Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:41 am GMT

PDB ID	:	6GOV
EMDB ID	:	EMD-0043
Title	:	Structure of THE RNA POLYMERASE LAMBDA-BASED ANTITERMINATION COMPLEX
Authors	:	Loll, B.; Krupp, F.; Said, N.; Huang, Y.; Buerger, J.; Mielke, T.; Spahn, C.M.T.; Wahl, M.C.
Deposited on	:	2018-06-04
Resolution	:	3.70 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:

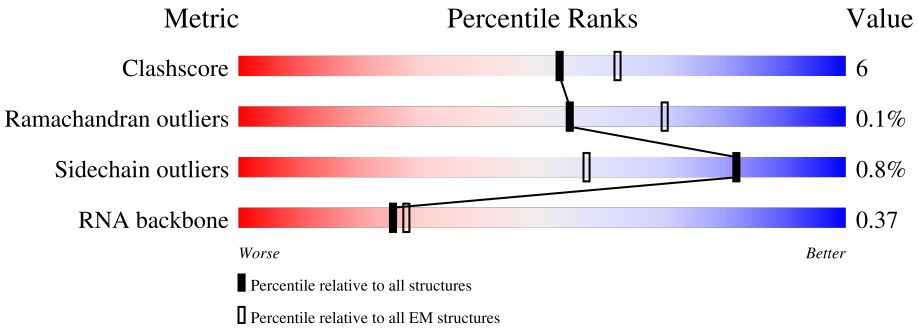
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.70 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	497	70% 68% 17% 15%
2	B	141	99% 83% 14% ••
3	E	106	91% 64% 26% 9%
4	G	184	39% 78% 15% • 7%
5	N	110	62% 91% 9%
6	U	329	62% 8% 30%
6	V	329	55% 12% 33%

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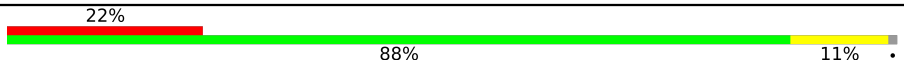
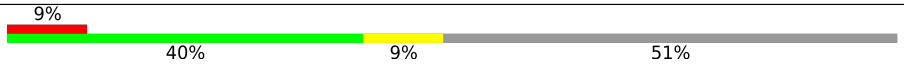
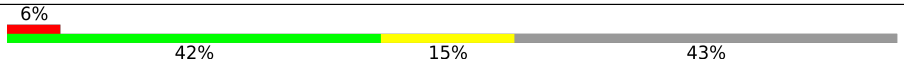
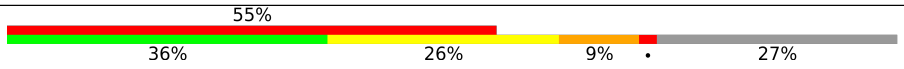
Mol	Chain	Length	Quality of chain
7	W	91	
8	X	1342	
9	Y	1417	
10	K	65	
11	L	65	
12	R	66	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 35040 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 Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3288	2050	576	652	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P0AFF8
A	0	ALA	-	expression tag	UNP P0AFF8
A	358	ALA	THR	conflict	UNP P0AFF8

- Molecule 2 is a protein called Transcription antitermination protein NusB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	139	Total	C	N	O	S	0	0
			1106	705	191	207	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P0A782
B	0	ALA	-	expression tag	UNP P0A782

- Molecule 3 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	96	Total	C	N	O	S	0	0
			771	482	147	141	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	LEU	-	expression tag	UNP P0A7R7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P0A7R7
E	0	SER	-	expression tag	UNP P0A7R7

- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	172	Total	C	N	O	S	0	0
			1377	875	243	252	7		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	LEU	-	expression tag	UNP P0AFG1
G	-1	GLY	-	expression tag	UNP P0AFG1
G	0	SER	-	expression tag	UNP P0AFG1
G	37	GLU	ASP	conflict	UNP P0AFG1

- Molecule 5 is a protein called Antitermination protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	110	Total	C	N	O	S	0	0
			882	547	177	156	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-2	LEU	-	expression tag	UNP P03045
N	-1	GLY	-	expression tag	UNP P03045
N	0	SER	-	expression tag	UNP P03045

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
6	V	220	Total	C	N	O	S	0	0
			1699	1061	299	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	1341	Total	C	N	O	S	0	0
			10575	6636	1842	2053	44		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	1339	Total	C	N	O	S	0	0
			10410	6539	1855	1966	50		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1	VAL	MET	conflict	UNP P0A8T8
Y	1408	HIS	-	expression tag	UNP P0A8T8
Y	1409	HIS	-	expression tag	UNP P0A8T8
Y	1410	HIS	-	expression tag	UNP P0A8T8
Y	1411	HIS	-	expression tag	UNP P0A8T8
Y	1412	HIS	-	expression tag	UNP P0A8T8
Y	1413	HIS	-	expression tag	UNP P0A8T8
Y	1414	HIS	-	expression tag	UNP P0A8T8
Y	1415	HIS	-	expression tag	UNP P0A8T8
Y	1416	HIS	-	expression tag	UNP P0A8T8
Y	1417	HIS	-	expression tag	UNP P0A8T8

- Molecule 10 is a DNA chain called DNA (I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	32	Total	C	N	O	P	0	0
			657	313	119	193	32		

- Molecule 11 is a DNA chain called DNA (II).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	37	Total	C	N	O	P	0	0
			748	356	139	217	36		

- Molecule 12 is a RNA chain called RNA (TRANSCRIPTION BUBBLE).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	48	Total	C	N	O	P	0	0
			1029	461	193	327	48		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	Y	1	Total	Mg	0
			1	1	

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

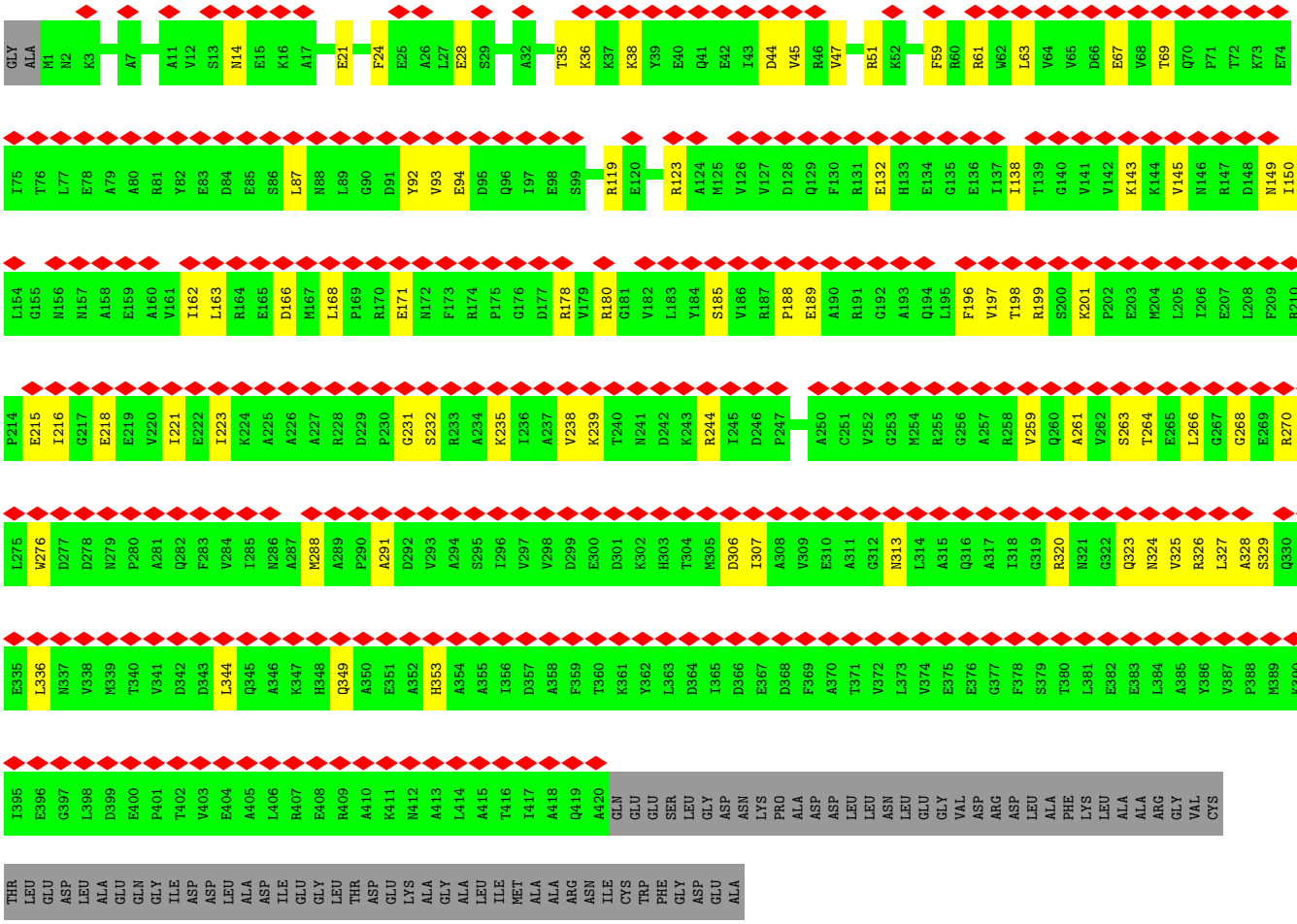
Mol	Chain	Residues	Atoms		AltConf
14	Y	2	Total	Zn	0
			2	2	

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.

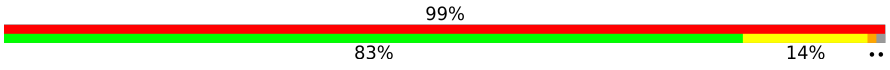
• Molecule 1: Transcription termination/antitermination protein NusA

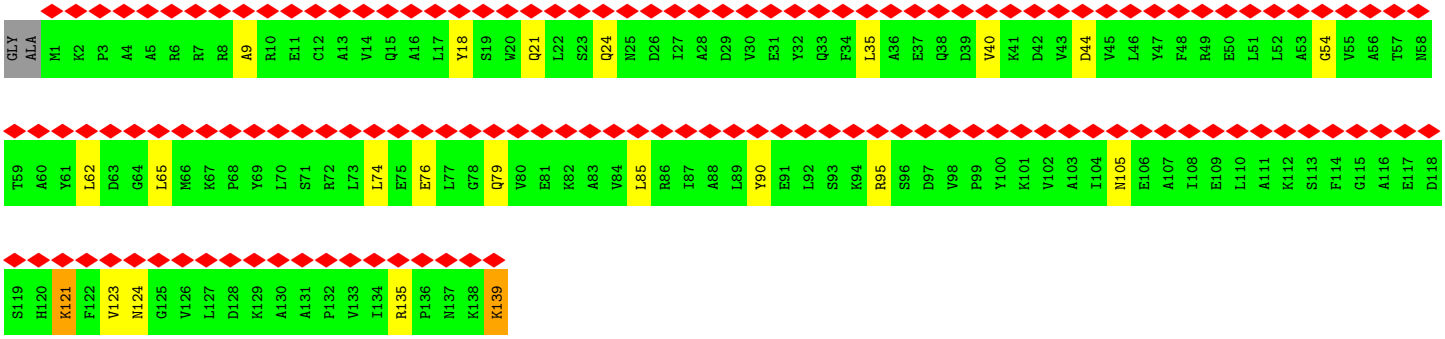
Chain A:



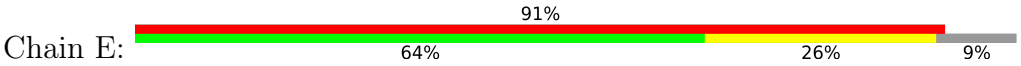
• Molecule 2: Transcription antitermination protein NusB

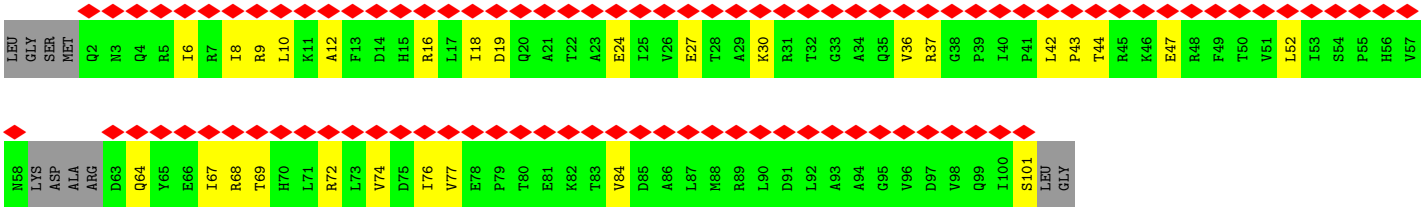
Chain B:



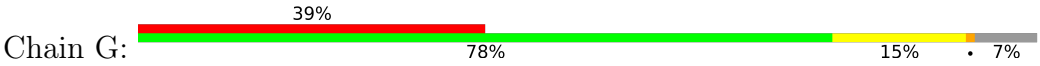


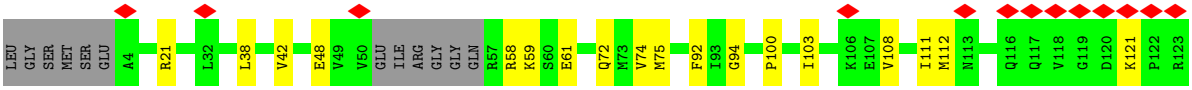
• Molecule 3: 30S ribosomal protein S10

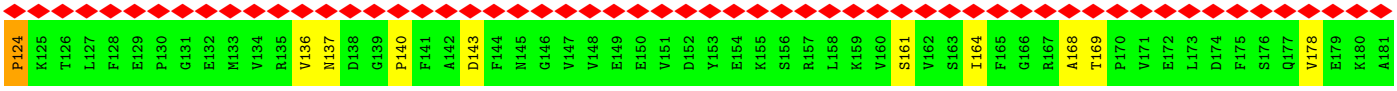




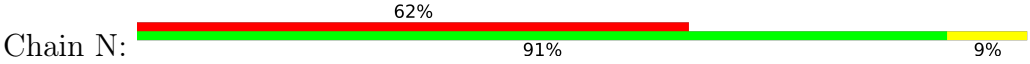
• Molecule 4: Transcription termination/antitermination protein NusG

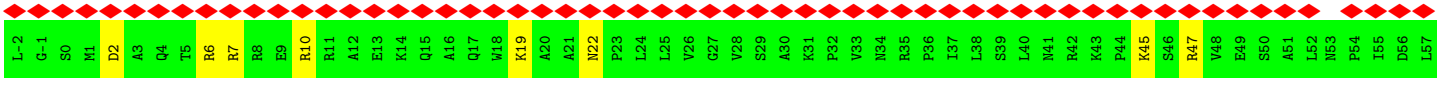


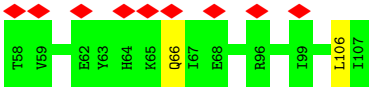




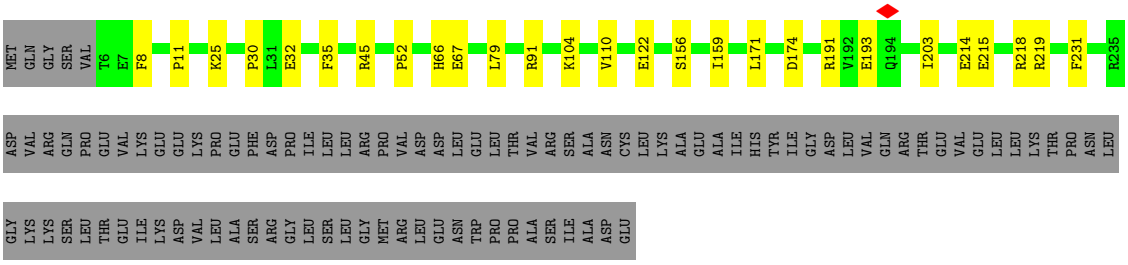
• Molecule 5: Antitermination protein N





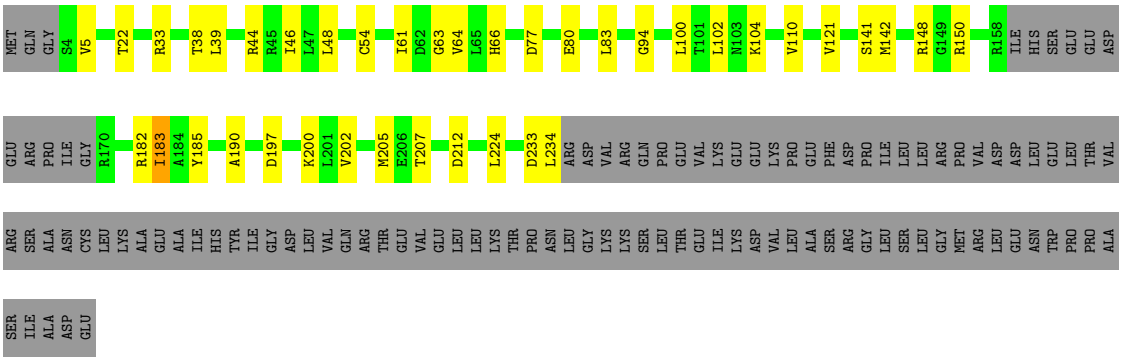


• Molecule 6: DNA-directed RNA polymerase subunit alpha



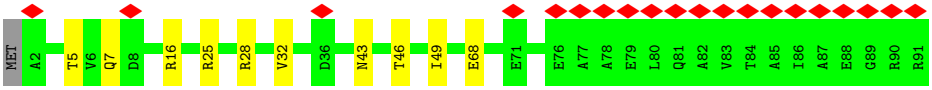
• Molecule 6: DNA-directed RNA polymerase subunit alpha

Chain V:



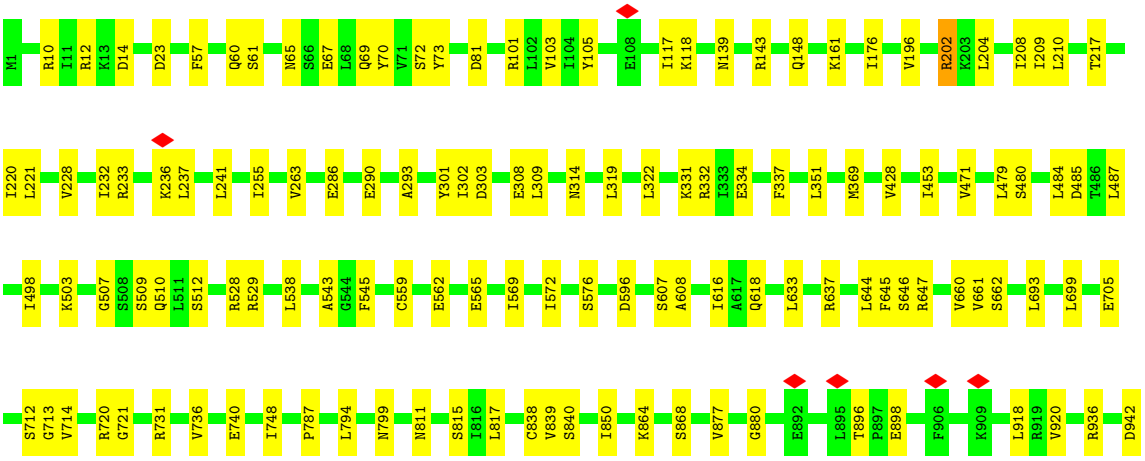
• Molecule 7: DNA-directed RNA polymerase subunit omega

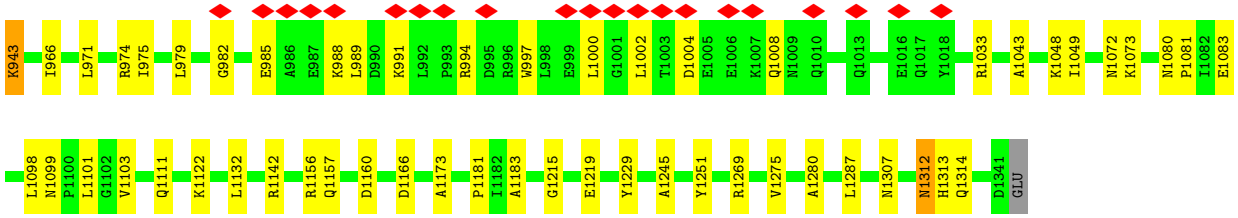
Chain W:



• Molecule 8: DNA-directed RNA polymerase subunit beta

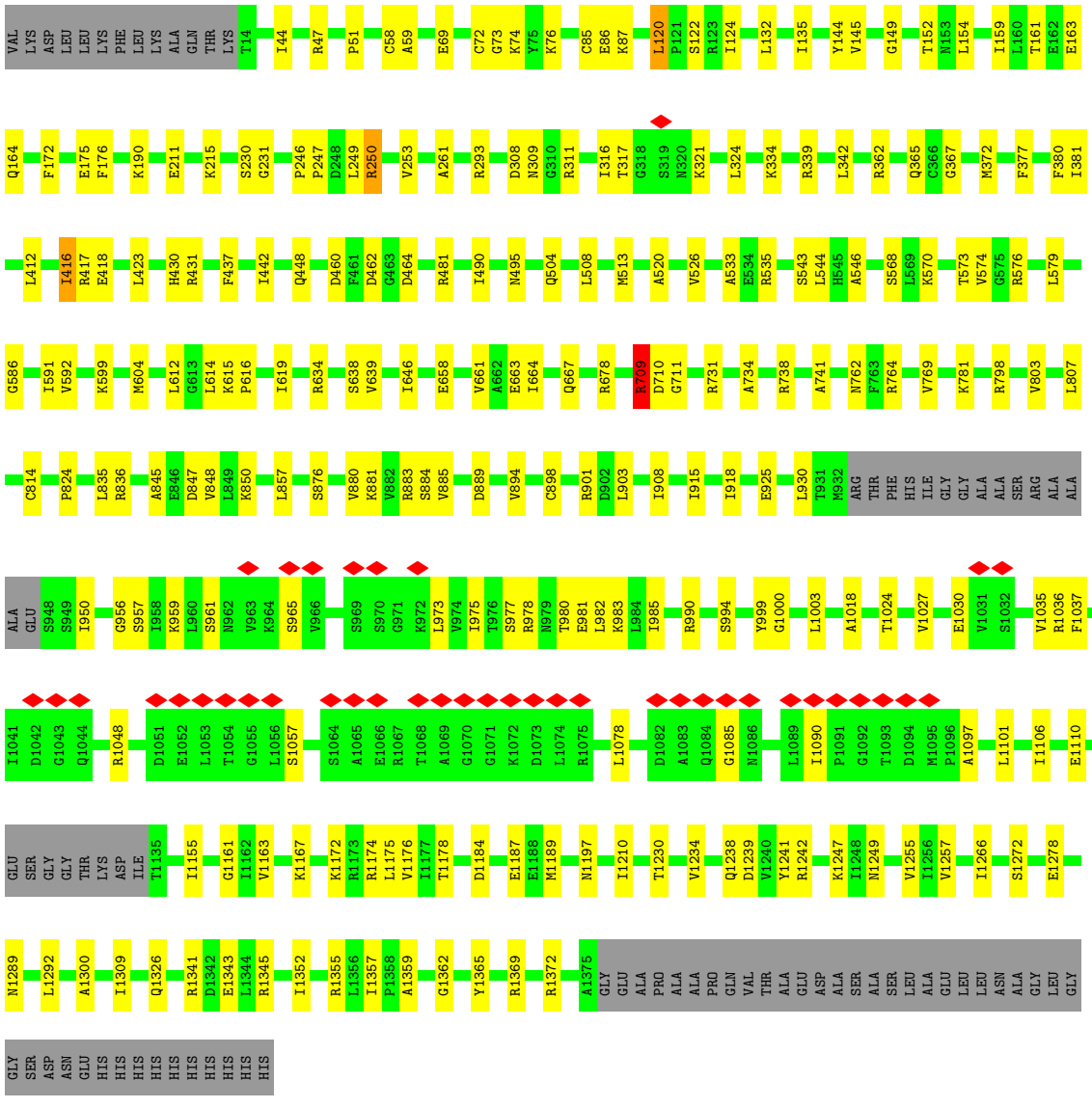
Chain X:





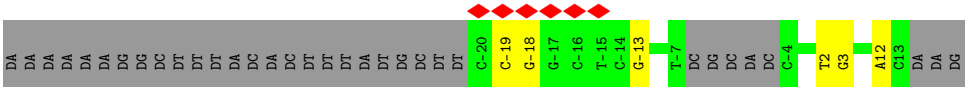
• Molecule 9: DNA-directed RNA polymerase subunit beta'

Chain Y:

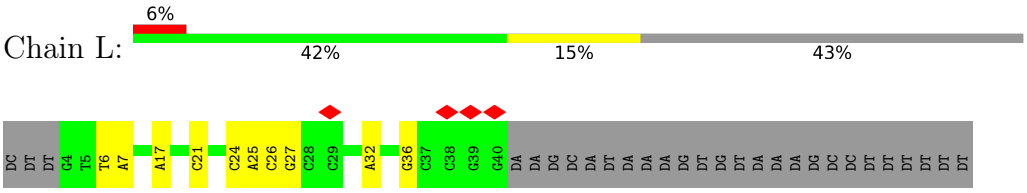


• Molecule 10: DNA (I)

