Full wwPDB EM Validation Report

Mar 3, 2024 – 07:56 AM EST

PDB ID	:	6C04
EMDB ID	:	EMD-7320
Title	:	Mtb RNAP Holo/RbpA/double fork DNA -closed clamp
Authors	:	Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.; Lilic, M.
Deposited on	:	2017-12-27
Resolution	:	3.27 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

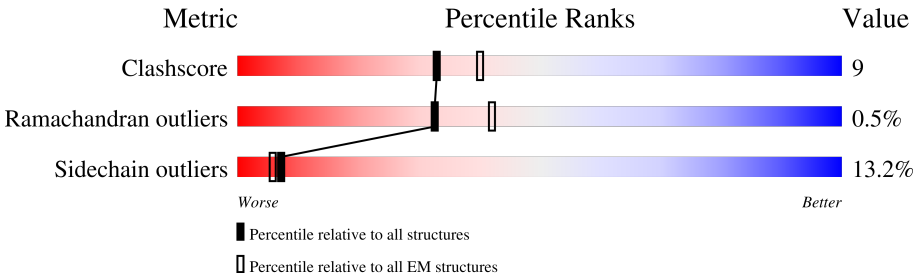
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.27 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	347	50% 13% • 35%
1	B	347	50% 15% • 32%
2	C	1179	70% 22% • 6%
3	D	1326	72% 19% • •
4	E	110	54% 15% 6% 25%
5	F	531	48% 11% • 40%
6	J	111	56% 25% 13% • •
7	H	31	52% 16% • 29%

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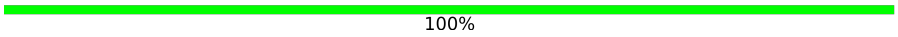
Mol	Chain	Length	Quality of chain
7	O	31	
8	G	26	
8	P	26	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27982 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	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	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
			8585	5378	1507	1661	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1267	Total	C	N	O	S	0	0
			9881	6190	1795	1854	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

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

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

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	319	Total	C	N	O	S	0	0
			2508	1566	453	480	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			881	543	168	167	3		

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	31	Total 634	C 305	N 114	O 185	P 30	0	0
7	H	22	Total 454	C 218	N 82	O 132	P 22	0	0

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	26	Total 526	C 254	N 94	O 153	P 25	0	0
8	G	18	Total 362	C 176	N 64	O 105	P 17	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

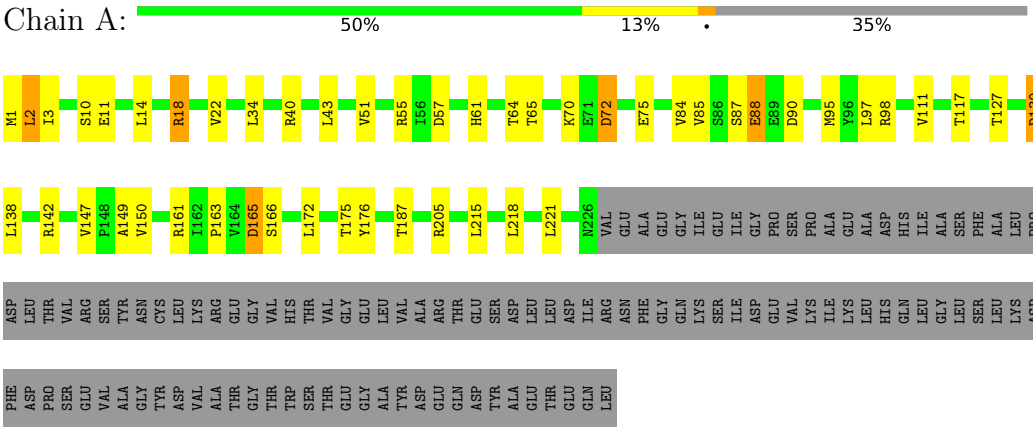
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total 1	Mg 1	0

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.

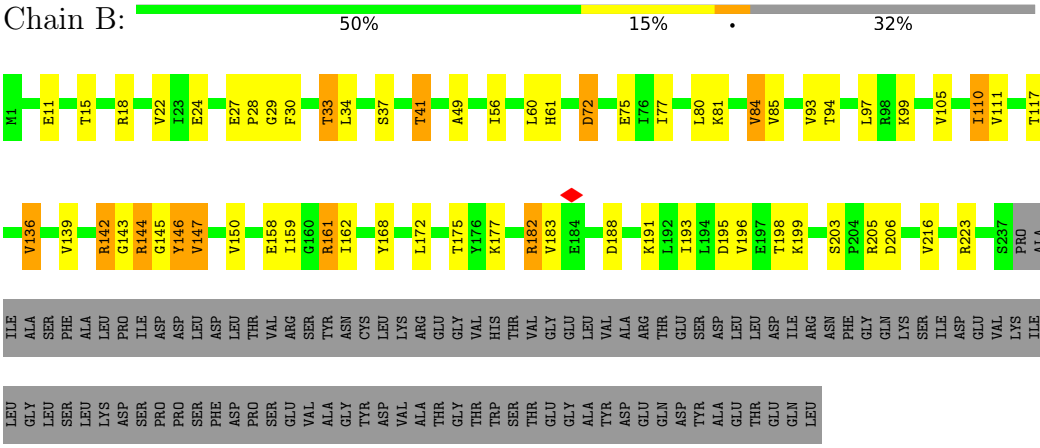
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



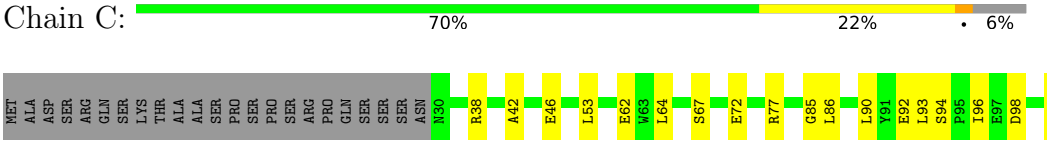
• Molecule 1: DNA-directed RNA polymerase subunit alpha

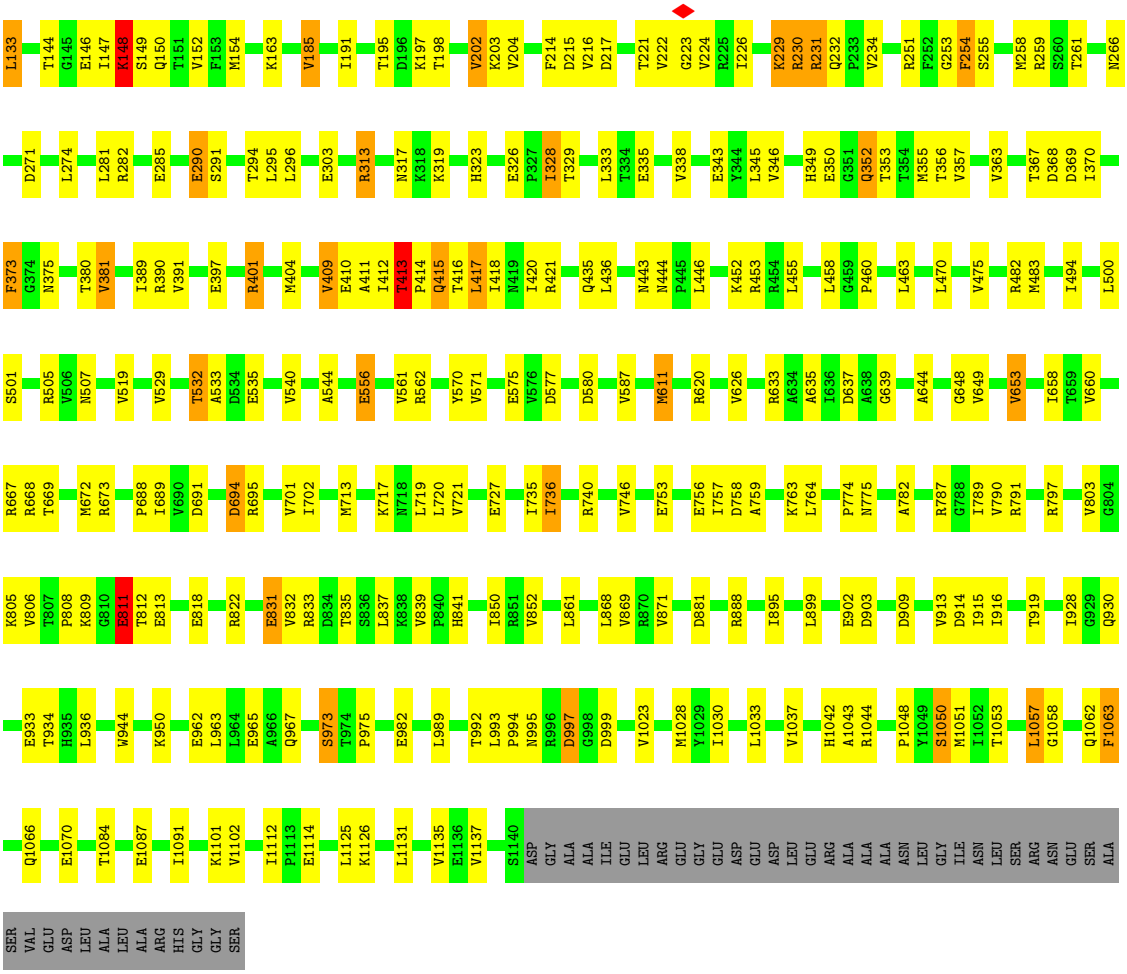
Chain B:



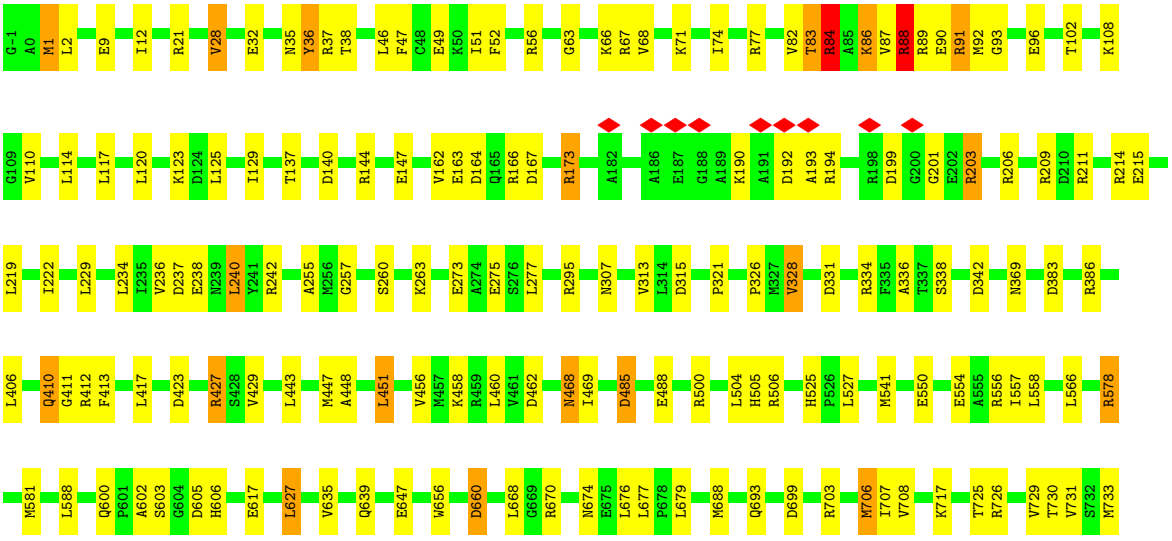
• Molecule 2: DNA-directed RNA polymerase subunit beta

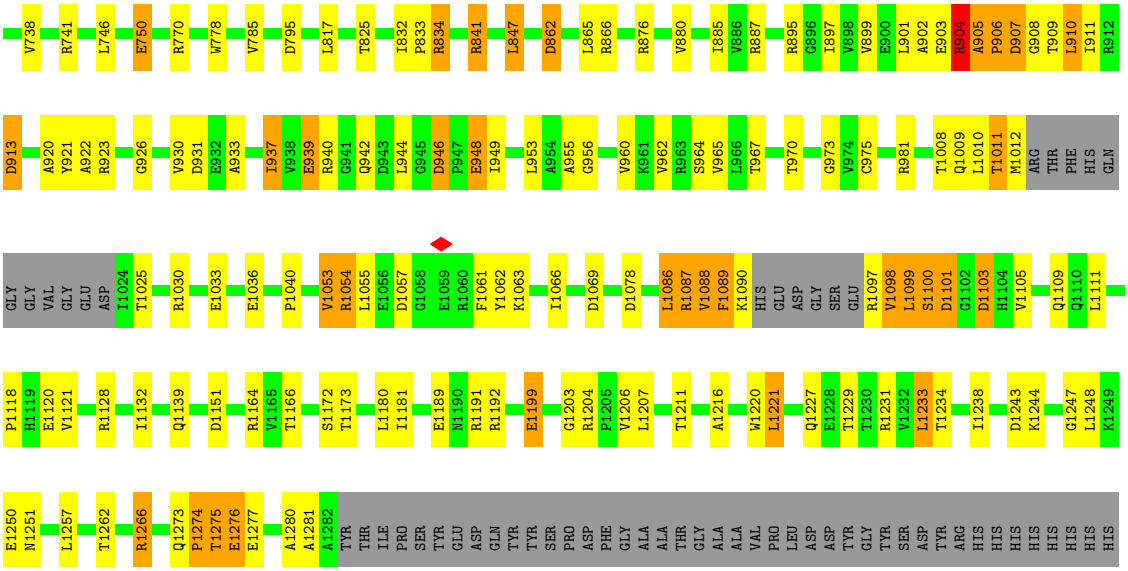
Chain C:





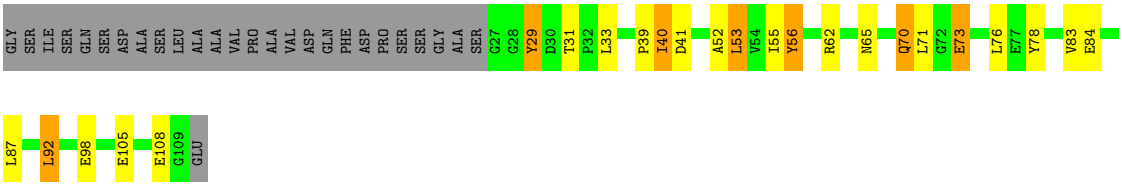
• Molecule 3: DNA-directed RNA polymerase subunit beta'





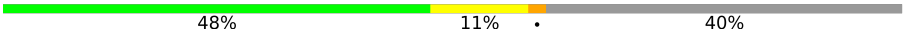
• Molecule 4: DNA-directed RNA polymerase subunit omega

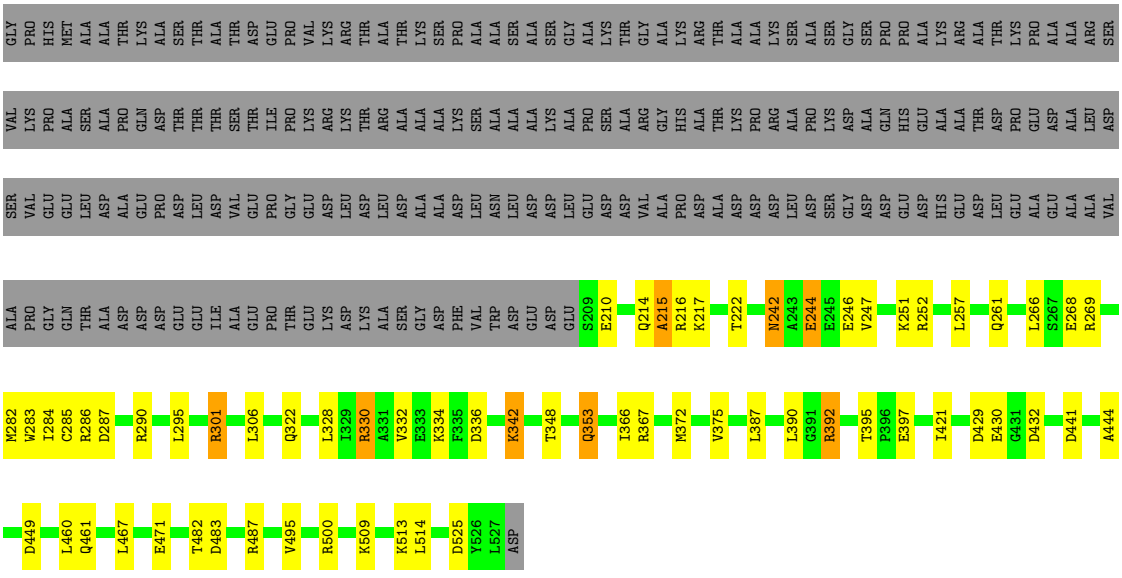
Chain E:



• Molecule 5: RNA polymerase sigma factor SigA

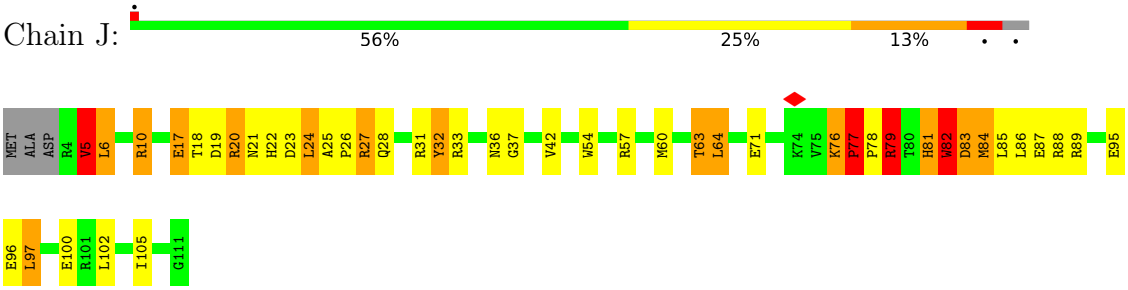
Chain F:





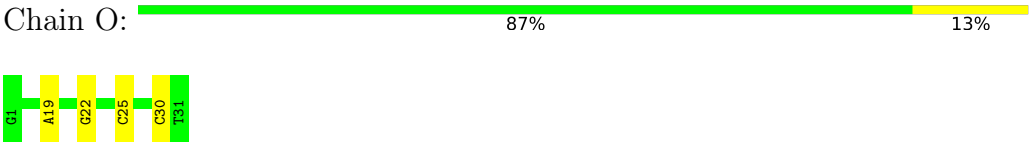
• Molecule 6: RNA polymerase-binding protein RbpA

Chain J:



• Molecule 7: DNA (31-MER)

Chain O:



• Molecule 7: DNA (31-MER)

Chain H:

• Molecule 8: DNA (26-MER)

Chain P:

There are no outlier residues recorded for this chain.

• Molecule 8: DNA (26-MER)

Chain G:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171547	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 ($e^-/Å^2$)	6.7	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	3.539	Depositor
Minimum map value	-1.657	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.372	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/1750	0.56	0/2380
1	B	0.73	9/1802 (0.5%)	0.61	1/2454 (0.0%)
2	C	0.44	0/8743	0.59	6/11859 (0.1%)
3	D	0.67	32/10045 (0.3%)	0.63	12/13581 (0.1%)
4	E	0.51	0/662	0.66	0/901
5	F	0.33	0/2539	0.47	0/3426
6	J	0.93	3/897 (0.3%)	1.13	5/1210 (0.4%)
7	H	0.75	1/509 (0.2%)	0.96	0/784
7	O	0.73	0/710	1.01	1/1095 (0.1%)
8	G	0.67	0/405	1.00	0/622
8	P	0.72	0/589	0.96	0/906
All	All	0.58	45/28651 (0.2%)	0.66	25/39218 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
3	D	0	4
All	All	0	7

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	TYR	CE1-CZ	-12.56	1.22	1.38
3	D	36	TYR	CE1-CZ	-9.97	1.25	1.38
3	D	52	PHE	CG-CD1	-9.75	1.24	1.38
3	D	88	ARG	C-O	-8.92	1.06	1.23
3	D	92	MET	C-O	-8.56	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	52	PHE	CG-CD2	-8.53	1.25	1.38
1	B	146	TYR	CG-CD2	-8.35	1.28	1.39
3	D	52	PHE	C-O	-8.28	1.07	1.23
1	B	145	GLY	C-O	-7.95	1.10	1.23
6	J	32	TYR	CE1-CZ	-7.81	1.28	1.38
3	D	88	ARG	CZ-NH1	-7.71	1.23	1.33
3	D	36	TYR	CG-CD1	-7.45	1.29	1.39
3	D	411	GLY	C-O	-7.24	1.12	1.23
3	D	88	ARG	CZ-NH2	-7.22	1.23	1.33
1	B	147	VAL	C-O	-7.09	1.09	1.23
7	H	27	DA	O3'-P	-7.02	1.52	1.61
1	B	146	TYR	CG-CD1	-6.83	1.30	1.39
3	D	36	TYR	CE2-CZ	-6.80	1.29	1.38
1	B	146	TYR	CE2-CZ	-6.75	1.29	1.38
3	D	413	PHE	CG-CD2	-6.45	1.29	1.38
6	J	32	TYR	CE2-CZ	-6.41	1.30	1.38
3	D	87	VAL	C-O	-6.17	1.11	1.23
3	D	91	ARG	C-O	-6.13	1.11	1.23
3	D	52	PHE	CE2-CZ	-6.06	1.25	1.37
3	D	51	ILE	C-O	-6.05	1.11	1.23
3	D	413	PHE	C-O	-6.05	1.11	1.23
3	D	93	GLY	C-O	-5.99	1.14	1.23
3	D	412	ARG	C-O	-5.99	1.11	1.23
3	D	413	PHE	CG-CD1	-5.97	1.29	1.38
1	B	146	TYR	C-O	-5.96	1.12	1.23
3	D	91	ARG	CA-CB	-5.88	1.41	1.53
3	D	83	THR	C-O	-5.71	1.12	1.23
6	J	32	TYR	CG-CD1	-5.65	1.31	1.39
3	D	87	VAL	CA-CB	-5.64	1.43	1.54
1	B	146	TYR	CD1-CE1	-5.56	1.31	1.39
3	D	1275	THR	CA-C	-5.53	1.38	1.52
1	B	146	TYR	CZ-OH	-5.46	1.28	1.37
3	D	49	GLU	CA-C	-5.36	1.39	1.52
3	D	1274	PRO	CA-C	-5.19	1.42	1.52
3	D	49	GLU	CD-OE1	-5.15	1.20	1.25
3	D	52	PHE	CE1-CZ	-5.15	1.27	1.37
3	D	87	VAL	CB-CG1	-5.14	1.42	1.52
3	D	86	LYS	C-O	-5.13	1.13	1.23
3	D	49	GLU	C-O	-5.12	1.13	1.23
3	D	88	ARG	N-CA	-5.02	1.36	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	77	PRO	C-N-CD	-20.77	74.89	120.60
6	J	77	PRO	C-N-CA	13.80	179.95	122.00
2	C	148	LYS	N-CA-C	-7.88	89.72	111.00
3	D	51	ILE	CG1-CB-CG2	-7.34	95.25	111.40
2	C	413	THR	C-N-CD	6.17	141.36	128.40
2	C	417	LEU	CB-CG-CD2	-6.10	100.64	111.00
3	D	92	MET	CG-SD-CE	-6.09	90.45	100.20
3	D	52	PHE	CA-C-N	6.03	128.26	116.20
3	D	834	ARG	C-N-CD	-5.96	107.48	120.60
2	C	413	THR	N-CA-C	-5.65	95.73	111.00
3	D	1207	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	146	TYR	N-CA-CB	-5.57	100.58	110.60
3	D	1011	THR	N-CA-C	5.54	125.95	111.00
3	D	37	ARG	CB-CA-C	-5.41	99.59	110.40
3	D	1275	THR	CB-CA-C	-5.40	97.02	111.60
6	J	20	ARG	CB-CA-C	-5.34	99.71	110.40
6	J	79	ARG	C-N-CA	-5.31	108.42	121.70
3	D	410	GLN	CB-CA-C	-5.23	99.93	110.40
2	C	811	GLU	N-CA-C	5.22	125.10	111.00
2	C	993	LEU	CA-CB-CG	5.21	127.29	115.30
3	D	140	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	1101	ASP	CB-CG-OD1	-5.17	113.65	118.30
7	O	19	DA	P-O3'-C3'	5.11	125.83	119.70
6	J	5	VAL	N-CA-C	-5.08	97.27	111.00
3	D	834	ARG	C-N-CA	5.05	143.22	122.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	229	LYS	Peptide
2	C	254	PHE	Peptide
2	C	774	PRO	Peptide
3	D	578	ARG	Peptide
3	D	600	GLN	Peptide
3	D	907	ASP	Peptide
3	D	933	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1768	28	0
1	B	1775	0	1809	27	0
2	C	8585	0	8508	156	0
3	D	9881	0	9949	214	0
4	E	649	0	645	18	0
5	F	2508	0	2525	44	0
6	J	881	0	861	54	0
7	H	454	0	251	12	0
7	O	634	0	350	4	0
8	G	362	0	206	1	0
8	P	526	0	296	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	27982	0	27168	509	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 9.

