Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 01:02 am GMT

PDB ID	:	7BEF
EMDB ID	:	EMD-12156
Title	:	Structures of class II bacterial transcription complexes
Authors	:	Hao, M.; Ye, F.Z.; Zhang, X.D.
Deposited on	:	2020-12-23
Resolution	:	4.50 Å(reported)
Based on initial model	:	4YLP

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:

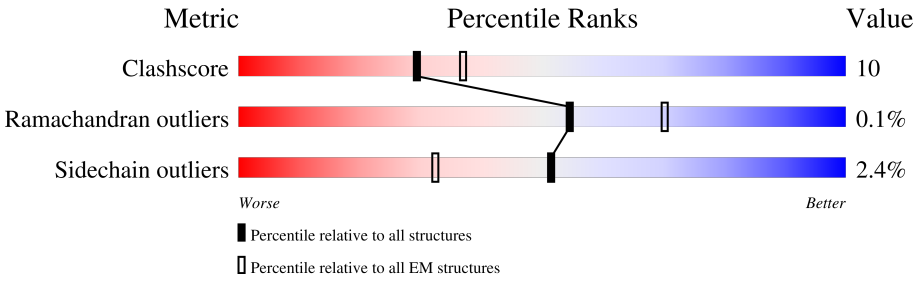
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.50 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

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	329	17% 74% 18% • 7%
1	B	329	7% 54% 15% • 31%
2	C	1342	10% 80% 19% •
3	D	1407	14% 75% 20% • •
4	E	91	75% 96% • •
5	F	630	39% 67% 12% 21%
6	G	130	5% 65% 14% • 18%
7	T	73	27% 42% 56% •

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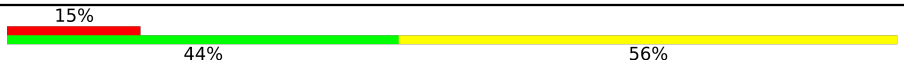
Mol	Chain	Length	Quality of chain
8	N	73	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	305	Total	C	N	O	S	0	0
			2376	1488	419	461	8		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10556	6621	1840	2052	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1362	Total	C	N	O	S	0	0
			10568	6633	1887	1998	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			708	430	136	141	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	496	Total	C	N	O	S	0	0
			4014	2508	717	766	23		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	MET	-	initiating methionine	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	ALA	-	expression tag	UNP P00579
F	-14	HIS	-	expression tag	UNP P00579
F	-13	HIS	-	expression tag	UNP P00579
F	-12	HIS	-	expression tag	UNP P00579
F	-11	HIS	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	SER	-	expression tag	UNP P00579
F	-7	SER	-	expression tag	UNP P00579
F	-6	GLY	-	expression tag	UNP P00579
F	-5	LEU	-	expression tag	UNP P00579
F	-4	GLU	-	expression tag	UNP P00579
F	-3	VAL	-	expression tag	UNP P00579
F	-2	LEU	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	GLN	-	expression tag	UNP P00579

- Molecule 6 is a protein called Transcriptional activator RamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	106	Total	C	N	O	S	0	0
			881	558	162	160	1		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	MET	-	initiating methionine	UNP Q48413
G	-15	ALA	-	expression tag	UNP Q48413
G	-14	HIS	-	expression tag	UNP Q48413
G	-13	HIS	-	expression tag	UNP Q48413
G	-12	HIS	-	expression tag	UNP Q48413
G	-11	HIS	-	expression tag	UNP Q48413
G	-10	HIS	-	expression tag	UNP Q48413
G	-9	HIS	-	expression tag	UNP Q48413
G	-8	SER	-	expression tag	UNP Q48413
G	-7	SER	-	expression tag	UNP Q48413
G	-6	GLY	-	expression tag	UNP Q48413
G	-5	LEU	-	expression tag	UNP Q48413
G	-4	GLU	-	expression tag	UNP Q48413
G	-3	VAL	-	expression tag	UNP Q48413
G	-2	LEU	-	expression tag	UNP Q48413
G	-1	PHE	-	expression tag	UNP Q48413

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLN	-	expression tag	UNP Q48413

- Molecule 7 is a DNA chain called pmicF promoter template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	73	Total	C	N	O	P	0	0
			1501	718	263	447	73		

- Molecule 8 is a DNA chain called pmicF promoter non-template DNA.

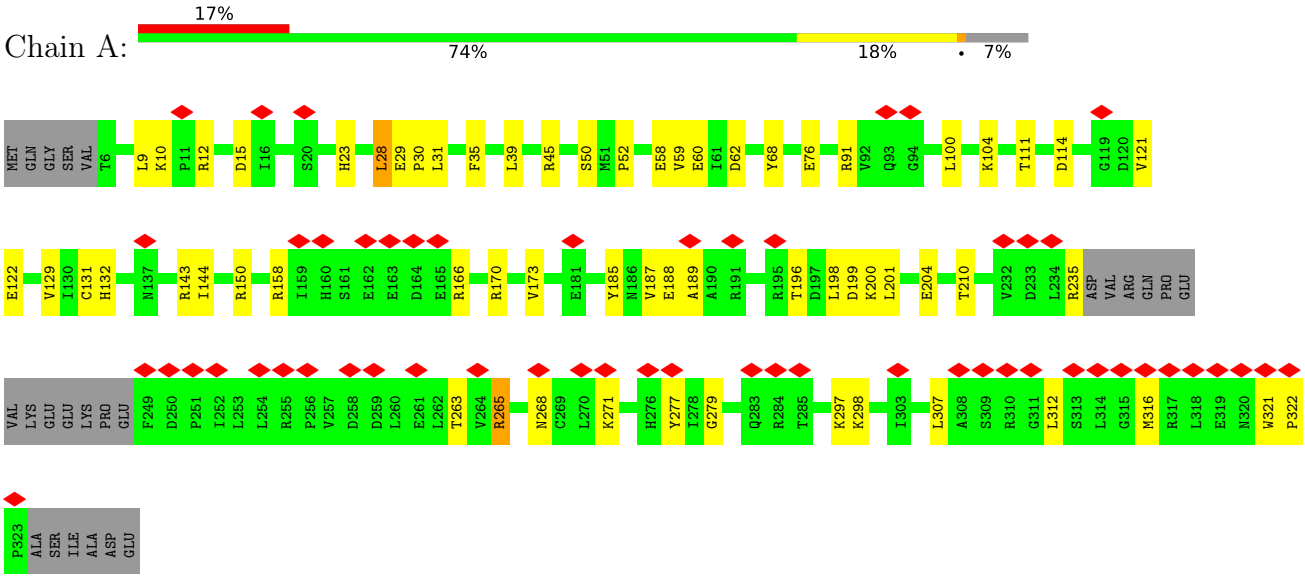
Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	73	Total	C	N	O	P	0	0
			1496	714	279	430	73		

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.

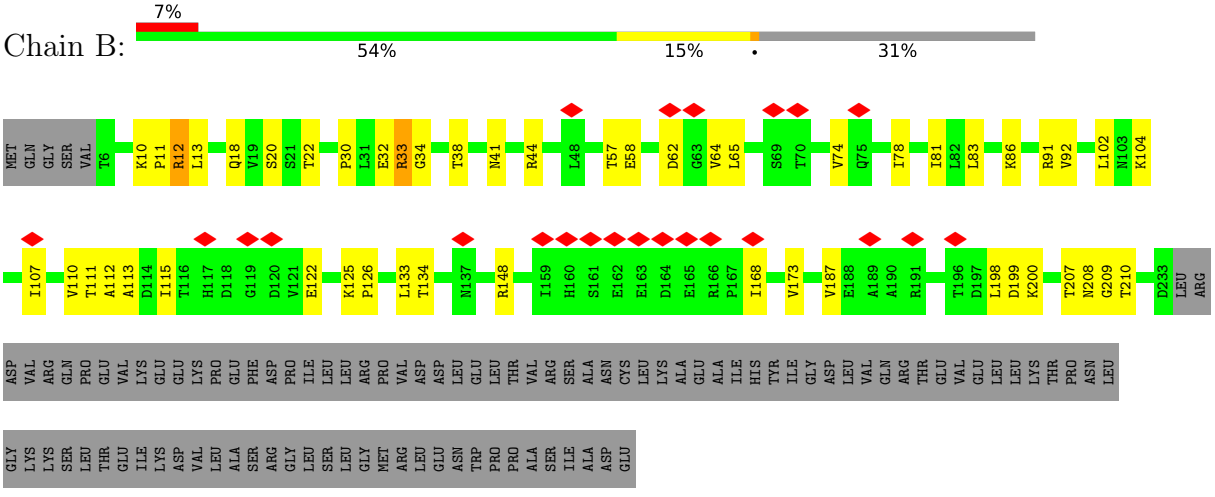
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



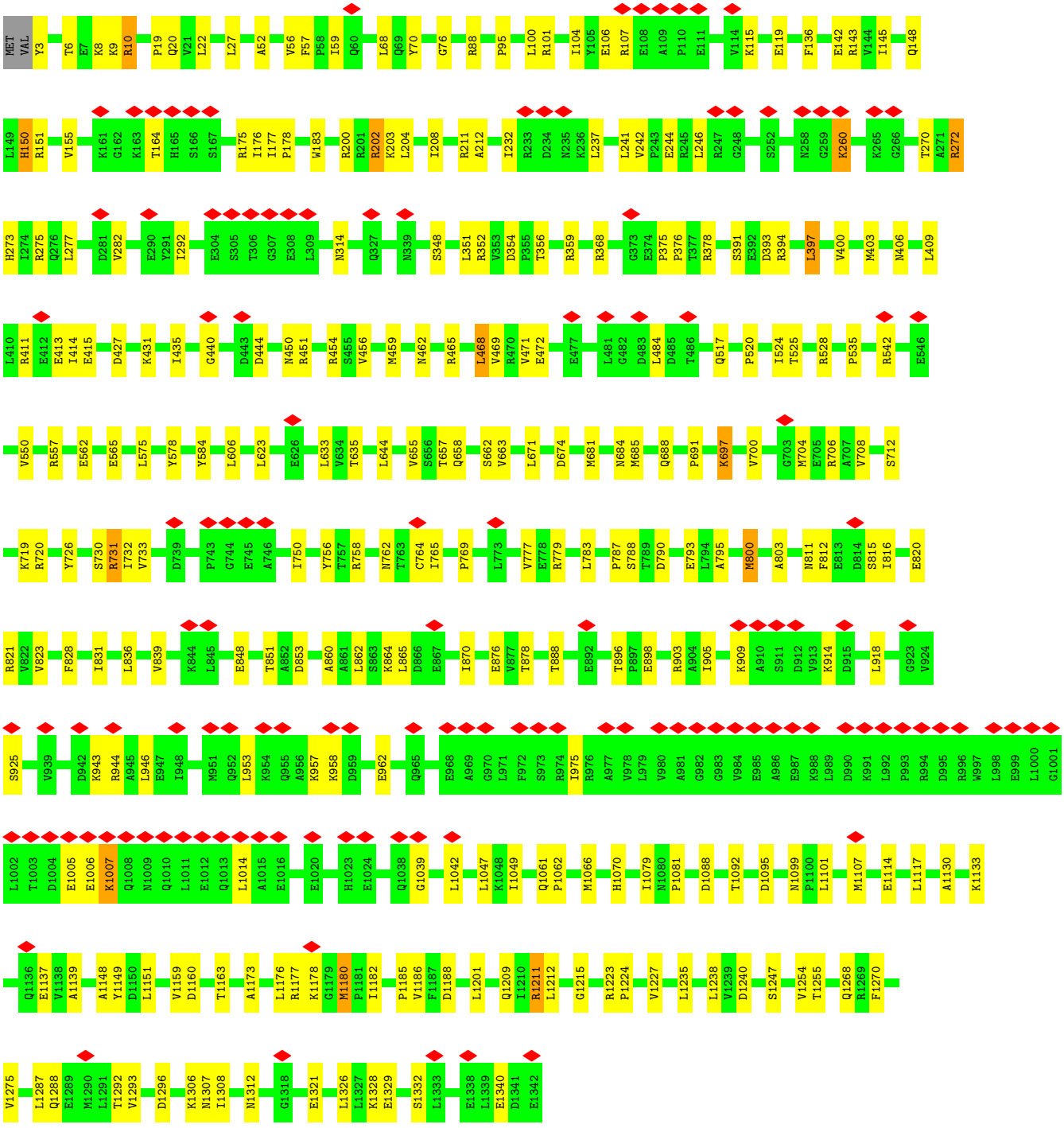
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

