



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:38 PM UTC

PDB ID : 6PTJ / pdb_00006ptj
EMDB ID : EMD-20471
Title : Structure of Ctf4 trimer in complex with one CMG helicase
Authors : Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.
Deposited on : 2019-07-15
Resolution : 3.80 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:

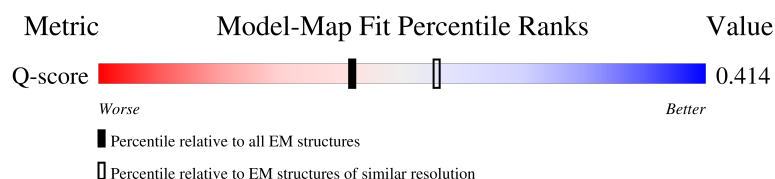
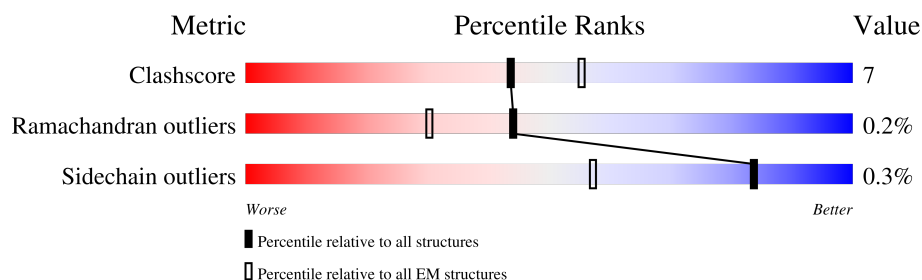
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	208	9% 88% 12%
2	B	213	78% 8% 13%
3	C	194	64% 18% 18%
4	D	294	65% 12% 22%

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Mol	Chain	Length	Quality of chain
5	c	650	76%9%15%
6	2	868	27%70%
7	3	971	23%5%72%
8	4	933	24%6%69%
9	5	775	25%7%67%
10	6	1017	23%73%
11	7	845	6%33%5%61%
12	E	927	41%54%
12	F	927	6%37%9%54%
12	G	927	11%40%6%54%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 34361 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 replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	186	Total	C	N	O	S	0	0
			1557	1005	271	277	4		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	230	Total	C	N	O	S	0	0
			1891	1206	309	364	12		

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 6 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	260	Total	C	N	O	S	0	0
			2025	1284	361	374	6		

- Molecule 7 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3	270	Total	C	N	O	S	0	0
			2139	1361	371	403	4		

- Molecule 8 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	285	Total	C	N	O	S	0	0
			2299	1450	400	432	17		

- Molecule 9 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	252	Total	C	N	O	S	0	0
			2006	1271	344	382	9		

- Molecule 10 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	6	273	Total	C	N	O	S	0	0
			2081	1314	371	390	6		

- Molecule 11 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	7	326	Total	C	N	O	S	0	0
			2615	1655	454	493	13		

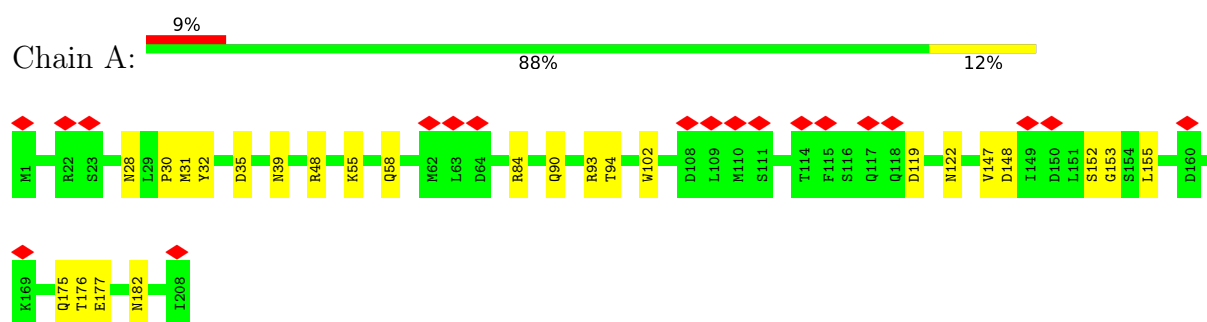
- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	424	Total	C	N	O	S	0	0
			3408	2189	564	640	15		
12	F	431	Total	C	N	O	S	1	0
			3472	2227	576	653	16		
12	G	423	Total	C	N	O	S	1	0
			3402	2186	563	638	15		

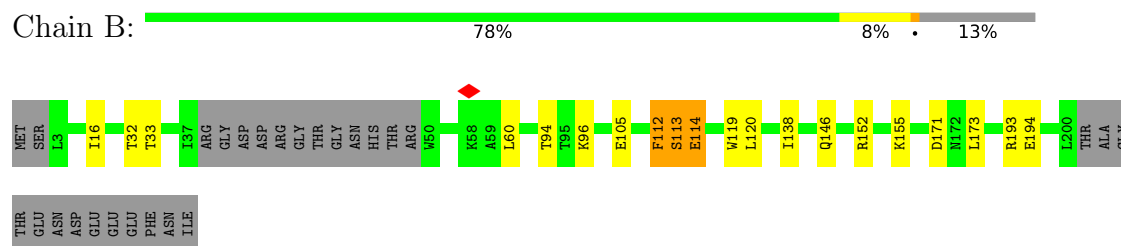
3 Residue-property plots [i](#)

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

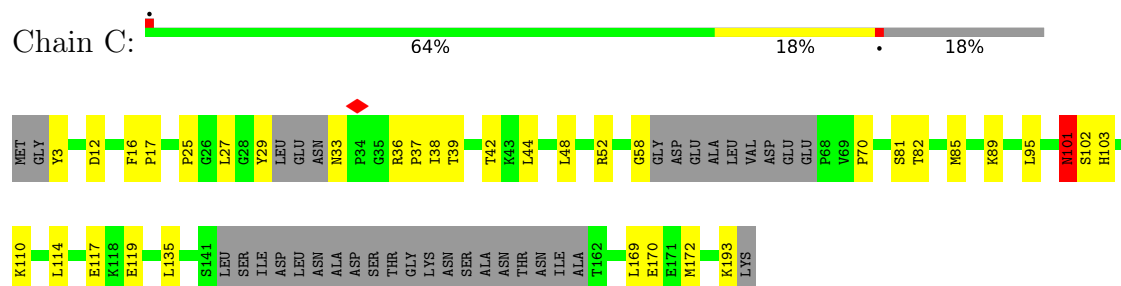
- Molecule 1: DNA replication complex GINS protein PSF1



- Molecule 2: DNA replication complex GINS protein PSF2



- Molecule 3: DNA replication complex GINS protein PSF3

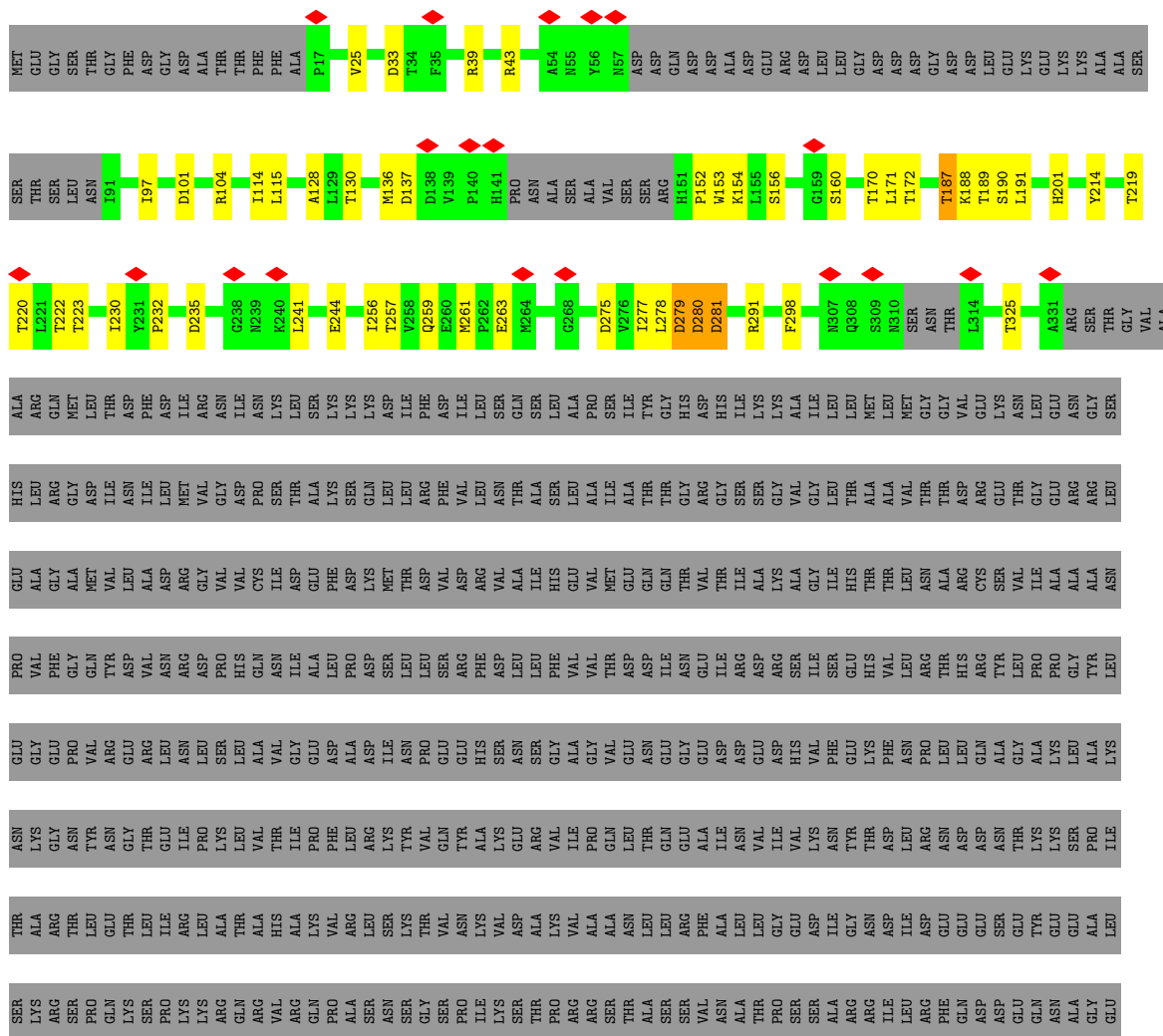


- Molecule 4: DNA replication complex GINS protein SLD5



[illegible]

- Molecule 7: DNA replication licensing factor MCM3



PRO	GLU	GLU	GLU	LYS	PHE	SER	ALA	GLN	GLU	TYR	LEU	ALA	GLY	LEU	LYS	ILE	MET	SER	ASP	ARG	ASN	ASN	LEU	MET	VAL	ALA	ASP	ASP	LYS	VAL	TRP	ARG	VAL
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- Molecule 8: DNA replication licensing factor MCM4

Chain 4: 24% 6% 69%

ASN ILE ARG ALA ALA ILE GLY SER SER PRO LEU ASN PHE PRO SER SER SER GLN ARG GLN GLN ASN ASN ASP VAL PHE GLN SER SER SER GLY ARG GLN GLY ARG ILE SER SER SER SER SER SER SER GLY ARG ARG ARG TYR HIS SER ASP ARG LEU ARG SER ASP ARG ALA ALA PRO THR SER SER

