



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 08:32 AM UTC

PDB ID : 8TVY / pdb_00008tvY
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

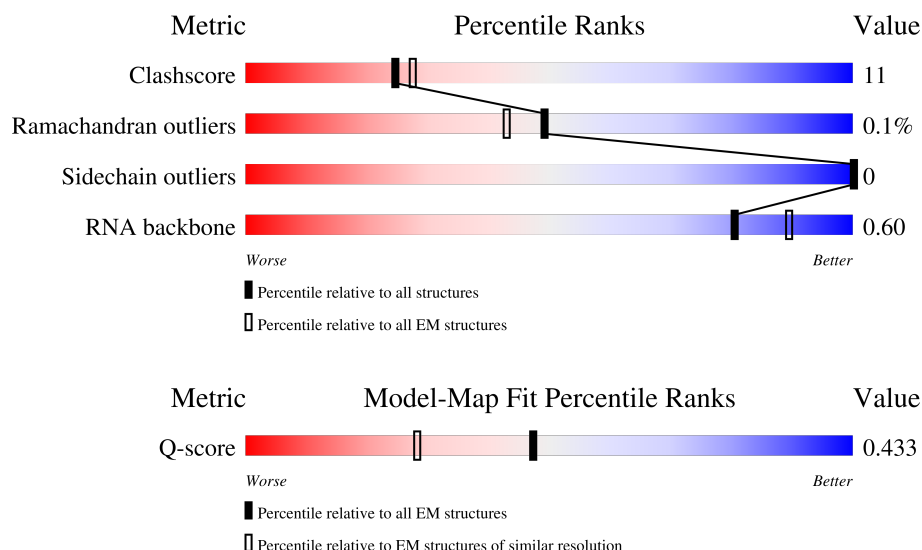
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



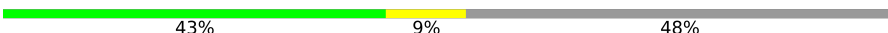
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
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 [i](#)

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
1	A	1448	Total	C	H	N	O	S	0	0
			22822	7168	11437	1988	2167	62		

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

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

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

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

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

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

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

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

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

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

- 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 (CCD ID: 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	

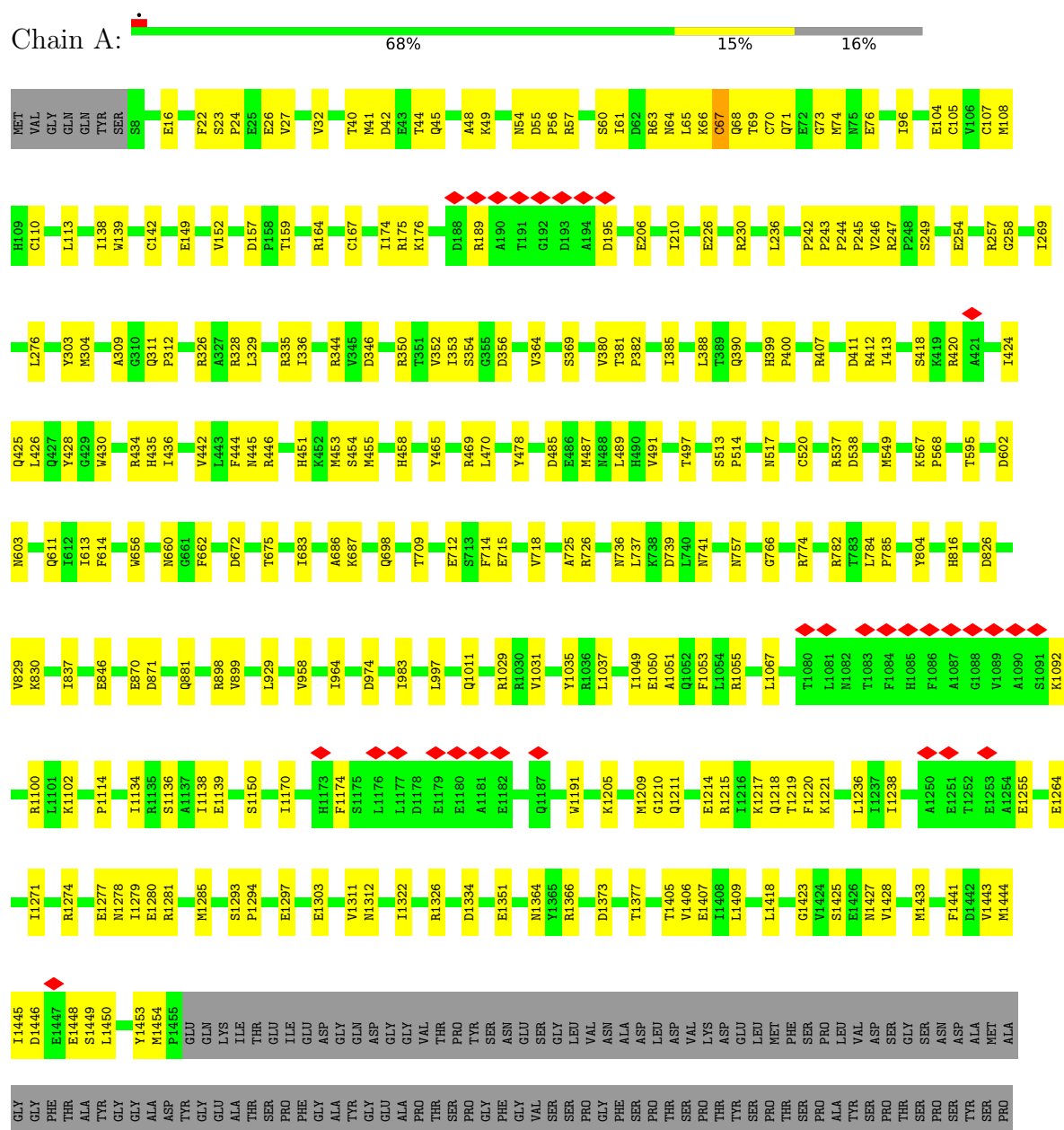
- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

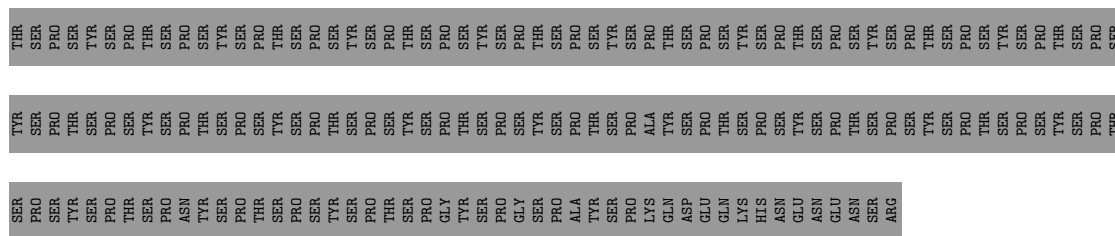
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

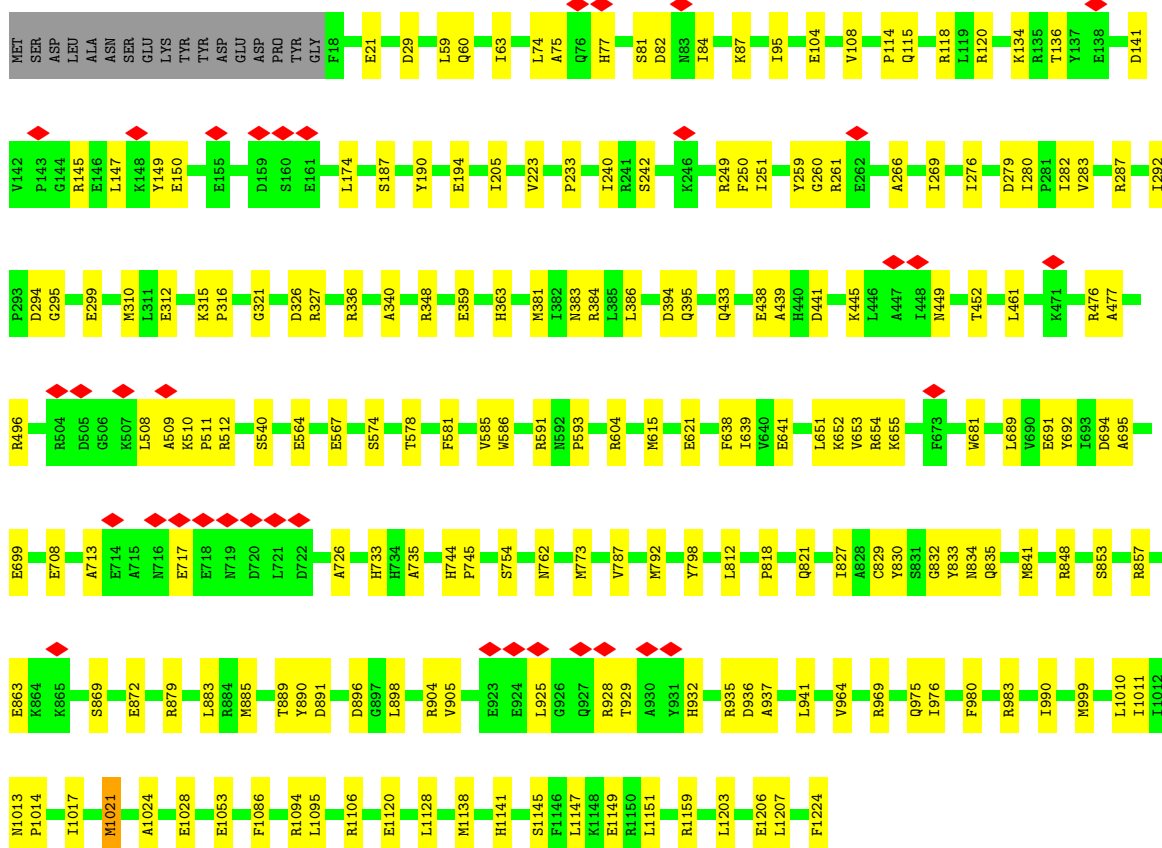
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





