Full wwPDB EM Validation Report ⓘ

Jan 28, 2025 – 12:31 pm GMT

PDB ID	:	8RWV
EMDB ID	:	EMD-19566
Title	:	Human OCCM DNA licensing intermediate
Authors	:	Wells, J.N.; Leber, V.; Edwards, L.V.; Allyjaun, S.; Peach, M.; Tomkins, J.; Kefala-Stavridi, A.; Faull, S.V.; Aramayo, R.; Pestana, C.M.; Ranjha, L.; Speck, C.
Deposited on	:	2024-02-05
Resolution	:	6.68 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:

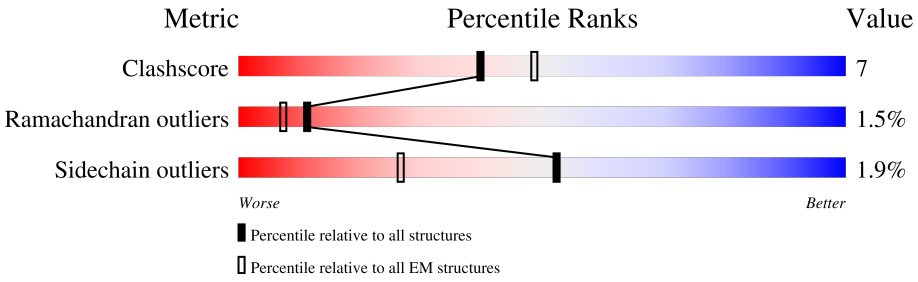
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 6.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	2	947	12% 58% 11% 31%
2	3	853	41% 67% 17% • 15%
3	4	883	13% 60% 11% 28%
4	6	821	7% 64% 16% • 20%
5	7	719	29% 83% 16% •
6	A	961	• 32% 8% 60%
7	B	577	6% 44% 10% 46%
8	C	712	12% 79% 16% 5%

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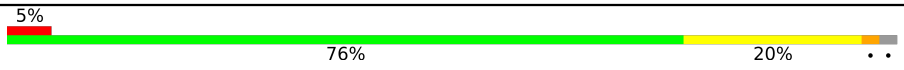
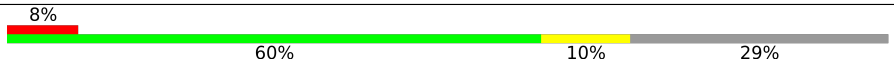
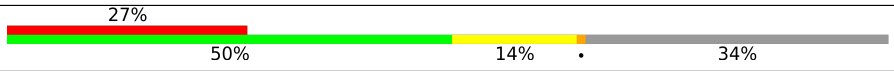
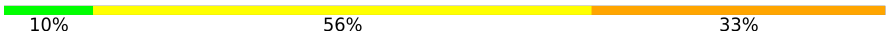
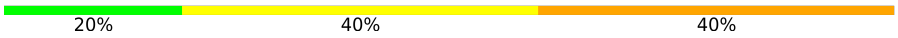
Mol	Chain	Length	Quality of chain
9	D	436	
10	E	435	
11	F	560	
12	G	410	
13	H	39	
14	J	40	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 51862 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 licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	653	5131	3221	913	966	31	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-42	MET	-	initiating methionine	UNP P49736
2	-41	SER	-	expression tag	UNP P49736
2	-40	ALA	-	expression tag	UNP P49736
2	-39	TRP	-	expression tag	UNP P49736
2	-38	SER	-	expression tag	UNP P49736
2	-37	HIS	-	expression tag	UNP P49736
2	-36	PRO	-	expression tag	UNP P49736
2	-35	GLN	-	expression tag	UNP P49736
2	-34	PHE	-	expression tag	UNP P49736
2	-33	GLU	-	expression tag	UNP P49736
2	-32	LYS	-	expression tag	UNP P49736
2	-31	GLY	-	expression tag	UNP P49736
2	-30	GLY	-	expression tag	UNP P49736
2	-29	GLY	-	expression tag	UNP P49736
2	-28	SER	-	expression tag	UNP P49736
2	-27	GLY	-	expression tag	UNP P49736
2	-26	GLY	-	expression tag	UNP P49736
2	-25	GLY	-	expression tag	UNP P49736
2	-24	SER	-	expression tag	UNP P49736
2	-23	GLY	-	expression tag	UNP P49736
2	-22	GLY	-	expression tag	UNP P49736
2	-21	SER	-	expression tag	UNP P49736
2	-20	ALA	-	expression tag	UNP P49736
2	-19	TRP	-	expression tag	UNP P49736
2	-18	SER	-	expression tag	UNP P49736
2	-17	HIS	-	expression tag	UNP P49736
2	-16	PRO	-	expression tag	UNP P49736
2	-15	GLN	-	expression tag	UNP P49736

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Chain	Residue	Modelled	Actual	Comment	Reference
2	-14	PHE	-	expression tag	UNP P49736
2	-13	GLU	-	expression tag	UNP P49736
2	-12	LYS	-	expression tag	UNP P49736
2	-11	GLU	-	expression tag	UNP P49736
2	-10	ASN	-	expression tag	UNP P49736
2	-9	LEU	-	expression tag	UNP P49736
2	-8	TYR	-	expression tag	UNP P49736
2	-7	PHE	-	expression tag	UNP P49736
2	-6	GLN	-	expression tag	UNP P49736
2	-5	GLY	-	expression tag	UNP P49736
2	-4	ALA	-	expression tag	UNP P49736
2	-3	GLY	-	expression tag	UNP P49736
2	-2	SER	-	expression tag	UNP P49736
2	-1	ALA	-	expression tag	UNP P49736
2	0	THR	-	expression tag	UNP P49736

- Molecule 2 is a protein called Isoform 2 of DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	724	Total	C	N	O	S	0	0
			5674	3541	994	1109	30		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	632	Total	C	N	O	S	0	0
			5017	3155	883	953	26		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-19	MET	-	initiating methionine	UNP P33991
4	-18	HIS	-	expression tag	UNP P33991
4	-17	HIS	-	expression tag	UNP P33991
4	-16	HIS	-	expression tag	UNP P33991
4	-15	HIS	-	expression tag	UNP P33991
4	-14	HIS	-	expression tag	UNP P33991
4	-13	HIS	-	expression tag	UNP P33991
4	-12	HIS	-	expression tag	UNP P33991
4	-11	HIS	-	expression tag	UNP P33991
4	-10	GLU	-	expression tag	UNP P33991
4	-9	ASN	-	expression tag	UNP P33991

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Chain	Residue	Modelled	Actual	Comment	Reference
4	-8	LEU	-	expression tag	UNP P33991
4	-7	TYR	-	expression tag	UNP P33991
4	-6	PHE	-	expression tag	UNP P33991
4	-5	GLN	-	expression tag	UNP P33991
4	-4	GLY	-	expression tag	UNP P33991
4	-3	SER	-	expression tag	UNP P33991
4	-2	SER	-	expression tag	UNP P33991
4	-1	ALA	-	expression tag	UNP P33991
4	0	THR	-	expression tag	UNP P33991

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	660	Total	C	N	O	S	0	0
			5311	3342	935	1007	27		

- Molecule 5 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	719	Total	C	N	O	S	0	0
			5698	3556	1023	1085	34		

- Molecule 6 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	387	Total	C	N	O	S	0	0
			3061	1919	542	577	23		

- Molecule 7 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	313	Total	C	N	O	S	0	0
			2575	1649	437	483	6		

- Molecule 8 is a protein called Isoform 2 of Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	678	Total	C	N	O	S	0	0
			5509	3525	930	1021	33		

- Molecule 9 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	428	Total	C	N	O	S	0	0
			3472	2206	607	637	22		

- Molecule 10 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	431	Total	C	N	O	S	0	0
			3514	2277	588	637	12		

- Molecule 11 is a protein called Cell division control protein 6 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	395	Total	C	N	O	S	0	0
			3105	1956	557	571	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	441	ILE	VAL	variant	UNP Q99741

- Molecule 12 is a protein called DNA replication factor Cdt1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	270	Total	C	N	O	S	0	0
			2175	1359	406	395	15		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	MET	-	initiating methionine	UNP Q9H211
G	138	GLY	-	expression tag	UNP Q9H211
G	139	SER	-	expression tag	UNP Q9H211
G	140	SER	-	expression tag	UNP Q9H211
G	141	HIS	-	expression tag	UNP Q9H211
G	142	HIS	-	expression tag	UNP Q9H211
G	143	HIS	-	expression tag	UNP Q9H211
G	144	HIS	-	expression tag	UNP Q9H211
G	145	HIS	-	expression tag	UNP Q9H211
G	146	HIS	-	expression tag	UNP Q9H211
G	147	SER	-	expression tag	UNP Q9H211
G	148	SER	-	expression tag	UNP Q9H211
G	149	GLY	-	expression tag	UNP Q9H211

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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	LEU	-	expression tag	UNP Q9H211
G	151	GLU	-	expression tag	UNP Q9H211
G	152	VAL	-	expression tag	UNP Q9H211
G	153	LEU	-	expression tag	UNP Q9H211
G	154	PHE	-	expression tag	UNP Q9H211
G	155	GLN	-	expression tag	UNP Q9H211
G	156	GLY	-	expression tag	UNP Q9H211
G	157	PRO	-	expression tag	UNP Q9H211

- Molecule 13 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	39	Total	C	N	O	P	0	0
			795	382	143	231	39		

- Molecule 14 is a DNA chain called DNA.

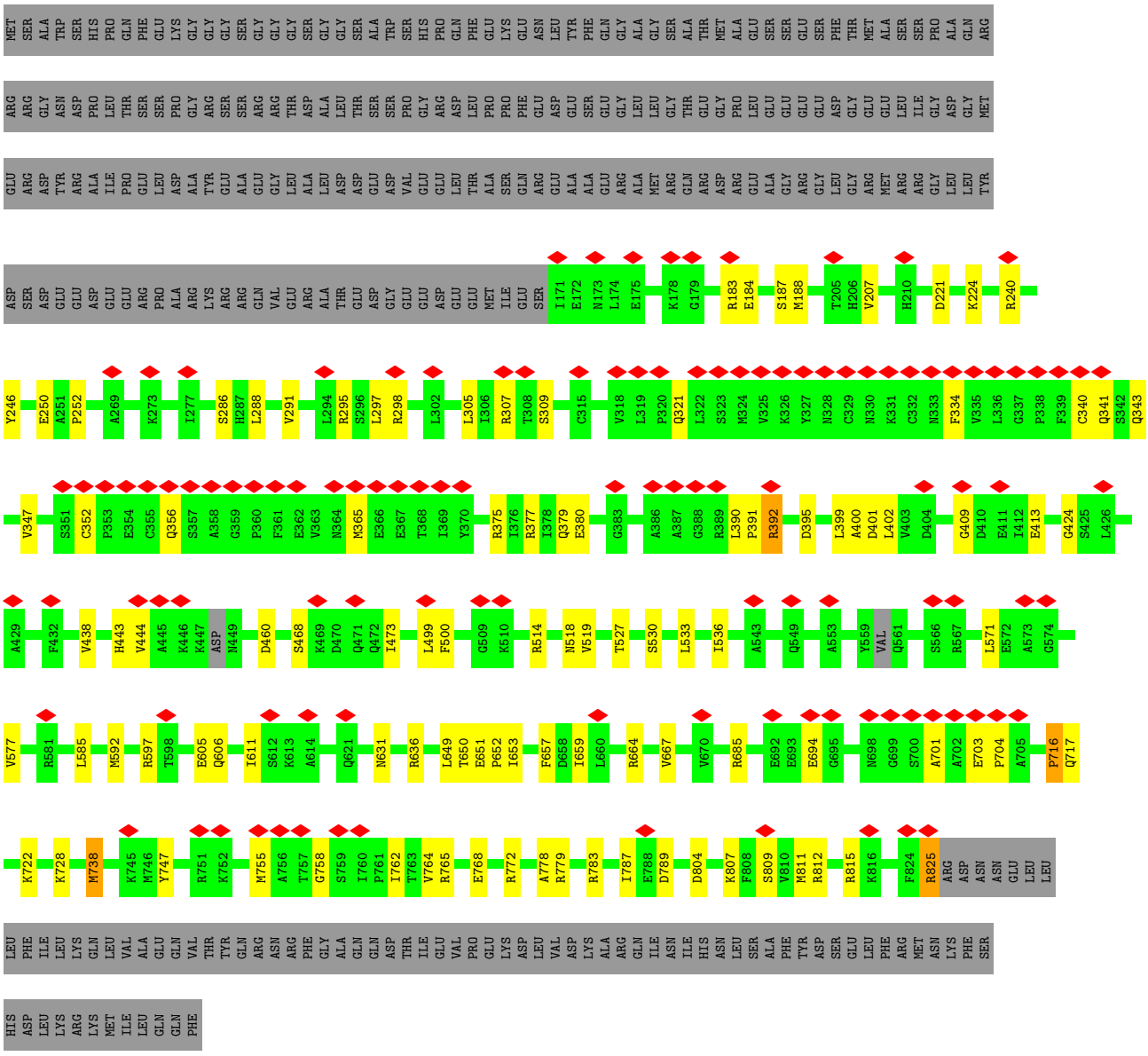
Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O	P	0	0
			825	396	147	242	40		

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 licensing factor MCM2

Chain 2:

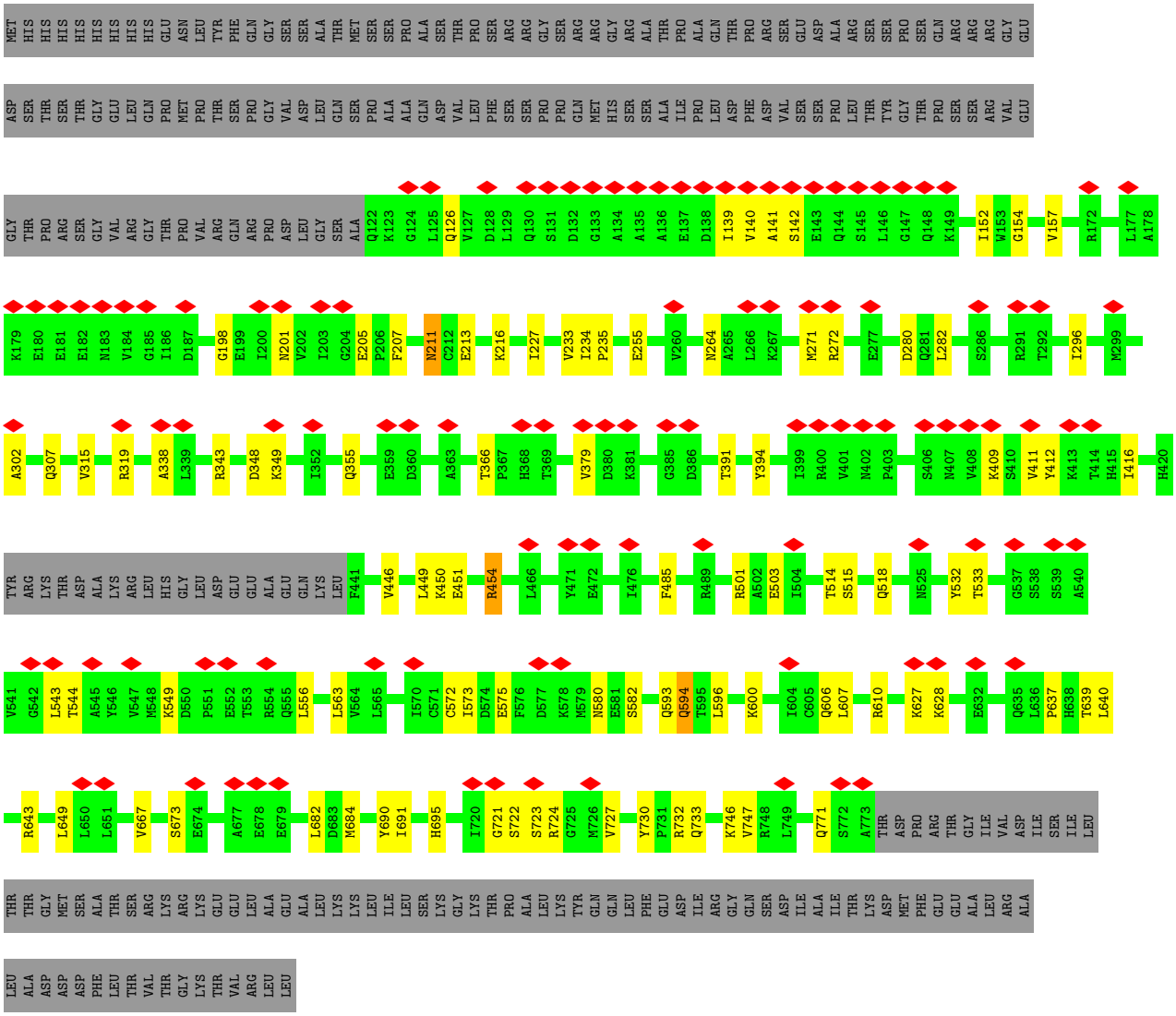


• Molecule 2: Isoform 2 of DNA replication licensing factor MCM3

Chain 3:

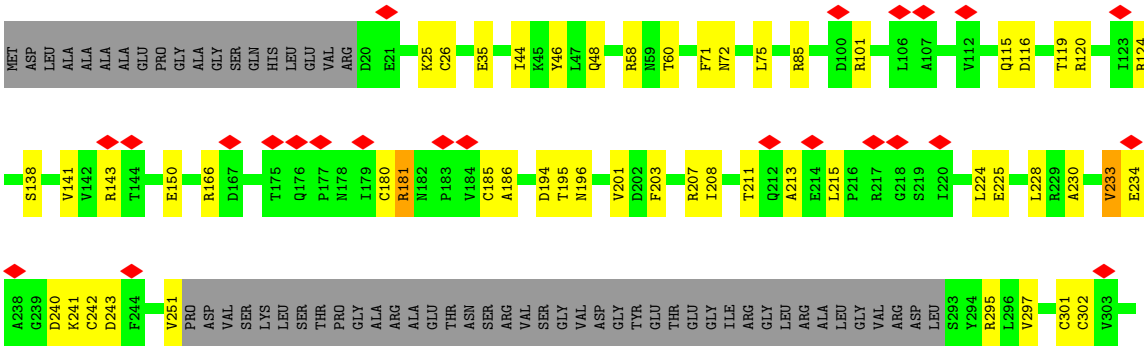
• Molecule 3: DNA replication licensing factor MCM4

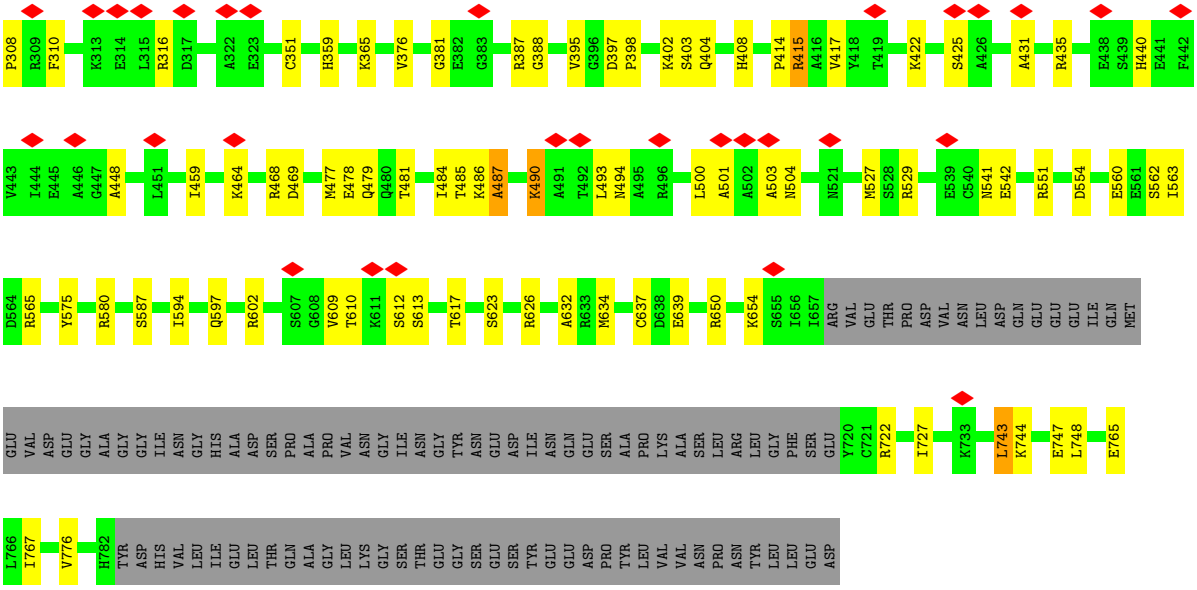
Chain 4:



