



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:38 AM UTC

PDB ID : 7VPZ / pdb_00007vpz
EMDB ID : EMD-32077
Title : Cryo-EM structure of Streptomyces coelicolor transcription initial complex with one Zur dimer
Authors : Yang, X.; Zheng, J.
Deposited on : 2021-10-18
Resolution : 4.14 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

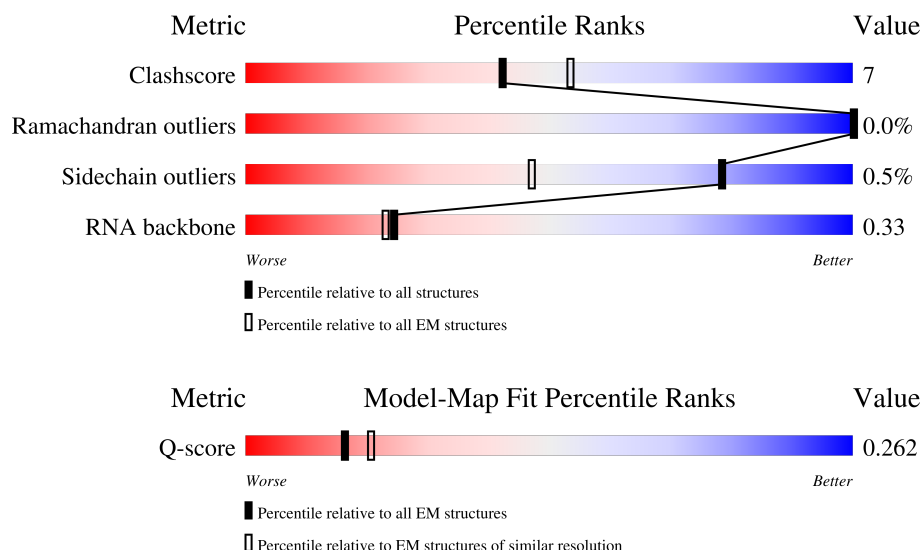
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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	-
RNA backbone	8273	3508	-
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	340	
1	B	340	
2	C	1161	

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Mol	Chain	Length	Quality of chain
3	D	1307	79% 17%
4	E	90	72% 13% 14%
5	F	531	46% 10% 43%
6	M	159	18% 70% 13% 18%
6	N	159	7% 70% 12% 18%
7	O	84	94% 6%
8	P	84	83% 17%
9	Q	5	80% 20%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 30593 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1742	1102	302	334	4		
1	B	233	Total	C	N	O	S	0	0
			1792	1131	309	347	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1116	Total	C	N	O	S	0	0
			8692	5450	1513	1698	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1259	Total	C	N	O	S	0	0
			9846	6161	1787	1857	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1300	HIS	-	expression tag	UNP Q8CJT1
D	1301	HIS	-	expression tag	UNP Q8CJT1
D	1302	HIS	-	expression tag	UNP Q8CJT1
D	1303	HIS	-	expression tag	UNP Q8CJT1
D	1304	HIS	-	expression tag	UNP Q8CJT1
D	1305	HIS	-	expression tag	UNP Q8CJT1
D	1306	HIS	-	expression tag	UNP Q8CJT1
D	1307	HIS	-	expression tag	UNP Q8CJT1

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	77	Total	C	N	O	0	0
			597	382	98	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	301	Total	C	N	O	S	0	0
			2396	1509	426	454	7		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P18183
F	-18	GLY	-	expression tag	UNP P18183
F	-17	SER	-	expression tag	UNP P18183
F	-16	SER	-	expression tag	UNP P18183
F	-15	HIS	-	expression tag	UNP P18183
F	-14	HIS	-	expression tag	UNP P18183
F	-13	HIS	-	expression tag	UNP P18183
F	-12	HIS	-	expression tag	UNP P18183
F	-11	HIS	-	expression tag	UNP P18183
F	-10	HIS	-	expression tag	UNP P18183
F	-9	SER	-	expression tag	UNP P18183
F	-8	SER	-	expression tag	UNP P18183
F	-7	GLY	-	expression tag	UNP P18183
F	-6	LEU	-	expression tag	UNP P18183
F	-5	VAL	-	expression tag	UNP P18183
F	-4	PRO	-	expression tag	UNP P18183
F	-3	ARG	-	expression tag	UNP P18183
F	-2	GLY	-	expression tag	UNP P18183
F	-1	SER	-	expression tag	UNP P18183
F	0	HIS	-	expression tag	UNP P18183

- Molecule 6 is a protein called Putative metal uptake regulation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	131	Total	C	N	O	S	0	0
			984	603	185	190	6		
6	N	131	Total	C	N	O	S	0	0
			984	603	185	190	6		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP Q9L2H5
M	-18	GLY	-	expression tag	UNP Q9L2H5
M	-17	SER	-	expression tag	UNP Q9L2H5
M	-16	SER	-	expression tag	UNP Q9L2H5
M	-15	HIS	-	expression tag	UNP Q9L2H5
M	-14	HIS	-	expression tag	UNP Q9L2H5
M	-13	HIS	-	expression tag	UNP Q9L2H5
M	-12	HIS	-	expression tag	UNP Q9L2H5
M	-11	HIS	-	expression tag	UNP Q9L2H5
M	-10	HIS	-	expression tag	UNP Q9L2H5
M	-9	SER	-	expression tag	UNP Q9L2H5
M	-8	SER	-	expression tag	UNP Q9L2H5
M	-7	GLY	-	expression tag	UNP Q9L2H5
M	-6	LEU	-	expression tag	UNP Q9L2H5
M	-5	VAL	-	expression tag	UNP Q9L2H5
M	-4	PRO	-	expression tag	UNP Q9L2H5
M	-3	ARG	-	expression tag	UNP Q9L2H5
M	-2	GLY	-	expression tag	UNP Q9L2H5
M	-1	SER	-	expression tag	UNP Q9L2H5
M	0	HIS	-	expression tag	UNP Q9L2H5
N	-19	MET	-	initiating methionine	UNP Q9L2H5
N	-18	GLY	-	expression tag	UNP Q9L2H5
N	-17	SER	-	expression tag	UNP Q9L2H5
N	-16	SER	-	expression tag	UNP Q9L2H5
N	-15	HIS	-	expression tag	UNP Q9L2H5
N	-14	HIS	-	expression tag	UNP Q9L2H5
N	-13	HIS	-	expression tag	UNP Q9L2H5
N	-12	HIS	-	expression tag	UNP Q9L2H5
N	-11	HIS	-	expression tag	UNP Q9L2H5
N	-10	HIS	-	expression tag	UNP Q9L2H5
N	-9	SER	-	expression tag	UNP Q9L2H5
N	-8	SER	-	expression tag	UNP Q9L2H5
N	-7	GLY	-	expression tag	UNP Q9L2H5
N	-6	LEU	-	expression tag	UNP Q9L2H5
N	-5	VAL	-	expression tag	UNP Q9L2H5
N	-4	PRO	-	expression tag	UNP Q9L2H5
N	-3	ARG	-	expression tag	UNP Q9L2H5
N	-2	GLY	-	expression tag	UNP Q9L2H5
N	-1	SER	-	expression tag	UNP Q9L2H5
N	0	HIS	-	expression tag	UNP Q9L2H5

- Molecule 7 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	84	Total	C	N	O	P	0	0
			1714	810	315	505	84		

- Molecule 8 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	84	Total	C	N	O	P	0	0
			1729	815	325	505	84		

- Molecule 9 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	5	Total	C	N	O	P	0	0
			108	49	22	33	4		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

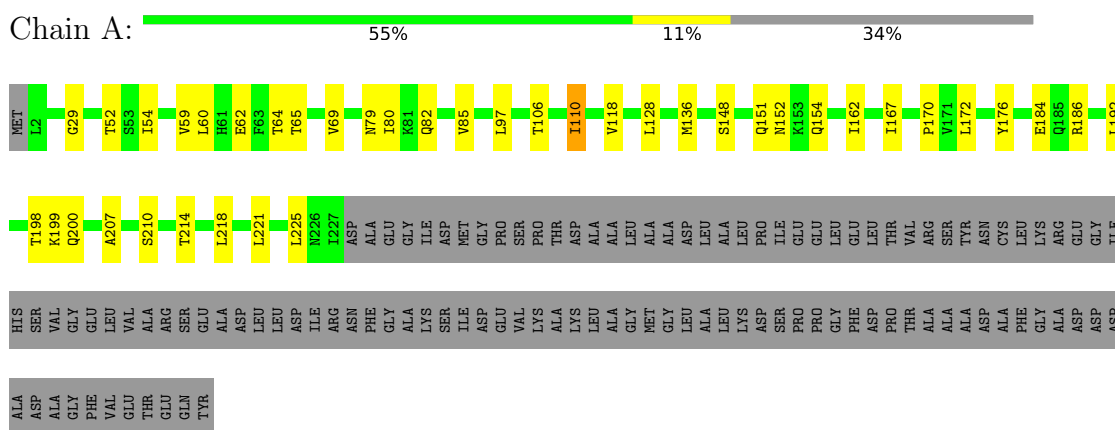
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	
11	M	3	Total	Zn	0
			3	3	
11	N	3	Total	Zn	0
			3	3	

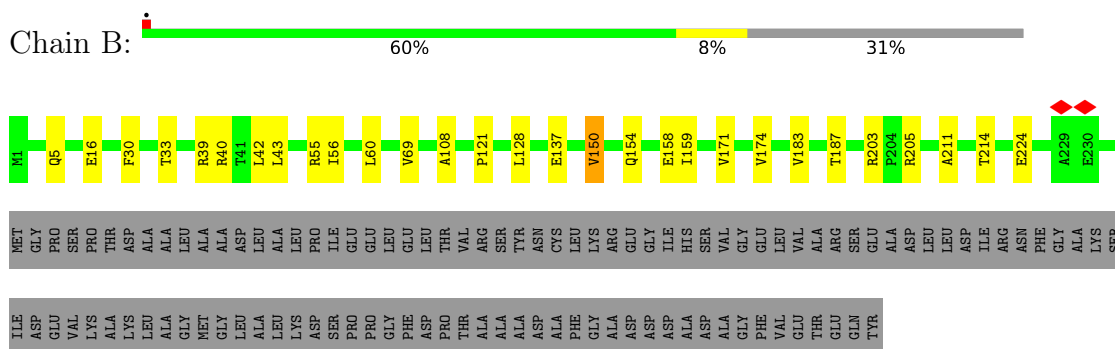
3 Residue-property plots

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.

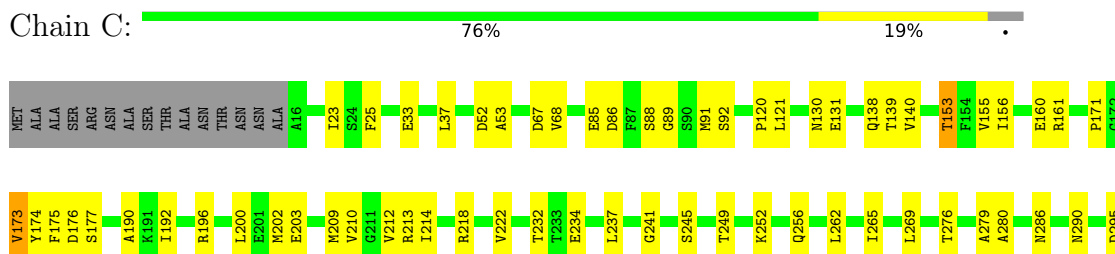
• Molecule 1: DNA-directed RNA polymerase subunit alpha



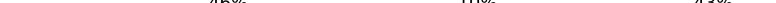
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



