Full wwPDB EM Validation Report ⓘ

Jan 16, 2024 – 10:37 AM EST

PDB ID	:	8TVY
EMDB ID	:	EMD-41655
Title	:	Cryo-EM structure of CPD lesion containing RNA Polymerase II elongation complex with Rad26 and Elf1 (closed state)
Authors	:	Sarsam, R.D.; Lahiri, I.; Leschziner, A.E.
Deposited on	:	2023-08-18
Resolution	:	3.10 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:

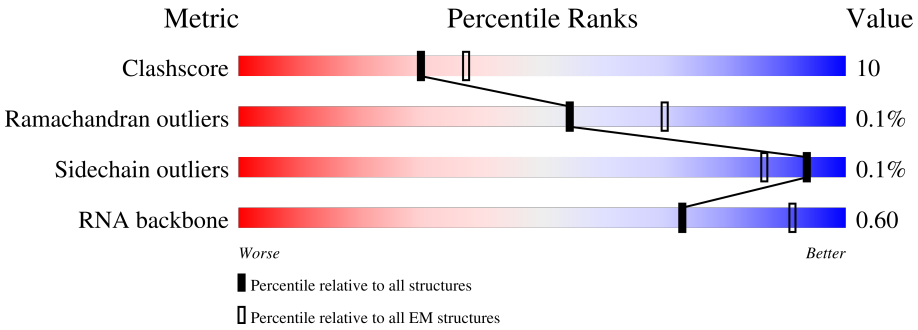
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1733	69% 14% 16%
2	B	1224	84% 15%
3	C	318	75% 10% 15%
4	D	221	62% 14% 24%
5	E	215	89% 11%
6	F	155	43% 9% 48%
7	G	171	66% 33%

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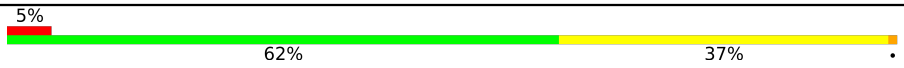
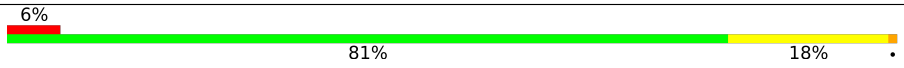
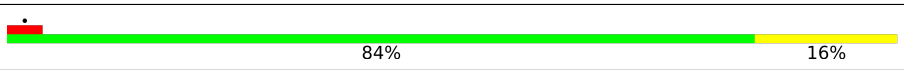
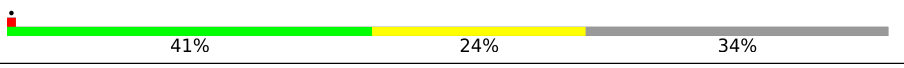
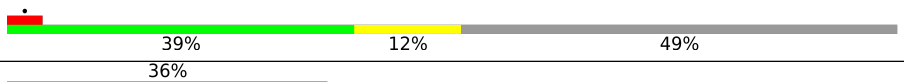
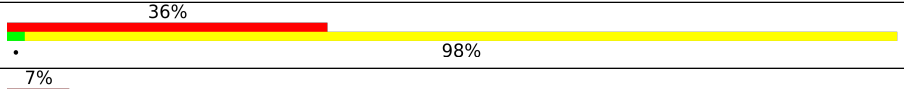
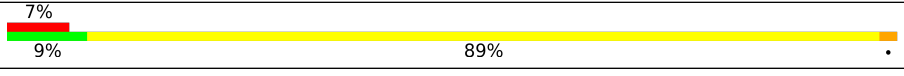
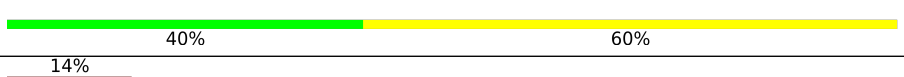
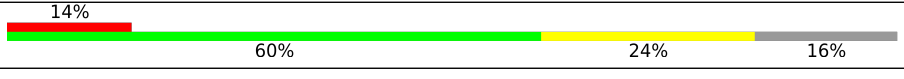
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	1085	
14	N	47	
15	T	46	
16	R	10	
17	O	85	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 76945 atoms, of which 37409 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1448	22822	7168	11437	1988	2167	62	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1207	19184	6062	9576	1678	1812	56	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	270	4212	1336	2087	353	422	14	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	167	2693	828	1353	236	274	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	215	3545	1116	1785	310	322	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	81	1330	419	673	111	124	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2694	861	1354	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	146	Total	C	H	N	O	S	0	0
			2282	726	1121	195	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	122	Total	C	H	N	O	S	0	0
			1947	613	950	182	191	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	70	Total	C	H	N	O	S	0	0
			1164	366	586	102	104	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	120	Total	C	H	N	O	S	0	0
			1920	616	958	162	182	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			750	224	386	72	64	4		

- Molecule 13 is a protein called RAD26 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	558	Total	C	H	N	O	S	0	0
			9170	2918	4606	808	819	19		

- Molecule 14 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			965	460	176	282	47		

- Molecule 15 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	46	Total	C	N	O	P	0	0
			947	454	155	291	47		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 17 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	O	71	Total	C	H	N	O	S	0	0
			1091	343	537	95	111	5		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	C	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

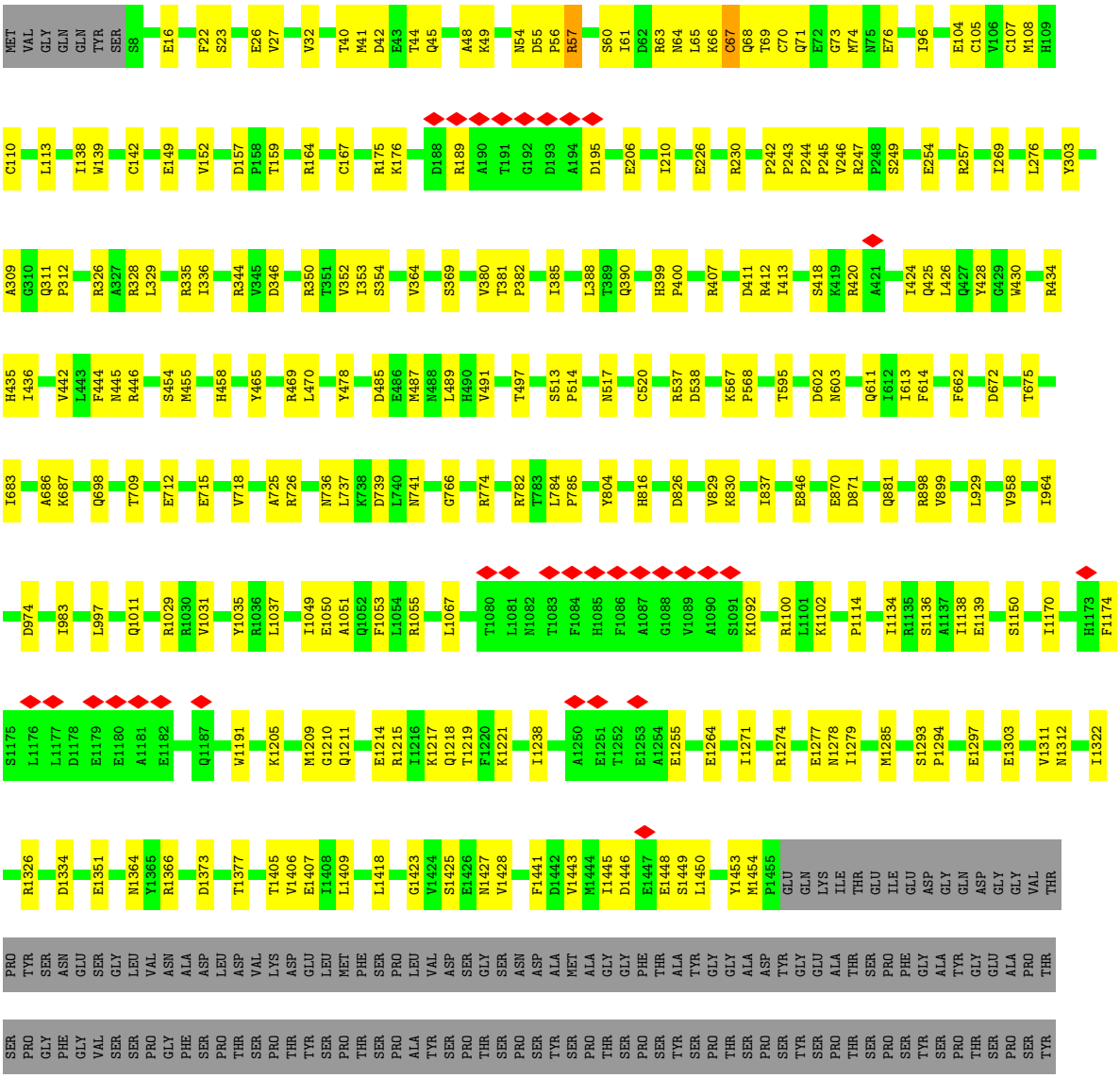
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

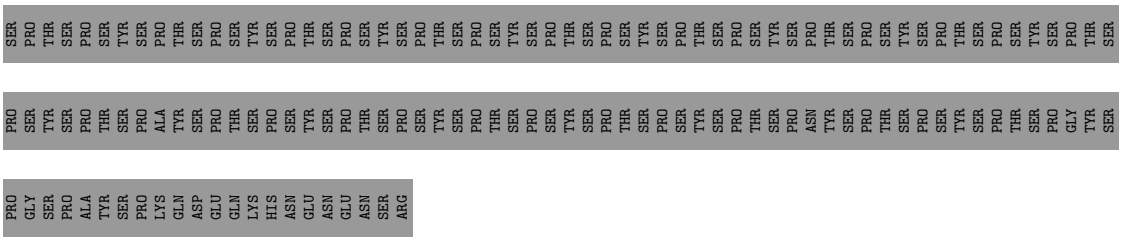
3 Residue-property plots (i)

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-directed RNA polymerase II subunit RPB1

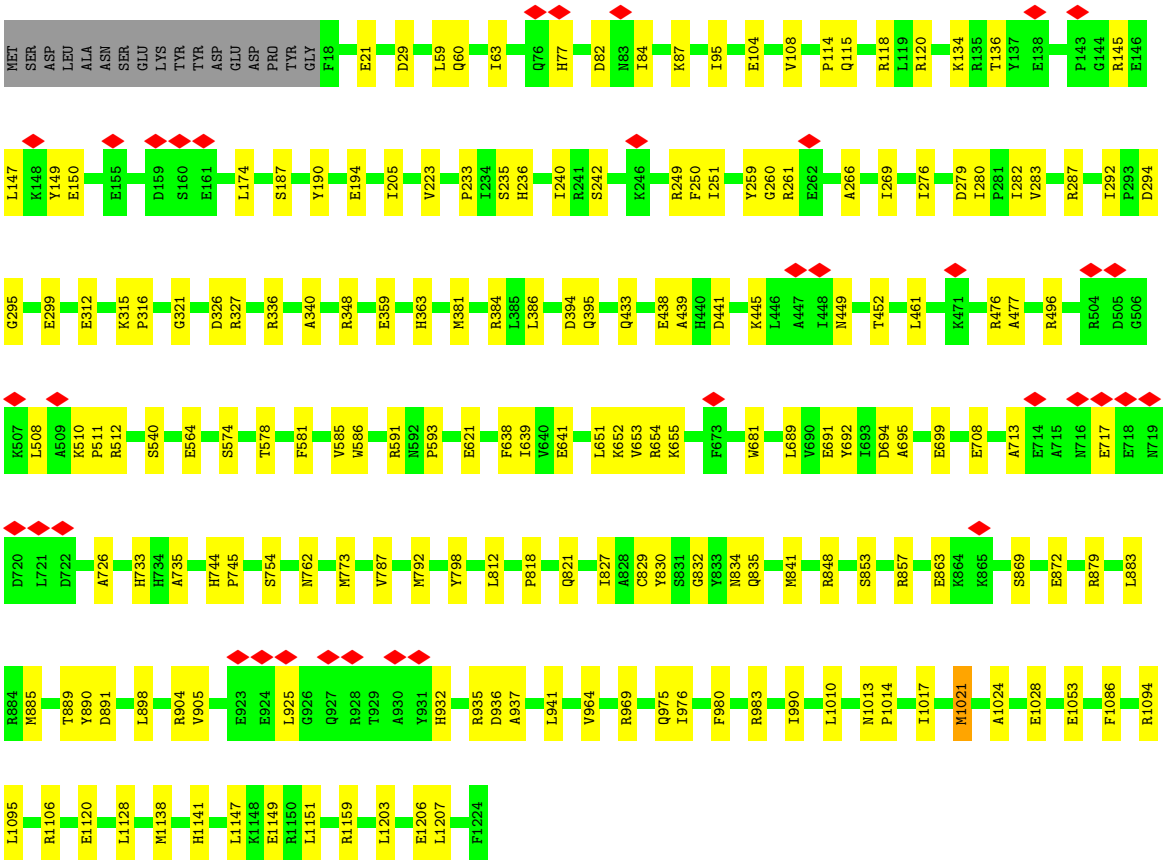
Chain A:





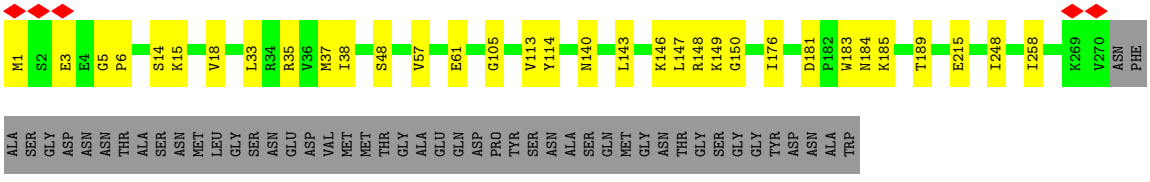
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



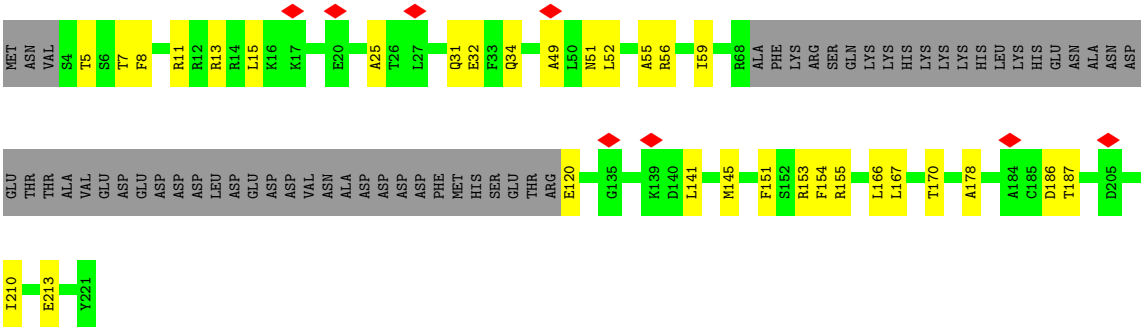
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



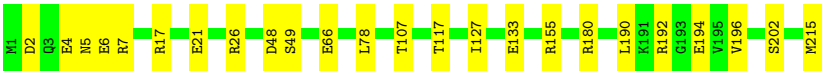
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



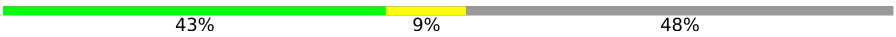
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

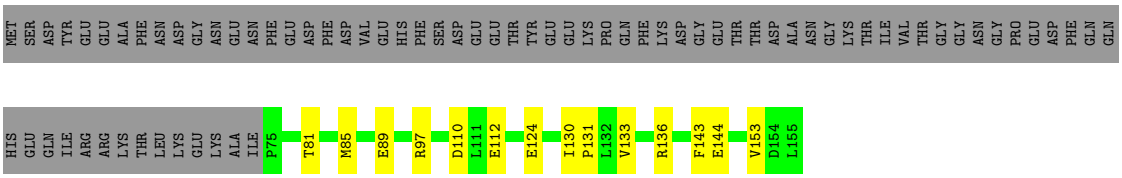
Chain E:



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

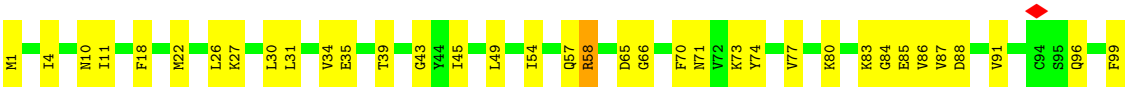
Chain F:

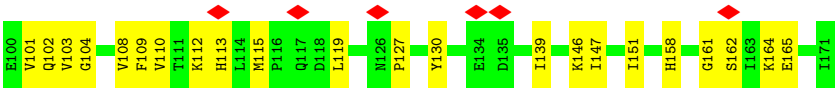




• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

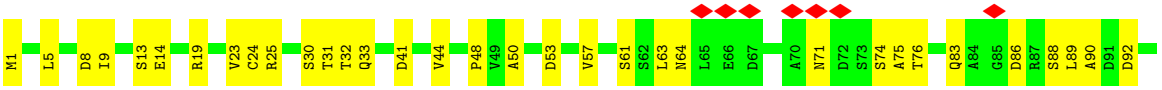
Chain G:

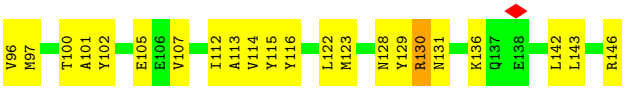




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

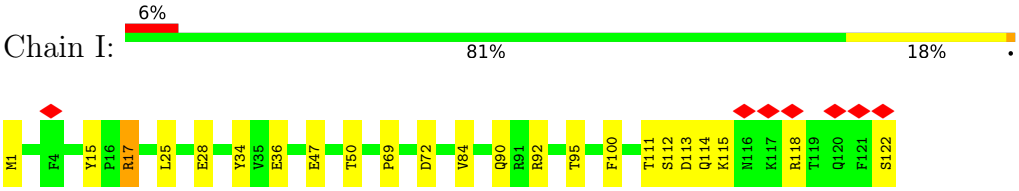
Chain H:





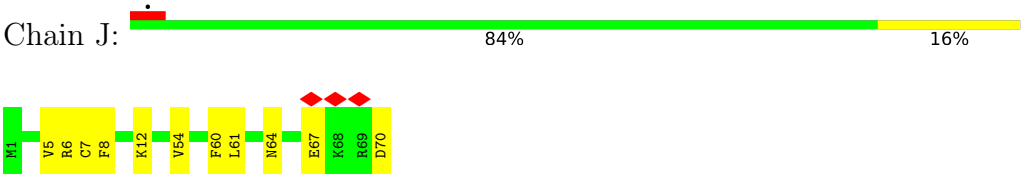
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



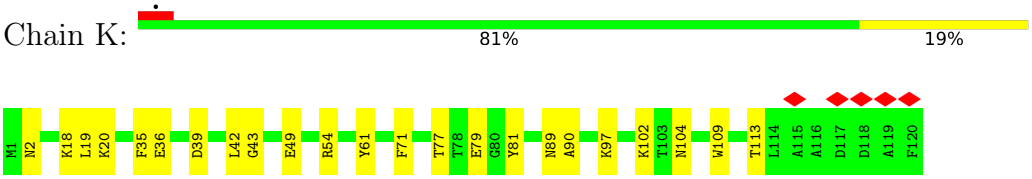
• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5

Chain J:



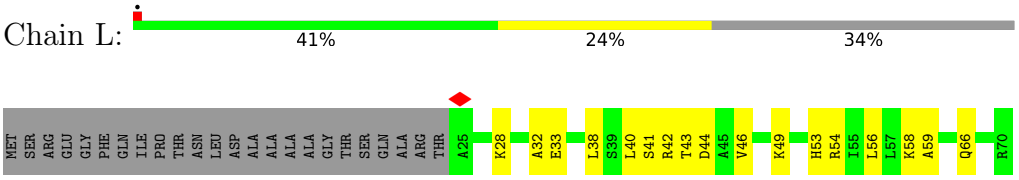
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



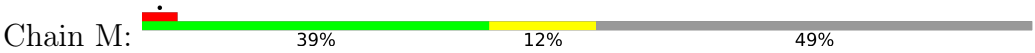
• Molecule 12: DNA-directed RNA polymerases II subunit RPABC4

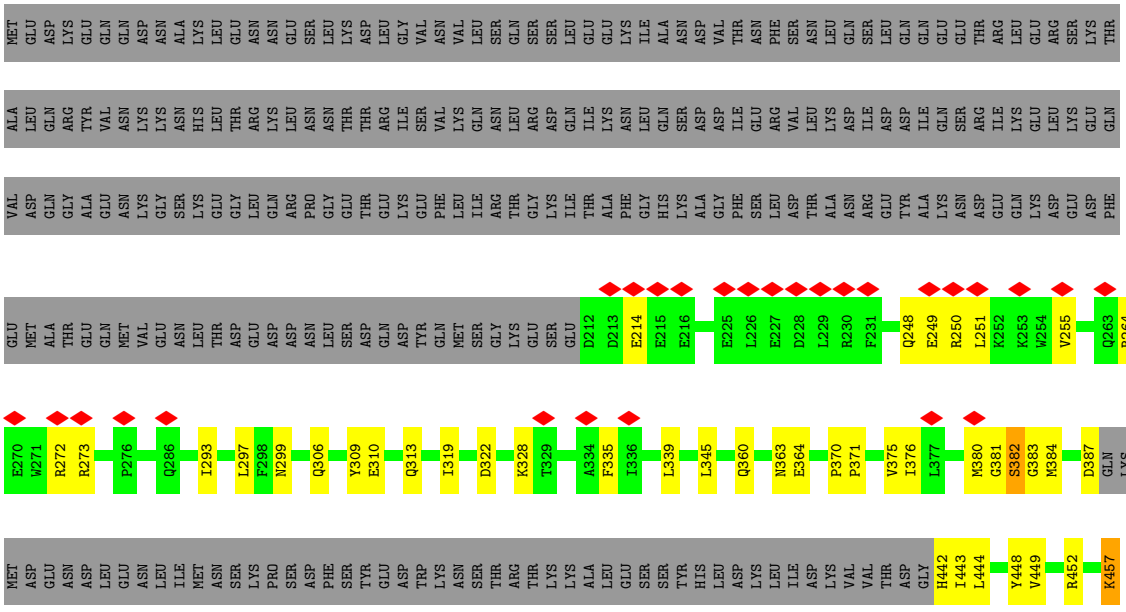
Chain L:

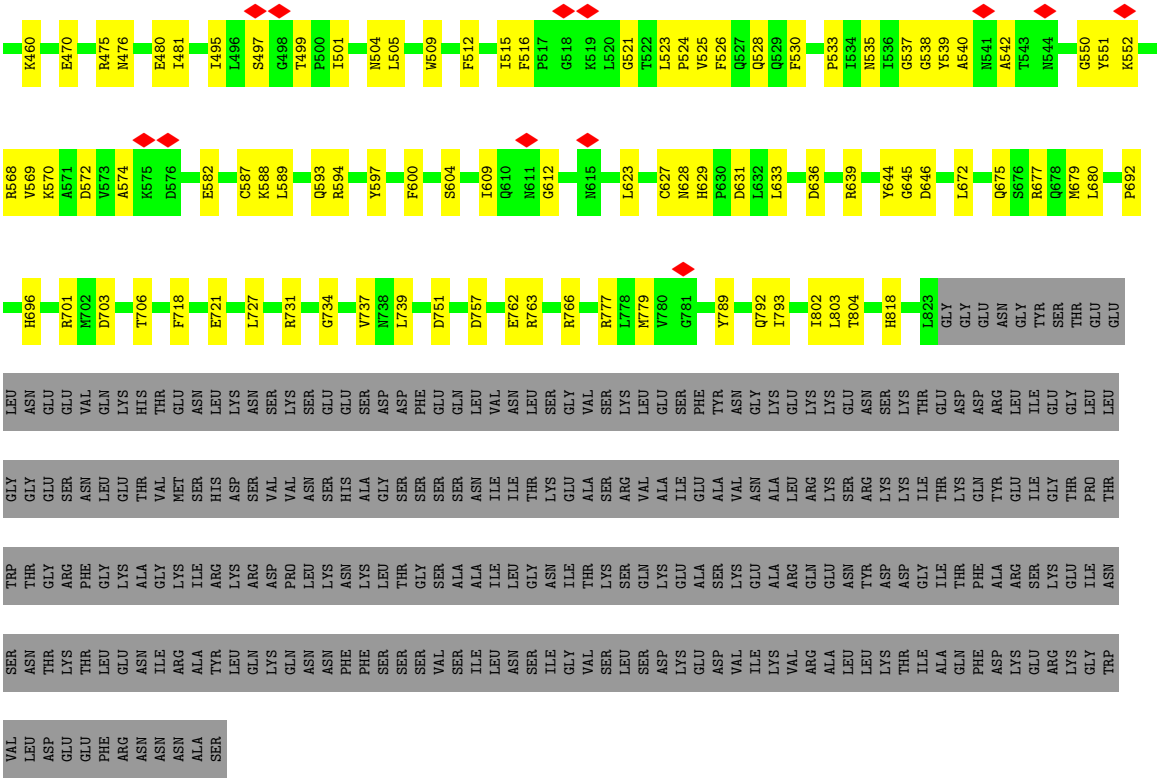


• Molecule 13: RAD26 isoform 1

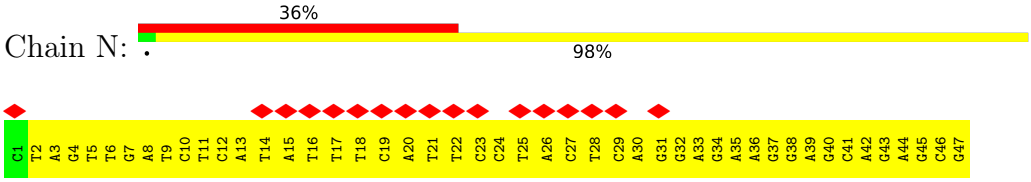
Chain M:



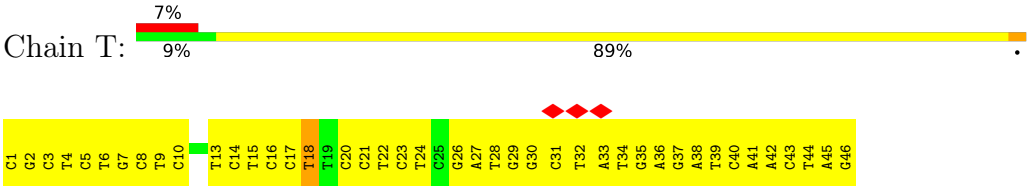




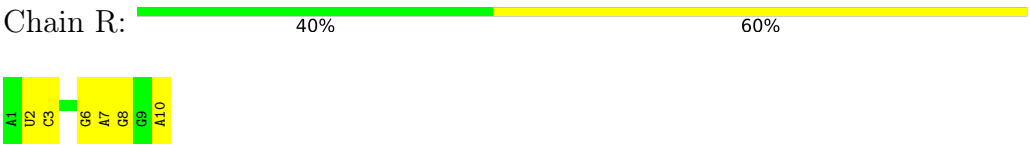
- Molecule 14: DNA (NTS)



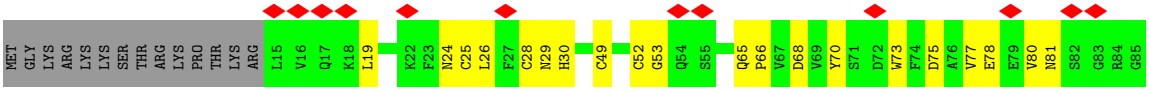
- Molecule 15: DNA (TS)



- Molecule 16: RNA



- Molecule 17: Transcription elongation factor 1 homolog


MET GLY LYS ARG LYS LYS SER THR ARG LYS PRO THR LYS ARG
L15 V16 Q17 K18 L19 K22 F23 N24 C25 L26 F27 C28 N29 H30 C49 C52 G53 Q54 S55 Q65 P66 V67 D68 V69 Y70 S71 D72 W73 F74 D75 A76 V77 E78 E79 V80 N81 S82 G83 R84 G85

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.275	Depositor
Minimum map value	-4.179	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.417	Depositor
Map size (Å)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTD, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/11592	0.51	0/15682
2	B	0.29	0/9799	0.51	0/13221
3	C	0.30	0/2163	0.48	0/2930
4	D	0.24	0/1349	0.48	0/1811
5	E	0.28	0/1796	0.49	0/2416
6	F	0.30	0/669	0.51	0/903
7	G	0.28	0/1368	0.49	0/1844
8	H	0.31	0/1181	0.56	0/1602
9	I	0.26	0/1016	0.53	0/1365
10	J	0.31	0/587	0.53	0/786
11	K	0.29	0/981	0.47	0/1324
12	L	0.27	0/366	0.61	0/485
13	M	0.24	0/4667	0.46	0/6301
14	N	0.48	0/1082	0.89	0/1668
15	T	0.49	0/1010	0.93	0/1551
16	R	0.39	0/247	0.70	0/384
17	O	0.28	0/562	0.53	0/755
All	All	0.30	0/40435	0.54	0/55028