• Molecule 4: DNA replication licensing factor MCM6

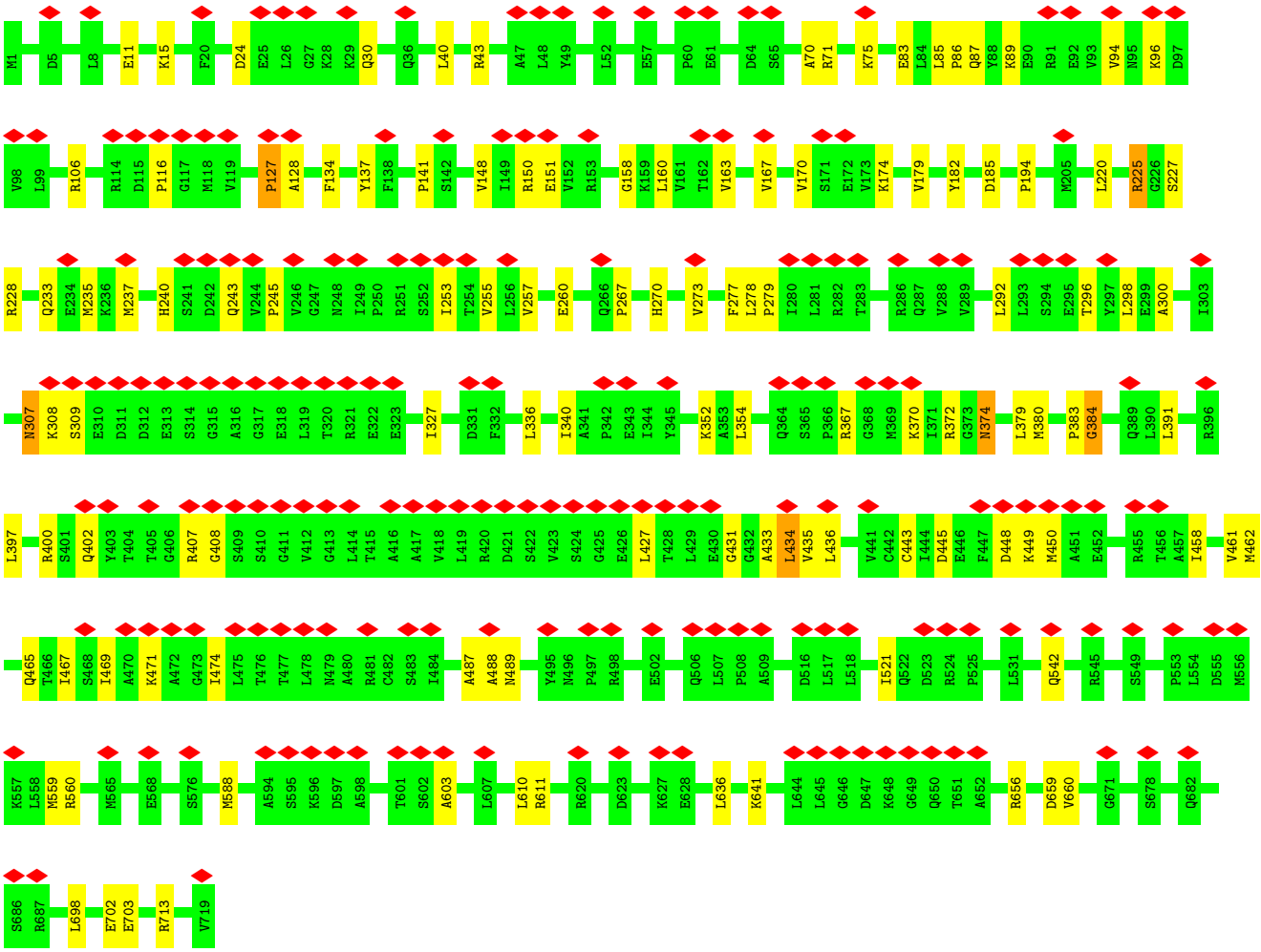
Chain 6:





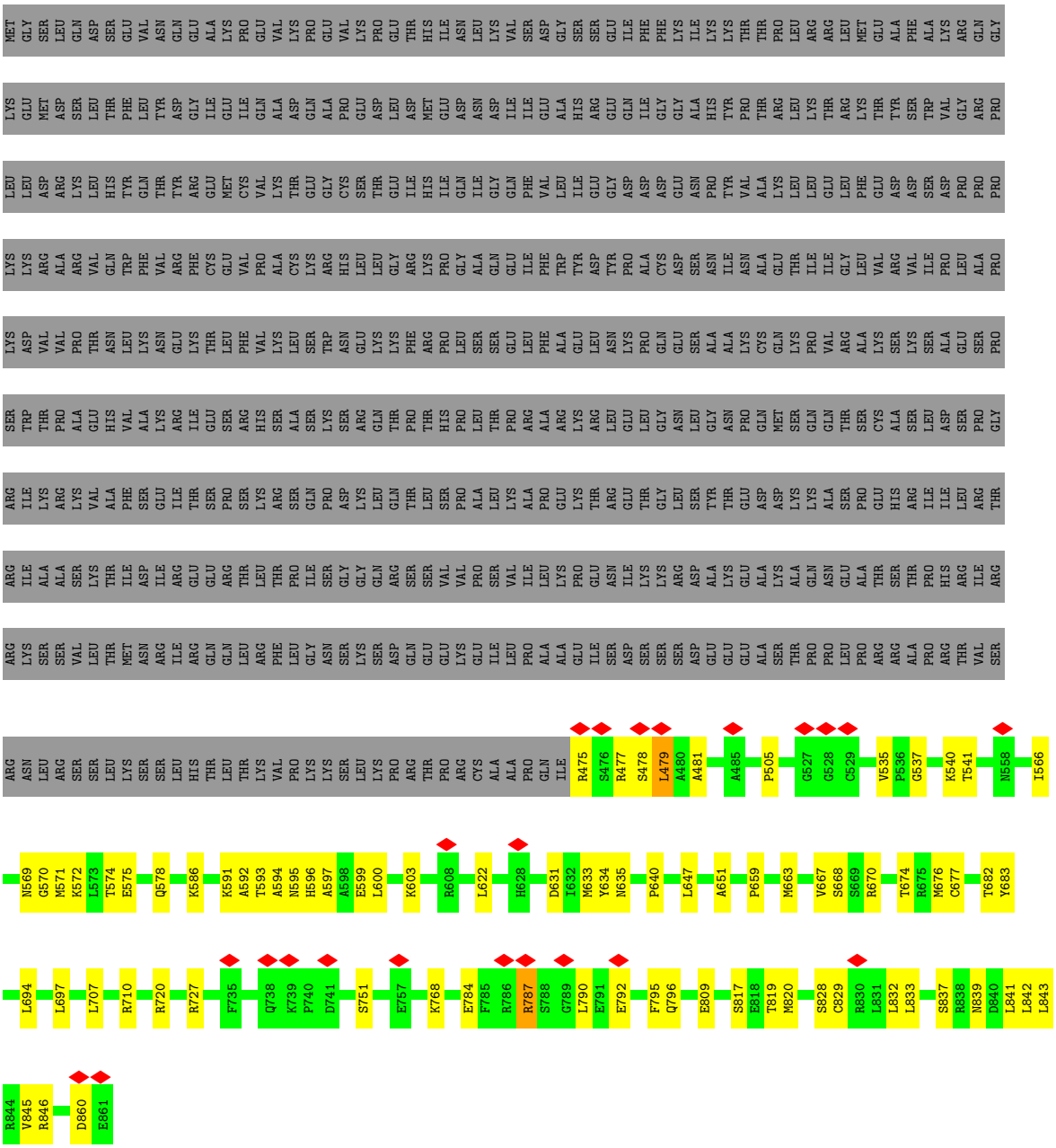
• Molecule 5: DNA replication licensing factor MCM7

Chain 7:



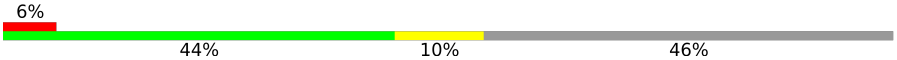
• Molecule 6: Origin recognition complex subunit 1

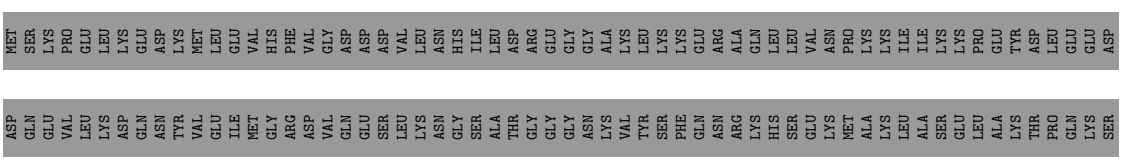
Chain A:

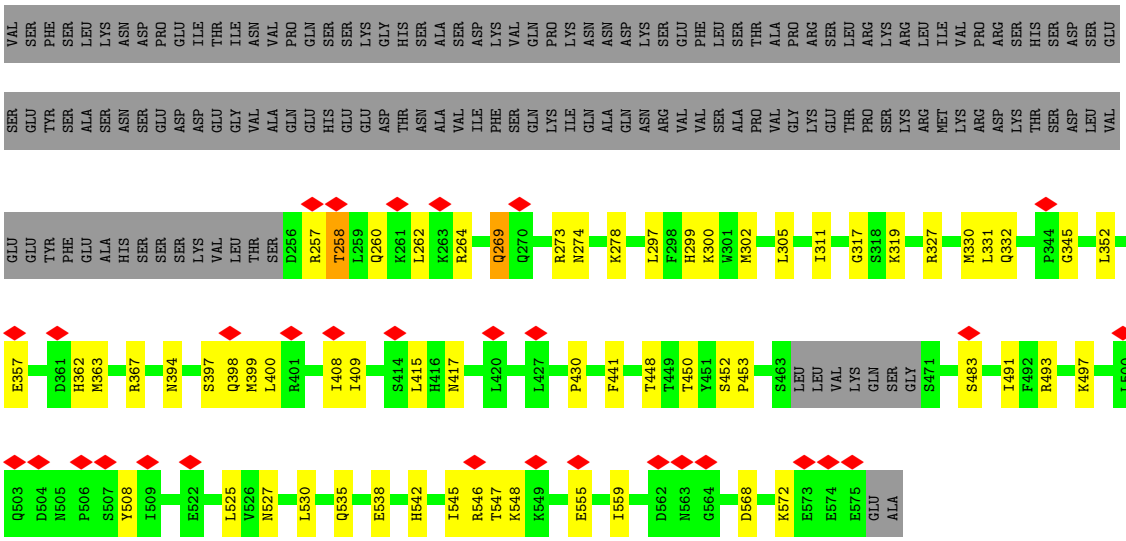


• Molecule 7: Origin recognition complex subunit 2

Chain B:

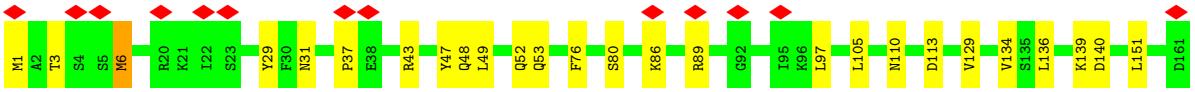


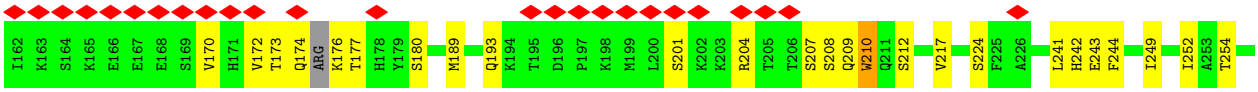


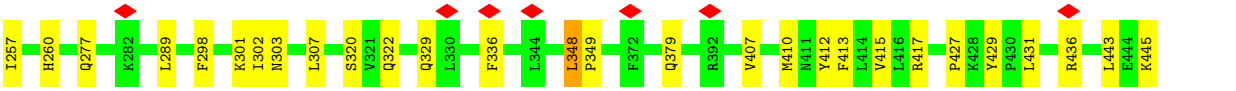


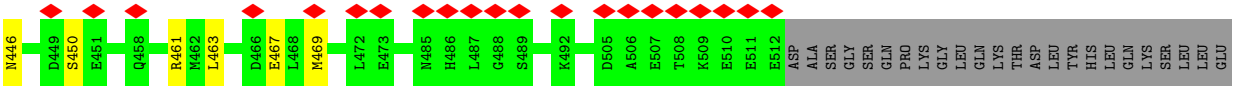
• Molecule 8: Isoform 2 of Origin recognition complex subunit 3

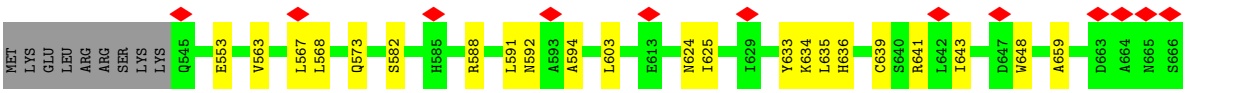
Chain C:

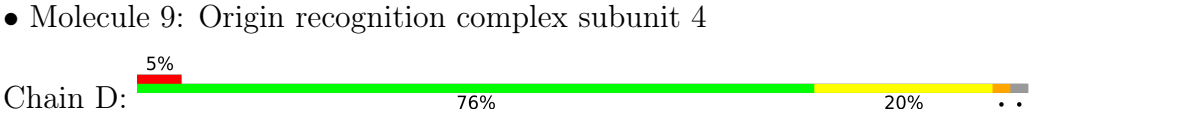


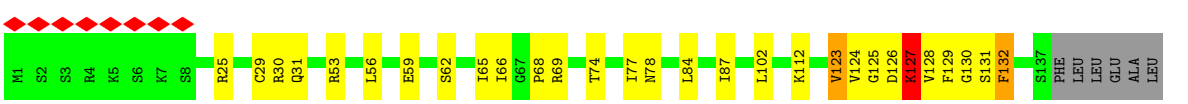






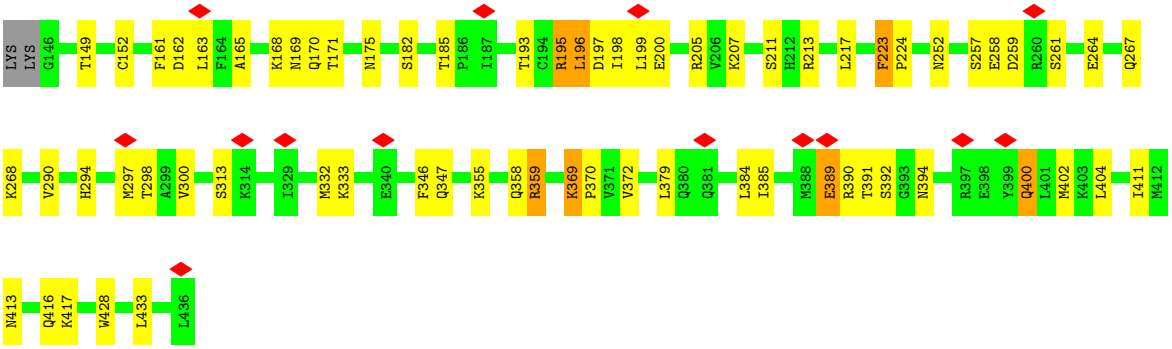




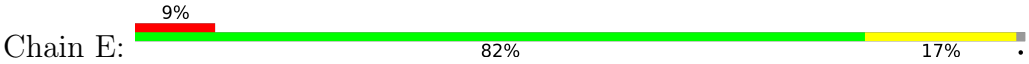


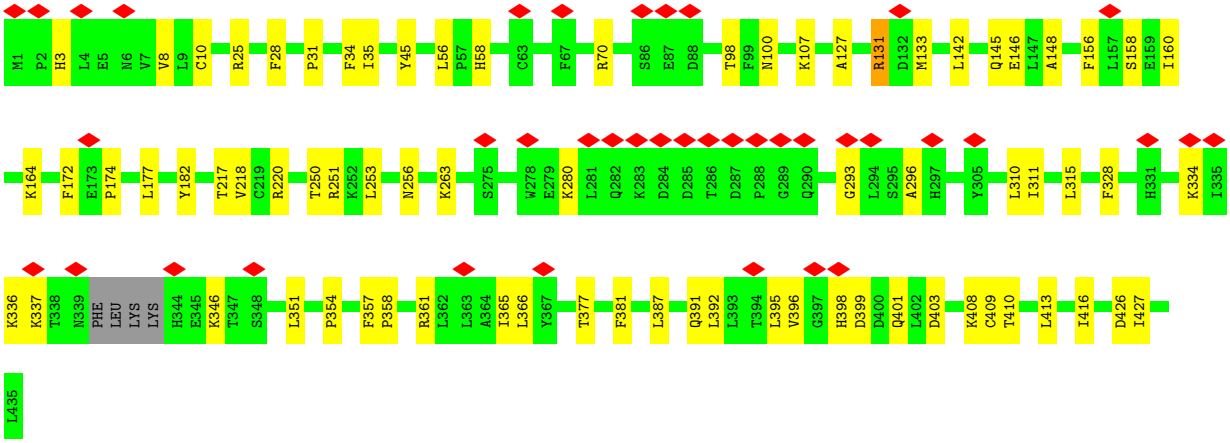
• Molecule 9: Origin recognition complex subunit 4

Chain D:

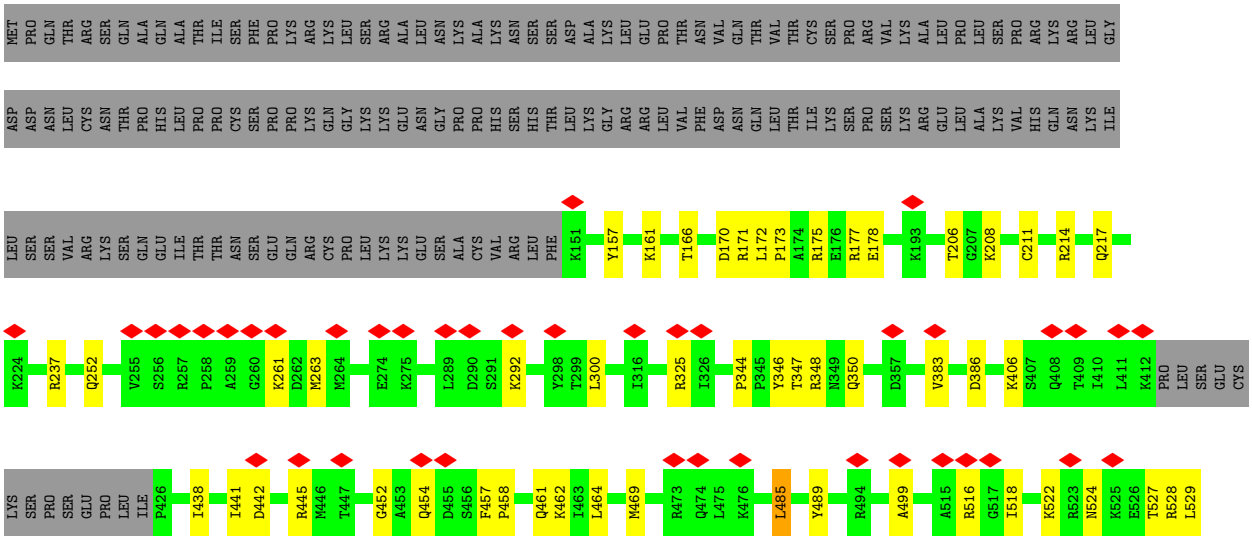


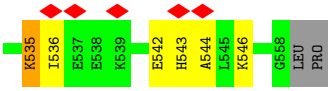
• Molecule 10: Origin recognition complex subunit 5