SER	SER	LEU	GLY	ARG	ASN	GLY	GLN	ASN	ASN	ARG	VAL	HIS	MET	ARG	ARG	ASN	ASP	ILE	HIS	THR	SER	ASP	LEU	SER	PRO	ARG	ARG	ILE	VAL	ASP	PHE	ASP	THR	ARG	SER	GLY	VAL	ASN	THR	LEU	ASP	THR	SER	SER	SER	ALA	PRO	PRO	SER	GLU	ALA	SER	GLU	PRO	L177	L178	L179	L180
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C311	C312	G313	M314	R315	I322	L325	K329	G330	F346	D353	V358	E359	I360	D361	R362	I365	R370	C371	E372	R373	I374	D375	C376	M377	E378	P379	C389	D393	E401	T402	P403	D404	F405	V406	P407	D408	G409	T410	T411	P412	H413	S414	I415	L423	V424	D425
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Category	Value	Color	Label
R428	428	Red	R428
R432	432	Green	R432
I433	433	Green	I433
E434	434	Green	E434
G437	437	Green	G437
I442	442	Green	I442
S448	448	Red	S448
R449	449	Red	R449
V452	452	Green	V452
V463	463	Yellow	V463
V464	464	Yellow	V464
H465	465	Yellow	H465
V466	466	Yellow	V466
K467	467	Yellow	K467
K468	468	Yellow	K468
V469	469	Yellow	V469
SER			SER
ASP			ASP
LYS			LYS
ARG			ARG
LEU			LEU
ASP			ASP
VAL			VAL
ASP			ASP
THR			THR
SER			SER
THR			THR
ILE			ILE
GLU			GLU
GLN			GLN
GLU			GLU
LEU			LEU
MET			MET
GLN			GLN
ASN			ASN
LYS			LYS
VAL			VAL
ASP			ASP
HIS			HIS
ASN			ASN
GLU			GLU
VAL			VAL
GLU			GLU
GLU			GLU
VAL			VAL
ARG			ARG
GLN			GLN
ILE			ILE
THR			THR
ASP			ASP
GLN			GLN
ASP			ASP
LEU			LEU
ALA			ALA

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

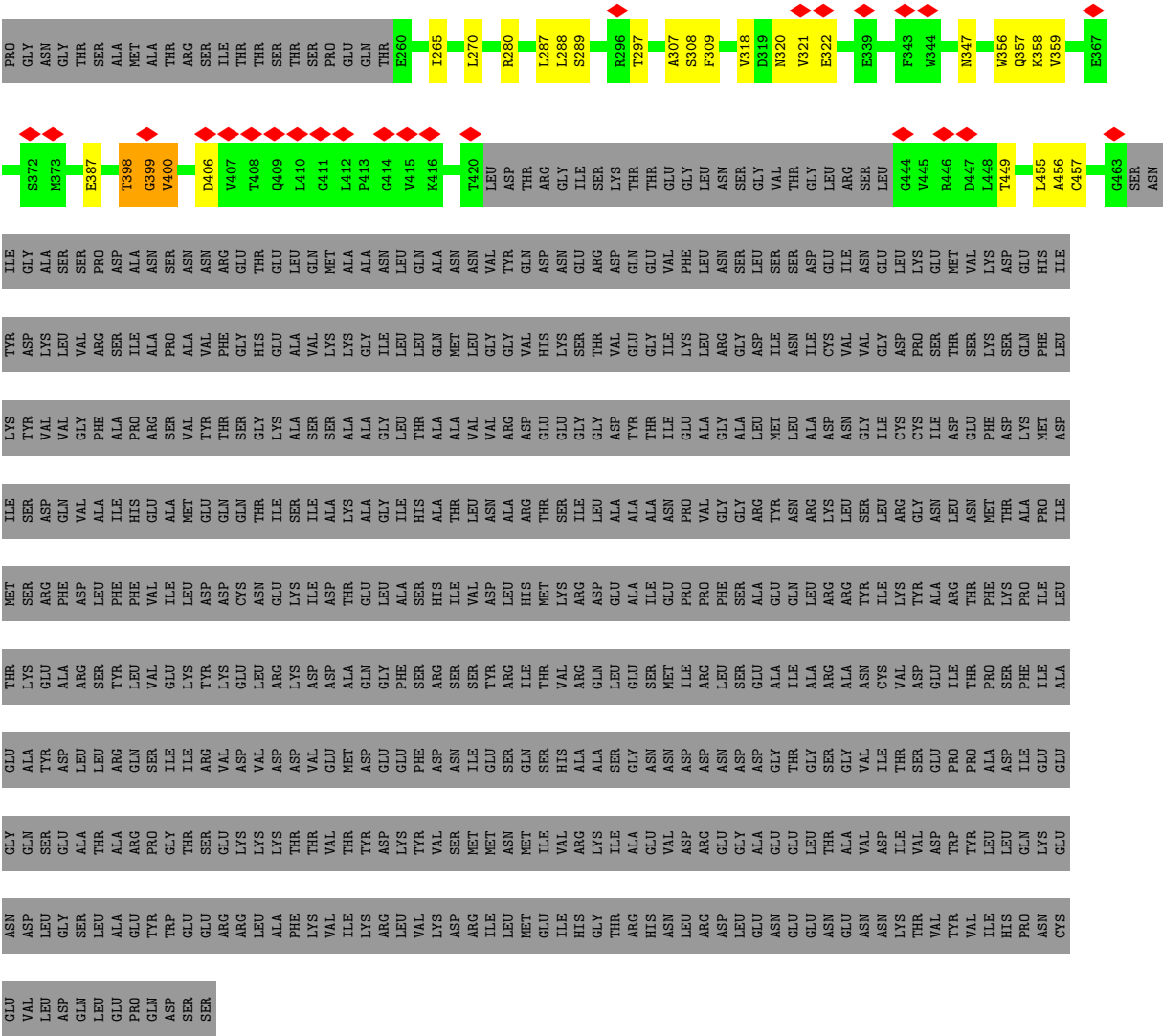
HIS	ALA	LYS	MET	LEU	LYS	ASN	VAL	VAL	GLU	LEU	GLU	ASP	VAL	GLN	GLU	ALA	VAL	ARG	LEU	ILE	ILE	ARG	SER	ALA	LYS	ASP	TYR	ALA	THR	GLY	LYS	ILE	ASP	MET	ASN	LEU	VAL	GLN	THR	GLY	LYS	SER	VAL	ILE	GLN	ARG	LYS	LEU	GLN	ASP	LEU	SER	ARG
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	GLU	ILE	MET	ASN	VAL	LEU	LYS	ASP	ASP	SER	MET	SER	PHE	ASN	GLU	LEU	ILE	LYS	GLN	GLN	SER	SER	ARG	VAL	GLU	GLY	VAL	ARG	SER	VAL
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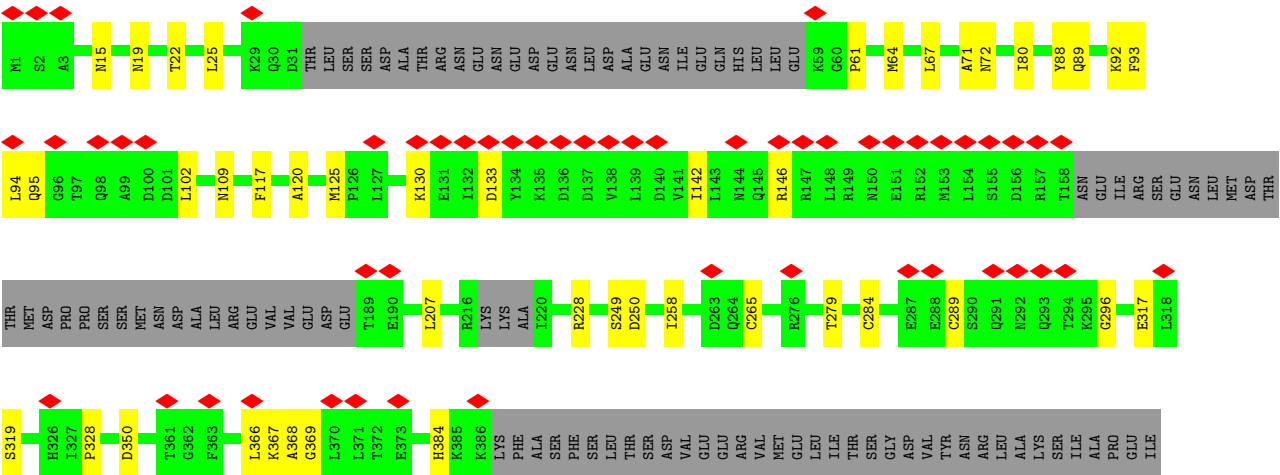
ARG
LEU
ASN
ASN
ARG
VAL

Chain 5: 25% 7% 67%





● Molecule 11: DNA replication licensing factor MCM7



[illegible]

- Molecule 12: DNA polymerase alpha-binding protein

[illegible]

L883	S884	L885	A886	H887	E888	L889	K890	Q891	D892	R893	A894	L895	E896	A897	A898	V899	K900	I901	S902	E903	R904	A905	E906	L907	P908	S909	L910	V911	K912	K913	I914	N915	N916	I917	R918	E919	A920	R921	Y922	E923	GLN	GLN	LYS												
THR	GLU	ALA	GLU	GLY	GLU	GLU	ASP	LYS	E814	I817	E825	E826	Y827	L833	L836	E842	N843	D844	G845	E846	N847	Y848	G849	N850	E851	N852	E853	V854	L855	L858	N859	G860	A861	Y862	D863	K864	A865	L866	L867	R868	L869	F870	A871	S872	A873	C874	S875	D876	Q877	N878	V879	E880			
ASN	SER	ASP	MET	LYS	D671	A672	F689	S690	S691	Y692	G693	L722	E727	K730	K735	E736	T737	T738	L745	Y749	N753	C754	P771	S772	E775	I776	R777	M778	P779	K783	E788	E789	N790	K791	A792	I793	LEU	ASN	LYS	ASN	GLU	ILE	GLY	ALA	ASP										
T495	M496	M497	E498	V499	S508	E509	T514	D519	V520	R524	D530	Y534	D535	L539	N540	E541	D560	S561	I562	A574	G575	E576	L594	N601	V605	F626	S631	Q632	F633	H634	L643	G644	T645	S646	S647	R653	M659	S660	N663	ILE															
SER	GLU	LYS	ARG	TRP	TYR	ASN	PHE	GLU	GLU	ASP	PHE	ILE	ASP	ASP	ASP	GLY	TYR	GLY	SER	GLY	LYS	LYS	PRO	HIS	ASN	GLU	VAL	ARG	ILE	ASN	VAL	HIS	LYS	F474	M477	P478	G487	F488																	
LEU	GLU	ASN	SER	ASP	GLU	THR	HIS	LYS	ALA	LYS	ALA	ILE	GLN	VAL	ASP	ASP	ASP	ASP	ASP	GLY	ALA	ASP	ASP	GLY	TYR	ASN	ILE	ASP	ALA	THR	GLN	THR	GLY	PHE	ASP	ILE	ALA	GLY	VAL	ASN	THR	ALA	ARG	HIS	VAL	ASP	GLU	LEU	ASN	ASP	TRP	HIS	PRO	GLY	ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200491	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.230	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	300.72, 300.72, 300.72	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