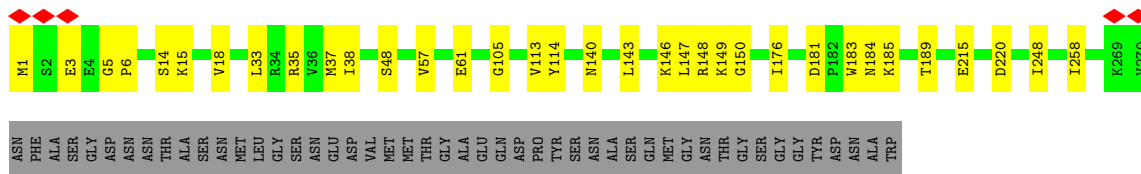
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B: 82% 16%



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

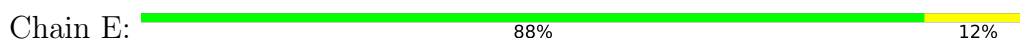
Chain C: 74% 11% 15%



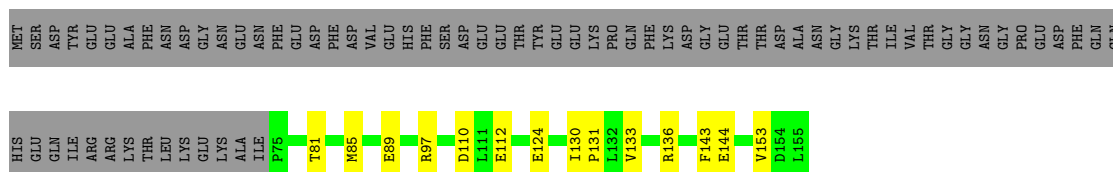
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 60% 15% 24%

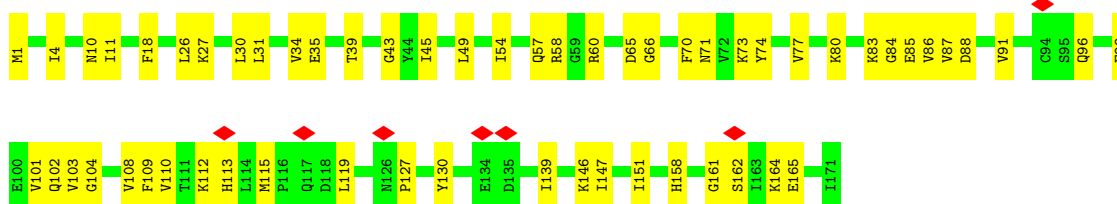
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



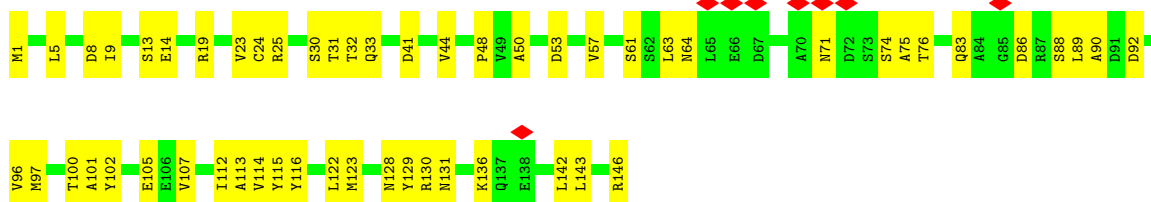
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



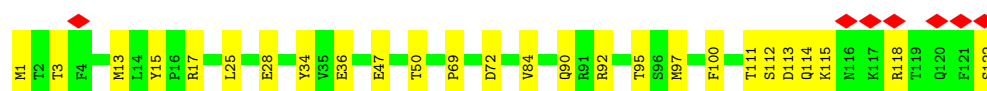
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



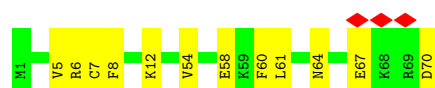
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

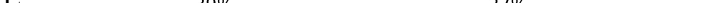


- Chain J: 83% 17%

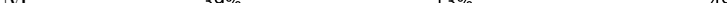


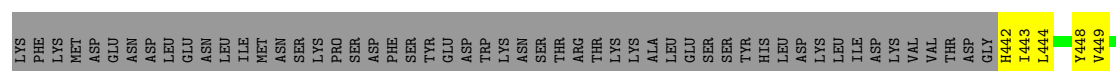
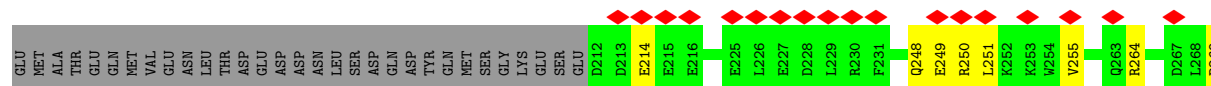
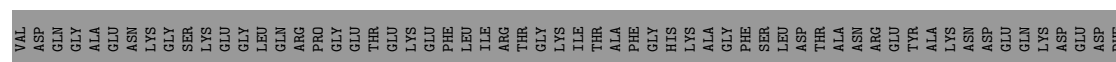
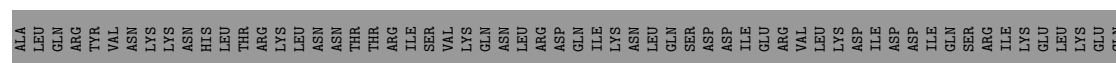
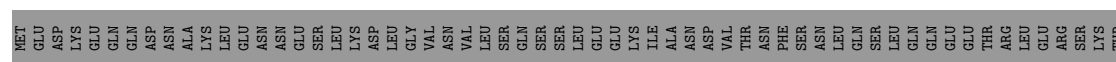
- Chain K: 

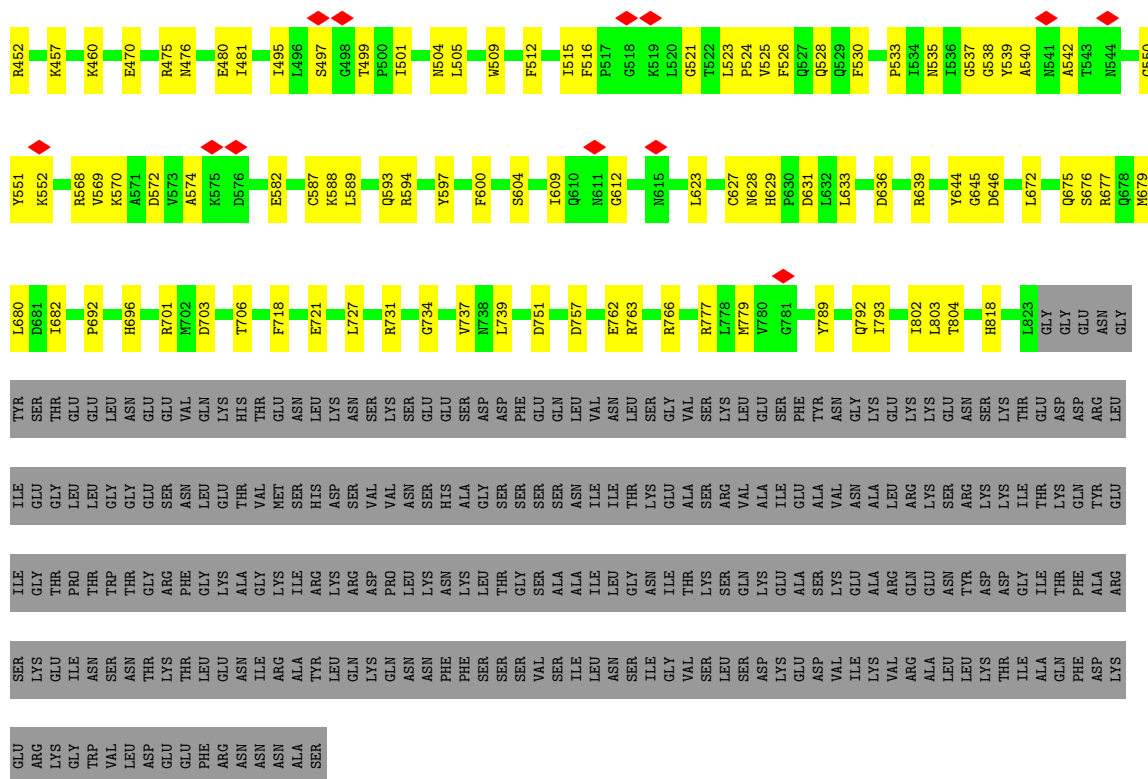


- Chain L:  39% 27% 34%



- Chain M: 