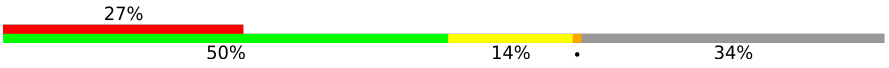
• Molecule 11: Cell division control protein 6 homolog

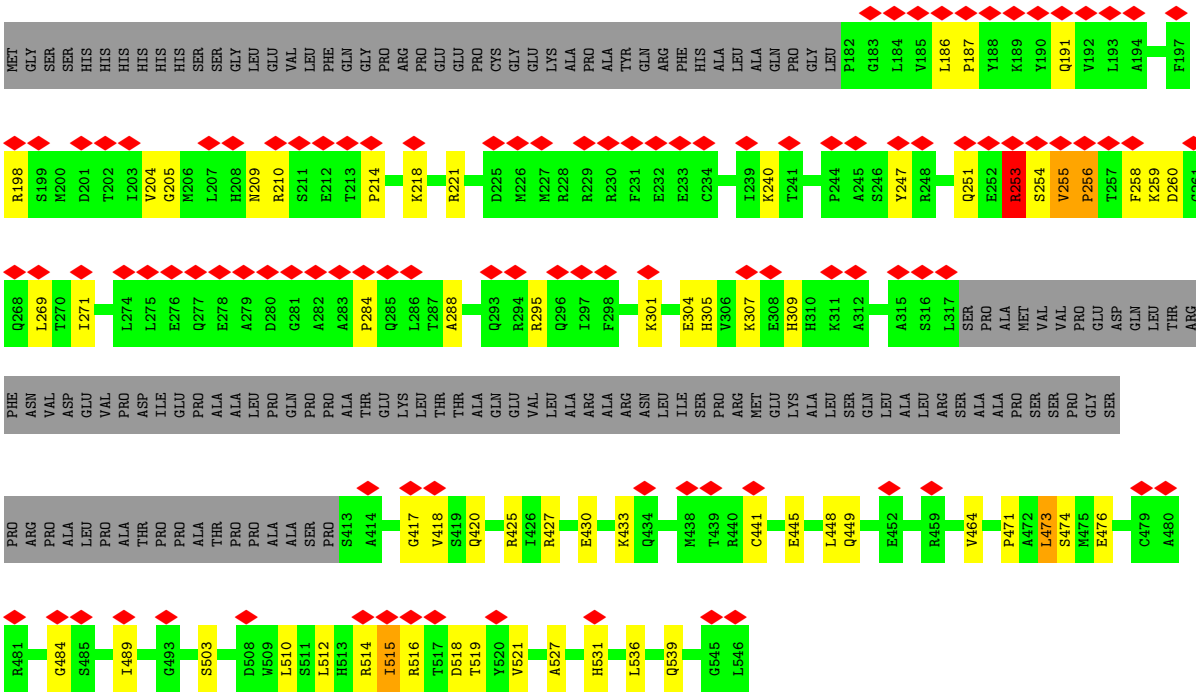




• Molecule 12: DNA replication factor Cdt1

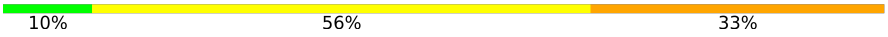
Chain G:

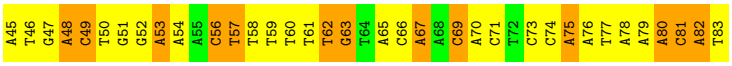




• Molecule 13: DNA

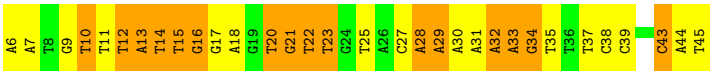
Chain H:





• Molecule 14: DNA

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8730	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.046	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	2	0.24	0/5227	0.47	0/7064
2	3	0.23	0/5759	0.47	0/7774
3	4	0.23	0/5104	0.46	0/6902
4	6	0.36	2/5397 (0.0%)	0.50	3/7276 (0.0%)
5	7	0.23	0/5788	0.49	0/7815
6	A	0.24	0/3114	0.47	0/4214
7	B	0.23	0/2628	0.45	0/3553
8	C	0.24	0/5622	0.43	0/7597
9	D	0.26	0/3537	0.45	0/4766
10	E	0.24	0/3601	0.44	0/4885
11	F	0.23	0/3140	0.48	0/4220
12	G	0.23	0/2209	0.50	0/2968
13	H	0.90	1/891 (0.1%)	1.63	27/1371 (2.0%)
14	J	0.80	1/925 (0.1%)	1.65	29/1427 (2.0%)
All	All	0.29	4/52942 (0.0%)	0.56	59/71832 (0.1%)

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
4	6	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	6	487	ALA	C-N	-16.28	1.03	1.33
13	H	47	DG	O3'-P	-12.81	1.45	1.61
4	6	485	THR	C-N	-12.21	1.05	1.34
14	J	43	DC	O3'-P	-5.29	1.54	1.61

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	43	DC	OP2-P-O3'	15.62	139.56	105.20
13	H	47	DG	P-O3'-C3'	12.82	135.09	119.70
14	J	43	DC	P-O3'-C3'	-12.82	104.31	119.70
13	H	49	DC	P-O3'-C3'	-10.93	106.59	119.70
14	J	23	DT	P-O3'-C3'	-10.32	107.31	119.70
13	H	71	DC	P-O3'-C3'	-10.04	107.65	119.70
13	H	67	DA	P-O3'-C3'	-9.97	107.73	119.70
13	H	53	DA	P-O3'-C3'	-9.67	108.09	119.70
13	H	62	DT	P-O3'-C3'	-9.53	108.27	119.70
14	J	15	DT	P-O3'-C3'	-9.22	108.64	119.70
14	J	32	DA	P-O3'-C3'	-9.04	108.85	119.70
13	H	57	DT	P-O3'-C3'	-8.89	109.03	119.70
13	H	47	DG	O3'-P-O5'	8.70	120.53	104.00
13	H	60	DT	P-O3'-C3'	-8.70	109.26	119.70
13	H	48	DA	P-O3'-C3'	-8.69	109.28	119.70
14	J	28	DA	P-O3'-C3'	-8.49	109.51	119.70
14	J	12	DT	P-O3'-C3'	-8.46	109.55	119.70
14	J	20	DT	P-O3'-C3'	-8.44	109.58	119.70
14	J	35	DT	P-O3'-C3'	-8.41	109.61	119.70
14	J	29	DA	P-O3'-C3'	-8.40	109.62	119.70
13	H	58	DT	P-O3'-C3'	-8.25	109.80	119.70
13	H	82	DA	P-O3'-C3'	-8.08	110.01	119.70
14	J	16	DG	P-O3'-C3'	-7.99	110.11	119.70
13	H	81	DC	P-O3'-C3'	-7.95	110.16	119.70
13	H	69	DC	P-O3'-C3'	-7.93	110.19	119.70
14	J	37	DT	P-O3'-C3'	-7.83	110.30	119.70
14	J	10	DT	P-O3'-C3'	-7.68	110.48	119.70
14	J	27	DC	P-O3'-C3'	-7.37	110.85	119.70
14	J	38	DC	P-O3'-C3'	-7.36	110.86	119.70
14	J	18	DA	P-O3'-C3'	-7.36	110.87	119.70
14	J	17	DG	P-O3'-C3'	-7.26	110.99	119.70
14	J	13	DA	P-O3'-C3'	-7.04	111.26	119.70
14	J	33	DA	P-O3'-C3'	-7.02	111.28	119.70
4	6	485	THR	O-C-N	7.02	133.93	122.70
13	H	51	DG	P-O3'-C3'	-7.00	111.30	119.70
14	J	22	DT	P-O3'-C3'	-6.93	111.39	119.70
14	J	43	DC	O3'-P-O5'	-6.82	91.04	104.00
14	J	25	DT	P-O3'-C3'	-6.78	111.57	119.70
13	H	75	DA	P-O3'-C3'	-6.76	111.58	119.70
13	H	50	DT	P-O3'-C3'	-6.61	111.77	119.70
13	H	63	DG	P-O3'-C3'	-6.50	111.90	119.70
14	J	21	DG	P-O3'-C3'	-6.38	112.04	119.70
4	6	485	THR	CA-C-N	-6.29	103.36	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	80	DA	P-O3'-C3'	-6.20	112.26	119.70
13	H	47	DG	OP1-P-O3'	-6.07	91.85	105.20
14	J	30	DA	P-O3'-C3'	-6.00	112.50	119.70
13	H	59	DT	P-O3'-C3'	-5.95	112.56	119.70
14	J	43	DC	OP1-P-O3'	-5.88	92.26	105.20
4	6	487	ALA	O-C-N	-5.76	113.40	123.20
13	H	66	DC	P-O3'-C3'	-5.58	113.00	119.70
13	H	65	DA	P-O3'-C3'	-5.55	113.04	119.70
13	H	54	DA	P-O3'-C3'	-5.37	113.26	119.70
13	H	73	DC	P-O3'-C3'	-5.36	113.27	119.70
14	J	39	DC	P-O3'-C3'	-5.25	113.40	119.70
13	H	56	DC	P-O3'-C3'	-5.21	113.45	119.70
14	J	6	DA	P-O3'-C3'	-5.12	113.56	119.70
14	J	34	DG	P-O3'-C3'	-5.10	113.58	119.70
14	J	14	DT	P-O3'-C3'	-5.08	113.61	119.70
13	H	61	DT	P-O3'-C3'	-5.07	113.62	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	6	487	ALA	Mainchain