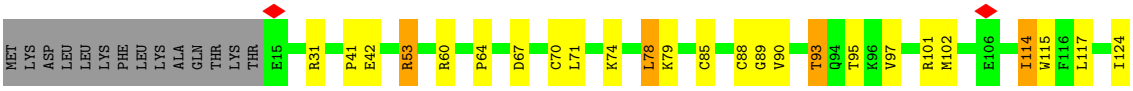


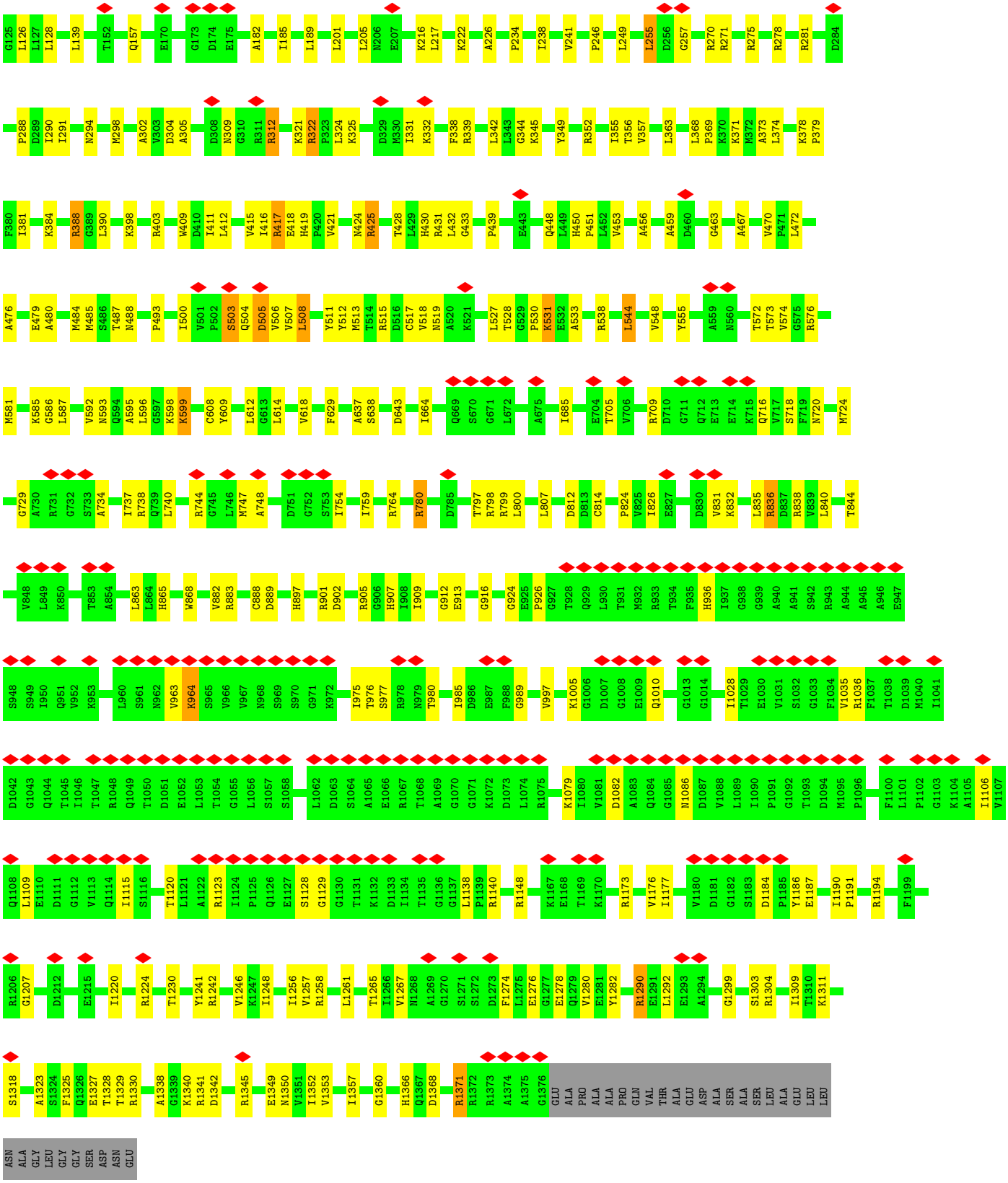
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

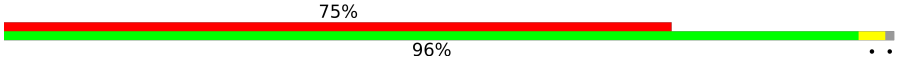


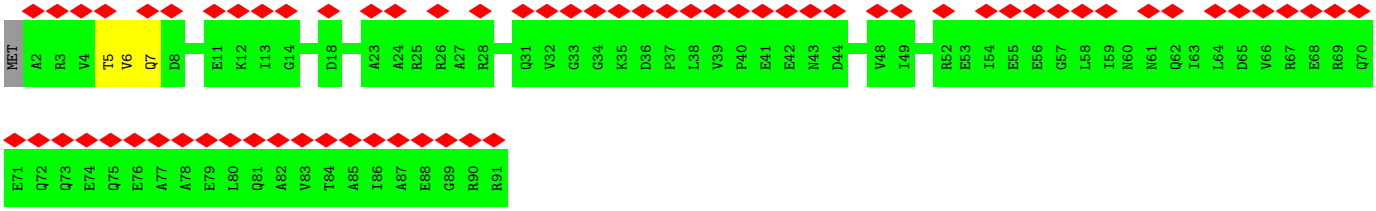
• Molecule 3: DNA-directed RNA polymerase subunit beta'





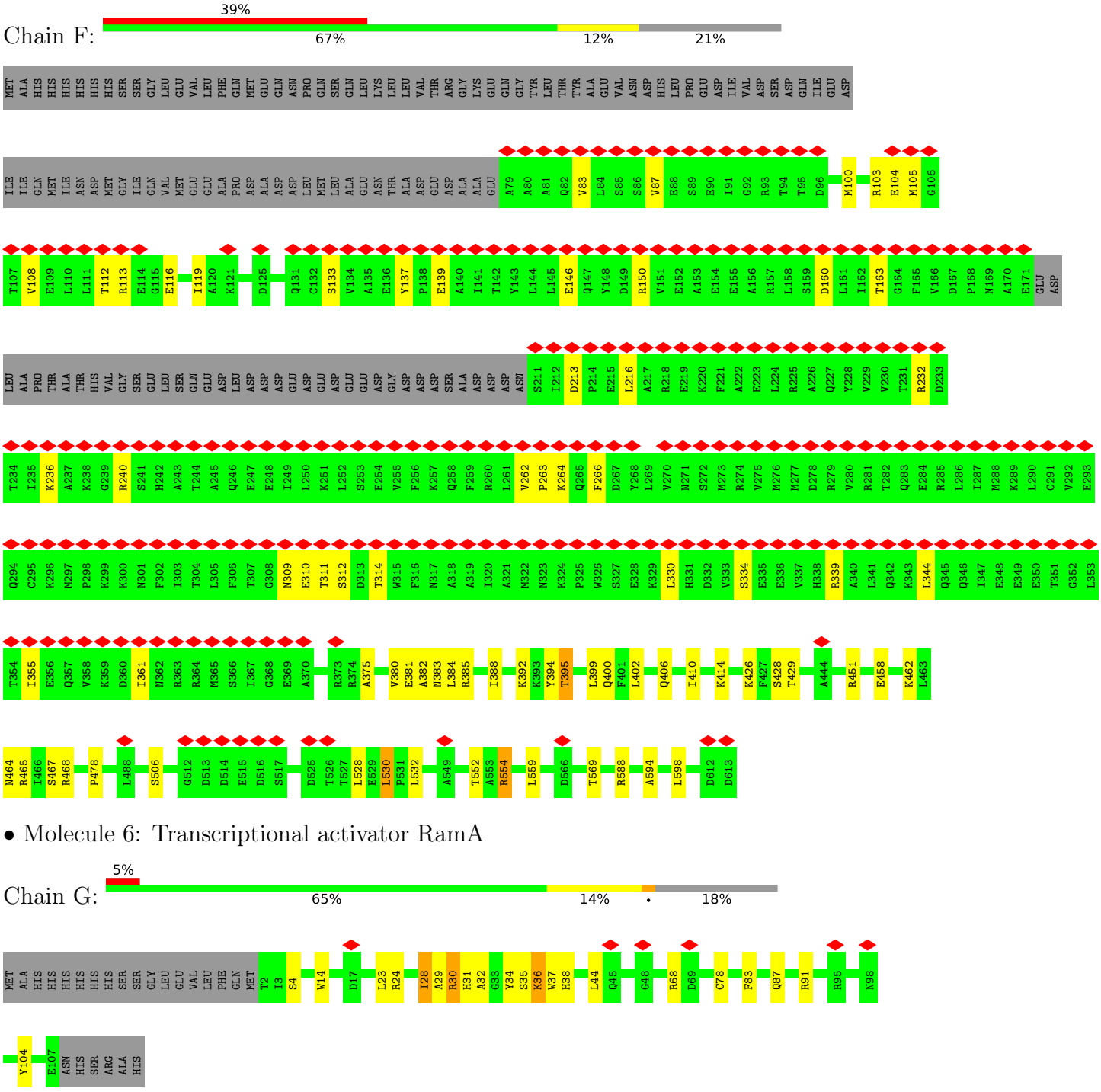
• Molecule 4: DNA-directed RNA polymerase subunit omega





• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:

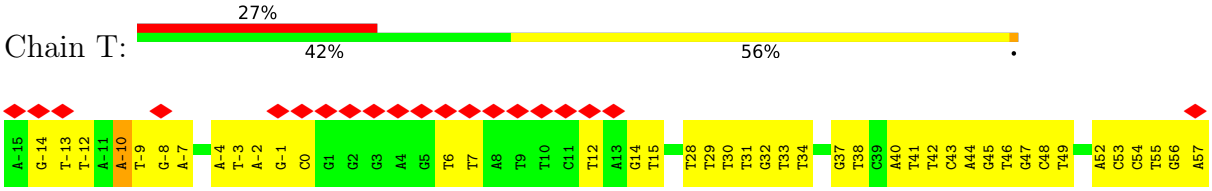


• Molecule 6: Transcriptional activator RamA

Chain G:

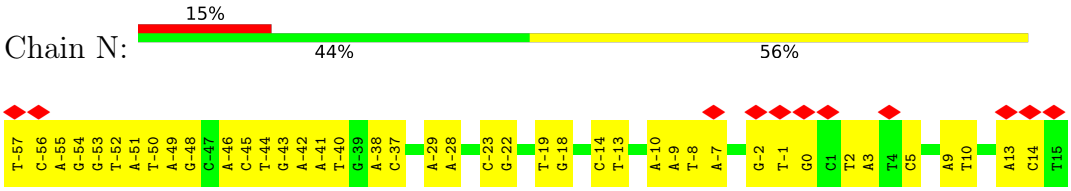
• Molecule 7: pmicF promoter template DNA

Chain T:



• Molecule 8: pmicF promoter non-template DNA

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	79.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	312.192, 312.192, 312.192	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/2407	0.44	0/3262
1	B	0.23	0/1789	0.41	0/2425
2	C	0.23	0/10723	0.40	0/14468
3	D	0.23	0/10729	0.40	0/14487
4	E	0.22	0/710	0.35	0/956
5	F	0.23	0/4068	0.37	0/5471
6	G	0.24	0/900	0.41	0/1216
7	T	0.50	0/1681	0.80	1/2595 (0.0%)
8	N	0.49	0/1680	0.79	0/2589
All	All	0.27	0/34687	0.46	1/47469 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	-10	DA	O4'-C1'-N9	5.07	111.55	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2376	0	2431	64	0
1	B	1767	0	1789	36	0
2	C	10556	0	10570	176	0
3	D	10568	0	10787	214	0
4	E	708	0	719	1	0
5	F	4014	0	4077	59	0
6	G	881	0	860	56	0
7	T	1501	0	830	95	0
8	N	1496	0	822	76	0
All	All	33867	0	32885	681	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 (681) 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)
7:T:6:DT:H72	7:T:7:DT:C5	1.42	1.54
7:T:6:DT:H72	7:T:7:DT:C6	1.52	1.43
7:T:6:DT:C7	7:T:7:DT:C5	2.00	1.42
7:T:-14:DG:H2"	7:T:-13:DT:C7	1.59	1.32
7:T:6:DT:H72	7:T:7:DT:C4	1.71	1.24
7:T:-13:DT:H2"	7:T:-12:DT:C7	1.67	1.23
6:G:24:ARG:O	6:G:28:ILE:HG12	1.39	1.20
7:T:-4:DA:C2'	7:T:-3:DT:H71	1.73	1.18
1:A:188:GLU:O	1:A:199:ASP:HB2	1.43	1.14
7:T:6:DT:C7	7:T:7:DT:C6	2.26	1.14
7:T:28:DT:C2'	7:T:29:DT:H71	1.76	1.14
7:T:28:DT:H2"	7:T:29:DT:H71	1.16	1.13
7:T:40:DA:H2'	7:T:41:DT:C7	1.78	1.12
7:T:-13:DT:C2'	7:T:-12:DT:H71	1.79	1.11
2:C:200:ARG:HH12	8:N:0:DG:N2	1.50	1.10
7:T:6:DT:C7	7:T:7:DT:C4	2.30	1.10
7:T:40:DA:C2'	7:T:41:DT:H72	1.81	1.09
7:T:40:DA:H2'	7:T:41:DT:H72	1.09	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:HB2	1:A:30:PRO:HG3	1.39	1.05
6:G:87:GLN:HE22	8:N:-37:DC:N4	1.53	1.04
7:T:45:DG:C8	7:T:46:DT:H72	1.92	1.04
7:T:-4:DA:H2"	7:T:-3:DT:C7	1.87	1.03
7:T:-14:DG:C2'	7:T:-13:DT:H71	1.90	1.00
6:G:14:TRP:CZ2	6:G:31:HIS:ND1	2.31	0.98
1:A:29:GLU:HA	1:A:31:LEU:CD2	1.94	0.98
7:T:28:DT:H2"	7:T:29:DT:C7	1.93	0.98
7:T:6:DT:H71	7:T:7:DT:C5	1.94	0.97
8:N:9:DA:H2'	8:N:10:DT:H72	1.45	0.97
6:G:14:TRP:HZ2	6:G:31:HIS:ND1	1.60	0.96
3:D:371:LYS:HA	3:D:374:LEU:CB	1.96	0.96
6:G:34:TYR:CB	6:G:38:HIS:CG	2.49	0.94
2:C:183:TRP:CB	8:N:0:DG:H22	1.81	0.94
6:G:4:SER:HB3	6:G:38:HIS:NE2	1.82	0.94
7:T:-14:DG:H2"	7:T:-13:DT:H71	0.95	0.94
6:G:23:LEU:HA	6:G:28:ILE:HD11	1.48	0.94
3:D:371:LYS:HD2	3:D:374:LEU:HD13	1.50	0.93
6:G:14:TRP:HZ2	6:G:31:HIS:HD1	1.09	0.92
7:T:40:DA:C2'	7:T:41:DT:C7	2.45	0.92
7:T:-14:DG:C2'	7:T:-13:DT:C7	2.46	0.92
7:T:-13:DT:H2"	7:T:-12:DT:H71	0.94	0.92
6:G:34:TYR:CB	6:G:38:HIS:HB3	2.00	0.91
6:G:87:GLN:NE2	8:N:-37:DC:H41	1.67	0.91
3:D:371:LYS:HA	3:D:374:LEU:HB3	1.54	0.86
6:G:34:TYR:CB	6:G:38:HIS:CB	2.53	0.86
7:T:-13:DT:C2'	7:T:-12:DT:C7	2.46	0.85
7:T:6:DT:H72	7:T:7:DT:N1	1.90	0.85
6:G:37:TRP:NE1	8:N:-48:DG:N7	2.25	0.84
7:T:-4:DA:H2"	7:T:-3:DT:H71	0.91	0.84
6:G:36:LYS:NZ	6:G:36:LYS:HB3	1.92	0.84
1:A:29:GLU:HA	1:A:31:LEU:HD22	1.60	0.84
1:A:10:LYS:CB	1:A:30:PRO:HG3	2.09	0.83
6:G:4:SER:HB3	6:G:38:HIS:CE1	2.11	0.83
2:C:200:ARG:NH1	8:N:0:DG:N2	2.27	0.83
7:T:28:DT:C2'	7:T:29:DT:C7	2.52	0.83
8:N:9:DA:C2'	8:N:10:DT:H72	2.09	0.81
6:G:23:LEU:CA	6:G:28:ILE:HD11	2.10	0.81
1:A:12:ARG:HG3	1:A:29:GLU:HG3	1.61	0.80
6:G:28:ILE:O	6:G:32:ALA:HB2	1.82	0.80
5:F:464:ASN:O	5:F:468:ARG:HG3	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:6:DT:H72	7:T:7:DT:C2	2.16	0.80
1:A:12:ARG:HD2	1:A:29:GLU:OE2	1.81	0.80
2:C:136:PHE:HB2	2:C:143:ARG:O	1.81	0.80
7:T:44:DA:C6	8:N:-43:DG:N2	2.51	0.79
6:G:87:GLN:HE22	8:N:-37:DC:H41	0.82	0.79
7:T:6:DT:H72	7:T:7:DT:N3	1.98	0.79
6:G:14:TRP:HZ2	6:G:31:HIS:CE1	2.00	0.78
7:T:32:DG:H2'	7:T:33:DT:H71	1.64	0.78
3:D:505:ASP:HA	3:D:508:LEU:HB3	1.66	0.78
8:N:9:DA:H2'	8:N:10:DT:C7	2.13	0.77
5:F:385:ARG:NH1	8:N:-8:DT:H72	2.00	0.77
3:D:371:LYS:HA	3:D:374:LEU:HB2	1.66	0.77
2:C:200:ARG:NH1	8:N:0:DG:C2	2.50	0.76
7:T:32:DG:C2'	7:T:33:DT:H71	2.15	0.76
1:A:12:ARG:CG	1:A:29:GLU:HG3	2.14	0.76
8:N:-51:DA:H2'	8:N:-50:DT:H71	1.66	0.76
8:N:-41:DA:H2'	8:N:-40:DT:H72	1.67	0.76
3:D:371:LYS:HD3	3:D:371:LYS:N	2.02	0.74
7:T:45:DG:N9	7:T:46:DT:H72	2.02	0.74
7:T:6:DT:H73	7:T:7:DT:C4	2.22	0.74
7:T:52:DA:H2"	7:T:53:DC:C5	2.22	0.74
1:A:189:ALA:HA	1:A:199:ASP:HB3	1.71	0.73
6:G:87:GLN:NE2	8:N:-37:DC:N4	2.30	0.73
6:G:35:SER:H	6:G:38:HIS:HB2	1.53	0.72
6:G:30:ARG:HA	6:G:30:ARG:HH21	1.55	0.72
6:G:37:TRP:CZ2	8:N:-48:DG:O6	2.43	0.72
2:C:1209:GLN:HG2	2:C:1224:PRO:HB2	1.72	0.71
6:G:4:SER:CB	6:G:38:HIS:CE1	2.73	0.71
7:T:28:DT:H2'	7:T:29:DT:H71	1.68	0.71
7:T:42:DT:H2"	7:T:43:DC:C5	2.26	0.71
8:N:-57:DT:H2"	8:N:-56:DC:C5	2.25	0.70
1:A:30:PRO:C	1:A:31:LEU:HD22	2.11	0.70
7:T:6:DT:H71	7:T:7:DT:C7	2.21	0.70
3:D:371:LYS:O	3:D:374:LEU:HB3	1.91	0.70
2:C:454:ARG:NH1	2:C:459:MET:SD	2.64	0.69
3:D:512:TYR:HA	3:D:515:ARG:HD3	1.73	0.69
8:N:13:DA:H2"	8:N:14:DC:C5	2.27	0.69
1:B:107:ILE:HA	1:B:133:LEU:O	1.92	0.69
6:G:35:SER:N	6:G:38:HIS:HB2	2.08	0.69
8:N:13:DA:H2"	8:N:14:DC:H5	1.57	0.68
5:F:382:ALA:O	8:N:-9:DA:H2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ARG:HH12	8:N:0:DG:H21	1.39	0.68
6:G:28:ILE:HD13	6:G:28:ILE:N	2.07	0.68
6:G:30:ARG:HA	6:G:30:ARG:NH2	2.08	0.67
7:T:37:DG:C8	7:T:38:DT:H72	2.29	0.67
2:C:56:VAL:HG11	2:C:468:LEU:HD12	1.76	0.67
3:D:332:LYS:HE3	3:D:1327:GLU:HA	1.77	0.67
3:D:902:ASP:HB2	3:D:909:ILE:HB	1.74	0.67
2:C:177:ILE:HG12	8:N:0:DG:O6	1.95	0.67
2:C:145:ILE:HG13	2:C:456:VAL:HG22	1.77	0.67
2:C:106:GLU:HG2	2:C:115:LYS:HE3	1.77	0.66
2:C:368:ARG:HE	2:C:376:PRO:HG3	1.60	0.66
3:D:371:LYS:CA	3:D:374:LEU:HB3	2.24	0.66
6:G:34:TYR:CB	6:G:38:HIS:ND1	2.58	0.66
5:F:468:ARG:HD2	7:T:12:DT:C7	2.26	0.66
7:T:-14:DG:H2"	7:T:-13:DT:H73	1.73	0.66
3:D:705:THR:HG21	3:D:716:GLN:H	1.60	0.66
1:A:91:ARG:HB2	1:A:122:GLU:HB3	1.77	0.65
3:D:117:LEU:HB3	3:D:124:ILE:HD12	1.78	0.65
8:N:9:DA:C2'	8:N:10:DT:C7	2.72	0.65
8:N:-8:DT:H2"	8:N:-7:DA:C2	2.32	0.65
2:C:200:ARG:NH1	8:N:0:DG:N3	2.44	0.65
2:C:1185:PRO:HG2	2:C:1188:ASP:HB3	1.78	0.65
1:A:31:LEU:HD22	1:A:31:LEU:N	2.11	0.65
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.70	0.64
6:G:91:ARG:NH2	7:T:38:DT:O4	2.29	0.64
3:D:384:LYS:HD2	3:D:388:ARG:HH12	1.63	0.64
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.80	0.64
7:T:-4:DA:C2'	7:T:-3:DT:C7	2.62	0.64
7:T:28:DT:H2"	7:T:29:DT:C5	2.32	0.64
3:D:373:ALA:HB1	3:D:412:LEU:HD11	1.80	0.63
2:C:435:ILE:HG12	2:C:440:GLY:HA3	1.79	0.63
6:G:35:SER:HB3	8:N:-49:DA:OP2	1.99	0.63
6:G:91:ARG:HH22	8:N:-38:DA:N6	1.95	0.63
1:A:12:ARG:HD2	1:A:29:GLU:CD	2.19	0.63
8:N:-45:DC:H2"	8:N:-44:DT:C5	2.33	0.63
1:B:30:PRO:HD3	1:B:200:LYS:HG2	1.79	0.63
6:G:36:LYS:HB3	6:G:36:LYS:HZ2	1.63	0.63
5:F:468:ARG:HD2	7:T:12:DT:H73	1.81	0.63
3:D:544:LEU:HA	3:D:574:VAL:HB	1.80	0.62
1:A:31:LEU:O	1:A:198:LEU:HD22	1.98	0.62
2:C:528:ARG:HH22	2:C:663:VAL:H	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:504:GLN:O	3:D:507:VAL:N	2.32	0.62
8:N:-51:DA:C2'	8:N:-50:DT:H71	2.29	0.62
3:D:275:ARG:NH2	5:F:400:GLN:OE1	2.33	0.62
6:G:35:SER:HB3	8:N:-49:DA:P	2.39	0.62
3:D:271:ARG:HG2	5:F:399:LEU:HD21	1.82	0.61
3:D:1207:GLY:O	3:D:1224:ARG:NH2	2.33	0.61
7:T:40:DA:H2"	7:T:41:DT:C7	2.31	0.61
2:C:6:THR:HA	2:C:9:LYS:HE2	1.83	0.61
1:B:102:LEU:HD13	1:B:115:ILE:HG13	1.81	0.61
2:C:1296:ASP:HB2	2:C:1321:GLU:HB2	1.81	0.61
8:N:-43:DG:H2"	8:N:-42:DA:C8	2.35	0.61
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.82	0.60
2:C:1061:GLN:NE2	2:C:1240:ASP:OD1	2.34	0.60
3:D:533:ALA:HB1	3:D:574:VAL:HG13	1.84	0.60
2:C:200:ARG:NH1	8:N:0:DG:H21	1.97	0.60
2:C:183:TRP:CB	8:N:0:DG:N2	2.60	0.60
1:A:28:LEU:O	1:A:31:LEU:HD21	2.02	0.60
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.34	0.60
1:B:12:ARG:NH1	1:B:13:LEU:O	2.35	0.59
2:C:454:ARG:NH2	2:C:462:ASN:OD1	2.35	0.59
3:D:85:CYS:HB3	3:D:89:GLY:H	1.68	0.59
3:D:322:ARG:NH2	5:F:506:SER:OG	2.36	0.59
6:G:91:ARG:HH22	8:N:-38:DA:H61	1.49	0.59
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.83	0.59
1:B:91:ARG:HH21	1:B:210:THR:HG22	1.68	0.59
2:C:1209:GLN:NE2	3:D:638:SER:OG	2.35	0.59
5:F:383:ASN:HA	8:N:-9:DA:C2	2.37	0.59
7:T:-13:DT:H2"	7:T:-12:DT:C5	2.35	0.59
3:D:309:ASN:ND2	3:D:324:LEU:O	2.36	0.59
3:D:374:LEU:HD12	3:D:409:TRP:HH2	1.66	0.59
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.36	0.59
5:F:530:LEU:HD13	5:F:532:LEU:HB3	1.83	0.59
1:B:57:THR:HG22	1:B:58:GLU:HG3	1.85	0.58
2:C:241:LEU:HD21	2:C:246:LEU:HD21	1.85	0.58
5:F:426:LYS:HG3	5:F:428:SER:H	1.68	0.58
5:F:462:LYS:HG2	5:F:465:ARG:HH21	1.67	0.58
2:C:765:ILE:HA	2:C:787:PRO:HB3	1.85	0.58
5:F:383:ASN:ND2	8:N:-9:DA:N1	2.51	0.58
2:C:52:ALA:HA	2:C:465:ARG:HE	1.68	0.58
7:T:48:DC:H2'	7:T:49:DT:H72	1.84	0.58
8:N:-23:DC:H2"	8:N:-22:DG:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:O	1:B:148:ARG:NH2	2.37	0.58
2:C:1292:THR:HG23	2:C:1293:VAL:HG13	1.85	0.58
8:N:2:DT:H2"	8:N:3:DA:H5'	1.84	0.58
2:C:444:ASP:O	2:C:450:ASN:ND2	2.36	0.58
3:D:31:ARG:HE	3:D:241:VAL:HG21	1.67	0.58
2:C:719:LYS:O	2:C:779:ARG:NH1	2.37	0.58
3:D:201:LEU:HD22	3:D:217:LEU:HD22	1.86	0.58
3:D:488:ASN:HA	3:D:614:LEU:HD21	1.86	0.58
3:D:390:LEU:HD12	3:D:411:ILE:HD11	1.85	0.58
2:C:528:ARG:NH1	2:C:575:LEU:O	2.37	0.57
2:C:691:PRO:HG3	2:C:788:SER:HB2	1.86	0.57
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.85	0.57
1:A:263:THR:OG1	1:A:265:ARG:NH1	2.37	0.57
1:A:50:SER:HA	1:A:150:ARG:HH21	1.69	0.57
1:A:158:ARG:NH2	1:A:173:VAL:O	2.37	0.57
1:B:44:ARG:NH2	3:D:538:ARG:O	2.36	0.57
5:F:385:ARG:NH1	8:N:-8:DT:C7	2.67	0.57
3:D:586:GLY:HA3	3:D:612:LEU:HD21	1.87	0.57
5:F:382:ALA:O	8:N:-9:DA:C2	2.56	0.57
1:B:187:VAL:HB	1:B:199:ASP:HB2	1.87	0.57
3:D:926:PRO:HG3	3:D:1248:ILE:HD11	1.87	0.57
1:A:297:LYS:CB	6:G:31:HIS:HA	2.35	0.57
3:D:1035:VAL:HG21	3:D:1115:ILE:HG12	1.87	0.57
8:N:-53:DG:H2'	8:N:-52:DT:C5	2.40	0.57
3:D:53:ARG:HB2	3:D:60:ARG:HH12	1.68	0.57
3:D:378:LYS:HG3	3:D:379:PRO:HD3	1.85	0.57
2:C:155:VAL:HG22	2:C:176:ILE:HG13	1.85	0.57
2:C:731:ARG:HH21	2:C:958:LYS:HE2	1.70	0.57
2:C:1270:PHE:O	3:D:344:GLY:CA	2.52	0.57
7:T:-14:DG:C2'	7:T:-13:DT:H73	2.30	0.57
1:A:297:LYS:O	6:G:31:HIS:CD2	2.58	0.56
1:B:91:ARG:HB3	1:B:122:GLU:HB3	1.86	0.56
8:N:-55:DA:C2	8:N:-54:DG:C6	2.93	0.56
3:D:363:LEU:HD13	3:D:618:VAL:HG13	1.87	0.56
5:F:263:PRO:HA	5:F:266:PHE:HB3	1.85	0.56
3:D:1109:LEU:HB2	3:D:1115:ILE:HG22	1.87	0.56
3:D:1177:ILE:HB	3:D:1186:TYR:HB2	1.87	0.56
5:F:458:GLU:CD	7:T:15:DT:C7	2.73	0.56
7:T:29:DT:C2'	7:T:30:DT:H72	2.36	0.56
2:C:1151:LEU:HD22	2:C:1201:LEU:HD22	1.87	0.56