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	0.36	0/1718	0.72	1/2314 (0.0%)
2	B	0.46	0/1589	0.82	2/2150 (0.1%)
3	C	0.39	0/1320	0.72	1/1784 (0.1%)
4	D	0.42	0/1923	0.82	4/2594 (0.2%)
5	c	0.41	0/4563	0.69	2/6173 (0.0%)
6	2	0.34	0/2063	0.72	2/2794 (0.1%)
7	3	0.39	0/2189	0.78	5/2975 (0.2%)
8	4	0.28	0/2336	0.80	4/3155 (0.1%)
9	5	0.46	0/2035	0.87	5/2752 (0.2%)
10	6	0.29	0/2114	0.77	6/2862 (0.2%)
11	7	0.29	0/2660	0.68	1/3595 (0.0%)
12	E	0.41	0/3493	0.62	3/4730 (0.1%)
12	F	0.28	0/3558	0.58	1/4817 (0.0%)
12	G	0.29	0/3487	0.60	0/4724
All	All	0.36	0/35048	0.71	37/47419 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	45	ILE	N-CA-C	16.83	127.79	110.62
8	4	373	ARG	N-CA-C	-16.59	90.28	111.02
10	6	399	GLY	N-CA-C	16.19	132.16	112.73
7	3	325	THR	CA-C-O	-12.06	105.72	119.95
9	5	265	VAL	N-CA-C	11.48	120.20	108.95
9	5	41	ASP	N-CA-C	10.08	122.26	111.28
9	5	264	LEU	N-CA-C	-9.95	92.08	108.49
12	E	507	ASN	N-CA-C	-9.78	92.96	108.90
2	B	113	SER	N-CA-C	9.43	121.56	111.28
7	3	187	THR	N-CA-C	9.02	127.13	113.61
10	6	320	ASN	N-CA-C	8.53	121.69	108.12
12	F	507	ASN	N-CA-C	-7.80	99.50	110.50
4	D	257	THR	N-CA-C	7.72	121.39	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	294	ASP	N-CA-C	7.64	120.78	109.24
4	D	221	GLU	CA-C-N	-7.37	110.63	119.84
4	D	221	GLU	C-N-CA	-7.37	110.63	119.84
10	6	321	VAL	N-CA-C	7.09	120.98	109.78
3	C	101	ASN	N-CA-C	-7.00	95.89	110.80
11	7	369	GLY	N-CA-C	-6.90	104.22	115.46
8	4	372	GLU	CA-C-N	-6.79	112.47	122.78
8	4	372	GLU	C-N-CA	-6.79	112.47	122.78
2	B	112	PHE	N-CA-C	-6.52	97.65	108.34
1	A	147	VAL	N-CA-C	-5.82	104.95	110.42
10	6	398	THR	CA-C-N	5.68	126.28	119.98
10	6	398	THR	C-N-CA	5.68	126.28	119.98
4	D	221	GLU	N-CA-C	5.51	123.81	112.40
10	6	400	VAL	N-CA-C	5.41	118.32	109.78
7	3	280	ASP	N-CA-C	5.40	121.06	113.56
9	5	45	ILE	CB-CA-C	-5.17	105.16	112.14
5	c	575	ASN	CA-C-N	5.16	131.15	123.05
5	c	575	ASN	C-N-CA	5.16	131.15	123.05
12	E	621	GLN	CA-C-N	5.14	128.54	120.82
12	E	621	GLN	C-N-CA	5.14	128.54	120.82
7	3	172	THR	CA-C-N	-5.09	114.63	121.71
7	3	172	THR	C-N-CA	-5.09	114.63	121.71
6	2	289	ILE	CA-C-N	5.01	131.11	121.54
6	2	289	ILE	C-N-CA	5.01	131.11	121.54

