Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 07:57 PM EDT

PDB ID	:	6EDT
EMDB ID	:	EMD-9037
Title	:	Mycobacterium tuberculosis RNAP open promoter complex with RbpA/CarD and AP3 promoter
Authors	:	Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.
Deposited on	:	2018-08-10
Resolution	:	3.60 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:

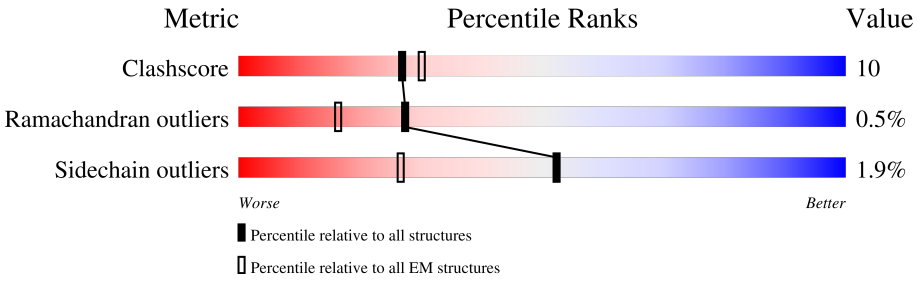
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	347	57% 7% • 35%
1	B	347	56% 12% 32%
2	C	1134	81% 16% • •
3	D	1371	75% 16% • 7%
4	E	110	62% 13% • 25%
5	F	531	54% 6% 39%
6	J	111	84% 13% • •
7	O	90	40% 32% 28%

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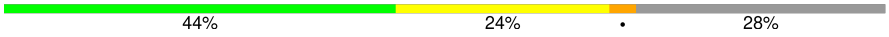
Mol	Chain	Length	Quality of chain
8	P	90	
9	M	162	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29979 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	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8606	5392	1511	1664	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-46	ASP	-	expression tag	UNP A5U053
D	-45	GLY	-	expression tag	UNP A5U053
D	-44	ALA	-	expression tag	UNP A5U053
D	-43	ALA	-	expression tag	UNP A5U053
D	-42	ILE	-	expression tag	UNP A5U053
D	-41	GLU	-	expression tag	UNP A5U053
D	-40	LEU	-	expression tag	UNP A5U053
D	-39	ARG	-	expression tag	UNP A5U053
D	-38	GLU	-	expression tag	UNP A5U053
D	-37	GLY	-	expression tag	UNP A5U053
D	-36	GLU	-	expression tag	UNP A5U053
D	-35	ASP	-	expression tag	UNP A5U053
D	-34	GLU	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-33	ASP	-	expression tag	UNP A5U053
D	-32	LEU	-	expression tag	UNP A5U053
D	-31	GLU	-	expression tag	UNP A5U053
D	-30	ARG	-	expression tag	UNP A5U053
D	-29	ALA	-	expression tag	UNP A5U053
D	-28	ALA	-	expression tag	UNP A5U053
D	-27	ALA	-	expression tag	UNP A5U053
D	-26	ASN	-	expression tag	UNP A5U053
D	-25	LEU	-	expression tag	UNP A5U053
D	-24	GLY	-	expression tag	UNP A5U053
D	-23	ILE	-	expression tag	UNP A5U053
D	-22	ASN	-	expression tag	UNP A5U053
D	-21	LEU	-	expression tag	UNP A5U053
D	-20	SER	-	expression tag	UNP A5U053
D	-19	ARG	-	expression tag	UNP A5U053
D	-18	ASN	-	expression tag	UNP A5U053
D	-17	GLU	-	expression tag	UNP A5U053
D	-16	SER	-	expression tag	UNP A5U053
D	-15	ALA	-	expression tag	UNP A5U053
D	-14	SER	-	expression tag	UNP A5U053
D	-13	VAL	-	expression tag	UNP A5U053
D	-12	GLU	-	expression tag	UNP A5U053
D	-11	ASP	-	expression tag	UNP A5U053
D	-10	LEU	-	expression tag	UNP A5U053
D	-9	ALA	-	expression tag	UNP A5U053
D	-8	LEU	-	expression tag	UNP A5U053
D	-7	ALA	-	expression tag	UNP A5U053
D	-6	ARG	-	expression tag	UNP A5U053
D	-5	HIS	-	expression tag	UNP A5U053
D	-4	GLY	-	expression tag	UNP A5U053
D	-3	GLY	-	expression tag	UNP A5U053
D	-2	SER	-	expression tag	UNP A5U053
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total 649	C 414	N 108	O 127	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	322	Total 2540	C 1583	N 459	O 489	S 9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	109	Total 880	C 543	N 166	O 168	S 3	0	0

- Molecule 7 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	65	Total 1336	C 633	N 243	O 395	P 65	0	0

- Molecule 8 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	65	Total 1329	C 629	N 250	O 385	P 65	0	0

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

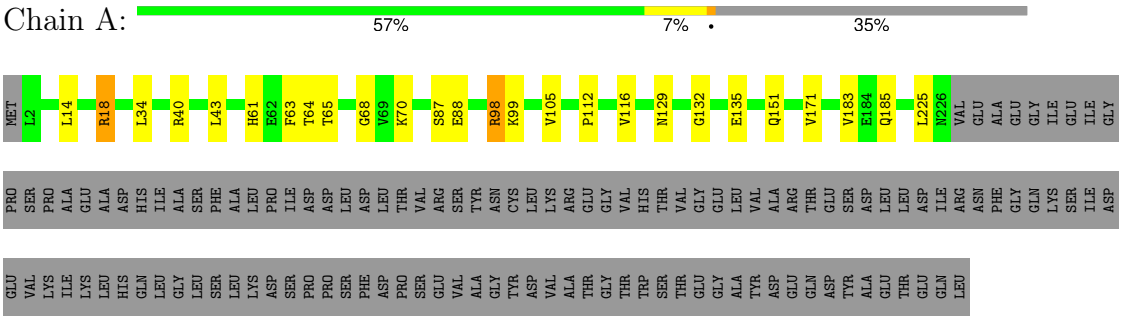
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

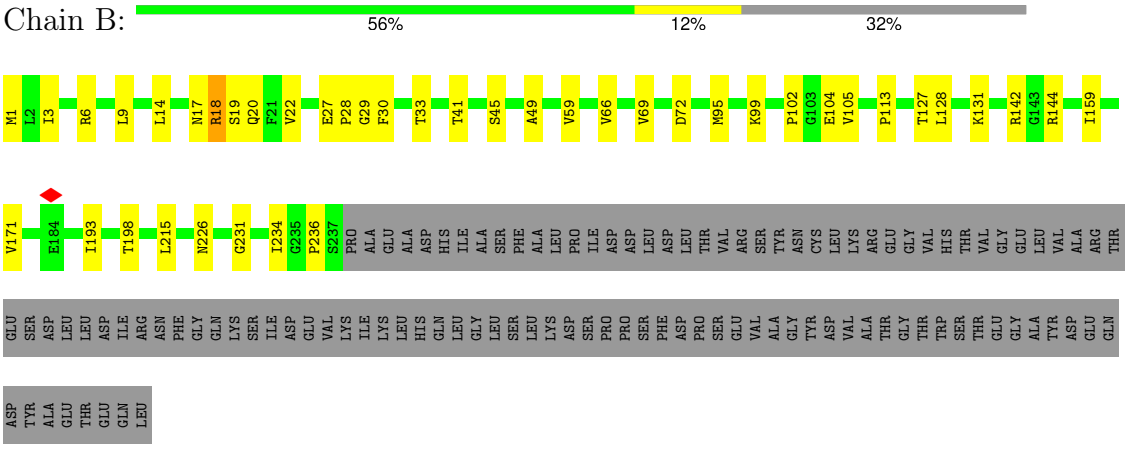
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



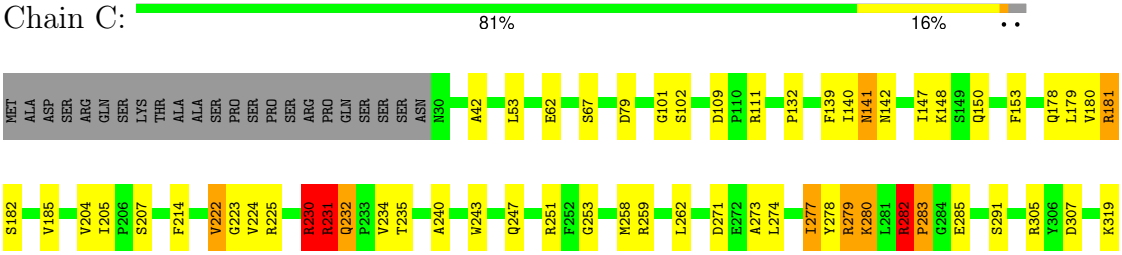
• Molecule 1: DNA-directed RNA polymerase subunit alpha

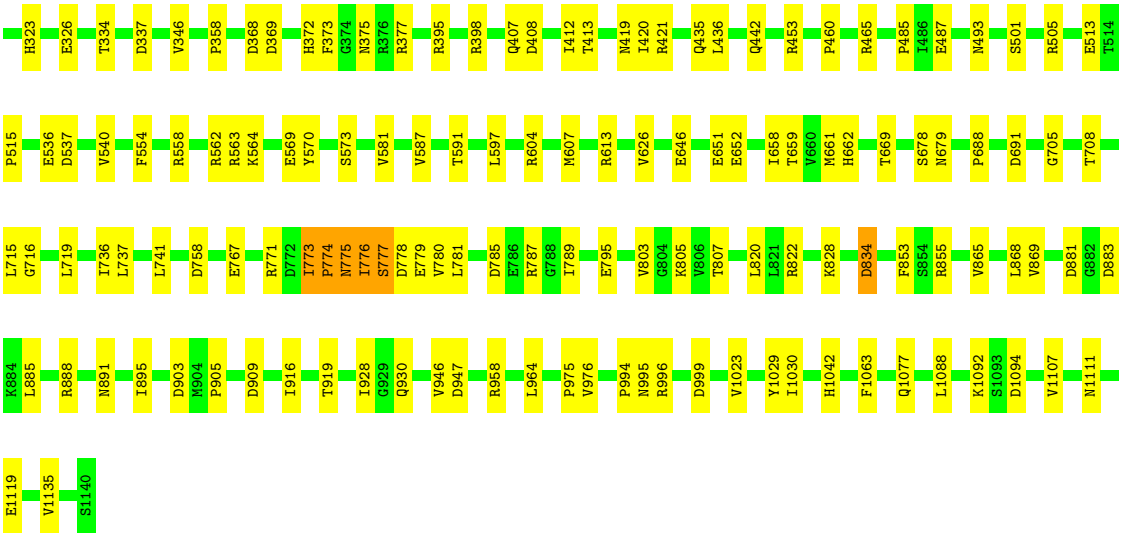
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

