



## Full wwPDB EM Validation Report ⓘ

Apr 10, 2025 – 01:33 PM JST

PDB ID : 9LXN / pdb\_00009lxn  
EMDB ID : EMD-63482  
Title : Human RNA Polymerase III de novo transcribing complex 5 (TC5)(without 3'dATP)  
Authors : Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.  
Deposited on : 2025-02-18  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

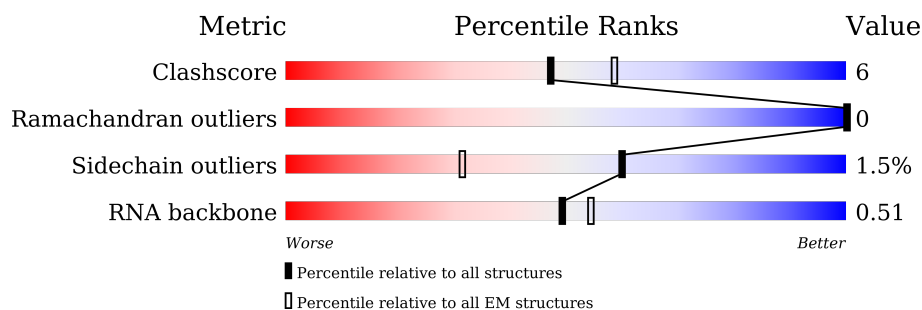
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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.



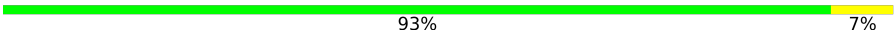









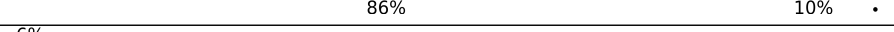
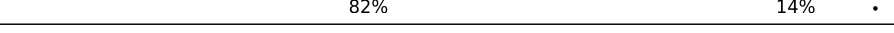
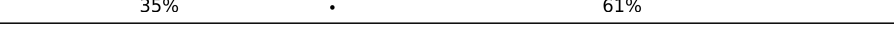
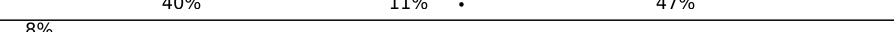

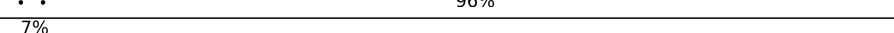



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1	368	<div> <div>30%</div> <div>29% 10% 60%</div> </div>
2	3	411	<div> <div>73%</div> <div>74% 16% 9%</div> </div>
3	4	1469	<div> <div>11%</div> <div>14% 83%</div> </div>
4	A	1390	<div> <div>87%</div> <div>12%</div> </div>
5	B	1133	<div> <div>84%</div> <div>12%</div> </div>
6	C	346	<div> <div>86%</div> <div>14%</div> </div>
7	D	148	<div> <div>68%</div> <div>14% 18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	398	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	127	
25	Y	127	
26	Z	4	

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 56785 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	374	Total	C	N	O	S	0	0
			3038	1925	521	571	21		

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	247	Total	C	N	O	S	0	0
			2066	1295	378	388	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1097	Total	C	N	O	S	0	0
			8680	5499	1516	1597	68		

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	178	Total	C	N	O	S	1	0
			1411	915	246	243	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (127-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	P	0	0
			1577	757	275	468	77		

- Molecule 25 is a DNA chain called DNA (127-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	77	Total	C	N	O	P	0	0
			1580	756	291	456	77		

- Molecule 26 is a RNA chain called RNA (5'-R(P\*UP\*GP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	4	Total	C	N	O	P	0	0
			83	37	12	30	4		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	I	1	Total	Zn	0
			1	1	

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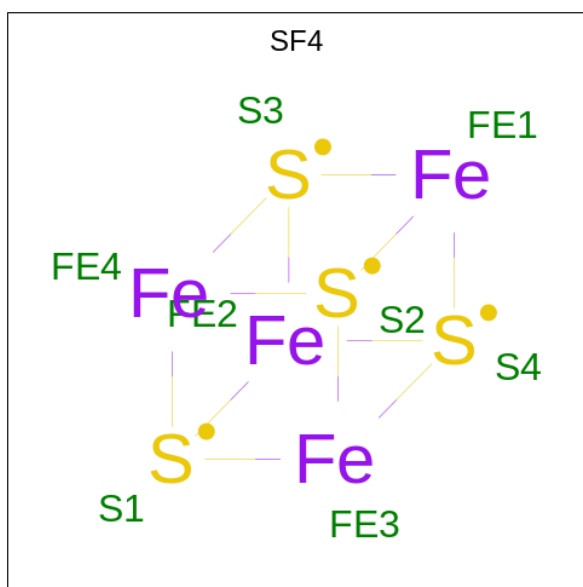
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Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	
27	V	1	Total	Zn	0
			1	1	

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

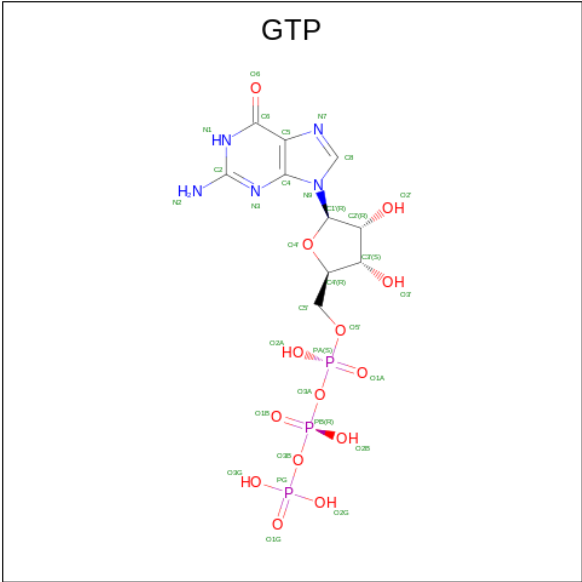
- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



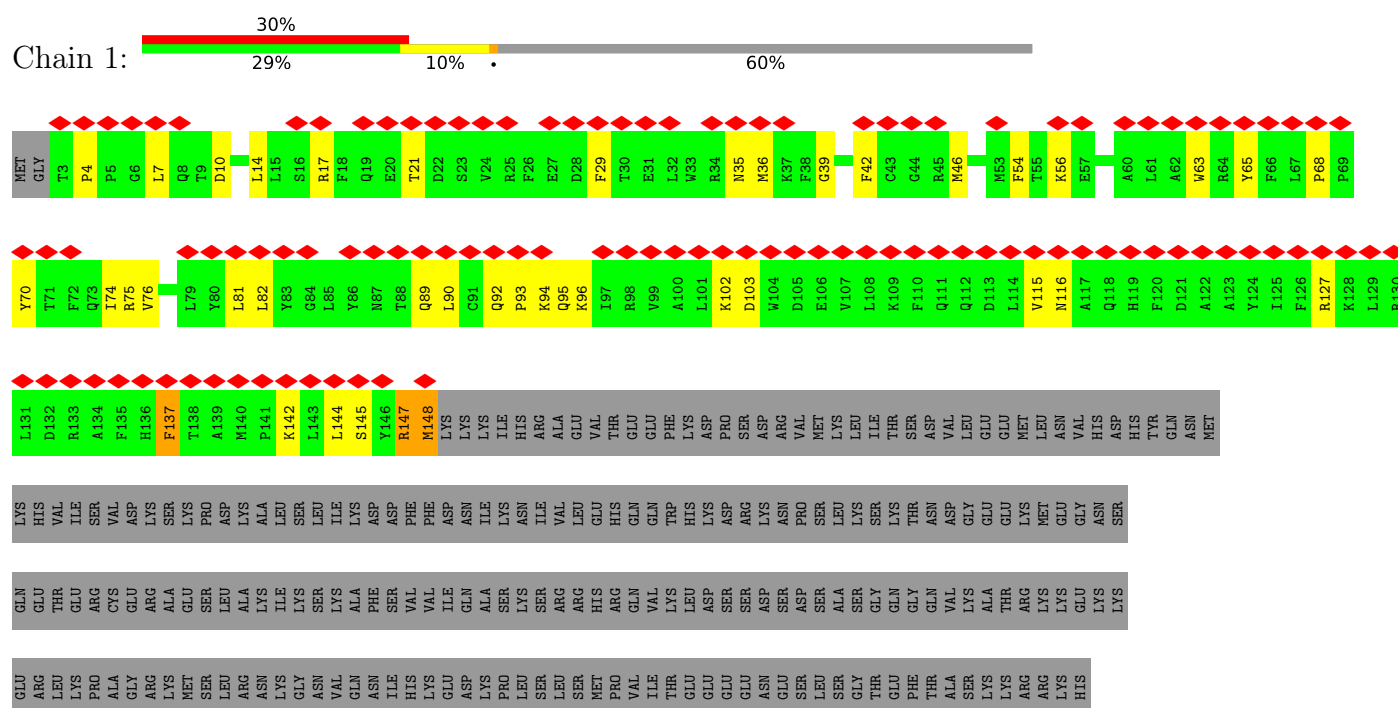


Mol	Chain	Residues	Atoms					AltConf
30	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

### 3 Residue-property plots

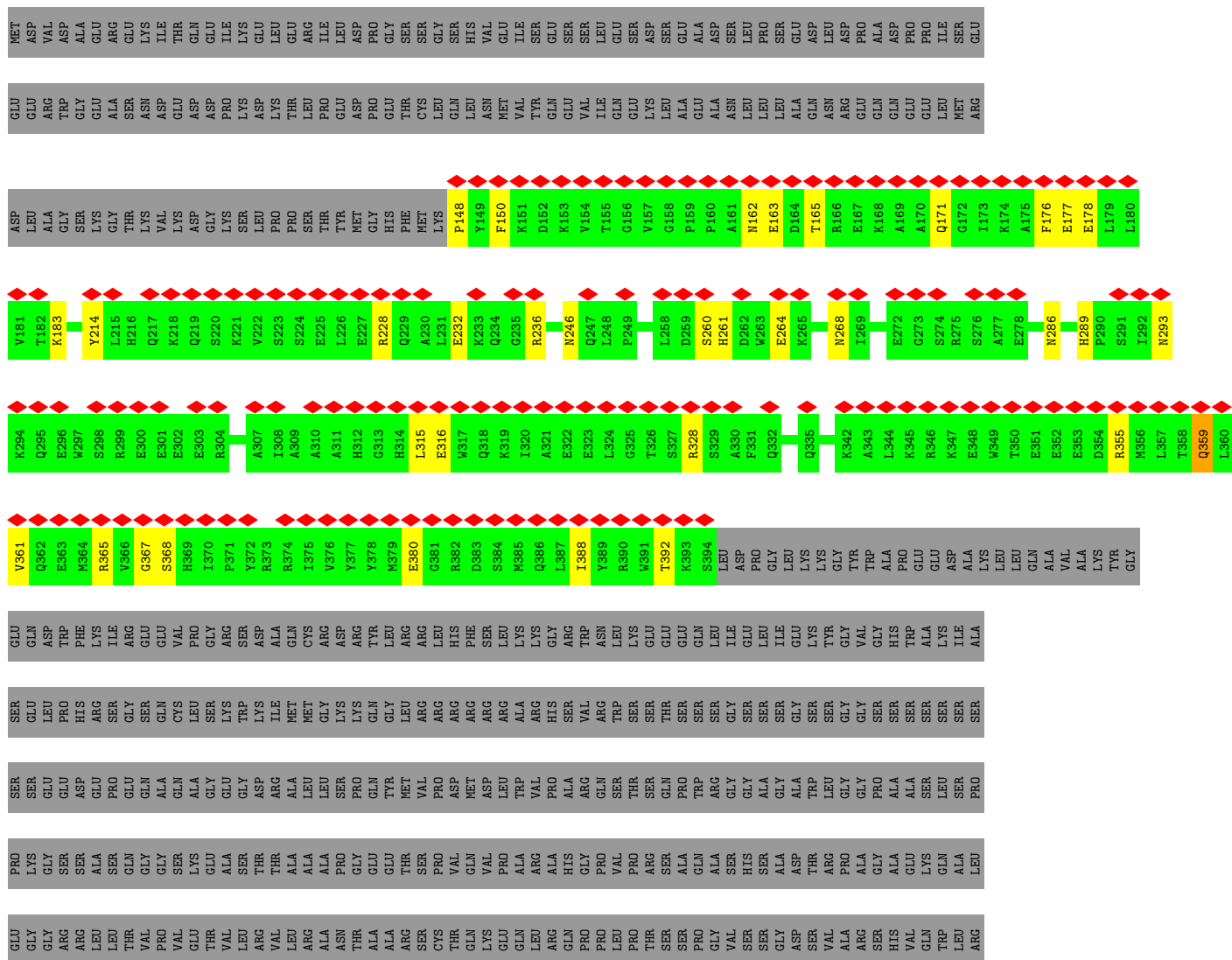
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: snRNA-activating protein complex subunit 1



#### • Molecule 2: snRNA-activating protein complex subunit 3

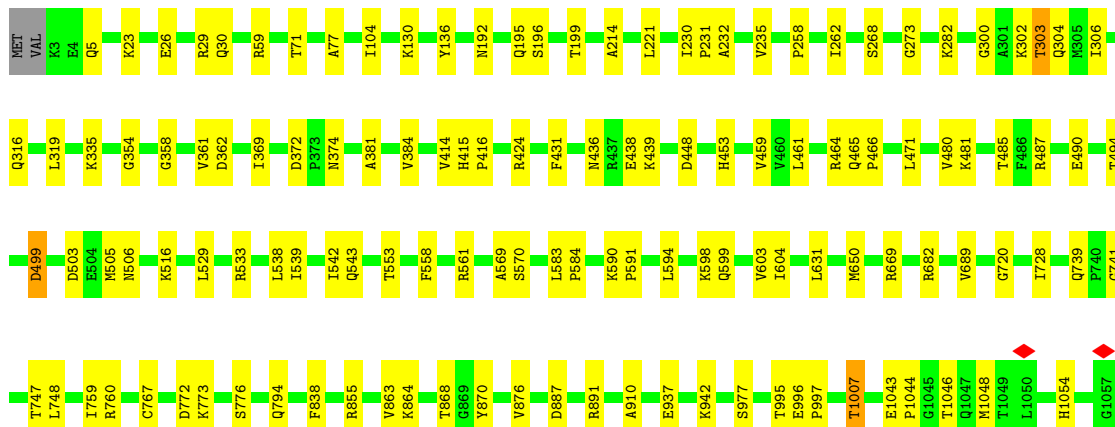


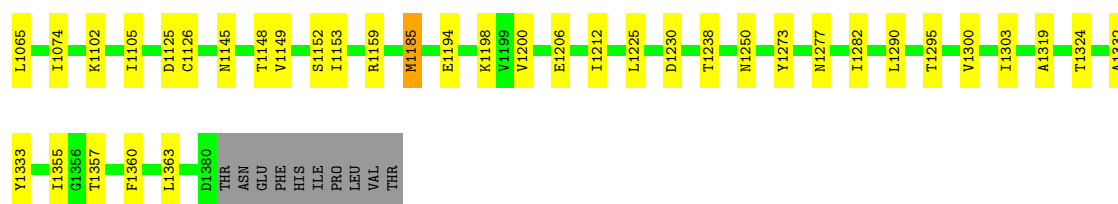


[illegible]