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	1696	0	1698	19	0
2	B	1557	0	1610	18	0
3	C	1288	0	1298	24	0
4	D	1891	0	1899	28	0
5	c	4482	0	4499	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2	2025	0	1993	20	0
7	3	2139	0	2112	38	0
8	4	2299	0	2292	59	0
9	5	2006	0	2038	41	0
10	6	2081	0	1987	35	0
11	7	2615	0	2627	30	0
12	E	3408	0	3351	24	0
12	F	3472	0	3418	63	0
12	G	3402	0	3345	37	0
All	All	34361	0	34167	448	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 (448) 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)
8:4:289:LEU:HD21	8:4:293:LEU:CD2	1.49	1.40
8:4:289:LEU:CD2	8:4:293:LEU:HD23	1.61	1.28
7:3:187:THR:HG21	7:3:259:GLN:NE2	1.46	1.26
8:4:370:ARG:HG2	8:4:378:GLU:CB	1.73	1.17
12:F:493:TYR:CZ	12:F:768:LEU:HD21	1.79	1.16
7:3:187:THR:CG2	7:3:259:GLN:HE21	1.63	1.11
8:4:465:HIS:NE2	8:4:467:LYS:HB2	1.66	1.11
10:6:288:LEU:H	10:6:399:GLY:HA2	1.08	1.08
4:D:256:TYR:OH	4:D:290:LYS:HD3	1.53	1.07
12:F:493:TYR:OH	12:F:768:LEU:HD21	1.51	1.06
10:6:288:LEU:H	10:6:399:GLY:CA	1.70	1.04
12:F:507:ASN:HD22	12:F:510:GLN:HG3	1.22	1.04
7:3:278:LEU:C	7:3:279:ASP:OD1	2.02	1.03
4:D:256:TYR:OH	4:D:290:LYS:CD	2.11	0.99
10:6:288:LEU:HD23	10:6:399:GLY:O	1.65	0.97
8:4:294:ASP:OD1	8:4:295:GLU:N	2.01	0.92
8:4:289:LEU:CD2	8:4:293:LEU:CD2	2.31	0.91
8:4:289:LEU:HD21	8:4:293:LEU:HD23	0.90	0.89
9:5:39:ARG:NH2	9:5:44:PHE:CE1	2.39	0.89
12:F:493:TYR:OH	12:F:768:LEU:CD2	2.20	0.89
8:4:294:ASP:OD2	8:4:297:GLU:HB2	1.71	0.89
10:6:287:LEU:HG	10:6:399:GLY:HA3	1.53	0.88
10:6:398:THR:HG21	10:6:457:CYS:SG	2.12	0.88
7:3:187:THR:HG21	7:3:259:GLN:HE21	0.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:39:ARG:HE	9:5:44:PHE:HD1	0.90	0.86
11:7:93:PHE:HD2	11:7:94:LEU:HG	1.40	0.86
12:F:493:TYR:CE2	12:F:768:LEU:HD21	2.11	0.86
3:C:193:LYS:NZ	9:5:41:ASP:OD2	2.08	0.85
9:5:39:ARG:NE	9:5:44:PHE:CD1	2.44	0.84
3:C:101:ASN:CG	3:C:102:SER:H	1.80	0.84
10:6:398:THR:OG1	10:6:456:ALA:HA	1.79	0.82
10:6:288:LEU:O	10:6:399:GLY:HA2	1.81	0.81
8:4:374:ILE:O	8:4:375:ASP:CB	2.25	0.81
10:6:288:LEU:N	10:6:399:GLY:HA2	1.92	0.81
8:4:465:HIS:CE1	8:4:467:LYS:HB2	2.17	0.80
8:4:372:GLU:O	8:4:373:ARG:C	2.19	0.80
7:3:188:LYS:HD2	7:3:257:THR:CG2	2.12	0.80
3:C:101:ASN:OD1	3:C:102:SER:N	2.16	0.79
9:5:39:ARG:NE	9:5:44:PHE:HD1	1.74	0.79
8:4:370:ARG:CG	8:4:378:GLU:CB	2.58	0.78
8:4:372:GLU:O	8:4:373:ARG:O	2.02	0.78
11:7:93:PHE:CE2	11:7:94:LEU:HD21	2.18	0.78
2:B:105:GLU:OE1	2:B:113:SER:OG	2.01	0.77
10:6:400:VAL:HG23	10:6:455:LEU:HB3	1.65	0.77
7:3:279:ASP:OD1	7:3:279:ASP:N	2.15	0.76
8:4:467:LYS:HD2	8:4:468:LYS:H	1.51	0.74
8:4:467:LYS:HD2	8:4:468:LYS:N	2.02	0.74
10:6:308:SER:HA	10:6:318:VAL:O	1.87	0.74
4:D:221:GLU:O	4:D:223:ASP:N	2.21	0.74
4:D:219:ILE:O	4:D:220:ASP:HB2	1.85	0.74
12:F:507:ASN:ND2	12:F:510:GLN:HG3	2.01	0.73
3:C:101:ASN:CG	3:C:102:SER:N	2.43	0.71
9:5:41:ASP:OD1	9:5:42:SER:N	2.23	0.71
7:3:280:ASP:O	7:3:281:ASP:CG	2.32	0.71
2:B:113:SER:O	2:B:114:GLU:HB2	1.91	0.71
8:4:289:LEU:HD21	8:4:293:LEU:HD22	1.69	0.70
7:3:188:LYS:HD2	7:3:257:THR:HG21	1.72	0.70
10:6:307:ALA:O	10:6:318:VAL:O	2.08	0.70
4:D:256:TYR:OH	4:D:290:LYS:HD2	1.91	0.70
4:D:221:GLU:O	4:D:222:PRO:C	2.29	0.70
11:7:93:PHE:CD2	11:7:94:LEU:HG	2.25	0.69
8:4:353:ASP:OD2	8:4:373:ARG:O	2.11	0.69
1:A:84:ARG:HD2	3:C:3:TYR:HB2	1.77	0.67
8:4:406:VAL:HG12	8:4:408:ASP:H	1.61	0.66
12:F:507:ASN:HD22	12:F:510:GLN:CG	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:507:ASN:ND2	12:F:510:GLN:HE21	1.93	0.66
8:4:304:ARG:HB3	8:4:465:HIS:HB2	1.78	0.66
11:7:93:PHE:CD2	11:7:94:LEU:CD2	2.80	0.65
10:6:288:LEU:N	10:6:399:GLY:CA	2.54	0.64
3:C:117:GLU:HG2	3:C:119:GLU:H	1.61	0.64
7:3:280:ASP:O	7:3:281:ASP:OD1	2.16	0.63
8:4:201:PHE:HB3	8:4:224:LEU:HD13	1.82	0.62
12:F:475:ARG:NH2	12:F:477:MET:SD	2.71	0.62
3:C:58:GLY:HA3	3:C:70:PRO:HA	1.81	0.62
2:B:113:SER:O	2:B:114:GLU:CB	2.48	0.62
12:F:558:PRO:HG2	12:F:563:HIS:HB2	1.82	0.62
8:4:467:LYS:O	8:4:468:LYS:HB2	2.00	0.61
7:3:137:ASP:N	7:3:137:ASP:OD1	2.33	0.61
10:6:287:LEU:HA	10:6:399:GLY:HA3	1.81	0.61
6:2:302:THR:HG22	6:2:303:ILE:HG13	1.83	0.60
8:4:329:LYS:HG2	8:4:434:GLU:HG2	1.83	0.60
10:6:400:VAL:CG2	10:6:455:LEU:HB3	2.31	0.60
5:c:146:GLY:HA2	5:c:149:ASP:HB3	1.83	0.60
7:3:188:LYS:HD2	7:3:257:THR:HG23	1.84	0.60
10:6:398:THR:HG1	10:6:456:ALA:HA	1.65	0.60
1:A:152:SER:O	4:D:145:ARG:NH1	2.35	0.60
7:3:43:ARG:HD3	7:3:136:MET:HE3	1.83	0.59
1:A:84:ARG:NH2	4:D:218:MET:SD	2.75	0.59
4:D:256:TYR:O	4:D:268:GLU:OE1	2.20	0.58
9:5:299:SER:OG	9:5:300:ILE:N	2.36	0.58
12:G:576:GLU:HG3	12:G:594:LEU:HD23	1.85	0.58
12:E:661:LEU:HD12	12:G:633:PHE:CE2	2.38	0.58
4:D:204:GLU:HA	4:D:207:GLN:HE21	1.69	0.58
12:F:754:CYS:SG	12:F:755:ILE:N	2.76	0.58
8:4:353:ASP:HB2	8:4:373:ARG:HB2	1.85	0.57
8:4:465:HIS:NE2	8:4:467:LYS:CB	2.57	0.57
8:4:437:GLY:HA2	8:4:464:VAL:HG12	1.86	0.57
8:4:469:VAL:O	8:4:469:VAL:HG22	2.05	0.57
9:5:39:ARG:NH2	9:5:44:PHE:CD1	2.68	0.57
4:D:261:PRO:HG2	4:D:264:LYS:HB2	1.87	0.57
8:4:294:ASP:OD2	8:4:297:GLU:CB	2.50	0.57
12:G:753[A]:ASN:HD21	12:G:771:PRO:HB3	1.70	0.56
6:2:334:LEU:HD23	9:5:322:ALA:HB1	1.88	0.56
8:4:372:GLU:O	8:4:373:ARG:HB2	2.05	0.56
2:B:193:ARG:NH2	4:D:225:ASN:OD1	2.39	0.56
12:E:507:ASN:O	12:E:510:GLN:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:THR:HG22	2:B:96:LYS:H	1.71	0.56
12:F:668:MET:HE1	12:F:673:ASN:HB2	1.87	0.56
6:2:298:SER:OG	6:2:299:ASP:N	2.39	0.56
12:F:706:LEU:HD21	12:F:836:LEU:HD21	1.88	0.56
8:4:360:ILE:HG13	8:4:365:ILE:HD13	1.88	0.56
5:c:5:ILE:N	5:c:144:ASP:O	2.39	0.55
12:G:495:THR:OG1	12:G:496:MET:N	2.39	0.55
7:3:277:ILE:HG22	7:3:279:ASP:OD1	2.07	0.55
9:5:64:ASN:ND2	9:5:66:GLU:OE1	2.39	0.55
11:7:133:ASP:OD1	11:7:133:ASP:N	2.39	0.55
3:C:33:ASN:O	3:C:36:ARG:NH1	2.40	0.55
12:F:493:TYR:CZ	12:F:768:LEU:CD2	2.71	0.55
12:F:631:SER:OG	12:F:632:GLN:N	2.39	0.55
11:7:228:ARG:NH1	11:7:317:GLU:OE2	2.40	0.54
2:B:105:GLU:OE1	2:B:152:ARG:NH2	2.40	0.54
5:c:306:SER:HB3	12:E:489:THR:HG22	1.89	0.54
6:2:210:GLU:O	6:2:253:LYS:NZ	2.41	0.54
12:F:490:ASP:HB3	12:F:506:LYS:HB3	1.89	0.54
5:c:396:LEU:HD22	5:c:401:LEU:HB2	1.90	0.54
12:E:490:ASP:N	12:E:490:ASP:OD1	2.39	0.54
7:3:244:GLU:OE1	11:7:109:ASN:ND2	2.41	0.53
5:c:76:ASP:OD1	5:c:76:ASP:N	2.41	0.53
5:c:486:ASP:OD1	5:c:486:ASP:N	2.41	0.53
6:2:201:PRO:HB2	6:2:203:VAL:HG22	1.90	0.53
12:G:497:ASN:ND2	12:G:539:LEU:O	2.38	0.53
4:D:215:SER:OG	4:D:216:VAL:N	2.41	0.53
4:D:262:ASP:HB2	4:D:263:LEU:HD12	1.90	0.53
3:C:12:ASP:OD1	3:C:110:LYS:NZ	2.42	0.53
10:6:288:LEU:H	10:6:399:GLY:HA3	1.68	0.53
12:F:642:GLU:OE1	12:F:651:TYR:OH	2.27	0.53
5:c:223:ARG:O	5:c:227:LYS:N	2.39	0.53
5:c:464:GLN:O	5:c:468:ASN:ND2	2.42	0.53
7:3:275:ASP:OD1	7:3:275:ASP:N	2.40	0.53
12:E:839:ASP:O	12:E:843:ASN:ND2	2.42	0.53
12:F:493:TYR:CE1	12:F:768:LEU:HD11	2.44	0.53
12:G:495:THR:HG21	12:G:539:LEU:HD13	1.91	0.53
7:3:33:ASP:OD1	7:3:33:ASP:N	2.39	0.53
1:A:55:LYS:HA	1:A:58:GLN:HE21	1.73	0.53
9:5:95:THR:HG22	9:5:135:PHE:HD2	1.74	0.52
12:F:524:ARG:NH1	12:F:525:GLU:O	2.42	0.52
2:B:146:GLN:HG2	9:5:44:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:276:MET:HG3	9:5:328:ILE:HB	1.90	0.52
10:6:308:SER:O	10:6:347:ASN:ND2	2.42	0.52
2:B:32:THR:OG1	2:B:33:THR:N	2.42	0.52
8:4:425:ASP:OD2	10:6:280:ARG:NH1	2.42	0.52
12:F:494:LEU:HB2	12:F:502:VAL:HG23	1.90	0.52
9:5:336:ASP:OD1	9:5:336:ASP:N	2.43	0.52
11:7:93:PHE:CD2	11:7:94:LEU:CG	2.93	0.52
2:B:171:ASP:OD1	2:B:171:ASP:N	2.40	0.52
11:7:93:PHE:CE2	11:7:94:LEU:CD2	2.89	0.52
1:A:28:ASN:ND2	1:A:119:ASP:OD1	2.42	0.52
5:c:224:LYS:HA	5:c:227:LYS:HB2	1.92	0.52
12:G:626:PHE:HB2	12:G:689:PHE:HE1	1.75	0.52
2:B:193:ARG:NH1	2:B:194:GLU:OE2	2.43	0.52
5:c:436:ASN:HD22	5:c:472:ARG:HD2	1.75	0.51
10:6:151:ILE:HD11	10:6:265:ILE:HG23	1.90	0.51
9:5:39:ARG:CZ	9:5:44:PHE:CD1	2.94	0.51
5:c:21:SER:OG	5:c:22:HIS:N	2.43	0.51
6:2:219:THR:HG22	6:2:225:SER:HB2	1.92	0.51
9:5:143:ALA:HB3	9:5:161:ARG:HH12	1.74	0.51
6:2:347:ILE:HG13	6:2:348:LEU:H	1.76	0.51
8:4:311:CYS:SG	8:4:312:LYS:N	2.84	0.51
8:4:330:GLY:HA3	8:4:401:GLU:HA	1.93	0.51
8:4:452:VAL:HG23	11:7:279:THR:HG22	1.92	0.50
12:F:839:ASP:O	12:F:843:ASN:ND2	2.43	0.50
2:B:105:GLU:OE2	2:B:155:LYS:NZ	2.41	0.50
12:G:883:LEU:O	12:G:913:LYS:NZ	2.43	0.50
12:E:482:ALA:HB1	12:E:743:TRP:HE1	1.76	0.50
11:7:228:ARG:HH12	11:7:328:PRO:HA	1.77	0.50
11:7:350:ASP:OD2	11:7:384:HIS:NE2	2.44	0.50
3:C:29:TYR:O	3:C:33:ASN:ND2	2.45	0.50
7:3:219:THR:OG1	7:3:220:THR:N	2.45	0.50
12:E:506:LYS:HG2	12:E:511:TYR:HE1	1.76	0.50
12:F:478:PRO:HB2	12:F:536:LEU:HD21	1.92	0.50
12:G:477:MET:HE3	12:G:478:PRO:HD2	1.93	0.50
12:G:601:ASN:HD21	12:G:605:VAL:HB	1.77	0.50
5:c:553:ILE:HD11	5:c:584:LEU:HB3	1.94	0.50
11:7:142:ILE:O	11:7:146:ARG:N	2.44	0.50
12:E:782:VAL:HG12	12:E:784:SER:H	1.77	0.50
10:6:309:PHE:H	10:6:318:VAL:CB	2.25	0.50
12:F:507:ASN:ND2	12:F:510:GLN:NE2	2.60	0.50
1:A:102:TRP:CD1	4:D:145:ARG:HH21	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:SER:OG	3:C:82:THR:N	2.44	0.49
8:4:238:THR:O	8:4:240:ASN:ND2	2.45	0.49
9:5:149:ARG:NH2	9:5:269:GLU:OE1	2.44	0.49
11:7:15:ASN:N	11:7:15:ASN:OD1	2.44	0.49
7:3:187:THR:CG2	7:3:259:GLN:NE2	2.41	0.49
7:3:130:THR:HG22	7:3:153:TRP:HB2	1.93	0.49
8:4:202:LYS:O	8:4:206:ARG:NH1	2.44	0.49
8:4:353:ASP:HB2	8:4:373:ARG:CB	2.42	0.49
5:c:341:SER:OG	5:c:342:ASN:N	2.45	0.49
9:5:261:ILE:HG22	9:5:263:GLU:H	1.78	0.49
4:D:281:VAL:HG23	4:D:282:ILE:HG23	1.93	0.49
6:2:245:ASN:HA	6:2:298:SER:HB3	1.95	0.49
12:E:909:SER:HA	12:E:912:LYS:HE2	1.94	0.49
3:C:52:ARG:HG3	3:C:114:LEU:HD11	1.95	0.49
7:3:214:TYR:OH	11:7:368:ALA:O	2.29	0.49
12:G:535:ASP:OD1	12:G:535:ASP:N	2.46	0.49
1:A:32:TYR:HA	1:A:93:ARG:HH12	1.77	0.49
12:E:885:LEU:HD21	12:G:605:VAL:HG21	1.94	0.49
12:G:778:MET:HB2	12:G:825:GLU:HG2	1.94	0.49
11:7:249:SER:OG	11:7:250:ASP:N	2.46	0.49
12:F:641:SER:OG	12:F:642:GLU:N	2.45	0.49
12:E:772:SER:OG	12:E:773:GLU:N	2.45	0.49
5:c:43:LYS:HG2	5:c:484:LEU:HD23	1.95	0.48
6:2:245:ASN:HD22	6:2:248:HIS:HD2	1.61	0.48
10:6:119:LEU:HD11	10:6:188:VAL:HG21	1.94	0.48
10:6:309:PHE:N	10:6:318:VAL:CB	2.76	0.48
12:E:702:ASN:HB3	12:E:724:SER:HB3	1.93	0.48
7:3:189:THR:HA	7:3:256:ILE:HG22	1.95	0.48
9:5:40:LEU:HD11	9:5:43:GLN:O	2.13	0.48
9:5:153:SER:O	9:5:153:SER:OG	2.29	0.48
5:c:246:THR:OG1	5:c:247:VAL:N	2.47	0.48
6:2:264:PRO:HA	6:2:267:MET:HB3	1.94	0.48
8:4:304:ARG:HE	8:4:423:LEU:HD11	1.78	0.48
12:F:543:GLY:HA2	12:F:558:PRO:HA	1.96	0.48
12:G:866:LEU:O	12:G:870:PHE:N	2.46	0.48
7:3:201:HIS:NE2	7:3:232:PRO:O	2.47	0.48
12:E:745:LEU:HD11	12:E:755:ILE:HD11	1.95	0.48
2:B:112:PHE:CZ	2:B:173:LEU:HD11	2.49	0.48
8:4:271:ILE:HG22	8:4:272:MET:HE2	1.95	0.48
3:C:89:LYS:HB2	7:3:104:ARG:HH11	1.78	0.48
5:c:80:SER:OG	5:c:81:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:39:ARG:HH22	7:3:136:MET:HE2	1.77	0.48
7:3:235:ASP:HB2	7:3:241:LEU:HD11	1.95	0.48
12:G:530:ASP:OD1	12:G:534:TYR:N	2.45	0.48
6:2:438:LEU:HD23	6:2:438:LEU:HA	1.79	0.47
7:3:101:ASP:OD1	7:3:104:ARG:NH2	2.46	0.47
9:5:24:ASN:OD1	9:5:24:ASN:N	2.47	0.47
10:6:287:LEU:HA	10:6:399:GLY:C	2.39	0.47
10:6:406:ASP:O	10:6:449:THR:OG1	2.32	0.47
12:F:588:VAL:HB	12:F:600:PHE:HB2	1.95	0.47
12:F:753[B]:ASN:N	12:F:753[B]:ASN:OD1	2.47	0.47
11:7:19:ASN:O	11:7:22:THR:OG1	2.27	0.47
12:F:537:CYS:SG	12:F:538:PHE:N	2.87	0.47
7:3:97:ILE:HA	7:3:156:SER:HB3	1.96	0.47
7:3:263:GLU:OE1	7:3:291:ARG:NH1	2.47	0.47
9:5:206:SER:OG	9:5:207:LEU:N	2.47	0.47
9:5:260:GLU:OE2	9:5:272:ARG:N	2.44	0.47
12:E:716:SER:O	12:G:653:ARG:NH1	2.48	0.47
1:A:153:GLY:O	4:D:141:ARG:NH1	2.48	0.47
4:D:258:VAL:HG23	4:D:266:GLU:HA	1.97	0.47
7:3:190:SER:OG	7:3:191:LEU:N	2.45	0.47
11:7:67:LEU:HD21	11:7:125:MET:HA	1.96	0.47
12:F:617:ALA:HB3	12:F:628:VAL:HB	1.96	0.47
12:F:866:LEU:HD12	12:F:869:LEU:HD13	1.96	0.47
12:F:533:GLY:O	12:F:548:GLN:NE2	2.48	0.47
4:D:221:GLU:O	4:D:221:GLU:HG3	2.15	0.47
12:G:514:THR:O	12:G:514:THR:OG1	2.31	0.47
4:D:269:LEU:HD13	4:D:275:TYR:HD2	1.80	0.47
12:G:883:LEU:HD12	12:G:913:LYS:HE3	1.97	0.47
11:7:72:ASN:HA	11:7:130:LYS:HB2	1.97	0.46
12:G:631:SER:OG	12:G:634:HIS:N	2.42	0.46
3:C:170:GLU:HG3	3:C:172:MET:H	1.79	0.46
9:5:319:SER:O	9:5:319:SER:OG	2.33	0.46
10:6:356:TRP:HZ3	10:6:358:LYS:HB2	1.79	0.46
12:G:889:LEU:O	12:G:921:ARG:NH2	2.38	0.46
11:7:61:PRO:HG2	11:7:64:MET:HB2	1.96	0.46
12:F:722:LEU:HD13	12:F:776:ILE:HA	1.96	0.46
8:4:315:ARG:HH21	8:4:411:THR:HG22	1.80	0.46
10:6:287:LEU:HA	10:6:399:GLY:CA	2.45	0.46
11:7:265:CYS:SG	11:7:289:CYS:N	2.87	0.46
8:4:201:PHE:HE1	8:4:251:TYR:HB2	1.80	0.46
8:4:234:ARG:HG3	8:4:291:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:ILE:HD12	4:D:8:ILE:HD12	1.97	0.46
7:3:223:THR:N	9:5:246:GLU:OE1	2.41	0.46
12:F:724:SER:HB2	12:F:742:VAL:HG21	1.97	0.46
7:3:160:SER:O	7:3:160:SER:OG	2.33	0.46
11:7:25:LEU:HD11	11:7:120:ALA:HB1	1.97	0.46
12:G:498:GLU:HG2	12:G:499:VAL:HG13	1.97	0.46
9:5:143:ALA:H	9:5:161:ARG:NH1	2.13	0.46
12:F:592:THR:OG1	12:F:593:SER:N	2.49	0.46
8:4:346:PHE:HB2	8:4:389:CYS:HB3	1.99	0.45
4:D:253:LYS:HG3	4:D:254:PRO:HD3	1.98	0.45
1:A:84:ARG:HH21	4:D:217:ASN:HB2	1.82	0.45
12:F:573:GLN:HB2	12:F:576:GLU:HG3	1.98	0.45
12:G:722:LEU:HD13	12:G:776:ILE:HG13	1.97	0.45
1:A:31:MET:HA	1:A:122:ASN:HB3	1.97	0.45
4:D:142:SER:O	4:D:142:SER:OG	2.35	0.45
5:c:8:PHE:HB3	5:c:258:LEU:HD12	1.99	0.45
8:4:373:ARG:N	8:4:373:ARG:HD3	2.29	0.45
8:4:432:ARG:O	8:4:469:VAL:C	2.60	0.45
9:5:143:ALA:H	9:5:161:ARG:CZ	2.30	0.45
10:6:287:LEU:CA	10:6:399:GLY:HA3	2.45	0.45
4:D:202:MET:HE2	4:D:202:MET:HB3	1.82	0.45
8:4:294:ASP:CG	8:4:295:GLU:N	2.74	0.45
10:6:297:THR:HA	10:6:359:VAL:HG12	1.98	0.45
6:2:438:LEU:HB3	6:2:441:LYS:HB2	1.99	0.45
10:6:270:LEU:HD12	10:6:289:SER:HB3	1.97	0.45
12:F:507:ASN:HB2	12:F:510:GLN:HG3	1.99	0.45
12:G:858:LEU:O	12:G:862:TYR:N	2.48	0.45
8:4:289:LEU:HD23	8:4:293:LEU:HD23	1.80	0.45
8:4:371:CYS:O	8:4:374:ILE:HA	2.17	0.45
12:F:652:LYS:NZ	12:F:713:PRO:O	2.48	0.45
1:A:175:GLN:OE1	1:A:177:GLU:N	2.46	0.45
5:c:218:ASN:O	5:c:221:SER:OG	2.32	0.45
7:3:152:PRO:HB2	7:3:154:LYS:HG3	1.99	0.45
9:5:178:TYR:HE1	9:5:191:SER:HB2	1.82	0.44
9:5:193:THR:O	9:5:193:THR:OG1	2.34	0.44
9:5:259:GLN:HE21	9:5:271:PRO:HB2	1.82	0.44
12:G:861:ALA:HA	12:G:864:LYS:HD2	1.98	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.83	0.44
5:c:229:GLN:HA	5:c:232:GLU:HG2	1.98	0.44
12:F:690:SER:OG	12:F:693:GLY:N	2.41	0.44
7:3:261:MET:HE2	7:3:261:MET:HB3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:265:VAL:HA	9:5:266:PRO:HD2	1.71	0.44
12:F:694:ASP:OD1	12:F:710:TRP:NE1	2.42	0.44
6:2:439:ASN:OD1	6:2:439:ASN:N	2.50	0.44
7:3:114:ILE:HG22	7:3:115:LEU:HD23	1.98	0.44
6:2:317:LEU:HD12	6:2:317:LEU:HA	1.88	0.44
12:F:619:THR:OG1	12:F:620:ALA:N	2.51	0.44
12:G:691:SER:HB2	12:G:749:TYR:HE2	1.83	0.44
12:G:887:HIS:O	12:G:921:ARG:NH2	2.50	0.44
1:A:148:ASP:OD1	1:A:148:ASP:N	2.50	0.44
3:C:25:PRO:HA	3:C:37:PRO:HA	2.00	0.44
1:A:182:ASN:HB3	5:c:74:LEU:HD13	2.00	0.44
12:F:484:THR:HG23	12:F:492:ARG:HB2	2.00	0.44
2:B:119:TRP:CD1	2:B:120:LEU:HG	2.53	0.44
12:F:553:GLN:HE21	12:F:567:THR:HG21	1.83	0.44
12:G:754:CYS:N	12:G:772:SER:O	2.43	0.44
6:2:268:LEU:HD21	6:2:297:ILE:HD11	2.00	0.43
6:2:340:ASN:HB3	6:2:374:ARG:H	1.82	0.43
9:5:65:MET:HE2	9:5:139:LEU:HD13	1.99	0.43
11:7:88:TYR:OH	11:7:92:LYS:NZ	2.48	0.43
1:A:48:ARG:HE	1:A:48:ARG:HB2	1.61	0.43
10:6:126:SER:OG	10:6:131:GLU:OE2	2.35	0.43
11:7:80:ILE:HG12	11:7:117:PHE:HE2	1.83	0.43
12:F:534:TYR:HB3	12:F:546:PHE:HB3	2.00	0.43
12:G:727:GLU:HA	12:G:730:LYS:HE3	1.99	0.43
12:F:888:GLU:N	12:F:888:GLU:OE1	2.51	0.43
2:B:171:ASP:HA	4:D:273:SER:HB2	2.00	0.43
5:c:396:LEU:HD23	5:c:396:LEU:HA	1.88	0.43
9:5:170:SER:OG	9:5:171:VAL:N	2.51	0.43
11:7:366:LEU:H	11:7:367:LYS:HZ2	1.65	0.43
3:C:135:LEU:HD21	3:C:169:LEU:HD21	2.00	0.43
5:c:537:ASP:OD1	5:c:537:ASP:N	2.51	0.43
5:c:28:VAL:HG22	5:c:57:GLN:HG3	1.99	0.43
5:c:155:GLN:H	5:c:155:GLN:HG2	1.66	0.43
12:E:631:SER:HG	12:E:634:HIS:H	1.62	0.43
12:F:889:LEU:HD22	12:F:894:ALA:HB1	2.00	0.43
3:C:27:LEU:HB2	3:C:38:ILE:HD11	2.00	0.43
12:F:909:SER:HA	12:F:912:LYS:HE2	2.00	0.43
11:7:319:SER:O	11:7:319:SER:OG	2.34	0.43
12:E:663:ASN:OD1	12:E:663:ASN:N	2.45	0.43
12:G:889:LEU:HD22	12:G:894:ALA:HB1	2.01	0.43
2:B:112:PHE:HD1	2:B:152:ARG:NH1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:180:ILE:HD12	8:4:185:VAL:HB	1.99	0.43
12:F:592:THR:HG23	12:F:594:LEU:H	1.84	0.43
3:C:39:THR:O	3:C:42:THR:OG1	2.33	0.42
5:c:222:LYS:O	5:c:226:ARG:N	2.45	0.42
10:6:398:THR:OG1	10:6:456:ALA:CA	2.60	0.42
11:7:89:GLN:NE2	11:7:102:LEU:H	2.16	0.42
12:F:570:ILE:HD13	12:F:570:ILE:HA	1.92	0.42
10:6:109:GLU:HA	10:6:112:ARG:HB3	2.02	0.42
12:E:642:GLU:OE1	12:E:651:TYR:OH	2.35	0.42
12:F:732:SER:HB2	12:F:735:LYS:HB2	2.01	0.42
3:C:85:MET:HE3	3:C:85:MET:HB3	1.89	0.42
12:F:587:ARG:HA	12:F:601:ASN:HA	2.01	0.42
9:5:279:ASP:OD2	9:5:280:ARG:N	2.52	0.42
12:F:493:TYR:CZ	12:F:768:LEU:HD11	2.55	0.42
5:c:569:LEU:HD23	5:c:569:LEU:HA	1.85	0.42
8:4:371:CYS:SG	8:4:372:GLU:N	2.92	0.42
9:5:49:GLN:HE22	9:5:62:THR:HB	1.83	0.42
10:6:288:LEU:O	10:6:399:GLY:CA	2.61	0.42
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.81	0.42
5:c:338:PHE:HD1	5:c:344:VAL:HG11	1.85	0.42
9:5:164:GLY:HA2	9:5:261:ILE:HG13	2.01	0.42
9:5:296:GLY:HA2	9:5:331:LEU:HD23	2.02	0.42
12:F:492:ARG:NH1	12:F:493:TYR:O	2.53	0.42
1:A:84:ARG:HA	1:A:84:ARG:HD3	1.78	0.42
7:3:278:LEU:O	7:3:279:ASP:OD1	2.33	0.42
8:4:437:GLY:HA3	8:4:463:VAL:HA	2.01	0.42
6:2:411:LEU:HD23	6:2:411:LEU:HA	1.92	0.42
7:3:171:LEU:HD13	7:3:298:PHE:HE1	1.84	0.42
9:5:258:LEU:HB2	9:5:276:MET:HE1	2.01	0.42
12:G:783:LYS:HE3	12:G:783:LYS:HB2	1.86	0.42
5:c:6:SER:OG	5:c:144:ASP:OD1	2.29	0.42
12:G:833:LEU:HA	12:G:836:LEU:HD12	2.01	0.42
3:C:27:LEU:HD21	3:C:29:TYR:HD2	1.85	0.42
3:C:44:LEU:HD23	3:C:44:LEU:HA	1.90	0.42
5:c:41:ALA:HB1	5:c:255:ILE:HD12	2.02	0.42
12:F:507:ASN:CB	12:F:510:GLN:HG3	2.50	0.42
12:F:601:ASN:OD1	12:F:605:VAL:N	2.43	0.42
12:F:896:THR:OG1	12:F:918:ARG:NH2	2.53	0.42
12:G:519:ASP:OD2	12:G:519:ASP:N	2.53	0.42
1:A:90:GLN:O	1:A:94:THR:OG1	2.38	0.41
8:4:322:ILE:HD13	8:4:322:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:273:ASN:OD1	9:5:273:ASN:N	2.53	0.41
12:G:659:MET:SD	12:G:660:SER:N	2.93	0.41
12:G:883:LEU:HB2	12:G:913:LYS:HD2	2.02	0.41
11:7:284:CYS:SG	11:7:296:GLY:N	2.93	0.41
11:7:71:ALA:HB2	11:7:125:MET:HE3	2.02	0.41
12:E:577:ARG:O	12:E:592:THR:OG1	2.31	0.41
10:6:165:ALA:HA	10:6:168:MET:HE2	2.02	0.41
12:F:560:ASP:HB2	12:F:562:ILE:HG23	2.02	0.41
5:c:388:LEU:HD12	5:c:388:LEU:HA	1.85	0.41
12:F:530:ASP:OD1	12:F:533:GLY:N	2.45	0.41
12:F:912:LYS:HB2	12:F:912:LYS:HE3	1.87	0.41
6:2:203:VAL:O	6:2:206:THR:OG1	2.32	0.41
1:A:35:ASP:O	1:A:39:ASN:ND2	2.54	0.41
5:c:502:LEU:HD12	5:c:502:LEU:HA	1.90	0.41
2:B:138:ILE:H	2:B:138:ILE:HG12	1.70	0.41
4:D:286:LEU:HA	4:D:286:LEU:HD23	1.87	0.41
11:7:92:LYS:HA	11:7:95:GLN:O	2.20	0.41
12:G:827:TYR:CZ	12:G:866:LEU:HD21	2.56	0.41
5:c:351:TRP:HB2	5:c:511:VAL:HG22	2.01	0.41
8:4:413:HIS:HD2	8:4:415:ILE:HG12	1.86	0.41
12:G:892:ASP:OD1	12:G:918:ARG:NH2	2.53	0.41
2:B:60:LEU:HD23	2:B:60:LEU:HA	1.94	0.40
6:2:348:LEU:HD23	6:2:351:PHE:HE2	1.86	0.40
8:4:375:ASP:O	8:4:379:PRO:O	2.39	0.40
12:F:694:ASP:HA	12:F:695:PRO:HD3	1.91	0.40
1:A:175:GLN:OE1	1:A:176:THR:N	2.54	0.40
7:3:25:VAL:HG13	7:3:128:ALA:HB2	2.02	0.40
8:4:467:LYS:HE3	8:4:468:LYS:HG3	2.03	0.40
12:E:479:PHE:O	12:E:580:SER:OG	2.34	0.40
12:F:601:ASN:OD1	12:F:601:ASN:N	2.54	0.40
12:G:496:MET:HB2	12:G:496:MET:HE3	1.79	0.40
3:C:16:PHE:HA	3:C:17:PRO:HD3	1.85	0.40
3:C:48:LEU:HD12	3:C:48:LEU:HA	1.93	0.40
5:c:298:GLU:OE1	5:c:301:ARG:NH1	2.54	0.40
7:3:222:THR:OG1	9:5:246:GLU:OE1	2.30	0.40
8:4:294:ASP:OD2	8:4:297:GLU:CG	2.69	0.40
8:4:358:VAL:HG13	8:4:365:ILE:HD11	2.03	0.40
9:5:36:LEU:HA	9:5:47:ARG:HD2	2.02	0.40
12:E:572:LEU:HD23	12:E:572:LEU:HA	1.97	0.40
12:E:673:ASN:HD21	12:E:762:ILE:HG23	1.85	0.40
12:F:516:SER:HA	12:F:525:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:760:LYS:HB3	12:F:760:LYS:HE2	1.79	0.40
3:C:101:ASN:ND2	3:C:103:HIS:O	2.36	0.40
5:c:129:TRP:HZ3	5:c:240:TYR:HB3	1.86	0.40
5:c:291:LEU:HD23	5:c:291:LEU:HA	1.90	0.40
6:2:245:ASN:HD22	6:2:248:HIS:CD2	2.39	0.40
8:4:256:ASP:OD1	8:4:256:ASP:N	2.53	0.40
8:4:262:LEU:HD23	8:4:325:LEU:HD12	2.03	0.40
8:4:442:ILE:HD13	8:4:442:ILE:HA	1.90	0.40
4:D:234:GLY:HA2	4:D:235:PRO:HD3	1.91	0.40
10:6:357:GLN:HE21	10:6:387:GLU:H	1.69	0.40
12:E:576:GLU:HG3	12:E:594:LEU:HG	2.03	0.40
12:E:712:SER:OG	12:E:715:GLU:OE1	2.33	0.40
12:E:898:ALA:HA	12:E:901:ILE:HD12	2.03	0.40
12:F:582:ALA:HB3	12:F:589:ILE:HB	2.02	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	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	24	57
2	B	182/213 (85%)	149 (82%)	32 (18%)	1 (0%)	24	57
3	C	151/194 (78%)	136 (90%)	14 (9%)	1 (1%)	18	51
4	D	222/294 (76%)	197 (89%)	24 (11%)	1 (0%)	24	57
5	c	543/650 (84%)	482 (89%)	61 (11%)	0	100	100
6	2	258/868 (30%)	218 (84%)	40 (16%)	0	100	100
7	3	262/971 (27%)	221 (84%)	40 (15%)	1 (0%)	30	62
8	4	281/933 (30%)	247 (88%)	31 (11%)	3 (1%)	11	41
9	5	242/775 (31%)	214 (88%)	28 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	6	267/1017 (26%)	221 (83%)	45 (17%)	1 (0%)	30	62
11	7	318/845 (38%)	282 (89%)	36 (11%)	0	100	100
12	E	418/927 (45%)	392 (94%)	26 (6%)	0	100	100
12	F	428/927 (46%)	404 (94%)	24 (6%)	0	100	100
12	G	418/927 (45%)	398 (95%)	20 (5%)	0	100	100
All	All	4196/9749 (43%)	3741 (89%)	446 (11%)	9 (0%)	44	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	114	GLU
8	4	375	ASP
8	4	378	GLU
7	3	281	ASP
3	C	101	ASN
8	4	379	PRO
10	6	322	GLU
4	D	222	PRO
1	A	30	PRO