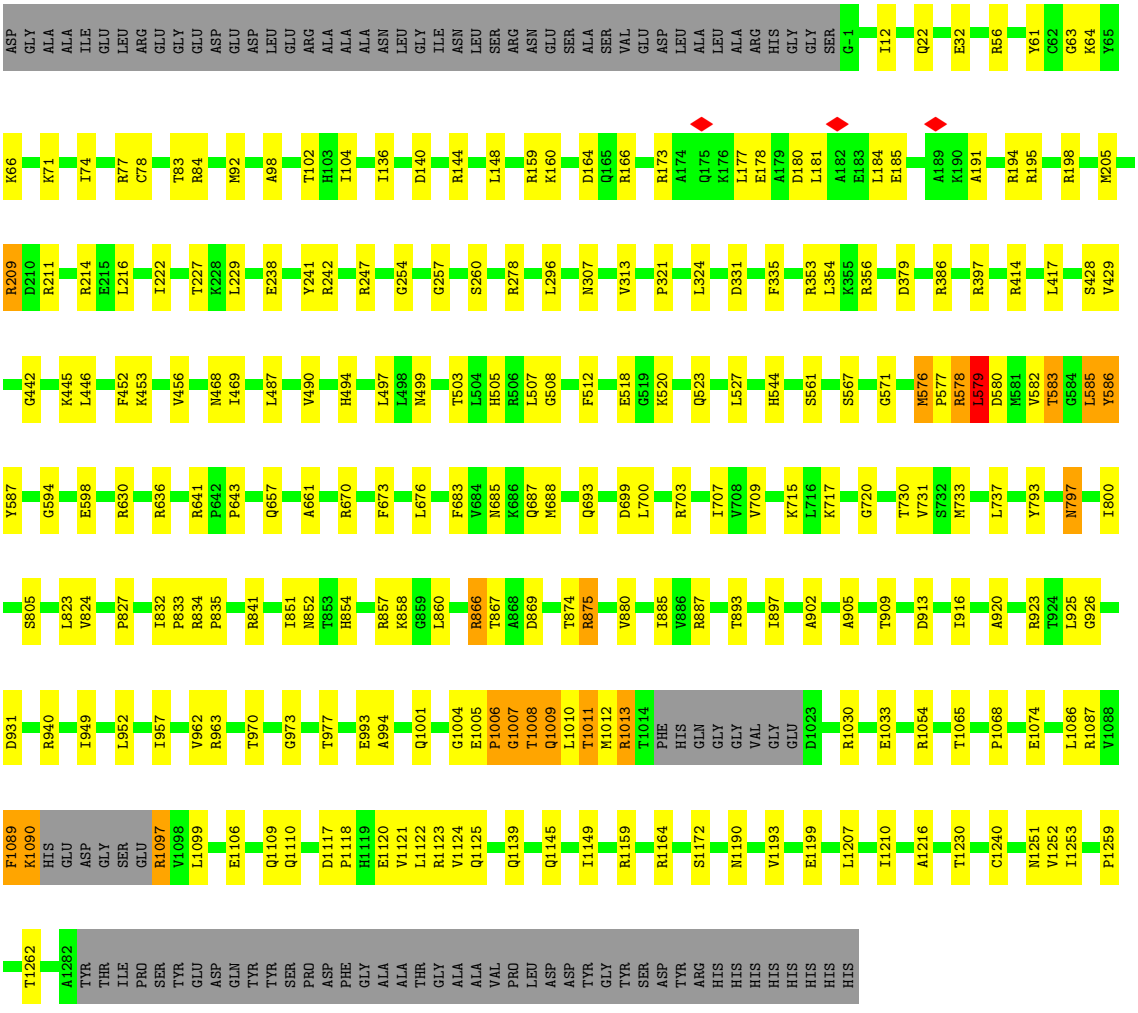
Chain C:





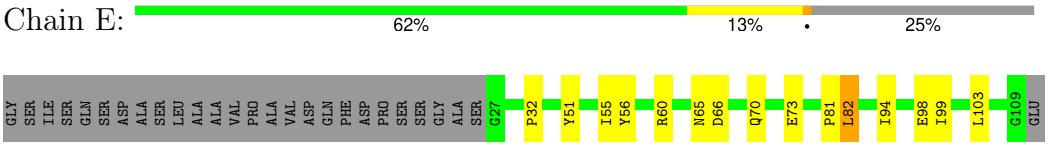
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



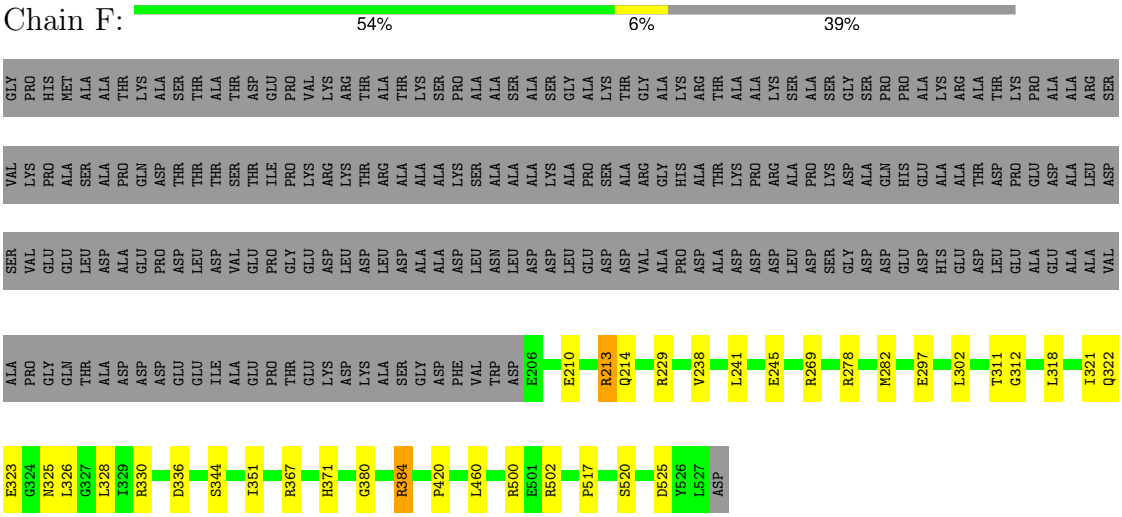
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



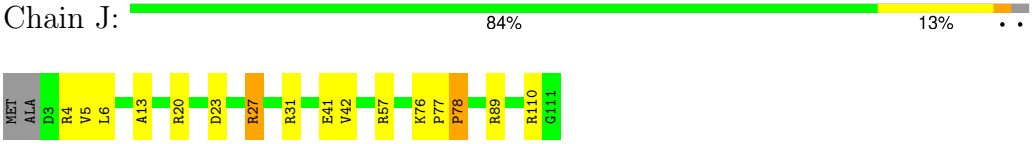
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



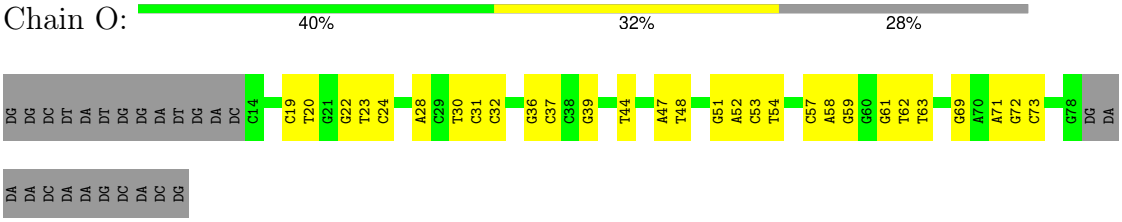
• Molecule 6: RNA polymerase-binding protein RbpA

Chain J:



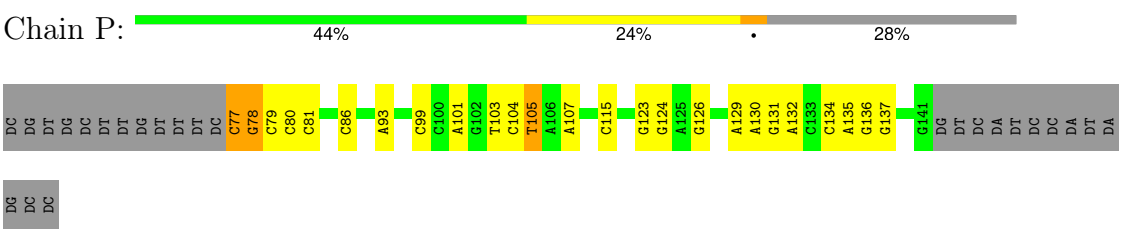
• Molecule 7: DNA (65-MER)

Chain O:



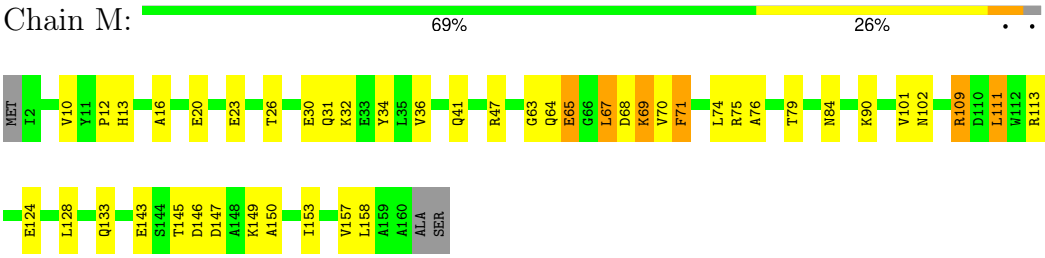
• Molecule 8: DNA (65-MER)

Chain P:



• Molecule 9: RNA polymerase-binding transcription factor CarD

Chain M:


69%
26%
MET I2 V10 Y11 P12 H13 A16 E20 E23 T26 E30 Q31 K32 E33 Y34 L35 V36 Q41 R47 G63 Q64 E65 G66 L67 D68 K69 V70 F71 L74 R75 A76 T79 N84 K90 V101 N102 R109 D110 L111 W112 R113 R114 L120 S121
E124 L128 Q133 E143 S144 T145 D146 D147 A148 K149 A150 I153 V157 L158 A159 A160 ALA SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211381	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	69.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.931	Depositor
Minimum map value	-0.730	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	325.0, 325.0, 325.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.44	0/1742	0.59	0/2370
1	B	0.45	0/1792	0.62	0/2442
2	C	0.50	0/8765	0.64	1/11885 (0.0%)
3	D	0.52	0/10078	0.63	4/13624 (0.0%)
4	E	0.40	0/662	0.64	0/901
5	F	0.37	0/2571	0.55	0/3468
6	J	0.38	0/896	0.62	0/1210
7	O	0.84	0/1497	0.96	0/2310
8	P	0.87	0/1491	1.04	5/2297 (0.2%)
9	M	0.39	0/1257	0.64	0/1700
All	All	0.53	0/30751	0.67	10/42207 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	77	DC	OP1-P-O3'	8.55	124.02	105.20
8	P	77	DC	P-O3'-C3'	7.37	128.54	119.70
3	D	583	THR	CB-CA-C	-6.80	93.24	111.60
2	C	231	ARG	N-CA-C	6.78	129.30	111.00
3	D	1007	GLY	N-CA-C	-6.60	96.60	113.10
8	P	78	DG	P-O3'-C3'	6.19	127.12	119.70
3	D	834	ARG	C-N-CD	-6.15	107.06	120.60
8	P	123	DG	O4'-C1'-N9	5.46	111.82	108.00
8	P	105	DT	OP1-P-O3'	5.33	116.92	105.20
3	D	140	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1716	0	1756	18	0
1	B	1765	0	1794	27	0
2	C	8606	0	8544	218	0
3	D	9914	0	9987	206	0
4	E	649	0	645	10	0
5	F	2540	0	2552	33	0
6	J	880	0	852	12	0
7	O	1336	0	732	37	0
8	P	1329	0	727	36	0
9	M	1241	0	1259	38	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	29979	0	28848	572	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 (572) 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)
2:C:776:ILE:CD1	2:C:780:VAL:HG21	1.23	1.59
2:C:231:ARG:CD	2:C:232:GLN:H	0.90	1.53
2:C:278:TYR:CE2	2:C:282:ARG:HG3	1.55	1.41
2:C:231:ARG:HD2	2:C:232:GLN:N	1.06	1.39
3:D:1010:LEU:CD1	3:D:1145:GLN:HG3	1.52	1.37
2:C:776:ILE:CD1	2:C:780:VAL:CG2	1.84	1.35
2:C:776:ILE:HD11	2:C:780:VAL:CG2	0.87	1.35
2:C:223:GLY:HA2	2:C:232:GLN:O	1.32	1.29
2:C:278:TYR:CZ	2:C:282:ARG:HG3	1.67	1.29
2:C:231:ARG:HD2	2:C:232:GLN:CA	1.62	1.27
2:C:278:TYR:CE2	2:C:282:ARG:CG	2.17	1.26
2:C:231:ARG:CG	2:C:232:GLN:H	1.46	1.23
3:D:866:ARG:HD2	3:D:1008:THR:O	1.08	1.22
3:D:866:ARG:CD	3:D:1008:THR:O	1.89	1.21
2:C:278:TYR:CE2	2:C:282:ARG:CB	2.26	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:80:DC:H2"	8:P:81:DC:C5'	1.73	1.16
2:C:776:ILE:HD11	2:C:780:VAL:HG22	1.22	1.14
2:C:230:ARG:HH11	2:C:230:ARG:HB2	1.10	1.14
2:C:231:ARG:CD	2:C:232:GLN:N	1.73	1.12
3:D:586:TYR:CE1	3:D:805:SER:HA	1.83	1.12
2:C:771:ARG:HD2	2:C:785:ASP:O	1.45	1.11
2:C:231:ARG:O	2:C:232:GLN:HG2	1.50	1.10
2:C:773:ILE:HD11	2:C:781:LEU:HD21	1.29	1.09
3:D:586:TYR:HE1	3:D:805:SER:HA	1.07	1.08
3:D:1010:LEU:HD11	3:D:1145:GLN:HG3	1.34	1.08
3:D:586:TYR:HD1	3:D:805:SER:HB2	1.11	1.07
8:P:80:DC:H2"	8:P:81:DC:O5'	1.47	1.06
3:D:1010:LEU:HD12	3:D:1145:GLN:HG3	1.16	1.06
2:C:776:ILE:HD11	2:C:780:VAL:HG23	1.36	1.04
2:C:773:ILE:CD1	2:C:781:LEU:HD21	1.86	1.04
3:D:587:TYR:HE1	3:D:630:ARG:CZ	1.69	1.04
3:D:586:TYR:CD1	3:D:805:SER:CB	2.41	1.03
2:C:231:ARG:CG	2:C:232:GLN:N	2.06	1.03
7:O:57:DC:H2"	7:O:58:DA:O5'	1.54	1.03
2:C:773:ILE:HD12	2:C:773:ILE:H	1.25	1.01
3:D:1089:PHE:O	3:D:1097:ARG:N	1.93	1.01
3:D:866:ARG:HD2	3:D:1008:THR:C	1.80	0.99
3:D:586:TYR:CD1	3:D:805:SER:HB2	1.97	0.99
2:C:214:PHE:CD1	2:C:224:VAL:HG13	1.97	0.98
2:C:278:TYR:HE2	2:C:282:ARG:CB	1.73	0.97
2:C:181:ARG:NH2	7:O:62:DT:C2	2.33	0.94
8:P:80:DC:H2"	8:P:81:DC:H5"	1.47	0.94
2:C:305:ARG:HH12	7:O:58:DA:H8	1.01	0.94
2:C:278:TYR:HE2	2:C:282:ARG:HB3	1.31	0.94
3:D:1013:ARG:NH1	3:D:1013:ARG:HB2	1.83	0.92
2:C:273:ALA:O	2:C:277:ILE:HG13	1.70	0.92
2:C:274:LEU:HA	2:C:277:ILE:HD12	1.50	0.91
2:C:230:ARG:HB2	2:C:230:ARG:NH1	1.84	0.90
3:D:586:TYR:HD1	3:D:805:SER:CB	1.78	0.90
2:C:278:TYR:CD2	2:C:282:ARG:HB2	2.07	0.90
3:D:1001:GLN:O	3:D:1005:GLU:HB2	1.74	0.88
3:D:586:TYR:HE2	3:D:687:GLN:HE21	1.21	0.87
3:D:587:TYR:CE1	3:D:630:ARG:HD3	2.10	0.87
3:D:586:TYR:CE1	3:D:805:SER:CA	2.58	0.87
9:M:65:GLU:N	9:M:65:GLU:OE1	2.07	0.87
2:C:776:ILE:HD13	2:C:780:VAL:HG21	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:586:TYR:HE1	3:D:805:SER:CA	1.88	0.86
3:D:1010:LEU:CD1	3:D:1145:GLN:CG	2.48	0.86
7:O:58:DA:H1'	7:O:59:DG:C5	2.09	0.86
7:O:57:DC:C2'	7:O:58:DA:O5'	2.24	0.86
5:F:384:ARG:HG2	5:F:384:ARG:HH21	1.38	0.85
3:D:1010:LEU:HD12	3:D:1145:GLN:CG	2.06	0.85
3:D:585:LEU:CD2	3:D:720:GLY:HA2	2.08	0.84
3:D:397:ARG:NH1	8:P:101:DA:C2	2.46	0.84
2:C:231:ARG:O	2:C:232:GLN:CG	2.24	0.84
2:C:181:ARG:NH2	7:O:62:DT:O2	2.12	0.82
2:C:231:ARG:HD2	2:C:232:GLN:C	1.99	0.82
2:C:278:TYR:CE2	2:C:282:ARG:HB2	2.14	0.82
5:F:502:ARG:NH2	7:O:23:DT:OP2	2.13	0.82
2:C:240:ALA:HB2	2:C:277:ILE:HD11	1.62	0.81
2:C:231:ARG:HB3	2:C:231:ARG:CZ	2.10	0.80
3:D:1013:ARG:HB2	3:D:1013:ARG:HH11	1.44	0.80
3:D:1010:LEU:HD11	3:D:1145:GLN:CG	2.11	0.79
2:C:231:ARG:HG2	2:C:232:GLN:N	1.96	0.78
7:O:58:DA:H1'	7:O:59:DG:C4	2.19	0.78
3:D:397:ARG:NH1	8:P:101:DA:H2	1.81	0.77
9:M:69:LYS:HD3	9:M:69:LYS:C	2.03	0.77
2:C:305:ARG:NH1	7:O:58:DA:C8	2.51	0.77
2:C:280:LYS:HZ3	2:C:280:LYS:HB2	1.48	0.77
3:D:144:ARG:O	3:D:148:LEU:HB2	1.85	0.75
2:C:305:ARG:NH1	7:O:58:DA:H8	1.82	0.75
9:M:68:ASP:HA	9:M:71:PHE:HB2	1.67	0.75
3:D:585:LEU:HD23	3:D:720:GLY:HA2	1.66	0.75
2:C:773:ILE:HD11	2:C:781:LEU:CD2	2.15	0.74
9:M:69:LYS:HD3	9:M:69:LYS:O	1.87	0.74
3:D:587:TYR:HE1	3:D:630:ARG:NH1	1.85	0.74
3:D:587:TYR:CE1	3:D:630:ARG:CZ	2.62	0.73
1:B:18:ARG:HG2	1:B:18:ARG:HH21	1.51	0.73
2:C:274:LEU:O	2:C:277:ILE:HB	1.89	0.73
1:B:18:ARG:HG2	1:B:18:ARG:NH2	2.02	0.72
2:C:273:ALA:O	2:C:277:ILE:CG1	2.37	0.72
3:D:577:PRO:O	3:D:582:VAL:HG23	1.88	0.72
3:D:1007:GLY:O	3:D:1009:GLN:N	2.22	0.72
2:C:224:VAL:HG21	2:C:234:VAL:HA	1.72	0.72
2:C:231:ARG:HD3	2:C:232:GLN:O	1.90	0.71
3:D:505:HIS:HB3	3:D:1005:GLU:HG3	1.72	0.71
2:C:214:PHE:CE1	2:C:224:VAL:HG13	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:ARG:CZ	2:C:279:ARG:HB3	2.21	0.71
2:C:231:ARG:CD	2:C:232:GLN:O	2.39	0.70
3:D:585:LEU:HD23	3:D:585:LEU:N	2.06	0.70
8:P:80:DC:C2'	8:P:81:DC:O5'	2.30	0.70
3:D:587:TYR:HE1	3:D:630:ARG:NE	1.89	0.70
8:P:80:DC:C2'	8:P:81:DC:H5"	2.22	0.70
3:D:307:ASN:HD21	3:D:1240:CYS:HB2	1.57	0.70
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.57	0.69
2:C:240:ALA:HB2	2:C:277:ILE:CD1	2.22	0.69
3:D:587:TYR:CE1	3:D:630:ARG:CD	2.74	0.69
3:D:587:TYR:CE1	3:D:630:ARG:NH1	2.61	0.69
5:F:384:ARG:HH21	5:F:384:ARG:CG	2.05	0.69
3:D:586:TYR:HE2	3:D:687:GLN:NE2	1.91	0.69
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.75	0.68
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	1.73	0.68
3:D:586:TYR:CD1	3:D:805:SER:HB3	2.28	0.68
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.76	0.67
2:C:279:ARG:HG2	2:C:279:ARG:HH11	1.59	0.67
2:C:223:GLY:HA3	2:C:231:ARG:HG3	1.75	0.67
2:C:280:LYS:HB2	2:C:280:LYS:NZ	2.08	0.67
2:C:231:ARG:HG3	2:C:231:ARG:HH11	1.60	0.67
2:C:222:VAL:HG22	2:C:234:VAL:HG13	1.77	0.67
3:D:866:ARG:HD2	3:D:1008:THR:CA	2.25	0.67
7:O:57:DC:O2	7:O:58:DA:H5'	1.95	0.66
3:D:1007:GLY:O	3:D:1009:GLN:HG3	1.94	0.66
3:D:867:THR:HG21	8:P:93:DA:N1	2.11	0.66
7:O:22:DG:H2"	7:O:23:DT:H5'	1.78	0.66
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.60	0.66
2:C:231:ARG:CD	2:C:232:GLN:C	2.64	0.64
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.78	0.64
2:C:181:ARG:NH2	7:O:62:DT:N3	2.45	0.64
2:C:214:PHE:CE1	2:C:224:VAL:CG1	2.80	0.64
2:C:282:ARG:N	2:C:283:PRO:CD	2.60	0.64
3:D:587:TYR:CE1	3:D:630:ARG:NE	2.65	0.64
3:D:585:LEU:HD21	3:D:720:GLY:CA	2.27	0.64
3:D:586:TYR:CE2	3:D:687:GLN:NE2	2.65	0.64
9:M:70:VAL:O	9:M:74:LEU:N	2.29	0.64
2:C:776:ILE:CD1	2:C:780:VAL:HG22	1.95	0.64
2:C:776:ILE:CG1	2:C:780:VAL:CG2	2.75	0.64
5:F:517:PRO:HA	5:F:520:SER:HB3	1.80	0.63
2:C:777:SER:C	2:C:779:GLU:H	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:77:DC:H3'	8:P:78:DG:C8	2.33	0.63
2:C:282:ARG:N	2:C:283:PRO:HD3	2.13	0.63
2:C:231:ARG:CG	2:C:231:ARG:HH11	2.12	0.63
3:D:897:ILE:HD11	3:D:923:ARG:HH12	1.64	0.62
3:D:586:TYR:CE1	3:D:805:SER:CB	2.79	0.62
3:D:397:ARG:HH11	8:P:101:DA:H2	1.44	0.62
3:D:585:LEU:HD21	3:D:720:GLY:HA2	1.80	0.62
6:J:20:ARG:NH1	6:J:23:ASP:OD1	2.33	0.62
2:C:773:ILE:HD12	2:C:773:ILE:N	2.07	0.62
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.82	0.62
1:A:18:ARG:HH12	2:C:996:ARG:HH12	1.48	0.61
4:E:70:GLN:NE2	4:E:73:GLU:OE2	2.33	0.61
3:D:177:LEU:HD11	3:D:198:ARG:HD3	1.83	0.61
3:D:1008:THR:HG22	3:D:1009:GLN:N	2.15	0.61
3:D:926:GLY:O	3:D:940:ARG:NH2	2.34	0.61
8:P:79:DC:H2"	8:P:80:DC:H5'	1.82	0.61
1:A:129:ASN:ND2	2:C:652:GLU:OE2	2.35	0.60
6:J:20:ARG:NH1	6:J:23:ASP:O	2.34	0.60
2:C:231:ARG:O	2:C:232:GLN:CB	2.49	0.60
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.82	0.60
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.84	0.60
2:C:279:ARG:HB3	2:C:279:ARG:NH1	2.17	0.59
2:C:776:ILE:HD11	2:C:780:VAL:HG21	0.61	0.59
3:D:335:PHE:HB2	5:F:420:PRO:HB3	1.83	0.59
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.35	0.59
9:M:70:VAL:HG12	9:M:102:ASN:HA	1.84	0.59
2:C:274:LEU:CA	2:C:277:ILE:HD12	2.26	0.59
2:C:777:SER:O	2:C:779:GLU:N	2.35	0.59
2:C:279:ARG:HH11	2:C:279:ARG:CG	2.15	0.58
5:F:384:ARG:NH1	8:P:104:DC:N3	2.51	0.58