- Molecule 4: DNA-directed RNA polymerase III subunit RPC1

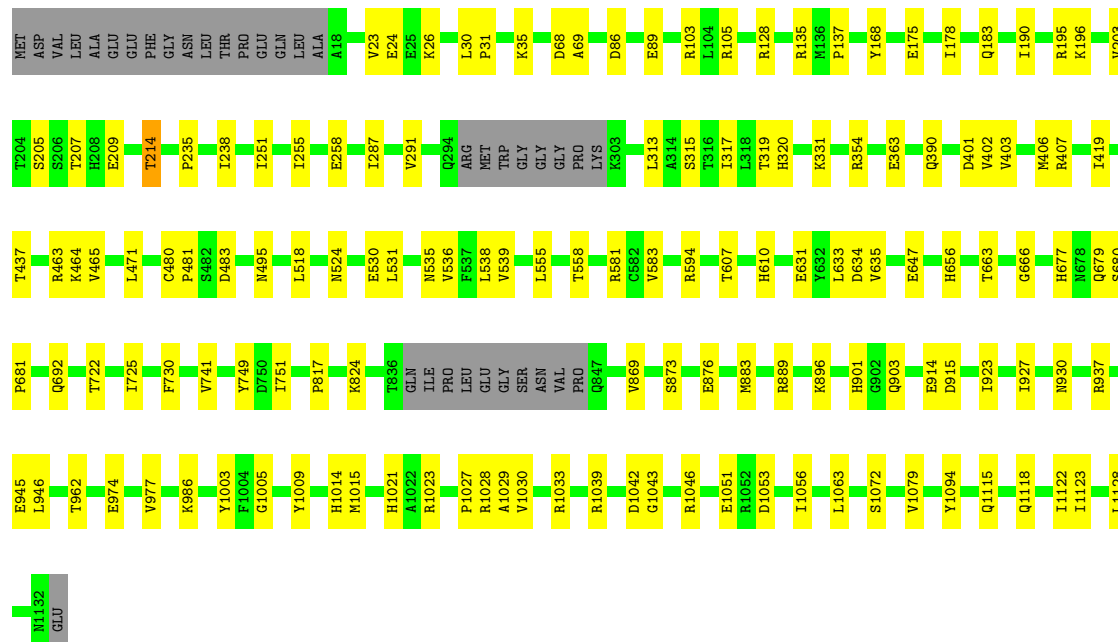
Chain A:  87% 12%





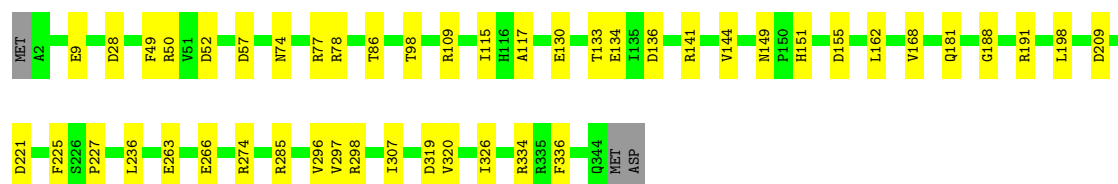
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B: 84% 12%



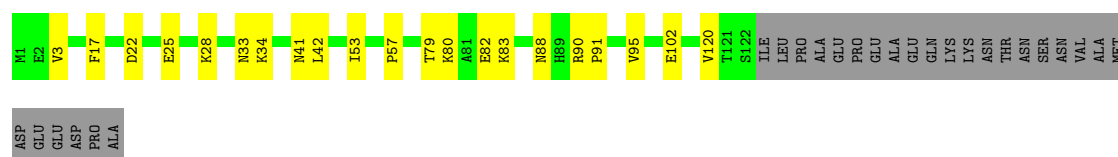
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 86% 14%



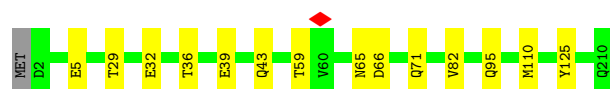
• Molecule 7: DNA-directed RNA polymerase III subunit RPC9

Chain D: 68% 14% 18%



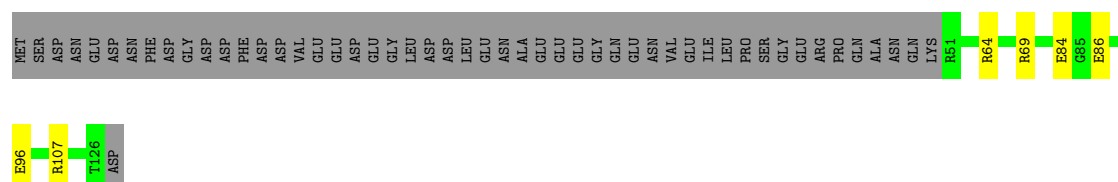
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  93% 7%



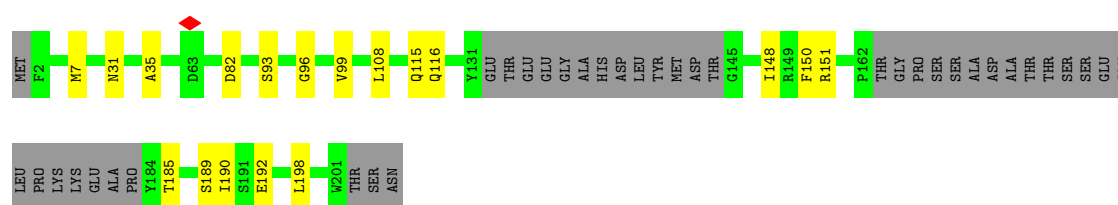
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  55% 5% 40%




- Molecule 10: DNA-directed RNA polymerase III subunit RPC8

Chain G:  73% 9% 19%



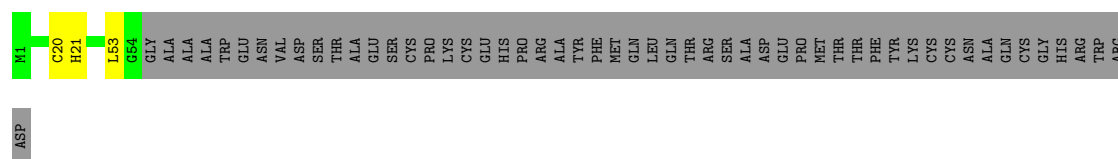
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  85% 13% .




- Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I:  47% . 50%



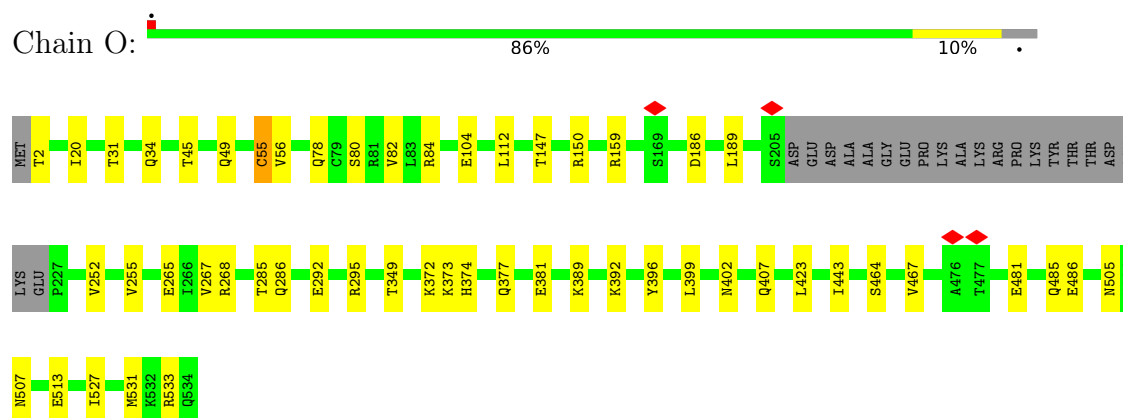
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  82% 13% . .

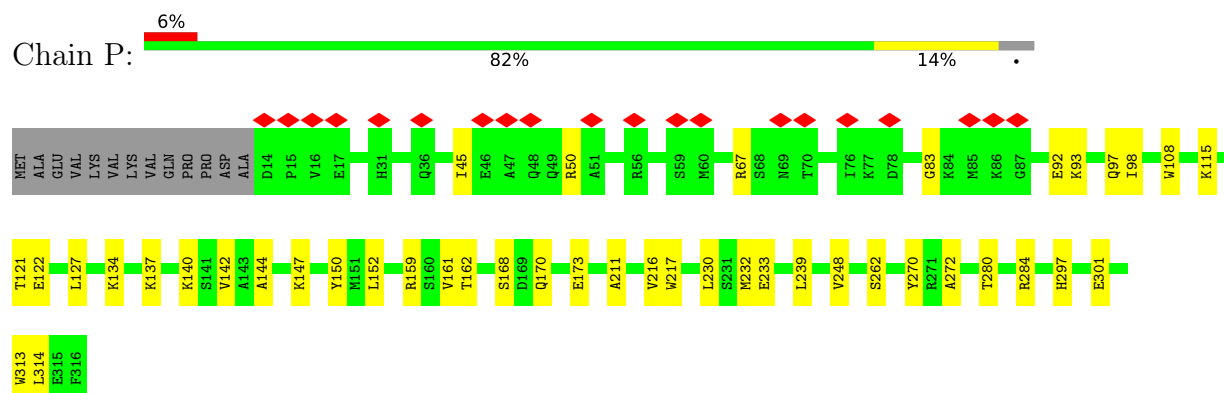


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |             |             |             |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | ASN | TRP | ASP | ASP | LYS | THR | VAL | ASP | ASP | MET | GLY | PRO | SER | HIS | <b>I137</b> | <b>R156</b> | <b>M157</b> | LEU | GLU | LYS | ASP | ASP | PHE | LEU | ASP | ASP | PRO | GLY | LEU | ARG | ASN | ASP | THR | ASP | GLN | VAL | PRO | PRO | LEU | LEU | ALA | HIS | SER | GLY | TRP | PHE | LYS | GLU | GLU | ASN | ASP | GLU | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

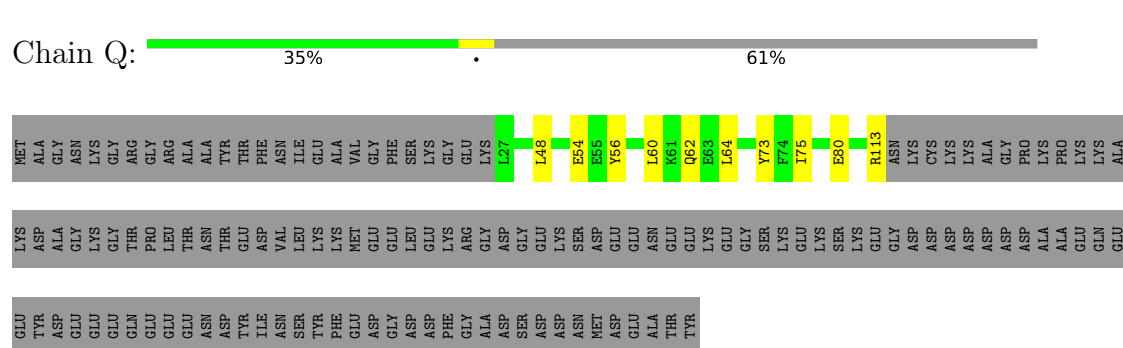
- Molecule 18: DNA-directed RNA polymerase III subunit RPC3



- Molecule 19: DNA-directed RNA polymerase III subunit RPC6



- Molecule 20: DNA-directed RNA polymerase III subunit RPC7



- Molecule 21: TATA-box-binding protein

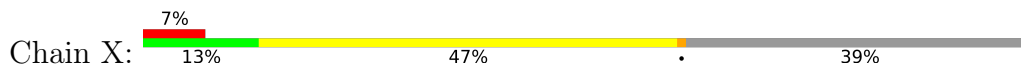








- Molecule 24: DNA (127-MER)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	341000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.436	Depositor
Minimum map value	-4.297	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.332538, 1.332538, 1.332538	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, GTP, 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	1	0.27	0/1266	0.49	0/1708
2	3	0.25	0/3113	0.49	0/4206
3	4	0.24	0/2107	0.47	0/2828
4	A	0.24	0/11008	0.46	0/14842
5	B	0.24	0/8845	0.47	0/11930
6	C	0.24	0/2790	0.49	0/3782
7	D	0.23	0/997	0.47	0/1343
8	E	0.24	0/1745	0.48	0/2358
9	F	0.23	0/620	0.49	0/839
10	G	0.25	0/1374	0.46	0/1868
11	H	0.24	0/1207	0.48	0/1628
12	I	0.29	0/434	0.52	0/584
13	J	0.23	0/521	0.44	0/703
14	K	0.24	0/837	0.47	0/1129
15	L	0.24	0/394	0.56	0/524
16	M	0.23	0/3455	0.45	0/4673
17	N	0.24	0/1137	0.49	0/1530
18	O	0.24	0/4141	0.47	0/5592
19	P	0.24	0/2446	0.42	0/3301
20	Q	0.24	0/777	0.49	0/1050
21	U	0.25	0/1439	0.50	0/1938
22	V	0.24	0/2904	0.48	0/3941
23	W	0.27	0/967	0.48	0/1293
24	X	0.60	0/1765	0.99	1/2720 (0.0%)
25	Y	0.56	0/1773	0.93	1/2731 (0.0%)
26	Z	0.59	0/91	1.25	0/139
All	All	0.28	0/58153	0.52	2/79180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	-48	DT	O4'-C1'-N1	5.80	112.06	108.00
25	Y	-3	DG	O4'-C4'-C3'	-5.05	102.48	104.50