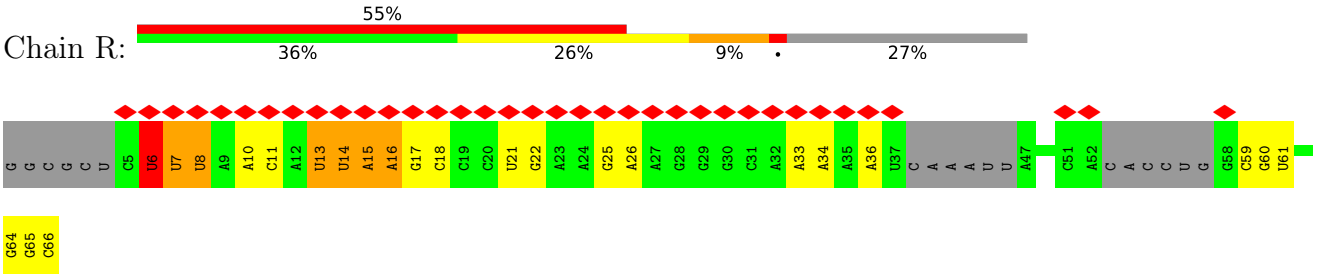
Chain K:



• Molecule 11: DNA (II)



• Molecule 12: RNA (TRANSCRIPTION BUBBLE)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	708030	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 ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0138	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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, 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	0.26	0/3328	0.49	0/4503
2	B	0.25	0/1124	0.43	0/1517
3	E	0.24	0/780	0.54	0/1055
4	G	0.29	0/1407	0.53	0/1895
5	N	0.27	0/895	0.54	0/1201
6	U	0.44	0/1808	0.61	0/2450
6	V	0.39	0/1718	0.59	0/2328
7	W	0.30	0/711	0.52	0/956
8	X	0.44	0/10744	0.59	0/14497
9	Y	0.40	0/10567	0.59	2/14268 (0.0%)
10	K	0.61	0/735	0.97	0/1130
11	L	0.75	0/838	1.02	3/1289 (0.2%)
12	R	0.36	0/1151	1.05	1/1787 (0.1%)
All	All	0.41	0/35806	0.62	6/48876 (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
4	G	0	1
8	X	0	2
9	Y	0	3
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	24	DC	O5'-P-OP1	8.00	120.30	110.70
9	Y	710	ASP	CB-CG-OD1	6.53	124.17	118.30
11	L	36	DG	O4'-C4'-C3'	-5.74	102.20	104.50
12	R	6	U	C2-N1-C1'	5.23	123.97	117.70
11	L	24	DC	O5'-P-OP2	-5.20	101.02	105.70
9	Y	709	ARG	C-N-CA	5.17	134.63	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	75	MET	Peptide
8	X	241	LEU	Peptide
8	X	81	ASP	Peptide
9	Y	120	LEU	Peptide
9	Y	416	ILE	Peptide
9	Y	709	ARG	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	3288	0	3297	54	0
2	B	1106	0	1129	15	0
3	E	771	0	803	20	0
4	G	1377	0	1373	16	0
5	N	882	0	938	8	0
6	U	1786	0	1813	21	0
6	V	1699	0	1734	25	0
7	W	709	0	719	7	0
8	X	10575	0	10597	107	0
9	Y	10410	0	10627	136	0
10	K	657	0	363	5	0
11	L	748	0	415	7	0
12	R	1029	0	522	18	0
13	Y	1	0	0	0	0
14	Y	2	0	0	0	0
All	All	35040	0	34330	387	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 (387) 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)
1:A:21:GLU:OE2	1:A:51:ARG:NH1	2.11	0.83
9:Y:1362:GLY:O	9:Y:1365:TYR:HB3	1.83	0.79
6:U:45:ARG:HD2	6:V:38:THR:HB	1.71	0.72
9:Y:903:LEU:HD11	9:Y:1249:ASN:HD22	1.57	0.69
1:A:138:ILE:O	1:A:180:ARG:HA	1.92	0.69
8:X:840:SER:HB2	8:X:850:ILE:HD11	1.76	0.68
4:G:121:LYS:HA	4:G:124:PRO:HD3	1.77	0.67
8:X:204:LEU:HD13	8:X:208:ILE:HD11	1.77	0.67
9:Y:334:LYS:HA	9:Y:339:ARG:HD2	1.78	0.66
9:Y:961:SER:O	9:Y:980:THR:HA	1.95	0.66
1:A:123:ARG:HG3	1:A:188:PRO:HB2	1.78	0.66
8:X:660:VAL:HG13	8:X:661:VAL:HG13	1.79	0.65
6:U:8:PHE:HB3	6:V:150:ARG:HH12	1.61	0.65
8:X:839:VAL:HG12	8:X:1049:ILE:HG12	1.77	0.65
9:Y:975:ILE:HG22	9:Y:977:SER:H	1.62	0.65
9:Y:152:THR:HG22	9:Y:154:LEU:H	1.62	0.64
9:Y:956:GLY:HA3	9:Y:985:ILE:O	1.98	0.64
4:G:48:GLU:HG2	4:G:61:GLU:HG2	1.80	0.63
6:U:66:HIS:ND1	6:U:67:GLU:O	2.27	0.63
8:X:65:ASN:HB3	8:X:105:TYR:HB2	1.78	0.63
1:A:239:LYS:HB2	1:A:276:TRP:HB3	1.81	0.63
9:Y:586:GLY:HA3	9:Y:612:LEU:HD11	1.81	0.63
9:Y:978:ARG:HA	9:Y:999:TYR:HB2	1.79	0.63
9:Y:58:CYS:SG	9:Y:59:ALA:N	2.73	0.62
8:X:528:ARG:NH2	8:X:576:SER:O	2.32	0.62
9:Y:1174:ARG:NH2	9:Y:1187:GLU:OE1	2.34	0.61
9:Y:803:VAL:HG21	9:Y:1309:ILE:HB	1.83	0.61
8:X:14:ASP:HA	8:X:1183:ALA:HB3	1.83	0.61
1:A:288:MET:HB3	1:A:291:ALA:HB3	1.84	0.59
9:Y:901:ARG:HA	9:Y:908:ILE:HA	1.83	0.59
8:X:538:LEU:HD13	8:X:543:ALA:HB2	1.84	0.58
3:E:12:ALA:HA	3:E:18:ILE:HG13	1.85	0.58
8:X:314:ASN:HD22	8:X:351:LEU:HD22	1.68	0.58
8:X:748:ILE:HD13	8:X:966:ILE:HD13	1.84	0.58
9:Y:172:PHE:HB3	9:Y:175:GLU:HB2	1.86	0.58
8:X:1072:ASN:ND2	8:X:1111:GLN:OE1	2.36	0.58
4:G:136:VAL:O	4:G:143:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:103:VAL:HG12	8:X:117:ILE:HG22	1.84	0.58
3:E:84:VAL:HB	4:G:140:PRO:HB3	1.86	0.58
6:U:91:ARG:NH1	6:U:122:GLU:OE2	2.37	0.58
8:X:143:ARG:NH2	8:X:512:SER:O	2.37	0.58
8:X:148:GLN:O	8:X:453:ILE:HA	2.04	0.58
9:Y:418:GLU:O	9:Y:481:ARG:NH2	2.37	0.58
8:X:936:ARG:NH2	8:X:1043:ALA:O	2.36	0.58
7:W:25:ARG:NH2	7:W:68:GLU:OE1	2.37	0.57
8:X:811:ASN:ND2	8:X:1098:LEU:O	2.37	0.57
8:X:975:ILE:HD11	8:X:994:ARG:HH21	1.69	0.57
9:Y:122:SER:HB3	9:Y:132:LEU:HD12	1.87	0.57
9:Y:573:THR:OG1	9:Y:576:ARG:NH1	2.38	0.57
1:A:168:LEU:HB2	1:A:171:GLU:HG3	1.86	0.57
8:X:868:SER:HB2	8:X:943:LYS:HE3	1.85	0.57
9:Y:883:ARG:NH2	9:Y:898:CYS:SG	2.76	0.57
1:A:307:ILE:HD11	1:A:336:LEU:HD22	1.85	0.57
9:Y:69:GLU:HG2	9:Y:76:LYS:HG3	1.87	0.57
9:Y:1078:LEU:HG	9:Y:1101:LEU:HD11	1.86	0.57
12:R:16:A:H5'	12:R:17:G:H5'	1.85	0.57
2:B:135:ARG:NH1	2:B:139:LYS:O	2.38	0.57
4:G:137:ASN:HA	4:G:143:ASP:H	1.70	0.57
1:A:145:VAL:HA	1:A:150:ILE:HG22	1.86	0.57
6:U:45:ARG:NH2	8:X:1215:GLY:O	2.37	0.57
8:X:143:ARG:NH1	8:X:507:GLY:O	2.38	0.56
8:X:714:VAL:HB	8:X:787:PRO:HD2	1.87	0.56
3:E:8:ILE:HB	3:E:74:VAL:HB	1.87	0.56
9:Y:1239:ASP:OD1	9:Y:1242:ARG:NH2	2.39	0.56
9:Y:568:SER:OG	9:Y:570:LYS:NZ	2.38	0.56
9:Y:709:ARG:HH21	9:Y:711:GLY:HA3	1.70	0.56
8:X:233:ARG:HB3	8:X:237:LEU:HA	1.87	0.56
9:Y:1035:VAL:HG23	9:Y:1115:ILE:HG12	1.86	0.56
6:U:11:PRO:HA	6:U:30:PRO:HG2	1.88	0.56
8:X:811:ASN:HA	8:X:815:SER:HB2	1.88	0.56
9:Y:1272:SER:HB2	9:Y:1292:LEU:HD11	1.88	0.56
9:Y:1024:THR:HG23	9:Y:1123:ARG:HA	1.88	0.56
9:Y:1036:ARG:NH2	9:Y:1085:GLY:O	2.38	0.56
1:A:28:GLU:HB2	1:A:47:VAL:HG13	1.89	0.55
9:Y:460:ASP:N	9:Y:464:ASP:OD2	2.37	0.55
8:X:232:ILE:HG12	8:X:237:LEU:HD22	1.89	0.55
9:Y:1176:VAL:HG22	9:Y:1187:GLU:HG2	1.86	0.55
6:U:45:ARG:HG3	8:X:1083:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:139:ASN:ND2	11:L:27:DG:OP1	2.40	0.55
9:Y:1289:ASN:HD21	9:Y:1300:ALA:H	1.55	0.55
1:A:21:GLU:HA	1:A:24:PHE:HD2	1.72	0.55
9:Y:1161:GLY:HA3	9:Y:1178:THR:O	2.07	0.55
1:A:36:LYS:HG3	1:A:44:ASP:HA	1.89	0.55
1:A:119:ARG:NH2	1:A:189:GLU:O	2.40	0.55
8:X:646:SER:OG	8:X:647:ARG:N	2.39	0.55
9:Y:638:SER:OG	9:Y:639:VAL:N	2.39	0.54
9:Y:959:LYS:HB3	9:Y:983:LYS:HB2	1.89	0.54
1:A:166:ASP:HB3	1:A:198:THR:HA	1.89	0.54
1:A:235:LYS:HG2	1:A:272:ASP:HB2	1.90	0.54
2:B:121:LYS:HB2	12:R:6:U:H5'	1.90	0.54
7:W:7:GLN:OE1	7:W:16:ARG:NH2	2.40	0.54
6:U:231:PHE:HE2	6:V:39:LEU:HD13	1.73	0.54
9:Y:950:ILE:HB	9:Y:1018:ALA:HB3	1.90	0.54
9:Y:975:ILE:H	9:Y:1000:GLY:HA2	1.73	0.54
8:X:720:ARG:HH21	8:X:736:VAL:HG21	1.73	0.54
2:B:21:GLN:O	2:B:24:GLN:NE2	2.40	0.54
3:E:6:ILE:HB	3:E:76:ILE:HB	1.88	0.54
4:G:42:VAL:HG12	4:G:72:GLN:H	1.72	0.54
1:A:239:LYS:HD2	1:A:276:TRP:HD1	1.73	0.53
8:X:176:ILE:HD11	8:X:428:VAL:HG21	1.90	0.53
8:X:1142:ARG:NH2	8:X:1166:ASP:OD1	2.41	0.53
8:X:633:LEU:HA	8:X:645:PHE:O	2.09	0.53
1:A:180:ARG:O	1:A:199:ARG:NH1	2.41	0.53
8:X:221:LEU:HD11	8:X:314:ASN:HB2	1.90	0.53
8:X:1219:GLU:OE1	9:Y:634:ARG:NH1	2.36	0.53
9:Y:1357:ILE:HG23	9:Y:1359:ALA:H	1.73	0.53
1:A:223:ILE:HG12	1:A:238:VAL:HG12	1.90	0.53
8:X:721:GLY:N	8:X:740:GLU:OE1	2.41	0.53
6:V:22:THR:HG1	6:V:207:THR:HG1	1.56	0.53
8:X:817:LEU:HD21	8:X:1080:ASN:HD22	1.72	0.53
9:Y:957:SER:HB3	9:Y:985:ILE:HB	1.91	0.53
3:E:44:THR:OG1	3:E:68:ARG:NH1	2.40	0.53
8:X:1004:ASP:OD1	8:X:1008:GLN:NE2	2.41	0.53
9:Y:741:ALA:O	9:Y:762:ASN:ND2	2.37	0.53
3:E:9:ARG:NH1	3:E:101:SER:OG	2.41	0.53
3:E:12:ALA:O	3:E:69:THR:HA	2.09	0.53
5:N:106:LEU:HD11	8:X:1251:TYR:HE2	1.74	0.53
9:Y:308:ASP:OD2	9:Y:311:ARG:NH1	2.42	0.53
3:E:36:VAL:HG23	3:E:76:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:896:THR:HG22	8:X:898:GLU:H	1.75	0.52
8:X:1313:HIS:HE2	9:Y:380:PHE:HE1	1.57	0.52
8:X:61:SER:HB3	8:X:479:LEU:HD23	1.90	0.52
9:Y:1037:PHE:HB3	9:Y:1040:MET:HB2	1.91	0.52
1:A:132:GLU:O	5:N:45:LYS:NZ	2.43	0.52
9:Y:884:SER:OG	9:Y:885:VAL:N	2.41	0.52
1:A:35:THR:HB	1:A:45:VAL:HG11	1.91	0.52
1:A:306:ASP:HB3	1:A:344:LEU:HD11	1.92	0.51
1:A:320:ARG:NH1	12:R:17:G:OP1	2.43	0.51
8:X:850:ILE:HG13	8:X:1048:LYS:HD2	1.91	0.51
1:A:215:GLU:HA	1:A:218:GLU:HB2	1.92	0.51
1:A:326:ARG:O	1:A:329:SER:HB3	2.10	0.51
9:Y:1167:LYS:NZ	10:K:12:DA:OP1	2.36	0.51
2:B:95:ARG:O	2:B:135:ARG:NH2	2.43	0.51
8:X:69:GLN:HE21	8:X:101:ARG:HD2	1.75	0.51
1:A:323:GLN:O	1:A:326:ARG:HB3	2.10	0.51
9:Y:591:ILE:HG23	9:Y:592:VAL:HG13	1.93	0.51
1:A:162:ILE:HB	1:A:197:VAL:HB	1.93	0.51
9:Y:495:ASN:ND2	9:Y:1247:LYS:O	2.42	0.51
8:X:1073:LYS:NZ	12:R:66:C:OP1	2.42	0.51
8:X:971:LEU:HD23	8:X:974:ARG:HD2	1.91	0.50
9:Y:211:GLU:HG2	9:Y:215:LYS:HE3	1.93	0.50
8:X:1269:ARG:HD3	11:L:21:DC:H5'	1.92	0.50
9:Y:85:CYS:SG	9:Y:87:LYS:N	2.81	0.50
3:E:10:LEU:HB3	3:E:72:ARG:HB2	1.93	0.50
6:U:67:GLU:HB2	6:U:171:LEU:HD22	1.93	0.50
6:V:54:CYS:SG	6:V:148:ARG:NE	2.83	0.50
9:Y:616:PRO:HA	9:Y:619:ILE:HG22	1.93	0.50
9:Y:161:THR:HG23	9:Y:163:GLU:H	1.76	0.50
9:Y:1048:ARG:NH1	9:Y:1110:GLU:OE2	2.43	0.50
1:A:149:ASN:HB3	1:A:163:LEU:HG	1.93	0.50
9:Y:1048:ARG:NH2	9:Y:1057:SER:OG	2.45	0.50
1:A:35:THR:HA	1:A:38:LYS:HD3	1.92	0.50
8:X:985:GLU:HB2	8:X:988:LYS:HE3	1.93	0.50
12:R:64:G:H2'	12:R:65:G:H8	1.76	0.50
9:Y:367:GLY:HA3	9:Y:448:GLN:HB2	1.94	0.50
9:Y:978:ARG:NH2	9:Y:1197:ASN:OD1	2.45	0.49
9:Y:144:TYR:OH	9:Y:293:ARG:NH2	2.46	0.49
4:G:136:VAL:HG22	4:G:178:VAL:HG12	1.93	0.49
6:U:215:GLU:OE2	6:U:219:ARG:NH2	2.46	0.49
8:X:545:PHE:HZ	9:Y:781:LYS:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:230:SER:OG	9:Y:231:GLY:N	2.45	0.49
4:G:94:GLY:HA3	4:G:100:PRO:HA	1.95	0.49
9:Y:44:ILE:HG22	9:Y:51:PRO:HA	1.94	0.49
6:U:32:GLU:HB2	6:U:35:PHE:HD2	1.78	0.49
1:A:320:ARG:NH1	5:N:2:ASP:OD1	2.45	0.49
9:Y:591:ILE:HD11	9:Y:604:MET:HA	1.94	0.49
3:E:44:THR:HG23	3:E:68:ARG:HG3	1.94	0.49
7:W:28:ARG:HH12	8:X:1314:GLN:HA	1.78	0.49
9:Y:814:CYS:SG	9:Y:883:ARG:NH2	2.85	0.49
6:U:214:GLU:OE2	6:U:218:ARG:NE	2.41	0.49
3:E:64:GLN:HG3	3:E:67:ILE:HD11	1.95	0.49
8:X:979:LEU:HD21	8:X:1000:LEU:HD23	1.94	0.49
1:A:185:SER:HB3	1:A:196:PHE:HB2	1.95	0.49
9:Y:381:ILE:HD11	9:Y:412:LEU:HD13	1.94	0.49
9:Y:490:ILE:HD13	9:Y:614:LEU:HD11	1.94	0.48
7:W:43:ASN:O	9:Y:417:ARG:NH1	2.46	0.48
8:X:705:GLU:HB3	8:X:794:LEU:H	1.78	0.48
9:Y:520:ALA:HB3	9:Y:546:ALA:HB2	1.96	0.48
8:X:236:LYS:HD3	8:X:286:GLU:HG2	1.94	0.48
