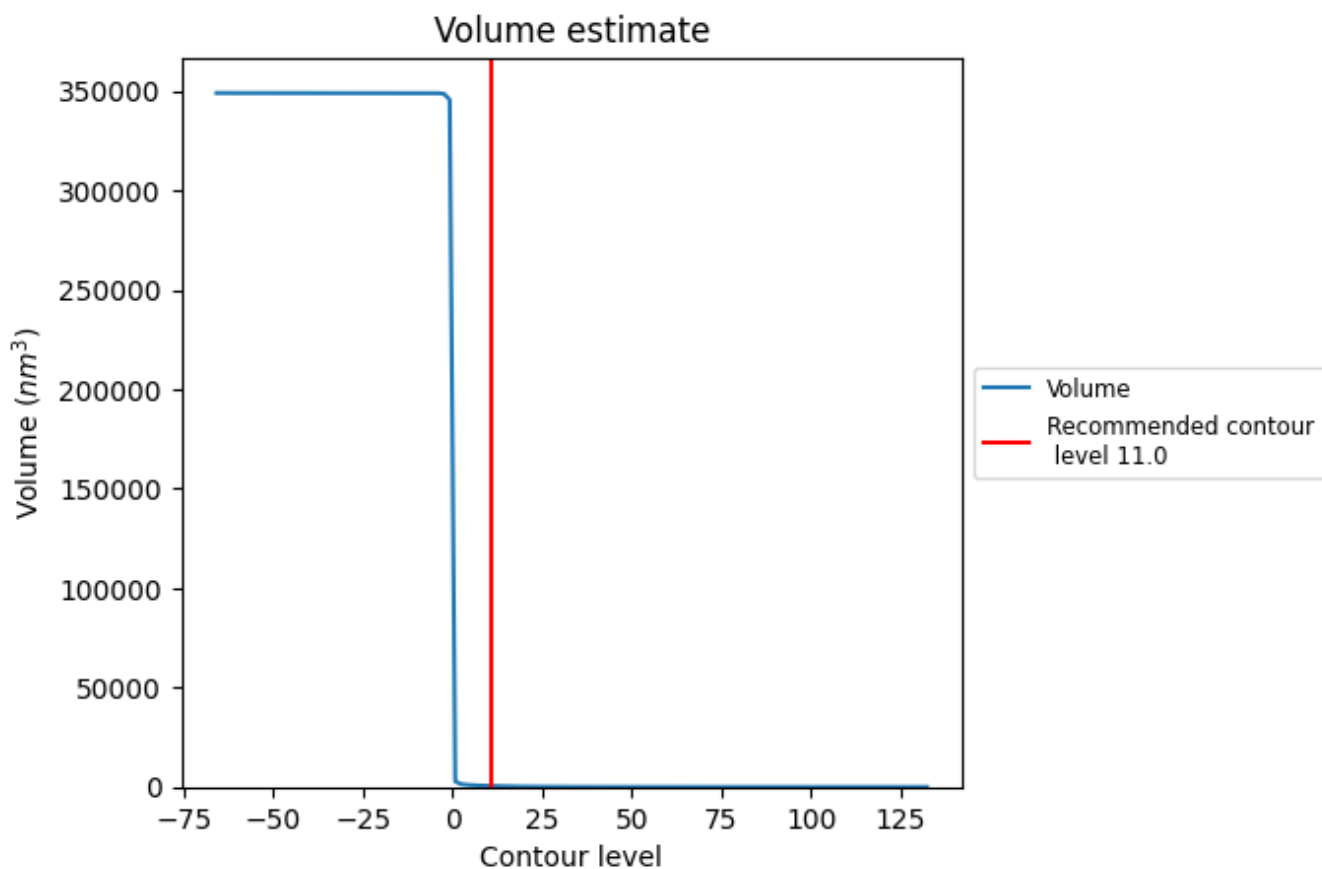
This section contains the results of statistical analysis of the map.

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.