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	2	5131	0	5126	61	0
2	3	5674	0	5688	79	0
3	4	5017	0	5038	66	0
4	6	5311	0	5334	79	0
5	7	5698	0	5726	71	0
6	A	3061	0	3076	45	0
7	B	2575	0	2572	41	0
8	C	5509	0	5564	64	0
9	D	3472	0	3511	72	0
10	E	3514	0	3529	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	3105	0	3272	50	0
12	G	2175	0	2232	35	0
13	H	795	0	441	85	0
14	J	825	0	456	73	0
All	All	51862	0	51565	714	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 (714) 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)
13:H:78:DA:N1	14:J:12:DT:N3	1.72	1.38
13:H:75:DA:N1	14:J:15:DT:N3	1.68	1.34
9:D:390:ARG:NH1	13:H:67:DA:H2"	1.45	1.31
3:4:549:LYS:HE3	14:J:45:DT:C5'	1.64	1.25
10:E:337:LYS:HE2	13:H:57:DT:OP2	1.30	1.25
13:H:77:DT:O4	14:J:13:DA:N6	1.66	1.24
9:D:390:ARG:HH12	13:H:67:DA:C2'	1.51	1.23
10:E:337:LYS:CE	13:H:57:DT:OP2	1.88	1.21
13:H:78:DA:N6	14:J:12:DT:O4	1.72	1.21
3:4:549:LYS:CE	14:J:45:DT:H5"	1.74	1.17
4:6:486:LYS:NZ	13:H:46:DT:O5'	1.80	1.13
10:E:337:LYS:NZ	13:H:57:DT:P	2.25	1.09
10:E:337:LYS:NZ	13:H:57:DT:OP1	1.87	1.06
13:H:77:DT:N3	14:J:13:DA:N1	2.02	1.06
9:D:390:ARG:NH1	13:H:67:DA:C2'	2.13	1.05
13:H:76:DA:N6	14:J:14:DT:O4	1.91	1.04
3:4:600:LYS:HE3	13:H:49:DC:OP2	1.58	1.01
11:F:292:LYS:NZ	14:J:20:DT:H4'	1.77	1.00
11:F:292:LYS:HZ2	14:J:20:DT:H4'	1.33	0.93
11:F:292:LYS:HE3	14:J:20:DT:H5'	1.52	0.91
13:H:76:DA:N1	14:J:14:DT:N3	2.18	0.90
10:E:337:LYS:HZ1	13:H:57:DT:P	1.91	0.90
4:6:425:SER:OG	13:H:48:DA:OP1	1.90	0.90
9:D:390:ARG:NH2	13:H:67:DA:H1'	1.87	0.89
13:H:76:DA:N6	14:J:14:DT:H3	1.71	0.88
10:E:337:LYS:NZ	13:H:57:DT:OP2	2.06	0.86
11:F:292:LYS:HE3	14:J:20:DT:C5'	2.07	0.85
13:H:76:DA:N6	14:J:14:DT:C4	2.40	0.85
3:4:600:LYS:CE	13:H:49:DC:OP2	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:78:DA:C2	14:J:13:DA:C2	2.66	0.83
13:H:78:DA:N1	14:J:12:DT:C2	2.46	0.82
9:D:390:ARG:NH1	13:H:67:DA:H4'	1.94	0.82
13:H:76:DA:N6	14:J:14:DT:N3	2.28	0.81
9:D:390:ARG:NH1	13:H:67:DA:C4'	2.44	0.81
10:E:337:LYS:HZ3	13:H:57:DT:P	1.97	0.78
13:H:75:DA:C2	14:J:16:DG:N2	2.52	0.78
13:H:75:DA:N1	14:J:15:DT:C2	2.51	0.77
9:D:390:ARG:HH12	13:H:67:DA:H2"	0.66	0.77
11:F:292:LYS:CE	14:J:20:DT:C5'	2.62	0.77
11:F:292:LYS:HD3	14:J:20:DT:H5"	1.67	0.76
4:6:486:LYS:HZ3	13:H:46:DT:C5'	1.98	0.76
3:4:211:ASN:HD22	3:4:213:GLU:H	1.33	0.75
3:4:549:LYS:HE3	14:J:45:DT:H5"	0.80	0.75
13:H:70:DA:H2	14:J:21:DG:H1	1.35	0.74
11:F:438:ILE:HG23	11:F:441:ILE:HD12	1.70	0.74
7:B:367:ARG:HH11	8:C:174:GLN:HE21	1.32	0.74
4:6:486:LYS:HG2	13:H:46:DT:H5"	1.73	0.70
11:F:292:LYS:CD	14:J:20:DT:H5"	2.23	0.68
8:C:698:GLN:HG3	8:C:699:LYS:HG2	1.76	0.67
11:F:292:LYS:NZ	14:J:20:DT:C4'	2.55	0.67
7:B:367:ARG:HH11	8:C:174:GLN:NE2	1.92	0.67
11:F:292:LYS:CE	14:J:20:DT:H5"	2.25	0.67
9:D:390:ARG:NH1	13:H:67:DA:C3'	2.57	0.67
9:D:390:ARG:HH11	13:H:67:DA:H4'	1.59	0.65
3:4:600:LYS:HZ3	13:H:48:DA:H5"	1.61	0.65
7:B:453:PRO:HB2	8:C:682:ARG:HH22	1.62	0.65
2:3:765:MET:SD	2:3:766:ASN:ND2	2.69	0.65
13:H:74:DC:H2"	13:H:75:DA:C8	2.32	0.65
13:H:78:DA:N6	14:J:12:DT:C4	2.44	0.65
3:4:643:ARG:HG2	3:4:732:ARG:HH12	1.60	0.64
11:F:438:ILE:HA	11:F:441:ILE:HD12	1.78	0.64
3:4:549:LYS:HD3	3:4:556:LEU:CD1	2.27	0.63
6:A:682:THR:HG22	11:F:454:GLN:H	1.63	0.63
12:G:253:ARG:HA	12:G:258:PHE:HA	1.80	0.63
13:H:78:DA:C2	14:J:12:DT:O2	2.52	0.63
3:4:600:LYS:NZ	13:H:49:DC:OP2	2.31	0.63
3:4:307:GLN:HE21	3:4:338:ALA:HB2	1.65	0.62
10:E:293:GLY:H	10:E:296:ALA:HB2	1.64	0.62
4:6:120:ARG:HD2	4:6:138:SER:HB3	1.82	0.62
11:F:292:LYS:HZ1	14:J:20:DT:H4'	1.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:76:DA:N1	14:J:14:DT:C2	2.68	0.62
8:C:257:ILE:O	8:C:260:HIS:ND1	2.33	0.62
7:B:264:ARG:HH21	8:C:673:ASN:HB3	1.65	0.62
13:H:52:DG:H2"	13:H:53:DA:C8	2.35	0.62
13:H:75:DA:N1	14:J:15:DT:C4	2.64	0.62
6:A:622:LEU:HD11	6:A:651:ALA:HB1	1.81	0.61
7:B:257:ARG:HB2	7:B:260:GLN:HE22	1.64	0.61
7:B:258:THR:HG22	8:C:700:THR:HG21	1.82	0.61
1:2:636:ARG:NH2	4:6:613:SER:O	2.33	0.61
4:6:387:ARG:HH21	4:6:478:GLU:HG3	1.64	0.61
11:F:175:ARG:NH1	11:F:211:CYS:SG	2.73	0.61
12:G:255:VAL:H	12:G:256:PRO:HD2	1.65	0.61
13:H:78:DA:H2	14:J:13:DA:C2	2.19	0.61
13:H:69:DC:H2"	13:H:70:DA:C5	2.36	0.61
7:B:305:LEU:HD21	7:B:311:ILE:HG12	1.83	0.60
8:C:252:ILE:HG22	8:C:254:THR:H	1.66	0.60
9:D:390:ARG:CZ	13:H:67:DA:C1'	2.79	0.60
8:C:568:LEU:HB2	8:C:573:GLN:HE22	1.66	0.60
2:3:762:SER:HB2	2:3:767:ARG:HH11	1.67	0.60
5:7:148:VAL:HG12	5:7:151:GLU:HG2	1.82	0.60
10:E:387:LEU:HG	10:E:392:LEU:HD12	1.84	0.60
4:6:251:VAL:HB	4:6:295:ARG:H	1.65	0.60
8:C:49:LEU:O	8:C:53:GLN:NE2	2.35	0.60
4:6:632:ALA:HB1	4:6:637:CYS:HB2	1.84	0.60
1:2:717:GLN:NE2	4:6:381:GLY:O	2.34	0.60
3:4:596:LEU:HB3	3:4:607:LEU:HB2	1.83	0.59
11:F:292:LYS:CE	14:J:20:DT:H5'	2.27	0.59
3:4:501:ARG:NH1	3:4:594:GLN:OE1	2.35	0.59
9:D:199:LEU:HB3	9:D:207:LYS:HE2	1.84	0.59
14:J:15:DT:H2"	14:J:16:DG:C8	2.37	0.59
11:F:206:THR:OG1	11:F:208:LYS:NZ	2.36	0.59
6:A:592:ALA:HB3	6:A:597:ALA:HB2	1.85	0.59
6:A:817:SER:HB3	9:D:313:SER:H	1.68	0.59
9:D:332:MET:HB3	9:D:404:LEU:HD21	1.85	0.58
10:E:182:TYR:O	10:E:220:ARG:NH2	2.37	0.58
2:3:381:ALA:HB3	2:3:394:GLU:HB2	1.86	0.58
8:C:298:PHE:O	8:C:301:LYS:NZ	2.37	0.58
11:F:524:ASN:ND2	11:F:529:LEU:O	2.37	0.58
2:3:604:SER:O	2:3:609:ARG:NH2	2.36	0.58
6:A:829:CYS:O	9:D:195:ARG:NH1	2.37	0.58
10:E:217:THR:HG23	10:E:218:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:171:ARG:HG3	11:F:173:PRO:HD2	1.85	0.58
2:3:464:THR:HG22	2:3:466:MET:H	1.68	0.58
5:7:71:ARG:HD2	5:7:278:LEU:HD13	1.85	0.58
7:B:317:GLY:HA3	7:B:450:THR:HB	1.85	0.58
5:7:379:LEU:HD11	5:7:521:ILE:HG12	1.86	0.58
3:4:549:LYS:HG3	14:J:45:DT:P	2.44	0.58
9:D:123:VAL:HG23	9:D:125:GLY:H	1.69	0.58
11:F:461:GLN:HE21	11:F:462:LYS:HG3	1.69	0.58
2:3:616:ARG:HE	5:7:384:GLY:HA3	1.69	0.57
5:7:233:GLN:HE22	5:7:235:MET:HB3	1.67	0.57
6:A:677:CYS:HB3	11:F:445:ARG:HH12	1.69	0.57
14:J:43:DC:H2"	14:J:44:DA:OP2	2.04	0.57
1:2:246:TYR:OH	12:G:209:ASN:ND2	2.36	0.57
6:A:784:GLU:O	6:A:787:ARG:NH1	2.37	0.57
12:G:301:LYS:O	12:G:305:HIS:ND1	2.37	0.57
13:H:83:DT:H3	14:J:7:DA:H2	1.50	0.57
1:2:246:TYR:HB3	12:G:288:ALA:HB2	1.85	0.57
9:D:390:ARG:HH22	13:H:67:DA:H1'	1.64	0.57
1:2:592:MET:O	1:2:597:ARG:NH1	2.38	0.57
4:6:404:GLN:O	4:6:408:HIS:ND1	2.37	0.57
7:B:415:LEU:HG	7:B:417:ASN:H	1.68	0.57
1:2:409:GLY:HA3	1:2:577:VAL:HG12	1.87	0.57
13:H:75:DA:C2	14:J:15:DT:O2	2.58	0.57
1:2:402:LEU:HD13	1:2:444:VAL:HG13	1.86	0.57
4:6:242:CYS:SG	4:6:243:ASP:N	2.78	0.57
9:D:390:ARG:CZ	13:H:67:DA:H2"	2.28	0.57
12:G:417:GLY:O	12:G:420:GLN:NE2	2.37	0.57
1:2:514:ARG:O	1:2:772:ARG:NH2	2.37	0.56
8:C:639:CYS:HB3	8:C:643:ILE:HG13	1.87	0.56
6:A:541:THR:OG1	6:A:720:ARG:NH2	2.38	0.56
4:6:208:ILE:HD11	4:6:224:LEU:HB3	1.86	0.56
10:E:35:ILE:HG12	10:E:177:LEU:HB3	1.87	0.56
5:7:11:GLU:O	5:7:15:LYS:NZ	2.38	0.56
5:7:462:MET:O	5:7:465:GLN:NE2	2.39	0.56
7:B:483:SER:HA	11:F:344:PRO:HA	1.87	0.56
4:6:71:PHE:HD2	4:6:72:ASN:HD22	1.53	0.56
8:C:705:ARG:NH1	8:C:707:THR:O	2.39	0.56
3:4:730:TYR:H	3:4:733:GLN:HE22	1.54	0.56
4:6:180:CYS:SG	4:6:181:ARG:N	2.77	0.56
5:7:43:ARG:NH2	5:7:94:VAL:O	2.38	0.56
6:A:634:TYR:OH	6:A:670:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:409:CYS:SG	10:E:410:THR:N	2.79	0.56
1:2:390:LEU:HD13	4:6:237:GLN:HB2	1.88	0.56
2:3:244:LEU:HD22	2:3:257:ARG:HD2	1.87	0.56
13:H:78:DA:C6	14:J:12:DT:N3	2.45	0.56
5:7:374:ASN:O	5:7:611:ARG:NH1	2.39	0.56
7:B:538:GLU:O	7:B:542:HIS:ND1	2.39	0.56
12:G:204:VAL:HG23	12:G:214:PRO:HG2	1.87	0.56
2:3:799:MET:SD	2:3:800:VAL:N	2.77	0.56
8:C:6:MET:SD	8:C:6:MET:N	2.79	0.56
14:J:20:DT:H2"	14:J:21:DG:C8	2.40	0.56
1:2:377:ARG:NH2	1:2:395:ASP:OD1	2.38	0.56
2:3:304:ALA:HB1	2:3:307:ILE:HB	1.88	0.55
5:7:24:ASP:OD2	5:7:30:GLN:NE2	2.39	0.55
5:7:83:GLU:O	5:7:87:GLN:NE2	2.39	0.55
7:B:367:ARG:HH22	8:C:173:THR:HG21	1.71	0.55
9:D:65:ILE:HG23	9:D:217:LEU:HD23	1.87	0.55
8:C:48:GLN:O	8:C:52:GLN:NE2	2.38	0.55
9:D:66:ILE:HG21	9:D:196:LEU:HD13	1.88	0.55
3:4:549:LYS:HD3	3:4:556:LEU:HD11	1.87	0.55
5:7:327:ILE:HD11	5:7:336:LEU:HD11	1.88	0.55
8:C:97:LEU:HA	8:C:241:LEU:HD23	1.87	0.55
9:D:347:GLN:NE2	10:E:351:LEU:O	2.39	0.55
2:3:336:ARG:HA	2:3:426:MET:HB2	1.87	0.55
3:4:296:ILE:HB	3:4:349:LYS:HB3	1.89	0.55
2:3:204:MET:SD	2:3:207:LYS:NZ	2.79	0.55
1:2:288:LEU:HD22	1:2:307:ARG:HB2	1.89	0.55
4:6:397:ASP:HB3	4:6:402:LYS:HE3	1.88	0.55
4:6:414:PRO:HG2	4:6:415:ARG:HD3	1.89	0.55
5:7:445:ASP:HA	5:7:487:ALA:HB3	1.89	0.55
9:D:112:LYS:NZ	9:D:129:PHE:O	2.33	0.55
2:3:791:LYS:O	2:3:793:GLN:N	2.39	0.55
3:4:639:THR:O	3:4:643:ARG:NH1	2.40	0.55
7:B:262:LEU:HG	7:B:264:ARG:H	1.72	0.55
12:G:515:ILE:HD11	12:G:519:THR:HA	1.88	0.55
3:4:271:MET:SD	3:4:271:MET:N	2.79	0.55
9:D:30:ARG:HE	9:D:31:GLN:H	1.55	0.54
2:3:792:MET:HB3	2:3:798:VAL:H	1.71	0.54
11:F:263:MET:SD	11:F:263:MET:N	2.81	0.54
1:2:291:VAL:O	12:G:221:ARG:NH2	2.39	0.54
8:C:303:ASN:HD22	8:C:582:SER:HB2	1.72	0.54
1:2:768:GLU:O	1:2:772:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:154:GLY:HA2	5:7:106:ARG:HH22	1.73	0.54
4:6:602:ARG:HH12	4:6:617:THR:HG22	1.72	0.54
9:D:379:LEU:HD12	9:D:384:LEU:HD22	1.89	0.54
9:D:390:ARG:NH1	13:H:67:DA:C1'	2.70	0.54
1:2:530:SER:OG	4:6:479:GLN:NE2	2.41	0.54
5:7:270:HIS:ND1	5:7:307:ASN:O	2.40	0.54
9:D:385:ILE:HD12	9:D:402:MET:HG3	1.90	0.54
11:F:292:LYS:HZ1	14:J:20:DT:C4'	2.19	0.54
1:2:789:ASP:O	1:2:825:ARG:NH1	2.41	0.54
2:3:333:SER:HB3	2:3:429:GLY:HA3	1.90	0.54
5:7:698:LEU:HD12	5:7:713:ARG:HH21	1.72	0.54
6:A:477:ARG:NH1	9:D:149:THR:O	2.41	0.54
3:4:485:PHE:HB3	3:4:746:LYS:HD3	1.90	0.54
5:7:588:MET:SD	5:7:641:LYS:NZ	2.80	0.54
8:C:695:PRO:HA	8:C:703:VAL:HA	1.89	0.54
9:D:30:ARG:NH2	10:E:146:GLU:OE2	2.41	0.54
12:G:304:GLU:HA	12:G:307:LYS:HE3	1.89	0.54
3:4:580:ASN:ND2	3:4:582:SER:OG	2.41	0.54
3:4:593:GLN:HE22	4:6:403:SER:HB3	1.72	0.54
1:2:187:SER:OG	1:2:188:MET:SD	2.64	0.54
14:J:33:DA:H3'	14:J:34:DG:H8	1.73	0.54
3:4:549:LYS:HG3	14:J:45:DT:OP1	2.08	0.53
7:B:568:ASP:O	7:B:572:LYS:NZ	2.40	0.53
8:C:594:ALA:HB2	10:E:377:THR:HG22	1.90	0.53
8:C:563:VAL:HG13	8:C:567:LEU:HD23	1.90	0.53
9:D:400:GLN:HB3	9:D:402:MET:HG2	1.90	0.53
5:7:397:LEU:HG	5:7:560:ARG:HE	1.74	0.53
1:2:694:GLU:HG2	1:2:701:ALA:HA	1.90	0.53
2:3:743:ARG:NH1	2:3:778:GLU:OE1	2.41	0.53
8:C:413:PHE:O	8:C:417:ARG:NH1	2.41	0.53
2:3:295:ILE:HD11	2:3:632:ARG:HA	1.90	0.53
4:6:44:ILE:HG22	4:6:46:TYR:H	1.73	0.53
13:H:80:DA:H2"	13:H:81:DC:C6	2.44	0.53
5:7:179:VAL:HA	5:7:194:PRO:HA	1.89	0.53
6:A:694:LEU:HA	6:A:697:LEU:HD23	1.89	0.53
4:6:143:ARG:HB3	4:6:207:ARG:HB3	1.89	0.53
4:6:563:ILE:HD11	4:6:565:ARG:HE	1.73	0.53
2:3:456:TYR:OH	2:3:468:ASN:ND2	2.42	0.53
6:A:707:LEU:HD22	6:A:751:SER:HB2	1.90	0.53
7:B:327:ARG:HA	7:B:331:LEU:HD23	1.89	0.53
8:C:43:ARG:HD3	8:C:336:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:640:PRO:HB3	6:A:647:LEU:HB2	1.90	0.52
8:C:189:MET:SD	8:C:193:GLN:NE2	2.82	0.52
9:D:413:ASN:O	9:D:417:LYS:NZ	2.42	0.52
13:H:78:DA:C2	14:J:12:DT:C2	2.97	0.52
2:3:309:GLY:O	2:3:314:LYS:NZ	2.35	0.52
3:4:198:GLY:HA2	3:4:201:ASN:HD21	1.74	0.52
4:6:486:LYS:NZ	13:H:46:DT:C5'	2.66	0.52
8:C:289:LEU:HD13	8:C:436:ARG:HG3	1.91	0.52
5:7:402:GLN:HE21	5:7:433:ALA:HA	1.75	0.52
8:C:603:LEU:O	8:C:634:LYS:NZ	2.40	0.52
3:4:343:ARG:HH21	4:6:85:ARG:HA	1.75	0.52
9:D:390:ARG:CZ	13:H:67:DA:H1'	2.40	0.52
3:4:348:ASP:HB2	3:4:379:VAL:HG21	1.91	0.52
5:7:279:PRO:HA	5:7:296:THR:HA	1.92	0.52
9:D:413:ASN:O	9:D:416:GLN:NE2	2.42	0.52
13:H:75:DA:C2	14:J:15:DT:C2	2.97	0.52
14:J:9:DG:H1'	14:J:10:DT:C6	2.43	0.52
1:2:365:MET:SD	1:2:365:MET:N	2.82	0.52
4:6:310:PHE:HB2	12:G:489:ILE:HD13	1.90	0.52
9:D:195:ARG:HB3	9:D:198:ILE:HD11	1.91	0.52
8:C:625:ILE:HG13	8:C:659:ALA:HB1	1.90	0.52
1:2:207:VAL:O	1:2:240:ARG:NH2	2.43	0.52
1:2:649:LEU:HB3	1:2:653:ILE:HD11	1.92	0.52
3:4:667:VAL:HG22	5:7:610:LEU:HD11	1.92	0.52
4:6:431:ALA:HB3	4:6:484:ILE:HD12	1.90	0.52
4:6:481:THR:OG1	4:6:493:LEU:O	2.27	0.52
6:A:475:ARG:NH2	6:A:478:SER:O	2.43	0.52
9:D:390:ARG:NH2	13:H:67:DA:C1'	2.65	0.52
12:G:186:LEU:HD11	12:G:191:GLN:HB3	1.92	0.52
3:4:227:ILE:HG23	3:4:282:LEU:HB3	1.92	0.52
7:B:330:MET:HG3	7:B:331:LEU:HD22	1.92	0.52
9:D:369:LYS:H	9:D:370:PRO:HD2	1.74	0.52
2:3:411:PHE:O	2:3:419:ARG:NH2	2.43	0.51
1:2:252:PRO:HG2	1:2:305:LEU:HD23	1.92	0.51
2:3:61:ARG:H	2:3:61:ARG:HD3	1.74	0.51
2:3:231:PRO:HG2	2:3:395:ALA:H	1.75	0.51
3:4:549:LYS:HD3	3:4:556:LEU:HD12	1.92	0.51
7:B:269:GLN:O	7:B:273:ARG:NH1	2.43	0.51
8:C:320:SER:OG	8:C:322:GLN:OE1	2.27	0.51
1:2:375:ARG:HE	1:2:377:ARG:HH12	1.58	0.51
6:A:819:THR:OG1	6:A:820:MET:SD	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:3:HIS:ND1	10:E:45:TYR:OH	2.42	0.51
3:4:157:VAL:HG11	3:4:233:VAL:HG22	1.92	0.51
5:7:233:GLN:HB3	5:7:257:VAL:HB	1.92	0.51
8:C:47:TYR:OH	8:C:329:GLN:NE2	2.43	0.51
4:6:541:ASN:OD1	4:6:542:GLU:N	2.44	0.51
9:D:165:ALA:O	9:D:170:GLN:NE2	2.44	0.51
9:D:197:ASP:OD1	9:D:197:ASP:N	2.44	0.51
13:H:79:DA:N6	14:J:10:DT:O4	2.43	0.51
2:3:420:THR:HB	5:7:408:GLY:H	1.74	0.51
3:4:409:LYS:HG2	3:4:411:VAL:H	1.73	0.51
6:A:833:LEU:HB2	6:A:846:ARG:HB2	1.92	0.51
9:D:394:ASN:ND2	10:E:395:LEU:O	2.42	0.51
10:E:142:LEU:HB3	10:E:172:PHE:HB3	1.92	0.51
11:F:171:ARG:O	11:F:175:ARG:NH2	2.41	0.51
12:G:198:ARG:HH21	12:G:295:ARG:HE	1.59	0.51
3:4:451:GLU:HA	3:4:454:ARG:HH21	1.76	0.51
9:D:290:VAL:HG13	9:D:294:HIS:HB2	1.93	0.51
10:E:310:LEU:HD11	10:E:392:LEU:HD13	1.93	0.51
1:2:379:GLN:HE21	1:2:391:PRO:HB2	1.76	0.51
7:B:363:MET:SD	7:B:363:MET:N	2.81	0.51
8:C:208:SER:O	8:C:210:TRP:N	2.44	0.50
5:7:352:LYS:HD2	5:7:636:LEU:HD21	1.94	0.50
13:H:75:DA:C2	14:J:16:DG:C2	3.00	0.50
3:4:649:LEU:O	3:4:771:GLN:NE2	2.42	0.50
4:6:141:VAL:HA	4:6:208:ILE:HA	1.92	0.50
4:6:634:MET:SD	4:6:634:MET:N	2.84	0.50
9:D:333:LYS:HE3	9:D:411:ILE:HG21	1.93	0.50
4:6:398:PRO:HA	4:6:504:ASN:HD21	1.76	0.50
5:7:70:ALA:O	5:7:75:LYS:NZ	2.43	0.50
5:7:240:HIS:HB3	5:7:243:GLN:HB2	1.94	0.50
7:B:297:LEU:HD12	7:B:300:LYS:HG3	1.92	0.50
13:H:77:DT:O4	14:J:13:DA:C6	2.58	0.50
3:4:272:ARG:NH2	3:4:366:THR:O	2.44	0.50
7:B:547:THR:OG1	7:B:555:GLU:OE1	2.30	0.50
11:F:535:LYS:HG3	11:F:536:ILE:HG22	1.93	0.50
13:H:77:DT:C4	14:J:13:DA:N1	2.77	0.50
9:D:171:THR:O	9:D:175:ASN:ND2	2.45	0.50
11:F:457:PHE:HB3	11:F:461:GLN:HE21	1.76	0.50
2:3:306:SER:O	2:3:500:HIS:NE2	2.41	0.50
4:6:727:ILE:HG21	4:6:776:VAL:HG11	1.93	0.50
4:6:744:LYS:HA	4:6:748:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:56:LEU:O	10:E:58:HIS:ND1	2.42	0.50
5:7:703:GLU:OE2	11:F:452:GLY:N	2.45	0.49
1:2:340:CYS:HB2	1:2:347:VAL:HG23	1.94	0.49
2:3:288:SER:OG	2:3:291:ARG:NH2	2.45	0.49
5:7:179:VAL:HG22	5:7:194:PRO:HB3	1.93	0.49
7:B:317:GLY:HA2	7:B:452:SER:H	1.77	0.49
8:C:224:SER:HA	10:E:391:GLN:HE21	1.77	0.49
12:G:251:GLN:HA	12:G:259:LYS:HD3	1.94	0.49
8:C:624:ASN:HB2	8:C:659:ALA:HB2	1.95	0.49
2:3:616:ARG:NH2	5:7:383:PRO:O	2.45	0.49
3:4:721:GLY:O	3:4:723:SER:N	2.44	0.49
5:7:148:VAL:HG13	5:7:150:ARG:H	1.78	0.49
11:F:292:LYS:NZ	14:J:20:DT:C5'	2.75	0.49
2:3:162:LEU:HD11	2:3:169:PRO:HG3	1.95	0.49
2:3:590:ILE:HG23	2:3:621:LEU:HD23	1.95	0.49
11:F:157:TYR:O	11:F:161:LYS:NZ	2.44	0.49
12:G:304:GLU:HG3	12:G:305:HIS:HD1	1.77	0.49
3:4:549:LYS:CD	3:4:556:LEU:HD11	2.43	0.49
7:B:493:ARG:O	7:B:497:LYS:NZ	2.42	0.49
5:7:253:ILE:HD11	5:7:298:LEU:HD13	1.93	0.49
10:E:398:HIS:CE1	13:H:67:DA:OP2	2.65	0.49
4:6:316:ARG:HH22	4:6:376:VAL:HG12	1.78	0.49
6:A:566:ILE:HG23	6:A:586:LYS:HG2	1.95	0.49
9:D:298:THR:HG23	9:D:300:VAL:H	1.78	0.49
12:G:474:SER:OG	12:G:476:GLU:OE1	2.31	0.49
4:6:301:CYS:SG	4:6:302:CYS:N	2.86	0.49
6:A:839:ASN:HB3	6:A:842:LEU:HB2	1.95	0.49
8:C:446:ASN:O	8:C:450:SER:OG	2.26	0.49
8:C:635:LEU:HB3	8:C:648:TRP:HE1	1.78	0.49
12:G:205:GLY:O	12:G:209:ASN:ND2	2.46	0.49
2:3:78:ARG:HH11	2:3:81:LYS:HE2	1.78	0.48
2:3:187:GLU:O	2:3:191:SER:OG	2.30	0.48
3:4:600:LYS:NZ	13:H:48:DA:H5"	2.28	0.48
4:6:115:GLN:HG3	4:6:116:ASP:H	1.78	0.48
8:C:105:LEU:HD23	8:C:249:ILE:HG23	1.95	0.48
3:4:319:ARG:NH1	5:7:185:ASP:OD2	2.46	0.48
3:4:501:ARG:HG2	3:4:503:GLU:H	1.76	0.48
11:F:527:THR:O	11:F:529:LEU:N	2.45	0.48
13:H:45:DA:C8	14:J:44:DA:N1	2.81	0.48
2:3:32:TYR:HE1	2:3:49:VAL:HG22	1.79	0.48
14:J:31:DA:H2'	14:J:32:DA:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:1:MET:HA	2:3:2:ALA:HA	1.57	0.48
2:3:740:SER:HB2	2:3:744:LEU:HB2	1.94	0.48
3:4:280:ASP:OD2	5:7:225:ARG:NH1	2.45	0.48
