



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 02:01 pm BST

PDB ID : 28OP / pdb_000028op
EMDB ID : EMD-56683
Title : Structure of the human inner kinetochore CCAN and CENP-C bound to DNA
Authors : Yu, C.; Barford, D.
Deposited on : 2026-02-11
Resolution : 2.70 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

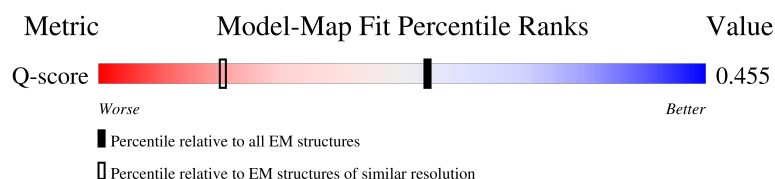
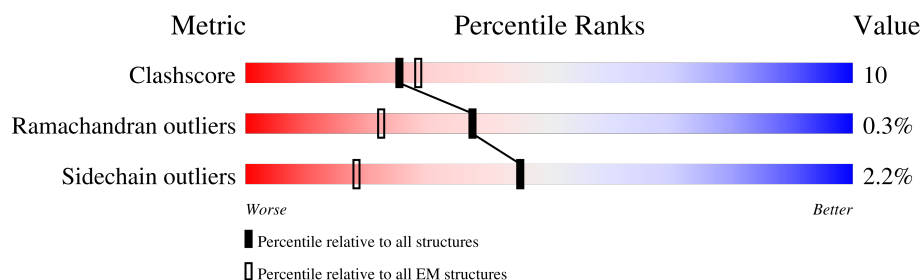
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	M	180	<div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	S	138	<div> <div>11%</div> <div>66%</div> <div>21%</div> <div>13%</div> </div>
3	T	777	<div> <div>10%</div> <div>86%</div> </div>
4	U	211	<div> <div>54%</div> <div>24%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	V	212	
6	W	88	
7	X	81	
8	Y	212	
9	H	247	
10	I	762	
11	K	269	
12	L	348	
13	N	347	
14	O	300	
15	P	288	
16	Q	215	
17	R	177	
18	C	775	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 27973 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 Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	172	Total	C	N	O	S	0	0
			1325	839	236	243	7		

- Molecule 2 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	120	Total	C	N	O	S	0	0
			982	607	174	195	6		

- Molecule 3 is a protein called Methylated-DNA--protein-cysteine methyltransferase, Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	112	Total	C	N	O	S	0	0
			915	586	163	159	7		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-215	MET	-	initiating methionine	UNP P16455
T	-214	SER	-	expression tag	UNP P16455
T	-213	TYR	-	expression tag	UNP P16455
T	-212	TYR	-	expression tag	UNP P16455
T	-211	HIS	-	expression tag	UNP P16455
T	-210	HIS	-	expression tag	UNP P16455
T	-209	HIS	-	expression tag	UNP P16455
T	-208	HIS	-	expression tag	UNP P16455
T	-207	HIS	-	expression tag	UNP P16455
T	-206	HIS	-	expression tag	UNP P16455
T	-205	ASP	-	expression tag	UNP P16455
T	-204	TYR	-	expression tag	UNP P16455
T	-203	ASP	-	expression tag	UNP P16455
T	-202	ILE	-	expression tag	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-201	PRO	-	expression tag	UNP P16455
T	-200	THR	-	expression tag	UNP P16455
T	-199	THR	-	expression tag	UNP P16455
T	-198	GLU	-	expression tag	UNP P16455
T	-197	ASN	-	expression tag	UNP P16455
T	-196	LEU	-	expression tag	UNP P16455
T	-195	TYR	-	expression tag	UNP P16455
T	-194	PHE	-	expression tag	UNP P16455
T	-193	GLN	-	expression tag	UNP P16455
T	-192	GLY	-	expression tag	UNP P16455
T	-162	ARG	GLU	conflict	UNP P16455
T	-160	ILE	LYS	conflict	UNP P16455
T	-159	PHE	LEU	conflict	UNP P16455
T	-130	ALA	CYS	conflict	UNP P16455
T	-77	SER	GLN	conflict	UNP P16455
T	-76	HIS	GLN	conflict	UNP P16455
T	-67	ALA	LYS	conflict	UNP P16455
T	-65	THR	ALA	conflict	UNP P16455
T	-64	ALA	ARG	conflict	UNP P16455
T	-61	LYS	GLY	conflict	UNP P16455
T	-60	THR	GLY	conflict	UNP P16455
T	-58	LEU	MET	conflict	UNP P16455
T	-57	SER	ARG	conflict	UNP P16455
T	-42	GLN	CYS	conflict	UNP P16455
T	-41	GLY	SER	conflict	UNP P16455
T	-40	ASP	SER	conflict	UNP P16455
T	-39	LEU	GLY	conflict	UNP P16455
T	-38	ASP	ALA	conflict	UNP P16455
T	-35	GLY	ASN	conflict	UNP P16455
T	-33	GLU	SER	conflict	UNP P16455
T	-9	SER	-	linker	UNP P16455
T	-8	ASP	-	linker	UNP P16455
T	-7	LEU	-	linker	UNP P16455
T	-6	GLU	-	linker	UNP P16455
T	-5	VAL	-	linker	UNP P16455
T	-4	LEU	-	linker	UNP P16455
T	-3	PHE	-	linker	UNP P16455
T	-2	GLN	-	linker	UNP P16455
T	-1	GLY	-	linker	UNP P16455
T	0	PRO	-	linker	UNP P16455

- Molecule 4 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	166	Total	C	N	O	S	0	0
			1369	864	243	257	5		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	419	GLU	-	expression tag	UNP Q71F23
U	420	ASN	-	expression tag	UNP Q71F23
U	421	LEU	-	expression tag	UNP Q71F23
U	422	TYR	-	expression tag	UNP Q71F23
U	423	PHE	-	expression tag	UNP Q71F23
U	424	GLN	-	expression tag	UNP Q71F23
U	425	SER	-	expression tag	UNP Q71F23
U	426	TRP	-	expression tag	UNP Q71F23
U	427	SER	-	expression tag	UNP Q71F23
U	428	HIS	-	expression tag	UNP Q71F23
U	429	PRO	-	expression tag	UNP Q71F23
U	430	GLN	-	expression tag	UNP Q71F23
U	431	PHE	-	expression tag	UNP Q71F23
U	432	GLU	-	expression tag	UNP Q71F23
U	433	LYS	-	expression tag	UNP Q71F23
U	434	GLY	-	expression tag	UNP Q71F23
U	435	GLY	-	expression tag	UNP Q71F23
U	436	GLY	-	expression tag	UNP Q71F23
U	437	SER	-	expression tag	UNP Q71F23
U	438	GLY	-	expression tag	UNP Q71F23
U	439	GLY	-	expression tag	UNP Q71F23
U	440	GLY	-	expression tag	UNP Q71F23
U	441	SER	-	expression tag	UNP Q71F23
U	442	GLY	-	expression tag	UNP Q71F23
U	443	GLY	-	expression tag	UNP Q71F23
U	444	GLY	-	expression tag	UNP Q71F23
U	445	SER	-	expression tag	UNP Q71F23
U	446	TRP	-	expression tag	UNP Q71F23
U	447	SER	-	expression tag	UNP Q71F23
U	448	HIS	-	expression tag	UNP Q71F23
U	449	PRO	-	expression tag	UNP Q71F23
U	450	GLN	-	expression tag	UNP Q71F23
U	451	PHE	-	expression tag	UNP Q71F23
U	452	GLU	-	expression tag	UNP Q71F23
U	453	LYS	-	expression tag	UNP Q71F23

- Molecule 5 is a DNA chain called DNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	59	Total	C	N	O	P	0	0
			1220	580	224	357	59		

- Molecule 6 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	85	Total	C	N	O	S	0	0
			683	431	140	109	3		

- Molecule 7 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 8 is a DNA chain called DNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	61	Total	C	N	O	P	0	0
			1239	591	225	362	61		

- Molecule 9 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	205	Total	C	N	O	S	0	0
			1669	1047	289	322	11		

- Molecule 10 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	630	Total	C	N	O	S	0	0
			5096	3334	828	905	29		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	757	GLU	-	expression tag	UNP Q92674
I	758	ASN	-	expression tag	UNP Q92674
I	759	LEU	-	expression tag	UNP Q92674
I	760	TYR	-	expression tag	UNP Q92674
I	761	PHE	-	expression tag	UNP Q92674
I	762	GLN	-	expression tag	UNP Q92674

- Molecule 11 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	233	Total	C	N	O	S	0	0
			1926	1222	318	376	10		

- Molecule 12 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	313	Total	C	N	O	S	0	0
			2509	1632	410	453	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q8N0S6
L	-2	PRO	-	expression tag	UNP Q8N0S6
L	-1	LEU	-	expression tag	UNP Q8N0S6
L	0	GLY	-	expression tag	UNP Q8N0S6

- Molecule 13 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	319	Total	C	N	O	S	0	0
			2629	1688	456	475	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	340	SER	-	expression tag	UNP Q96H22
N	341	ASP	-	expression tag	UNP Q96H22
N	342	LEU	-	expression tag	UNP Q96H22
N	343	GLU	-	expression tag	UNP Q96H22
N	344	VAL	-	expression tag	UNP Q96H22
N	345	LEU	-	expression tag	UNP Q96H22
N	346	PHE	-	expression tag	UNP Q96H22
N	347	GLN	-	expression tag	UNP Q96H22

- Molecule 14 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	214	Total	C	N	O	S	0	0
			1664	1073	281	303	7		

- Molecule 15 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	224	Total	C	N	O	S	0	0
			1788	1141	310	329	8		

- Molecule 16 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	189	Total	C	N	O	S	0	0
			1514	945	256	302	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	54	MET	-	initiating methionine	UNP Q7L2Z9

- Molecule 17 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	80	Total	C	N	O	S	0	0
			649	412	105	125	7		

- Molecule 18 is a protein called Centromere protein C,Methylated-DNA--protein-cysteine methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	C	26	Total	C	N	O	0	0
			206	132	32	42		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	546	ASP	-	linker	UNP Q03188
C	547	LEU	-	linker	UNP Q03188
C	548	GLU	-	linker	UNP Q03188
C	549	VAL	-	linker	UNP Q03188
C	550	LEU	-	linker	UNP Q03188
C	551	PHE	-	linker	UNP Q03188
C	552	GLN	-	linker	UNP Q03188
C	553	GLY	-	linker	UNP Q03188
C	554	PRO	-	linker	UNP Q03188
C	555	LEU	-	linker	UNP Q03188
C	556	GLY	-	linker	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
C	586	ARG	GLU	conflict	UNP P16455
C	588	ILE	LYS	conflict	UNP P16455
C	589	PHE	LEU	conflict	UNP P16455
C	618	ALA	CYS	conflict	UNP P16455
C	671	SER	GLN	conflict	UNP P16455
C	672	HIS	GLN	conflict	UNP P16455
C	681	ALA	LYS	conflict	UNP P16455
C	683	THR	ALA	conflict	UNP P16455
C	684	ALA	ARG	conflict	UNP P16455
C	687	LYS	GLY	conflict	UNP P16455
C	688	THR	GLY	conflict	UNP P16455
C	690	LEU	MET	conflict	UNP P16455
C	691	SER	ARG	conflict	UNP P16455
C	706	GLN	CYS	conflict	UNP P16455
C	707	GLY	SER	conflict	UNP P16455
C	708	ASP	SER	conflict	UNP P16455
C	709	LEU	GLY	conflict	UNP P16455
C	710	ASP	ALA	conflict	UNP P16455
C	713	GLY	ASN	conflict	UNP P16455
C	715	GLU	SER	conflict	UNP P16455
C	739	GLU	-	expression tag	UNP P16455
C	740	ASN	-	expression tag	UNP P16455
C	741	LEU	-	expression tag	UNP P16455
C	742	TYR	-	expression tag	UNP P16455
C	743	PHE	-	expression tag	UNP P16455
C	744	GLN	-	expression tag	UNP P16455
C	745	SER	-	expression tag	UNP P16455
C	746	SER	-	expression tag	UNP P16455
C	747	ALA	-	expression tag	UNP P16455
C	748	TRP	-	expression tag	UNP P16455
C	749	SER	-	expression tag	UNP P16455
C	750	HIS	-	expression tag	UNP P16455
C	751	PRO	-	expression tag	UNP P16455
C	752	GLN	-	expression tag	UNP P16455
C	753	PHE	-	expression tag	UNP P16455
C	754	GLU	-	expression tag	UNP P16455
C	755	LYS	-	expression tag	UNP P16455
C	756	GLY	-	expression tag	UNP P16455
C	757	GLY	-	expression tag	UNP P16455
C	758	GLY	-	expression tag	UNP P16455
C	759	SER	-	expression tag	UNP P16455
C	760	GLY	-	expression tag	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
C	761	GLY	-	expression tag	UNP P16455
C	762	GLY	-	expression tag	UNP P16455
C	763	SER	-	expression tag	UNP P16455
C	764	GLY	-	expression tag	UNP P16455
C	765	GLY	-	expression tag	UNP P16455
C	766	SER	-	expression tag	UNP P16455
C	767	ALA	-	expression tag	UNP P16455
C	768	TRP	-	expression tag	UNP P16455
C	769	SER	-	expression tag	UNP P16455
C	770	HIS	-	expression tag	UNP P16455
C	771	PRO	-	expression tag	UNP P16455
C	772	GLN	-	expression tag	UNP P16455
C	773	PHE	-	expression tag	UNP P16455
C	774	GLU	-	expression tag	UNP P16455
C	775	LYS	-	expression tag	UNP P16455

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.

