Full wwPDB EM Validation Report ⓘ

Jun 12, 2023 – 10:22 PM JST

PDB ID	:	8HYJ
EMDB ID	:	EMD-35086
Title	:	A cryo-EM structure of KTF1-bound polymerase V transcription elongation complex
Authors	:	Zhang, H.; Zhang, Y.
Deposited on	:	2023-01-06
Resolution	:	4.30 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 ⓘ 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:

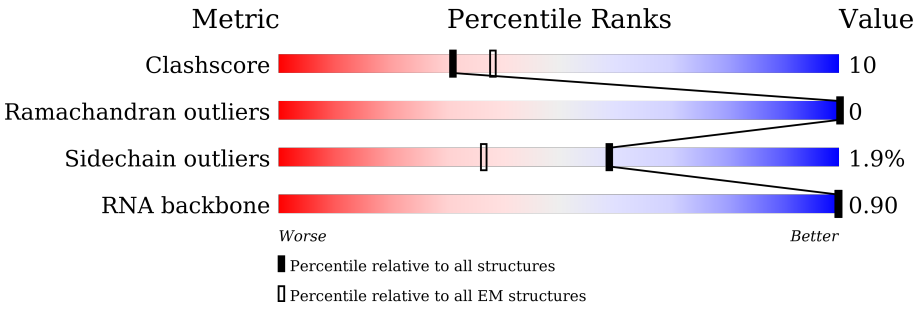
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 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	1976	45% 13% 42%
2	B	1172	73% 16% • 10%
3	C	319	70% 18% • 11%
4	D	205	7% 39% 18% 43%
5	E	222	71% 23% 6%
6	F	144	43% 10% 47%
7	G	178	15% 75% 25%

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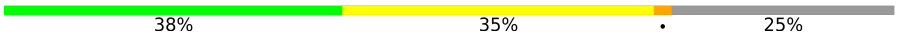
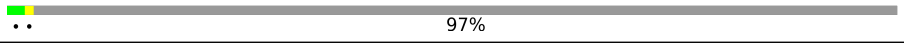
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	114	
10	J	71	
11	K	116	
12	L	51	
13	N	48	
14	P	30	
15	T	48	
16	W	1493	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 28568 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 V subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1141	8794	5540	1526	1672	56	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerases IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1054	7912	5047	1426	1400	39	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases IV and V subunit 3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	285	2123	1351	360	398	14	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases IV and V subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	117	896	566	142	181	7	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase V subunit 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1652	1050	283	316	3	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases II, IV and V subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	76	554	355	97	99	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	178	Total	C	N	O	S	0	0
			1417	926	227	253	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases II and V subunit 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			904	597	142	160	5		

- Molecule 9 is a protein called DNA-directed RNA polymerases II, IV and V subunit 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	98	Total	C	N	O	S	0	0
			702	436	131	124	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	62	Total	C	N	O	S	0	0
			484	316	83	79	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases II, IV and V subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			756	482	138	135	1		

- Molecule 12 is a protein called DNA-directed RNA polymerases II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	42	Total	C	N	O	S	0	0
			309	192	54	59	4		

- Molecule 13 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	36	Total	C	N	O	P	0	0
			749	356	139	218	36		

- Molecule 14 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	10	Total	C	N	O	P	0	0
			218	97	42	69	10		

- Molecule 15 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	37	Total	C	N	O	P	0	0
			746	356	133	220	37		

- Molecule 16 is a protein called Protein RNA-directed DNA methylation 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	44	Total	C	N	O	S	0	0
			347	223	63	60	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

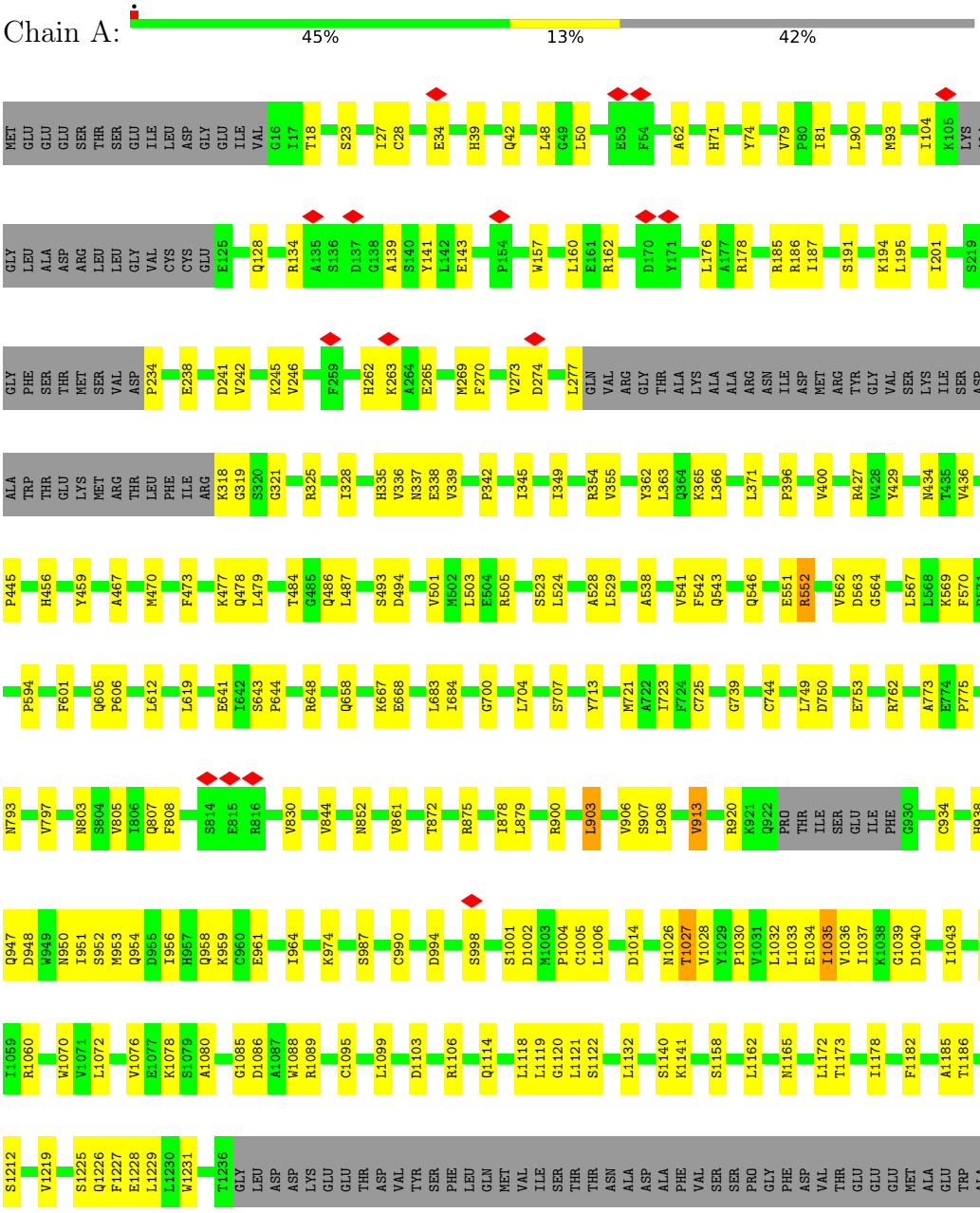
Mol	Chain	Residues	Atoms		AltConf
18	C	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

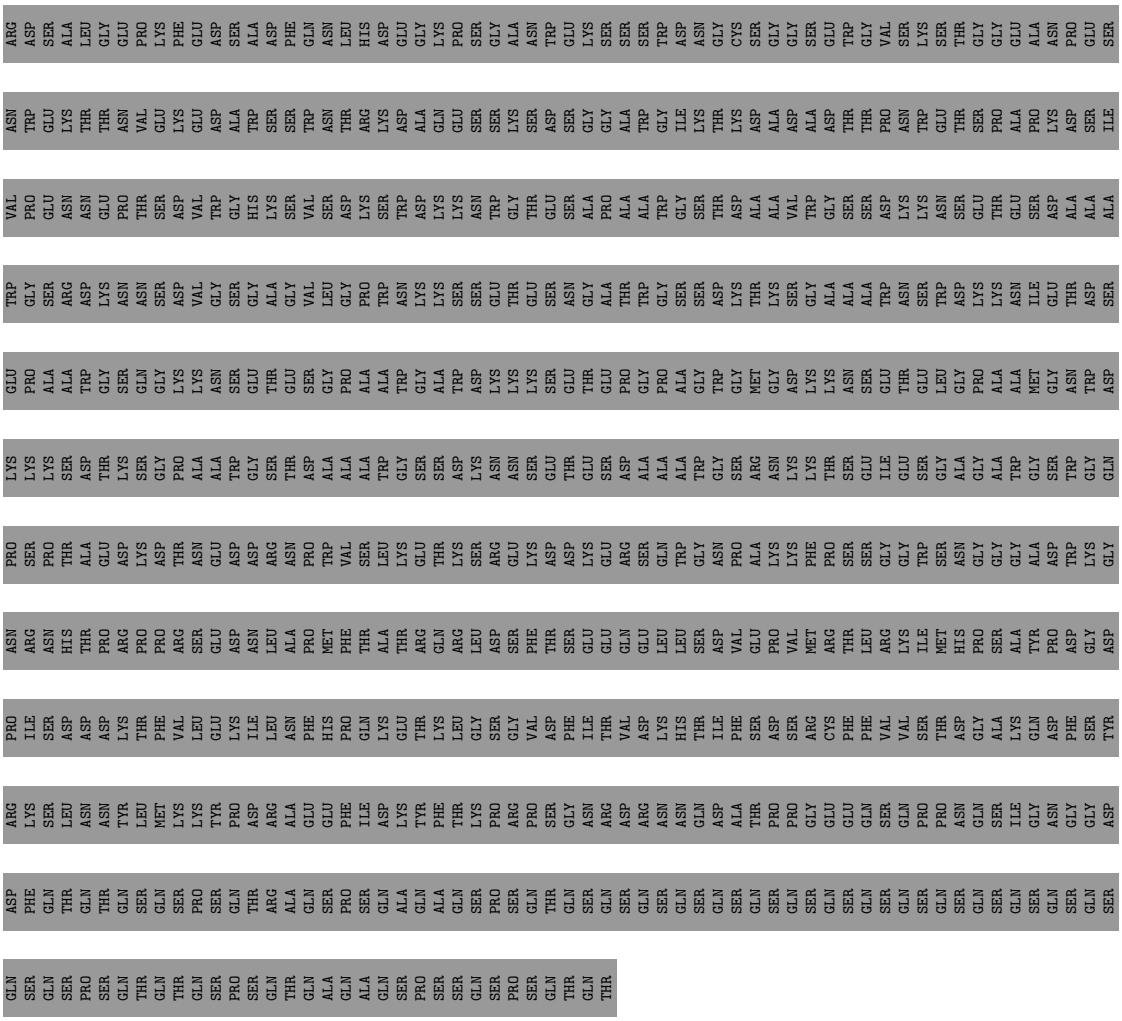
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase V subunit 1

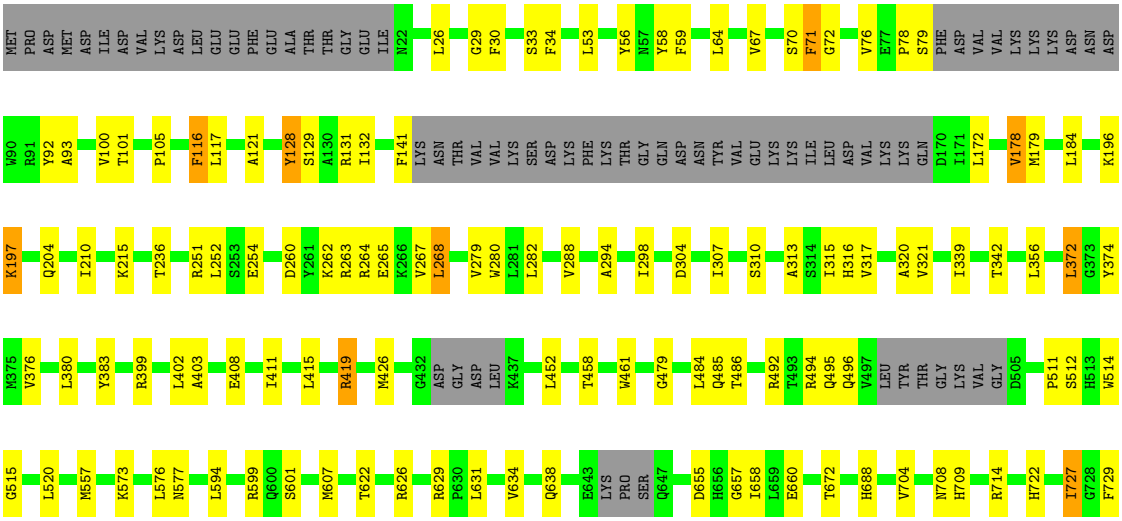
Chain A:

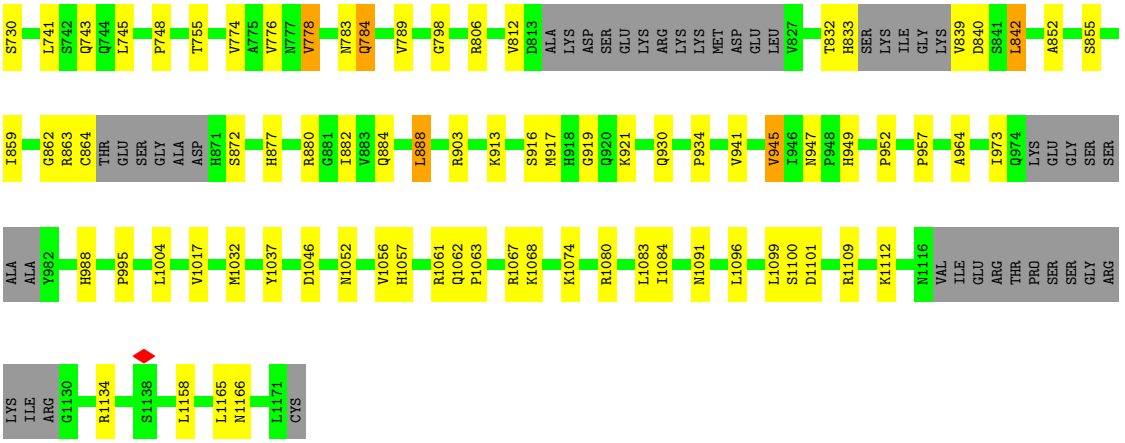




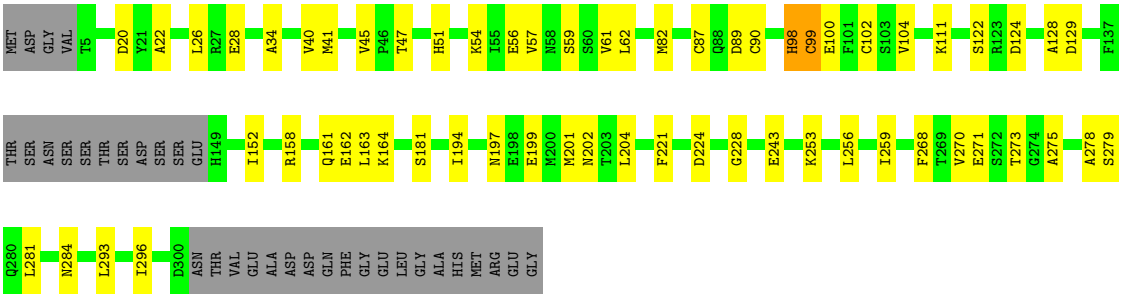
• Molecule 2: DNA-directed RNA polymerases IV and V subunit 2