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	1	1233	0	1231	25	0
2	3	3038	0	2911	55	0
3	4	2066	0	2049	20	0
4	A	10814	0	11057	115	0
5	B	8680	0	8805	99	0
6	C	2736	0	2712	32	0
7	D	985	0	1006	14	0
8	E	1715	0	1733	8	0
9	F	610	0	642	5	0
10	G	1337	0	1306	13	0
11	H	1186	0	1147	14	0
12	I	426	0	428	2	0
13	J	512	0	525	7	0
14	K	822	0	810	12	0
15	L	388	0	393	3	0
16	M	3382	0	3376	34	0
17	N	1128	0	1181	8	0
18	O	4075	0	4149	40	0
19	P	2403	0	2406	35	0
20	Q	754	0	759	10	0
21	U	1411	0	1501	31	0
22	V	2853	0	2890	34	0
23	W	943	0	924	12	0
24	X	1577	0	877	78	0
25	Y	1580	0	871	94	0
26	Z	83	0	41	5	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	I	1	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	V	1	0	0	0	0
28	A	1	0	0	0	0
29	P	8	0	0	0	0
30	Z	32	0	11	1	0
All	All	56785	0	55741	651	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 (651) 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)
24:X:-49:DG:H22	25:Y:49:DC:H42	1.15	0.93
24:X:-48:DT:H4'	24:X:-47:DA:H5'	1.58	0.85
24:X:-43:DC:O2	25:Y:43:DG:N2	2.10	0.84
1:1:46:MET:HG3	2:3:140:ARG:HH22	1.43	0.83
25:Y:36:DA:H2''	25:Y:37:DG:H5''	1.61	0.82
24:X:5:DA:H2''	24:X:6:DA:H5''	1.63	0.80
24:X:-43:DC:N3	25:Y:43:DG:N1	2.29	0.80
2:3:193:HIS:HE1	24:X:-50:DA:H8	1.31	0.78
25:Y:53:DC:H2''	25:Y:54:DA:C8	2.19	0.76
5:B:692:GLN:NE2	26:Z:3:G:O3'	2.18	0.75
25:Y:25:DA:H2''	25:Y:26:DT:H5'	1.66	0.75
2:3:193:HIS:CE1	24:X:-50:DA:H8	2.03	0.74
1:1:147:ARG:HB3	2:3:198:HIS:HB3	1.67	0.74
24:X:1:DT:H2''	24:X:2:DG:H5''	1.69	0.73
2:3:193:HIS:HE1	24:X:-50:DA:C8	2.06	0.73
24:X:11:DG:H1	25:Y:-10:DG:H21	1.36	0.73
4:A:414:VAL:HG12	4:A:416:PRO:HD2	1.72	0.72
25:Y:58:DT:H1'	25:Y:59:DA:H5'	1.73	0.71
2:3:245:ASP:OD1	16:M:312:ARG:NH1	2.24	0.71
2:3:266:GLU:OE2	16:M:312:ARG:NH2	2.23	0.70
4:A:485:THR:OG1	4:A:487:ARG:NH1	2.24	0.70
22:V:173:VAL:HG21	22:V:208:VAL:HG21	1.74	0.69
22:V:202:SER:O	22:V:206:GLN:NE2	2.24	0.69
19:P:98:ILE:HD13	19:P:115:LYS:HD3	1.75	0.69
25:Y:23:DA:H2''	25:Y:24:DT:H5''	1.75	0.69
18:O:374:HIS:HB3	18:O:423:LEU:HD23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:159:ARG:NH1	19:P:233:GLU:OE2	2.26	0.68
25:Y:30:DA:H2'	25:Y:31:DA:C8	2.28	0.68
4:A:465:GLN:OE1	4:A:506:ASN:ND2	2.26	0.68
19:P:140:LYS:NZ	25:Y:16:DC:OP1	2.26	0.68
21:U:171:THR:HG22	21:U:220:VAL:HG22	1.76	0.68
24:X:-49:DG:H22	25:Y:49:DC:N4	1.89	0.67
5:B:105:ARG:NH2	5:B:873:SER:O	2.27	0.67
8:E:95:GLN:OE1	8:E:125:TYR:OH	2.13	0.67
25:Y:-8:DA:H2''	25:Y:-7:DG:C8	2.30	0.67
4:A:995:THR:HG22	4:A:997:PRO:HD2	1.76	0.67
4:A:1074:ILE:HB	4:A:1303:ILE:HD12	1.77	0.67
25:Y:52:DT:H2''	25:Y:53:DC:C6	2.29	0.67
4:A:855:ARG:NH2	5:B:481:PRO:O	2.28	0.67
5:B:1023:ARG:NH2	5:B:1027:PRO:O	2.28	0.66
23:W:299:TYR:OH	25:Y:36:DA:O4'	2.13	0.66
4:A:760:ARG:NH2	4:A:794:GLN:OE1	2.29	0.66
19:P:137:LYS:NZ	19:P:152:LEU:O	2.28	0.66
19:P:216:VAL:HG21	19:P:239:LEU:HD11	1.76	0.66
22:V:267:GLN:NE2	24:X:-38:DT:OP1	2.29	0.66
2:3:193:HIS:NE2	24:X:-50:DA:H5''	2.12	0.65
2:3:55:LEU:HD13	2:3:57:GLY:H	1.61	0.65
4:A:374:ASN:ND2	5:B:749:TYR:OH	2.30	0.65
4:A:471:LEU:HD22	4:A:538:LEU:HD12	1.79	0.65
24:X:11:DG:H4'	24:X:12:DG:H5''	1.79	0.65
4:A:720:GLY:HA3	4:A:759:ILE:HD11	1.79	0.65
5:B:190:ILE:HG21	5:B:354:ARG:HE	1.62	0.65
5:B:401:ASP:OD1	22:V:143:TYR:OH	2.12	0.64
18:O:147:THR:HG22	18:O:150:ARG:HH22	1.62	0.64
18:O:159:ARG:NH2	18:O:189:LEU:O	2.29	0.64
4:A:1273:TYR:O	4:A:1277:ASN:ND2	2.30	0.64
2:3:247:TYR:OH	3:4:171:GLN:NE2	2.31	0.64
18:O:381:GLU:OE2	18:O:392:LYS:NZ	2.26	0.64
3:4:365:ARG:NH1	3:4:367:GLY:O	2.31	0.63
25:Y:-14:DT:H2''	25:Y:-13:DG:C8	2.33	0.63
21:U:167:ASN:HD21	21:U:169:VAL:HG23	1.63	0.63
4:A:1185:MET:SD	4:A:1185:MET:N	2.72	0.63
5:B:896:LYS:NZ	26:Z:5:U:OP1	2.32	0.63
24:X:-14:DA:H2''	24:X:-13:DA:H5'	1.80	0.63
22:V:43:THR:HG22	22:V:46:ASP:HB2	1.80	0.63
1:1:35:ASN:OD1	1:1:36:MET:N	2.32	0.62
21:U:174:LEU:HD12	21:U:178:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1230:ASP:OD1	4:A:1250:ASN:ND2	2.32	0.62
5:B:1014:HIS:CE1	26:Z:4:C:H4'	2.35	0.62
5:B:313:LEU:O	5:B:331:LYS:NZ	2.29	0.62
13:J:36:ASP:OD1	13:J:46:ARG:NH1	2.33	0.62
4:A:1152:SER:OG	4:A:1200:VAL:O	2.17	0.62
25:Y:-18:DG:H1'	25:Y:-17:DT:H5'	1.82	0.62
4:A:26:GLU:HG2	19:P:297:HIS:HB2	1.82	0.62
4:A:533:ARG:NH1	4:A:1043:GLU:OE1	2.33	0.62
16:M:171:LYS:HG3	19:P:67:ARG:HD3	1.80	0.61
5:B:915:ASP:OD1	6:C:78:ARG:NH2	2.33	0.61
5:B:1023:ARG:NH1	5:B:1042:ASP:O	2.32	0.61
19:P:83:GLY:N	19:P:92:GLU:OE2	2.30	0.61
25:Y:-7:DG:H2'	25:Y:-6:DT:C6	2.34	0.61
7:D:41:ASN:ND2	10:G:35:ALA:O	2.34	0.61
23:W:379:GLU:OE2	23:W:383:GLN:NE2	2.34	0.61
9:F:69:ARG:NE	9:F:96:GLU:OE1	2.34	0.61
21:U:199:ALA:HB2	21:U:214:PHE:CE1	2.36	0.61
19:P:284:ARG:HD3	20:Q:48:LEU:HA	1.81	0.61
24:X:22:DT:H2''	24:X:23:DA:C8	2.36	0.61
25:Y:-21:DT:H2''	25:Y:-20:DA:C8	2.36	0.61
24:X:20:DT:H2''	24:X:21:DA:N7	2.15	0.60
11:H:112:LEU:HD13	11:H:129:ALA:HB2	1.83	0.60
24:X:6:DA:H2''	24:X:7:DC:H6	1.64	0.60
3:4:232:GLU:OE1	3:4:236:ARG:NH1	2.34	0.60
4:A:230:ILE:O	18:O:2:THR:N	2.35	0.60
22:V:278:GLU:OE2	22:V:287:ARG:NH2	2.34	0.60
25:Y:0:DC:H2'	25:Y:1:DG:O4'	2.02	0.60
4:A:461:LEU:HD21	5:B:1063:LEU:HD21	1.84	0.60
6:C:149:ASN:ND2	6:C:151:HIS:O	2.35	0.60
5:B:183:GLN:NE2	5:B:363:GLU:OE2	2.34	0.60
18:O:507:ASN:OD1	20:Q:62:GLN:NE2	2.33	0.60
24:X:11:DG:H4'	24:X:12:DG:C5'	2.31	0.60
25:Y:28:DT:H2''	25:Y:29:DA:N7	2.17	0.60
16:M:225:LEU:HD11	17:N:376:LEU:HD13	1.84	0.60
5:B:692:GLN:HE22	26:Z:4:C:H5'	1.66	0.60
16:M:50:LYS:NZ	16:M:200:HIS:O	2.34	0.60
3:4:264:GLU:O	3:4:268:ASN:ND2	2.34	0.60
4:A:499:ASP:OD1	4:A:499:ASP:N	2.34	0.60
5:B:903:GLN:OE1	5:B:937:ARG:NH1	2.36	0.59
23:W:299:TYR:CE1	25:Y:35:DA:H1'	2.37	0.59
16:M:177:PHE:HE1	19:P:97:GLN:HB2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:203:VAL:HG13	5:B:214:THR:HG23	1.84	0.59
4:A:741:GLY:HA3	12:I:53:LEU:HD21	1.83	0.59
24:X:10:DC:H2'	24:X:11:DG:C8	2.37	0.59
25:Y:-10:DG:H2''	25:Y:-9:DA:N7	2.17	0.59
2:3:198:HIS:CD2	3:4:148:PRO:HG2	2.38	0.59
11:H:20:LYS:NZ	11:H:22:PHE:O	2.36	0.59
22:V:238:GLN:OE1	22:V:242:ARG:NH2	2.36	0.59
24:X:-28:DA:C8	24:X:-27:DT:H72	2.37	0.58
3:4:293:ASN:O	3:4:328:ARG:NH1	2.36	0.58
13:J:28:GLU:OE2	16:M:397:GLY:N	2.37	0.58
21:U:309:LYS:HD3	25:Y:30:DA:H5''	1.85	0.58
2:3:304:LYS:N	2:3:309:TYR:OH	2.36	0.58
4:A:1054:HIS:HD2	4:A:1065:LEU:HD12	1.69	0.58
5:B:536:VAL:O	5:B:581:ARG:NH1	2.36	0.58
6:C:109:ARG:NH2	6:C:198:LEU:O	2.36	0.58
24:X:-24:DA:H2''	24:X:-23:DT:C5	2.39	0.57
7:D:17:PHE:HB2	7:D:53:ILE:HG21	1.85	0.57
19:P:147:LYS:HG3	25:Y:14:DT:H4'	1.86	0.57
25:Y:55:DA:H2''	25:Y:56:DG:C8	2.39	0.57
7:D:3:VAL:HG12	10:G:7:MET:HG2	1.86	0.57
3:4:355:ARG:O	3:4:359:GLN:NE2	2.37	0.57
4:A:529:LEU:HA	4:A:539:ILE:HD13	1.85	0.57
6:C:9:GLU:OE2	6:C:298:ARG:NH1	2.38	0.57
5:B:463:ARG:HE	5:B:465:VAL:HG22	1.70	0.57
24:X:-32:DC:C6	24:X:-31:DT:H72	2.39	0.57
4:A:937:GLU:OE1	4:A:1007:THR:OG1	2.22	0.57
17:N:254:LEU:HD12	17:N:331:ILE:HD11	1.87	0.57
5:B:89:GLU:OE2	15:L:42:ARG:NE	2.38	0.57
5:B:524:ASN:O	16:M:134:GLN:NE2	2.38	0.57
16:M:347:GLU:OE2	16:M:351:ARG:NH2	2.38	0.57
6:C:188:GLY:O	6:C:191:ARG:NH1	2.38	0.56
21:U:189:ASN:ND2	21:U:203:ARG:O	2.39	0.56
16:M:171:LYS:HZ3	19:P:67:ARG:HB2	1.70	0.56
6:C:50:ARG:NH1	6:C:52:ASP:OD2	2.37	0.56
10:G:115:GLN:NE2	10:G:192:GLU:O	2.38	0.56
22:V:76:VAL:HG22	22:V:118:VAL:HG13	1.87	0.56
16:M:409:ILE:HG23	16:M:416:VAL:HG21	1.87	0.56
21:U:295:MET:HB2	21:U:298:PRO:HD2	1.88	0.56
4:A:1044:PRO:HG2	4:A:1282:ILE:HD11	1.87	0.56
6:C:141:ARG:NH1	6:C:209:ASP:OD1	2.38	0.56
4:A:303:THR:OG1	18:O:377:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:177:PHE:CZ	19:P:98:ILE:HB	2.40	0.56
24:X:8:DT:H2''	24:X:9:DT:C6	2.41	0.56
2:3:350:TRP:NE1	24:X:-50:DA:OP1	2.38	0.56
25:Y:46:DA:C8	25:Y:47:DT:H72	2.41	0.56
5:B:313:LEU:HD23	5:B:317:ILE:HD12	1.88	0.56
18:O:45:THR:OG1	18:O:49:GLN:OE1	2.23	0.56
24:X:-27:DT:H2'	24:X:-26:DA:C8	2.41	0.56
18:O:112:LEU:HD11	20:Q:64:LEU:HD22	1.88	0.55
24:X:-58:DA:H2''	24:X:-57:DA:C8	2.41	0.55
19:P:121:THR:OG1	19:P:122:GLU:OE1	2.24	0.55
21:U:298:PRO:HB3	21:U:324:ALA:CB	2.35	0.55
25:Y:-20:DA:H2''	25:Y:-19:DT:H71	1.86	0.55
7:D:33:ASN:OD1	7:D:34:LYS:N	2.40	0.55
19:P:313:TRP:HZ2	20:Q:48:LEU:HD21	1.71	0.55
25:Y:-15:DC:H2'	25:Y:-14:DT:H71	1.88	0.55
4:A:542:ILE:HG13	4:A:543:GLN:H	1.71	0.55
24:X:-35:DT:H2'	24:X:-34:DG:C8	2.41	0.55
25:Y:37:DG:H2''	25:Y:38:DA:C8	2.42	0.55
1:1:148:MET:SD	1:1:148:MET:N	2.78	0.55
4:A:5:GLN:HB2	10:G:185:THR:HG21	1.89	0.55
11:H:8:ASP:OD1	11:H:9:ILE:N	2.39	0.55
19:P:168:SER:OG	19:P:173:GLU:OE2	2.23	0.55
16:M:134:GLN:OE1	16:M:136:ARG:NH2	2.39	0.55
18:O:349:THR:HG23	19:P:280:THR:HG21	1.88	0.55
21:U:297:LYS:HB2	21:U:298:PRO:HD3	1.89	0.55
25:Y:47:DT:H2''	25:Y:48:DA:C8	2.41	0.55
2:3:198:HIS:CG	3:4:148:PRO:HG2	2.42	0.54
24:X:-52:DA:H4'	24:X:-51:DA:OP1	2.06	0.54
4:A:838:PHE:O	5:B:677:HIS:ND1	2.36	0.54
16:M:327:VAL:O	16:M:353:ARG:NH1	2.38	0.54
25:Y:-20:DA:H2''	25:Y:-19:DT:C7	2.37	0.54
25:Y:45:DA:H2''	25:Y:46:DA:N7	2.22	0.54
4:A:558:PHE:HB3	4:A:594:LEU:HD13	1.90	0.54
6:C:326:ILE:HG21	14:K:111:LEU:HB2	1.90	0.54
16:M:221:GLU:HB3	17:N:374:THR:HG21	1.89	0.54
19:P:147:LYS:CG	25:Y:14:DT:H4'	2.37	0.54
4:A:361:VAL:HG12	5:B:1072:SER:HB3	1.89	0.54
13:J:3:ILE:HD12	13:J:4:PRO:HD2	1.90	0.54
5:B:634:ASP:OD1	5:B:635:VAL:N	2.39	0.53
16:M:117:ALA:HB1	16:M:124:LEU:HD11	1.90	0.53
19:P:108:TRP:HD1	19:P:147:LYS:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:298:TYR:CE2	24:X:-32:DC:H4'	2.43	0.53
3:4:260:SER:O	3:4:261:HIS:ND1	2.41	0.53
2:3:260:ASN:ND2	2:3:269:ASP:OD1	2.42	0.53
1:1:115:VAL:HG22	2:3:90:LEU:HD22	1.89	0.53
16:M:53:GLN:OE1	16:M:200:HIS:ND1	2.41	0.53
24:X:-53:DG:H2''	24:X:-52:DA:C8	2.44	0.53
4:A:29:ARG:NH1	19:P:301:GLU:OE1	2.41	0.53
1:1:63:TRP:NE1	1:1:103:ASP:OD2	2.42	0.53
4:A:232:ALA:HA	4:A:235:VAL:HG23	1.91	0.53
5:B:390:GLN:NE2	25:Y:12:DC:OP1	2.42	0.53
24:X:12:DG:H4'	24:X:13:DC:OP1	2.08	0.53
24:X:15:DG:H1'	24:X:16:DC:H5'	1.91	0.53
6:C:74:ASN:OD1	6:C:77:ARG:NH2	2.41	0.53
6:C:133:THR:OG1	6:C:136:ASP:OD1	2.25	0.53
6:C:296:VAL:HG23	6:C:297:VAL:HG13	1.91	0.53
13:J:28:GLU:OE2	16:M:396:LYS:N	2.41	0.53
5:B:1021:HIS:NE2	5:B:1043:GLY:O	2.40	0.53
22:V:145:ASP:OD1	22:V:146:LEU:N	2.42	0.53
5:B:463:ARG:CZ	24:X:6:DA:H4'	2.39	0.52
4:A:221:LEU:HB3	18:O:402:ASN:HD21	1.74	0.52
16:M:322:GLN:NE2	16:M:360:PHE:O	2.42	0.52
4:A:772:ASP:OD1	4:A:773:LYS:N	2.42	0.52
18:O:255:VAL:HG21	18:O:267:VAL:HG11	1.91	0.52
1:1:63:TRP:HE3	1:1:82:LEU:HD13	1.74	0.52
9:F:84:GLU:N	9:F:86:GLU:OE1	2.42	0.52
22:V:384:ILE:HD12	22:V:385:SER:H	1.74	0.52
4:A:1105:ILE:HG22	4:A:1238:THR:HG21	1.92	0.52
11:H:98:ARG:HB3	11:H:115:TYR:HB2	1.92	0.52
4:A:30:GLN:NE2	5:B:1094:TYR:O	2.43	0.52
24:X:-31:DT:H2'	24:X:-30:DT:C6	2.45	0.52
25:Y:16:DC:H4'	25:Y:17:DC:OP1	2.10	0.52
1:1:68:PRO:HA	1:1:75:ARG:CZ	2.40	0.52
2:3:192:PHE:HZ	2:3:198:HIS:NE2	2.06	0.52
5:B:986:LYS:O	6:C:285:ARG:NH2	2.42	0.52
21:U:298:PRO:HB3	21:U:324:ALA:HB2	1.92	0.52
24:X:17:DA:H1'	24:X:18:DC:C5	2.45	0.52
25:Y:45:DA:H2''	25:Y:46:DA:C8	2.45	0.52
2:3:251:PHE:HE1	2:3:270:LEU:HD12	1.75	0.51
16:M:276:LEU:O	16:M:281:GLN:NE2	2.42	0.51
22:V:101:TYR:OH	24:X:-16:DG:OP2	2.28	0.51
25:Y:20:DA:H2''	25:Y:21:DA:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:722:THR:HG23	5:B:962:THR:HA	1.91	0.51
24:X:-1:DC:H2''	24:X:0:DG:H3'	1.92	0.51
4:A:282:LYS:HZ1	4:A:319:LEU:HB2	1.75	0.51
19:P:248:VAL:HG12	19:P:272:ALA:HA	1.91	0.51
25:Y:16:DC:H1'	25:Y:17:DC:O5'	2.10	0.51
1:1:14:LEU:HD23	1:1:81:LEU:HD22	1.90	0.51
3:4:183:LYS:HD2	24:X:-48:DT:OP1	2.11	0.51
4:A:354:GLY:HA2	5:B:1046:ARG:HH22	1.74	0.51
7:D:88:ASN:O	7:D:90:ARG:NH2	2.43	0.51
4:A:863:VAL:HG22	5:B:464:LYS:HB3	1.92	0.51
5:B:741:VAL:HG22	5:B:927:ILE:HB	1.92	0.51
25:Y:49:DC:H2'	25:Y:50:DT:H71	1.93	0.51
4:A:1145:ASN:N	4:A:1148:THR:OG1	2.41	0.51
6:C:115:ILE:HG22	6:C:117:ALA:H	1.76	0.51
18:O:292:GLU:HA	18:O:295:ARG:HG2	1.93	0.51
5:B:751:ILE:O	5:B:930:ASN:ND2	2.44	0.51
1:1:17:ARG:O	1:1:21:THR:HG23	2.11	0.51
5:B:471:LEU:HD21	5:B:481:PRO:HB3	1.93	0.51
6:C:144:VAL:HG21	6:C:168:VAL:HG13	1.92	0.51
18:O:31:THR:HB	18:O:34:GLN:NE2	2.26	0.51
5:B:463:ARG:NE	5:B:465:VAL:HG22	2.25	0.51
1:1:137:PHE:HB2	2:3:51:TRP:HZ2	1.76	0.50
5:B:205:SER:OG	5:B:320:HIS:N	2.43	0.50
11:H:58:LEU:HD11	11:H:143:LEU:HD11	1.93	0.50
23:W:299:TYR:OH	25:Y:36:DA:O5'	2.30	0.50
24:X:-36:DT:H2'	24:X:-35:DT:C6	2.46	0.50
25:Y:50:DT:H2''	25:Y:51:DT:H71	1.93	0.50
5:B:235:PRO:HD2	5:B:238:ILE:HD12	1.94	0.50
5:B:741:VAL:HG21	5:B:1009:TYR:CE1	2.47	0.50
15:L:36:CYS:HB3	15:L:39:CYS:SG	2.52	0.50
4:A:1125:ASP:OD1	4:A:1126:CYS:N	2.44	0.50
4:A:1360:PHE:O	9:F:64:ARG:NH1	2.42	0.50
5:B:483:ASP:OD2	5:B:495:ASN:ND2	2.44	0.50
5:B:607:THR:HG1	5:B:610:HIS:HD1	1.59	0.50
16:M:218:SER:HA	17:N:374:THR:HG23	1.93	0.50
16:M:249:LEU:HD12	16:M:250:MET:HG2	1.94	0.50
24:X:-18:DT:H2'	24:X:-17:DG:C8	2.46	0.50
4:A:424:ARG:N	4:A:448:ASP:OD1	2.44	0.50
4:A:1102:LYS:HB2	4:A:1212:ILE:HD11	1.92	0.50
5:B:914:GLU:O	6:C:78:ARG:NH1	2.44	0.50
19:P:284:ARG:HB3	20:Q:48:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:268:SER:OG	4:A:273:GLY:O	2.29	0.50
24:X:-45:DT:H2''	24:X:-44:DT:C6	2.47	0.50
10:G:148:ILE:HG23	10:G:190:ILE:HG23	1.94	0.50
21:U:171:THR:HG23	21:U:256:GLN:HG3	1.94	0.50
13:J:10:CYS:SG	13:J:11:GLY:N	2.85	0.50
19:P:144:ALA:HB1	24:X:-12:DG:H5''	1.92	0.50
4:A:23:LYS:HG3	5:B:1123:ILE:HG13	1.93	0.50
11:H:70:LEU:HD23	11:H:70:LEU:H	1.76	0.50
2:3:375:ASP:HB3	2:3:376:PRO:HD3	1.93	0.49
4:A:262:ILE:HD11	5:B:1115:GLN:HB3	1.94	0.49
5:B:1030:VAL:HG23	22:V:41:THR:O	2.12	0.49
4:A:887:ASP:OD2	4:A:891:ARG:NH2	2.45	0.49
5:B:631:GLU:OE2	5:B:656:HIS:NE2	2.39	0.49
5:B:901:HIS:NE2	5:B:945:GLU:OE1	2.45	0.49
6:C:134:GLU:O	6:C:181:GLN:NE2	2.43	0.49
22:V:195:GLU:OE1	22:V:242:ARG:NH2	2.45	0.49
6:C:86:THR:HG21	6:C:227:PRO:HB3	1.94	0.49
22:V:176:TYR:CD1	22:V:223:LEU:HD11	2.48	0.49
24:X:14:DA:H2''	24:X:15:DG:C8	2.46	0.49
25:Y:25:DA:H2'	25:Y:26:DT:H71	1.94	0.49
25:Y:33:DC:H2''	25:Y:34:DC:C6	2.48	0.49
25:Y:39:DA:H1'	25:Y:40:DA:H5'	1.94	0.49
5:B:1028:ARG:NH1	5:B:1072:SER:O	2.46	0.49
19:P:122:GLU:OE1	19:P:122:GLU:N	2.46	0.49
25:Y:31:DA:H2''	25:Y:32:DG:C8	2.48	0.49
5:B:594:ARG:NH2	5:B:663:THR:OG1	2.39	0.49
8:E:39:GLU:OE2	8:E:43:GLN:NE2	2.46	0.49
25:Y:-10:DG:H2''	25:Y:-9:DA:C5	2.47	0.49
5:B:531:LEU:HD22	5:B:538:LEU:HD21	1.95	0.49
5:B:633:LEU:HD11	5:B:656:HIS:CD2	2.47	0.49
5:B:824:LYS:NZ	22:V:18:ASP:OD1	2.45	0.49
17:N:253:GLU:OE2	17:N:256:ARG:NH2	2.45	0.49
6:C:86:THR:OG1	6:C:225:PHE:O	2.30	0.48
24:X:-27:DT:H2''	24:X:-26:DA:O4'	2.12	0.48
5:B:889:ARG:NH1	5:B:1015:MET:SD	2.84	0.48
24:X:25:DT:H2''	24:X:26:DA:N7	2.28	0.48
4:A:465:GLN:HG3	25:Y:-3:DG:C2'	2.43	0.48
19:P:127:LEU:HD13	19:P:150:TYR:CZ	2.49	0.48
24:X:18:DC:H1'	24:X:19:DA:H5'	1.95	0.48
2:3:390:ASP:HA	3:4:315:LEU:HD22	1.96	0.48
4:A:300:GLY:HA3	18:O:389:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:222:PRO:O	22:V:226:ILE:HG12	2.13	0.48
4:A:876:VAL:HG11	5:B:1053:ASP:CG	2.34	0.48
18:O:252:VAL:HG22	18:O:267:VAL:HG13	1.95	0.48
24:X:-57:DA:H2''	24:X:-56:DC:C5	2.49	0.48
25:Y:-19:DT:H2''	25:Y:-18:DG:O4'	2.13	0.48
14:K:64:GLU:OE1	14:K:64:GLU:N	2.47	0.48
2:3:371:PHE:CE1	3:4:316:GLU:HA	2.49	0.48
6:C:263:GLU:OE2	6:C:274:ARG:NH1	2.42	0.48
25:Y:-26:DT:H2''	25:Y:-25:DA:N7	2.29	0.48
4:A:77:ALA:O	5:B:1033:ARG:NH1	2.43	0.48
5:B:23:VAL:HG23	5:B:26:LYS:HB2	1.96	0.48
24:X:12:DG:H1'	24:X:13:DC:O4'	2.14	0.48
5:B:137:PRO:HG2	5:B:419:ILE:HD12	1.94	0.48
5:B:539:VAL:HG12	5:B:583:VAL:HB	1.96	0.48
6:C:28:ASP:O	14:K:61:LYS:NZ	2.47	0.48
21:U:211:ALA:HB2	21:U:237:TYR:CE2	2.49	0.48
25:Y:-11:DC:H2''	25:Y:-10:DG:C8	2.48	0.48
4:A:669:ARG:NH2	4:A:910:ALA:O	2.46	0.47
5:B:679:GLN:HG2	5:B:681:PRO:HD2	1.96	0.47
6:C:144:VAL:HG11	6:C:168:VAL:HG22	1.96	0.47
4:A:282:LYS:NZ	4:A:316:GLN:OE1	2.29	0.47
10:G:93:SER:OG	10:G:96:GLY:O	2.21	0.47
18:O:80:SER:O	18:O:84:ARG:HG2	2.14	0.47
22:V:110:ARG:HD3	25:Y:22:DG:H4'	1.96	0.47