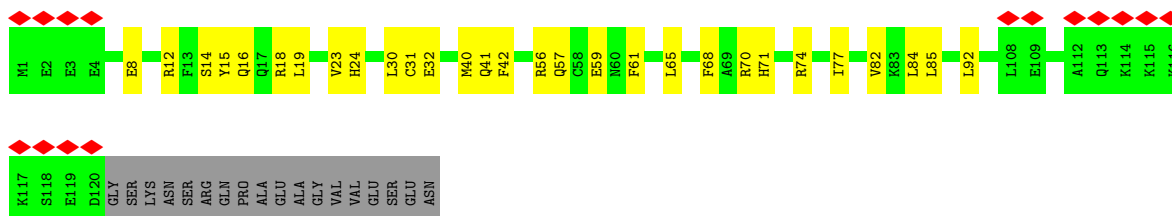
- Molecule 1: Centromere protein M

Chain M: 



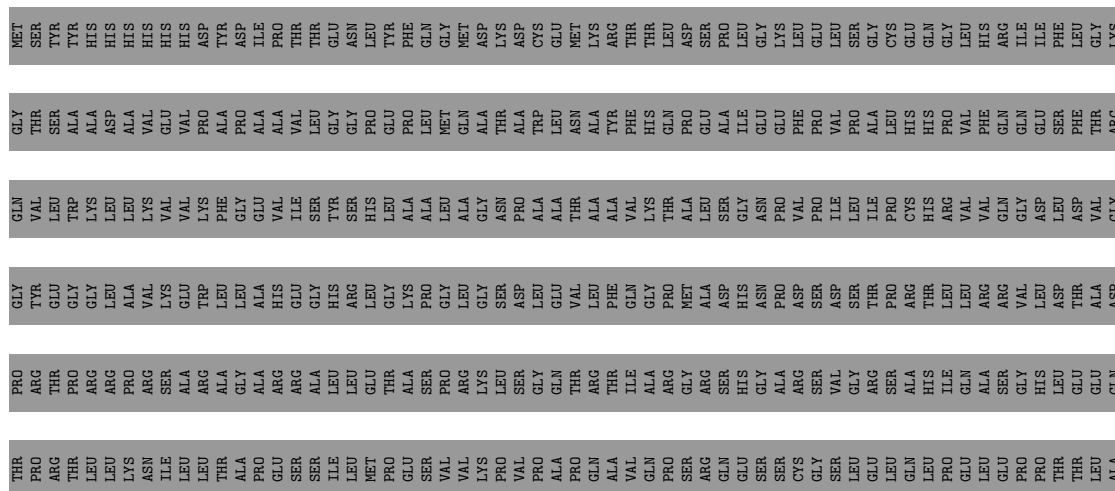
- Molecule 2: Centromere protein S

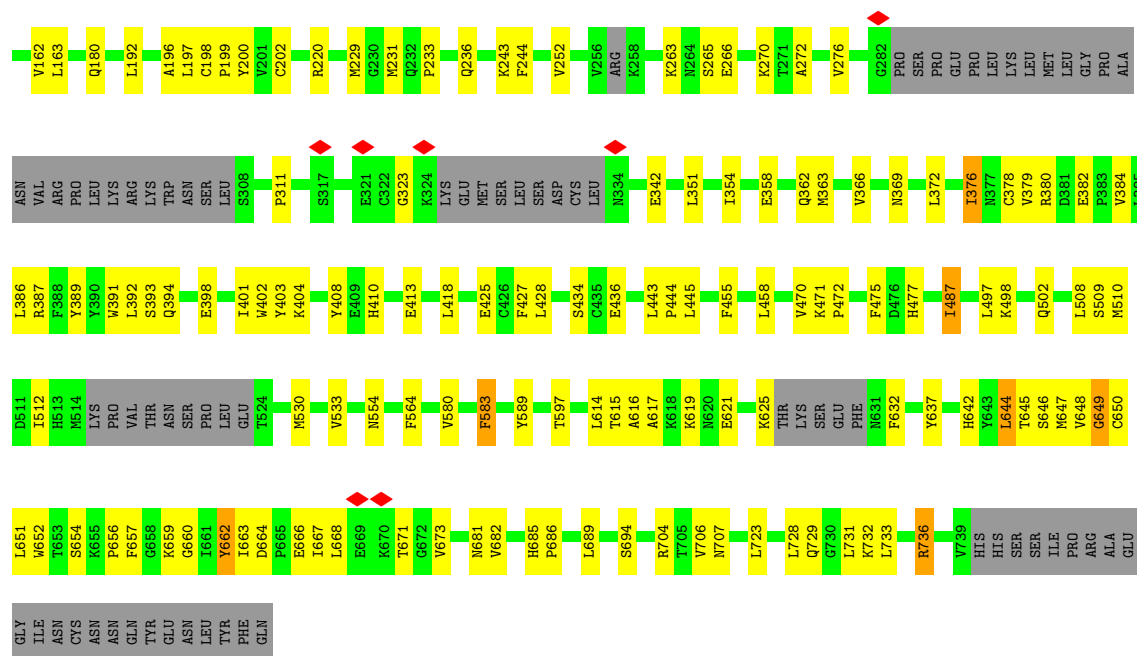
Chain S: 



- Molecule 3: Methylated-DNA--protein-cysteine methyltransferase, Centromere protein T

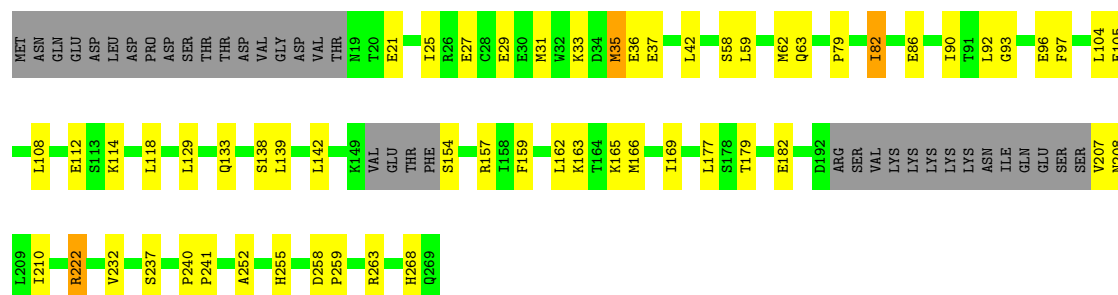
Chain T: 





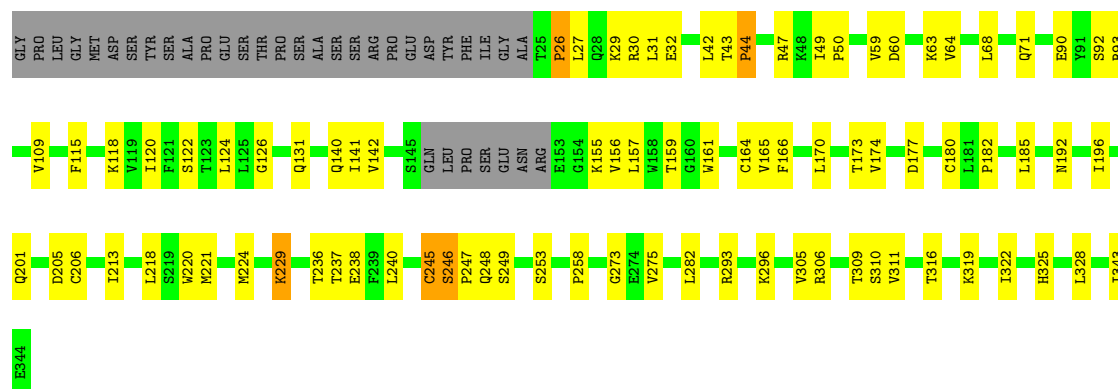
• Molecule 11: Centromere protein K

Chain K: 65% 20% 13%

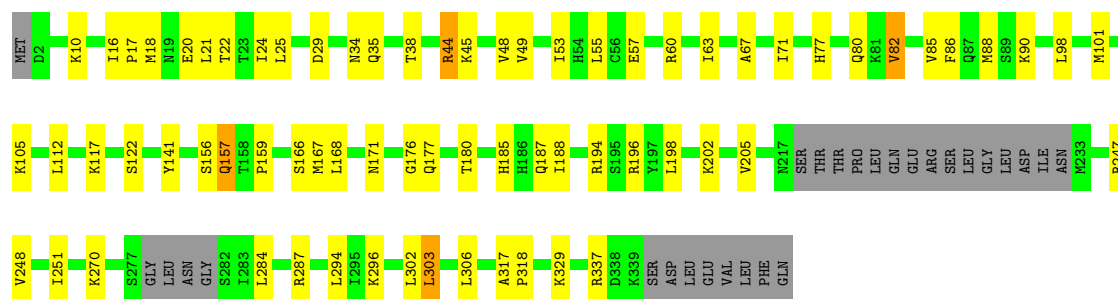


• Molecule 12: Centromere protein L

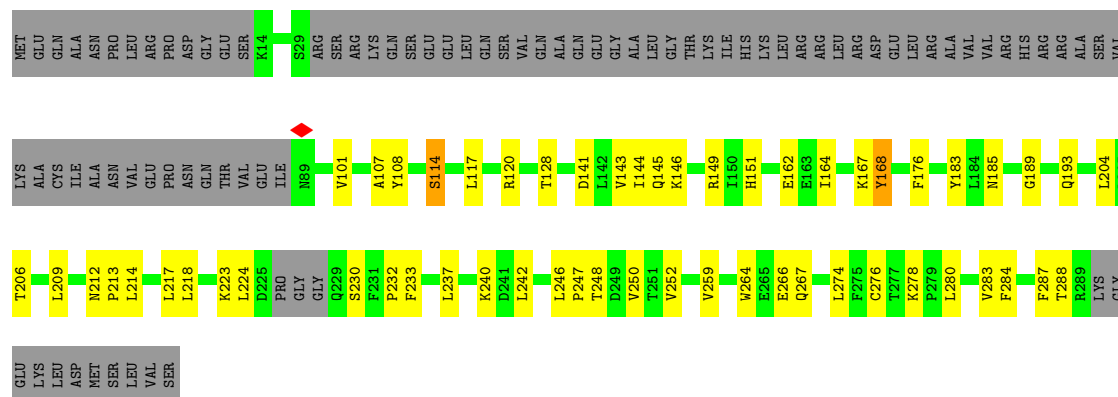
Chain L: 66% 23% 10%



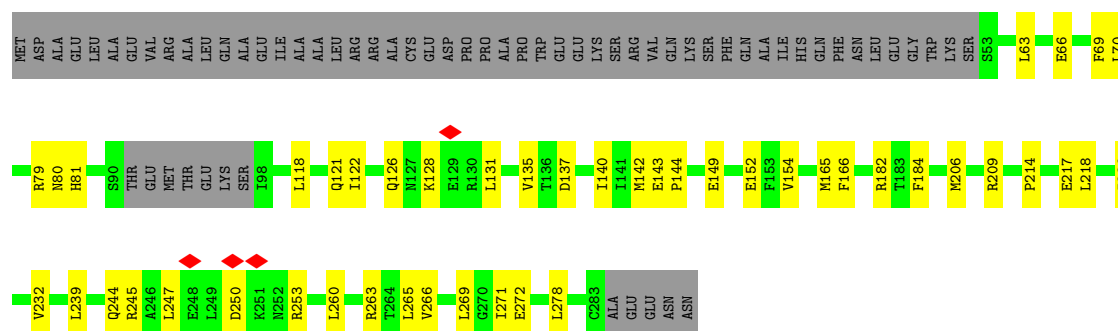
• Molecule 13: Centromere protein N



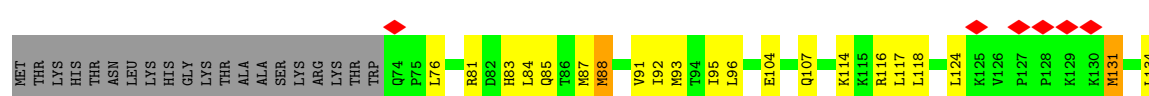
- Molecule 14: Centromere protein O



- Molecule 15: Centromere protein P



- Molecule 16: Centromere protein Q



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1260362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.646	Depositor
Minimum map value	-2.544	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.0759	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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	M	0.31	0/1347	0.48	0/1827
2	S	0.22	0/991	0.55	0/1322
3	T	0.24	0/937	0.47	0/1263
4	U	0.18	0/1387	0.49	0/1860
5	V	0.21	0/1369	0.45	0/2114
6	W	0.20	0/690	0.47	0/916
7	X	0.18	0/596	0.42	0/801
8	Y	0.23	0/1388	0.48	0/2136
9	H	0.24	0/1677	0.48	0/2238
10	I	0.26	0/5222	0.50	0/7069
11	K	0.24	0/1957	0.49	0/2639
12	L	0.32	0/2576	0.59	1/3496 (0.0%)
13	N	0.29	0/2686	0.54	0/3625
14	O	0.18	0/1700	0.46	0/2310
15	P	0.16	0/1820	0.50	0/2451
16	Q	0.22	0/1526	0.62	3/2045 (0.1%)
17	R	0.22	0/653	0.73	3/865 (0.3%)
18	C	0.19	0/207	0.45	0/274
All	All	0.24	0/28729	0.52	7/39251 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
2	S	0	2
3	T	0	2
4	U	0	1
6	W	0	1
7	X	0	2
9	H	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	I	0	2
12	L	0	2
13	N	0	2
14	O	0	2
All	All	0	19

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	254	MET	N-CA-CB	6.62	120.53	110.28
16	Q	254	MET	CA-CB-CG	6.30	126.69	114.10
12	L	229	LYS	CA-CB-CG	6.20	126.50	114.10
17	R	136	MET	CA-CB-CG	5.89	125.89	114.10
17	R	136	MET	N-CA-CB	5.82	119.31	110.28
17	R	101	MET	CA-CB-CG	5.29	124.68	114.10
16	Q	131	MET	CB-CG-SD	5.07	127.91	112.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	H	107	ARG	Sidechain
9	H	45	ARG	Sidechain
10	I	128	ARG	Sidechain
10	I	220	ARG	Sidechain
12	L	293	ARG	Sidechain
12	L	47	ARG	Sidechain
1	M	5	ARG	Sidechain
13	N	196	ARG	Sidechain
13	N	44	ARG	Sidechain
14	O	120	ARG	Sidechain
14	O	146	LYS	Peptide
2	S	56	ARG	Sidechain
2	S	74	ARG	Sidechain
3	T	507	ARG	Sidechain
3	T	544	ARG	Sidechain
4	U	329	ARG	Sidechain
6	W	24	ARG	Sidechain
7	X	45	ARG	Sidechain
7	X	48	ARG	Sidechain

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	M	1325	0	1370	8	0
2	S	982	0	987	35	0
3	T	915	0	924	30	0
4	U	1369	0	1407	53	0
5	V	1220	0	667	30	0
6	W	683	0	761	16	0
7	X	590	0	623	17	0
8	Y	1239	0	686	25	0
9	H	1669	0	1756	42	0
10	I	5096	0	5125	114	0
11	K	1926	0	1928	38	0
12	L	2509	0	2498	50	0
13	N	2629	0	2653	45	0
14	O	1664	0	1635	42	0
15	P	1788	0	1791	40	0
16	Q	1514	0	1575	69	0
17	R	649	0	673	28	0
18	C	206	0	199	4	0
All	All	27973	0	27258	576	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 10.

