Full wwPDB EM Validation Report (i)

Aug 26, 2021 – 06:25 am BST

PDB ID	:	7OKX
EMDB ID	:	EMD-12969
Title	:	Structure of active transcription elongation complex Pol II-DSIF (SPT5-KOW5)-ELL2-EAF1 (composite structure)
Authors	:	Chen, Y.; Vos, S.M.; Dienemann, C.; Ninov, M.; Urlaub, H.; Cramer, P.
Deposited on	:	2021-05-18
Resolution	:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

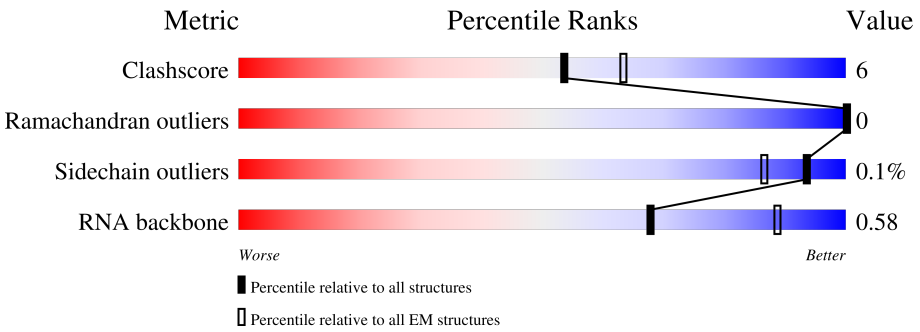
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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
RNA backbone	4643	859

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	1970	61% 11% 29%
2	B	1251	76% 14% 10%
3	C	275	78% 16% 6%
4	D	184	55% 9% 36%
5	E	210	89% 11%
6	F	127	55% 6% 39%
7	G	172	81% 18%

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Mol	Chain	Length	Quality of chain
8	H	150	81% 17%
9	I	125	10% 76% 17% 7%
10	J	67	81% 18%
11	K	117	94%
12	L	58	67% 9% 24%
13	M	640	18% 78%
14	N	48	23% 40% 17% 44%
15	O	268	34% 5% 60%
16	P	47	6% 21% 6% 72%
17	T	48	17% 50% 31% 19%
18	Z	1087	95%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 34834 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	1407	11149	7018	1998	2062	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9047	5721	1592	1670	64	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	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	118	967	608	167	188	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1721	1089	300	324	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1347	872	218	249	8	0	0

- Molecule 8 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		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	932	577	165	179	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	367	228	69	64	6	0	0

- Molecule 13 is a protein called RNA polymerase II elongation factor ELL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	139	1106	686	201	213	6	0	0

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	27	549	264	96	162	27	0	0

- Molecule 15 is a protein called ELL-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	106	832	523	149	156	4	0	0

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	P	13	279	125	54	87	13	0	0

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	T	39	808	385	149	235	39	0	0

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	51	393	241	72	79	1	0	0

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	A	2	2	2	0
20	B	1	1	1	0
20	C	1	1	1	0

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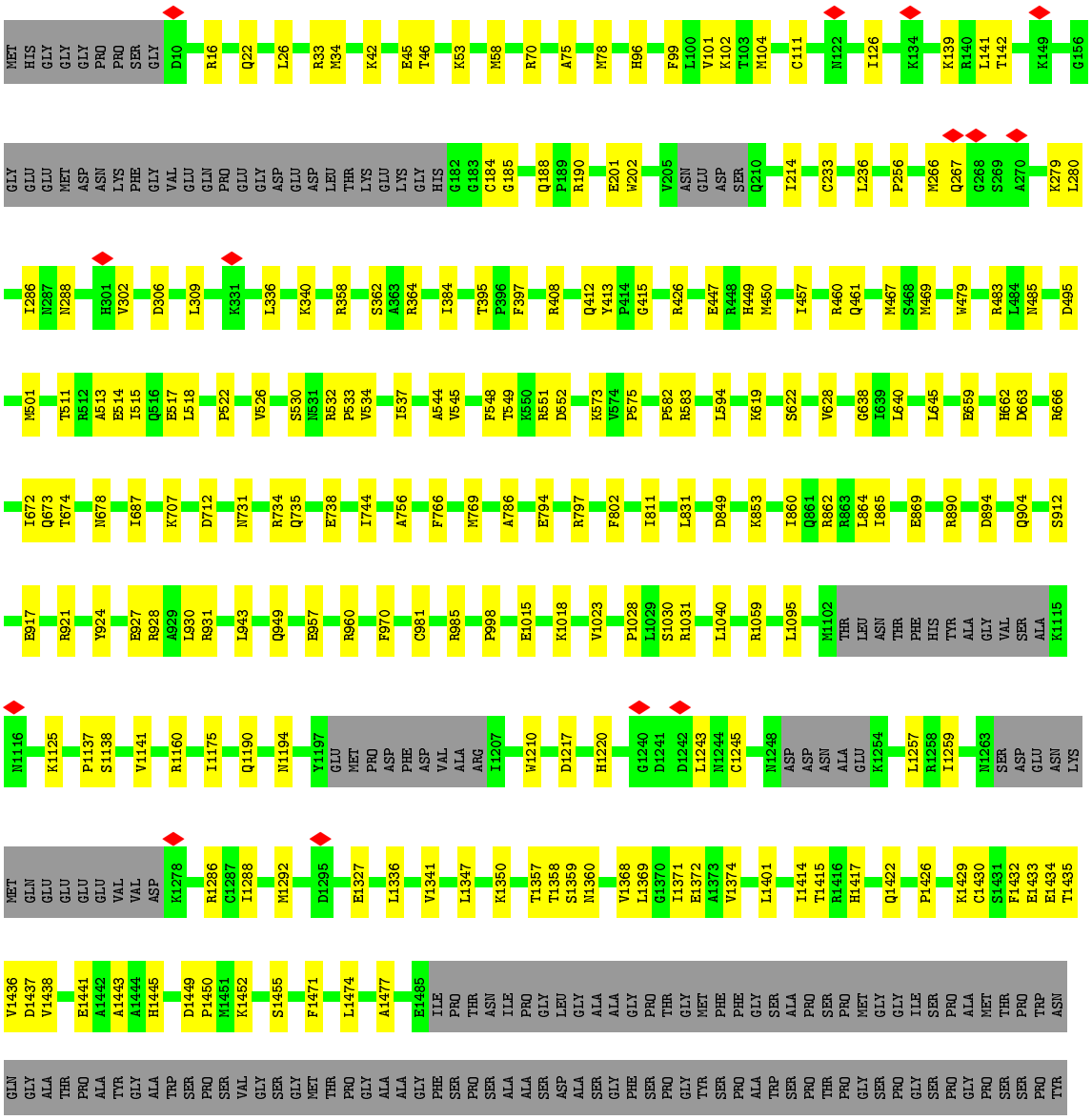
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	I	2	2	2	0
			Total	Zn	
20	J	1	1	1	0
			Total	Zn	
20	L	1	1	1	0

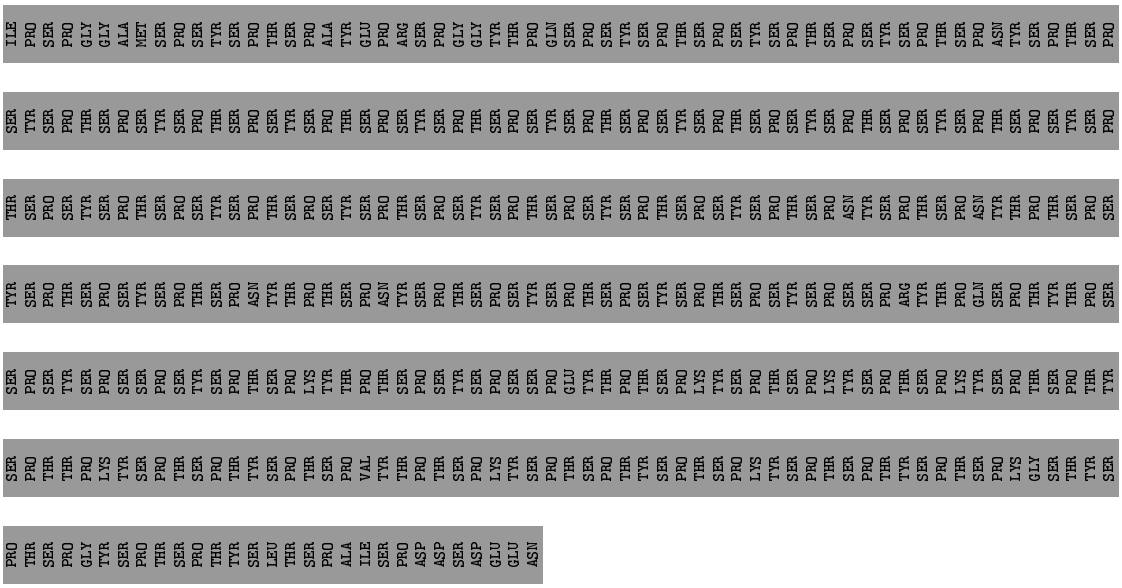
3 Residue-property plots (i)