3:D:184:LEU:O	3:D:194:ARG:NH1	2.36	0.58
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.32	0.58
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.30	0.58
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.36	0.58
3:D:885:ILE:HD11	3:D:887:ARG:HH21	1.69	0.58
2:C:223:GLY:CA	2:C:232:GLN:O	2.27	0.58
2:C:224:VAL:HG12	2:C:224:VAL:O	2.03	0.57
1:B:45:SER:O	1:B:144:ARG:NH1	2.37	0.57
3:D:159:ARG:HE	3:D:216:LEU:HD22	1.69	0.57
3:D:63:GLY:O	3:D:66:LYS:NZ	2.37	0.57
5:F:384:ARG:HH12	8:P:104:DC:N4	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:771:ARG:O	2:C:773:ILE:HD12	2.04	0.57
3:D:1005:GLU:H	3:D:1006:PRO:HD2	1.70	0.57
1:A:183:VAL:HG13	1:A:185:GLN:H	1.70	0.56
2:C:453:ARG:NH2	2:C:501:SER:O	2.38	0.56
3:D:148:LEU:HD21	3:D:227:THR:HG22	1.87	0.56
3:D:866:ARG:O	3:D:867:THR:C	2.39	0.56
5:F:344:SER:OG	7:O:53:DC:OP2	2.17	0.56
2:C:223:GLY:HA3	2:C:231:ARG:CG	2.35	0.56
6:J:5:VAL:O	8:P:99:DC:N4	2.38	0.56
2:C:776:ILE:HG12	2:C:781:LEU:CD1	2.36	0.56
2:C:773:ILE:HG22	2:C:774:PRO:HD2	1.87	0.56
3:D:22:GLN:O	6:J:57:ARG:NH2	2.38	0.56
3:D:1089:PHE:N	3:D:1089:PHE:CD2	2.72	0.56
1:B:104:GLU:HG2	1:B:127:THR:HG22	1.87	0.56
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.88	0.56
2:C:214:PHE:HD1	2:C:224:VAL:HG13	1.67	0.56
9:M:64:GLN:O	9:M:65:GLU:C	2.40	0.56
2:C:678:SER:OG	2:C:679:ASN:N	2.38	0.56
2:C:369:ASP:O	2:C:375:ASN:ND2	2.38	0.55
3:D:1120:GLU:OE2	3:D:1123:ARG:NH2	2.33	0.55
1:A:151:GLN:NE2	2:C:795:GLU:OE2	2.39	0.55
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.88	0.55
3:D:963:ARG:NH1	3:D:977:THR:OG1	2.39	0.55
8:P:107:DA:OP1	9:M:121:SER:OG	2.24	0.55
3:D:866:ARG:O	3:D:869:ASP:N	2.39	0.55
2:C:775:ASN:N	2:C:775:ASN:OD1	2.34	0.55
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.40	0.54
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.89	0.54
2:C:398:ARG:NH1	7:O:58:DA:OP2	2.40	0.54
2:C:604:ARG:NH1	2:C:607:MET:SD	2.80	0.54
3:D:866:ARG:NH1	3:D:1010:LEU:O	2.40	0.54
2:C:102:SER:O	2:C:141:ASN:ND2	2.40	0.54
2:C:771:ARG:O	2:C:773:ILE:CD1	2.55	0.54
3:D:64:LYS:HD3	3:D:77:ARG:HH21	1.72	0.54
5:F:384:ARG:HG2	5:F:384:ARG:NH2	2.17	0.54
3:D:1030:ARG:NH1	3:D:1033:GLU:OE2	2.39	0.54
2:C:319:LYS:NZ	2:C:368:ASP:OD2	2.36	0.54
2:C:659:THR:HG22	2:C:669:THR:HG22	1.90	0.54
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.72	0.54
3:D:173:ARG:HG2	3:D:205:MET:HG2	1.90	0.54
3:D:468:ASN:HD21	5:F:525:ASP:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.73	0.54
9:M:30:GLU:OE1	9:M:32:LYS:NZ	2.41	0.54
3:D:173:ARG:NH2	3:D:180:ASP:OD2	2.41	0.53
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.41	0.53
9:M:10:VAL:HA	9:M:16:ALA:HA	1.89	0.53
9:M:71:PHE:CZ	9:M:157:VAL:HG11	2.42	0.53
9:M:76:ALA:O	9:M:113:ARG:NH2	2.42	0.53
2:C:822:ARG:NH1	2:C:828:LYS:O	2.41	0.53
2:C:278:TYR:OH	2:C:282:ARG:HG3	2.04	0.53
3:D:916:ILE:HG23	3:D:920:ALA:HB3	1.89	0.53
7:O:58:DA:C1'	7:O:59:DG:C4	2.91	0.53
1:B:49:ALA:HA	1:B:142:ARG:HA	1.91	0.53
3:D:1013:ARG:HB2	3:D:1013:ARG:CZ	2.39	0.53
5:F:241:LEU:HD22	5:F:245:GLU:HG2	1.90	0.53
5:F:384:ARG:CG	5:F:384:ARG:NH2	2.67	0.53
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.91	0.53
9:M:111:LEU:HD12	9:M:128:LEU:HB2	1.91	0.53
2:C:214:PHE:CD1	2:C:224:VAL:CG1	2.82	0.53
2:C:855:ARG:NH1	2:C:865:VAL:O	2.42	0.52
1:B:22:VAL:HG12	1:B:193:ILE:HG12	1.90	0.52
3:D:577:PRO:O	3:D:582:VAL:CG2	2.55	0.52
9:M:26:THR:HB	9:M:31:GLN:HG3	1.91	0.52
3:D:700:LEU:HD23	3:D:709:VAL:HG22	1.91	0.52
9:M:41:GLN:OE1	9:M:133:GLN:NE2	2.42	0.52
2:C:222:VAL:HG22	2:C:222:VAL:O	2.09	0.52
2:C:285:GLU:OE1	5:F:229:ARG:NH1	2.42	0.52
2:C:395:ARG:HG2	2:C:398:ARG:HH21	1.74	0.52
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.42	0.52
9:M:71:PHE:O	9:M:75:ARG:N	2.30	0.52
3:D:136:ILE:HG13	3:D:229:LEU:HD11	1.91	0.52
2:C:777:SER:OG	2:C:779:GLU:HB3	2.09	0.52
3:D:1005:GLU:H	3:D:1006:PRO:CD	2.22	0.52
2:C:253:GLY:O	2:C:259:ARG:NH1	2.34	0.52
1:B:19:SER:OG	1:B:20:GLN:N	2.42	0.52
2:C:240:ALA:CB	2:C:277:ILE:CD1	2.87	0.52
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.92	0.52
2:C:777:SER:C	2:C:779:GLU:N	2.63	0.52
3:D:74:ILE:HD12	6:J:42:VAL:HG13	1.91	0.52
9:M:23:GLU:N	9:M:34:TYR:O	2.43	0.52
2:C:515:PRO:HB2	2:C:581:VAL:HG11	1.90	0.52
2:C:181:ARG:HG3	2:C:181:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:651:GLU:HG2	2:C:661:MET:HB2	1.92	0.51
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.41	0.51
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.92	0.51
5:F:330:ARG:NH2	7:O:48:DT:OP2	2.42	0.51
2:C:140:ILE:HG12	2:C:147:ILE:HG22	1.92	0.51
2:C:774:PRO:HD2	2:C:834:ASP:HB2	1.93	0.51
3:D:577:PRO:O	3:D:577:PRO:HG2	2.11	0.51
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.40	0.51
3:D:586:TYR:CD1	3:D:805:SER:HA	2.38	0.51
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.93	0.51
2:C:773:ILE:HG22	2:C:774:PRO:CD	2.41	0.51
8:P:115:DC:H2'	8:P:115:DC:OP2	2.11	0.51
3:D:586:TYR:HD2	3:D:586:TYR:C	2.14	0.51
3:D:1139:GLN:HE22	3:D:1149:ILE:HB	1.76	0.51
2:C:231:ARG:NH1	2:C:231:ARG:CB	2.74	0.50
2:C:279:ARG:CZ	2:C:279:ARG:CB	2.85	0.50
3:D:102:THR:HG22	3:D:313:VAL:HG12	1.93	0.50
1:A:98:ARG:HG3	1:A:135:GLU:HG2	1.91	0.50
2:C:147:ILE:HD11	9:M:47:ARG:HD3	1.91	0.50
3:D:331:ASP:OD1	3:D:331:ASP:N	2.44	0.50
1:A:61:HIS:HD2	1:A:63:PHE:H	1.59	0.50
7:O:63:DT:OP1	7:O:63:DT:H2'	2.12	0.50
3:D:586:TYR:CD1	3:D:805:SER:CA	2.85	0.50
2:C:767:GLU:HG2	2:C:807:THR:HG22	1.94	0.50
3:D:503:THR:HG23	3:D:508:GLY:HA3	1.94	0.50
2:C:273:ALA:O	2:C:277:ILE:CD1	2.59	0.50
4:E:82:LEU:HB3	4:E:103:LEU:HD23	1.94	0.50
1:A:225:LEU:HD21	1:B:9:LEU:HD23	1.93	0.50
2:C:485:PRO:O	3:D:857:ARG:NH2	2.43	0.50
2:C:716:GLY:N	2:C:1029:TYR:OH	2.44	0.50
3:D:1117:ASP:OD1	3:D:1117:ASP:N	2.44	0.50
2:C:334:THR:HG23	2:C:337:ASP:H	1.75	0.50
2:C:737:LEU:HB3	2:C:741:LEU:HD12	1.93	0.50
2:C:853:PHE:HB2	2:C:868:LEU:HB3	1.93	0.50
5:F:318:LEU:HD23	5:F:321:ILE:HD12	1.94	0.50
7:O:30:DT:H1'	7:O:31:DC:H5'	1.94	0.50
1:A:43:LEU:HA	1:A:171:VAL:HG11	1.94	0.49
1:B:3:ILE:HG21	1:B:234:ILE:HG23	1.94	0.49
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.94	0.49
3:D:1005:GLU:N	3:D:1006:PRO:CD	2.73	0.49
5:F:371:HIS:NE2	7:O:44:DT:OP2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:32:DC:H2'	7:O:32:DC:OP2	2.11	0.49
2:C:421:ARG:HH22	8:P:103:DT:H3'	1.77	0.49
7:O:19:DC:H2"	7:O:20:DT:OP2	2.12	0.49
9:M:121:SER:HB3	9:M:124:GLU:HB2	1.95	0.49
2:C:231:ARG:CG	2:C:231:ARG:NH1	2.72	0.49
3:D:1262:THR:HB	4:E:55:ILE:HD11	1.93	0.49
2:C:274:LEU:HA	2:C:277:ILE:CD1	2.35	0.49
2:C:558:ARG:HE	2:C:570:TYR:HB3	1.77	0.49
3:D:594:GLY:N	3:D:598:GLU:OE2	2.45	0.49
2:C:323:HIS:HB3	2:C:326:GLU:HB2	1.95	0.49
2:C:442:GLN:O	2:C:678:SER:OG	2.22	0.49
3:D:585:LEU:CD2	3:D:720:GLY:CA	2.81	0.49
2:C:101:GLY:O	2:C:142:ASN:ND2	2.46	0.49
1:B:69:VAL:HG12	1:B:128:LEU:HG	1.95	0.49
2:C:278:TYR:CD2	2:C:282:ARG:CG	2.90	0.49
5:F:328:LEU:HD23	5:F:351:ILE:HD11	1.94	0.49
2:C:776:ILE:O	2:C:776:ILE:HG13	2.08	0.49
8:P:134:DC:H2'	8:P:135:DA:C8	2.47	0.49
2:C:563:ARG:NH2	2:C:569:GLU:OE1	2.46	0.48
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.43	0.48
6:J:31:ARG:NH1	6:J:41:GLU:OE2	2.45	0.48
2:C:407:GLN:HB3	2:C:412:ILE:HG21	1.95	0.48
5:F:502:ARG:NE	7:O:24:DC:OP2	2.46	0.48
2:C:773:ILE:HD13	2:C:781:LEU:HD11	1.95	0.48
2:C:789:ILE:HG21	2:C:869:VAL:HG21	1.95	0.48
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.95	0.48
3:D:1172:SER:OG	3:D:1199:GLU:OE2	2.31	0.48
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.40	0.48
3:D:905:ALA:HB3	3:D:909:THR:H	1.78	0.48
5:F:500:ARG:NH1	8:P:126:DG:O6	2.46	0.48
2:C:909:ASP:OD2	2:C:995:ASN:ND2	2.47	0.48
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.47	0.48
2:C:207:SER:OG	2:C:307:ASP:O	2.29	0.48
2:C:279:ARG:NH1	2:C:279:ARG:CG	2.73	0.48
2:C:435:GLN:HE21	2:C:460:PRO:HD3	1.78	0.48
3:D:586:TYR:C	3:D:586:TYR:CD2	2.85	0.48
9:M:20:GLU:HB3	9:M:36:VAL:HG13	1.95	0.48
1:B:27:GLU:O	1:B:30:PHE:N	2.47	0.47
1:B:72:ASP:N	1:B:72:ASP:OD1	2.47	0.47
2:C:280:LYS:NZ	2:C:280:LYS:CB	2.73	0.47
3:D:166:ARG:HH21	3:D:209:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:GLU:HB2	3:D:1109:GLN:HB2	1.96	0.47
3:D:579:LEU:HB3	3:D:580:ASP:H	1.41	0.47
3:D:56:ARG:HG2	6:J:13:ALA:H	1.80	0.47
3:D:1005:GLU:HB3	3:D:1006:PRO:CD	2.44	0.47
1:B:18:ARG:HH21	1:B:18:ARG:CG	2.19	0.47
2:C:271:ASP:OD1	2:C:271:ASP:N	2.48	0.47
3:D:414:ARG:CZ	3:D:875:ARG:HH12	2.27	0.47
3:D:583:THR:O	3:D:583:THR:HG22	2.13	0.47
2:C:278:TYR:HD2	2:C:278:TYR:O	1.97	0.47
3:D:32:GLU:OE2	5:F:367:ARG:NE	2.47	0.47
2:C:372:HIS:NE2	2:C:537:ASP:OD2	2.47	0.47
3:D:61:TYR:HB3	3:D:78:CYS:HB2	1.97	0.47
3:D:194:ARG:HG3	3:D:195:ARG:HG2	1.96	0.47
3:D:1090:LYS:HZ3	3:D:1090:LYS:HB3	1.79	0.47
3:D:1090:LYS:NZ	3:D:1090:LYS:CB	2.77	0.47
1:A:87:SER:OG	1:A:88:GLU:N	2.48	0.47
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.97	0.47
2:C:994:PRO:HB3	2:C:999:ASP:H	1.79	0.47
3:D:893:THR:O	3:D:940:ARG:NH1	2.48	0.47
5:F:238:VAL:HG11	5:F:297:GLU:HB3	1.97	0.47
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.51	0.47
2:C:224:VAL:O	2:C:225:ARG:C	2.53	0.47
3:D:587:TYR:O	3:D:587:TYR:CD1	2.68	0.47
3:D:874:THR:OG1	3:D:1004:GLY:O	2.33	0.47
1:A:40:ARG:HE	1:B:33:THR:HG22	1.80	0.47
1:A:68:GLY:HA3	1:A:132:GLY:HA2	1.97	0.47
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.96	0.47
9:M:63:GLY:C	9:M:65:GLU:OE1	2.53	0.47
2:C:705:GLY:N	2:C:708:THR:OG1	2.41	0.46
3:D:587:TYR:CD1	3:D:630:ARG:HD3	2.50	0.46
