Full wwPDB EM Validation Report ⓘ

Sep 2, 2026 – 02:13 PM EDT

PDB ID	:	36RS / pdb_000036rs
EMDB ID	:	EMD-77811
Title	:	Cryo-EM structure of Saccharomyces cerevisiae RNA polymerase II without stalk (no Rpb4/Rpb7)
Authors	:	Fordjour, G.N.R.; Murakami, K.; Armache, J.-P.; Murakami, K.S.
Deposited on	:	2026-06-29
Resolution	:	6.75 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:

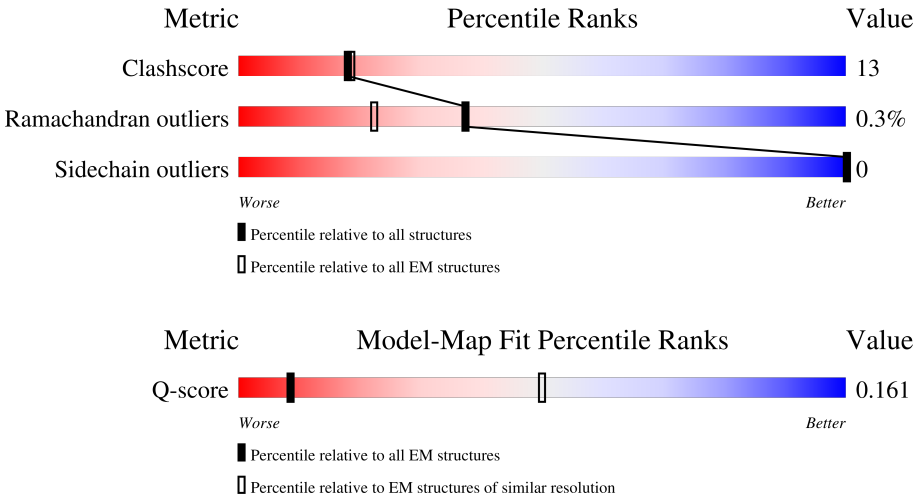
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 6.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	480 (6.25 - 7.25)

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

Mol	Chain	Length	Quality of chain
1	A	1733	55% 26% 18%
2	B	1224	65% 28% 6%
3	C	318	56% 28% 17%
4	E	215	74% 26%

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Mol	Chain	Length	Quality of chain
5	F	155	35% 21% 44%
6	H	146	64% 29% 7%
7	I	122	60% 34% 7%
8	J	70	71% 23% 6%
9	K	120	12% 69% 27%
10	L	70	47% 16% 37%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28625 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1419	11135	7014	1944	2115	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1148	9107	5755	1592	1705	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	265	2086	1312	347	414	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	214	1752	1111	309	321	11	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	87	705	451	119	132	3	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	136	1089	685	184	215	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

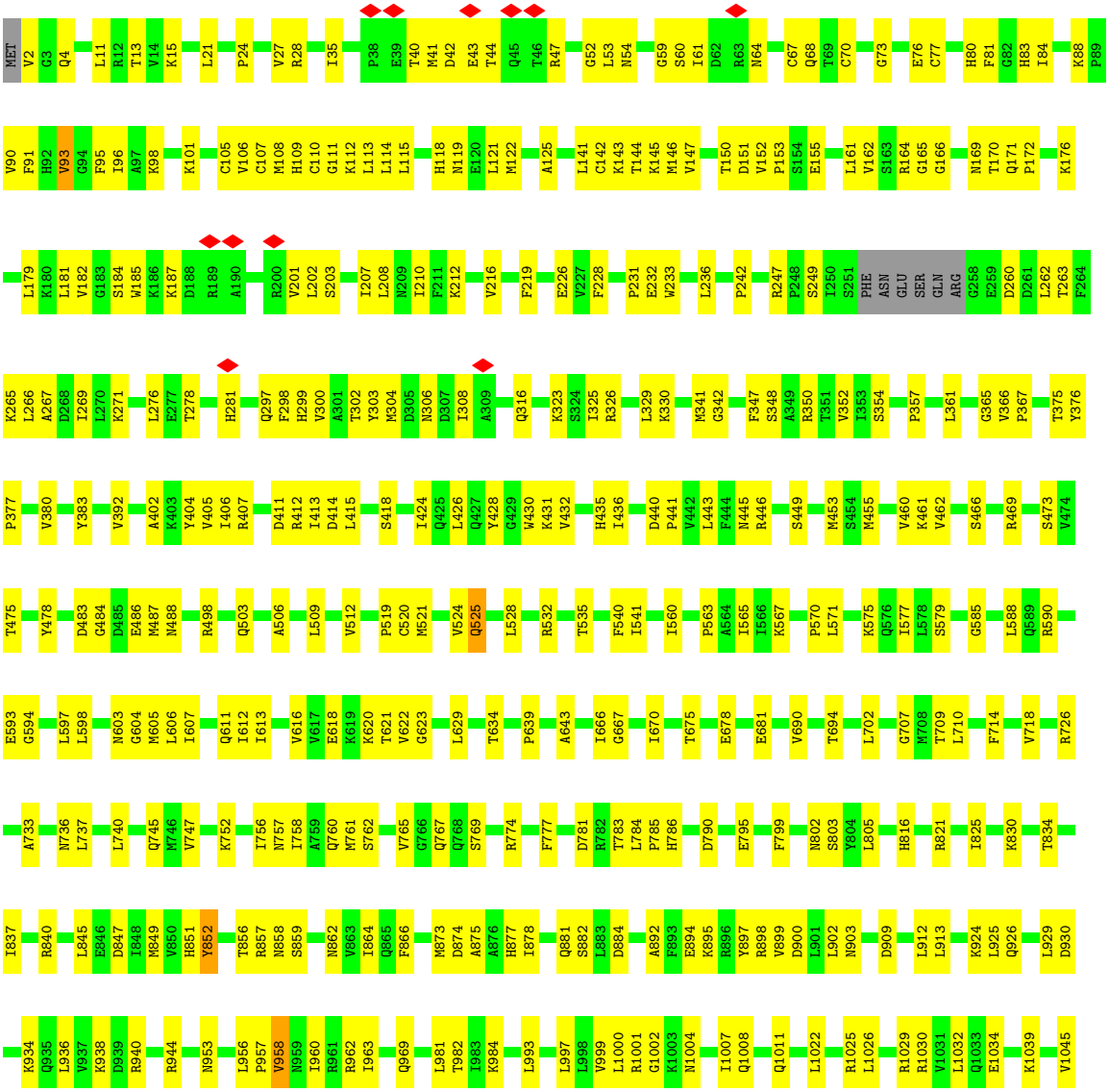
3 Residue-property plots (i)

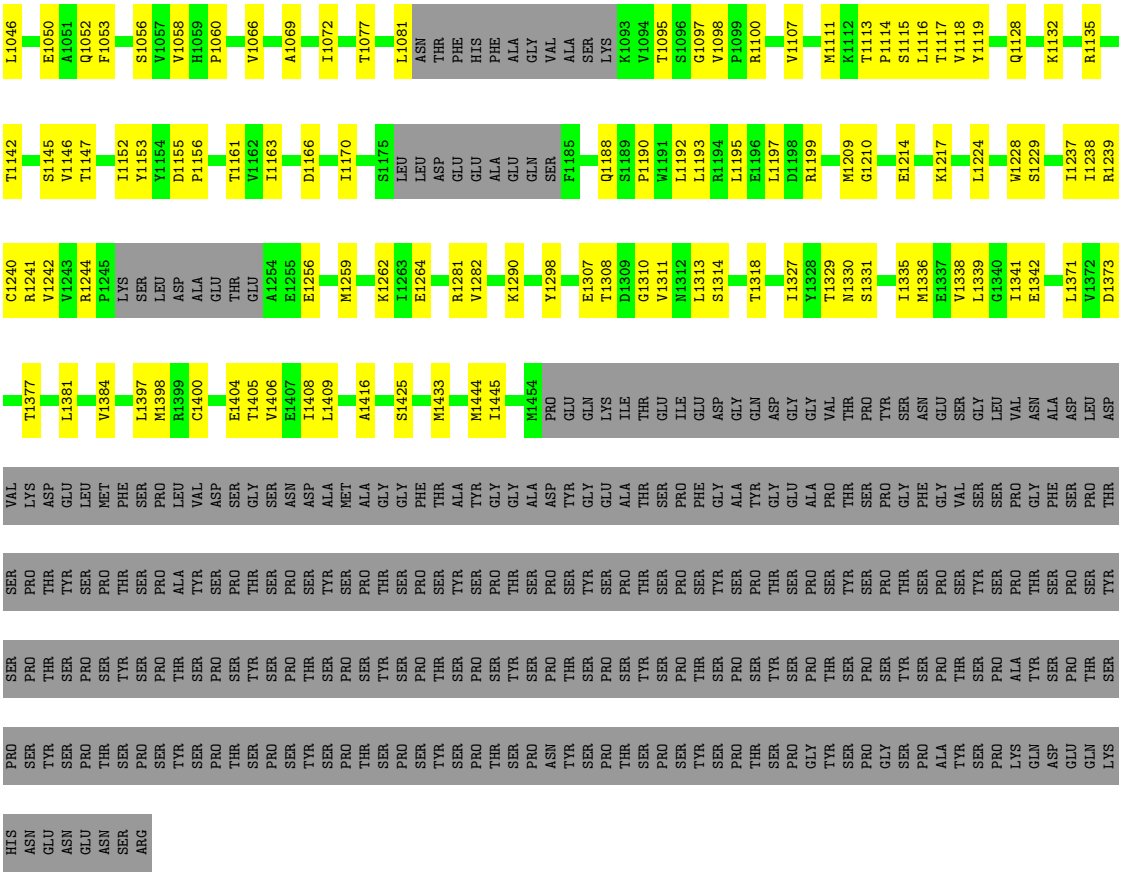
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:



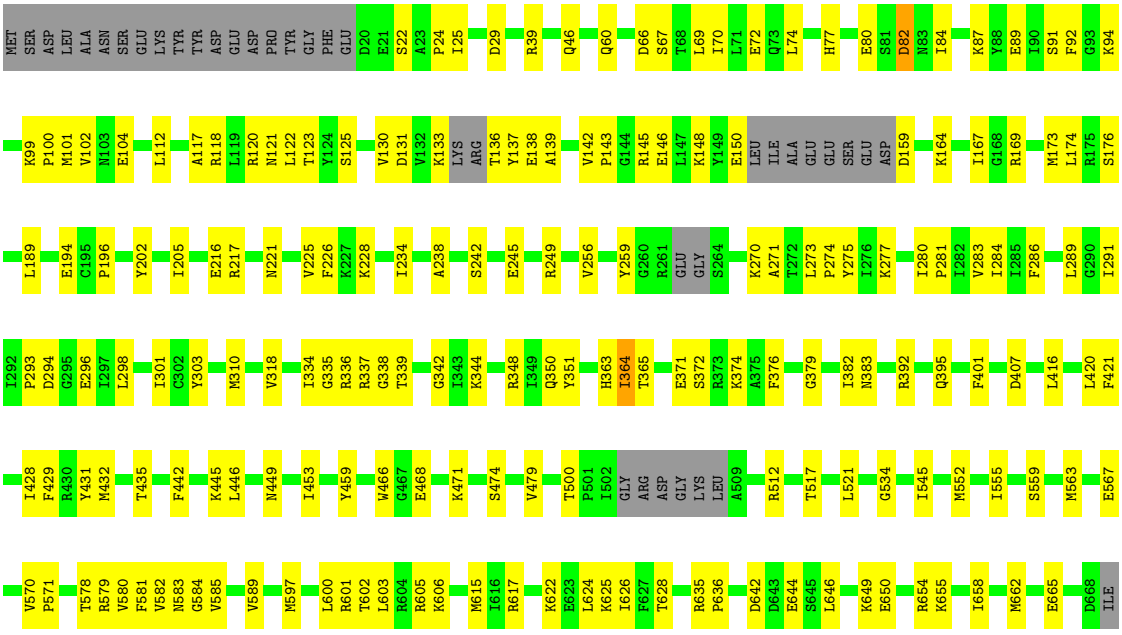


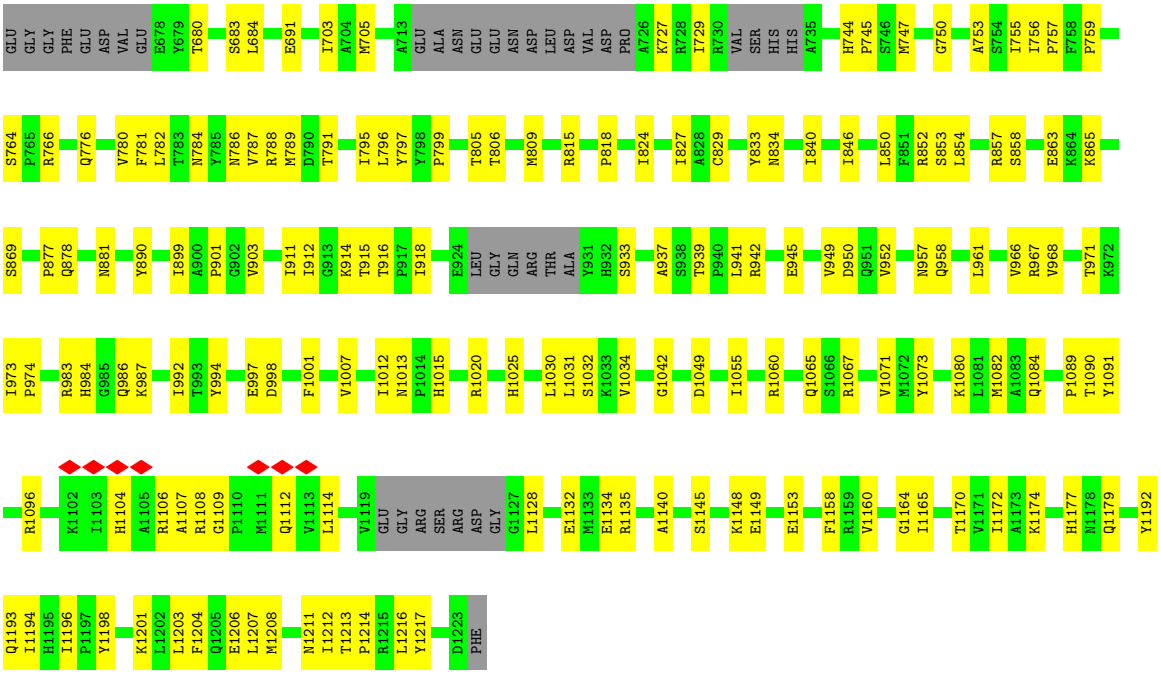


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



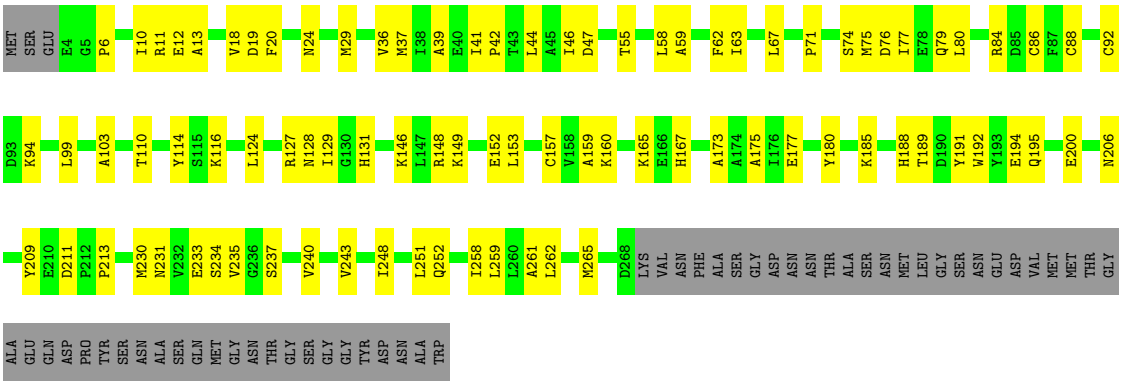




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

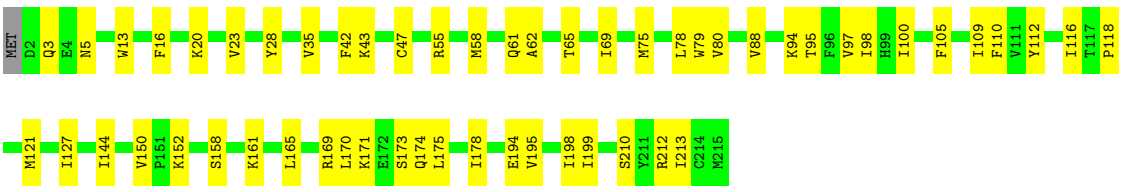




• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

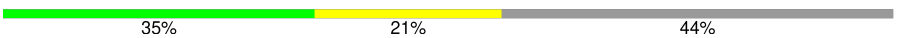
Chain E:

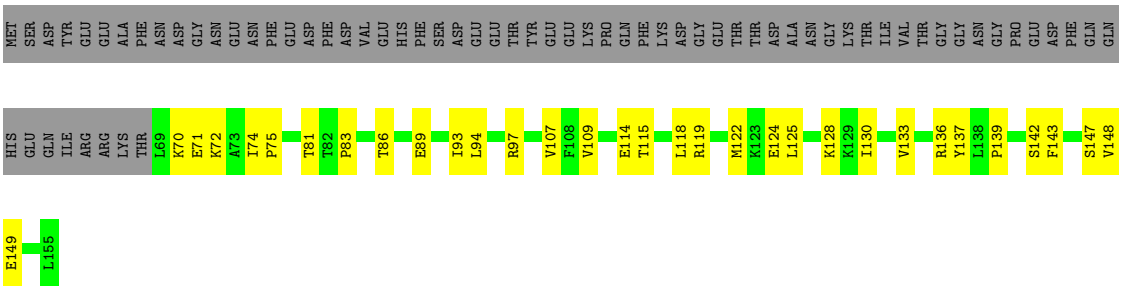




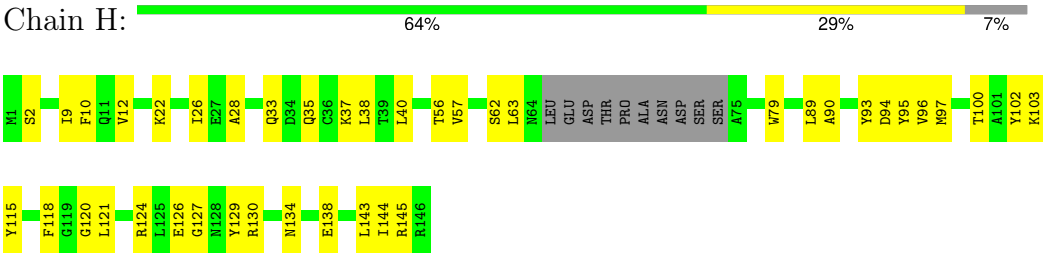
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

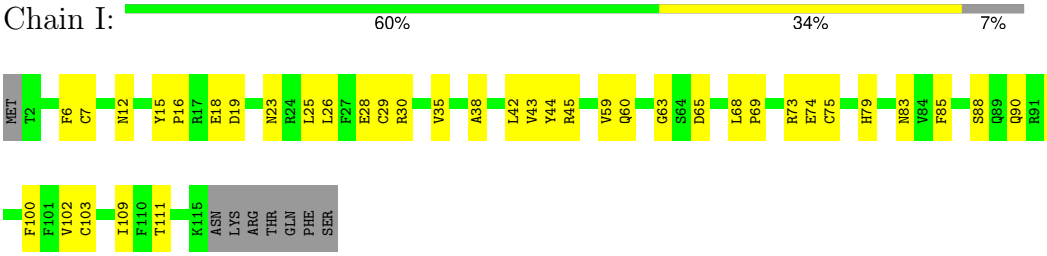




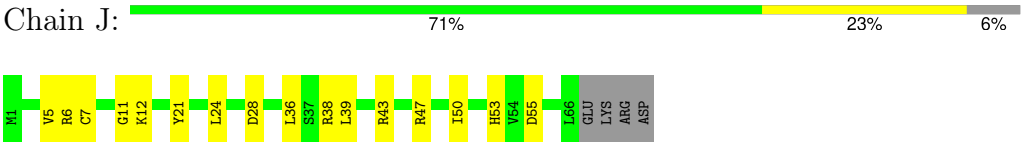
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



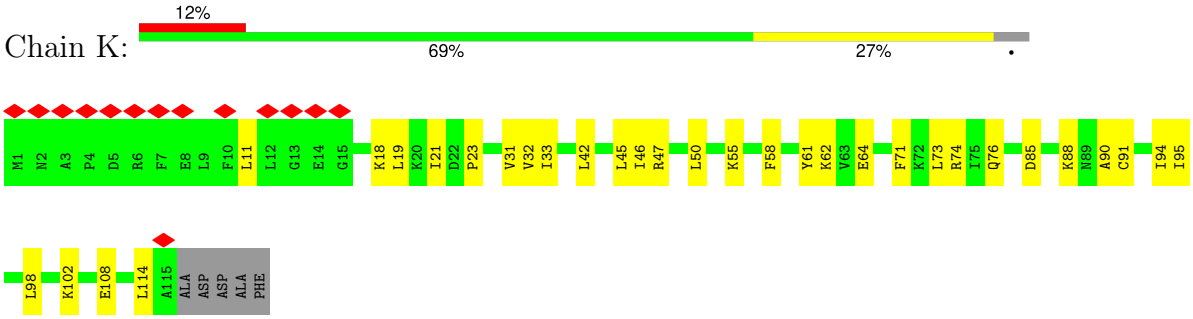
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



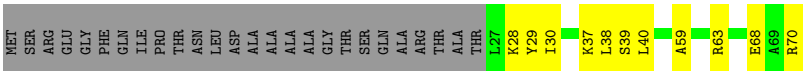
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:


47%
16%
37%


MET
SER
ARG
GLU
GLY
PHE
GLN
ILE
PRO
THR
ASN
LEU
ASP
ALA
ALA
ALA
ALA
GLY
THR
SER
GLN
ALA
ARG
THR
ALA
THR
L27
K28
Y29
I30
K37
L38
S39
L40
A59
R63
E68
A69
R70

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.582	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.944, 0.944, 0.944	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.15	0/11334	0.44	2/15332 (0.0%)
2	B	0.13	0/9280	0.38	0/12516
3	C	0.12	0/2124	0.34	0/2879
4	E	0.12	0/1788	0.36	0/2406
5	F	0.14	0/717	0.45	0/967
6	H	0.13	0/1107	0.39	0/1498
7	I	0.11	0/945	0.32	0/1273
8	J	0.12	0/549	0.35	0/738
9	K	0.11	0/942	0.30	0/1272
10	L	0.14	0/354	0.46	0/468
All	All	0.14	0/29140	0.40	2/39349 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	CYS	CA-C-N	5.04	131.17	121.54
1	A	67	CYS	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11135	0	11177	354	0
2	B	9107	0	9091	245	0
3	C	2086	0	2045	66	0
4	E	1752	0	1776	39	0
5	F	705	0	731	23	0
6	H	1089	0	1063	36	0
7	I	927	0	880	30	0
8	J	540	0	553	12	0
9	K	924	0	934	26	0
10	L	352	0	374	9	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
All	All	28625	0	28624	759	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 13.