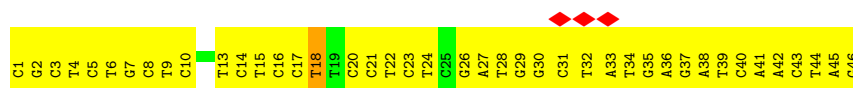




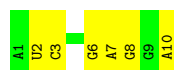
- Molecule 14: DNA (NTS)



- Molecule 15: DNA (TS)



- Molecule 16: RNA



- Molecule 17: Transcription elongation factor 1 homolog





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.18	0/11592	0.33	0/15682
2	B	0.19	0/9799	0.30	0/13221
3	C	0.20	0/2163	0.31	0/2930
4	D	0.09	0/1349	0.25	0/1811
5	E	0.15	0/1796	0.24	0/2416
6	F	0.19	0/669	0.30	0/903
7	G	0.14	0/1368	0.31	0/1844
8	H	0.19	0/1181	0.38	0/1602
9	I	0.12	0/1016	0.27	0/1365
10	J	0.21	0/587	0.30	0/786
11	K	0.18	0/981	0.24	0/1324
12	L	0.16	0/366	0.46	0/485
13	M	0.10	0/4667	0.28	0/6301
14	N	0.17	0/1082	0.32	0/1668
15	T	0.19	0/1010	0.35	0/1551
16	R	0.18	0/247	0.24	0/384
17	O	0.15	0/562	0.41	0/755
All	All	0.17	0/40435	0.31	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

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	216	0
2	B	9608	9576	9576	138	0
3	C	2125	2087	2090	30	0
4	D	1340	1353	1352	25	0
5	E	1760	1785	1788	18	0
6	F	657	673	673	11	0
7	G	1340	1354	1357	51	0
8	H	1161	1121	1124	50	0
9	I	997	950	954	21	0
10	J	578	586	590	11	0
11	K	962	958	961	21	0
12	L	364	386	388	13	0
13	M	4564	4606	4605	96	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	811	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 11.

All (811) 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
3:C:1:MET:HE3	11:K:97:LYS:HD2	1.49	0.94
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:10:DC:H2'	14:N:11:DT:H71	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:841:MET:HE2	2:B:1010:LEU:HD21	1.74	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
13:M:353:CYS:HG	13:M:361:TRP:CD1	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:H:75:ALA:O	8:H:76:THR:OG1	2.12	0.65
15:T:44:DT:H2''	15:T:45:DA:C8	2.32	0.65
1:A:1444:MET:HE2	7:G:60:ARG:HB3	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
2:B:438:GLU:OE1	2:B:445:LYS:NZ	2.28	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
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
8:H:31:THR:O	8:H:32:THR:OG1	2.16	0.62
8:H:123:MET:HE2	8:H:142:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
14:N:10:DC:C2'	14:N:11:DT:H71	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:G:96:GLN:O	7:G:112:LYS:NZ	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
6:F:85:MET:HE2	6:F:153:VAL:HG22	1.84	0.58
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
14:N:42:DA:H2'	14:N:42:DA:OP2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.40	0.57
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.86	0.57
13:M:322:ASP:O	13:M:328:LYS:NZ	2.35	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
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
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
2:B:604:ARG:HD3	2:B:615:MET:HE2	1.87	0.56
9:I:113:ASP:OD1	9:I:114:GLN:N	2.39	0.56
7:G:113:HIS:O	7:G:164:LYS:NZ	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: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
1:A:66:LYS:O	1:A:67:CYS:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:41:DA:H2''	15:T:42:DA:H8	1.70	0.55
1:A:757:ASN:HA	2:B:1021:MET:HE2	1.89	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
3:C:114:TYR:HH	3:C:140:ASN:CG	2.10	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
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
9:I:1:MET:HE3	9:I:3:THR:O	2.08	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
7:G:30:LEU:C	7:G:30:LEU:HD23	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.17	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
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.23	0.52
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.10	0.52
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.91	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
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:108:MET:HE2	1:A:174:ILE:HD11	1.93	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
2:B:773:MET:HE3	2:B:1095:LEU:HD11	1.93	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:375:VAL:HG21	13:M:380:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:870:GLU:OE1	5:E:202:SER:OG	2.21	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:375:VAL:HG11	13:M:380:MET:HE1	1.94	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
2:B:681:TRP:NE1	2:B:692:TYR:OH	2.41	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
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
13:M:679:MET:HE3	13:M:679:MET:HA	1.95	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
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
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
1:A:56:PRO:C	1:A:57:ARG:HE	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:SER:OG	2:B:141:ASP:OD1	2.29	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
9:I:72:ASP:C	9:I:72:ASP:OD2	2.57	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
13:M:381:GLY:O	13:M:382:SER:C	2.57	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
2:B:869:SER:OG	13:M:633:LEU:O	2.29	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
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
17:O:26:LEU:C	17:O:28:CYS:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:ARG:NH1	7:G:70:PHE:CE1	2.82	0.47
13:M:524:PRO:O	13:M:525:VAL:C	2.58	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
1:A:1446:ASP:C	7:G:58:ARG:HD2	2.40	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:444:PHE:HD1	1:A:487:MET:HE3	1.80	0.46
1:A:614:PHE:CD1	8:H:122:LEU:HD11	2.50	0.46
8:H:101:ALA:HA	8:H:115:TYR:HB3	1.97	0.46
13:M:703:ASP:OD1	13:M:706:THR:OG1	2.31	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
2:B:641:GLU:OE1	2:B:652:LYS:NZ	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:MET:HE2	1:A:1236:LEU:HB3	1.96	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
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
2:B:476:ARG:O	2:B:477:ALA:C	2.59	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
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:13:SER:HG	8:H:14:GLU:CD	2.14	0.45
8:H:83:GLN:OE1	11:K:54:ARG:NE	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:249:ARG:O	2:B:250:PHE:C	2.59	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:74:LEU:O	2:B:75:ALA:C	2.60	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
7:G:91:VAL:HG13	7:G:99:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:130:ARG:O	8:H:131:ASN:C	2.61	0.44
14:N:8:DA:H2'	14:N:9:DT:H71	1.98	0.44
1:A:61:ILE:C	1:A:74:MET:HE3	2.43	0.44
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.99	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
5:E:74:ASP:OD2	5:E:74:ASP:C	2.61	0.44
9:I:113:ASP:OD1	9:I:113:ASP:C	2.61	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
8:H:5:LEU:HD13	8:H:61:SER:H	1.84	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
1:A:356:ASP:OD1	2:B:833:TYR:OH	2.34	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
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:257:ARG:O	1:A:258:GLY:C	2.62	0.43
1:A:1191:TRP:NE1	1:A:1255:GLU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1220:PHE:O	1:A:1221:LYS:C	2.62	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
1:A:311:GLN:N	1:A:312:PRO:CD	2.82	0.43
3:C:220:ASP:C	3:C:220:ASP:OD1	2.62	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
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:360:GLN:O	13:M:361:TRP:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:928:ARG:O	2:B:929:THR:C	2.61	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: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:310:MET:HE1	2:B:383:ASN:OD1	2.19	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
2:B:282:ILE:HG13	2:B:283:VAL:N	2.35	0.42
2:B:315:LYS:CD	9:I:13:MET:HE1	2.49	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
1:A:1303:GLU:OE2	1:A:1326:ARG:NH1	2.44	0.42
1:A:1433:MET:HE2	2:B:1145:SER:OG	2.20	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:41:MET:HE2	1:A:42:ASP:OD1	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:VAL:HG12	12:L:46:VAL:O	2.17	0.42
12:L:59:ALA:O	12:L:60:ARG:C	2.63	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:485:ASP:OD1	16:R:10:A:O3'	2.35	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
2:B:615:MET:HE3	2:B:615:MET:HB2	1.95	0.42
4:D:220:LEU:O	4:D:221:TYR:C	2.63	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:660:ASN:OD1	1:A:660:ASN:C	2.62	0.41
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
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:23:SER:O	1:A:24:PRO:C	2.63	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
10:J:6:ARG:O	10:J:7:CYS:C	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:ILE:HG21	4:D:145:MET:SD	2.60	0.41
9:I:13:MET:HE2	9:I:15:TYR:CE1	2.56	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:549:MET:HE1	1:A:656:TRP:HD1	1.85	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
4:D:33:PHE:O	4:D:34:GLN:C	2.63	0.41
13:M:382:SER:OG	13:M:383:GLY:N	2.46	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
1:A:1280:GLU:O	1:A:1281:ARG:C	2.63	0.41
3:C:113:VAL:CG2	3:C:147:LEU:HD11	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
2:B:1224:PHE:OXT	5:E:171:LYS:NZ	2.47	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:48:ALA:C	1:A:49:LYS:HD3	2.46	0.41
1:A:714:PHE:CD2	9:I:97:MET:HE1	2.56	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
2:B:896:ASP:CG	12:L:29:TYR:HH	2.29	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
13:M:679:MET:HE3	13:M:682:ILE:HB	2.03	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
11:K:7:PHE:CD1	11:K:7:PHE:C	2.99	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:675:GLN:O	13:M:676:SER:C	2.64	0.40
2:B:509:ALA:C	2:B:511:PRO:HD2	2.46	0.40
8:H:96:VAL:HG12	8:H:97:MET:N	2.35	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:567:GLU:H	2:B:567:GLU:CD	2.29	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
8:H:1:MET:HE3	8:H:90:ALA:HB2	2.03	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1446/1733 (83%)	1336 (92%)	109 (8%)	1 (0%)	48	78
2	B	1205/1224 (98%)	1112 (92%)	92 (8%)	1 (0%)	48	78
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%)	43	73
17	O	69/85 (81%)	59 (86%)	10 (14%)	0	100	100
All	All	4660/5735 (81%)	4291 (92%)	366 (8%)	3 (0%)	49	78