25:Y:-21:DT:H2''	25:Y:-20:DA:N7	2.28	0.47
4:A:590:LYS:HB3	4:A:591:PRO:HD3	1.94	0.47
4:A:868:THR:HG21	4:A:1046:THR:HG23	1.96	0.47
5:B:287:ILE:O	5:B:291:VAL:HG23	2.13	0.47
1:1:46:MET:HG3	2:3:140:ARG:NH2	2.22	0.47
2:3:150:CYS:HB2	2:3:153:GLU:HB2	1.95	0.47
2:3:181:ILE:HD13	2:3:340:TYR:OH	2.13	0.47
2:3:216:ARG:HE	2:3:250:ALA:HB3	1.78	0.47
2:3:305:LEU:HD21	2:3:326:ILE:HG13	1.97	0.47
5:B:923:ILE:HD11	13:J:42:ARG:HB2	1.95	0.47
25:Y:34:DC:H2''	25:Y:35:DA:H8	1.79	0.47
1:1:92:GLN:HB3	1:1:93:PRO:HD3	1.95	0.47
6:C:319:ASP:OD1	6:C:320:VAL:N	2.46	0.47
16:M:9:VAL:HG23	16:M:10:VAL:HG22	1.95	0.47
24:X:8:DT:H2''	24:X:9:DT:N1	2.30	0.47
25:Y:49:DC:H6	25:Y:49:DC:H5'	1.78	0.47
1:1:89:GLN:HG2	1:1:94:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:870:TYR:CD1	25:Y:-5:DT:H5'	2.49	0.47
11:H:14:ASP:OD1	11:H:15:ILE:N	2.48	0.47
21:U:325:PHE:HA	21:U:328:ILE:HG22	1.97	0.47
24:X:1:DT:H4'	24:X:1:DT:OP1	2.14	0.47
2:3:241:HIS:NE2	16:M:312:ARG:HG2	2.30	0.47
4:A:258:PRO:HB2	4:A:262:ILE:HD12	1.96	0.47
16:M:173:ILE:HG22	16:M:175:VAL:HG22	1.96	0.47
16:M:308:VAL:O	16:M:312:ARG:HG3	2.15	0.47
25:Y:-3:DG:N3	25:Y:-3:DG:H2'	2.29	0.47
18:O:104:GLU:OE2	20:Q:56:TYR:OH	2.24	0.47
19:P:108:TRP:CD1	19:P:147:LYS:HB2	2.50	0.47
2:3:184:VAL:HG22	2:3:323:ILE:HG12	1.95	0.47
2:3:187:LEU:HD23	2:3:198:HIS:HE1	1.80	0.47
2:3:193:HIS:NE2	24:X:-50:DA:H2'	2.30	0.47
4:A:104:ILE:HD11	4:A:1333:TYR:HE1	1.80	0.47
5:B:178:ILE:HG12	5:B:437:THR:HG22	1.96	0.47
16:M:161:SER:OG	16:M:164:ASP:OD1	2.33	0.46
16:M:171:LYS:HZ2	19:P:67:ARG:HD2	1.79	0.46
21:U:293:TYR:HE1	21:U:295:MET:HB3	1.79	0.46
24:X:17:DA:H1'	24:X:18:DC:C6	2.50	0.46
25:Y:-23:DT:H2''	25:Y:-22:DA:C8	2.50	0.46
25:Y:40:DA:H2''	25:Y:41:DT:C6	2.50	0.46
4:A:599:GLN:O	4:A:603:VAL:HG23	2.15	0.46
1:1:7:LEU:HD11	1:1:54:PHE:CE2	2.51	0.46
4:A:1054:HIS:CD2	4:A:1065:LEU:HD12	2.50	0.46
1:1:46:MET:HA	2:3:140:ARG:HH12	1.81	0.46
2:3:188:TYR:HH	3:4:176:PHE:HE1	1.62	0.46
4:A:304:GLN:OE1	4:A:304:GLN:N	2.46	0.46
7:D:95:VAL:HG11	10:G:198:LEU:HD22	1.98	0.46
25:Y:19:DC:H2''	25:Y:20:DA:O4'	2.14	0.46
21:U:203:ARG:NH1	25:Y:27:DA:OP1	2.48	0.46
23:W:297:ASN:OD1	23:W:298:TYR:N	2.49	0.46
5:B:535:ASN:HD21	17:N:247:LYS:HE2	1.81	0.46
22:V:116:VAL:HG11	22:V:152:THR:HB	1.98	0.46
25:Y:-2:DC:H2'	25:Y:-1:DA:C8	2.51	0.46
25:Y:16:DC:P	25:Y:16:DC:H3'	2.56	0.46
7:D:25:GLU:HA	7:D:28:LYS:HG2	1.98	0.46
11:H:33:GLU:OE1	11:H:33:GLU:N	2.49	0.46
21:U:188:ARG:NH1	22:V:391:GLN:O	2.49	0.46
2:3:34:LEU:HD12	2:3:38:ASN:HD21	1.81	0.46
4:A:372:ASP:N	4:A:490:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1206:GLU:OE1	4:A:1206:GLU:N	2.49	0.46
21:U:204:ILE:HG21	21:U:236:LYS:HD3	1.97	0.46
25:Y:53:DC:H2''	25:Y:54:DA:H8	1.79	0.46
30:Z:101:GTP:O5'	30:Z:101:GTP:H8	1.99	0.46
4:A:465:GLN:HG3	25:Y:-3:DG:H2''	1.98	0.45
17:N:251:VAL:HG11	17:N:335:GLY:HA2	1.98	0.45
25:Y:-23:DT:H2''	25:Y:-22:DA:N7	2.32	0.45
2:3:193:HIS:CE1	24:X:-50:DA:H2'	2.51	0.45
4:A:583:LEU:HD12	4:A:584:PRO:HD2	1.98	0.45
5:B:103:ARG:NE	5:B:175:GLU:OE2	2.47	0.45
5:B:480:CYS:SG	5:B:666:GLY:N	2.84	0.45
25:Y:17:DC:H2''	25:Y:18:DA:C8	2.51	0.45
4:A:631:LEU:HD11	11:H:115:TYR:HE2	1.82	0.45
7:D:79:THR:HG23	7:D:82:GLU:H	1.81	0.45
8:E:65:ASN:OD1	8:E:66:ASP:N	2.50	0.45
11:H:96:VAL:HA	11:H:116:VAL:HG22	1.98	0.45
25:Y:15:DT:C2	25:Y:16:DC:C5	3.05	0.45
2:3:187:LEU:HD23	2:3:198:HIS:CE1	2.50	0.45
3:4:388:ILE:O	3:4:392:THR:OG1	2.28	0.45
4:A:436:ASN:OD1	4:A:439:LYS:N	2.42	0.45
5:B:876:GLU:N	5:B:876:GLU:OE1	2.50	0.45
5:B:530:GLU:OE1	5:B:530:GLU:N	2.50	0.45
10:G:115:GLN:HG3	10:G:116:GLN:H	1.82	0.45
19:P:45:ILE:O	19:P:50:ARG:NH1	2.50	0.45
21:U:242:GLN:NE2	21:U:248:ALA:O	2.46	0.45
21:U:305:PHE:CZ	25:Y:30:DA:H1'	2.52	0.45
5:B:647:GLU:N	5:B:647:GLU:OE1	2.50	0.45
5:B:817:PRO:HG3	5:B:869:VAL:HG23	1.98	0.45
14:K:66:GLU:HG2	14:K:87:ARG:HG2	1.98	0.45
16:M:56:VAL:N	16:M:104:SER:OG	2.49	0.45
24:X:-48:DT:H1'	24:X:-47:DA:C8	2.52	0.45
24:X:0:DG:H1'	24:X:1:DT:H5''	1.98	0.45
2:3:371:PHE:HE1	3:4:316:GLU:HA	1.81	0.45
4:A:1332:ALA:HB2	5:B:1122:ILE:HG23	1.99	0.45
8:E:29:THR:HG23	8:E:32:GLU:H	1.81	0.45
4:A:604:ILE:HG23	4:A:682:ARG:HB2	1.98	0.45
7:D:91:PRO:HD2	7:D:120:VAL:HG21	1.99	0.45
18:O:485:GLN:N	18:O:485:GLN:OE1	2.50	0.45
21:U:208:ARG:HA	21:U:208:ARG:NE	2.31	0.45
4:A:415:HIS:CE1	4:A:480:VAL:HG11	2.52	0.45
5:B:1079:VAL:HB	5:B:1128:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:42:DC:H2''	25:Y:43:DG:C8	2.51	0.45
5:B:258:GLU:OE1	5:B:258:GLU:N	2.49	0.45
5:B:946:LEU:HD22	5:B:1003:TYR:CE2	2.52	0.45
24:X:25:DT:H2''	24:X:26:DA:C8	2.53	0.45
2:3:148:ARG:NH1	3:4:368:SER:OG	2.51	0.44
4:A:384:VAL:HG13	4:A:415:HIS:CD2	2.52	0.44
4:A:1355:ILE:HD11	5:B:1056:ILE:HG23	1.98	0.44
6:C:57:ASP:N	6:C:57:ASP:OD1	2.50	0.44
10:G:82:ASP:OD1	10:G:151:ARG:NH2	2.51	0.44
25:Y:29:DA:H62	25:Y:30:DA:N6	2.14	0.44
4:A:870:TYR:HD1	25:Y:-5:DT:H5'	1.83	0.44
4:A:1149:VAL:O	4:A:1153:ILE:HG13	2.18	0.44
22:V:147:ASP:OD1	22:V:148:VAL:N	2.50	0.44
25:Y:34:DC:H2''	25:Y:35:DA:C8	2.52	0.44
25:Y:36:DA:H2''	25:Y:37:DG:H8	1.82	0.44
5:B:518:LEU:HD13	5:B:555:LEU:HD12	1.99	0.44
2:3:390:ASP:OD1	2:3:394:ASN:N	2.49	0.44
18:O:486:GLU:N	18:O:486:GLU:OE1	2.51	0.44
21:U:188:ARG:NE	22:V:393:LEU:O	2.50	0.44
1:1:39:GLY:O	2:3:110:LYS:HD2	2.17	0.44
5:B:315:SER:O	5:B:319:THR:HG22	2.17	0.44
5:B:1118:GLN:HA	5:B:1123:ILE:HD13	2.00	0.44
6:C:336:PHE:HE2	14:K:44:LEU:HD22	1.81	0.44
16:M:215:ASP:OD1	16:M:216:SER:N	2.50	0.44
18:O:265:GLU:OE1	18:O:268:ARG:NH1	2.50	0.44
21:U:209:THR:HG21	21:U:233:ALA:CB	2.48	0.44
24:X:-27:DT:OP2	24:X:-27:DT:H3'	2.18	0.44
25:Y:37:DG:H2''	25:Y:38:DA:H8	1.83	0.44
1:1:4:PRO:HB2	1:1:7:LEU:HB2	2.00	0.44
6:C:236:LEU:HD12	6:C:307:ILE:HD11	1.99	0.44
19:P:217:TRP:NE1	19:P:230:LEU:O	2.45	0.44
1:1:127:ARG:NH1	2:3:89:ASP:OD2	2.51	0.44
4:A:1363:LEU:HD11	9:F:107:ARG:HD2	2.00	0.44
5:B:68:ASP:OD1	5:B:69:ALA:N	2.50	0.44
10:G:108:LEU:HD22	10:G:190:ILE:HD11	2.00	0.44
18:O:159:ARG:NH1	18:O:186:ASP:OD2	2.50	0.44
25:Y:28:DT:OP2	25:Y:28:DT:H3'	2.18	0.44
4:A:1194:GLU:O	4:A:1198:LYS:NZ	2.51	0.44
4:A:1290:LEU:HD11	4:A:1303:ILE:HD11	1.99	0.44
25:Y:-19:DT:H2'	25:Y:-18:DG:C8	2.53	0.44
4:A:369:ILE:HD13	4:A:505:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:402:VAL:O	5:B:406:MET:HG2	2.18	0.44
6:C:49:PHE:CZ	14:K:110:VAL:HG23	2.52	0.44
18:O:527:ILE:O	18:O:531:MET:HG3	2.18	0.44
23:W:294:PHE:CE1	24:X:-31:DT:H4'	2.52	0.44
1:1:145:SER:HB2	1:1:147:ARG:HD3	1.99	0.43
4:A:598:LYS:HD2	11:H:120:GLY:HA3	2.00	0.43
19:P:108:TRP:HB3	19:P:147:LYS:HE2	1.99	0.43
21:U:296:ILE:O	21:U:299:ARG:HG2	2.17	0.43
4:A:631:LEU:HD11	11:H:124:ARG:HD3	1.98	0.43
6:C:334:ARG:NH2	14:K:104:MET:SD	2.91	0.43
7:D:57:PRO:HB2	7:D:90:ARG:HE	1.83	0.43
24:X:3:DC:O3'	24:X:4:DT:H4'	2.18	0.43
2:3:253:TYR:HB3	2:3:310:LEU:HB3	2.00	0.43
5:B:1039:ARG:HB3	25:Y:0:DC:P	2.59	0.43
12:I:20:CYS:SG	12:I:21:HIS:N	2.92	0.43
22:V:80:CYS:SG	22:V:85:LEU:HB2	2.58	0.43
5:B:207:THR:HG23	5:B:209:GLU:H	1.84	0.43
14:K:28:GLU:N	14:K:28:GLU:OE1	2.52	0.43
17:N:367:ASP:OD1	17:N:368:SER:N	2.51	0.43
21:U:304:ILE:HG13	21:U:310:VAL:HG13	1.99	0.43
22:V:221:HIS:CD2	25:Y:33:DC:H5''	2.54	0.43
23:W:295:ARG:CZ	25:Y:32:DG:H21	2.31	0.43
24:X:9:DT:H1'	24:X:10:DC:C6	2.54	0.43
4:A:59:ARG:O	4:A:71:THR:OG1	2.33	0.43
5:B:518:LEU:HD21	5:B:558:THR:HG21	2.00	0.43
8:E:82:VAL:HB	8:E:110:MET:SD	2.59	0.43
4:A:221:LEU:HB3	18:O:402:ASN:ND2	2.33	0.43
4:A:561:ARG:NH1	14:K:60:MET:SD	2.91	0.43
24:X:0:DG:C1'	24:X:1:DT:H5''	2.48	0.43
3:4:162:ASN:ND2	3:4:165:THR:H	2.17	0.43
4:A:130:LYS:HD3	4:A:130:LYS:HA	1.87	0.43
8:E:36:THR:HG23	8:E:39:GLU:H	1.83	0.43
18:O:55:CYS:SG	18:O:56:VAL:N	2.91	0.43
22:V:98:GLN:O	22:V:102:ARG:HG3	2.18	0.43
24:X:-50:DA:H2''	24:X:-49:DG:C8	2.54	0.43
2:3:266:GLU:N	2:3:266:GLU:OE1	2.52	0.43
7:D:42:LEU:HD11	10:G:31:ASN:HB3	2.01	0.43
16:M:6:ASP:N	16:M:6:ASP:OD1	2.52	0.43
16:M:246:LEU:HD12	16:M:249:LEU:HD11	2.01	0.43
21:U:187:ALA:HB3	21:U:190:ALA:HB2	2.00	0.43
23:W:325:ILE:HG22	23:W:337:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:32:DG:H2''	25:Y:33:DC:H6	1.83	0.43
25:Y:42:DC:H2''	25:Y:43:DG:H8	1.83	0.43
2:3:193:HIS:CE1	24:X:-50:DA:H5''	2.54	0.43
4:A:438:GLU:OE1	4:A:438:GLU:N	2.51	0.43
5:B:974:GLU:HA	5:B:977:VAL:HG12	2.01	0.43
16:M:273:LEU:HD11	16:M:281:GLN:HA	2.00	0.43
18:O:20:ILE:HD11	20:Q:75:ILE:HG13	2.01	0.43
25:Y:-26:DT:H2''	25:Y:-25:DA:C8	2.54	0.43
2:3:187:LEU:HB3	3:4:150:PHE:HE1	1.83	0.43
3:4:380:GLU:OE1	3:4:380:GLU:N	2.51	0.43
24:X:22:DT:H2''	24:X:23:DA:N7	2.33	0.43
2:3:146:ILE:HG13	2:3:147:ASP:H	1.84	0.42
4:A:381:ALA:HB3	4:A:487:ARG:HB2	1.99	0.42
10:G:151:ARG:HB2	10:G:189:SER:OG	2.19	0.42
4:A:996:GLU:HB3	4:A:997:PRO:HD3	2.02	0.42
4:A:1105:ILE:HD13	4:A:1225:LEU:HD13	2.01	0.42
5:B:946:LEU:HD22	5:B:1003:TYR:CZ	2.54	0.42
11:H:87:GLN:N	11:H:87:GLN:OE1	2.52	0.42
20:Q:80:GLU:N	20:Q:80:GLU:OE1	2.52	0.42
25:Y:51:DT:H2''	25:Y:52:DT:C6	2.54	0.42
5:B:86:ASP:O	5:B:135:ARG:NH2	2.49	0.42
5:B:103:ARG:NH2	5:B:168:TYR:OH	2.53	0.42
5:B:195:ARG:HH22	24:X:6:DA:H5'	1.84	0.42
7:D:22:ASP:O	7:D:25:GLU:HG3	2.20	0.42
7:D:80:LYS:HD2	7:D:83:LYS:HD2	2.01	0.42
8:E:59:THR:OG1	8:E:71:GLN:OE1	2.37	0.42
18:O:56:VAL:HG23	20:Q:73:TYR:HD1	1.85	0.42
22:V:281:ALA:O	22:V:284:ARG:HG2	2.20	0.42
24:X:6:DA:C4	24:X:7:DC:C5	3.07	0.42
25:Y:32:DG:H2''	25:Y:33:DC:C6	2.55	0.42
2:3:192:PHE:CZ	2:3:200:PRO:HB3	2.55	0.42
4:A:358:GLY:O	5:B:1046:ARG:NH1	2.53	0.42
5:B:30:LEU:HB3	5:B:31:PRO:HD3	2.01	0.42
18:O:505:ASN:HB3	19:P:314:LEU:HD13	2.02	0.42
21:U:197:PHE:CE2	21:U:199:ALA:HB3	2.54	0.42
21:U:220:VAL:HG11	24:X:-26:DA:H2	1.84	0.42
23:W:328:LEU:HD13	23:W:367:PHE:CZ	2.54	0.42
25:Y:31:DA:H2''	25:Y:32:DG:H8	1.83	0.42
22:V:186:SER:OG	22:V:189:VAL:HG12	2.19	0.42
4:A:214:ALA:HB1	18:O:407:GLN:HE21	1.84	0.42
5:B:883:MET:SD	5:B:883:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:5:GLU:N	8:E:5:GLU:OE1	2.52	0.42
10:G:99:VAL:HG11	10:G:148:ILE:HD11	2.01	0.42
19:P:232:MET:SD	19:P:262:SER:OG	2.62	0.42
4:A:306:ILE:HG13	18:O:396:TYR:CZ	2.55	0.42
24:X:-52:DA:H2''	24:X:-51:DA:C8	2.54	0.42
23:W:299:TYR:HE1	25:Y:35:DA:H1'	1.81	0.42
24:X:4:DT:H3'	24:X:5:DA:H3'	2.02	0.42
4:A:553:THR:HG21	4:A:650:MET:HG2	2.02	0.42
4:A:942:LYS:HG3	4:A:977:SER:HB2	2.01	0.42
19:P:142:VAL:HG23	19:P:170:GLN:HA	2.01	0.42
4:A:464:ARG:HG2	4:A:466:PRO:HD2	2.01	0.41
5:B:31:PRO:O	5:B:35:LYS:HG2	2.19	0.41
14:K:50:THR:OG1	14:K:51:LEU:N	2.53	0.41
21:U:232:LEU:HD22	22:V:379:THR:HG23	2.02	0.41
1:1:10:ASP:OD2	2:3:129:THR:OG1	2.22	0.41
1:1:56:LYS:NZ	1:1:95:GLN:OE1	2.32	0.41
2:3:334:CYS:HB3	2:3:340:TYR:CE1	2.55	0.41
6:C:49:PHE:HZ	14:K:110:VAL:HG23	1.85	0.41
18:O:443:ILE:HG23	18:O:513:GLU:HG3	2.02	0.41
22:V:193:TYR:HA	22:V:242:ARG:NH1	2.35	0.41
22:V:309:ARG:O	22:V:313:ARG:HG3	2.20	0.41
24:X:-29:DT:H2'	24:X:-28:DA:C4	2.55	0.41
4:A:1319:ALA:O	4:A:1324:THR:HG22	2.21	0.41
5:B:1029:ALA:HA	22:V:41:THR:O	2.19	0.41
6:C:155:ASP:HB3	16:M:348:VAL:HG21	2.02	0.41
25:Y:18:DA:H2''	25:Y:19:DC:C5	2.55	0.41
25:Y:28:DT:H1'	25:Y:29:DA:C4	2.55	0.41
4:A:196:SER:HB2	18:O:373:LYS:CB	2.50	0.41
4:A:503:ASP:OD1	26:Z:5:U:H4'	2.19	0.41
4:A:1357:THR:O	9:F:64:ARG:NH1	2.54	0.41
7:D:102:GLU:OE1	7:D:102:GLU:N	2.51	0.41
18:O:78:GLN:O	18:O:82:VAL:HG23	2.21	0.41
24:X:-1:DC:H6	24:X:-1:DC:H2'	1.69	0.41
25:Y:-11:DC:H2''	25:Y:-10:DG:N7	2.35	0.41
4:A:196:SER:O	18:O:373:LYS:HB2	2.21	0.41
4:A:231:PRO:HA	18:O:2:THR:OG1	2.21	0.41
4:A:739:GLN:HG3	4:A:747:THR:HG23	2.02	0.41
24:X:-47:DA:H2''	24:X:-46:DT:C5	2.56	0.41
3:4:361:VAL:O	3:4:365:ARG:HB3	2.20	0.41
4:A:199:THR:OG1	18:O:372:LYS:HD2	2.20	0.41
4:A:1159:ARG:NH2	24:X:19:DA:OP2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:130:GLU:OE1	6:C:130:GLU:N	2.52	0.41
18:O:285:THR:OG1	18:O:286:GLN:N	2.53	0.41
21:U:295:MET:HE2	21:U:298:PRO:HG2	2.03	0.41
22:V:72:GLY:O	22:V:76:VAL:HG23	2.21	0.41
1:1:70:TYR:HB3	1:1:74:ILE:HB	2.03	0.41
4:A:864:LYS:NZ	4:A:1048:MET:O	2.52	0.41
5:B:128:ARG:HH12	5:B:403:VAL:HG11	1.86	0.41
6:C:221:ASP:OD2	15:L:58:ARG:NH2	2.53	0.41
19:P:211:ALA:N	19:P:270:TYR:O	2.51	0.41
24:X:0:DG:H4'	24:X:1:DT:OP1	2.20	0.41
25:Y:51:DT:H6	25:Y:51:DT:H2'	1.75	0.41
1:1:29:PHE:CZ	1:1:76:VAL:HG12	2.56	0.41
1:1:42:PHE:HB2	1:1:90:LEU:HD12	2.03	0.41
4:A:415:HIS:O	4:A:453:HIS:ND1	2.53	0.41
4:A:481:LYS:HB2	4:A:487:ARG:HH21	1.85	0.41
4:A:590:LYS:NZ	11:H:88:PHE:O	2.54	0.41
5:B:1051:GLU:OE1	5:B:1051:GLU:N	2.52	0.41
6:C:266:GLU:OE1	6:C:266:GLU:N	2.54	0.41
13:J:30:THR:HG22	13:J:31:GLU:H	1.85	0.41
23:W:288:THR:HG23	23:W:289:THR:H	1.86	0.41
24:X:-43:DC:H2''	24:X:-42:DG:C8	2.55	0.41
4:A:728:ILE:HD13	4:A:748:LEU:HD21	2.03	0.41
22:V:273:LEU:HD13	22:V:297:ILE:HG12	2.03	0.41
2:3:127:LEU:HD13	2:3:130:LEU:HD23	2.02	0.40
2:3:140:ARG:HG3	2:3:144:ILE:HB	2.03	0.40
2:3:313:HIS:HD1	2:3:314:GLN:HG3	1.84	0.40
2:3:406:ASP:O	2:3:409:THR:OG1	2.37	0.40
4:A:221:LEU:HD13	18:O:399:LEU:O	2.21	0.40
5:B:24:GLU:OE1	5:B:24:GLU:N	2.53	0.40
5:B:946:LEU:HD21	5:B:1005:GLY:HA3	2.03	0.40
18:O:464:SER:HA	18:O:467:VAL:HG22	2.03	0.40
18:O:481:GLU:OE2	18:O:485:GLN:NE2	2.49	0.40
19:P:161:VAL:HG23	19:P:162:THR:HG22	2.03	0.40
21:U:169:VAL:HG13	21:U:222:THR:HG22	2.03	0.40
25:Y:52:DT:H2''	25:Y:53:DC:H5''	2.03	0.40
2:3:163:ALA:HB1	2:3:334:CYS:HB2	2.03	0.40
20:Q:54:GLU:OE1	20:Q:54:GLU:N	2.52	0.40
22:V:173:VAL:HG22	22:V:226:ILE:HD12	2.03	0.40
22:V:388:GLU:O	22:V:391:GLN:HG2	2.21	0.40
25:Y:-9:DA:H2''	25:Y:-8:DA:O4'	2.22	0.40
4:A:192:ASN:HA	4:A:195:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:569:ALA:HB2	14:K:67:PHE:HZ	1.87	0.40
4:A:570:SER:HB2	4:A:689:VAL:HG21	2.03	0.40
5:B:725:ILE:HG23	5:B:730:PHE:HB3	2.03	0.40
21:U:313:THR:HG21	24:X:-28:DA:H1'	2.04	0.40
4:A:459:VAL:HB	4:A:516:LYS:HG3	2.03	0.40
24:X:-53:DG:H2''	24:X:-52:DA:N7	2.36	0.40
25:Y:41:DT:H2''	25:Y:42:DC:C5	2.57	0.40
2:3:394:ASN:OD1	2:3:395:LYS:N	2.55	0.40
4:A:1295:THR:HG22	4:A:1300:VAL:HG22	2.03	0.40
5:B:251:ILE:O	5:B:255:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1	144/368 (39%)	137 (95%)	7 (5%)	0	100	100
2	3	368/411 (90%)	346 (94%)	22 (6%)	0	100	100
3	4	245/1469 (17%)	232 (95%)	13 (5%)	0	100	100
4	A	1376/1390 (99%)	1345 (98%)	31 (2%)	0	100	100
5	B	1091/1133 (96%)	1061 (97%)	30 (3%)	0	100	100
6	C	341/346 (99%)	338 (99%)	3 (1%)	0	100	100
7	D	120/148 (81%)	116 (97%)	4 (3%)	0	100	100
8	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
9	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
10	G	160/204 (78%)	149 (93%)	11 (7%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	52/108 (48%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	418/708 (59%)	404 (97%)	14 (3%)	0	100	100
17	N	140/398 (35%)	140 (100%)	0	0	100	100
18	O	508/534 (95%)	496 (98%)	12 (2%)	0	100	100
19	P	301/316 (95%)	292 (97%)	9 (3%)	0	100	100
20	Q	85/223 (38%)	83 (98%)	2 (2%)	0	100	100
21	U	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
22	V	358/419 (85%)	342 (96%)	16 (4%)	0	100	100
23	W	109/2624 (4%)	102 (94%)	7 (6%)	0	100	100
All	All	6628/11883 (56%)	6429 (97%)	199 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	1	130/334 (39%)	121 (93%)	9 (7%)	13	38
2	3	330/356 (93%)	315 (96%)	15 (4%)	23	52
3	4	221/1213 (18%)	212 (96%)	9 (4%)	26	54
4	A	1200/1212 (99%)	1188 (99%)	12 (1%)	73	84
5	B	959/988 (97%)	955 (100%)	4 (0%)	89	93
6	C	299/302 (99%)	297 (99%)	2 (1%)	81	88
7	D	114/136 (84%)	114 (100%)	0	100	100
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	52 (98%)	1 (2%)	52	72
14	K	92/119 (77%)	91 (99%)	1 (1%)	70	82
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/347 (38%)	129 (98%)	2 (2%)	60	77
18	O	458/476 (96%)	456 (100%)	2 (0%)	89	93
19	P	269/280 (96%)	267 (99%)	2 (1%)	81	88
20	Q	84/195 (43%)	82 (98%)	2 (2%)	44	68
21	U	154/293 (53%)	146 (95%)	8 (5%)	19	47
22	V	325/365 (89%)	313 (96%)	12 (4%)	29	56
23	W	102/2381 (4%)	93 (91%)	9 (9%)	8	28
All	All	5924/10438 (57%)	5833 (98%)	91 (2%)	60	77