3:4:690:TYR:OH	3:4:747:VAL:O	2.32	0.48
6:A:535:VAL:O	6:A:540:LYS:NZ	2.46	0.48
8:C:461:ARG:NH1	8:C:553:GLU:OE1	2.47	0.48
4:6:359:HIS:HB2	4:6:551:ARG:HG3	1.96	0.48
4:6:435:ARG:HH21	4:6:440:HIS:HB3	1.78	0.48
4:6:650:ARG:HH22	4:6:722:ARG:HH21	1.62	0.48
6:A:599:GLU:O	6:A:603:LYS:NZ	2.47	0.48
7:B:274:ASN:O	7:B:278:LYS:NZ	2.45	0.48
11:F:445:ARG:HH21	11:F:516:ARG:HG2	1.79	0.48
1:2:286:SER:OG	1:2:443:HIS:NE2	2.45	0.48
1:2:352:CYS:HB2	1:2:356:GLN:HA	1.96	0.48
3:4:205:GLU:HB2	3:4:207:PHE:HD2	1.79	0.48
7:B:367:ARG:HH22	8:C:173:THR:CG2	2.27	0.48
8:C:110:ASN:ND2	8:C:113:ASP:OD2	2.38	0.48
8:C:348:LEU:HB2	8:C:349:PRO:HD3	1.96	0.48
10:E:160:ILE:HD11	10:E:164:LYS:HG3	1.94	0.48
10:E:396:VAL:HG12	10:E:408:LYS:HE2	1.94	0.48
3:4:412:TYR:H	5:7:174:LYS:HE3	1.79	0.48
5:7:450:MET:SD	5:7:450:MET:N	2.87	0.48
8:C:172:VAL:HG22	8:C:174:GLN:H	1.78	0.48
1:2:288:LEU:HB2	1:2:307:ARG:HD2	1.95	0.48
1:2:571:LEU:H	1:2:571:LEU:HD23	1.78	0.48
13:H:77:DT:C4	14:J:13:DA:N6	2.64	0.48
2:3:322:LEU:HD23	2:3:572:ILE:HG23	1.95	0.48
6:A:820:MET:SD	6:A:820:MET:N	2.87	0.48
8:C:302:ILE:HD11	8:C:307:LEU:HD13	1.95	0.48
2:3:368:THR:HB	2:3:408:ILE:HA	1.96	0.47
8:C:86:LYS:HD2	8:C:89:ARG:HD2	1.96	0.47
14:J:23:DT:H2'	14:J:23:DT:O2	2.14	0.47
5:7:559:MET:SD	5:7:559:MET:N	2.87	0.47
9:D:252:ASN:HD21	9:D:297:MET:H	1.62	0.47
13:H:56:DC:H1'	13:H:57:DT:C6	2.48	0.47
4:6:554:ASP:O	4:6:562:SER:OG	2.32	0.47
10:E:395:LEU:HD21	10:E:399:ASP:HA	1.97	0.47
11:F:214:ARG:HD3	11:F:217:GLN:HE21	1.78	0.47
12:G:259:LYS:HG2	12:G:269:LEU:H	1.80	0.47
4:6:194:ASP:OD1	4:6:195:THR:N	2.45	0.47
5:7:448:ASP:OD1	5:7:448:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:458:ILE:HA	5:7:461:VAL:HG22	1.96	0.47
8:C:641:ARG:NH1	8:C:705:ARG:O	2.47	0.47
8:C:1:MET:HG3	8:C:3:THR:H	1.79	0.47
1:2:728:LYS:HG2	1:2:779:ARG:HH11	1.79	0.47
2:3:174:TYR:HB3	5:7:292:LEU:HB3	1.97	0.47
2:3:472:GLN:H	2:3:475:LEU:HD12	1.78	0.47
6:A:574:THR:OG1	6:A:575:GLU:OE1	2.31	0.47
6:A:828:SER:OG	9:D:69:ARG:NH2	2.48	0.47
4:6:422:LYS:HE2	4:6:464:LYS:HB2	1.97	0.47
2:3:796:ASN:O	2:3:797:GLN:NE2	2.48	0.47
5:7:370:LYS:O	5:7:372:ARG:NH2	2.48	0.47
1:2:221:ASP:HA	1:2:224:LYS:HE2	1.97	0.47
2:3:362:ALA:HB3	2:3:365:ALA:HB2	1.97	0.47
3:4:264:ASN:H	3:4:391:THR:HG21	1.80	0.47
5:7:427:LEU:HG	5:7:474:ILE:HD11	1.96	0.47
2:3:369:THR:HG22	2:3:371:ARG:H	1.80	0.46
8:C:207:SER:HB3	8:C:212:SER:HA	1.97	0.46
11:F:292:LYS:HE3	14:J:20:DT:H5”	1.88	0.46
2:3:799:MET:HB2	2:3:808:ILE:HB	1.96	0.46
6:A:600:LEU:HD13	6:A:603:LYS:HD2	1.95	0.46
6:A:631:ASP:O	6:A:635:ASN:ND2	2.48	0.46
8:C:289:LEU:O	8:C:436:ARG:NH1	2.47	0.46
10:E:328:PHE:HZ	10:E:365:ILE:HG22	1.80	0.46
11:F:464:LEU:HD12	11:F:485:LEU:HD12	1.96	0.46
14:J:22:DT:H2”	14:J:23:DT:H6	1.80	0.46
1:2:747:TYR:OH	1:2:762:ILE:O	2.25	0.46
1:2:787:ILE:HG23	1:2:789:ASP:H	1.79	0.46
2:3:151:THR:O	2:3:153:LYS:NZ	2.48	0.46
12:G:247:TYR:HB3	12:G:271:ILE:HD11	1.96	0.46
2:3:807:LEU:HD22	2:3:808:ILE:HG13	1.97	0.46
6:A:659:PRO:O	6:A:668:SER:OG	2.34	0.46
6:A:790:LEU:HG	6:A:792:GLU:H	1.80	0.46
7:B:299:HIS:HB3	8:C:29:TYR:HB3	1.96	0.46
3:4:126:GLN:HG2	3:4:152:ILE:HG12	1.96	0.46
4:6:486:LYS:HZ3	13:H:46:DT:P	2.26	0.46
2:3:267:GLN:NE2	2:3:271:ASP:OD2	2.49	0.46
2:3:490:ASP:OD1	2:3:490:ASP:N	2.49	0.46
2:3:578:ILE:O	2:3:630:LYS:NZ	2.49	0.46
4:6:211:THR:HG22	4:6:213:ALA:H	1.81	0.46
4:6:650:ARG:HG2	4:6:654:LYS:HE3	1.97	0.46
12:G:253:ARG:HB2	12:G:254:SER:H	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:500:PHE:O	1:2:728:LYS:NZ	2.45	0.46
2:3:28:ASP:O	2:3:30:GLY:N	2.48	0.46
2:3:751:LEU:HA	2:3:754:VAL:HG12	1.97	0.46
4:6:767:ILE:HG13	12:G:427:ARG:HH12	1.80	0.46
8:C:463:LEU:HD22	8:C:467:GLU:HG3	1.98	0.46
1:2:807:LYS:HG3	1:2:809:SER:H	1.81	0.46
2:3:340:ASN:ND2	2:3:478:ARG:O	2.46	0.46
4:6:185:CYS:SG	4:6:186:ALA:N	2.88	0.46
5:7:167:VAL:HA	5:7:237:MET:HG2	1.97	0.46
10:E:334:LYS:HG3	10:E:336:LYS:H	1.79	0.46
1:2:518:ASN:HB2	1:2:657:PHE:HA	1.97	0.46
11:F:457:PHE:HB3	11:F:461:GLN:NE2	2.31	0.45
11:F:469:MET:SD	11:F:469:MET:N	2.89	0.45
12:G:527:ALA:HB1	12:G:531:HIS:HE1	1.81	0.45
4:6:417:VAL:HG11	4:6:448:ALA:HB1	1.97	0.45
4:6:481:THR:HA	4:6:494:ASN:HA	1.97	0.45
8:C:204:ARG:NH2	8:C:243:GLU:OE1	2.49	0.45
10:E:31:PRO:HB3	10:E:145:GLN:HB2	1.98	0.45
2:3:802:GLU:OE1	2:3:803:GLY:N	2.49	0.45
3:4:684:MET:SD	3:4:684:MET:N	2.80	0.45
10:E:98:THR:HG22	10:E:100:ASN:H	1.81	0.45
2:3:581:VAL:HG11	5:7:542:GLN:HE21	1.80	0.45
5:7:163:VAL:O	5:7:273:VAL:N	2.47	0.45
7:B:430:PRO:HG2	10:E:381:PHE:HB2	1.99	0.45
7:B:530:LEU:HD11	11:F:442:ASP:HA	1.99	0.45
12:G:474:SER:OG	12:G:519:THR:N	2.49	0.45
13:H:78:DA:N6	14:J:12:DT:N3	2.56	0.45
4:6:201:VAL:HG13	4:6:230:ALA:HB2	1.98	0.45
9:D:53:ARG:HB3	9:D:59:GLU:HB3	1.98	0.45
13:H:78:DA:C6	14:J:12:DT:C4	2.99	0.45
3:4:514:THR:HG23	5:7:603:ALA:HB3	1.98	0.45
1:2:755:MET:SD	1:2:755:MET:N	2.90	0.45
4:6:119:THR:HG23	12:G:464:VAL:HG12	1.99	0.45
4:6:395:VAL:HB	4:6:503:ALA:HB3	1.99	0.45
4:6:743:LEU:HD21	4:6:747:GLU:HB2	1.98	0.45
1:2:183:ARG:HG2	4:6:196:ASN:HD22	1.81	0.45
1:2:664:ARG:NH2	1:2:804:ASP:O	2.43	0.45
1:2:716:PRO:HB2	1:2:717:GLN:H	1.58	0.45
3:4:533:THR:HG23	3:4:573:ILE:HD13	1.99	0.45
4:6:35:GLU:OE2	4:6:101:ARG:NH2	2.39	0.45
9:D:168:LYS:NZ	9:D:169:ASN:OD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:685:ARG:NH1	1:2:703:GLU:O	2.49	0.45
1:2:778:ALA:HB1	1:2:783:ARG:HB2	1.99	0.45
2:3:161:ASP:H	2:3:167:ALA:HB1	1.81	0.45
2:3:321:LEU:HD23	2:3:405:VAL:HG21	1.98	0.45
6:A:571:MET:SD	6:A:572:LYS:NZ	2.77	0.45
6:A:768:LYS:HE3	6:A:860:ASP:HB2	1.98	0.45
7:B:409:ILE:HG23	7:B:441:PHE:HZ	1.82	0.45
8:C:699:LYS:HG3	8:C:702:HIS:HB2	1.98	0.45
11:F:489:TYR:OH	11:F:499:ALA:O	2.34	0.45
4:6:233:VAL:O	4:6:235:SER:N	2.50	0.44
5:7:158:GLY:H	5:7:277:PHE:HB3	1.82	0.44
1:2:380:GLU:OE1	1:2:392:ARG:NH1	2.51	0.44
2:3:777:GLU:OE1	2:3:778:GLU:N	2.50	0.44
3:4:730:TYR:O	3:4:733:GLN:NE2	2.50	0.44
6:A:479:LEU:HD22	9:D:56:LEU:HA	1.99	0.44
7:B:302:MET:SD	7:B:302:MET:N	2.91	0.44
8:C:427:PRO:C	8:C:429:TYR:H	2.21	0.44
9:D:132:PHE:HD1	9:D:132:PHE:HA	1.72	0.44
2:3:341:ILE:HG13	2:3:481:LEU:HD11	1.98	0.44
2:3:777:GLU:HB3	2:3:778:GLU:H	1.57	0.44
7:B:535:GLN:HE22	11:F:383:VAL:HA	1.81	0.44
10:E:357:PHE:HB2	10:E:361:ARG:HD3	1.98	0.44
5:7:137:TYR:HH	5:7:260:GLU:H	1.64	0.44
11:F:346:TYR:HB3	11:F:350:GLN:HB2	1.98	0.44
3:4:140:VAL:O	3:4:142:SER:N	2.50	0.44
3:4:450:LYS:O	3:4:454:ARG:NE	2.50	0.44
6:A:633:MET:SD	6:A:633:MET:N	2.91	0.44
13:H:62:DT:H2'	13:H:63:DG:C8	2.53	0.44
1:2:291:VAL:H	12:G:221:ARG:HH22	1.63	0.44
1:2:657:PHE:O	1:2:765:ARG:NH2	2.50	0.44
6:A:593:THR:HG23	6:A:595:ASN:H	1.82	0.44
8:C:633:TYR:HA	8:C:636:HIS:CE1	2.53	0.44
9:D:128:VAL:HG13	9:D:130:GLY:H	1.82	0.44
10:E:127:ALA:HB3	10:E:158:SER:HB3	2.00	0.44
2:3:340:ASN:HB2	2:3:479:PHE:HA	2.00	0.44
2:3:603:MET:SD	2:3:603:MET:N	2.79	0.44
4:6:26:CYS:HA	4:6:75:LEU:HD11	1.99	0.44
8:C:588:ARG:HH21	8:C:592:ASN:HD22	1.66	0.44
4:6:25:LYS:HE3	4:6:25:LYS:HB3	1.91	0.44
4:6:124:ARG:HE	4:6:215:LEU:HD22	1.83	0.44
5:7:43:ARG:HH21	5:7:96:LYS:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:575:GLU:OE1	6:A:578:GLN:NE2	2.51	0.44
7:B:258:THR:OG1	7:B:260:GLN:OE1	2.26	0.44
2:3:74:VAL:HG22	2:3:166:VAL:HG22	2.00	0.43
2:3:508:ARG:NH1	2:3:516:ASP:O	2.51	0.43
5:7:255:VAL:HG13	5:7:300:ALA:HB2	2.00	0.43
8:C:412:TYR:HA	8:C:415:VAL:HG22	2.00	0.43
13:H:76:DA:N1	14:J:14:DT:O2	2.51	0.43
1:2:184:GLU:O	1:2:187:SER:OG	2.35	0.43
1:2:460:ASP:HB2	1:2:722:LYS:HD2	2.00	0.43
1:2:650:THR:HB	1:2:652:PRO:HD2	1.99	0.43
4:6:308:PRO:HG2	4:6:415:ARG:HD2	2.00	0.43
9:D:428:TRP:HE1	9:D:433:LEU:HD13	1.82	0.43
5:7:431:GLY:H	5:7:435:VAL:HG21	1.82	0.43
6:A:592:ALA:HB1	6:A:596:HIS:HB2	2.00	0.43
6:A:795:PHE:HB2	6:A:843:LEU:HB2	1.99	0.43
7:B:319:LYS:NZ	7:B:448:THR:OG1	2.42	0.43
13:H:57:DT:O4	14:J:32:DA:N6	2.51	0.43
2:3:194:LYS:HD2	2:3:223:ASP:HB2	1.99	0.43
2:3:292:SER:O	2:3:294:ASP:N	2.52	0.43
5:7:434:LEU:HD12	5:7:435:VAL:HG13	2.01	0.43
6:A:683:TYR:OH	6:A:710:ARG:NH2	2.50	0.43
9:D:161:PHE:HD1	9:D:193:THR:HB	1.83	0.43
9:D:390:ARG:HD3	13:H:67:DA:H4'	2.00	0.43
10:E:8:VAL:HG12	10:E:10:CYS:H	1.83	0.43
13:H:81:DC:H2"	13:H:82:DA:H8	1.83	0.43
1:2:468:SER:HA	1:2:473:ILE:HG21	2.00	0.43
2:3:239:GLY:HA2	2:3:262:ALA:HA	2.01	0.43
5:7:40:LEU:HD11	5:7:134:PHE:HB3	1.99	0.43
8:C:31:ASN:HD22	8:C:37:PRO:HA	1.83	0.43
9:D:84:LEU:HD12	9:D:87:ILE:HD11	2.00	0.43
1:2:519:VAL:HG22	1:2:659:ILE:HB	2.00	0.43
3:4:627:LYS:HG3	3:4:628:LYS:HG3	2.01	0.43
7:B:545:ILE:HG22	7:B:559:ILE:HG13	1.99	0.43
9:D:223:PHE:HB3	9:D:224:PRO:HD3	2.01	0.43
9:D:257:SER:OG	9:D:258:GLU:OE1	2.31	0.43
1:2:533:LEU:HD23	1:2:585:LEU:HD22	2.01	0.43
2:3:140:LYS:HB2	2:3:196:HIS:HB2	2.01	0.43
4:6:237:GLN:NE2	4:6:240:ASP:OD1	2.51	0.43
4:6:351:CYS:HB3	4:6:365:LYS:HB3	2.00	0.43
8:C:445:LYS:HG3	8:C:446:ASN:H	1.84	0.43
10:E:354:PRO:HB2	10:E:408:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:449:LEU:HD22	3:4:690:TYR:HD1	1.82	0.43
6:A:663:MET:HG2	6:A:667:VAL:HG11	1.99	0.43
7:B:491:ILE:HG12	7:B:525:LEU:HD13	2.00	0.43
9:D:259:ASP:OD2	9:D:261:SER:OG	2.32	0.43
1:2:395:ASP:HB3	1:2:438:VAL:HG12	2.00	0.43
1:2:811:MET:HB3	1:2:815:ARG:HH12	1.83	0.43
2:3:338:ASP:OD1	2:3:338:ASP:N	2.48	0.43
4:6:587:SER:HB3	4:6:639:GLU:HB3	2.01	0.43
9:D:30:ARG:NH2	9:D:31:GLN:OE1	2.46	0.43
9:D:66:ILE:HG21	9:D:196:LEU:HA	2.01	0.43
10:E:34:PHE:HA	10:E:156:PHE:HB2	2.00	0.43
11:F:172:LEU:HB2	11:F:173:PRO:HD3	2.00	0.43
13:H:78:DA:N1	14:J:12:DT:C4	2.74	0.43
1:2:309:SER:HB3	1:2:413:GLU:HG2	2.00	0.43
2:3:325:VAL:HG21	2:3:579:LYS:HG2	2.01	0.43
3:4:691:ILE:O	3:4:695:HIS:ND1	2.52	0.43
10:E:107:LYS:NZ	10:E:148:ALA:O	2.49	0.43
12:G:503:SER:HB2	12:G:510:LEU:HD23	2.01	0.43
3:4:302:ALA:HB3	3:4:315:VAL:HB	2.00	0.42
3:4:543:LEU:HG	3:4:563:LEU:HD22	2.01	0.42
3:4:544:THR:HG22	3:4:563:LEU:HD21	2.00	0.42
3:4:724:ARG:HE	3:4:727:VAL:HG21	1.84	0.42
4:6:765:GLU:N	4:6:765:GLU:OE1	2.52	0.42
5:7:391:LEU:HD11	5:7:443:CYS:HB3	2.00	0.42
9:D:29:CYS:SG	9:D:30:ARG:N	2.92	0.42
12:G:305:HIS:O	12:G:309:HIS:ND1	2.47	0.42
9:D:65:ILE:HG13	9:D:77:ILE:HD11	2.00	0.42
13:H:78:DA:N6	14:J:11:DT:O4	2.52	0.42
2:3:135:SER:HA	2:3:392:ARG:HG2	2.01	0.42
2:3:277:SER:OG	2:3:278:ALA:N	2.53	0.42
2:3:322:LEU:HD11	2:3:631:ALA:HB2	2.02	0.42
5:7:379:LEU:O	5:7:488:ALA:N	2.51	0.42
13:H:75:DA:H2	14:J:15:DT:O2	2.02	0.42
5:7:85:LEU:HB3	5:7:86:PRO:HD3	2.00	0.42
5:7:170:VAL:HG13	5:7:267:PRO:HG3	2.02	0.42
8:C:445:LYS:HD2	8:C:445:LYS:HA	1.96	0.42
3:4:216:LYS:HE2	3:4:216:LYS:HB3	1.94	0.42
3:4:446:VAL:HG12	3:4:450:LYS:HE3	2.02	0.42
4:6:459:ILE:HG23	4:6:501:ALA:HA	2.01	0.42
5:7:469:ILE:HA	5:7:471:LYS:HZ3	1.84	0.42
9:D:355:LYS:HZ2	9:D:433:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:164:THR:OG1	2:3:165:LEU:N	2.51	0.42
2:3:743:ARG:NH2	2:3:784:GLU:OE2	2.53	0.42
3:4:532:TYR:HA	3:4:572:CYS:HB2	2.01	0.42
12:G:512:LEU:HD12	12:G:514:ARG:HH22	1.84	0.42
12:G:536:LEU:O	12:G:539:GLN:NE2	2.53	0.42
13:H:81:DC:H2"	13:H:82:DA:C8	2.55	0.42
2:3:806:PHE:HB2	7:B:527:ASN:HB2	2.02	0.42
7:B:356:THR:O	7:B:362:HIS:N	2.51	0.42
10:E:365:ILE:HG13	10:E:366:LEU:HD22	2.02	0.42
2:3:561:LYS:HB3	2:3:562:MET:H	1.72	0.42
4:6:150:GLU:HB2	4:6:203:PHE:HE1	1.85	0.42
4:6:743:LEU:HD23	4:6:748:LEU:HG	2.01	0.42
5:7:380:MET:HG3	5:7:488:ALA:HB3	2.01	0.42
7:B:398:GLN:HG2	7:B:399:MET:HG3	2.00	0.42
8:C:407:VAL:HA	8:C:410:MET:HG2	2.02	0.42
10:E:311:ILE:HG12	10:E:416:ILE:HG23	2.02	0.42
2:3:151:THR:OG1	2:3:182:ASN:ND2	2.53	0.42
3:4:515:SER:O	3:4:518:GLN:NE2	2.53	0.42
4:6:469:ASP:OD1	4:6:469:ASP:N	2.53	0.42
5:7:702:GLU:O	6:A:710:ARG:NH1	2.51	0.42
6:A:727:ARG:HG2	9:D:213:ARG:HH22	1.85	0.42
11:F:206:THR:HA	11:F:386:ASP:HA	2.02	0.42
12:G:430:GLU:HA	12:G:433:LYS:HE3	2.02	0.42
4:6:225:GLU:HB3	4:6:297:VAL:HA	2.02	0.41
4:6:594:ILE:HG23	4:6:597:GLN:HE21	1.85	0.41
9:D:162:ASP:N	9:D:162:ASP:OD1	2.52	0.41
9:D:358:GLN:O	9:D:359:ARG:HG3	2.20	0.41
10:E:315:LEU:HD21	10:E:427:ILE:HD11	2.01	0.41
13:H:70:DA:H2	14:J:21:DG:N1	2.10	0.41
13:H:79:DA:H2"	13:H:80:DA:C8	2.55	0.41
1:2:499:LEU:HD22	1:2:536:ILE:HD11	2.01	0.41
1:2:651:GLU:N	1:2:652:PRO:HD2	2.35	0.41
5:7:308:LYS:HG3	5:7:400:ARG:HG2	2.01	0.41
6:A:832:LEU:HD11	6:A:845:VAL:HG23	2.01	0.41
9:D:400:GLN:HE21	9:D:400:GLN:HB2	1.68	0.41
11:F:542:GLU:O	11:F:544:ALA:N	2.53	0.41
12:G:514:ARG:HH21	12:G:519:THR:HG21	1.85	0.41
1:2:321:GLN:NE2	1:2:343:GLN:H	2.19	0.41
6:A:596:HIS:O	6:A:600:LEU:HD23	2.20	0.41
8:C:134:VAL:HB	8:C:217:VAL:HG12	2.02	0.41
8:C:277:GLN:HB2	10:E:280:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:605:GLU:HG3	1:2:606:GLN:HG3	2.02	0.41
2:3:346:ASP:HB2	2:3:349:VAL:HG11	2.02	0.41
5:7:656:ARG:HB3	5:7:659:ASP:HB3	2.02	0.41
8:C:242:HIS:CD2	8:C:243:GLU:HG2	2.55	0.41
9:D:25:ARG:NH1	10:E:28:PHE:O	2.51	0.41
9:D:197:ASP:HB2	9:D:200:GLU:OE1	2.21	0.41
14:J:28:DA:H2"	14:J:29:DA:C8	2.56	0.41
4:6:241:LYS:HD2	4:6:308:PRO:HD3	2.03	0.41
5:7:127:PRO:HB2	5:7:128:ALA:H	1.66	0.41
5:7:435:VAL:HG23	5:7:436:LEU:HG	2.02	0.41
6:A:796:GLN:HB2	6:A:841:LEU:HD12	2.03	0.41
9:D:264:GLU:HG2	9:D:267:GLN:HE21	1.85	0.41
14:J:10:DT:H2'	14:J:11:DT:O4'	2.20	0.41
1:2:812:ARG:HH22	10:E:426:ASP:H	1.68	0.41
6:A:569:ASN:OD1	6:A:570:GLY:N	2.53	0.41
10:E:131:ARG:H	10:E:131:ARG:HD3	1.86	0.41
1:2:571:LEU:HD13	1:2:611:ILE:HG21	2.03	0.41
3:4:234:ILE:HB	3:4:235:PRO:HD3	2.03	0.41
9:D:74:THR:O	9:D:78:ASN:ND2	2.45	0.41
10:E:250:THR:OG1	10:E:251:ARG:NH1	2.53	0.41
10:E:253:LEU:HA	10:E:256:ASN:HD21	1.85	0.41
11:F:406:LYS:HE2	11:F:406:LYS:HB2	1.94	0.41
12:G:240:LYS:HE3	12:G:240:LYS:HB3	1.88	0.41
13:H:75:DA:H2	14:J:16:DG:N2	2.12	0.41
4:6:623:SER:HA	4:6:626:ARG:HE	1.86	0.41
8:C:76:PHE:O	8:C:80:SER:OG	2.37	0.41
9:D:346:PHE:HZ	9:D:372:VAL:HG12	1.84	0.41
14:J:15:DT:H2"	14:J:16:DG:N7	2.35	0.41
14:J:33:DA:H3'	14:J:34:DG:C8	2.52	0.41
2:3:253:SER:OG	2:3:254:GLY:N	2.54	0.41
2:3:801:SER:HB2	2:3:805:ILE:HG22	2.03	0.41
4:6:477:MET:SD	4:6:477:MET:N	2.89	0.41
4:6:490:LYS:HE3	4:6:490:LYS:HB3	1.92	0.41
5:7:383:PRO:HD3	5:7:489:ASN:HB3	2.03	0.41
7:B:548:LYS:HE2	7:B:548:LYS:HB2	1.91	0.41
9:D:62:SER:O	9:D:211:SER:OG	2.30	0.41
9:D:102:LEU:HA	9:D:163:LEU:HD22	2.02	0.41
11:F:177:ARG:NE	11:F:178:GLU:OE2	2.54	0.41
12:G:445:GLU:HA	12:G:448:LEU:HG	2.03	0.41
12:G:473:LEU:HD12	12:G:521:VAL:HB	2.03	0.41
2:3:133:LYS:HE2	2:3:133:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:676:MET:SD	6:A:676:MET:N	2.94	0.41
7:B:352:LEU:HD11	7:B:408:ILE:HG21	2.03	0.41
11:F:347:THR:OG1	11:F:348:ARG:N	2.50	0.40
13:H:83:DT:N3	14:J:7:DA:H2	2.15	0.40
1:2:631:ASN:HD21	4:6:529:ARG:HH22	1.68	0.40
3:4:394:TYR:HA	3:4:416:ILE:HG12	2.02	0.40
5:7:407:ARG:HH11	5:7:449:LYS:HE3	1.85	0.40
7:B:399:MET:HB2	7:B:399:MET:HE3	1.97	0.40
8:C:136:LEU:HD13	8:C:151:LEU:HD21	2.04	0.40
8:C:172:VAL:C	8:C:174:GLN:H	2.24	0.40
14:J:12:DT:H6	14:J:12:DT:H2'	1.72	0.40
2:3:426:MET:SD	2:3:426:MET:N	2.85	0.40
5:7:340:ILE:HD13	5:7:354:LEU:HD23	2.03	0.40
9:D:127:LYS:H	9:D:127:LYS:HG3	1.52	0.40
11:F:170:ASP:OD2	11:F:214:ARG:NH2	2.54	0.40
1:2:400:ALA:O	1:2:402:LEU:N	2.54	0.40
2:3:412:ASP:OD1	2:3:412:ASP:N	2.52	0.40
5:7:182:TYR:HB3	5:7:220:LEU:HB3	2.03	0.40
5:7:227:SER:OG	5:7:228:ARG:N	2.49	0.40
5:7:659:ASP:OD1	5:7:660:VAL:N	2.54	0.40
10:E:403:ASP:OD1	10:E:403:ASP:N	2.55	0.40
11:F:438:ILE:CG2	11:F:441:ILE:HD12	2.46	0.40
3:4:637:PRO:HD2	3:4:640:LEU:HD22	2.03	0.40
4:6:120:ARG:NH2	12:G:484:GLY:O	2.54	0.40
4:6:609:VAL:HG12	4:6:610:THR:HG23	2.02	0.40
5:7:461:VAL:HG12	5:7:467:ILE:HA	2.03	0.40
6:A:594:ALA:HB1	11:F:237:ARG:HH22	1.86	0.40
7:B:357:GLU:HA	7:B:362:HIS:H	1.85	0.40
11:F:461:GLN:NE2	11:F:462:LYS:HG3	2.35	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	2	647/947 (68%)	547 (84%)	92 (14%)	8 (1%)	11	44
2	3	720/853 (84%)	602 (84%)	99 (14%)	19 (3%)	4	25
3	4	628/883 (71%)	573 (91%)	49 (8%)	6 (1%)	13	49
4	6	654/821 (80%)	562 (86%)	87 (13%)	5 (1%)	16	55
5	7	717/719 (100%)	612 (85%)	97 (14%)	8 (1%)	12	47
6	A	385/961 (40%)	343 (89%)	38 (10%)	4 (1%)	13	49
7	B	309/577 (54%)	272 (88%)	33 (11%)	4 (1%)	10	43
8	C	672/712 (94%)	608 (90%)	55 (8%)	9 (1%)	10	43
9	D	424/436 (97%)	359 (85%)	56 (13%)	9 (2%)	5	30
10	E	427/435 (98%)	379 (89%)	44 (10%)	4 (1%)	14	51
11	F	391/560 (70%)	333 (85%)	51 (13%)	7 (2%)	7	35
12	G	266/410 (65%)	223 (84%)	32 (12%)	11 (4%)	2	18
All	All	6240/8314 (75%)	5413 (87%)	733 (12%)	94 (2%)	11	40