1:A:235:ARG:HH12	1:B:12:ARG:HH12	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:GLN:NE2	2:C:535:PRO:O	2.39	0.56
4:E:5:THR:HG22	4:E:7:GLN:H	1.70	0.56
1:A:131:CYS:SG	1:A:132:HIS:N	2.78	0.56
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.88	0.56
7:T:30:DT:C6	7:T:31:DT:H72	2.41	0.56
3:D:513:MET:HA	3:D:544:LEU:HD13	1.88	0.56
3:D:255:LEU:HD23	3:D:257:GLY:H	1.72	0.55
3:D:278:ARG:HG2	3:D:281:ARG:HH21	1.71	0.55
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.87	0.55
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.88	0.55
3:D:1106:ILE:H	3:D:1120:THR:HG22	1.70	0.55
3:D:1191:PRO:HG2	3:D:1194:ARG:HB2	1.88	0.55
5:F:108:VAL:HG21	5:F:381:GLU:HB3	1.88	0.55
1:A:268:ASN:HA	1:A:271:LYS:HE3	1.87	0.55
2:C:3:TYR:O	2:C:8:LYS:NZ	2.39	0.55
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.88	0.55
7:T:28:DT:H2'	7:T:29:DT:C7	2.32	0.55
8:N:-46:DA:C6	8:N:-45:DC:N4	2.74	0.55
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.39	0.55
7:T:40:DA:H2'	7:T:41:DT:H73	1.82	0.55
3:D:800:LEU:HD22	3:D:1256:ILE:HD13	1.89	0.55
2:C:142:GLU:OE1	2:C:517:GLN:NE2	2.40	0.55
3:D:424:ASN:HB3	3:D:467:ALA:HB3	1.89	0.55
3:D:485:MET:HG2	3:D:487:THR:H	1.72	0.55
8:N:-13:DT:H6	8:N:-13:DT:H5'	1.72	0.55
2:C:59:ILE:HD12	2:C:472:GLU:HB2	1.88	0.55
5:F:310:GLU:HB3	5:F:355:ILE:HD13	1.89	0.55
1:A:29:GLU:HA	1:A:31:LEU:HD21	1.87	0.55
3:D:865:HIS:H	3:D:868:TRP:HD1	1.55	0.55
2:C:6:THR:OG1	2:C:706:ARG:NH1	2.40	0.54
2:C:204:LEU:HD13	2:C:208:ILE:HD13	1.89	0.54
2:C:145:ILE:HD11	2:C:456:VAL:HG13	1.89	0.54
7:T:-10:DA:H2'	7:T:-9:DT:H72	1.88	0.54
3:D:371:LYS:O	3:D:374:LEU:N	2.40	0.54
1:B:18:GLN:NE2	1:B:20:SER:O	2.41	0.54
3:D:416:ILE:HD11	3:D:439:PRO:HB2	1.88	0.54
7:T:29:DT:C6	7:T:30:DT:H72	2.42	0.54
6:G:31:HIS:ND1	6:G:31:HIS:O	2.41	0.54
1:A:52:PRO:HB3	1:A:150:ARG:HB3	1.89	0.54
2:C:270:THR:OG1	2:C:273:HIS:ND1	2.41	0.54
3:D:1241:TYR:HB3	3:D:1246:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD12	3:D:528:THR:HG23	1.90	0.54
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.90	0.54
2:C:557:ARG:NH2	2:C:606:LEU:O	2.41	0.53
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.42	0.53
3:D:599:LYS:H	3:D:599:LYS:HD3	1.74	0.53
8:N:-1:DT:C5	8:N:0:DG:H1'	2.42	0.53
3:D:1176:VAL:HG22	3:D:1187:GLU:HG2	1.89	0.53
3:D:432:LEU:HB3	3:D:456:ALA:HB1	1.89	0.53
3:D:102:MET:SD	3:D:102:MET:N	2.81	0.53
5:F:309:ASN:ND2	5:F:312:SER:H	2.07	0.53
2:C:815:SER:HB3	3:D:357:VAL:HG21	1.91	0.53
2:C:1307:ASN:HB3	2:C:1312:ASN:HB3	1.89	0.53
3:D:288:PRO:HD2	3:D:291:ILE:HD12	1.91	0.53
1:B:10:LYS:HD2	1:B:11:PRO:HD2	1.91	0.53
2:C:10:ARG:HH22	2:C:706:ARG:HH21	1.57	0.53
6:G:28:ILE:O	6:G:32:ALA:CB	2.54	0.53
7:T:28:DT:H2"	7:T:29:DT:C6	2.43	0.52
1:A:189:ALA:O	1:A:200:LYS:NZ	2.43	0.52
8:N:-46:DA:C2	8:N:-45:DC:N3	2.78	0.52
1:A:76:GLU:OE2	1:A:132:HIS:ND1	2.42	0.52
2:C:756:TYR:N	2:C:765:ILE:O	2.42	0.52
2:C:764:CYS:HB2	2:C:831:ILE:HB	1.90	0.52
5:F:410:ILE:HG22	5:F:414:LYS:HE3	1.89	0.52
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.90	0.52
3:D:814:CYS:HB2	3:D:889:ASP:HB3	1.92	0.52
5:F:458:GLU:OE2	7:T:15:DT:C7	2.57	0.52
7:T:54:DC:H2"	7:T:55:DT:C6	2.45	0.52
1:A:28:LEU:HB3	1:A:201:LEU:HB3	1.91	0.52
2:C:1254:VAL:HG23	2:C:1255:THR:HG23	1.92	0.52
8:N:-2:DG:H4'	8:N:-1:DT:C6	2.44	0.52
3:D:975:ILE:HD12	3:D:997:VAL:HG11	1.92	0.52
6:G:14:TRP:CZ2	6:G:31:HIS:CE1	2.87	0.52
3:D:42:GLU:OE2	5:F:451:ARG:NH1	2.43	0.52
1:A:297:LYS:HB2	6:G:31:HIS:HA	1.92	0.52
3:D:748:ALA:HA	3:D:754:ILE:HA	1.90	0.52
2:C:812:PHE:O	3:D:504:GLN:NE2	2.42	0.52
2:C:562:GLU:OE1	2:C:662:SER:OG	2.28	0.51
2:C:888:THR:HB	2:C:914:LYS:HB2	1.92	0.51
3:D:222:LYS:HE2	3:D:1278:GLU:HG2	1.91	0.51
6:G:4:SER:HB3	6:G:38:HIS:CD2	2.44	0.51
3:D:1005:LYS:NZ	3:D:1010:GLN:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.92	0.51
2:C:88:ARG:NH1	2:C:1039:GLY:O	2.43	0.51
2:C:413:GLU:HG2	2:C:415:GLU:H	1.75	0.51
3:D:812:ASP:O	3:D:897:HIS:ND1	2.43	0.51
3:D:126:LEU:HD22	3:D:216:LYS:HE2	1.92	0.51
3:D:836:ARG:HH12	3:D:840:LEU:HD13	1.76	0.51
3:D:290:ILE:HD12	5:F:104:GLU:HB3	1.93	0.51
3:D:305:ALA:HA	3:D:309:ASN:HA	1.92	0.51
3:D:485:MET:SD	3:D:487:THR:OG1	2.62	0.51
3:D:517:CYS:SG	3:D:518:VAL:N	2.81	0.51
1:A:307:LEU:HA	1:A:312:LEU:HD12	1.93	0.51
2:C:104:ILE:HD13	2:C:484:LEU:HB3	1.93	0.51
2:C:348:SER:OG	2:C:352:ARG:NH1	2.43	0.51
2:C:375:PRO:HB3	5:F:83:VAL:HG13	1.92	0.51
2:C:565:GLU:OE2	2:C:684:ASN:ND2	2.44	0.51
3:D:288:PRO:HG2	5:F:380:VAL:HG11	1.93	0.51
3:D:798:ARG:HH21	3:D:1325:PHE:HA	1.75	0.51
2:C:1101:LEU:HD23	3:D:505:ASP:H	1.76	0.51
3:D:41:PRO:HB2	3:D:270:ARG:HG3	1.92	0.51
3:D:531:LYS:H	3:D:531:LYS:HD2	1.76	0.51
2:C:860:ALA:O	2:C:864:LYS:NZ	2.39	0.51
3:D:814:CYS:H	3:D:883:ARG:HH22	1.59	0.51
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.93	0.50
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.93	0.50
3:D:1082:ASP:OD1	3:D:1086:ASN:N	2.44	0.50
2:C:1328:LYS:HE3	3:D:249:LEU:HD11	1.93	0.50
2:C:878:THR:HG23	2:C:925:SER:HB2	1.94	0.50
2:C:260:LYS:H	2:C:260:LYS:HD2	1.76	0.50
2:C:975:ILE:HG12	2:C:1014:LEU:HD13	1.94	0.50
2:C:1211:ARG:H	2:C:1211:ARG:HD3	1.76	0.50
3:D:205:LEU:HD21	3:D:217:LEU:HB2	1.94	0.50
3:D:294:ASN:OD1	5:F:406:GLN:NE2	2.42	0.50
5:F:385:ARG:CZ	8:N:-8:DT:H72	2.41	0.50
1:B:111:THR:OG1	1:B:126:PRO:O	2.29	0.50
2:C:905:ILE:HD11	5:F:598:LEU:HD13	1.93	0.50
3:D:476:ALA:HA	3:D:479:GLU:HG2	1.93	0.50
3:D:322:ARG:HH12	3:D:324:LEU:HD13	1.77	0.49
3:D:555:TYR:HD2	3:D:585:LYS:HB3	1.76	0.49
6:G:29:ALA:O	6:G:30:ARG:O	2.30	0.49
7:T:-14:DG:H2"	7:T:-13:DT:C5	2.41	0.49
3:D:312:ARG:H	3:D:312:ARG:HD3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:799:ARG:HB3	3:D:1309:ILE:HD13	1.95	0.49
7:T:-1:DG:N3	7:T:0:DC:H5	2.09	0.49
1:B:64:VAL:HG13	1:B:78:ILE:HD13	1.93	0.49
5:F:262:VAL:HG12	5:F:264:LYS:H	1.76	0.49
6:G:35:SER:CB	8:N:-49:DA:P	3.00	0.49
3:D:572:THR:OG1	3:D:573:THR:N	2.45	0.49
1:B:111:THR:HG23	1:B:113:ALA:H	1.78	0.49
2:C:409:LEU:HA	2:C:431:LYS:HE3	1.95	0.49
2:C:520:PRO:HD2	2:C:788:SER:HB3	1.94	0.49
3:D:352:ARG:HH11	3:D:467:ALA:HB2	1.77	0.49
3:D:1184:ASP:OD1	3:D:1184:ASP:N	2.46	0.49
5:F:588:ARG:HH22	7:T:33:DT:H2'	1.76	0.49
7:T:29:DT:H2'	7:T:30:DT:H72	1.93	0.49
2:C:68:LEU:HD21	2:C:100:LEU:HD13	1.95	0.49
2:C:803:ALA:HB2	2:C:1227:VAL:HG13	1.94	0.49
2:C:277:LEU:HD12	2:C:282:VAL:HG21	1.94	0.49
3:D:888:CYS:SG	3:D:889:ASP:N	2.85	0.49
8:N:13:DA:C4	8:N:14:DC:N4	2.81	0.49
6:G:4:SER:O	6:G:38:HIS:CE1	2.66	0.49
1:B:208:ASN:OD1	1:B:209:GLY:N	2.45	0.48
3:D:977:SER:HG	3:D:980:THR:HG1	1.51	0.48
5:F:146:GLU:OE2	5:F:150:ARG:NH2	2.46	0.48
2:C:756:TYR:HA	2:C:765:ILE:O	2.12	0.48
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.95	0.48
3:D:863:LEU:HD11	3:D:901:ARG:HB2	1.95	0.48
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.93	0.48
8:N:-14:DC:P	8:N:-13:DT:H73	2.52	0.48
3:D:511:TYR:HE1	3:D:595:ALA:HB1	1.78	0.48
3:D:889:ASP:OD2	3:D:1290:ARG:NH2	2.44	0.48
3:D:909:ILE:HD11	3:D:913:GLU:HB3	1.94	0.48
8:N:-57:DT:H2"	8:N:-56:DC:C6	2.48	0.48
8:N:-45:DC:H2"	8:N:-44:DT:C7	2.43	0.48
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.94	0.48
3:D:905:ARG:HG3	3:D:907:HIS:H	1.77	0.48
5:F:87:VAL:HG11	5:F:103:ARG:HD3	1.94	0.48
6:G:36:LYS:NZ	6:G:36:LYS:CB	2.73	0.48
1:A:166:ARG:NH2	2:C:876:GLU:OE1	2.46	0.48
1:B:65:LEU:HD22	1:B:168:ILE:HG22	1.95	0.48
3:D:298:MET:HG2	5:F:402:LEU:HD13	1.95	0.48
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.78	0.48
7:T:-8:DG:H2"	7:T:-7:DA:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1230:THR:HG23	3:D:1257:VAL:HG11	1.95	0.48
2:C:811:ASN:HB2	2:C:1099:ASN:HB2	1.95	0.48
3:D:371:LYS:CD	3:D:374:LEU:HD13	2.32	0.48
7:T:32:DG:H2"	7:T:33:DT:H71	1.93	0.48
1:A:187:VAL:HG22	1:A:201:LEU:HD13	1.95	0.48
1:A:189:ALA:HA	1:A:199:ASP:CB	2.41	0.48
3:D:342:LEU:HB3	3:D:1352:ILE:HG12	1.96	0.48
3:D:1342:ASP:OD1	3:D:1345:ARG:NE	2.39	0.48
7:T:47:DG:N2	8:N:-46:DA:C6	2.80	0.48
2:C:524:ILE:HD11	2:C:712:SER:HA	1.95	0.48
8:N:-41:DA:H2'	8:N:-40:DT:C7	2.41	0.48
2:C:777:VAL:HG21	2:C:783:LEU:HD11	1.96	0.48
3:D:368:LEU:HD13	3:D:439:PRO:HB3	1.96	0.48
5:F:392:LYS:HA	5:F:395:THR:HG23	1.95	0.48
1:A:31:LEU:CD2	1:A:31:LEU:N	2.76	0.47
1:B:107:ILE:HG23	1:B:134:THR:HA	1.95	0.47
2:C:19:PRO:HD2	2:C:623:LEU:HD12	1.95	0.47
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.95	0.47
2:C:272:ARG:H	2:C:272:ARG:HD2	1.79	0.47
3:D:508:LEU:HD11	3:D:724:MET:HB3	1.96	0.47
5:F:100:MET:SD	5:F:103:ARG:NH1	2.78	0.47
5:F:133:SER:HB3	5:F:361:ILE:HG23	1.96	0.47
7:T:37:DG:N9	7:T:38:DT:H72	2.28	0.47
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.96	0.47
2:C:756:TYR:CA	2:C:765:ILE:O	2.62	0.47
2:C:1329:GLU:O	2:C:1332:SER:OG	2.26	0.47
3:D:530:PRO:HB2	3:D:581:MET:HB2	1.95	0.47
3:D:1292:LEU:HD13	3:D:1299:GLY:HA2	1.96	0.47
2:C:816:ILE:HD12	2:C:1066:MET:HB2	1.97	0.47
3:D:1368:ASP:O	3:D:1371:ARG:HG3	2.15	0.47
7:T:-1:DG:N3	7:T:0:DC:C5	2.83	0.47
8:N:-19:DT:H2"	8:N:-18:DG:C8	2.50	0.47
3:D:832:LYS:HG2	3:D:1242:ARG:HD3	1.96	0.47
8:N:-13:DT:H5'	8:N:-13:DT:C6	2.49	0.47
1:A:12:ARG:CB	1:A:29:GLU:HG3	2.44	0.47
2:C:1176:LEU:HD22	2:C:1180:MET:HA	1.97	0.47
3:D:97:VAL:HG12	3:D:101:ARG:HD2	1.97	0.47
3:D:275:ARG:HD2	3:D:302:ALA:HB2	1.96	0.47
7:T:-1:DG:C2	7:T:0:DC:N4	2.83	0.47
8:N:-1:DT:C7	8:N:0:DG:H1'	2.45	0.47
2:C:1247:SER:HA	3:D:349:TYR:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1326:LEU:HD22	3:D:342:LEU:HD11	1.97	0.47
3:D:419:HIS:HE1	3:D:470:VAL:HG13	1.80	0.47
3:D:226:ALA:HB1	3:D:1338:ALA:HA	1.97	0.47
2:C:27:LEU:HD11	2:C:708:VAL:HG22	1.97	0.47
2:C:896:THR:OG1	2:C:898:GLU:OE1	2.32	0.47
3:D:912:GLY:O	3:D:1360:GLY:N	2.47	0.47
6:G:78:CYS:HB2	6:G:83:PHE:HB2	1.97	0.47
1:B:83:LEU:HD13	1:B:86:LYS:HD2	1.96	0.46
2:C:400:VAL:HG22	2:C:584:TYR:HD1	1.79	0.46
2:C:958:LYS:NZ	2:C:962:GLU:OE2	2.46	0.46
3:D:1282:TYR:OH	3:D:1304:ARG:NH2	2.48	0.46
1:A:28:LEU:C	1:A:31:LEU:HD21	2.35	0.46
2:C:211:ARG:HH21	2:C:351:LEU:HD22	1.80	0.46
3:D:985:ILE:HD11	3:D:989:GLY:HA2	1.97	0.46
3:D:1173:ARG:HB2	3:D:1190:ILE:HB	1.96	0.46
1:A:45:ARG:NH1	1:B:38:THR:HG1	2.13	0.46
1:A:111:THR:HG22	1:A:129:VAL:HA	1.96	0.46
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.96	0.46
2:C:719:LYS:HG3	2:C:720:ARG:HG3	1.98	0.46
3:D:139:LEU:HD21	3:D:185:ILE:HD12	1.97	0.46
3:D:643:ASP:O	3:D:720:ASN:ND2	2.47	0.46
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.48	0.46
2:C:20:GLN:NE2	2:C:22:LEU:O	2.48	0.46
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.97	0.46
2:C:943:LYS:HA	2:C:946:LEU:HD12	1.98	0.46
3:D:609:TYR:HE1	3:D:614:LEU:HD13	1.80	0.46
7:T:44:DA:H2'	7:T:45:DG:C8	2.50	0.46
2:C:848:GLU:HB3	2:C:1047:LEU:HD12	1.97	0.46