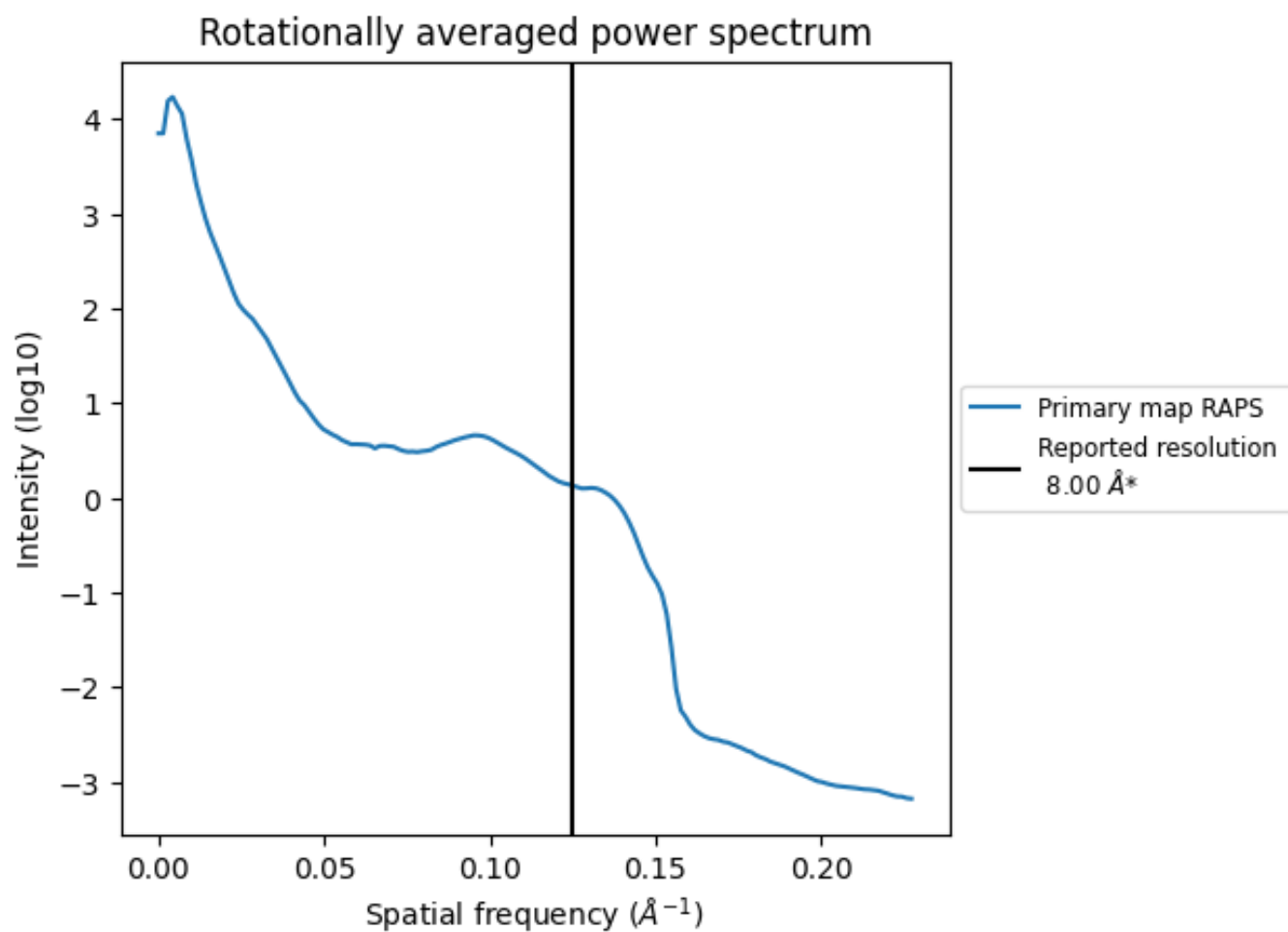
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm³; this corresponds to an approximate mass of 452 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 0.125\AA^{-1}