ME1	SE1	SE2	SE3	SE4	SE5	SE6	SE7	SE8	SE9	SE10	SE11	SE12	SE13	SE14	SE15	SE16	SE17	SE18	SE19	SE20	SE21	SE22	SE23	SE24	SE25	SE26	SE27	SE28	SE29	SE30	SE31	SE32	SE33	SE34	SE35	SE36	SE37	SE38	SE39	SE40	SE41	SE42	SE43	SE44	SE45	SE46	SE47	SE48	SE49	SE50	SE51	SE52	SE53	SE54	SE55	SE56	SE57	SE58	SE59	SE60	SE61	SE62	SE63	SE64	SE65	SE66	SE67	SE68	SE69	SE70	SE71	SE72	SE73	SE74	SE75	SE76	SE77	SE78	SE79	SE80	SE81	SE82	SE83	SE84	SE85	SE86	SE87	SE88	SE89	SE90	SE91	SE92	SE93	SE94	SE95	SE96	SE97	SE98	SE99	SE100	SE101	SE102	SE103	SE104	SE105	SE106	SE107	SE108	SE109	SE110	SE111	SE112	SE113	SE114	SE115	SE116	SE117	SE118	SE119	SE120	SE121	SE122	SE123	SE124	SE125	SE126	SE127	SE128	SE129	SE130	SE131	SE132	SE133	SE134	SE135	SE136	SE137	SE138	SE139	SE140	SE141	SE142	SE143	SE144	SE145	SE146	SE147	SE148	SE149	SE150	SE151	SE152	SE153	SE154	SE155	SE156	SE157	SE158	SE159	SE160	SE161	SE162	SE163	SE164	SE165	SE166	SE167	SE168	SE169	SE170	SE171	SE172	SE173	SE174	SE175	SE176	SE177	SE178	SE179	SE180	SE181	SE182	SE183	SE184	SE185	SE186	SE187	SE188	SE189	SE190	SE191	SE192	SE193	SE194	SE195	SE196	SE197	SE198	SE199	SE200	SE201	SE202	SE203	SE204	SE205	SE206	SE207	SE208	SE209	SE210	SE211	SE212	SE213	SE214	SE215	SE216	SE217	SE218	SE219	SE220	SE221	SE222	SE223	SE224	SE225	SE226	SE227	SE228	SE229	SE230	SE231	SE232	SE233	SE234	SE235	SE236	SE237	SE238	SE239	SE240	SE241	SE242	SE243	SE244	SE245	SE246	SE247	SE248	SE249	SE250	SE251	SE252	SE253	SE254	SE255	SE256	SE257	SE258	SE259	SE260	SE261	SE262	SE263	SE264	SE265	SE266	SE267	SE268	SE269	SE270	SE271	SE272	SE273	SE274	SE275	SE276	SE277	SE278	SE279	SE280	SE281	SE282	SE283	SE284	SE285	SE286	SE287	SE288	SE289	SE290	SE291	SE292	SE293	SE294	SE295	SE296	SE297	SE298	SE299	SE300	SE301	SE302	SE303	SE304	SE305	SE306	SE307	SE308	SE309	SE310	SE311	SE312	SE313	SE314	SE315	SE316	SE317	SE318	SE319	SE320	SE321	SE322	SE323	SE324	SE325	SE326	SE327	SE328	SE329	SE330	SE331	SE332	SE333	SE334	SE335	SE336	SE337	SE338	SE339	SE340	SE341	SE342	SE343	SE344	SE345	SE346	SE347	SE348	SE349	SE350	SE351	SE352	SE353	SE354	SE355	SE356	SE357	SE358	SE359	SE360	SE361	SE362	SE363	SE364	SE365	SE366	SE367	SE368	SE369	SE370	SE371	SE372	SE373	SE374	SE375	SE376	SE377	SE378	SE379	SE380	SE381	SE382	SE383	SE384	SE385	SE386	SE387	SE388	SE389	SE390	SE391	SE392	SE393	SE394	SE395	SE396	SE397	SE398	SE399	SE400	SE401	SE402	SE403	SE404	SE405	SE406	SE407	SE408	SE409	SE410	SE411	SE412	SE413	SE414	SE415	SE416	SE417	SE418	SE419	SE420	SE421	SE422	SE423	SE424	SE425	SE426	SE427	SE428	SE429	SE430	SE431	SE432	SE433	SE434	SE435	SE436	SE437	SE438	SE439	SE440	SE441	SE442	SE443	SE444	SE445	SE446	SE447	SE448	SE449	SE450	SE451	SE452	SE453	SE454	SE455	SE456	SE457	SE458	SE459	SE460	SE461	SE462	SE463	SE464	SE465	SE
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- Chain F:  46% 10% 43%

MET	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	VAL	VAL	PRO	ARG	GLY	SER	HIS	HIS	MET	SER	ALA	SER	THR	ARG	SER	THR	LEU	PRO	PRO	GLU	ILE	ALA	ALA	GLU	SER	VAL	VAL	SER	MET	LEU	ILE	GLU	GLY	GLY	GLN	GLY	ASP	VAL	ARG	ARG	ALA
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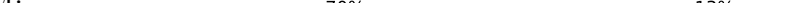
PHE	GLU	ALA	GLN	ASP	GLY	THR	LEU	VAL	SER	ASN	ARG	GLY	GLU	GLY	THR	MET	VAL	SER	ALA	ALA	GLY	PRO	LYS	ARG	THR	ARG	LYS	SER	VAL	ALA	ALA	LYS	PRO	ALA	LYS	THR	ALA	ALA	VAL	VAL	ALA	ALA	LYS
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[illegible]

LYS	GLU	ASP	GLY	GLU	LEU	LEU	GLU	ASP	GLU	ALA	THR	GLU	GLU	PRO	LYS	ALA	ALA	THR	GLU	GLU	PRO	PRO	GLY	GLY	THR	GLU	ASN	ALA	GLY	PHE	VAL	LEU	SER	ASP	GLU	ASP	GLU	ASP	ASP	ASP	ALA	ALA	PRO	ALA	ALA	GLN	GLN	VAL	ALA	ALA	ALA	ALA	GLY	A210	V215	N229	A230	E231	Q232	E233	T240
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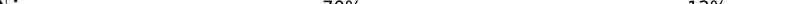
K275	L279	E280	L283	R284	V287	L301	D302	L303	L309	G310	L311	Q345	T348	H354	K355	V358	T359	K360	K361	L362	V365	E391	V396	E402	T408	D413	S416	D424	V428	D432	S435	V457	S458	Q462
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D466	G467	Q468	P469	K470	T471	L472	D473	R485	I486	R487	Q488	I489	E490	S491	K492	T493	M494	S495	L510	ASP
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- Chain M: 

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	MET	THR	THR	ALA	GLY	P6	G9	R10	R11	R16	A22	E27	E28	F29	R30	H36	D37	M38	L39	K40	H41	K42	G43	D44	A45	L48	V51	Y52	L55	Q56	S57
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D60	A61	V66	Y76	R77	D83	H84	H85	A92	C93	P102	A113	E114	V118	M119	H122	T123	T129	C130	A131	D132	C133	A134	C135	A136	SER	GLY	GLY
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- Chain N: 

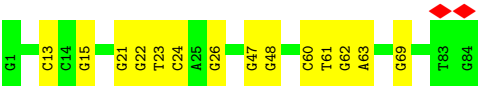
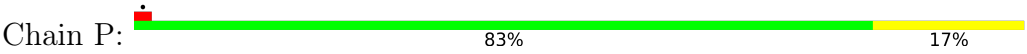
MET	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	HIS	THR	THR	ALA	GLY	P6	Q15	E27	E28	F29	R30	L35	M38	G43	L55	R68	G72	Y76	R77	R78	C79	S80	T81	G82	D83	H84	H85	E98
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acids: Y, I, E, I, T, C, A, D, C, A, G, A, S, R, G, G. The 'Y' and 'I' positions show high information content, with 'Y' being the most conserved. The 'T', 'C', 'A', 'D', 'C', 'A', 'G', and 'A' positions also show significant conservation. The 'S', 'R', 'G', and 'G' positions show very low information content.

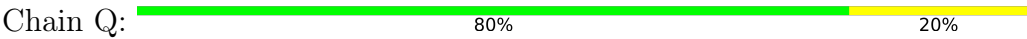
- 
- WORLDWIDE
PDB
PROTEIN DATA BANK



● Molecule 8: DNA (84-MER)



● Molecule 9: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21494	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.751	Depositor
Minimum map value	-1.584	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.24	0/1768	0.48	0/2400
1	B	0.20	0/1818	0.44	0/2467
2	C	0.23	0/8848	0.46	4/11982 (0.0%)
3	D	0.21	0/9998	0.46	3/13490 (0.0%)
4	E	0.18	0/607	0.39	0/826
5	F	0.22	0/2431	0.49	3/3277 (0.1%)
6	M	0.18	0/1001	0.35	0/1355
6	N	0.10	0/1001	0.25	0/1355
7	O	0.30	0/1920	0.56	0/2959
8	P	0.30	0/1940	0.52	0/2994
9	Q	0.40	0/121	0.71	0/188
All	All	0.23	0/31453	0.47	10/43293 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	286	GLY	N-CA-C	7.55	125.54	111.80
2	C	1036	MET	N-CA-C	7.19	118.91	111.14
3	D	134	TYR	N-CA-C	6.74	119.65	110.55
3	D	130	TYR	N-CA-C	-6.60	100.07	109.96
2	C	872	ALA	N-CA-C	5.49	117.44	108.55
5	F	408	THR	CA-C-N	-5.39	113.60	120.23
5	F	408	THR	C-N-CA	-5.39	113.60	120.23
5	F	416	SER	CB-CA-C	-5.37	110.40	116.63
2	C	742	GLU	N-CA-C	5.15	117.24	109.41
2	C	153	THR	N-CA-C	5.07	117.16	108.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1742	0	1796	24	0
1	B	1792	0	1841	23	0
2	C	8692	0	8632	143	0
3	D	9846	0	10017	158	0
4	E	597	0	604	10	0
5	F	2396	0	2453	35	0
6	M	984	0	947	14	0
6	N	984	0	947	13	0
7	O	1714	0	940	7	0
8	P	1729	0	940	17	0
9	Q	108	0	55	0	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
11	M	3	0	0	0	0
11	N	3	0	0	0	0
All	All	30593	0	29172	401	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 7.