3:D:1148:ARG:NH2	8:N:5:DC:O3'	2.48	0.46
3:D:1220:ILE:HG23	3:D:1224:ARG:HH11	1.81	0.46
1:A:277:TYR:HD2	1:A:279:GLY:H	1.64	0.46
1:A:297:LYS:HE3	6:G:30:ARG:HH22	1.81	0.46
3:D:342:LEU:HD22	3:D:1352:ILE:HG23	1.98	0.46
5:F:467:SER:HB3	5:F:478:PRO:HG3	1.98	0.46
1:B:32:GLU:HG2	1:B:33:ARG:HD3	1.98	0.46
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.97	0.46
3:D:576:ARG:NH1	3:D:593:ASN:O	2.49	0.46
7:T:-1:DG:H1'	7:T:0:DC:C5	2.51	0.46
3:D:78:LEU:HD12	3:D:78:LEU:H	1.80	0.46
3:D:371:LYS:C	3:D:374:LEU:HB3	2.36	0.46
3:D:417:ARG:HD3	3:D:418:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:559:LEU:HD11	5:F:594:ALA:HB1	1.98	0.46
7:T:44:DA:H61	8:N:-44:DT:H3	1.62	0.46
7:T:48:DC:C2'	7:T:49:DT:H72	2.45	0.46
1:A:60:GLU:HB2	1:A:170:ARG:HD3	1.98	0.46
3:D:450:HIS:HD2	3:D:453:VAL:HG13	1.81	0.46
3:D:592:VAL:HG23	3:D:596:LEU:HD11	1.98	0.46
6:G:36:LYS:HB3	6:G:36:LYS:HZ3	1.77	0.46
8:N:-52:DT:H2"	8:N:-51:DA:C8	2.51	0.46
1:B:30:PRO:HB2	1:B:198:LEU:HB3	1.98	0.45
2:C:76:GLY:HA3	2:C:95:PRO:HG2	1.99	0.45
3:D:844:THR:HG22	3:D:882:VAL:HG12	1.98	0.45
3:D:863:LEU:HG	3:D:901:ARG:HH21	1.81	0.45
3:D:1267:VAL:HG13	3:D:1276:GLU:HG3	1.97	0.45
7:T:14:DG:H2"	7:T:15:DT:H5"	1.97	0.45
2:C:1288:GLN:O	2:C:1292:THR:HG22	2.16	0.45
3:D:744:ARG:HD3	3:D:759:ILE:HG21	1.98	0.45
5:F:588:ARG:NH1	7:T:34:DT:OP2	2.48	0.45
1:A:321:TRP:CD2	1:A:322:PRO:HD3	2.50	0.45
3:D:1036:ARG:HB3	3:D:1079:LYS:HB3	1.98	0.45
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.51	0.45
5:F:309:ASN:HD22	5:F:311:THR:H	1.64	0.45
1:A:45:ARG:NH1	1:B:34:GLY:O	2.42	0.45
3:D:398:LYS:HE3	5:F:532:LEU:HG	1.96	0.45
6:G:37:TRP:CH2	7:T:47:DG:O6	2.69	0.45
3:D:1340:LYS:HB3	3:D:1340:LYS:HZ2	1.81	0.45
1:A:12:ARG:HB3	1:A:29:GLU:CG	2.46	0.45
2:C:68:LEU:HD11	2:C:100:LEU:HB3	1.98	0.45
2:C:812:PHE:CE1	3:D:451:PRO:HB3	2.52	0.45
2:C:1268:GLN:HG2	3:D:352:ARG:HG2	1.99	0.45
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.98	0.45
3:D:71:LEU:HB2	3:D:90:VAL:HG21	1.99	0.45
5:F:388:ILE:HG12	5:F:392:LYS:HE2	1.99	0.45
1:A:298:LYS:HA	6:G:31:HIS:NE2	2.32	0.45
3:D:664:ILE:HD11	3:D:685:ILE:HD12	1.99	0.45
2:C:943:LYS:HD2	2:C:946:LEU:HD12	1.98	0.45
3:D:506:VAL:HG11	3:D:629:PHE:HD1	1.81	0.45
7:T:56:DG:H2"	7:T:57:DA:C8	2.52	0.45
3:D:368:LEU:HA	3:D:369:PRO:HD3	1.69	0.45
7:T:52:DA:H2"	7:T:53:DC:C6	2.51	0.45
1:B:44:ARG:HH21	3:D:538:ARG:HG3	1.82	0.44
3:D:963:VAL:HG23	3:D:975:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:68:ARG:NH2	6:G:104:TYR:OH	2.49	0.44
2:C:212:ALA:HA	2:C:359:ARG:HG3	1.99	0.44
2:C:1005:GLU:HB3	2:C:1007:LYS:HD2	1.99	0.44
3:D:182:ALA:HB1	3:D:238:ILE:HD11	1.99	0.44
3:D:1265:THR:OG1	3:D:1303:SER:OG	2.35	0.44
7:T:48:DC:C6	7:T:49:DT:H72	2.52	0.44
1:B:86:LYS:HG2	1:B:173:VAL:HG13	1.99	0.44
2:C:354:ASP:OD2	2:C:356:THR:OG1	2.31	0.44
3:D:515:ARG:NH2	3:D:718:SER:O	2.50	0.44
3:D:807:LEU:HD13	3:D:916:GLY:HA3	1.99	0.44
5:F:309:ASN:OD1	5:F:314:THR:OG1	2.35	0.44
5:F:429:THR:HG23	8:N:-10:DA:H62	1.82	0.44
7:T:29:DT:C2'	7:T:30:DT:C7	2.95	0.44
7:T:40:DA:H2"	7:T:41:DT:C6	2.51	0.44
2:C:862:LEU:HD23	2:C:865:LEU:HD12	1.99	0.44
3:D:115:TRP:HZ2	3:D:1329:THR:HG1	1.64	0.44
7:T:-1:DG:H1'	7:T:0:DC:H5	1.82	0.44
7:T:40:DA:C2'	7:T:41:DT:H73	2.39	0.44
2:C:1062:PRO:HG3	2:C:1079:ILE:HG13	2.00	0.44
3:D:70:CYS:SG	3:D:74:LYS:N	2.89	0.44
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.53	0.44
2:C:525:THR:OG1	2:C:562:GLU:OE2	2.29	0.44
2:C:697:LYS:N	2:C:790:ASP:OD2	2.50	0.44
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.99	0.44
3:D:747:MET:SD	3:D:747:MET:N	2.89	0.44
3:D:1350:ASN:HA	3:D:1353:VAL:HG22	1.99	0.44
2:C:10:ARG:HH21	2:C:793:GLU:HG3	1.81	0.44
2:C:1270:PHE:O	3:D:344:GLY:HA2	2.16	0.44
6:G:44:LEU:HD13	7:T:46:DT:OP2	2.17	0.44
2:C:151:ARG:HA	2:C:451:ARG:HA	1.99	0.44
2:C:726:TYR:H	2:C:733:VAL:HG22	1.82	0.44
3:D:128:LEU:O	3:D:157:GLN:NE2	2.51	0.44
3:D:431:ARG:HD3	3:D:493:PRO:HB3	2.00	0.44
6:G:4:SER:HB2	6:G:38:HIS:CE1	2.49	0.44
1:B:199:ASP:OD1	1:B:199:ASP:N	2.50	0.44
2:C:101:ARG:HG2	2:C:119:GLU:HB3	2.00	0.44
2:C:232:ILE:HG12	2:C:237:LEU:HD23	2.00	0.44
2:C:1005:GLU:HG2	2:C:1006:GLU:H	1.83	0.44
3:D:1129:GLY:HA3	3:D:1140:ARG:HH11	1.82	0.44
7:T:48:DC:H2"	7:T:49:DT:C6	2.53	0.44
2:C:550:VAL:HG23	3:D:780:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:554:ARG:H	5:F:554:ARG:HD3	1.83	0.43
7:T:-3:DT:H2'	7:T:-2:DA:C8	2.53	0.43
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.52	0.43
2:C:633:LEU:HB3	2:C:644:LEU:HB3	2.01	0.43
2:C:953:LEU:HD12	2:C:957:LYS:HE3	2.00	0.43
1:B:22:THR:OG1	1:B:207:THR:O	2.30	0.43
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.82	0.43
2:C:903:ARG:NH2	2:C:909:LYS:O	2.51	0.43
8:N:-52:DT:H2"	8:N:-51:DA:H8	1.83	0.43
2:C:22:LEU:HD23	2:C:22:LEU:H	1.84	0.43
2:C:788:SER:OG	2:C:795:ALA:O	2.34	0.43
3:D:67:ASP:OD1	3:D:95:THR:OG1	2.29	0.43
5:F:458:GLU:CD	7:T:15:DT:H71	2.39	0.43
1:A:59:VAL:HG23	1:A:144:ILE:HG12	2.00	0.43
2:C:663:VAL:HG11	2:C:708:VAL:HG21	1.99	0.43
2:C:823:VAL:HG21	2:C:1079:ILE:HD13	2.00	0.43
3:D:826:ILE:HG23	3:D:831:VAL:HA	2.00	0.43
5:F:160:ASP:OD1	5:F:163:THR:OG1	2.34	0.43
7:T:44:DA:C5	8:N:-43:DG:N2	2.86	0.43
3:D:503:SER:O	3:D:504:GLN:HB2	2.18	0.43
6:G:37:TRP:CD1	8:N:-49:DA:C8	3.06	0.43
7:T:6:DT:C5	7:T:7:DT:C6	3.01	0.43
2:C:178:PRO:HA	2:C:397:LEU:HD22	2.01	0.43
5:F:116:GLU:OE2	8:N:-9:DA:N6	2.51	0.43
3:D:114:ILE:HG21	3:D:304:ASP:HA	2.01	0.43
3:D:734:ALA:HA	3:D:737:ILE:HD12	2.01	0.43
3:D:1128:SER:OG	3:D:1129:GLY:N	2.51	0.43
1:A:58:GLU:OE2	1:A:170:ARG:NH1	2.46	0.43
3:D:338:PHE:HA	3:D:342:LEU:HD12	2.01	0.43
5:F:380:VAL:O	5:F:384:LEU:HG	2.18	0.43
8:N:-14:DC:P	8:N:-13:DT:C7	3.07	0.43
2:C:800:MET:HG3	2:C:828:PHE:HE2	1.84	0.42
2:C:1308:ILE:HD11	3:D:472:LEU:HB3	2.01	0.42
5:F:383:ASN:HA	8:N:-9:DA:H2	1.81	0.42
6:G:31:HIS:O	6:G:31:HIS:CG	2.70	0.42
2:C:1223:ARG:HH21	3:D:637:ALA:HB2	1.85	0.42
3:D:421:VAL:HG11	3:D:439:PRO:HG3	2.01	0.42
3:D:1274:PHE:HE1	3:D:1280:VAL:HG11	1.83	0.42
2:C:22:LEU:HD22	2:C:655:VAL:HB	2.00	0.42
2:C:150:HIS:CE1	2:C:454:ARG:HD2	2.54	0.42
2:C:391:SER:OG	2:C:393:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:-57:DT:H2”	8:N:-56:DC:H5	1.80	0.42
2:C:733:VAL:HG12	2:C:750:ILE:HD13	2.00	0.42
3:D:411:ILE:O	3:D:415:VAL:HG23	2.19	0.42
8:N:-41:DA:H2”	8:N:-40:DT:C6	2.53	0.42
1:A:23:HIS:CE1	1:A:204:GLU:HB3	2.54	0.42
5:F:112:THR:HB	5:F:113:ARG:HD2	2.01	0.42
1:A:166:ARG:HD2	1:A:170:ARG:HB3	2.02	0.42
3:D:425:ARG:HG3	3:D:459:ALA:HB2	2.02	0.42
3:D:964:LYS:O	3:D:976:THR:OG1	2.37	0.42
2:C:758:ARG:NE	2:C:762:ASN:OD1	2.52	0.42
2:C:1130:ALA:HA	2:C:1133:LYS:HE2	2.02	0.42
3:D:531:LYS:HE3	3:D:531:LYS:HB3	1.91	0.42
7:T:6:DT:C7	7:T:7:DT:C7	2.80	0.42
8:N:-53:DG:C2’	8:N:-52:DT:C6	3.03	0.42
2:C:1224:PRO:O	3:D:638:SER:OG	2.32	0.42
3:D:60:ARG:NH2	3:D:88:CYS:O	2.53	0.42
3:D:331:ILE:HG23	3:D:338:PHE:HE1	1.85	0.42
3:D:587:LEU:HD21	3:D:608:CYS:HA	2.01	0.42
6:G:23:LEU:HD22	6:G:28:ILE:HD12	2.02	0.42
1:A:15:ASP:N	1:A:15:ASP:OD1	2.52	0.42
2:C:1160:ASP:OD2	2:C:1163:THR:OG1	2.28	0.41
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	2.02	0.41
3:D:339:ARG:NH2	7:T:0:DC:OP1	2.50	0.41
8:N:-53:DG:H2’	8:N:-52:DT:C6	2.55	0.41
2:C:403:MET:HG3	2:C:414:ILE:HB	2.02	0.41
2:C:1088:ASP:CG	2:C:1092:THR:H	2.22	0.41
2:C:1107:MET:HA	3:D:740:LEU:HD21	2.01	0.41
2:C:1148:ALA:HA	2:C:1201:LEU:HD21	2.02	0.41
3:D:527:LEU:HG	3:D:548:VAL:HG11	2.02	0.41
3:D:865:HIS:HA	3:D:901:ARG:HH22	1.85	0.41
3:D:1327:GLU:HG2	3:D:1330:ARG:HB2	2.02	0.41
8:N:-29:DA:H2”	8:N:-28:DA:C8	2.54	0.41
5:F:213:ASP:OD1	5:F:216:LEU:HB3	2.21	0.41
7:T:37:DG:C2’	7:T:38:DT:H72	2.51	0.41
1:B:62:ASP:N	1:B:62:ASP:OD1	2.53	0.41
2:C:57:PHE:HD2	2:C:70:TYR:HB2	1.85	0.41
3:D:298:MET:SD	5:F:402:LEU:HB3	2.61	0.41
3:D:598:LYS:HE3	3:D:729:GLY:O	2.20	0.41
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.02	0.41
5:F:330:LEU:O	5:F:334:SER:OG	2.32	0.41
1:A:68:TYR:HE1	2:C:831:ILE:HG12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1329:GLU:HG2	3:D:331:ILE:HD11	2.01	0.41
2:C:1340:GLU:OE2	3:D:1341:ARG:NH2	2.53	0.41
5:F:236:LYS:HD3	5:F:240:ARG:HH12	1.85	0.41
3:D:64:PRO:HG3	3:D:93:THR:H	1.84	0.41
1:A:104:LYS:HB2	1:A:114:ASP:HB3	2.03	0.41
3:D:1261:LEU:HB3	3:D:1304:ARG:HD3	2.03	0.41
7:T:37:DG:H2'	7:T:38:DT:H72	2.02	0.41
2:C:657:THR:OG1	2:C:1186:VAL:O	2.26	0.41
3:D:1318:SER:OG	3:D:1349:GLU:OE2	2.32	0.41
1:A:28:LEU:O	1:A:31:LEU:CD2	2.68	0.41
1:A:188:GLU:O	1:A:199:ASP:CB	2.37	0.41
1:B:74:VAL:HG11	1:B:81:ILE:HD11	2.03	0.41
2:C:469:VAL:HA	2:C:472:GLU:HG2	2.03	0.41
2:C:851:THR:HG22	2:C:853:ASP:H	1.85	0.41
2:C:1173:ALA:O	2:C:1177:ARG:HG3	2.21	0.41
2:C:1212:LEU:HD21	2:C:1227:VAL:HG21	2.03	0.41
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	2.02	0.41
3:D:480:ALA:HA	3:D:484:MET:HG2	2.03	0.41
2:C:578:TYR:OH	2:C:658:GLN:NE2	2.52	0.41
3:D:356:THR:HB	3:D:448:GLN:HG2	2.03	0.41
3:D:976:THR:HG22	3:D:1028:ILE:HD13	2.03	0.41
1:A:321:TRP:N	1:A:322:PRO:HD2	2.36	0.40
2:C:242:VAL:HG12	2:C:244:GLU:HG2	2.02	0.40
2:C:730:SER:OG	2:C:731:ARG:NH1	2.54	0.40
2:C:821:ARG:NH2	2:C:1095:ASP:OD2	2.54	0.40
1:A:62:ASP:OD1	1:A:62:ASP:N	2.54	0.40
1:A:91:ARG:HD3	1:A:210:THR:HA	2.02	0.40
1:A:297:LYS:HG3	6:G:30:ARG:O	2.22	0.40
2:C:431:LYS:HE2	2:C:431:LYS:HB2	1.96	0.40
3:D:518:VAL:HG12	3:D:519:ASN:H	1.86	0.40
7:T:54:DC:C2'	7:T:55:DT:H71	2.51	0.40
8:N:-8:DT:H2"	8:N:-7:DA:N3	2.37	0.40
1:B:86:LYS:HE2	1:B:173:VAL:HG13	2.03	0.40
2:C:391:SER:HB3	2:C:394:ARG:HB3	2.02	0.40
2:C:870:ILE:HB	2:C:944:ARG:HE	1.86	0.40
2:C:1117:LEU:HG	2:C:1182:ILE:HG21	2.04	0.40
3:D:324:LEU:HD22	3:D:324:LEU:H	1.86	0.40
3:D:450:HIS:CD2	3:D:453:VAL:HG13	2.56	0.40
8:N:-49:DA:C2	8:N:-48:DG:C6	3.10	0.40
1:A:35:PHE:HB3	1:A:39:LEU:HD13	2.03	0.40
1:A:58:GLU:HG2	1:A:170:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:ARG:NH1	2:C:203:LYS:O	2.55	0.40
2:C:681:MET:O	2:C:685:MET:HG2	2.22	0.40
3:D:79:LYS:HZ3	5:F:569:THR:HA	1.86	0.40
3:D:356:THR:HB	3:D:448:GLN:HA	2.03	0.40
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.41	0.40
3:D:355:ILE:HD11	3:D:463:GLY:H	1.87	0.40
3:D:504:GLN:C	3:D:506:VAL:N	2.75	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	301/329 (92%)	294 (98%)	7 (2%)	0	100	100
1	B	226/329 (69%)	218 (96%)	8 (4%)	0	100	100
2	C	1338/1342 (100%)	1293 (97%)	45 (3%)	0	100	100
3	D	1360/1407 (97%)	1298 (95%)	59 (4%)	3 (0%)	47	81
4	E	88/91 (97%)	86 (98%)	2 (2%)	0	100	100
5	F	492/630 (78%)	473 (96%)	19 (4%)	0	100	100
6	G	104/130 (80%)	96 (92%)	7 (7%)	1 (1%)	15	54
All	All	3909/4258 (92%)	3758 (96%)	147 (4%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	30	ARG
3	D	505	ASP
3	D	78	LEU
3	D	503	SER