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	193/193 (100%)	193 (100%)	0	100	100
2	B	176/198 (89%)	176 (100%)	0	100	100
3	C	144/173 (83%)	143 (99%)	1 (1%)	76	77
4	D	221/279 (79%)	221 (100%)	0	100	100
5	c	499/586 (85%)	498 (100%)	1 (0%)	87	87
6	2	212/770 (28%)	212 (100%)	0	100	100
7	3	236/835 (28%)	233 (99%)	3 (1%)	61	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	4	260/848 (31%)	259 (100%)	1 (0%)	84	83
9	5	237/688 (34%)	233 (98%)	4 (2%)	53	67
10	6	210/886 (24%)	209 (100%)	1 (0%)	81	81
11	7	296/753 (39%)	294 (99%)	2 (1%)	76	77
12	E	376/825 (46%)	376 (100%)	0	100	100
12	F	384/825 (46%)	384 (100%)	0	100	100
12	G	375/825 (46%)	375 (100%)	0	100	100
All	All	3819/8684 (44%)	3806 (100%)	13 (0%)	84	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	95	LEU
5	c	601	ILE
7	3	170	THR
7	3	230	ILE
7	3	279	ASP
8	4	466	VAL
9	5	40	LEU
9	5	45	ILE
9	5	159	ILE
9	5	162	LEU
10	6	129	THR
11	7	207	LEU
11	7	258	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	58	GLN
1	A	121	ASN
1	A	201	GLN
2	B	61	ASN
2	B	118	ASN
2	B	164	ASN
3	C	21	GLN
3	C	33	ASN