Chain B:

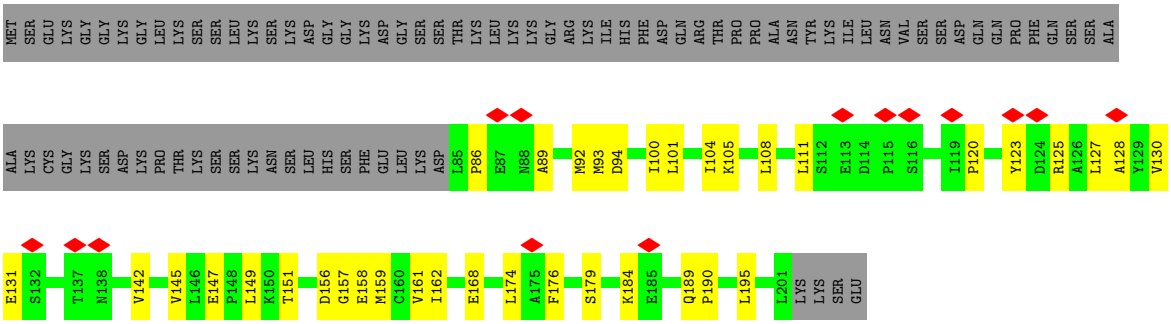




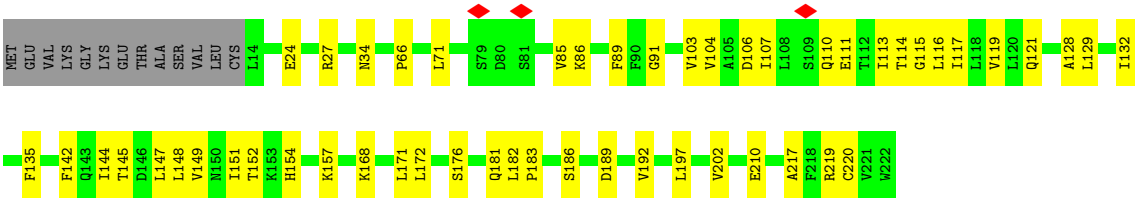
• Molecule 3: DNA-directed RNA polymerases IV and V subunit 3B



• Molecule 4: DNA-directed RNA polymerases IV and V subunit 4

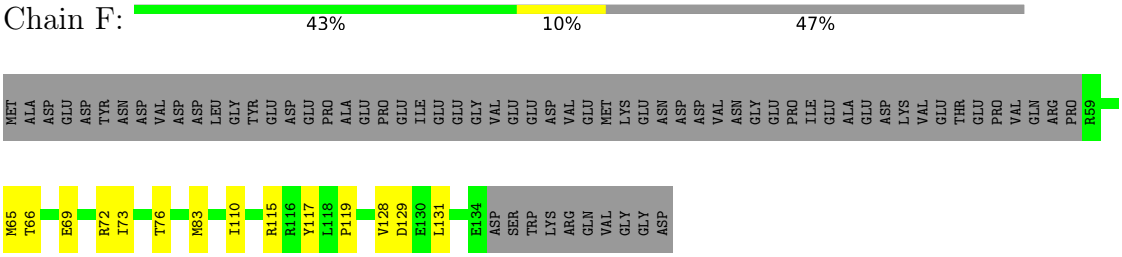


• Molecule 5: DNA-directed RNA polymerase V subunit 5A



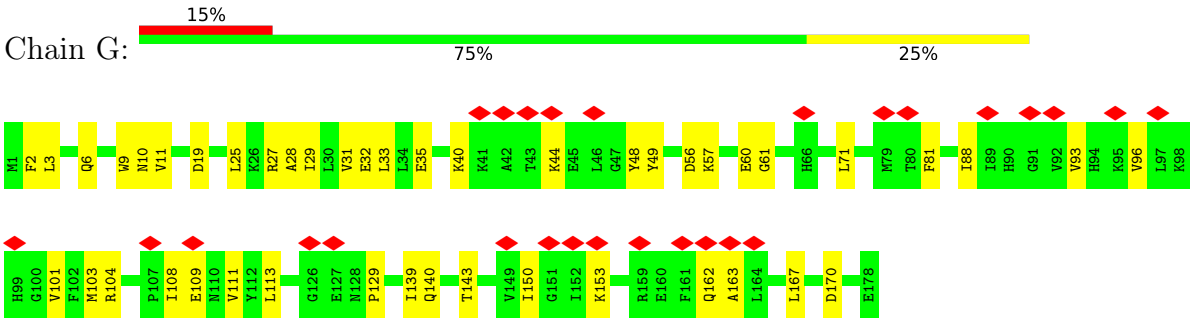
• Molecule 6: DNA-directed RNA polymerases II, IV and V subunit 6A

Chain F:



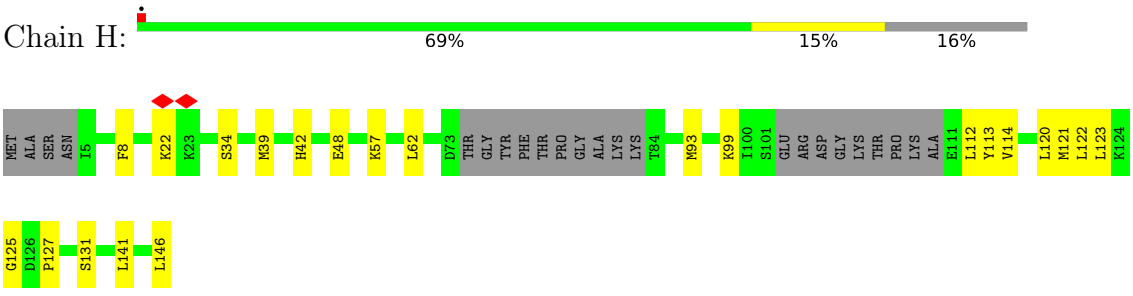
• Molecule 7: DNA-directed RNA polymerase V subunit 7

Chain G:



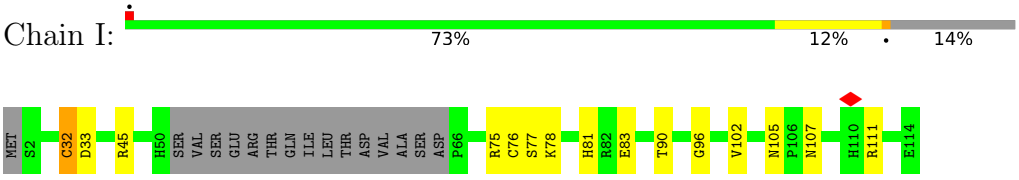
• Molecule 8: DNA-directed RNA polymerases II and V subunit 8A

Chain H:



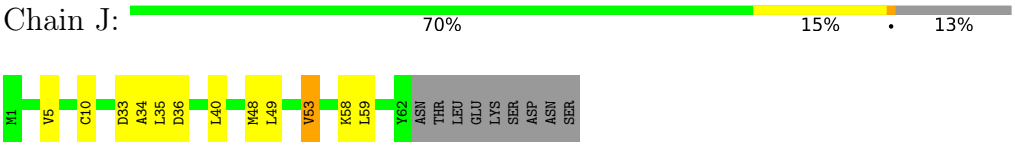
• Molecule 9: DNA-directed RNA polymerases II, IV and V subunit 9A

Chain I:



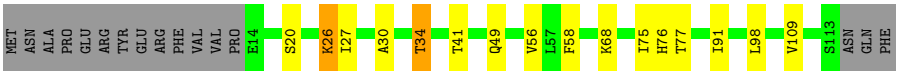
• Molecule 10: DNA-directed RNA polymerases II, IV and V subunit 10

Chain J:



• Molecule 11: DNA-directed RNA polymerases II, IV and V subunit 11

Chain K:

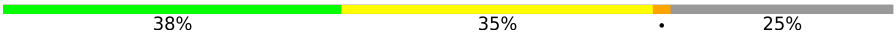


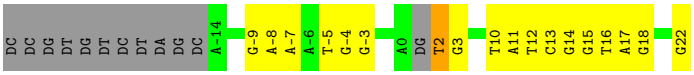
• Molecule 12: DNA-directed RNA polymerases II, IV and V subunit 12

Chain L:

• Molecule 13: DNA (48-MER)

Chain N:



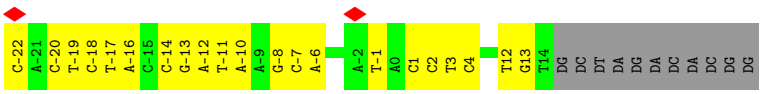


• Molecule 14: RNA (30-MER)

Chain P:

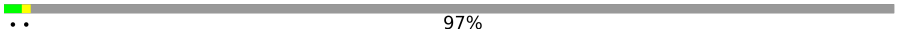
• Molecule 15: DNA (48-MER)

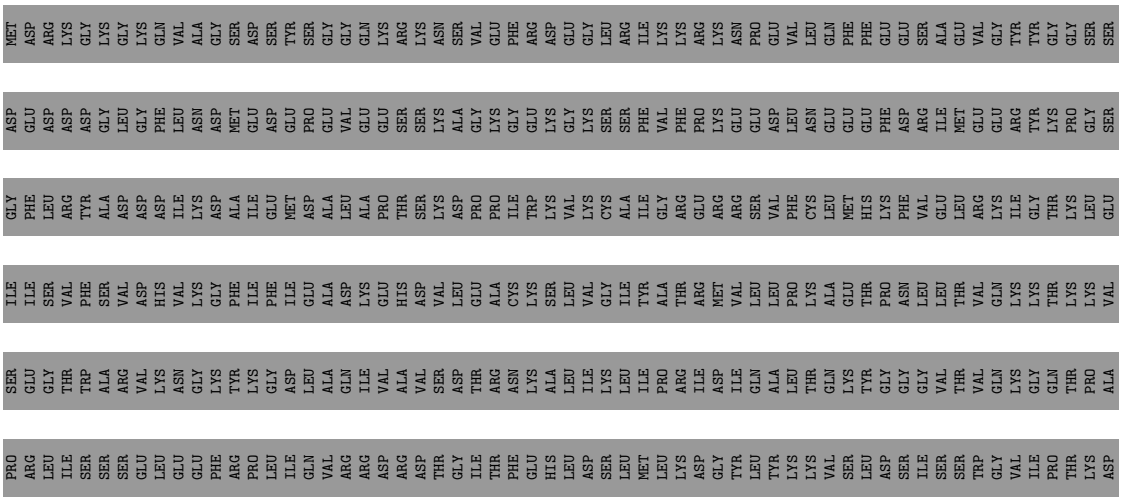
Chain T:

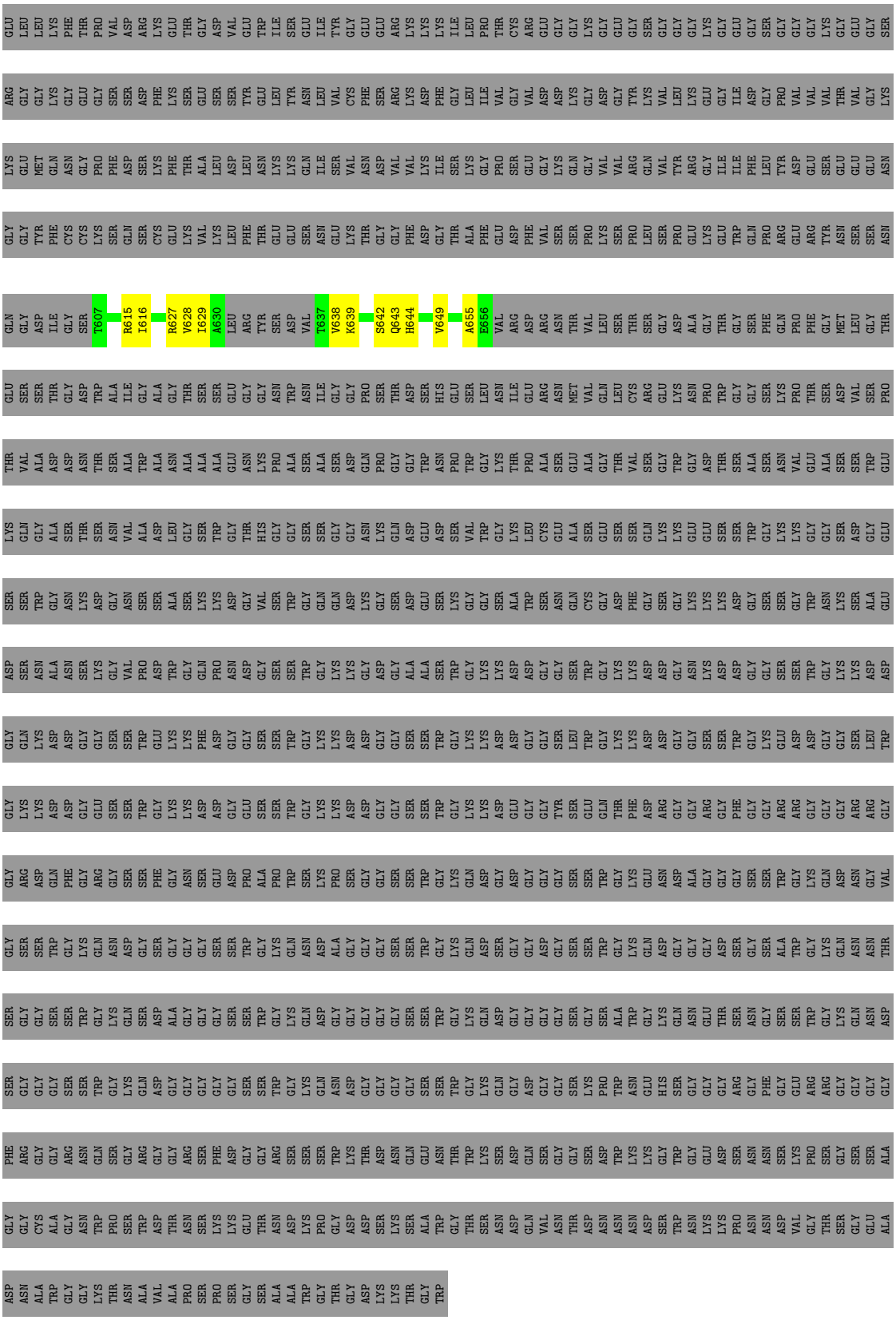


• Molecule 16: Protein RNA-directed DNA methylation 3

Chain W:






T607
R615
I616
R627
V628
I629
A630
T637
V638
K639
S642
Q643
H644
V649
A655
E656

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/8949	0.52	4/12093 (0.0%)
2	B	1.02	0/8074	0.90	15/10929 (0.1%)
3	C	1.11	0/2156	0.93	3/2929 (0.1%)
4	D	0.27	0/909	0.45	0/1232
5	E	0.24	0/1678	0.42	0/2271
6	F	0.25	0/564	0.41	0/767
7	G	0.27	0/1448	0.46	0/1951
8	H	0.26	0/919	0.42	0/1244
9	I	0.28	0/716	0.52	0/973
10	J	1.20	0/492	1.01	2/666 (0.3%)
11	K	1.06	0/770	0.82	0/1045
12	L	1.07	0/312	1.05	2/420 (0.5%)
13	N	0.54	1/840 (0.1%)	0.83	1/1295 (0.1%)
14	P	0.25	0/244	0.66	0/379
15	T	0.54	0/834	0.85	0/1281
16	W	0.88	1/351 (0.3%)	0.98	1/470 (0.2%)
All	All	0.73	2/29256 (0.0%)	0.72	28/39945 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	642	SER	CA-CB	-5.84	1.44	1.52
13	N	2	DT	O3'-P	5.41	1.67	1.61