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	F	458	PRO
12	G	256	PRO
1	2	401	ASP
1	2	704	PRO
1	2	716	PRO
1	2	758	GLY
2	3	209	PRO
2	3	293	LYS
2	3	305	PRO
2	3	458	ARG
5	7	127	PRO
5	7	245	PRO
8	C	140	ASP
8	C	209	GLN
8	C	210	TRP
9	D	68	PRO
9	D	127	LYS
9	D	196	LEU
9	D	369	LYS
9	D	389	GLU
10	E	133	MET
11	F	543	HIS

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Mol	Chain	Res	Type
12	G	187	PRO
12	G	471	PRO
12	G	515	ILE
12	G	518	ASP
2	3	29	GLN
2	3	30	GLY
2	3	165	LEU
2	3	410	GLU
2	3	515	GLY
2	3	546	GLU
3	4	141	ALA
3	4	575	GLU
3	4	673	SER
3	4	722	SER
4	6	234	GLU
5	7	141	PRO
5	7	309	SER
5	7	374	ASN
6	A	537	GLY
8	C	201	SER
8	C	379	GLN
9	D	182	SER
10	E	358	PRO
11	F	252	GLN
11	F	528	ARG
11	F	546	LYS
12	G	260	ASP
1	2	250	GLU
1	2	424	GLY
1	2	738	MET
2	3	521	GLY
2	3	777	GLU
3	4	255	GLU
5	7	307	ASN
6	A	481	ALA
7	B	345	GLY
7	B	397	SER
8	C	177	THR
8	C	180	SER
8	C	348	LEU
9	D	223	PHE
10	E	174	PRO

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Mol	Chain	Res	Type
10	E	401	GLN
12	G	253	ARG
12	G	266	ASP
12	G	441	CYS
1	2	295	ARG
2	3	773	ASN
2	3	778	GLU
4	6	233	VAL
4	6	612	SER
4	6	743	LEU
6	A	505	PRO
6	A	837	SER
7	B	258	THR
7	B	394	ASN
11	F	535	LYS
2	3	55	ARG
2	3	801	SER
3	4	139	ILE
5	7	384	GLY
8	C	129	VAL
2	3	349	VAL
4	6	388	GLY
12	G	255	VAL
9	D	123	VAL
9	D	152	CYS
2	3	211	GLY
5	7	116	PRO
11	F	518	ILE
12	G	284	PRO
2	3	510	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2	565/810 (70%)	554 (98%)	11 (2%)	52 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	3	626/742 (84%)	612 (98%)	14 (2%)	47 65
3	4	556/771 (72%)	549 (99%)	7 (1%)	65 77
4	6	594/724 (82%)	580 (98%)	14 (2%)	44 62
5	7	619/619 (100%)	614 (99%)	5 (1%)	79 85
6	A	340/854 (40%)	335 (98%)	5 (2%)	60 75
7	B	292/529 (55%)	287 (98%)	5 (2%)	56 72
8	C	628/659 (95%)	619 (99%)	9 (1%)	62 75
9	D	396/403 (98%)	382 (96%)	14 (4%)	31 51
10	E	394/399 (99%)	388 (98%)	6 (2%)	60 75
11	F	346/499 (69%)	340 (98%)	6 (2%)	56 72
12	G	237/351 (68%)	228 (96%)	9 (4%)	28 49
All	All	5593/7360 (76%)	5488 (98%)	105 (2%)	52 69

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	297	LEU
1	2	298	ARG
1	2	334	PHE
1	2	341	GLN
1	2	392	ARG
1	2	399	LEU
1	2	527	THR
1	2	667	VAL
1	2	738	MET
1	2	764	VAL
1	2	825	ARG
2	3	61	ARG
2	3	83	PHE
2	3	176	THR
2	3	193	TYR
2	3	204	MET
2	3	290	THR
2	3	441	ARG
2	3	461	GLN
2	3	745	LYS
2	3	765	MET
2	3	792	MET

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Mol	Chain	Res	Type
2	3	799	MET
2	3	802	GLU
2	3	807	LEU
3	4	211	ASN
3	4	355	GLN
3	4	454	ARG
3	4	594	GLN
3	4	606	GLN
3	4	610	ARG
3	4	682	LEU
4	6	48	GLN
4	6	58	ARG
4	6	60	THR
4	6	166	ARG
4	6	181	ARG
4	6	228	LEU
4	6	415	ARG
4	6	468	ARG
4	6	490	LYS
4	6	500	LEU
4	6	527	MET
4	6	560	GLU
4	6	575	TYR
4	6	580	ARG
5	7	89	LYS
5	7	160	LEU
5	7	225	ARG
5	7	367	ARG
5	7	434	LEU
6	A	479	LEU
6	A	591	LYS
6	A	674	THR
6	A	787	ARG
6	A	809	GLU
7	B	269	GLN
7	B	332	GLN
7	B	400	LEU
7	B	508	TYR
7	B	546	ARG
8	C	6	MET
8	C	139	LYS
8	C	170	VAL

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Mol	Chain	Res	Type
8	C	176	LYS
8	C	244	PHE
8	C	431	LEU
8	C	443	LEU
8	C	469	MET
8	C	591	LEU
9	D	124	VAL
9	D	126	ASP
9	D	127	LYS
9	D	131	SER
9	D	132	PHE
9	D	185	THR
9	D	195	ARG
9	D	205	ARG
9	D	268	LYS
9	D	359	ARG
9	D	389	GLU
9	D	391	THR
9	D	392	SER
9	D	400	GLN
10	E	25	ARG
10	E	70	ARG
10	E	131	ARG
10	E	263	LYS
10	E	346	LYS
10	E	413	LEU
11	F	166	THR
11	F	261	LYS
11	F	300	LEU
11	F	325	ARG
11	F	485	LEU
11	F	522	LYS
12	G	210	ARG
12	G	218	LYS
12	G	253	ARG
12	G	267	TYR
12	G	418	VAL
12	G	425	ARG
12	G	449	GLN
12	G	473	LEU
12	G	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116)

such sidechains are listed below:

Mol	Chain	Res	Type
1	2	343	GLN
1	2	356	GLN
1	2	379	GLN
1	2	471	GLN
1	2	472	GLN
1	2	549	GLN
1	2	561	GLN
1	2	595	GLN
1	2	631	ASN
1	2	646	ASN
1	2	683	HIS
2	3	182	ASN
2	3	212	GLN
2	3	267	GLN
2	3	331	ASN
2	3	353	GLN
2	3	468	ASN
2	3	488	GLN
2	3	584	GLN
2	3	766	ASN
2	3	786	GLN
2	3	797	GLN
3	4	171	GLN
3	4	195	GLN
3	4	201	ASN
3	4	211	ASN
3	4	214	HIS
3	4	231	GLN
3	4	257	GLN
3	4	259	GLN
3	4	270	ASN
3	4	305	GLN
3	4	307	GLN
3	4	355	GLN
3	4	521	GLN
3	4	531	GLN
3	4	580	ASN
3	4	606	GLN
3	4	623	GLN
3	4	638	HIS
3	4	665	HIS
3	4	672	GLN

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Mol	Chain	Res	Type
4	6	48	GLN
4	6	72	ASN
4	6	74	GLN
4	6	328	GLN
4	6	342	GLN
4	6	470	GLN
4	6	479	GLN
4	6	504	ASN
4	6	518	GLN
4	6	519	ASN
5	7	87	GLN
5	7	123	GLN
5	7	124	ASN
5	7	186	GLN
5	7	196	GLN
5	7	243	GLN
5	7	290	GLN
5	7	389	GLN
5	7	504	ASN
5	7	542	GLN
5	7	655	GLN
5	7	682	GLN
6	A	496	HIS
6	A	553	GLN
6	A	564	GLN
6	A	630	GLN
6	A	679	GLN
6	A	688	GLN
7	B	269	GLN
7	B	291	ASN
7	B	293	GLN
7	B	332	GLN
7	B	438	GLN
7	B	499	GLN
8	C	53	GLN
8	C	78	GLN
8	C	154	GLN
8	C	174	GLN
8	C	193	GLN
8	C	312	ASN
8	C	329	GLN
8	C	360	ASN

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Mol	Chain	Res	Type
8	C	379	GLN
8	C	406	HIS
8	C	486	HIS
8	C	500	GLN
8	C	698	GLN
9	D	57	HIS
9	D	61	ASN
9	D	170	GLN
9	D	175	ASN
9	D	252	ASN
9	D	347	GLN
9	D	427	GLN
10	E	75	GLN
10	E	81	ASN
10	E	232	ASN
10	E	256	ASN
10	E	331	HIS
10	E	391	GLN
11	F	158	GLN
11	F	217	GLN
11	F	240	GLN
11	F	288	GLN
11	F	339	GLN
11	F	356	GLN
11	F	361	GLN
11	F	496	GLN
11	F	497	GLN
12	G	209	ASN
12	G	277	GLN
12	G	300	GLN
12	G	449	GLN
12	G	531	HIS

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	6	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	6	485:THR	C	486:LYS	N	1.06
1	6	487:ALA	C	488:GLY	N	1.03

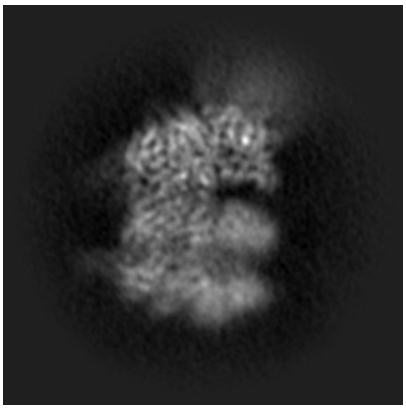
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19566. These allow visual inspection of the internal detail of the map and identification of artifacts.