All (509) 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)
3:D:1089:PHE:CE1	3:D:1109:GLN:NE2	1.91	1.38
6:J:76:LYS:HB2	6:J:77:PRO:CD	1.67	1.23
3:D:1089:PHE:CD1	3:D:1109:GLN:NE2	2.09	1.20
5:F:261:GLN:HG2	6:J:82:TRP:CZ2	1.78	1.17
6:J:76:LYS:HB2	6:J:77:PRO:HD3	1.16	1.15
6:J:17:GLU:OE1	6:J:17:GLU:N	1.85	1.07
3:D:1055:LEU:N	3:D:1101:ASP:OD2	1.86	1.07
5:F:210:GLU:OE1	5:F:210:GLU:N	1.86	1.07
2:C:809:LYS:NZ	2:C:831:GLU:O	1.90	1.05
3:D:1277:GLU:O	3:D:1280:ALA:HB3	1.57	1.03
3:D:1221:LEU:CD2	3:D:1250:GLU:HG2	1.89	1.02
5:F:214:GLN:O	5:F:217:LYS:N	1.93	1.00
3:D:1221:LEU:HD21	3:D:1250:GLU:HG2	1.46	0.97
3:D:1089:PHE:HE1	3:D:1109:GLN:NE2	1.45	0.96
2:C:809:LYS:HB3	2:C:831:GLU:O	1.66	0.95
2:C:409:VAL:HG22	2:C:410:GLU:H	1.29	0.93
3:D:1221:LEU:CG	3:D:1250:GLU:HG2	1.99	0.93
5:F:261:GLN:OE1	6:J:82:TRP:NE1	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:76:LYS:CB	6:J:77:PRO:CD	2.41	0.92
6:J:76:LYS:CB	6:J:77:PRO:HD3	2.02	0.90
3:D:1087:ARG:HG2	3:D:1087:ARG:HH11	1.35	0.90
6:J:81:HIS:O	6:J:84:MET:N	2.05	0.90
3:D:1221:LEU:HD23	3:D:1243:ASP:OD2	1.73	0.88
6:J:6:LEU:HD12	6:J:6:LEU:H	1.38	0.87
3:D:905:ALA:HB1	3:D:906:PRO:CD	2.07	0.85
3:D:1128:ARG:O	3:D:1128:ARG:NH1	2.10	0.84
3:D:903:GLU:O	3:D:904:ARG:O	1.95	0.84
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.11	0.84
3:D:1276:GLU:O	3:D:1280:ALA:HB2	1.77	0.83
5:F:334:LYS:NZ	7:O:25:DC:OP2	2.10	0.83
3:D:1221:LEU:HD21	3:D:1250:GLU:CG	2.08	0.83
2:C:414:PRO:HG2	2:C:415:GLN:H	1.42	0.82
3:D:905:ALA:HB1	3:D:906:PRO:HD2	1.62	0.82
3:D:63:GLY:O	3:D:66:LYS:NZ	2.12	0.82
3:D:1221:LEU:HG	3:D:1250:GLU:HG2	1.61	0.81
2:C:813:GLU:N	2:C:813:GLU:OE1	2.14	0.81
3:D:1221:LEU:HD11	3:D:1250:GLU:CB	2.09	0.80
3:D:1221:LEU:HD21	3:D:1250:GLU:CB	2.12	0.80
2:C:414:PRO:HG2	2:C:415:GLN:N	1.97	0.79
3:D:1276:GLU:O	3:D:1280:ALA:CB	2.30	0.79
2:C:648:GLY:O	2:C:695:ARG:NH1	2.16	0.79
3:D:1221:LEU:HD21	3:D:1250:GLU:HB3	1.64	0.79
3:D:1089:PHE:HD1	3:D:1109:GLN:HE22	1.29	0.78
6:J:23:ASP:C	6:J:24:LEU:HD13	2.02	0.78
1:A:75:GLU:OE2	2:C:620:ARG:NH1	2.16	0.78
3:D:1086:LEU:HD23	3:D:1099:LEU:HB3	1.65	0.78
5:F:261:GLN:HG2	6:J:82:TRP:HZ2	1.46	0.78
3:D:1128:ARG:HH12	3:D:1132:ILE:HG12	1.48	0.78
3:D:199:ASP:O	3:D:203:ARG:NH1	2.17	0.77
5:F:261:GLN:HG2	6:J:82:TRP:CE2	2.19	0.77
2:C:146:GLU:HB3	2:C:148:LYS:CE	2.15	0.77
6:J:6:LEU:HD12	6:J:6:LEU:N	1.96	0.77
2:C:414:PRO:O	2:C:417:LEU:HB2	1.85	0.77
2:C:409:VAL:HG22	2:C:410:GLU:N	2.00	0.77
7:H:28:DT:H3'	7:H:28:DT:H6	1.48	0.76
6:J:76:LYS:HB2	6:J:77:PRO:HD2	1.62	0.76
6:J:19:ASP:OD1	6:J:20:ARG:N	2.18	0.76
3:D:904:ARG:HH11	3:D:904:ARG:HB2	1.50	0.75
4:E:71:LEU:HD13	4:E:71:LEU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:27:ARG:HH11	6:J:27:ARG:HB3	1.51	0.74
6:J:32:TYR:CE2	6:J:54:TRP:HB2	2.22	0.74
3:D:163:GLU:OE2	3:D:166:ARG:NH1	2.21	0.73
3:D:905:ALA:CB	3:D:906:PRO:CD	2.67	0.73
3:D:237:ASP:OD2	3:D:240:LEU:N	2.22	0.72
2:C:319:LYS:NZ	2:C:368:ASP:OD1	2.23	0.72
3:D:1089:PHE:HE1	3:D:1109:GLN:CD	1.92	0.72
2:C:414:PRO:O	2:C:417:LEU:N	2.23	0.71
3:D:1030:ARG:NH1	3:D:1033:GLU:OE2	2.22	0.71
3:D:88:ARG:HH11	3:D:88:ARG:CG	2.03	0.71
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.71	0.71
3:D:706:MET:N	4:E:41:ASP:OD2	2.24	0.70
3:D:1009:GLN:O	3:D:1010:LEU:HD12	1.91	0.70
3:D:1011:THR:O	3:D:1012:MET:HB3	1.92	0.70
3:D:904:ARG:HH11	3:D:904:ARG:CG	2.05	0.70
1:B:143:GLY:C	1:B:144:ARG:HG3	2.12	0.69
3:D:108:LYS:O	3:D:386:ARG:NH1	2.25	0.69
5:F:483:ASP:OD2	5:F:487:ARG:NH2	2.25	0.69
3:D:1054:ARG:HA	3:D:1101:ASP:OD2	1.92	0.69
3:D:1277:GLU:C	3:D:1280:ALA:HB3	2.13	0.69
7:H:27:DA:N3	7:H:28:DT:O2	2.25	0.69
1:B:81:LYS:NZ	3:D:617:GLU:OE2	2.21	0.69
3:D:1221:LEU:CG	3:D:1250:GLU:CG	2.70	0.68
2:C:413:THR:CG2	2:C:416:THR:HG23	2.22	0.68
6:J:79:ARG:CB	6:J:79:ARG:HH11	2.06	0.68
6:J:79:ARG:HH11	6:J:79:ARG:HB3	1.58	0.68
1:A:2:LEU:N	1:A:2:LEU:HD12	2.08	0.68
5:F:242:ASN:ND2	5:F:244:GLU:OE2	2.26	0.68
2:C:410:GLU:N	2:C:411:ALA:HA	2.08	0.67
2:C:414:PRO:HA	2:C:417:LEU:HD12	1.75	0.67
2:C:413:THR:HG23	2:C:416:THR:HG23	1.77	0.67
5:F:210:GLU:O	5:F:214:GLN:HB2	1.93	0.67
6:J:97:LEU:O	6:J:100:GLU:HB3	1.94	0.67
3:D:1221:LEU:HD11	3:D:1250:GLU:HB3	1.76	0.67
3:D:1087:ARG:HG2	3:D:1087:ARG:NH1	2.09	0.67
5:F:471:GLU:OE2	5:F:509:LYS:NZ	2.27	0.67
3:D:905:ALA:CB	3:D:906:PRO:HD2	2.25	0.66
1:B:182:ARG:NH2	3:D:488:GLU:OE2	2.29	0.66
3:D:9:GLU:OE2	3:D:1244:LYS:NZ	2.21	0.66
3:D:1063:LYS:NZ	3:D:1078:ASP:OD2	2.29	0.65
3:D:904:ARG:HH11	3:D:904:ARG:CB	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.79	0.65
6:J:82:TRP:O	6:J:83:ASP:C	2.32	0.65
6:J:82:TRP:O	6:J:85:LEU:N	2.31	0.64
1:A:98:ARG:HG2	1:A:135:GLU:HG2	1.79	0.64
3:D:1276:GLU:O	3:D:1280:ALA:N	2.31	0.64
2:C:397:GLU:OE2	2:C:401:ARG:NH1	2.30	0.64
2:C:740:ARG:NH2	2:C:914:ASP:OD2	2.25	0.63
3:D:905:ALA:HB3	3:D:908:GLY:HA3	1.81	0.63
2:C:809:LYS:NZ	2:C:809:LYS:HB3	2.14	0.63
3:D:1088:VAL:HG23	3:D:1098:VAL:HG23	1.80	0.63
7:H:28:DT:H3'	7:H:28:DT:C6	2.32	0.63
3:D:1277:GLU:CA	3:D:1280:ALA:HB3	2.30	0.62
3:D:923:ARG:HH11	3:D:962:VAL:HG11	1.62	0.62
3:D:468:ASN:ND2	5:F:525:ASP:OD2	2.31	0.62
3:D:1221:LEU:HG	3:D:1250:GLU:CG	2.28	0.62
3:D:550:GLU:OE1	4:E:62:ARG:NH1	2.33	0.62
3:D:1012:MET:O	3:D:1012:MET:HG2	1.99	0.62
2:C:150:GLN:HB2	2:C:414:PRO:HG3	1.82	0.61
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.33	0.61
6:J:79:ARG:HH11	6:J:79:ARG:CG	2.14	0.61
3:D:1273:GLN:NE2	4:E:105:GLU:OE2	2.33	0.61
3:D:173:ARG:NH1	3:D:201:GLY:HA2	2.16	0.60
5:F:214:GLN:O	5:F:216:ARG:N	2.34	0.60
2:C:809:LYS:HD3	2:C:833:ARG:HG3	1.84	0.60
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.35	0.60
6:J:76:LYS:HG3	6:J:77:PRO:HD2	1.83	0.60
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.84	0.60
1:B:72:ASP:OD1	1:B:72:ASP:N	2.33	0.60
3:D:199:ASP:HB3	3:D:203:ARG:HH22	1.67	0.60
7:H:28:DT:C6	7:H:28:DT:C3'	2.84	0.60
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.82	0.60
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.84	0.59
2:C:222:VAL:HG21	2:C:234:VAL:HG22	1.83	0.59
2:C:611:MET:HG2	2:C:1033:LEU:HD21	1.85	0.59
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.35	0.59
1:B:183:VAL:HA	1:B:188:ASP:H	1.67	0.59
3:D:904:ARG:HH11	3:D:904:ARG:HG2	1.67	0.59
3:D:1053:VAL:HG13	3:D:1103:ASP:HB2	1.83	0.59
2:C:150:GLN:NE2	2:C:415:GLN:OE1	2.31	0.58
2:C:577:ASP:OD1	2:C:577:ASP:N	2.35	0.58
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:25:ALA:HB1	6:J:26:PRO:HD2	1.84	0.58
1:B:11:GLU:OE1	1:B:205:ARG:NH2	2.36	0.58
2:C:1062:GLN:HG3	6:J:5:VAL:HG13	1.85	0.58
2:C:412:ILE:HG13	2:C:412:ILE:O	2.03	0.58
3:D:699:ASP:OD1	3:D:703:ARG:NH1	2.35	0.58
6:J:32:TYR:CD1	6:J:32:TYR:N	2.71	0.57
2:C:255:SER:HB3	2:C:258:MET:HB2	1.85	0.57
3:D:1089:PHE:N	3:D:1089:PHE:CD2	2.72	0.57
3:D:707:ILE:HD12	4:E:39:PRO:HB3	1.84	0.57
3:D:1221:LEU:HD11	3:D:1250:GLU:CG	2.34	0.57
2:C:215:ASP:HB2	2:C:223:GLY:HA3	1.87	0.57
3:D:1277:GLU:O	3:D:1281:ALA:N	2.38	0.57
6:J:81:HIS:O	6:J:84:MET:HB2	2.05	0.57
3:D:1221:LEU:HD11	3:D:1250:GLU:HA	1.86	0.56
1:A:3:ILE:HG13	1:A:3:ILE:O	2.05	0.56
3:D:277:LEU:HD11	3:D:295:ARG:NH1	2.21	0.56
3:D:1221:LEU:HD11	3:D:1250:GLU:CA	2.34	0.56
2:C:251:ARG:NH2	2:C:343:GLU:OE2	2.39	0.56
3:D:1277:GLU:HA	3:D:1280:ALA:HB3	1.86	0.56
7:H:28:DT:H6	7:H:28:DT:C3'	2.18	0.56
2:C:217:ASP:OD2	2:C:231:ARG:NH1	2.39	0.56
2:C:994:PRO:HB3	2:C:999:ASP:H	1.70	0.56
2:C:995:ASN:OD1	2:C:995:ASN:N	2.39	0.55
3:D:1277:GLU:O	3:D:1280:ALA:CB	2.44	0.55
5:F:483:ASP:OD1	5:F:483:ASP:N	2.38	0.55
2:C:202:VAL:HG12	2:C:214:PHE:H	1.71	0.55
2:C:146:GLU:HB3	2:C:148:LYS:HE3	1.88	0.55
2:C:413:THR:HG23	2:C:416:THR:H	1.70	0.55
6:J:76:LYS:CB	6:J:77:PRO:HD2	2.27	0.55
7:H:27:DA:N3	7:H:28:DT:C2	2.75	0.55
3:D:885:ILE:HD11	3:D:887:ARG:NH1	2.22	0.55
6:J:79:ARG:HD3	6:J:84:MET:SD	2.47	0.55
2:C:414:PRO:CG	2:C:415:GLN:N	2.66	0.55
2:C:453:ARG:NH2	2:C:501:SER:O	2.40	0.55
3:D:1053:VAL:CG1	3:D:1103:ASP:HB2	2.37	0.55
2:C:133:LEU:HB3	2:C:154:MET:HB2	1.88	0.55
7:H:27:DA:C2	7:H:28:DT:O2	2.60	0.55
1:B:77:ILE:HD11	1:B:162:ILE:HD12	1.89	0.54
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.88	0.54
1:B:158:GLU:HB3	1:B:161:ARG:HB3	1.89	0.54
2:C:414:PRO:O	2:C:415:GLN:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:79:ARG:HB3	6:J:84:MET:SD	2.47	0.54
2:C:997:ASP:N	2:C:997:ASP:OD1	2.38	0.54
3:D:1089:PHE:N	3:D:1089:PHE:HD2	2.06	0.54
6:J:36:ASN:ND2	6:J:60:MET:SD	2.81	0.54
3:D:21:ARG:NH2	3:D:96:GLU:OE2	2.39	0.54
3:D:273:GLU:OE1	3:D:295:ARG:NH2	2.41	0.54
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.88	0.54
3:D:144:ARG:HH12	3:D:229:LEU:H	1.56	0.54
3:D:129:ILE:HA	3:D:257:GLY:HA2	1.90	0.54
3:D:32:GLU:OE2	5:F:367:ARG:NE	2.41	0.53
3:D:605:ASP:OD1	3:D:605:ASP:N	2.40	0.53
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.89	0.53
3:D:602:ALA:HB3	3:D:606:HIS:HE1	1.74	0.53
5:F:242:ASN:OD1	5:F:242:ASN:N	2.35	0.53
6:J:20:ARG:NH1	6:J:23:ASP:O	2.41	0.53
2:C:62:GLU:HB2	2:C:67:SER:HB3	1.90	0.53
2:C:809:LYS:CB	2:C:831:GLU:O	2.49	0.53
5:F:252:ARG:NH2	5:F:287:ASP:OD1	2.42	0.53
2:C:758:ASP:N	2:C:758:ASP:OD1	2.42	0.53
2:C:809:LYS:NZ	2:C:809:LYS:CB	2.71	0.53
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.42	0.53
3:D:1089:PHE:HE2	3:D:1099:LEU:HD13	1.74	0.53
7:H:28:DT:H2'	7:H:29:DA:C4	2.43	0.53
2:C:532:THR:OG1	2:C:533:ALA:N	2.42	0.53
2:C:811:GLU:OE2	2:C:811:GLU:HA	2.09	0.53
2:C:850:ILE:HG12	2:C:871:VAL:HG22	1.91	0.53
2:C:409:VAL:CG2	2:C:410:GLU:H	2.10	0.52
3:D:964:SER:OG	3:D:965:VAL:N	2.40	0.52
1:A:40:ARG:HE	1:B:33:THR:HG22	1.74	0.52
2:C:224:VAL:HB	2:C:232:GLN:HB3	1.92	0.52
2:C:653:VAL:HG12	2:C:658:ILE:HG12	1.90	0.52
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.74	0.52
6:J:22:HIS:ND1	6:J:23:ASP:N	2.57	0.52
2:C:1048:PRO:HD2	2:C:1063:PHE:HB2	1.91	0.52
3:D:1033:GLU:OE2	3:D:1040:PRO:HB3	2.09	0.52
3:D:1221:LEU:HD23	3:D:1243:ASP:CG	2.29	0.52
5:F:261:GLN:OE1	6:J:82:TRP:CD1	2.62	0.52
5:F:441:ASP:OD1	6:J:10:ARG:NH1	2.42	0.52
6:J:76:LYS:CG	6:J:77:PRO:HD2	2.40	0.52
2:C:350:GLU:OE1	2:C:352:GLN:NE2	2.42	0.52
2:C:809:LYS:HB3	2:C:809:LYS:HZ2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASP:N	2:C:881:ASP:OD1	2.43	0.52
2:C:98:ASP:OD1	2:C:98:ASP:N	2.40	0.52
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.43	0.52
3:D:447:MET:O	3:D:451:LEU:HB2	2.09	0.52
3:D:1166:THR:O	3:D:1203:GLY:CA	2.58	0.52
6:J:32:TYR:CE2	6:J:54:TRP:CB	2.93	0.52
3:D:1276:GLU:HG3	3:D:1277:GLU:N	2.25	0.51
2:C:152:VAL:HG11	2:C:418:ILE:HG21	1.92	0.51
3:D:1066:ILE:HD11	3:D:1111:LEU:HD21	1.91	0.51
3:D:443:LEU:HD23	3:D:448:ALA:HB2	1.92	0.51
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.44	0.51
2:C:146:GLU:HB3	2:C:148:LYS:HE2	1.93	0.51
2:C:147:ILE:HG13	2:C:147:ILE:O	2.10	0.51
3:D:904:ARG:HB2	3:D:904:ARG:NH1	2.23	0.51
2:C:809:LYS:CB	2:C:809:LYS:HZ2	2.24	0.51
2:C:455:LEU:HD21	2:C:500:LEU:HG	1.93	0.51
3:D:102:THR:HG22	3:D:313:VAL:HG12	1.93	0.51
2:C:782:ALA:O	2:C:791:ARG:NH2	2.45	0.50
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.44	0.50
3:D:88:ARG:HH11	3:D:88:ARG:HG2	1.77	0.50
1:A:72:ASP:OD1	1:A:72:ASP:N	2.32	0.50
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.92	0.50
2:C:77:ARG:NH2	2:C:505:ARG:HH12	2.08	0.50
2:C:313:ARG:O	2:C:317:ASN:ND2	2.44	0.50
3:D:190:LYS:O	3:D:194:ARG:NE	2.44	0.50
3:D:557:ILE:HD13	4:E:53:LEU:HD13	1.93	0.50
3:D:1166:THR:O	3:D:1203:GLY:HA2	2.10	0.50
1:B:22:VAL:HG12	1:B:193:ILE:HG12	1.92	0.50
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.94	0.50
3:D:1089:PHE:CD2	3:D:1089:PHE:C	2.85	0.50
1:A:130:ASP:OD1	1:A:130:ASP:N	2.43	0.50
2:C:811:GLU:CD	2:C:812:THR:H	2.15	0.50
2:C:818:GLU:OE2	2:C:822:ARG:NH2	2.44	0.50
3:D:173:ARG:HH11	3:D:201:GLY:HA2	1.76	0.50
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.93	0.50