All (759) 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:B:583:ASN:HD21	2:B:628:THR:H	1.26	0.83
4:E:43:LYS:O	4:E:47:CYS:HB2	1.78	0.82
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.62	0.81
2:B:117:ALA:O	2:B:121:ASN:HA	1.84	0.78
1:A:326:ARG:O	1:A:330:LYS:HB3	1.86	0.76
1:A:1224:LEU:HD13	1:A:1240:CYS:HB2	1.67	0.75
2:B:833:TYR:H	2:B:840:ILE:HD11	1.51	0.74
1:A:73:GLY:H	1:A:77:CYS:HB2	1.52	0.73
3:C:110:THR:HB	3:C:146:LYS:HB3	1.69	0.73
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.70	0.73
2:B:1080:LYS:HE3	3:C:188:HIS:HB2	1.70	0.72
1:A:415:LEU:HA	1:A:418:SER:HB3	1.72	0.72
2:B:348:ARG:HG2	2:B:351:TYR:H	1.53	0.72
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.72	0.72
1:A:512:VAL:HA	1:A:519:PRO:HA	1.72	0.71
1:A:718:VAL:HG23	1:A:774:ARG:HH12	1.55	0.71
6:H:37:LYS:H	6:H:126:GLU:HB2	1.54	0.71
2:B:829:CYS:HA	2:B:834:ASN:HD21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:175:LEU:HD22	4:E:213:ILE:HG13	1.73	0.71
1:A:618:GLU:HB2	1:A:620:LYS:HG2	1.71	0.70
5:F:125:LEU:HA	5:F:130:ILE:HD11	1.73	0.69
1:A:2:VAL:HA	2:B:1193:GLN:HB2	1.73	0.69
1:A:1114:PRO:HG2	1:A:1310:GLY:HA2	1.74	0.69
2:B:125:SER:HB2	2:B:169:ARG:HB3	1.74	0.69
1:A:21:LEU:HD23	2:B:1212:ILE:HG12	1.75	0.69
2:B:789:MET:HG3	2:B:967:ARG:HD2	1.75	0.68
1:A:341:MET:HB3	2:B:1135:ARG:HH12	1.59	0.68
1:A:1135:ARG:HG2	1:A:1282:VAL:HG23	1.73	0.68
1:A:383:TYR:HB3	5:F:115:THR:HB	1.76	0.68
1:A:1156:PRO:HG2	7:I:23:ASN:HB3	1.76	0.68
2:B:77:HIS:HB3	2:B:80:GLU:HB2	1.75	0.68
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.75	0.68
7:I:42:LEU:HD21	7:I:45:ARG:HG2	1.77	0.67
1:A:898:ARG:HH12	1:A:930:ASP:HA	1.60	0.67
2:B:824:ILE:HA	2:B:1089:PRO:HA	1.74	0.67
1:A:326:ARG:HH11	1:A:330:LYS:HA	1.58	0.67
2:B:766:ARG:HE	2:B:1020:ARG:HG2	1.60	0.67
1:A:845:LEU:HB2	1:A:1069:ALA:HB2	1.77	0.67
1:A:1192:LEU:HB3	1:A:1241:ARG:HH21	1.60	0.67
1:A:35:ILE:HA	1:A:52:GLY:HA2	1.77	0.66
6:H:57:VAL:HG12	6:H:144:ILE:HG22	1.77	0.66
7:I:73:ARG:HB2	7:I:83:ASN:HD21	1.59	0.66
8:J:7:CYS:HB3	8:J:11:GLY:H	1.60	0.66
2:B:228:LYS:HG2	2:B:234:ILE:HG13	1.77	0.66
1:A:352:VAL:HG13	1:A:484:GLY:HA2	1.77	0.66
1:A:262:LEU:HD11	1:A:303:TYR:HD1	1.61	0.66
1:A:851:HIS:HB3	5:F:139:PRO:HG3	1.76	0.66
2:B:597:MET:HG2	2:B:617:ARG:HD3	1.78	0.66
7:I:65:ASP:HB3	7:I:68:LEU:HB2	1.77	0.66
3:C:251:LEU:HD22	9:K:98:LEU:HD21	1.78	0.66
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.62	0.65
5:F:86:THR:HG23	5:F:89:GLU:H	1.62	0.65
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.77	0.65
1:A:565:ILE:HD12	1:A:571:LEU:HD23	1.79	0.65
1:A:882:SER:HA	1:A:953:ASN:HA	1.78	0.65
1:A:1290:LYS:HB3	1:A:1298:TYR:HB3	1.79	0.64
2:B:348:ARG:HE	2:B:350:GLN:HB3	1.62	0.64
2:B:786:ASN:HA	2:B:967:ARG:HH12	1.61	0.64
1:A:767:GLN:HA	1:A:799:PHE:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:GLY:H	2:B:753:ALA:HB3	1.62	0.64
1:A:329:LEU:HB3	2:B:1203:LEU:HD12	1.79	0.64
1:A:781:ASP:HB3	1:A:790:ASP:H	1.62	0.64
7:I:92:ARG:HE	7:I:93:LYS:H	1.46	0.64
1:A:567:LYS:HB2	6:H:96:VAL:HG23	1.80	0.64
2:B:912:ILE:HG22	2:B:914:LYS:H	1.62	0.64
2:B:82:ASP:H	2:B:142:VAL:HA	1.62	0.64
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.78	0.63
2:B:221:ASN:HB3	2:B:584:GLY:HA3	1.79	0.63
6:H:9:ILE:HA	6:H:56:THR:HA	1.79	0.63
2:B:559:SER:HA	2:B:563:MET:HB2	1.79	0.63
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.81	0.63
1:A:1329:THR:HG22	1:A:1331:SER:H	1.63	0.63
2:B:432:MET:HA	2:B:435:THR:HG22	1.80	0.63
2:B:1204:PHE:HA	2:B:1207:LEU:HD12	1.81	0.63
1:A:143:LYS:HA	1:A:146:MET:HE3	1.81	0.63
7:I:18:GLU:HA	7:I:25:LEU:HA	1.81	0.63
1:A:40:THR:HG22	1:A:41:MET:H	1.64	0.62
1:A:1400:CYS:HA	1:A:1404:GLU:HB2	1.82	0.62
7:I:7:CYS:HB2	7:I:29:CYS:SG	2.39	0.62
1:A:108:MET:HA	1:A:210:ILE:HG12	1.81	0.62
6:H:35:GLN:HB2	6:H:111:LEU:HD11	1.81	0.62
10:L:68:GLU:HG3	10:L:70:ARG:H	1.65	0.62
1:A:181:LEU:HD11	1:A:207:ILE:HD11	1.82	0.62
2:B:578:THR:HA	2:B:622:LYS:HB3	1.81	0.62
6:H:111:LEU:HG	6:H:127:GLY:H	1.63	0.62
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.61
1:A:588:LEU:HD22	1:A:629:LEU:HB3	1.83	0.61
2:B:580:VAL:HA	2:B:624:LEU:HB3	1.82	0.61
2:B:1149:GLU:HA	2:B:1153:GLU:HB2	1.83	0.61
1:A:443:LEU:HG	1:A:445:ASN:HD21	1.65	0.61
1:A:1095:THR:H	1:A:1113:THR:HG21	1.65	0.61
2:B:1030:LEU:HB3	2:B:1055:ILE:HG21	1.81	0.61
2:B:1071:VAL:HB	2:B:1084:GLN:HG3	1.83	0.61
1:A:506:ALA:H	1:A:509:LEU:HD12	1.65	0.61
1:A:446:ARG:HA	1:A:487:MET:HG2	1.82	0.60
2:B:680:THR:HG23	2:B:683:SER:H	1.65	0.60
1:A:153:PRO:HD3	1:A:164:ARG:HD2	1.83	0.60
1:A:840:ARG:HH21	1:A:1384:VAL:HB	1.66	0.60
1:A:585:GLY:HA2	1:A:969:GLN:HE22	1.67	0.60
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:MET:HE2	1:A:1229:SER:H	1.65	0.60
1:A:348:SER:HB2	2:B:1128:LEU:HD22	1.83	0.60
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.60
1:A:367:PRO:HB3	1:A:466:SER:HA	1.83	0.60
2:B:123:THR:HG23	2:B:205:ILE:HG22	1.84	0.60
2:B:776:GLN:HG3	2:B:1096:ARG:HE	1.66	0.60
1:A:115:LEU:HD13	1:A:125:ALA:HB1	1.84	0.60
1:A:1081:LEU:HD22	1:A:1097:GLY:HA2	1.83	0.60
3:C:177:GLU:HB2	3:C:231:ASN:H	1.67	0.59
1:A:13:THR:HA	2:B:1194:ILE:HD13	1.83	0.59
1:A:47:ARG:HE	1:A:61:ILE:HD11	1.68	0.59
2:B:459:TYR:HB3	2:B:468:GLU:HB2	1.84	0.59
4:E:88:VAL:HB	4:E:116:ILE:HG23	1.84	0.59
1:A:404:TYR:HA	1:A:414:ASP:HA	1.84	0.59
2:B:1177:HIS:HB2	2:B:1179:GLN:HG2	1.85	0.59
3:C:6:PRO:HA	3:C:24:ASN:HB2	1.85	0.59
5:F:137:TYR:HA	5:F:143:PHE:HA	1.82	0.59
2:B:429:PHE:HA	2:B:432:MET:HG2	1.85	0.59
2:B:603:LEU:HA	2:B:606:LYS:HD2	1.85	0.59
1:A:208:LEU:HG	1:A:212:LYS:HE2	1.84	0.59
2:B:727:LYS:HE3	2:B:1049:ASP:HB3	1.85	0.59
2:B:580:VAL:HG23	2:B:624:LEU:HD23	1.85	0.58
2:B:118:ARG:HH21	2:B:788:ARG:HB3	1.68	0.58
3:C:185:LYS:HG2	3:C:213:PRO:HB3	1.85	0.58
1:A:445:ASN:HB2	1:A:488:ASN:HD22	1.69	0.58
1:A:1338:VAL:HG12	1:A:1339:LEU:HD23	1.85	0.58
2:B:857:ARG:HD3	2:B:942:ARG:HH12	1.69	0.58
1:A:121:LEU:HD23	1:A:144:THR:HG21	1.84	0.58
1:A:579:SER:HB2	1:A:611:GLN:HA	1.85	0.58
7:I:7:CYS:CB	7:I:29:CYS:SG	2.91	0.58
3:C:39:ALA:HB1	3:C:165:LYS:HG3	1.85	0.58
9:K:64:GLU:HG2	9:K:71:PHE:HA	1.86	0.58
1:A:702:LEU:HB3	1:A:710:LEU:HD22	1.86	0.58
2:B:796:LEU:HD23	2:B:853:SER:HB3	1.85	0.58
7:I:74:GLU:HB3	7:I:79:HIS:HA	1.86	0.58
2:B:334:ILE:HG21	2:B:336:ARG:HH21	1.68	0.58
2:B:642:ASP:HA	2:B:649:LYS:HG3	1.86	0.57
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.85	0.57
5:F:124:GLU:HG2	5:F:130:ILE:HG13	1.85	0.57
1:A:666:ILE:HD13	2:B:1030:LEU:HD21	1.86	0.57
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	1.85	0.57
1:A:151:ASP:HB2	1:A:161:LEU:HB3	1.86	0.57
1:A:825:ILE:HG12	2:B:512:ARG:HB3	1.86	0.57
1:A:1433:MET:HA	2:B:1148:LYS:HD2	1.86	0.57
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.85	0.57
2:B:277:LYS:HE3	2:B:335:GLY:HA3	1.85	0.57
4:E:94:LYS:HA	4:E:97:VAL:HG12	1.87	0.57
1:A:606:LEU:HB3	1:A:613:ILE:HB	1.85	0.57
1:A:999:VAL:HG22	1:A:1053:PHE:HZ	1.69	0.57
2:B:601:ARG:HB3	2:B:605:ARG:HH21	1.69	0.57
2:B:173:MET:HB3	2:B:176:SER:HB3	1.87	0.57
2:B:69:LEU:HB3	2:B:432:MET:HE1	1.87	0.57
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.86	0.57
1:A:405:VAL:HA	1:A:432:VAL:HG13	1.87	0.57
2:B:644:GLU:HG3	2:B:646:LEU:H	1.68	0.57
7:I:25:LEU:HG	7:I:38:ALA:HB3	1.87	0.57
2:B:301:ILE:HD12	2:B:379:GLY:HA2	1.86	0.57
4:E:3:GLN:HG2	4:E:5:ASN:H	1.68	0.57
1:A:21:LEU:HA	2:B:1212:ILE:HA	1.87	0.56
10:L:30:ILE:HD11	10:L:37:LYS:HD3	1.87	0.56
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.86	0.56
1:A:899:VAL:HG13	1:A:929:LEU:HD13	1.87	0.56
1:A:1117:THR:HG23	1:A:1307:GLU:HB3	1.87	0.56
2:B:67:SER:HA	2:B:92:PHE:HD2	1.69	0.56
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.86	0.56
3:C:86:CYS:HB3	3:C:88:CYS:SG	2.45	0.56
5:F:72:LYS:HB3	5:F:142:SER:HA	1.87	0.56
1:A:785:PRO:HB2	2:B:703:ILE:HD13	1.87	0.56
2:B:581:PHE:HB3	2:B:625:LYS:HD2	1.87	0.56
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.70	0.56
7:I:102:VAL:HG12	7:I:109:ILE:HA	1.88	0.56
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.86	0.56
6:H:114:VAL:HG11	6:H:134:ASN:HD21	1.71	0.56
7:I:75:CYS:HB2	7:I:79:HIS:H	1.71	0.56
2:B:298:LEU:HA	2:B:301:ILE:HG22	1.88	0.56
3:C:55:THR:HG22	3:C:152:GLU:H	1.70	0.56
1:A:325:ILE:HG13	2:B:1206:GLU:HG2	1.87	0.56
2:B:863:GLU:HB2	2:B:961:LEU:HB3	1.87	0.56
6:H:143:LEU:HB3	6:H:145:ARG:HH22	1.70	0.56
1:A:765:VAL:HG23	1:A:803:SER:HA	1.88	0.56
1:A:894:GLU:O	1:A:898:ARG:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:HB2	1:A:323:LYS:HE3	1.88	0.55
8:J:24:LEU:HD21	8:J:38:ARG:HH11	1.71	0.55
1:A:821:ARG:HH21	2:B:534:GLY:HA2	1.70	0.55
1:A:1128:GLN:HG3	1:A:1132:LYS:HE2	1.87	0.55
6:H:95:TYR:HE2	6:H:97:MET:HB2	1.72	0.55
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.89	0.55
2:B:846:ILE:HD13	2:B:850:LEU:HB3	1.88	0.55
1:A:593:GLU:CD	1:A:594:GLY:H	2.15	0.55
1:A:830:LYS:HG2	1:A:1098:VAL:HG21	1.88	0.55
1:A:837:ILE:HD13	1:A:840:ARG:HD3	1.88	0.55
1:A:41:MET:HE1	1:A:247:ARG:HH21	1.72	0.55
1:A:326:ARG:HD3	1:A:330:LYS:HA	1.88	0.55
1:A:909:ASP:HB3	1:A:912:LEU:HB2	1.88	0.55
2:B:102:VAL:HB	2:B:112:LEU:HD22	1.89	0.55
2:B:139:ALA:HB2	2:B:150:GLU:HG2	1.87	0.55
2:B:805:THR:HG21	2:B:815:ARG:HH12	1.71	0.55
3:C:173:ALA:HA	3:C:234:SER:HA	1.87	0.55
4:E:118:PRO:HA	4:E:121:MET:HE2	1.89	0.55
1:A:563:PRO:HG3	1:A:570:PRO:HB3	1.88	0.55
1:A:91:PHE:H	1:A:297:GLN:HG2	1.72	0.55
2:B:277:LYS:HD2	2:B:337:ARG:HE	1.72	0.55
2:B:806:THR:HG23	2:B:809:MET:HE3	1.89	0.55
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.47	0.54
1:A:376:TYR:HB2	1:A:436:ILE:HG13	1.89	0.54
1:A:524:VAL:HB	1:A:528:LEU:HD22	1.89	0.54
1:A:247:ARG:HG3	1:A:262:LEU:HB3	1.88	0.54
1:A:579:SER:HB3	1:A:612:ILE:HG12	1.89	0.54
1:A:1444:MET:HE3	1:A:1445:ILE:H	1.72	0.54
2:B:298:LEU:HD12	7:I:6:PHE:HZ	1.72	0.54
1:A:114:LEU:HD22	1:A:146:MET:HG3	1.89	0.54
2:B:1132:GLU:HA	2:B:1135:ARG:HE	1.72	0.54
2:B:555:ILE:HG12	2:B:582:VAL:HG21	1.89	0.54
10:L:29:TYR:HB2	10:L:38:LEU:HB2	1.89	0.54
1:A:357:PRO:HD2	2:B:833:TYR:HD1	1.73	0.54
2:B:70:ILE:HG22	2:B:89:GLU:HA	1.90	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.89	0.54
3:C:167:HIS:HD2	10:L:70:ARG:HG2	1.72	0.54
1:A:106:VAL:HG13	1:A:111:GLY:HA2	1.88	0.54
1:A:565:ILE:HB	1:A:571:LEU:HB3	1.90	0.54
1:A:1100:ARG:HH22	1:A:1111:MET:HE3	1.73	0.54
1:A:795:GLU:HA	1:A:799:PHE:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:PRO:HD2	5:F:86:THR:HB	1.89	0.54
2:B:336:ARG:HH22	2:B:351:TYR:HB3	1.73	0.54
1:A:892:ALA:HA	1:A:895:LYS:HG2	1.90	0.54
1:A:1116:LEU:HB3	1:A:1329:THR:HG23	1.89	0.54
3:C:11:ARG:HH22	3:C:230:MET:H	1.56	0.54
4:E:100:ILE:HA	4:E:105:PHE:HD2	1.73	0.54
5:F:70:LYS:O	5:F:71:GLU:HG3	2.08	0.54
1:A:607:ILE:HA	1:A:612:ILE:HA	1.89	0.53
1:A:902:LEU:HB3	1:A:926:GLN:HG2	1.89	0.53
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.74	0.53
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.90	0.53
1:A:1072:ILE:HD13	1:A:1371:LEU:HD12	1.90	0.53
3:C:75:MET:HB2	3:C:128:ASN:HB3	1.88	0.53
1:A:308:ILE:HG22	1:A:326:ARG:HH21	1.74	0.53
1:A:622:VAL:HG13	1:A:623:GLY:H	1.72	0.53
2:B:101:MET:HA	2:B:112:LEU:H	1.73	0.53
5:F:93:ILE:HG22	5:F:125:LEU:HD21	1.90	0.53
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.91	0.53
4:E:165:LEU:HD13	4:E:170:LEU:HB2	1.91	0.53
1:A:999:VAL:HG12	1:A:1000:LEU:HD22	1.91	0.53
5:F:133:VAL:HA	5:F:147:SER:HA	1.91	0.53
1:A:88:LYS:HB2	1:A:276:LEU:HD11	1.89	0.53
1:A:107:CYS:CB	1:A:110:CYS:HB3	2.39	0.53
1:A:118:HIS:HE1	1:A:164:ARG:HE	1.57	0.53
2:B:1034:VAL:HG21	2:B:1055:ILE:HG23	1.90	0.53
2:B:310:MET:HE1	2:B:383:ASN:HA	1.91	0.52
1:A:93:VAL:HG23	1:A:95:PHE:H	1.73	0.52
2:B:428:ILE:HD11	2:B:446:LEU:HB3	1.91	0.52
3:C:59:ALA:HB3	3:C:62:PHE:HB3	1.91	0.52
1:A:70:CYS:HA	2:B:1174:LYS:HG3	1.90	0.52
1:A:1022:LEU:O	1:A:1026:LEU:HB3	2.10	0.52
9:K:91:CYS:HA	9:K:94:ILE:HD12	1.90	0.52
1:A:98:LYS:HA	1:A:101:LYS:HE2	1.92	0.52
1:A:802:ASN:HD21	2:B:729:ILE:H	1.58	0.52
2:B:24:PRO:HB3	2:B:650:GLU:HG2	1.91	0.52
9:K:32:VAL:HG12	9:K:74:ARG:HB2	1.91	0.52
7:I:15:TYR:HB2	7:I:30:ARG:HE	1.73	0.52
1:A:60:SER:HB2	1:A:64:ASN:HB3	1.92	0.52
2:B:22:SER:HA	2:B:654:ARG:HD3	1.91	0.52
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.90	0.52
2:B:912:ILE:HB	2:B:939:THR:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HB2	1:A:110:CYS:HB3	1.90	0.52
2:B:1158:PHE:HB3	2:B:1198:TYR:H	1.73	0.52
2:B:123:THR:HA	2:B:205:ILE:HA	1.91	0.52
2:B:903:VAL:HG22	10:L:63:ARG:HH12	1.75	0.52
1:A:24:PRO:HA	1:A:27:VAL:HG22	1.91	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CD1	2.45	0.52
1:A:1152:ILE:HG22	7:I:44:TYR:HB3	1.90	0.52
1:A:121:LEU:HG	1:A:141:LEU:HD21	1.92	0.51
1:A:1339:LEU:HD22	4:E:144:ILE:HG23	1.91	0.51
2:B:225:VAL:HG12	2:B:238:ALA:HA	1.92	0.51
1:A:616:VAL:HG12	1:A:618:GLU:HG2	1.91	0.51
2:B:512:ARG:HA	2:B:534:GLY:HA3	1.92	0.51
2:B:1160:VAL:HG11	2:B:1201:LYS:HG3	1.91	0.51
1:A:96:ILE:HD13	1:A:179:LEU:HA	1.92	0.51
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.75	0.51
2:B:289:LEU:HD21	2:B:374:LYS:HB2	1.92	0.51
3:C:44:LEU:HD22	3:C:129:ILE:HG23	1.92	0.51
8:J:24:LEU:O	8:J:28:ASP:CB	2.58	0.51
1:A:866:PHE:HE2	4:E:210:SER:HA	1.75	0.51
2:B:957:ASN:HD21	2:B:961:LEU:HD12	1.75	0.51
1:A:767:GLN:HE21	1:A:769:SER:HB3	1.74	0.51
2:B:984:HIS:HB2	2:B:986:GLN:HE22	1.75	0.51
1:A:483:ASP:HB3	2:B:987:LYS:HE2	1.92	0.51
2:B:136:THR:HG22	2:B:138:GLU:HB3	1.93	0.51
2:B:364:ILE:HG21	2:B:585:VAL:HB	1.93	0.51
1:A:524:VAL:HG23	1:A:525:GLN:H	1.75	0.51
1:A:525:GLN:HE21	2:B:1015:HIS:CD2	2.28	0.51
1:A:1405:THR:HG22	1:A:1406:VAL:H	1.75	0.51
2:B:122:LEU:HD11	2:B:958:GLN:HB2	1.93	0.51
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	1.92	0.51
8:J:36:LEU:HD22	8:J:47:ARG:HG3	1.93	0.51
3:C:124:LEU:HB3	3:C:127:ARG:HG2	1.93	0.51
3:C:10:ILE:HG12	9:K:108:GLU:HG3	1.93	0.50
3:C:194:GLU:HG2	3:C:195:GLN:HG2	1.93	0.50
1:A:392:VAL:HG21	1:A:426:LEU:HD21	1.92	0.50
1:A:925:LEU:HD21	1:A:984:LYS:HB3	1.93	0.50
2:B:1160:VAL:HG21	2:B:1201:LYS:HG3	1.93	0.50
3:C:58:LEU:HD23	3:C:63:ILE:HD11	1.93	0.50
1:A:406:ILE:HG23	1:A:412:ARG:HG2	1.93	0.50
6:H:33:GLN:HG2	6:H:129:TYR:CE1	2.46	0.50
1:A:726:ARG:NH2	1:A:767:GLN:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:ARG:HG3	3:C:129:ILE:HB	1.94	0.50
3:C:148:ARG:HD2	3:C:149:LYS:HG2	1.92	0.50
1:A:475:THR:HA	1:A:478:TYR:HB2	1.93	0.50
1:A:407:ARG:HB2	1:A:411:ASP:HB3	1.94	0.50
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.50
3:C:13:ALA:HB3	9:K:114:LEU:HD21	1.94	0.50
1:A:119:ASN:H	1:A:122:MET:HB2	1.76	0.50
1:A:1341:ILE:HG21	4:E:212:ARG:HH12	1.77	0.50
4:E:97:VAL:HG22	4:E:127:ILE:HD12	1.94	0.50
1:A:119:ASN:HD21	1:A:155:GLU:HB2	1.77	0.49
3:C:240:VAL:HA	3:C:243:VAL:HG22	1.94	0.49
6:H:12:VAL:HG21	6:H:26:ILE:HD12	1.94	0.49
9:K:85:ASP:HA	9:K:88:LYS:HG2	1.94	0.49
1:A:579:SER:HB2	1:A:612:ILE:H	1.77	0.49
2:B:1160:VAL:HG21	2:B:1201:LYS:HE2	1.94	0.49
1:A:300:VAL:HG22	1:A:304:MET:HE2	1.92	0.49
1:A:525:GLN:HE22	2:B:1013:ASN:HD21	1.60	0.49
1:A:1166:ASP:HB2	1:A:1237:ILE:HG21	1.93	0.49
2:B:256:VAL:HG13	2:B:271:ALA:HB2	1.94	0.49
2:B:602:THR:HA	2:B:605:ARG:HD2	1.92	0.49
1:A:849:MET:HB3	1:A:851:HIS:CD2	2.47	0.49
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.47	0.49
6:H:56:THR:HB	6:H:145:ARG:HB2	1.94	0.49
3:C:265:MET:HE1	9:K:21:ILE:H	1.77	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.95	0.49
2:B:446:LEU:HA	2:B:449:ASN:HB2	1.95	0.49
2:B:781:PHE:HD1	2:B:782:LEU:HD23	1.78	0.49
2:B:952:VAL:HG22	2:B:966:VAL:HG23	1.94	0.49
9:K:61:TYR:HB3	9:K:73:LEU:HD13	1.95	0.49
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.94	0.48
1:A:958:VAL:HA	1:A:962:ARG:HH21	1.78	0.48
1:A:1029:ARG:HA	1:A:1032:LEU:HB2	1.95	0.48
1:A:1188:GLN:HA	1:A:1244:ARG:H	1.77	0.48
1:A:709:THR:HG22	1:A:710:LEU:HG	1.95	0.48
2:B:392:ARG:HG2	7:I:90:GLN:HG2	1.94	0.48
5:F:130:ILE:HB	5:F:148:VAL:HG11	1.94	0.48
1:A:28:ARG:HD3	1:A:83:HIS:CE1	2.48	0.48
6:H:63:LEU:HD12	6:H:90:ALA:H	1.78	0.48
1:A:308:ILE:HG22	1:A:326:ARG:NH2	2.28	0.48
1:A:1066:VAL:HG12	2:B:1140:ALA:HB2	1.95	0.48
2:B:145:ARG:HE	2:B:146:GLU:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.77	0.48
9:K:42:LEU:O	9:K:46:ILE:HG12	2.13	0.48
1:A:13:THR:HG23	1:A:15:LYS:HZ2	1.77	0.48
1:A:176:LYS:HA	1:A:181:LEU:HA	1.96	0.48
1:A:232:GLU:HG2	1:A:233:TRP:HD1	1.78	0.48
1:A:350:ARG:HE	1:A:486:GLU:HB3	1.78	0.48
1:A:375:THR:HA	1:A:435:HIS:HA	1.95	0.48
2:B:91:SER:H	2:B:133:LYS:C	2.22	0.48
2:B:283:VAL:HG21	2:B:318:VAL:HA	1.94	0.48
2:B:916:THR:HG23	2:B:918:ILE:HG12	1.95	0.48
6:H:95:TYR:CE2	6:H:97:MET:HB2	2.48	0.48
1:A:413:ILE:HG13	1:A:418:SER:HB2	1.95	0.48
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.94	0.48
2:B:301:ILE:HD11	2:B:382:ILE:HB	1.96	0.48
9:K:23:PRO:HA	9:K:31:VAL:HG22	1.95	0.48
1:A:216:VAL:HG13	1:A:226:GLU:HG3	1.96	0.48
1:A:733:ALA:O	1:A:737:LEU:HG	2.13	0.48
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.94	0.48
2:B:376:PHE:HE1	2:B:571:PRO:HG3	1.79	0.48
2:B:901:PRO:HB3	2:B:950:ASP:HA	1.96	0.48
2:B:949:VAL:HG12	2:B:968:VAL:HG12	1.96	0.48
2:B:1214:PRO:HG2	2:B:1216:LEU:HD22	1.95	0.48
1:A:302:THR:HA	1:A:306:ASN:HA	1.96	0.48
2:B:449:ASN:O	2:B:453:ILE:HG12	2.14	0.48
3:C:103:ALA:HB3	3:C:153:LEU:HB3	1.95	0.48
7:I:42:LEU:HD11	7:I:45:ARG:HD3	1.95	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.47
3:C:13:ALA:HA	3:C:18:VAL:HG12	1.94	0.47
3:C:185:LYS:HZ3	3:C:211:ASP:H	1.60	0.47
1:A:4:GLN:HG3	1:A:76:GLU:HA	1.95	0.47
1:A:678:GLU:HA	1:A:681:GLU:HG3	1.96	0.47
2:B:1032:SER:HB3	2:B:1089:PRO:HB2	1.95	0.47
9:K:32:VAL:HA	9:K:74:ARG:HA	1.97	0.47
1:A:690:VAL:O	1:A:694:THR:HG23	2.15	0.47
1:A:1118:VAL:HA	1:A:1327:ILE:HG12	1.96	0.47
2:B:137:TYR:H	2:B:159:ASP:HA	1.79	0.47
1:A:147:VAL:HA	1:A:170:THR:HG23	1.96	0.47
2:B:1145:SER:HA	2:B:1148:LYS:HD3	1.95	0.47
4:E:152:LYS:HB2	4:E:199:ILE:HB	1.96	0.47