1:A:63:LEU:HA	1:A:92:TYR:HB3	1.94	0.48
5:N:6:ARG:NH2	12:R:18:C:OP1	2.41	0.48
1:A:244:ARG:HB3	2:B:74:LEU:HA	1.96	0.48
10:K:-19:DC:H2"	10:K:-18:DG:C8	2.48	0.48
9:Y:663:GLU:OE2	9:Y:667:GLN:NE2	2.47	0.48
8:X:712:SER:OG	8:X:713:GLY:N	2.47	0.48
1:A:235:LYS:HB3	1:A:331:LEU:HD22	1.96	0.47
6:V:104:LYS:HD3	6:V:110:VAL:HG22	1.95	0.47
9:Y:1106:ILE:O	9:Y:1122:ALA:HA	2.14	0.47
9:Y:1343:GLU:HG2	9:Y:1345:ARG:HE	1.79	0.47
4:G:161:SER:HB2	4:G:168:ALA:HB1	1.96	0.47
6:V:77:ASP:H	6:V:80:GLU:HB2	1.79	0.47
5:N:19:LYS:HA	5:N:22:ASN:HB2	1.96	0.47
6:V:44:ARG:HG3	6:V:183:ILE:HD13	1.96	0.47
9:Y:1178:THR:HA	9:Y:1184:ASP:HB3	1.97	0.47
4:G:21:ARG:NH1	11:L:32:DA:OP1	2.45	0.47
6:U:79:LEU:HD21	8:X:693:LEU:HD11	1.96	0.47
9:Y:734:ALA:O	9:Y:738:ARG:HB2	2.14	0.47
9:Y:73:GLY:O	9:Y:76:LYS:NZ	2.43	0.47
6:V:64:VAL:HG12	6:V:66:HIS:H	1.79	0.47
8:X:302:ILE:HG22	8:X:309:LEU:HA	1.97	0.47
8:X:1275:VAL:HG13	8:X:1287:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:253:VAL:HB	9:Y:261:ALA:HB3	1.96	0.47
9:Y:807:LEU:HD11	9:Y:894:VAL:HG23	1.96	0.47
1:A:216:ILE:HG12	1:A:221:ILE:HB	1.96	0.47
9:Y:1172:LYS:HB2	9:Y:1189:MET:HB3	1.97	0.47
9:Y:930:LEU:HD11	9:Y:1241:TYR:HE1	1.80	0.47
6:U:174:ASP:OD1	6:U:174:ASP:N	2.48	0.47
8:X:232:ILE:HB	8:X:331:LYS:HG2	1.95	0.46
8:X:1245:ALA:HB2	9:Y:372:MET:HG3	1.97	0.46
9:Y:72:CYS:CB	9:Y:87:LYS:HB3	2.45	0.46
4:G:108:VAL:HA	4:G:111:ILE:HG22	1.96	0.46
6:V:102:LEU:O	6:V:141:SER:HA	2.15	0.46
9:Y:1326:GLN:HB2	11:L:17:DA:OP2	2.15	0.46
1:A:266:LEU:HD12	1:A:271:ILE:HD11	1.96	0.46
9:Y:847:ASP:OD1	9:Y:847:ASP:N	2.48	0.46
1:A:261:ALA:O	1:A:264:THR:HB	2.15	0.46
6:V:46:ILE:HD11	6:V:224:LEU:HD13	1.98	0.46
9:Y:1163:VAL:HG13	9:Y:1175:LEU:HD11	1.97	0.46
10:K:2:DT:H2'	10:K:3:DG:C8	2.50	0.46
9:Y:646:ILE:HD11	9:Y:764:ARG:HD3	1.97	0.46
9:Y:1355:ARG:NH1	9:Y:1369:ARG:HH12	2.14	0.46
2:B:121:LYS:NZ	12:R:7:U:O3'	2.48	0.46
6:U:218:ARG:HB3	6:V:234:LEU:HD21	1.98	0.46
3:E:37:ARG:HH22	3:E:77:VAL:H	1.63	0.46
8:X:210:LEU:HD12	8:X:220:ILE:HG12	1.98	0.46
8:X:1072:ASN:N	8:X:1072:ASN:OD1	2.48	0.46
8:X:1101:LEU:HD21	9:Y:508:LEU:HD22	1.98	0.46
9:Y:342:LEU:HD23	9:Y:1352:ILE:HG23	1.98	0.46
9:Y:1230:THR:HG22	9:Y:1257:VAL:HG11	1.97	0.46
1:A:14:ASN:HA	5:N:66:GLN:HE22	1.80	0.46
9:Y:246:PRO:HA	9:Y:247:PRO:HD3	1.78	0.46
9:Y:1027:VAL:HG21	9:Y:1122:ALA:HB3	1.98	0.46
8:X:509:SER:OG	8:X:510:GLN:N	2.49	0.45
1:A:166:ASP:OD1	1:A:201:LYS:NZ	2.50	0.45
9:Y:845:ALA:HA	9:Y:883:ARG:HG3	1.98	0.45
1:A:61:ARG:HG2	1:A:94:GLU:HG3	1.97	0.45
2:B:62:LEU:HD23	2:B:65:LEU:HD12	1.98	0.45
3:E:24:GLU:OE2	5:N:47:ARG:NH2	2.49	0.45
9:Y:74:LYS:NZ	9:Y:86:GLU:OE2	2.50	0.45
9:Y:885:VAL:HG11	9:Y:1255:VAL:HG23	1.97	0.45
4:G:38:LEU:HD12	4:G:74:VAL:HG21	1.98	0.45
9:Y:149:GLY:HA2	9:Y:176:PHE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:824:PRO:HD3	9:Y:835:LEU:HD12	1.97	0.45
1:A:327:LEU:O	1:A:331:LEU:N	2.50	0.45
8:X:228:VAL:HG23	8:X:337:PHE:HB2	1.99	0.45
8:X:607:SER:OG	8:X:608:ALA:N	2.50	0.45
9:Y:973:LEU:HB3	9:Y:1003:LEU:HB2	1.98	0.45
12:R:64:G:H2'	12:R:65:G:C8	2.52	0.45
1:A:232:SER:O	12:R:15:A:N6	2.49	0.45
2:B:9:ALA:HB2	2:B:44:ASP:H	1.81	0.45
8:X:57:PHE:HD2	8:X:70:TYR:HB2	1.82	0.45
8:X:559:CYS:HB2	8:X:662:SER:HB3	1.99	0.45
9:Y:317:THR:HB	9:Y:324:LEU:HD11	1.98	0.45
9:Y:543:SER:OG	9:Y:544:LEU:N	2.49	0.45
9:Y:664:ILE:HG22	9:Y:678:ARG:HG2	1.99	0.45
9:Y:1030:GLU:HG3	9:Y:1090:ILE:HG12	1.99	0.45
6:V:61:ILE:HG22	6:V:63:GLY:H	1.81	0.45
8:X:202:ARG:NH1	8:X:369:MET:O	2.50	0.45
3:E:52:LEU:HD23	12:R:14:U:H3	1.82	0.45
6:V:48:LEU:HD22	9:Y:535:ARG:HG3	1.97	0.45
8:X:290:GLU:O	8:X:293:ALA:HB2	2.17	0.45
9:Y:504:GLN:OE1	9:Y:731:ARG:NH1	2.40	0.44
1:A:349:GLN:O	1:A:353:HIS:ND1	2.37	0.44
9:Y:362:ARG:H	9:Y:365:GLN:HE21	1.65	0.44
9:Y:513:MET:HE1	9:Y:579:LEU:HD13	1.99	0.44
3:E:27:GLU:HA	3:E:30:LYS:HE3	1.99	0.44
8:X:61:SER:HB2	8:X:480:SER:HA	1.99	0.44
2:B:85:LEU:HD21	2:B:123:VAL:HA	1.99	0.44
9:Y:1266:ILE:HD12	9:Y:1278:GLU:HB3	2.00	0.44
9:Y:850:LYS:HB2	9:Y:857:LEU:HB2	1.98	0.44
8:X:319:LEU:HD23	8:X:322:LEU:HD12	1.99	0.44
1:A:59:PHE:HD2	1:A:61:ARG:HH21	1.64	0.44
8:X:23:ASP:OD1	8:X:23:ASP:N	2.51	0.44
8:X:838:CYS:HB2	8:X:918:LEU:HD22	1.98	0.44
1:A:178:ARG:HD3	4:G:164:ILE:HG13	1.99	0.44
6:U:191:ARG:HH12	6:U:193:GLU:HA	1.82	0.44
9:Y:915:ILE:HA	9:Y:918:ILE:HG12	2.00	0.44
8:X:982:GLY:HA3	8:X:1002:LEU:HD21	2.00	0.44
9:Y:876:SER:HB2	9:Y:990:ARG:HE	1.83	0.44
9:Y:983:LYS:HB3	9:Y:985:ILE:HD11	2.00	0.44
8:X:12:ARG:O	8:X:1157:GLN:NE2	2.50	0.43
8:X:303:ASP:N	8:X:308:GLU:O	2.45	0.43
8:X:864:LYS:HD3	8:X:877:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:25:DA:H2'	11:L:26:DC:C6	2.53	0.43
12:R:33:A:H2'	12:R:34:A:H8	1.82	0.43
8:X:1160:ASP:OD1	8:X:1160:ASP:N	2.51	0.43
9:Y:85:CYS:SG	9:Y:86:GLU:N	2.91	0.43
9:Y:249:LEU:HD13	9:Y:249:LEU:HA	1.89	0.43
8:X:484:LEU:HB2	8:X:487:LEU:HG	2.00	0.43
8:X:1280:ALA:HB1	9:Y:918:ILE:HG22	2.00	0.43
9:Y:1155:ILE:HB	9:Y:1210:ILE:HB	2.01	0.43
1:A:67:GLU:HG2	1:A:69:THR:H	1.84	0.43
1:A:268:GLY:O	12:R:15:A:N6	2.51	0.43
2:B:76:GLU:OE2	3:E:16:ARG:NH2	2.51	0.43
6:V:33:ARG:NH1	8:X:1081:PRO:HG3	2.34	0.43
8:X:1132:LEU:HD11	8:X:1173:ALA:HB1	2.00	0.43
11:L:7:DA:H8	11:L:7:DA:OP2	2.00	0.43
6:U:25:LYS:HA	6:U:203:ILE:O	2.19	0.43
8:X:562:GLU:OE1	8:X:662:SER:OG	2.29	0.43
9:Y:982:LEU:O	9:Y:994:SER:HA	2.19	0.43
2:B:18:TYR:OH	3:E:19:ASP:OD1	2.37	0.43
9:Y:377:PHE:HE2	9:Y:416:ILE:HD13	1.84	0.43
1:A:232:SER:HA	12:R:16:A:H61	1.84	0.43
8:X:618:GLN:HE21	9:Y:769:VAL:HB	1.84	0.43
8:X:880:GLY:H	8:X:920:VAL:HB	1.84	0.42
9:Y:1369:ARG:O	9:Y:1372:ARG:HB3	2.18	0.42
6:V:212:ASP:N	6:V:212:ASP:OD1	2.50	0.42
8:X:565:GLU:HA	8:X:569:ILE:HG12	2.01	0.42
7:W:32:VAL:HG21	8:X:1312:ASN:ND2	2.35	0.42
8:X:633:LEU:HD13	8:X:644:LEU:HD23	2.00	0.42
2:B:35:LEU:HA	2:B:40:VAL:HG11	2.01	0.42
6:V:190:ALA:HB2	6:V:200:LYS:HB2	2.01	0.42
9:Y:460:ASP:HB3	9:Y:462:ASP:CG	2.40	0.42
9:Y:845:ALA:HB3	9:Y:881:LYS:HG2	2.02	0.42
1:A:270:ARG:NH2	12:R:13:U:O2	2.52	0.42
1:A:324:ASN:O	1:A:327:LEU:HB2	2.19	0.42
2:B:54:GLY:HA3	2:B:90:TYR:CZ	2.55	0.42
6:U:218:ARG:NH1	6:V:233:ASP:O	2.52	0.42
8:X:301:TYR:OH	8:X:334:GLU:OE1	2.36	0.42
8:X:699:LEU:HG	8:X:799:ASN:ND2	2.34	0.42
9:Y:1234:VAL:O	9:Y:1238:GLN:HB2	2.20	0.42
8:X:596:ASP:OD1	8:X:596:ASP:N	2.53	0.42
8:X:616:ILE:HG21	8:X:637:ARG:HH21	1.85	0.42
8:X:1103:VAL:HG22	8:X:1111:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:LEU:HD12	3:E:43:PRO:HD2	2.02	0.42
6:U:104:LYS:HG2	6:U:110:VAL:HG22	2.00	0.42
9:Y:423:LEU:HD13	9:Y:437:PHE:HD2	1.85	0.42
2:B:74:LEU:HD12	12:R:8:U:H3'	2.01	0.41
5:N:7:ARG:NH2	12:R:21:U:OP2	2.36	0.41
8:X:60:GLN:HB3	8:X:67:GLU:HG3	2.02	0.41
8:X:1122:LYS:HE3	8:X:1229:TYR:CE2	2.55	0.41
9:Y:430:HIS:HB3	9:Y:925:GLU:HG3	2.01	0.41
8:X:471:VAL:HG21	8:X:498:ILE:HG13	2.03	0.41
8:X:989:LEU:O	8:X:997:TRP:NE1	2.53	0.41
9:Y:848:VAL:HG21	9:Y:880:VAL:HG13	2.01	0.41
2:B:21:GLN:NE2	2:B:79:GLN:O	2.50	0.41
6:V:197:ASP:N	6:V:197:ASP:OD1	2.52	0.41
8:X:1122:LYS:HE3	8:X:1229:TYR:HE2	1.85	0.41
9:Y:1161:GLY:CA	9:Y:1178:THR:O	2.67	0.41
8:X:118:LYS:NZ	8:X:485:ASP:O	2.39	0.41
8:X:196:VAL:HG21	8:X:209:ILE:HG21	2.02	0.41
6:U:52:PRO:HB3	6:V:5:VAL:HG11	2.02	0.41
8:X:811:ASN:O	8:X:1099:ASN:ND2	2.53	0.41
9:Y:247:PRO:HA	9:Y:250:ARG:HD3	2.01	0.41
6:V:182:ARG:O	6:V:205:MET:HA	2.20	0.41
7:W:5:THR:HG21	9:Y:615:LYS:HD3	2.01	0.41
8:X:529:ARG:HH11	8:X:572:ILE:HG22	1.85	0.41
9:Y:145:VAL:HG12	9:Y:159:ILE:HG22	2.03	0.41
9:Y:814:CYS:HB2	9:Y:889:ASP:HB3	2.01	0.41
10:K:-13:DG:H8	10:K:-13:DG:OP2	2.03	0.41
3:E:47:GLU:OE2	3:E:69:THR:HG21	2.21	0.41
4:G:103:ILE:HD12	4:G:103:ILE:HA	1.94	0.41
4:G:161:SER:HA	4:G:169:THR:O	2.21	0.41
1:A:143:LYS:HD3	1:A:153:ASP:HB2	2.03	0.41
1:A:231:GLY:O	12:R:16:A:N6	2.54	0.41
1:A:259:VAL:O	1:A:263:SER:N	2.52	0.41
8:X:255:ILE:HB	8:X:263:VAL:HB	2.02	0.41
1:A:87:LEU:HD11	1:A:93:VAL:HB	2.02	0.41
1:A:325:VAL:O	1:A:328:ALA:HB3	2.21	0.41
6:U:156:SER:HA	6:U:159:ILE:HD12	2.02	0.41
6:V:83:LEU:HD11	9:Y:526:VAL:HB	2.02	0.41
6:V:102:LEU:HB3	6:V:142:MET:HG2	2.02	0.41
9:Y:316:ILE:HD12	9:Y:321:LYS:HD2	2.02	0.41
9:Y:1090:ILE:HD11	9:Y:1097:ALA:HB2	2.02	0.41
9:Y:1184:ASP:OD1	9:Y:1184:ASP:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:6:DT:H2'	11:L:6:DT:OP2	2.20	0.41
6:V:100:LEU:HD21	6:V:121:VAL:HG11	2.03	0.41
7:W:46:THR:HA	7:W:49:ILE:HG22	2.03	0.41
8:X:503:LYS:HE2	8:X:503:LYS:HB3	1.94	0.41
9:Y:161:THR:HG22	9:Y:164:GLN:NE2	2.35	0.41
9:Y:533:ALA:HB1	9:Y:574:VAL:HG13	2.03	0.41
9:Y:658:GLU:HA	9:Y:661:VAL:HG22	2.03	0.41
9:Y:965:SER:HB3	9:Y:975:ILE:HG12	2.02	0.41
8:X:217:THR:HG23	8:X:351:LEU:HD11	2.03	0.40
9:Y:442:ILE:HD13	9:Y:442:ILE:HA	1.83	0.40
12:R:22:G:H21	12:R:26:A:H62	1.69	0.40
4:G:92:PHE:HD2	4:G:100:PRO:HG3	1.87	0.40
6:V:185:TYR:HA	6:V:202:VAL:O	2.21	0.40
8:X:72:SER:OG	8:X:73:TYR:N	2.54	0.40
8:X:868:SER:OG	8:X:942:ASP:OD2	2.32	0.40
9:Y:961:SER:HB2	9:Y:981:GLU:HB3	2.02	0.40
3:E:47:GLU:HB2	3:E:67:ILE:HB	2.03	0.40
8:X:10:ARG:HD3	8:X:1181:PRO:HG2	2.03	0.40
1:A:36:LYS:HB2	1:A:45:VAL:HG12	2.02	0.40
8:X:1307:ASN:OD1	8:X:1312:ASN:HB3	2.22	0.40
9:Y:47:ARG:HH22	10:K:-13:DG:H4'	1.86	0.40
9:Y:124:ILE:HG22	9:Y:135:ILE:HD13	2.03	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	418/497 (84%)	401 (96%)	17 (4%)	0	100	100
2	B	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
3	E	92/106 (87%)	85 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	G	168/184 (91%)	154 (92%)	13 (8%)	1 (1%)	25 62
5	N	108/110 (98%)	100 (93%)	8 (7%)	0	100 100
6	U	228/329 (69%)	203 (89%)	25 (11%)	0	100 100
6	V	216/329 (66%)	201 (93%)	14 (6%)	1 (0%)	29 66
7	W	88/91 (97%)	83 (94%)	5 (6%)	0	100 100
8	X	1339/1342 (100%)	1224 (91%)	115 (9%)	0	100 100
9	Y	1333/1417 (94%)	1219 (91%)	113 (8%)	1 (0%)	51 83
All	All	4127/4546 (91%)	3805 (92%)	319 (8%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	V	94	GLY
4	G	124	PRO
9	Y	120	LEU