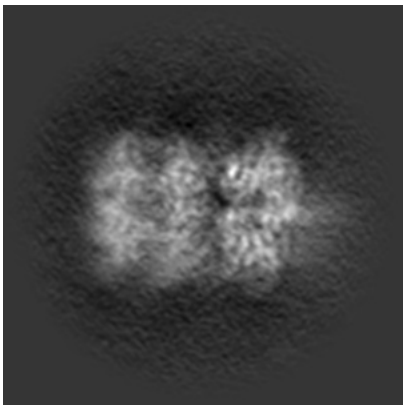
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

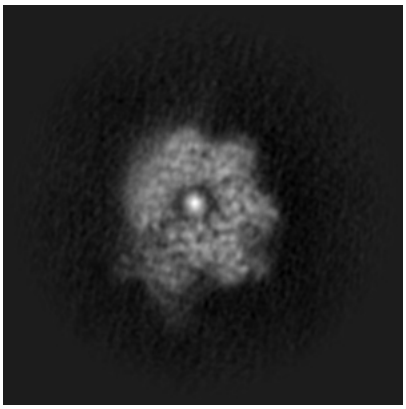
6.1.1 Primary map



X

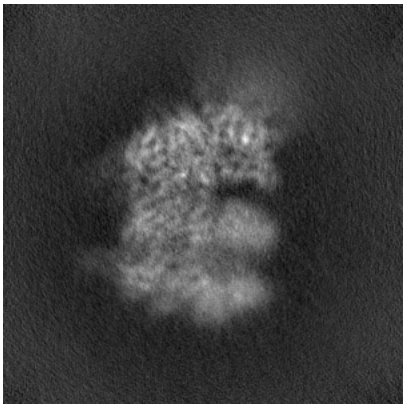


Y

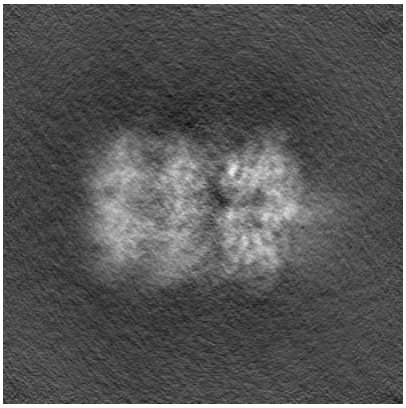


Z

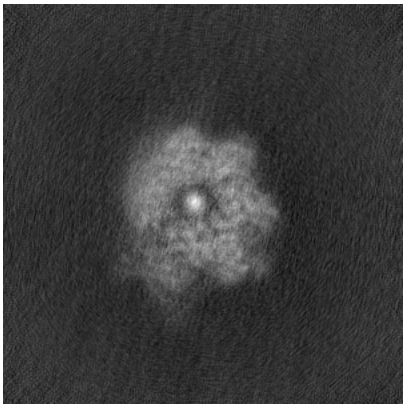
6.1.2 Raw map



X



Y

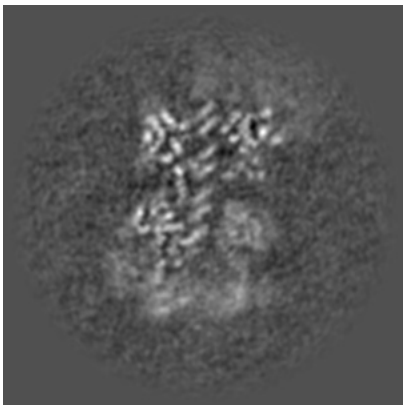


Z

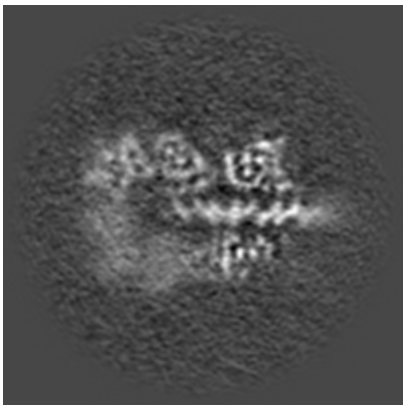
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

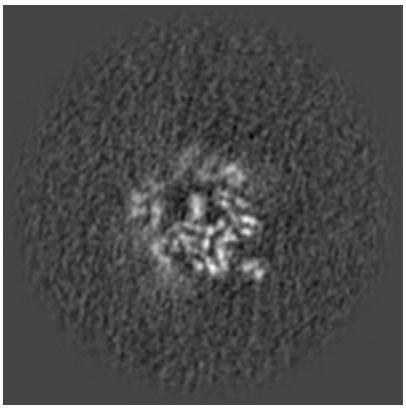
6.2.1 Primary map



X Index: 150

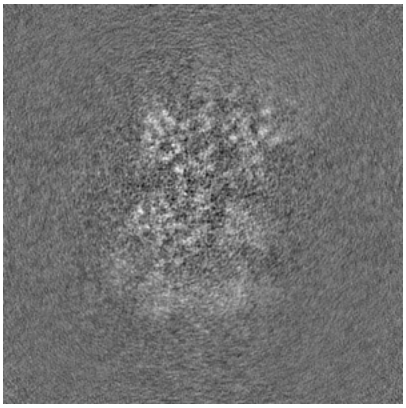


Y Index: 150

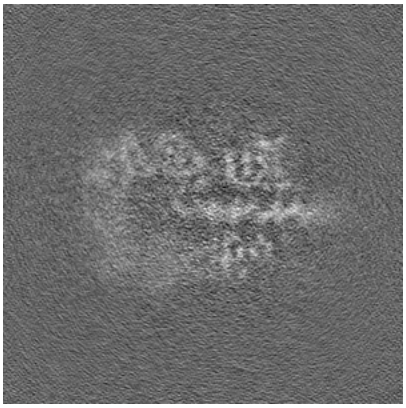


Z Index: 150

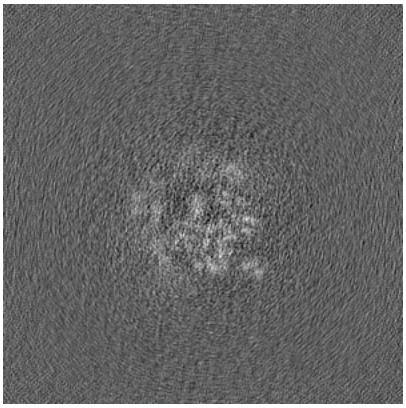
6.2.2 Raw map



X Index: 150



Y Index: 150

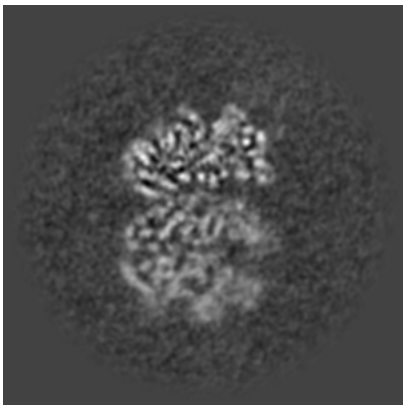


Z Index: 150

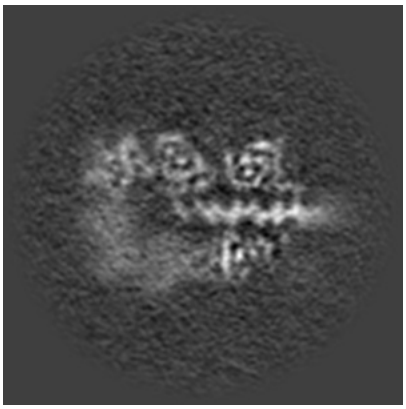
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

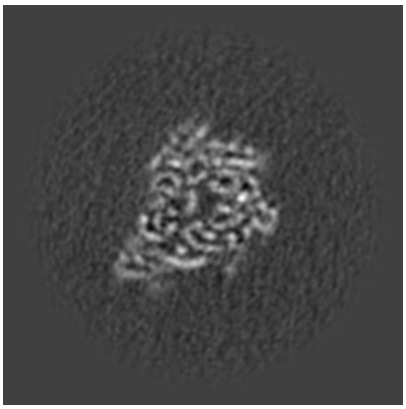
6.3.1 Primary map



X Index: 172

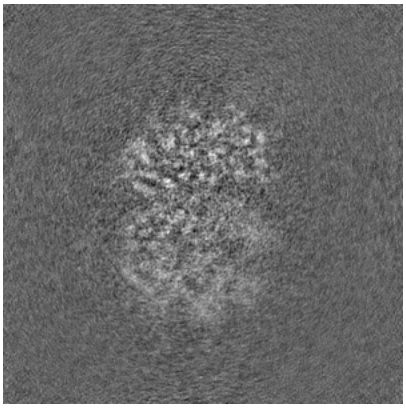


Y Index: 151

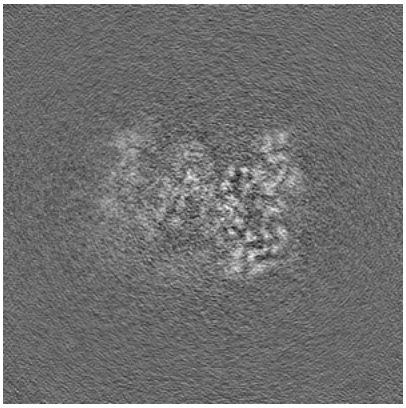


Z Index: 198

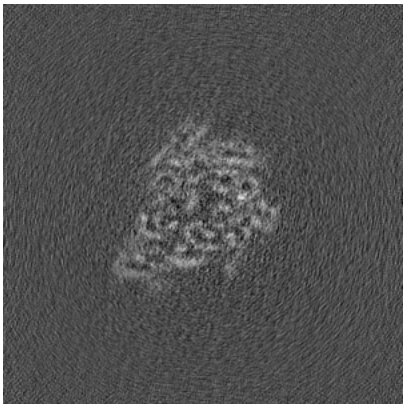
6.3.2 Raw map



X Index: 171



Y Index: 133

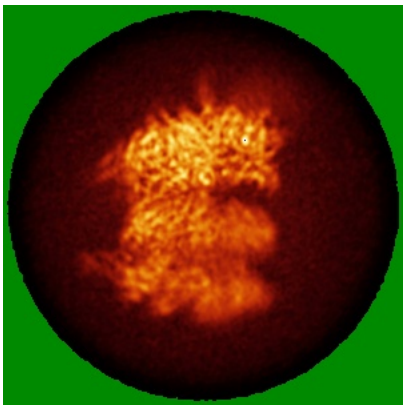


Z Index: 197

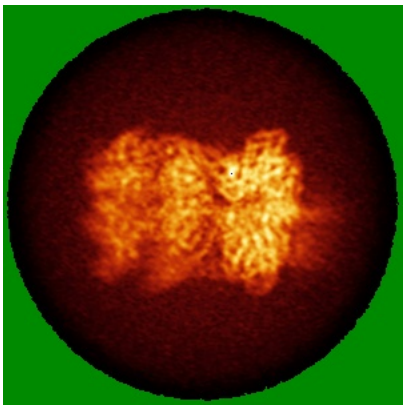
The images above show the largest variance slices of the map in three orthogonal directions.

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

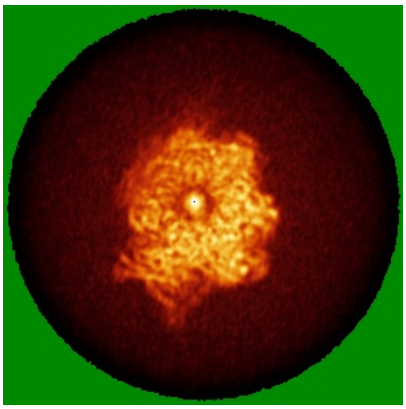
6.4.1 Primary map



X

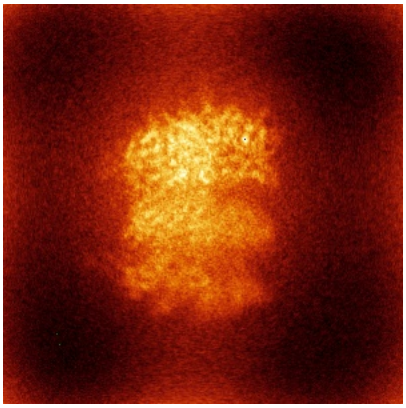


Y

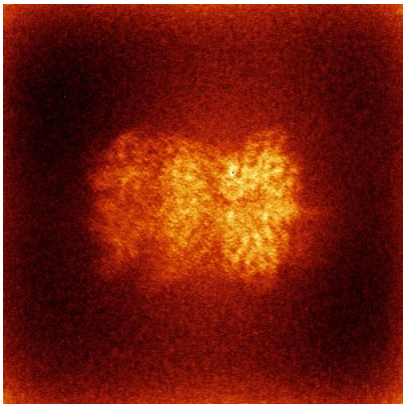


Z

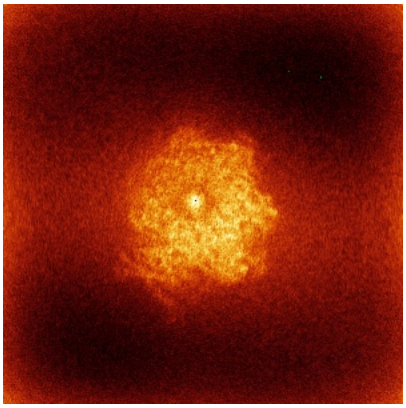
6.4.2 Raw map



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.

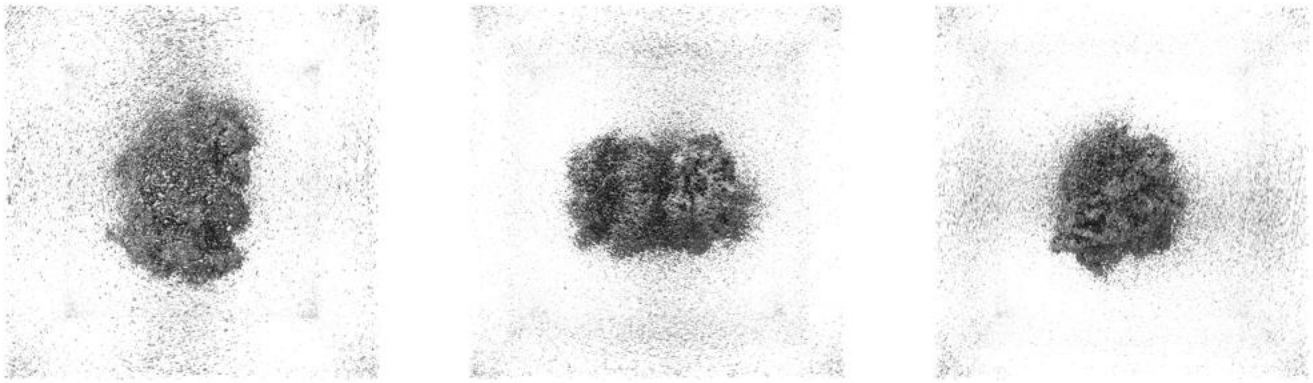
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



X Y Z

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

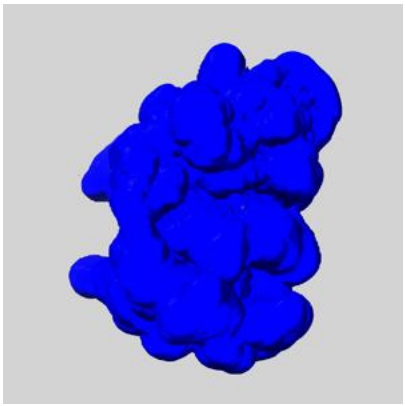
6.6 Mask visualisation (i)

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

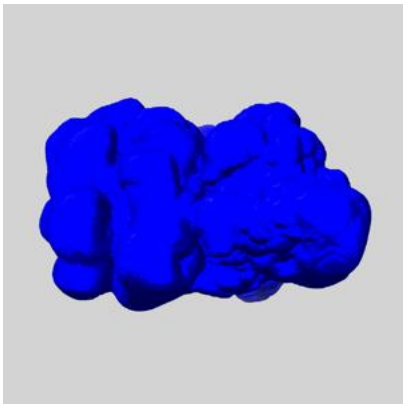
A mask typically either:

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

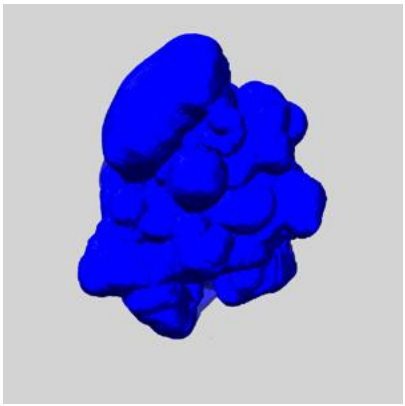
6.6.1 emd_19566_msk_1.map (i)