1:A:350:ARG:HB3	1:A:486:GLU:HB3	1.96	0.47
1:A:377:PRO:HB2	1:A:431:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:HB3	1:A:607:ILE:HD12	1.97	0.47
2:B:39:ARG:HH22	2:B:665:GLU:HG2	1.79	0.47
2:B:471:LYS:HA	2:B:474:SER:HB3	1.96	0.47
1:A:150:THR:HA	1:A:166:GLY:HA2	1.96	0.47
1:A:267:ALA:O	1:A:271:LYS:HG2	2.15	0.47
1:A:1214:GLU:HA	1:A:1217:LYS:HG2	1.95	0.47
7:I:19:ASP:HB2	7:I:26:LEU:HD23	1.96	0.47
1:A:118:HIS:CE1	1:A:164:ARG:HE	2.31	0.47
2:B:139:ALA:HB1	2:B:148:LYS:HB3	1.96	0.47
1:A:449:SER:HB3	2:B:1134:GLU:HG3	1.96	0.47
1:A:857:ARG:HH22	4:E:169:ARG:HB2	1.80	0.47
2:B:74:LEU:HG	2:B:143:PRO:HG3	1.96	0.47
3:C:11:ARG:HH21	3:C:20:PHE:H	1.63	0.47
3:C:88:CYS:HB3	3:C:92:CYS:H	1.79	0.47
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.97	0.47
2:B:1001:PHE:HB3	2:B:1007:VAL:HG12	1.97	0.47
1:A:958:VAL:HG22	1:A:1052:GLN:HG3	1.97	0.46
1:A:1114:PRO:HB2	1:A:1311:VAL:H	1.79	0.46
2:B:600:LEU:HG	2:B:615:MET:HE3	1.97	0.46
2:B:787:VAL:HG12	2:B:788:ARG:H	1.81	0.46
3:C:175:ALA:HB3	3:C:233:GLU:HB3	1.96	0.46
8:J:12:LYS:HD2	8:J:43:ARG:HH21	1.80	0.46
1:A:361:LEU:HD13	1:A:643:ALA:HB1	1.96	0.46
1:A:666:ILE:HD13	2:B:1030:LEU:HD11	1.96	0.46
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.15	0.46
2:B:755:ILE:HA	2:B:809:MET:HE2	1.97	0.46
4:E:23:VAL:HG22	4:E:28:TYR:HB2	1.96	0.46
4:E:80:VAL:HG12	4:E:109:ILE:HB	1.97	0.46
1:A:757:ASN:HB3	1:A:761:MET:HE2	1.97	0.46
1:A:784:LEU:HD23	1:A:786:HIS:HB2	1.95	0.46
1:A:874:ASP:HB2	1:A:1058:VAL:HA	1.97	0.46
1:A:1209:MET:HG2	1:A:1229:SER:HB3	1.98	0.46
2:B:91:SER:HB3	2:B:133:LYS:HB2	1.97	0.46
4:E:178:ILE:HB	4:E:212:ARG:HB3	1.96	0.46
2:B:420:LEU:HB3	2:B:453:ILE:HD12	1.97	0.46
3:C:114:TYR:HD2	3:C:116:LYS:HE3	1.79	0.46
5:F:114:GLU:HG3	5:F:119:ARG:HH21	1.79	0.46
1:A:278:THR:HA	1:A:281:HIS:CD2	2.51	0.46
1:A:675:THR:O	1:A:678:GLU:HG2	2.15	0.46
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.81	0.46
2:B:1112:GLN:HG3	2:B:1114:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:MET:HE1	3:C:243:VAL:HG23	1.96	0.46
8:J:36:LEU:HD11	8:J:50:ILE:HG21	1.97	0.46
2:B:364:ILE:HG23	2:B:365:THR:H	1.80	0.46
2:B:852:ARG:HD2	2:B:973:ILE:HA	1.96	0.46
1:A:80:HIS:ND1	2:B:1172:ILE:HA	2.31	0.46
1:A:265:LYS:HE3	1:A:316:GLN:HA	1.98	0.46
1:A:588:LEU:H	1:A:607:ILE:HB	1.81	0.46
1:A:777:PHE:HA	1:A:783:THR:HG22	1.97	0.46
2:B:1208:MET:C	2:B:1211:ASN:H	2.24	0.46
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.97	0.46
4:E:116:ILE:HB	4:E:121:MET:SD	2.56	0.46
5:F:119:ARG:HA	5:F:122:MET:HE3	1.97	0.46
5:F:128:LYS:HD2	5:F:149:GLU:HA	1.98	0.46
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.98	0.46
2:B:46:GLN:HG2	2:B:545:ILE:HG12	1.96	0.46
2:B:338:GLY:HA2	2:B:339:THR:HA	1.53	0.46
2:B:915:THR:HA	2:B:937:ALA:H	1.80	0.46
7:I:25:LEU:HD13	7:I:43:VAL:HG22	1.98	0.46
1:A:380:VAL:HG12	1:A:428:TYR:HD1	1.80	0.46
2:B:348:ARG:HD3	2:B:351:TYR:HB2	1.97	0.46
2:B:552:MET:HA	2:B:555:ILE:HD12	1.98	0.46
1:A:11:LEU:HD12	2:B:1193:GLN:HG3	1.96	0.46
1:A:118:HIS:HB2	1:A:122:MET:HG2	1.98	0.46
2:B:854:LEU:HD23	2:B:971:THR:HA	1.97	0.46
2:B:1160:VAL:HG12	2:B:1196:ILE:HB	1.98	0.46
6:H:2:SER:HB3	6:H:62:SER:HB3	1.98	0.46
1:A:153:PRO:HD2	1:A:162:VAL:O	2.16	0.45
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	1.99	0.45
2:B:806:THR:H	2:B:809:MET:HE3	1.80	0.45
4:E:20:LYS:HB3	4:E:35:VAL:HG12	1.97	0.45
1:A:634:THR:HG22	1:A:639:PRO:HA	1.98	0.45
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.98	0.45
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.51	0.45
8:J:53:HIS:HE1	8:J:55:ASP:HB3	1.79	0.45
2:B:431:TYR:CD2	2:B:445:LYS:HG2	2.51	0.45
2:B:941:LEU:HG	2:B:945:GLU:HB2	1.99	0.45
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.45
2:B:1106:ARG:HH12	2:B:1109:GLY:H	1.64	0.45
1:A:532:ARG:HA	1:A:535:THR:HG22	1.98	0.45
1:A:1156:PRO:HA	1:A:1190:PRO:HA	1.98	0.45
7:I:28:GLU:HB2	7:I:35:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:HB3	10:L:40:LEU:HG	1.98	0.45
1:A:88:LYS:H	1:A:276:LEU:HD21	1.82	0.45
1:A:412:ARG:HH12	2:B:1108:ARG:HD2	1.81	0.45
1:A:858:ASN:ND2	1:A:862:ASN:HB2	2.30	0.45
3:C:235:VAL:HG11	8:J:6:ARG:HH22	1.81	0.45
3:C:252:GLN:HG3	9:K:95:ILE:HD11	1.98	0.45
4:E:62:ALA:HB3	4:E:78:LEU:HD22	1.98	0.45
8:J:21:TYR:HB2	8:J:39:LEU:HD22	1.98	0.45
1:A:575:LYS:HD2	6:H:120:GLY:HA3	1.99	0.45
4:E:158:SER:HA	4:E:161:LYS:HD3	1.98	0.45
2:B:104:GLU:HB2	2:B:120:ARG:HH22	1.81	0.45
5:F:94:LEU:HD22	5:F:125:LEU:HG	1.98	0.45
1:A:1030:ARG:O	1:A:1034:GLU:HB3	2.17	0.45
3:C:259:LEU:O	3:C:262:LEU:HG	2.17	0.45
4:E:95:THR:HA	4:E:98:ILE:HG12	1.99	0.45
1:A:878:ILE:HG12	1:A:957:PRO:HD3	1.99	0.45
1:A:1193:LEU:HB3	1:A:1240:CYS:SG	2.57	0.45
1:A:1210:GLY:HA2	1:A:1228:TRP:HD1	1.82	0.45
2:B:615:MET:HG3	2:B:626:ILE:HG23	1.98	0.45
9:K:62:LYS:O	9:K:71:PHE:HB2	2.17	0.45
1:A:900:ASP:HB3	1:A:903:ASN:HB3	1.99	0.44
1:A:934:LYS:O	1:A:938:LYS:HG2	2.17	0.44
2:B:416:LEU:HG	2:B:466:TRP:NE1	2.32	0.44
1:A:560:ILE:HB	6:H:79:TRP:H	1.82	0.44
1:A:666:ILE:O	1:A:670:ILE:HG12	2.17	0.44
2:B:744:HIS:HB3	2:B:747:MET:HG2	1.98	0.44
3:C:29:MET:HA	9:K:45:LEU:HD12	1.99	0.44
1:A:1329:THR:HB	1:A:1335:ILE:HD11	1.99	0.44
6:H:38:LEU:HD21	6:H:40:LEU:HB2	1.99	0.44
1:A:726:ARG:HH21	1:A:767:GLN:HB3	1.82	0.44
1:A:1199:ARG:HH12	1:A:1209:MET:H	1.66	0.44
2:B:344:LYS:HD3	2:B:344:LYS:HA	1.85	0.44
2:B:521:LEU:HD23	2:B:635:ARG:HD3	1.99	0.44
2:B:846:ILE:HD12	2:B:974:PRO:HG2	1.99	0.44
2:B:994:TYR:HB3	2:B:998:ASP:HB2	2.00	0.44
3:C:84:ARG:HD2	9:K:11:LEU:HD11	1.98	0.44
1:A:1001:ARG:CZ	5:F:83:PRO:HD3	2.47	0.44
1:A:1116:LEU:HD23	1:A:1311:VAL:HG12	2.00	0.44
1:A:114:LEU:HB2	1:A:145:LYS:O	2.18	0.44
1:A:593:GLU:OE2	1:A:603:ASN:HB3	2.16	0.44
1:A:834:THR:HB	1:A:1077:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HA	1:A:1039:LYS:HD3	2.00	0.44
1:A:35:ILE:HB	1:A:84:ILE:HA	2.00	0.44
2:B:245:GLU:HA	2:B:249:ARG:HG2	1.99	0.44
1:A:169:ASN:HB2	1:A:187:LYS:HD3	1.99	0.44
1:A:326:ARG:O	1:A:330:LYS:CB	2.62	0.44
1:A:866:PHE:CE2	4:E:210:SER:HA	2.53	0.44
1:A:1152:ILE:HG23	7:I:43:VAL:HB	1.99	0.44
1:A:1193:LEU:HD21	1:A:1264:GLU:HB2	2.00	0.44
2:B:286:PHE:HD1	2:B:291:ILE:HD13	1.82	0.44
3:C:71:PRO:HB2	3:C:237:SER:HB3	2.00	0.44
6:H:94:ASP:HB2	6:H:145:ARG:HE	1.83	0.44
1:A:506:ALA:HB3	1:A:509:LEU:HG	1.98	0.44
2:B:342:GLY:H	2:B:348:ARG:HB2	1.82	0.44
2:B:420:LEU:HD12	2:B:453:ILE:HD13	2.00	0.44
2:B:579:ARG:HA	2:B:589:VAL:HG12	2.00	0.44
2:B:899:ILE:HD11	2:B:903:VAL:HG11	1.99	0.44
6:H:111:LEU:HB3	6:H:126:GLU:OE1	2.17	0.44
7:I:100:PHE:HA	7:I:111:THR:HA	2.00	0.44
1:A:152:VAL:HB	1:A:153:PRO:HD3	1.99	0.43
1:A:532:ARG:NH2	1:A:745:GLN:HB3	2.33	0.43
2:B:130:VAL:HB	2:B:167:ILE:HG13	1.99	0.43
2:B:174:LEU:HG	2:B:202:TYR:CZ	2.53	0.43
2:B:273:LEU:HD13	2:B:280:ILE:HD13	1.99	0.43
7:I:92:ARG:HB3	7:I:95:THR:HG23	2.00	0.43
1:A:43:GLU:OE1	1:A:44:THR:HG23	2.19	0.43
1:A:402:ALA:HB3	1:A:415:LEU:HD12	2.00	0.43
1:A:1313:LEU:HD23	1:A:1313:LEU:HA	1.83	0.43
3:C:76:ASP:HB3	3:C:79:GLN:HB2	1.99	0.43
1:A:308:ILE:HA	1:A:326:ARG:HH21	1.82	0.43
1:A:862:ASN:HA	4:E:174:GLN:O	2.19	0.43
2:B:881:ASN:O	2:B:933:SER:HB2	2.18	0.43
4:E:161:LYS:NZ	4:E:194:GLU:HA	2.33	0.43
5:F:81:THR:HB	5:F:136:ARG:HH11	1.84	0.43
6:H:100:THR:HG23	6:H:138:GLU:HB2	2.00	0.43
1:A:445:ASN:ND2	1:A:455:MET:HG3	2.33	0.43
2:B:442:PHE:H	2:B:445:LYS:HE2	1.84	0.43
2:B:1132:GLU:HA	2:B:1135:ARG:NE	2.33	0.43
3:C:206:ASN:HA	3:C:209:TYR:HD2	1.83	0.43
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.00	0.43
1:A:202:LEU:HD12	1:A:203:SER:H	1.83	0.43
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:903:VAL:HA	10:L:63:ARG:HH22	1.83	0.43
2:B:1207:LEU:HB3	2:B:1213:THR:HB	2.01	0.43
1:A:53:LEU:HD21	1:A:267:ALA:HA	1.99	0.43
1:A:114:LEU:HD13	1:A:146:MET:HA	2.01	0.43
1:A:242:PRO:HA	1:A:303:TYR:OH	2.19	0.43
1:A:406:ILE:HB	1:A:431:LYS:HB3	2.01	0.43
1:A:440:ASP:O	1:A:460:VAL:HG23	2.18	0.43
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.84	0.43
2:B:1080:LYS:HG3	3:C:180:TYR:CZ	2.53	0.43
1:A:207:ILE:HD13	1:A:210:ILE:HD12	2.00	0.43
1:A:1170:ILE:HD11	1:A:1239:ARG:HD3	1.99	0.43
1:A:1259:MET:HA	1:A:1262:LYS:HE3	2.00	0.43
2:B:878:GLN:HG2	2:B:881:ASN:HB2	2.00	0.43
3:C:12:GLU:HG3	3:C:19:ASP:HB2	2.00	0.43
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.84	0.43
1:A:733:ALA:HA	1:A:736:ASN:ND2	2.33	0.43
1:A:849:MET:O	1:A:856:THR:HA	2.19	0.43
1:A:873:MET:HE2	1:A:873:MET:HB2	1.95	0.43
2:B:281:PRO:HD2	2:B:284:ILE:HD12	2.00	0.43
4:E:144:ILE:HG22	4:E:150:VAL:HG21	2.00	0.43
7:I:83:ASN:HA	7:I:103:CYS:HA	1.99	0.43
1:A:108:MET:HE1	1:A:185:TRP:CD1	2.53	0.43
1:A:453:MET:HG2	1:A:520:CYS:HB3	2.01	0.43
1:A:540:PHE:CE2	6:H:22:LYS:HD2	2.53	0.43
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.84	0.43
2:B:797:TYR:CZ	3:C:62:PHE:HB2	2.54	0.43
4:E:13:TRP:HB2	4:E:42:PHE:CD2	2.54	0.43
6:H:28:ALA:HB3	6:H:38:LEU:HD22	2.00	0.43
6:H:93:TYR:HD2	6:H:143:LEU:HD13	1.84	0.43
1:A:881:GLN:HB3	1:A:956:LEU:HB2	2.01	0.43
2:B:901:PRO:HD2	10:L:59:ALA:O	2.18	0.43
4:E:65:THR:O	4:E:69:ILE:HD12	2.18	0.43
1:A:28:ARG:HD3	1:A:83:HIS:HE1	1.84	0.42
1:A:107:CYS:SG	1:A:110:CYS:HB3	2.59	0.42
1:A:597:LEU:HG	6:H:103:LYS:HG2	2.00	0.42
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.84	0.42
2:B:1104:HIS:HB3	2:B:1128:LEU:HD11	2.01	0.42
1:A:216:VAL:HA	1:A:219:PHE:CD2	2.54	0.42
1:A:913:LEU:HD22	1:A:982:THR:HA	2.00	0.42
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.53	0.42
5:F:74:ILE:HG13	5:F:75:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:50:LEU:HD13	9:K:90:ALA:HB2	2.01	0.42
1:A:795:GLU:HG3	1:A:799:PHE:HD2	1.85	0.42
2:B:1065:GLN:HE22	3:C:200:GLU:HB3	1.84	0.42
3:C:11:ARG:CZ	3:C:19:ASP:HB3	2.49	0.42
1:A:114:LEU:HD23	1:A:171:GLN:OE1	2.20	0.42
1:A:219:PHE:CE1	1:A:231:PRO:HD2	2.54	0.42
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.18	0.42
1:A:981:LEU:HB3	1:A:1039:LYS:HA	2.02	0.42
2:B:131:ASP:HA	2:B:164:LYS:H	1.82	0.42
2:B:216:GLU:HB3	2:B:500:THR:HB	2.00	0.42
10:L:28:LYS:H	10:L:39:SER:HA	1.85	0.42
1:A:90:VAL:HG23	1:A:236:LEU:HB2	2.01	0.42
1:A:913:LEU:HD23	1:A:1032:LEU:HD21	2.02	0.42
1:A:1153:TYR:HB2	1:A:1192:LEU:HG	2.02	0.42
2:B:401:PHE:H	2:B:517:THR:HG21	1.84	0.42
2:B:840:ILE:HG12	2:B:992:ILE:HG22	2.00	0.42
2:B:1158:PHE:CD2	2:B:1198:TYR:HB2	2.55	0.42
1:A:847:ASP:HB2	1:A:859:SER:HB2	2.02	0.42
1:A:930:ASP:O	1:A:934:LYS:HG2	2.19	0.42
1:A:940:ARG:O	1:A:944:ARG:HG2	2.20	0.42
1:A:1155:ASP:HB3	1:A:1241:ARG:HH22	1.84	0.42
2:B:865:LYS:HD3	2:B:869:SER:HA	2.02	0.42
2:B:983:ARG:HD3	2:B:1091:TYR:HD2	1.83	0.42
2:B:1165:ILE:HG23	2:B:1217:TYR:HE1	1.83	0.42
3:C:11:ARG:NH2	3:C:230:MET:H	2.18	0.42
5:F:97:ARG:HD2	5:F:97:ARG:HA	1.85	0.42
6:H:63:LEU:HG	6:H:89:LEU:HG	2.01	0.42
9:K:19:LEU:HD23	9:K:19:LEU:H	1.85	0.42
1:A:59:GLY:CA	1:A:80:HIS:HD2	2.32	0.42
1:A:424:ILE:HG22	1:A:426:LEU:HG	2.01	0.42
1:A:858:ASN:HD22	1:A:864:ILE:HD11	1.85	0.42
1:A:993:LEU:O	1:A:997:LEU:HG	2.19	0.42
2:B:99:LYS:HE3	2:B:100:PRO:HD2	2.01	0.42
2:B:791:THR:HA	2:B:858:SER:H	1.85	0.42
1:A:60:SER:HB2	1:A:64:ASN:HD22	1.85	0.42
1:A:185:TRP:CH2	1:A:202:LEU:HD13	2.55	0.42
1:A:598:LEU:HD11	6:H:124:ARG:HD2	2.02	0.42
1:A:756:ILE:O	1:A:760:GLN:HG2	2.20	0.42
1:A:1115:SER:O	1:A:1330:ASN:HB2	2.20	0.42
1:A:1398:MET:HB3	1:A:1425:SER:HB2	2.02	0.42
2:B:25:ILE:HD12	2:B:655:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:THR:O	2:B:684:LEU:HG	2.20	0.42
1:A:41:MET:HG3	1:A:42:ASP:H	1.85	0.42
1:A:109:HIS:H	1:A:210:ILE:HG12	1.84	0.42
1:A:714:PHE:O	1:A:718:VAL:HG22	2.20	0.42
1:A:1192:LEU:HD22	1:A:1239:ARG:HE	1.84	0.42
1:A:1256:GLU:HA	1:A:1259:MET:HE2	2.02	0.42
1:A:1313:LEU:HB3	1:A:1314:SER:H	1.59	0.42
1:A:179:LEU:HG	1:A:298:PHE:HA	2.01	0.42
1:A:228:PHE:HE1	1:A:1416:ALA:HB1	1.85	0.42
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.20	0.42
1:A:1341:ILE:HG21	4:E:212:ARG:NH1	2.35	0.42
2:B:66:ASP:HB2	2:B:421:PHE:CE2	2.55	0.42
3:C:80:LEU:HD23	3:C:80:LEU:HA	1.94	0.42
3:C:248:ILE:HG21	9:K:102:LYS:HB3	2.02	0.42
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.79	0.41
1:A:247:ARG:HD2	1:A:263:THR:HA	2.02	0.41
1:A:269:ILE:HG13	1:A:299:HIS:HB3	2.01	0.41
4:E:43:LYS:O	4:E:47:CYS:CB	2.61	0.41
5:F:107:VAL:HG22	5:F:109:VAL:H	1.85	0.41
6:H:129:TYR:CZ	6:H:130:ARG:HD2	2.55	0.41
1:A:473:SER:HB2	1:A:521:MET:HE1	2.01	0.41
1:A:1224:LEU:HB3	1:A:1242:VAL:HA	2.01	0.41
2:B:552:MET:HE3	2:B:552:MET:HB3	1.83	0.41
2:B:636:PRO:HA	2:B:691:GLU:O	2.20	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.02	0.41
3:C:92:CYS:SG	3:C:94:LYS:HG2	2.60	0.41
5:F:70:LYS:C	5:F:72:LYS:H	2.27	0.41
6:H:35:GLN:HG3	6:H:127:GLY:HA2	2.02	0.41
6:H:93:TYR:HB3	6:H:145:ARG:CZ	2.50	0.41
1:A:304:MET:O	1:A:325:ILE:HG21	2.21	0.41
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.20	0.41
1:A:1282:VAL:HG12	1:A:1308:THR:HB	2.00	0.41
2:B:827:ILE:HG23	2:B:1012:ILE:HG23	2.01	0.41
2:B:242:SER:HB2	2:B:363:HIS:HB3	2.02	0.41
2:B:756:ILE:HB	2:B:759:PRO:HG3	2.02	0.41
3:C:74:SER:HB3	3:C:77:ILE:HB	2.02	0.41
3:C:258:ILE:HD12	3:C:258:ILE:HA	1.89	0.41
1:A:503:GLN:HE22	5:F:118:LEU:HD11	1.86	0.41
2:B:662:MET:HE2	2:B:662:MET:HB2	1.87	0.41
2:B:705:MET:HE2	2:B:745:PRO:HB3	2.02	0.41
2:B:1164:GLY:HA2	2:B:1192:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:24:LEU:O	8:J:28:ASP:HB3	2.20	0.41
9:K:55:LYS:HB3	9:K:55:LYS:HE3	1.86	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD13	2.03	0.41
1:A:1408:ILE:HD12	1:A:1408:ILE:HA	1.93	0.41
2:B:74:LEU:HD21	2:B:143:PRO:HA	2.03	0.41
2:B:259:TYR:CE1	2:B:270:LYS:HB2	2.56	0.41
4:E:16:PHE:CZ	4:E:20:LYS:HD2	2.56	0.41
4:E:55:ARG:HA	4:E:58:MET:HE3	2.02	0.41
4:E:75:MET:HE3	4:E:75:MET:HB2	1.90	0.41
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.03	0.41
1:A:182:VAL:HA	1:A:201:VAL:HA	2.03	0.41
1:A:325:ILE:HG23	2:B:1206:GLU:HB3	2.02	0.41
1:A:740:LEU:HG	3:C:192:TRP:CD1	2.56	0.41
1:A:924:LYS:HB2	1:A:924:LYS:HE2	1.88	0.41
1:A:1142:THR:HG23	1:A:1145:SER:H	1.85	0.41
1:A:1155:ASP:HB3	1:A:1192:LEU:HD23	2.03	0.41
1:A:1373:ASP:O	1:A:1377:THR:HB	2.20	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD3	1.95	0.41
2:B:757:PRO:HG3	2:B:983:ARG:NH2	2.36	0.41
2:B:780:VAL:HG12	2:B:795:ILE:HD12	2.03	0.41
3:C:47:ASP:HB3	3:C:160:LYS:HD2	2.03	0.41
3:C:261:ALA:HB2	9:K:18:LYS:HD2	2.03	0.41
7:I:88:SER:HA	7:I:100:PHE:HE2	1.85	0.41
1:A:105:CYS:O	1:A:113:LEU:HD13	2.21	0.41
1:A:242:PRO:HG2	1:A:266:LEU:HD22	2.01	0.41
1:A:960:ILE:HD12	1:A:1025:ARG:HG3	2.02	0.41
1:A:1000:LEU:H	1:A:1011:GLN:HG2	1.85	0.41
1:A:1314:SER:O	1:A:1318:THR:HG23	2.20	0.41
2:B:274:PRO:HA	2:B:275:TYR:HA	1.71	0.41
2:B:857:ARG:HB3	2:B:968:VAL:HG22	2.03	0.41
6:H:97:MET:HG2	6:H:118:PHE:HB3	2.02	0.41
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.34	0.41
7:I:59:VAL:HG22	7:I:60:GLN:H	1.86	0.41
7:I:69:PRO:HB2	7:I:85:PHE:CZ	2.55	0.41
1:A:524:VAL:HB	1:A:528:LEU:HB2	2.02	0.41
1:A:1153:TYR:CG	1:A:1163:ILE:HD11	2.56	0.41
2:B:217:ARG:HD3	2:B:407:ASP:OD2	2.21	0.41
6:H:102:TYR:CZ	6:H:115:TYR:HB3	2.56	0.41
9:K:42:LEU:HA	9:K:42:LEU:HD23	1.86	0.41
1:A:91:PHE:HD2	1:A:96:ILE:HG22	1.86	0.40
1:A:407:ARG:HG3	1:A:430:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HG21	1:A:577:ILE:HG13	2.02	0.40
1:A:620:LYS:HG3	1:A:621:THR:HG23	2.03	0.40
1:A:1119:TYR:HD1	1:A:1327:ILE:HA	1.86	0.40
2:B:877:PRO:HD2	2:B:890:TYR:HD2	1.85	0.40
3:C:262:LEU:HA	9:K:19:LEU:HD21	2.03	0.40
4:E:171:LYS:C	4:E:173:SER:H	2.29	0.40
1:A:81:PHE:HD2	2:B:1170:THR:HG22	1.85	0.40
1:A:112:LYS:HB3	1:A:165:GLY:HA3	2.02	0.40
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	2.02	0.40
1:A:1397:LEU:HD23	1:A:1409:LEU:HD11	2.02	0.40
2:B:911:ILE:HD11	2:B:941:LEU:HB2	2.02	0.40
3:C:41:ILE:HD12	3:C:42:PRO:HD2	2.03	0.40
3:C:128:ASN:HA	3:C:131:HIS:HE1	1.86	0.40
7:I:15:TYR:HA	7:I:16:PRO:HD3	1.96	0.40
8:J:53:HIS:CE1	8:J:55:ASP:HB3	2.57	0.40
9:K:47:ARG:HH21	9:K:61:TYR:HE1	1.69	0.40
1:A:172:PRO:HB2	1:A:184:SER:HB3	2.03	0.40
1:A:354:SER:HB2	1:A:469:ARG:HD2	2.03	0.40
1:A:366:VAL:H	1:A:462:VAL:HA	1.86	0.40
1:A:461:LYS:HA	1:A:461:LYS:HD2	1.88	0.40
1:A:707:GLY:HA3	1:A:1281:ARG:CZ	2.51	0.40
1:A:816:HIS:CD2	2:B:764:SER:H	2.39	0.40
1:A:877:HIS:CG	1:A:1056:SER:HA	2.56	0.40
1:A:993:LEU:HD13	1:A:1046:LEU:HB3	2.03	0.40
1:A:1259:MET:HG3	1:A:1262:LYS:HE3	2.03	0.40
2:B:136:THR:HG23	2:B:159:ASP:HB3	2.04	0.40
3:C:46:ILE:HD11	3:C:67:LEU:HB3	2.03	0.40
7:I:63:GLY:HA2	7:I:68:LEU:HD23	2.02	0.40
1:A:61:ILE:HD12	1:A:249:SER:HB2	2.03	0.40
1:A:667:GLY:HA2	2:B:1067:ARG:HD3	2.03	0.40
1:A:873:MET:HG3	1:A:1056:SER:O	2.21	0.40
1:A:884:ASP:CG	1:A:1025:ARG:HH22	2.29	0.40
2:B:277:LYS:HD2	2:B:337:ARG:NE	2.36	0.40
2:B:1082:MET:HE2	2:B:1082:MET:HB2	1.81	0.40
4:E:161:LYS:HE3	4:E:195:VAL:HG23	2.02	0.40
9:K:21:ILE:HG22	9:K:33:ILE:HD12	2.04	0.40
1:A:342:GLY:H	2:B:1135:ARG:NH1	2.19	0.40
1:A:440:ASP:H	1:A:460:VAL:H	1.69	0.40
1:A:441:PRO:HD2	1:A:498:ARG:HH21	1.86	0.40
1:A:762:SER:HA	1:A:805:LEU:HG	2.04	0.40
2:B:72:GLU:HB3	2:B:87:LYS:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:SER:OG	2:B:567:GLU:HG3	2.21	0.40
4:E:110:PHE:HE1	4:E:112:TYR:HB3	1.87	0.40
6:H:94:ASP:HB2	6:H:144:ILE:O	2.22	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	1409/1733 (81%)	1244 (88%)	158 (11%)	7 (0%)	24	63
2	B	1128/1224 (92%)	1000 (89%)	123 (11%)	5 (0%)	30	67
3	C	263/318 (83%)	245 (93%)	18 (7%)	0	100	100
4	E	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
5	F	85/155 (55%)	79 (93%)	6 (7%)	0	100	100
6	H	132/146 (90%)	115 (87%)	17 (13%)	0	100	100
7	I	112/122 (92%)	107 (96%)	5 (4%)	0	100	100
8	J	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
9	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	36 (86%)	6 (14%)	0	100	100
All	All	3560/4173 (85%)	3193 (90%)	355 (10%)	12 (0%)	37	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	525	GLN
1	A	1107	VAL
2	B	364	ILE