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	351/408 (86%)	350 (100%)	1 (0%)	92 96
2	B	116/116 (100%)	112 (97%)	4 (3%)	37 64
3	E	85/92 (92%)	85 (100%)	0	100 100
4	G	151/160 (94%)	148 (98%)	3 (2%)	55 74
5	N	96/96 (100%)	95 (99%)	1 (1%)	76 86
6	U	198/286 (69%)	198 (100%)	0	100 100
6	V	189/286 (66%)	188 (100%)	1 (0%)	88 94
7	W	74/75 (99%)	74 (100%)	0	100 100
8	X	1156/1157 (100%)	1147 (99%)	9 (1%)	81 89
9	Y	1122/1178 (95%)	1114 (99%)	8 (1%)	84 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3538/3854 (92%)	3511 (99%)	27 (1%)	82 89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
2	B	105	ASN
2	B	121	LYS
2	B	124	ASN
2	B	139	LYS
4	G	58	ARG
4	G	59	LYS
4	G	112	MET
5	N	10	ARG
6	V	183	ILE
8	X	161	LYS
8	X	202	ARG
8	X	332	ARG
8	X	731	ARG
8	X	943	LYS
8	X	991	LYS
8	X	1033	ARG
8	X	1156	ARG
8	X	1312	ASN
9	Y	190	LYS
9	Y	250	ARG
9	Y	309	ASN
9	Y	431	ARG
9	Y	599	LYS
9	Y	798	ARG
9	Y	836	ARG
9	Y	1341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
2	B	105	ASN
3	E	3	ASN
5	N	15	GLN
6	V	132	HIS

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Mol	Chain	Res	Type
8	X	69	GLN
8	X	437	ASN
8	X	618	GLN
8	X	1080	ASN
8	X	1312	ASN
9	Y	164	GLN
9	Y	1289	ASN
9	Y	1350	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	45/66 (68%)	14 (31%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	6	U
12	R	7	U
12	R	8	U
12	R	10	A
12	R	11	C
12	R	13	U
12	R	14	U
12	R	15	A
12	R	16	A
12	R	25	G
12	R	36	A
12	R	59	C
12	R	60	G
12	R	61	U

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

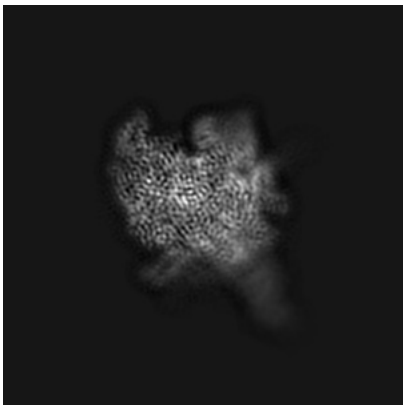
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0043. These allow visual inspection of the internal detail of the map and identification of artifacts.