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	65	TYR
1	1	96	LYS
1	1	102	LYS
1	1	116	ASN
1	1	137	PHE
1	1	142	LYS
1	1	144	LEU
1	1	147	ARG
1	1	148	MET
2	3	55	LEU
2	3	56	ARG
2	3	61	LEU
2	3	108	LYS
2	3	109	LEU
2	3	110	LYS
2	3	130	LEU
2	3	133	ARG
2	3	148	ARG
2	3	158	GLU

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Mol	Chain	Res	Type
2	3	342	LEU
2	3	343	LEU
2	3	374	GLU
2	3	377	CYS
2	3	386	MET
3	4	163	GLU
3	4	177	GLU
3	4	178	GLU
3	4	214	TYR
3	4	228	ARG
3	4	246	ASN
3	4	286	ASN
3	4	289	HIS
3	4	359	GLN
4	A	136	TYR
4	A	302	LYS
4	A	303	THR
4	A	335	LYS
4	A	362	ASP
4	A	431	PHE
4	A	494	THR
4	A	499	ASP
4	A	767	CYS
4	A	776	SER
4	A	1007	THR
4	A	1185	MET
5	B	196	LYS
5	B	214	THR
5	B	407	ARG
5	B	680	SER
6	C	98	THR
6	C	162	LEU
10	G	150	PHE
13	J	30	THR
14	K	66	GLU
17	N	156	ARG
17	N	251	VAL
18	O	55	CYS
18	O	533	ARG
19	P	93	LYS
19	P	134	LYS
20	Q	60	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	Q	113	ARG
21	U	167	ASN
21	U	205	ARG
21	U	206	GLU
21	U	208	ARG
21	U	209	THR
21	U	295	MET
21	U	296	ILE
21	U	323	GLU
22	V	43	THR
22	V	106	ILE
22	V	120	CYS
22	V	128	GLN
22	V	243	LEU
22	V	247	LEU
22	V	287	ARG
22	V	356	LEU
22	V	357	LEU
22	V	367	LYS
22	V	368	ARG
22	V	384	ILE
23	W	288	THR
23	W	289	THR
23	W	291	TYR
23	W	294	PHE
23	W	301	LYS
23	W	341	PHE
23	W	351	ARG
23	W	357	GLN
23	W	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	52	ASN
1	1	92	GLN
1	1	118	GLN
2	3	38	ASN
2	3	193	HIS
2	3	195	HIS
2	3	210	GLN
2	3	226	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	4	162	ASN
3	4	171	GLN
3	4	229	GLN
3	4	234	GLN
3	4	247	GLN
3	4	268	ASN
3	4	295	GLN
3	4	362	GLN
3	4	369	HIS
4	A	17	HIS
4	A	44	GLN
4	A	119	GLN
4	A	374	ASN
4	A	415	HIS
4	A	423	GLN
4	A	739	GLN
4	A	1054	HIS
4	A	1364	HIS
5	B	273	GLN
5	B	616	GLN
5	B	692	GLN
5	B	959	HIS
6	C	160	ASN
8	E	108	GLN
11	H	29	HIS
16	M	197	GLN
18	O	34	GLN
18	O	68	HIS
18	O	402	ASN
18	O	407	GLN
18	O	457	ASN
18	O	497	GLN
19	P	182	GLN
21	U	166	GLN
22	V	49	ASN
22	V	112	GLN
22	V	129	HIS
22	V	155	GLN
22	V	212	ASN
22	V	406	GLN
23	W	357	GLN
23	W	383	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	Z	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	GTP	Z	101	26	26,34,34	1.15	2 (7%)	32,54,54	1.70	6 (18%)
29	SF4	P	401	19	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GTP	Z	101	26	-	5/18/38/38	0/3/3/3
29	SF4	P	401	19	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z	101	GTP	C5-C6	-3.99	1.39	1.47
30	Z	101	GTP	C2-N3	2.44	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z	101	GTP	PA-O3A-PB	-4.64	116.90	132.83
30	Z	101	GTP	PB-O3B-PG	-3.88	119.52	132.83
30	Z	101	GTP	C3'-C2'-C1'	3.16	105.73	100.98
30	Z	101	GTP	C2-N1-C6	-2.89	119.77	125.10
30	Z	101	GTP	C5-C6-N1	2.85	118.99	113.95
30	Z	101	GTP	C8-N7-C5	2.40	107.56	102.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