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

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%)	1264 (100%)	0	100	100
2	B	1046/1061 (99%)	1046 (100%)	0	100	100
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%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	128/128 (100%)	128 (100%)	0	100	100
9	I	116/116 (100%)	116 (100%)	0	100	100
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%)	504 (100%)	0	100	100
17	O	66/79 (84%)	66 (100%)	0	100	100
All	All	4140/5066 (82%)	4140 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	299	HIS
1	A	490	HIS
1	A	517	ASN
1	A	736	ASN
1	A	969	GLN
1	A	1048	ASN
1	A	1364	ASN
1	A	1387	HIS
2	B	110	HIS
2	B	255	GLN
2	B	300	HIS
2	B	433	GLN
2	B	465	ASN

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Mol	Chain	Res	Type
2	B	494	HIS
2	B	932	HIS
2	B	1097	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	65	HIS
5	E	32	GLN
5	E	101	GLN
7	G	153	GLN
7	G	158	HIS
8	H	134	ASN
11	K	52	ASN
13	M	313	GLN
13	M	615	ASN
13	M	628	ASN
13	M	808	GLN

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	1.30	6 (14%)	61,74,77	2.14	15 (24%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	18	TTD	C2T-N1T	3.19	1.42	1.36
15	T	18	TTD	C4T-N3T	-3.05	1.32	1.37
15	T	18	TTD	C2T-N3T	-2.95	1.32	1.38
15	T	18	TTD	C2-N3	-2.93	1.32	1.38
15	T	18	TTD	C4-N3	-2.65	1.33	1.37
15	T	18	TTD	C5T-C6T	-2.00	1.52	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	18	TTD	C2'-C1'-N1	-9.73	102.44	115.59
15	T	18	TTD	C4-N3-C2	-4.98	119.16	126.67
15	T	18	TTD	C4T-N3T-C2T	-4.75	119.50	126.67
15	T	18	TTD	N3T-C2T-N1T	4.29	121.28	116.78
15	T	18	TTD	O4R-C1R-N1T	4.26	113.70	108.65
15	T	18	TTD	O2T-C2T-N1T	-3.75	117.83	123.44
15	T	18	TTD	C2R-C1R-N1T	-3.01	111.52	115.59
15	T	18	TTD	O4'-C1'-N1	2.72	111.88	108.65
15	T	18	TTD	C5-C5T-C6T	2.54	91.34	88.36
15	T	18	TTD	O4-C4-C5	-2.33	120.54	122.71
15	T	18	TTD	C6T-C6-N1	-2.29	109.97	118.51
15	T	18	TTD	C6-C6T-N1T	-2.13	110.53	118.51
15	T	18	TTD	C5'-C4R-C3R	-2.07	109.68	114.57
15	T	18	TTD	C3R-C2'-C1'	2.02	106.74	102.89
15	T	18	TTD	C5M-C5T-C5	-2.01	110.69	116.61

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	O4R-C4'-C5R-O5R

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Mol	Chain	Res	Type	Atoms
15	T	18	TTD	O4'-C4R-C5'-O5'
15	T	18	TTD	C3R-C4R-C5'-O5'
15	T	18	TTD	C2'-C1'-N1-C6
15	T	18	TTD	C3'-C4'-C5R-O5R
15	T	18	TTD	O4'-C1'-N1-C2
15	T	18	TTD	C2'-C1'-N1-C2
15	T	18	TTD	O4'-C1'-N1-C6
15	T	18	TTD	C5R-O5R-PB-O3R
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

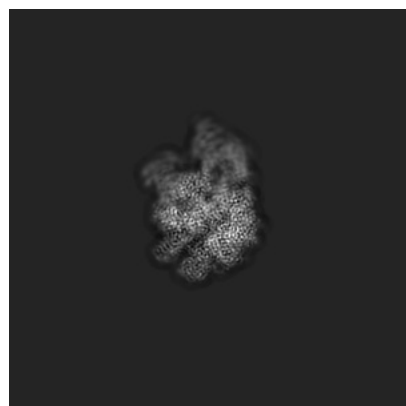
6 Map visualisation [i](#)

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.

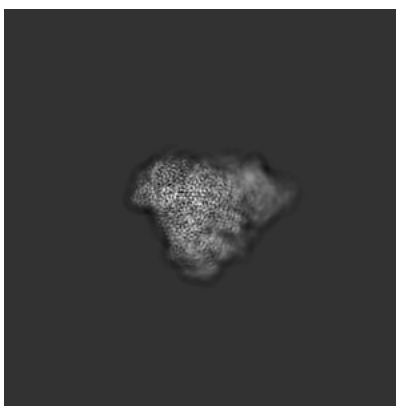
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

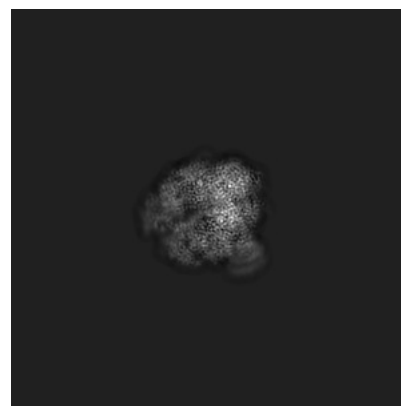
6.1.1 Primary map



X

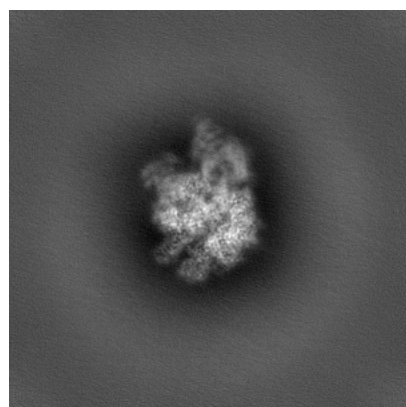


Y

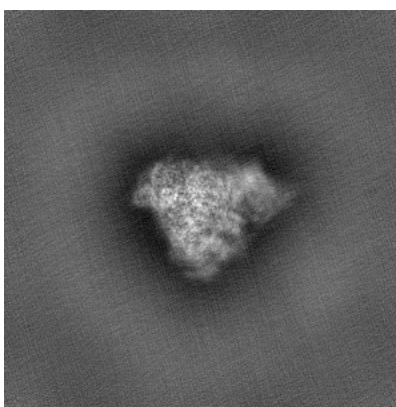


Z

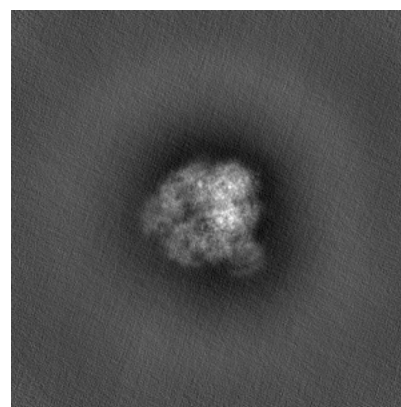
6.1.2 Raw map



X



Y



Z

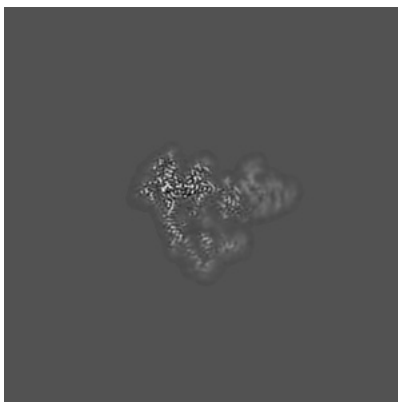
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