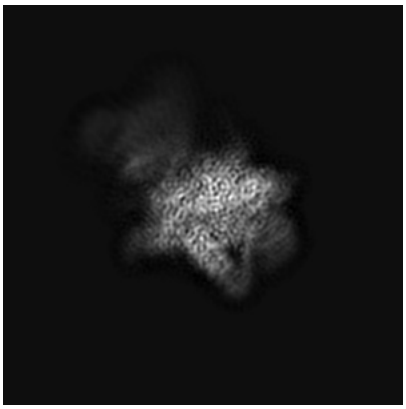
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

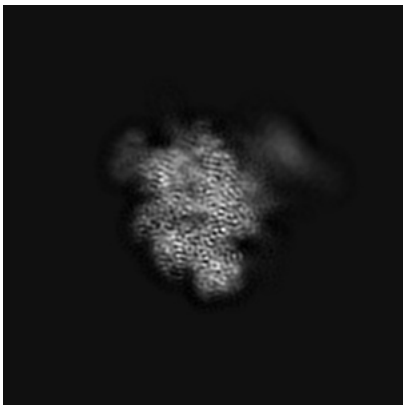
6.1.1 Primary map



X

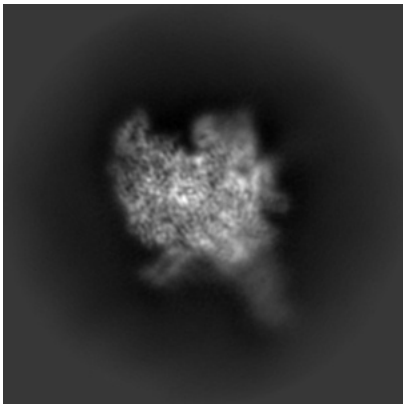


Y

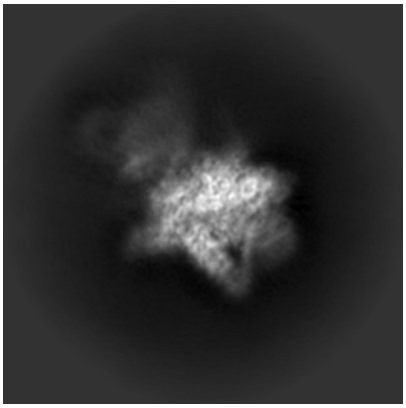


Z

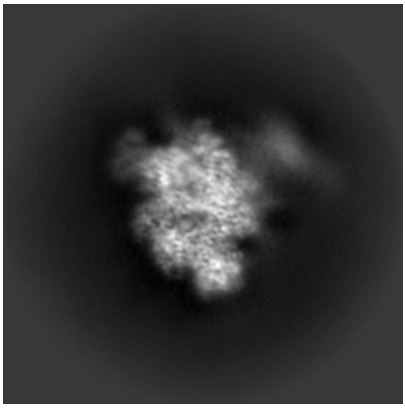
6.1.2 Raw map



X



Y

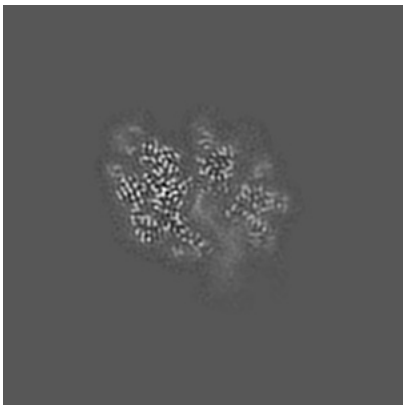


Z

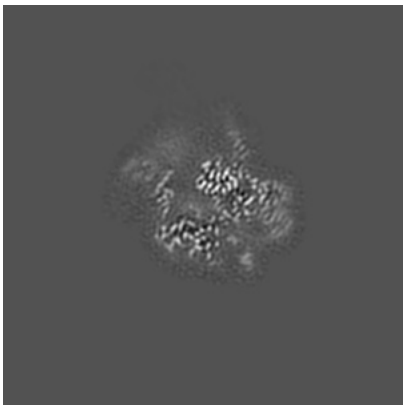
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

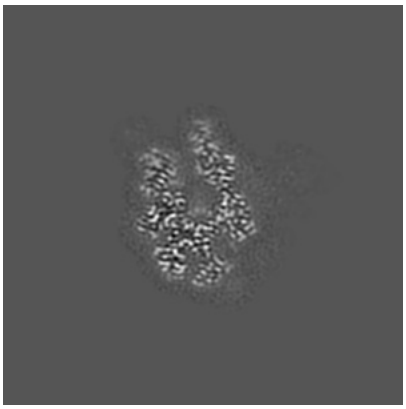
6.2.1 Primary map



X Index: 120

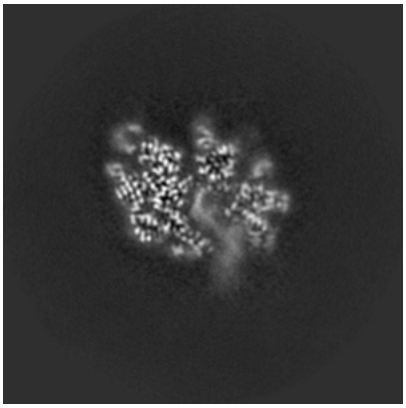


Y Index: 120

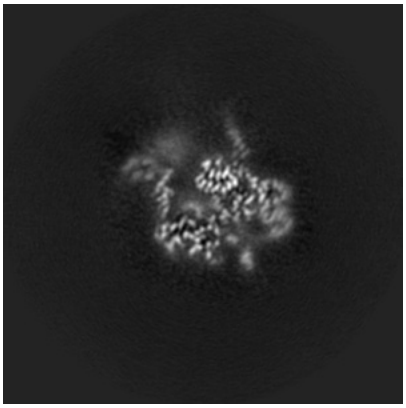


Z Index: 120

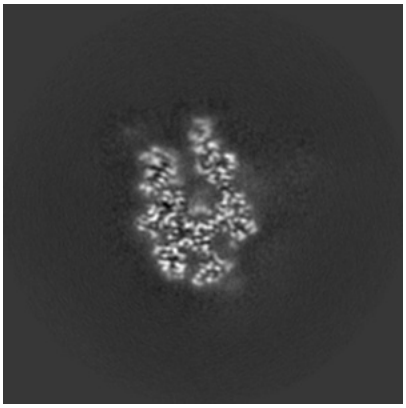
6.2.2 Raw map



X Index: 120



Y Index: 120

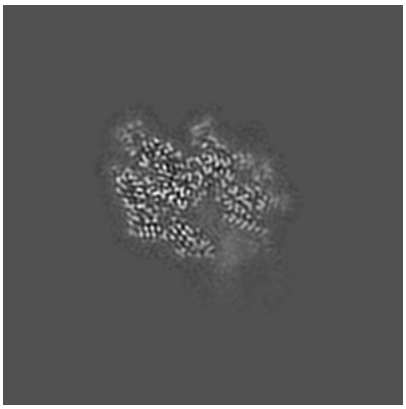


Z Index: 120

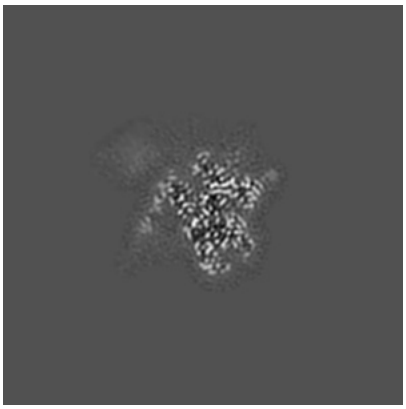
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

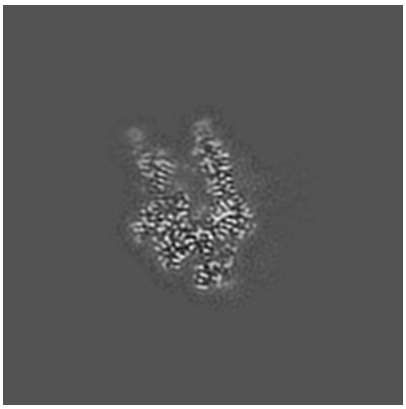
6.3.1 Primary map



X Index: 124

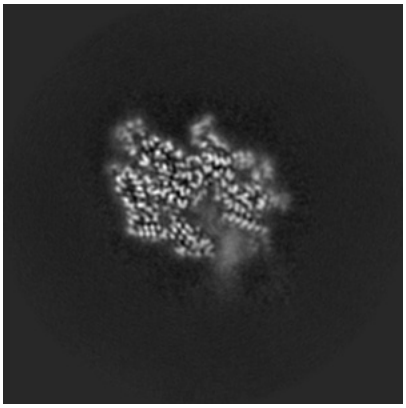


Y Index: 105

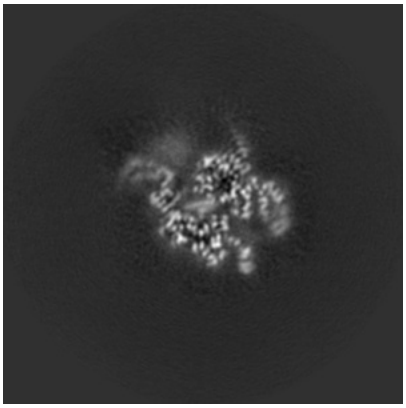


Z Index: 124

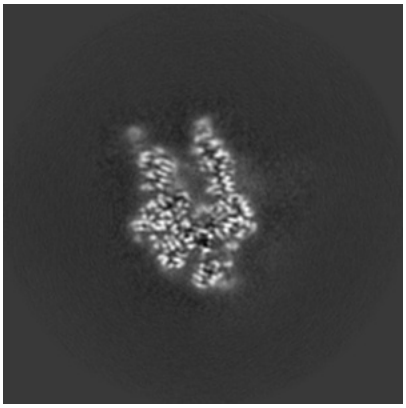
6.3.2 Raw map



X Index: 124



Y Index: 117



Z Index: 123

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

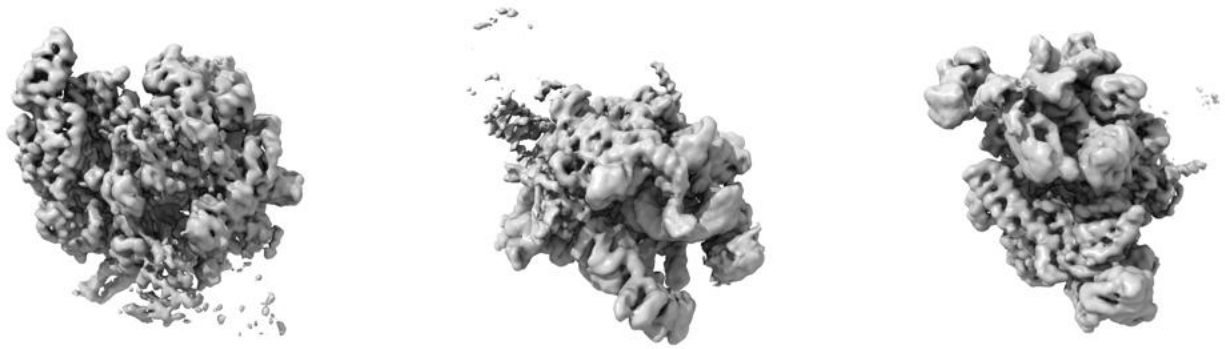
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

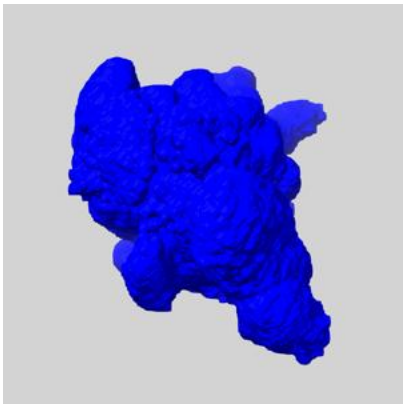
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