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	265/286 (93%)	260 (98%)	5 (2%)	57 75
1	B	196/286 (68%)	193 (98%)	3 (2%)	65 80
2	C	1153/1157 (100%)	1126 (98%)	27 (2%)	50 70
3	D	1135/1168 (97%)	1102 (97%)	33 (3%)	42 64
4	E	74/75 (99%)	73 (99%)	1 (1%)	67 81
5	F	438/555 (79%)	428 (98%)	10 (2%)	50 70
6	G	92/116 (79%)	90 (98%)	2 (2%)	52 71
All	All	3353/3643 (92%)	3272 (98%)	81 (2%)	51 69

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	28	LEU
1	A	143	ARG
1	A	265	ARG
1	A	316	MET
1	B	12	ARG
1	B	33	ARG
1	B	125	LYS
2	C	10	ARG
2	C	107	ARG
2	C	150	HIS
2	C	164	THR
2	C	175	ARG
2	C	202	ARG
2	C	260	LYS
2	C	272	ARG
2	C	275	ARG
2	C	314	ASN
2	C	378	ARG
2	C	397	LEU

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Mol	Chain	Res	Type
2	C	468	LEU
2	C	542	ARG
2	C	635	THR
2	C	671	LEU
2	C	697	LYS
2	C	704	MET
2	C	731	ARG
2	C	800	MET
2	C	1007	LYS
2	C	1042	LEU
2	C	1178	LYS
2	C	1180	MET
2	C	1211	ARG
2	C	1238	LEU
2	C	1306	LYS
3	D	53	ARG
3	D	93	THR
3	D	114	ILE
3	D	255	LEU
3	D	312	ARG
3	D	321	LYS
3	D	322	ARG
3	D	325	LYS
3	D	345	LYS
3	D	388	ARG
3	D	403	ARG
3	D	417	ARG
3	D	425	ARG
3	D	500	ILE
3	D	508	LEU
3	D	531	LYS
3	D	544	LEU
3	D	599	LYS
3	D	709	ARG
3	D	738	ARG
3	D	764	ARG
3	D	780	ARG
3	D	836	ARG
3	D	838	ARG
3	D	936	HIS
3	D	964	LYS
3	D	1123	ARG

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Mol	Chain	Res	Type
3	D	1138	LEU
3	D	1258	ARG
3	D	1290	ARG
3	D	1311	LYS
3	D	1366	HIS
3	D	1371	ARG
4	E	6	VAL
5	F	105	MET
5	F	232	ARG
5	F	339	ARG
5	F	344	LEU
5	F	394	TYR
5	F	395	THR
5	F	528	LEU
5	F	530	LEU
5	F	552	THR
5	F	554	ARG
6	G	28	ILE
6	G	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	658	GLN
3	D	419	HIS
3	D	450	HIS
5	F	309	ASN
6	G	87	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

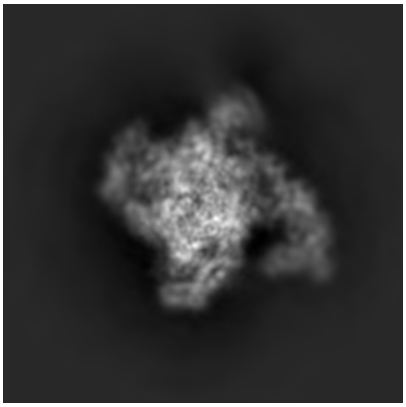
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12156. These allow visual inspection of the internal detail of the map and identification of artifacts.