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	A	0	1
12	L	0	1
17	O	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	THR	Peptide
12	L	58	LYS	Peptide
17	O	53	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11385	11437	11436	199	0
2	B	9608	9576	9576	126	0
3	C	2125	2087	2090	29	0
4	D	1340	1353	1352	23	0
5	E	1760	1785	1788	16	0
6	F	657	673	673	11	0
7	G	1340	1354	1357	51	0
8	H	1161	1121	1124	46	0
9	I	997	950	954	16	0
10	J	578	586	590	9	0
11	K	962	958	961	21	0
12	L	364	386	388	11	0
13	M	4564	4606	4605	89	0
14	N	965	0	531	117	0
15	T	947	0	534	73	0
16	R	220	0	110	4	0
17	O	554	537	536	12	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
All	All	39536	37409	38605	764	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 (764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:O	1:A:69:THR:N	1.88	1.05
15:T:15:DT:H2"	15:T:16:DC:H5'	1.39	1.01
9:I:17:ARG:NH2	9:I:28:GLU:O	1.93	1.01
8:H:105:GLU:OE2	8:H:116:TYR:OH	1.80	0.98
14:N:12:DC:H1'	14:N:13:DA:H5'	1.44	0.96
14:N:23:DC:H2"	14:N:24:DC:H5'	1.43	0.96
2:B:315:LYS:NZ	9:I:1:MET:SD	2.40	0.93
1:A:346:ASP:OD1	2:B:1106:ARG:NH1	2.03	0.92
2:B:792:MET:SD	2:B:857:ARG:NH2	2.43	0.92
14:N:16:DT:H2"	14:N:17:DT:H5"	1.55	0.87
1:A:595:THR:OG1	1:A:603:ASN:O	1.94	0.85
14:N:21:DT:H3'	14:N:22:DT:H71	1.56	0.85
1:A:709:THR:OG1	1:A:712:GLU:OE1	1.91	0.85
13:M:818:HIS:ND1	14:N:19:DC:OP1	2.10	0.85
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.10	0.84
1:A:517:ASN:OD1	1:A:1364:ASN:ND2	2.10	0.84
4:D:11:ARG:NH2	4:D:13:ARG:O	2.09	0.84
2:B:449:ASN:O	2:B:452:THR:OG1	1.97	0.82
3:C:48:SER:OG	12:L:66:GLN:OE1	1.99	0.80
1:A:1449:SER:O	1:A:1453:TYR:N	2.16	0.79
17:O:25:CYS:O	17:O:29:ASN:N	2.15	0.78
15:T:36:DA:H1'	15:T:37:DG:H5'	1.64	0.78
14:N:27:DC:H2"	14:N:28:DT:H5"	1.65	0.78
1:A:997:LEU:HD23	1:A:1053:PHE:CZ	2.20	0.76
1:A:189:ARG:NE	1:A:195:ASP:OD2	2.19	0.76
14:N:46:DC:H6	14:N:46:DC:H5'	1.52	0.74
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.19	0.74
14:N:22:DT:C3'	14:N:23:DC:H4'	2.18	0.74
2:B:744:HIS:ND1	2:B:745:PRO:O	2.21	0.74
4:D:153:ARG:NH2	7:G:88:ASP:OD2	2.21	0.74
3:C:150:GLY:N	10:J:67:GLU:OE1	2.21	0.73
17:O:77:VAL:O	17:O:81:ASN:N	2.22	0.73
5:E:192:ARG:NH1	5:E:215:MET:OXT	2.22	0.73
1:A:380:VAL:HG22	1:A:388:LEU:HD23	1.69	0.72
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.90	0.72
4:D:151:PHE:O	4:D:153:ARG:NH1	2.23	0.72
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:SER:OG	8:H:33:GLN:O	2.08	0.71
7:G:101:VAL:O	7:G:108:VAL:N	2.22	0.71
14:N:19:DC:H1'	14:N:20:DA:H5'	1.73	0.71
1:A:537:ARG:NH2	1:A:602:ASP:OD1	2.24	0.71
2:B:841:MET:CE	2:B:1010:LEU:HD21	2.21	0.70
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.09	0.70
15:T:18:TTD:H2'	15:T:18:TTD:O4R	1.91	0.70
7:G:109:PHE:O	7:G:161:GLY:N	2.25	0.70
1:A:242:PRO:O	1:A:247:ARG:NH1	2.24	0.69
1:A:1277:GLU:O	1:A:1312:ASN:ND2	2.24	0.69
7:G:1:MET:N	7:G:80:LYS:O	2.24	0.69
15:T:6:DT:H2"	15:T:7:DG:C8	2.26	0.69
4:D:167:LEU:O	4:D:170:THR:OG1	2.10	0.69
13:M:249:GLU:OE1	13:M:249:GLU:N	2.26	0.69
13:M:309:TYR:O	13:M:313:GLN:NE2	2.26	0.69
13:M:452:ARG:NH2	13:M:480:GLU:OE1	2.26	0.69
13:M:449:VAL:HG11	15:T:39:DT:H5'	1.74	0.69
1:A:1448:GLU:HB2	6:F:133:VAL:HG11	1.75	0.68
8:H:50:ALA:N	8:H:53:ASP:OD2	2.25	0.68
1:A:1373:ASP:O	1:A:1377:THR:HG23	1.94	0.68
7:G:102:GLN:NE2	7:G:104:GLY:O	2.27	0.68
14:N:23:DC:C2'	14:N:24:DC:H5'	2.23	0.68
14:N:12:DC:H2"	14:N:13:DA:O4'	1.94	0.68
13:M:587:CYS:N	13:M:779:MET:O	2.25	0.67
1:A:76:GLU:OE1	2:B:1159:ARG:NH2	2.27	0.67
15:T:41:DA:H2"	15:T:42:DA:C8	2.29	0.67
15:T:8:DC:H2'	15:T:9:DT:H71	1.77	0.67
14:N:12:DC:C1'	14:N:13:DA:H5'	2.20	0.67
1:A:249:SER:OG	1:A:257:ARG:O	2.08	0.67
1:A:411:ASP:OD1	1:A:412:ARG:N	2.27	0.67
8:H:8:ASP:OD1	8:H:9:ILE:N	2.26	0.67
14:N:24:DC:H4'	14:N:25:DT:C2	2.30	0.67
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.76	0.67
14:N:32:DG:O6	15:T:16:DC:N4	2.28	0.67
2:B:223:VAL:HG22	2:B:240:ILE:HD11	1.77	0.66
14:N:43:DG:H2"	14:N:44:DA:H8	1.60	0.66
15:T:21:DC:H2"	15:T:22:DT:H5'	1.76	0.66
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.28	0.66
2:B:639:ILE:HD11	2:B:691:GLU:OE2	1.96	0.66
14:N:41:DC:H2"	14:N:42:DA:C8	2.30	0.66
13:M:677:ARG:NH2	15:T:36:DA:OP2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:SER:OG	1:A:1264:GLU:OE1	2.05	0.65
14:N:39:DA:OP2	14:N:39:DA:H2'	1.95	0.65
5:E:17:ARG:NH1	5:E:21:GLU:OE2	2.28	0.65
8:H:13:SER:OG	8:H:14:GLU:OE1	2.10	0.65
8:H:83:GLN:NE2	8:H:86:ASP:OD2	2.30	0.65
14:N:43:DG:H2"	14:N:44:DA:C8	2.31	0.65
1:A:1445:ILE:HG23	7:G:58:ARG:NH1	2.10	0.65
14:N:20:DA:H1'	14:N:21:DT:C6	2.32	0.65
15:T:3:DC:H2'	15:T:4:DT:H71	1.79	0.65
15:T:44:DT:H2"	15:T:45:DA:C8	2.32	0.65
2:B:841:MET:HE2	2:B:1010:LEU:HD21	1.79	0.65
17:O:49:CYS:SG	17:O:52:CYS:N	2.70	0.65
5:E:48:ASP:OD1	5:E:49:SER:N	2.31	0.64
14:N:35:DA:H2"	14:N:36:DA:H5'	1.79	0.64
13:M:762:GLU:O	13:M:766:ARG:NH1	2.30	0.64
15:T:6:DT:OP2	15:T:6:DT:H2'	1.97	0.64
15:T:9:DT:H2"	15:T:10:DC:C5'	2.27	0.64
5:E:155:ARG:NH1	5:E:194:GLU:OE2	2.30	0.64
1:A:899:VAL:HG11	1:A:929:LEU:HD22	1.79	0.64
8:H:75:ALA:O	8:H:76:THR:OG1	2.12	0.64
2:B:438:GLU:OE1	2:B:445:LYS:NZ	2.28	0.64
8:H:31:THR:O	8:H:32:THR:OG1	2.16	0.64
8:H:105:GLU:O	8:H:107:VAL:HG23	1.98	0.64
3:C:184:ASN:ND2	3:C:189:THR:O	2.32	0.63
13:M:731:ARG:NH1	15:T:36:DA:H5"	2.13	0.63
14:N:24:DC:H2"	14:N:25:DT:C5	2.33	0.63
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.31	0.63
7:G:27:LYS:O	7:G:31:LEU:HD23	1.97	0.63
14:N:26:DA:H1'	14:N:27:DC:C4	2.34	0.63
2:B:641:GLU:OE1	2:B:652:LYS:NZ	2.21	0.63
15:T:40:DC:H2"	15:T:41:DA:C8	2.33	0.63
1:A:1445:ILE:O	7:G:58:ARG:NE	2.32	0.63
1:A:66:LYS:O	1:A:68:GLN:N	2.32	0.62
3:C:6:PRO:O	11:K:104:ASN:ND2	2.31	0.62
16:R:6:G:O2'	16:R:7:A:H5'	1.99	0.62
15:T:18:TTD:H2'	15:T:18:TTD:O5R	1.98	0.62
1:A:42:ASP:OD2	1:A:257:ARG:NH1	2.33	0.62
2:B:287:ARG:NH1	2:B:292:ILE:O	2.33	0.62
14:N:38:DG:H2"	14:N:39:DA:H8	1.65	0.62
15:T:26:DG:H4'	15:T:27:DA:OP1	1.98	0.62
14:N:22:DT:C2'	14:N:23:DC:H4'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG23	1:A:41:MET:HG2	1.83	0.61
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.33	0.61
1:A:226:GLU:O	1:A:230:ARG:NH2	2.30	0.61
1:A:444:PHE:CE2	1:A:489:LEU:HD13	2.34	0.61
17:O:19:LEU:O	17:O:70:TYR:OH	2.19	0.61
13:M:264:ARG:NH2	13:M:387:ASP:O	2.34	0.61
1:A:380:VAL:HG23	1:A:430:TRP:O	2.00	0.61
1:A:1050:GLU:HA	1:A:1053:PHE:CE1	2.36	0.61
2:B:733:HIS:NE2	2:B:735:ALA:O	2.33	0.61
2:B:312:GLU:OE2	9:I:1:MET:N	2.31	0.61
3:C:15:LYS:HA	3:C:15:LYS:HE3	1.82	0.61
2:B:1017:ILE:O	2:B:1021:MET:N	2.34	0.61
15:T:5:DC:H2"	15:T:6:DT:C6	2.36	0.61
15:T:42:DA:H2"	15:T:43:DC:C6	2.35	0.61
2:B:242:SER:OG	2:B:363:HIS:ND1	2.22	0.61
17:O:24:ASN:OD1	17:O:25:CYS:N	2.34	0.61
2:B:1138:MET:HB2	2:B:1147:LEU:HD21	1.83	0.61
14:N:31:DG:H22	15:T:17:DC:H42	1.47	0.60
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.60
13:M:269:PRO:O	13:M:273:ARG:NH1	2.34	0.60
1:A:881:GLN:NE2	1:A:958:VAL:O	2.34	0.60
13:M:636:ASP:O	13:M:639:ARG:NH1	2.35	0.60
14:N:9:DT:H2"	14:N:10:DC:C6	2.37	0.60
1:A:898:ARG:O	1:A:1029:ARG:NH2	2.35	0.60
14:N:17:DT:H2"	14:N:18:DT:H72	1.82	0.60
14:N:46:DC:H5'	14:N:46:DC:C6	2.36	0.60
15:T:36:DA:H5'	15:T:36:DA:H8	1.66	0.60
1:A:309:ALA:HB1	15:T:15:DT:H5'	1.82	0.60
14:N:10:DC:H2'	14:N:11:DT:H72	1.83	0.60
14:N:22:DT:O3'	14:N:23:DC:H4'	2.02	0.60
1:A:344:ARG:NH1	15:T:21:DC:OP1	2.35	0.60
8:H:14:GLU:OE1	8:H:14:GLU:N	2.34	0.59
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.19	0.59
12:L:41:SER:N	12:L:44:ASP:OD2	2.35	0.59
14:N:42:DA:H2"	14:N:43:DG:C8	2.38	0.59
1:A:614:PHE:CE1	8:H:122:LEU:HD11	2.37	0.59
2:B:115:GLN:NE2	2:B:787:VAL:HG12	2.18	0.59
2:B:694:ASP:OD1	2:B:695:ALA:N	2.36	0.59
4:D:25:ALA:N	7:G:83:LYS:O	2.36	0.59
15:T:28:DT:H3'	15:T:29:DG:H5"	1.85	0.59
1:A:425:GLN:OE1	1:A:426:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:638:PHE:HB3	2:B:651:LEU:HD11	1.83	0.59
7:G:65:ASP:OD1	7:G:66:GLY:N	2.36	0.59
13:M:757:ASP:OD2	13:M:792:GLN:NE2	2.35	0.59
1:A:718:VAL:HG11	1:A:774:ARG:HH12	1.67	0.59
1:A:1445:ILE:HG23	7:G:58:ARG:CZ	2.33	0.59
2:B:134:LYS:NZ	2:B:136:THR:OG1	2.35	0.59
13:M:512:PHE:O	13:M:516:PHE:N	2.30	0.59
15:T:7:DG:H2"	15:T:8:DC:C6	2.38	0.59
2:B:496:ARG:NH2	2:B:540:SER:O	2.36	0.59
7:G:96:GLN:N	7:G:96:GLN:OE1	2.34	0.58
2:B:835:GLN:O	2:B:1013:ASN:ND2	2.35	0.58
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.34	0.58
13:M:375:VAL:HG11	13:M:380:MET:HE1	1.85	0.58
14:N:42:DA:H2'	14:N:42:DA:OP2	2.02	0.58
2:B:681:TRP:HE1	2:B:692:TYR:HH	1.50	0.58
2:B:905:VAL:HG23	2:B:941:LEU:HD11	1.86	0.58
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.85	0.58
14:N:19:DC:H2"	14:N:20:DA:O5'	2.04	0.58
15:T:4:DT:H2"	15:T:5:DC:C6	2.39	0.58
1:A:369:SER:OG	11:K:2:ASN:ND2	2.33	0.58
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.34	0.58
13:M:475:ARG:NH2	13:M:499:THR:O	2.36	0.58
15:T:13:DT:H2"	15:T:14:DC:H5'	1.84	0.58
13:M:629:HIS:ND1	13:M:629:HIS:O	2.36	0.58
5:E:190:LEU:HD11	5:E:196:VAL:HG21	1.86	0.58
7:G:54:ILE:HG23	7:G:74:TYR:HE1	1.68	0.58
9:I:34:TYR:OH	9:I:36:GLU:OE1	2.17	0.58
13:M:452:ARG:NH1	14:N:11:DT:O3'	2.35	0.58
1:A:538:ASP:OD1	8:H:23:VAL:HG22	2.04	0.58
13:M:734:GLY:O	13:M:763:ARG:NH1	2.35	0.58
5:E:2:ASP:N	5:E:5:ASN:OD1	2.35	0.58
11:K:77:THR:OG1	11:K:81:TYR:O	2.20	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.57
15:T:7:DG:H2"	15:T:8:DC:H6	1.69	0.57
15:T:9:DT:H2"	15:T:10:DC:H5'	1.85	0.57
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.86	0.57
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.34	0.57
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.40	0.57
14:N:47:DG:H5'	14:N:47:DG:C8	2.39	0.57
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.85	0.57
14:N:14:DT:H1'	14:N:15:DA:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HD13	1:A:741:ASN:ND2	2.20	0.57
1:A:54:ASN:OD1	1:A:247:ARG:NH2	2.38	0.57
1:A:1449:SER:HB2	6:F:133:VAL:HG13	1.87	0.57
3:C:35:ARG:NH2	11:K:39:ASP:OD2	2.38	0.56
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.17	0.56
15:T:28:DT:H5'	15:T:29:DG:OP2	2.04	0.56
13:M:569:VAL:N	13:M:572:ASP:OD2	2.38	0.56
14:N:36:DA:H2"	14:N:37:DG:OP2	2.04	0.56
9:I:113:ASP:OD1	9:I:114:GLN:N	2.39	0.56
13:M:449:VAL:CG1	15:T:39:DT:H5'	2.36	0.56
2:B:713:ALA:O	2:B:717:GLU:N	2.38	0.56
1:A:870:GLU:OE1	5:E:202:SER:OG	2.21	0.56
1:A:1311:VAL:HG21	1:A:1334:ASP:OD2	2.05	0.56
1:A:60:SER:OG	1:A:61:ILE:N	2.38	0.56
2:B:295:GLY:O	2:B:299:GLU:N	2.36	0.56
1:A:1136:SER:O	1:A:1274:ARG:NE	2.38	0.56
1:A:1445:ILE:O	7:G:58:ARG:CD	2.54	0.56
7:G:99:PHE:O	7:G:110:VAL:N	2.37	0.56
7:G:30:LEU:HD22	7:G:74:TYR:HE2	1.70	0.56
14:N:22:DT:H2'	14:N:23:DC:H1'	1.86	0.56
2:B:21:GLU:N	2:B:21:GLU:OE1	2.39	0.56
2:B:283:VAL:HG11	2:B:321:GLY:HA3	1.88	0.56
2:B:798:TYR:O	2:B:821:GLN:NE2	2.39	0.56
1:A:276:LEU:HD23	1:A:276:LEU:O	2.06	0.55
14:N:34:DG:H2"	14:N:35:DA:H8	1.70	0.55
1:A:55:ASP:O	1:A:57:ARG:N	2.40	0.55
15:T:39:DT:H2"	15:T:40:DC:C6	2.41	0.55
17:O:73:TRP:O	17:O:77:VAL:HG23	2.05	0.55
1:A:672:ASP:OD1	1:A:675:THR:OG1	2.20	0.55
7:G:110:VAL:HG12	7:G:115:MET:SD	2.46	0.55
2:B:564:GLU:OE1	2:B:591:ARG:NH1	2.39	0.55
14:N:15:DA:H3'	14:N:16:DT:C5'	2.37	0.55
14:N:40:DG:H2"	14:N:41:DC:C6	2.41	0.55
2:B:754:SER:OG	2:B:812:LEU:HD11	2.05	0.55
15:T:41:DA:H2"	15:T:42:DA:H8	1.70	0.55
4:D:170:THR:HG21	4:D:210:ILE:HD12	1.88	0.55
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.89	0.55
13:M:476:ASN:OD1	14:N:14:DT:H5'	2.06	0.55
14:N:40:DG:H2"	14:N:41:DC:OP2	2.06	0.55
1:A:65:LEU:HD22	1:A:73:GLY:H	1.71	0.54
13:M:537:GLY:O	13:M:540:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:6:DT:H2"	14:N:7:DG:C8	2.42	0.54
1:A:899:VAL:CG1	1:A:929:LEU:HD22	2.37	0.54
11:K:109:TRP:O	11:K:113:THR:HG23	2.06	0.54
14:N:2:DT:H2"	14:N:3:DA:C8	2.43	0.54
14:N:8:DA:C2'	14:N:9:DT:H71	2.37	0.54
1:A:68:GLN:O	1:A:69:THR:OG1	2.25	0.54
2:B:87:LYS:NZ	2:B:150:GLU:OE1	2.39	0.54
2:B:581:PHE:HB3	2:B:586:TRP:HA	1.90	0.54
4:D:31:GLN:NE2	4:D:34:GLN:OE1	2.40	0.54
1:A:1443:VAL:HG12	1:A:1443:VAL:O	2.07	0.54
4:D:51:ASN:OD1	4:D:52:LEU:N	2.41	0.54
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	0.54
6:F:97:ARG:NE	6:F:124:GLU:OE2	2.40	0.54
14:N:38:DG:H2"	14:N:39:DA:C8	2.43	0.54
13:M:589:LEU:O	13:M:594:ARG:NE	2.41	0.54
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.89	0.54
9:I:113:ASP:OD1	9:I:115:LYS:N	2.34	0.54
13:M:299:ASN:O	13:M:568:ARG:NH1	2.41	0.54
14:N:39:DA:H2"	14:N:40:DG:OP2	2.08	0.53
8:H:105:GLU:HB2	8:H:113:ALA:HB3	1.91	0.53
1:A:1209:MET:SD	1:A:1238:ILE:HD11	2.48	0.53
15:T:36:DA:H2"	15:T:37:DG:O5'	2.08	0.53
2:B:104:GLU:OE2	2:B:120:ARG:NH1	2.38	0.53
2:B:651:LEU:O	2:B:654:ARG:NH1	2.42	0.53
3:C:1:MET:CE	11:K:97:LYS:HD2	2.39	0.53
7:G:57:GLN:O	7:G:58:ARG:HB2	2.09	0.53
7:G:151:ILE:N	7:G:158:HIS:O	2.39	0.53
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.91	0.53
9:I:118:ARG:O	9:I:122:SER:N	2.41	0.53
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.90	0.53
2:B:976:ILE:O	2:B:990:ILE:O	2.27	0.53
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.91	0.53
8:H:64:ASN:O	8:H:89:LEU:HD22	2.08	0.53
9:I:90:GLN:HG3	9:I:95:THR:HG21	1.90	0.53
13:M:449:VAL:HG21	15:T:38:DA:H4'	1.89	0.53
13:M:501:ILE:HG21	13:M:802:ILE:HG21	1.91	0.52
14:N:18:DT:H2"	14:N:19:DC:C5	2.44	0.52
2:B:925:LEU:HD22	2:B:932:HIS:CD2	2.43	0.52
13:M:526:PHE:O	13:M:530:PHE:N	2.42	0.52
1:A:675:THR:HG21	1:A:736:ASN:HB2	1.91	0.52
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.10	0.52
14:N:15:DA:H3'	14:N:16:DT:H5"	1.91	0.52
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.42	0.52
13:M:322:ASP:O	13:M:328:LYS:NZ	2.35	0.52
14:N:19:DC:H2"	14:N:20:DA:C5'	2.39	0.52
13:M:442:HIS:CG	13:M:443:ILE:HD12	2.45	0.52
14:N:39:DA:H2"	14:N:40:DG:H8	1.74	0.52
2:B:511:PRO:O	2:B:512:ARG:HG2	2.09	0.52
14:N:44:DA:H2"	14:N:45:DG:H8	1.75	0.52
7:G:84:GLY:N	7:G:147:ILE:O	2.41	0.52
13:M:504:ASN:OD1	13:M:505:LEU:N	2.43	0.52
1:A:1215:ARG:NH1	1:A:1218:GLN:OE1	2.42	0.52
2:B:359:GLU:OE1	2:B:359:GLU:N	2.41	0.52
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.92	0.52
5:E:78:LEU:HD12	5:E:107:THR:HG23	1.92	0.51
7:G:30:LEU:CD2	7:G:74:TYR:HE2	2.23	0.51
7:G:127:PRO:HB2	7:G:139:ILE:HD12	1.91	0.51
14:N:40:DG:H2"	14:N:41:DC:H6	1.75	0.51
15:T:39:DT:H2"	15:T:40:DC:H6	1.75	0.51
3:C:148:ARG:NH2	10:J:70:ASP:OD2	2.40	0.51
14:N:34:DG:H2"	14:N:35:DA:C8	2.44	0.51
13:M:319:ILE:HB	13:M:515:ILE:HD13	1.91	0.51
13:M:570:LYS:O	13:M:574:ALA:N	2.43	0.51
13:M:644:TYR:HB3	13:M:645:GLY:HA2	1.92	0.51
14:N:14:DT:H1'	14:N:15:DA:N9	2.25	0.51
14:N:36:DA:H2"	14:N:37:DG:H8	1.74	0.51
1:A:1170:ILE:O	1:A:1174:PHE:N	2.42	0.51
2:B:240:ILE:HD12	2:B:381:MET:SD	2.50	0.51
14:N:8:DA:H2"	14:N:9:DT:H71	1.93	0.51
1:A:686:ALA:HB2	1:A:725:ALA:HB2	1.92	0.51
2:B:29:ASP:OD2	2:B:655:LYS:NZ	2.43	0.51
2:B:235:SER:HG	2:B:236:HIS:CE1	2.28	0.51
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.91	0.51
1:A:66:LYS:O	1:A:67:CYS:C	2.48	0.51
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.93	0.51
1:A:672:ASP:OD1	1:A:736:ASN:ND2	2.44	0.51
13:M:360:GLN:O	13:M:364:GLU:OE1	2.29	0.51
15:T:15:DT:H4'	15:T:15:DT:OP1	2.10	0.51
4:D:13:ARG:NH2	4:D:15:LEU:O	2.38	0.51
5:E:6:GLU:N	5:E:6:GLU:OE1	2.42	0.51
15:T:23:DC:C2'	15:T:24:DT:H5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:40:DC:H2”	15:T:41:DA:H8	1.75	0.51
1:A:829:VAL:HG13	2:B:508:LEU:HD13	1.91	0.51
1:A:64:ASN:OD1	1:A:64:ASN:O	2.29	0.50
1:A:997:LEU:HD23	1:A:1053:PHE:CE1	2.46	0.50
2:B:578:THR:HG21	2:B:593:PRO:HB3	1.93	0.50
6:F:110:ASP:OD1	6:F:110:ASP:O	2.29	0.50
13:M:737:VAL:O	13:M:766:ARG:NH2	2.42	0.50
1:A:329:LEU:HD11	2:B:1203:LEU:HD13	1.92	0.50
4:D:56:ARG:NH2	4:D:154:PHE:O	2.44	0.50
13:M:335:PHE:CE2	13:M:339:LEU:HD11	2.46	0.50
13:M:370:PRO:N	13:M:371:PRO:HD2	2.26	0.50
14:N:10:DC:H2”	14:N:11:DT:C6	2.47	0.50
14:N:19:DC:C1’	14:N:20:DA:H5’	2.40	0.50
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.37	0.50
8:H:116:TYR:CB	8:H:123:MET:O	2.59	0.50
3:C:114:TYR:HH	3:C:140:ASN:CG	2.10	0.50
14:N:22:DT:H2’	14:N:23:DC:H4’	1.94	0.50
15:T:34:DT:H5’	15:T:35:DG:OP2	2.11	0.50
13:M:539:TYR:O	13:M:542:ALA:N	2.44	0.50
14:N:46:DC:H2”	14:N:47:DG:H5’	1.93	0.50
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.93	0.50
2:B:975:GLN:O	2:B:990:ILE:HD12	2.12	0.50
13:M:609:ILE:O	13:M:612:GLY:N	2.45	0.50
15:T:15:DT:H2”	15:T:16:DC:C5’	2.27	0.50
1:A:105:CYS:O	1:A:113:LEU:HD23	2.11	0.49
3:C:18:VAL:O	3:C:18:VAL:HG13	2.11	0.49
13:M:680:LEU:HD12	13:M:727:LEU:CD2	2.42	0.49
14:N:21:DT:H3’	14:N:22:DT:C7	2.35	0.49
8:H:63:LEU:HD12	8:H:63:LEU:H	1.77	0.49
15:T:21:DC:C2’	15:T:22:DT:H5’	2.40	0.49
15:T:36:DA:H5’	15:T:36:DA:C8	2.44	0.49
14:N:12:DC:C2’	14:N:13:DA:H5’	2.42	0.49
7:G:27:LYS:HE2	7:G:54:ILE:HD12	1.95	0.49
13:M:672:LEU:HB2	13:M:727:LEU:HD12	1.95	0.49
13:M:701:ARG:NH1	13:M:703:ASP:OD2	2.42	0.49
14:N:38:DG:H2”	14:N:39:DA:OP2	2.13	0.49
1:A:55:ASP:N	1:A:56:PRO:CD	2.75	0.49
3:C:215:GLU:OE1	3:C:215:GLU:N	2.43	0.49
13:M:593:GLN:NE2	13:M:627:CYS:O	2.46	0.49
12:L:53:HIS:CD2	12:L:54:ARG:H	2.30	0.49
11:K:79:GLU:OE1	11:K:79:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:306:GLN:NE2	13:M:310:GLU:OE2	2.42	0.49
1:A:1139:GLU:OE2	1:A:1205:LYS:NZ	2.45	0.49
8:H:63:LEU:HD13	8:H:71:ASN:O	2.12	0.49
14:N:44:DA:H2"	14:N:45:DG:C8	2.48	0.49
2:B:883:LEU:HD21	2:B:932:HIS:CE1	2.48	0.49
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.11	0.49
13:M:631:ASP:OD2	13:M:646:ASP:N	2.44	0.49
1:A:418:SER:OG	1:A:420:ARG:NE	2.38	0.48
1:A:1210:GLY:O	1:A:1214:GLU:OE1	2.31	0.48
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.43	0.48
5:E:66:GLU:OE1	5:E:66:GLU:N	2.45	0.48
1:A:67:CYS:O	1:A:68:GLN:HB3	2.14	0.48
1:A:364:VAL:HG21	1:A:444:PHE:CE2	2.48	0.48
2:B:326:ASP:OD1	2:B:327:ARG:N	2.46	0.48
2:B:818:PRO:HG3	10:J:54:VAL:HG21	1.95	0.48
14:N:41:DC:H2"	14:N:42:DA:H8	1.79	0.48
1:A:336:ILE:HD12	1:A:1405:THR:CG2	2.44	0.48
2:B:681:TRP:NE1	2:B:692:TYR:OH	2.41	0.48
3:C:14:SER:OG	3:C:15:LYS:N	2.46	0.48
4:D:186:ASP:OD1	4:D:187:THR:N	2.47	0.48
14:N:17:DT:H2"	14:N:18:DT:C7	2.42	0.48
14:N:36:DA:H2"	14:N:37:DG:C8	2.48	0.48
7:G:30:LEU:C	7:G:30:LEU:HD23	2.34	0.48
14:N:9:DT:H2"	14:N:10:DC:C5	2.48	0.48
14:N:37:DG:H2"	14:N:38:DG:C8	2.48	0.48
1:A:49:LYS:HE3	1:A:61:ILE:CD1	2.44	0.48
13:M:803:LEU:CD2	13:M:804:THR:HG23	2.43	0.48
15:T:13:DT:H2"	15:T:14:DC:C5'	2.43	0.48
4:D:32:GLU:OE1	4:D:32:GLU:N	2.46	0.48
14:N:14:DT:H1'	14:N:15:DA:C4	2.48	0.48
1:A:67:CYS:HB2	1:A:71:GLN:O	2.14	0.48
5:E:4:GLU:OE1	5:E:4:GLU:N	2.46	0.48
13:M:631:ASP:OD1	13:M:631:ASP:N	2.46	0.48
3:C:1:MET:HE3	11:K:97:LYS:HD2	1.94	0.48
14:N:10:DC:C6	14:N:11:DT:H72	2.48	0.48
15:T:38:DA:H2'	15:T:39:DT:H72	1.95	0.48
1:A:175:ARG:HH22	14:N:38:DG:H5"	1.78	0.48
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.96	0.48
1:A:353:ILE:CG2	1:A:487:MET:HG3	2.44	0.47
1:A:354:SER:OG	1:A:469:ARG:NH1	2.47	0.47
1:A:964:ILE:HG21	1:A:1035:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ASN:HA	7:G:70:PHE:O	2.14	0.47
11:K:43:GLY:HA3	11:K:71:PHE:CE1	2.49	0.47
13:M:452:ARG:HD2	13:M:481:ILE:HD13	1.96	0.47