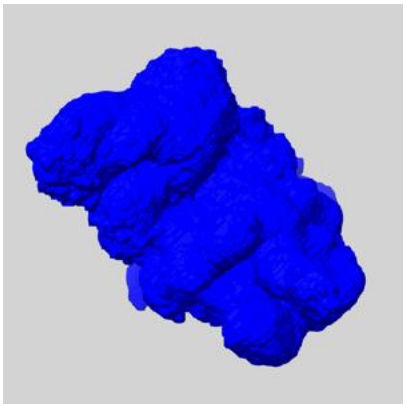
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

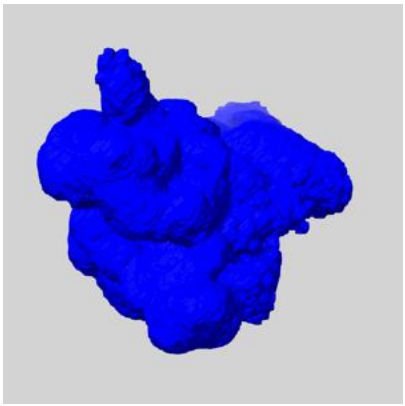
6.5.1 emd_0043_msk_1.map (i)



X



Y

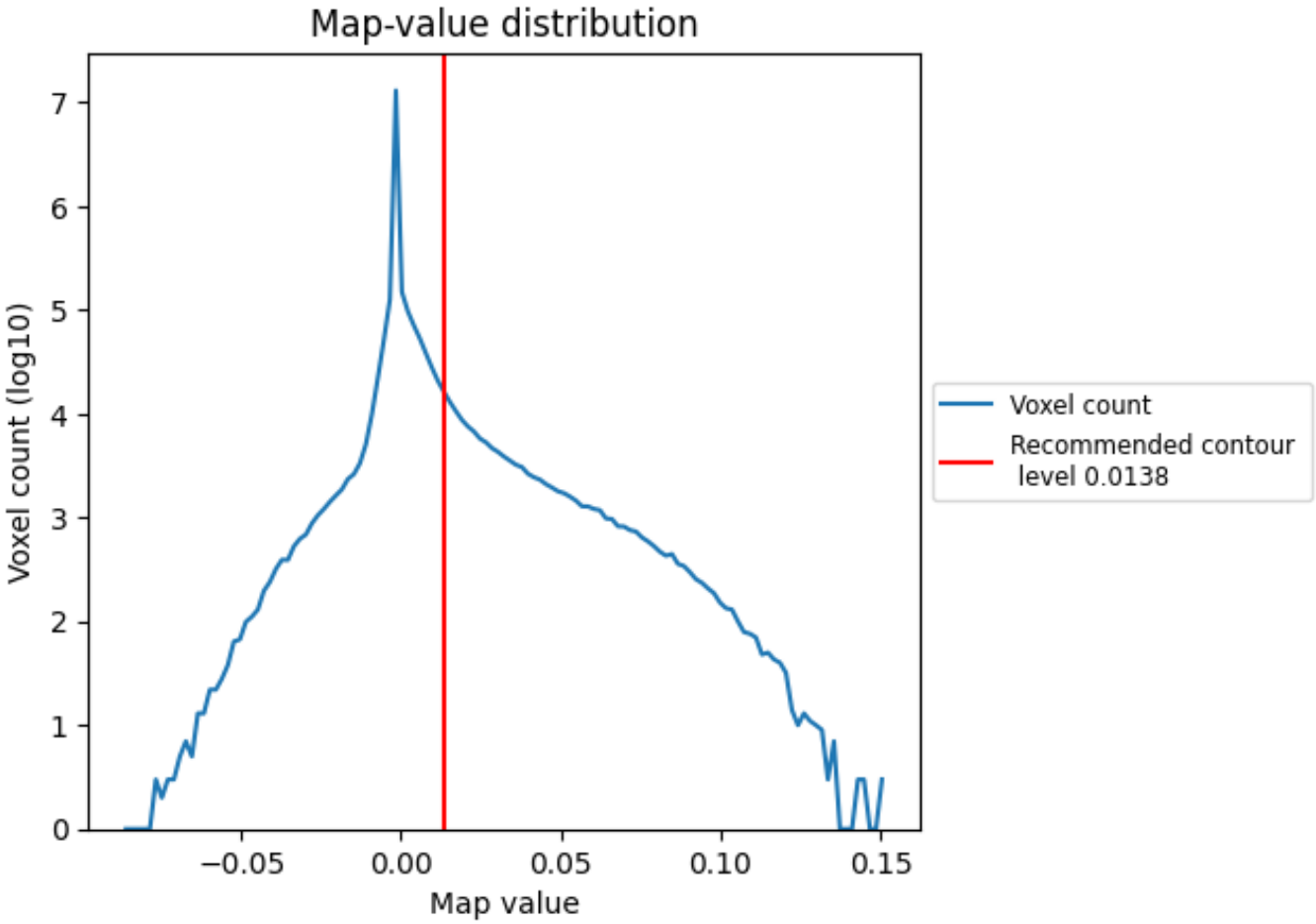


Z

7 Map analysis

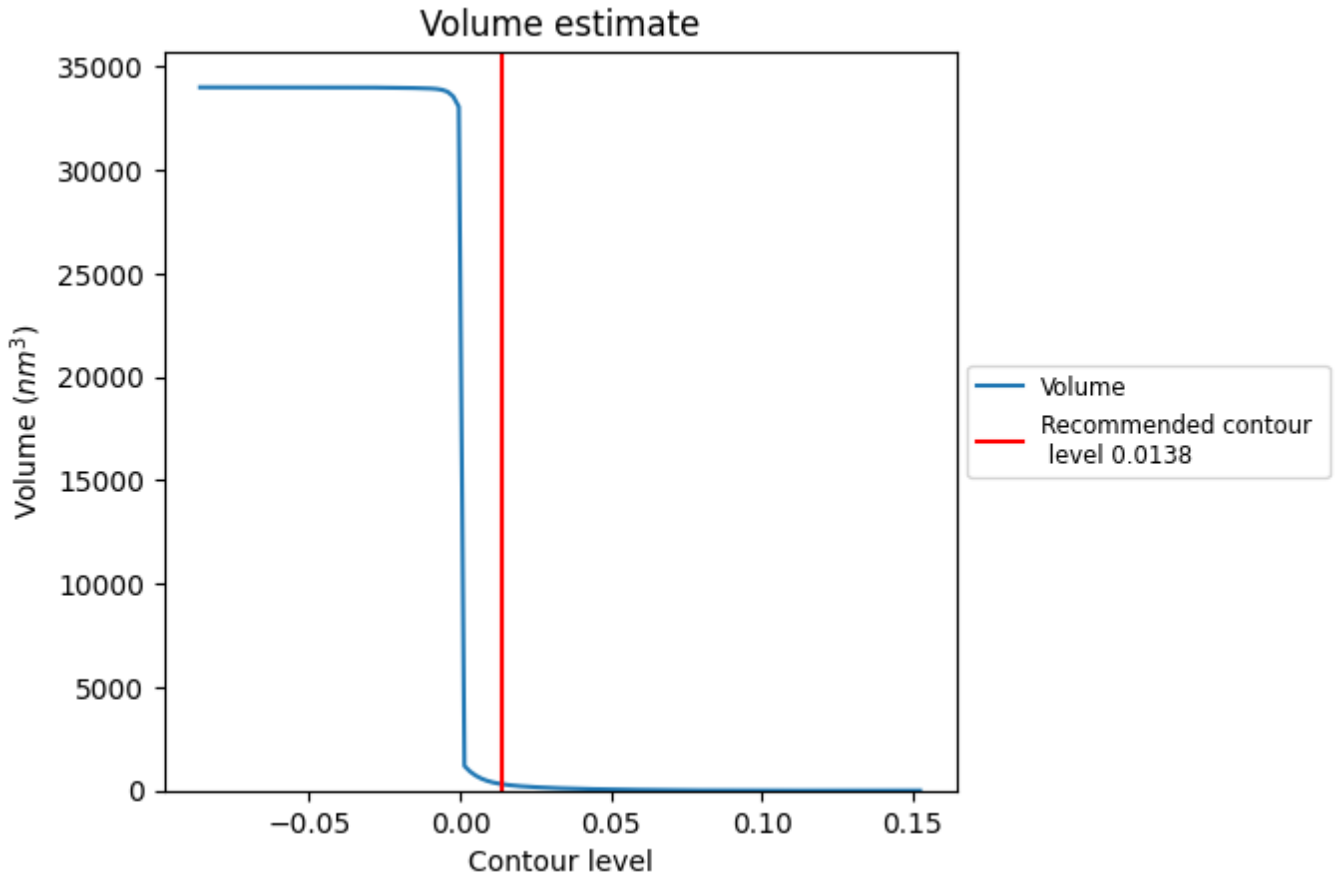
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

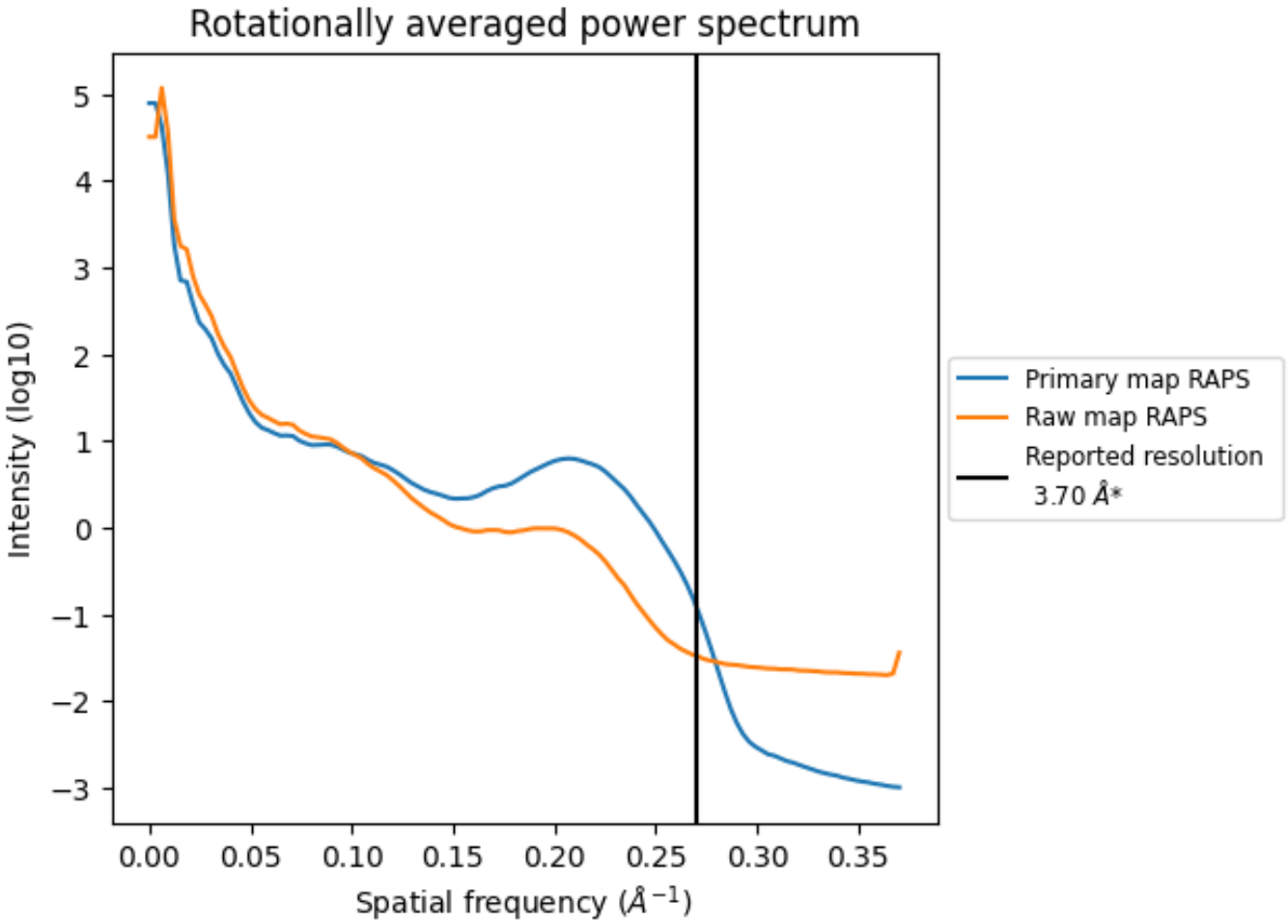
7.2 Volume estimate



The volume at the recommended contour level is 314 nm^3; this corresponds to an approximate mass of 284 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)