All (576) 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)
12:L:141:ILE:HD11	12:L:196:ILE:HD11	1.60	0.84
9:H:159:LYS:HG3	10:I:510:MET:HE1	1.60	0.83
13:N:248:VAL:HG22	13:N:317:ALA:HB2	1.60	0.83
10:I:243:LYS:HD3	10:I:252:VAL:HG12	1.61	0.80
2:S:82:VAL:HG12	7:X:31:MET:HE3	1.65	0.79
14:O:259:VAL:HG23	14:O:264:TRP:HB2	1.66	0.78
14:O:145:GLN:HE22	14:O:149:ARG:HB2	1.50	0.77
9:H:206:ILE:HD13	9:H:244:VAL:HG13	1.65	0.76
2:S:40:MET:HE1	7:X:57:ARG:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:17:PRO:HG2	13:N:20:GLU:HG2	1.69	0.75
12:L:229:LYS:HD2	12:L:229:LYS:O	1.86	0.75
14:O:274:LEU:HD12	14:O:283:VAL:HG23	1.67	0.75
12:L:164:CYS:HB2	12:L:182:PRO:HD2	1.70	0.74
15:P:218:LEU:HD11	15:P:278:LEU:HD21	1.71	0.72
10:I:125:VAL:O	10:I:129:ILE:HG13	1.90	0.72
4:U:358:LEU:HD22	16:Q:201:HIS:HE1	1.53	0.71
12:L:246:SER:HB2	12:L:247:PRO:HD3	1.73	0.71
10:I:616:ALA:HA	10:I:619:LYS:HE2	1.73	0.71
16:Q:251:MET:HA	16:Q:254:MET:SD	2.31	0.70
15:P:209:ARG:HD3	15:P:214:PRO:HA	1.73	0.69
14:O:117:LEU:HD21	15:P:69:PHE:HD2	1.57	0.69
14:O:168:TYR:HB2	14:O:176:PHE:HB2	1.74	0.69
6:W:34:ARG:HG2	6:W:34:ARG:HH11	1.58	0.69
12:L:29:LYS:HA	12:L:32:GLU:HG3	1.74	0.68
12:L:63:LYS:HD3	12:L:124:LEU:HD23	1.76	0.68
3:T:453:GLN:HE22	5:V:146:DG:H4'	1.60	0.67
11:K:210:ILE:HG23	11:K:237:SER:HB3	1.77	0.67
10:I:112:LEU:HB3	10:I:133:MET:HE1	1.77	0.67
16:Q:162:ILE:O	16:Q:166:VAL:HG23	1.95	0.67
4:U:407:ILE:HG23	16:Q:265:LEU:HD11	1.77	0.66
4:U:364:LEU:HD11	15:P:253:ARG:HH12	1.61	0.66
16:Q:197:VAL:HG13	16:Q:201:HIS:HD2	1.60	0.66
10:I:129:ILE:HG22	10:I:133:MET:HE2	1.77	0.65
4:U:409:HIS:CE1	4:U:413:LYS:HE3	2.32	0.65
3:T:508:LYS:HE3	6:W:34:ARG:HE	1.61	0.65
12:L:50:PRO:HD3	12:L:224:MET:HE2	1.79	0.65
16:Q:88:MET:HA	16:Q:91:VAL:HG12	1.78	0.65
16:Q:142:ASN:HB3	16:Q:143:MET:HE2	1.79	0.64
11:K:207:VAL:HG12	11:K:208:ASN:H	1.62	0.64
14:O:214:LEU:HD21	14:O:242:LEU:HD21	1.80	0.64
15:P:142:MET:HA	15:P:142:MET:HE2	1.79	0.64
11:K:159:PHE:O	11:K:163:LYS:HE3	1.98	0.64
10:I:642:HIS:HB3	10:I:659:LYS:HG2	1.79	0.63
3:T:518:LEU:O	3:T:522:GLN:HG3	1.97	0.63
9:H:207:LYS:HD3	11:K:268:HIS:HD2	1.62	0.63
10:I:92:LEU:HA	10:I:95:VAL:HG22	1.80	0.63
10:I:369:ASN:HB3	10:I:372:LEU:HD12	1.81	0.63
17:R:98:GLU:HA	17:R:101:MET:SD	2.39	0.63
4:U:375:GLU:HB2	15:P:245:ARG:HH12	1.63	0.63
15:P:122:ILE:HG22	15:P:135:VAL:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:24:HIS:CD2	16:Q:93:MET:HE1	2.34	0.62
4:U:358:LEU:HD22	16:Q:201:HIS:CE1	2.33	0.62
9:H:227:TRP:CE3	9:H:237:VAL:HG21	2.34	0.62
10:I:389:TYR:CE2	12:L:30:ARG:HD3	2.34	0.62
13:N:21:LEU:HD23	13:N:25:LEU:HD23	1.82	0.62
12:L:59:VAL:HG22	12:L:126:GLY:HA3	1.80	0.61
12:L:253:SER:HB3	13:N:296:LYS:HB2	1.82	0.61
2:S:57:GLN:HG3	2:S:61:PHE:CE1	2.35	0.61
3:T:515:LEU:O	3:T:519:MET:HG3	2.00	0.61
4:U:408:ASN:HD21	17:R:139:THR:HG22	1.66	0.61
9:H:61:VAL:HG12	11:K:42:LEU:HG	1.82	0.61
5:V:147:DA:H2"	5:V:148:DG:C8	2.34	0.61
13:N:35:GLN:HB3	13:N:55:LEU:HD21	1.83	0.61
17:R:98:GLU:O	17:R:102:GLU:HG2	1.99	0.61
10:I:664:ASP:HB3	10:I:666:GLU:OE1	2.01	0.61
2:S:82:VAL:CG1	7:X:31:MET:HE3	2.31	0.60
3:T:544:ARG:HG3	3:T:548:ILE:HD12	1.83	0.60
10:I:663:ILE:HG23	10:I:668:LEU:HD21	1.83	0.60
10:I:475:PHE:HE1	10:I:497:LEU:HD11	1.65	0.60
16:Q:214:LEU:HD21	16:Q:218:THR:HG21	1.81	0.60
9:H:201:ASN:HB3	11:K:166:MET:HE1	1.83	0.60
13:N:82:VAL:HG21	13:N:194:ARG:HH21	1.67	0.60
14:O:237:LEU:HD23	14:O:247:PRO:HG3	1.83	0.60
10:I:394:GLN:O	10:I:398:GLU:HG2	2.01	0.60
2:S:40:MET:HE3	2:S:41:GLN:N	2.16	0.59
5:V:146:DG:H2"	5:V:147:DA:C8	2.37	0.59
4:U:309:MET:HE2	4:U:309:MET:HA	1.84	0.59
8:Y:-123:DA:H2"	8:Y:-122:DC:C5	2.37	0.59
10:I:471:LYS:HA	10:I:475:PHE:HD2	1.67	0.59
10:I:614:LEU:HB3	10:I:637:TYR:HE2	1.67	0.59
4:U:269:ILE:HG12	4:U:274:CYS:SG	2.42	0.59
2:S:40:MET:HE3	2:S:41:GLN:H	1.67	0.59
8:Y:-164:DC:H2"	8:Y:-163:DG:N7	2.17	0.59
11:K:154:SER:HA	11:K:157:ARG:HD3	1.85	0.59
10:I:362:GLN:HA	12:L:205:ASP:OD1	2.02	0.59
10:I:363:MET:HE3	10:I:384:VAL:HG23	1.84	0.59
13:N:44:ARG:O	13:N:48:VAL:HG23	2.03	0.58
14:O:101:VAL:HG11	15:P:63:LEU:HB3	1.86	0.58
12:L:237:THR:HG23	12:L:309:THR:HG22	1.86	0.58
1:M:78:LEU:O	1:M:82:GLU:HG3	2.03	0.58
11:K:21:GLU:O	11:K:25:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ARG:CZ	12:L:173:THR:HG22	2.34	0.58
14:O:108:TYR:CZ	15:P:70:LEU:HD21	2.38	0.58
16:Q:259:GLU:HB3	16:Q:263:LYS:HZ3	1.68	0.58
17:R:89:LEU:HA	17:R:92:LYS:HG2	1.85	0.58
17:R:120:GLU:HB3	17:R:126:SER:HA	1.84	0.58
15:P:126:GLN:HG2	15:P:131:LEU:HD22	1.86	0.58
8:Y:-140:DG:H2'	8:Y:-139:DT:H71	1.85	0.58
10:I:158:GLY:O	10:I:162:VAL:HG23	2.03	0.58
14:O:206:THR:HG21	14:O:223:LYS:HE2	1.86	0.57
5:V:122:DG:H2''	5:V:123:DT:H72	1.85	0.57
17:R:136:MET:O	17:R:140:LYS:HG2	2.04	0.57
16:Q:197:VAL:HG13	16:Q:201:HIS:CD2	2.40	0.57
14:O:144:ILE:HG23	17:R:172:LEU:HD13	1.86	0.57
5:V:147:DA:H2''	5:V:148:DG:H8	1.70	0.57
10:I:382:GLU:OE1	12:L:26:PRO:HB2	2.05	0.57
12:L:236:THR:HA	12:L:258:PRO:HG3	1.87	0.57
13:N:166:SER:C	13:N:168:LEU:H	2.09	0.57
1:M:10:LEU:HD11	11:K:36:GLU:HG2	1.85	0.57
10:I:162:VAL:HG13	10:I:200:TYR:CE2	2.39	0.57
1:M:67:VAL:HG22	1:M:98:CYS:SG	2.45	0.57
16:Q:81:ARG:HA	16:Q:84:LEU:HG	1.87	0.56
2:S:40:MET:HE2	7:X:58:VAL:HG23	1.85	0.56
9:H:103:LEU:HB2	10:I:663:ILE:HD12	1.88	0.56
9:H:246:MET:HE3	9:H:246:MET:HA	1.86	0.56
16:Q:189:GLU:O	16:Q:192:GLU:HG3	2.06	0.56
11:K:165:LYS:O	11:K:169:ILE:HG12	2.05	0.56
13:N:284:LEU:HD13	13:N:287:ARG:HD3	1.88	0.56
15:P:121:GLN:HG2	15:P:137:ASP:HB3	1.87	0.56
10:I:78:ILE:HG13	10:I:84:LYS:HZ3	1.71	0.56
14:O:107:ALA:HB2	15:P:81:HIS:CG	2.41	0.56
14:O:224:LEU:O	14:O:230:SER:HA	2.06	0.56
16:Q:88:MET:HE2	16:Q:114:LYS:HZ3	1.70	0.56
10:I:127:THR:HG23	10:I:163:LEU:HD11	1.88	0.55
13:N:88:MET:O	13:N:159:PRO:HB3	2.06	0.55
18:C:305:ILE:HG22	18:C:307:GLU:HG2	1.88	0.55
9:H:233:LEU:O	9:H:237:VAL:HG13	2.06	0.55
4:U:411:LEU:HD22	17:R:146:VAL:HG21	1.88	0.55
8:Y:-158:DC:H1'	8:Y:-157:DC:H5'	1.88	0.55
4:U:351:LEU:HD22	16:Q:193:GLU:HB3	1.89	0.55
4:U:408:ASN:HD22	17:R:142:LEU:HD21	1.71	0.55
9:H:131:LYS:HE3	9:H:135:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:162:LEU:HB3	10:I:510:MET:HE3	1.87	0.55
13:N:198:LEU:HG	13:N:202:LYS:HE2	1.89	0.55
2:S:57:GLN:HG3	2:S:61:PHE:HE1	1.71	0.55
10:I:652:TRP:HZ3	10:I:731:LEU:HD11	1.72	0.55
9:H:232:ALA:O	9:H:235:GLU:HG3	2.07	0.54
14:O:209:LEU:HD12	14:O:218:LEU:HD22	1.89	0.54
10:I:386:LEU:HD23	12:L:27:LEU:HD13	1.88	0.54
6:W:24:ARG:O	6:W:28:ARG:HG3	2.07	0.54
7:X:31:MET:HE2	7:X:31:MET:HA	1.90	0.54
11:K:207:VAL:HG12	11:K:208:ASN:N	2.23	0.54
12:L:192:ASN:O	12:L:196:ILE:HD12	2.08	0.54
2:S:65:LEU:HB3	2:S:77:ILE:HD13	1.90	0.54
10:I:78:ILE:HB	10:I:84:LYS:HD3	1.90	0.54
10:I:732:LYS:HE2	10:I:736:ARG:HH12	1.72	0.54
15:P:226:ILE:HG12	15:P:232:VAL:HG22	1.90	0.54
4:U:313:ILE:HD11	13:N:141:TYR:CD2	2.43	0.54
10:I:681:ASN:O	10:I:685:HIS:HB2	2.08	0.54
3:T:473:MET:O	3:T:475:MET:HE2	2.08	0.54
10:I:104:LEU:HD12	10:I:108:GLU:HG3	1.88	0.54
17:R:133:LYS:HA	17:R:136:MET:SD	2.47	0.54
3:T:540:PRO:HD2	3:T:543:TYR:CD2	2.43	0.53
4:U:408:ASN:ND2	17:R:139:THR:HG22	2.23	0.53
8:Y:-155:DC:H1'	8:Y:-154:DA:C4	2.43	0.53
7:X:45:ARG:HB3	7:X:66:VAL:HG21	1.89	0.53
12:L:245:CYS:HB2	12:L:248:GLN:HB2	1.91	0.53
10:I:617:ALA:O	10:I:621:GLU:HG3	2.08	0.53
12:L:213:ILE:HD13	12:L:221:MET:HE1	1.89	0.53
12:L:246:SER:CB	12:L:247:PRO:HD3	2.37	0.53
8:Y:-162:DA:H1'	8:Y:-161:DA:H5'	1.89	0.53
13:N:98:LEU:HB3	14:O:217:LEU:HD12	1.90	0.53
14:O:108:TYR:CE2	15:P:70:LEU:HD21	2.43	0.53
4:U:408:ASN:ND2	17:R:142:LEU:HD21	2.23	0.53
16:Q:235:GLN:HB3	16:Q:239:LEU:HD23	1.90	0.53
9:H:174:GLU:O	9:H:177:THR:HG22	2.08	0.53
3:T:541:LEU:O	3:T:545:GLN:HG3	2.09	0.53
14:O:280:LEU:O	14:O:283:VAL:HG12	2.09	0.53
2:S:59:GLU:HG2	7:X:15:HIS:ND1	2.24	0.52
11:K:82:ILE:O	11:K:82:ILE:HD12	2.09	0.52
4:U:334:LEU:HD13	16:Q:172:MET:HG2	1.91	0.52
17:R:99:GLU:O	17:R:103:ILE:HG12	2.09	0.52
4:U:409:HIS:NE2	15:P:144:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:162:LEU:HD23	10:I:510:MET:HG2	1.92	0.52
12:L:201:GLN:HG2	12:L:206:CYS:O	2.08	0.52
14:O:117:LEU:HD23	15:P:66:GLU:HG3	1.90	0.52
16:Q:85:GLN:HA	16:Q:114:LYS:HZ1	1.75	0.52
2:S:65:LEU:HD21	2:S:85:LEU:HD22	1.91	0.52
5:V:126:DT:H2''	5:V:127:DA:C8	2.44	0.52
8:Y:-163:DG:H2''	8:Y:-162:DA:OP2	2.10	0.52
13:N:29:ASP:O	13:N:29:ASP:OD2	2.28	0.52
14:O:232:PRO:C	14:O:233:PHE:HD1	2.17	0.52
3:T:482:MET:HA	3:T:482:MET:HE2	1.92	0.52
9:H:164:LEU:HD11	11:K:133:GLN:HG3	1.91	0.52
10:I:648:VAL:HG23	10:I:652:TRP:HE1	1.74	0.52
16:Q:182:LYS:O	16:Q:185:ILE:HG13	2.10	0.52
3:T:508:LYS:HE3	6:W:34:ARG:NE	2.24	0.52
4:U:265:HIS:CD2	16:Q:116:ARG:HH22	2.28	0.52
10:I:530:MET:HA	10:I:533:VAL:HG22	1.91	0.52
13:N:45:LYS:O	13:N:49:VAL:HG23	2.10	0.52
14:O:108:TYR:HE2	14:O:114:SER:HA	1.75	0.52
17:R:146:VAL:HG13	17:R:151:LEU:HB2	1.91	0.52
2:S:71:HIS:CD2	3:T:517:LEU:HD22	2.44	0.52
10:I:366:VAL:HG22	10:I:372:LEU:HD13	1.92	0.52
15:P:266:VAL:HG23	15:P:271:ILE:HA	1.92	0.52
5:V:152:DT:H3	8:Y:-151:DG:N2	2.08	0.51
12:L:322:ILE:HD12	12:L:328:LEU:HD12	1.92	0.51
17:R:169:TYR:O	17:R:172:LEU:HD12	2.09	0.51
4:U:358:LEU:HD22	16:Q:200:MET:HE1	1.92	0.51
10:I:149:SER:O	10:I:153:VAL:HG23	2.11	0.51
10:I:198:CYS:O	10:I:199:PRO:C	2.52	0.51
10:I:392:LEU:HD23	10:I:434:SER:HB2	1.91	0.51
5:V:144:DC:H2''	5:V:145:DG:C8	2.46	0.51
10:I:530:MET:HA	10:I:530:MET:HE2	1.93	0.51
13:N:18:MET:HG2	13:N:45:LYS:HD3	1.93	0.51
13:N:317:ALA:HB3	13:N:318:PRO:HD3	1.93	0.51
15:P:118:LEU:HB2	15:P:140:ILE:HG22	1.93	0.51
2:S:23:VAL:HG23	7:X:7:LEU:HD11	1.93	0.51
10:I:509:SER:O	10:I:512:ILE:HG12	2.10	0.51
10:I:125:VAL:HG12	10:I:129:ILE:HD11	1.92	0.51
13:N:77:HIS:HB3	13:N:80:GLN:HG3	1.91	0.51
4:U:313:ILE:HG22	16:Q:155:LEU:HD13	1.92	0.51
10:I:657:PHE:HB3	10:I:662:TYR:CD2	2.46	0.51
17:R:91:SER:O	17:R:95:LYS:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:252:ALA:HA	11:K:263:ARG:O	2.10	0.50
12:L:30:ARG:NH1	12:L:173:THR:HG22	2.26	0.50
10:I:351:LEU:HA	10:I:354:ILE:HD12	1.93	0.50
10:I:498:LYS:O	10:I:502:GLN:HG3	2.11	0.50
4:U:292:MET:HG3	16:Q:134:LEU:HG	1.94	0.50
6:W:18:PRO:HB2	6:W:21:PHE:HB3	1.94	0.50
13:N:156:SER:HB2	14:O:213:PRO:HG2	1.93	0.50
15:P:271:ILE:HD11	16:Q:211:LEU:HG	1.93	0.50
16:Q:169:THR:O	16:Q:173:THR:HG22	2.11	0.50
16:Q:231:LEU:HG	16:Q:232:ILE:HG23	1.92	0.50
16:Q:259:GLU:HB3	16:Q:263:LYS:NZ	2.25	0.50
5:V:133:DA:H2''	5:V:134:DA:C8	2.46	0.50
5:V:134:DA:H2''	5:V:135:DG:C8	2.47	0.50
9:H:175:ILE:O	9:H:178:GLU:HG3	2.12	0.50
10:I:233:PRO:HA	10:I:236:GLN:HG3	1.93	0.50
14:O:162:GLU:H	14:O:162:GLU:CD	2.20	0.50
2:S:68:PHE:CE1	3:T:521:ARG:HD2	2.47	0.49
4:U:309:MET:O	4:U:313:ILE:HG23	2.12	0.49
5:V:145:DG:H2''	5:V:146:DG:C8	2.47	0.49
11:K:138:SER:O	11:K:142:LEU:HD13	2.12	0.49
11:K:222:ARG:HG2	11:K:232:VAL:HG22	1.94	0.49
4:U:325:ASP:O	4:U:329:ARG:HG2	2.12	0.49
9:H:136:LEU:HD11	11:K:105:GLU:OE1	2.12	0.49
9:H:195:ILE:HG22	9:H:199:ARG:HD3	1.94	0.49
12:L:42:LEU:HG	12:L:44:PRO:HD3	1.93	0.49
13:N:157:GLN:HE22	14:O:212:ASN:ND2	2.10	0.49
15:P:271:ILE:HG13	15:P:272:GLU:H	1.77	0.49
16:Q:142:ASN:HB3	16:Q:143:MET:CE	2.42	0.49
5:V:155:DG:H22	8:Y:-154:DA:H2	1.60	0.49
10:I:358:GLU:HA	10:I:358:GLU:OE1	2.11	0.49
13:N:90:LYS:HG3	13:N:185:HIS:CD2	2.48	0.49
12:L:140:GLN:HG3	12:L:159:THR:HG23	1.94	0.49
17:R:94:GLU:HG3	17:R:140:LYS:HE3	1.95	0.49
9:H:148:TRP:O	9:H:152:GLU:HG3	2.13	0.49
16:Q:84:LEU:HA	16:Q:87:MET:HG2	1.95	0.49
2:S:84:LEU:HD11	3:T:504:HIS:CG	2.48	0.49
15:P:79:ARG:HG3	15:P:80:ASN:H	1.77	0.49
11:K:179:THR:HA	11:K:182:GLU:HG3	1.95	0.49
12:L:218:LEU:HD11	12:L:316:THR:HG23	1.95	0.49
12:L:246:SER:HB2	12:L:247:PRO:CD	2.42	0.49
8:Y:-140:DG:C2'	8:Y:-139:DT:H71	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:85:GLU:HA	17:R:88:MET:HG3	1.95	0.49
4:U:329:ARG:HH12	13:N:187:GLN:HG2	1.78	0.48
4:U:258:PHE:HD2	4:U:286:LYS:HD3	1.77	0.48
4:U:340:LYS:O	4:U:343:GLU:HG2	2.13	0.48
5:V:124:DA:H2''	5:V:125:DG:C8	2.47	0.48
5:V:168:DG:H4'	13:N:167:MET:HG2	1.94	0.48
10:I:508:LEU:O	10:I:512:ILE:HG23	2.13	0.48
15:P:209:ARG:HB2	15:P:217:GLU:HG3	1.94	0.48
5:V:153:DT:H2''	5:V:154:DT:C6	2.48	0.48
11:K:92:LEU:O	11:K:96:GLU:HG3	2.14	0.48
12:L:224:MET:HE3	12:L:224:MET:HA	1.95	0.48
9:H:57:TYR:O	9:H:61:VAL:HG13	2.14	0.48
16:Q:226:LYS:O	16:Q:230:ALA:HB2	2.12	0.48
3:T:482:MET:SD	6:W:76:LEU:HD23	2.52	0.48
9:H:84:ASP:O	9:H:88:GLU:HG3	2.14	0.48
10:I:436:GLU:OE1	12:L:31:LEU:HD21	2.14	0.48
15:P:253:ARG:HG2	15:P:253:ARG:HH11	1.79	0.48
16:Q:200:MET:SD	16:Q:201:HIS:CE1	3.07	0.48
2:S:68:PHE:HE1	3:T:521:ARG:HD2	1.78	0.48
10:I:471:LYS:HB3	10:I:472:PRO:HD3	1.95	0.48
5:V:136:DT:H2''	5:V:137:DG:C8	2.48	0.48
10:I:418:LEU:HD12	10:I:458:LEU:HD11	1.95	0.48
10:I:704:ARG:O	10:I:706:VAL:HG13	2.14	0.48
8:Y:-151:DG:C8	8:Y:-150:DT:H72	2.49	0.48
12:L:60:ASP:O	12:L:64:VAL:HG23	2.14	0.48
10:I:648:VAL:HG23	10:I:652:TRP:NE1	2.29	0.47
10:I:729:GLN:O	10:I:733:LEU:HD13	2.13	0.47
15:P:263:ARG:O	15:P:266:VAL:HG12	2.13	0.47
3:T:453:GLN:NE2	5:V:146:DG:H4'	2.26	0.47
7:X:8:VAL:HG23	7:X:28:LEU:HD22	1.97	0.47
10:I:311:PRO:HD3	10:I:391:TRP:NE1	2.29	0.47
3:T:540:PRO:HD2	3:T:543:TYR:HD2	1.78	0.47
10:I:580:VAL:HG23	10:I:632:PHE:HE2	1.78	0.47
11:K:29:GLU:OE2	18:C:261:SER:HB2	2.14	0.47
10:I:111:ILE:O	10:I:115:ILE:HG12	2.14	0.47
15:P:263:ARG:HA	15:P:266:VAL:HG12	1.97	0.47
7:X:33:GLU:O	7:X:37:VAL:HG23	2.15	0.47
10:I:192:LEU:HD22	10:I:202:CYS:SG	2.54	0.47
11:K:58:SER:O	11:K:62:MET:HG3	2.14	0.47
11:K:255:HIS:HB3	11:K:258:ASP:O	2.14	0.47
4:U:272:LYS:O	4:U:275:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:348:LYS:HB2	16:Q:190:VAL:HG22	1.95	0.47