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Mol	Chain	Res	Type
3	C	103	HIS
4	D	207	GLN
5	c	26	GLN
5	c	133	ASN
5	c	218	ASN
5	c	254	GLN
5	c	266	ASN
6	2	245	ASN
6	2	294	HIS
6	2	454	ASN
7	3	164	HIS
7	3	259	GLN
7	3	310	ASN
8	4	387	ASN
9	5	43	GLN
9	5	49	GLN
9	5	64	ASN
9	5	254	GLN
9	5	259	GLN
9	5	284	ASN
10	6	149	ASN
10	6	156	GLN
10	6	274	HIS
10	6	347	ASN
11	7	107	GLN
11	7	112	HIS
11	7	150	ASN
11	7	210	ASN
11	7	320	GLN
11	7	379	GLN
12	E	621	GLN
12	E	673	ASN
12	E	702	ASN
12	E	877	GLN
12	E	916	ASN
12	E	924	GLN
12	F	507	ASN
12	F	553	GLN
12	F	573	GLN
12	F	665	ASN
12	F	877	GLN
12	F	915	ASN

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Mol	Chain	Res	Type
12	G	527	HIS
12	G	678	ASN
12	G	859	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

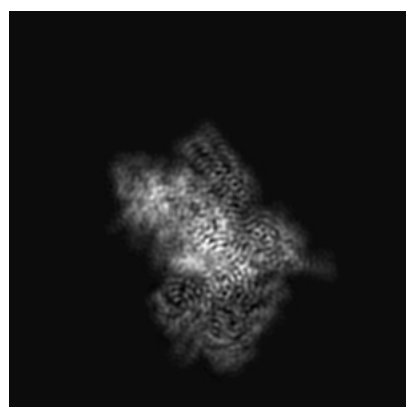
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20471. These allow visual inspection of the internal detail of the map and identification of artifacts.

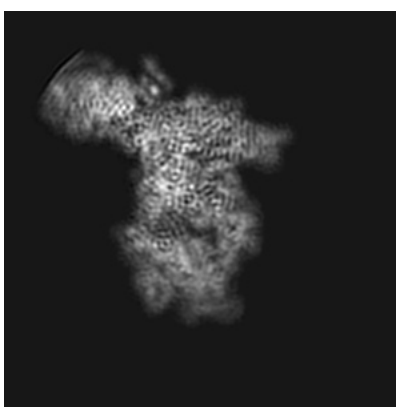
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

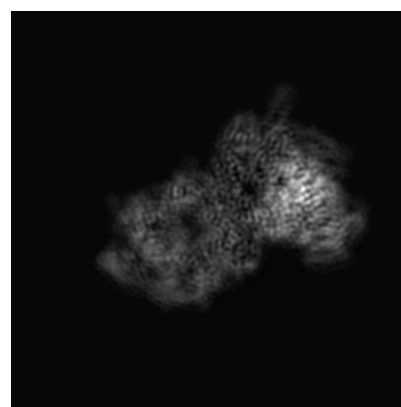
6.1.1 Primary map



X



Y



Z

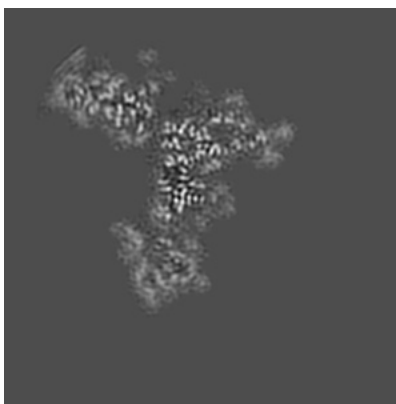
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

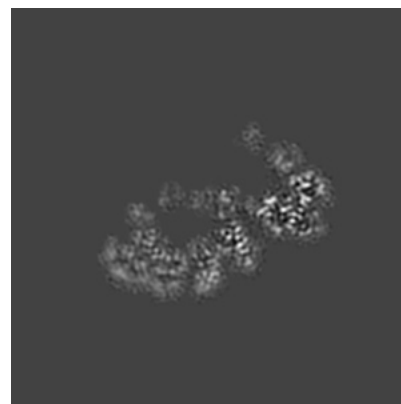
6.2.1 Primary map



X Index: 140



Y Index: 140

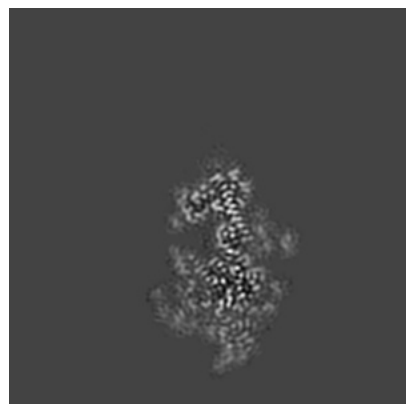


Z Index: 140

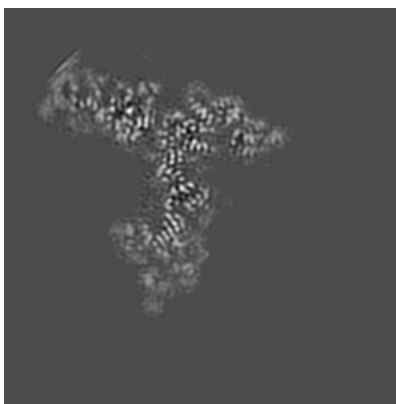
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

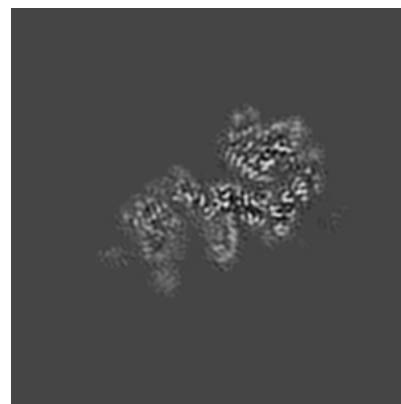
6.3.1 Primary map



X Index: 204



Y Index: 146

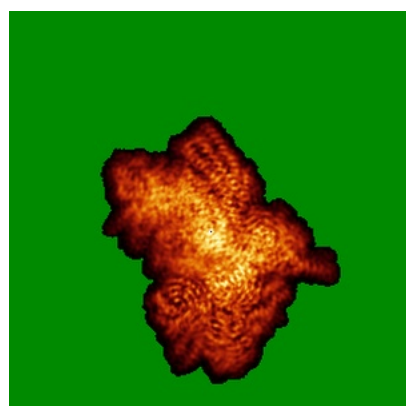


Z Index: 121

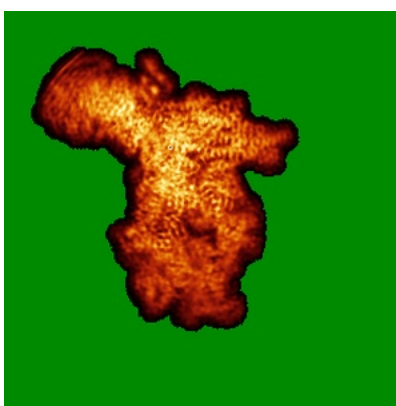
The images above show the largest variance slices of the map in three orthogonal directions.