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	304	ASP	N-CA-C	-7.36	91.14	111.00
2	B	72	GLY	N-CA-C	7.34	131.45	113.10
2	B	798	GLY	N-CA-C	6.89	130.33	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	44	ARG	N-CA-C	-6.70	92.92	111.00
1	A	903	LEU	CA-CB-CG	6.40	130.02	115.30
16	W	627	ARG	N-CA-C	6.39	128.25	111.00
3	C	99	CYS	N-CA-C	-6.38	93.76	111.00
2	B	197	LYS	N-CA-C	-6.26	94.11	111.00
2	B	252	LEU	CA-CB-CG	6.17	129.49	115.30
10	J	33	ASP	N-CA-C	-5.92	95.01	111.00
2	B	778	VAL	CB-CA-C	-5.76	100.45	111.40
2	B	727	ILE	CB-CA-C	-5.75	100.11	111.60
2	B	116	PHE	N-CA-C	-5.67	95.70	111.00
1	A	913	VAL	CB-CA-C	-5.64	100.68	111.40
2	B	356	LEU	N-CA-C	5.63	126.20	111.00
1	A	619	LEU	CA-CB-CG	5.54	128.05	115.30
2	B	268	LEU	CA-CB-CG	5.53	128.03	115.30
2	B	634	VAL	N-CA-C	5.53	125.93	111.00
2	B	842	LEU	CA-CB-CG	5.47	127.89	115.30
3	C	102	CYS	N-CA-C	5.45	125.71	111.00
2	B	730	SER	N-CA-C	5.39	125.56	111.00
10	J	59	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	1039	GLY	N-CA-C	5.27	126.27	113.10
2	B	128	TYR	N-CA-C	-5.22	96.90	111.00
12	L	26	VAL	N-CA-C	-5.17	97.03	111.00
3	C	129	ASP	C-N-CD	5.16	139.23	128.40
13	N	2	DT	P-O3'-C3'	5.09	125.81	119.70
2	B	557	MET	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8794	0	8748	214	0
2	B	7912	0	7591	148	0
3	C	2123	0	2089	42	0
4	D	896	0	899	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1652	0	1634	58	0
6	F	554	0	516	12	0
7	G	1417	0	1459	31	0
8	H	904	0	851	13	0
9	I	702	0	609	9	0
10	J	484	0	486	7	0
11	K	756	0	716	9	0
12	L	309	0	282	5	0
13	N	749	0	409	20	0
14	P	218	0	109	3	0
15	T	746	0	416	31	0
16	W	347	0	366	6	0
17	A	1	0	0	0	0
18	C	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	28568	0	27180	541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:CZ	2:B:121:ALA:HB2	1.36	1.56
1:A:1060:ARG:NH2	5:E:210:GLU:HG2	1.47	1.29
1:A:1060:ARG:HH22	5:E:210:GLU:CG	1.47	1.27
2:B:116:PHE:CZ	2:B:121:ALA:CB	2.20	1.25
2:B:116:PHE:HZ	2:B:121:ALA:CB	1.51	1.23
13:N:-9:DG:H4'	13:N:-8:DA:H5'	1.18	1.14
2:B:116:PHE:CD2	2:B:128:TYR:HD1	1.65	1.12
2:B:116:PHE:CD2	2:B:128:TYR:CD1	2.38	1.10
2:B:116:PHE:CE2	2:B:128:TYR:HD1	1.72	1.08
1:A:1060:ARG:CZ	5:E:210:GLU:HG2	1.92	0.98
2:B:116:PHE:HD2	2:B:128:TYR:CD1	1.78	0.98
2:B:116:PHE:CE2	2:B:121:ALA:HB2	2.00	0.97
2:B:92:TYR:HB2	2:B:141:PHE:HB2	1.44	0.97
1:A:1060:ARG:HH22	5:E:210:GLU:HG2	1.00	0.96
2:B:116:PHE:CE2	2:B:128:TYR:CD1	2.52	0.94
13:N:-9:DG:C4'	13:N:-8:DA:H5'	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PHE:HD2	2:B:128:TYR:CE1	1.90	0.89
1:A:1085:GLY:HA3	1:A:1114:GLN:HE22	1.37	0.89
15:T:-12:DA:H2"	15:T:-11:DT:O4'	1.73	0.88
1:A:950:ASN:C	1:A:952:SER:H	1.76	0.88
2:B:672:THR:HG22	2:B:688:HIS:HB2	1.57	0.85
3:C:34:ALA:HB1	3:C:268:PHE:HE1	1.43	0.83
3:C:34:ALA:HB1	3:C:268:PHE:CE1	2.14	0.82
1:A:1060:ARG:NH2	5:E:210:GLU:CG	2.20	0.82
3:C:54:LYS:HG3	12:L:47:GLN:HG2	1.61	0.82
1:A:1085:GLY:HA3	1:A:1114:GLN:NE2	1.96	0.80
2:B:76:VAL:HB	2:B:93:ALA:HB3	1.64	0.80
1:A:908:LEU:HB3	1:A:1030:PRO:HA	1.64	0.80
15:T:-1:DT:H5"	15:T:-1:DT:C6	2.17	0.79
4:D:168:GLU:HB2	4:D:195:LEU:HD13	1.66	0.77
1:A:805:VAL:HB	5:E:181:GLN:O	1.84	0.77
1:A:1060:ARG:HH22	5:E:210:GLU:CD	1.87	0.77
15:T:-19:DT:H2"	15:T:-18:DC:H5'	1.66	0.77
4:D:101:LEU:HB3	4:D:127:LEU:HD12	1.67	0.76
3:C:98:HIS:CE1	3:C:128:ALA:HB3	2.21	0.76
1:A:1060:ARG:NH1	5:E:210:GLU:HG2	2.00	0.76
2:B:714:ARG:HG3	2:B:919:GLY:HA3	1.66	0.75
15:T:-7:DC:H2'	15:T:-6:DA:C8	2.24	0.73
1:A:950:ASN:C	1:A:952:SER:N	2.40	0.72
1:A:808:PHE:HE2	5:E:217:ALA:O	1.72	0.72
1:A:325:ARG:HH22	15:T:3:DT:H5'	1.55	0.72
2:B:515:GLY:HA3	2:B:629:ARG:HH11	1.58	0.69
1:A:808:PHE:CZ	5:E:183:PRO:HD2	2.28	0.69
1:A:775:PRO:HG2	1:A:844:VAL:HG11	1.75	0.69
7:G:96:VAL:HG13	7:G:101:VAL:HG12	1.75	0.69
4:D:92:MET:HB2	7:G:2:PHE:HB2	1.75	0.69
5:E:24:GLU:HB3	5:E:66:PRO:HG2	1.75	0.68
2:B:236:THR:HG22	2:B:251:ARG:HG3	1.76	0.68
4:D:89:ALA:HB1	7:G:3:LEU:HD11	1.76	0.68
1:A:1048:ILE:HB	1:A:1070:TRP:HB3	1.77	0.67
2:B:855:SER:HA	16:W:644:HIS:CE1	2.30	0.67
1:A:725:CYS:SG	2:B:511:PRO:HB3	2.35	0.66
1:A:808:PHE:CE2	5:E:217:ALA:O	2.48	0.66
1:A:954:GLN:HE21	1:A:958:GLN:HE21	1.44	0.66
1:A:487:LEU:HD23	1:A:586:THR:HG22	1.77	0.66
1:A:721:MET:HB3	2:B:511:PRO:HG2	1.77	0.66
4:D:105:LYS:HD2	4:D:127:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:MET:HG2	4:D:94:ASP:H	1.62	0.65
2:B:116:PHE:HE2	2:B:128:TYR:CD1	2.09	0.65
1:A:808:PHE:HZ	5:E:182:LEU:HG	1.60	0.65
7:G:10:ASN:HD21	7:G:71:LEU:HD13	1.62	0.65
3:C:54:LYS:HG2	12:L:45:VAL:HG22	1.79	0.65
1:A:134:ARG:NH1	1:A:143:GLU:OE2	2.30	0.64
13:N:-4:DG:H2"	13:N:-3:DG:C8	2.32	0.64
6:F:110:ILE:HB	6:F:128:VAL:HG21	1.80	0.64
2:B:67:VAL:HG21	2:B:411:ILE:HD11	1.80	0.64
5:E:71:LEU:HD22	5:E:89:PHE:HB2	1.80	0.64
1:A:808:PHE:CZ	5:E:182:LEU:HG	2.32	0.64
15:T:-1:DT:H5"	15:T:-1:DT:H6	1.63	0.64
9:I:75:ARG:NH2	9:I:76:CYS:O	2.31	0.63
1:A:950:ASN:HB3	1:A:952:SER:HB3	1.81	0.63
7:G:48:TYR:HB3	7:G:81:PHE:HB3	1.80	0.63
6:F:65:MET:HB2	6:F:131:LEU:HD21	1.80	0.62
3:C:26:LEU:CB	3:C:268:PHE:HE2	2.13	0.62
2:B:862:GLY:HA2	2:B:872:SER:HB3	1.82	0.61
1:A:90:LEU:HA	1:A:93:MET:HG2	1.81	0.61
8:H:112:LEU:HB2	8:H:123:LEU:HB2	1.82	0.61
1:A:141:TYR:HE1	1:A:269:MET:HG2	1.65	0.61
2:B:949:HIS:H	2:B:949:HIS:CD2	2.16	0.61
1:A:903:LEU:O	1:A:1043:ILE:HD12	2.01	0.61
2:B:741:LEU:HD12	2:B:806:ARG:HG2	1.81	0.60
13:N:-9:DG:H4'	13:N:-8:DA:C5'	2.13	0.60
2:B:930:GLN:HG3	2:B:941:VAL:HG21	1.84	0.60
3:C:26:LEU:HB3	3:C:268:PHE:HE2	1.66	0.60
1:A:176:LEU:HG	1:A:178:ARG:H	1.67	0.60
1:A:1106:ARG:H	5:E:154:HIS:CD2	2.19	0.60
1:A:1229:LEU:HD21	6:F:76:THR:HG21	1.83	0.60
3:C:253:LYS:H	3:C:253:LYS:HD2	1.65	0.60
1:A:319:GLY:HA3	2:B:1063:PRO:HD2	1.84	0.60
15:T:-20:DC:H2'	15:T:-19:DT:C6	2.36	0.60
1:A:270:PHE:O	1:A:274:ASP:HB2	2.01	0.59
1:A:569:LYS:HB3	8:H:120:LEU:HD21	1.84	0.59
2:B:988:HIS:O	2:B:995:PRO:HD3	2.03	0.58
2:B:116:PHE:CZ	2:B:121:ALA:CA	2.86	0.58
2:B:116:PHE:HZ	2:B:121:ALA:HB1	1.57	0.58
1:A:1086:ASP:HA	1:A:1089:ARG:HD2	1.86	0.58
1:A:1058:TRP:HE3	5:E:210:GLU:CB	2.18	0.57
2:B:131:ARG:HB3	2:B:172:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ARG:HH22	1:A:1078:LYS:HD3	1.69	0.57
2:B:268:LEU:HD12	2:B:315:ILE:HD11	1.86	0.57
1:A:1118:LEU:HG	1:A:1119:LEU:HD12	1.86	0.57
1:A:875:ARG:HH21	1:A:1080:ALA:HB3	1.69	0.57
2:B:880:ARG:HB2	16:W:644:HIS:CD2	2.40	0.57
1:A:337:ASN:O	1:A:427:ARG:N	2.36	0.56
7:G:96:VAL:HB	7:G:129:PRO:HG2	1.87	0.56
1:A:913:VAL:HG22	1:A:940:HIS:O	2.06	0.56
2:B:745:LEU:HB3	2:B:748:PRO:HG3	1.87	0.56
3:C:201:MET:HB2	3:C:256:LEU:HD11	1.87	0.56
1:A:808:PHE:HZ	5:E:183:PRO:HD2	1.71	0.56
5:E:192:VAL:HG23	5:E:197:LEU:HD12	1.87	0.56
2:B:784:GLN:HA	2:B:947:ASN:ND2	2.20	0.56
5:E:151:ILE:HG22	5:E:152:THR:H	1.69	0.56
7:G:32:GLU:HA	7:G:35:GLU:HG2	1.87	0.56
13:N:17:DA:H2"	13:N:18:DG:H5"	1.88	0.56
1:A:328:ILE:HG22	1:A:436:VAL:HB	1.88	0.56
13:N:2:DT:H2"	13:N:3:DG:O5'	2.06	0.56
13:N:-8:DA:H2"	13:N:-7:DA:H5'	1.87	0.56
4:D:174:LEU:HD13	4:D:184:LYS:HE3	1.87	0.56
4:D:100:ILE:O	4:D:104:ILE:HG12	2.06	0.55
1:A:951:ILE:C	1:A:953:MET:H	2.07	0.55
2:B:26:LEU:HD11	2:B:638:GLN:HA	1.87	0.55
5:E:121:GLN:HG2	5:E:144:ILE:HG21	1.86	0.55
9:I:81:HIS:HB3	9:I:83:GLU:HG2	1.88	0.55
1:A:707:SER:O	1:A:713:TYR:OH	2.20	0.55
2:B:1112:LYS:HB3	2:B:1166:ASN:HD22	1.71	0.55
4:D:127:LEU:HA	4:D:130:VAL:HG12	1.89	0.55
2:B:1057:HIS:N	2:B:1062:GLN:O	2.40	0.55
1:A:1026:ASN:O	1:A:1030:PRO:HD2	2.07	0.55
2:B:116:PHE:CD2	2:B:128:TYR:CE1	2.78	0.55
1:A:494:ASP:OD2	2:B:784:GLN:HB3	2.07	0.54
1:A:1027:THR:HG21	2:B:263:ARG:CZ	2.37	0.54
2:B:934:PRO:HB3	2:B:1017:VAL:CG1	2.37	0.54
1:A:18:THR:HB	2:B:1166:ASN:HB3	1.89	0.54
3:C:204:LEU:HD21	3:C:253:LYS:HD3	1.89	0.54
8:H:39:MET:HG2	8:H:125:GLY:HA2	1.89	0.54
1:A:793:ASN:ND2	6:F:117:TYR:O	2.41	0.54
2:B:279:VAL:HG13	2:B:280:TRP:HD1	1.73	0.54
2:B:260:ASP:HB2	2:B:264:ARG:HB2	1.88	0.54
4:D:108:LEU:HD23	4:D:111:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:-8:DG:H2”	15:T:-7:DC:H5”	1.90	0.54
1:A:938:HIS:CE1	1:A:1004:PRO:HB3	2.42	0.54
13:N:15:DG:H2”	13:N:16:DT:H5”	1.89	0.54
1:A:1120:GLY:HA2	5:E:189:ASP:HB3	1.90	0.54
2:B:722:HIS:HE1	2:B:921:LYS:HD2	1.72	0.54
1:A:951:ILE:C	1:A:953:MET:N	2.58	0.54
1:A:683:LEU:HD23	2:B:952:PRO:HG2	1.90	0.54
2:B:265:GLU:HB3	2:B:310:SER:HB3	1.90	0.54
1:A:1122:SER:HA	5:E:219:ARG:HH12	1.74	0.53
7:G:29:ILE:O	7:G:33:LEU:HG	2.08	0.53
1:A:1182:PHE:O	1:A:1186:THR:HG23	2.09	0.53
2:B:298:ILE:HG23	2:B:376:VAL:HG23	1.88	0.53
15:T:-14:DC:H2’	15:T:-13:DG:C8	2.44	0.53
1:A:1158:SER:HB3	1:A:1172:LEU:HD23	1.90	0.53
5:E:34:ASN:ND2	5:E:147:LEU:O	2.41	0.53
2:B:408:GLU:O	2:B:411:ILE:HG12	2.08	0.53
1:A:319:GLY:HA2	2:B:1074:LYS:HA	1.89	0.53
1:A:325:ARG:NH2	15:T:3:DT:H5’	2.24	0.53
4:D:157:GLY:O	4:D:161:VAL:HG23	2.09	0.53
1:A:354:ARG:NH1	6:F:83:MET:SD	2.82	0.53
1:A:501:VAL:HG21	1:A:612:LEU:HD13	1.91	0.53
1:A:505:ARG:NH2	8:H:48:GLU:OE2	2.41	0.53
5:E:119:VAL:HG12	5:E:142:PHE:HB2	1.90	0.53
1:A:1060:ARG:HH12	5:E:210:GLU:HG2	1.69	0.53
7:G:28:ALA:O	7:G:32:GLU:HG3	2.09	0.53
1:A:342:PRO:HB3	1:A:434:ASN:HA	1.91	0.52
1:A:456:HIS:HE1	15:T:1:DC:H2”	1.74	0.52
4:D:105:LYS:HA	4:D:108:LEU:HD12	1.91	0.52
7:G:93:VAL:HA	7:G:103:MET:HA	1.91	0.52
15:T:-12:DA:C5	15:T:-11:DT:C4	2.97	0.52
1:A:1001:SER:OG	1:A:1002:ASP:N	2.43	0.52
1:A:773:ALA:HA	15:T:-1:DT:C5	2.45	0.52
3:C:82:MET:HG3	3:C:284:ASN:HD21	1.74	0.52
1:A:1121:LEU:HD23	5:E:219:ARG:HD3	1.92	0.52
1:A:1225:SER:OG	1:A:1226:GLN:N	2.42	0.52
2:B:655:ASP:C	2:B:657:GLY:H	2.12	0.52
1:A:563:ASP:N	1:A:563:ASP:OD1	2.43	0.51
5:E:106:ASP:O	5:E:110:GLN:HB2	2.10	0.51
4:D:105:LYS:HG2	4:D:108:LEU:HD12	1.92	0.51
1:A:1088:TRP:CD1	1:A:1118:LEU:HD13	2.45	0.51
2:B:832:THR:O	2:B:833:HIS:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:ILE:HG13	11:K:91:ILE:HD13	1.93	0.51
8:H:93:MET:HB2	8:H:141:LEU:HB3	1.91	0.51
3:C:122:SER:C	3:C:124:ASP:H	2.14	0.51
5:E:172:LEU:HA	5:E:176:SER:HA	1.92	0.51
11:K:56:VAL:HA	11:K:77:THR:HG22	1.91	0.51
15:T:-12:DA:C8	15:T:-11:DT:C7	2.93	0.51
1:A:1060:ARG:NH2	5:E:210:GLU:CB	2.74	0.51
1:A:34:GLU:O	1:A:74:TYR:OH	2.29	0.51
1:A:648:ARG:NH1	1:A:658:GLN:OE1	2.43	0.50
3:C:158:ARG:H	3:C:161:GLN:NE2	2.09	0.50
2:B:1158:LEU:HD13	2:B:1165:LEU:HD21	1.93	0.50
10:J:34:ALA:C	10:J:36:ASP:H	2.15	0.50
2:B:1112:LYS:HB3	2:B:1166:ASN:ND2	2.25	0.50
3:C:20:ASP:O	3:C:271:GLU:HA	2.12	0.50
11:K:20:SER:HB2	11:K:34:THR:HG23	1.94	0.50
1:A:191:SER:HA	1:A:194:LYS:HG2	1.93	0.50
1:A:1122:SER:CA	5:E:219:ARG:HH12	2.24	0.50
1:A:956:ILE:HA	1:A:959:LYS:HG2	1.92	0.50
7:G:93:VAL:HG21	7:G:139:ILE:HD11	1.93	0.50
2:B:880:ARG:HB2	16:W:644:HIS:NE2	2.27	0.50
2:B:210:ILE:HG12	2:B:215:LYS:HG3	1.93	0.50
13:N:2:DT:H2'	13:N:3:DG:C8	2.47	0.50
16:W:629:ILE:HD11	16:W:639:LYS:HB2	1.94	0.50
1:A:805:VAL:CG2	5:E:181:GLN:CB	2.90	0.49
1:A:48:LEU:HA	1:A:71:HIS:HB2	1.95	0.49
1:A:938:HIS:HA	1:A:1005:CYS:H	1.76	0.49
1:A:1226:GLN:HB2	6:F:117:TYR:HB3	1.93	0.49
2:B:372:LEU:O	2:B:376:VAL:HG22	2.12	0.49
7:G:153:LYS:N	7:G:162:GLN:O	2.44	0.49
9:I:77:SER:OG	9:I:107:ASN:OD1	2.24	0.49
1:A:1058:TRP:HE3	5:E:210:GLU:HB2	1.77	0.49
6:F:129:ASP:OD1	6:F:129:ASP:N	2.45	0.49
1:A:1033:LEU:HB3	1:A:1036:VAL:HG13	1.94	0.49
1:A:50:LEU:HD13	1:A:62:ALA:O	2.12	0.49
1:A:139:ALA:HA	1:A:273:VAL:HG21	1.94	0.49
1:A:269:MET:O	1:A:273:VAL:HG22	2.13	0.49
1:A:723:ILE:H	1:A:723:ILE:HD12	1.78	0.49
1:A:805:VAL:HG23	5:E:181:GLN:CB	2.42	0.49
2:B:607:MET:HG3	2:B:622:THR:CG2	2.43	0.49
5:E:27:ARG:HG3	5:E:148:LEU:HD21	1.94	0.49
10:J:34:ALA:C	10:J:36:ASP:N	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:32:CYS:SG	9:I:33:ASP:N	2.84	0.49
1:A:1212:SER:HB2	1:A:1219:VAL:HG22	1.94	0.49
2:B:53:LEU:HD23	2:B:179:MET:SD	2.53	0.49
2:B:100:VAL:HG12	2:B:132:ILE:HD11	1.94	0.49
2:B:629:ARG:HH21	2:B:631:LEU:HD21	1.77	0.49
12:L:12:CYS:HA	12:L:37:LEU:HD23	1.95	0.49
2:B:839:VAL:HG12	2:B:842:LEU:HG	1.95	0.48
1:A:1103:ASP:OD1	5:E:149:VAL:HG22	2.13	0.48
2:B:704:VAL:HG13	2:B:917:MET:HG3	1.93	0.48
2:B:877:HIS:HB3	2:B:1068:LYS:O	2.12	0.48
7:G:40:LYS:HZ3	7:G:49:TYR:HD2	1.61	0.48
1:A:773:ALA:CA	15:T:-1:DT:H72	2.43	0.48
7:G:48:TYR:O	7:G:81:PHE:N	2.45	0.48
1:A:1194:PHE:HD2	2:B:1158:LEU:HD21	1.78	0.48
5:E:128:ALA:O	5:E:132:ILE:HG23	2.12	0.48
7:G:108:ILE:HD12	7:G:108:ILE:H	1.79	0.48
1:A:788:ASP:OD1	1:A:788:ASP:N	2.45	0.48
1:A:1058:TRP:CE3	5:E:210:GLU:HB3	2.49	0.48
1:A:920:ARG:H	1:A:934:CYS:HB2	1.77	0.48
2:B:774:VAL:O	2:B:1032:MET:HA	2.14	0.48
8:H:42:HIS:HD2	8:H:122:LEU:HD22	1.78	0.48
2:B:863:ARG:O	2:B:864:CYS:C	2.51	0.48
4:D:156:ASP:HA	4:D:159:MET:HB2	1.94	0.48
1:A:523:SER:OG	1:A:524:LEU:N	2.44	0.47
1:A:79:VAL:HG23	1:A:81:ILE:HD11	1.94	0.47
1:A:808:PHE:CZ	5:E:183:PRO:CD	2.95	0.47
1:A:906:VAL:HB	1:A:1037:ILE:O	2.14	0.47
1:A:1162:LEU:HD11	1:A:1172:LEU:HG	1.95	0.47
2:B:842:LEU:HD21	2:B:859:ILE:O	2.14	0.47
5:E:145:THR:HG23	5:E:148:LEU:HD12	1.96	0.47
1:A:964:ILE:HG21	1:A:974:LYS:HE3	1.96	0.47
1:A:1028:VAL:O	1:A:1032:LEU:HB2	2.15	0.47
15:T:3:DT:H2'	15:T:4:DC:C6	2.49	0.47
1:A:195:LEU:HD13	1:A:201:ILE:HA	1.96	0.47
1:A:762:ARG:HH22	2:B:520:LEU:C	2.18	0.47
4:D:149:LEU:HB2	4:D:159:MET:HE1	1.97	0.47
5:E:85:VAL:HA	5:E:115:GLY:O	2.14	0.47
1:A:349:ILE:HG21	1:A:459:TYR:CZ	2.49	0.47
1:A:938:HIS:N	1:A:1005:CYS:O	2.46	0.47
2:B:1080:ARG:O	2:B:1084:ILE:HG12	2.14	0.47
4:D:142:VAL:HA	4:D:145:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.74	0.47
2:B:374:TYR:HD1	2:B:573:LYS:HZ2	1.63	0.47
6:F:73:ILE:HA	6:F:76:THR:HG22	1.97	0.47