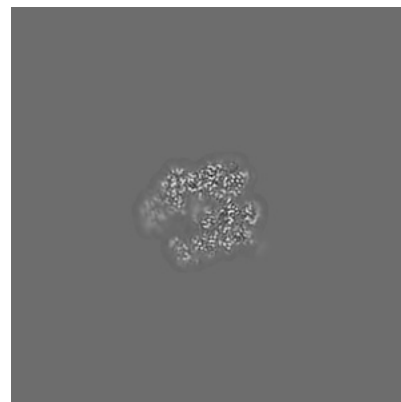
6.2.1 Primary map



X Index: 192

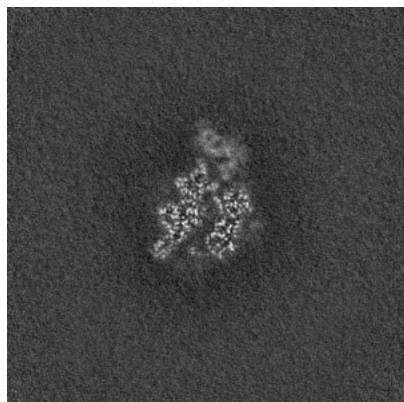


Y Index: 192

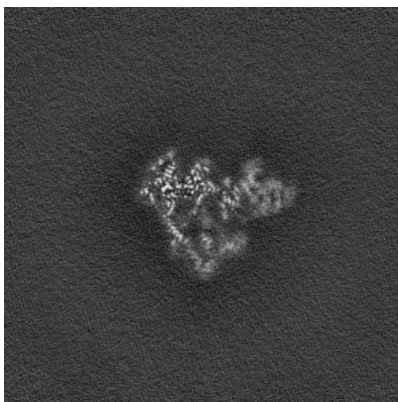


Z Index: 192

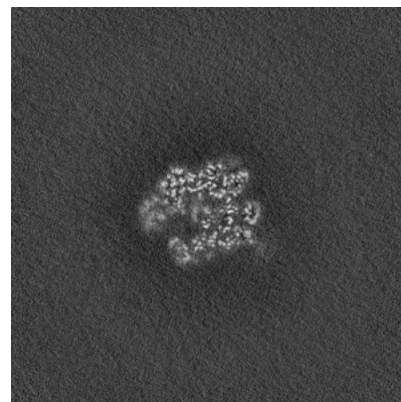
6.2.2 Raw map



X Index: 192



Y Index: 192

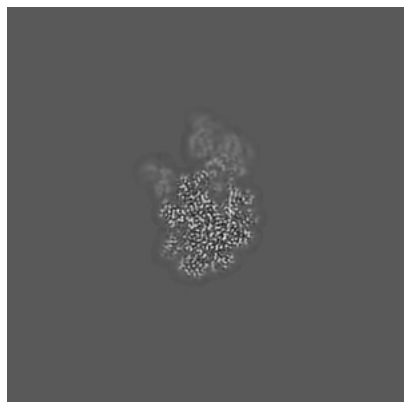


Z Index: 192

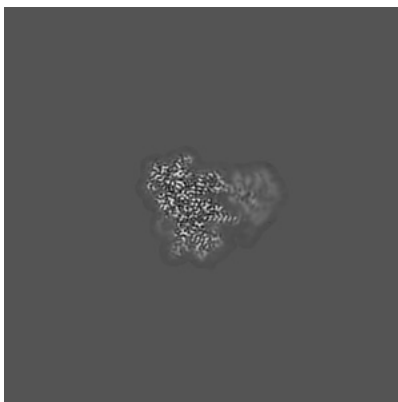
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

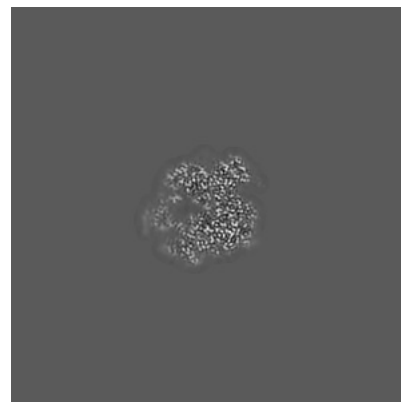
6.3.1 Primary map



X Index: 209

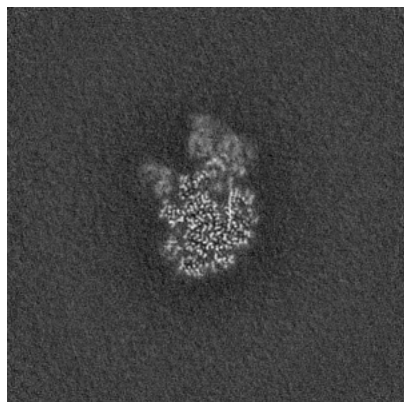


Y Index: 215

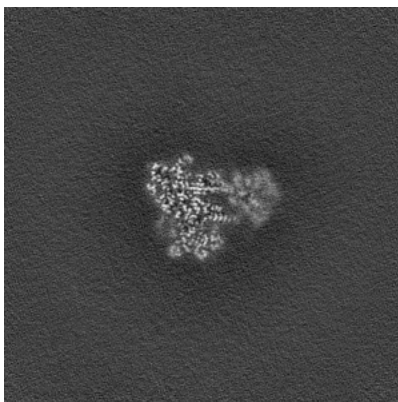


Z Index: 182

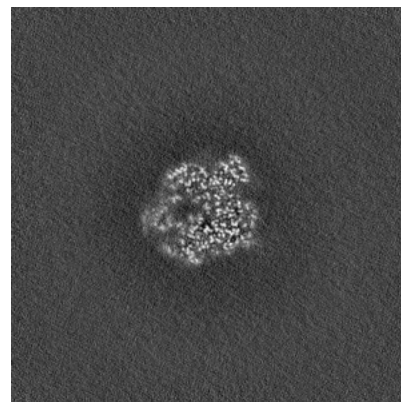
6.3.2 Raw map



X Index: 209



Y Index: 214

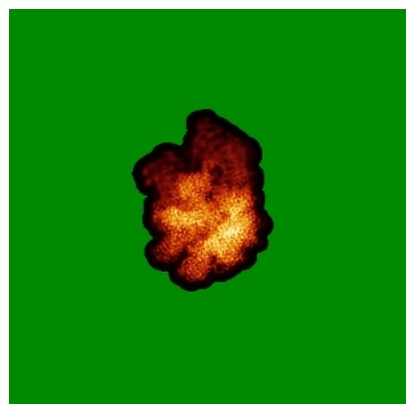


Z Index: 182

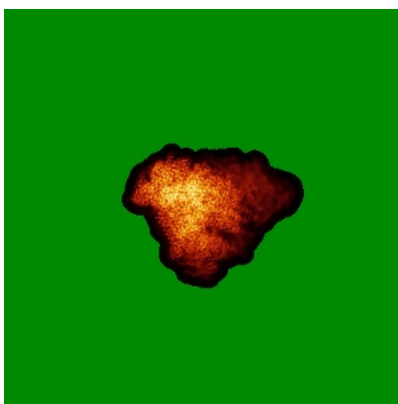
The images above show the largest variance slices of the map in three orthogonal directions.

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

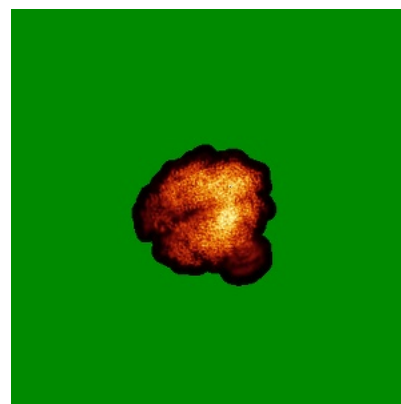
6.4.1 Primary map



X

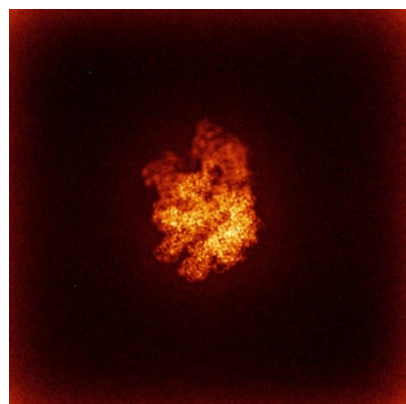


Y

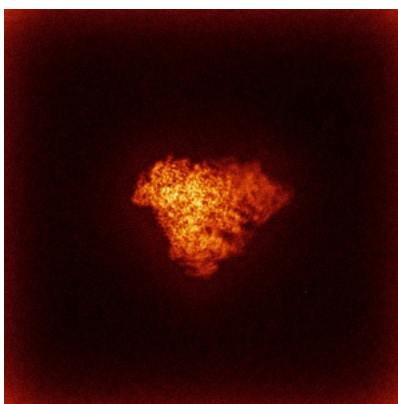


Z

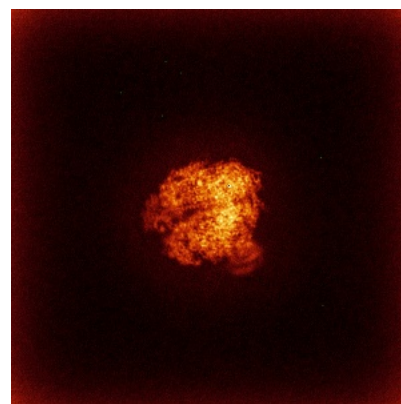
6.4.2 Raw map



X



Y

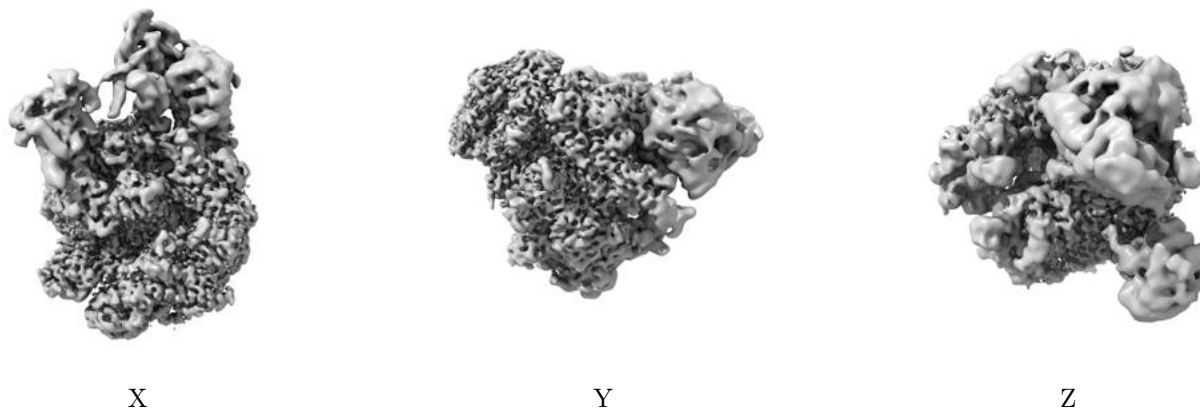


Z

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.