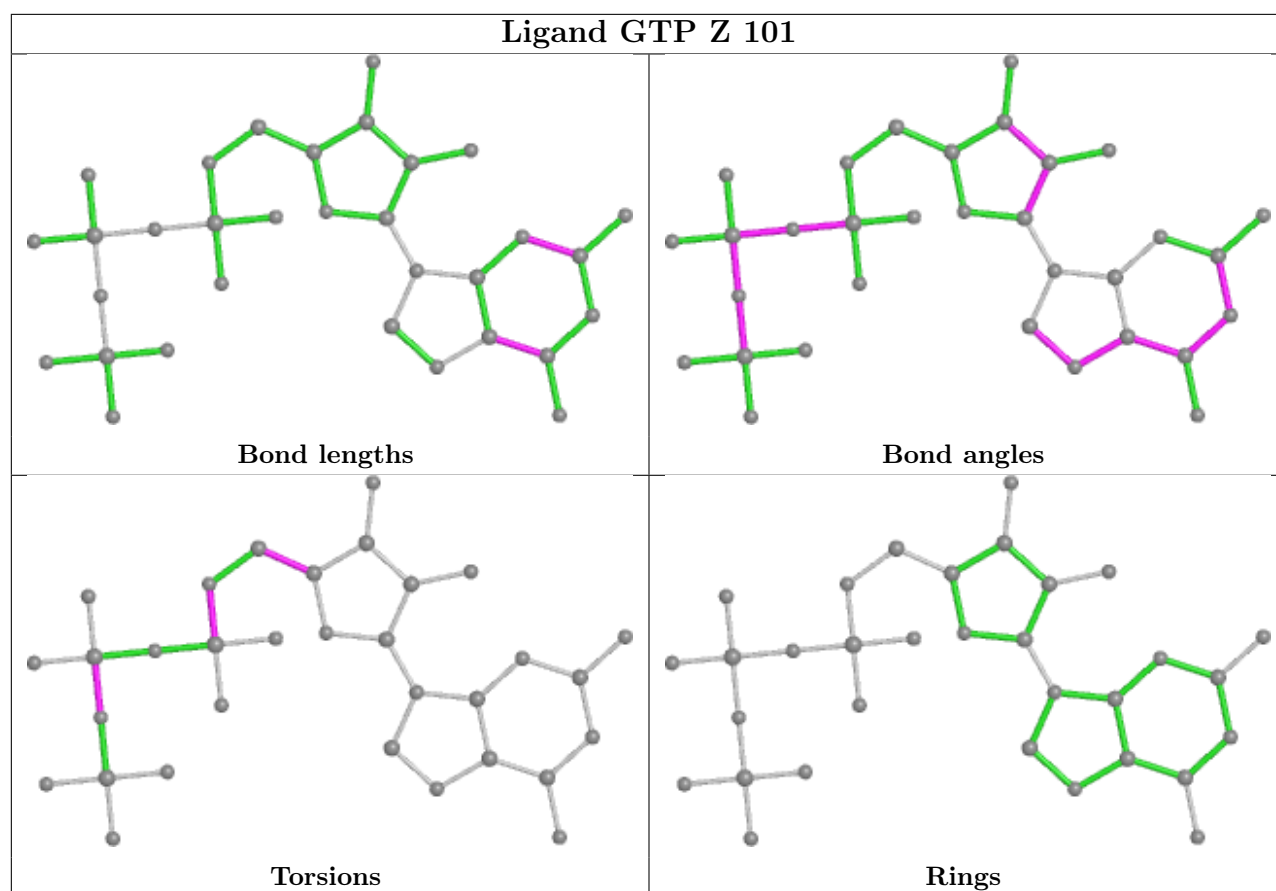
Mol	Chain	Res	Type	Atoms
30	Z	101	GTP	C5'-O5'-PA-O3A
30	Z	101	GTP	C5'-O5'-PA-O1A
30	Z	101	GTP	O4'-C4'-C5'-O5'
30	Z	101	GTP	C3'-C4'-C5'-O5'
30	Z	101	GTP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	Z	101	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