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 II subunit RPB1

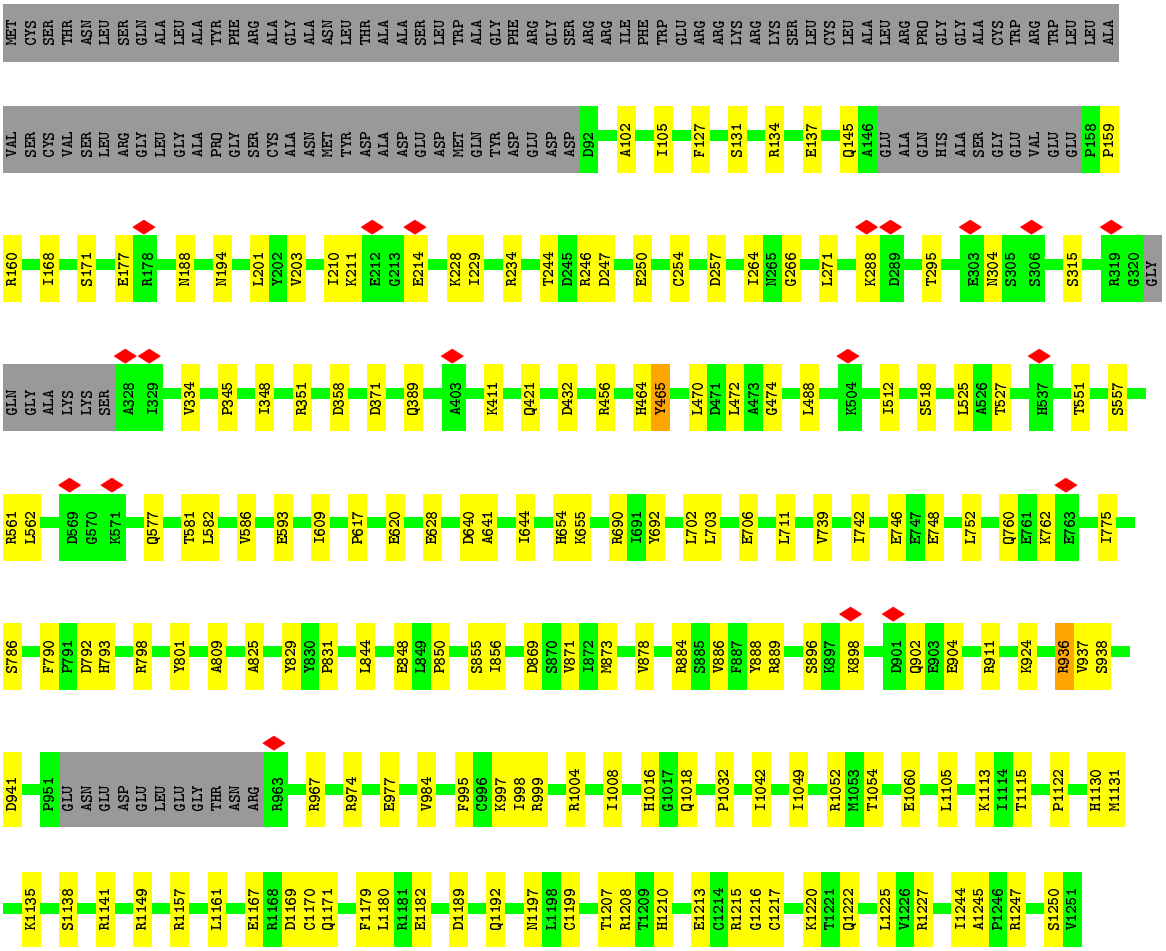
Chain A: 61% 11% 29%





- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



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

Chain C: 78% 16% 6%

MET P2 N5 Q6 P7 E13 V19 K20 T26 V37 F38 E41 D48 I52 S56 L59 H60 D61 R67 R86 E91 E92 F93 V105 E109 D110 Q111 V115 R126 R133 ASN ARG ASP ASN ASP PRO SER ASP TYR VAL GLU Q145

L149 I150 V151 K152 L153 R154 E158 E172 K175 A183 N190 R193 H194 T195 V196 Y197 D212 Q217 P222 N232 P241 V245 D270 VAL LEU THR ILE ASN

- Molecule 4: RNA polymerase II subunit D

Chain D: 55% 9% 36%

MET TRP GLY PRO ALA GLN PRO TYR SER ASP SER ALA LEU SER PRO LYS PRO ARG PRO PHE ARG ALA VAL PHE ARG GLY SER ALA LEU PRO PHE PRO ALA VAL ARG VAL GLU VAL ARG GLY ARG SER MET ALA ALA GLY GLY SER ASP PRO ARG ALA GLY ASP VAL GLU GLU ASP ALA S60

P65 K66 E67 L75 N76 S77 E78 A93 GLU ASP GLU Q97 T110 A111 R112 L134 E138 L142 A143 N144 L145 L156 E165 E168 I176 R180 SER PHE GLN TYR

- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 89% 11%

MET D2 L10 I13 R14 I17 M18 R55 L58 H64 N65 D66 V74 V82 Q95 L103 M110 Y125 Q132 Q133 E134 I137 R162 R166 R181 I193 A200 Q210

- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 55% 6% 39%

MET SER ASP ASN GLU ASP ASN PHE ASP GLY ASP ASP PHE ASP ASP VAL GLU GLU ASP GLU GLY LEU ASP ASP LEU GLU ASN ALA GLU GLU GLU GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO GLN ALA ASN GLN K50 R62 A63 R64 V79 M80 V81 L90

R100 I105 L123 D127

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

Chain G: 81% 18%

M1 L22 L30 V34 T39 Y42 T49 T50 I54 V70 K81 V84 A87 V88 V89 T90 Q91 F98 T99 E100 I101 C106 M117 E118 F119 N124 K129 V136 E142 I143 R144 L145 K146 A159 D165 D166 Y167 L168 V171

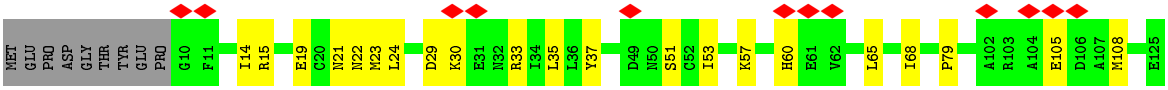
SER

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

Chain H: 81% 17%

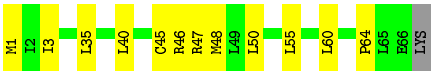
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



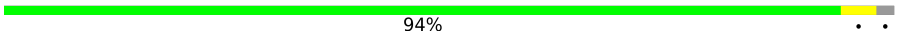
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

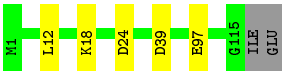
Chain J:



- Molecule 11: RNA_pol_L_2 domain-containing protein

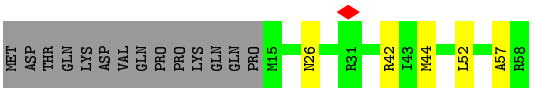
Chain K:





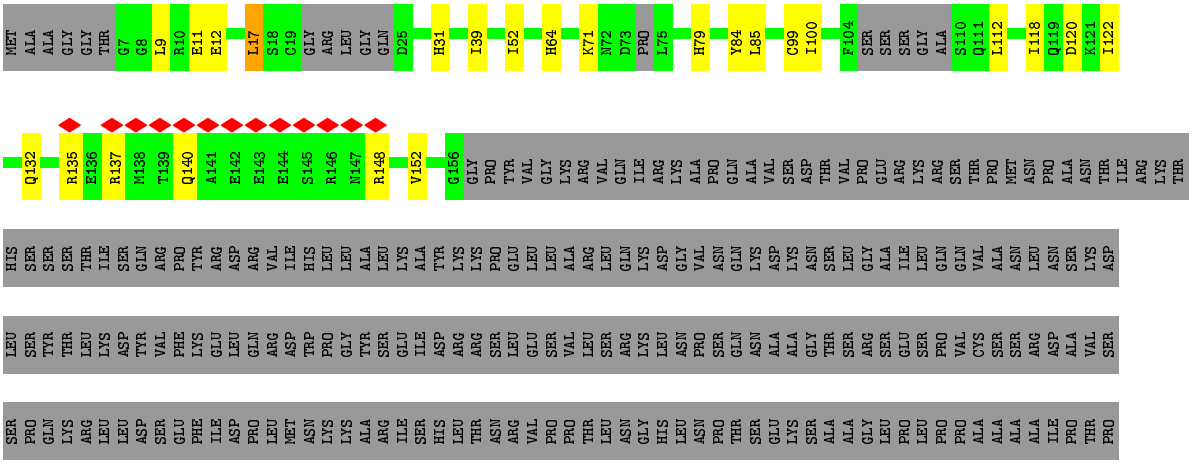
- Molecule 12: RNA polymerase II subunit K

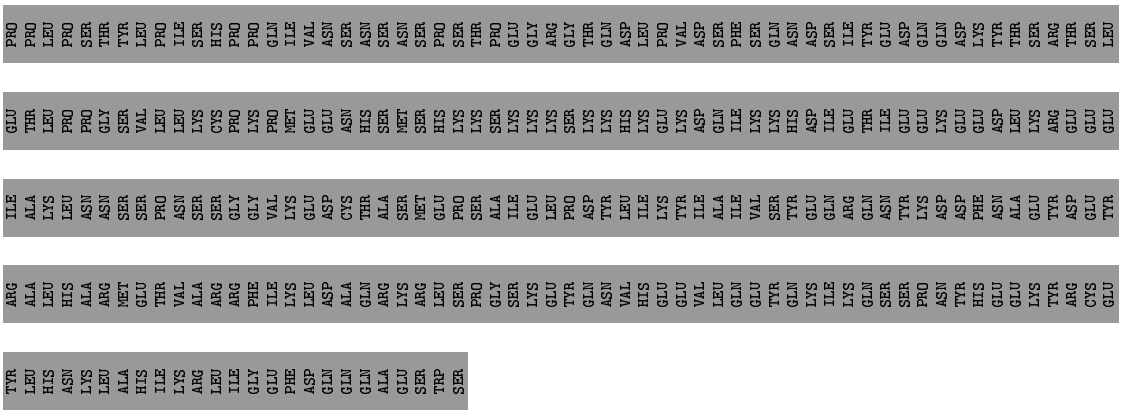
Chain L:



- Molecule 13: RNA polymerase II elongation factor ELL2

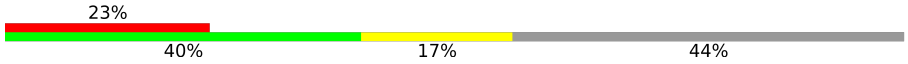
Chain M:

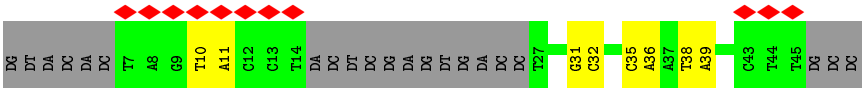




- Molecule 14: Non-template DNA

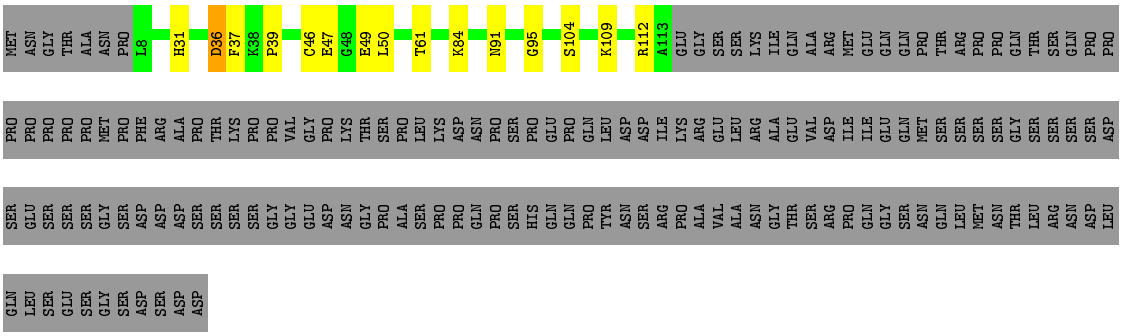
Chain N:





- Molecule 15: ELL-associated factor 1

Chain O:



- Molecule 16: RNA

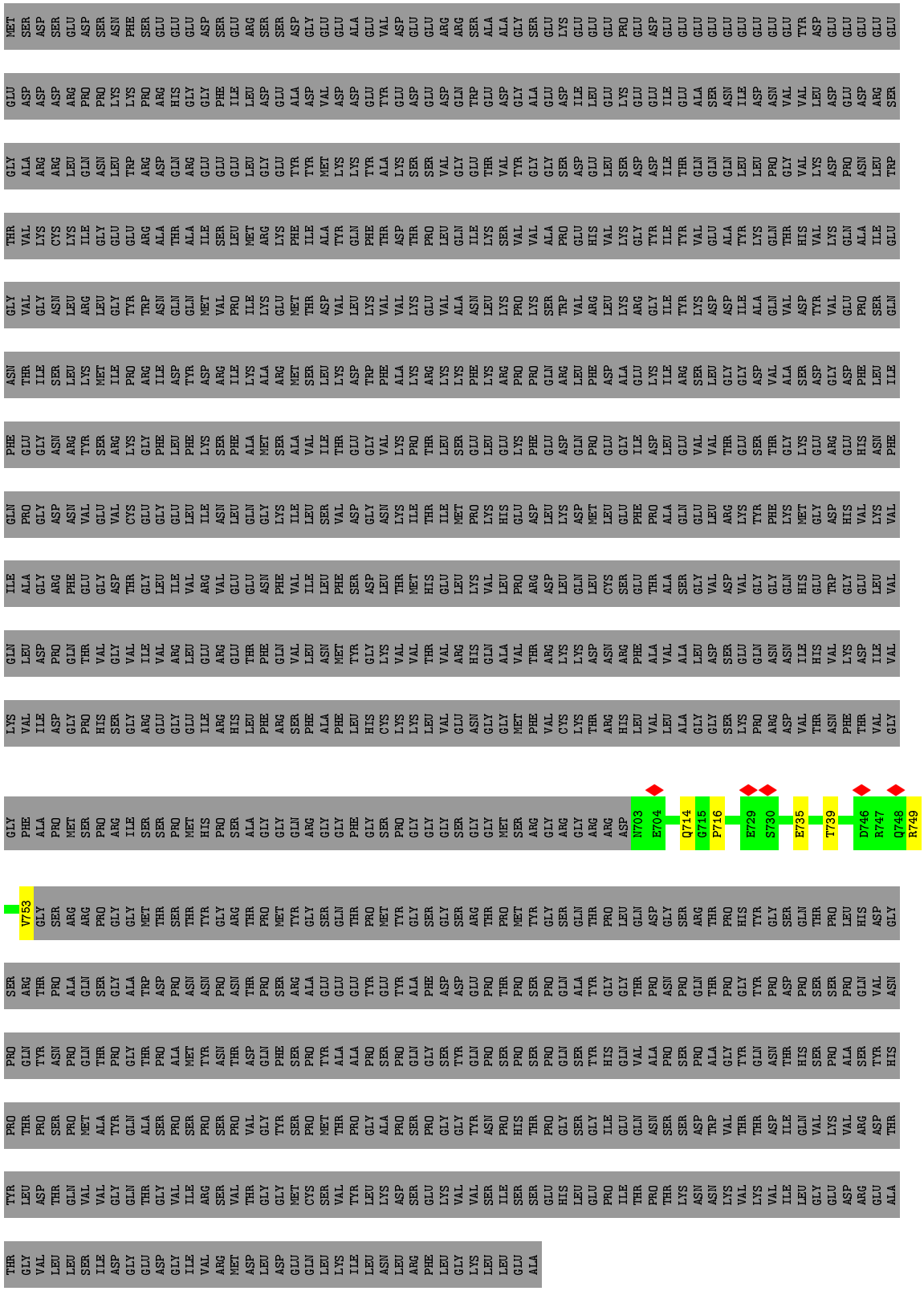
Chain P:

- Molecule 17: Template DNA

Chain T:

- Molecule 18: Transcription elongation factor SPT5

Chain Z: 95%


V753
N703
E704
Q714
G715
P716
E729
S730
E735
T739
D746
R747
Q748
R749

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364641	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 ($e^-/Å^2$)	43.21	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	56.269	Depositor
Minimum map value	-31.934	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.104	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.28	0/11350	0.49	0/15314
2	B	0.29	0/9227	0.49	1/12454 (0.0%)
3	C	0.29	0/2115	0.50	1/2873 (0.0%)
4	D	0.31	0/979	0.59	1/1312 (0.1%)
5	E	0.27	0/1752	0.50	1/2366 (0.0%)
6	F	0.29	0/636	0.51	0/859
7	G	0.37	0/1378	0.61	0/1870
8	H	0.29	0/1207	0.51	0/1628
9	I	0.31	0/954	0.57	0/1293
10	J	0.31	0/533	0.47	0/719
11	K	0.29	0/939	0.45	0/1271
12	L	0.31	0/372	0.57	0/493
13	M	0.28	0/1121	0.60	2/1507 (0.1%)
14	N	0.54	0/613	0.95	0/940
15	O	0.32	0/849	0.62	1/1145 (0.1%)
16	P	0.22	0/312	0.78	0/484
17	T	0.55	0/907	0.93	0/1400
18	Z	0.25	0/396	0.46	0/536
All	All	0.30	0/35640	0.54	7/48464 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	36	ASP	CB-CG-OD1	6.31	123.98	118.30
2	B	640	ASP	CB-CG-OD1	5.91	123.62	118.30
3	C	126	ARG	NE-CZ-NH1	5.17	122.89	120.30
13	M	120	ASP	CB-CG-OD1	5.15	122.94	118.30
13	M	17	LEU	CA-CB-CG	5.10	127.03	115.30
4	D	142	LEU	CA-CB-CG	5.01	126.83	115.30
5	E	166	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	117	MET	Peptide
7	G	124	ASN	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	11149	0	11300	143	0
2	B	9047	0	9080	122	0
3	C	2072	0	2019	33	0
4	D	967	0	973	13	0
5	E	1721	0	1737	14	0
6	F	626	0	657	6	0
7	G	1347	0	1347	18	0
8	H	1186	0	1147	16	0
9	I	932	0	856	16	0
10	J	524	0	540	11	0
11	K	920	0	942	4	0
12	L	367	0	367	4	0
13	M	1106	0	1082	17	0
14	N	549	0	308	4	0
15	O	832	0	832	14	0
16	P	279	0	142	2	0
17	T	808	0	442	12	0
18	Z	393	0	400	6	0
19	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
All	All	34834	0	34171	378	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 6.