8:P:124:DG:OP2	8:P:124:DG:H2'	2.15	0.46
1:B:171:VAL:HG12	1:B:198:THR:HG22	1.97	0.46
2:C:235:THR:HG21	2:C:262:LEU:HA	1.97	0.46
2:C:278:TYR:CD2	2:C:278:TYR:O	2.68	0.46
8:P:135:DA:OP2	8:P:135:DA:H2'	2.16	0.46
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.97	0.46
9:M:74:LEU:HD21	9:M:158:LEU:HD23	1.97	0.46
8:P:105:DT:O4	9:M:90:LYS:NZ	2.41	0.46
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.96	0.46
3:D:417:LEU:HD12	3:D:1253:ILE:HG23	1.98	0.46
3:D:567:SER:HB2	3:D:571:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:179:LEU:C	2:C:180:VAL:HG13	2.36	0.46
3:D:707:ILE:HD11	4:E:32:PRO:HB3	1.98	0.46
3:D:866:ARG:NE	3:D:1008:THR:O	2.46	0.46
2:C:881:ASP:N	2:C:881:ASP:OD1	2.49	0.46
3:D:587:TYR:O	3:D:587:TYR:CG	2.69	0.46
3:D:866:ARG:HD2	3:D:1008:THR:HA	1.98	0.46
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	1.98	0.46
1:B:14:LEU:HD13	1:B:18:ARG:HH22	1.81	0.46
2:C:626:VAL:HG13	2:C:888:ARG:HH22	1.80	0.46
3:D:576:MET:HG2	3:D:577:PRO:HD2	1.98	0.46
8:P:137:DG:OP2	8:P:137:DG:H8	1.99	0.46
2:C:109:ASP:OD2	2:C:111:ARG:NH1	2.49	0.45
2:C:251:ARG:HH12	2:C:358:PRO:HG3	1.81	0.45
3:D:512:PHE:CE1	3:D:561:SER:HB2	2.51	0.45
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.31	0.45
2:C:883:ASP:HB2	2:C:895:ILE:HD12	1.97	0.45
3:D:222:ILE:HD13	3:D:247:ARG:HH21	1.81	0.45
3:D:970:THR:OG1	3:D:973:GLY:O	2.28	0.45
3:D:1010:LEU:HD12	3:D:1010:LEU:HA	1.42	0.45
3:D:241:TYR:OH	3:D:254:GLY:O	2.34	0.45
8:P:80:DC:H2'	8:P:81:DC:C6	2.51	0.45
3:D:1006:PRO:O	3:D:1006:PRO:HG2	2.16	0.45
5:F:380:GLY:O	5:F:384:ARG:HB2	2.16	0.45
9:M:67:LEU:CD2	9:M:67:LEU:C	2.84	0.45
9:M:79:THR:OG1	9:M:109:ARG:NH2	2.49	0.45
2:C:282:ARG:HB3	2:C:285:GLU:HB3	1.98	0.45
2:C:282:ARG:HA	2:C:282:ARG:HD3	1.60	0.45
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.48	0.45
2:C:891:ASN:OD1	2:C:891:ASN:N	2.50	0.45
3:D:160:LYS:NZ	3:D:164:ASP:OD1	2.49	0.45
3:D:257:GLY:O	3:D:260:SER:OG	2.28	0.45
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.52	0.45
7:O:58:DA:C4	7:O:59:DG:C2	3.04	0.45
3:D:925:LEU:HD23	3:D:962:VAL:HG23	1.99	0.45
1:B:17:ASN:OD1	1:B:17:ASN:N	2.44	0.45
3:D:397:ARG:NH1	8:P:101:DA:N1	2.54	0.45
9:M:71:PHE:CE1	9:M:157:VAL:HG11	2.52	0.45
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.99	0.45
3:D:238:GLU:OE2	3:D:242:ARG:NE	2.47	0.45
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	1.99	0.45
3:D:578:ARG:H	3:D:578:ARG:HG2	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:ARG:HD2	2:C:205:ILE:HD12	1.99	0.44
2:C:223:GLY:CA	2:C:231:ARG:CG	2.95	0.44
8:P:129:DA:OP2	8:P:129:DA:H2'	2.16	0.44
1:B:6:ARG:NH1	1:B:236:PRO:O	2.50	0.44
2:C:278:TYR:O	2:C:282:ARG:HB2	2.17	0.44
3:D:585:LEU:CD1	3:D:673:PHE:HE1	2.30	0.44
3:D:1090:LYS:HB3	3:D:1090:LYS:NZ	2.33	0.44
5:F:210:GLU:O	5:F:214:GLN:HB2	2.17	0.44
6:J:4:ARG:HA	6:J:5:VAL:HA	1.60	0.44
9:M:146:ASP:O	9:M:149:LYS:N	2.49	0.44
2:C:231:ARG:HB3	2:C:231:ARG:NH1	2.31	0.44
8:P:78:DG:OP2	8:P:78:DG:H8	2.00	0.44
2:C:178:GLN:HB2	2:C:436:LEU:HD21	1.98	0.44
3:D:931:ASP:N	3:D:931:ASP:OD1	2.50	0.44
8:P:136:DG:H2"	8:P:137:DG:C8	2.51	0.44
1:A:61:HIS:CD2	1:A:63:PHE:H	2.35	0.44
3:D:178:GLU:HA	3:D:181:LEU:HD12	1.99	0.44
9:M:114:ARG:HB3	9:M:120:LEU:HD11	1.99	0.44
2:C:758:ASP:O	2:C:805:LYS:NZ	2.51	0.44
2:C:62:GLU:HB2	2:C:67:SER:HB3	1.99	0.44
7:O:61:DG:H2'	7:O:61:DG:OP2	2.18	0.44
1:B:59:VAL:HG21	1:B:66:VAL:HG22	2.00	0.43
1:B:159:ILE:H	1:B:159:ILE:HG13	1.65	0.43
2:C:1107:VAL:HG11	3:D:469:ILE:HD12	1.99	0.43
3:D:278:ARG:HE	3:D:296:LEU:HD11	1.83	0.43
3:D:1122:LEU:HD22	3:D:1207:LEU:HB2	2.00	0.43
1:B:1:MET:N	1:B:231:GLY:O	2.51	0.43
1:B:102:PRO:HD3	1:B:131:LYS:H	1.82	0.43
2:C:181:ARG:HD2	2:C:205:ILE:CD1	2.48	0.43
3:D:527:LEU:HD11	3:D:717:LYS:HB2	2.00	0.43
2:C:820:LEU:HD11	5:F:460:LEU:HD21	2.00	0.43
2:C:1023:VAL:HA	3:D:730:THR:HG21	2.00	0.43
9:M:65:GLU:H	9:M:65:GLU:CD	2.22	0.43
3:D:71:LYS:O	6:J:27:ARG:NH1	2.51	0.43
3:D:579:LEU:HD23	3:D:579:LEU:HA	1.75	0.43
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	1.99	0.43
3:D:866:ARG:NH1	3:D:1010:LEU:C	2.71	0.43
9:M:67:LEU:C	9:M:67:LEU:HD22	2.39	0.43
3:D:83:THR:OG1	3:D:84:ARG:N	2.52	0.43
3:D:211:ARG:HD3	3:D:214:ARG:HH21	1.83	0.43
3:D:324:LEU:HD23	3:D:324:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:81:PRO:HB3	4:E:94:ILE:HG21	2.01	0.43
1:A:64:THR:OG1	1:A:65:THR:N	2.51	0.43
3:D:214:ARG:NH1	5:F:213:ARG:HH22	2.17	0.43
3:D:824:VAL:HG11	3:D:852:ASN:HA	2.01	0.43
3:D:1001:GLN:O	3:D:1005:GLU:CB	2.56	0.42
7:O:39:DG:H8	7:O:39:DG:OP2	2.02	0.42
1:B:41:THR:HG21	1:B:215:LEU:HG	2.01	0.42
2:C:182:SER:HB3	2:C:377:ARG:HD2	2.01	0.42
2:C:231:ARG:CZ	2:C:231:ARG:CB	2.84	0.42
2:C:420:ILE:H	2:C:420:ILE:HG13	1.66	0.42
7:O:69:DG:H8	7:O:69:DG:OP2	2.01	0.42
2:C:222:VAL:O	2:C:222:VAL:CG2	2.67	0.42
2:C:885:LEU:HD13	2:C:895:ILE:HD11	2.01	0.42
5:F:322:GLN:HA	5:F:325:ASN:HD22	1.84	0.42
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.43	0.42
2:C:587:VAL:HG22	2:C:591:THR:HB	2.02	0.42
1:A:99:LYS:HG2	1:A:105:VAL:HG22	2.01	0.42
2:C:230:ARG:NH2	8:P:86:DC:H4'	2.34	0.42
3:D:1013:ARG:CZ	3:D:1013:ARG:CB	2.97	0.42
4:E:56:TYR:CE2	4:E:99:ILE:HD12	2.54	0.42
6:J:77:PRO:HA	6:J:78:PRO:HD3	1.90	0.42
1:A:112:PRO:HB2	1:A:116:VAL:HG23	2.00	0.42
3:D:699:ASP:OD1	3:D:703:ARG:NH1	2.53	0.42
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.87	0.42
5:F:311:THR:OG1	5:F:312:GLY:N	2.53	0.42
3:D:641:ARG:O	3:D:683:PHE:N	2.52	0.42
9:M:70:VAL:HG11	9:M:101:VAL:HG12	2.02	0.42
2:C:758:ASP:OD1	2:C:758:ASP:N	2.48	0.42
2:C:1063:PHE:HD1	2:C:1063:PHE:HA	1.75	0.42
3:D:446:LEU:HD13	3:D:520:LYS:HE2	2.02	0.42
9:M:67:LEU:HD23	9:M:67:LEU:HA	1.70	0.42
2:C:1111:ASN:OD1	4:E:65:ASN:ND2	2.53	0.42
3:D:452:PHE:HE1	3:D:494:HIS:HD2	1.66	0.42
3:D:453:LYS:HA	3:D:456:VAL:HG12	2.02	0.42
7:O:57:DC:C1'	7:O:58:DA:O5'	2.67	0.42
9:M:67:LEU:HD22	9:M:67:LEU:O	2.20	0.42
9:M:143:GLU:HB3	9:M:145:THR:HG22	2.01	0.42
2:C:273:ALA:C	2:C:277:ILE:HD12	2.40	0.42
2:C:563:ARG:HG3	2:C:564:LYS:H	1.84	0.42
2:C:715:LEU:N	2:C:1029:TYR:OH	2.52	0.42
3:D:353:ARG:NE	5:F:323:GLU:OE2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:CD1	1:B:18:ARG:HH22	2.33	0.41
2:C:278:TYR:CD2	2:C:278:TYR:C	2.94	0.41
2:C:919:THR:HG23	3:D:731:VAL:HG23	2.02	0.41
3:D:902:ALA:HA	3:D:913:ASP:H	1.84	0.41
7:O:71:DA:H1'	7:O:72:DG:H5'	2.01	0.41
3:D:428:SER:OG	3:D:429:VAL:N	2.53	0.41
6:J:5:VAL:H	6:J:6:LEU:HA	1.84	0.41
2:C:139:PHE:HB3	2:C:148:LYS:HB2	2.02	0.41
2:C:646:GLU:HB3	2:C:662:HIS:CE1	2.56	0.41
3:D:98:ALA:HB3	3:D:354:LEU:HD23	2.02	0.41
3:D:1068:PRO:HD3	3:D:1074:GLU:HG2	2.02	0.41
8:P:80:DC:H3'	8:P:80:DC:H6	1.86	0.41
1:A:14:LEU:HB2	1:A:18:ARG:HD3	2.03	0.41
2:C:278:TYR:HE1	2:C:291:SER:HG	1.69	0.41
2:C:1077:GLN:HE21	3:D:1252:VAL:HG21	1.85	0.41
3:D:356:ARG:HE	5:F:326:LEU:HD11	1.85	0.41
3:D:866:ARG:HH12	3:D:1011:THR:HA	1.84	0.41
7:O:32:DC:O2	8:P:124:DG:N2	2.53	0.41
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.85	0.41
3:D:636:ARG:HD3	3:D:661:ALA:HB1	2.02	0.41
3:D:827:PRO:O	3:D:858:LYS:NZ	2.34	0.41
9:M:150:ALA:HA	9:M:153:ILE:HG22	2.02	0.41
2:C:258:MET:HG2	2:C:346:VAL:HG21	2.03	0.41
3:D:191:ALA:HA	3:D:194:ARG:HE	1.85	0.41
3:D:952:LEU:HD22	3:D:957:ILE:HD11	2.03	0.41
3:D:1106:GLU:H	3:D:1109:GLN:HB2	1.85	0.41
5:F:302:LEU:N	7:O:54:DT:O2	2.54	0.41
8:P:131:DG:H2"	8:P:132:DA:C8	2.56	0.41
2:C:554:PHE:HD2	2:C:573:SER:HB2	1.86	0.41
2:C:885:LEU:HD23	2:C:1030:ILE:HD12	2.02	0.41
3:D:497:LEU:HB2	3:D:544:HIS:HB2	2.03	0.41
3:D:797:ASN:HB3	3:D:800:ILE:HG22	2.03	0.41
3:D:832:ILE:HA	3:D:833:PRO:HD3	1.85	0.41
3:D:867:THR:HG21	8:P:93:DA:C2	2.55	0.41
7:O:28:DA:OP2	7:O:28:DA:H8	2.03	0.41
7:O:36:DG:H2"	7:O:37:DC:H5"	2.01	0.41
8:P:129:DA:H2"	8:P:130:DA:OP2	2.20	0.41
9:M:71:PHE:CE1	9:M:157:VAL:HG21	2.56	0.41
2:C:928:ILE:HD11	3:D:841:ARG:HA	2.03	0.41
2:C:946:VAL:N	2:C:964:LEU:O	2.49	0.41
7:O:57:DC:H1'	7:O:58:DA:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:PHE:O	2:C:148:LYS:N	2.54	0.40
3:D:1251:ASN:HD22	3:D:1259:PRO:HD3	1.85	0.40
4:E:60:ARG:NE	4:E:98:GLU:OE1	2.45	0.40
5:F:384:ARG:NH1	8:P:104:DC:C4	2.89	0.40
9:M:12:PRO:HA	9:M:13:HIS:HA	1.83	0.40
2:C:243:TRP:HE3	2:C:247:GLN:HB3	1.86	0.40
3:D:104:ILE:HD12	3:D:379:ASP:HB3	2.04	0.40
3:D:386:ARG:HH22	3:D:1230:THR:HG21	1.86	0.40
5:F:330:ARG:HH22	7:O:47:DA:H3'	1.85	0.40
2:C:408:ASP:OD1	2:C:408:ASP:N	2.54	0.40
2:C:774:PRO:CD	2:C:834:ASP:HB2	2.51	0.40
2:C:905:PRO:HD2	2:C:916:ILE:HD11	2.02	0.40
3:D:487:LEU:HA	3:D:490:VAL:HG22	2.02	0.40
3:D:851:ILE:HA	3:D:854:HIS:HD2	1.86	0.40
7:O:73:DC:H6	7:O:73:DC:OP2	2.04	0.40
2:C:230:ARG:O	2:C:230:ARG:HG2	2.22	0.40
2:C:1111:ASN:ND2	4:E:66:ASP:OD1	2.55	0.40
3:D:866:ARG:HG2	3:D:867:THR:N	2.36	0.40
3:D:1086:LEU:HD23	3:D:1099:LEU:HD23	2.04	0.40
7:O:51:DG:H2"	7:O:52:DA:C8	2.56	0.40
2:C:947:ASP:OD1	2:C:947:ASP:N	2.54	0.40
3:D:185:GLU:OE2	3:D:195:ARG:NH2	2.45	0.40
8:P:132:DA:H8	8:P:132:DA:OP2	2.04	0.40
9:M:71:PHE:O	9:M:74:LEU:N	2.55	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	223/347 (64%)	207 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	235/347 (68%)	210 (89%)	24 (10%)	1 (0%)	30 63
2	C	1109/1134 (98%)	991 (89%)	107 (10%)	11 (1%)	13 46
3	D	1264/1371 (92%)	1183 (94%)	77 (6%)	4 (0%)	37 67
4	E	81/110 (74%)	73 (90%)	8 (10%)	0	100 100
5	F	320/531 (60%)	303 (95%)	17 (5%)	0	100 100
6	J	107/111 (96%)	95 (89%)	11 (10%)	1 (1%)	14 48
9	M	157/162 (97%)	147 (94%)	9 (6%)	1 (1%)	22 55
All	All	3496/4113 (85%)	3209 (92%)	269 (8%)	18 (0%)	27 59