1:A:611:GLN:O	1:A:613:ILE:HG12	2.15	0.47
3:C:114:TYR:HB3	3:C:143:LEU:HA	1.96	0.47
1:A:399:HIS:CG	1:A:400:PRO:HD3	2.49	0.47
13:M:524:PRO:O	13:M:528:GLN:OE1	2.31	0.47
14:N:27:DC:H2"	14:N:28:DT:O4'	2.14	0.47
14:N:28:DT:H2'	14:N:29:DC:C6	2.50	0.47
14:N:37:DG:H2"	14:N:38:DG:H8	1.80	0.47
1:A:613:ILE:CG2	8:H:102:TYR:HE1	2.27	0.47
1:A:1217:LYS:O	1:A:1221:LYS:N	2.47	0.47
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.45	0.47
13:M:538:GLY:O	13:M:550:GLY:N	2.47	0.47
1:A:66:LYS:O	1:A:69:THR:CA	2.61	0.47
1:A:175:ARG:NH2	14:N:38:DG:H5"	2.30	0.47
2:B:904:ARG:NH2	12:L:66:GLN:O	2.47	0.47
14:N:4:DG:H2'	14:N:5:DT:H72	1.95	0.47
14:N:11:DT:H2"	14:N:12:DC:OP2	2.11	0.47
14:N:24:DC:H2"	14:N:25:DT:C7	2.45	0.47
1:A:385:ILE:HD11	1:A:428:TYR:CE1	2.50	0.47
1:A:739:ASP:OD2	8:H:19:ARG:NH1	2.46	0.47
1:A:1092:LYS:NZ	1:A:1285:MET:SD	2.85	0.47
7:G:58:ARG:NH1	7:G:70:PHE:CE1	2.82	0.47
7:G:113:HIS:O	7:G:164:LYS:NZ	2.39	0.47
15:T:6:DT:H2"	15:T:7:DG:N7	2.29	0.47
15:T:13:DT:H4'	15:T:13:DT:OP1	2.13	0.47
1:A:246:VAL:O	1:A:328:ARG:NH2	2.43	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:OE1	2.40	0.47
1:A:67:CYS:CB	1:A:71:GLN:O	2.63	0.47
2:B:82:ASP:O	2:B:147:LEU:HD13	2.14	0.47
2:B:223:VAL:O	2:B:384:ARG:NH1	2.48	0.47
4:D:141:LEU:HD11	7:G:35:GLU:HG3	1.97	0.47
1:A:434:ARG:NH1	1:A:435:HIS:O	2.48	0.47
1:A:1134:ILE:HG23	1:A:1322:ILE:HD11	1.96	0.47
2:B:853:SER:OG	2:B:1094:ARG:NH1	2.48	0.47
10:J:64:ASN:ND2	10:J:70:ASP:OD1	2.48	0.47
13:M:737:VAL:O	13:M:766:ARG:NE	2.45	0.47
14:N:33:DA:H2"	14:N:34:DG:H8	1.80	0.47
15:T:45:DA:H2"	15:T:46:DG:C8	2.50	0.47
1:A:614:PHE:CD1	8:H:122:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:101:ALA:HA	8:H:115:TYR:HB3	1.97	0.46
14:N:22:DT:H71	14:N:22:DT:OP2	2.15	0.46
15:T:14:DC:H2"	15:T:15:DT:O5'	2.14	0.46
1:A:247:ARG:O	1:A:247:ARG:HG3	2.15	0.46
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.96	0.46
8:H:128:ASN:OD1	8:H:130:ARG:HD3	2.14	0.46
14:N:22:DT:H2'	14:N:23:DC:C4'	2.45	0.46
14:N:24:DC:H4'	14:N:25:DT:N1	2.30	0.46
1:A:1049:ILE:O	1:A:1053:PHE:CD1	2.69	0.46
13:M:789:TYR:CE2	13:M:793:ILE:HD11	2.50	0.46
14:N:47:DG:H5'	14:N:47:DG:H8	1.79	0.46
16:R:2:U:H2'	16:R:3:C:C6	2.50	0.46
2:B:433:GLN:NE2	14:N:21:DT:O5'	2.49	0.46
11:K:20:LYS:NZ	11:K:36:GLU:OE2	2.46	0.46
14:N:39:DA:H2"	14:N:40:DG:C8	2.51	0.46
1:A:352:VAL:HG12	1:A:353:ILE:N	2.30	0.46
1:A:1051:ALA:O	1:A:1055:ARG:HD3	2.16	0.46
8:H:101:ALA:HB1	8:H:115:TYR:CG	2.50	0.46
11:K:19:LEU:HD22	11:K:35:PHE:CD1	2.51	0.46
2:B:134:LYS:HE3	2:B:439:ALA:HB1	1.97	0.46
14:N:5:DT:H2"	14:N:6:DT:C6	2.51	0.46
2:B:773:MET:HE3	2:B:1095:LEU:HD11	1.97	0.46
3:C:113:VAL:HG21	3:C:147:LEU:HD11	1.98	0.46
4:D:120:GLU:OE1	4:D:155:ARG:NH1	2.49	0.46
7:G:54:ILE:HG23	7:G:74:TYR:CE1	2.50	0.46
11:K:49:GLU:HG3	11:K:90:ALA:HB1	1.96	0.46
15:T:5:DC:OP2	15:T:5:DC:H6	1.98	0.46
2:B:708:GLU:OE1	2:B:708:GLU:N	2.44	0.46
3:C:183:TRP:O	3:C:185:LYS:N	2.48	0.46
8:H:114:VAL:O	8:H:116:TYR:HD1	1.99	0.46
13:M:509:TRP:NE1	13:M:521:GLY:O	2.44	0.46
14:N:17:DT:C2'	14:N:18:DT:H72	2.46	0.46
14:N:27:DC:H6	14:N:27:DC:H2'	1.61	0.46
15:T:3:DC:C2'	15:T:4:DT:H71	2.45	0.46
1:A:1450:LEU:HD22	7:G:58:ARG:HG3	1.98	0.46
4:D:166:LEU:HD22	4:D:213:GLU:HG2	1.97	0.46
15:T:7:DG:H2"	15:T:8:DC:OP2	2.16	0.46
13:M:448:TYR:OH	13:M:470:GLU:N	2.44	0.46
13:M:628:ASN:HB3	13:M:679:MET:SD	2.56	0.46
2:B:869:SER:OG	13:M:633:LEU:O	2.29	0.45
7:G:96:GLN:O	7:G:112:LYS:NZ	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:92:ARG:O	9:I:95:THR:HG23	2.16	0.45
14:N:31:DG:H22	15:T:17:DC:N4	2.14	0.45
1:A:107:CYS:SG	1:A:167:CYS:SG	3.14	0.45
1:A:329:LEU:CD1	2:B:1203:LEU:HD13	2.46	0.45
5:E:127:ILE:O	5:E:127:ILE:HG13	2.17	0.45
13:M:582:GLU:OE2	13:M:777:ARG:NH1	2.48	0.45
14:N:27:DC:C2'	14:N:28:DT:H5"	2.43	0.45
15:T:42:DA:OP2	15:T:42:DA:H2'	2.16	0.45
2:B:340:ALA:O	2:B:348:ARG:NH1	2.49	0.45
7:G:10:ASN:OD1	7:G:71:ASN:ND2	2.44	0.45
15:T:18:TTD:H2"	15:T:18:TTD:H6	1.18	0.45
1:A:1445:ILE:O	1:A:1449:SER:HB3	2.17	0.45
2:B:394:ASP:OD1	2:B:395:GLN:N	2.49	0.45
2:B:621:GLU:OE2	2:B:621:GLU:HA	2.16	0.45
2:B:726:ALA:HB1	2:B:1053:GLU:OE1	2.15	0.45
4:D:8:PHE:O	4:D:8:PHE:CG	2.70	0.45
13:M:214:GLU:OE1	13:M:250:ARG:NH2	2.43	0.45
13:M:375:VAL:HG13	13:M:444:LEU:HD12	1.98	0.45
8:H:83:GLN:OE1	11:K:54:ARG:NE	2.50	0.45
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.15	0.45
2:B:233:PRO:O	2:B:260:GLY:N	2.48	0.45
4:D:25:ALA:HB2	7:G:85:GLU:HB2	1.99	0.45
9:I:47:GLU:HG2	9:I:50:THR:HG22	1.97	0.45
15:T:23:DC:H2"	15:T:24:DT:H5'	1.98	0.45
17:O:75:ASP:HA	17:O:78:GLU:OE1	2.16	0.45
1:A:698:GLN:O	9:I:112:SER:OG	2.34	0.45
5:E:117:THR:CG2	14:N:44:DA:H5"	2.47	0.45
8:H:63:LEU:HD23	8:H:74:SER:HB2	1.98	0.45
8:H:88:SER:O	8:H:89:LEU:HD23	2.16	0.45
11:K:49:GLU:HG3	11:K:90:ALA:CB	2.47	0.45
14:N:22:DT:H2'	14:N:23:DC:C1'	2.46	0.45
1:A:1114:PRO:HB2	1:A:1311:VAL:HG13	1.98	0.45
2:B:63:ILE:HG13	2:B:95:ILE:HD12	1.99	0.45
2:B:889:THR:HG22	2:B:891:ASP:H	1.82	0.45
3:C:33:LEU:O	3:C:37:MET:HG3	2.17	0.45
8:H:96:VAL:HG13	8:H:143:LEU:HD23	1.99	0.45
13:M:597:TYR:OH	13:M:623:LEU:HD23	2.17	0.45
4:D:51:ASN:O	4:D:55:ALA:N	2.40	0.45
8:H:48:PRO:O	8:H:146:ARG:NH1	2.41	0.45
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.99	0.44
5:E:180:ARG:HB3	5:E:180:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:91:VAL:HG13	7:G:99:PHE:CE2	2.51	0.44
13:M:382:SER:OG	13:M:383:GLY:N	2.46	0.44
13:M:457:LYS:O	13:M:460:LYS:N	2.41	0.44
14:N:11:DT:H2"	14:N:12:DC:C6	2.52	0.44
1:A:1191:TRP:HH2	9:I:25:LEU:HD13	1.83	0.44
9:I:15:TYR:HB2	9:I:17:ARG:NH1	2.32	0.44
1:A:22:PHE:HB3	1:A:27:VAL:CG2	2.48	0.44
1:A:1454:MET:O	1:A:1454:MET:HG2	2.18	0.44
7:G:165:GLU:N	7:G:165:GLU:OE1	2.50	0.44
11:K:81:TYR:OH	11:K:89:ASN:ND2	2.45	0.44
14:N:15:DA:H5'	14:N:16:DT:H2'	2.00	0.44
15:T:8:DC:H6	15:T:8:DC:OP2	2.01	0.44
1:A:1445:ILE:O	1:A:1445:ILE:HG12	2.17	0.44
2:B:315:LYS:HB2	2:B:316:PRO:HD3	1.99	0.44
7:G:39:THR:O	7:G:43:GLY:N	2.50	0.44
1:A:784:LEU:HD12	1:A:785:PRO:HD2	2.00	0.44
2:B:574:SER:OG	2:B:591:ARG:NH2	2.50	0.44
2:B:905:VAL:CG2	2:B:941:LEU:HD11	2.48	0.44
14:N:32:DG:H2"	14:N:33:DA:OP2	2.18	0.44
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.42	0.44
1:A:567:LYS:HB3	1:A:568:PRO:HD3	2.00	0.44
1:A:686:ALA:CB	1:A:725:ALA:HB2	2.46	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.99	0.44
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.47	0.44
4:D:166:LEU:HD21	4:D:210:ILE:HG13	2.00	0.44
8:H:19:ARG:CG	8:H:19:ARG:O	2.65	0.44
8:H:92:ASP:OD1	8:H:92:ASP:N	2.49	0.44
14:N:8:DA:H2'	14:N:9:DT:H71	1.98	0.44
14:N:21:DT:H5'	14:N:22:DT:OP1	2.18	0.44
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.98	0.44
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.17	0.44
6:F:112:GLU:OE2	6:F:112:GLU:HA	2.18	0.44
13:M:675:GLN:NE2	13:M:751:ASP:OD1	2.50	0.44
14:N:33:DA:OP2	14:N:33:DA:H8	2.01	0.44
15:T:20:DC:H2"	15:T:21:DC:H5'	1.99	0.44
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.99	0.44
1:A:105:CYS:SG	1:A:139:TRP:HA	2.58	0.44
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.43	0.44
3:C:3:GLU:O	3:C:5:GLY:N	2.49	0.43
1:A:175:ARG:HH12	14:N:38:DG:H5"	1.83	0.43
1:A:718:VAL:HG11	1:A:774:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:LEU:HD13	8:H:61:SER:H	1.84	0.43
1:A:56:PRO:C	1:A:57:ARG:HE	2.21	0.43
2:B:841:MET:HE3	2:B:1010:LEU:HD21	1.97	0.43
7:G:26:LEU:HD11	7:G:70:PHE:CE2	2.53	0.43
8:H:101:ALA:CB	8:H:115:TYR:HB3	2.48	0.43
15:T:32:DT:OP1	15:T:32:DT:H4'	2.17	0.43
1:A:254:GLU:OE2	2:B:935:ARG:NH1	2.51	0.43
1:A:344:ARG:NH2	2:B:1120:GLU:OE1	2.51	0.43
8:H:96:VAL:HG22	8:H:143:LEU:HD23	2.00	0.43
8:H:112:ILE:HD12	8:H:129:TYR:O	2.19	0.43
9:I:72:ASP:C	9:I:72:ASP:OD2	2.57	0.43
13:M:360:GLN:O	13:M:363:ASN:N	2.51	0.43
15:T:1:DC:H2"	15:T:2:DG:C8	2.53	0.43
1:A:1191:TRP:NE1	1:A:1255:GLU:O	2.51	0.43
4:D:49:ALA:HB1	4:D:178:ALA:HB2	2.00	0.43
12:L:28:LYS:HA	12:L:59:ALA:CB	2.47	0.43
1:A:32:VAL:HG22	1:A:32:VAL:O	2.18	0.43
1:A:152:VAL:HG21	1:A:164:ARG:HE	1.84	0.43
1:A:364:VAL:HG23	1:A:470:LEU:HD23	1.99	0.43
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.34	0.43
1:A:1211:GLN:HA	1:A:1214:GLU:OE1	2.18	0.43
1:A:1449:SER:OG	6:F:131:PRO:O	2.35	0.43
2:B:510:LYS:N	2:B:511:PRO:HD2	2.34	0.43
13:M:381:GLY:O	13:M:382:SER:C	2.57	0.43
1:A:513:SER:HB3	1:A:520:CYS:SG	2.58	0.43
2:B:863:GLU:HG2	2:B:872:GLU:O	2.18	0.43
8:H:114:VAL:O	8:H:116:TYR:CD1	2.72	0.43
13:M:803:LEU:HD23	13:M:804:THR:HG23	2.00	0.43
14:N:30:DA:H2"	14:N:31:DG:O4'	2.19	0.43
15:T:31:DC:H4'	15:T:32:DT:H4'	2.01	0.43
2:B:249:ARG:O	2:B:251:ILE:N	2.51	0.43
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.18	0.43
8:H:57:VAL:HG13	8:H:142:LEU:HD11	2.00	0.43
14:N:20:DA:H1'	14:N:21:DT:N1	2.33	0.43
17:O:26:LEU:C	17:O:28:CYS:H	2.22	0.43
1:A:311:GLN:N	1:A:312:PRO:CD	2.82	0.43
7:G:30:LEU:HD23	7:G:30:LEU:O	2.19	0.43
7:G:73:LYS:O	7:G:74:TYR:CD1	2.72	0.43
7:G:86:VAL:HG22	7:G:146:LYS:HD3	2.01	0.43
10:J:7:CYS:N	10:J:12:LYS:O	2.47	0.43
14:N:42:DA:H2"	14:N:43:DG:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:N	1:A:149:GLU:OE1	2.52	0.42
1:A:829:VAL:HG22	2:B:508:LEU:HD22	2.00	0.42
1:A:1035:TYR:O	1:A:1037:LEU:N	2.51	0.42
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.00	0.42
3:C:1:MET:HG3	11:K:49:GLU:OE1	2.19	0.42
8:H:1:MET:CE	8:H:90:ALA:HB2	2.49	0.42
12:L:32:ALA:O	12:L:33:GLU:HG2	2.19	0.42
13:M:495:ILE:HG22	13:M:497:SER:H	1.83	0.42
1:A:446:ARG:HB2	1:A:487:MET:SD	2.59	0.42
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.54	0.42
2:B:936:ASP:OD1	2:B:937:ALA:N	2.52	0.42
14:N:46:DC:H2"	14:N:47:DG:C8	2.54	0.42
17:O:25:CYS:HB3	17:O:30:HIS:N	2.34	0.42
1:A:42:ASP:O	1:A:45:GLN:HA	2.19	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.19	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HH11	1.84	0.42
2:B:108:VAL:HG13	2:B:108:VAL:O	2.18	0.42
2:B:848:ARG:NH1	10:J:8:PHE:O	2.52	0.42
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.59	0.42
15:T:38:DA:H2"	15:T:39:DT:C6	2.54	0.42
1:A:683:ILE:O	1:A:687:LYS:HG2	2.19	0.42
1:A:1277:GLU:HG3	1:A:1278:ASN:OD1	2.20	0.42
1:A:1297:GLU:OE2	1:A:1297:GLU:HA	2.20	0.42
8:H:130:ARG:HH11	8:H:131:ASN:H	1.66	0.42
14:N:11:DT:H3	15:T:36:DA:H61	1.66	0.42
15:T:29:DG:H1'	15:T:30:DG:P	2.60	0.42
1:A:485:ASP:OD1	16:R:10:A:O3'	2.35	0.42
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	2.02	0.42
2:B:114:PRO:HB3	2:B:174:LEU:HD21	2.01	0.42
2:B:187:SER:HA	2:B:190:TYR:CE1	2.55	0.42
2:B:282:ILE:HG13	2:B:283:VAL:N	2.35	0.42
13:M:524:PRO:O	13:M:525:VAL:C	2.58	0.42
14:N:5:DT:H2'	14:N:6:DT:H72	2.01	0.42
15:T:32:DT:H2"	15:T:33:DA:O5'	2.19	0.42
1:A:175:ARG:NH1	14:N:38:DG:H5"	2.33	0.42
13:M:339:LEU:O	13:M:345:LEU:N	2.50	0.42
1:A:70:CYS:HB3	1:A:71:GLN:OE1	2.20	0.42
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.19	0.42
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.50	0.42
9:I:100:PHE:CD2	9:I:111:THR:HG22	2.55	0.42
1:A:206:GLU:O	1:A:210:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:GLU:OE2	1:A:1326:ARG:NH1	2.44	0.42
7:G:11:ILE:HD11	7:G:30:LEU:HD12	2.02	0.42
11:K:18:LYS:O	11:K:19:LEU:HD23	2.20	0.42
13:M:600:PHE:O	13:M:604:SER:N	2.53	0.42
13:M:718:PHE:HA	13:M:721:GLU:HB3	2.02	0.42
1:A:107:CYS:O	1:A:108:MET:HB2	2.20	0.42
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.42
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.19	0.42
1:A:1446:ASP:C	7:G:58:ARG:HD2	2.40	0.42
4:D:166:LEU:HD22	4:D:213:GLU:CG	2.49	0.42
9:I:69:PRO:O	9:I:84:VAL:HG23	2.19	0.42
12:L:46:VAL:HG12	12:L:46:VAL:O	2.17	0.42
13:M:269:PRO:HA	13:M:272:ARG:HD3	2.02	0.42
1:A:63:ARG:NE	1:A:63:ARG:HA	2.35	0.42
1:A:445:ASN:HA	1:A:454:SER:O	2.20	0.42
1:A:662:PHE:O	2:B:829:CYS:N	2.49	0.42
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.83	0.42
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.00	0.42
10:J:5:VAL:HG12	10:J:6:ARG:HG2	2.01	0.42
12:L:40:LEU:HD11	12:L:56:LEU:CD2	2.50	0.42
14:N:12:DC:H6	14:N:12:DC:H2'	1.75	0.42
14:N:15:DA:H5'	14:N:16:DT:H5"	2.01	0.42
1:A:846:GLU:OE2	1:A:1425:SER:OG	2.37	0.41
2:B:441:ASP:OD1	2:B:441:ASP:O	2.38	0.41
15:T:26:DG:H1'	15:T:27:DA:C8	2.54	0.41
1:A:837:ILE:HD11	1:A:1102:LYS:HG3	2.02	0.41
3:C:181:ASP:OD2	3:C:185:LYS:N	2.53	0.41
8:H:96:VAL:HG12	8:H:97:MET:N	2.35	0.41
13:M:293:ILE:O	13:M:297:LEU:N	2.47	0.41
13:M:739:LEU:HD12	13:M:763:ARG:HB3	2.00	0.41
17:O:80:VAL:O	17:O:80:VAL:HG12	2.19	0.41
1:A:61:ILE:C	1:A:74:MET:HE3	2.41	0.41
1:A:107:CYS:HB2	1:A:110:CYS:H	1.84	0.41
1:A:974:ASP:OD2	8:H:136:LYS:NZ	2.53	0.41
2:B:59:LEU:O	2:B:63:ILE:HG12	2.20	0.41
13:M:251:LEU:HD11	13:M:255:VAL:HG12	2.02	0.41
13:M:376:ILE:O	13:M:380:MET:HB3	2.19	0.41
13:M:551:TYR:O	13:M:552:LYS:HB2	2.20	0.41
14:N:42:DA:H2"	14:N:43:DG:H8	1.80	0.41
15:T:9:DT:H2"	15:T:10:DC:O5'	2.21	0.41
17:O:65:GLN:HB3	17:O:66:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG21	1:A:176:LYS:HE2	2.02	0.41
1:A:138:ILE:O	1:A:142:CYS:SG	2.78	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.54	0.41
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.53	0.41
2:B:261:ARG:O	2:B:266:ALA:HB3	2.21	0.41
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.41
4:D:59:ILE:HG21	4:D:145:MET:SD	2.60	0.41
15:T:4:DT:H2"	15:T:5:DC:OP2	2.20	0.41
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	2.02	0.41
1:A:407:ARG:NE	1:A:413:ILE:HD11	2.36	0.41
1:A:1453:TYR:OH	7:G:18:PHE:HB3	2.20	0.41
2:B:827:ILE:HD13	2:B:1017:ILE:HD11	2.02	0.41
3:C:146:LYS:HB2	10:J:61:LEU:HD11	2.02	0.41
13:M:533:PRO:O	13:M:535:ASN:N	2.53	0.41
13:M:731:ARG:NH2	15:T:35:DG:O3'	2.53	0.41
1:A:23:SER:O	1:A:26:GLU:N	2.54	0.41
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.41
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.56	0.41
7:G:87:VAL:HG11	7:G:103:VAL:CG2	2.50	0.41
14:N:11:DT:H3	15:T:36:DA:N6	2.19	0.41
14:N:16:DT:H1'	14:N:17:DT:O4'	2.20	0.41
1:A:42:ASP:HA	1:A:48:ALA:O	2.21	0.41
1:A:381:THR:HB	1:A:382:PRO:HD2	2.03	0.41
2:B:476:ARG:O	2:B:477:ALA:C	2.59	0.41
3:C:113:VAL:CG2	3:C:147:LEU:HD11	2.51	0.41
6:F:85:MET:CE	6:F:153:VAL:HG22	2.51	0.41
14:N:8:DA:H2"	14:N:9:DT:C6	2.56	0.41
1:A:157:ASP:OD1	1:A:159:THR:OG1	2.31	0.41
1:A:244:PRO:N	1:A:245:PRO:CD	2.84	0.41
1:A:455:MET:O	2:B:1141:HIS:NE2	2.49	0.41
1:A:1450:LEU:HD13	7:G:22:MET:HE1	2.01	0.41
3:C:258:ILE:CG1	11:K:42:LEU:HD21	2.51	0.41
5:E:78:LEU:CD1	5:E:107:THR:HG23	2.51	0.41
7:G:88:ASP:OD1	7:G:88:ASP:N	2.46	0.41
11:K:61:TYR:HB2	11:K:71:PHE:CE1	2.56	0.41
12:L:46:VAL:O	12:L:56:LEU:HD22	2.21	0.41
14:N:10:DC:OP2	14:N:10:DC:H6	2.02	0.41
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	2.02	0.41
2:B:77:HIS:O	2:B:84:ILE:N	2.54	0.41
2:B:145:ARG:NH2	2:B:149:TYR:OH	2.49	0.41
2:B:336:ARG:HD2	17:O:68:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:42:DA:H2"	15:T:43:DC:H6	1.83	0.41
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.86	0.41
6:F:136:ARG:O	6:F:143:PHE:HA	2.21	0.41
7:G:146:LYS:O	7:G:162:SER:N	2.55	0.41
13:M:633:LEU:O	13:M:633:LEU:HD23	2.21	0.41
1:A:1450:LEU:HA	1:A:1453:TYR:HB2	2.02	0.40
4:D:5:THR:HG22	4:D:7:THR:HG23	2.02	0.40
8:H:100:THR:OG1	8:H:101:ALA:N	2.51	0.40
13:M:248:GLN:O	13:M:384:MET:SD	2.79	0.40
13:M:475:ARG:NH2	13:M:499:THR:OG1	2.50	0.40
13:M:523:LEU:HB2	13:M:524:PRO:HD3	2.03	0.40
13:M:692:PRO:O	13:M:696:HIS:ND1	2.54	0.40
2:B:564:GLU:OE1	2:B:591:ARG:NH2	2.50	0.40
2:B:581:PHE:CB	2:B:586:TRP:HA	2.51	0.40
2:B:830:TYR:O	2:B:832:GLY:N	2.53	0.40
3:C:105:GLY:O	3:C:149:LYS:O	2.39	0.40
12:L:38:LEU:HD11	12:L:49:LYS:H	1.86	0.40
13:M:515:ILE:HG13	13:M:516:PHE:N	2.37	0.40
1:A:390:GLN:OE1	1:A:390:GLN:HA	2.21	0.40
1:A:1407:GLU:OE1	1:A:1407:GLU:N	2.46	0.40
2:B:249:ARG:O	2:B:250:PHE:C	2.59	0.40
2:B:879:ARG:CZ	2:B:885:MET:CE	3.00	0.40
14:N:28:DT:C3'	14:N:29:DC:H5'	2.52	0.40
16:R:7:A:H2'	16:R:8:G:O4'	2.22	0.40
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.51	0.40
1:A:826:ASP:O	1:A:830:LYS:HG2	2.22	0.40
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.54	0.40
13:M:587:CYS:SG	13:M:588:LYS:N	2.95	0.40
13:M:703:ASP:OD1	13:M:706:THR:N	2.55	0.40
13:M:731:ARG:HB3	15:T:36:DA:H4'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1446/1733 (83%)	1336 (92%)	109 (8%)	1 (0%)	51 83
2	B	1205/1224 (98%)	1112 (92%)	92 (8%)	1 (0%)	51 83
3	C	268/318 (84%)	251 (94%)	17 (6%)	0	100 100
4	D	163/221 (74%)	149 (91%)	14 (9%)	0	100 100
5	E	213/215 (99%)	210 (99%)	3 (1%)	0	100 100
6	F	79/155 (51%)	75 (95%)	4 (5%)	0	100 100
7	G	169/171 (99%)	161 (95%)	8 (5%)	0	100 100
8	H	144/146 (99%)	119 (83%)	25 (17%)	0	100 100
9	I	120/122 (98%)	110 (92%)	10 (8%)	0	100 100
10	J	68/70 (97%)	62 (91%)	6 (9%)	0	100 100
11	K	118/120 (98%)	115 (98%)	3 (2%)	0	100 100
12	L	44/70 (63%)	33 (75%)	11 (25%)	0	100 100
13	M	554/1085 (51%)	499 (90%)	54 (10%)	1 (0%)	47 79
17	O	69/85 (81%)	59 (86%)	10 (14%)	0	100 100
All	All	4660/5735 (81%)	4291 (92%)	366 (8%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	382	SER
1	A	67	CYS
2	B	1021	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1264/1520 (83%)	1263 (100%)	1 (0%)	93 98
2	B	1046/1061 (99%)	1046 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	238/274 (87%)	238 (100%)	0	100 100
4	D	150/200 (75%)	150 (100%)	0	100 100
5	E	197/197 (100%)	196 (100%)	1 (0%)	88 94
6	F	72/137 (53%)	72 (100%)	0	100 100
7	G	152/152 (100%)	151 (99%)	1 (1%)	84 93
8	H	128/128 (100%)	127 (99%)	1 (1%)	81 92
9	I	116/116 (100%)	115 (99%)	1 (1%)	78 91
10	J	65/65 (100%)	65 (100%)	0	100 100
11	K	102/102 (100%)	102 (100%)	0	100 100
12	L	40/57 (70%)	40 (100%)	0	100 100
13	M	504/978 (52%)	503 (100%)	1 (0%)	93 97
17	O	66/79 (84%)	66 (100%)	0	100 100
All	All	4140/5066 (82%)	4134 (100%)	6 (0%)	93 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
5	E	7	ARG
7	G	58	ARG
8	H	130	ARG
9	I	17	ARG
13	M	457	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	517	ASN
1	A	736	ASN
1	A	1364	ASN
2	B	110	HIS
2	B	932	HIS
13	M	313	GLN
13	M	367	HIS
13	M	610	GLN
13	M	615	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	R	9/10 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	TTD	T	18	15	42,45,46	1.27	5 (11%)	62,74,77	2.12	14 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TTD	T	18	15	-	11/22/109/110	0/5/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	18	TTD	C4T-N3T	-3.09	1.32	1.37
15	T	18	TTD	C2T-N1T	2.99	1.42	1.36
15	T	18	TTD	C2T-N3T	-2.88	1.32	1.38
15	T	18	TTD	C2-N3	-2.87	1.32	1.38
15	T	18	TTD	C4-N3	-2.69	1.33	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	18	TTD	C2'-C1'-N1	-9.73	102.44	115.59
15	T	18	TTD	C4-N3-C2	-4.89	119.16	126.67
15	T	18	TTD	C4T-N3T-C2T	-4.66	119.50	126.67
15	T	18	TTD	N3T-C2T-N1T	4.42	121.28	116.69
15	T	18	TTD	O4R-C1R-N1T	4.26	113.70	108.65
15	T	18	TTD	O2T-C2T-N1T	-3.65	117.83	123.49
15	T	18	TTD	C2R-C1R-N1T	-3.01	111.52	115.59
15	T	18	TTD	O4-C4-C5	-2.93	120.54	122.88
15	T	18	TTD	O4'-C1'-N1	2.72	111.88	108.65
15	T	18	TTD	C5-C5T-C6T	2.38	91.34	88.38
15	T	18	TTD	O4T-C4T-C5T	-2.19	121.12	122.88
15	T	18	TTD	C5'-C4R-C3R	-2.12	109.68	114.53
15	T	18	TTD	C6T-C6-N1	-2.06	109.97	118.20
15	T	18	TTD	C3R-C2'-C1'	2.00	106.74	102.91