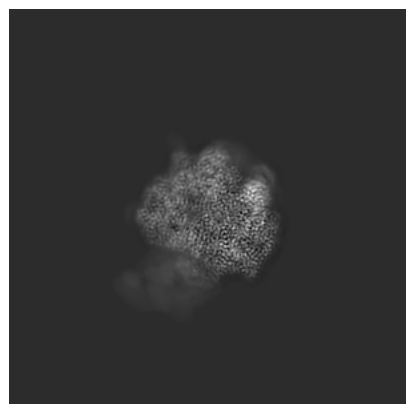
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63482. These allow visual inspection of the internal detail of the map and identification of artifacts.

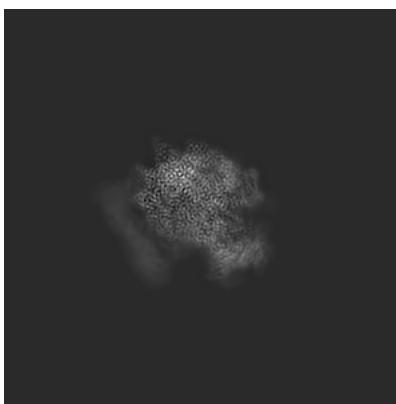
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

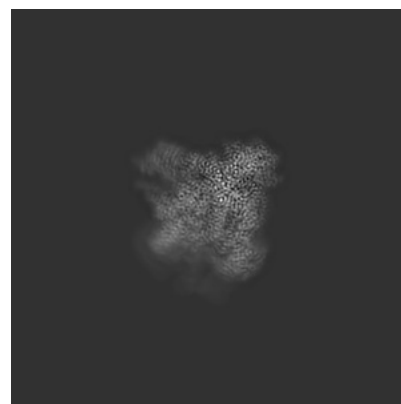
#### 6.1.1 Primary map



X

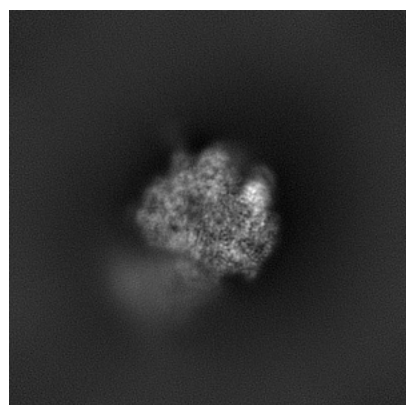


Y

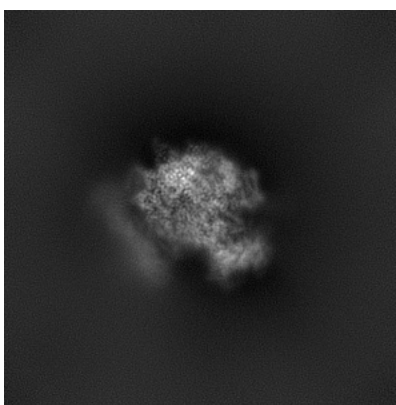


Z

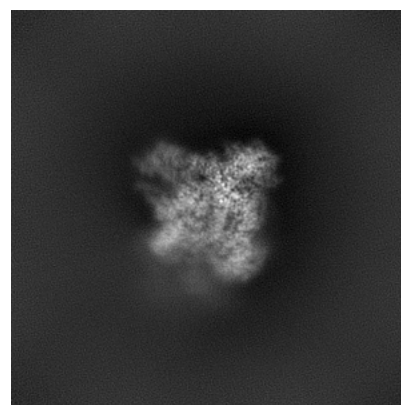
#### 6.1.2 Raw map



X



Y

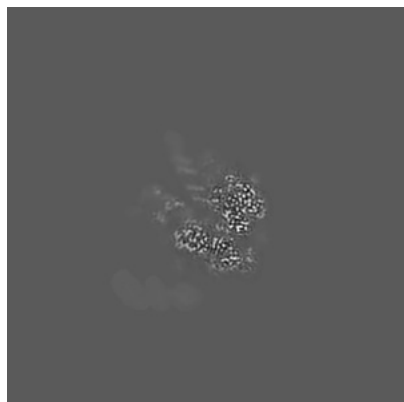


Z

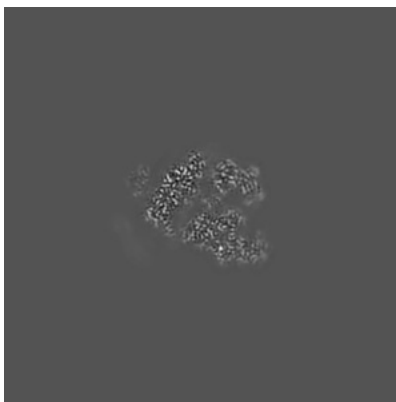
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 161

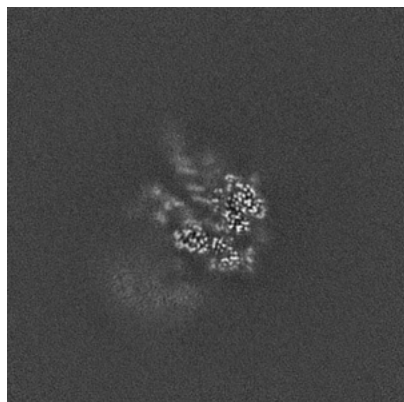


Y Index: 161

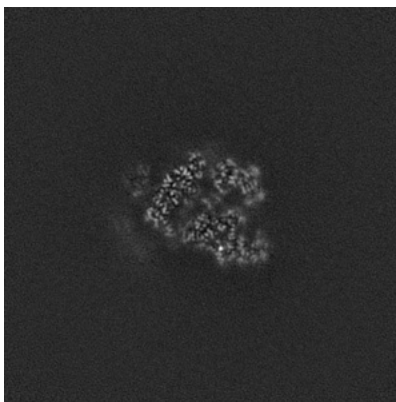


Z Index: 161

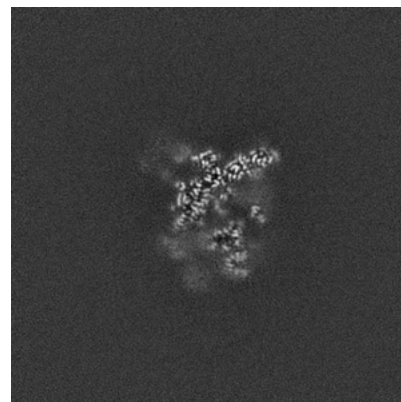
### 6.2.2 Raw map



X Index: 161



Y Index: 161

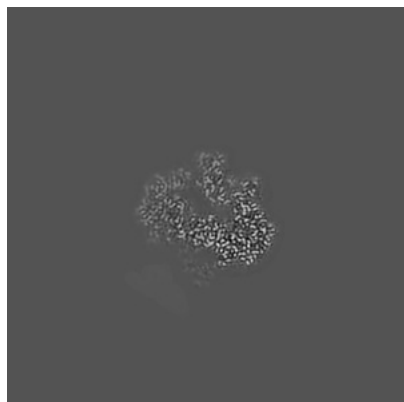


Z Index: 161

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

## 6.3 Largest variance slices [i](#)

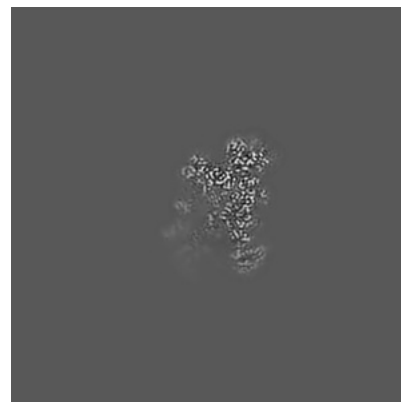
### 6.3.1 Primary map



X Index: 181

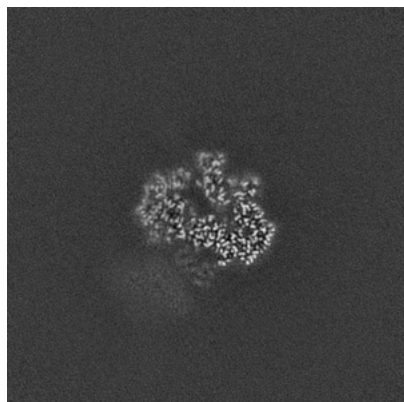


Y Index: 191

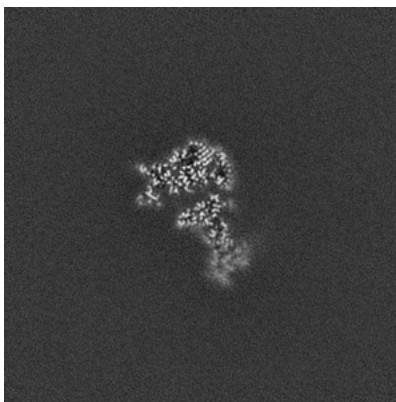


Z Index: 145

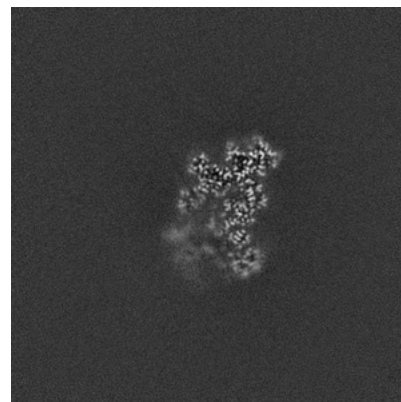
### 6.3.2 Raw map



X Index: 181



Y Index: 198

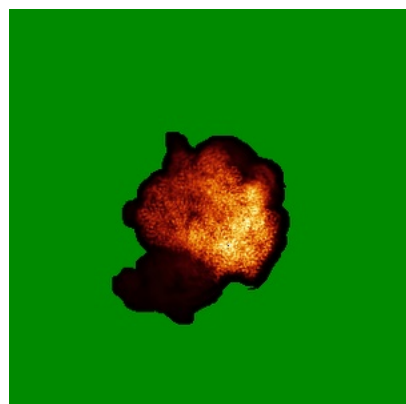


Z Index: 149

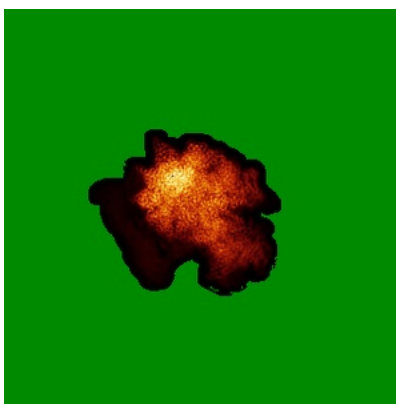
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