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	231	ARG
3	D	1008	THR
3	D	1011	THR
2	C	230	ARG
2	C	775	ASN
2	C	778	ASP
1	B	18	ARG
2	C	232	GLN
2	C	774	PRO
3	D	579	LEU
9	M	147	ASP
2	C	53	LEU
2	C	282	ARG
2	C	79	ASP
2	C	283	PRO
3	D	1006	PRO
6	J	78	PRO
2	C	277	ILE

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	194/297 (65%)	191 (98%)	3 (2%)	60	78
1	B	195/297 (66%)	194 (100%)	1 (0%)	86	93
2	C	937/965 (97%)	920 (98%)	17 (2%)	54	74
3	D	1048/1135 (92%)	1029 (98%)	19 (2%)	54	74
4	E	69/89 (78%)	68 (99%)	1 (1%)	62	79
5	F	266/429 (62%)	261 (98%)	5 (2%)	52	73
6	J	92/97 (95%)	89 (97%)	3 (3%)	33	61
9	M	129/131 (98%)	122 (95%)	7 (5%)	18	48
All	All	2930/3440 (85%)	2874 (98%)	56 (2%)	52	73

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	34	LEU
1	A	98	ARG
1	B	226	ASN
2	C	141	ASN
2	C	181	ARG
2	C	222	VAL
2	C	230	ARG
2	C	231	ARG
2	C	279	ARG
2	C	280	LYS
2	C	282	ARG
2	C	373	PHE
2	C	419	ASN
2	C	540	VAL
2	C	773	ILE
2	C	776	ILE
2	C	777	SER
2	C	787	ARG
2	C	834	ASP
2	C	958	ARG
3	D	209	ARG
3	D	499	ASN
3	D	576	MET
3	D	578	ARG
3	D	579	LEU
3	D	585	LEU

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Mol	Chain	Res	Type
3	D	586	TYR
3	D	733	MET
3	D	797	ASN
3	D	860	LEU
3	D	866	ARG
3	D	875	ARG
3	D	1009	GLN
3	D	1012	MET
3	D	1013	ARG
3	D	1089	PHE
3	D	1090	LYS
3	D	1097	ARG
3	D	1159	ARG
4	E	82	LEU
5	F	213	ARG
5	F	269	ARG
5	F	278	ARG
5	F	282	MET
5	F	384	ARG
6	J	27	ARG
6	J	76	LYS
6	J	110	ARG
9	M	65	GLU
9	M	67	LEU
9	M	69	LYS
9	M	71	PHE
9	M	84	ASN
9	M	109	ARG
9	M	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	151	GLN
1	B	79	ASN
1	B	226	ASN
2	C	141	ASN
2	C	150	GLN
2	C	200	HIS
2	C	317	ASN
2	C	419	ASN

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Mol	Chain	Res	Type
2	C	435	GLN
2	C	662	HIS
2	C	875	GLN
2	C	920	HIS
2	C	1066	GLN
3	D	307	ASN
3	D	494	HIS
3	D	657	GLN
3	D	687	GLN
3	D	693	GLN
3	D	771	ASN
3	D	797	ASN
3	D	1139	GLN
3	D	1251	ASN
4	E	70	GLN
5	F	322	GLN
5	F	325	ASN
5	F	388	GLN
9	M	13	HIS
9	M	133	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

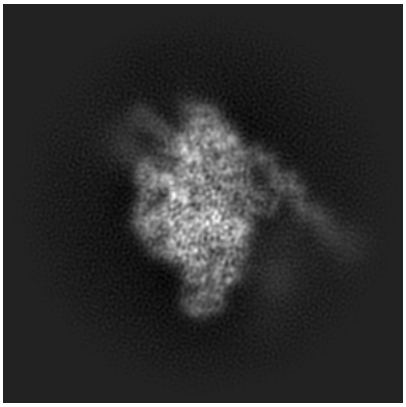
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9037. These allow visual inspection of the internal detail of the map and identification of artifacts.

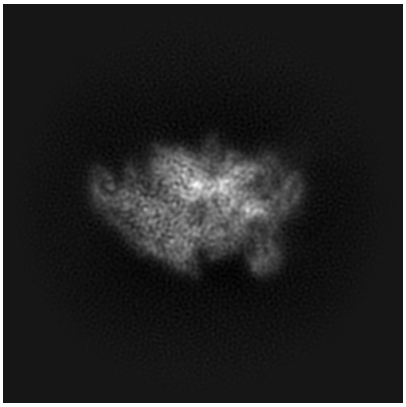
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

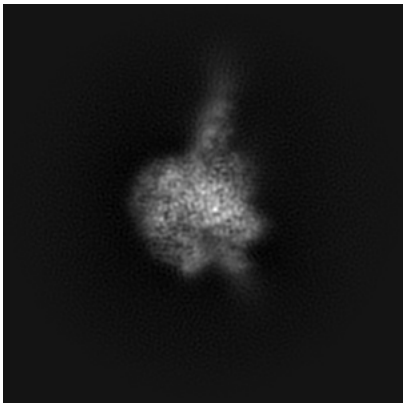
6.1.1 Primary map



X



Y

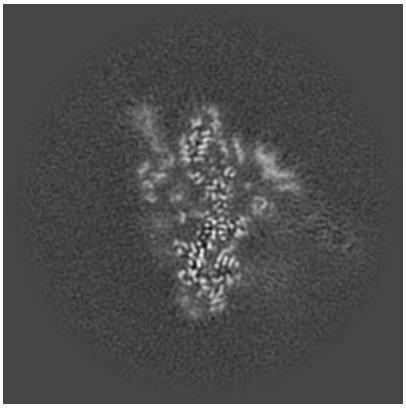


Z

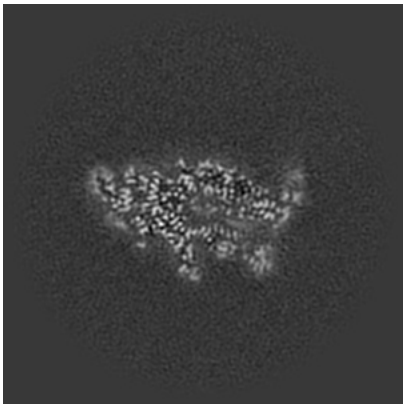
The images above show the map projected in three orthogonal directions.