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Mol	Chain	Res	Type
1	A	93	VAL
2	B	479	VAL
1	A	142	CYS
1	A	852	TYR
2	B	82	ASP
2	B	371	GLU
1	A	958	VAL
2	B	84	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	1234/1520 (81%)	1234 (100%)	0	100	100
2	B	991/1061 (93%)	991 (100%)	0	100	100
3	C	233/274 (85%)	233 (100%)	0	100	100
4	E	196/197 (100%)	196 (100%)	0	100	100
5	F	77/137 (56%)	77 (100%)	0	100	100
6	H	119/128 (93%)	119 (100%)	0	100	100
7	I	108/116 (93%)	108 (100%)	0	100	100
8	J	61/65 (94%)	61 (100%)	0	100	100
9	K	99/102 (97%)	99 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3157/3657 (86%)	3157 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	80	HIS
1	A	390	GLN
1	A	394	ASN
1	A	445	ASN
1	A	503	GLN
1	A	525	GLN
1	A	611	GLN
1	A	741	ASN
1	A	862	ASN
1	A	877	HIS
1	A	935	GLN
1	A	965	GLN
1	A	969	GLN
1	A	1033	GLN
1	A	1052	GLN
1	A	1203	ASN
1	A	1218	GLN
1	A	1222	ASN
1	A	1278	ASN
2	B	103	ASN
2	B	350	GLN
2	B	573	GLN
2	B	583	ASN
2	B	686	ASN
2	B	767	ASN
2	B	881	ASN
2	B	986	GLN
2	B	1176	ASN
3	C	24	ASN
3	C	242	GLN
4	E	106	GLN
6	H	52	GLN
6	H	134	ASN
7	I	114	GLN
9	K	92	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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.