1:A:321:GLY:HA3	2:B:1099:LEU:HD12	1.96	0.47
2:B:254:GLU:HG2	2:B:262:LYS:HA	1.97	0.47
2:B:1100:SER:OG	2:B:1101:ASP:N	2.47	0.47
4:D:176:PHE:CD2	7:G:88:ILE:HD13	2.50	0.47
13:N:11:DA:H2'	13:N:12:DT:H71	1.97	0.47
1:A:479:LEU:HD12	1:A:594:PRO:HB3	1.97	0.47
1:A:1058:TRP:HE3	5:E:210:GLU:HB3	1.79	0.47
8:H:127:PRO:O	8:H:131:SER:OG	2.28	0.47
14:P:5:A:H2'	14:P:6:G:C8	2.50	0.47
1:A:444:SER:OG	1:A:445:PRO:HD3	2.15	0.47
2:B:729:PHE:HZ	10:J:53:VAL:HG21	1.79	0.47
2:B:1056:VAL:HG21	2:B:1061:ARG:HD2	1.97	0.47
1:A:241:ASP:O	1:A:245:LYS:HG2	2.15	0.46
1:A:339:VAL:O	1:A:429:TYR:N	2.47	0.46
1:A:503:LEU:HD22	1:A:572:PHE:HE1	1.78	0.46
2:B:934:PRO:HB3	2:B:1017:VAL:HG13	1.96	0.46
2:B:105:PRO:HB3	2:B:129:SER:O	2.16	0.46
7:G:111:VAL:HG13	7:G:163:ALA:HB3	1.98	0.46
13:N:13:DC:H2"	13:N:14:DG:C8	2.50	0.46
3:C:194:ILE:HG12	3:C:259:ILE:HG23	1.96	0.46
4:D:128:ALA:O	4:D:131:GLU:HG2	2.16	0.46
13:N:2:DT:H3'	13:N:2:DT:H6	1.80	0.46
1:A:552:ARG:HA	1:A:564:GLY:HA2	1.97	0.46
1:A:750:ASP:HB2	1:A:753:GLU:HG3	1.96	0.46
15:T:-17:DT:H2"	15:T:-16:DA:C8	2.50	0.46
15:T:-14:DC:H2'	15:T:-13:DG:H8	1.81	0.46
2:B:56:TYR:C	2:B:58:TYR:H	2.18	0.46
2:B:660:GLU:OE2	2:B:688:HIS:HE1	1.99	0.46
3:C:22:ALA:HB3	3:C:270:VAL:HG22	1.97	0.46
1:A:683:LEU:HD21	2:B:949:HIS:HA	1.98	0.46
4:D:86:PRO:HG3	7:G:6:GLN:H	1.81	0.46
1:A:773:ALA:HB2	15:T:-1:DT:H72	1.98	0.46
5:E:111:GLU:HG3	5:E:113:ILE:HG12	1.97	0.46
7:G:19:ASP:H	7:G:25:LEU:HD11	1.80	0.46
10:J:48:MET:HE3	10:J:48:MET:HB3	1.67	0.46
3:C:34:ALA:HB2	3:C:268:PHE:HZ	1.81	0.46
3:C:59:SER:HB2	3:C:162:GLU:H	1.81	0.46
3:C:111:LYS:HB2	3:C:162:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD11	1:A:400:VAL:HG21	1.96	0.46
1:A:440:PRO:HG2	2:B:784:GLN:NE2	2.31	0.46
1:A:503:LEU:HD23	1:A:541:VAL:HG21	1.98	0.46
1:A:1040:ASP:HB2	1:A:1043:ILE:HD11	1.97	0.46
1:A:1225:SER:HB3	1:A:1227:PHE:HE1	1.81	0.46
2:B:415:LEU:HG	2:B:419:ARG:HD2	1.98	0.46
1:A:875:ARG:HH22	1:A:1078:LYS:HA	1.81	0.45
2:B:320:ALA:O	2:B:321:VAL:C	2.55	0.45
2:B:916:SER:OG	2:B:917:MET:N	2.49	0.45
1:A:242:VAL:O	1:A:246:VAL:HG13	2.16	0.45
1:A:493:SER:OG	2:B:949:HIS:ND1	2.48	0.45
1:A:879:LEU:HB3	1:A:1072:LEU:HB2	1.97	0.45
9:I:77:SER:HB3	9:I:78:LYS:HE2	1.99	0.45
1:A:28:CYS:O	2:B:1134:ARG:NH1	2.50	0.45
1:A:473:PHE:O	1:A:478:GLN:NE2	2.50	0.45
1:A:335:HIS:HB2	1:A:338:GLU:HG2	1.97	0.45
2:B:1083:LEU:HD21	2:B:1091:ASN:HD21	1.81	0.45
3:C:41:MET:HE2	3:C:281:LEU:HG	1.99	0.45
5:E:103:VAL:O	5:E:107:ILE:HG12	2.17	0.45
2:B:727:ILE:HG23	2:B:743:GLN:HB3	1.99	0.45
1:A:1229:LEU:HD13	6:F:72:ARG:NH2	2.32	0.45
3:C:34:ALA:CB	3:C:268:PHE:CE1	2.95	0.45
7:G:44:LYS:HB3	7:G:44:LYS:HE2	1.73	0.45
7:G:170:ASP:N	7:G:170:ASP:OD1	2.50	0.45
1:A:781:ASN:HD21	1:A:1165:ASN:HA	1.82	0.45
1:A:907:SER:HA	1:A:1034:GLU:HA	1.98	0.45
1:A:947:GLN:O	1:A:948:ASP:HB2	2.17	0.45
1:A:1194:PHE:CD2	2:B:1158:LEU:HD21	2.51	0.45
1:A:362:TYR:HD1	1:A:365:LYS:HE2	1.82	0.45
1:A:528:ALA:HB2	1:A:543:GLN:HE21	1.82	0.45
1:A:185:ARG:NH1	1:A:186:ARG:HG3	2.32	0.45
1:A:542:PHE:HE1	1:A:570:PHE:HB3	1.81	0.45
1:A:773:ALA:HA	15:T:-1:DT:C6	2.52	0.45
1:A:1140:SER:OG	1:A:1141:LYS:N	2.49	0.45
2:B:729:PHE:CZ	10:J:53:VAL:HG11	2.52	0.45
2:B:888:LEU:HG	12:L:27:ILE:HG12	1.99	0.45
2:B:884:GLN:OE1	2:B:903:ARG:HB2	2.16	0.45
2:B:964:ALA:O	2:B:1004:LEU:HD11	2.16	0.45
3:C:34:ALA:CB	3:C:268:PHE:CZ	2.99	0.45
3:C:89:ASP:O	3:C:90:CYS:C	2.56	0.45
3:C:278:ALA:O	3:C:279:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:SER:O	4:D:179:SER:OG	2.33	0.45
7:G:9:TRP:HD1	7:G:11:VAL:HG22	1.82	0.45
1:A:749:LEU:H	2:B:708:ASN:HD22	1.65	0.44
1:A:1106:ARG:N	5:E:154:HIS:NE2	2.53	0.44
2:B:59:PHE:HZ	2:B:411:ILE:HD13	1.82	0.44
7:G:140:GLN:O	7:G:143:THR:OG1	2.28	0.44
1:A:467:ALA:HA	1:A:470:MET:HG3	1.98	0.44
2:B:494:ARG:HG2	2:B:495:GLN:N	2.32	0.44
3:C:224:ASP:HB3	3:C:228:GLY:H	1.81	0.44
9:I:105:ASN:OD1	9:I:111:ARG:NH1	2.50	0.44
1:A:773:ALA:HA	15:T:-1:DT:H72	1.98	0.44
1:A:1185:ALA:HB1	1:A:1190:PRO:HB3	1.98	0.44
3:C:98:HIS:CE1	3:C:104:VAL:HG13	2.52	0.44
3:C:197:ASN:O	3:C:199:GLU:N	2.51	0.44
3:C:221:PHE:HZ	3:C:259:ILE:HD11	1.82	0.44
4:D:189:GLN:HB3	4:D:190:PRO:HD3	2.00	0.44
11:K:26:LYS:H	11:K:26:LYS:HG2	1.56	0.44
1:A:700:GLY:HA2	1:A:744:CYS:HB3	1.99	0.44
1:A:1173:THR:HG22	1:A:1178:ILE:HB	2.00	0.44
14:P:3:C:H2'	14:P:4:G:C8	2.53	0.44
1:A:684:ILE:HD11	2:B:952:PRO:HB3	2.00	0.44
2:B:196:LYS:O	2:B:197:LYS:C	2.53	0.44
3:C:56:GLU:HG3	3:C:164:LYS:HB3	1.99	0.44
3:C:57:VAL:O	3:C:163:LEU:HA	2.18	0.44
13:N:-8:DA:OP2	13:N:-8:DA:C8	2.70	0.44
1:A:875:ARG:HB2	1:A:1076:VAL:HB	1.99	0.44
3:C:61:VAL:HG23	3:C:62:LEU:HG	2.00	0.44
1:A:366:LEU:HG	1:A:371:LEU:HD21	2.00	0.44
2:B:402:LEU:HB3	2:B:403:ALA:H	1.60	0.44
2:B:1109:ARG:HD2	2:B:1109:ARG:HA	1.82	0.44
1:A:141:TYR:CE1	1:A:269:MET:HG2	2.49	0.43
1:A:245:LYS:HA	1:A:245:LYS:HD3	1.85	0.43
1:A:484:THR:HG23	1:A:486:GLN:H	1.83	0.43
1:A:683:LEU:HD11	2:B:949:HIS:ND1	2.33	0.43
5:E:86:LYS:H	5:E:116:LEU:HA	1.83	0.43
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.84	0.43
12:L:21:LEU:HD12	12:L:21:LEU:HA	1.74	0.43
2:B:655:ASP:C	2:B:657:GLY:N	2.71	0.43
7:G:56:ASP:O	7:G:57:LYS:HD2	2.18	0.43
1:A:234:PRO:O	1:A:238:GLU:HG2	2.17	0.43
1:A:325:ARG:HB3	2:B:1067:ARG:HH12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:LEU:HB2	1:A:1033:LEU:HB2	2.00	0.43
4:D:158:GLU:O	4:D:162:ILE:HG12	2.18	0.43
6:F:66:THR:HG23	6:F:69:GLU:H	1.82	0.43
1:A:878:ILE:HD12	1:A:878:ILE:HA	1.91	0.43
2:B:29:GLY:O	2:B:30:PHE:C	2.56	0.43
2:B:267:VAL:CG2	2:B:315:ILE:HD12	2.49	0.43
2:B:514:TRP:HD1	2:B:629:ARG:HH12	1.64	0.43
2:B:789:VAL:HB	2:B:945:VAL:HG13	2.00	0.43
3:C:87:CYS:C	3:C:89:ASP:N	2.71	0.43
5:E:86:LYS:O	5:E:117:ILE:N	2.42	0.43
1:A:585:VAL:HG21	1:A:601:PHE:HE2	1.82	0.43
1:A:704:LEU:HG	1:A:739:GLY:HA3	2.01	0.43
1:A:1231:TRP:N	7:G:61:GLY:O	2.35	0.43
3:C:45:VAL:HG11	3:C:281:LEU:HD12	1.99	0.43
15:T:-11:DT:H2'	15:T:-10:DA:C8	2.53	0.43
1:A:830:VAL:HG11	2:B:1084:ILE:HD12	2.01	0.43
1:A:1035:ILE:H	1:A:1035:ILE:HG13	1.53	0.43
11:K:68:LYS:HE3	11:K:68:LYS:HB2	1.62	0.43
14:P:4:G:H2'	14:P:5:A:C8	2.54	0.43
1:A:956:ILE:HG13	1:A:1036:VAL:HA	2.00	0.43
1:A:958:GLN:O	1:A:961:GLU:HG2	2.18	0.43
1:A:1027:THR:HG21	2:B:263:ARG:NH2	2.33	0.43
2:B:267:VAL:HG23	2:B:315:ILE:HD12	2.00	0.43
5:E:152:THR:HA	5:E:157:LYS:HD2	2.01	0.43
1:A:529:LEU:HB3	1:A:538:ALA:HB3	2.01	0.43
1:A:605:GLN:HB3	1:A:606:PRO:HD3	2.00	0.43
1:A:861:VAL:HG11	1:A:1132:LEU:HD11	2.01	0.43
7:G:113:LEU:HD11	7:G:167:LEU:HD21	2.00	0.43
1:A:994:ASP:OD2	9:I:45:ARG:NH2	2.52	0.43
5:E:104:VAL:HG11	5:E:135:PHE:CD1	2.54	0.43
5:E:202:VAL:HG12	5:E:220:CYS:HB3	2.01	0.43
13:N:14:DG:H1	15:T:-14:DC:H42	1.67	0.43
15:T:-18:DC:H2'	15:T:-17:DT:C6	2.54	0.43
1:A:1014:ASP:N	1:A:1014:ASP:OD1	2.51	0.42
2:B:178:VAL:HG11	2:B:184:LEU:HB3	2.00	0.42
3:C:26:LEU:HB2	3:C:268:PHE:HE2	1.82	0.42
3:C:34:ALA:HB1	3:C:268:PHE:CZ	2.54	0.42
11:K:58:PHE:HB3	11:K:76:HIS:HB2	2.00	0.42
1:A:349:ILE:HD12	2:B:1052:ASN:HD22	1.84	0.42
1:A:562:VAL:HG12	1:A:567:LEU:HA	2.02	0.42
1:A:908:LEU:HD22	1:A:1033:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:LEU:HD23	1:A:1099:LEU:H	1.84	0.42
2:B:288:VAL:HG11	2:B:294:ALA:HB2	2.01	0.42
13:N:10:DT:H2"	13:N:11:DA:C8	2.54	0.42
1:A:262:HIS:HA	1:A:265:GLU:HB2	2.00	0.42
1:A:342:PRO:HG2	1:A:345:ILE:HB	2.02	0.42
1:A:641:GLU:O	1:A:644:PRO:HD2	2.19	0.42
2:B:70:SER:O	2:B:71:PHE:C	2.56	0.42
7:G:11:VAL:HG11	7:G:33:LEU:HD23	2.00	0.42
8:H:114:VAL:HG13	8:H:121:MET:HB3	2.01	0.42
1:A:23:SER:O	1:A:27:ILE:HG13	2.20	0.42
2:B:479:GLY:O	2:B:486:THR:HG22	2.19	0.42
3:C:51:HIS:O	3:C:51:HIS:CG	2.71	0.42
3:C:293:LEU:O	3:C:296:ILE:HG12	2.19	0.42
15:T:3:DT:H2'	15:T:4:DC:H6	1.84	0.42
1:A:277:LEU:HD23	1:A:277:LEU:H	1.85	0.42
1:A:987:SER:O	1:A:987:SER:OG	2.34	0.42
1:A:1106:ARG:CB	5:E:154:HIS:CE1	3.03	0.42
1:A:803:ASN:ND2	6:F:119:PRO:O	2.52	0.42
1:A:667:LYS:NZ	1:A:668:GLU:OE2	2.53	0.42
2:B:268:LEU:HB2	2:B:315:ILE:HD11	2.02	0.42
2:B:307:ILE:HG21	2:B:383:TYR:HD2	1.85	0.42
9:I:102:VAL:HG13	9:I:111:ARG:HE	1.84	0.42
13:N:-8:DA:OP2	13:N:-8:DA:H8	2.03	0.42
13:N:2:DT:C3'	13:N:2:DT:C6	3.02	0.42
1:A:104:ILE:HG13	1:A:186:ARG:HH21	1.85	0.42
1:A:355:VAL:HB	1:A:396:PRO:HA	2.01	0.42
2:B:56:TYR:O	2:B:58:TYR:N	2.51	0.42
2:B:515:GLY:HA3	2:B:629:ARG:NH1	2.29	0.42
2:B:852:ALA:O	2:B:882:ILE:HA	2.20	0.42
7:G:104:ARG:NE	7:G:109:GLU:HA	2.35	0.42
1:A:945:LEU:HA	1:A:945:LEU:HD23	1.63	0.41
2:B:452:LEU:HD23	2:B:452:LEU:HA	1.92	0.41
2:B:947:ASN:CG	2:B:949:HIS:HD2	2.24	0.41
8:H:22:LYS:HA	8:H:22:LYS:HD2	1.90	0.41
1:A:157:TRP:HE3	1:A:160:LEU:HB2	1.85	0.41
1:A:1141:LYS:HA	1:A:1141:LYS:HD3	1.94	0.41
2:B:282:LEU:HD23	2:B:372:LEU:HD11	2.01	0.41
2:B:399:ARG:CZ	2:B:626:ARG:HH11	2.33	0.41
5:E:129:LEU:O	5:E:132:ILE:HG12	2.19	0.41
8:H:99:LYS:HB3	8:H:113:TYR:HB2	2.02	0.41
1:A:998:SER:O	1:A:998:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:90:THR:HG23	9:I:96:GLY:H	1.85	0.41
15:T:-8:DG:H2"	15:T:-7:DC:H6	1.85	0.41
15:T:2:DC:H2'	15:T:3:DT:H71	2.01	0.41
1:A:128:GLN:N	1:A:128:GLN:OE1	2.54	0.41
1:A:345:ILE:O	1:A:349:ILE:HG22	2.21	0.41
1:A:773:ALA:HB1	15:T:-1:DT:OP1	2.21	0.41
2:B:512:SER:C	2:B:514:TRP:H	2.23	0.41
2:B:709:HIS:O	2:B:957:PRO:HD2	2.20	0.41
4:D:147:GLU:O	4:D:151:THR:HG23	2.21	0.41
1:A:551:GLU:HG2	1:A:552:ARG:H	1.85	0.41
2:B:204:GLN:H	2:B:204:GLN:HG2	1.70	0.41
2:B:839:VAL:HG22	2:B:840:ASP:H	1.86	0.41
5:E:107:ILE:HD12	5:E:114:THR:HA	2.02	0.41
8:H:34:SER:OG	8:H:39:MET:HB2	2.20	0.41
10:J:35:LEU:HD22	10:J:40:LEU:HD12	2.01	0.41
13:N:13:DC:H2"	13:N:14:DG:H5"	2.03	0.41
1:A:336:VAL:HA	1:A:439:ASN:ND2	2.35	0.41
1:A:477:LYS:HE3	1:A:477:LYS:HB3	1.92	0.41
1:A:797:VAL:HB	1:A:807:GLN:H	1.84	0.41
2:B:778:VAL:HA	2:B:783:ASN:HD21	1.85	0.41
1:A:900:ARG:HG3	1:A:1046:ALA:HB3	2.02	0.41
2:B:78:PRO:O	2:B:79:SER:C	2.58	0.41
2:B:399:ARG:HD3	2:B:399:ARG:HA	1.89	0.41
5:E:85:VAL:HG13	5:E:116:LEU:HA	2.02	0.41
7:G:60:GLU:CD	7:G:60:GLU:H	2.24	0.41
1:A:39:HIS:HB2	1:A:42:GLN:HG2	2.03	0.41
1:A:643:SER:HB2	1:A:644:PRO:HD3	2.01	0.41
1:A:1033:LEU:HD23	1:A:1033:LEU:HA	1.70	0.41
1:A:1086:ASP:HA	1:A:1089:ARG:CD	2.49	0.41
2:B:315:ILE:HG22	2:B:316:HIS:N	2.36	0.41
2:B:599:ARG:HE	2:B:599:ARG:HB3	1.70	0.41
3:C:273:THR:HG23	3:C:275:ALA:H	1.86	0.41
4:D:120:PRO:HG2	4:D:123:TYR:CE2	2.55	0.41
8:H:57:LYS:HB3	8:H:146:LEU:HD11	2.02	0.41
11:K:26:LYS:HE3	11:K:26:LYS:HB3	1.87	0.41
13:N:22:DG:H21	15:T:-22:DC:H42	1.67	0.41
15:T:12:DT:H2"	15:T:13:DG:C8	2.56	0.41
1:A:546:GLN:HG2	1:A:567:LEU:H	1.86	0.41
1:A:1228:GLU:HB2	6:F:115:ARG:HB3	2.03	0.41
2:B:178:VAL:CG1	2:B:184:LEU:HB3	2.51	0.41
2:B:916:SER:HB2	2:B:1037:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:150:ILE:HD12	7:G:150:ILE:HA	1.95	0.41
8:H:8:PHE:HB3	8:H:62:LEU:HB2	2.03	0.41
1:A:187:ILE:O	1:A:187:ILE:HG13	2.21	0.41
3:C:99:CYS:O	3:C:100:GLU:C	2.58	0.41
5:E:91:GLY:O	5:E:121:GLN:HB2	2.21	0.41
5:E:186:SER:O	5:E:192:VAL:HG11	2.21	0.41
13:N:-5:DT:H6	13:N:-5:DT:H2'	1.67	0.41
16:W:615:ARG:N	16:W:655:ALA:O	2.53	0.41
1:A:773:ALA:HA	15:T:-1:DT:C7	2.51	0.40
1:A:990:CYS:HB3	1:A:1004:PRO:HG3	2.02	0.40
2:B:33:SER:O	2:B:34:PHE:C	2.58	0.40
2:B:117:LEU:HD23	2:B:117:LEU:HA	1.65	0.40
2:B:268:LEU:HD12	2:B:315:ILE:CD1	2.50	0.40
5:E:171:LEU:HD23	5:E:171:LEU:HA	1.91	0.40
7:G:27:ARG:O	7:G:31:VAL:HG13	2.21	0.40
1:A:1048:ILE:HD12	1:A:1070:TRP:CG	2.57	0.40
2:B:71:PHE:O	2:B:419:ARG:NH1	2.55	0.40
2:B:484:LEU:O	2:B:485:GLN:C	2.57	0.40
2:B:594:LEU:HD12	2:B:594:LEU:HA	1.88	0.40
2:B:280:TRP:HB2	2:B:315:ILE:HG23	2.03	0.40
2:B:576:LEU:O	2:B:577:ASN:C	2.60	0.40
4:D:125:ARG:HA	4:D:125:ARG:HD2	1.94	0.40
16:W:628:VAL:HG22	16:W:638:VAL:HG12	2.03	0.40
1:A:318:LYS:HD3	2:B:1096:LEU:HD11	2.04	0.40
1:A:903:LEU:HD11	1:A:1095:CYS:SG	2.62	0.40
1:A:990:CYS:SG	1:A:1006:LEU:HD11	2.62	0.40
2:B:913:LYS:HD3	2:B:921:LYS:HZ1	1.86	0.40
3:C:152:ILE:HG21	10:J:5:VAL:HG13	2.02	0.40
2:B:313:ALA:O	2:B:317:VAL:HG23	2.22	0.40
2:B:339:ILE:O	2:B:342:THR:HG22	2.22	0.40
3:C:26:LEU:HB2	3:C:268:PHE:CE2	2.56	0.40
5:E:168:LYS:HE3	5:E:202:VAL:HG13	2.04	0.40
11:K:30:ALA:HA	11:K:75:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1131/1976 (57%)	1077 (95%)	54 (5%)	0	100	100
2	B	1032/1172 (88%)	966 (94%)	66 (6%)	0	100	100
3	C	281/319 (88%)	233 (83%)	48 (17%)	0	100	100
4	D	115/205 (56%)	109 (95%)	6 (5%)	0	100	100
5	E	207/222 (93%)	189 (91%)	18 (9%)	0	100	100
6	F	74/144 (51%)	74 (100%)	0	0	100	100
7	G	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
8	H	117/146 (80%)	114 (97%)	3 (3%)	0	100	100
9	I	94/114 (82%)	86 (92%)	8 (8%)	0	100	100
10	J	60/71 (84%)	52 (87%)	8 (13%)	0	100	100
11	K	98/116 (84%)	96 (98%)	2 (2%)	0	100	100
12	L	40/51 (78%)	40 (100%)	0	0	100	100
16	W	40/1493 (3%)	39 (98%)	1 (2%)	0	100	100
All	All	3465/6207 (56%)	3241 (94%)	224 (6%)	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	974/1710 (57%)	967 (99%)	7 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	786/1029 (76%)	764 (97%)	22 (3%)	43 65
3	C	221/282 (78%)	214 (97%)	7 (3%)	39 62
4	D	103/181 (57%)	103 (100%)	0	100 100
5	E	181/204 (89%)	181 (100%)	0	100 100
6	F	50/128 (39%)	50 (100%)	0	100 100
7	G	154/155 (99%)	154 (100%)	0	100 100
8	H	84/127 (66%)	84 (100%)	0	100 100
9	I	66/104 (64%)	65 (98%)	1 (2%)	65 80
10	J	49/66 (74%)	45 (92%)	4 (8%)	11 37
11	K	72/105 (69%)	66 (92%)	6 (8%)	11 37
12	L	30/45 (67%)	28 (93%)	2 (7%)	16 43
16	W	38/1156 (3%)	35 (92%)	3 (8%)	12 38
All	All	2808/5292 (53%)	2756 (98%)	52 (2%)	59 75