All (401) 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)
2:C:140:VAL:HG21	2:C:404:ILE:HD11	1.57	0.87
2:C:912:MET:SD	3:D:811:GLN:NE2	2.50	0.84
2:C:364:ILE:HD11	2:C:492:ILE:HD12	1.64	0.78
2:C:572:MET:HE1	3:D:845:PHE:HB2	1.67	0.77
1:B:55:ARG:NH1	1:B:56:ILE:O	2.18	0.77
3:D:502:PRO:HG3	8:P:15:DG:H22	1.51	0.74
3:D:665:ARG:NE	3:D:680:ASP:O	2.21	0.74
3:D:579:GLN:OE1	3:D:803:ARG:NH1	2.21	0.73
2:C:549:ARG:NH2	2:C:555:ASP:OD2	2.21	0.73
2:C:841:ARG:NH2	2:C:848:PRO:O	2.22	0.72
3:D:751:VAL:HG11	3:D:768:GLU:OE2	1.88	0.72
4:E:10:GLY:N	4:E:13:ASN:OD1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:LEU:HD13	2:C:214:ILE:HD13	1.71	0.72
6:M:27:GLU:O	6:M:77:ARG:NE	2.22	0.72
2:C:1072:GLU:OE2	3:D:547:LEU:N	2.23	0.72
3:D:76:GLU:OE2	3:D:76:GLU:N	2.23	0.72
6:N:78:ARG:NH1	6:N:79:CYS:O	2.23	0.72
6:N:15:GLN:NE2	7:O:11:DG:OP2	2.24	0.70
2:C:765:GLU:N	2:C:765:GLU:OE1	2.24	0.70
2:C:771:ASP:N	2:C:775:ILE:O	2.23	0.70
3:D:1048:VAL:O	3:D:1085:GLY:N	2.25	0.70
2:C:1029:ARG:NH1	2:C:1048:PHE:O	2.25	0.70
6:N:77:ARG:NH1	6:N:79:CYS:SG	2.65	0.69
2:C:339:THR:OG1	2:C:340:GLU:OE1	2.11	0.69
2:C:800:LEU:HD12	2:C:804:GLU:OE1	1.92	0.69
3:D:357:LEU:HD21	5:F:309:LEU:HD21	1.74	0.69
4:E:65:GLU:OE1	4:E:65:GLU:N	2.26	0.68
2:C:617:GLU:OE1	2:C:617:GLU:N	2.27	0.67
3:D:143:ARG:NH1	3:D:250:THR:O	2.28	0.67
2:C:924:TRP:HZ3	2:C:977:THR:HG21	1.60	0.67
5:F:301:LEU:HA	5:F:304:ILE:HD12	1.77	0.67
2:C:256:GLN:N	2:C:256:GLN:OE1	2.29	0.66
3:D:920:LEU:HG	3:D:938:LEU:HD21	1.77	0.66
3:D:923:ASP:OD1	3:D:934:ALA:N	2.28	0.66
2:C:33:GLU:OE1	2:C:33:GLU:N	2.29	0.66
2:C:161:ARG:NH2	2:C:423:SER:O	2.29	0.66
2:C:364:ILE:CD1	2:C:492:ILE:HD12	2.27	0.65
3:D:963:GLU:OE2	3:D:965:GLN:NE2	2.30	0.64
2:C:1079:ASP:OD2	3:D:420:LYS:NZ	2.28	0.64
3:D:345:ARG:NH2	5:F:348:THR:O	2.31	0.64
3:D:973:TYR:O	3:D:1135:LYS:NZ	2.20	0.64
2:C:822:SER:O	2:C:824:LYS:NZ	2.31	0.64
3:D:173:ARG:NE	3:D:208:LEU:HD23	2.12	0.64
3:D:96:GLU:O	3:D:351:ASN:ND2	2.31	0.63
2:C:724:SER:OG	2:C:890:MET:SD	2.53	0.63
2:C:432:LEU:HB2	2:C:699:MET:HE3	1.80	0.63
6:N:28:GLU:OE1	6:N:30:ARG:NH2	2.32	0.62
1:B:224:GLU:N	1:B:224:GLU:OE1	2.32	0.62
2:C:358:HIS:NE2	2:C:519:ALA:O	2.31	0.62
3:D:502:PRO:HB3	8:P:15:DG:N2	2.14	0.61
2:C:453:ARG:HA	7:O:71:DG:H1'	1.81	0.61
2:C:523:ASP:OD2	2:C:550:ARG:NE	2.33	0.61
2:C:1128:MET:N	2:C:1128:MET:HE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:508:GLY:N	2:C:560:ASP:OD1	2.34	0.60
5:F:472:LEU:HD12	8:P:48:DG:OP2	2.00	0.60
1:A:152:ASN:ND2	1:A:152:ASN:O	2.33	0.60
3:D:587:PHE:O	3:D:622:GLN:NE2	2.33	0.60
4:E:36:ARG:NE	4:E:74:GLU:OE1	2.35	0.60
3:D:671:LEU:HD21	3:D:714:ALA:CB	2.31	0.60
1:B:108:ALA:N	1:B:121:PRO:O	2.35	0.60
2:C:196:ARG:HB3	2:C:295:ASP:HB3	1.82	0.60
3:D:1044:ALA:HA	3:D:1090:VAL:HG12	1.84	0.60
2:C:980:ASN:OD1	2:C:981:ARG:N	2.34	0.60
3:D:1189:GLN:OE1	3:D:1191:MET:HE3	2.01	0.60
2:C:608:GLU:OE2	2:C:609:SER:N	2.35	0.60
2:C:1077:LYS:NZ	3:D:545:LEU:O	2.25	0.60
2:C:1116:LEU:HD13	3:D:105:TRP:CH2	2.37	0.60
2:C:716:ASN:O	2:C:904:ASN:ND2	2.35	0.59
3:D:1189:GLN:NE2	3:D:1190:LEU:O	2.35	0.59
3:D:884:GLU:OE2	3:D:884:GLU:N	2.32	0.59
2:C:952:GLU:OE1	2:C:952:GLU:N	2.35	0.59
2:C:650:ASP:OD1	2:C:651:GLY:N	2.35	0.59
3:D:618:ASP:OD1	3:D:619:LEU:N	2.36	0.59
6:M:55:LEU:HD13	6:M:76:TYR:HE2	1.66	0.59
3:D:1029:LEU:HD12	3:D:1117:LEU:HD23	1.85	0.59
2:C:23:ILE:O	2:C:958:ALA:N	2.36	0.59
6:M:28:GLU:OE2	6:M:30:ARG:NH2	2.36	0.59
2:C:444:LEU:HD21	2:C:482:LEU:HD13	1.83	0.58
2:C:631:GLU:N	2:C:631:GLU:OE1	2.36	0.58
3:D:586:PHE:O	3:D:590:THR:OG1	2.21	0.58
3:D:671:LEU:HD21	3:D:714:ALA:HB3	1.84	0.58
3:D:493:GLU:OE2	4:E:10:GLY:N	2.37	0.58
3:D:527:LEU:HD21	3:D:712:LYS:HB2	1.84	0.58
1:B:154:GLN:N	1:B:154:GLN:OE1	2.37	0.58
7:O:72:DG:H1	8:P:13:DC:H42	1.52	0.57
2:C:992:LYS:NZ	3:D:725:THR:OG1	2.36	0.57
2:C:173:VAL:HG12	2:C:192:ILE:HG22	1.87	0.57
2:C:341:THR:N	2:C:348:GLU:OE2	2.36	0.57
2:C:882:SER:OG	3:D:432:VAL:O	2.22	0.57
3:D:626:ASP:OD1	3:D:627:ILE:N	2.38	0.57
6:N:27:GLU:OE1	6:N:77:ARG:NH2	2.37	0.57
2:C:731:ASP:OD1	2:C:864:LYS:NZ	2.27	0.57
3:D:525:HIS:CE1	3:D:527:LEU:HD23	2.40	0.57
3:D:238:GLU:OE1	3:D:238:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1036:MET:HB3	5:F:424:ASP:HB3	1.87	0.56
3:D:502:PRO:CG	8:P:15:DG:H22	2.18	0.56
5:F:359:ILE:HD13	5:F:396:VAL:HG12	1.87	0.56
3:D:487:LEU:HD22	3:D:516:LEU:HD11	1.88	0.56
2:C:949:ASP:OD1	2:C:950:LYS:N	2.39	0.55
3:D:1058:LYS:NZ	3:D:1059:ILE:O	2.40	0.55
2:C:352:GLU:N	2:C:352:GLU:OE1	2.40	0.55
2:C:671:ASN:OD1	2:C:672:GLN:N	2.39	0.55
2:C:942:ARG:NH2	2:C:969:GLU:OE2	2.40	0.55
6:M:123:THR:OG1	6:N:125:GLU:O	2.25	0.55
3:D:502:PRO:CB	8:P:15:DG:N2	2.69	0.55
5:F:229:ASN:O	5:F:232:GLN:N	2.40	0.55
8:P:21:DG:H2'	8:P:22:DG:C8	2.41	0.55
2:C:430:ASN:HD22	2:C:701:LEU:HD22	1.72	0.54
2:C:472:ILE:CD1	2:C:577:THR:HG21	2.37	0.54
1:A:79:ASN:O	1:A:82:GLN:NE2	2.40	0.54
3:D:770:ILE:HD12	3:D:826:THR:HG21	1.88	0.54
3:D:1261:ALA:HB2	4:E:79:LEU:HD21	1.88	0.54
5:F:354:HIS:O	5:F:358:VAL:HG23	2.07	0.54
1:A:184:GLU:OE2	1:A:184:GLU:N	2.35	0.54
1:A:200:GLN:OE1	1:A:200:GLN:N	2.41	0.54
3:D:277:LEU:HD21	3:D:295:ARG:HE	1.72	0.54
2:C:212:VAL:O	2:C:213:ARG:NE	2.40	0.54
1:A:154:GLN:OE1	1:A:154:GLN:N	2.40	0.54
3:D:1060:VAL:HG13	3:D:1069:GLU:OE2	2.08	0.54
3:D:938:LEU:HD22	3:D:942:LEU:HD22	1.91	0.53
6:M:66:VAL:HG12	6:M:76:TYR:CE1	2.43	0.53
2:C:888:GLU:OE2	2:C:888:GLU:N	2.40	0.53
1:A:170:PRO:O	1:A:198:THR:OG1	2.21	0.53
2:C:209:MET:SD	2:C:252:LYS:NZ	2.77	0.53
6:N:81:THR:OG1	6:N:98:GLU:OE1	2.27	0.53
2:C:138:GLN:NE2	2:C:139:THR:O	2.41	0.53
5:F:413:ASP:O	5:F:416:SER:OG	2.20	0.53
3:D:349:ASN:ND2	5:F:345:GLN:OE1	2.41	0.52
3:D:434:PRO:O	3:D:712:LYS:NZ	2.32	0.52
3:D:763:GLU:O	3:D:766:THR:OG1	2.22	0.52
3:D:1256:GLU:OE1	3:D:1256:GLU:N	2.43	0.52
4:E:32:TYR:CE2	4:E:75:ILE:HD12	2.44	0.52
6:N:83:ASP:O	6:N:85:HIS:ND1	2.42	0.52
5:F:215:VAL:HG22	5:F:301:LEU:HB2	1.92	0.52
2:C:472:ILE:HD13	2:C:577:THR:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:GLU:N	2:C:203:GLU:OE1	2.43	0.51
3:D:128:VAL:HG21	3:D:135:MET:SD	2.50	0.51
2:C:85:GLU:O	2:C:387:ARG:NH1	2.43	0.51
2:C:461:VAL:HG23	3:D:852:ARG:HD2	1.92	0.51
6:M:83:ASP:O	6:M:85:HIS:ND1	2.37	0.51
1:A:69:VAL:HG13	1:A:128:LEU:HD23	1.92	0.51
2:C:579:MET:O	2:C:614:THR:OG1	2.20	0.51
5:F:459:SER:O	5:F:463:GLY:N	2.43	0.51
2:C:237:LEU:O	2:C:241:GLY:N	2.43	0.51
2:C:469:MET:HE3	2:C:484:GLY:HA3	1.91	0.51
3:D:809:MET:HA	3:D:812:ILE:HG22	1.91	0.51
2:C:175:PHE:CE1	2:C:190:ALA:HB2	2.46	0.51
5:F:485:ARG:HB2	7:O:34:DT:H71	1.92	0.51
3:D:879:VAL:O	3:D:879:VAL:HG13	2.11	0.51
2:C:872:ALA:HB3	2:C:1018:LEU:HD11	1.93	0.50
1:B:158:GLU:OE1	1:B:158:GLU:N	2.44	0.50
8:P:62:DG:H2''	8:P:63:DA:C8	2.46	0.50
3:D:888:THR:OG1	3:D:889:GLU:N	2.44	0.50
2:C:213:ARG:NH2	2:C:218:ARG:O	2.40	0.50
3:D:576:MET:HE2	3:D:688:LEU:CD2	2.41	0.50
5:F:490:GLU:O	5:F:493:THR:OG1	2.28	0.50
2:C:156:ILE:HD13	2:C:417:PHE:HB3	1.94	0.50
4:E:9:GLU:N	4:E:9:GLU:OE1	2.45	0.50
2:C:676:VAL:HG21	2:C:688:LEU:CD1	2.42	0.50
3:D:210:ASP:O	3:D:213:GLN:NE2	2.44	0.49
1:A:186:ARG:HG3	1:B:150:VAL:HG21	1.93	0.49
3:D:644:ARG:HE	3:D:645:GLU:H	1.60	0.49
2:C:330:TYR:CZ	2:C:351:VAL:HG23	2.46	0.49
2:C:1064:TYR:OH	3:D:506:ARG:O	2.20	0.49
5:F:391:GLU:OE1	5:F:391:GLU:N	2.45	0.49
5:F:457:VAL:HB	5:F:486:ILE:HD11	1.94	0.49
1:B:60:LEU:HD22	1:B:159:ILE:HD13	1.93	0.49
2:C:408:PRO:HG3	8:P:26:DG:H8	1.76	0.49
3:D:93:GLY:C	3:D:319:VAL:HG22	2.37	0.49
1:B:39:ARG:O	1:B:43:LEU:HD23	2.12	0.49
2:C:530:ALA:HB2	2:C:566:ASP:HB2	1.94	0.49
3:D:588:LEU:HD21	3:D:664:GLY:O	2.12	0.49
3:D:976:SER:HB2	3:D:983:VAL:HG12	1.93	0.49
6:M:22:ALA:HB1	6:M:38:MET:HE3	1.94	0.49
6:M:55:LEU:HD13	6:M:76:TYR:CE2	2.45	0.49
3:D:278:ARG:HH21	3:D:296:LEU:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:OG1	1:A:65:THR:N	2.46	0.48
1:A:207:ALA:O	1:A:210:SER:OG	2.27	0.48
1:B:69:VAL:HG22	1:B:128:LEU:CD1	2.43	0.48
3:D:576:MET:HE3	3:D:577:PRO:O	2.13	0.48
3:D:876:SER:O	3:D:879:VAL:HG12	2.12	0.48
6:N:55:LEU:HD21	6:N:76:TYR:CD1	2.47	0.48
6:N:68:ARG:NH2	6:N:72:GLY:O	2.46	0.48
3:D:89:ARG:N	3:D:323:ASP:OD2	2.46	0.48
2:C:808:ARG:O	2:C:812:GLY:N	2.47	0.48
2:C:1106:PHE:CZ	3:D:10:LEU:HD21	2.48	0.48
3:D:107:PHE:HB3	3:D:108:LYS:HZ2	1.79	0.48
3:D:334:ARG:NH2	5:F:402:GLU:O	2.47	0.48
3:D:807:MET:SD	3:D:807:MET:N	2.86	0.48
1:B:39:ARG:NE	1:B:174:VAL:O	2.47	0.48
3:D:1203:TRP:NE1	3:D:1226:ASP:HB2	2.29	0.48
3:D:1233:GLU:OE1	3:D:1233:GLU:N	2.41	0.48
2:C:633:ALA:N	2:C:684:GLU:OE2	2.47	0.48
3:D:1218:ASP:HA	3:D:1221:ILE:HG22	1.95	0.48
2:C:262:LEU:HD21	2:C:280:ALA:HB3	1.94	0.48
2:C:723:LEU:HD23	2:C:881:ILE:HD12	1.96	0.48
2:C:959:THR:HG23	2:C:959:THR:O	2.14	0.48
3:D:501:ALA:HB3	3:D:502:PRO:HD3	1.96	0.48
2:C:286:ASN:HA	2:C:290:ASN:HB2	1.96	0.48
2:C:493:ASN:N	2:C:497:PHE:O	2.40	0.48
2:C:914:PRO:O	2:C:917:VAL:HG12	2.14	0.48
3:D:1203:TRP:CD1	3:D:1226:ASP:HB2	2.49	0.48
5:F:279:LEU:HD23	5:F:311:LEU:HD22	1.96	0.48
5:F:488:GLN:O	5:F:491:SER:OG	2.30	0.48
2:C:160:GLU:O	2:C:426:MET:HB3	2.14	0.47
2:C:641:ALA:HB1	2:C:660:LYS:NZ	2.29	0.47
2:C:91:MET:SD	2:C:92:SER:N	2.87	0.47
2:C:505:VAL:HG11	2:C:562:VAL:HG23	1.96	0.47
3:D:596:SER:O	3:D:598:LYS:N	2.47	0.47
3:D:1089:GLU:N	3:D:1089:GLU:OE1	2.46	0.47
1:B:42:LEU:HD23	1:B:171:VAL:HG21	1.96	0.47
3:D:27:GLU:N	3:D:51:ILE:HD12	2.30	0.47
3:D:740:ILE:HD12	3:D:779:GLU:OE1	2.15	0.47
4:E:32:TYR:CZ	4:E:75:ILE:HD12	2.49	0.47
8:P:62:DG:H2"	8:P:63:DA:N7	2.30	0.47
1:A:52:THR:OG1	1:A:152:ASN:OD1	2.26	0.47
2:C:707:VAL:HG21	2:C:903:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:506:ARG:N	3:D:995:GLN:OE1	2.48	0.47
3:D:1162:GLU:N	3:D:1162:GLU:OE1	2.48	0.47
3:D:1172:GLU:OE1	3:D:1175:ARG:NH1	2.47	0.47
7:O:71:DG:OP1	7:O:72:DG:P	2.72	0.47
2:C:330:TYR:CE1	2:C:351:VAL:HG23	2.50	0.47
2:C:767:LEU:HD12	2:C:767:LEU:O	2.14	0.47
3:D:304:GLN:NE2	3:D:305:THR:HG23	2.29	0.47
2:C:25:PHE:HD2	2:C:965:ALA:HB2	1.79	0.47
3:D:498:LEU:HB3	3:D:541:MET:HE3	1.97	0.47
3:D:830:PRO:O	3:D:832:LYS:NZ	2.40	0.47
8:P:60:DC:H2'	8:P:61:DT:H72	1.97	0.47
2:C:200:LEU:HD12	2:C:213:ARG:O	2.15	0.46
2:C:468:ARG:HG2	2:C:498:ILE:HB	1.97	0.46
1:B:69:VAL:HG22	1:B:128:LEU:HD13	1.97	0.46
2:C:388:GLU:O	2:C:391:THR:OG1	2.32	0.46
1:B:39:ARG:HE	1:B:43:LEU:HD21	1.79	0.46
1:B:137:GLU:OE1	1:B:137:GLU:N	2.49	0.46
2:C:209:MET:SD	2:C:249:THR:HG22	2.56	0.46
1:A:214:THR:O	1:A:218:LEU:HD23	2.16	0.46
2:C:1047:GLN:N	2:C:1047:GLN:OE1	2.49	0.46
3:D:142:GLU:OE1	3:D:142:GLU:N	2.43	0.46
3:D:674:GLU:N	3:D:674:GLU:OE1	2.44	0.46
2:C:86:ASP:OD2	2:C:88:SER:OG	2.34	0.46
2:C:636:VAL:HG11	2:C:639:VAL:HG13	1.98	0.46
1:A:148:SER:OG	1:A:151:GLN:OE1	2.34	0.46
2:C:265:ILE:O	2:C:269:LEU:HD23	2.16	0.46
5:F:355:MET:HE1	5:F:396:VAL:HG22	1.96	0.46
2:C:140:VAL:CG2	2:C:404:ILE:HD11	2.35	0.46
2:C:917:VAL:HA	2:C:920:ILE:HG22	1.97	0.46
2:C:1108:VAL:HG13	3:D:324:LEU:HD22	1.97	0.46
5:F:466:ASP:OD1	5:F:470:LYS:NZ	2.49	0.46
1:A:62:GLU:OE1	1:A:62:GLU:N	2.39	0.45
1:A:85:VAL:HG12	1:A:118:VAL:HG22	1.97	0.45
3:D:502:PRO:CB	8:P:15:DG:H22	2.30	0.45
5:F:280:GLU:HA	5:F:283:LEU:HG	1.96	0.45
6:M:27:GLU:OE1	6:M:27:GLU:N	2.48	0.45
2:C:932:VAL:HG13	2:C:935:LEU:HD22	1.98	0.45
2:C:1095:GLU:OE2	2:C:1095:GLU:HA	2.17	0.45
3:D:751:VAL:HG11	3:D:768:GLU:CD	2.42	0.45
1:A:221:LEU:O	1:A:225:LEU:HD13	2.15	0.45
2:C:176:ASP:OD1	2:C:177:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:938:GLU:OE2	2:C:942:ARG:NE	2.50	0.45
1:B:5:GLN:CD	1:B:183:VAL:HG11	2.42	0.45
4:E:60:ASP:OD1	4:E:60:ASP:N	2.48	0.45
6:N:35:LEU:HD12	6:N:38:MET:HE3	1.98	0.45
2:C:648:ASN:ND2	2:C:650:ASP:OD2	2.46	0.45
3:D:116:TYR:HB2	3:D:295:ARG:HG2	1.99	0.45
3:D:293:LEU:HG	3:D:1159:LEU:HD12	1.98	0.45
3:D:894:LEU:HD13	3:D:956:THR:OG1	2.17	0.45
2:C:776:ILE:HG21	2:C:788:LEU:CD1	2.46	0.45
2:C:516:TYR:C	2:C:517:LEU:HD12	2.41	0.45
3:D:320:ILE:O	3:D:325:ARG:NH2	2.49	0.45
1:B:203:ARG:HD3	1:B:205:ARG:HE	1.83	0.45
3:D:1153:SER:OG	3:D:1158:LEU:O	2.28	0.45
5:F:492:LYS:O	5:F:495:SER:OG	2.23	0.45
3:D:180:ASP:OD1	3:D:181:LEU:N	2.49	0.44
5:F:428:VAL:O	5:F:428:VAL:HG23	2.17	0.44
6:M:36:HIS:HA	6:M:39:LEU:HG	1.98	0.44
2:C:86:ASP:OD1	2:C:89:GLY:N	2.50	0.44
2:C:173:VAL:HG23	2:C:307:LYS:HG2	1.99	0.44
3:D:58:TRP:CE3	3:D:68:VAL:HG22	2.52	0.44
2:C:1116:LEU:HD21	3:D:402:LEU:HD12	2.00	0.44
3:D:20:ILE:HD13	3:D:316:CYS:O	2.17	0.44
3:D:170:LEU:HD12	3:D:173:ARG:NH2	2.33	0.44
5:F:466:ASP:OD2	5:F:468:GLN:NE2	2.50	0.44
1:A:176:TYR:HB2	1:A:192:LEU:HD11	1.98	0.44
2:C:1056:MET:HA	2:C:1056:MET:HE3	1.99	0.44
3:D:356:ARG:NE	3:D:356:ARG:O	2.50	0.44
3:D:583:LEU:HD21	3:D:724:VAL:HG11	1.99	0.44
3:D:915:VAL:HG23	3:D:956:THR:HG21	1.99	0.44
2:C:155:VAL:HG22	2:C:160:GLU:OE2	2.17	0.44
3:D:663:LEU:O	3:D:667:LEU:HD23	2.18	0.44
3:D:1074:ILE:HD12	3:D:1078:ALA:HB2	2.00	0.44
3:D:67:ARG:HD3	3:D:67:ARG:HA	1.86	0.44
2:C:232:THR:OG1	2:C:234:GLU:OE1	2.23	0.44
2:C:974:LEU:HD22	2:C:989:PRO:HA	2.00	0.44
5:F:472:LEU:HD13	5:F:487:ARG:HB2	2.00	0.44
1:B:30:PHE:O	1:B:33:THR:OG1	2.33	0.43
2:C:1104:GLU:OE2	2:C:1105:SER:OG	2.36	0.43
3:D:1051:GLU:N	3:D:1051:GLU:OE1	2.51	0.43
5:F:284:ARG:O	5:F:287:VAL:HG12	2.18	0.43
1:A:29:GLY:O	1:B:40:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:ASN:OD1	2:C:131:GLU:N	2.51	0.43
3:D:353:ARG:O	3:D:357:LEU:HD23	2.18	0.43
2:C:210:VAL:HG12	2:C:249:THR:HG21	1.99	0.43
3:D:337:THR:HG23	3:D:341:ASN:HD22	1.84	0.43
3:D:468:ASN:O	3:D:471:SER:OG	2.29	0.43
5:F:486:ILE:HD12	5:F:489:ILE:HD11	2.00	0.43
3:D:133:ALA:C	3:D:256:MET:HE1	2.44	0.43
3:D:920:LEU:CG	3:D:938:LEU:HD21	2.44	0.43
6:M:48:LEU:O	6:M:51:VAL:HG22	2.19	0.43
3:D:155:VAL:HG21	3:D:223:TRP:CH2	2.54	0.43
6:M:122:HIS:HA	6:N:126:ILE:HG22	1.99	0.43
2:C:37:LEU:O	2:C:439:ARG:NE	2.52	0.43
1:B:16:GLU:OE1	1:B:16:GLU:N	2.44	0.43
3:D:151:LEU:HD13	3:D:223:TRP:HH2	1.83	0.43
3:D:583:LEU:HD11	3:D:724:VAL:HG11	2.01	0.43
1:B:5:GLN:OE1	1:B:183:VAL:HG11	2.19	0.43
2:C:943:LEU:O	2:C:947:GLY:N	2.51	0.43
3:D:592:SER:OG	3:D:593:GLU:N	2.52	0.43
3:D:999:GLU:HG3	3:D:1000:PRO:HD3	2.01	0.43
2:C:171:PRO:HB2	2:C:300:GLY:HA3	2.00	0.43
2:C:574:SER:OG	2:C:575:VAL:N	2.52	0.43
2:C:627:VAL:CG2	2:C:687:VAL:HG13	2.49	0.43
2:C:1097:ILE:HD13	3:D:548:SER:HA	2.01	0.43
3:D:911:VAL:HG22	3:D:915:VAL:HG12	2.01	0.43
3:D:1206:ALA:HB3	3:D:1215:VAL:HG21	2.00	0.43
8:P:60:DC:C2'	8:P:61:DT:H72	2.49	0.43
2:C:690:ASP:OD2	2:C:696:ASN:N	2.49	0.42
3:D:959:ILE:HD11	3:D:968:THR:HG21	2.00	0.42
1:A:80:ILE:HG21	1:A:136:MET:HE1	2.00	0.42
3:D:296:LEU:HD23	3:D:296:LEU:HA	1.91	0.42
3:D:621:LEU:HD11	3:D:664:GLY:CA	2.49	0.42
5:F:240:ILE:HD12	5:F:275:LYS:HD3	2.01	0.42
3:D:893:LYS:C	3:D:894:LEU:HD12	2.43	0.42
3:D:1158:LEU:H	3:D:1158:LEU:HD23	1.85	0.42
2:C:174:TYR:HE1	2:C:303:LYS:HE3	1.83	0.42
2:C:202:MET:HE1	2:C:222:VAL:HG22	2.00	0.42
3:D:763:GLU:OE2	3:D:767:GLN:NE2	2.52	0.42
4:E:17:ASP:OD1	4:E:18:GLU:N	2.51	0.42
2:C:276:THR:HB	2:C:279:ALA:HB3	2.02	0.42
3:D:738:LYS:O	3:D:741:VAL:HG12	2.19	0.42
5:F:360:ASN:OD1	5:F:361:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:473:ASP:OD2	8:P:47:DG:OP2	2.37	0.42
2:C:1030:SER:OG	2:C:1031:THR:N	2.53	0.42
3:D:249:GLY:O	3:D:250:THR:OG1	2.26	0.42
6:M:11:ARG:O	6:M:16:ARG:NH2	2.53	0.42
1:B:211:ALA:O	1:B:214:THR:OG1	2.29	0.42
2:C:245:SER:O	2:C:249:THR:HG23	2.20	0.42
2:C:333:LYS:HE2	2:C:341:THR:HG21	2.01	0.42
2:C:604:LEU:HD23	2:C:604:LEU:H	1.85	0.42
1:A:97:LEU:HB2	1:A:110:ILE:HG13	2.01	0.42
5:F:432:ASP:O	5:F:435:SER:OG	2.26	0.42
2:C:120:PRO:O	2:C:121:LEU:HD22	2.19	0.42
3:D:176:LYS:NZ	3:D:204:GLU:OE1	2.31	0.42
3:D:671:LEU:HD23	3:D:711:LEU:HA	2.00	0.42
3:D:868:LEU:O	3:D:872:LEU:HD23	2.20	0.42
1:A:54:ILE:HD11	1:A:162:ILE:HD11	2.02	0.41
3:D:846:ILE:O	3:D:849:HIS:HB2	2.20	0.41
3:D:1121:VAL:HG11	3:D:1137:ILE:HD12	2.02	0.41
7:O:71:DG:H2'	7:O:71:DG:N3	2.34	0.41
2:C:1116:LEU:CD2	3:D:402:LEU:HD12	2.50	0.41
3:D:735:ASP:O	3:D:738:LYS:NZ	2.53	0.41
2:C:1106:PHE:HZ	3:D:10:LEU:HD21	1.85	0.41
3:D:810:ARG:O	3:D:814:GLY:N	2.53	0.41
6:M:52:TYR:O	6:M:55:LEU:HG	2.21	0.41
6:N:35:LEU:HD12	6:N:38:MET:CE	2.50	0.41
1:A:172:LEU:HD21	1:A:199:LYS:HG2	2.01	0.41
2:C:757:ARG:NH2	2:C:768:ALA:O	2.53	0.41
5:F:362:LEU:HA	5:F:365:VAL:HG22	2.02	0.41
2:C:52:ASP:OD1	2:C:53:ALA:N	2.54	0.41
2:C:644:ILE:HG22	2:C:658:LEU:HD11	2.02	0.41
1:A:59:VAL:C	1:A:60:LEU:HD22	2.46	0.41
2:C:518:THR:OG1	2:C:519:ALA:N	2.53	0.41
3:D:846:ILE:HD12	3:D:846:ILE:HA	1.85	0.41
3:D:102:THR:HG21	3:D:129:ILE:HD13	2.01	0.41
2:C:880:VAL:HG23	3:D:537:ASP:O	2.21	0.41
3:D:184:LEU:HD22	3:D:197:VAL:HB	2.02	0.41
3:D:288:LYS:HB3	3:D:288:LYS:HE3	1.78	0.41
3:D:768:GLU:OE2	3:D:769:LEU:HG	2.21	0.41
7:O:15:DA:N6	8:P:69:DG:O6	2.54	0.41
8:P:21:DG:H2'	8:P:22:DG:H8	1.84	0.41
1:A:167:ILE:HG13	1:A:167:ILE:O	2.21	0.41
1:B:42:LEU:HD21	1:B:171:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:578:THR:HG21	3:D:685:LYS:HD3	2.03	0.41
3:D:821:ASN:HD22	3:D:821:ASN:HA	1.63	0.41
5:F:230:ALA:HA	5:F:233:GLU:OE2	2.21	0.41
2:C:67:ASP:OD1	2:C:68:VAL:N	2.54	0.40
2:C:1060:ALA:HB3	3:D:509:ILE:HD13	2.03	0.40
3:D:353:ARG:NH1	5:F:302:ASP:OD1	2.54	0.40
2:C:676:VAL:HG21	2:C:688:LEU:HD13	2.02	0.40
3:D:255:SER:OG	3:D:256:MET:N	2.54	0.40
3:D:619:LEU:HD21	3:D:663:LEU:HD13	2.03	0.40
2:C:596:ASN:C	2:C:597:MET:HE2	2.46	0.40
3:D:93:GLY:O	3:D:319:VAL:HG22	2.22	0.40
8:P:23:DT:H2'	8:P:24:DC:C2	2.57	0.40
1:B:187:THR:O	1:B:187:THR:HG22	2.22	0.40
2:C:1039:GLN:O	2:C:1040:GLN:C	2.65	0.40
3:D:184:LEU:HD22	3:D:197:VAL:CG1	2.51	0.40
3:D:305:THR:HG22	3:D:1223:ALA:HB3	2.03	0.40
3:D:868:LEU:HD22	3:D:1023:LEU:HD11	2.03	0.40
3:D:1030:PHE:CE1	3:D:1140:ILE:HG21	2.56	0.40
3:D:1048:VAL:O	3:D:1085:GLY:CA	2.70	0.40
3:D:1081:LEU:H	3:D:1081:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/340 (66%)	215 (96%)	9 (4%)	0	100	100
1	B	231/340 (68%)	224 (97%)	7 (3%)	0	100	100
2	C	1114/1161 (96%)	1064 (96%)	50 (4%)	0	100	100
3	D	1257/1307 (96%)	1207 (96%)	49 (4%)	1 (0%)	48	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	75/90 (83%)	74 (99%)	1 (1%)	0	100	100
5	F	299/531 (56%)	292 (98%)	7 (2%)	0	100	100
6	M	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
6	N	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
All	All	3458/4087 (85%)	3331 (96%)	126 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	132	ALA