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

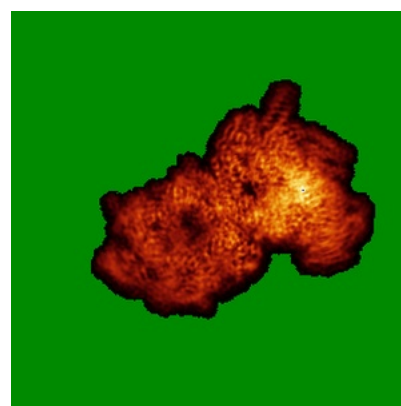
6.4.1 Primary map



X



Y

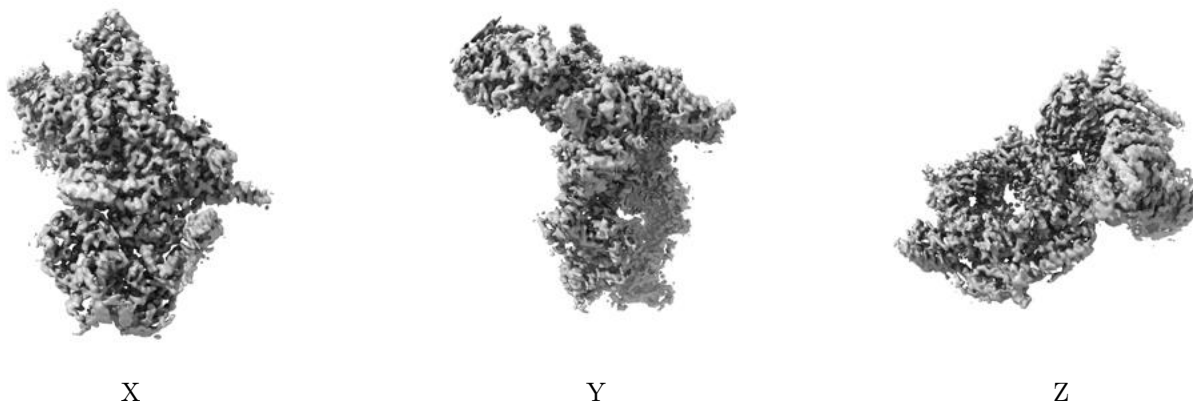


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

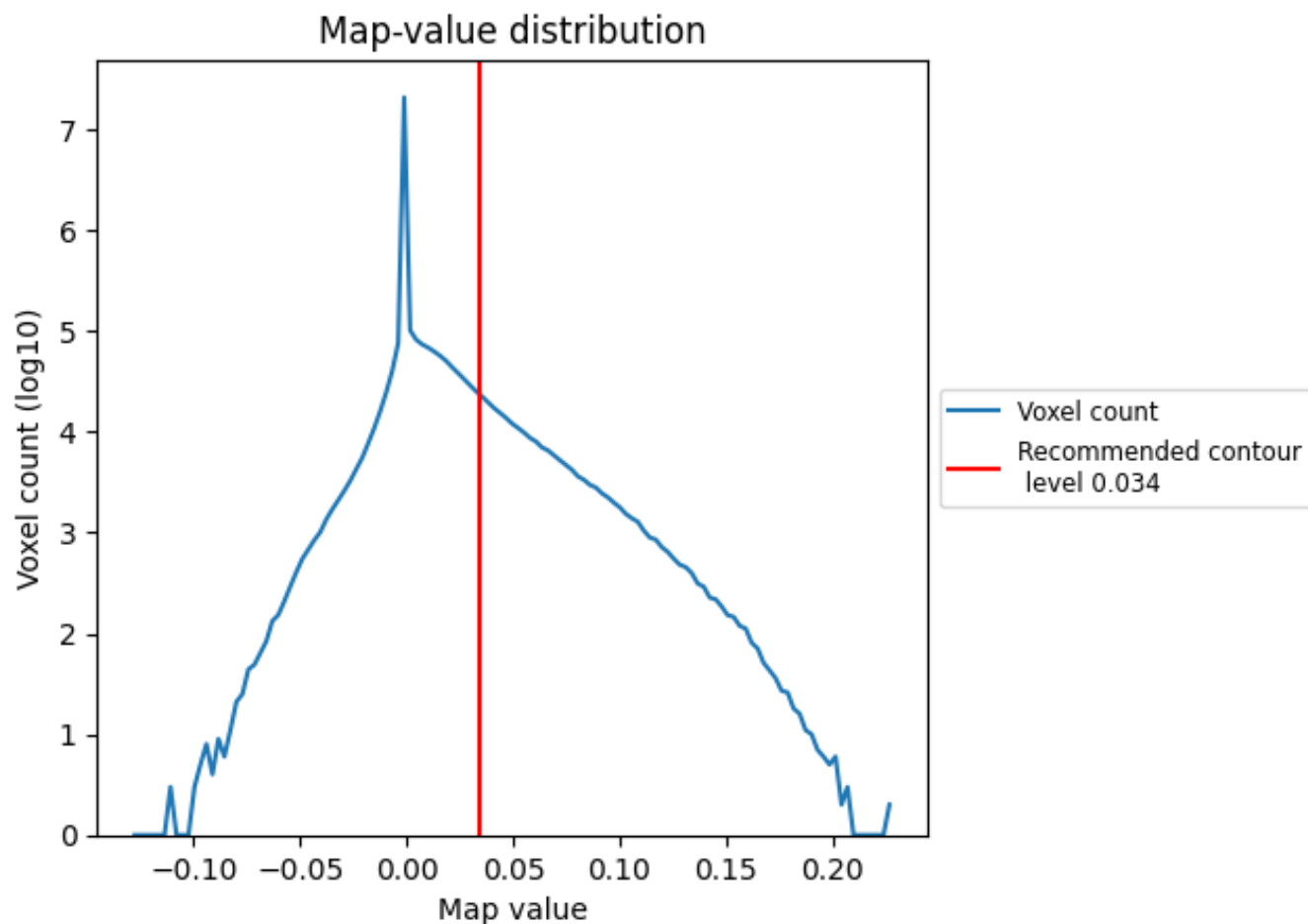
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

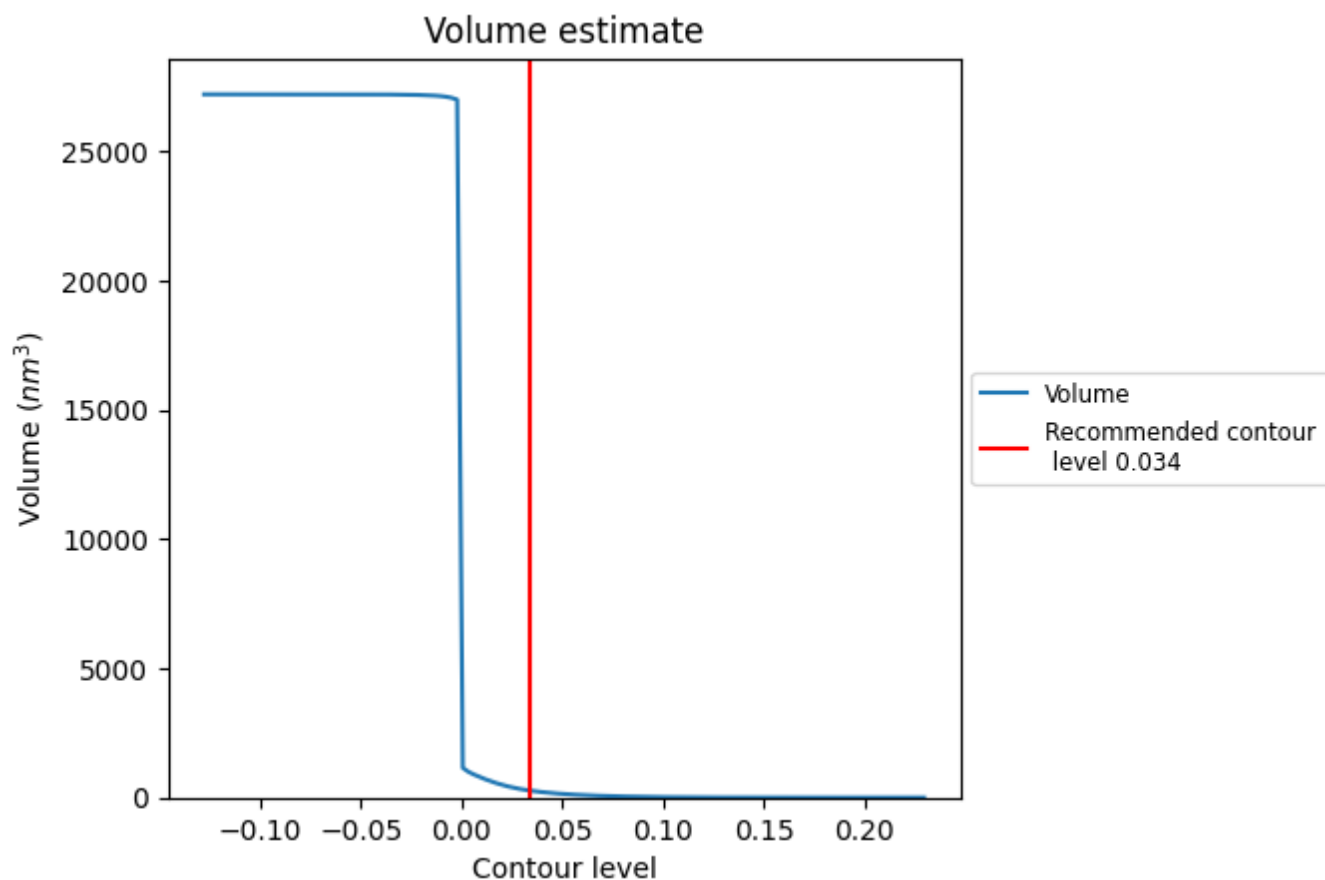
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