All (378) 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:C:91:GLU:HG2	3:C:92:GLU:OE1	1.46	1.14
15:O:31:HIS:ND1	15:O:104:SER:OG	2.10	0.84
3:C:91:GLU:CG	3:C:92:GLU:OE1	2.29	0.80
3:C:92:GLU:HG2	3:C:93:PHE:N	1.97	0.77
2:B:134:ARG:HD3	2:B:304:ASN:HB3	1.71	0.73
15:O:31:HIS:CE1	15:O:104:SER:OG	2.45	0.70
1:A:912:SER:HB3	1:A:1327:GLU:HG3	1.75	0.69
13:M:11:GLU:HG2	13:M:12:GLU:HG3	1.76	0.68
3:C:92:GLU:HG2	3:C:93:PHE:H	1.60	0.67
1:A:734:ARG:NH2	9:I:108:MET:SD	2.68	0.67
13:M:39:ILE:HD11	15:O:84:LYS:HA	1.77	0.65
3:C:56:SER:HB2	3:C:158:GLU:H	1.60	0.65
1:A:1433:GLU:HG2	17:T:21:DA:H5"	1.77	0.65
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.79	0.64
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.80	0.64
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.79	0.64
8:H:32:SER:HB3	8:H:37:MET:H	1.63	0.63
1:A:1471:PHE:O	6:F:64:ARG:NH2	2.32	0.63
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.63
2:B:159:PRO:HB3	2:B:211:LYS:HG2	1.80	0.63
10:J:1:MET:HA	10:J:55:LEU:HB2	1.80	0.62
1:A:1415:THR:HG23	1:A:1417:HIS:H	1.63	0.62
2:B:1245:ALA:HB1	2:B:1247:ARG:HE	1.63	0.62
2:B:1157:ARG:NH1	16:P:38:A:OP2	2.30	0.61
3:C:109:GLU:OE1	3:C:111:GLN:NE2	2.33	0.61
1:A:928:ARG:NH1	8:H:106:THR:O	2.34	0.61
9:I:29:ASP:O	9:I:33:ARG:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.83	0.60
7:G:129:LYS:HD2	7:G:136:VAL:HG22	1.84	0.60
1:A:22:GLN:HB3	2:B:1247:ARG:HB2	1.84	0.59
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.83	0.59
1:A:511:THR:HG21	2:B:1182:GLU:HG2	1.82	0.59
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.82	0.59
17:T:21:DA:H2'	17:T:22:DA:C8	2.38	0.59
3:C:86:ARG:NH2	18:Z:716:PRO:O	2.36	0.59
1:A:864:LEU:HD23	1:A:1414:ILE:HG21	1.85	0.58
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.84	0.58
13:M:132:GLN:O	13:M:135:ARG:HB2	2.02	0.58
2:B:702:LEU:HD13	2:B:752:LEU:HD21	1.85	0.58
1:A:794:GLU:OE2	2:B:577:GLN:NE2	2.36	0.58
2:B:889:ARG:NH2	17:T:29:DG:OP1	2.35	0.58
2:B:246:ARG:NH1	2:B:250:GLU:OE1	2.37	0.58
13:M:9:LEU:HD23	15:O:31:HIS:CE1	2.39	0.58
2:B:924:LYS:NZ	2:B:941:ASP:OD2	2.37	0.58
7:G:91:GLN:HB2	7:G:98:PHE:HB2	1.86	0.58
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.85	0.58
4:D:76:ASN:O	4:D:110:THR:OG1	2.22	0.58
1:A:413:TYR:O	1:A:449:HIS:ND1	2.37	0.57
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.86	0.57
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.85	0.57
7:G:49:THR:HG22	7:G:50:THR:HG23	1.85	0.57
1:A:485:ASN:ND2	1:A:673:GLN:OE1	2.32	0.57
2:B:334:VAL:HA	2:B:345:PRO:HA	1.85	0.57
2:B:160:ARG:HG3	2:B:210:ILE:HB	1.85	0.57
15:O:46:CYS:SG	15:O:47:GLU:N	2.78	0.57
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.37	0.57
2:B:760:GLN:O	2:B:762:LYS:NZ	2.38	0.57
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.37	0.57
8:H:96:VAL:HA	8:H:116:VAL:HA	1.87	0.56
1:A:184:CYS:SG	1:A:185:GLY:N	2.77	0.56
2:B:938:SER:OG	18:Z:735:GLU:OE2	2.21	0.56
1:A:461:GLN:NE2	2:B:1167:GLU:OE2	2.39	0.56
1:A:514:GLU:OE2	2:B:1179:PHE:N	2.34	0.56
1:A:1028:PRO:HA	1:A:1031:ARG:HG2	1.87	0.56
1:A:34:MET:HA	2:B:1215:ARG:HG3	1.86	0.56
7:G:165:ASP:HB2	7:G:168:LEU:HD22	1.88	0.56
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.36	0.56
1:A:904:GLN:NE2	1:A:981:CYS:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:GLU:OE1	1:A:1018:LYS:NZ	2.39	0.56
14:N:38:DT:H2"	14:N:39:DA:H5'	1.89	0.56
5:E:82:VAL:HB	5:E:110:MET:HG2	1.87	0.55
1:A:46:THR:HB	1:A:58:MET:HB2	1.88	0.55
1:A:831:LEU:HB2	2:B:792:ASP:HB2	1.88	0.55
2:B:464:HIS:CD2	2:B:581:THR:HG21	2.42	0.55
1:A:426:ARG:HH22	2:B:1141:ARG:HH21	1.55	0.55
5:E:10:LEU:HD23	5:E:58:LEU:HD11	1.89	0.55
1:A:467:MET:HG3	1:A:534:VAL:HG11	1.87	0.55
1:A:102:LYS:NZ	1:A:1441:GLU:OE1	2.36	0.54
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.89	0.54
15:O:36:ASP:OD2	15:O:109:LYS:NZ	2.39	0.54
1:A:1175:ILE:HD12	1:A:1286:ARG:HG2	1.88	0.54
1:A:267:GLN:O	2:B:967:ARG:NH1	2.41	0.54
1:A:1288:ILE:O	1:A:1292:MET:HB2	2.08	0.54
2:B:641:ALA:HB2	2:B:655:LYS:HD3	1.88	0.54
1:A:1030:SER:OG	5:E:162:ARG:NE	2.40	0.54
1:A:687:ILE:HD13	2:B:1049:ILE:HB	1.89	0.54
2:B:1213:GLU:OE1	2:B:1220:LYS:NZ	2.38	0.54
1:A:917:GLU:OE2	1:A:921:ARG:NE	2.41	0.54
3:C:197:TYR:HD2	3:C:217:GLN:HE21	1.55	0.53
9:I:19:GLU:HA	15:O:39:PRO:HB3	1.90	0.53
2:B:127:PHE:HA	2:B:131:SER:HB2	1.89	0.53
4:D:156:LEU:HD22	7:G:84:VAL:HG11	1.89	0.53
1:A:998:PRO:O	1:A:1059:ARG:NH2	2.42	0.53
1:A:1422:GLN:O	1:A:1429:LYS:NZ	2.41	0.53
1:A:1477:ALA:HA	7:G:22:LEU:HD23	1.89	0.53
1:A:233:CYS:HA	1:A:236:LEU:HD12	1.92	0.52
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.90	0.52
10:J:35:LEU:HD11	10:J:50:LEU:HD13	1.90	0.52
2:B:1018:GLN:NE2	2:B:1054:THR:OG1	2.41	0.52
2:B:628:GLU:OE2	2:B:655:LYS:NZ	2.41	0.52
5:E:13:ILE:HD11	5:E:132:GLN:HG3	1.90	0.52
1:A:362:SER:HB2	2:B:1161:LEU:HD12	1.92	0.52
7:G:146:LYS:HB2	7:G:168:LEU:HD21	1.92	0.52
1:A:860:ILE:HD11	1:A:1125:LYS:HB2	1.92	0.51
1:A:78:MET:O	2:B:1149:ARG:NH2	2.43	0.51
1:A:479:TRP:HB2	1:A:483:ARG:HH21	1.75	0.51
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.92	0.51
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.92	0.51
8:H:57:ARG:O	8:H:145:MET:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ALA:O	1:A:548:PHE:HB2	2.11	0.51
1:A:811:ILE:HD12	9:I:79:PRO:HG3	1.92	0.51
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.92	0.51
2:B:703:LEU:HD23	2:B:739:VAL:HG12	1.91	0.51
2:B:790:PHE:HB3	2:B:793:HIS:CD2	2.45	0.51
2:B:1199:CYS:HB3	2:B:1217:CYS:SG	2.50	0.51
3:C:86:ARG:HD3	18:Z:716:PRO:HA	1.92	0.51
1:A:101:VAL:HA	1:A:104:MET:HE2	1.92	0.51
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.92	0.51
2:B:1004:ARG:NH1	2:B:1131:MET:SD	2.80	0.51
9:I:14:ILE:HD11	9:I:23:MET:HG2	1.92	0.51
1:A:33:ARG:HD2	2:B:1216:GLY:HA2	1.93	0.50
3:C:86:ARG:NH1	3:C:172:GLU:OE2	2.44	0.50
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.94	0.50
1:A:849:ASP:O	1:A:853:LYS:HB3	2.12	0.50
2:B:871:VAL:HG13	2:B:1042:ILE:HG23	1.92	0.50
2:B:936:ARG:NH2	18:Z:739:THR:O	2.43	0.50
13:M:85:LEU:HA	13:M:122:ILE:HG22	1.94	0.50
1:A:583:ARG:NH1	3:C:222:PRO:O	2.44	0.50
3:C:175:LYS:NZ	12:L:57:ALA:O	2.40	0.50
13:M:100:ILE:HD12	13:M:112:LEU:HD13	1.93	0.50
2:B:1130:HIS:HB3	2:B:1135:LYS:HE3	1.94	0.50
1:A:1243:LEU:HD13	1:A:1259:ILE:HG23	1.94	0.50
1:A:927:GLU:HG2	1:A:931:ARG:HH12	1.76	0.49
2:B:201:LEU:HD22	2:B:229:ILE:HD11	1.94	0.49
2:B:389:GLN:O	15:O:112:ARG:NH2	2.45	0.49
2:B:1192:GLN:HB3	2:B:1225:LEU:HD11	1.94	0.49
2:B:936:ARG:NH1	2:B:937:VAL:O	2.45	0.49
3:C:19:VAL:HG13	3:C:241:PRO:HB2	1.94	0.49
8:H:40:ILE:O	8:H:123:MET:HA	2.12	0.49
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.93	0.49
7:G:118:GLU:HG2	7:G:119:PHE:H	1.77	0.49
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.95	0.49
2:B:351:ARG:NH2	2:B:358:ASP:OD1	2.45	0.49
1:A:802:PHE:HD2	2:B:748:GLU:HG2	1.77	0.49
2:B:234:ARG:NH2	2:B:254:CYS:O	2.46	0.49
1:A:447:GLU:OE2	2:B:1141:ARG:NH2	2.46	0.49
15:O:31:HIS:CE1	15:O:104:SER:HG	2.25	0.49
1:A:286:ILE:HD13	1:A:309:LEU:HD23	1.94	0.49
13:M:99:CYS:HB2	13:M:118:ILE:HD11	1.94	0.49
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:ASN:ND2	12:L:44:MET:SD	2.84	0.48
1:A:1474:LEU:HB2	6:F:105:ILE:HB	1.95	0.48
14:N:35:DC:H2'	14:N:36:DA:C8	2.47	0.48
2:B:742:ILE:HG23	2:B:746:GLU:HB3	1.95	0.48
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.96	0.48
2:B:171:SER:HA	13:M:152:VAL:HG13	1.96	0.48
2:B:896:SER:OG	2:B:904:GLU:OE2	2.31	0.48
9:I:29:ASP:O	9:I:33:ARG:CA	2.62	0.48
1:A:1443:ALA:HB2	2:B:1244:ILE:HG23	1.93	0.48
2:B:889:ARG:O	2:B:999:ARG:HA	2.13	0.48
16:P:46:A:H61	17:T:24:DC:H42	1.60	0.48
1:A:45:GLU:OE2	1:A:53:LYS:NZ	2.40	0.48
17:T:28:DG:H2'	17:T:29:DG:C8	2.49	0.48
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.46	0.48
2:B:177:GLU:OE2	12:L:42:ARG:NH1	2.47	0.47
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.96	0.47
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.96	0.47
1:A:738:GLU:OE1	1:A:797:ARG:NH1	2.44	0.47
2:B:1016:HIS:NE2	2:B:1060:GLU:OE1	2.37	0.47
2:B:211:LYS:HB2	2:B:214:GLU:HB2	1.95	0.47
2:B:264:ILE:HG13	2:B:525:LEU:HB3	1.97	0.47
11:K:39:ASP:OD1	11:K:39:ASP:N	2.47	0.47
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.96	0.47
2:B:1192:GLN:HG2	2:B:1227:ARG:HD2	1.96	0.47
7:G:166:ASP:N	7:G:166:ASP:OD1	2.48	0.47
8:H:63:THR:HG23	8:H:65:TYR:H	1.79	0.47
1:A:70:ARG:HH12	2:B:1208:ARG:NH1	2.13	0.47
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.43	0.47
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.97	0.47
6:F:100:ARG:NH2	6:F:123:LEU:O	2.47	0.47
9:I:57:LYS:HD2	9:I:60:HIS:HB3	1.97	0.47
1:A:943:LEU:O	1:A:949:GLN:NE2	2.47	0.47
1:A:957:GLU:OE1	1:A:960:ARG:NH1	2.48	0.47
2:B:690:ARG:NH1	2:B:692:TYR:OH	2.47	0.47
2:B:1197:ASN:HB2	2:B:1222:GLN:HB3	1.97	0.47
1:A:1437:ASP:O	1:A:1441:GLU:HG2	2.14	0.47
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.97	0.47
1:A:279:LYS:HD3	1:A:336:LEU:HD12	1.98	0.46
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.97	0.46
2:B:211:LYS:HE2	2:B:214:GLU:HG3	1.96	0.46
1:A:384:ILE:HG12	2:B:1138:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1113:LYS:HB2	3:C:194:HIS:HB3	1.97	0.46
3:C:190:ASN:O	3:C:193:ARG:NH1	2.42	0.46
13:M:64:HIS:HA	13:M:84:TYR:HA	1.97	0.46
17:T:33:DC:H3'	17:T:34:DA:H3'	1.97	0.46
2:B:421:GLN:NE2	2:B:432:ASP:OD1	2.48	0.46
3:C:5:ASN:HB2	11:K:97:GLU:HG3	1.97	0.46
2:B:703:LEU:HG	2:B:775:ILE:HG12	1.97	0.46
2:B:829:TYR:HE1	2:B:886:VAL:HG13	1.80	0.46
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.80	0.46