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	194/279 (70%)	192 (99%)	2 (1%)	68	76
1	B	199/279 (71%)	198 (100%)	1 (0%)	81	81
2	C	942/979 (96%)	935 (99%)	7 (1%)	76	79
3	D	1054/1095 (96%)	1050 (100%)	4 (0%)	84	83
4	E	64/74 (86%)	64 (100%)	0	100	100
5	F	258/430 (60%)	257 (100%)	1 (0%)	84	83
6	M	99/120 (82%)	99 (100%)	0	100	100
6	N	99/120 (82%)	99 (100%)	0	100	100
All	All	2909/3376 (86%)	2894 (100%)	15 (0%)	78	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	110	ILE
1	B	150	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	153	THR
2	C	173	VAL
2	C	308	LEU
2	C	639	VAL
2	C	743	VAL
2	C	1038	THR
2	C	1109	LEU
3	D	287	GLN
3	D	819	VAL
3	D	821	ASN
3	D	842	LEU
5	F	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	129	ASN
1	B	185	GLN
2	C	665	ASN
2	C	852	ASN
2	C	1051	GLN
3	D	103	HIS
3	D	287	GLN
3	D	368	ASN
3	D	494	HIS
3	D	525	HIS
3	D	540	GLN
3	D	767	GLN
3	D	821	ASN
5	F	282	ASN
5	F	354	HIS
5	F	499	HIS
6	M	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	5	G