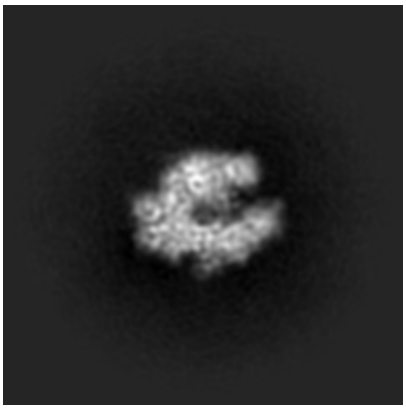
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77811. These allow visual inspection of the internal detail of the map and identification of artifacts.

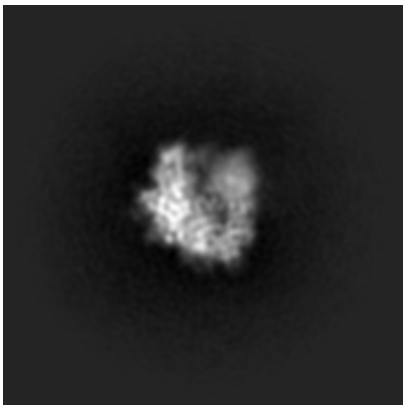
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

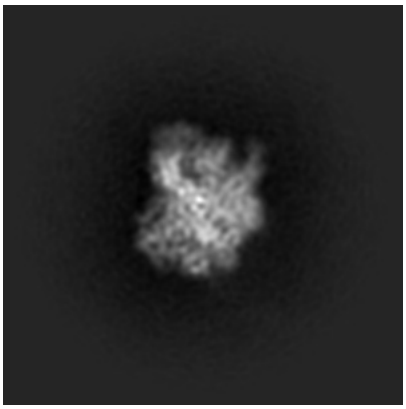
6.1.1 Primary map



X

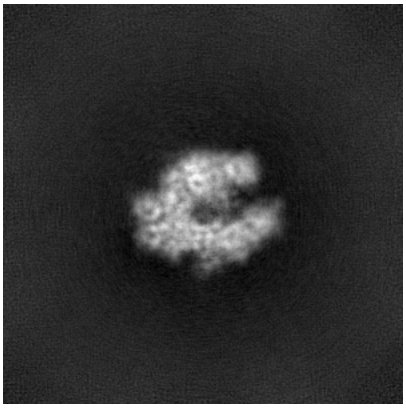


Y

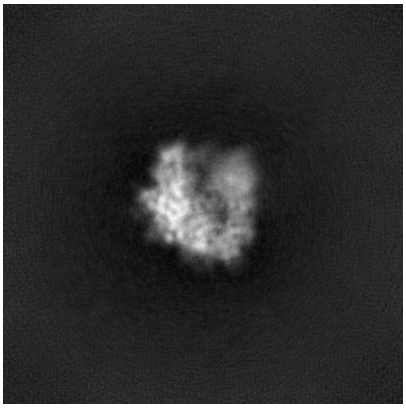


Z

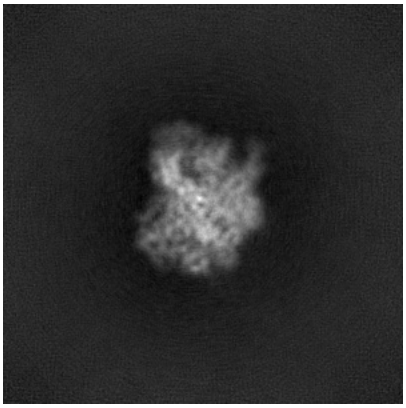
6.1.2 Raw map



X



Y



Z

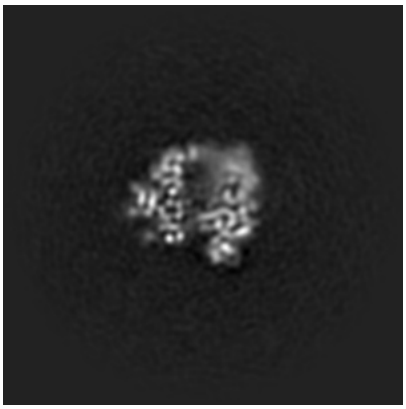
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

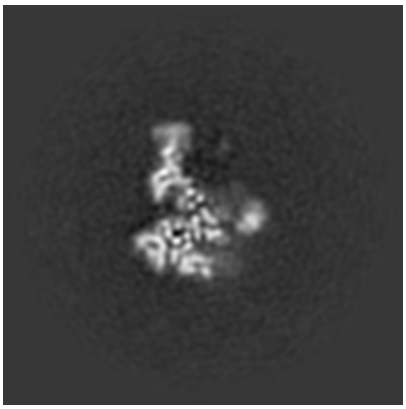
6.2.1 Primary map



X Index: 200

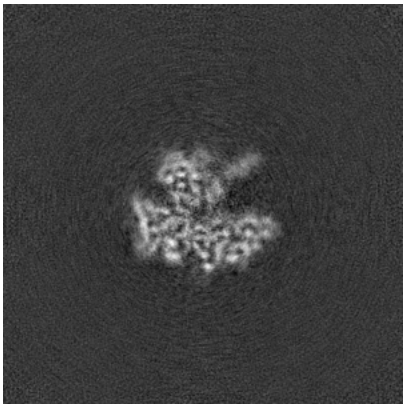


Y Index: 200

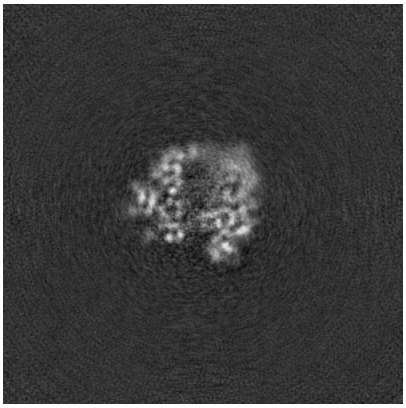


Z Index: 200

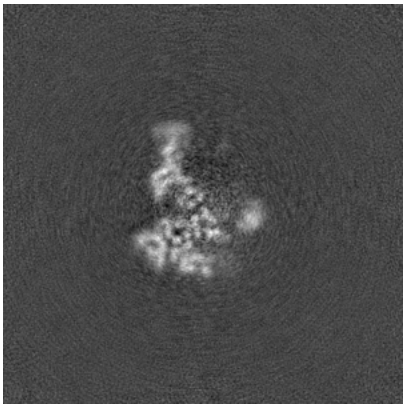
6.2.2 Raw map



X Index: 200



Y Index: 200

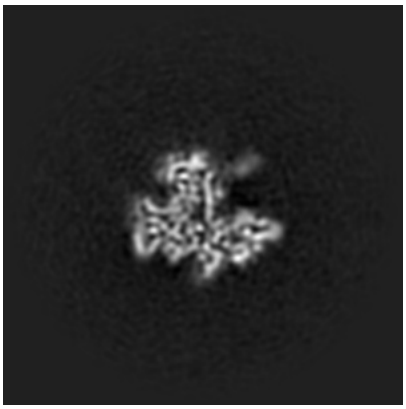


Z Index: 200

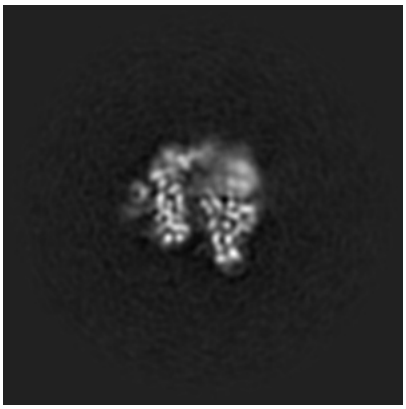
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