9:H:112:LEU:C	9:H:114:LYS:H	2.22	0.47
5:V:140:DC:H2"	5:V:141:DA:C8	2.49	0.47
10:I:231:MET:HG2	10:I:236:GLN:NE2	2.30	0.47
13:N:303:LEU:HD23	13:N:306:LEU:HD12	1.96	0.47
10:I:363:MET:HE2	10:I:387:ARG:CZ	2.44	0.47
10:I:645:THR:O	10:I:646:SER:C	2.57	0.47
12:L:240:LEU:HB3	12:L:306:ARG:HB3	1.97	0.47
14:O:164:ILE:HG22	14:O:176:PHE:CD1	2.50	0.47
3:T:470:TYR:O	3:T:472:LYS:HG3	2.14	0.47
10:I:379:VAL:HG13	10:I:380:ARG:N	2.29	0.47
4:U:391:LEU:HD11	16:Q:228:ILE:HD13	1.97	0.46
5:V:155:DG:N2	8:Y:-154:DA:H2	2.13	0.46
12:L:30:ARG:HH22	12:L:174:VAL:HG13	1.80	0.46
2:S:14:SER:O	2:S:18:ARG:HG3	2.16	0.46
4:U:331:GLU:HB3	4:U:332:PRO:HD3	1.97	0.46
6:W:34:ARG:HG2	6:W:34:ARG:NH1	2.26	0.46
2:S:19:LEU:HD11	7:X:10:ARG:HB2	1.96	0.46
16:Q:166:VAL:HA	16:Q:169:THR:HG22	1.97	0.46
16:Q:257:PHE:O	16:Q:260:GLU:HG3	2.16	0.46
1:M:5:ARG:HA	1:M:89:ASP:OD1	2.16	0.46
2:S:31:CYS:HB3	2:S:42:PHE:HD2	1.81	0.46
3:T:457:LYS:O	3:T:461:SER:HB3	2.16	0.46
4:U:398:LEU:HD13	17:R:127:CYS:SG	2.56	0.46
15:P:244:GLN:HA	15:P:247:LEU:HD12	1.96	0.46
17:R:86:PHE:O	17:R:89:LEU:HG	2.15	0.46
4:U:257:GLU:O	4:U:260:LYS:HG2	2.16	0.46
4:U:348:LYS:HE3	4:U:348:LYS:HB3	1.80	0.46
4:U:354:ALA:HB1	15:P:265:LEU:HD13	1.97	0.46
10:I:323:GLY:HA3	12:L:90:GLU:OE2	2.14	0.46
10:I:401:ILE:HG23	10:I:408:TYR:HA	1.97	0.46
13:N:10:LYS:HA	13:N:53:ILE:HD11	1.96	0.46
16:Q:143:MET:HE2	16:Q:143:MET:N	2.31	0.46
4:U:308:LYS:HE3	4:U:308:LYS:HB3	1.77	0.46
9:H:244:VAL:HA	9:H:247:MET:HG2	1.98	0.46
11:K:59:LEU:O	11:K:63:GLN:HG3	2.16	0.46
15:P:165:MET:HE3	15:P:166:PHE:N	2.31	0.46
2:S:30:LEU:HD11	7:X:36:LYS:HE3	1.98	0.46
10:I:263:LYS:HE2	10:I:265:SER:HB3	1.97	0.46
5:V:135:DG:H1'	5:V:136:DT:OP2	2.16	0.46
10:I:671:THR:HG23	10:I:673:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:284:PHE:O	14:O:288:THR:HG23	2.16	0.46
15:P:184:PHE:CD1	15:P:206:MET:HE2	2.50	0.46
2:S:24:HIS:CG	16:Q:93:MET:HE1	2.51	0.45
5:V:173:DG:C2	8:Y:-172:DG:C2	3.04	0.45
10:I:379:VAL:HG13	10:I:380:ARG:H	1.81	0.45
16:Q:83:HIS:O	16:Q:87:MET:HG2	2.16	0.45
16:Q:172:MET:O	16:Q:176:ILE:HG13	2.16	0.45
3:T:450:ARG:HH22	8:Y:-145:DC:H4'	1.80	0.45
7:X:36:LYS:O	7:X:40:VAL:HG13	2.16	0.45
13:N:16:ILE:HG23	13:N:24:ILE:HD12	1.99	0.45
13:N:302:LEU:O	13:N:303:LEU:HB2	2.15	0.45
2:S:70:ARG:HB3	2:S:70:ARG:HH11	1.82	0.45
4:U:261:THR:O	4:U:264:GLU:HG2	2.16	0.45
10:I:363:MET:CE	10:I:384:VAL:HG23	2.46	0.45
11:K:114:LYS:NZ	11:K:118:LEU:HD11	2.32	0.45
15:P:128:LYS:H	15:P:128:LYS:HD3	1.80	0.45
6:W:5:THR:O	6:W:6:ILE:HD13	2.16	0.45
9:H:194:ARG:HB3	11:K:159:PHE:CZ	2.52	0.45
14:O:274:LEU:HB3	14:O:283:VAL:HG21	1.98	0.45
14:O:274:LEU:HD13	14:O:278:LYS:HD2	1.98	0.45
10:I:112:LEU:CB	10:I:133:MET:HE1	2.46	0.45
10:I:129:ILE:HG22	10:I:133:MET:CE	2.44	0.45
16:Q:239:LEU:HA	16:Q:242:LEU:HG	1.98	0.45
16:Q:239:LEU:HD12	16:Q:240:LYS:HD2	1.98	0.45
17:R:135:GLU:O	17:R:139:THR:HG23	2.16	0.45
2:S:19:LEU:HD12	7:X:11:LEU:HG	1.99	0.45
10:I:134:ILE:HD12	10:I:272:ALA:CB	2.46	0.45
10:I:266:GLU:HG2	10:I:270:LYS:HZ2	1.82	0.45
10:I:272:ALA:O	10:I:276:VAL:HG23	2.17	0.45
13:N:85:VAL:HG11	13:N:205:VAL:HG21	1.98	0.45
2:S:57:GLN:CG	2:S:61:PHE:HE1	2.30	0.45
8:Y:-164:DC:H2''	8:Y:-163:DG:C8	2.51	0.45
8:Y:-132:DG:H2''	8:Y:-131:DC:C6	2.51	0.45
17:R:120:GLU:HA	17:R:123:ILE:HG22	1.99	0.45
9:H:160:LYS:HE3	11:K:129:LEU:HD21	1.99	0.45
10:I:403:TYR:HD1	10:I:445:LEU:HD12	1.82	0.45
11:K:114:LYS:HZ2	11:K:118:LEU:HD11	1.81	0.45
12:L:68:LEU:HD11	12:L:325:HIS:HB3	1.98	0.45
13:N:166:SER:C	13:N:168:LEU:N	2.74	0.45
16:Q:250:GLN:HG2	17:R:96:LEU:HD11	1.99	0.45
5:V:151:DC:H2''	5:V:152:DT:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:363:MET:HE3	10:I:384:VAL:HA	1.97	0.44
10:I:621:GLU:O	10:I:625:LYS:HG3	2.17	0.44
12:L:49:ILE:HD12	12:L:273:GLY:C	2.42	0.44
14:O:143:VAL:CG2	14:O:151:HIS:HB2	2.48	0.44
16:Q:140:LEU:O	16:Q:144:GLU:HG2	2.18	0.44
10:I:363:MET:SD	10:I:384:VAL:HG23	2.57	0.44
12:L:174:VAL:HG21	12:L:180:CYS:SG	2.57	0.44
12:L:220:TRP:O	12:L:224:MET:HG2	2.18	0.44
13:N:167:MET:SD	13:N:167:MET:O	2.75	0.44
15:P:260:LEU:HD22	16:Q:223:THR:HG21	1.99	0.44
4:U:329:ARG:HH12	13:N:187:GLN:CG	2.30	0.44
7:X:5:LYS:HE2	7:X:29:GLN:HB2	1.98	0.44
12:L:71:GLN:OE1	12:L:319:LYS:HB3	2.17	0.44
2:S:14:SER:HB2	16:Q:107:GLN:CD	2.43	0.44
4:U:316:LYS:HG3	16:Q:155:LEU:HD11	1.98	0.44
10:I:402:TRP:HZ2	10:I:455:PHE:CZ	2.35	0.44
10:I:487:ILE:HD12	10:I:554:ASN:HD22	1.82	0.44
12:L:43:THR:N	12:L:44:PRO:HD3	2.32	0.44
14:O:167:LYS:HB3	14:O:168:TYR:CD2	2.52	0.44
16:Q:158:LEU:O	16:Q:162:ILE:HG13	2.18	0.44
10:I:644:LEU:O	10:I:648:VAL:HG12	2.18	0.44
13:N:176:GLY:O	13:N:180:THR:HG23	2.17	0.44
14:O:240:LYS:HB2	14:O:248:THR:OG1	2.17	0.44
4:U:302:LEU:HD22	16:Q:145:ARG:HD2	1.99	0.44
9:H:57:TYR:CD2	11:K:35:MET:HG2	2.53	0.44
10:I:114:ASN:ND2	10:I:146:LYS:HE3	2.32	0.44
4:U:338:GLN:HA	16:Q:179:LEU:HD21	1.99	0.44
15:P:269:LEU:HD13	15:P:269:LEU:O	2.18	0.44
2:S:15:TYR:O	2:S:19:LEU:HD23	2.17	0.44
8:Y:-155:DC:C2	8:Y:-154:DA:C2	3.05	0.44
10:I:66:LEU:HD12	10:I:95:VAL:HG12	1.99	0.44
4:U:287:GLU:O	4:U:290:ILE:HG12	2.18	0.44
9:H:199:ARG:O	9:H:203:GLN:HG2	2.18	0.44
10:I:266:GLU:HG2	10:I:270:LYS:NZ	2.33	0.44
11:K:86:GLU:O	11:K:90:ILE:HG12	2.18	0.44
16:Q:231:LEU:HD23	16:Q:231:LEU:H	1.83	0.44
3:T:463:TYR:HB3	6:W:51:VAL:HG21	1.99	0.43
10:I:427:PHE:O	10:I:428:LEU:HB2	2.17	0.43
14:O:189:GLY:O	14:O:193:GLN:HG3	2.18	0.43
14:O:204:LEU:HD11	14:O:288:THR:HG22	1.99	0.43
14:O:284:PHE:HA	14:O:287:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:10:ARG:HH11	6:W:10:ARG:CB	2.31	0.43
12:L:118:LYS:HG2	12:L:120:ILE:HD11	2.01	0.43
12:L:296:LYS:HA	12:L:296:LYS:HD3	1.72	0.43
2:S:8:GLU:OE2	2:S:12:ARG:HG3	2.19	0.43
4:U:310:ILE:O	4:U:313:ILE:HG12	2.18	0.43
5:V:143:DT:H2"	5:V:144:DC:C6	2.54	0.43
9:H:202:LEU:HD23	9:H:202:LEU:HA	1.83	0.43
10:I:410:HIS:O	10:I:413:GLU:HG2	2.19	0.43
13:N:270:LYS:HG3	13:N:294:LEU:HD13	2.00	0.43
8:Y:-141:DT:H2"	8:Y:-140:DG:C8	2.53	0.43
10:I:99:ALA:HB1	10:I:134:ILE:CG1	2.48	0.43
12:L:90:GLU:HG3	12:L:93:ARG:NH2	2.33	0.43
16:Q:234:ASN:O	16:Q:238:LEU:HD13	2.19	0.43
9:H:198:ILE:HD13	11:K:162:LEU:HB3	2.00	0.43
9:H:237:VAL:HG23	9:H:238:LEU:HD22	2.01	0.43
10:I:648:VAL:HG13	10:I:649:GLY:N	2.34	0.43
11:K:33:LYS:O	11:K:37:GLU:HG3	2.18	0.43
13:N:247:ARG:O	13:N:251:ILE:HG12	2.18	0.43
16:Q:224:LEU:HA	16:Q:227:GLU:OE1	2.18	0.43
2:S:32:GLU:OE1	2:S:32:GLU:HA	2.19	0.43
9:H:119:ILE:HG22	9:H:120:SER:O	2.18	0.43
10:I:196:ALA:O	10:I:197:LEU:HD12	2.19	0.43
13:N:34:ASN:O	13:N:38:THR:HG23	2.18	0.43
16:Q:114:LYS:O	16:Q:118:LEU:HD23	2.19	0.43
2:S:65:LEU:CD2	2:S:85:LEU:HD22	2.48	0.43
5:V:142:DT:H2'	5:V:143:DT:H72	1.99	0.43
9:H:234:LYS:O	9:H:237:VAL:HG22	2.18	0.43
13:N:86:PHE:HD1	13:N:188:ILE:HG12	1.83	0.43
10:I:425:GLU:OE2	10:I:458:LEU:HD23	2.19	0.43
12:L:131:GLN:N	12:L:131:GLN:CD	2.77	0.43
14:O:223:LYS:HG2	14:O:232:PRO:HB3	2.00	0.43
16:Q:84:LEU:O	16:Q:88:MET:SD	2.77	0.43
1:M:146:LEU:HD23	1:M:146:LEU:HA	1.85	0.43
2:S:71:HIS:CE1	3:T:505:ALA:HB2	2.54	0.43
7:X:12:LEU:HD11	7:X:31:MET:HG3	2.01	0.43
9:H:181:LYS:HE3	9:H:181:LYS:HB3	1.85	0.43
10:I:686:PRO:HA	10:I:689:LEU:HD12	2.01	0.43
11:K:240:PRO:HB2	11:K:241:PRO:HD3	1.99	0.43
3:T:499:GLU:OE1	6:W:30:LYS:HD2	2.19	0.42
17:R:97:SER:O	17:R:101:MET:SD	2.77	0.42
5:V:134:DA:H2"	5:V:135:DG:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:156:DT:H2''	5:V:157:DG:N7	2.34	0.42
8:Y:-143:DA:H4'	8:Y:-142:DA:OP1	2.19	0.42
9:H:83:GLU:O	9:H:86:GLU:HG2	2.18	0.42
10:I:650:CYS:HB3	10:I:656:PRO:HA	2.01	0.42
3:T:499:GLU:HA	6:W:33:LEU:HD21	2.00	0.42
10:I:498:LYS:HD3	10:I:564:PHE:HA	2.01	0.42
13:N:329:LYS:NZ	18:C:305:ILE:HD12	2.34	0.42
15:P:140:ILE:HD11	15:P:154:VAL:HG13	2.00	0.42
8:Y:-165:DA:H2''	8:Y:-164:DC:C6	2.55	0.42
8:Y:-127:DT:H2''	8:Y:-126:DA:C8	2.54	0.42
10:I:366:VAL:HG11	10:I:376:ILE:HG13	2.01	0.42
10:I:402:TRP:CZ2	10:I:455:PHE:CZ	3.07	0.42
3:T:473:MET:SD	6:W:59:ARG:HG3	2.59	0.42
3:T:529:VAL:HG22	11:K:259:PRO:HG2	2.00	0.42
3:T:549:PRO:HA	3:T:559:PRO:HD2	2.00	0.42
16:Q:76:LEU:HB3	16:Q:81:ARG:NH1	2.33	0.42
17:R:96:LEU:O	17:R:100:ILE:HG12	2.20	0.42
3:T:483:VAL:HA	3:T:486:CYS:SG	2.59	0.42
3:T:486:CYS:SG	6:W:54:LEU:HD21	2.60	0.42
6:W:57:GLU:HB3	6:W:78:ALA:HB1	2.01	0.42
9:H:192:SER:HB3	9:H:195:ILE:HG12	2.02	0.42
10:I:72:TYR:OH	10:I:88:LEU:HB2	2.20	0.42
10:I:651:LEU:HB3	10:I:652:TRP:CE3	2.54	0.42
10:I:707:ASN:OD1	10:I:707:ASN:C	2.63	0.42
13:N:63:ILE:HD12	13:N:63:ILE:HA	1.94	0.42
16:Q:224:LEU:HD23	17:R:122:LEU:HD12	2.02	0.42
2:S:71:HIS:HE1	3:T:505:ALA:HB2	1.84	0.42
4:U:282:TYR:O	4:U:286:LYS:HG2	2.20	0.42
15:P:182:ARG:HD3	16:Q:209:LEU:HD22	2.01	0.42
16:Q:165:MET:O	16:Q:169:THR:HG22	2.19	0.42
16:Q:192:GLU:OE2	16:Q:193:GLU:HG2	2.19	0.42
4:U:409:HIS:HE1	4:U:413:LYS:HE3	1.84	0.42
5:V:143:DT:H2''	5:V:144:DC:C5	2.54	0.42
12:L:161:TRP:HB3	12:L:185:LEU:HB2	2.02	0.42
4:U:313:ILE:HG22	16:Q:155:LEU:HB2	2.01	0.42
8:Y:-134:DT:H2''	8:Y:-133:DT:O4'	2.19	0.42
9:H:130:MET:HE3	10:I:694:SER:HB2	2.01	0.42
10:I:141:GLU:CD	10:I:180:GLN:HB2	2.45	0.42
10:I:244:PHE:HZ	10:I:342:GLU:HG3	1.84	0.42
10:I:659:LYS:HG3	10:I:660:GLY:H	1.85	0.42
10:I:667:ILE:HD13	11:K:79:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:PRO:HB3	12:L:173:THR:O	2.20	0.42
13:N:157:GLN:OE1	14:O:213:PRO:HD2	2.20	0.42
12:L:170:LEU:HD22	12:L:343:ILE:HD11	2.01	0.42
14:O:141:ASP:OD1	14:O:141:ASP:C	2.63	0.42
4:U:409:HIS:CE1	15:P:144:PRO:HD2	2.54	0.41
13:N:101:MET:HG3	13:N:105:LYS:HE3	2.01	0.41
16:Q:124:LEU:HD12	16:Q:124:LEU:HA	1.88	0.41
1:M:22:GLY:O	1:M:50:LYS:HA	2.20	0.41
4:U:388:PRO:HB2	15:P:239:LEU:HD22	2.02	0.41
15:P:143:GLU:HA	15:P:144:PRO:HD3	1.93	0.41
15:P:182:ARG:HG3	16:Q:209:LEU:HD13	2.00	0.41
17:R:88:MET:HE2	17:R:88:MET:C	2.45	0.41
4:U:268:ARG:HH22	16:Q:116:ARG:NH2	2.18	0.41
10:I:444:PRO:HG3	10:I:477:HIS:CE1	2.55	0.41
14:O:266:GLU:OE1	14:O:267:GLN:HG2	2.20	0.41
4:U:297:GLN:OE1	4:U:297:GLN:HA	2.20	0.41
9:H:227:TRP:HA	9:H:233:LEU:HD23	2.02	0.41
12:L:49:ILE:HG13	12:L:275:VAL:HG23	2.02	0.41
15:P:149:GLU:O	15:P:152:GLU:HG3	2.20	0.41
7:X:67:LEU:N	7:X:68:PRO:HD2	2.35	0.41
17:R:94:GLU:CG	17:R:140:LYS:HE3	2.50	0.41
5:V:151:DC:H2''	5:V:152:DT:C7	2.51	0.41
9:H:193:GLU:OE2	9:H:193:GLU:HA	2.20	0.41
11:K:108:LEU:O	11:K:112:GLU:HG2	2.21	0.41
2:S:70:ARG:HH11	2:S:70:ARG:CB	2.33	0.41
4:U:265:HIS:NE2	16:Q:117:LEU:HD21	2.35	0.41
4:U:321:ILE:HG23	13:N:177:GLN:NE2	2.35	0.41
8:Y:-164:DC:H4'	8:Y:-163:DG:OP1	2.20	0.41
9:H:220:ILE:HD13	9:H:237:VAL:HG12	2.03	0.41
10:I:71:GLY:O	10:I:75:LYS:HG3	2.21	0.41
10:I:82:GLN:O	10:I:85:ASP:HB2	2.21	0.41
9:H:101:LEU:O	9:H:105:ARG:HG2	2.20	0.41
9:H:137:ASN:O	9:H:141:MET:HG3	2.21	0.41
2:S:12:ARG:O	2:S:16:GLN:HG3	2.21	0.41
6:W:73:GLU:HG2	6:W:74:HIS:N	2.36	0.41
10:I:615:THR:O	10:I:619:LYS:HG3	2.20	0.41
11:K:93:GLY:O	11:K:97:PHE:HD2	2.04	0.41
13:N:60:ARG:HA	13:N:60:ARG:CZ	2.50	0.41
13:N:117:LYS:HA	13:N:117:LYS:HD2	1.85	0.41
14:O:128:THR:HA	14:O:185:ASN:OD1	2.21	0.41
14:O:164:ILE:HD11	14:O:183:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:250:ASP:HB3	15:P:253:ARG:HH12	1.85	0.41
1:M:85:LEU:HD13	1:M:124:TYR:CE2	2.56	0.41
5:V:161:DT:H1'	5:V:162:DT:H5'	2.03	0.41
5:V:172:DC:C2	5:V:173:DG:N7	2.89	0.41
10:I:366:VAL:HG13	10:I:372:LEU:HB2	2.02	0.41
12:L:142:VAL:HG22	12:L:156:VAL:HG22	2.03	0.41
14:O:108:TYR:CE2	14:O:114:SER:HA	2.55	0.41
14:O:250:VAL:HG11	14:O:276:CYS:HB2	2.03	0.41
16:Q:92:ILE:O	16:Q:96:LEU:HD23	2.21	0.41
1:M:129:LEU:HB3	1:M:142:MET:CE	2.51	0.40
4:U:262:HIS:CE1	4:U:278:ILE:HG22	2.57	0.40
8:Y:-157:DC:H6	8:Y:-157:DC:H2'	1.72	0.40
10:I:87:THR:HA	10:I:90:LYS:HE3	2.03	0.40
10:I:723:LEU:HB3	10:I:728:LEU:HD22	2.02	0.40
11:K:27:GLU:HG2	11:K:31:MET:HE2	2.03	0.40
11:K:104:LEU:HD23	11:K:104:LEU:HA	1.90	0.40
16:Q:88:MET:HE2	16:Q:114:LYS:NZ	2.35	0.40
16:Q:131:MET:O	16:Q:131:MET:SD	2.79	0.40
18:C:269:THR:O	18:C:273:LYS:HG2	2.22	0.40
10:I:583:PHE:CD1	10:I:583:PHE:N	2.88	0.40
12:L:165:VAL:HG12	12:L:166:PHE:CD2	2.55	0.40
13:N:57:GLU:HA	13:N:57:GLU:OE2	2.19	0.40
14:O:246:LEU:HD23	14:O:246:LEU:HA	1.97	0.40
16:Q:92:ILE:HA	16:Q:95:ILE:HG12	2.03	0.40
2:S:61:PHE:O	2:S:65:LEU:HD23	2.21	0.40
4:U:344:LEU:HD12	4:U:344:LEU:HA	1.96	0.40
10:I:589:TYR:OH	10:I:659:LYS:HG3	2.22	0.40
10:I:651:LEU:O	10:I:682:VAL:N	2.55	0.40
13:N:67:ALA:O	13:N:71:ILE:HG13	2.21	0.40
8:Y:-153:DA:H2''	8:Y:-152:DA:O4'	2.22	0.40
9:H:164:LEU:HD23	9:H:164:LEU:HA	1.95	0.40
10:I:135:PRO:HB3	10:I:139:ILE:HG12	2.04	0.40
10:I:728:LEU:HD23	10:I:731:LEU:HD22	2.03	0.40
12:L:155:LYS:HE3	12:L:157:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	170/180 (94%)	168 (99%)	2 (1%)	0	100	100
2	S	118/138 (86%)	118 (100%)	0	0	100	100
3	T	110/777 (14%)	104 (94%)	6 (6%)	0	100	100
4	U	164/211 (78%)	159 (97%)	5 (3%)	0	100	100
6	W	83/88 (94%)	82 (99%)	1 (1%)	0	100	100
7	X	72/81 (89%)	72 (100%)	0	0	100	100
9	H	201/247 (81%)	195 (97%)	6 (3%)	0	100	100
10	I	618/762 (81%)	583 (94%)	29 (5%)	6 (1%)	12	32
11	K	227/269 (84%)	221 (97%)	6 (3%)	0	100	100
12	L	309/348 (89%)	296 (96%)	11 (4%)	2 (1%)	21	44
13	N	313/347 (90%)	299 (96%)	13 (4%)	1 (0%)	36	60
14	O	208/300 (69%)	202 (97%)	6 (3%)	0	100	100
15	P	220/288 (76%)	211 (96%)	9 (4%)	0	100	100
16	Q	185/215 (86%)	181 (98%)	4 (2%)	0	100	100
17	R	76/177 (43%)	71 (93%)	5 (7%)	0	100	100
18	C	22/775 (3%)	22 (100%)	0	0	100	100
All	All	3096/5203 (60%)	2984 (96%)	103 (3%)	9 (0%)	37	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	I	654	SER
12	L	44	PRO
12	L	246	SER
10	I	84	LYS
10	I	649	GLY
10	I	404	LYS