2:B:168:ILE:HG22	2:B:203:VAL:HG23	1.97	0.46
7:G:89:VAL:HG12	7:G:99:THR:HG22	1.97	0.46
9:I:65:LEU:HA	9:I:68:ILE:HD12	1.98	0.46
14:N:10:DT:H2"	14:N:11:DA:C8	2.51	0.46
1:A:70:ARG:NH1	1:A:75:ALA:O	2.49	0.46
1:A:479:TRP:CD1	2:B:1008:ILE:HD12	2.51	0.46
4:D:145:LEU:HD22	7:G:144:ARG:HD3	1.98	0.46
14:N:31:DG:H2'	14:N:32:DC:C6	2.51	0.46
2:B:856:ILE:HG12	10:J:47:ARG:HH21	1.81	0.46
1:A:495:ASP:OD1	1:A:495:ASP:N	2.49	0.45
5:E:14:ARG:O	5:E:18:MET:HG2	2.15	0.45
1:A:537:ILE:HG13	1:A:672:ILE:HG21	1.98	0.45
1:A:924:TYR:HA	1:A:930:LEU:HD11	1.97	0.45
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.97	0.45
2:B:869:ASP:OD1	2:B:1052:ARG:NH2	2.49	0.45
9:I:35:LEU:HD11	9:I:51:SER:HA	1.98	0.45
2:B:137:GLU:OE1	13:M:148:ARG:NE	2.39	0.45
2:B:898:LYS:HB3	2:B:902:GLN:HB2	1.98	0.45
7:G:87:ALA:HB2	7:G:101:ILE:HG12	1.98	0.45
8:H:58:LEU:HD12	8:H:145:MET:HB3	1.98	0.45
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.99	0.45
2:B:855:SER:O	2:B:1122:PRO:HA	2.17	0.45
2:B:1115:THR:HA	3:C:195:THR:HA	1.98	0.45
1:A:1175:ILE:CD1	1:A:1286:ARG:HG2	2.47	0.45
1:A:1372:GLU:HG3	5:E:193:ILE:HG21	1.99	0.45
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.77	0.45
4:D:112:ARG:NH2	7:G:142:GLU:OE1	2.46	0.45
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.99	0.45
1:A:102:LYS:HB2	1:A:102:LYS:HE2	1.74	0.45
12:L:52:LEU:HD13	18:Z:753:VAL:HG11	1.98	0.45
2:B:194:ASN:HA	2:B:266:GLY:HA3	1.99	0.45
17:T:24:DC:H2'	17:T:25:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:ARG:O	10:J:50:LEU:HB2	2.17	0.45
5:E:74:VAL:HG22	5:E:103:LEU:HD12	1.98	0.44
6:F:79:VAL:HG12	6:F:81:VAL:H	1.82	0.44
1:A:302:VAL:O	1:A:306:ASP:HB2	2.18	0.44
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.81	0.44
3:C:67:ARG:NH1	10:J:3:ILE:O	2.40	0.44
8:H:2:ALA:O	8:H:84:ARG:NH1	2.50	0.44
1:A:514:GLU:O	1:A:518:LEU:HB2	2.17	0.44
1:A:1190:GLN:NE2	1:A:1194:ASN:OD1	2.46	0.44
2:B:488:LEU:HD11	2:B:512:ILE:HG23	1.99	0.44
2:B:593:GLU:HG2	2:B:801:TYR:HE1	1.81	0.44
3:C:212:ASP:OD1	3:C:212:ASP:N	2.48	0.44
1:A:1095:LEU:HD13	1:A:1401:LEU:HD22	1.99	0.44
1:A:1210:TRP:HZ3	9:I:53:ILE:HG13	1.82	0.44
2:B:617:PRO:HA	2:B:620:GLU:HG2	1.98	0.44
2:B:825:ALA:HB3	2:B:888:TYR:HB2	2.00	0.44
2:B:878:VAL:O	2:B:884:ARG:NH2	2.45	0.44
2:B:389:GLN:OE1	9:I:22:ASN:ND2	2.40	0.44
2:B:1032:PRO:HB2	2:B:1105:LEU:HD13	2.00	0.44
2:B:1189:ASP:OD1	2:B:1189:ASP:N	2.51	0.44
13:M:52:ILE:HD13	13:M:71:LYS:HA	1.99	0.44
13:M:112:LEU:HD21	15:O:50:LEU:HD23	2.00	0.44
1:A:890:ARG:HH21	1:A:1023:VAL:HA	1.83	0.44
2:B:873:MET:HG2	2:B:1042:ILE:HG12	1.99	0.44
3:C:92:GLU:OE1	3:C:92:GLU:N	2.50	0.44
15:O:91:ASN:O	15:O:95:GLY:N	2.50	0.44
2:B:244:THR:OG1	2:B:247:ASP:OD1	2.35	0.44
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.51	0.44
3:C:92:GLU:CG	3:C:93:PHE:N	2.74	0.44
1:A:42:LYS:O	1:A:288:ASN:ND2	2.46	0.43
1:A:141:LEU:HD22	1:A:1445:HIS:HE1	1.84	0.43
2:B:295:THR:HA	2:B:315:SER:HA	2.00	0.43
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.99	0.43
4:D:75:LEU:HB2	4:D:78:GLU:HG2	2.00	0.43
18:Z:714:GLN:HB2	18:Z:749:ARG:HG2	1.98	0.43
2:B:974:ARG:HB2	2:B:977:GLU:HG3	2.01	0.43
1:A:1358:THR:OG1	1:A:1359:SER:N	2.52	0.43
11:K:24:ASP:OD1	11:K:24:ASP:N	2.51	0.43
1:A:674:THR:O	1:A:678:ASN:ND2	2.40	0.43
2:B:786:SER:HB2	2:B:844:LEU:HD11	2.01	0.43
1:A:1450:PRO:HB2	1:A:1452:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:CYS:SG	1:A:1257:LEU:HD11	2.58	0.42
2:B:345:PRO:HG2	2:B:348:ILE:HD12	1.99	0.42
2:B:551:THR:OG1	2:B:809:ALA:O	2.31	0.42
13:M:17:LEU:HD23	15:O:50:LEU:HB2	2.00	0.42
13:M:137:ARG:O	13:M:140:GLN:HG2	2.20	0.42
4:D:112:ARG:HE	4:D:112:ARG:HB3	1.64	0.42
1:A:279:LYS:HA	1:A:279:LYS:HD2	1.70	0.42
1:A:469:MET:HB2	2:B:1170:CYS:SG	2.59	0.42
1:A:619:LYS:HE3	1:A:619:LYS:HB2	1.86	0.42
1:A:756:ALA:HB2	1:A:786:ALA:HB2	2.00	0.42
1:A:869:GLU:OE1	1:A:1455:SER:OG	2.35	0.42
1:A:1217:ASP:OD2	1:A:1220:HIS:ND1	2.52	0.42
1:A:16:ARG:HG3	2:B:1250:SER:HB2	2.02	0.42
1:A:190:ARG:NH1	1:A:201:GLU:OE1	2.46	0.42
1:A:266:MET:HE2	1:A:266:MET:HB3	1.95	0.42
1:A:426:ARG:HH22	2:B:1141:ARG:NH2	2.18	0.42
1:A:517:GLU:OE2	6:F:62:ARG:NE	2.50	0.42
2:B:228:LYS:N	2:B:518:SER:OG	2.53	0.42
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.01	0.42
1:A:413:TYR:O	1:A:415:GLY:N	2.52	0.42
1:A:712:ASP:HB3	1:A:744:ILE:HD13	2.02	0.42
3:C:149:LEU:HD21	3:C:152:LYS:HE3	2.01	0.42
17:T:10:DT:H2"	17:T:11:DA:C8	2.54	0.42
2:B:889:ARG:NH1	2:B:977:GLU:OE1	2.53	0.42
9:I:21:ASN:HB2	15:O:37:PHE:CE2	2.55	0.42
17:T:23:DG:H2'	17:T:24:DC:C6	2.54	0.42
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.93	0.42
1:A:1426:PRO:HD2	1:A:1449:ASP:HB2	2.00	0.42
2:B:102:ALA:O	2:B:105:ILE:HB	2.20	0.42
2:B:798:ARG:CZ	2:B:1052:ARG:HD3	2.50	0.42
3:C:7:PRO:HB3	3:C:26:THR:HB	2.01	0.42
5:E:95:GLN:OE1	5:E:125:TYR:OH	2.38	0.42
10:J:47:ARG:NH1	10:J:48:MET:SD	2.93	0.42
1:A:687:ILE:HD12	1:A:769:MET:HE3	2.02	0.42
3:C:154:ARG:HB2	10:J:60:LEU:HD22	2.01	0.42
9:I:15:ARG:HB2	9:I:24:LEU:HD12	2.01	0.42
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.90	0.42
1:A:139:LYS:HA	1:A:142:THR:HG22	2.01	0.42
1:A:731:ASN:HB3	1:A:735:GLN:HB2	2.02	0.42
2:B:145:GLN:HB3	2:B:160:ARG:HB3	2.02	0.42
2:B:1207:THR:O	2:B:1210:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:49:GLU:HB3	15:O:61:THR:HB	2.00	0.42
2:B:465:TYR:CE1	2:B:582:LEU:HD21	2.55	0.41
2:B:644:ILE:HD11	2:B:654:HIS:HB2	2.02	0.41
7:G:54:ILE:HD13	7:G:70:VAL:HG13	2.02	0.41
2:B:371:ASP:OD2	2:B:456:ARG:NH1	2.41	0.41
7:G:30:LEU:O	7:G:34:VAL:HG22	2.19	0.41
1:A:530:SER:HB2	1:A:532:ARG:HG2	2.01	0.41
1:A:1286:ARG:HE	1:A:1286:ARG:HB3	1.62	0.41
2:B:582:LEU:HD22	2:B:586:VAL:HB	2.02	0.41
2:B:1199:CYS:O	2:B:1247:ARG:HD2	2.20	0.41
1:A:551:ARG:NH2	1:A:622:SER:O	2.40	0.41
4:D:176:ILE:O	4:D:180:ARG:N	2.48	0.41
8:H:91:VAL:HG22	8:H:144:LEU:HG	2.01	0.41
1:A:26:LEU:HG	2:B:1245:ALA:HB2	2.02	0.41
1:A:1368:VAL:HG12	1:A:1369:LEU:HG	2.02	0.41
2:B:557:SER:OG	2:B:561:ARG:NH2	2.54	0.41
13:M:31:HIS:HB2	13:M:118:ILE:HG21	2.00	0.41
1:A:358:ARG:NH1	17:T:26:DG:OP1	2.53	0.41
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.55	0.41
1:A:707:LYS:HB3	1:A:707:LYS:HE2	1.86	0.41
1:A:734:ARG:HG2	9:I:105:GLU:HA	2.03	0.41
1:A:865:ILE:HD12	2:B:1169:ASP:HB3	2.02	0.41
1:A:1138:SER:N	1:A:1360:ASN:OD1	2.53	0.41
2:B:706:GLU:HB2	2:B:711:LEU:HD21	2.02	0.41
4:D:65:PRO:HB2	4:D:67:GLU:HG2	2.02	0.41
1:A:413:TYR:OH	1:A:450:MET:O	2.29	0.41
2:B:911:ARG:HD2	2:B:911:ARG:HA	1.91	0.41
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.49	0.41
4:D:145:LEU:HD23	4:D:145:LEU:HA	1.93	0.41
1:A:96:HIS:HB3	1:A:99:PHE:HB2	2.03	0.41
1:A:526:VAL:HA	1:A:533:PRO:HA	2.02	0.41
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.56	0.41
13:M:132:GLN:HA	13:M:135:ARG:HD3	2.01	0.41
1:A:395:THR:HG22	1:A:397:PHE:H	1.86	0.41
1:A:1141:VAL:HA	1:A:1357:THR:HG23	2.03	0.41
1:A:1434:GLU:HG3	1:A:1438:VAL:HG23	2.03	0.41
2:B:288:LYS:HD3	2:B:288:LYS:HA	1.89	0.41
2:B:470:LEU:HD22	2:B:562:LEU:HD22	2.02	0.41
2:B:848:GLU:O	10:J:55:LEU:HD21	2.21	0.41
2:B:984:VAL:HG13	2:B:998:ILE:HG12	2.03	0.41
2:B:1171:GLN:HB2	2:B:1180:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.97	0.41
9:I:30:LYS:H	9:I:30:LYS:HG2	1.71	0.41
13:M:71:LYS:HD3	13:M:79:HIS:CE1	2.56	0.41
1:A:202:TRP:HZ3	1:A:214:ILE:HG12	1.86	0.41
1:A:970:PHE:HE2	1:A:1040:LEU:HD11	1.86	0.41
2:B:472:LEU:HD21	2:B:609:ILE:HD13	2.02	0.41
4:D:165:GLU:OE1	4:D:168:GLU:N	2.46	0.41
1:A:364:ARG:HB2	2:B:1161:LEU:HD11	2.02	0.40
1:A:513:ALA:HB2	6:F:90:LEU:HD21	2.02	0.40
1:A:573:LYS:HB2	8:H:74:GLU:HG3	2.03	0.40
2:B:411:LYS:HA	2:B:411:LYS:HD3	1.91	0.40
4:D:76:ASN:OD1	4:D:144:ASN:ND2	2.46	0.40
3:C:52:ILE:HD12	3:C:61:ASP:HB3	2.02	0.40
4:D:145:LEU:HD13	4:D:156:LEU:HD13	2.04	0.40
7:G:106:CYS:HB2	7:G:159:ALA:HB3	2.02	0.40
17:T:36:DG:H2'	17:T:37:DG:C8	2.55	0.40
4:D:134:LEU:HD22	4:D:138:GLU:HG3	2.03	0.40
2:B:527:THR:HG22	17:T:31:DT:H4'	2.03	0.40
2:B:995:PHE:HZ	2:B:997:LYS:HE3	1.86	0.40
7:G:39:THR:HG23	7:G:42:TYR:H	1.87	0.40
1:A:460:ARG:HB2	1:A:501:MET:HE3	2.02	0.40
2:B:127:PHE:HB2	2:B:474:GLY:HA2	2.03	0.40
2:B:254:CYS:HB3	2:B:257:ASP:HB2	2.02	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	1393/1970 (71%)	1360 (98%)	33 (2%)	0	100	100
2	B	1123/1251 (90%)	1092 (97%)	31 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	254/275 (92%)	249 (98%)	5 (2%)	0	100	100
4	D	114/184 (62%)	109 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
8	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
9	I	114/125 (91%)	109 (96%)	5 (4%)	0	100	100
10	J	64/67 (96%)	64 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
13	M	131/640 (20%)	128 (98%)	3 (2%)	0	100	100
15	O	104/268 (39%)	99 (95%)	5 (5%)	0	100	100
18	Z	49/1087 (4%)	49 (100%)	0	0	100	100
All	All	4099/6701 (61%)	3989 (97%)	110 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1239/1749 (71%)	1239 (100%)	0	100	100
2	B	991/1084 (91%)	988 (100%)	3 (0%)	92	96
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	150 (99%)	1 (1%)	84	90
8	H	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55 (73%)	40 (100%)	0	100	100
13	M	124/575 (22%)	124 (100%)	0	100	100
15	O	93/240 (39%)	93 (100%)	0	100	100
18	Z	45/940 (5%)	45 (100%)	0	100	100
All	All	3676/5916 (62%)	3672 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	188	ASN
2	B	465	TYR
2	B	936	ARG
7	G	81	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	12/47 (25%)	1 (8%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	36	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