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 9 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.

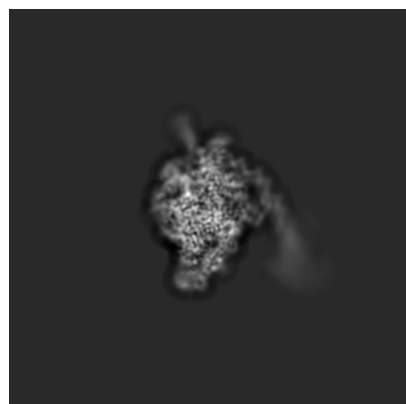
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32077. These allow visual inspection of the internal detail of the map and identification of artifacts.

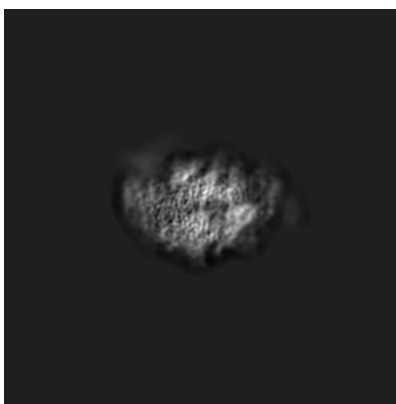
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

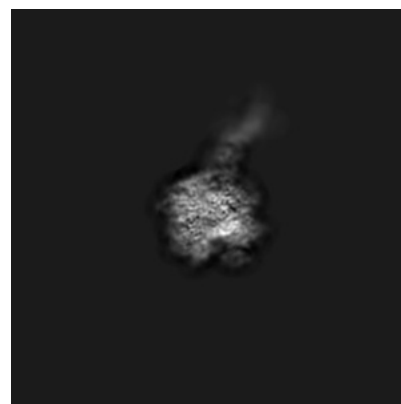
6.1.1 Primary map



X

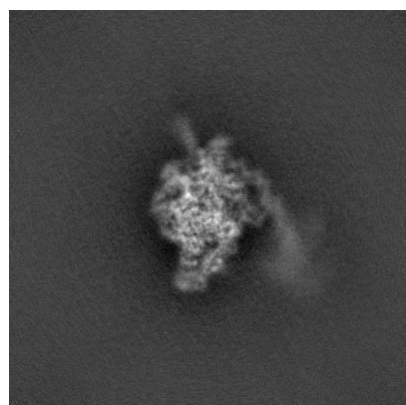


Y

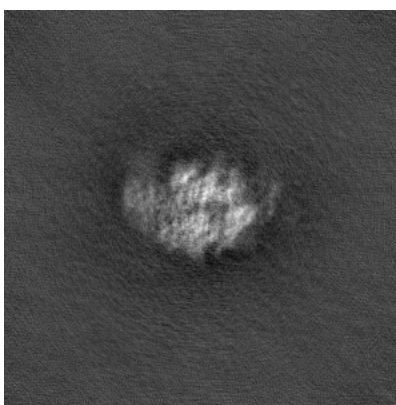


Z

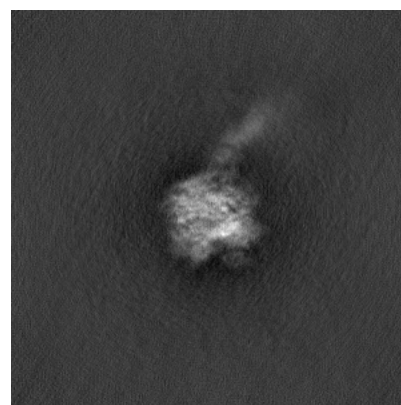
6.1.2 Raw map



X



Y

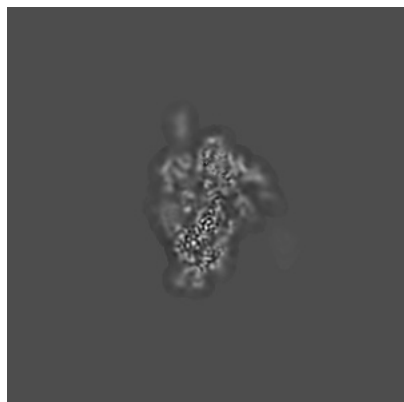


Z

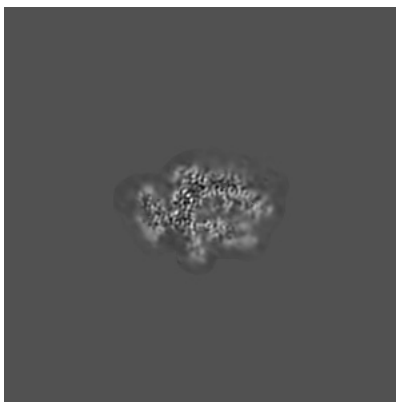
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