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	18	TTD	C5R-O5R-PB-O4P
15	T	18	TTD	O4'-C4R-C5'-O5'
15	T	18	TTD	O4R-C4'-C5R-O5R
15	T	18	TTD	C3R-C4R-C5'-O5'
15	T	18	TTD	C3'-C4'-C5R-O5R
15	T	18	TTD	C2'-C1'-N1-C6
15	T	18	TTD	O4'-C1'-N1-C2
15	T	18	TTD	C2'-C1'-N1-C2
15	T	18	TTD	C5R-O5R-PB-O3R
15	T	18	TTD	O4'-C1'-N1-C6
15	T	18	TTD	C5R-O5R-PB-O5P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	18	TTD	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

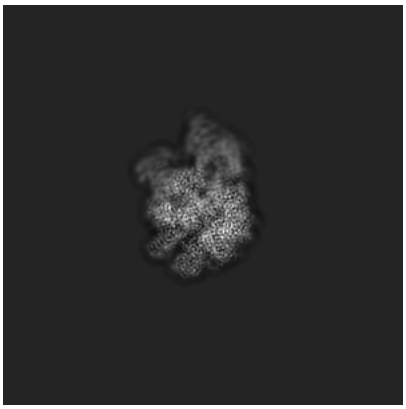
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41655. These allow visual inspection of the internal detail of the map and identification of artifacts.