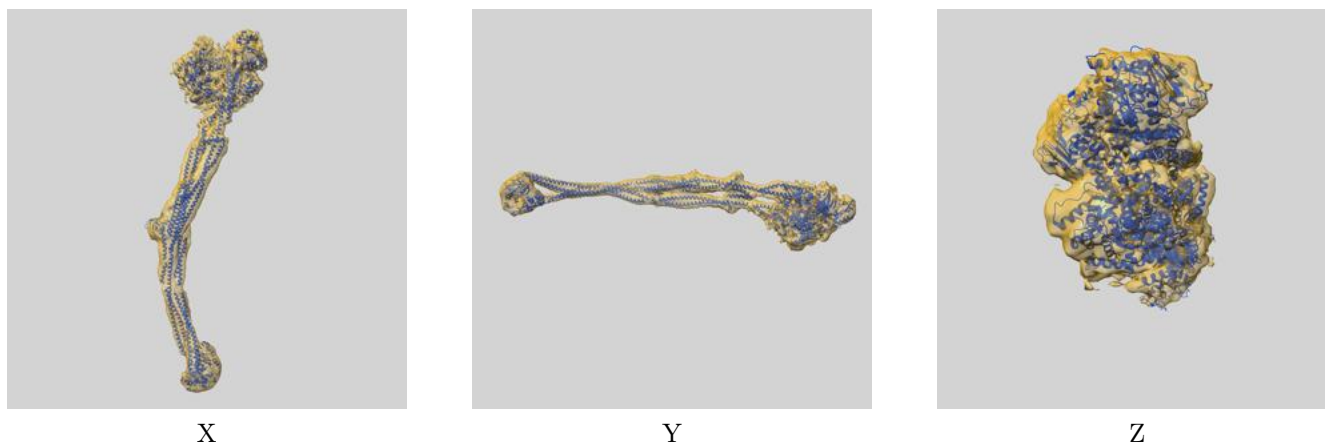
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

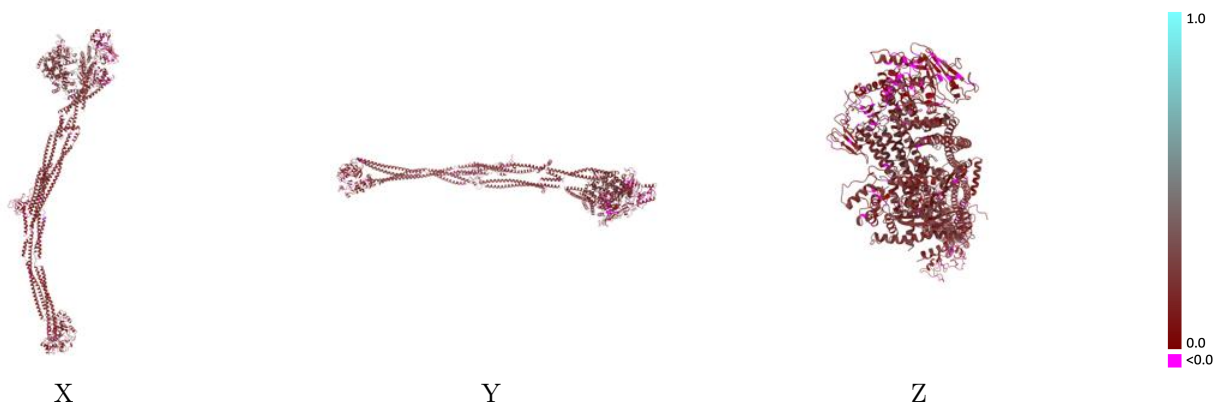
This section contains information regarding the fit between EMDB map EMD-13895 and PDB model 7QCD. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



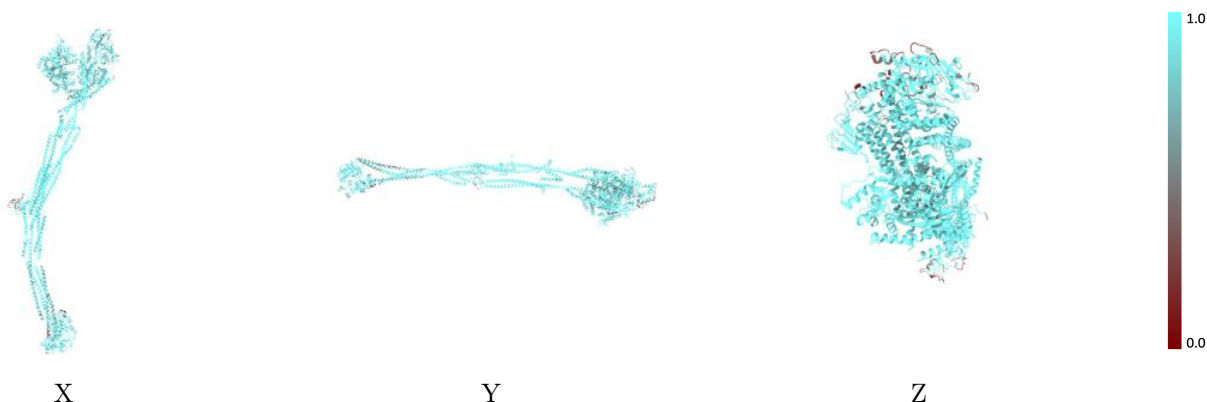
The images above show the 3D surface view of the map at the recommended contour level 11.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