3:D:427:ARG:HH11	3:D:427:ARG:HB2	1.77	0.50
2:C:930:GLN:O	2:C:934:THR:OG1	2.30	0.49
1:A:161:ARG:HB2	1:A:161:ARG:HH11	1.77	0.49
3:D:939:GLU:HG2	3:D:942:GLN:HE21	1.77	0.49
3:D:383:ASP:OD2	3:D:386:ARG:NE	2.45	0.49
6:J:32:TYR:N	6:J:32:TYR:HD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:ASN:OD1	2:C:443:ASN:N	2.45	0.49
2:C:694:ASP:OD1	2:C:694:ASP:N	2.43	0.49
2:C:944:TRP:NE1	2:C:963:LEU:O	2.42	0.49
5:F:286:ARG:HG2	5:F:290:ARG:NH1	2.27	0.49
3:D:1229:THR:O	3:D:1233:LEU:HB2	2.13	0.49
3:D:369:ASN:ND2	5:F:322:GLN:OE1	2.46	0.49
6:J:33:ARG:NH1	6:J:37:GLY:HA2	2.27	0.49
1:A:97:LEU:HB3	1:A:136:VAL:HG13	1.94	0.49
3:D:1087:ARG:NH1	3:D:1087:ARG:CG	2.72	0.49
6:J:23:ASP:O	6:J:24:LEU:HD13	2.13	0.49
3:D:970:THR:OG1	3:D:973:GLY:O	2.30	0.49
1:A:14:LEU:HD12	1:A:18:ARG:HH11	1.78	0.48
1:A:95:MET:HG3	1:A:138:LEU:HB2	1.94	0.48
2:C:446:LEU:HB2	2:C:713:MET:HE1	1.95	0.48
3:D:144:ARG:NH2	3:D:229:LEU:O	2.40	0.48
2:C:835:THR:O	2:C:835:THR:OG1	2.29	0.48
3:D:903:GLU:C	3:D:904:ARG:O	2.52	0.48
3:D:1054:ARG:CA	3:D:1101:ASP:OD2	2.60	0.48
5:F:390:LEU:HB3	5:F:392:ARG:HG3	1.95	0.48
2:C:92:GLU:OE2	2:C:390:ARG:NH2	2.39	0.48
2:C:380:THR:OG1	2:C:381:VAL:N	2.42	0.48
3:D:328:VAL:HG13	3:D:336:ALA:HB3	1.95	0.48
3:D:1221:LEU:CD2	3:D:1250:GLU:HB3	2.38	0.48
5:F:214:GLN:C	5:F:216:ARG:N	2.67	0.48
3:D:88:ARG:HG2	3:D:88:ARG:NH1	2.29	0.48
1:A:2:LEU:HD12	1:A:2:LEU:H	1.78	0.48
1:B:18:ARG:NH2	1:B:195:ASP:OD1	2.47	0.48
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.42	0.48
6:J:31:ARG:HB2	6:J:31:ARG:CZ	2.43	0.48
1:A:1:MET:SD	1:A:1:MET:C	2.93	0.48
1:B:94:THR:HG22	1:B:139:VAL:HG22	1.95	0.48
3:D:910:LEU:HD21	3:D:956:GLY:HA2	1.96	0.48
3:D:1036:GLU:OE2	3:D:1211:THR:OG1	2.29	0.48
3:D:746:LEU:O	3:D:750:GLU:HB2	2.14	0.47
3:D:1231:ARG:HA	3:D:1234:THR:HG22	1.95	0.47
3:D:897:ILE:HB	3:D:1128:ARG:HH21	1.79	0.47
3:D:931:ASP:OD1	3:D:931:ASP:N	2.38	0.47
3:D:1172:SER:N	3:D:1199:GLU:OE2	2.48	0.47
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.96	0.47
1:B:158:GLU:OE2	1:B:161:ARG:NH2	2.47	0.47
2:C:444:ASN:N	2:C:444:ASN:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:717:LYS:NZ	2:C:746:VAL:O	2.48	0.47
3:D:926:GLY:O	3:D:940:ARG:NH2	2.41	0.47
3:D:1221:LEU:CD1	3:D:1250:GLU:CG	2.92	0.47
2:C:689:ILE:HD11	2:C:701:VAL:HG12	1.94	0.47
2:C:919:THR:HG21	3:D:729:VAL:HG12	1.96	0.47
3:D:211:ARG:HA	3:D:214:ARG:NH1	2.29	0.47
1:A:165:ASP:N	1:A:165:ASP:OD1	2.45	0.47
2:C:253:GLY:O	2:C:259:ARG:NH2	2.47	0.47
2:C:644:ALA:HB2	2:C:702:ILE:HD12	1.96	0.47
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.50	0.47
3:D:904:ARG:HG2	3:D:904:ARG:NH1	2.27	0.47
3:D:660:ASP:OD1	3:D:660:ASP:N	2.48	0.47
1:B:56:ILE:HG12	1:B:136:VAL:HG13	1.97	0.46
2:C:1023:VAL:HA	3:D:730:THR:HG21	1.96	0.46
4:E:52:ALA:O	4:E:56:TYR:HB2	2.16	0.46
8:G:13:DC:H2'	8:G:14:DA:C8	2.51	0.46
2:C:413:THR:HG22	2:C:416:THR:HG23	1.97	0.46
4:E:71:LEU:O	4:E:71:LEU:HD22	2.15	0.46
1:A:64:THR:OG1	1:A:65:THR:N	2.47	0.46
3:D:255:ALA:HB3	3:D:260:SER:HB3	1.97	0.46
2:C:759:ALA:HA	2:C:805:LYS:HZ3	1.81	0.46
3:D:1099:LEU:HD12	3:D:1099:LEU:HA	1.56	0.46
1:B:37:SER:O	1:B:41:THR:OG1	2.27	0.46
3:D:1:MET:SD	3:D:1:MET:N	2.77	0.46
3:D:35:ASN:CG	3:D:38:THR:HG22	2.36	0.46
3:D:211:ARG:HG3	3:D:214:ARG:HH12	1.80	0.46
3:D:1139:GLN:NE2	3:D:1151:ASP:OD1	2.40	0.46
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.97	0.46
3:D:1227:GLN:HE22	7:H:25:DC:H4'	1.81	0.46
5:F:261:GLN:CG	6:J:82:TRP:CE2	2.97	0.46
2:C:369:ASP:O	2:C:375:ASN:ND2	2.38	0.46
3:D:88:ARG:CG	3:D:88:ARG:NH1	2.69	0.46
3:D:485:ASP:N	3:D:485:ASP:OD1	2.48	0.46
3:D:895:ARG:HH11	3:D:967:THR:HB	1.81	0.46
2:C:735:ILE:O	2:C:895:ILE:HA	2.16	0.46
1:A:2:LEU:HD12	1:A:2:LEU:O	2.16	0.45
2:C:1112:ILE:O	4:E:62:ARG:NH2	2.49	0.45
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.81	0.45
3:D:1088:VAL:CG2	3:D:1098:VAL:HG23	2.46	0.45
2:C:290:GLU:O	2:C:294:THR:OG1	2.28	0.45
2:C:1044:ARG:NH2	3:D:423:ASP:OD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1088:VAL:O	3:D:1088:VAL:HG13	2.15	0.45
5:F:471:GLU:OE1	5:F:513:LYS:NZ	2.41	0.45
2:C:1084:THR:OG1	3:D:554:GLU:OE1	2.32	0.45
3:D:307:ASN:ND2	3:D:1238:ILE:O	2.50	0.45
3:D:1086:LEU:CD2	3:D:1099:LEU:HB3	2.43	0.45
5:F:301:ARG:HB2	5:F:301:ARG:NH1	2.32	0.45
2:C:96:ILE:HB	2:C:105:LEU:HB3	1.99	0.45
2:C:373:PHE:HD2	2:C:482:ARG:HD3	1.82	0.45
3:D:1089:PHE:CD2	3:D:1089:PHE:O	2.70	0.45
5:F:334:LYS:HE3	5:F:334:LYS:HB2	1.83	0.45
1:A:161:ARG:HB2	1:A:161:ARG:NH1	2.32	0.45
2:C:335:GLU:O	2:C:338:VAL:HB	2.16	0.45
2:C:1050:SER:OG	2:C:1051:MET:N	2.49	0.45
3:D:904:ARG:HD3	3:D:904:ARG:HA	1.69	0.45
3:D:1180:LEU:HD22	3:D:1206:VAL:HG21	1.97	0.45
3:D:904:ARG:CG	3:D:904:ARG:NH1	2.72	0.45
2:C:759:ALA:HA	2:C:805:LYS:NZ	2.32	0.45
2:C:811:GLU:OE2	2:C:812:THR:N	2.35	0.45
2:C:86:LEU:HD21	2:C:389:ILE:HD13	1.98	0.44
3:D:28:VAL:HG21	3:D:46:LEU:HD23	2.00	0.44
3:D:960:VAL:HG12	3:D:962:VAL:HG23	1.98	0.44
2:C:185:VAL:HG12	2:C:204:VAL:HG22	2.00	0.44
3:D:91:ARG:O	3:D:321:PRO:HG3	2.18	0.44
3:D:708:VAL:HG22	4:E:29:TYR:HB3	1.98	0.44
2:C:562:ARG:HD3	3:D:847:LEU:HD11	1.97	0.44
3:D:162:VAL:HG13	3:D:215:GLU:OE2	2.17	0.44
3:D:937:ILE:HD13	3:D:955:ALA:HB2	2.00	0.44
7:H:27:DA:H2"	7:H:28:DT:O5'	2.18	0.44
1:A:55:ARG:NH2	1:A:137:GLU:OE2	2.51	0.44
2:C:455:LEU:HD12	2:C:483:MET:HG3	2.00	0.44
4:E:40:ILE:H	4:E:40:ILE:HG13	1.56	0.44
1:B:146:TYR:O	1:B:146:TYR:CD2	2.70	0.44
3:D:1088:VAL:CB	3:D:1098:VAL:HG23	2.47	0.44
5:F:467:LEU:HD11	5:F:514:LEU:HD21	2.00	0.44
1:B:84:VAL:HB	1:B:199:LYS:HE2	1.98	0.44
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.99	0.44
6:J:79:ARG:CG	6:J:79:ARG:NH1	2.73	0.44
2:C:635:ALA:HB2	2:C:713:MET:HG2	2.00	0.44
5:F:334:LYS:HE2	6:J:84:MET:HG2	2.00	0.44
1:B:143:GLY:O	1:B:144:ARG:HG3	2.16	0.43
3:D:556:ARG:HD3	4:E:92:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.00	0.43
6:J:79:ARG:NH1	6:J:79:ARG:HG2	2.33	0.43
2:C:230:ARG:NH1	7:H:21:DT:OP1	2.51	0.43
3:D:725:THR:HG23	3:D:726:ARG:HD2	2.00	0.43
2:C:303:GLU:H	2:C:303:GLU:HG2	1.56	0.43
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.99	0.43
3:D:83:THR:HG23	3:D:84:ARG:O	2.19	0.43
1:A:11:GLU:OE1	1:A:205:ARG:NH2	2.52	0.43
1:A:87:SER:OG	1:A:88:GLU:N	2.51	0.43
2:C:64:LEU:HA	2:C:85:GLY:HA3	2.01	0.43
2:C:532:THR:HG23	2:C:535:GLU:HG2	2.00	0.43
5:F:214:GLN:O	5:F:215:ALA:C	2.55	0.43
5:F:246:GLU:H	5:F:246:GLU:HG3	1.68	0.43
2:C:216:VAL:HG11	2:C:349:HIS:HD2	1.83	0.43
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	2.01	0.43
3:D:1089:PHE:CE2	3:D:1099:LEU:HD13	2.54	0.43
2:C:191:ILE:HG12	2:C:198:THR:HG22	2.01	0.43
3:D:1128:ARG:NH1	3:D:1132:ILE:HG12	2.26	0.42
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	2.01	0.42
3:D:47:PHE:O	3:D:88:ARG:NH2	2.49	0.42
3:D:922:ALA:HB1	3:D:981:ARG:HB3	2.01	0.42
5:F:247:VAL:HG12	5:F:251:LYS:HE3	2.02	0.42
5:F:430:GLU:HG3	5:F:432:ASP:OD2	2.19	0.42
6:J:24:LEU:HD13	6:J:24:LEU:N	2.32	0.42
2:C:222:VAL:HG22	2:C:261:THR:HG21	2.00	0.42
3:D:948:GLU:H	3:D:948:GLU:HG2	1.56	0.42
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	2.00	0.42
1:A:175:THR:OG1	1:A:176:TYR:N	2.52	0.42
2:C:229:LYS:NZ	2:C:281:LEU:O	2.45	0.42
3:D:164:ASP:HA	3:D:167:ASP:OD2	2.19	0.42
3:D:410:GLN:CA	3:D:410:GLN:OE1	2.67	0.42
4:E:83:VAL:HG23	4:E:98:GLU:HG2	2.02	0.42
5:F:261:GLN:CD	6:J:82:TRP:HE1	2.21	0.42
3:D:71:LYS:HE3	3:D:71:LYS:HB2	1.88	0.42
3:D:326:PRO:O	3:D:338:SER:OG	2.37	0.42
3:D:944:LEU:HD23	3:D:944:LEU:HA	1.94	0.42
4:E:71:LEU:HD13	4:E:71:LEU:C	2.38	0.42
2:C:775:ASN:OD1	2:C:775:ASN:N	2.50	0.42
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	2.00	0.42
3:D:190:LYS:NZ	3:D:193:ALA:H	2.18	0.42
3:D:921:TYR:OH	3:D:946:ASP:OD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1088:VAL:O	3:D:1088:VAL:CG1	2.67	0.42
2:C:282:ARG:HA	2:C:282:ARG:HD3	1.81	0.42
3:D:211:ARG:HA	3:D:214:ARG:HH12	1.84	0.42
3:D:342:ASP:N	3:D:342:ASP:OD1	2.52	0.42
3:D:902:ALA:H	3:D:913:ASP:HB2	1.85	0.42
5:F:342:LYS:HZ2	7:O:30:DC:P	2.42	0.42
1:B:30:PHE:HA	1:B:33:THR:HG23	2.01	0.42
2:C:1057:LEU:HD23	2:C:1062:GLN:HG2	2.02	0.42
5:F:353:GLN:HE21	5:F:353:GLN:HB3	1.60	0.42
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.55	0.41
1:B:49:ALA:HA	1:B:142:ARG:HA	2.02	0.41
2:C:721:VAL:HG11	2:C:1028:MET:HB2	2.02	0.41
3:D:410:GLN:OE1	3:D:410:GLN:HA	2.19	0.41
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.53	0.41
3:D:1276:GLU:HG3	3:D:1277:GLU:H	1.84	0.41
5:F:342:LYS:HG2	7:O:30:DC:OP2	2.20	0.41
2:C:809:LYS:HB3	2:C:809:LYS:HZ3	1.85	0.41
3:D:238:GLU:O	3:D:242:ARG:NH1	2.53	0.41
3:D:456:VAL:HG22	3:D:460:LEU:HD23	2.02	0.41
3:D:627:LEU:HD13	3:D:668:LEU:HD12	2.02	0.41
3:D:1262:THR:HB	4:E:55:ILE:HD11	2.02	0.41
5:F:367:ARG:NH2	7:O:22:DG:OP1	2.53	0.41
5:F:441:ASP:OD2	5:F:444:ALA:HB2	2.19	0.41
6:J:25:ALA:HA	6:J:26:PRO:HD3	1.82	0.41
2:C:195:THR:HG23	2:C:197:LYS:HG2	2.03	0.41
2:C:281:LEU:HD23	2:C:295:LEU:HD21	2.02	0.41
3:D:1089:PHE:HD2	3:D:1089:PHE:O	2.03	0.41
1:A:149:ALA:HB1	1:A:163:PRO:HB2	2.03	0.41
2:C:417:LEU:HA	2:C:417:LEU:HD23	1.88	0.41
2:C:909:ASP:OD2	2:C:995:ASN:ND2	2.53	0.41
6:J:63:THR:OG1	6:J:64:LEU:N	2.52	0.41
2:C:326:GLU:HB3	2:C:328:ILE:HG13	2.01	0.41
2:C:727:GLU:OE2	3:D:725:THR:HG21	2.21	0.41
4:E:87:LEU:HD23	4:E:87:LEU:HA	1.91	0.41
5:F:372:MET:HA	5:F:375:VAL:HG22	2.02	0.41
1:A:40:ARG:NH1	2:C:903:ASP:HB3	2.35	0.41
2:C:38:ARG:HG2	2:C:973:SER:HB3	2.02	0.41
2:C:401:ARG:HA	2:C:404:MET:HB2	2.02	0.41
2:C:414:PRO:O	2:C:417:LEU:CB	2.63	0.41
2:C:556:GLU:H	2:C:556:GLU:HG2	1.43	0.41
2:C:808:PRO:O	2:C:808:PRO:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.93	0.41
1:A:40:ARG:HG2	2:C:902:GLU:HB2	2.03	0.41
1:A:57:ASP:N	1:A:57:ASP:OD1	2.51	0.41
3:D:190:LYS:HZ2	3:D:193:ALA:H	1.69	0.41
3:D:1089:PHE:HD2	3:D:1089:PHE:H	1.66	0.41
3:D:1221:LEU:CD1	3:D:1250:GLU:HB3	2.46	0.41
1:B:24:GLU:HB3	1:B:191:LYS:HG3	2.02	0.41
2:C:435:GLN:HE21	2:C:460:PRO:HG3	1.86	0.41
2:C:809:LYS:O	2:C:809:LYS:CG	2.69	0.41
3:D:725:THR:HG23	3:D:726:ARG:HH11	1.86	0.41
5:F:330:ARG:NE	5:F:334:LYS:HZ1	2.18	0.41
1:A:3:ILE:O	1:A:3:ILE:CG1	2.69	0.41
1:B:206:ASP:N	1:B:206:ASP:OD1	2.53	0.41
3:D:110:VAL:HG11	7:H:23:DT:H4'	2.02	0.41
5:F:283:TRP:HE3	5:F:284:ILE:HD12	1.85	0.41
1:B:80:LEU:HD21	1:B:125:ILE:HD12	2.03	0.41
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.02	0.40
3:D:1266:ARG:NH1	4:E:108:GLU:OE1	2.54	0.40
1:B:143:GLY:HA3	1:B:168:TYR:CD2	2.56	0.40
2:C:163:LYS:NZ	2:C:639:GLY:O	2.49	0.40
3:D:89:ARG:HH11	3:D:89:ARG:HD2	1.61	0.40
3:D:862:ASP:O	3:D:866:ARG:HB2	2.21	0.40
6:J:82:TRP:HB3	6:J:83:ASP:H	1.73	0.40
1:A:3:ILE:H	1:A:3:ILE:HG12	1.65	0.40
2:C:42:ALA:HB2	2:C:975:PRO:HG2	2.03	0.40
3:D:74:ILE:HD12	6:J:42:VAL:HG13	2.03	0.40
3:D:257:GLY:O	3:D:260:SER:OG	2.32	0.40
3:D:725:THR:CG2	3:D:726:ARG:HH11	2.34	0.40
3:D:750:GLU:HG2	3:D:778:TRP:HH2	1.87	0.40
3:D:832:ILE:HA	3:D:833:PRO:HD3	1.93	0.40
3:D:923:ARG:HH11	3:D:923:ARG:HG3	1.87	0.40
3:D:1128:ARG:HA	3:D:1128:ARG:HD2	1.74	0.40
2:C:216:VAL:HG11	2:C:349:HIS:CD2	2.56	0.40
2:C:494:ILE:H	2:C:494:ILE:HG13	1.67	0.40
2:C:756:GLU:OE2	2:C:868:LEU:HD21	2.21	0.40
2:C:757:ILE:HD12	2:C:757:ILE:HA	1.96	0.40
2:C:1126:LYS:HD3	2:C:1126:LYS:HA	1.85	0.40
3:D:670:ARG:O	3:D:674:ASN:ND2	2.46	0.40
4:E:70:GLN:O	4:E:70:GLN:CG	2.70	0.40
6:J:20:ARG:NH1	6:J:23:ASP:HB3	2.36	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	224/347 (65%)	206 (92%)	18 (8%)	0	100 100
1	B	235/347 (68%)	205 (87%)	30 (13%)	0	100 100
2	C	1109/1179 (94%)	1001 (90%)	106 (10%)	2 (0%)	47 77
3	D	1261/1326 (95%)	1171 (93%)	83 (7%)	7 (1%)	25 58
4	E	81/110 (74%)	71 (88%)	9 (11%)	1 (1%)	13 44
5	F	317/531 (60%)	307 (97%)	9 (3%)	1 (0%)	41 72
6	J	106/111 (96%)	91 (86%)	11 (10%)	4 (4%)	3 20
All	All	3333/3951 (84%)	3052 (92%)	266 (8%)	15 (0%)	32 62