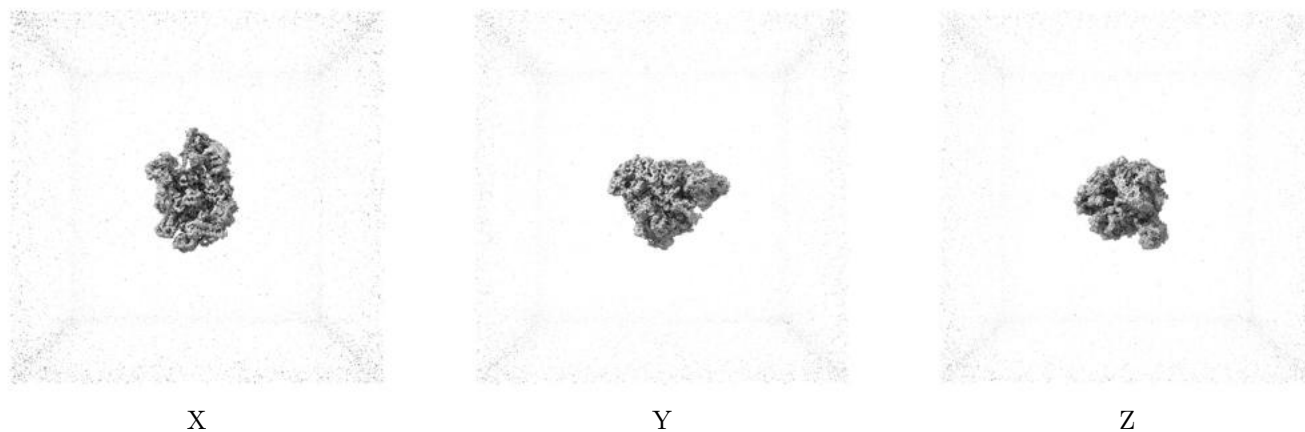
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

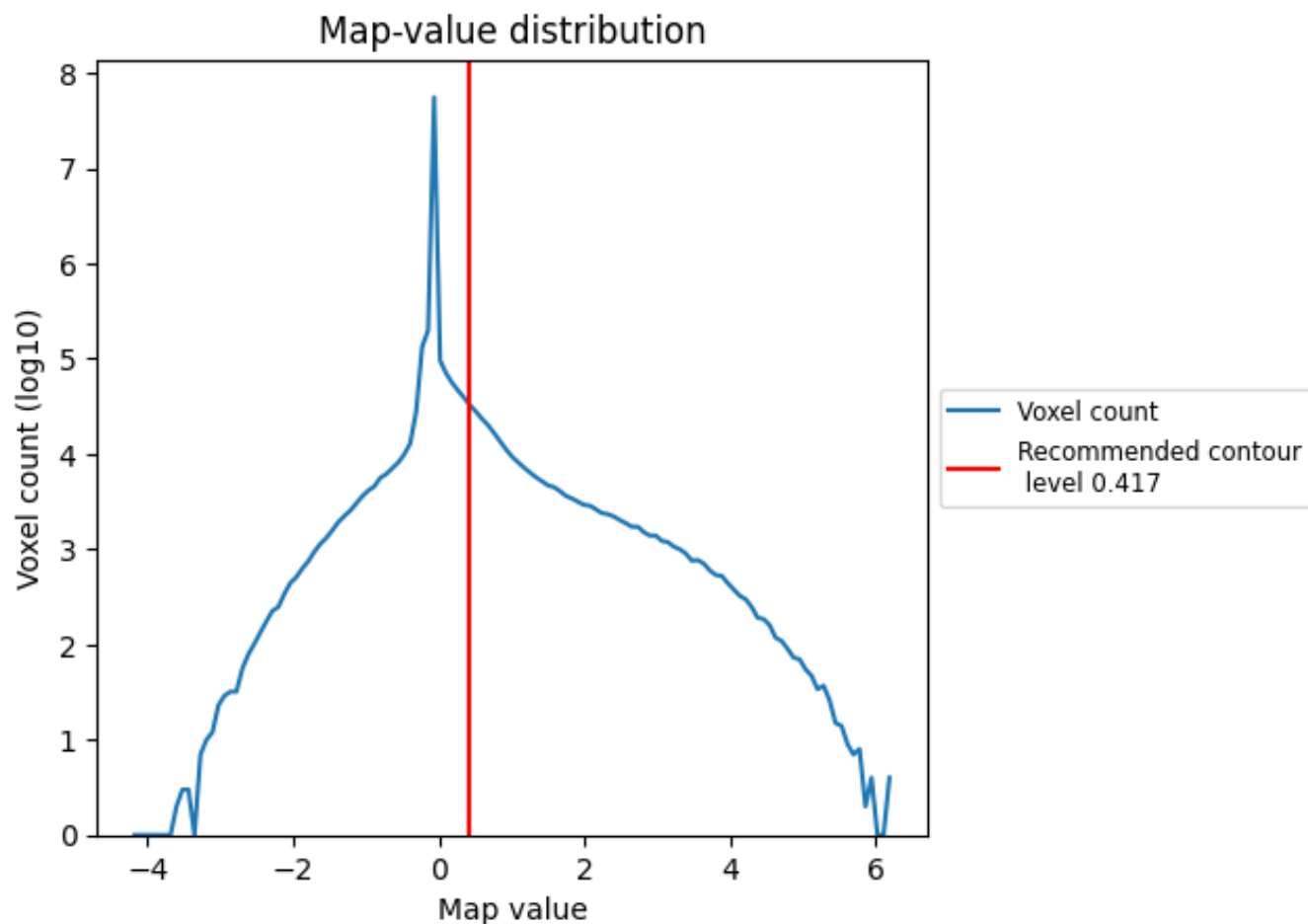
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

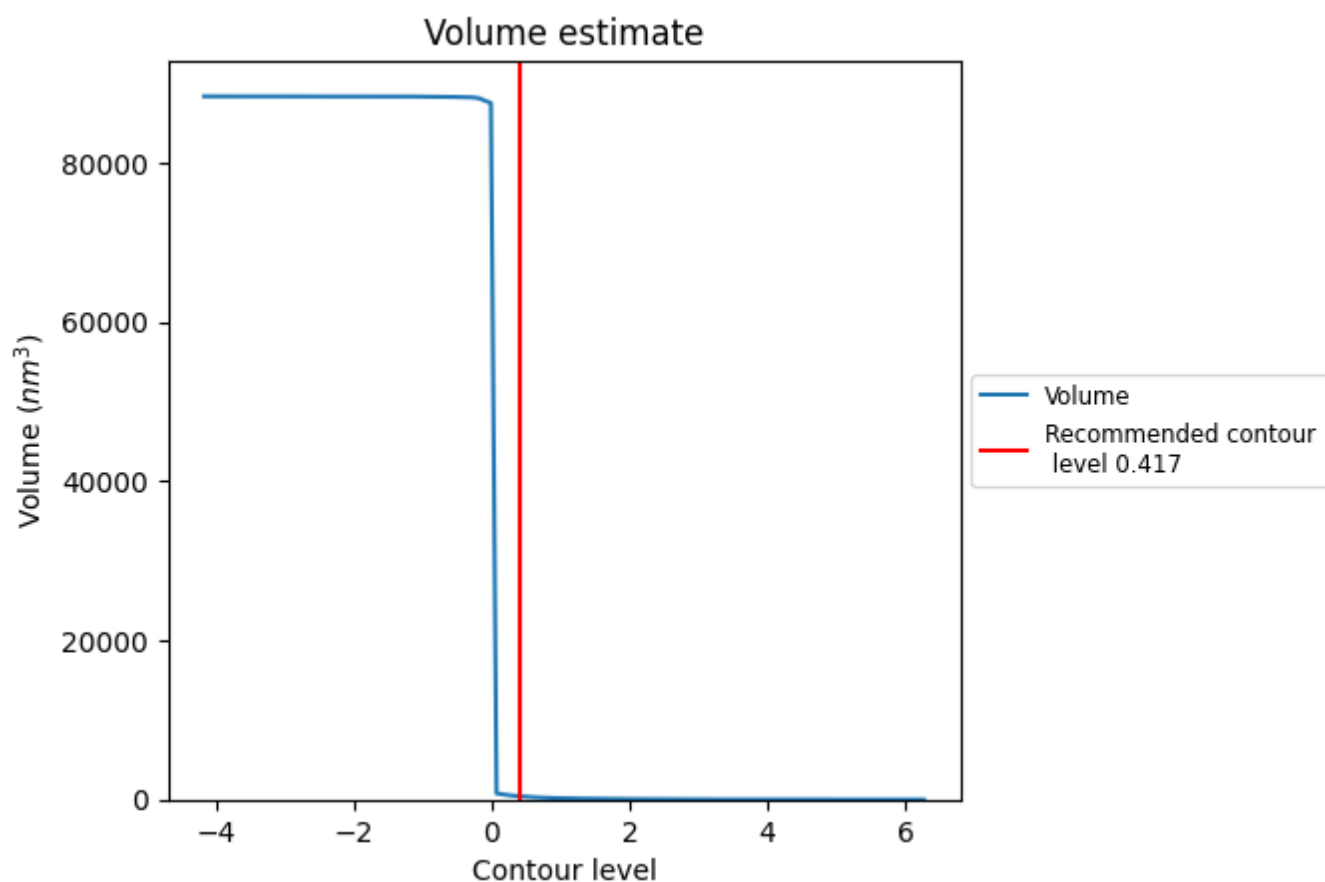
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