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ARG
1	A	552	ARG
1	A	852	ASN
1	A	872	THR
1	A	946	LEU
1	A	1027	THR
1	A	1035	ILE
2	B	64	LEU
2	B	71	PHE
2	B	101	THR
2	B	178	VAL
2	B	372	LEU
2	B	380	LEU
2	B	419	ARG
2	B	426	MET
2	B	458	THR
2	B	461	TRP
2	B	492	ARG
2	B	496	GLN
2	B	601	SER
2	B	658	ILE

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Mol	Chain	Res	Type
2	B	755	THR
2	B	776	VAL
2	B	784	GLN
2	B	812	VAL
2	B	888	LEU
2	B	945	VAL
2	B	973	ILE
2	B	1046	ASP
3	C	28	GLU
3	C	40	VAL
3	C	47	THR
3	C	98	HIS
3	C	181	SER
3	C	202	ASN
3	C	243	GLU
9	I	32	CYS
10	J	10	CYS
10	J	49	LEU
10	J	53	VAL
10	J	58	LYS
11	K	26	LYS
11	K	27	ILE
11	K	34	THR
11	K	41	THR
11	K	49	GLN
11	K	109	VAL
12	L	15	CYS
12	L	18	GLU
16	W	616	ILE
16	W	643	GLN
16	W	649	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	258	ASN
1	A	364	GLN
1	A	391	HIS
1	A	424	GLN
1	A	456	HIS
1	A	478	GLN