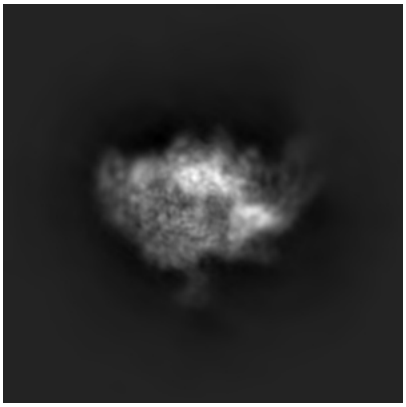
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

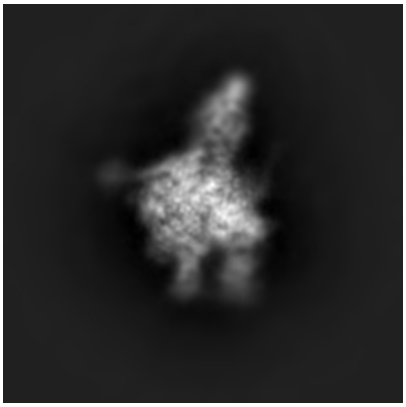
6.1.1 Primary map



X



Y

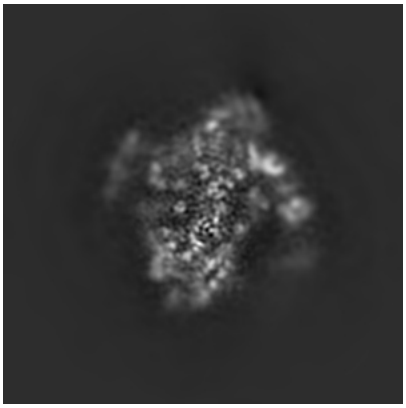


Z

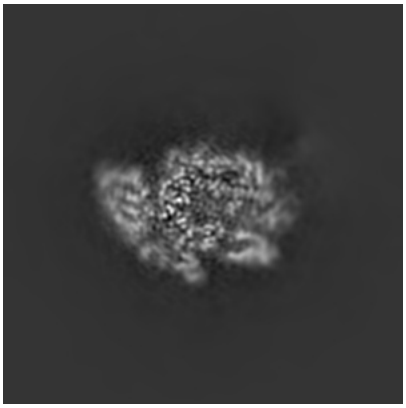
The images above show the map projected in three orthogonal directions.

6.2 Central slices

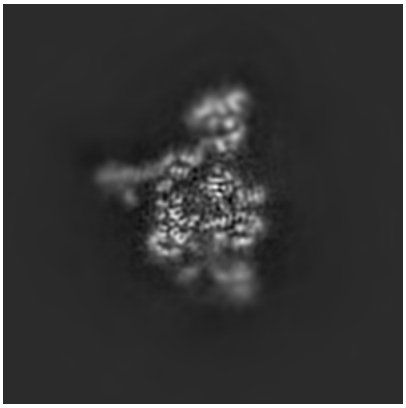
6.2.1 Primary map



X Index: 144



Y Index: 144

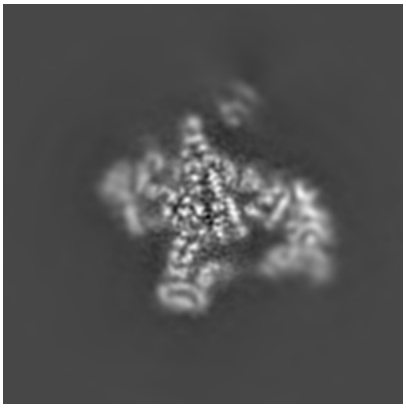


Z Index: 144

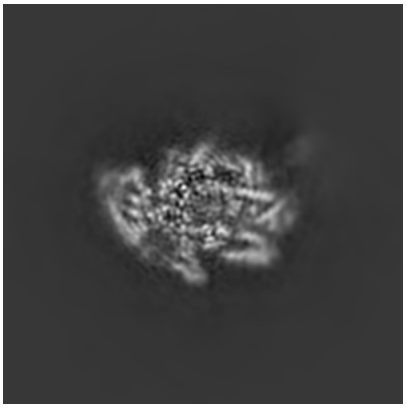
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

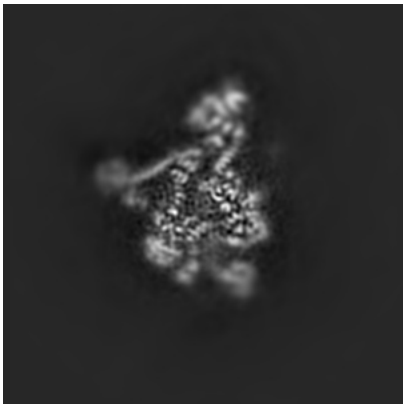
6.3.1 Primary map



X Index: 162



Y Index: 146

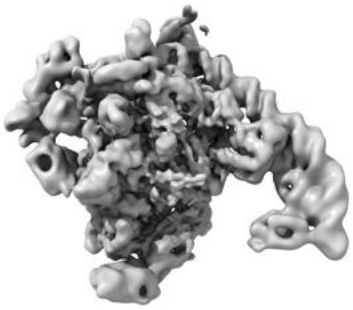


Z Index: 140

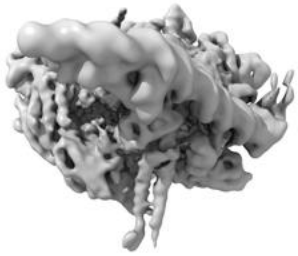
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

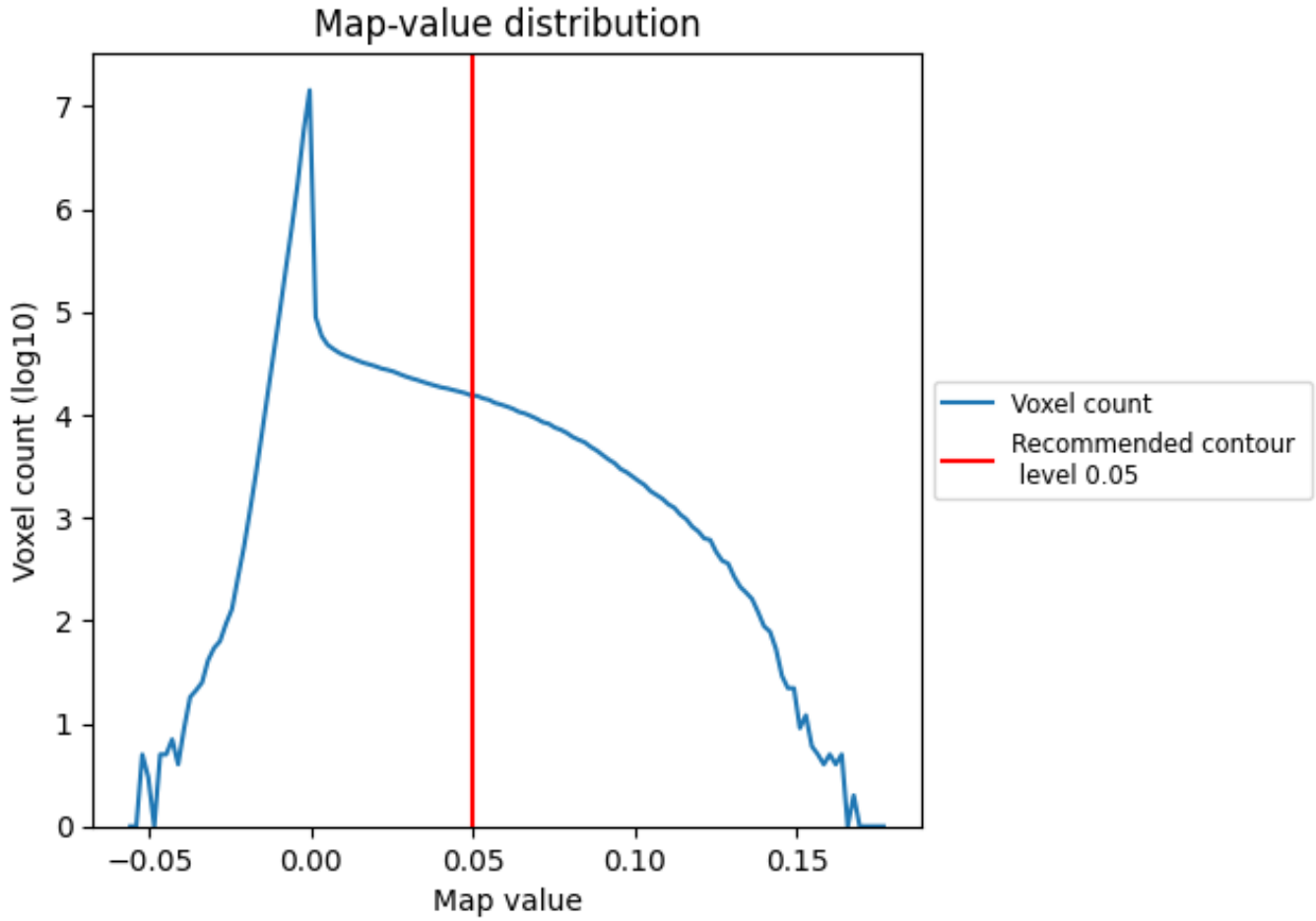
6.5 Mask visualisation (i)

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

7 Map analysis

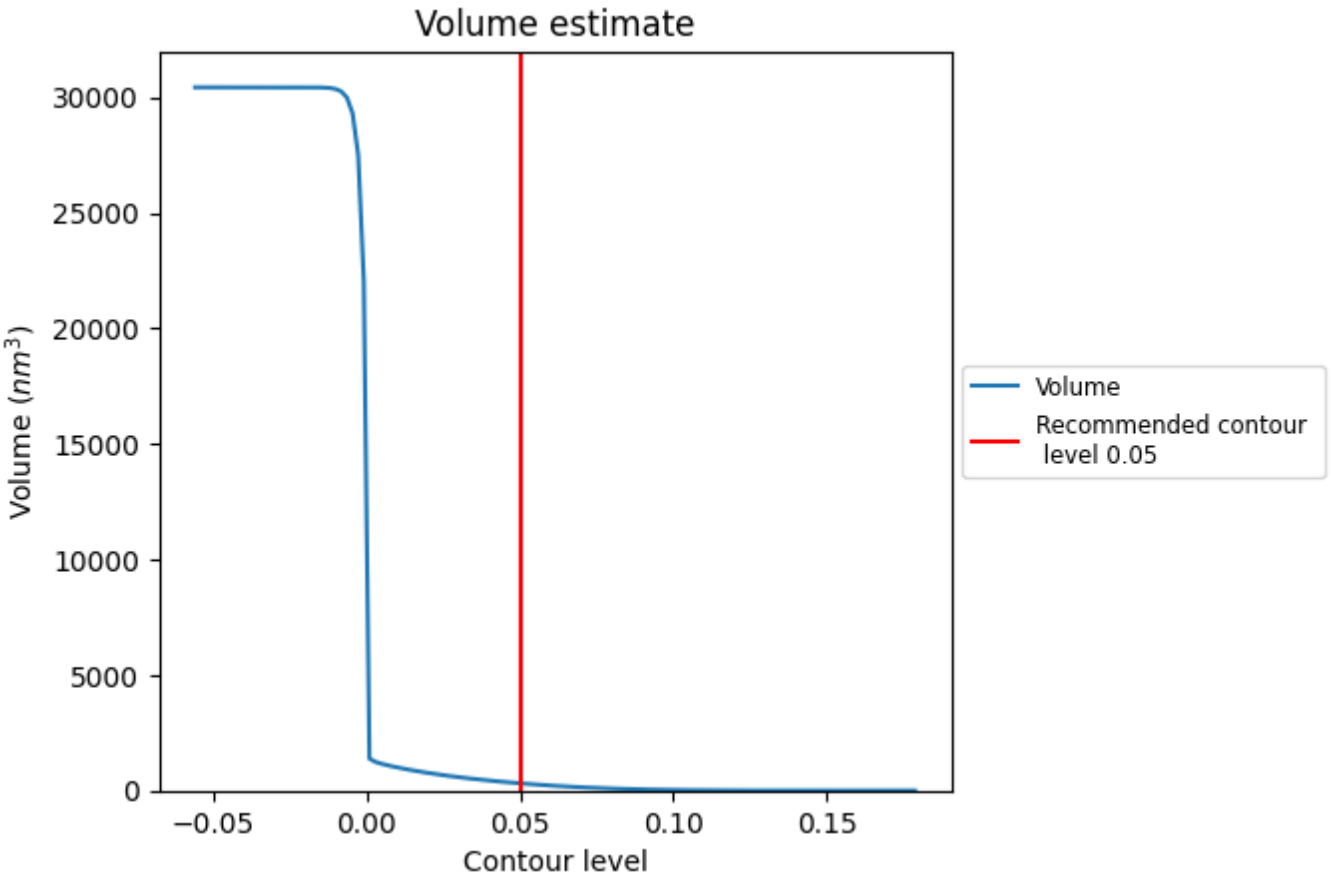
This section contains the results of statistical analysis of the map.