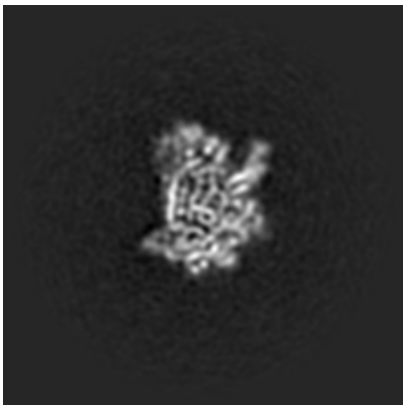
6.3.1 Primary map



X Index: 196

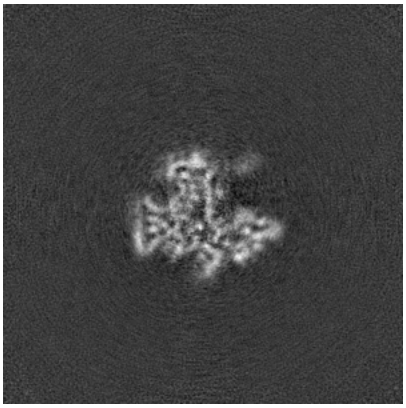


Y Index: 193

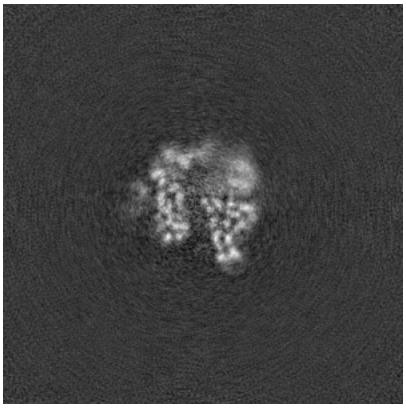


Z Index: 176

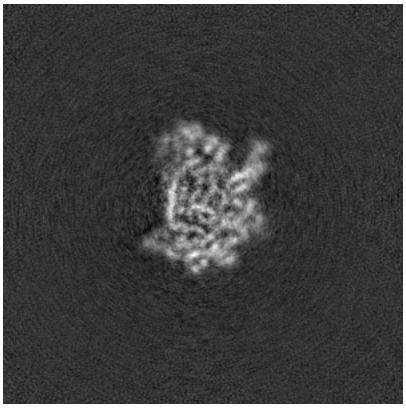
6.3.2 Raw map



X Index: 195



Y Index: 192

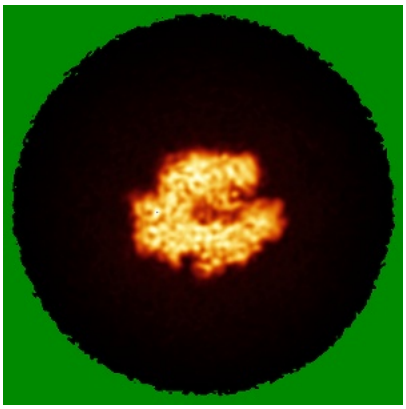


Z Index: 176

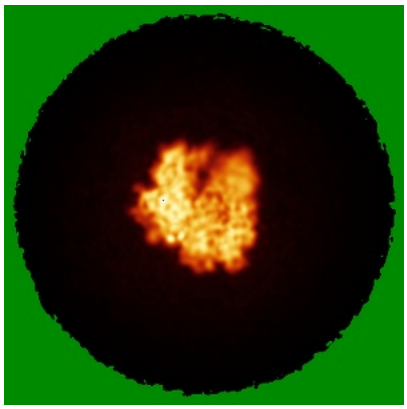
The images above show the largest variance slices of the map in three orthogonal directions.

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

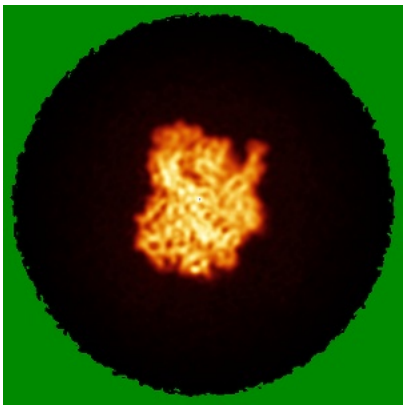
6.4.1 Primary map



X

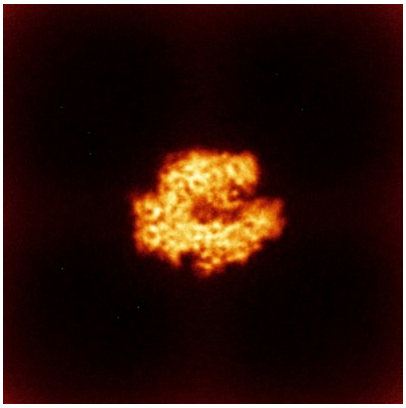


Y

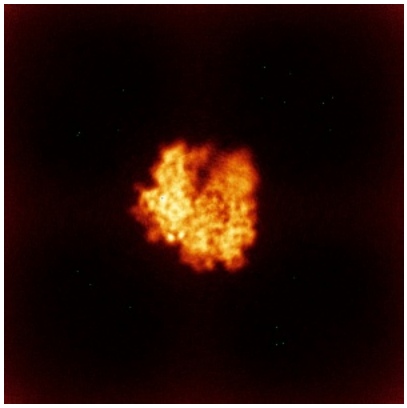


Z

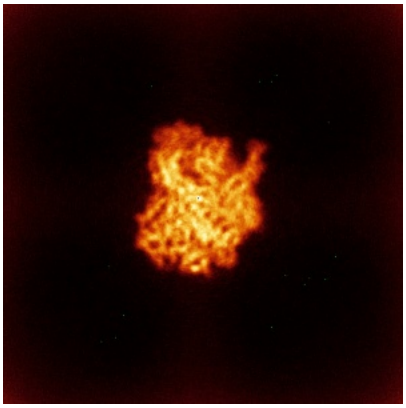
6.4.2 Raw map



X



Y

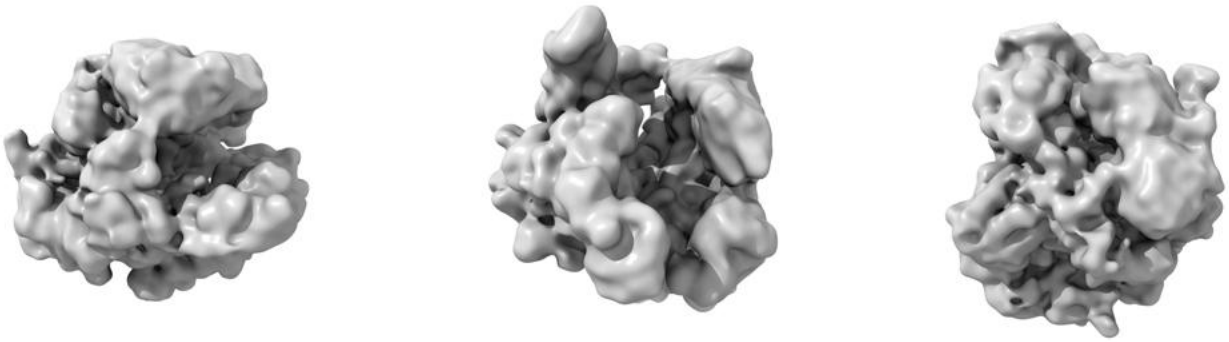


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

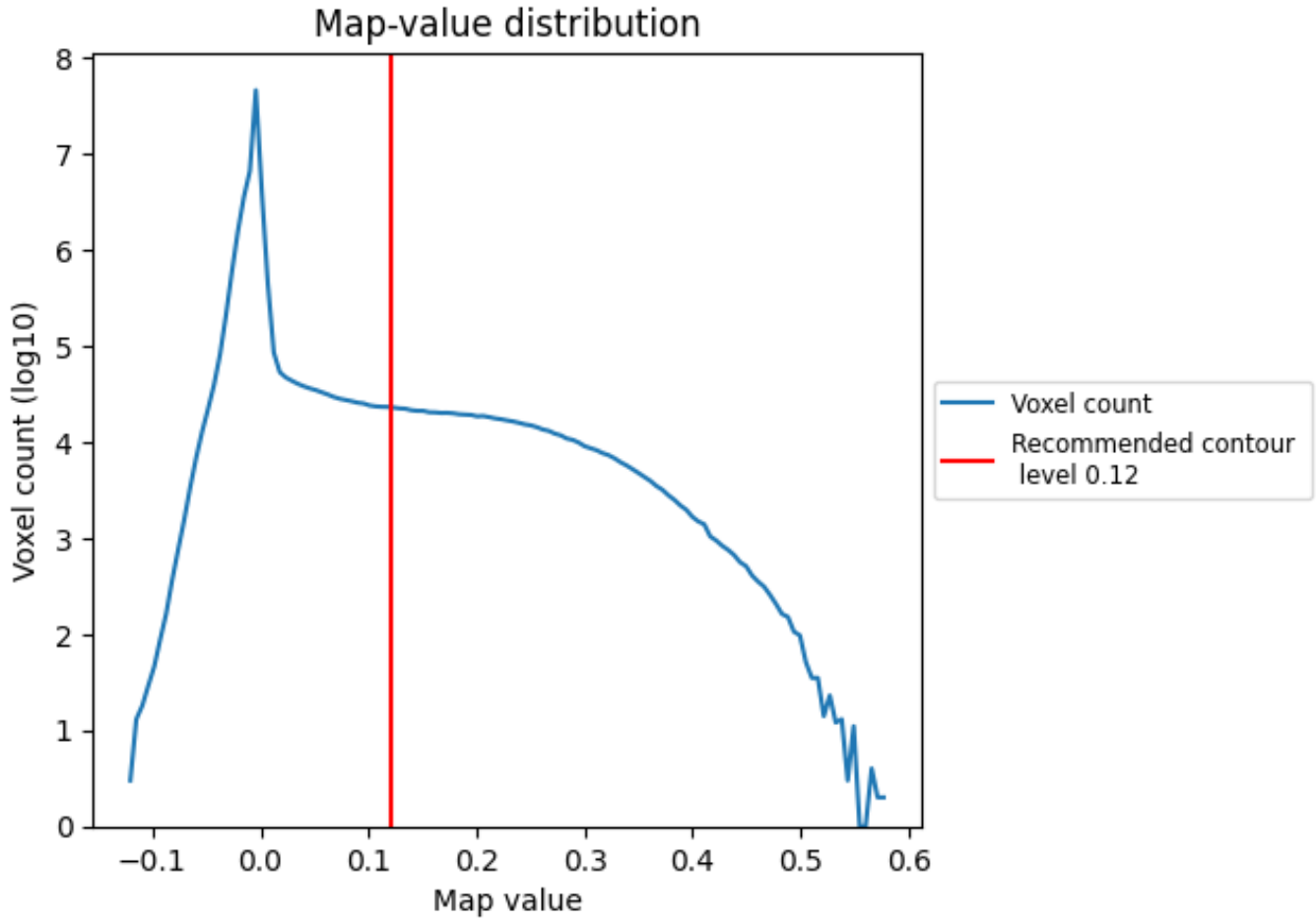
6.6 Mask visualisation (i)

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

7 Map analysis

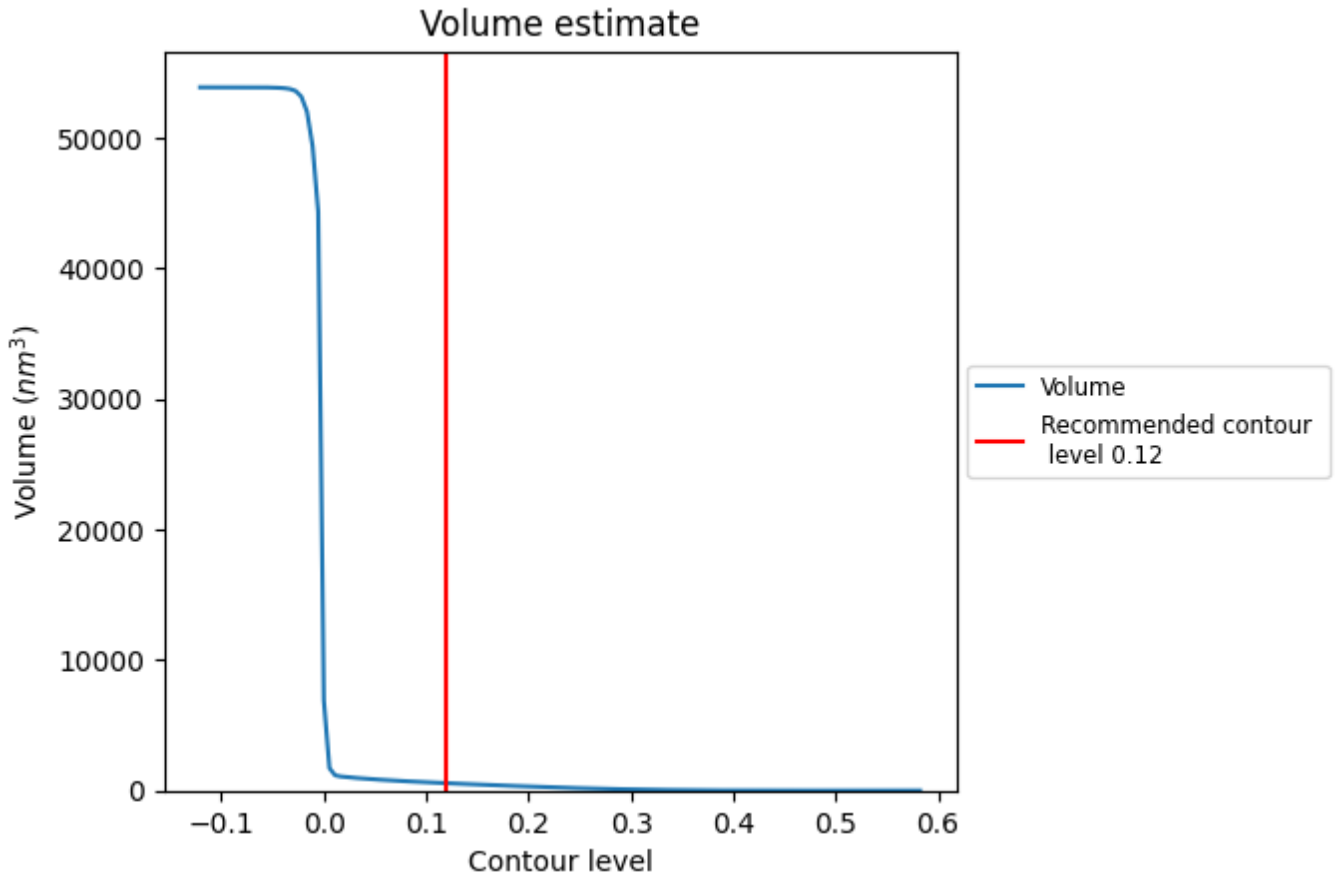
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