X



Y

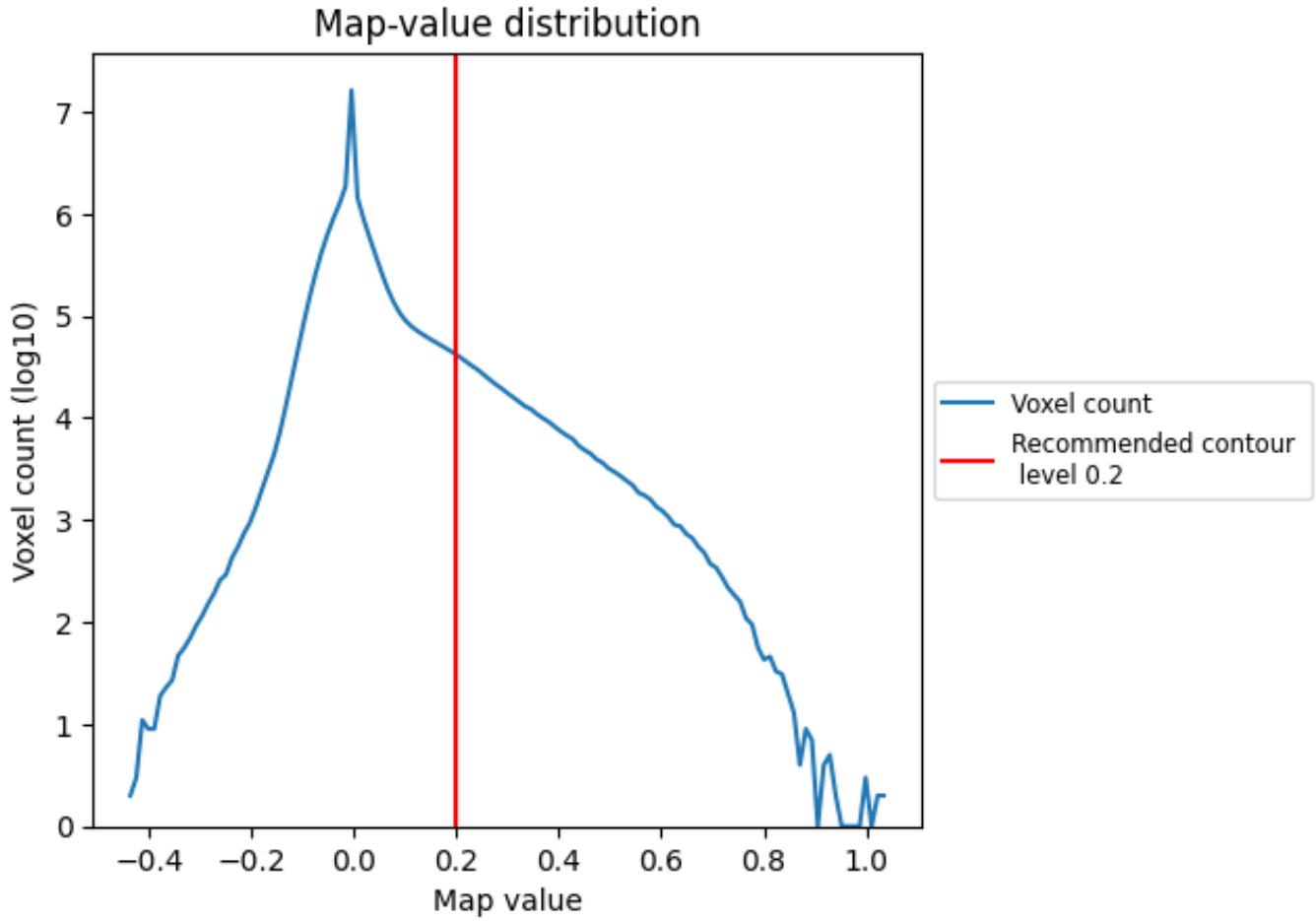


Z

7 Map analysis

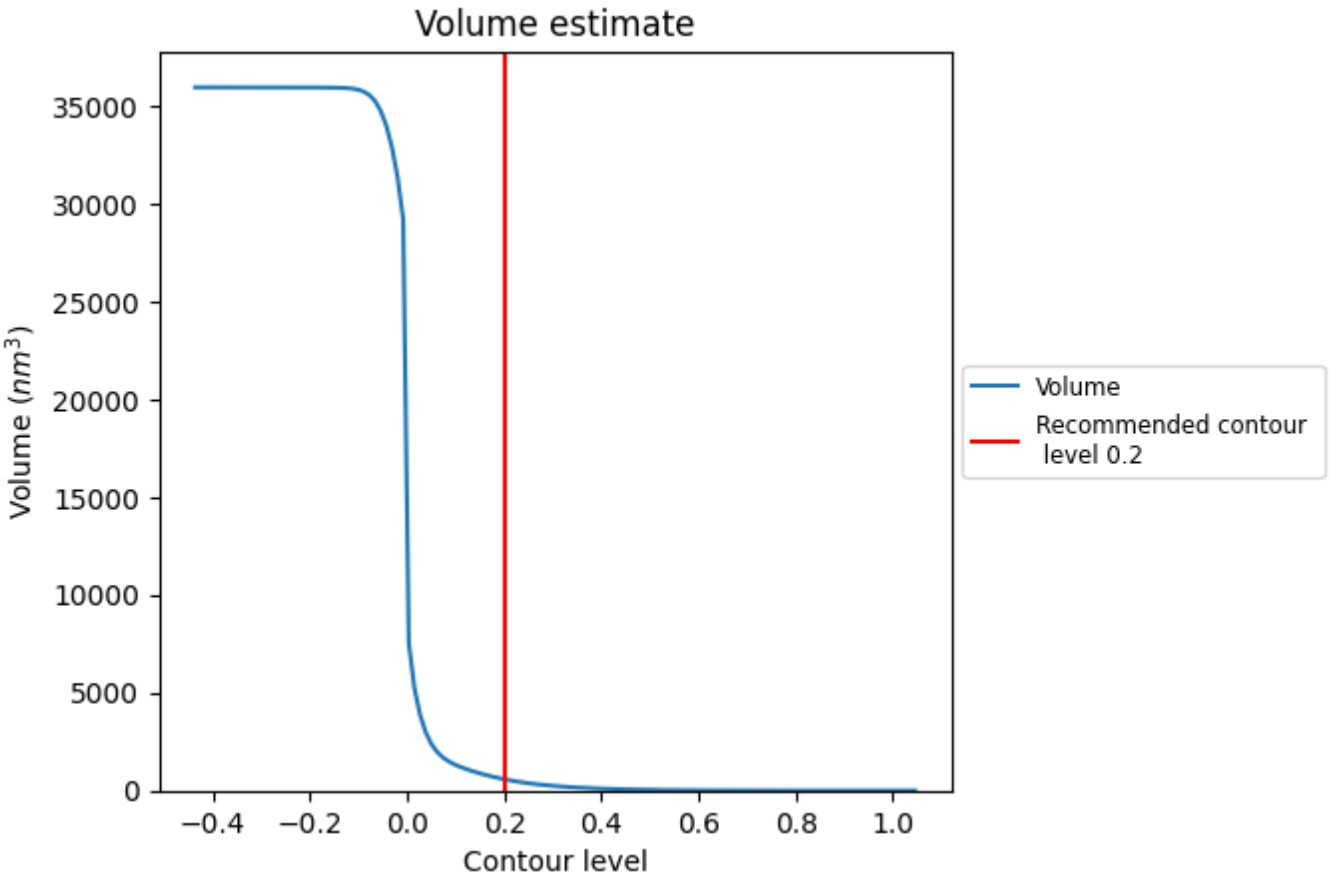
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

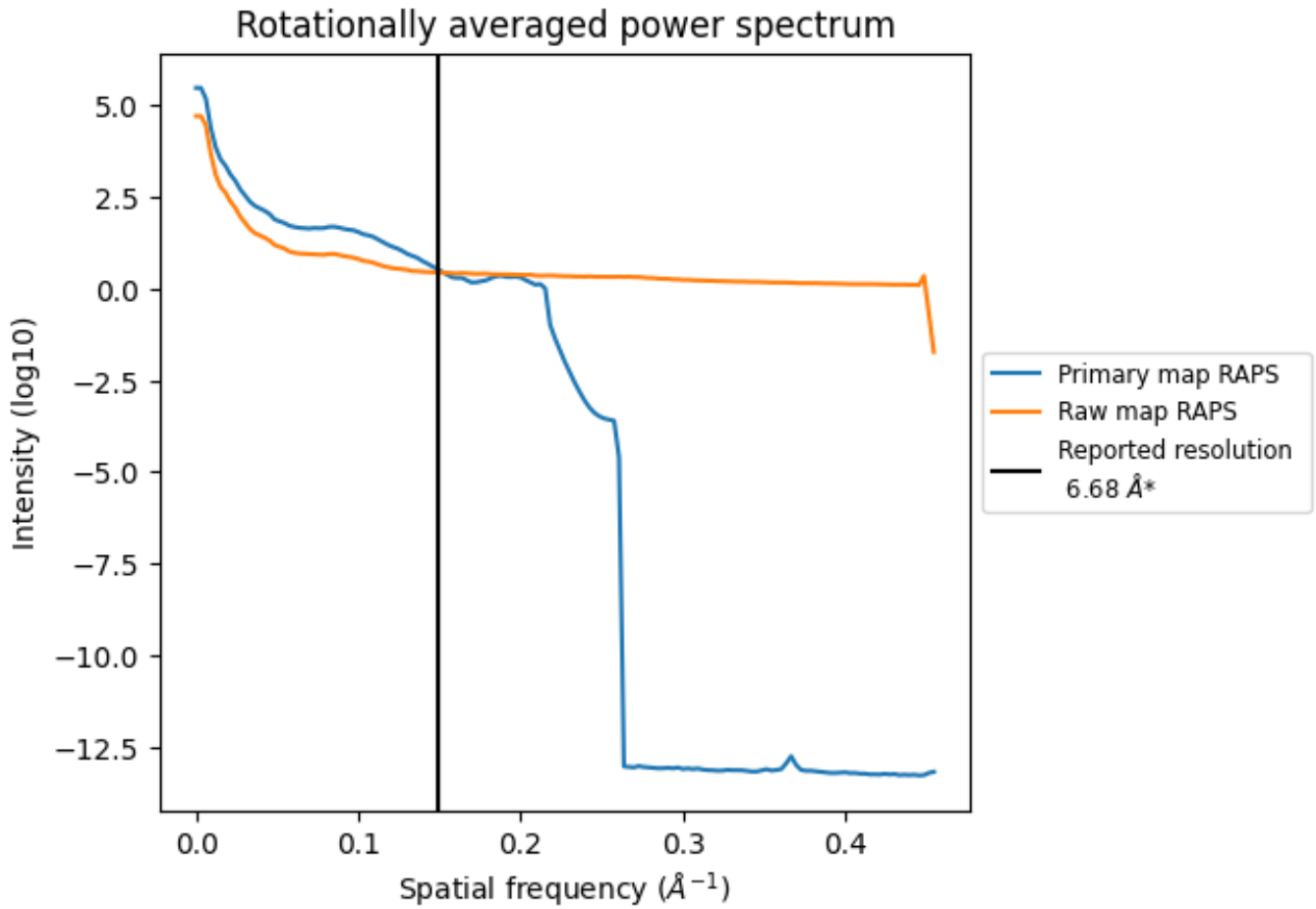
7.2 Volume estimate (i)



The volume at the recommended contour level is 578 nm^3; this corresponds to an approximate mass of 522 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

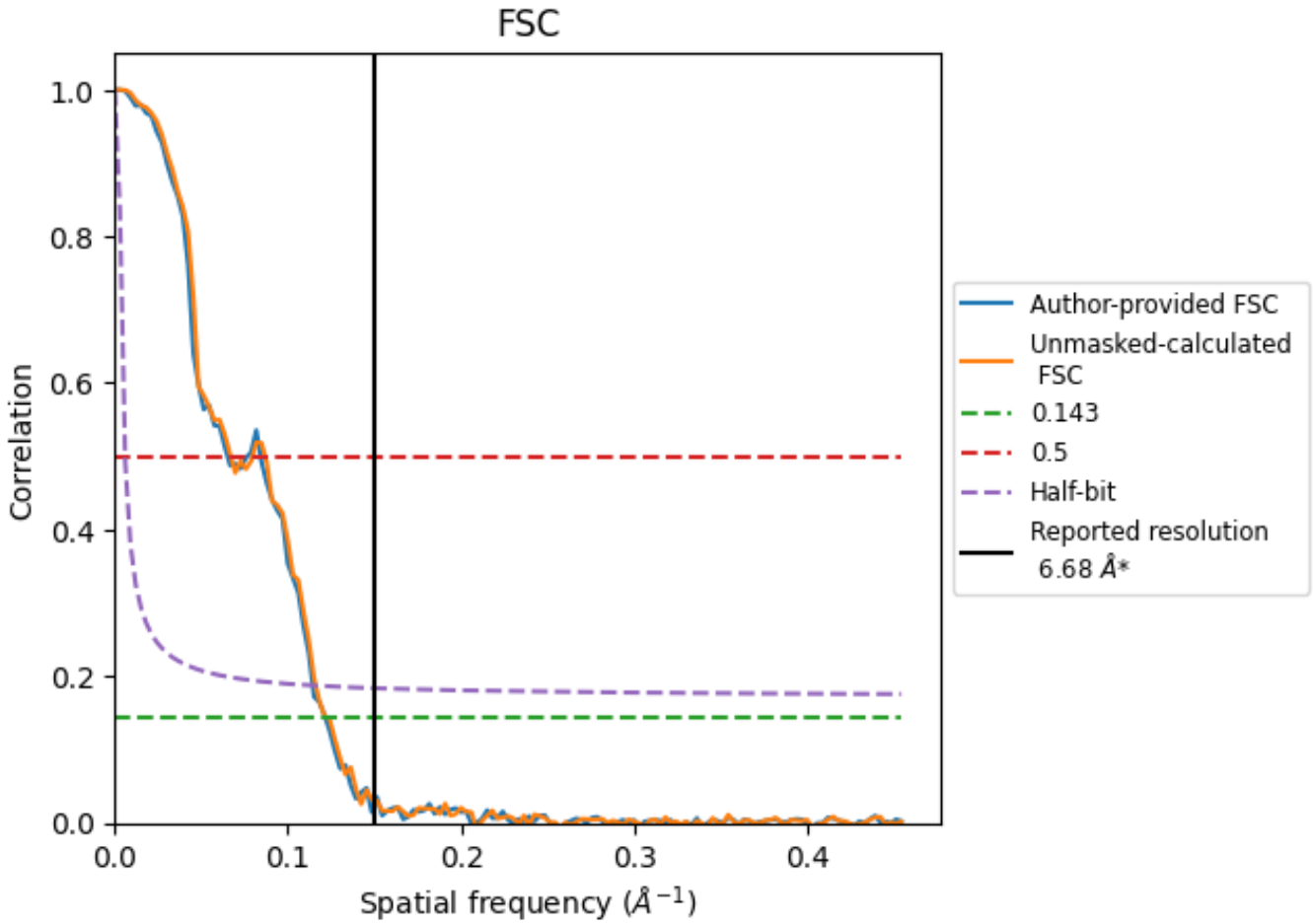


*Reported resolution corresponds to spatial frequency of 0.150 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.150 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.68	-	-
Author-provided FSC curve	8.22	15.34	8.74
Unmasked-calculated*	8.14	14.95	8.61

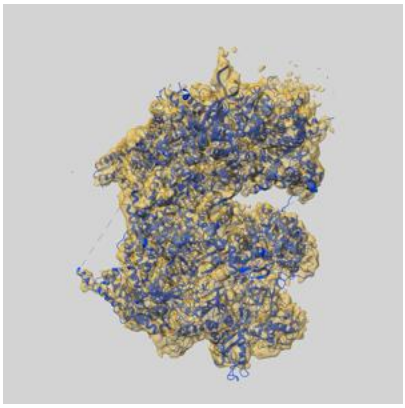
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.22 differs from the reported value 6.68 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.14 differs from the reported value 6.68 by more than 10 %

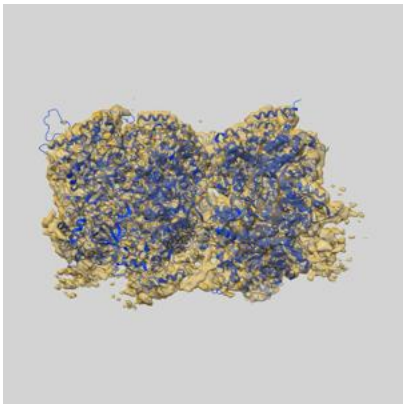
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19566 and PDB model 8RWV. Per-residue inclusion information can be found in section 3 on page 9.

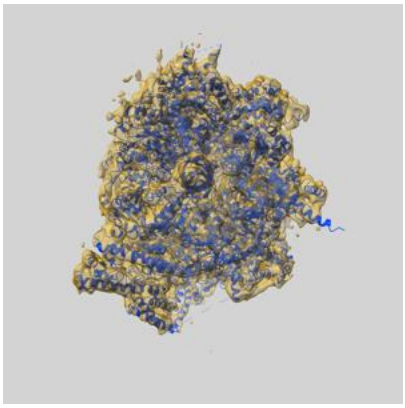
9.1 Map-model overlay



X



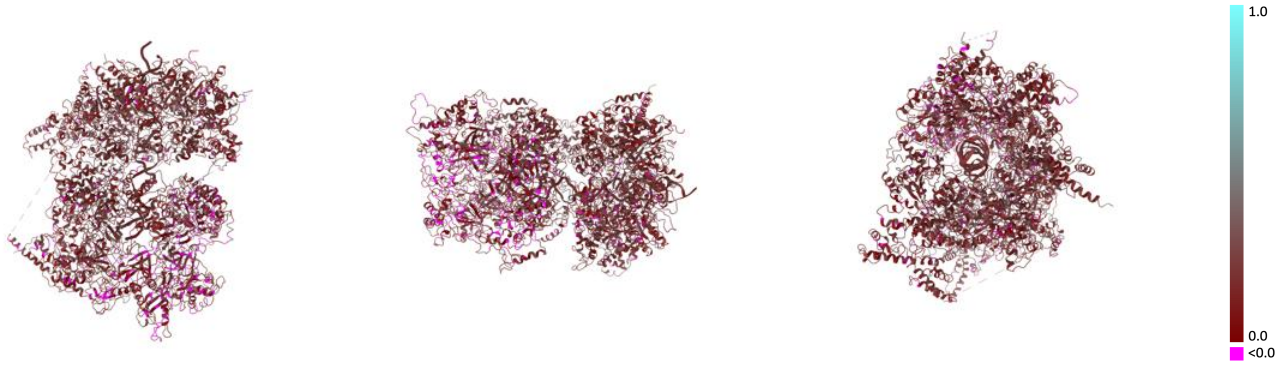
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

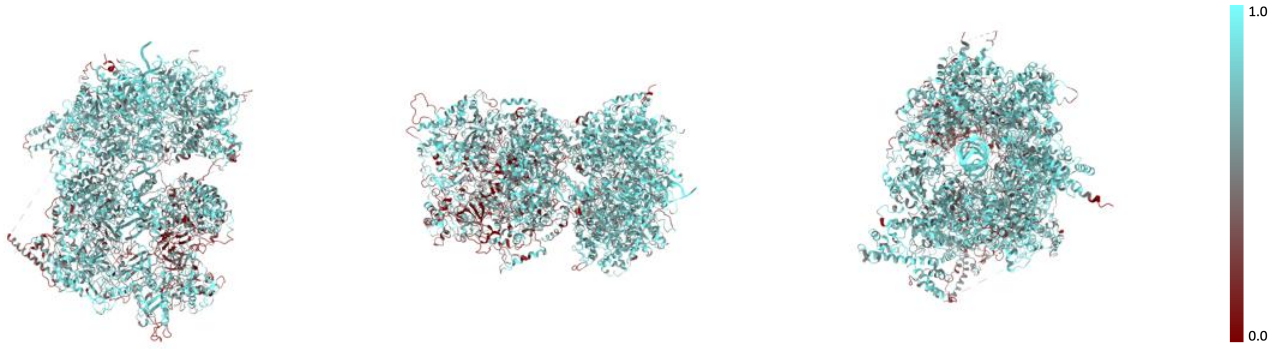
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

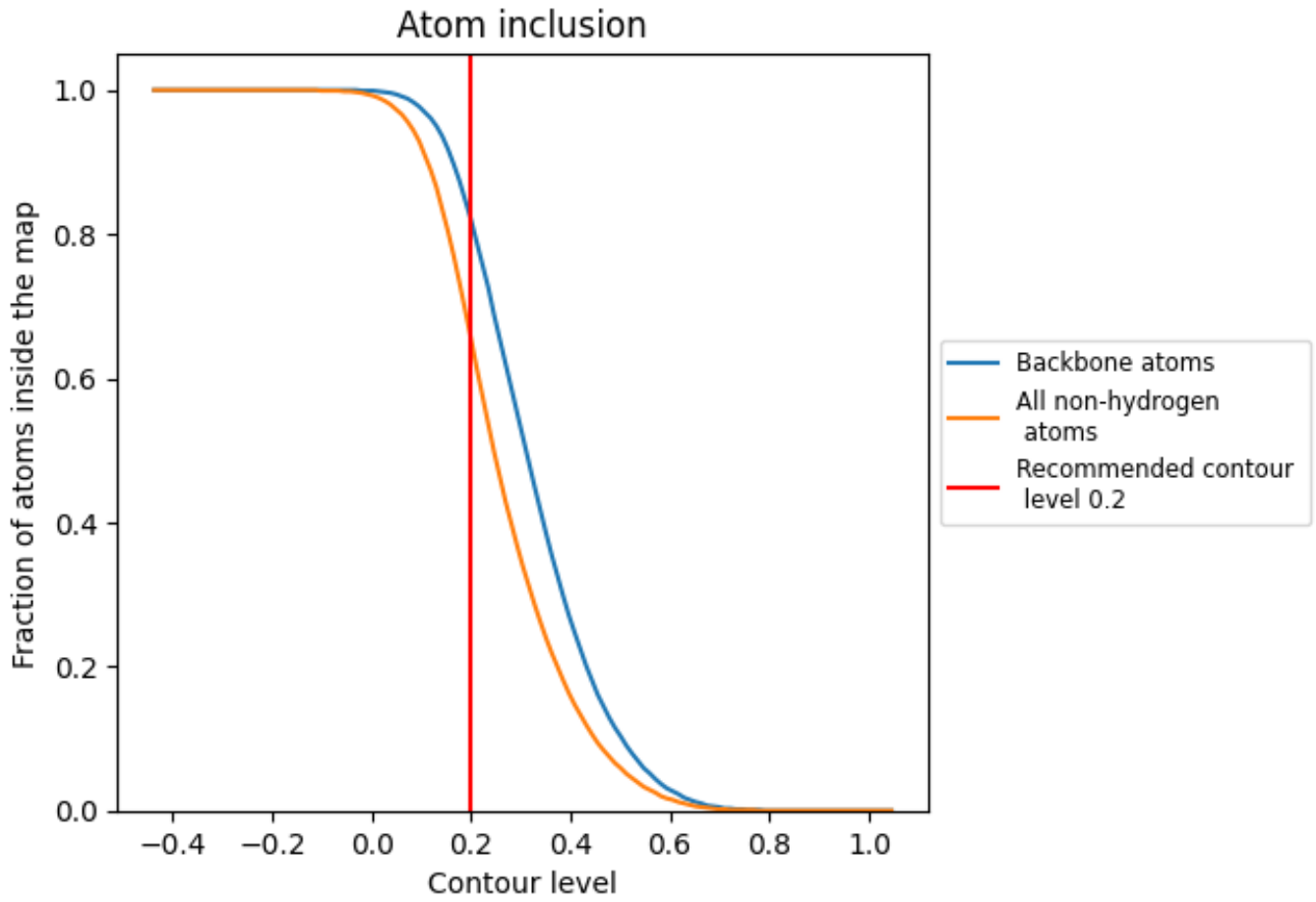
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.1860
2	0.6490	0.1960
3	0.4400	0.1290
4	0.6450	0.1730
6	0.7150	0.2000
7	0.5950	0.1530
A	0.7480	0.2060
B	0.6900	0.1970
C	0.6910	0.1920
D	0.7530	0.2180
E	0.7170	0.2150
F	0.6910	0.1980
G	0.5000	0.1710
H	0.9120	0.2440
J	0.9390	0.2400