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Mol	Chain	Res	Type
1	A	664	HIS
1	A	781	ASN
1	A	869	GLN
1	A	947	GLN
1	A	958	GLN
1	A	1100	HIS
1	A	1114	GLN
1	A	1153	ASN
1	A	1165	ASN
1	A	1226	GLN
2	B	54	ASN
2	B	57	ASN
2	B	65	GLN
2	B	69	GLN
2	B	135	ASN
2	B	204	GLN
2	B	246	ASN
2	B	397	ASN
2	B	441	HIS
2	B	510	HIS
2	B	513	HIS
2	B	678	GLN
2	B	688	HIS
2	B	711	HIS
2	B	722	HIS
2	B	768	ASN
2	B	770	GLN
2	B	932	ASN
2	B	955	GLN
2	B	1038	GLN
2	B	1052	ASN
2	B	1057	HIS
2	B	1156	GLN
2	B	1166	ASN
3	C	7	GLN
3	C	88	GLN
3	C	161	GLN
3	C	280	GLN
3	C	284	ASN
3	C	291	GLN
4	D	164	ASN
7	G	128	ASN

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Mol	Chain	Res	Type
8	H	46	ASN
8	H	67	ASN
9	I	11	ASN
9	I	88	GLN
10	J	16	ASN
10	J	61	ASN
11	K	55	ASN
12	L	47	GLN
16	W	612	GLN
16	W	644	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/30 (30%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G
14	P	9	G
14	P	10	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 5 ligands modelled in this entry, 5 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.

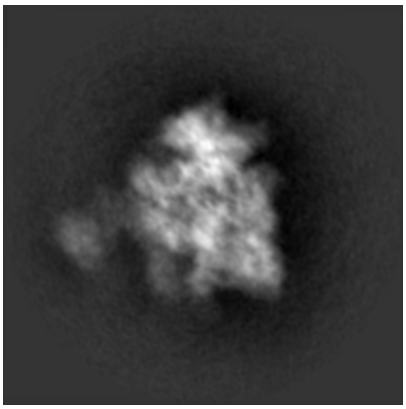
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35086. These allow visual inspection of the internal detail of the map and identification of artifacts.

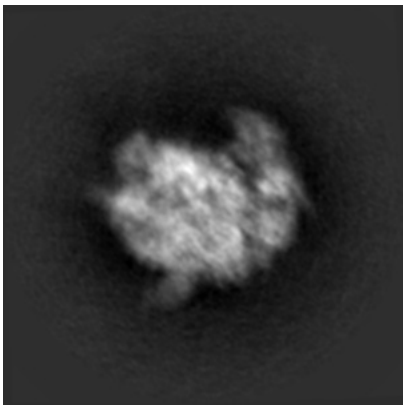
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

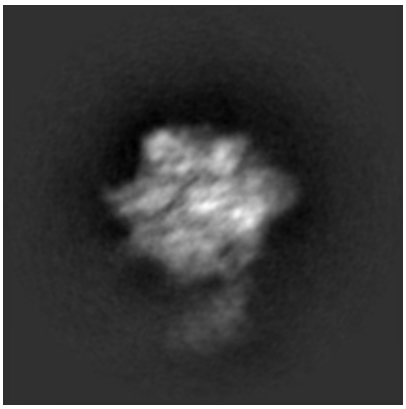
6.1.1 Primary map



X

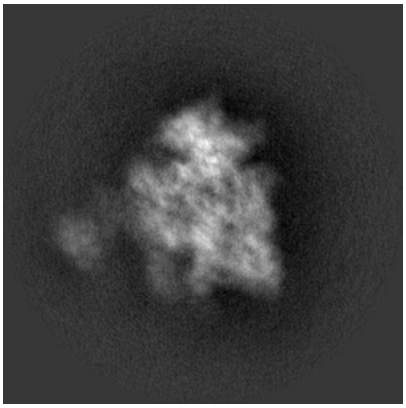


Y

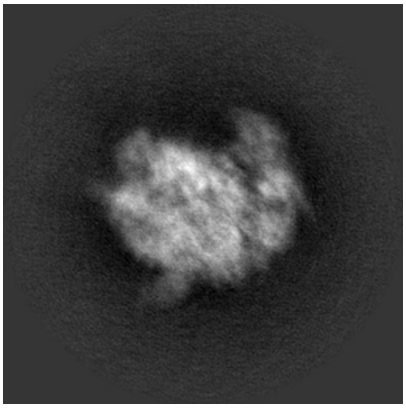


Z

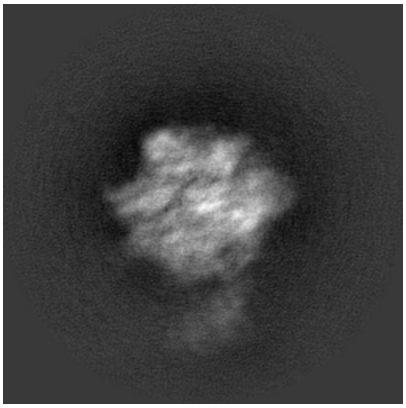
6.1.2 Raw map



X



Y

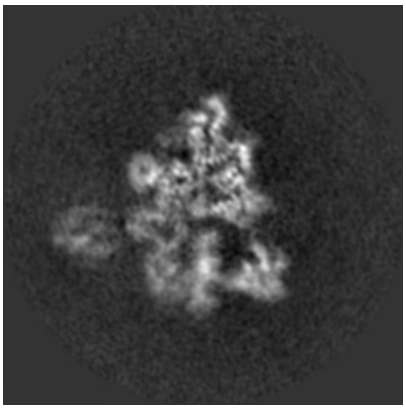


Z

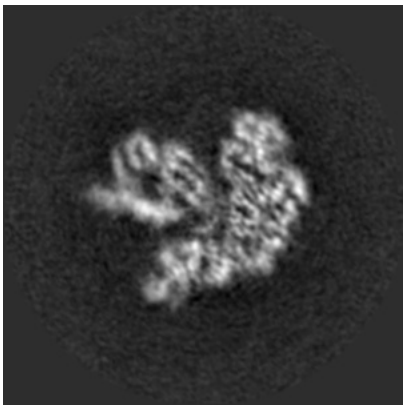
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

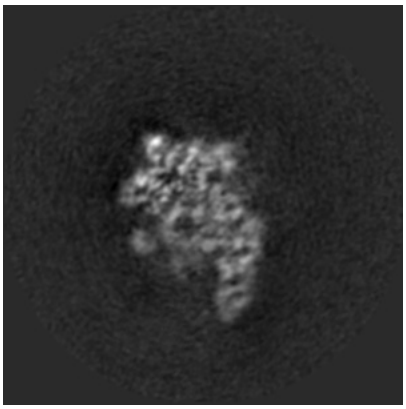
6.2.1 Primary map



X Index: 128

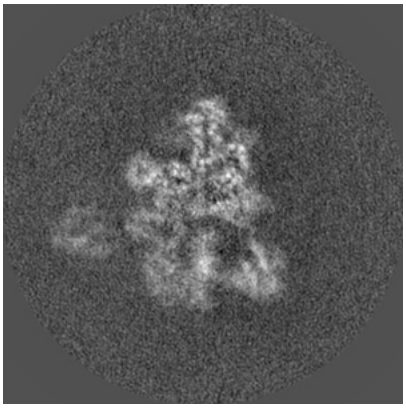


Y Index: 128

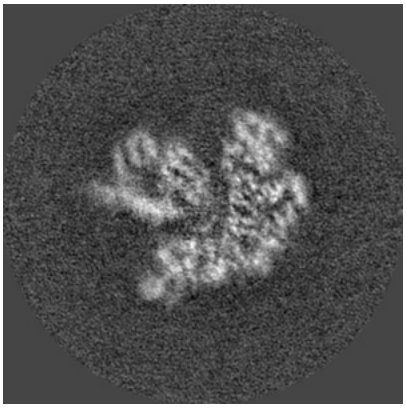


Z Index: 128

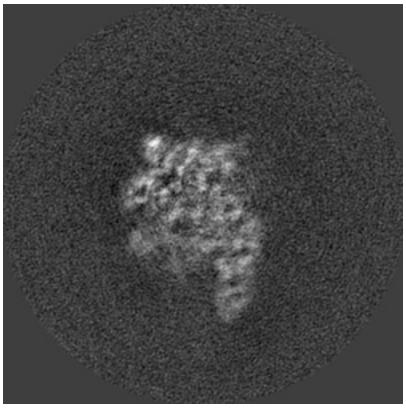
6.2.2 Raw map



X Index: 128



Y Index: 128

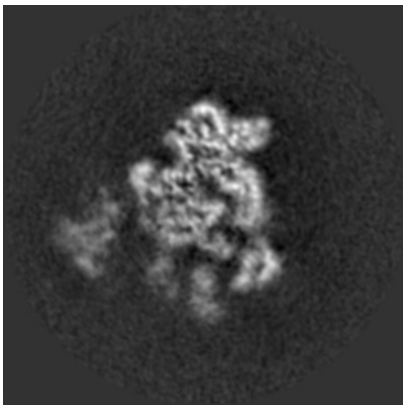


Z Index: 128

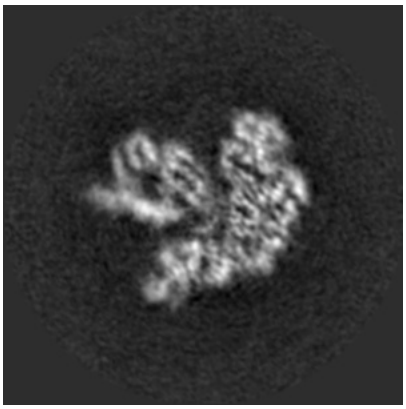
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