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	904	ARG
3	D	905	ALA
3	D	909	THR
6	J	78	PRO
3	D	1100	SER
3	D	84	ARG
3	D	907	ASP
5	F	215	ALA
6	J	77	PRO
6	J	81	HIS
6	J	82	TRP
4	E	73	GLU
2	C	53	LEU
2	C	409	VAL
3	D	906	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	195/297 (66%)	167 (86%)	28 (14%)	3 15
1	B	197/297 (66%)	164 (83%)	33 (17%)	2 9
2	C	932/997 (94%)	816 (88%)	116 (12%)	4 20
3	D	1043/1103 (95%)	919 (88%)	124 (12%)	5 21
4	E	69/89 (78%)	56 (81%)	13 (19%)	1 7
5	F	262/429 (61%)	233 (89%)	29 (11%)	6 24
6	J	93/97 (96%)	67 (72%)	26 (28%)	0 1
All	All	2791/3309 (84%)	2422 (87%)	369 (13%)	7 17

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	10	SER
1	A	18	ARG
1	A	22	VAL
1	A	34	LEU
1	A	43	LEU
1	A	51	VAL
1	A	61	HIS
1	A	72	ASP
1	A	84	VAL
1	A	85	VAL
1	A	88	GLU
1	A	90	ASP
1	A	111	VAL
1	A	117	THR
1	A	127	THR
1	A	130	ASP
1	A	136	VAL
1	A	142	ARG
1	A	147	VAL