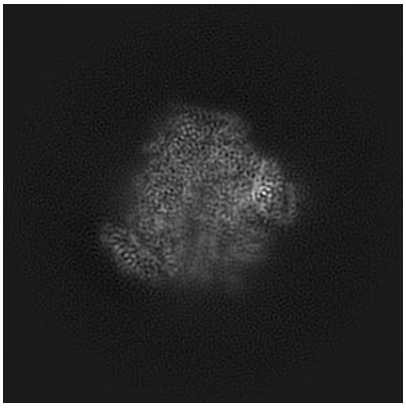
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12969. These allow visual inspection of the internal detail of the map and identification of artifacts.

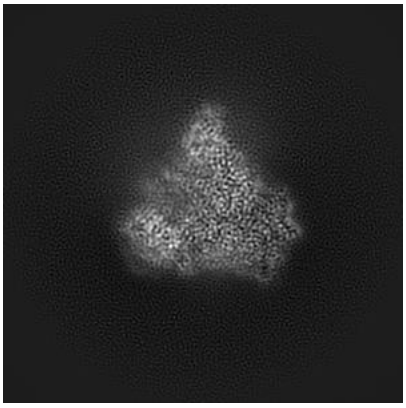
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

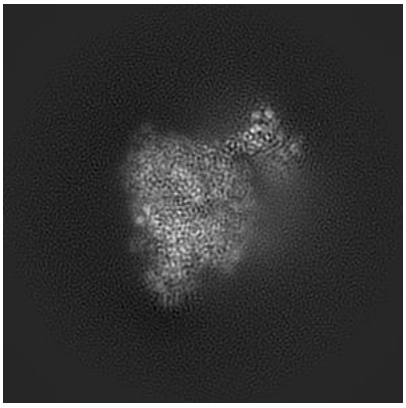
6.1.1 Primary map



X



Y

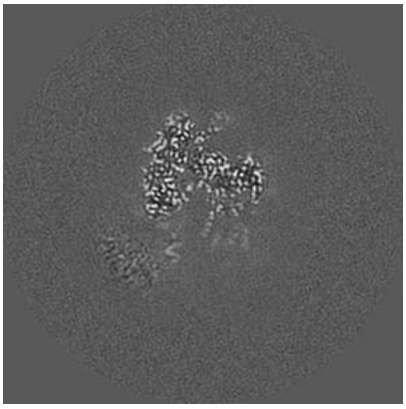


Z

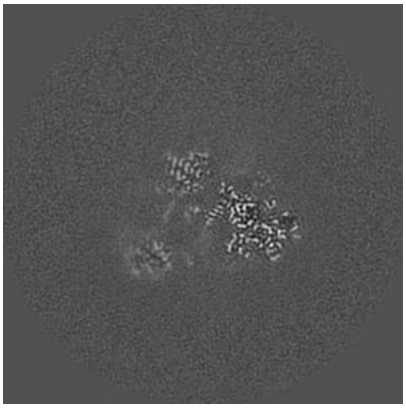
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