6.2 Central slices

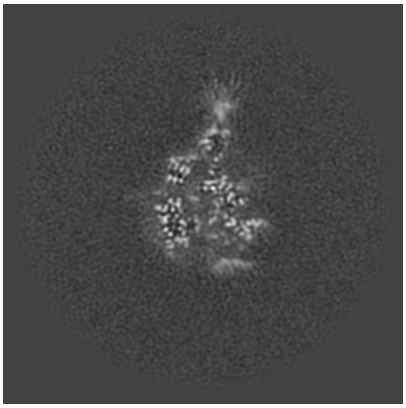
6.2.1 Primary map



X Index: 125



Y Index: 125

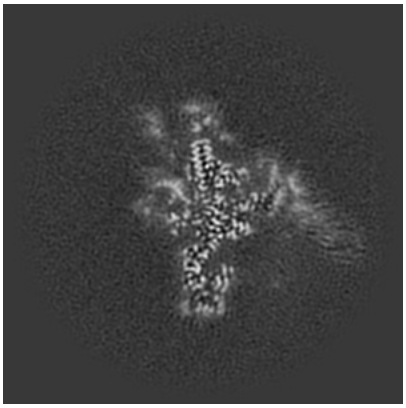


Z Index: 125

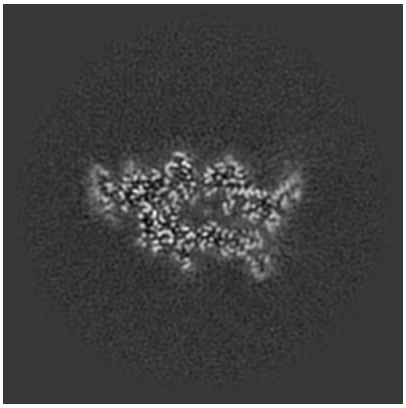
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

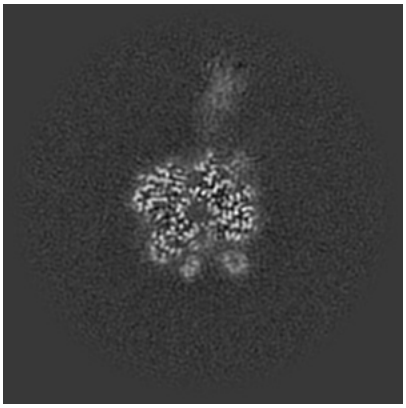
6.3.1 Primary map



X Index: 132



Y Index: 121

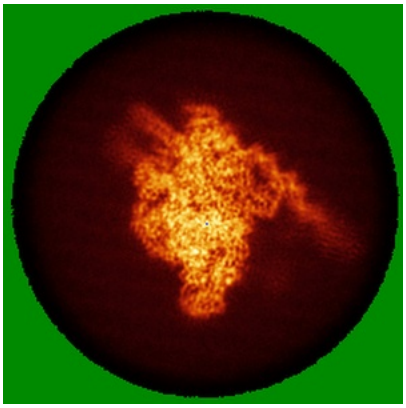


Z Index: 113

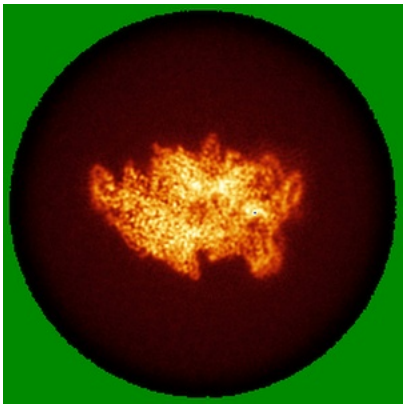
The images above show the largest variance slices of the map in three orthogonal directions.

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

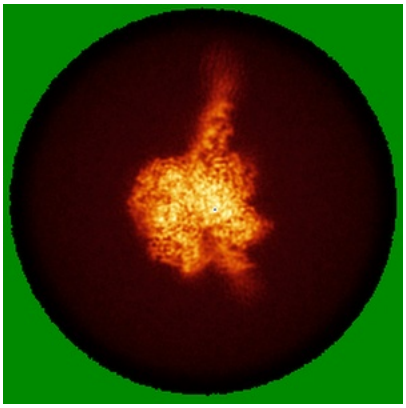
6.4.1 Primary map



X



Y

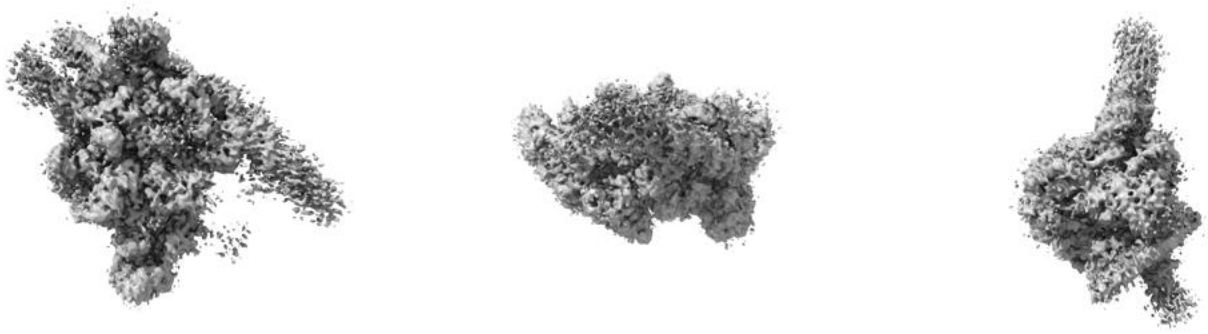


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

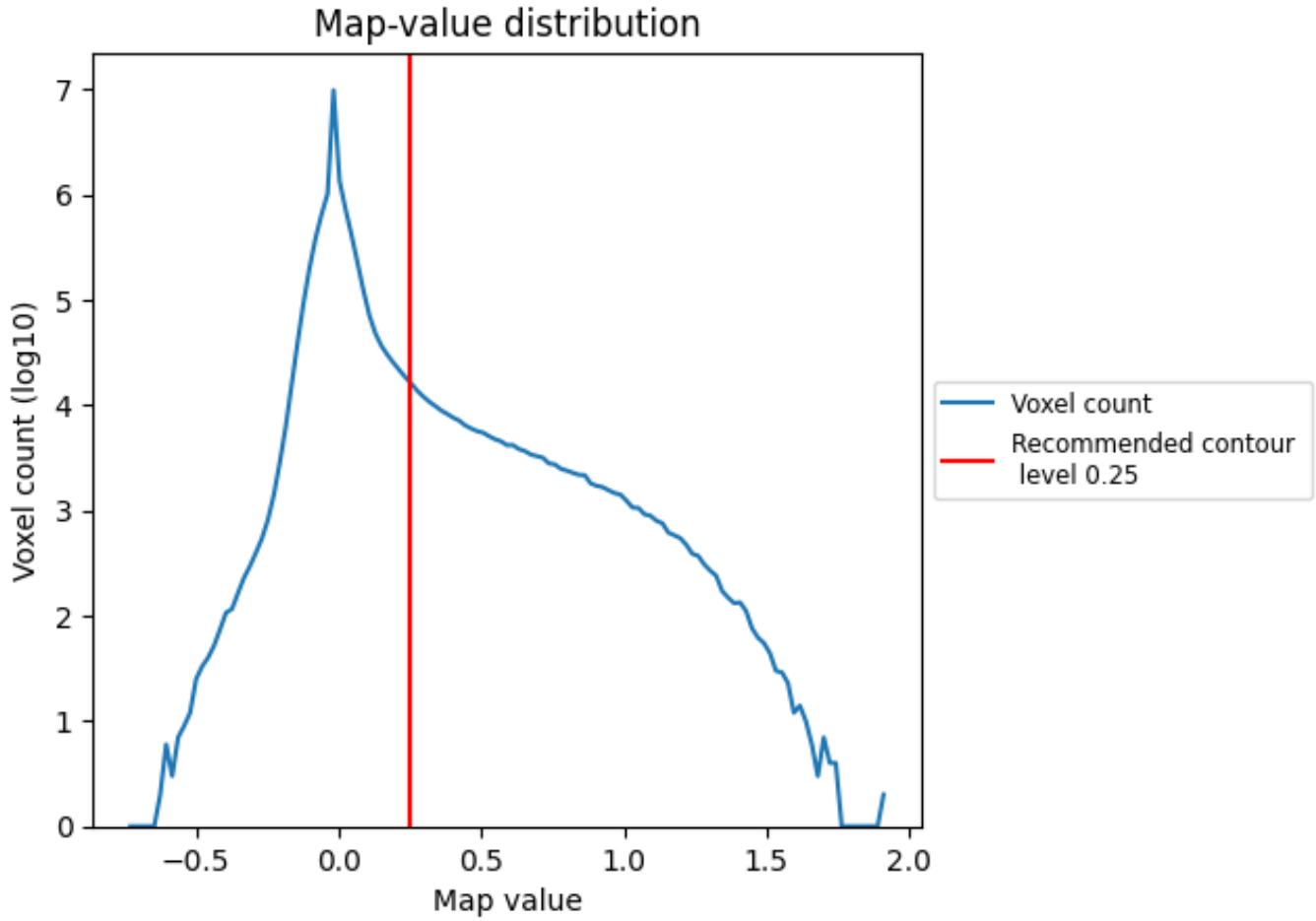
6.6 Mask visualisation (i)

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

7 Map analysis

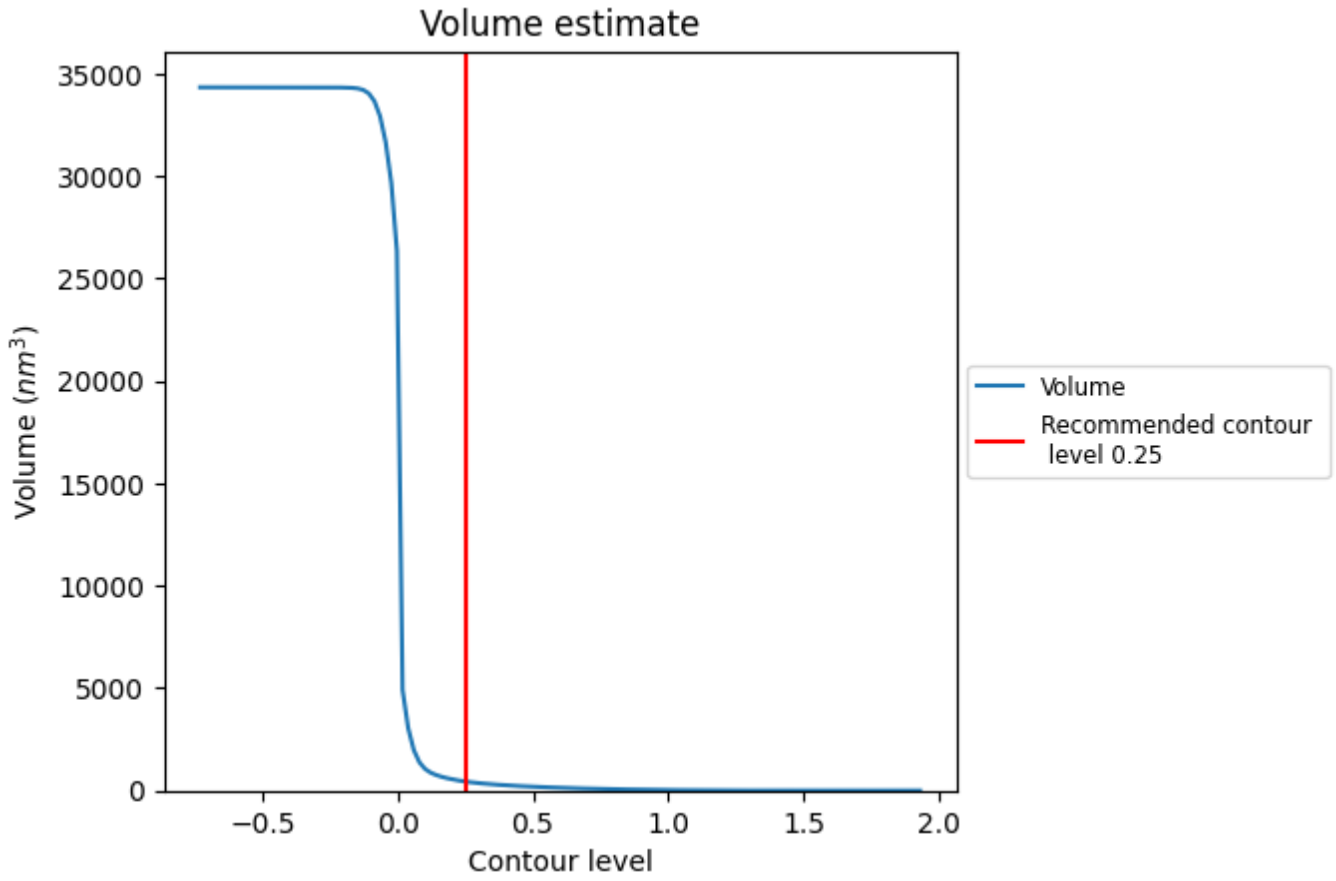
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