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Mol	Chain	Res	Type
1	A	150	VAL
1	A	165	ASP
1	A	166	SER
1	A	172	LEU
1	A	187	THR
1	A	215	LEU
1	A	218	LEU
1	A	221	LEU
1	B	15	THR
1	B	27	GLU
1	B	33	THR
1	B	34	LEU
1	B	41	THR
1	B	60	LEU
1	B	61	HIS
1	B	72	ASP
1	B	75	GLU
1	B	84	VAL
1	B	85	VAL
1	B	93	VAL
1	B	110	ILE
1	B	111	VAL
1	B	117	THR
1	B	123	MET
1	B	125	ILE
1	B	136	VAL
1	B	142	ARG
1	B	144	ARG
1	B	147	VAL
1	B	150	VAL
1	B	159	ILE
1	B	161	ARG
1	B	172	LEU
1	B	175	THR
1	B	177	LYS
1	B	182	ARG
1	B	196	VAL
1	B	198	THR
1	B	203	SER
1	B	216	VAL
1	B	223	ARG
2	C	46	GLU

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Mol	Chain	Res	Type
2	C	72	GLU
2	C	90	LEU
2	C	93	LEU
2	C	94	SER
2	C	128	THR
2	C	133	LEU
2	C	144	THR
2	C	148	LYS
2	C	149	SER
2	C	185	VAL
2	C	202	VAL
2	C	203	LYS
2	C	221	THR
2	C	226	ILE
2	C	230	ARG
2	C	231	ARG
2	C	254	PHE
2	C	266	ASN
2	C	271	ASP
2	C	274	LEU
2	C	285	GLU
2	C	290	GLU
2	C	291	SER
2	C	296	LEU
2	C	313	ARG
2	C	323	HIS
2	C	328	ILE
2	C	329	THR
2	C	333	LEU
2	C	345	LEU
2	C	346	VAL
2	C	352	GLN
2	C	353	THR
2	C	355	MET
2	C	356	THR
2	C	357	VAL
2	C	363	VAL
2	C	367	THR
2	C	370	ILE
2	C	373	PHE
2	C	381	VAL
2	C	391	VAL

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Mol	Chain	Res	Type
2	C	401	ARG
2	C	413	THR
2	C	415	GLN
2	C	420	ILE
2	C	421	ARG
2	C	436	LEU
2	C	452	LYS
2	C	458	LEU
2	C	463	LEU
2	C	470	LEU
2	C	475	VAL
2	C	507	ASN
2	C	519	VAL
2	C	529	VAL
2	C	532	THR
2	C	540	VAL
2	C	556	GLU
2	C	561	VAL
2	C	570	TYR
2	C	571	VAL
2	C	575	GLU
2	C	587	VAL
2	C	611	MET
2	C	626	VAL
2	C	649	VAL
2	C	653	VAL
2	C	660	VAL
2	C	667	ARG
2	C	668	ARG
2	C	669	THR
2	C	672	MET
2	C	673	ARG
2	C	694	ASP
2	C	736	ILE
2	C	753	GLU
2	C	763	LYS
2	C	764	LEU
2	C	787	ARG
2	C	790	VAL
2	C	797	ARG
2	C	806	VAL
2	C	811	GLU

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Mol	Chain	Res	Type
2	C	831	GLU
2	C	839	VAL
2	C	841	HIS
2	C	852	VAL
2	C	861	LEU
2	C	869	VAL
2	C	888	ARG
2	C	899	LEU
2	C	928	ILE
2	C	933	GLU
2	C	936	LEU
2	C	950	LYS
2	C	962	GLU
2	C	965	GLU
2	C	967	GLN
2	C	973	SER
2	C	989	LEU
2	C	992	THR
2	C	997	ASP
2	C	1037	VAL
2	C	1050	SER
2	C	1053	THR
2	C	1057	LEU
2	C	1063	PHE
2	C	1066	GLN
2	C	1070	GLU
2	C	1101	LYS
2	C	1114	GLU
2	C	1125	LEU
2	C	1131	LEU
2	C	1137	VAL
3	D	1	MET
3	D	2	LEU
3	D	28	VAL
3	D	36	TYR
3	D	56	ARG
3	D	67	ARG
3	D	68	VAL
3	D	77	ARG
3	D	82	VAL
3	D	84	ARG
3	D	86	LYS

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Mol	Chain	Res	Type
3	D	88	ARG
3	D	90	GLU
3	D	117	LEU
3	D	120	LEU
3	D	123	LYS
3	D	137	THR
3	D	147	GLU
3	D	173	ARG
3	D	192	ASP
3	D	203	ARG
3	D	206	ARG
3	D	209	ARG
3	D	219	LEU
3	D	222	ILE
3	D	234	LEU
3	D	236	VAL
3	D	240	LEU
3	D	263	LYS
3	D	275	GLU
3	D	315	ASP
3	D	328	VAL
3	D	331	ASP
3	D	334	ARG
3	D	406	LEU
3	D	417	LEU
3	D	427	ARG
3	D	429	VAL
3	D	451	LEU
3	D	468	ASN
3	D	469	ILE
3	D	485	ASP
3	D	504	LEU
3	D	505	HIS
3	D	506	ARG
3	D	558	LEU
3	D	566	LEU
3	D	578	ARG
3	D	581	MET
3	D	588	LEU
3	D	603	SER
3	D	627	LEU
3	D	635	VAL

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Mol	Chain	Res	Type
3	D	639	GLN
3	D	647	GLU
3	D	656	TRP
3	D	660	ASP
3	D	676	LEU
3	D	677	LEU
3	D	679	LEU
3	D	706	MET
3	D	717	LYS
3	D	733	MET
3	D	738	VAL
3	D	741	ARG
3	D	750	GLU
3	D	770	ARG
3	D	785	VAL
3	D	795	ASP
3	D	817	LEU
3	D	825	THR
3	D	834	ARG
3	D	841	ARG
3	D	847	LEU
3	D	862	ASP
3	D	865	LEU
3	D	880	VAL
3	D	901	LEU
3	D	904	ARG
3	D	910	LEU
3	D	911	ILE
3	D	913	ASP
3	D	930	VAL
3	D	937	ILE
3	D	939	GLU
3	D	946	ASP
3	D	948	GLU
3	D	953	LEU
3	D	975	CYS
3	D	1008	THR
3	D	1025	THR
3	D	1053	VAL
3	D	1054	ARG
3	D	1057	ASP
3	D	1061	PHE

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Mol	Chain	Res	Type
3	D	1062	TYR
3	D	1069	ASP
3	D	1086	LEU
3	D	1087	ARG
3	D	1088	VAL
3	D	1089	PHE
3	D	1090	LYS
3	D	1097	ARG
3	D	1098	VAL
3	D	1099	LEU
3	D	1100	SER
3	D	1103	ASP
3	D	1105	VAL
3	D	1120	GLU
3	D	1173	THR
3	D	1181	ILE
3	D	1189	GLU
3	D	1191	ARG
3	D	1192	ARG
3	D	1199	GLU
3	D	1204	ARG
3	D	1221	LEU
3	D	1233	LEU
3	D	1248	LEU
3	D	1257	LEU
3	D	1266	ARG
3	D	1274	PRO
3	D	1275	THR
3	D	1276	GLU
4	E	29	TYR
4	E	31	THR
4	E	33	LEU
4	E	40	ILE
4	E	53	LEU
4	E	56	TYR
4	E	65	ASN
4	E	70	GLN
4	E	73	GLU
4	E	76	LEU
4	E	78	TYR
4	E	84	GLU
4	E	92	LEU

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Mol	Chain	Res	Type
5	F	222	THR
5	F	242	ASN
5	F	244	GLU
5	F	257	LEU
5	F	266	LEU
5	F	268	GLU
5	F	269	ARG
5	F	282	MET
5	F	285	CYS
5	F	295	LEU
5	F	301	ARG
5	F	328	LEU
5	F	330	ARG
5	F	332	VAL
5	F	342	LYS
5	F	353	GLN
5	F	366	ILE
5	F	387	LEU
5	F	392	ARG
5	F	395	THR
5	F	397	GLU
5	F	421	ILE
5	F	429	ASP
5	F	449	ASP
5	F	460	LEU
5	F	461	GLN
5	F	482	THR
5	F	495	VAL
5	F	500	ARG
6	J	5	VAL
6	J	6	LEU
6	J	10	ARG
6	J	17	GLU
6	J	18	THR
6	J	21	ASN
6	J	24	LEU
6	J	27	ARG
6	J	28	GLN
6	J	57	ARG
6	J	63	THR
6	J	64	LEU
6	J	71	GLU

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Mol	Chain	Res	Type
6	J	76	LYS
6	J	79	ARG
6	J	82	TRP
6	J	83	ASP
6	J	84	MET
6	J	86	LEU
6	J	87	GLU
6	J	88	ARG
6	J	95	GLU
6	J	96	GLU
6	J	97	LEU
6	J	102	LEU
6	J	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	B	124	HIS
1	B	226	ASN
2	C	57	GLN
2	C	141	ASN
2	C	142	ASN
2	C	169	ASN
2	C	200	HIS
2	C	349	HIS
2	C	352	GLN
2	C	372	HIS
2	C	435	GLN
2	C	442	GLN
2	C	476	HIS
2	C	479	HIS
2	C	585	GLN
2	C	920	HIS
2	C	1035	HIS
2	C	1062	GLN
3	D	287	GLN
3	D	329	GLN
3	D	368	ASN
3	D	606	HIS
3	D	639	GLN
3	D	693	GLN

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Mol	Chain	Res	Type
3	D	766	ASN
3	D	1145	GLN
3	D	1227	GLN
4	E	65	ASN
4	E	70	GLN
5	F	353	GLN
5	F	425	GLN
5	F	457	GLN
5	F	516	HIS
6	J	21	ASN
6	J	28	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

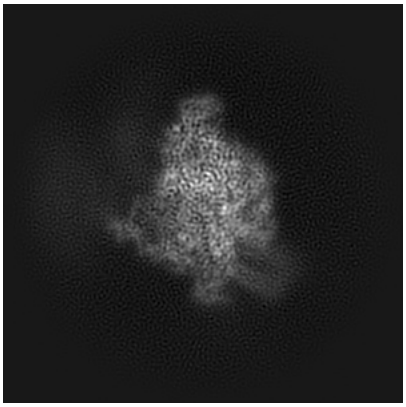
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7320. These allow visual inspection of the internal detail of the map and identification of artifacts.

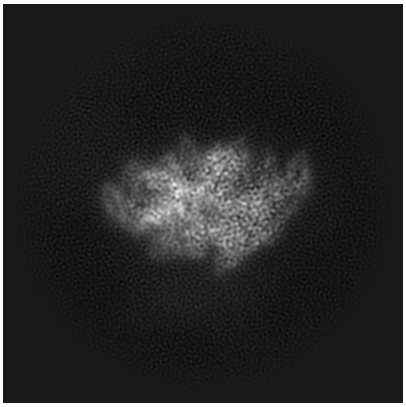
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

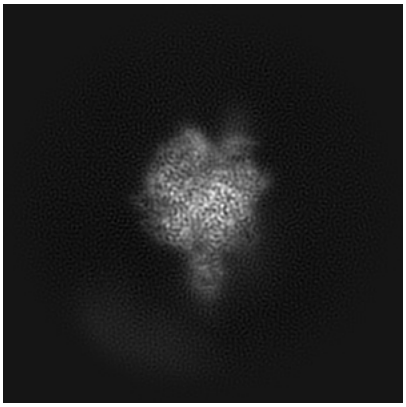
6.1.1 Primary map



X



Y

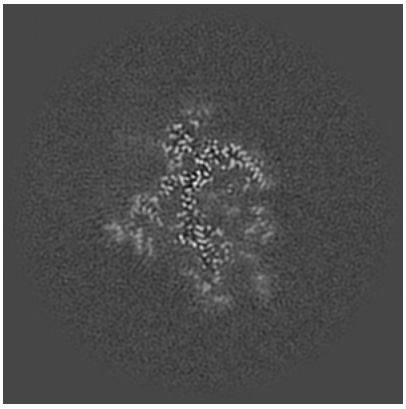


Z

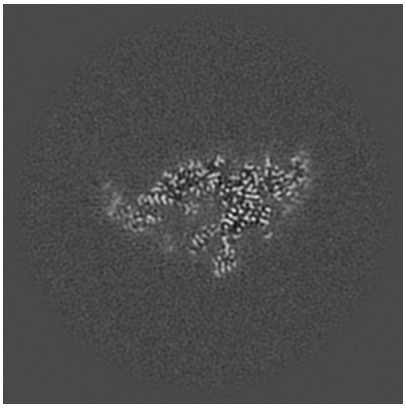
The images above show the map projected in three orthogonal directions.