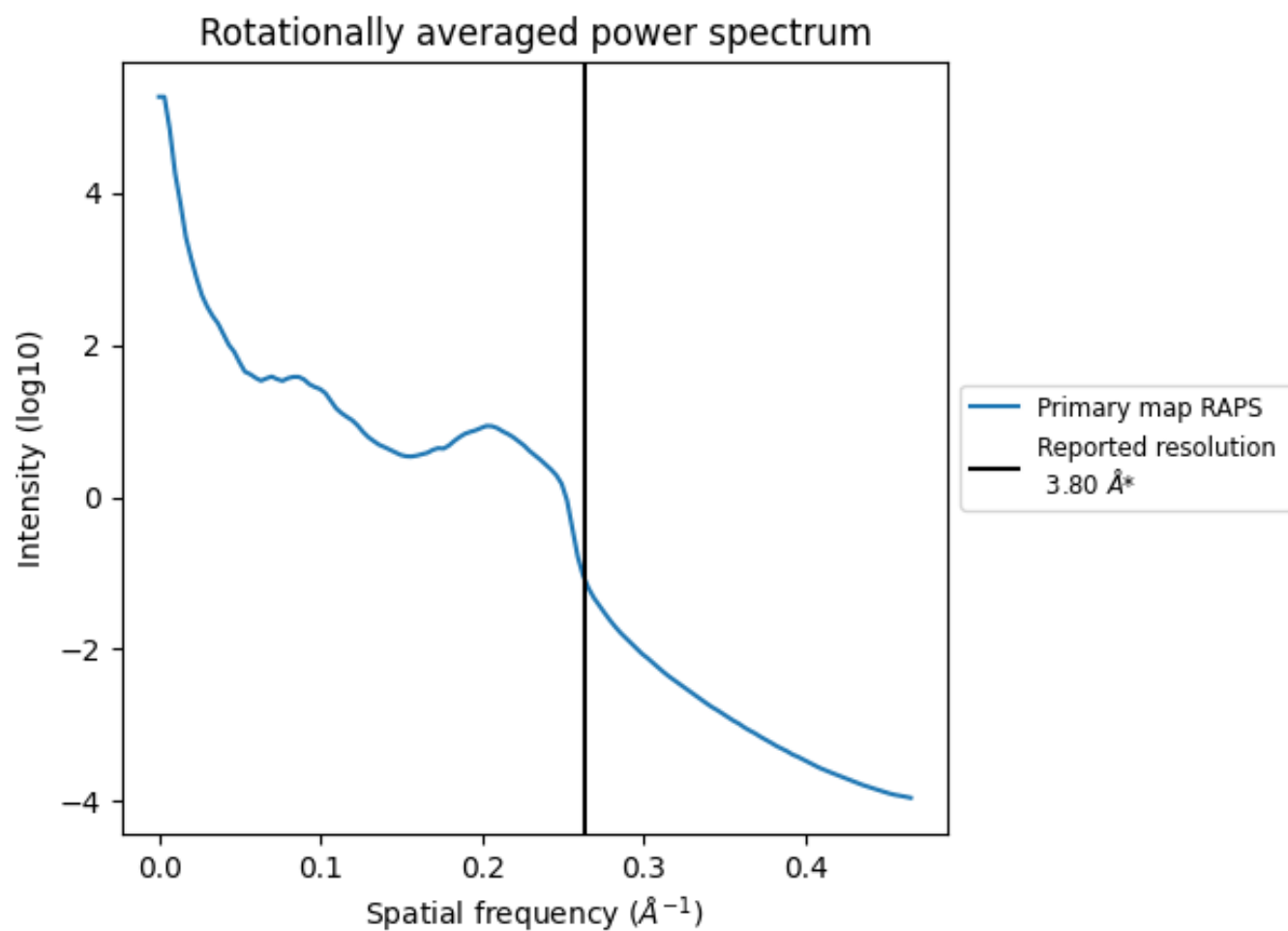
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 Å⁻¹

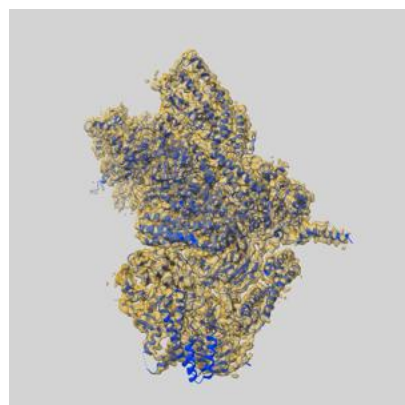
8 Fourier-Shell correlation ⓘ

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

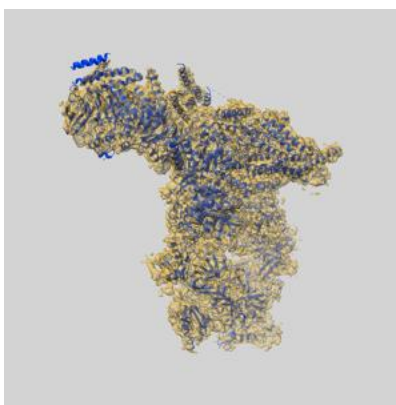
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20471 and PDB model 6PTJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

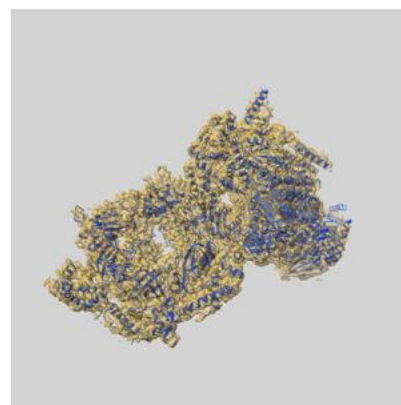
9.1 Map-model overlay [i](#)



X



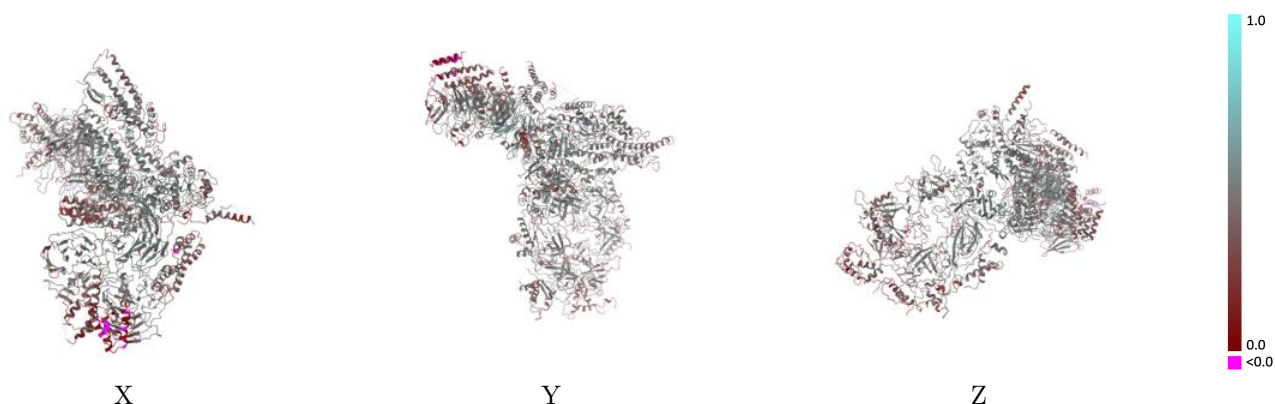
Y



Z

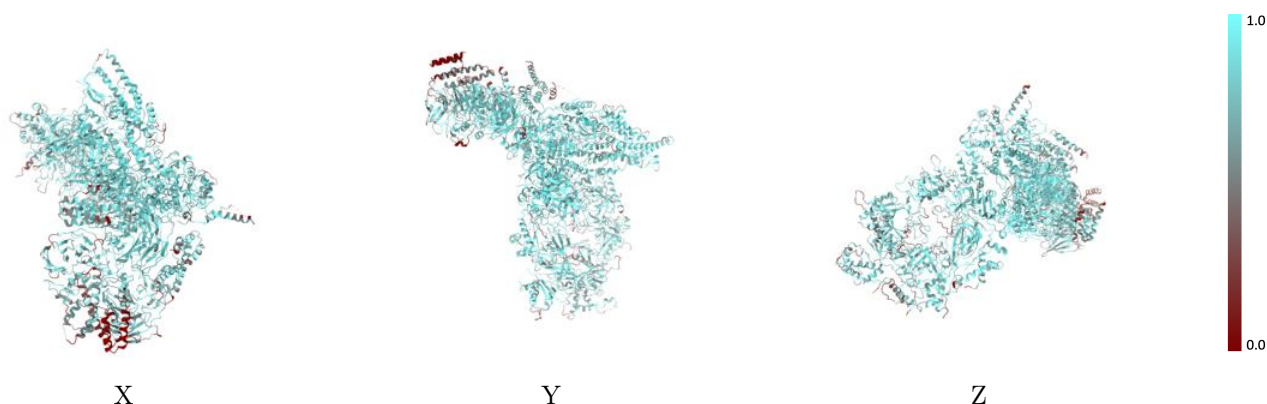
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



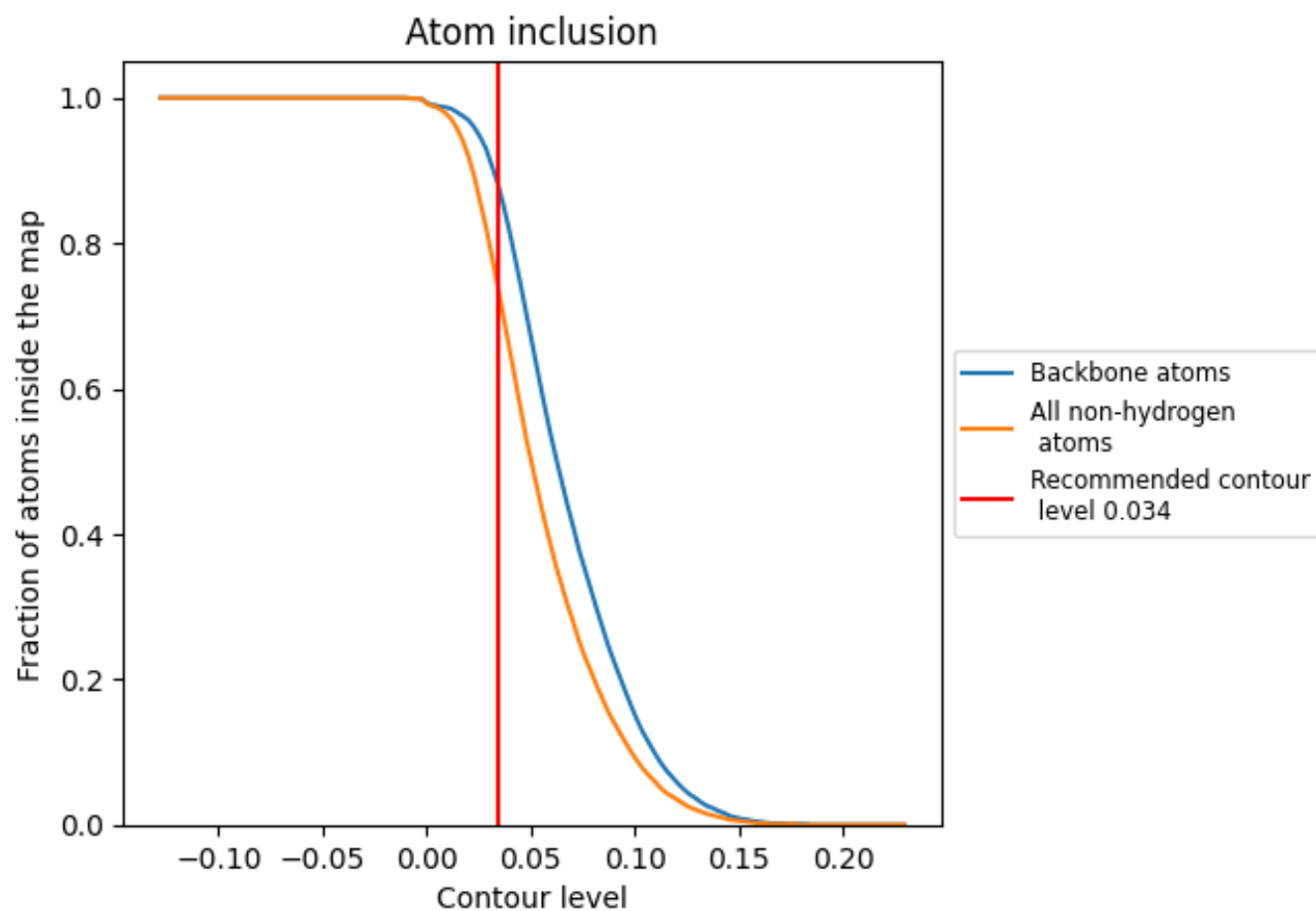
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 74% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.4140
2	 0.7350	 0.4080
3	 0.7820	 0.4310
4	 0.6830	 0.3360
5	 0.8300	 0.4740
6	 0.7020	 0.3820
7	 0.6650	 0.3640
A	 0.7460	 0.4030
B	 0.8420	 0.4790
C	 0.8430	 0.4660
D	 0.7880	 0.4380
E	 0.8070	 0.4620
F	 0.6930	 0.3990
G	 0.6120	 0.3620
c	 0.8000	 0.4380