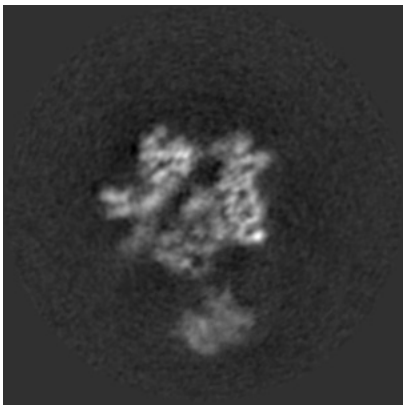
6.3.1 Primary map



X Index: 137

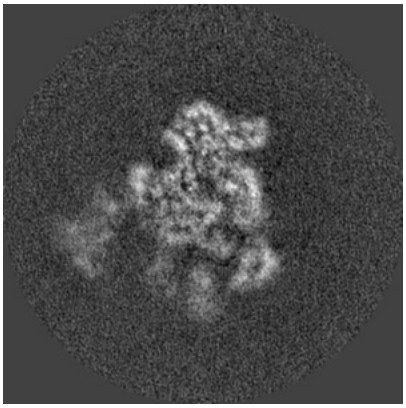


Y Index: 128

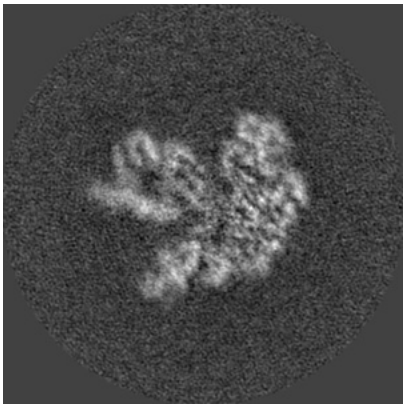


Z Index: 105

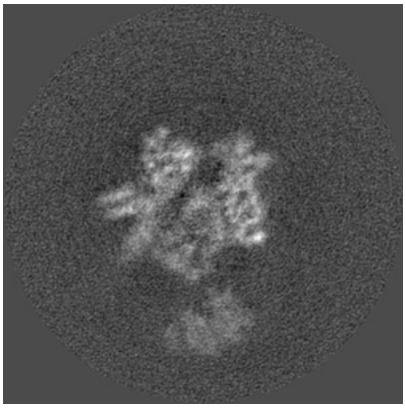
6.3.2 Raw map



X Index: 138



Y Index: 126

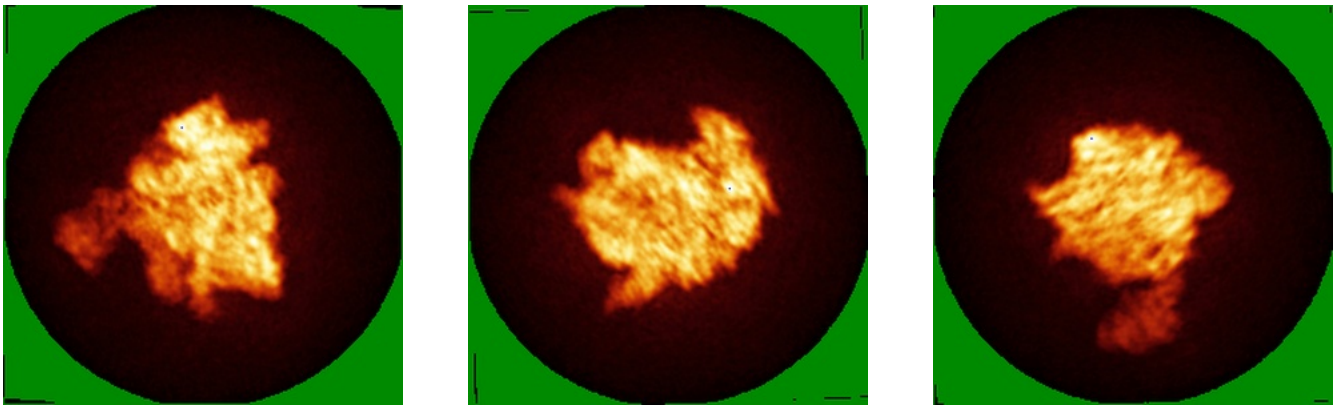


Z Index: 106

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

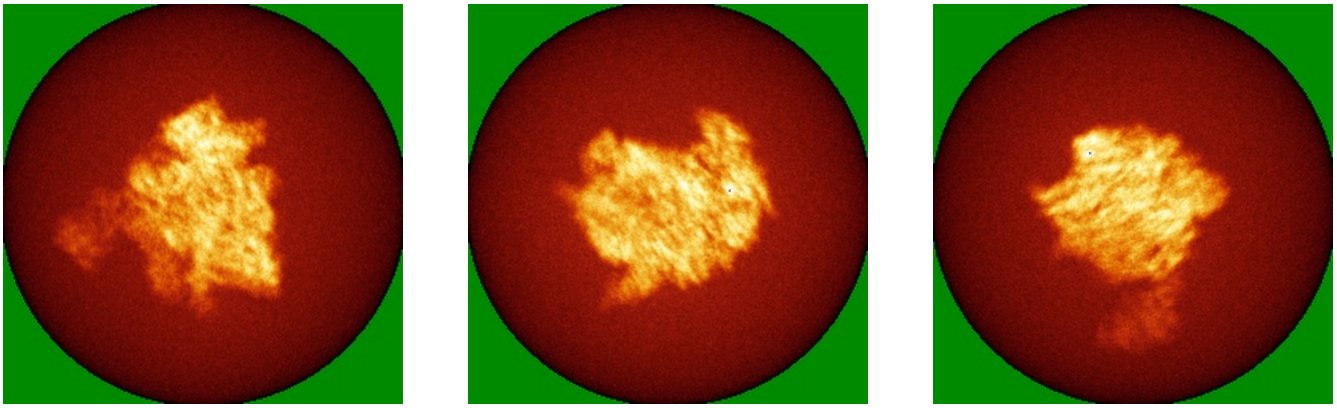
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

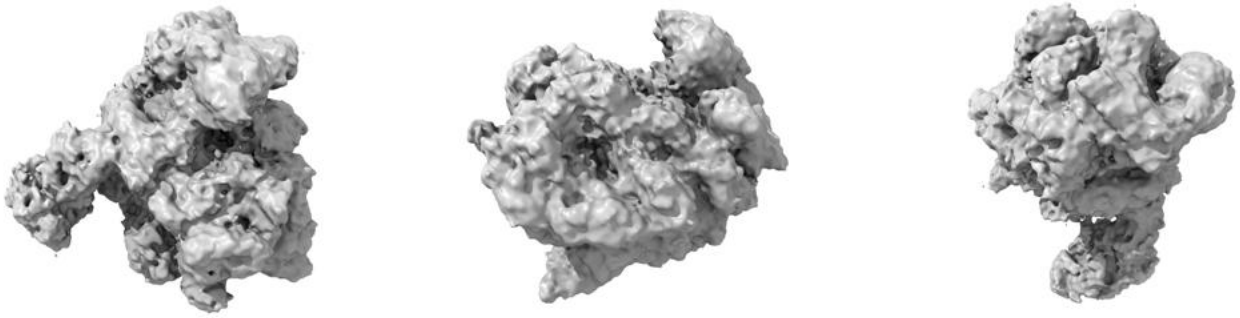


X Y Z

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

6.5 Orthogonal surface views (i)

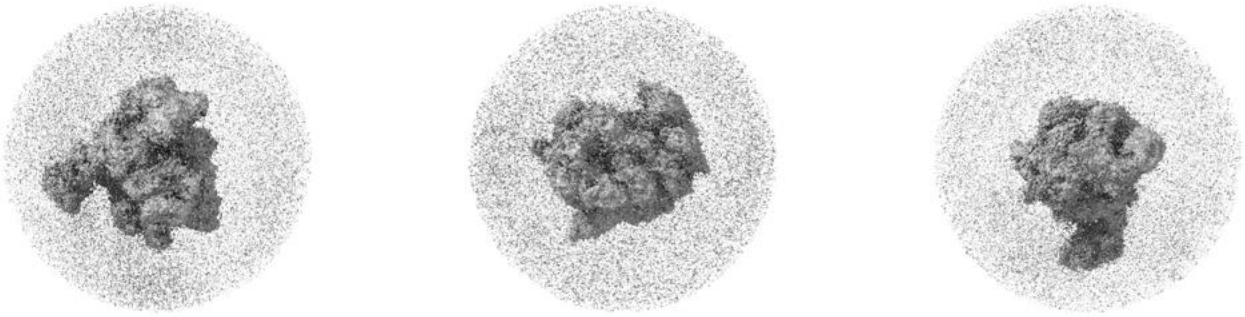
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

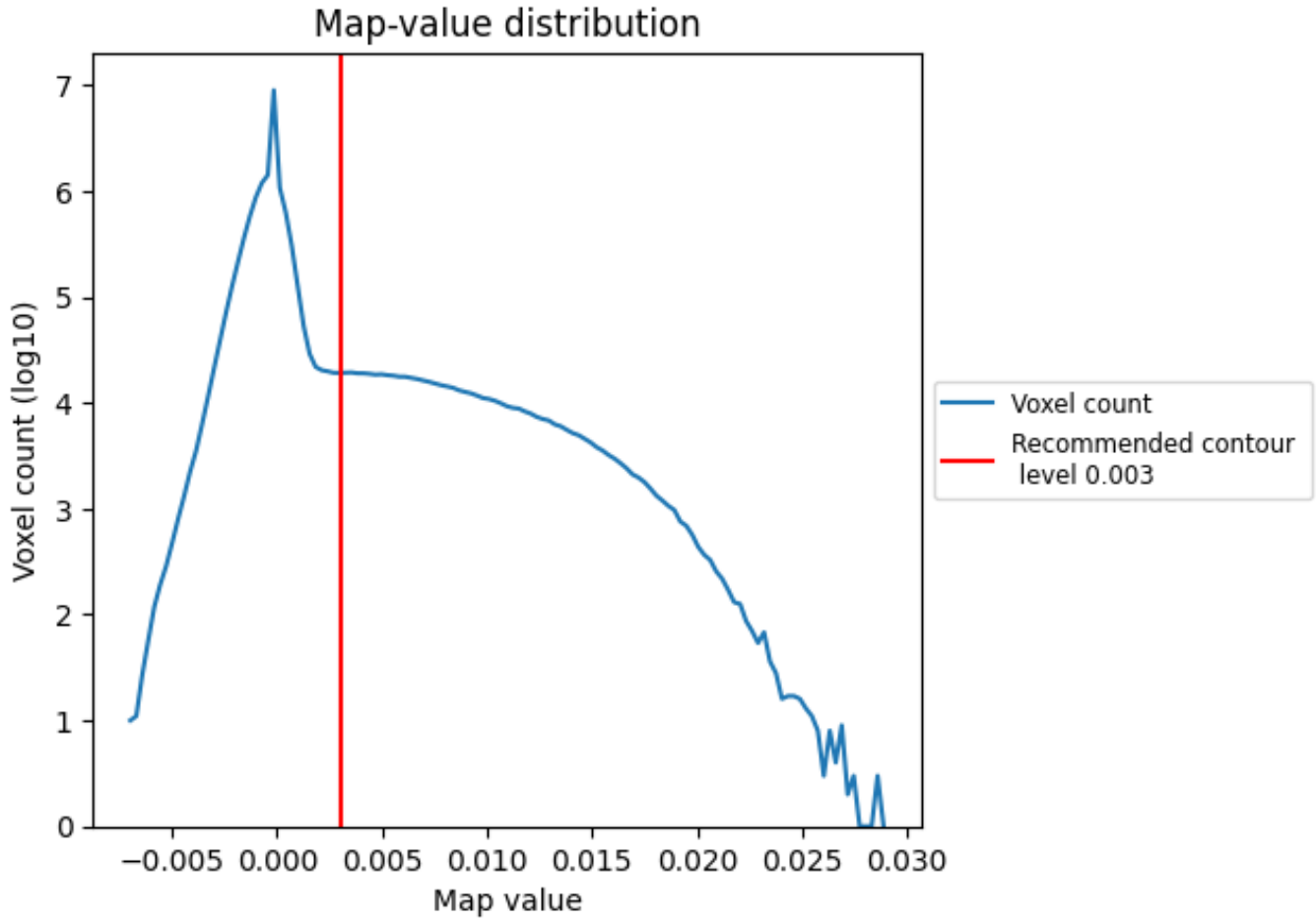
6.6 Mask visualisation (i)

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

7 Map analysis

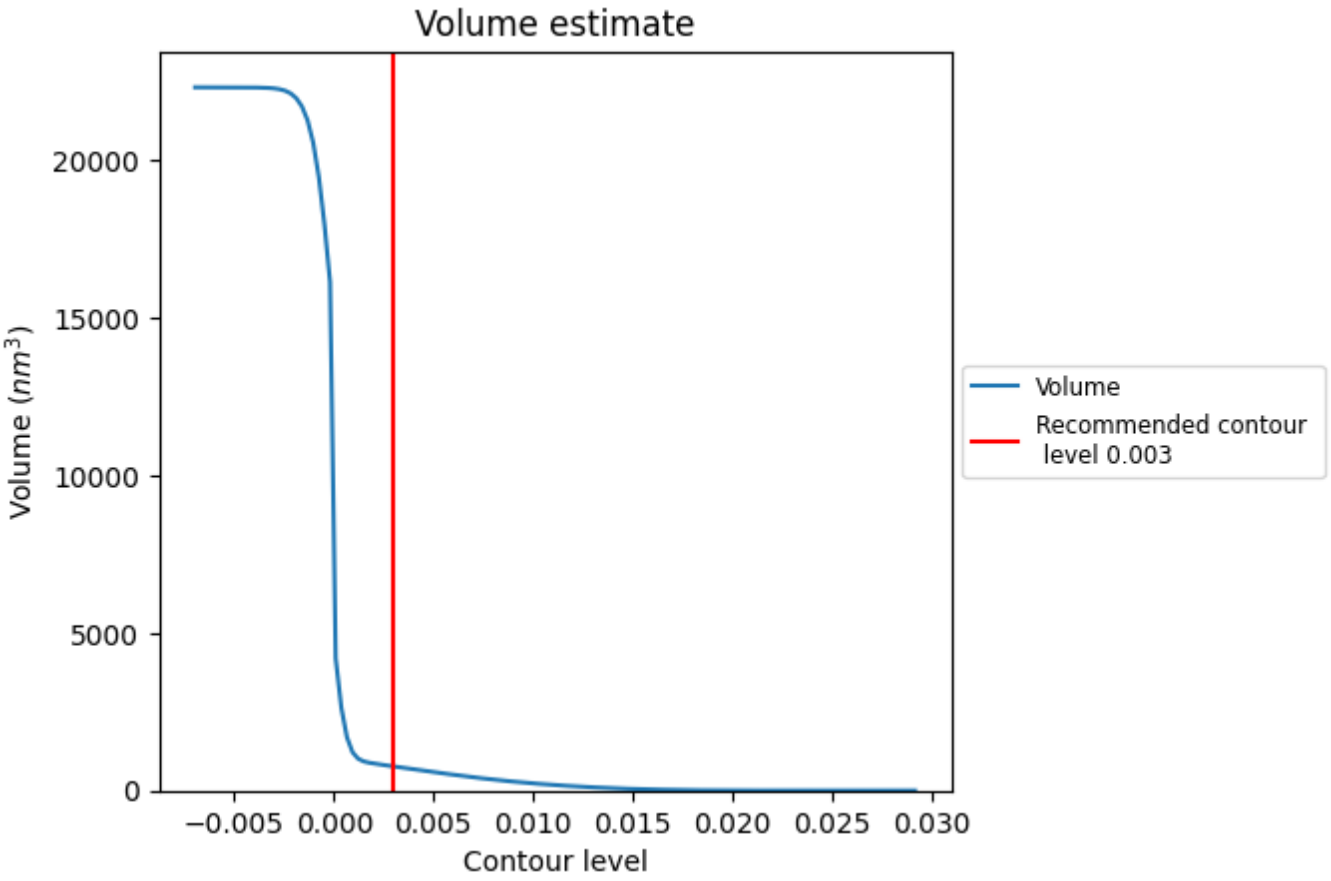
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