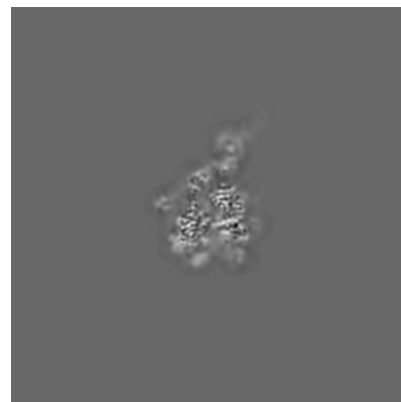
6.2.1 Primary map



X Index: 192

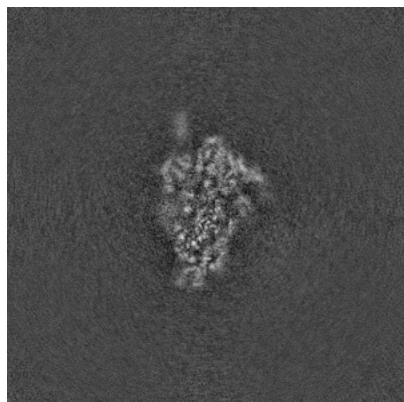


Y Index: 192

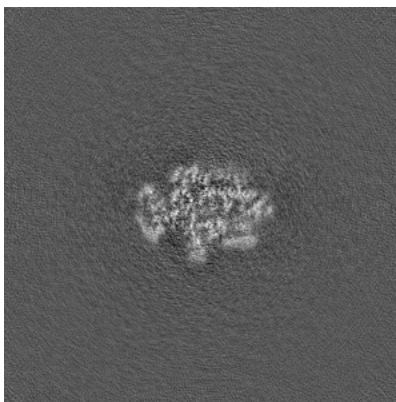


Z Index: 192

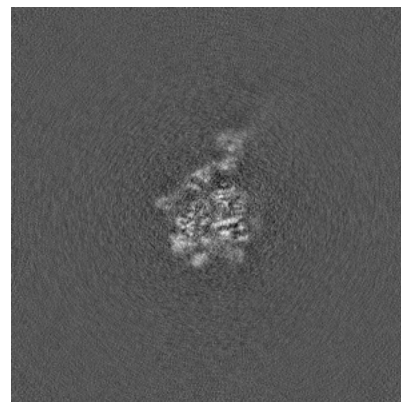
6.2.2 Raw map



X Index: 192



Y Index: 192

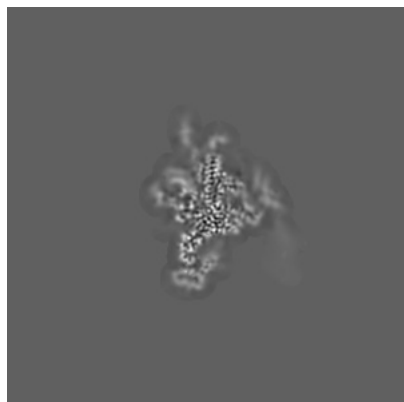


Z Index: 192

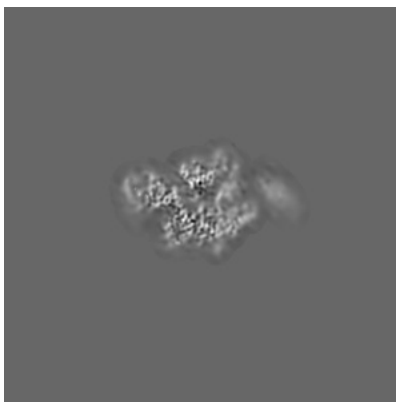
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

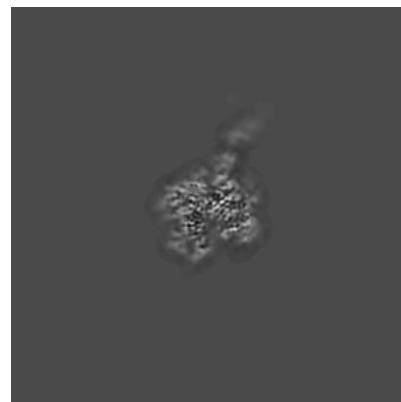
6.3.1 Primary map



X Index: 204

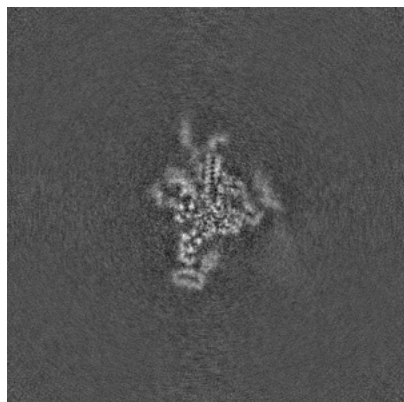


Y Index: 171

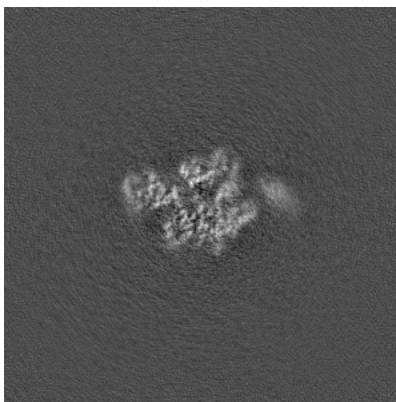


Z Index: 179

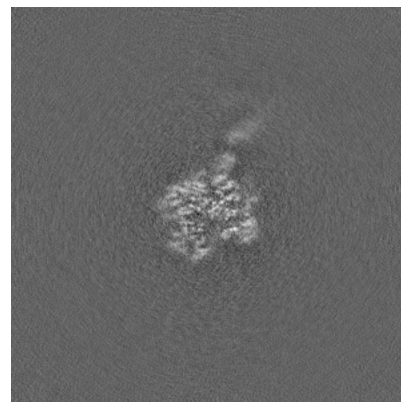
6.3.2 Raw map



X Index: 204



Y Index: 171

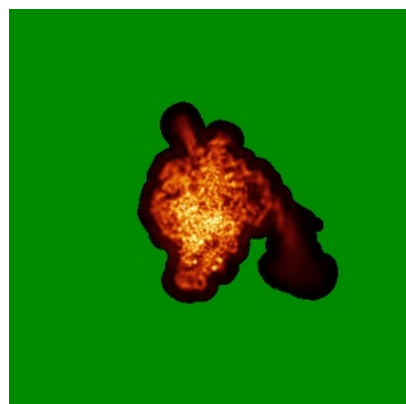


Z Index: 179

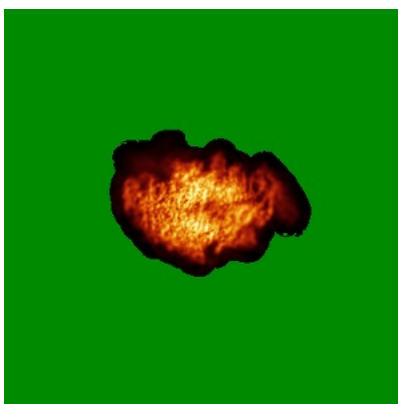
The images above show the largest variance slices of the map in three orthogonal directions.

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

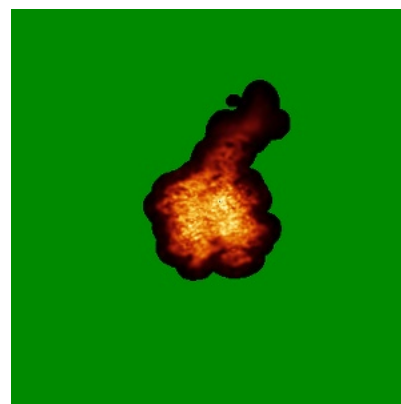
6.4.1 Primary map



X

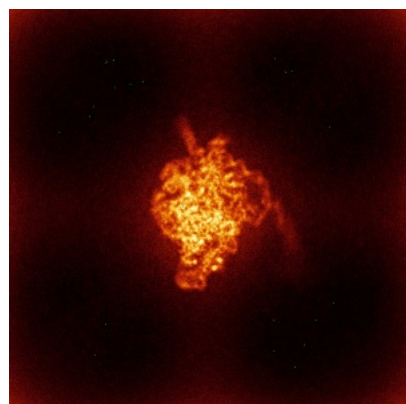


Y

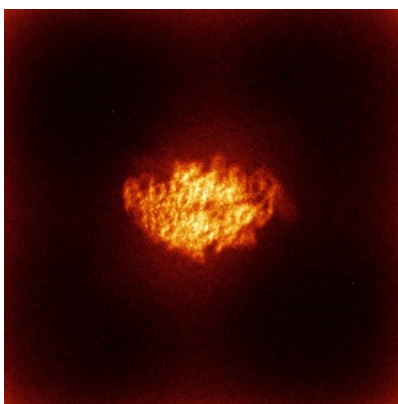


Z

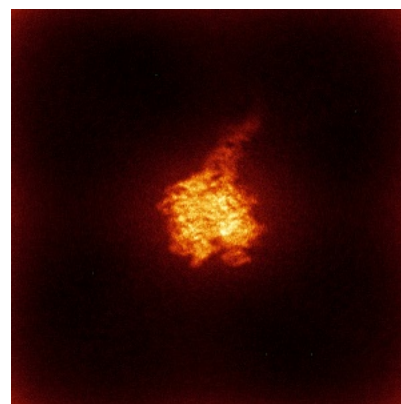
6.4.2 Raw map



X



Y

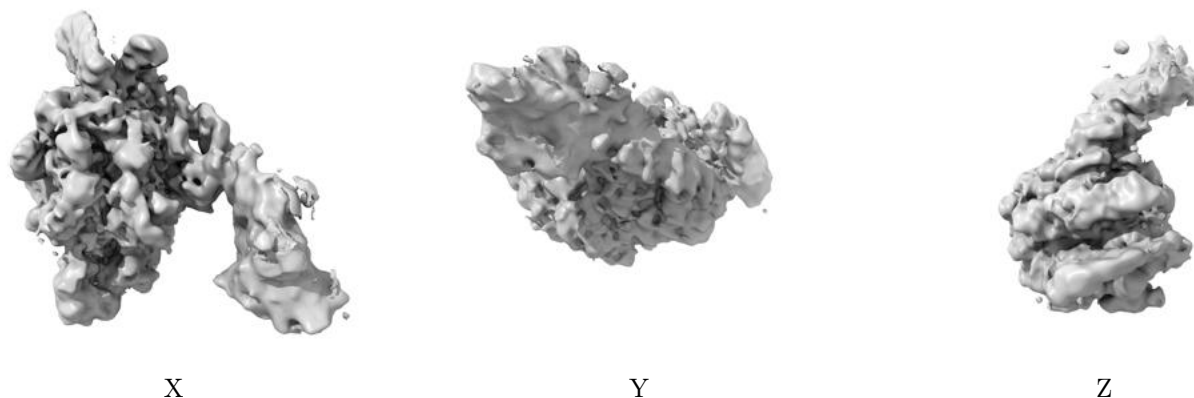


Z

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.

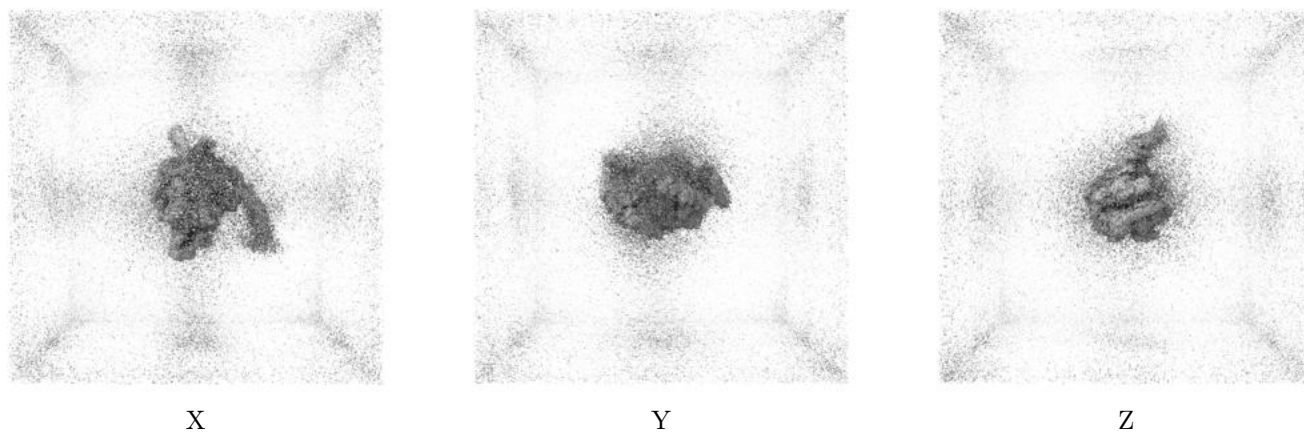
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