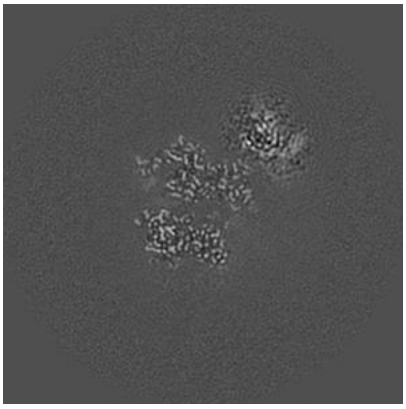
6.2.1 Primary map



X Index: 150



Y Index: 150

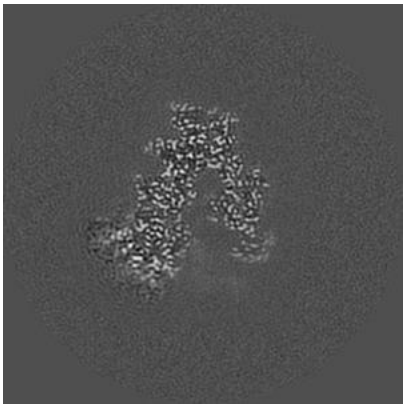


Z Index: 150

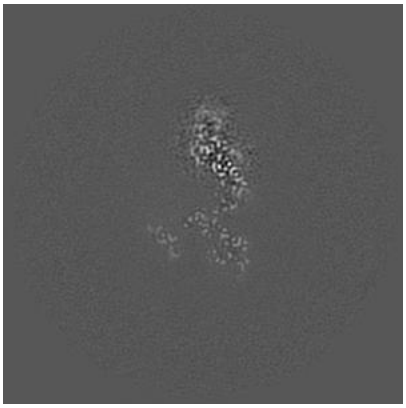
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

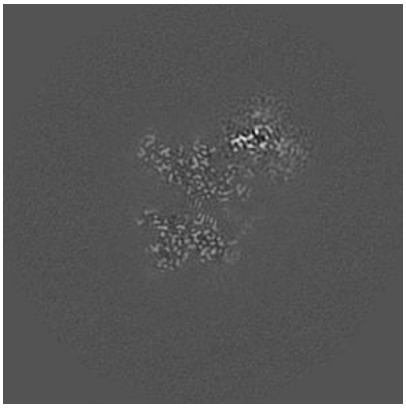
6.3.1 Primary map



X Index: 128



Y Index: 194

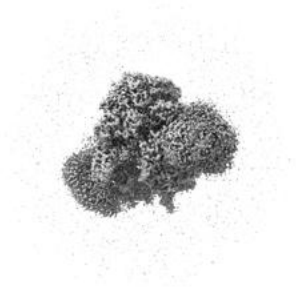


Z Index: 161

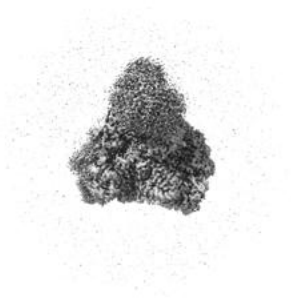
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

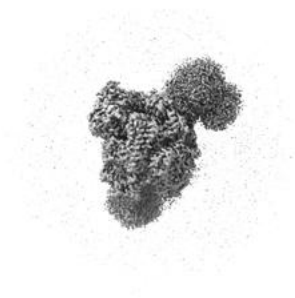
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

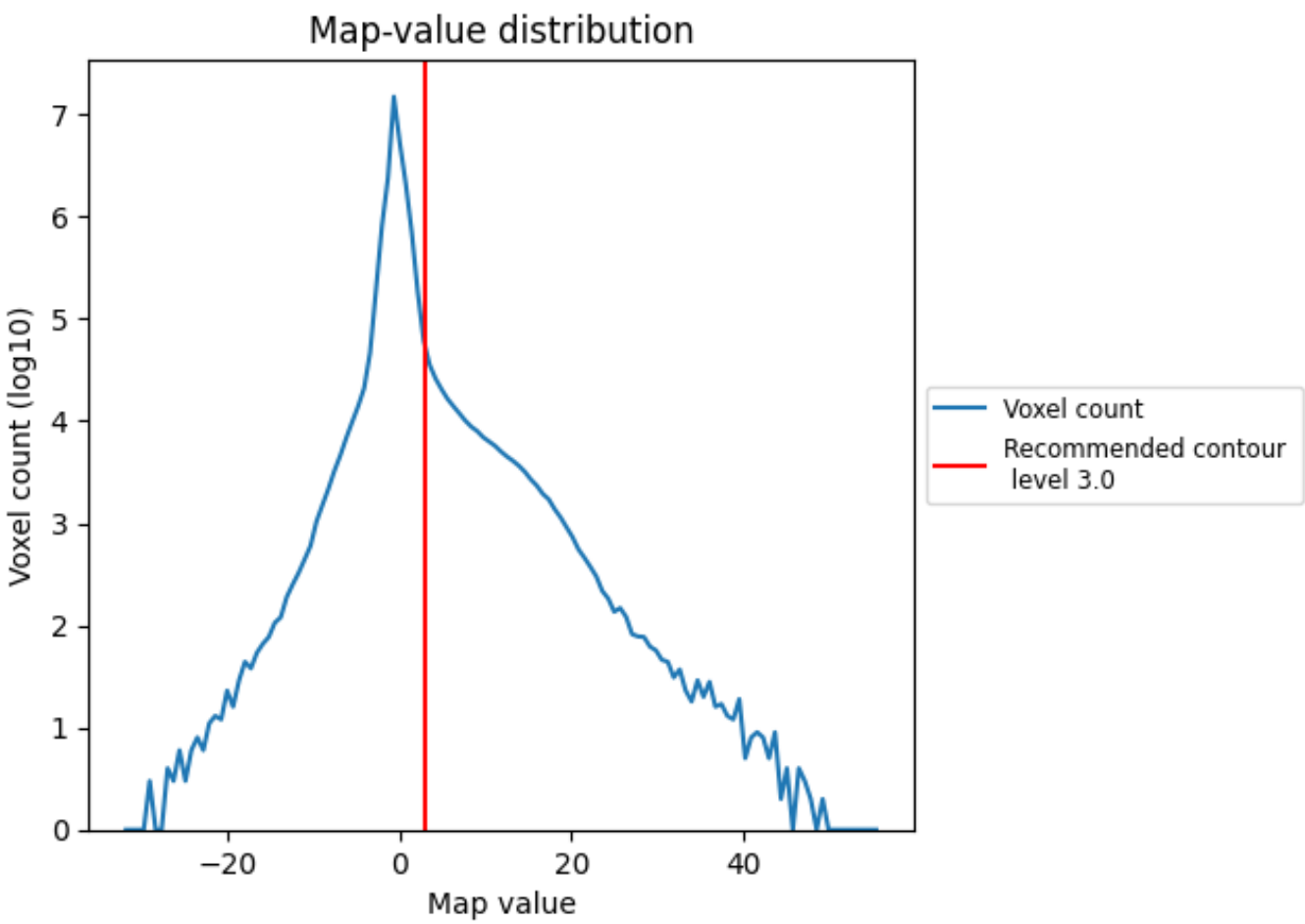
6.5 Mask visualisation (i)

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

7 Map analysis (i)

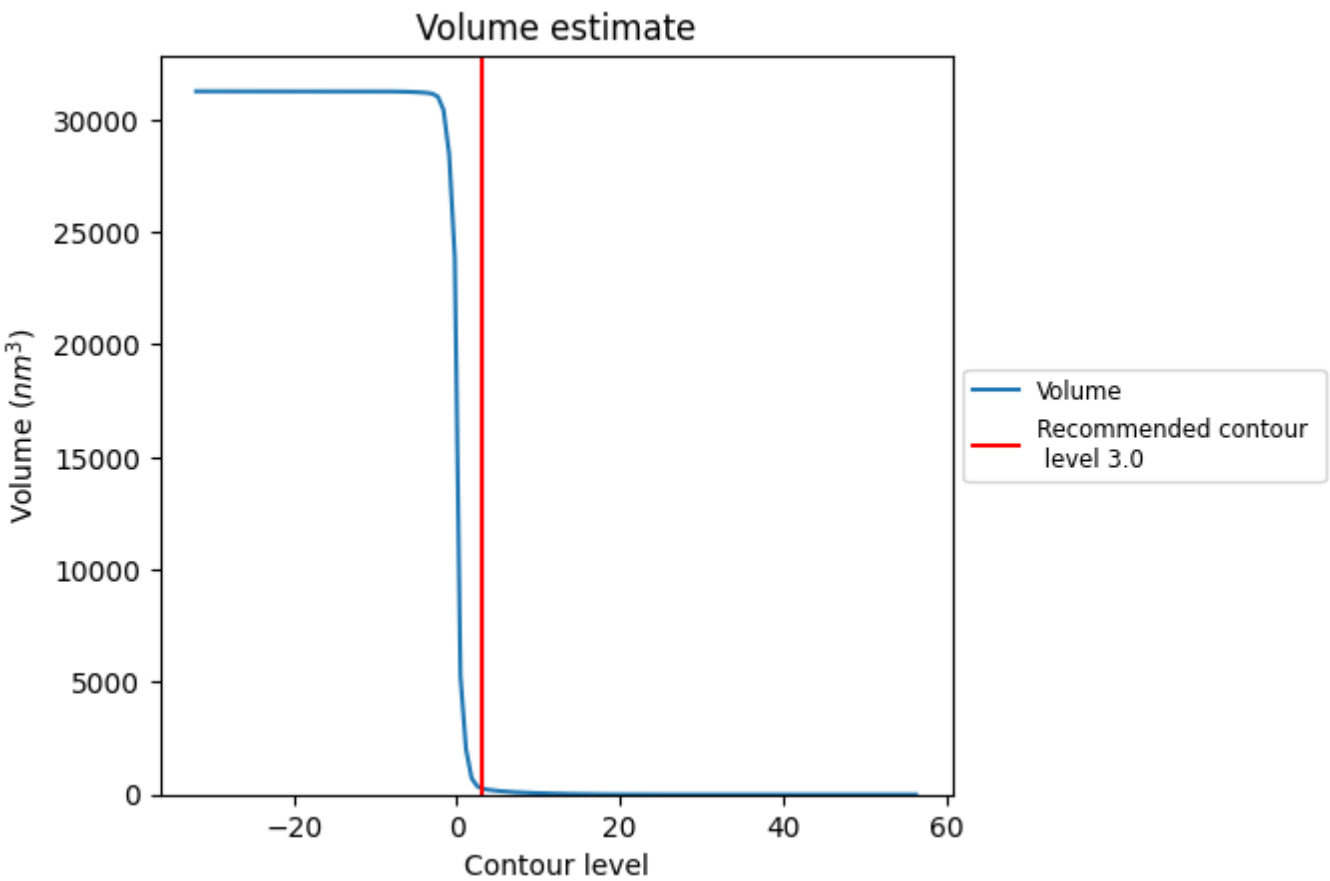
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