6.2 Central slices

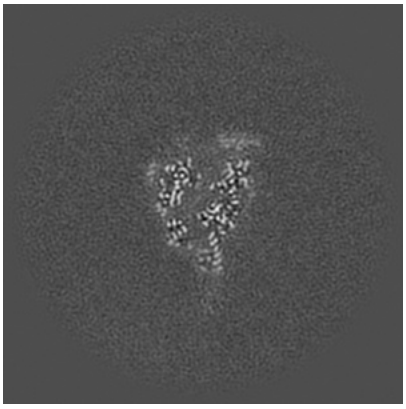
6.2.1 Primary map



X Index: 150



Y Index: 150

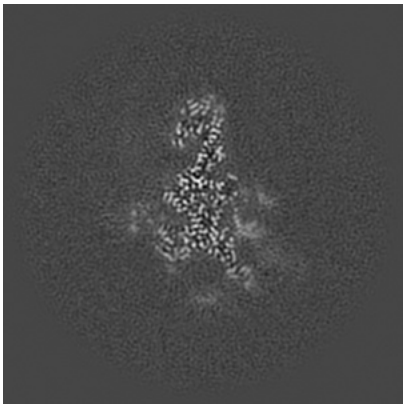


Z Index: 150

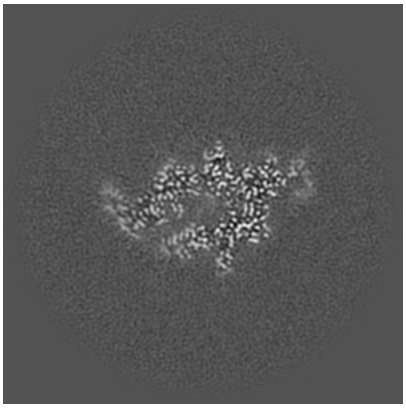
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

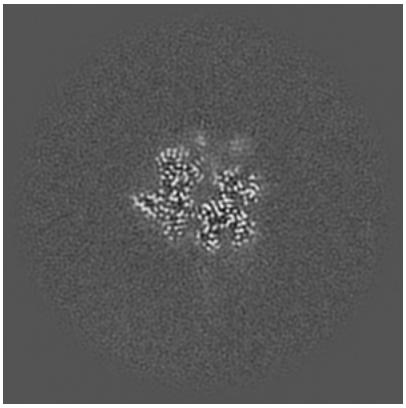
6.3.1 Primary map



X Index: 164



Y Index: 156

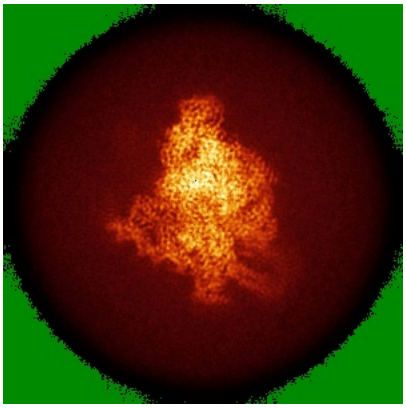


Z Index: 164

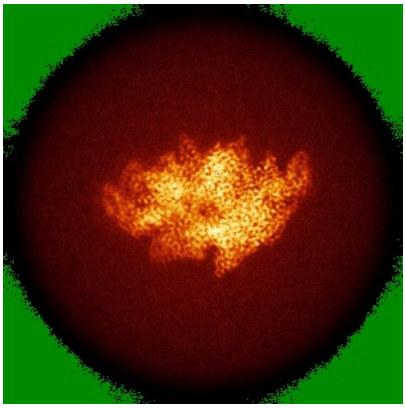
The images above show the largest variance slices of the map in three orthogonal directions.

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

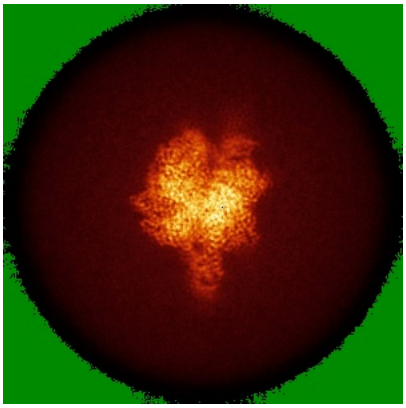
6.4.1 Primary map



X



Y

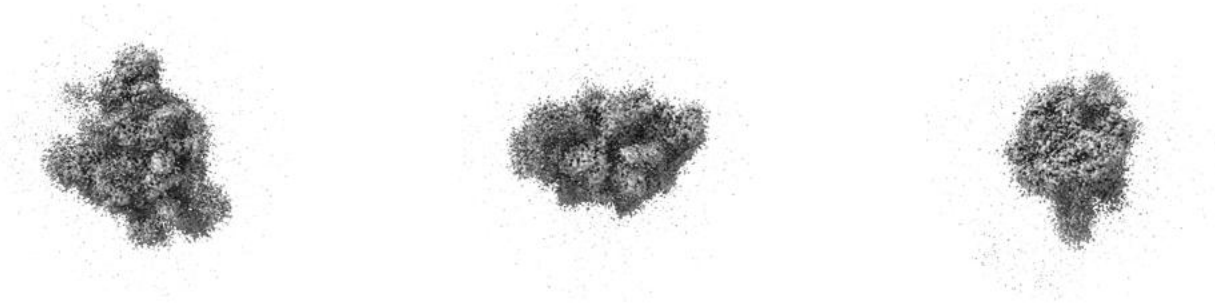


Z

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 0.372. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

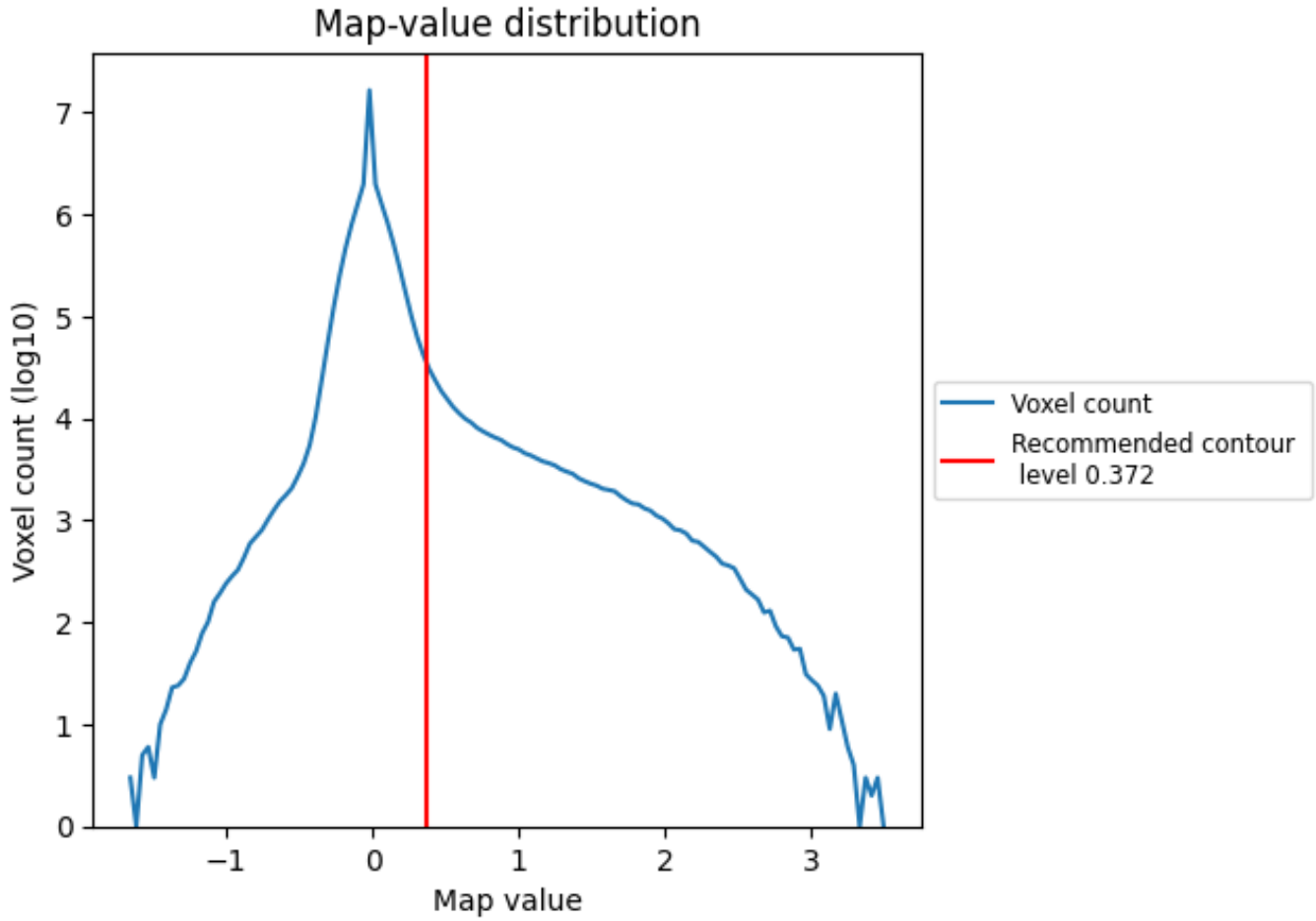
6.6 Mask visualisation (i)

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

7 Map analysis

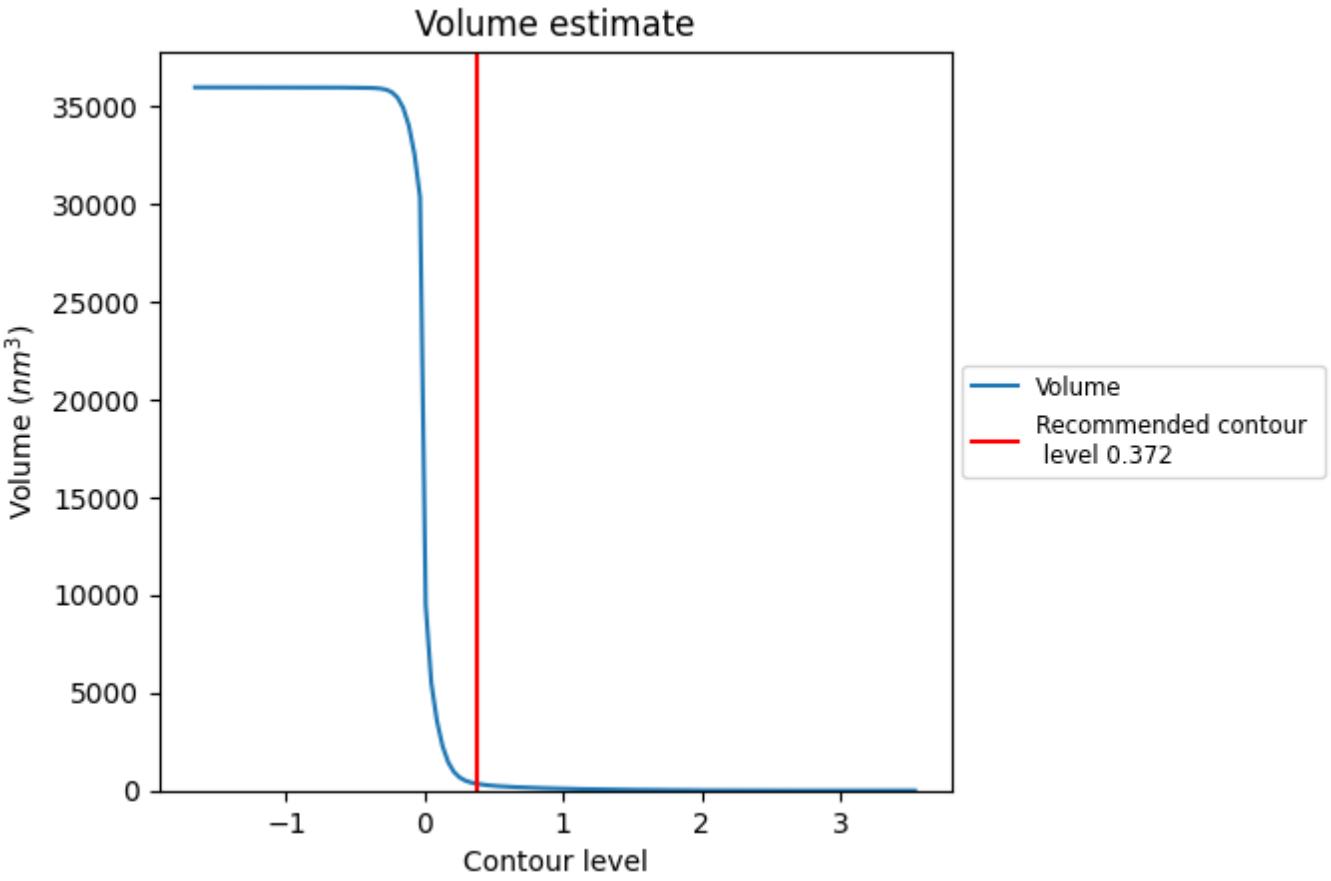
This section contains the results of statistical analysis of the map.