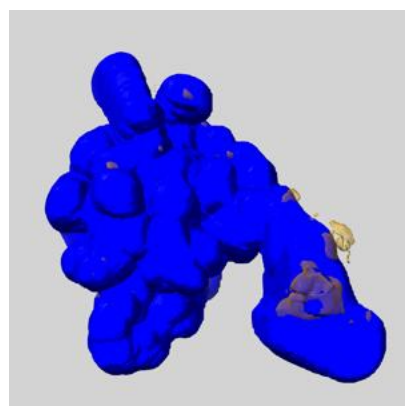
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

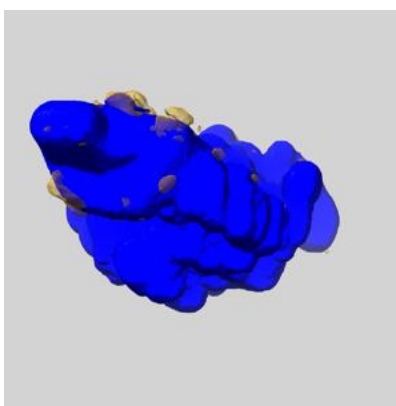
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

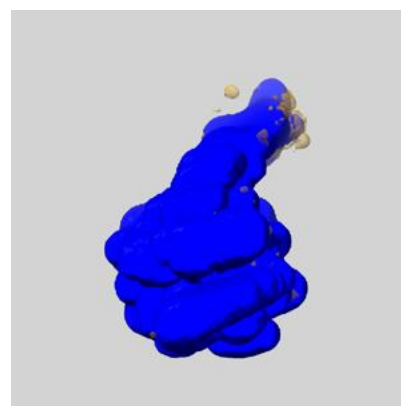
6.6.1 emd_32077_msk_1.map [i](#)



X



Y

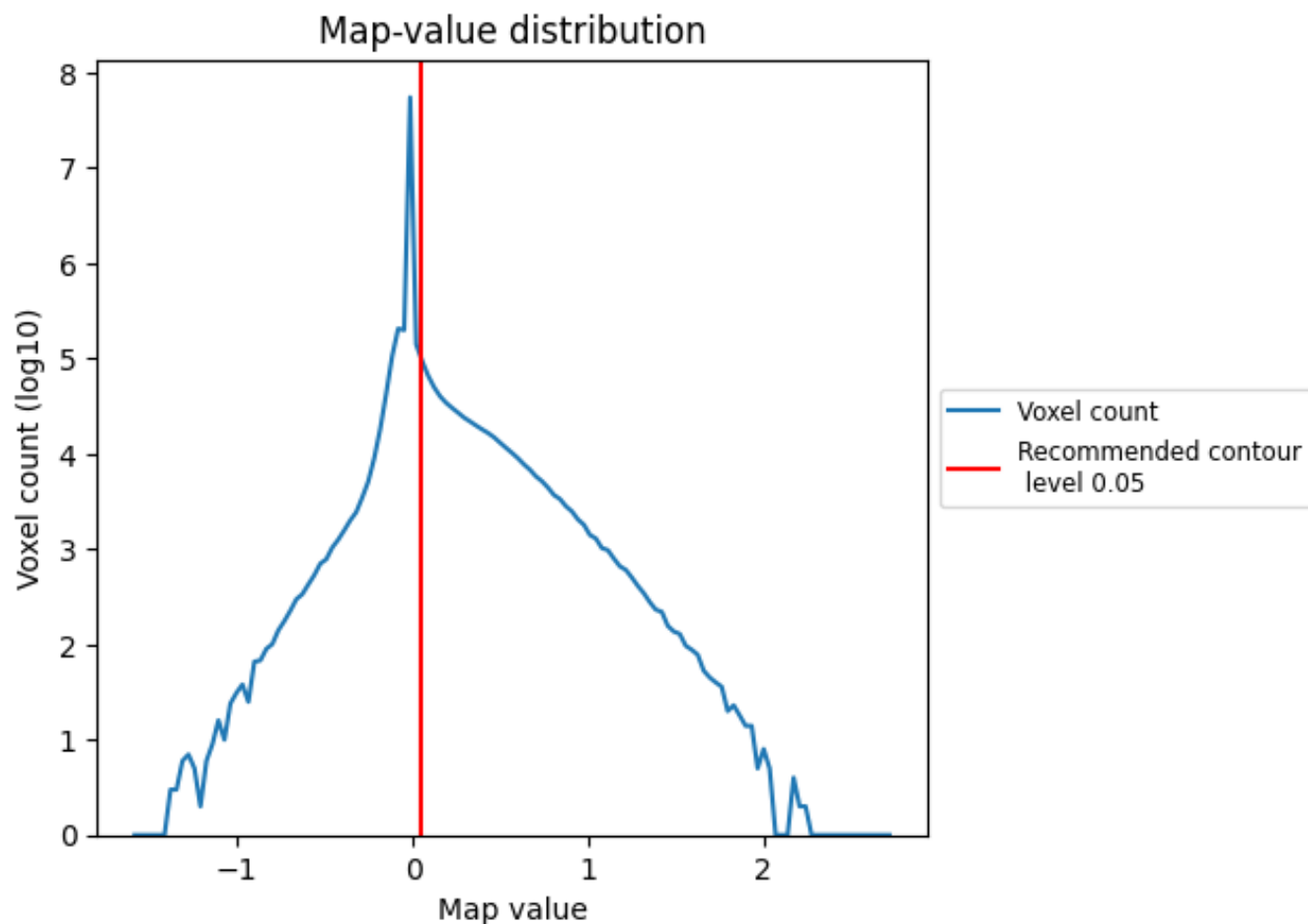


Z

7 Map analysis [i](#)

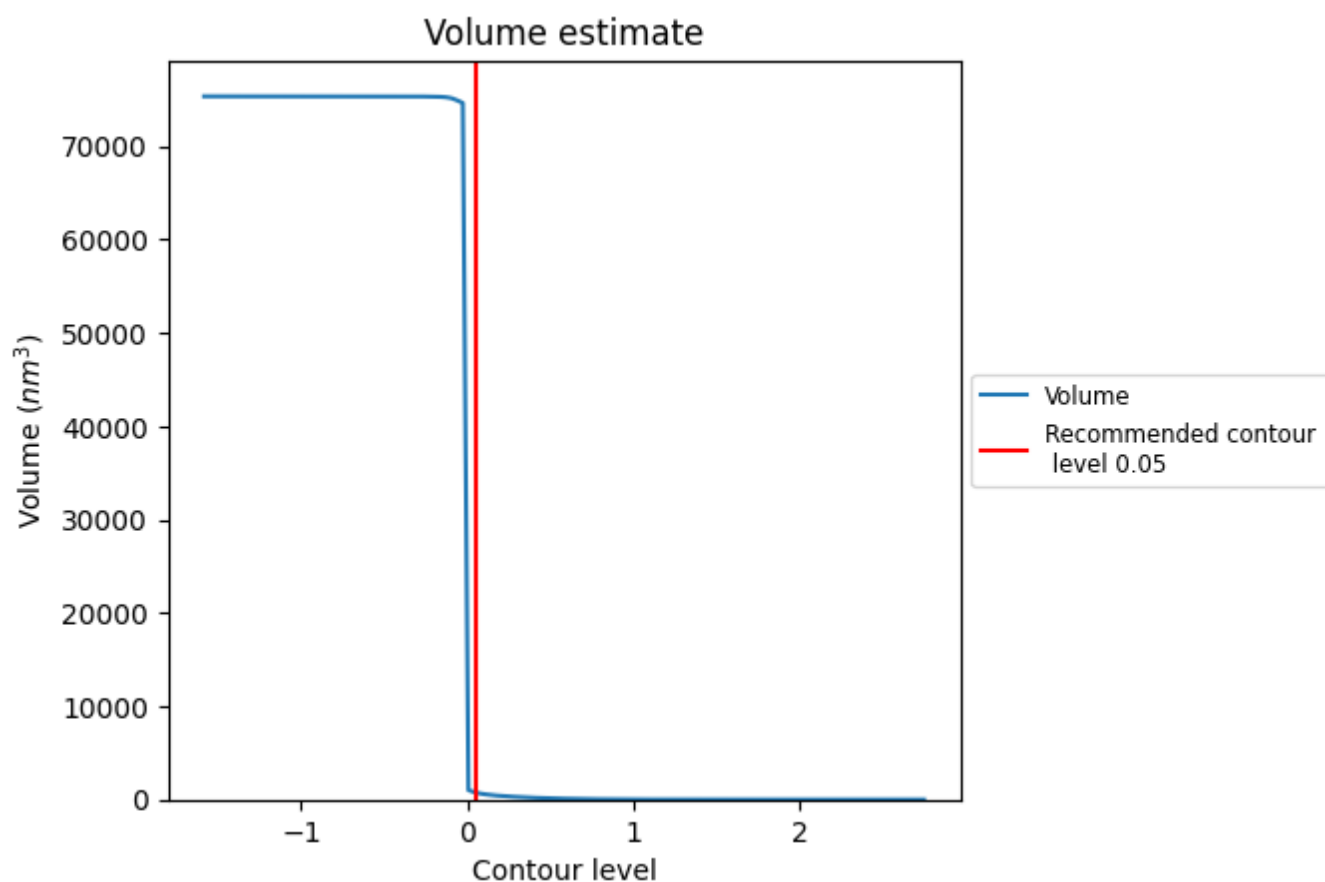
This section contains the results of statistical analysis of the map.

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.

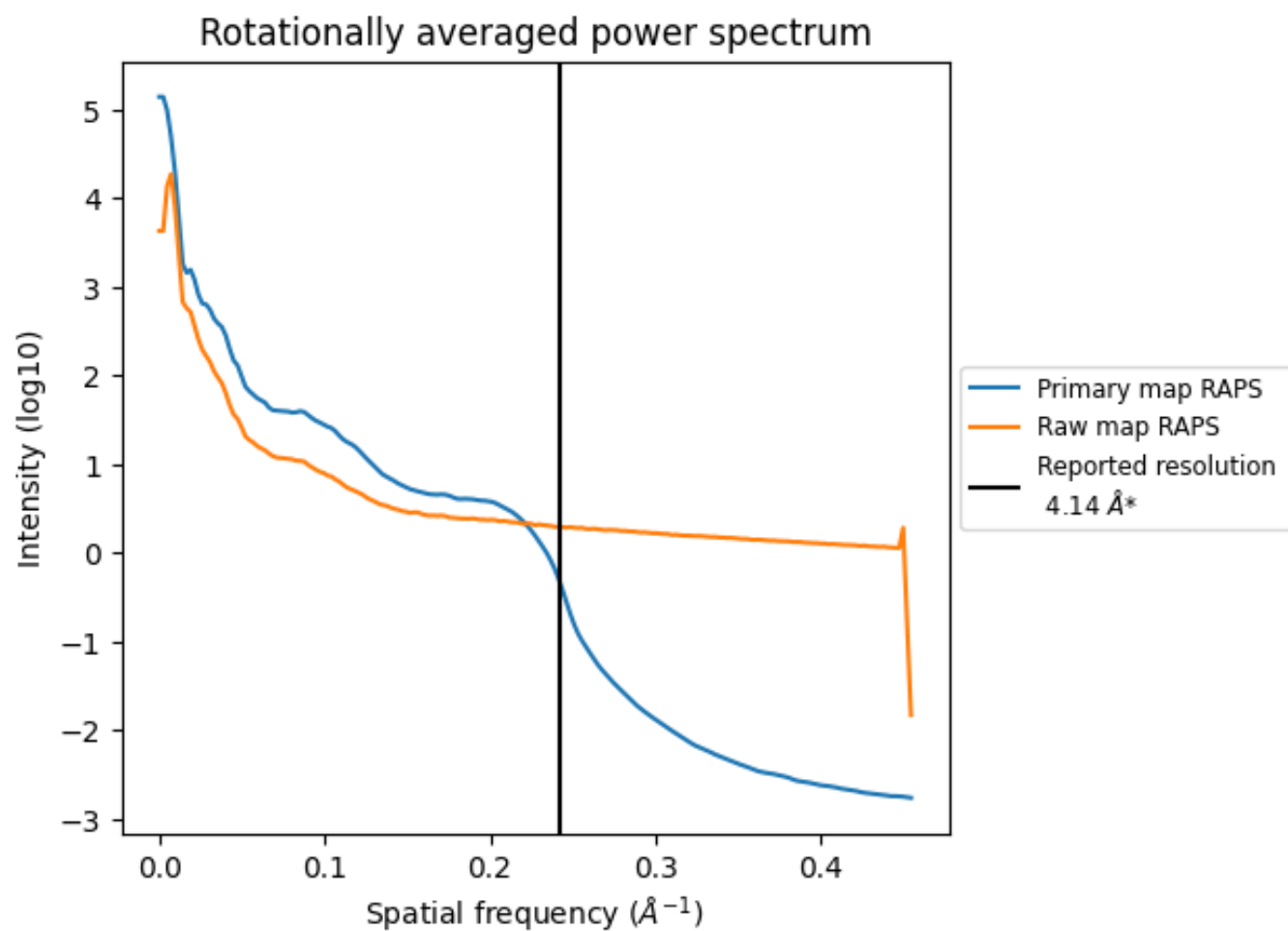
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 770 nm^3 ; this corresponds to an approximate mass of 695 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](#)