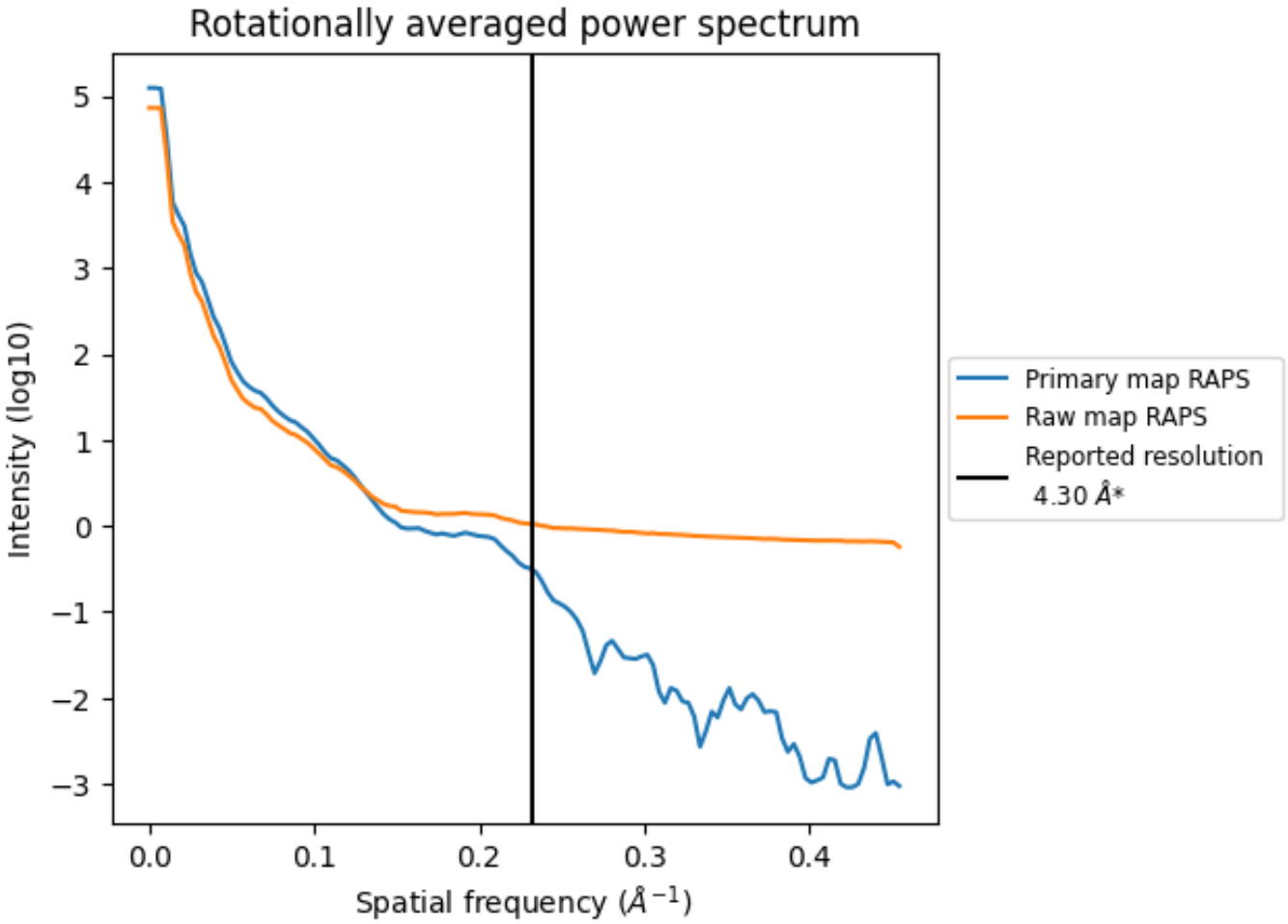
7.2 Volume estimate



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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)

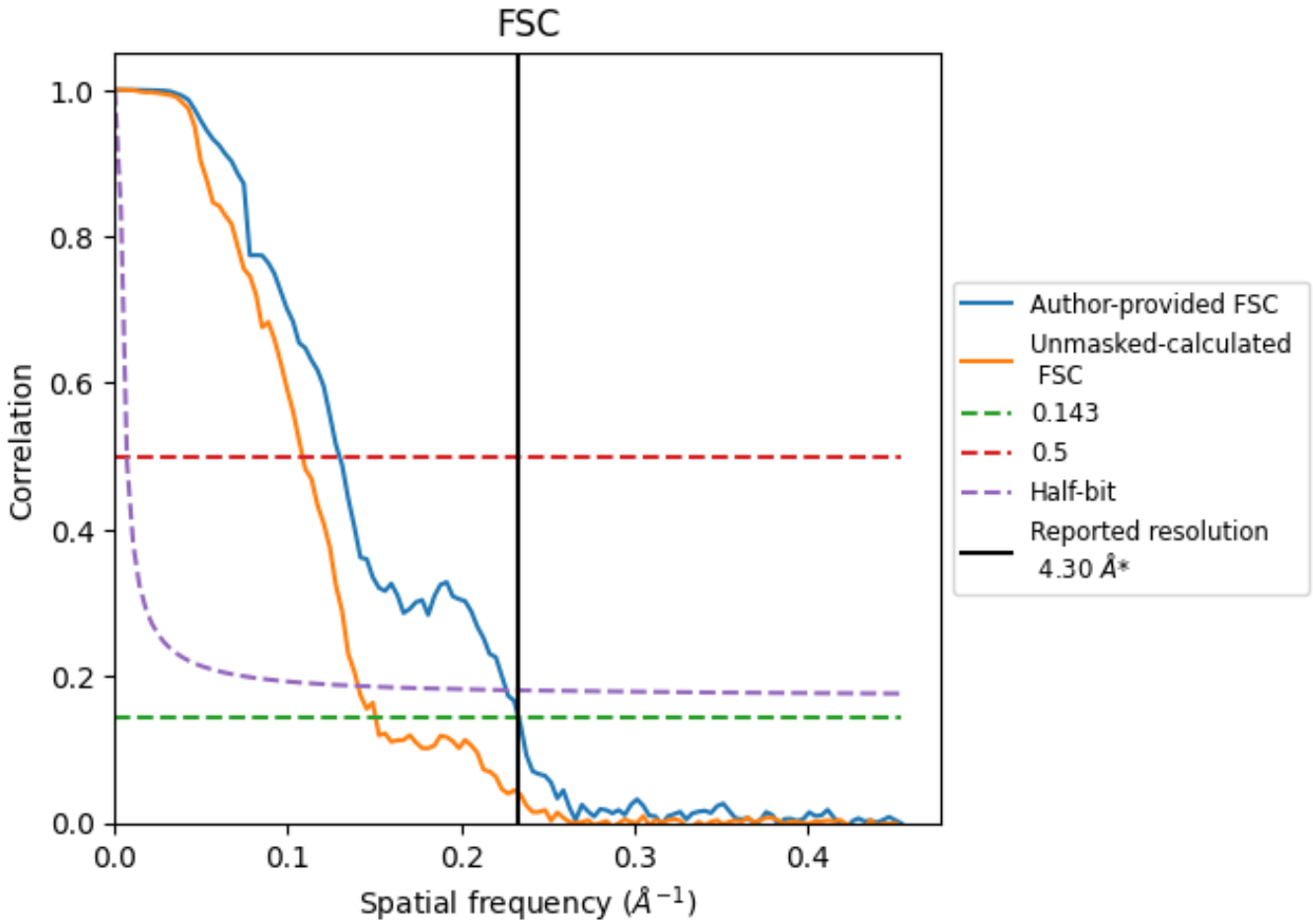


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

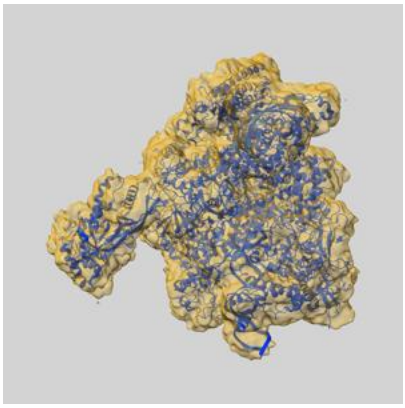
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.28	7.70	4.42
Unmasked-calculated*	6.63	9.22	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.63 differs from the reported value 4.3 by more than 10 %

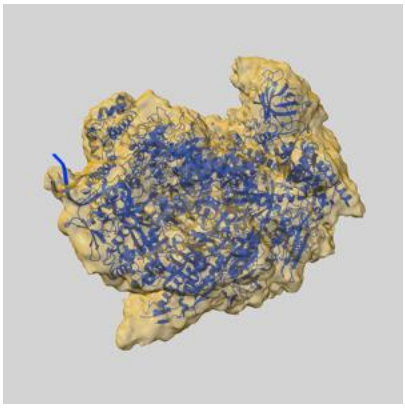
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35086 and PDB model 8HYJ. Per-residue inclusion information can be found in section 3 on page 7.

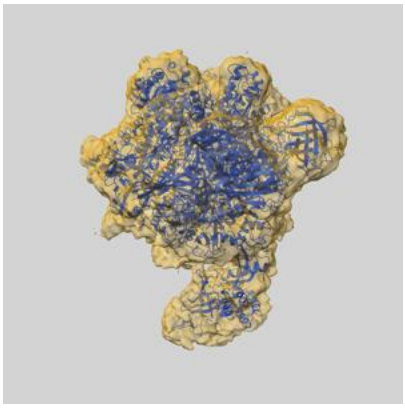
9.1 Map-model overlay



X



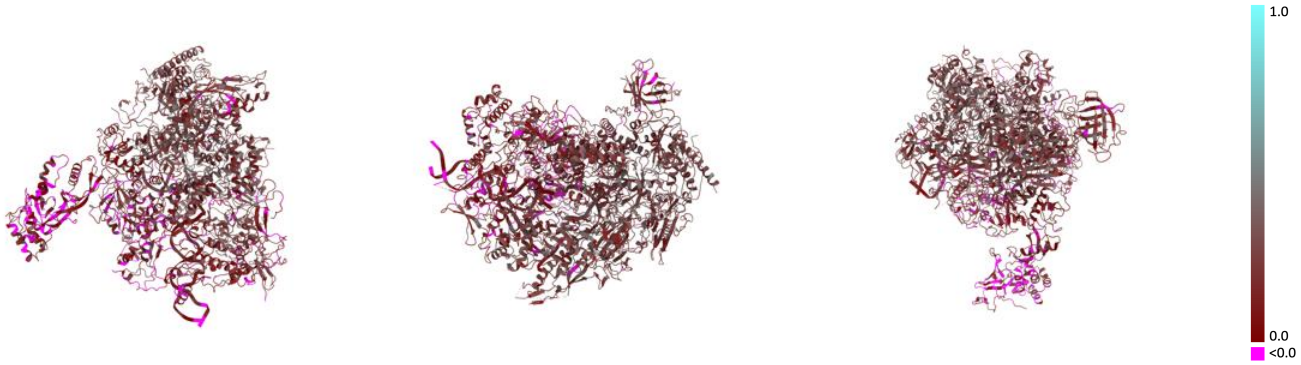
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

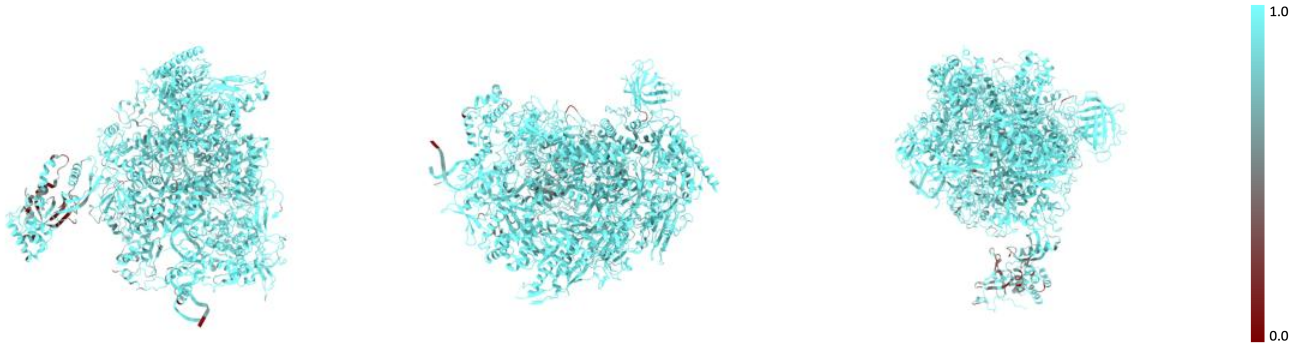
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

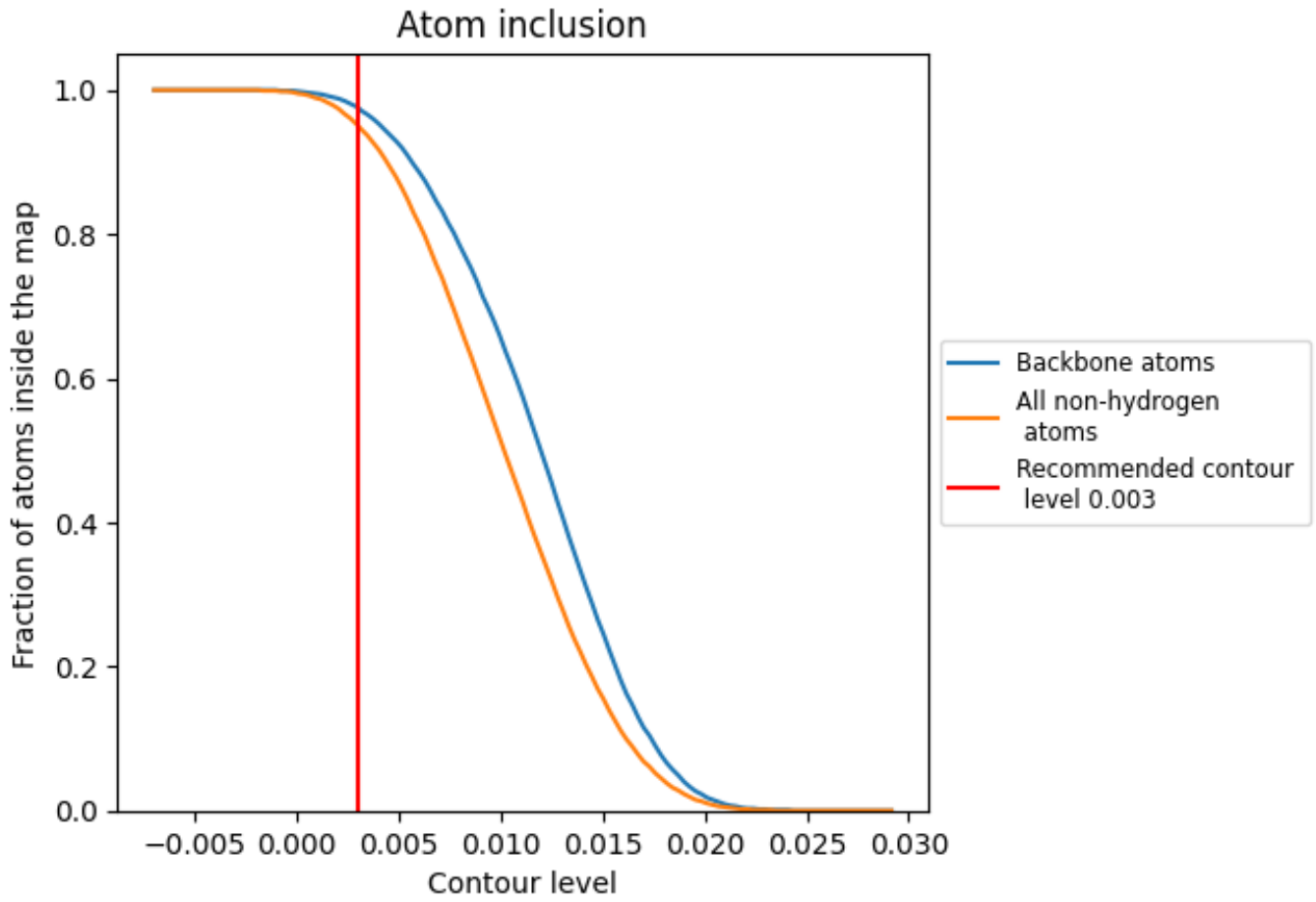
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9510	0.2050
A	0.9540	0.1860
B	0.9800	0.2720
C	0.9860	0.2680
D	0.8040	0.0480
E	0.9590	0.1390
F	0.9800	0.1900
G	0.7720	0.0680
H	0.9780	0.1910
I	0.9840	0.1480
J	0.9940	0.3120
K	0.9890	0.2870
L	0.9930	0.2440
N	0.9470	0.1140
P	0.9910	0.2590
T	0.8750	0.1340
W	0.8910	0.1890