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Mol	Chain	Res	Type
10	I	647	MET
10	I	662	TYR
13	N	303	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	151/158 (96%)	145 (96%)	6 (4%)	28	56
2	S	107/121 (88%)	106 (99%)	1 (1%)	70	87
3	T	100/635 (16%)	98 (98%)	2 (2%)	48	76
4	U	153/190 (80%)	149 (97%)	4 (3%)	40	70
6	W	75/77 (97%)	74 (99%)	1 (1%)	61	83
7	X	65/67 (97%)	65 (100%)	0	100	100
9	H	191/224 (85%)	186 (97%)	5 (3%)	40	70
10	I	570/697 (82%)	558 (98%)	12 (2%)	47	75
11	K	222/260 (85%)	217 (98%)	5 (2%)	44	73
12	L	278/308 (90%)	265 (95%)	13 (5%)	23	51
13	N	290/319 (91%)	283 (98%)	7 (2%)	43	72
14	O	179/263 (68%)	176 (98%)	3 (2%)	53	79
15	P	197/259 (76%)	197 (100%)	0	100	100
16	Q	178/200 (89%)	174 (98%)	4 (2%)	45	74
17	R	75/166 (45%)	75 (100%)	0	100	100
18	C	23/687 (3%)	22 (96%)	1 (4%)	26	54
All	All	2854/4631 (62%)	2790 (98%)	64 (2%)	45	74