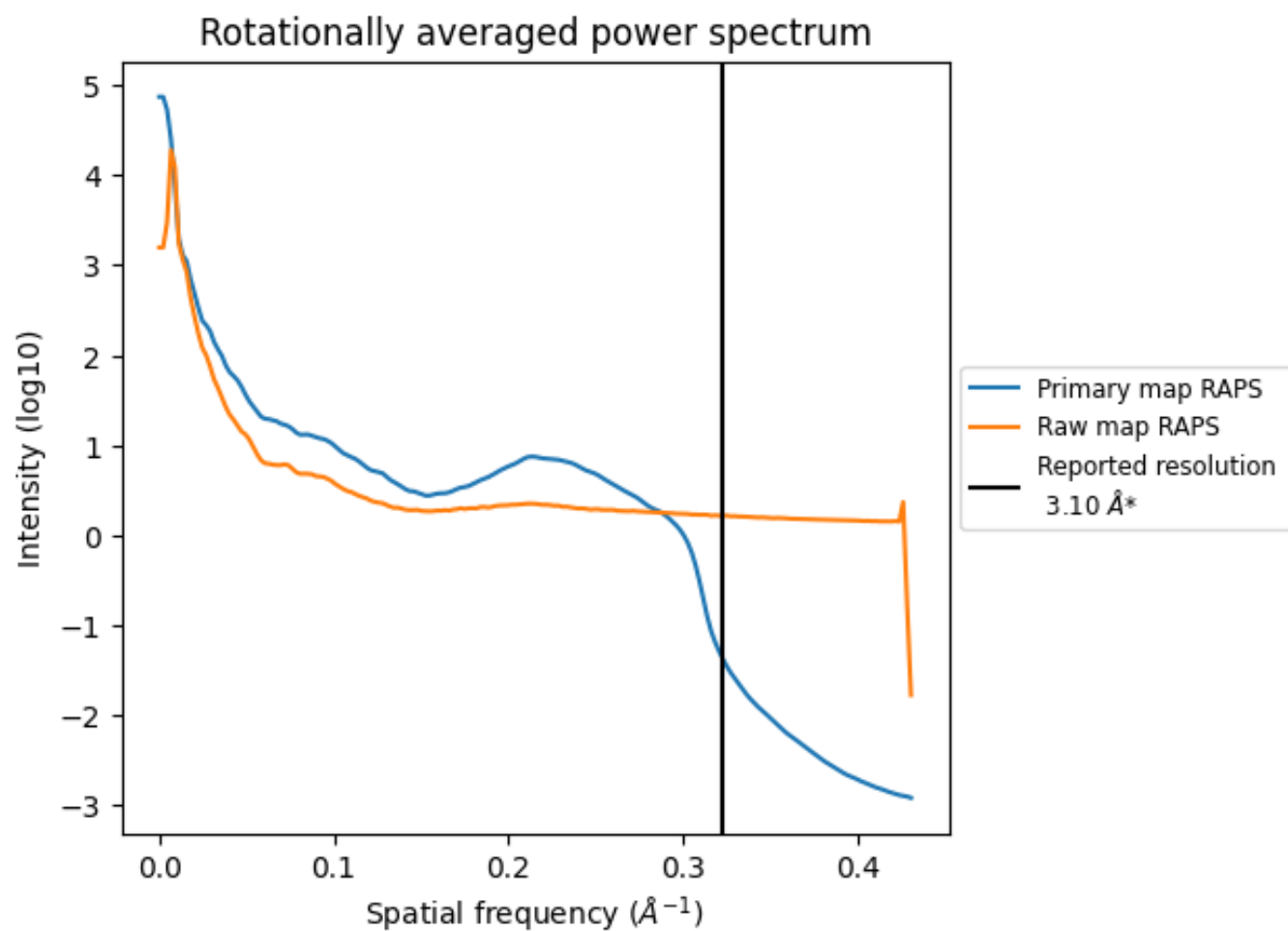
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm³; 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 ⓘ

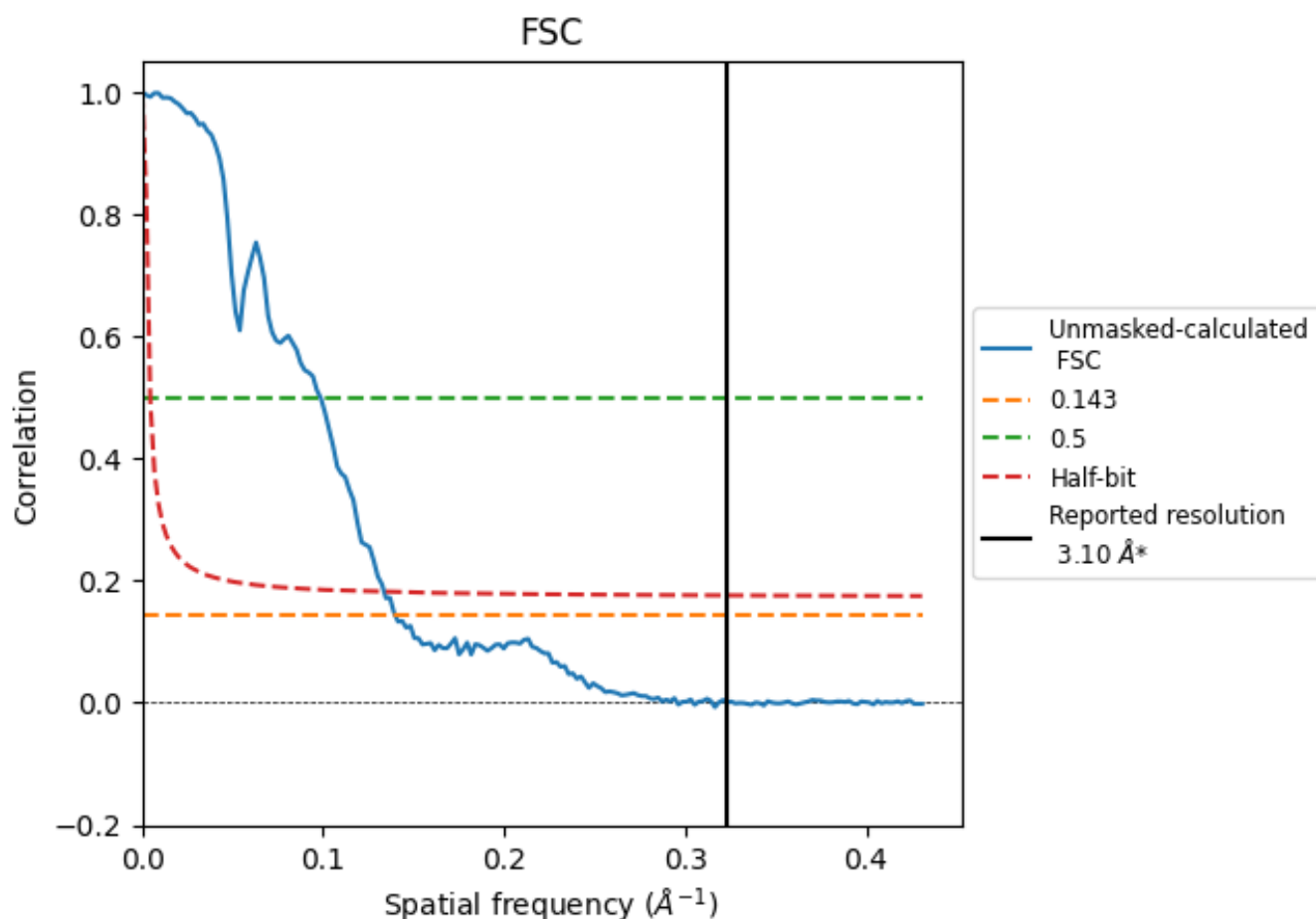


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

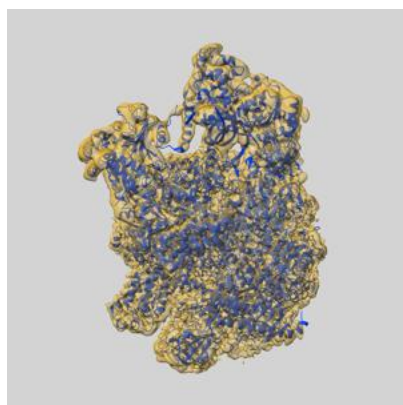
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.15	10.16	7.48

*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 %

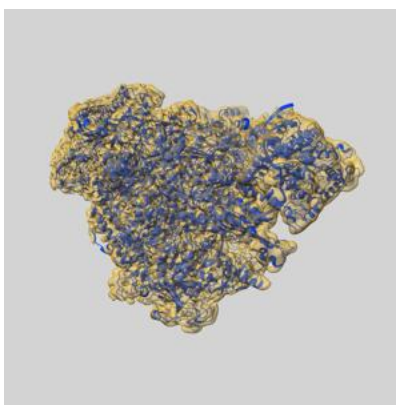
9 Map-model fit [i](#)

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](#).