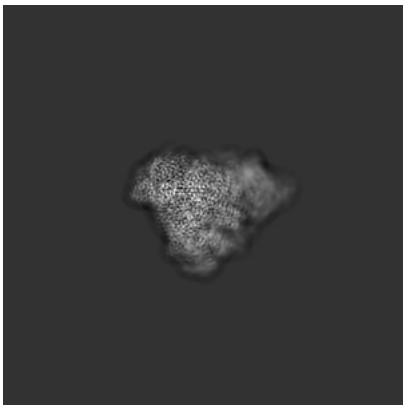
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

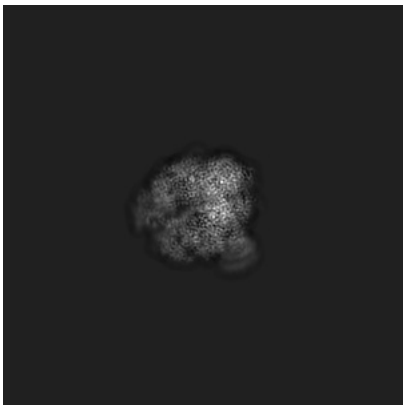
6.1.1 Primary map



X

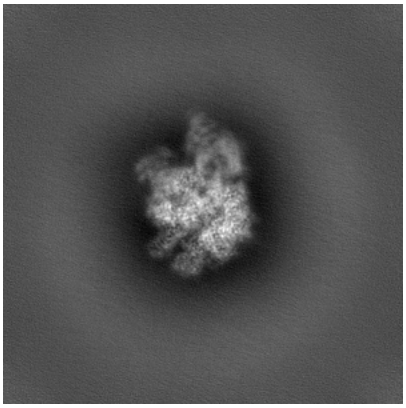


Y

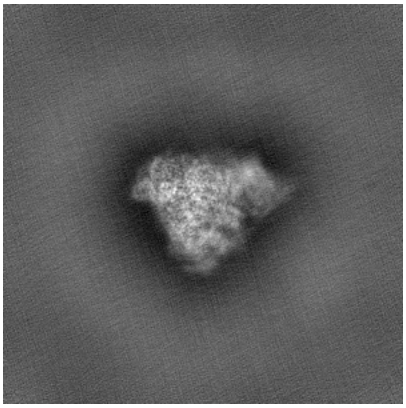


Z

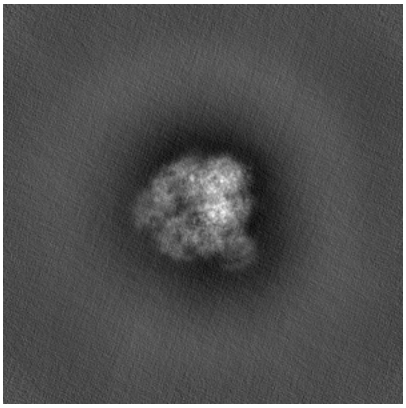
6.1.2 Raw map



X



Y



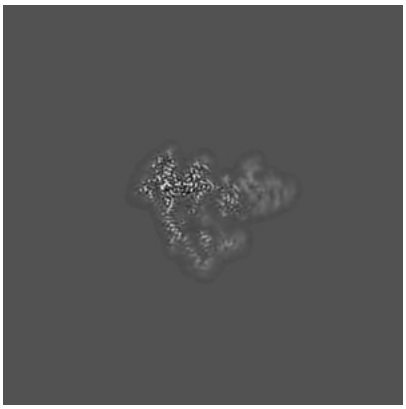
Z

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

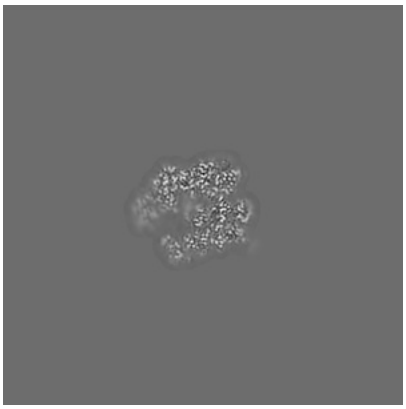
6.2 Central slices (i)