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	88	VAL

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Mol	Chain	Res	Type
1	M	92	PHE
1	M	109	HIS
1	M	111	SER
1	M	167	SER
1	M	171	SER
2	S	92	LEU
3	T	461	SER
3	T	494	LEU
4	U	296	SER
4	U	361	LEU
4	U	364	LEU
4	U	402	SER
6	W	76	LEU
9	H	77	GLN
9	H	107	ARG
9	H	127	MET
9	H	177	THR
9	H	219	LEU
10	I	156	CYS
10	I	229	MET
10	I	376	ILE
10	I	378	CYS
10	I	393	SER
10	I	443	LEU
10	I	470	VAL
10	I	487	ILE
10	I	583	PHE
10	I	597	THR
10	I	644	LEU
10	I	736	ARG
11	K	35	MET
11	K	82	ILE
11	K	139	LEU
11	K	177	LEU
11	K	222	ARG
12	L	26	PRO
12	L	92	SER
12	L	109	VAL
12	L	115	PHE
12	L	122	SER
12	L	177	ASP
12	L	238	GLU

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Mol	Chain	Res	Type
12	L	245	CYS
12	L	249	SER
12	L	282	LEU
12	L	305	VAL
12	L	310	SER
12	L	311	VAL
13	N	22	THR
13	N	82	VAL
13	N	112	LEU
13	N	122	SER
13	N	157	GLN
13	N	171	ASN
13	N	337	ARG
14	O	114	SER
14	O	168	TYR
14	O	252	VAL
16	Q	88	MET
16	Q	104	GLU
16	Q	163	ASP
16	Q	167	GLU
18	C	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	87	HIS
1	M	125	GLN
1	M	151	GLN
2	S	71	HIS
3	T	453	GLN
3	T	532	HIS
4	U	408	ASN
4	U	409	HIS
7	X	49	GLN
9	H	239	GLN
10	I	477	HIS
10	I	613	ASN
10	I	678	ASN
10	I	729	GLN
11	K	126	GLN
11	K	213	HIS
11	K	249	ASN

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Mol	Chain	Res	Type
12	L	37	GLN
12	L	342	GLN
13	N	113	GLN
13	N	261	GLN
14	O	145	GLN
14	O	185	ASN
14	O	212	ASN
15	P	186	HIS
15	P	225	GLN
15	P	252	ASN
16	Q	177	GLN
16	Q	201	HIS
16	Q	236	ASN
17	R	147	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.

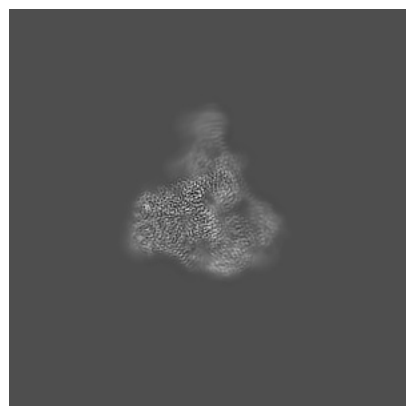
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56683. These allow visual inspection of the internal detail of the map and identification of artifacts.

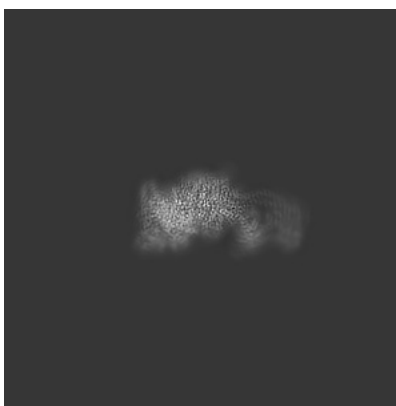
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

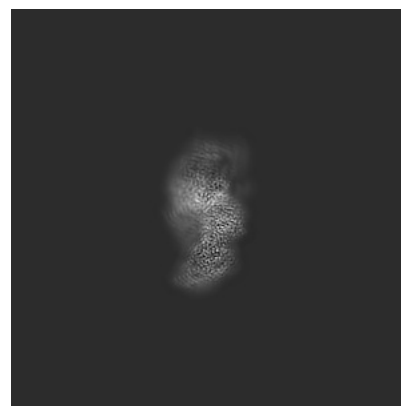
6.1.1 Primary map



X

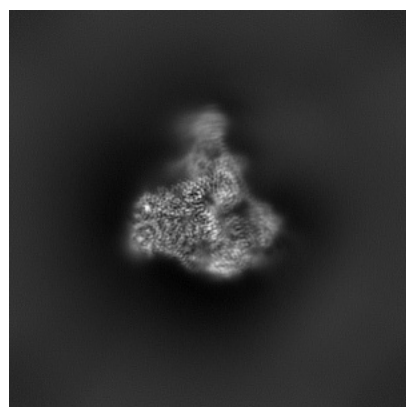


Y

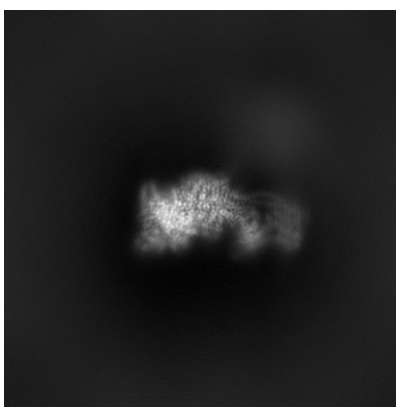


Z

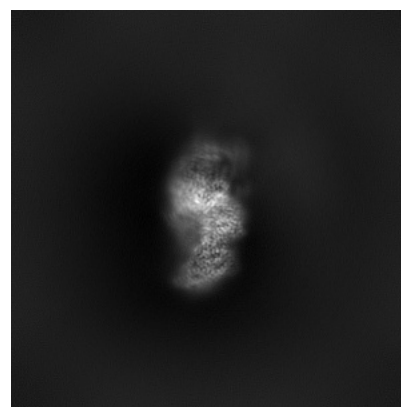
6.1.2 Raw map



X



Y

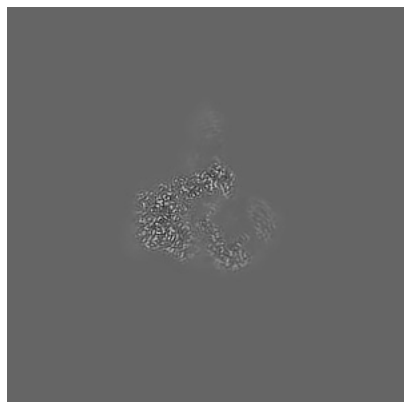


Z

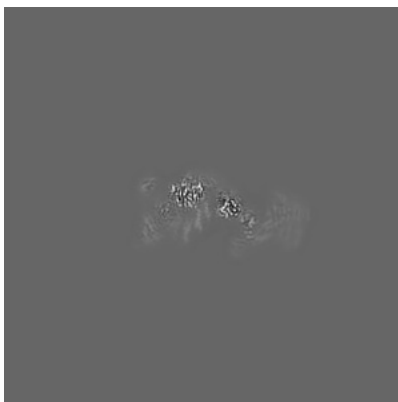
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

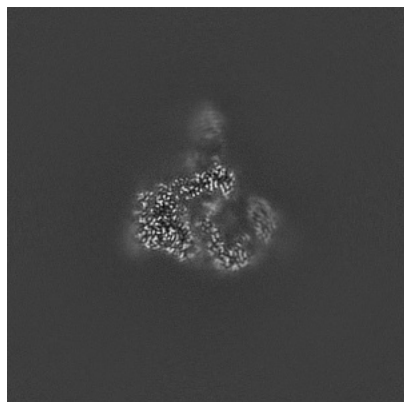


Y Index: 200

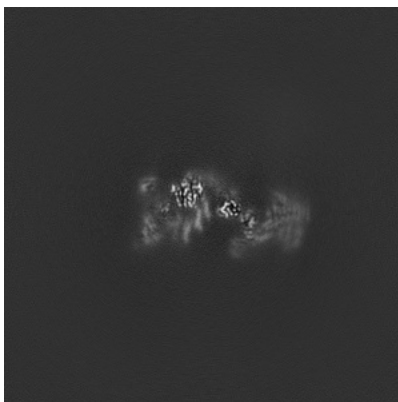


Z Index: 200

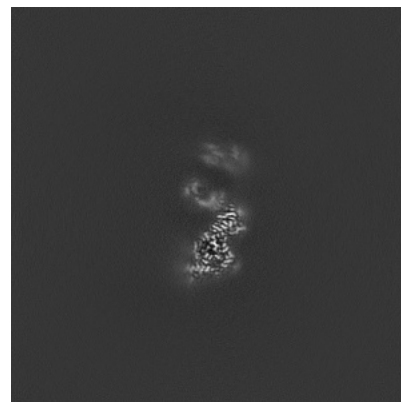
6.2.2 Raw map



X Index: 200



Y Index: 200

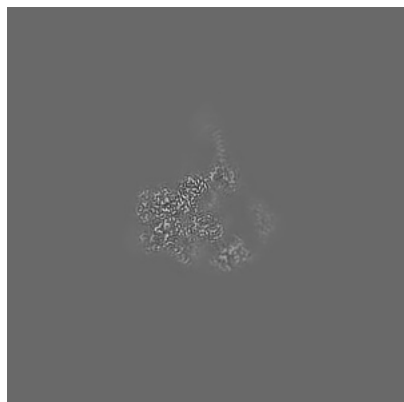


Z Index: 200

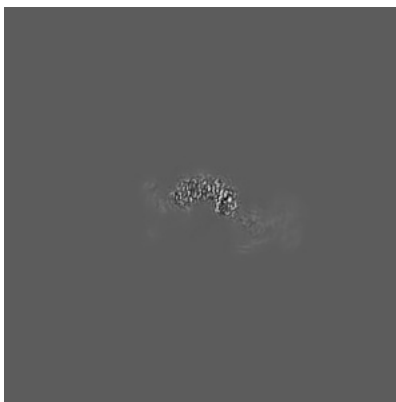
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 206

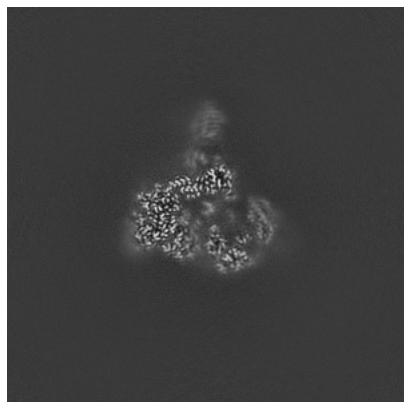


Y Index: 191

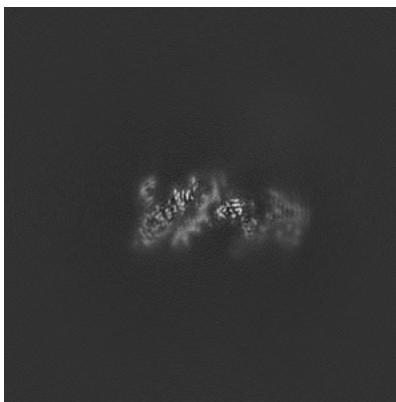


Z Index: 200

6.3.2 Raw map



X Index: 197



Y Index: 205

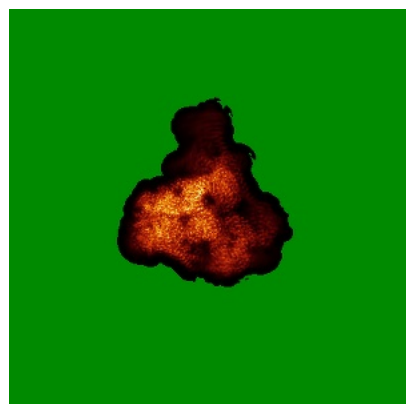


Z Index: 178

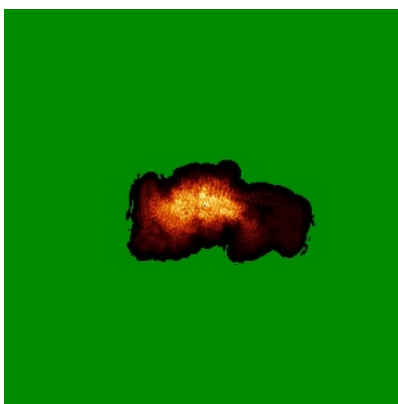
The images above show the largest variance slices of the map in three orthogonal directions.