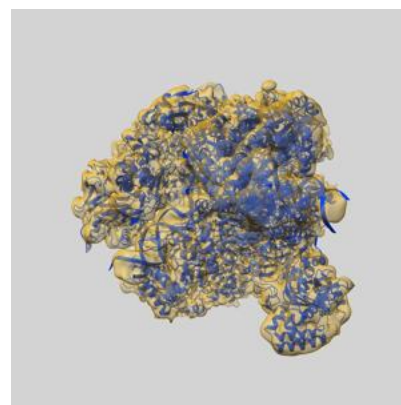
9.1 Map-model overlay [i](#)



X



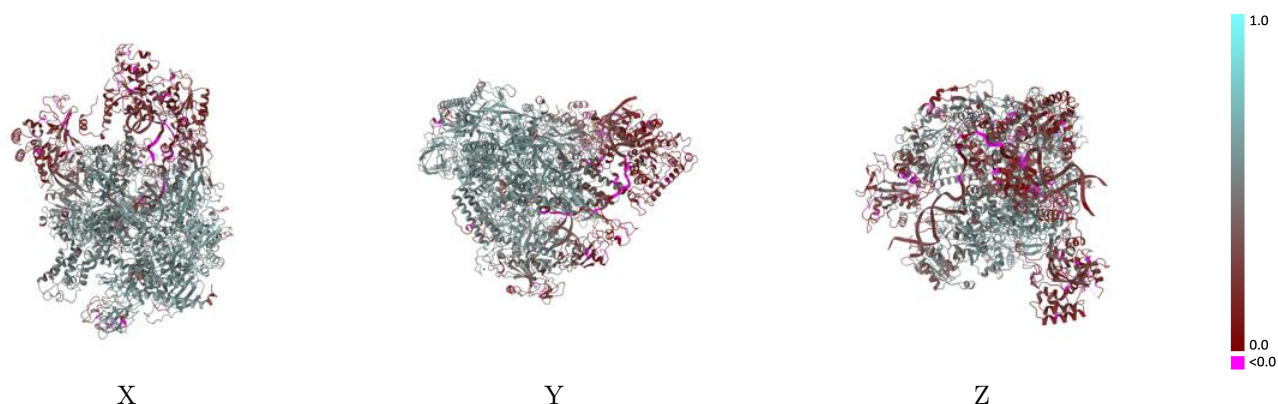
Y



Z

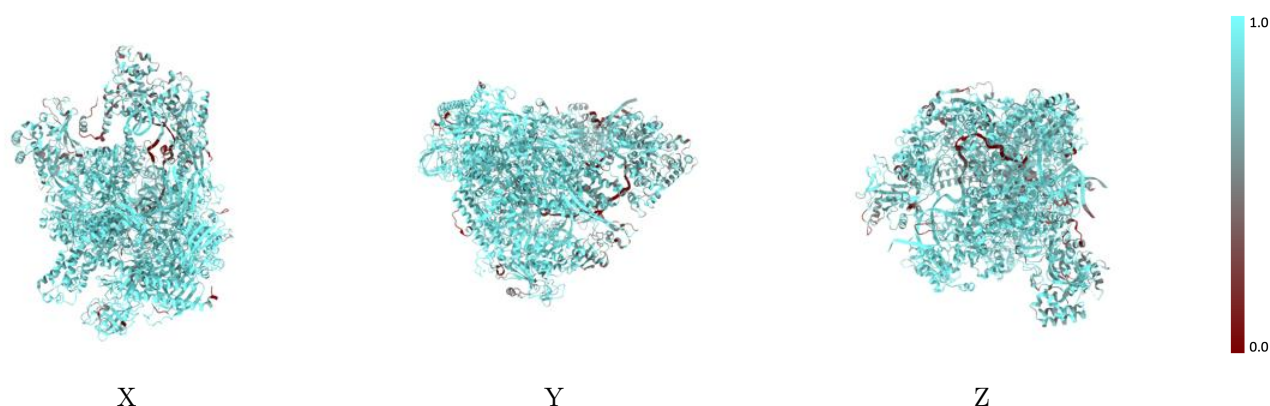
The images above show the 3D surface view of the map at the recommended contour level 0.417 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



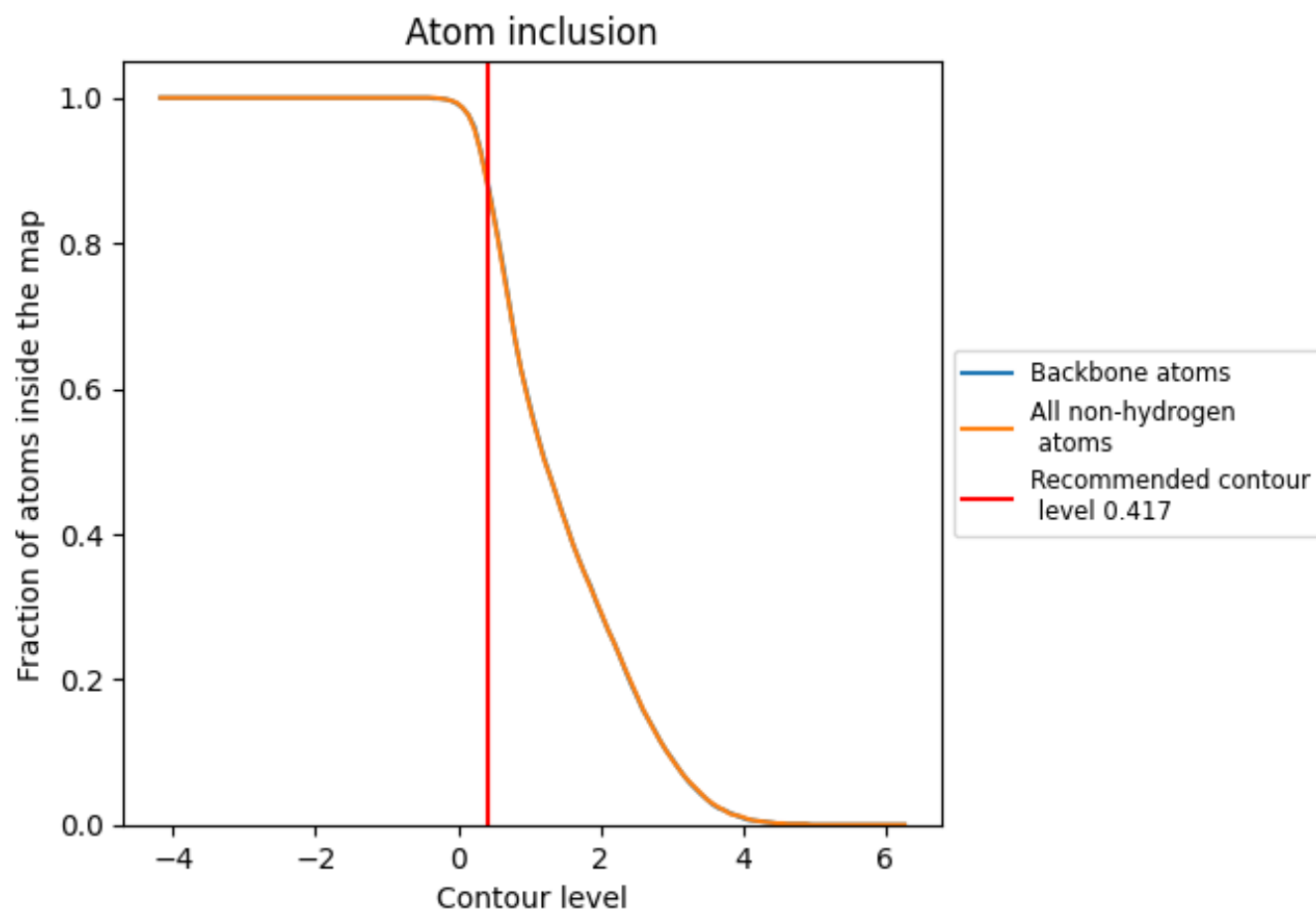
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.417).

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