6.2.1 Primary map

X Index: 192

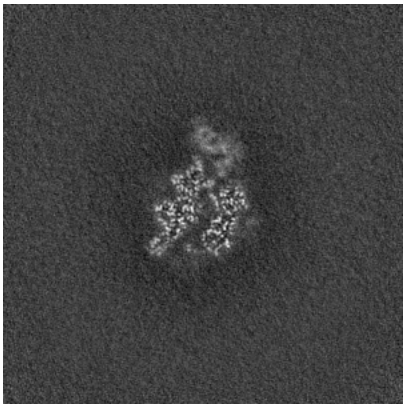


Y Index: 192

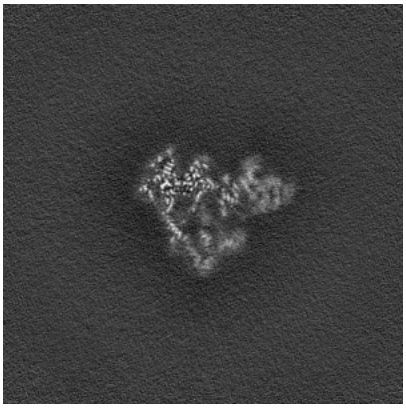


Z Index: 192

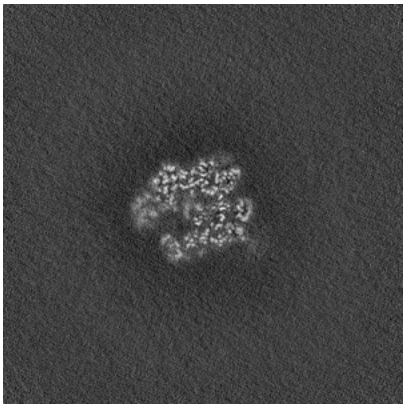
6.2.2 Raw map



X Index: 192



Y Index: 192



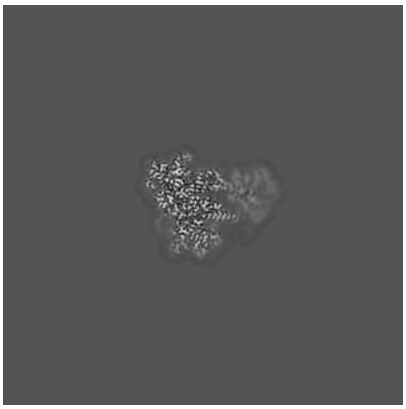
Z Index: 192

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

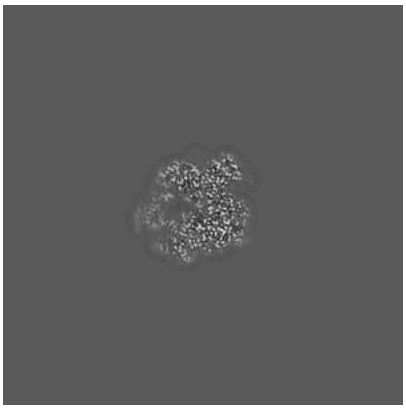
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 209

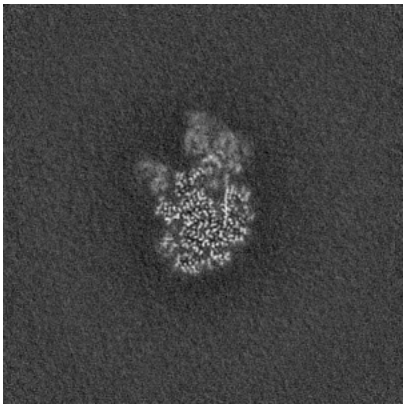


Y Index: 215

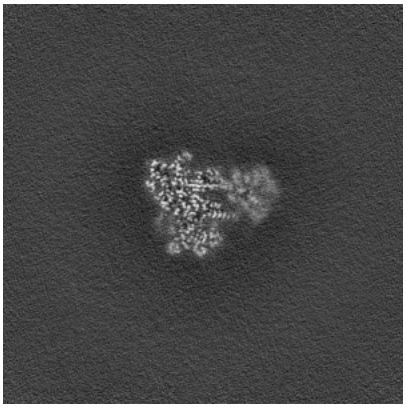


Z Index: 182

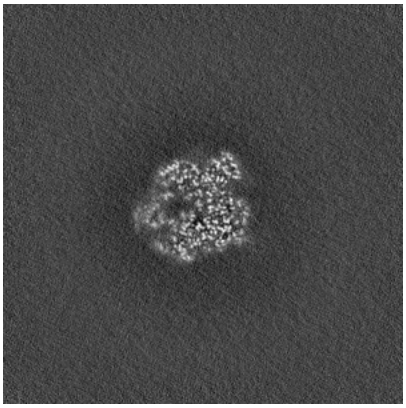
6.3.2 Raw map



X Index: 209



Y Index: 214

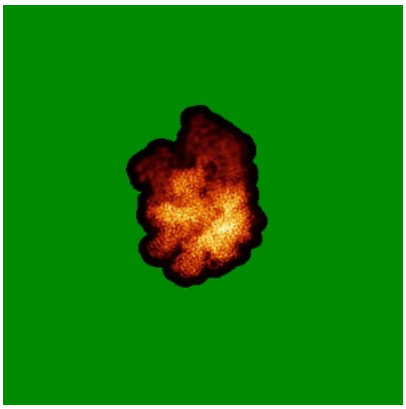


Z Index: 182

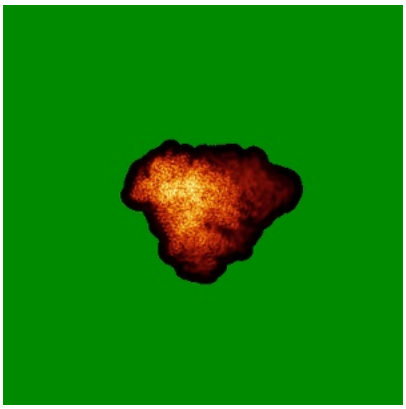
The images above show the largest variance slices of the map in three orthogonal directions.

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

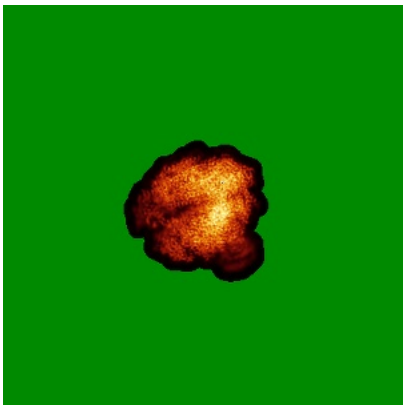
6.4.1 Primary map



X

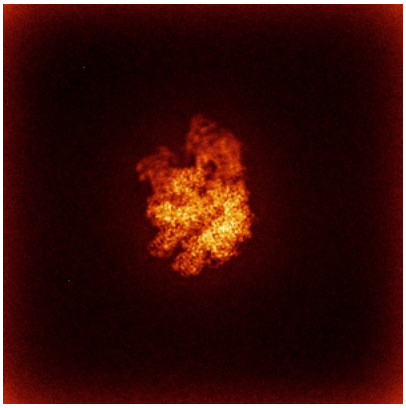


Y

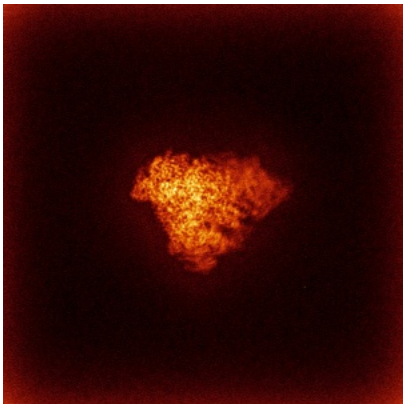


Z

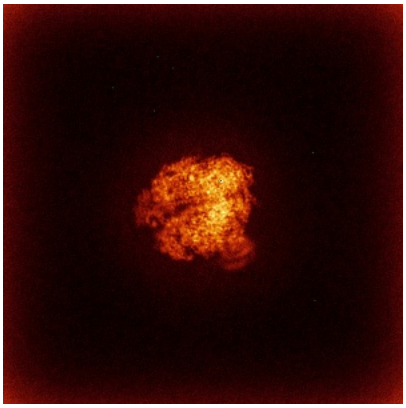
6.4.2 Raw map



X



Y

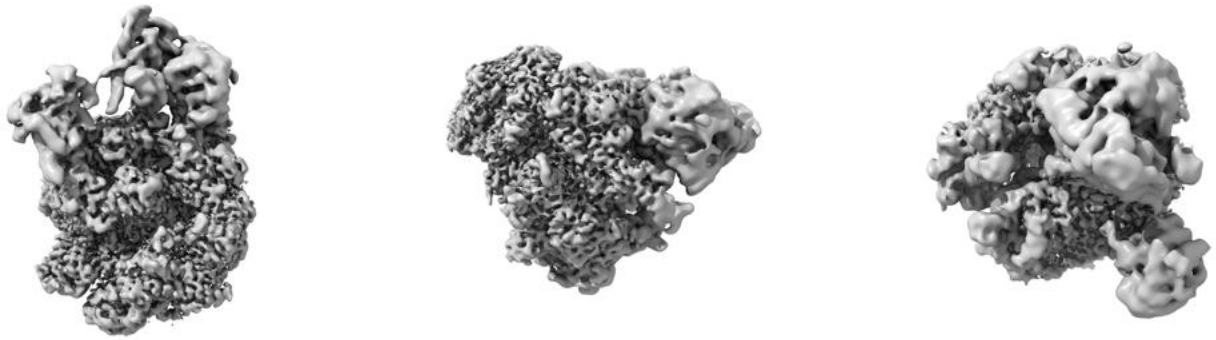


Z

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 0.417. 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.

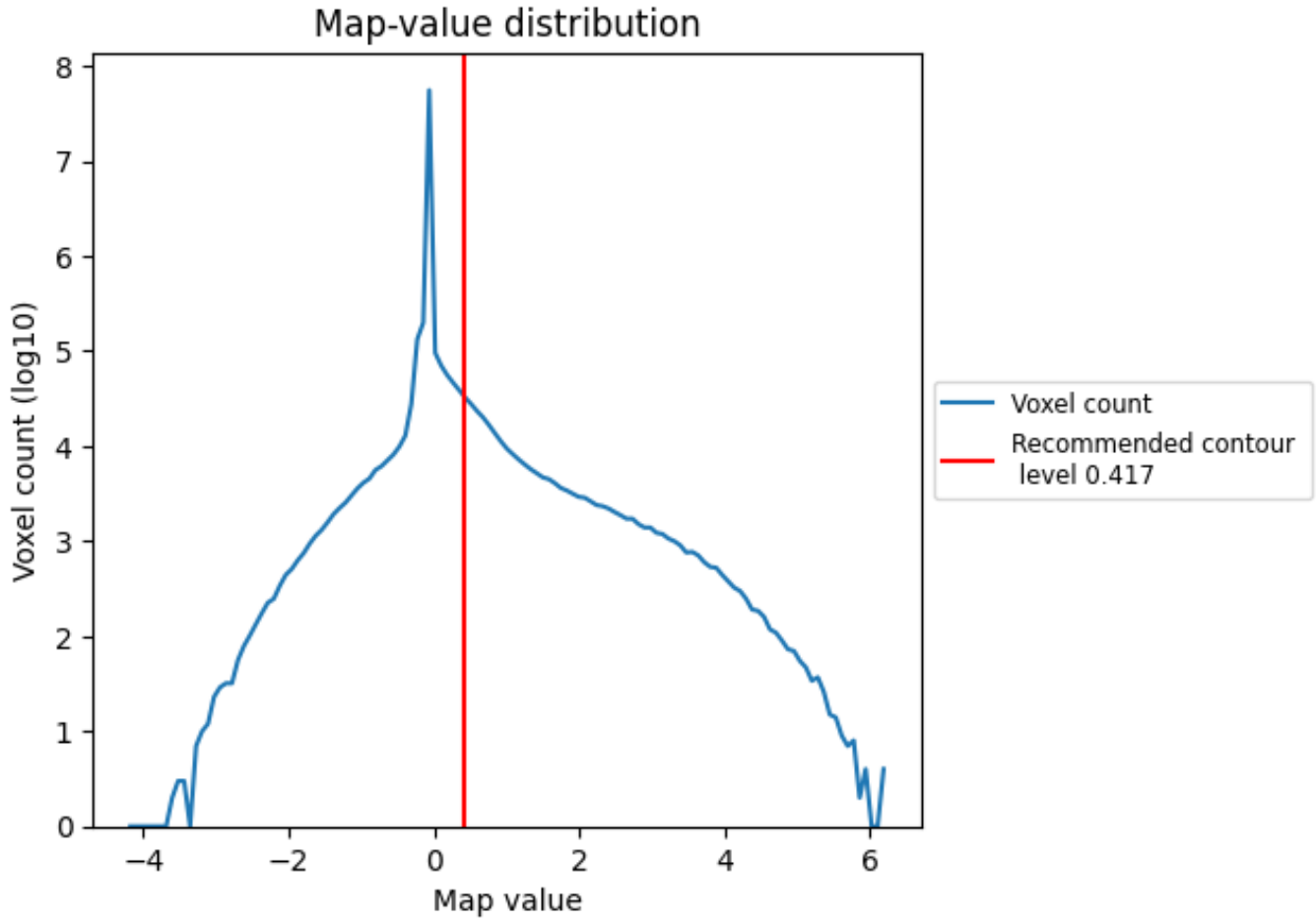
6.6 Mask visualisation (i)

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

7 Map analysis

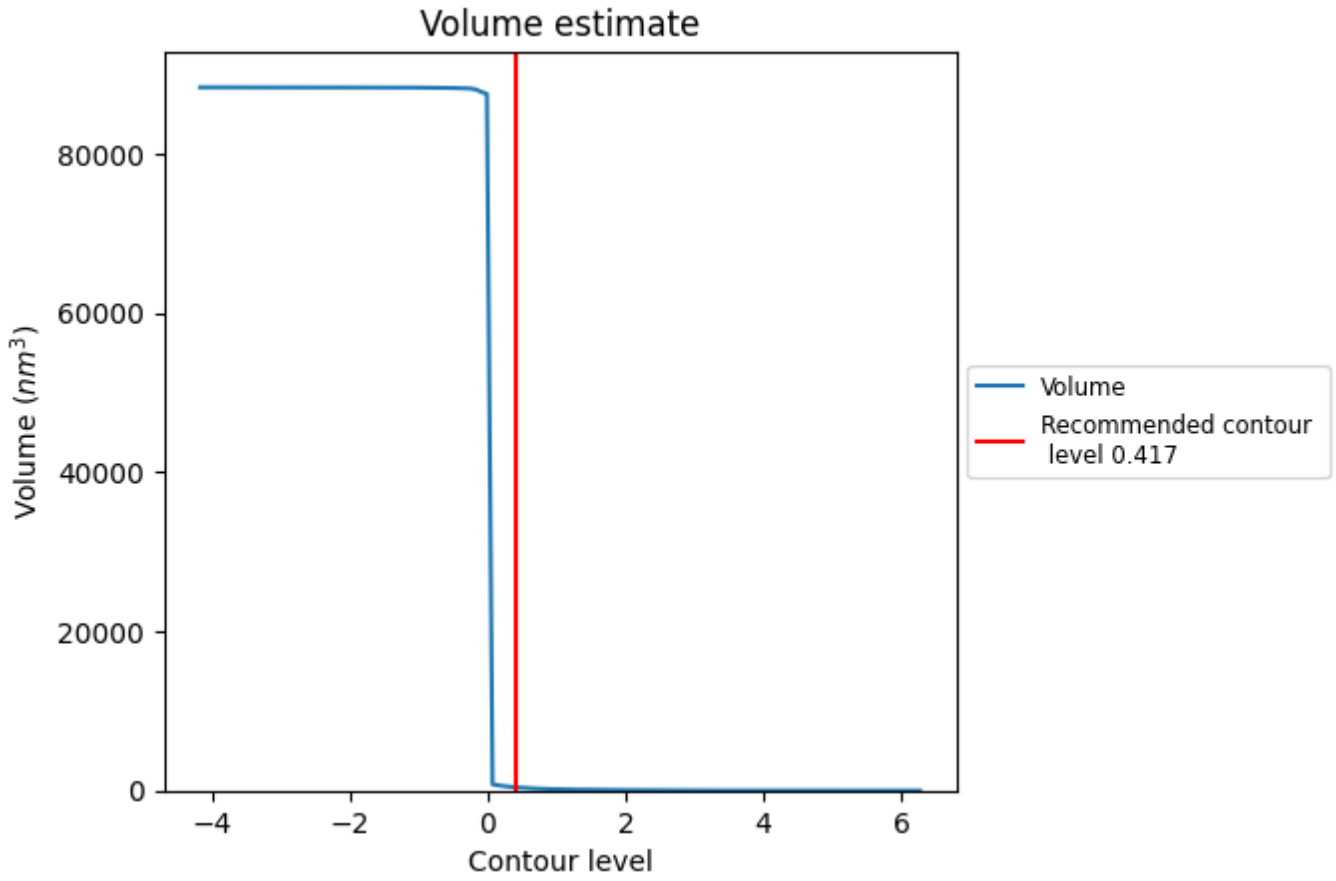
This section contains the results of statistical analysis of the map.

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.