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

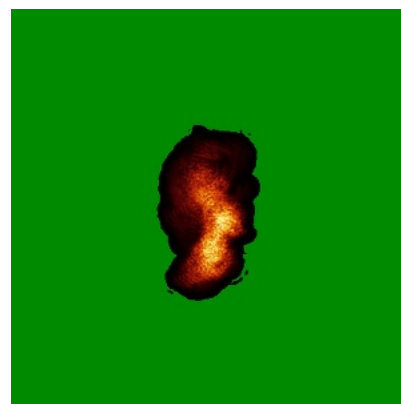
6.4.1 Primary map



X

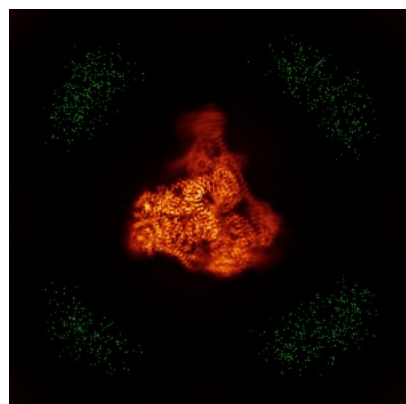


Y

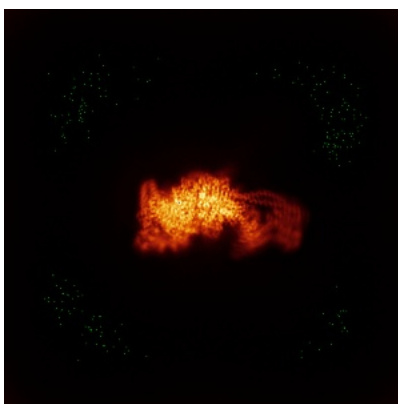


Z

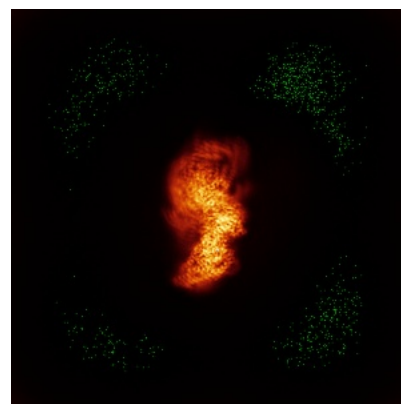
6.4.2 Raw map



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.

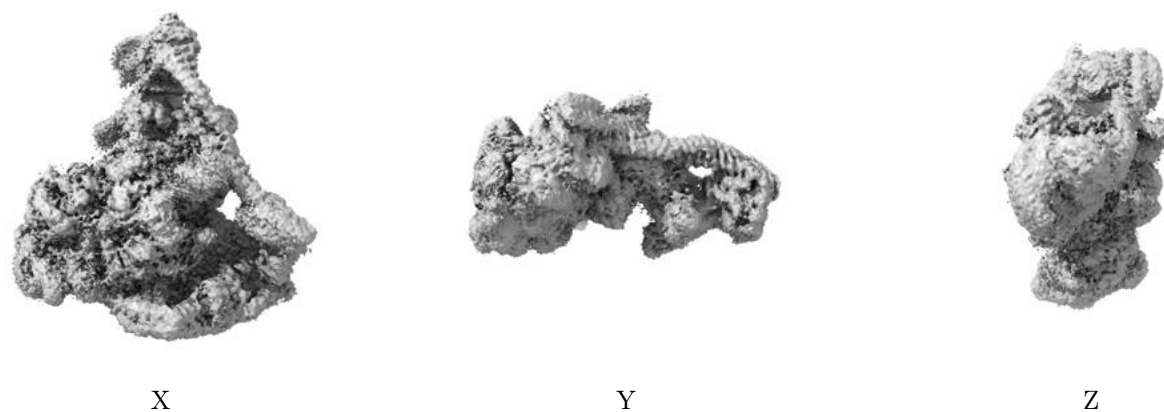
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0759. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

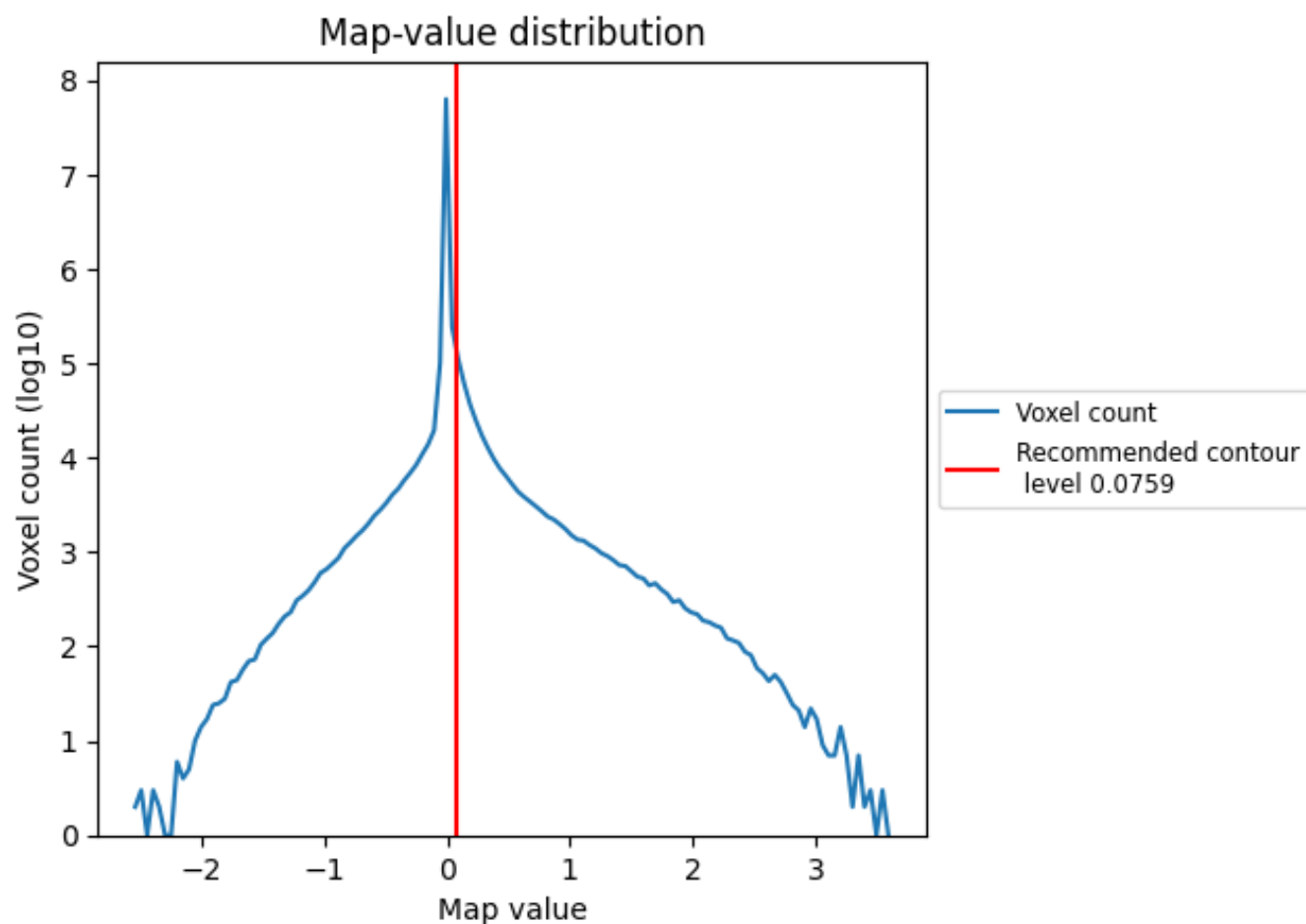
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

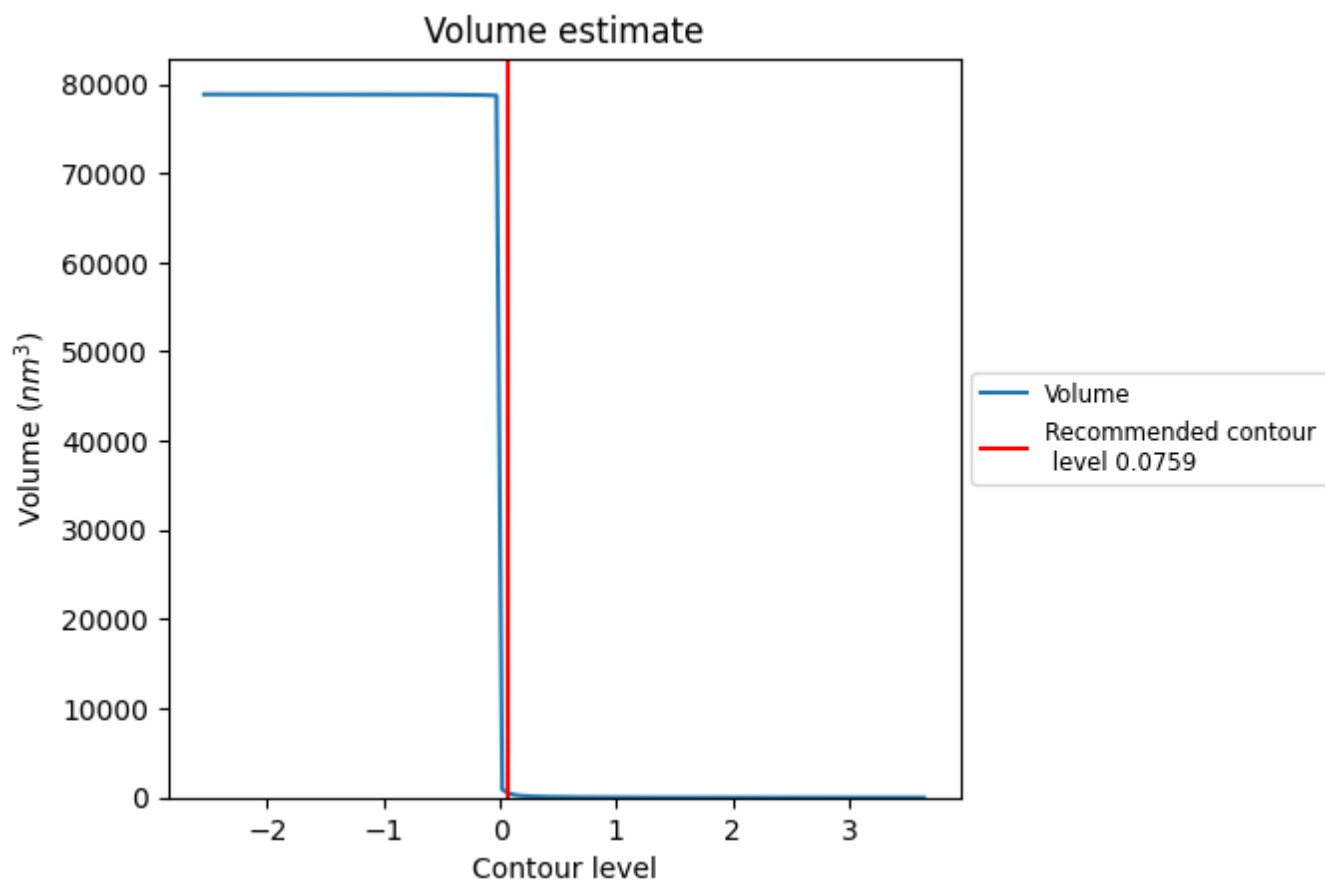
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

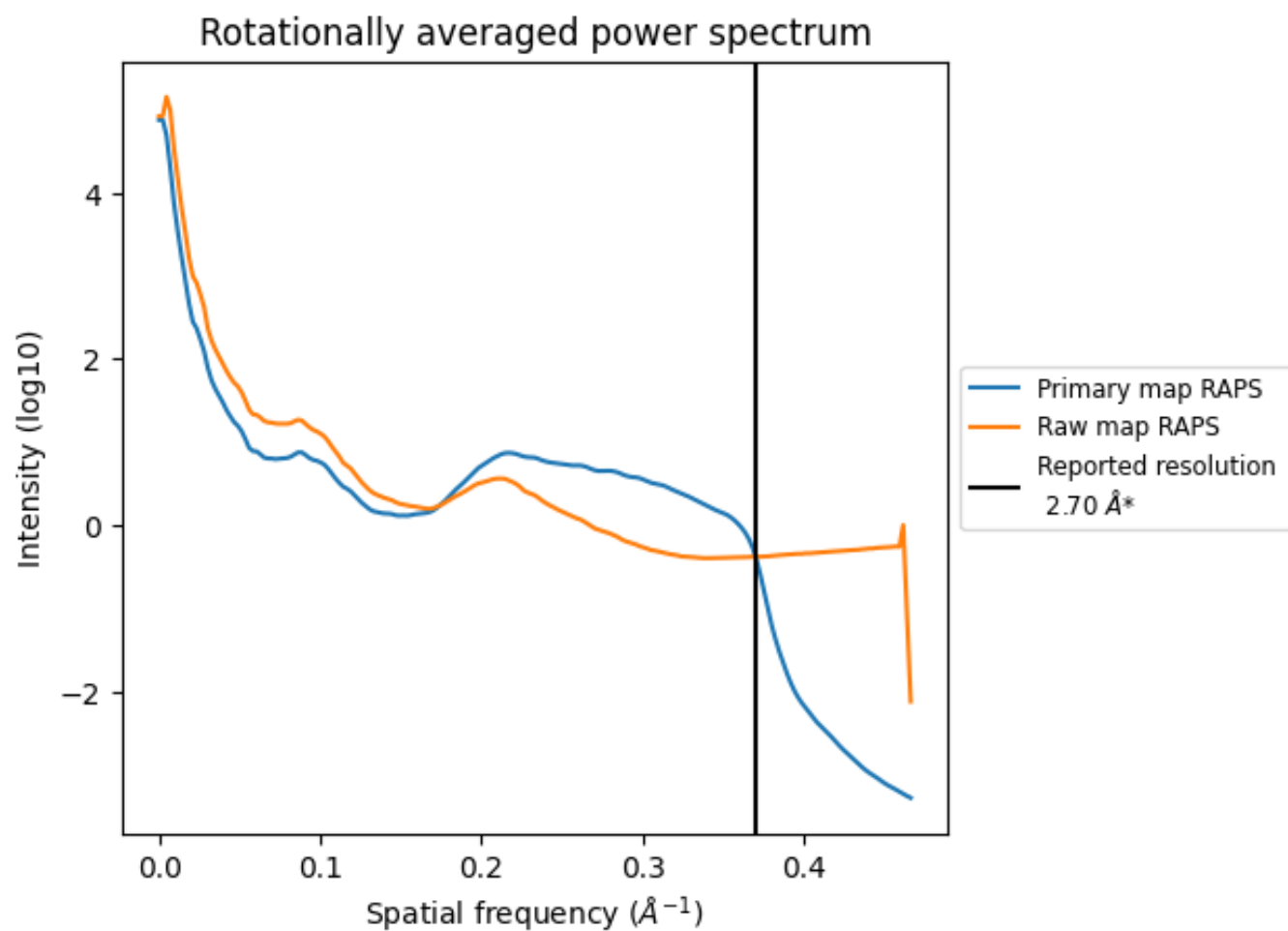
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 435 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 ⓘ