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.

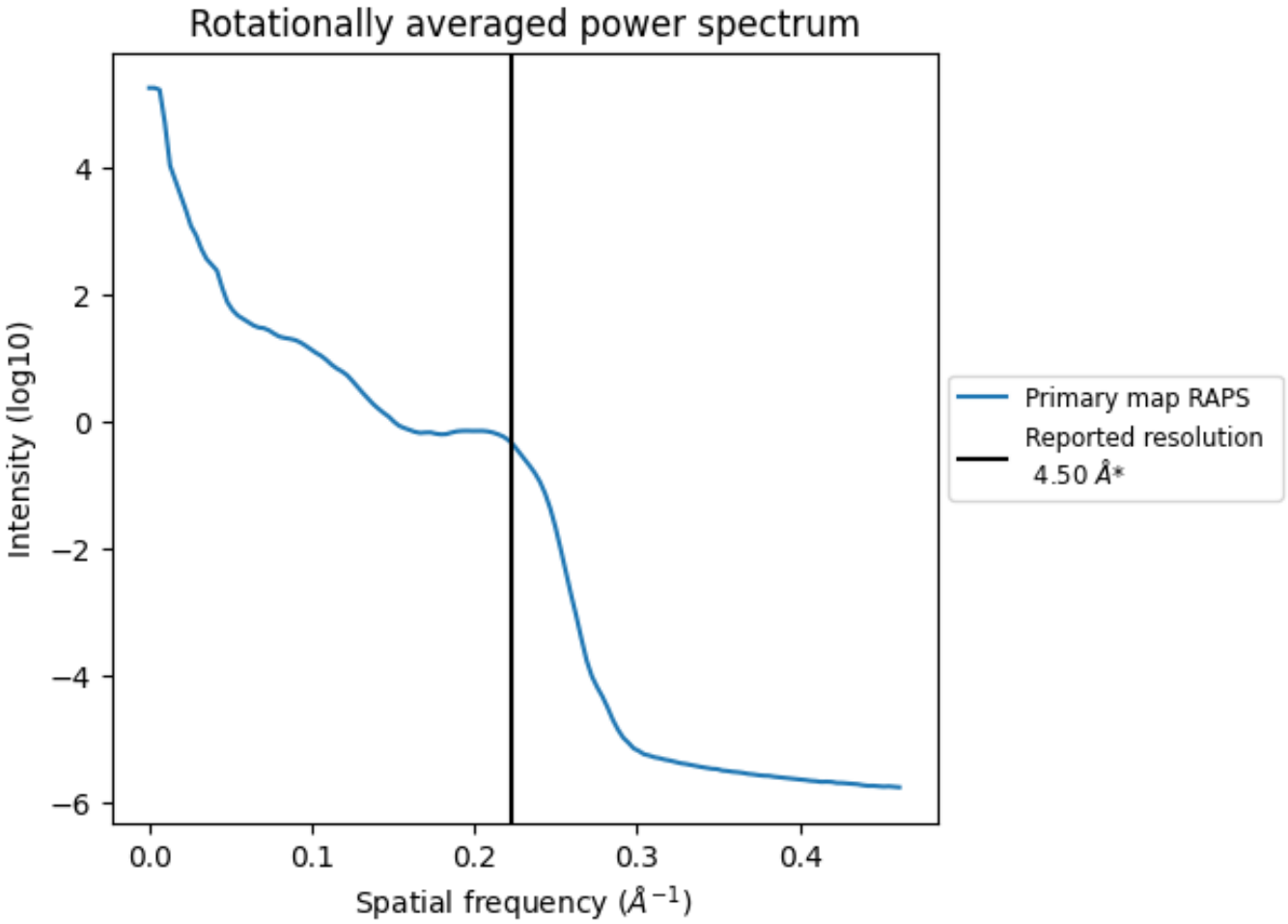
7.2 Volume estimate



The volume at the recommended contour level is 314 nm^3; this corresponds to an approximate mass of 283 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 0.222 Å^{-1}

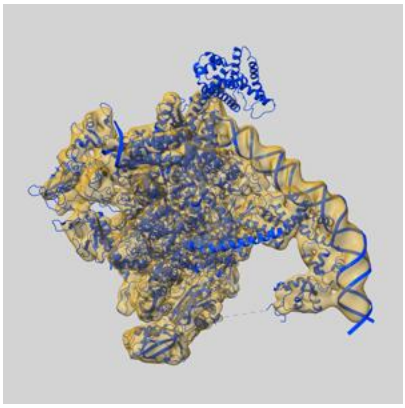
8 Fourier-Shell correlation

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

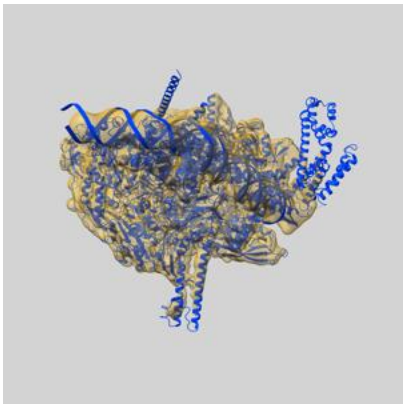
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12156 and PDB model 7BEF. Per-residue inclusion information can be found in section 3 on page 7.

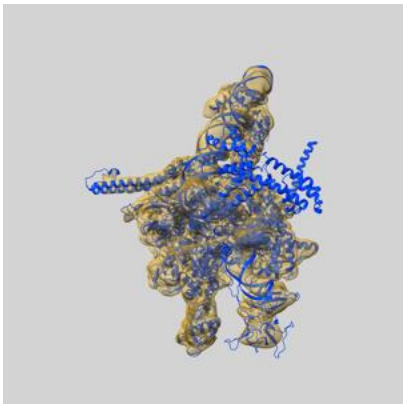
9.1 Map-model overlay



X



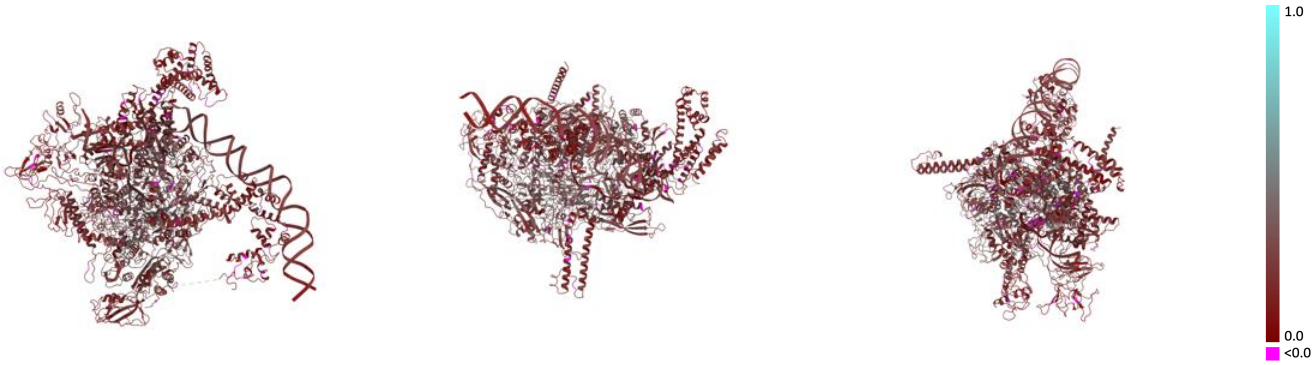
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

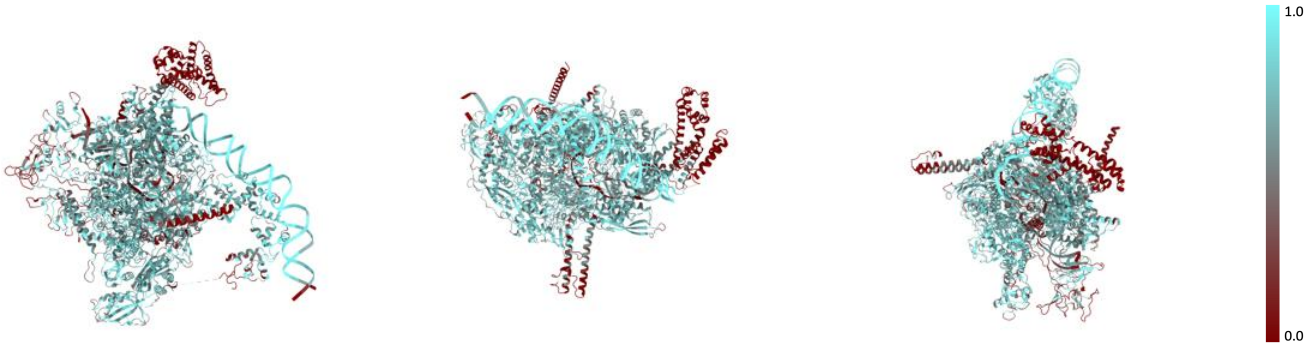
9.2 Q-score mapped to coordinate model (i)



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.

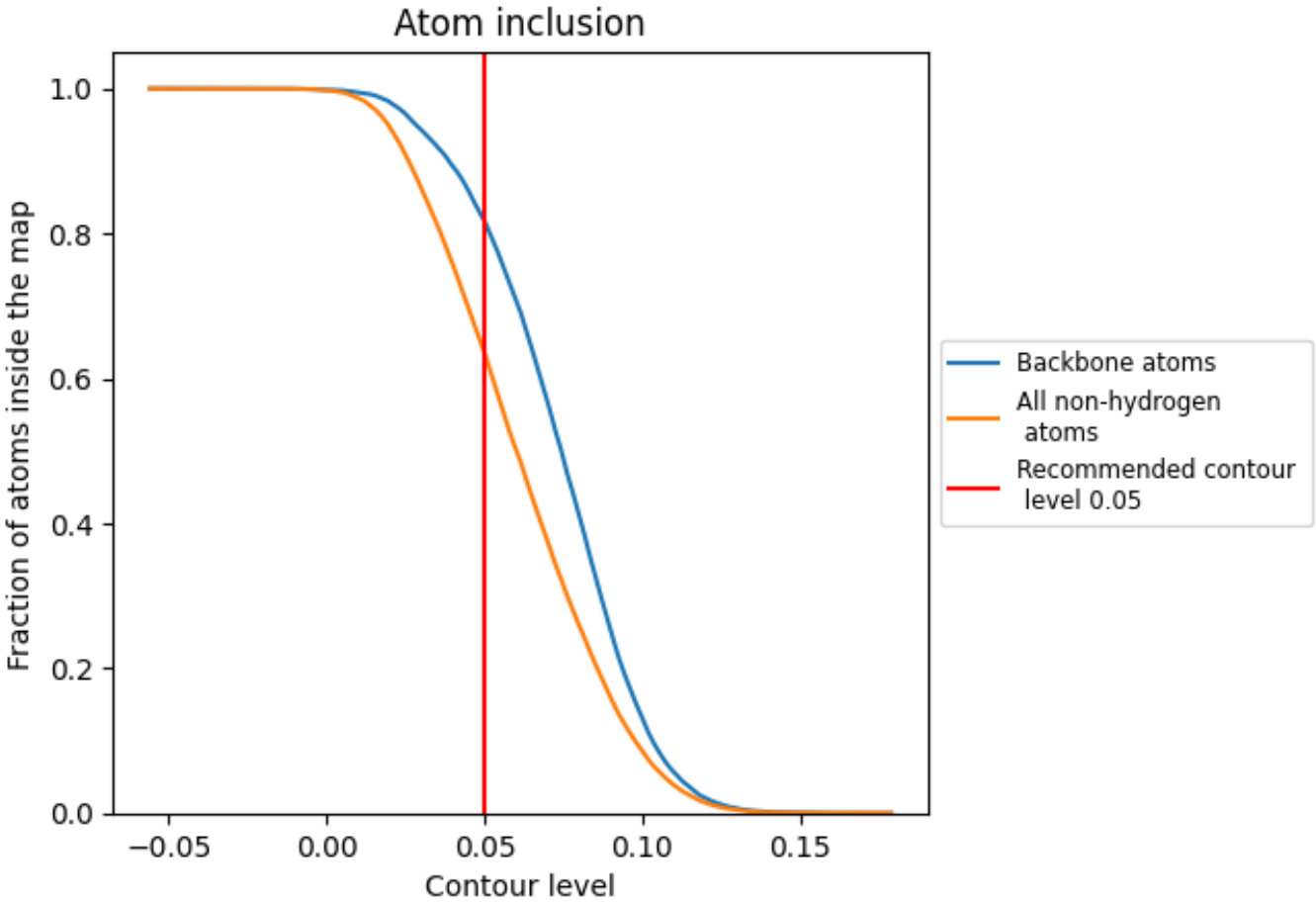
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 63% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6345	0.2290
A	0.6488	0.2200
B	0.7083	0.2130
C	0.6959	0.2630
D	0.6521	0.2360
E	0.2326	0.2160
F	0.3842	0.1760
G	0.7746	0.1420
N	0.7507	0.2160
T	0.6236	0.1950