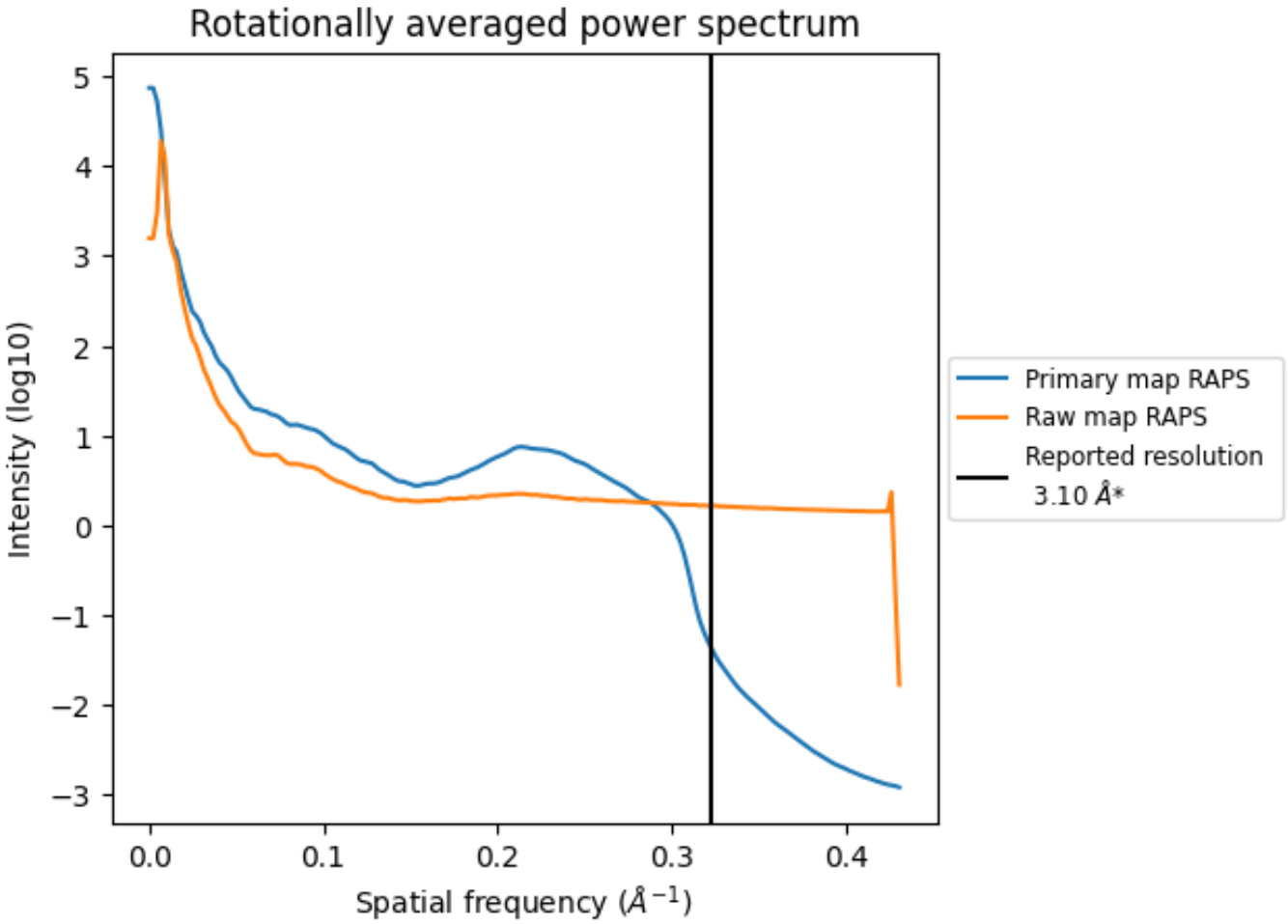
7.2 Volume estimate



The volume at the recommended contour level is 401 nm^3; this corresponds to an approximate mass of 362 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)

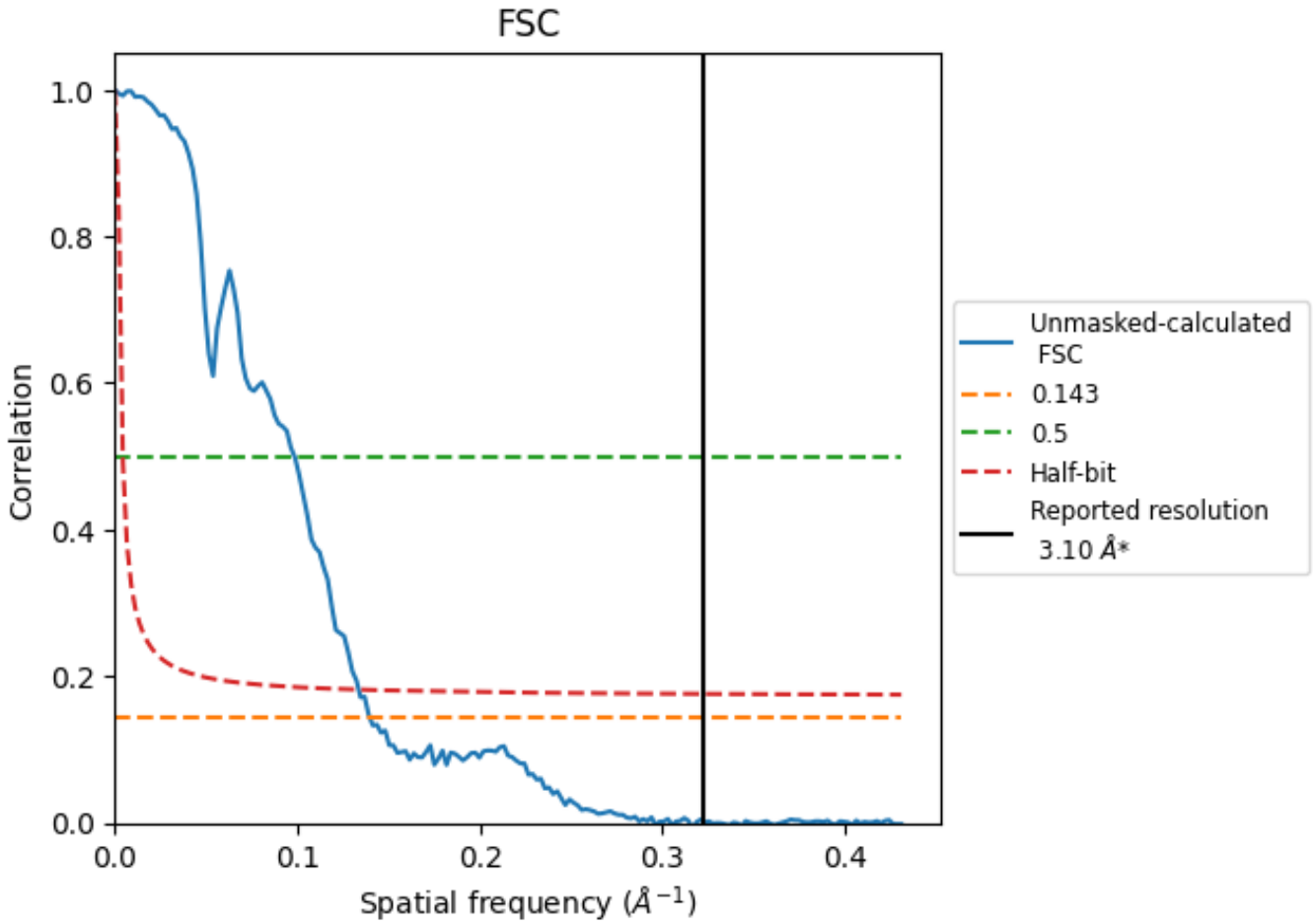


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

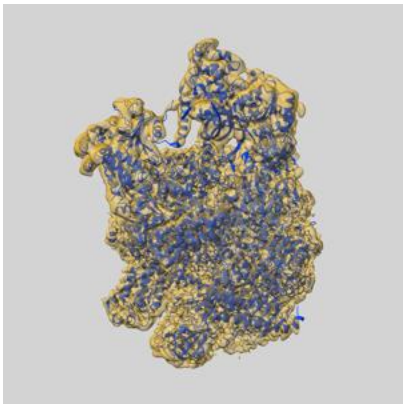
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.15	10.16	7.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 3.1 by more than 10 %

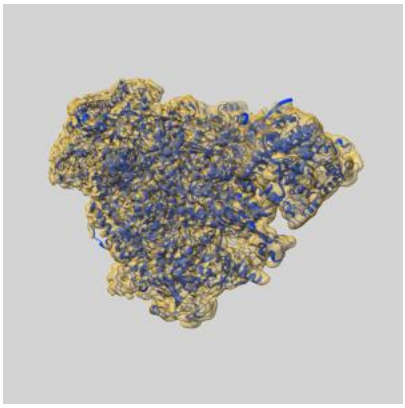
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41655 and PDB model 8TVY. Per-residue inclusion information can be found in section 3 on page 7.

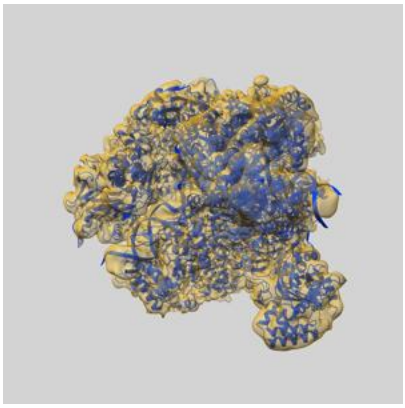
9.1 Map-model overlay



X



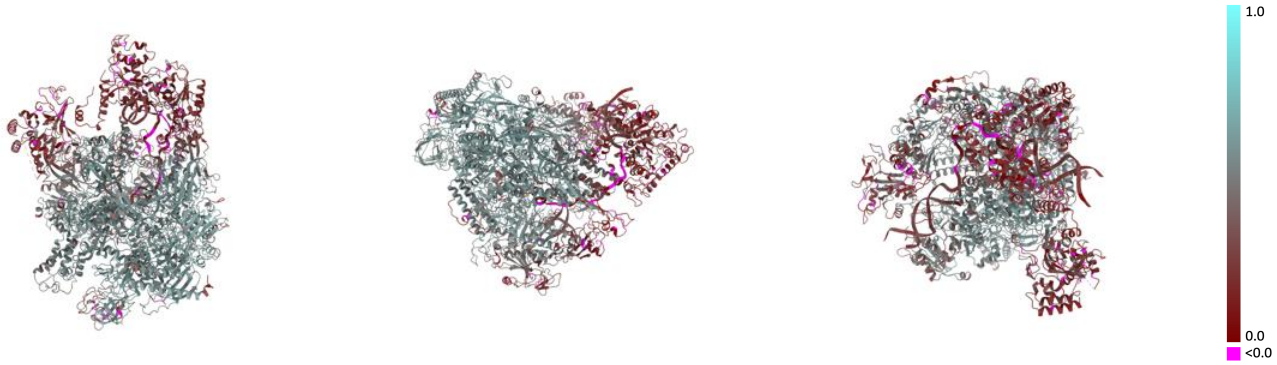
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.417 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.

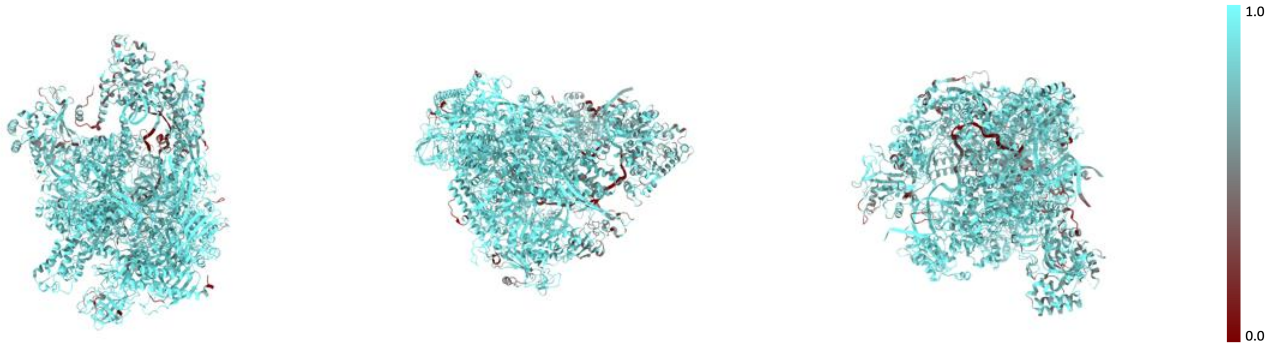
9.2 Q-score mapped to coordinate model (i)



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.

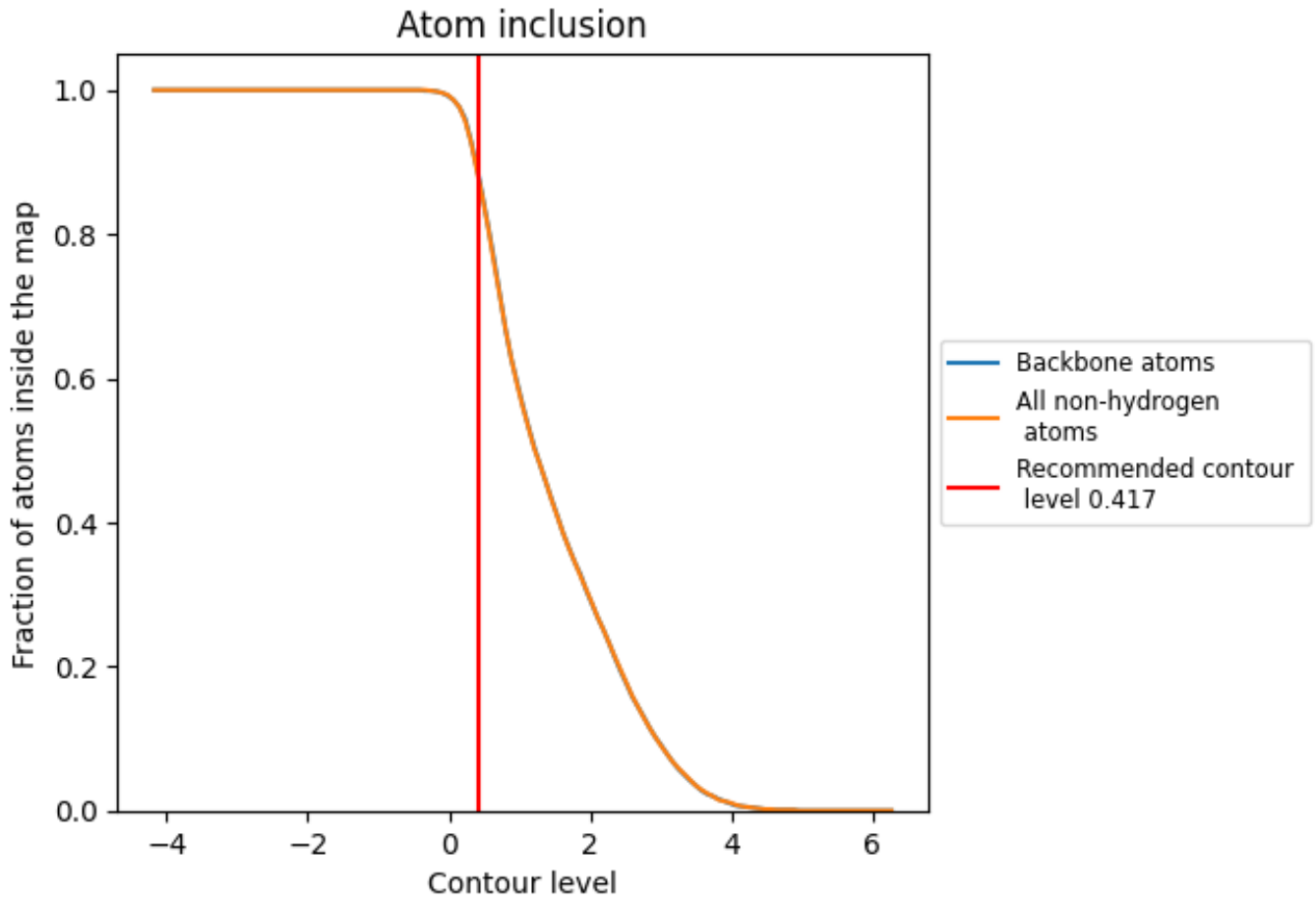
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.417).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.417) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.4330
A	0.9190	0.5000
B	0.9200	0.5020
C	0.9570	0.5510
D	0.7580	0.2400
E	0.9490	0.4920
F	0.9640	0.5490
G	0.8060	0.3050
H	0.8830	0.4440
I	0.8640	0.4030
J	0.9180	0.5240
K	0.9350	0.5390
L	0.9380	0.4960
M	0.7560	0.1930
N	0.6290	0.1580
O	0.6820	0.1650
R	0.9730	0.5240
T	0.8650	0.3180