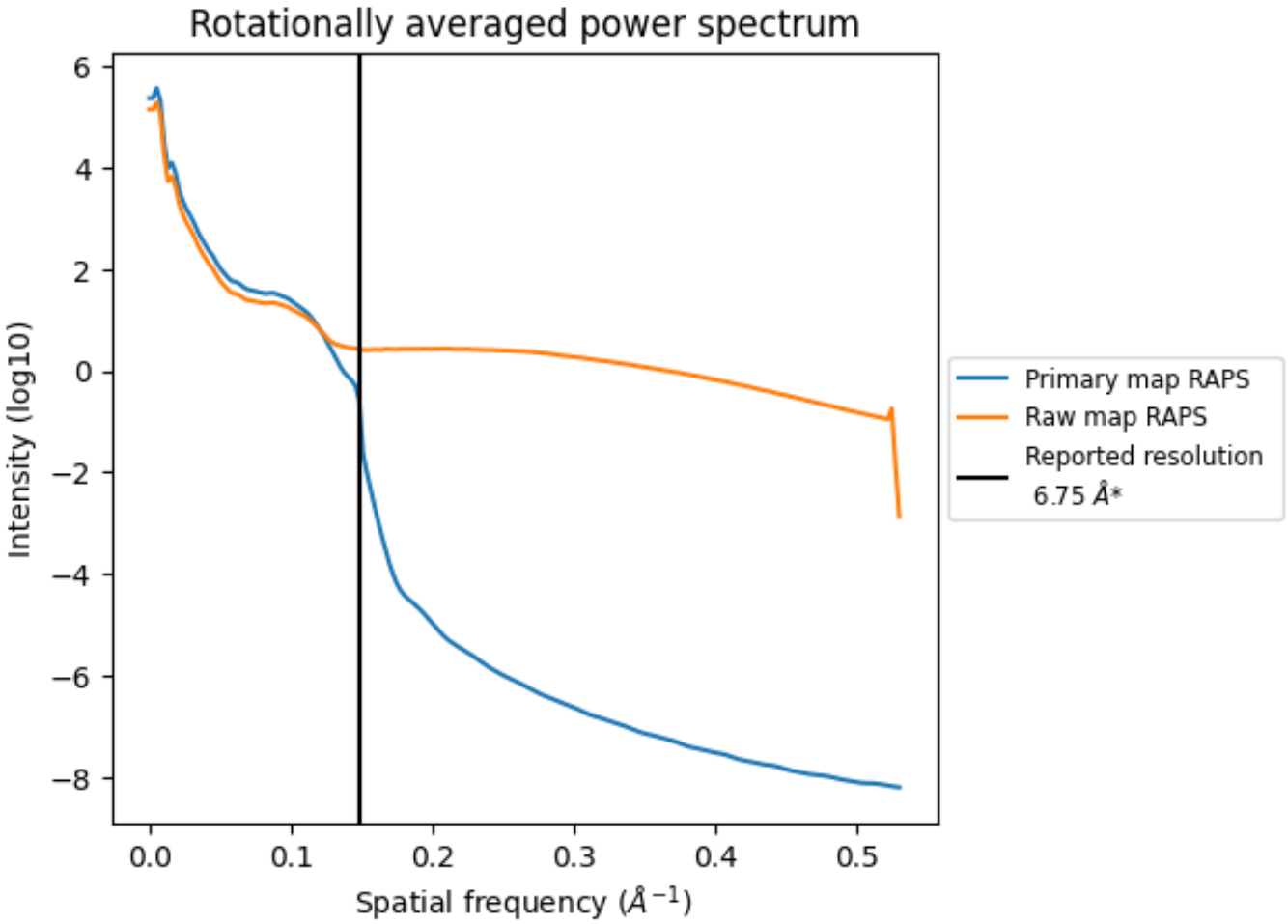
7.2 Volume estimate



The volume at the recommended contour level is 565 nm^3; this corresponds to an approximate mass of 510 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)

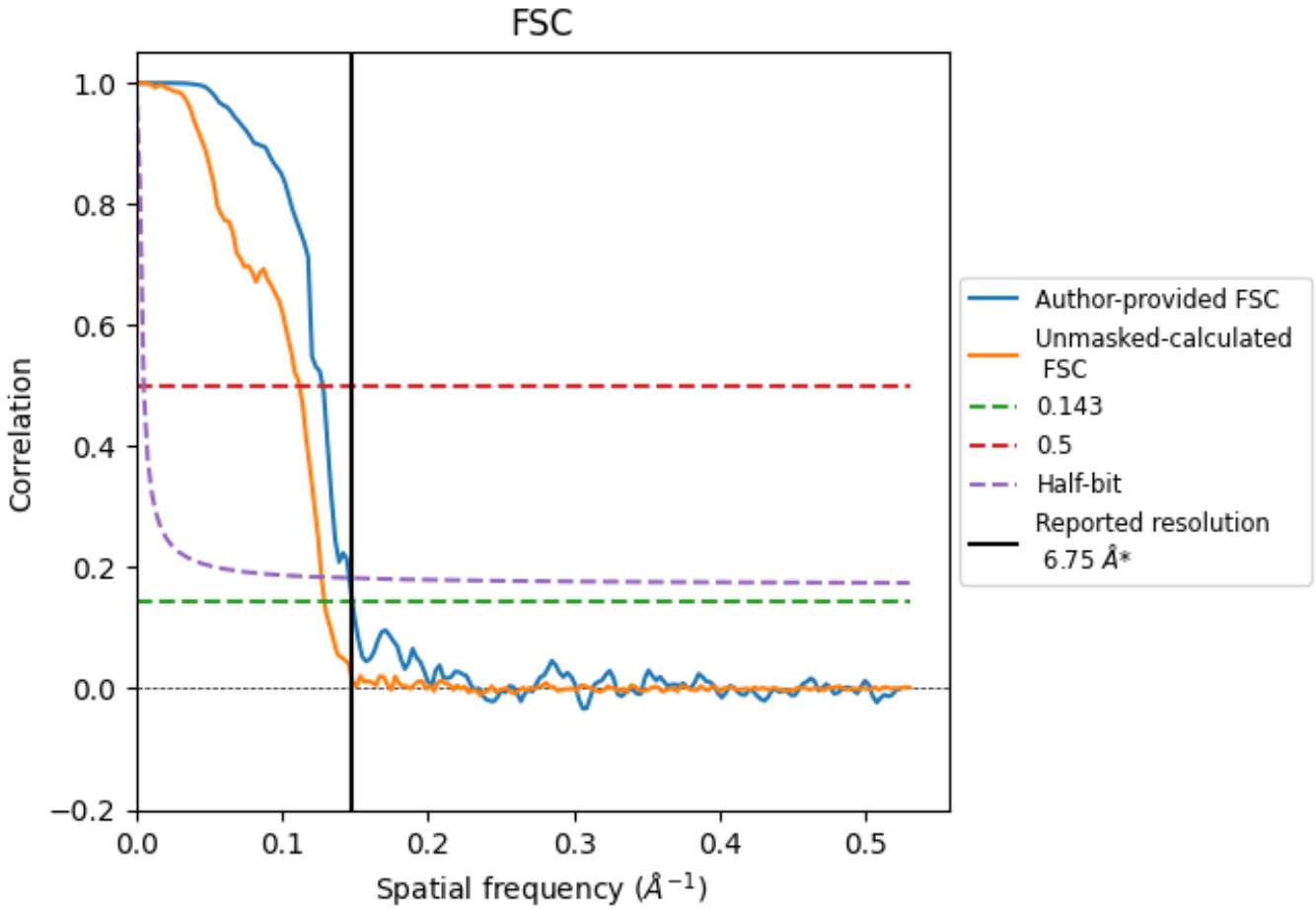


*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

8.2 Resolution estimates (i)

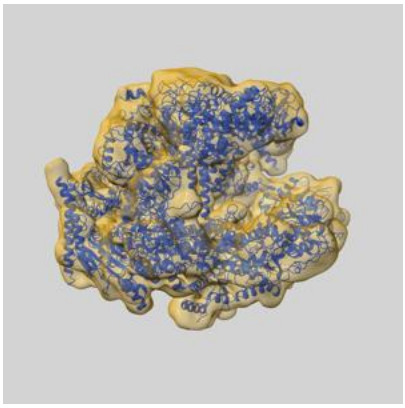
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.75	-	-
Author-provided FSC curve	6.75	7.82	6.84
Unmasked-calculated*	7.75	8.94	7.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.75 differs from the reported value 6.75 by more than 10 %

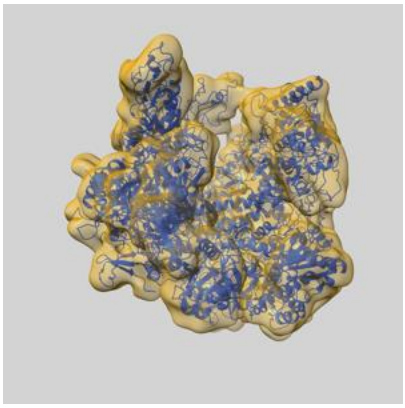
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77811 and PDB model 36RS. Per-residue inclusion information can be found in section 3 on page 6.

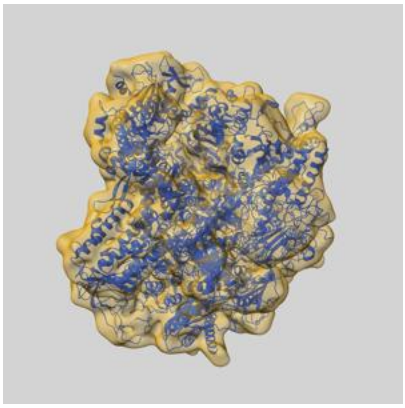
9.1 Map-model overlay



X



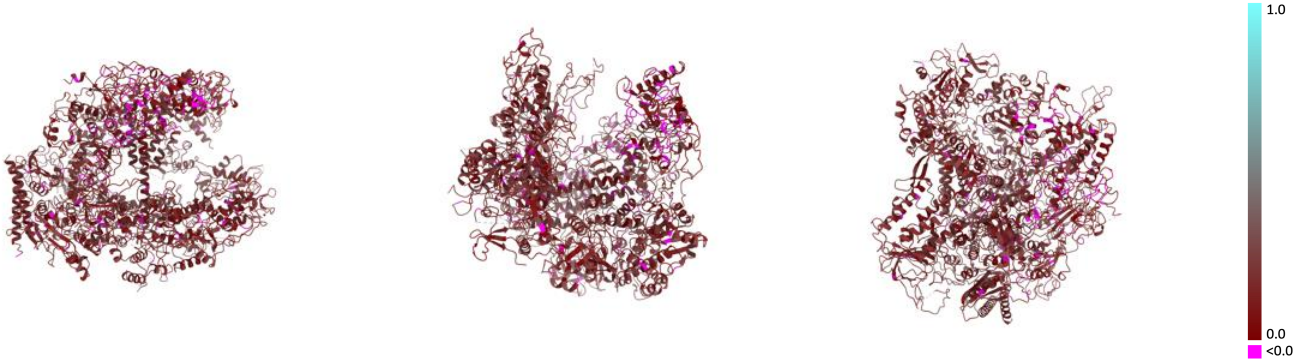
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

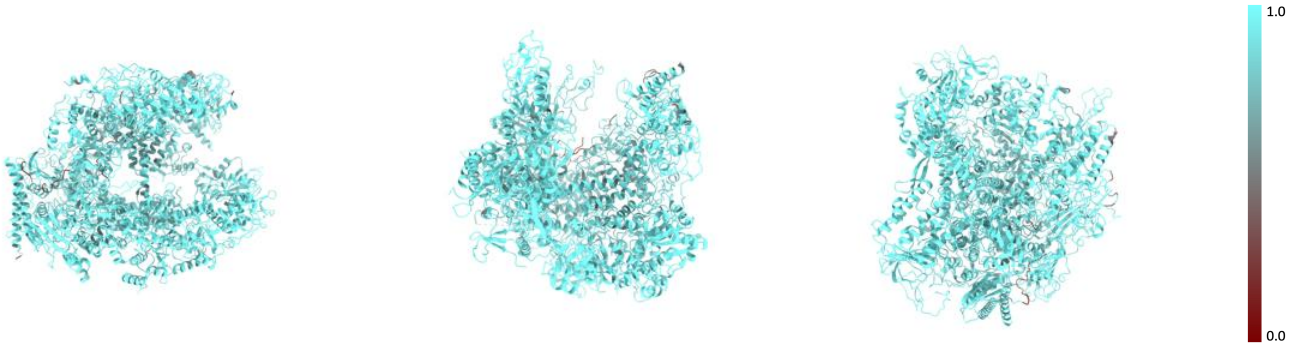
9.2 Q-score mapped to coordinate model (i)



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.

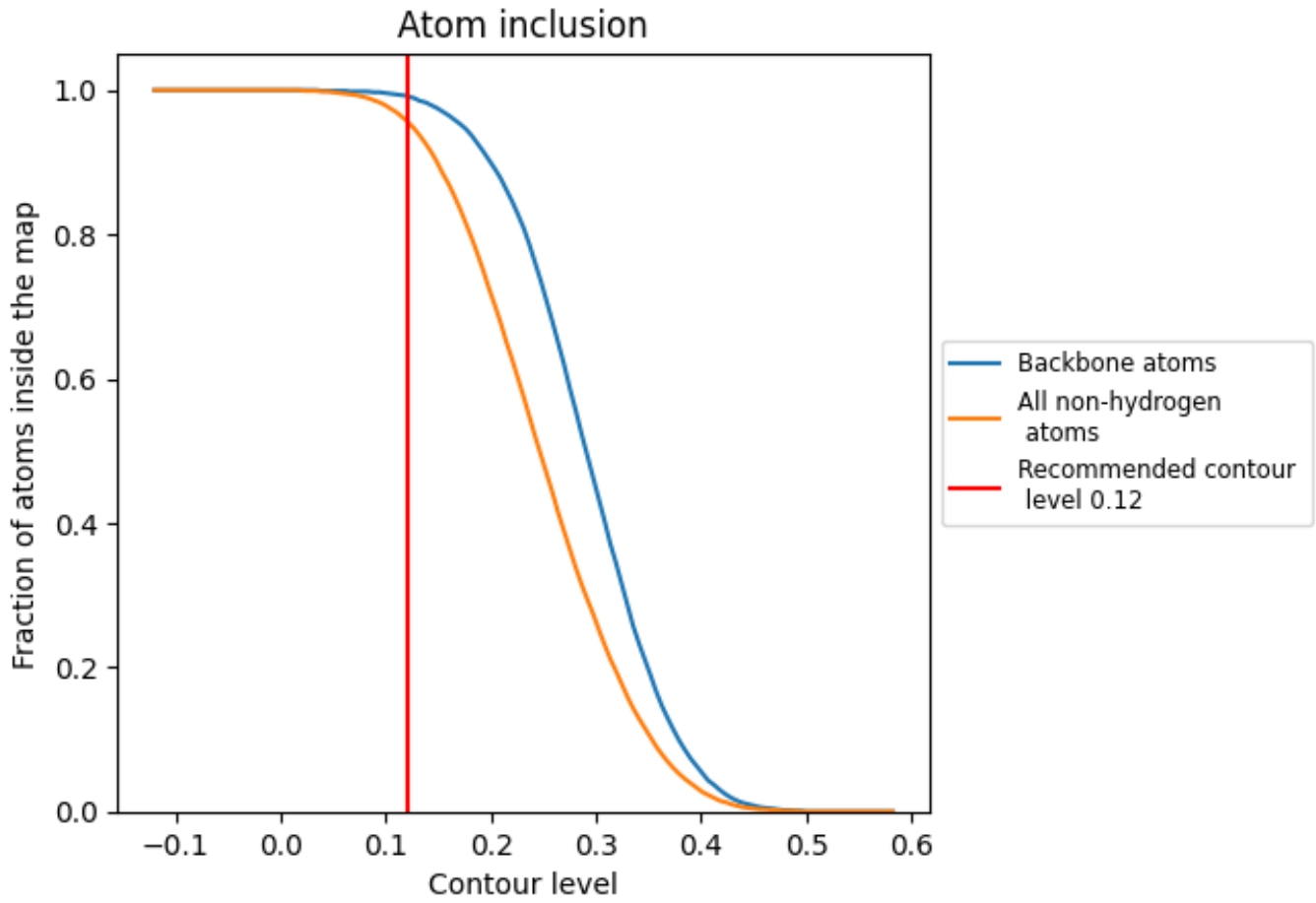
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 99% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.1610
A	0.9580	0.1510
B	0.9550	0.1620
C	0.9630	0.1830
E	0.9780	0.1720
F	0.9670	0.1850
H	0.9760	0.1890
I	0.9740	0.1610
J	0.9620	0.1590
K	0.8570	0.1610
L	0.9850	0.1600