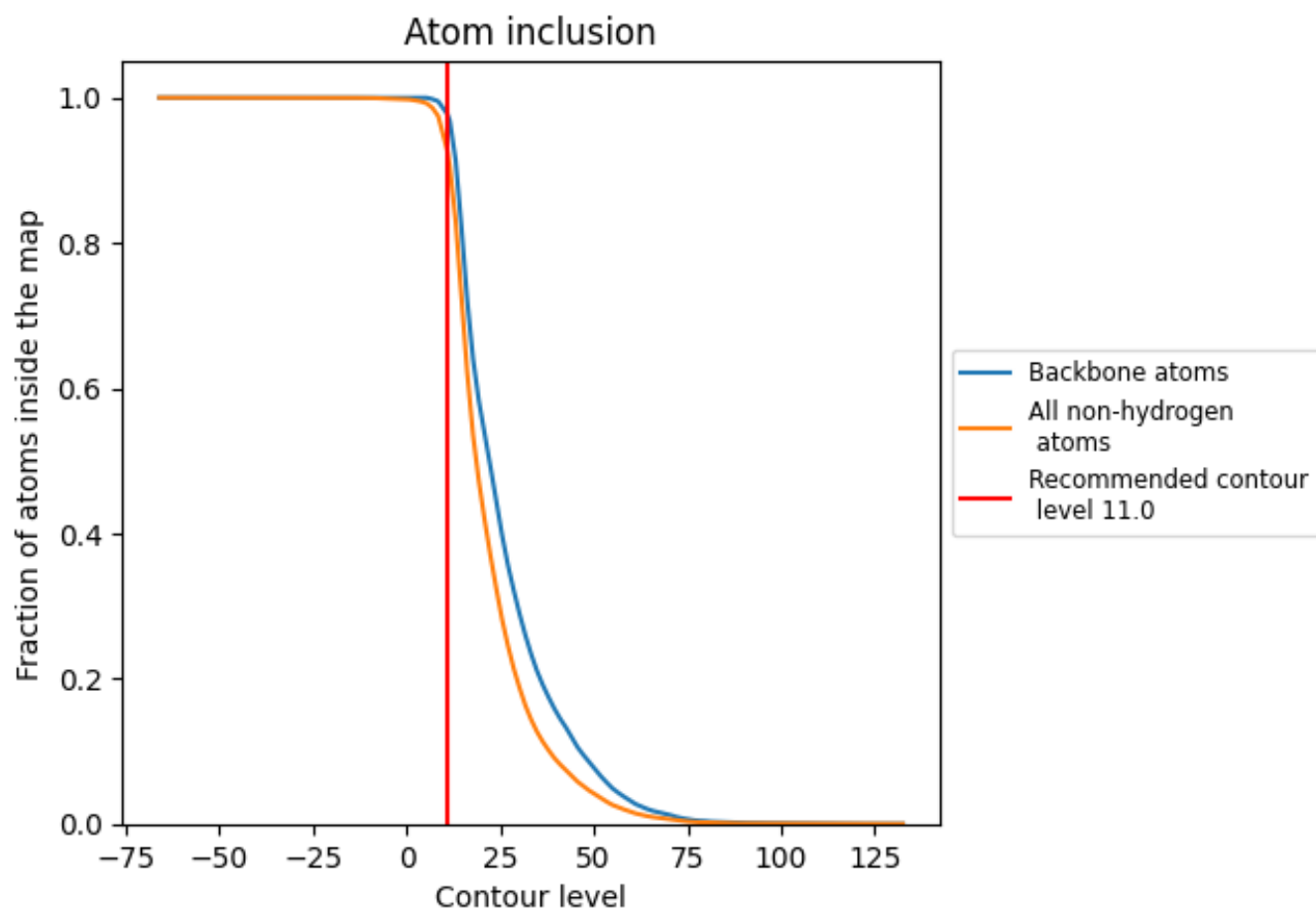
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (11.0).















9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (11.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9253	 0.1650
A	 0.9290	 0.1640
B	 0.9349	 0.1520
C	 0.8919	 0.1160
D	 0.9428	 0.2050
E	 0.9301	 0.2190
F	 0.8797	 0.1580