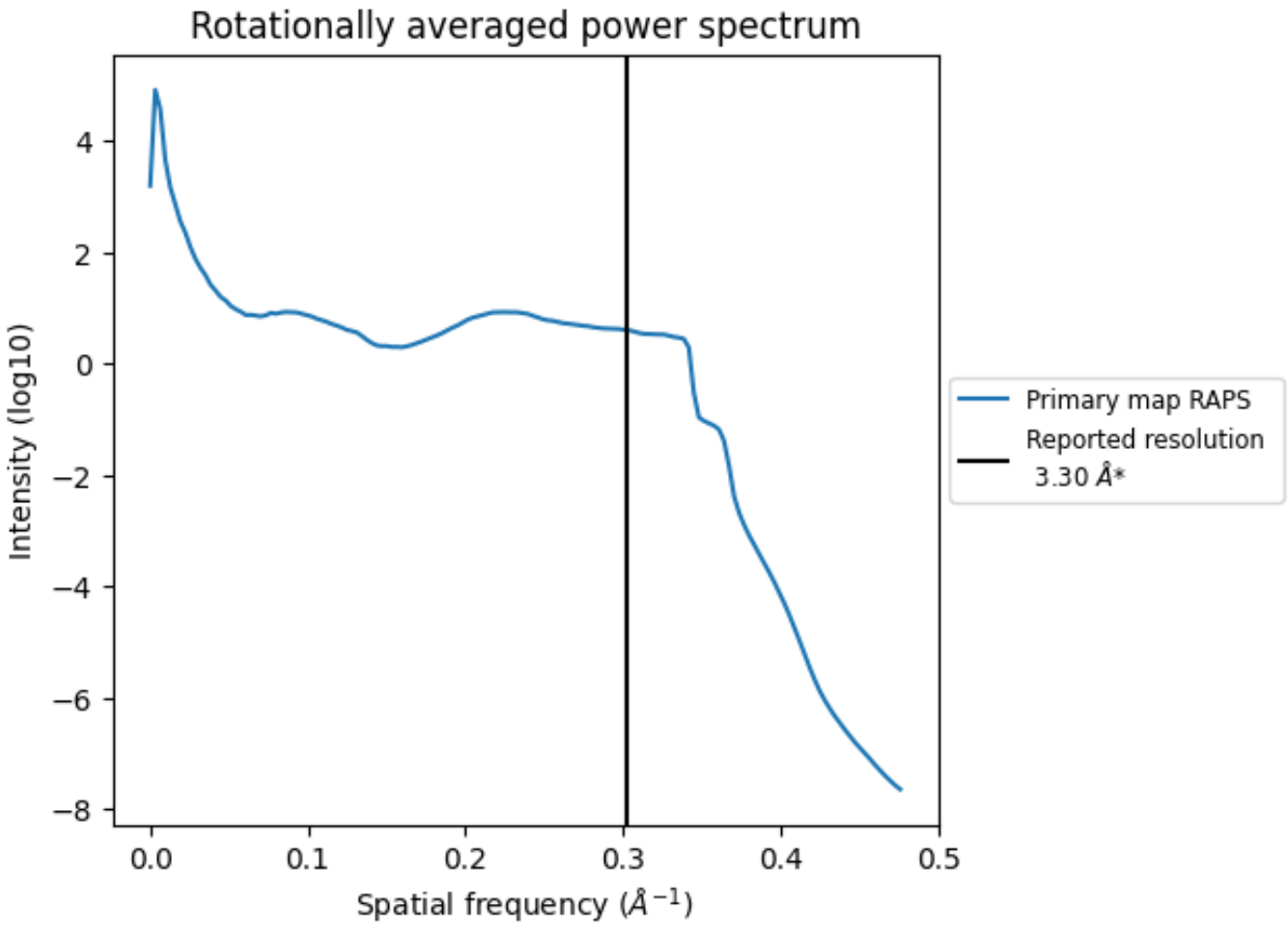
7.2 Volume estimate (i)



The volume at the recommended contour level is 293 nm^3; this corresponds to an approximate mass of 264 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 0.303 Å^{-1}

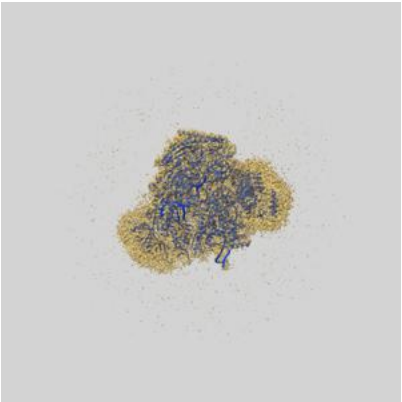
8 Fourier-Shell correlation (i)

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

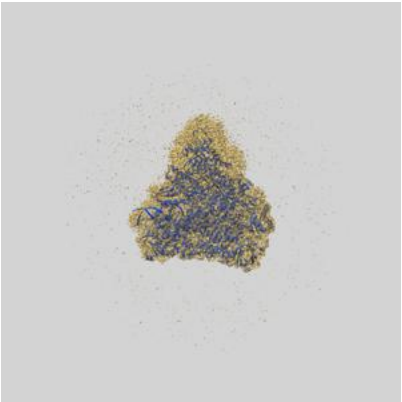
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12969 and PDB model 7OKX. Per-residue inclusion information can be found in section 3 on page 8.

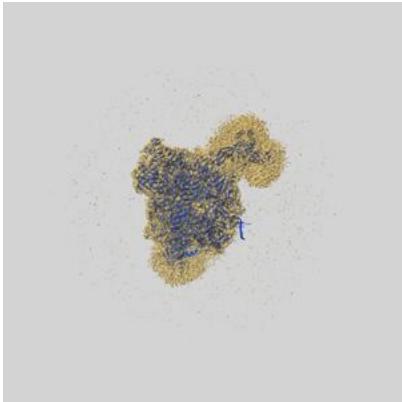
9.1 Map-model overlay (i)



X



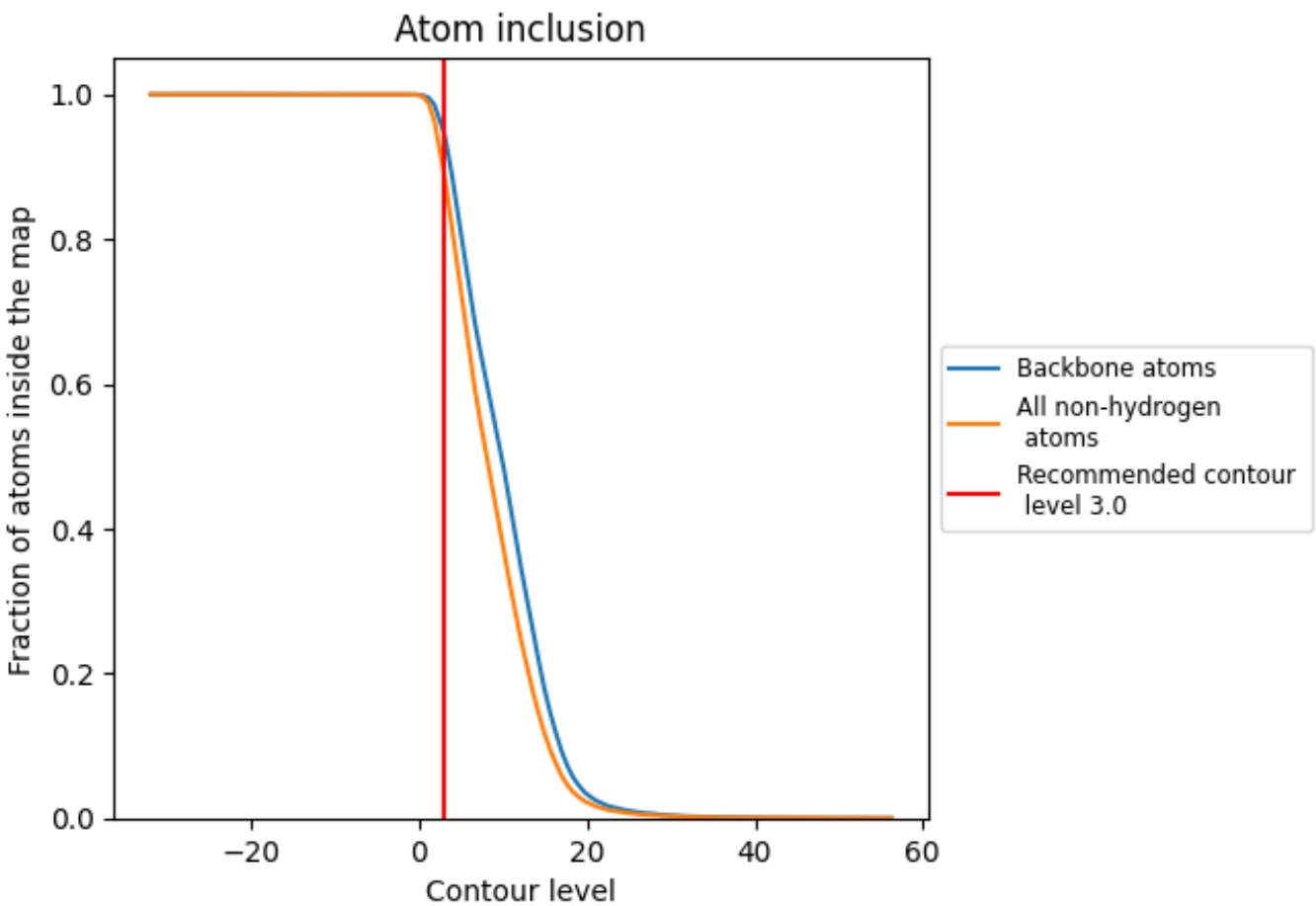
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.