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.

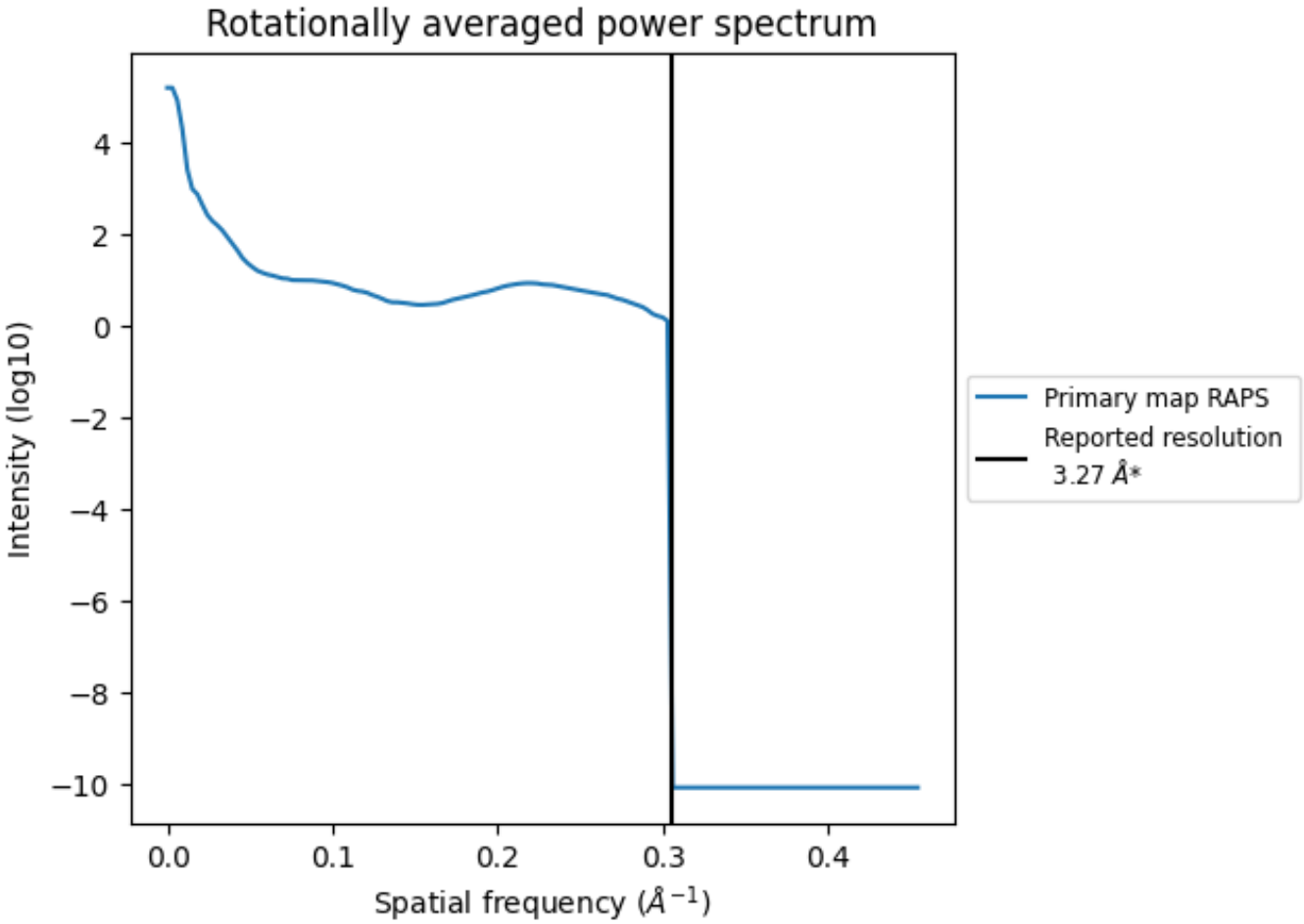
7.2 Volume estimate



The volume at the recommended contour level is 354 nm^3; this corresponds to an approximate mass of 319 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 0.306 Å^{-1}

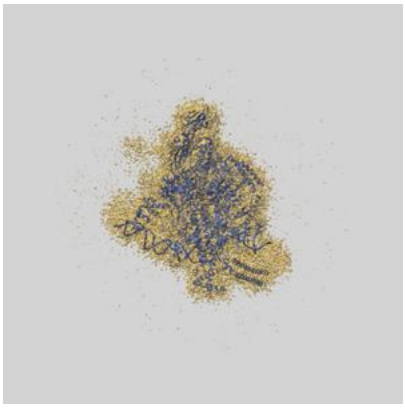
8 Fourier-Shell correlation (i)

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

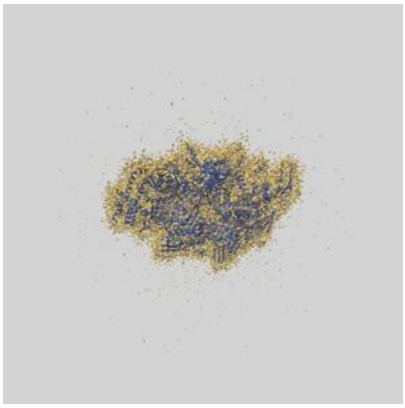
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7320 and PDB model 6C04. Per-residue inclusion information can be found in section 3 on page 7.

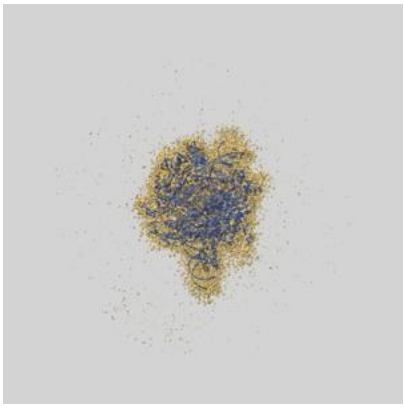
9.1 Map-model overlay



X



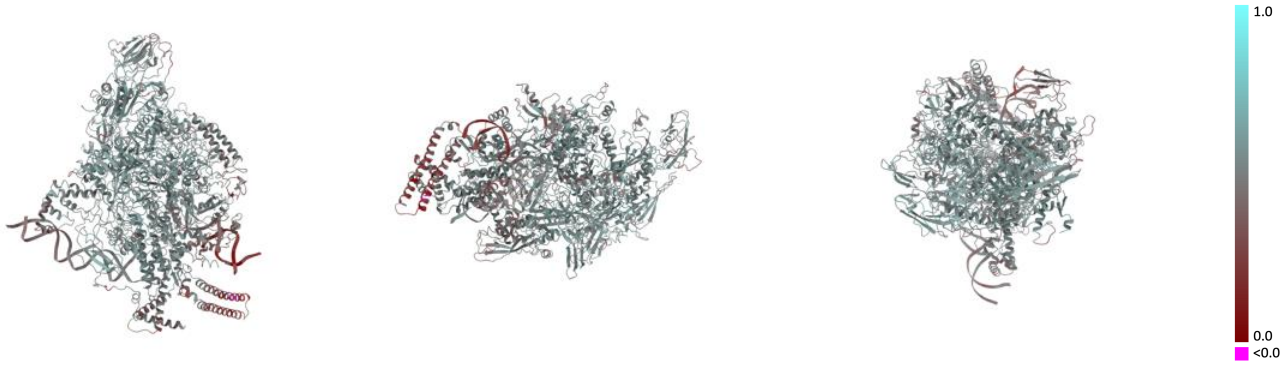
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.372 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.

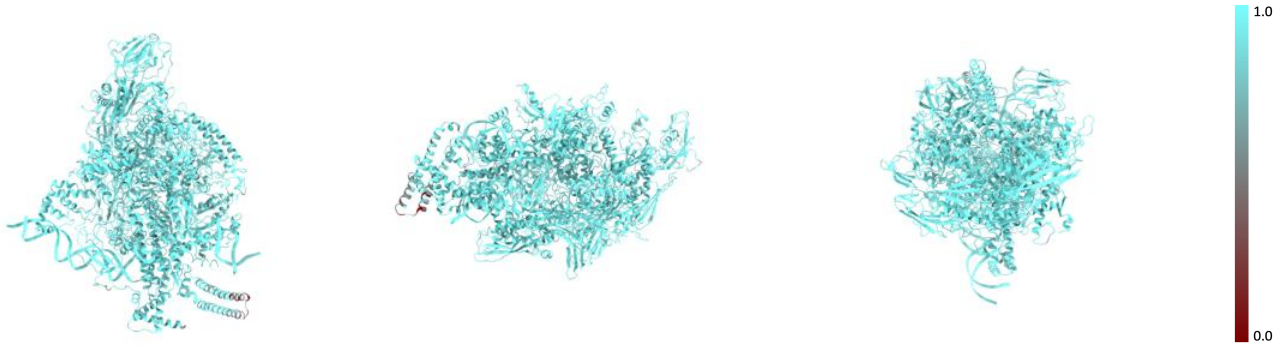
9.2 Q-score mapped to coordinate model (i)



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.

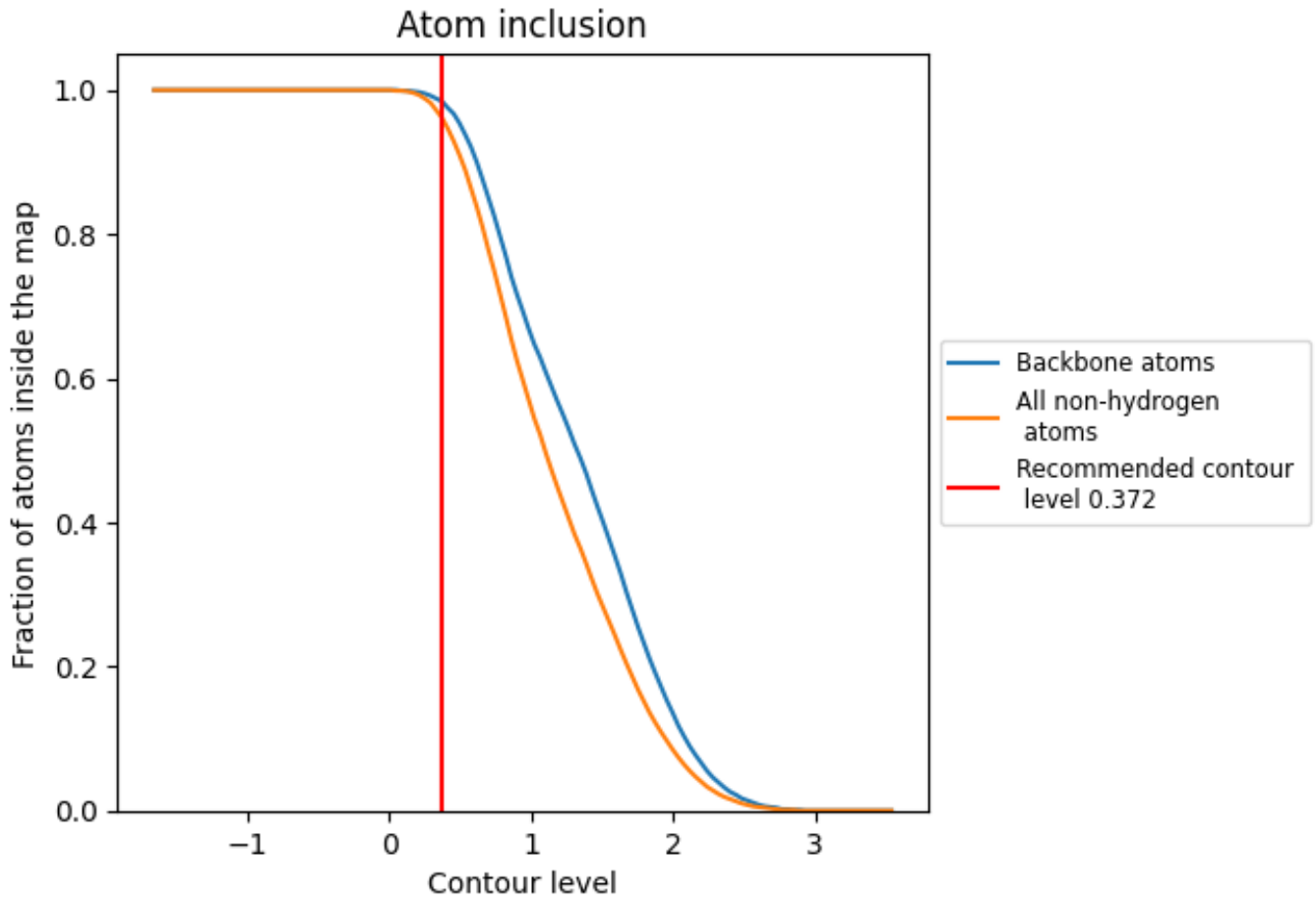
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.372).

9.4 Atom inclusion (i)



At the recommended contour level, 98% 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 (0.372) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.5150
A	0.9700	0.5410
B	0.9510	0.5090
C	0.9660	0.5300
D	0.9560	0.5220
E	0.9640	0.5370
F	0.9580	0.4940
G	0.9420	0.3330
H	0.9540	0.3970
J	0.9420	0.5010
O	0.9950	0.4560
P	0.9870	0.4520