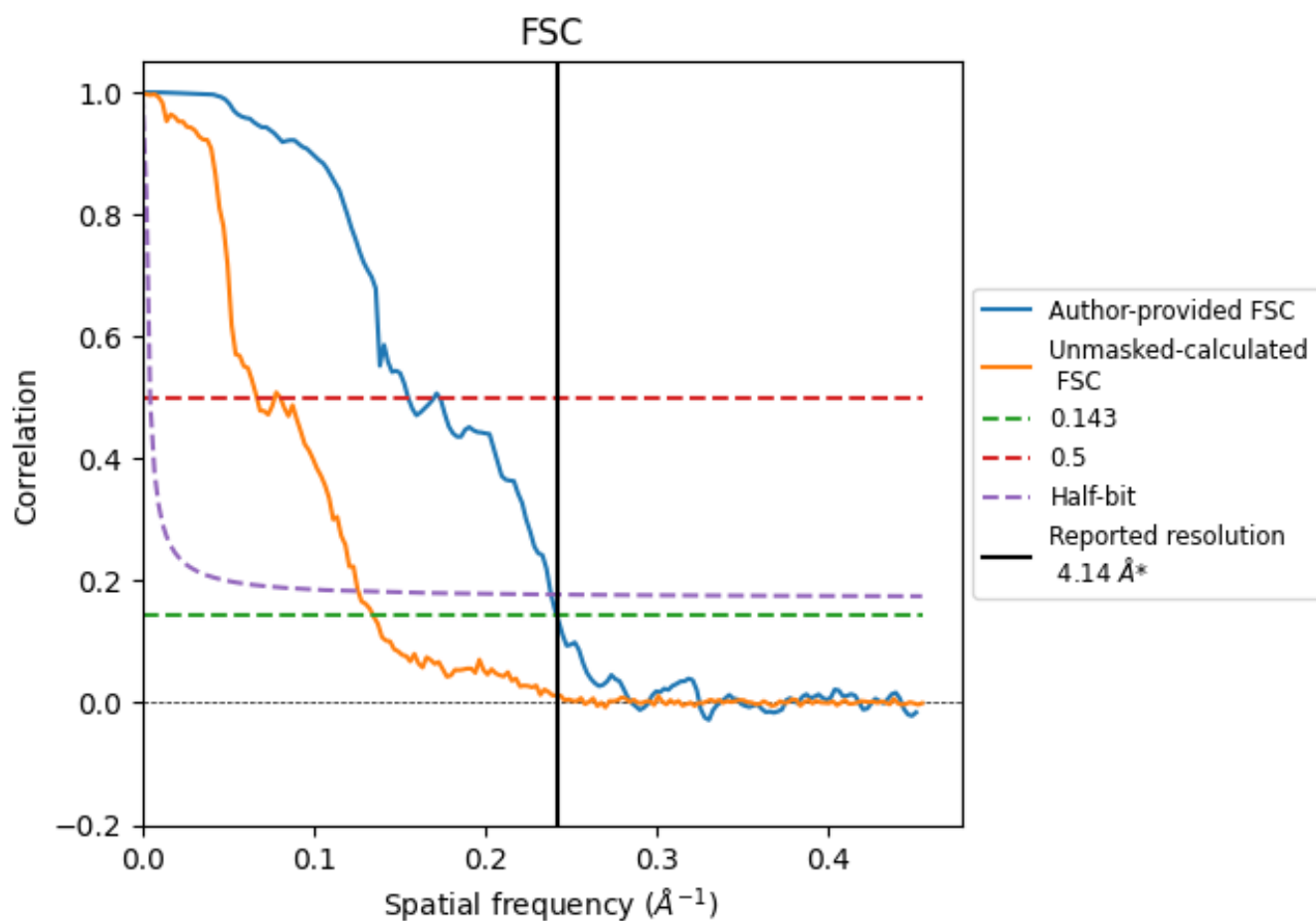


*Reported resolution corresponds to spatial frequency of 0.242 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

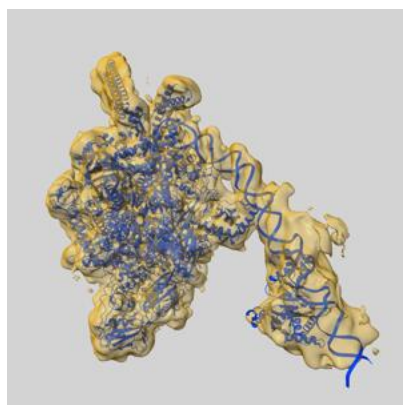
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.14	6.46	4.20
Unmasked-calculated*	7.43	14.99	7.95

*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 7.43 differs from the reported value 4.14 by more than 10 %

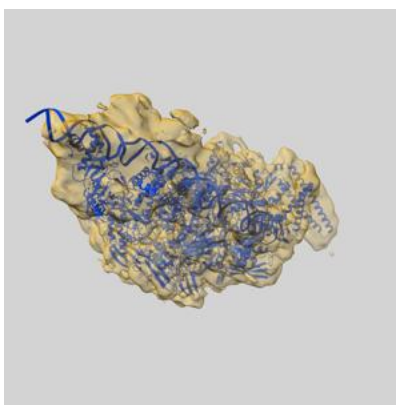
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32077 and PDB model 7VPZ. Per-residue inclusion information can be found in section 3 on page 8.

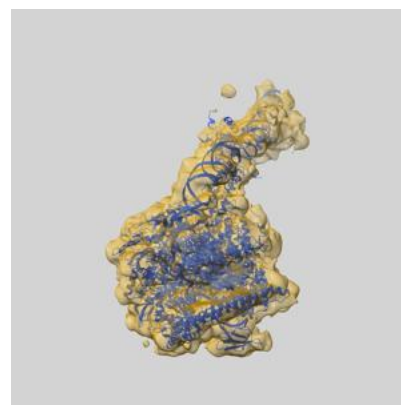
9.1 Map-model overlay [i](#)



X



Y



Z

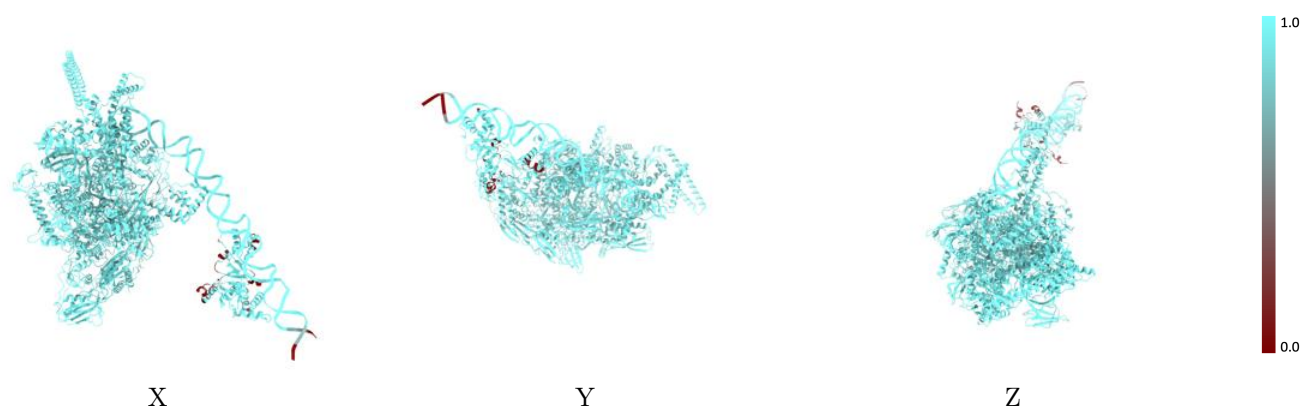
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



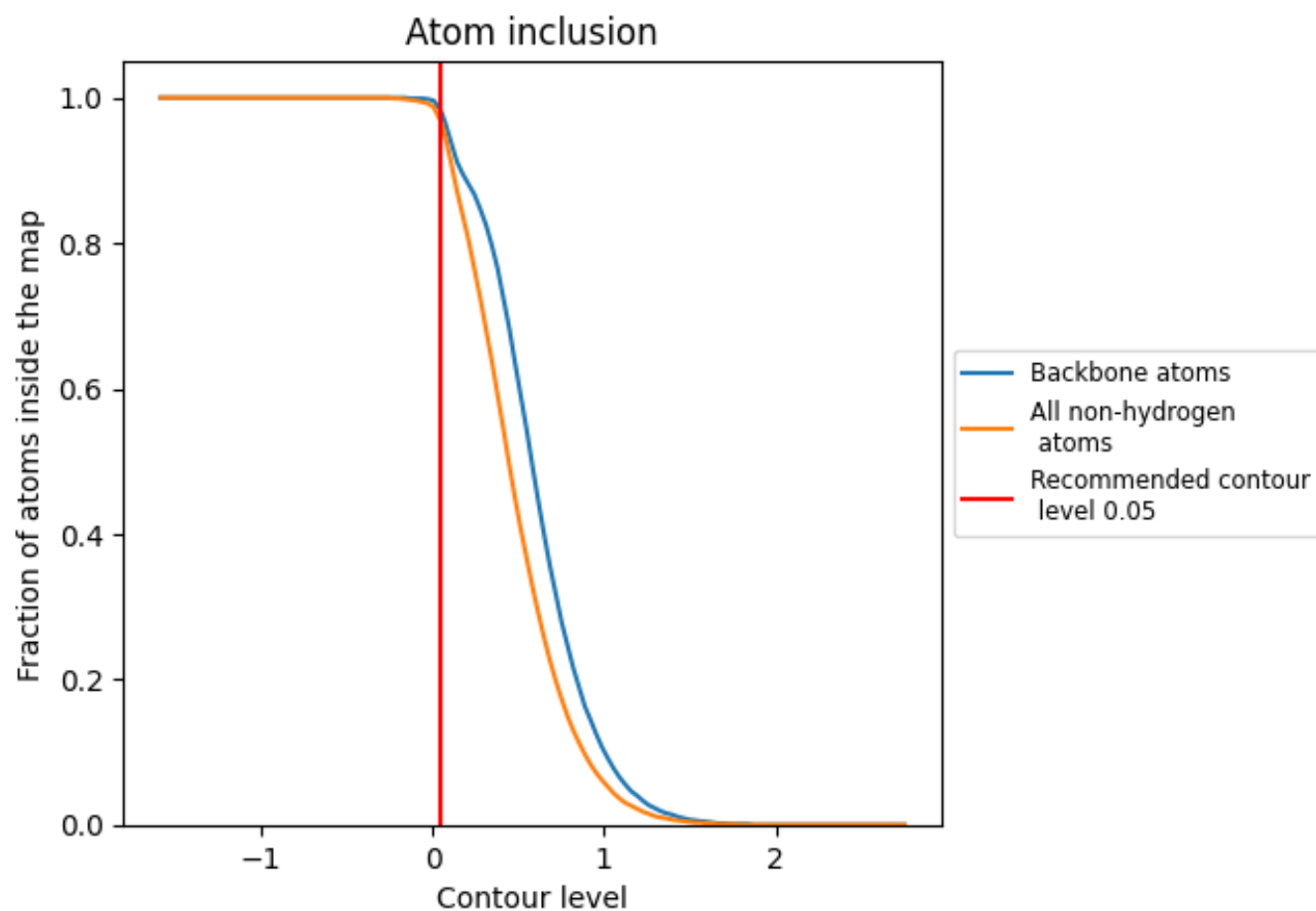
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.2620
A	0.9770	0.2750
B	0.9800	0.2360
C	0.9830	0.3180
D	0.9780	0.3000
E	0.9490	0.2760
F	0.9710	0.2160
M	0.7750	0.0390
N	0.9020	0.0610
O	0.9600	0.1780
P	0.9530	0.1570
Q	0.9540	0.2760

1.0

0.0

<0.0