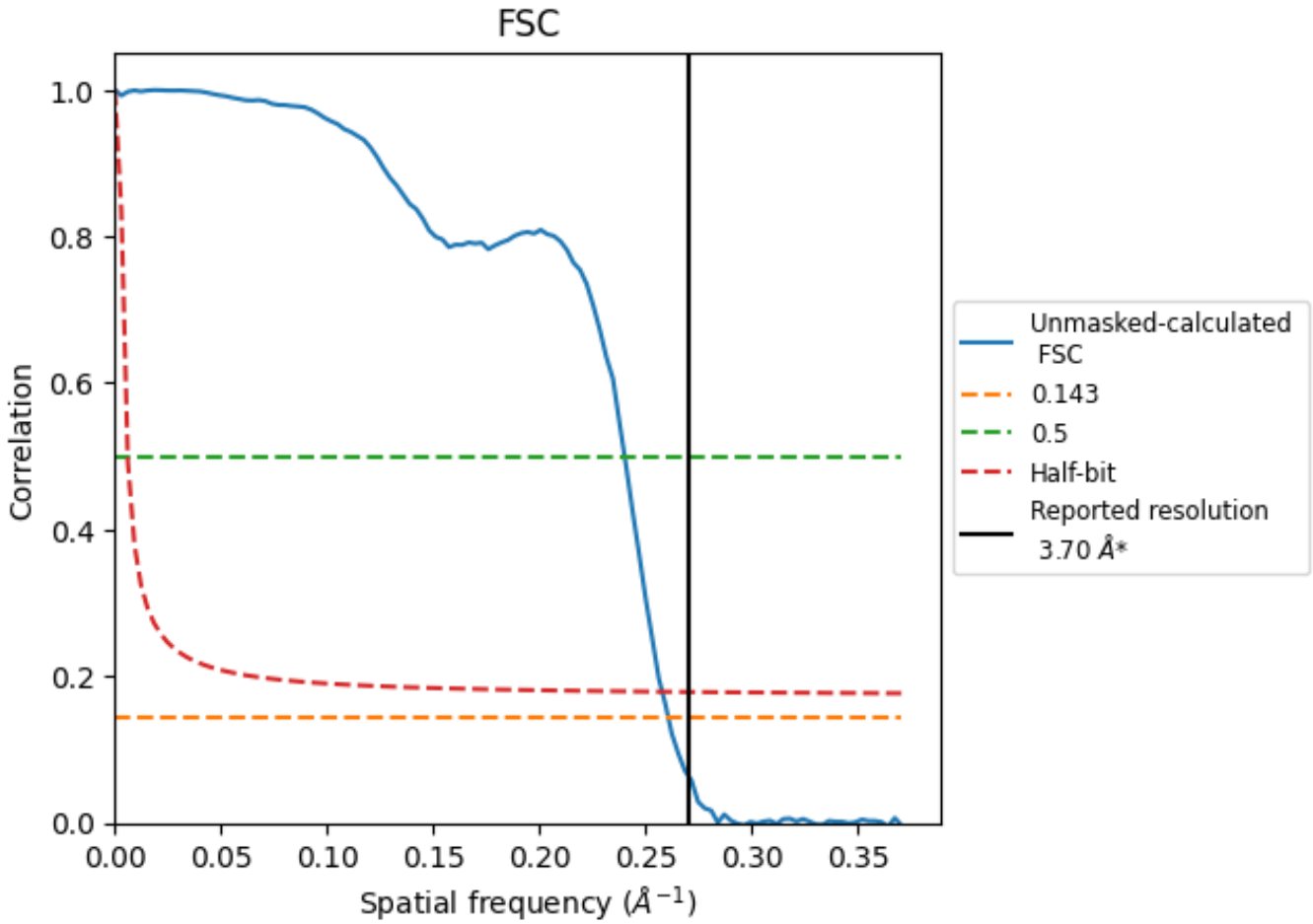


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

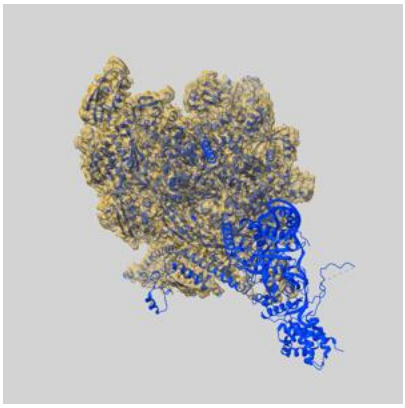
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	4.16	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

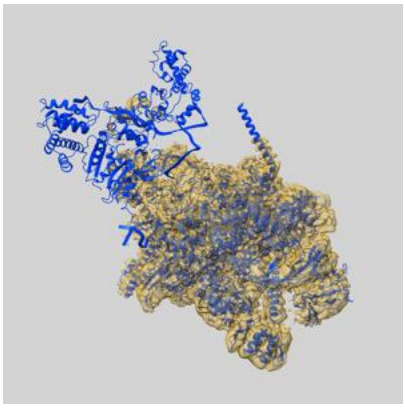
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0043 and PDB model 6GOV. Per-residue inclusion information can be found in section 3 on page 8.

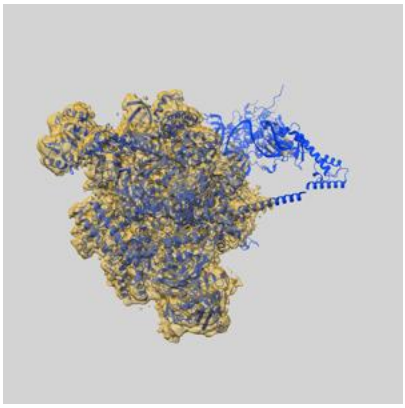
9.1 Map-model overlay



X



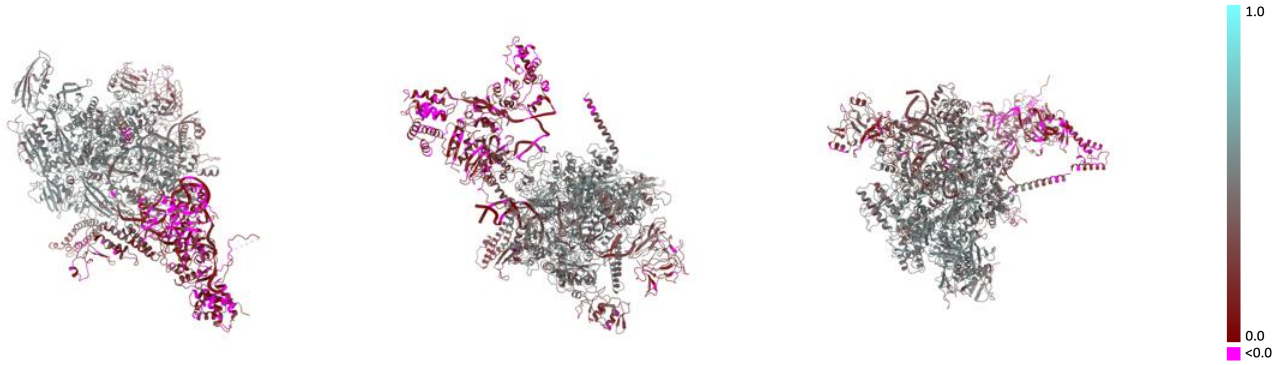
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138 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.

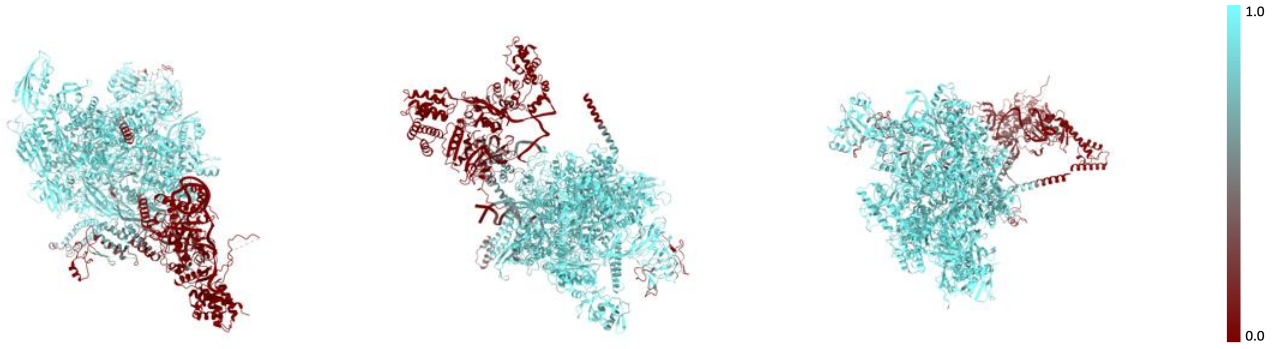
9.2 Q-score mapped to coordinate model



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.

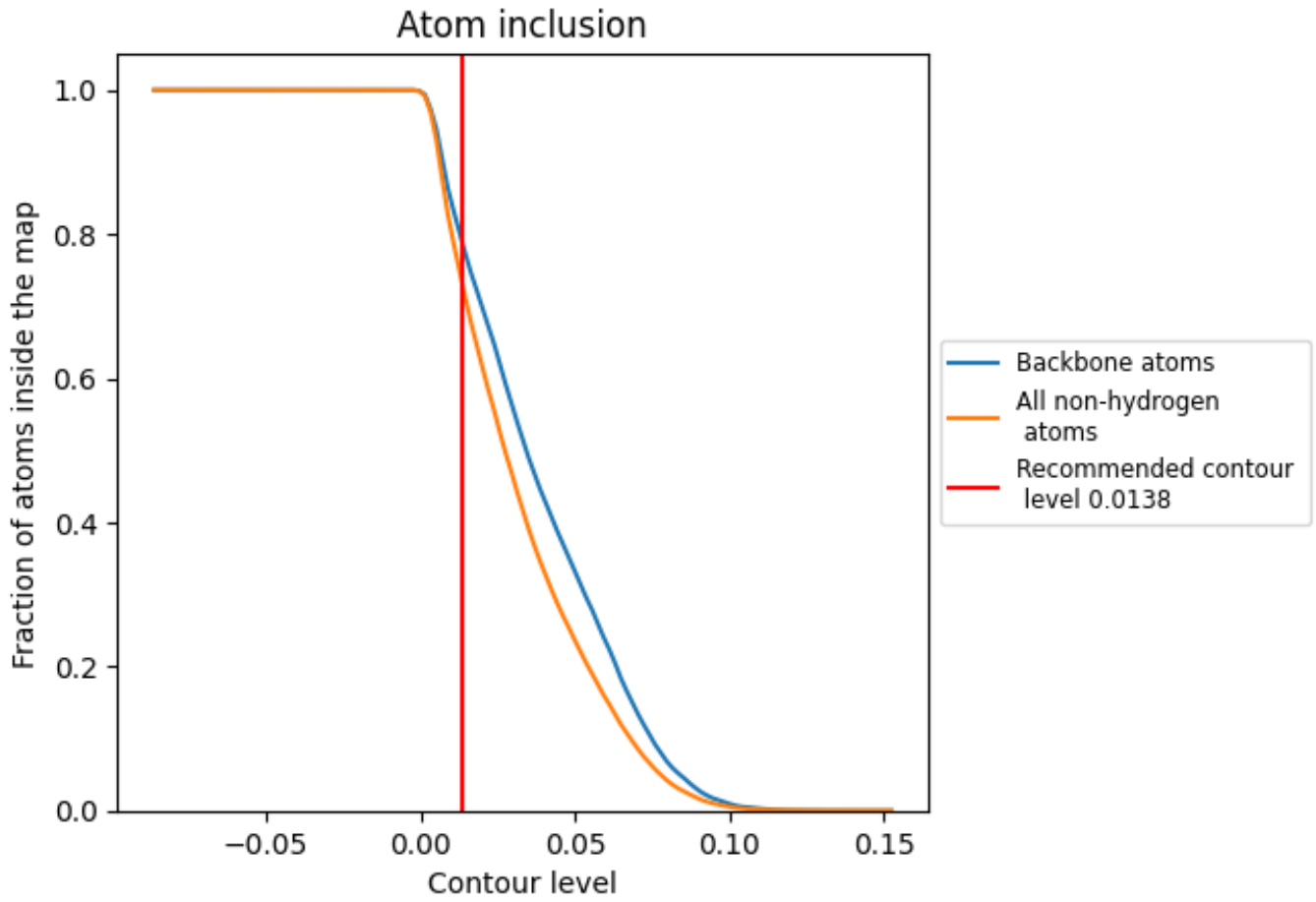
9.3 Atom inclusion mapped to coordinate model



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 (0.0138).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.0138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7256	0.3690
A	0.1401	0.1290
B	0.0000	0.0810
E	0.0053	0.0740
G	0.4710	0.2960
K	0.7504	0.2330
L	0.7995	0.2830
N	0.3345	0.2290
R	0.2138	0.1440
U	0.9451	0.4910
V	0.9273	0.4590
W	0.6604	0.4120
X	0.9109	0.4510
Y	0.8972	0.4320