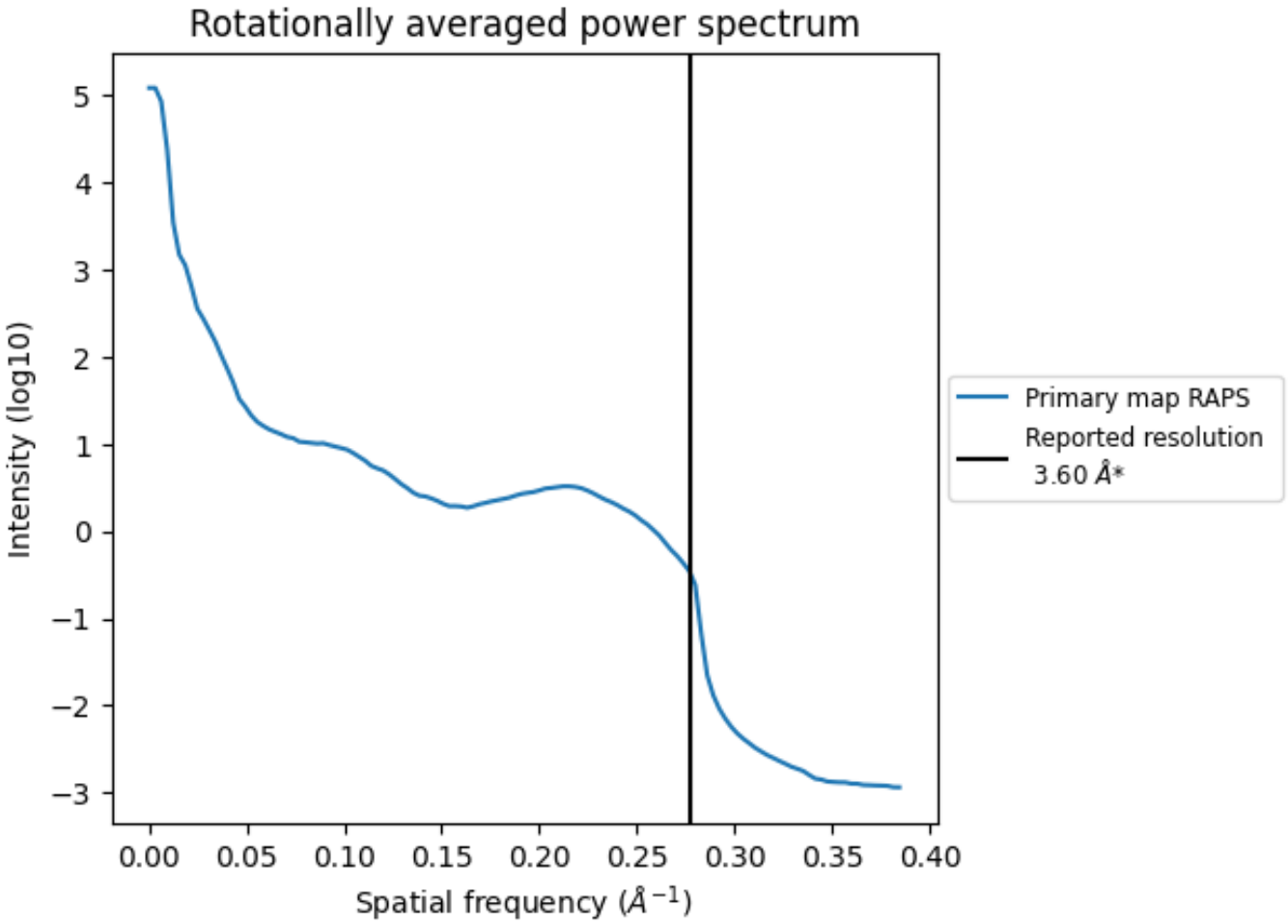
7.2 Volume estimate



The volume at the recommended contour level is 442 nm^3; this corresponds to an approximate mass of 399 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 0.278 Å^{-1}

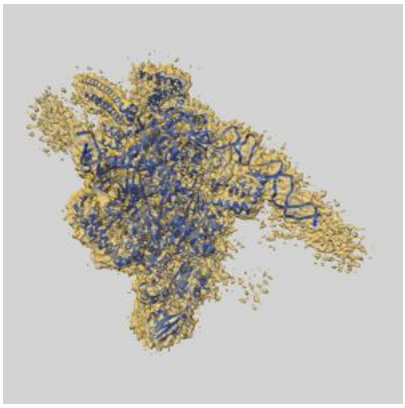
8 Fourier-Shell correlation (i)

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

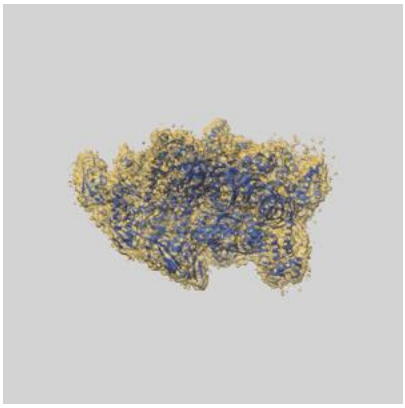
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9037 and PDB model 6EDT. Per-residue inclusion information can be found in section 3 on page 8.

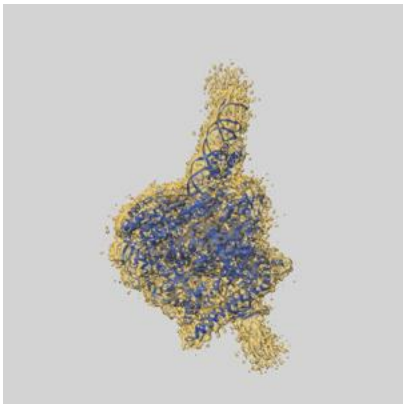
9.1 Map-model overlay



X



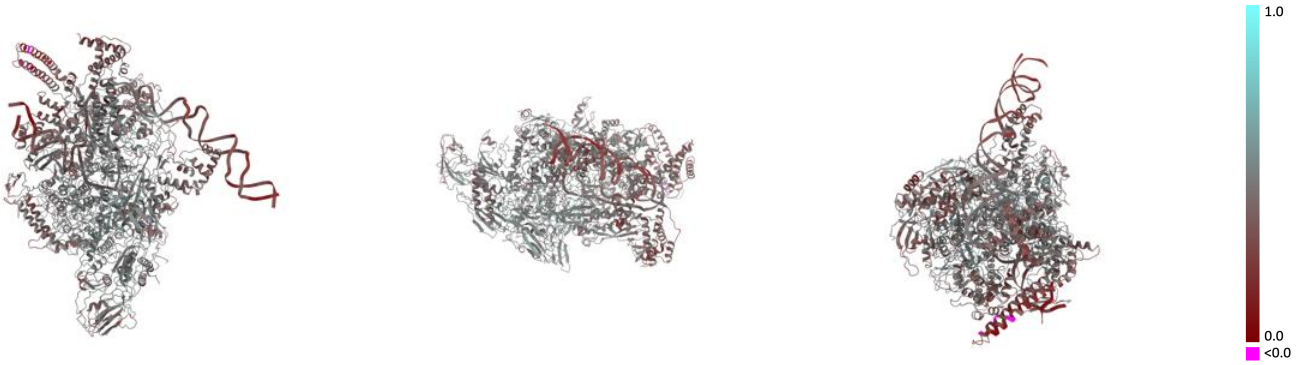
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

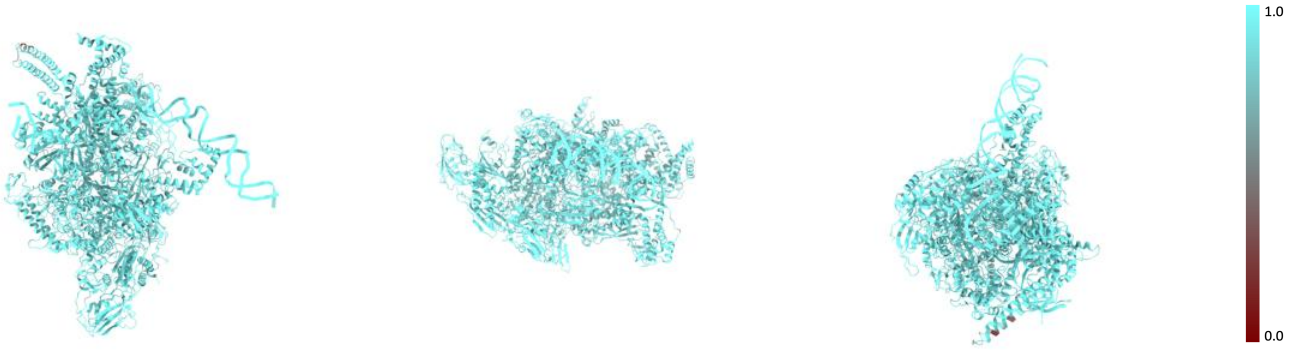
9.2 Q-score mapped to coordinate model (i)



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.

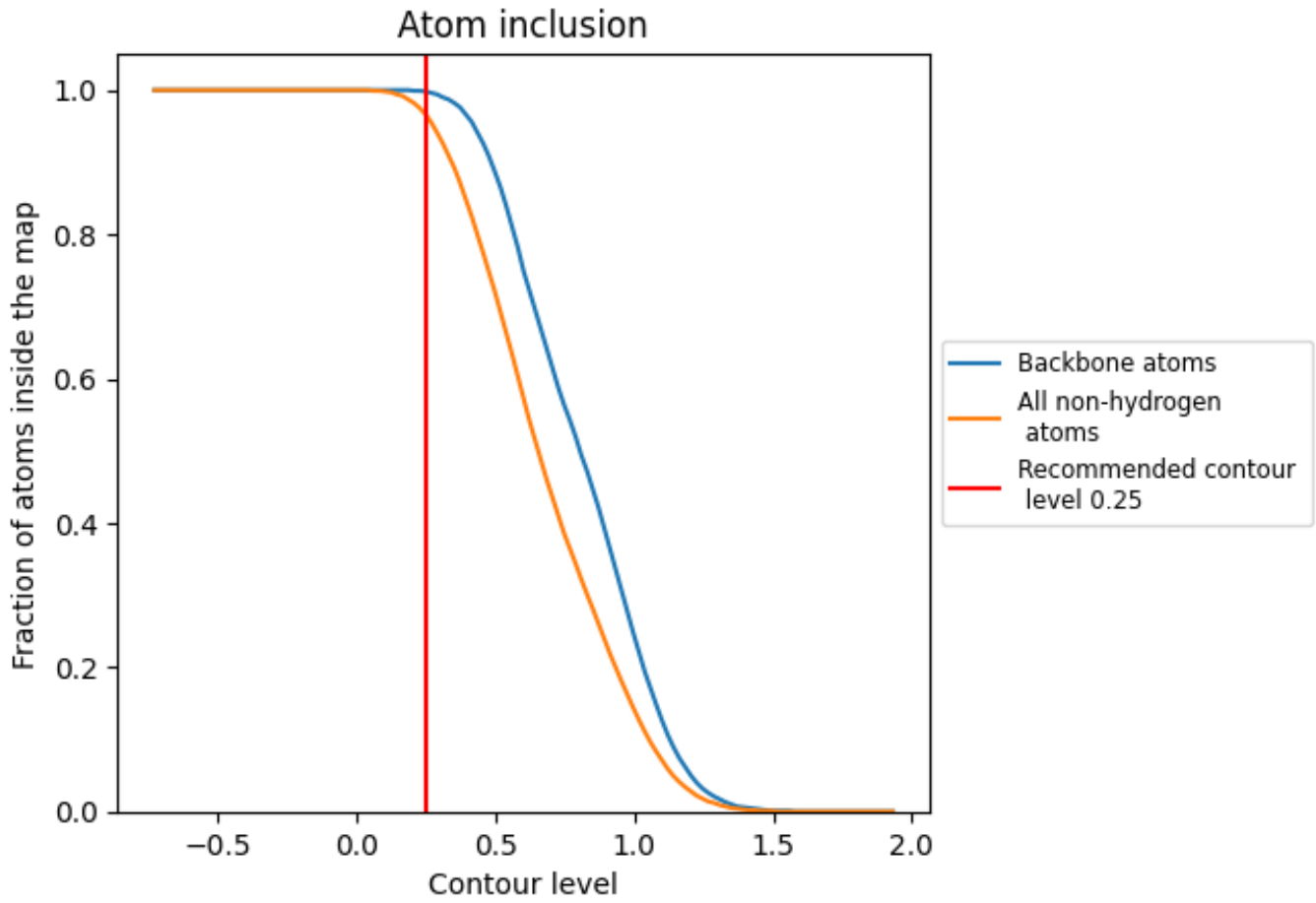
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.4370
A	0.9780	0.4790
B	0.9650	0.4440
C	0.9630	0.4690
D	0.9610	0.4490
E	0.9480	0.4570
F	0.9610	0.4020
J	0.9540	0.4070
M	0.9540	0.3620
O	0.9900	0.3260
P	0.9950	0.3320