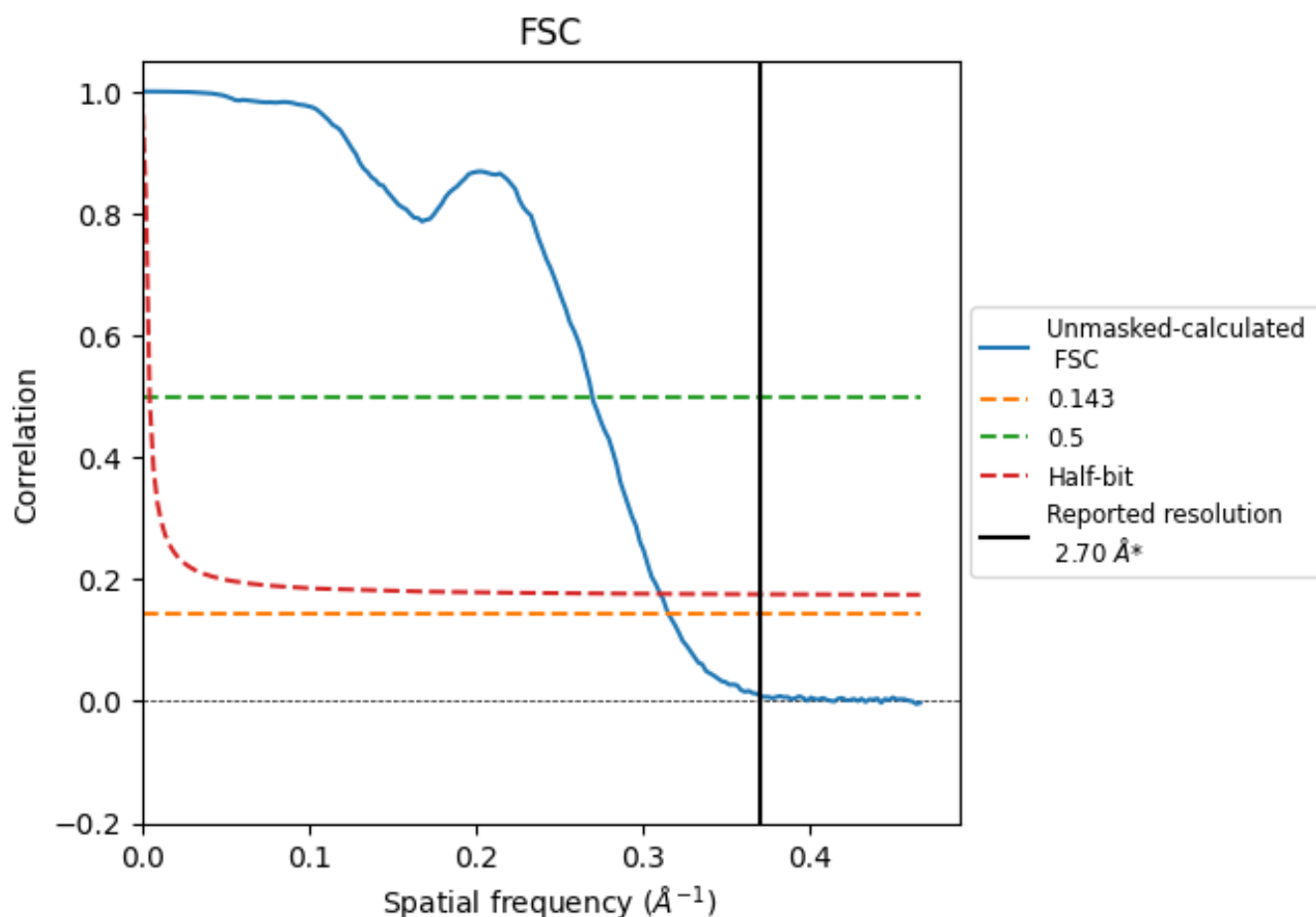


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

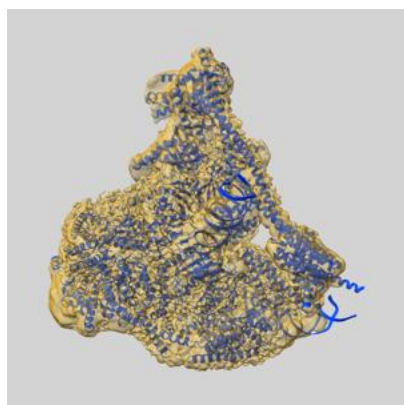
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.70	3.22

*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 3.17 differs from the reported value 2.7 by more than 10 %

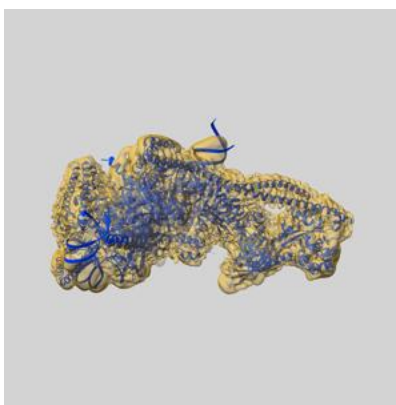
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56683 and PDB model 28OP. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

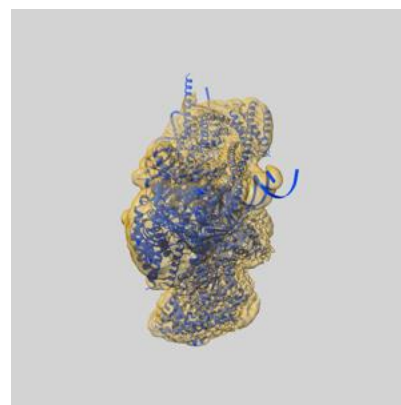
9.1 Map-model overlay [i](#)



X



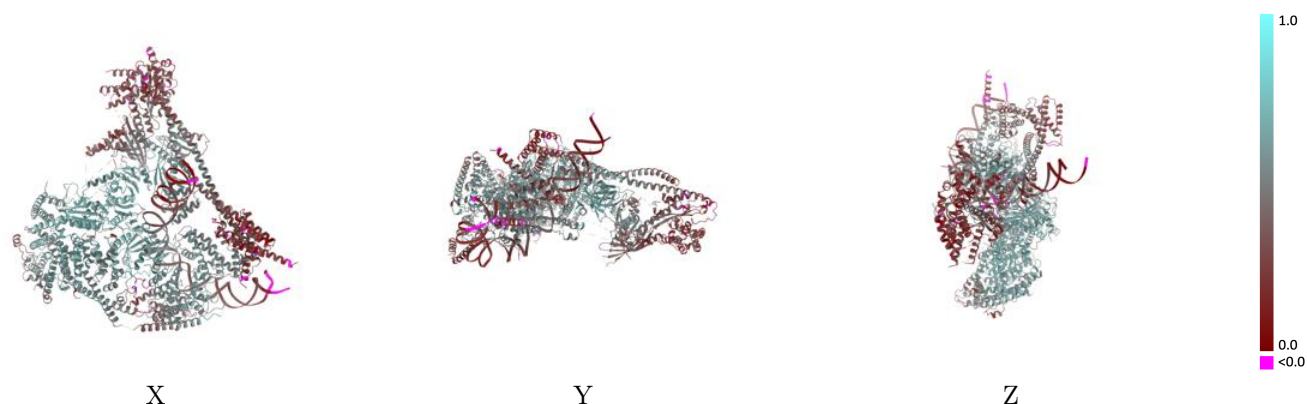
Y



Z

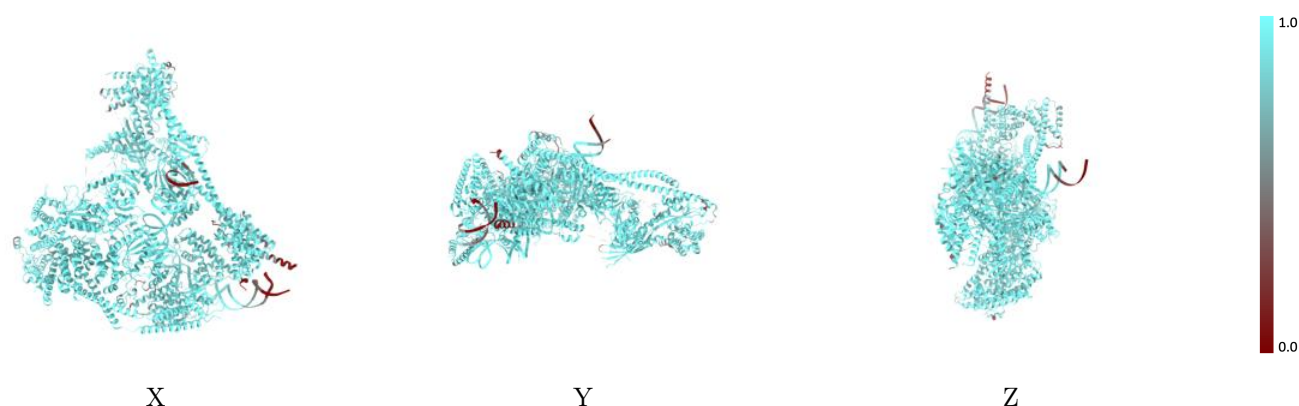
The images above show the 3D surface view of the map at the recommended contour level 0.0759 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



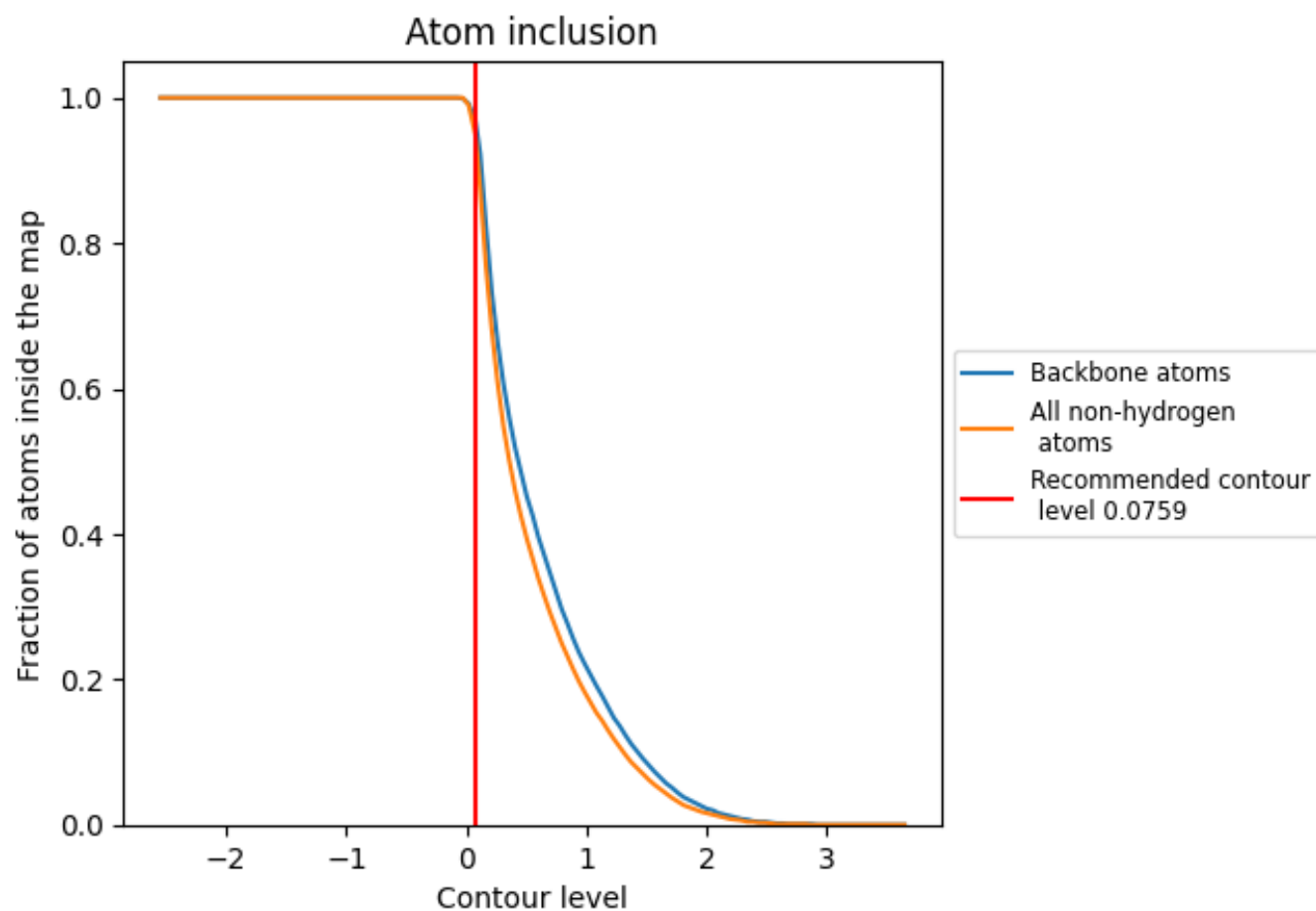
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0759).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.0759) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.4550
C	 0.9610	 0.4760
H	 0.9890	 0.5320
I	 0.9680	 0.5030
K	 0.9930	 0.5550
L	 0.9940	 0.6200
M	 0.9990	 0.6600
N	 0.9890	 0.5950
O	 0.9840	 0.4470
P	 0.9580	 0.2950
Q	 0.8890	 0.2580
R	 0.8820	 0.1750
S	 0.8120	 0.3200
T	 0.9770	 0.5250
U	 0.9040	 0.2930
V	 0.8470	 0.2310
W	 0.9880	 0.5580
X	 0.9480	 0.3870
Y	 0.7930	 0.2070