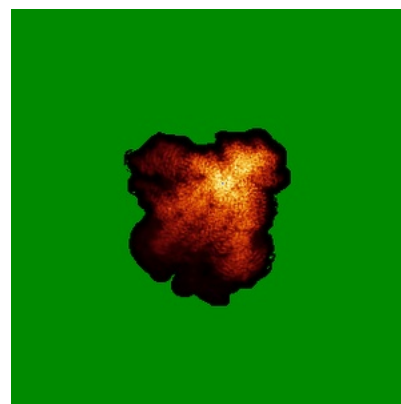
### 6.4.1 Primary map



X

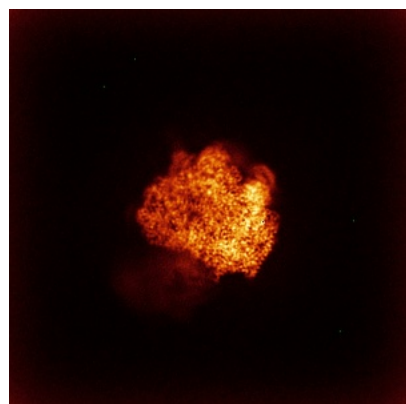


Y

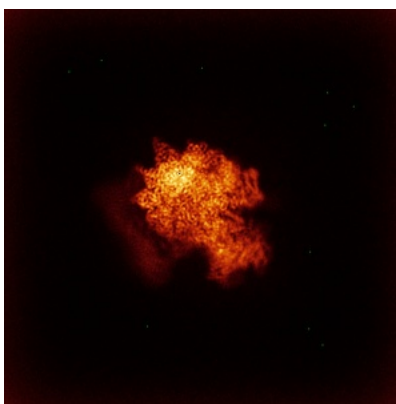


Z

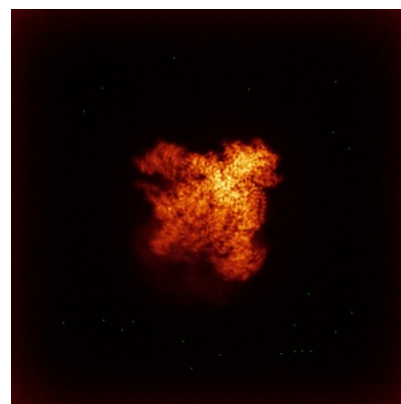
### 6.4.2 Raw map



X



Y

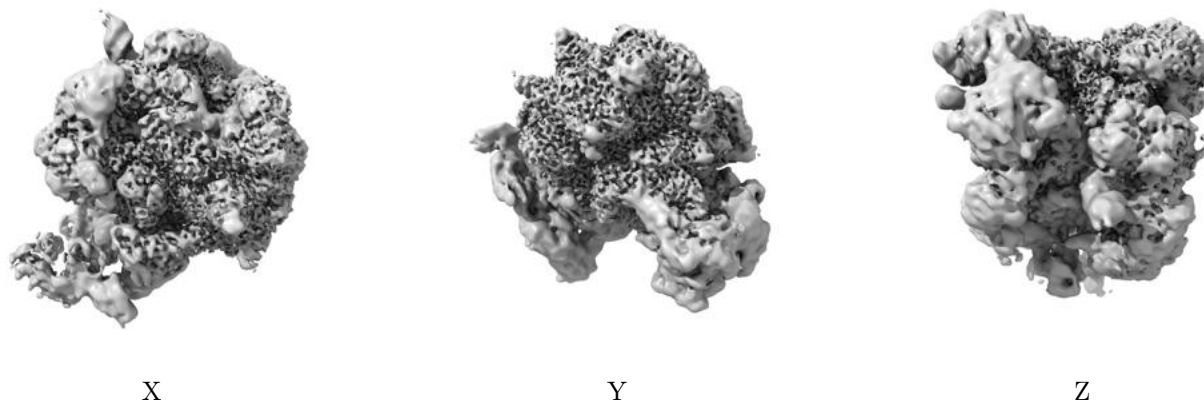


Z

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.

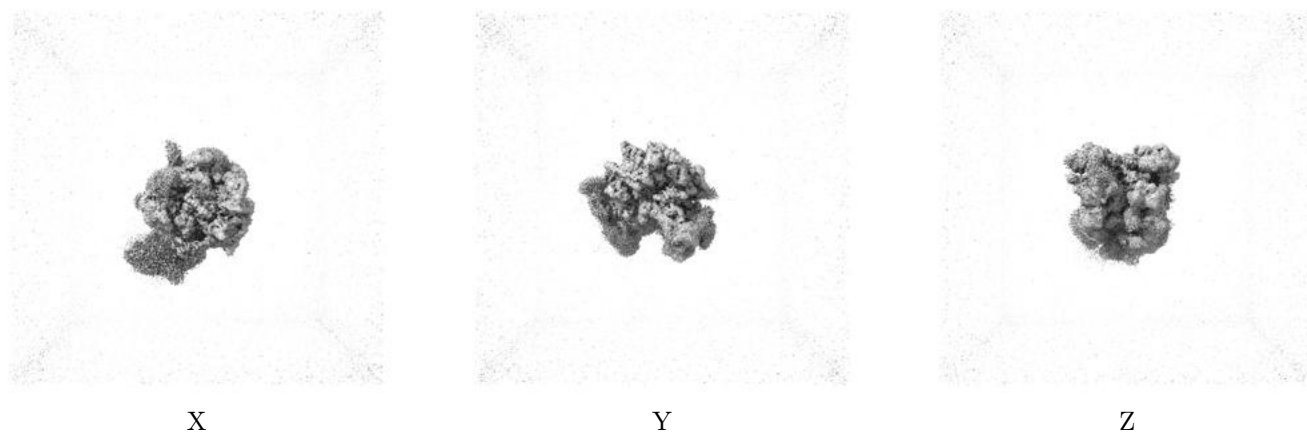
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



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.

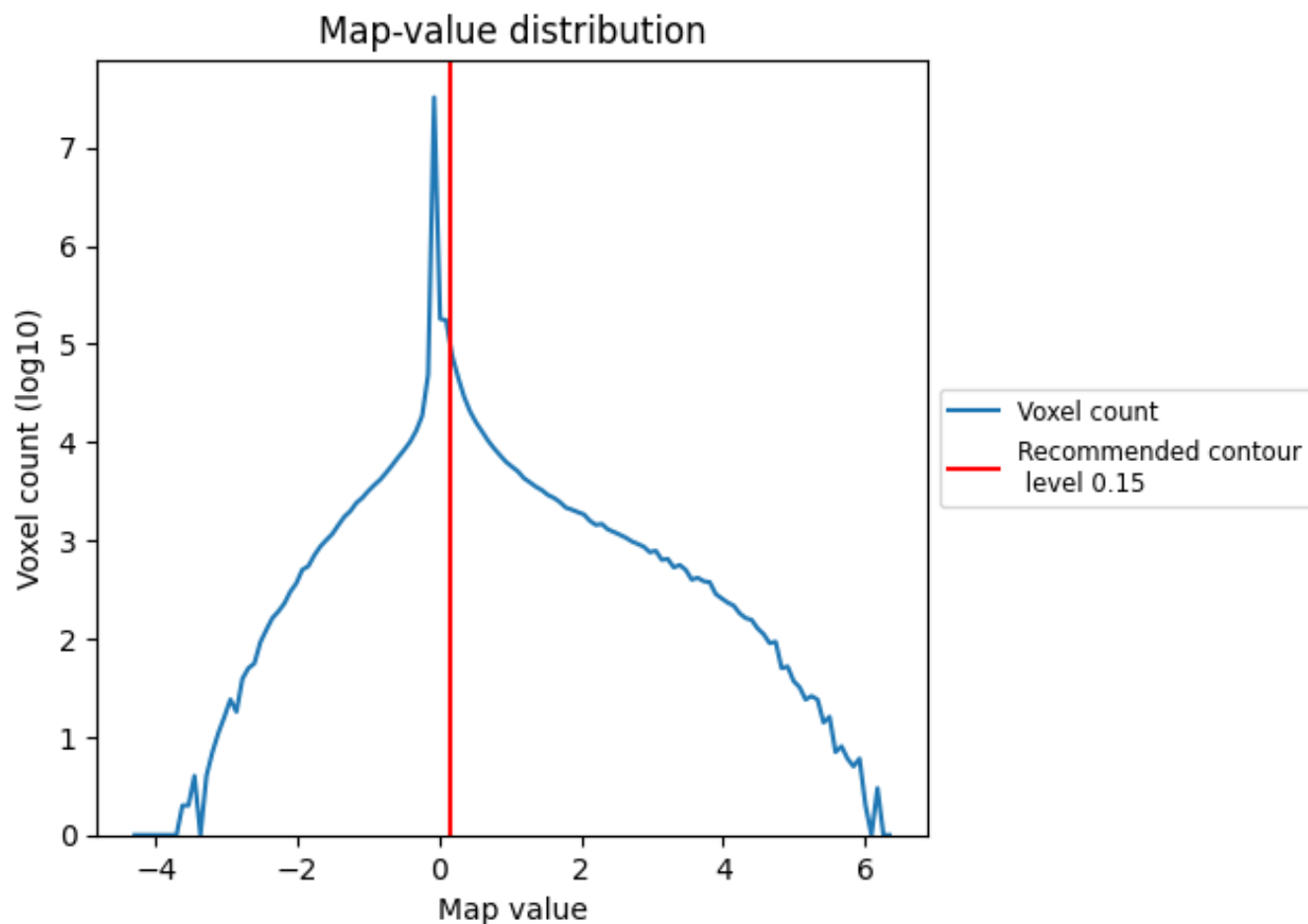
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

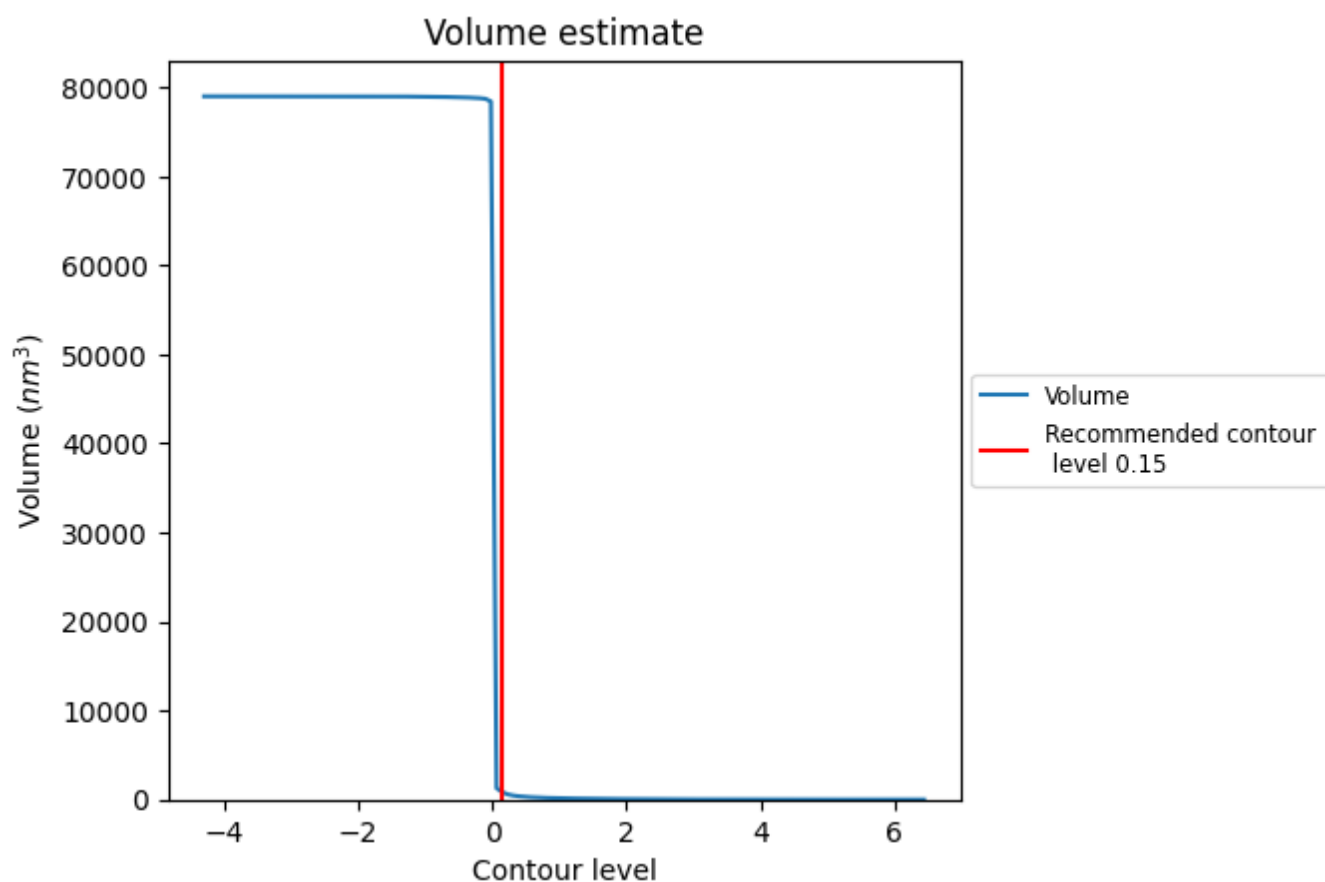
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

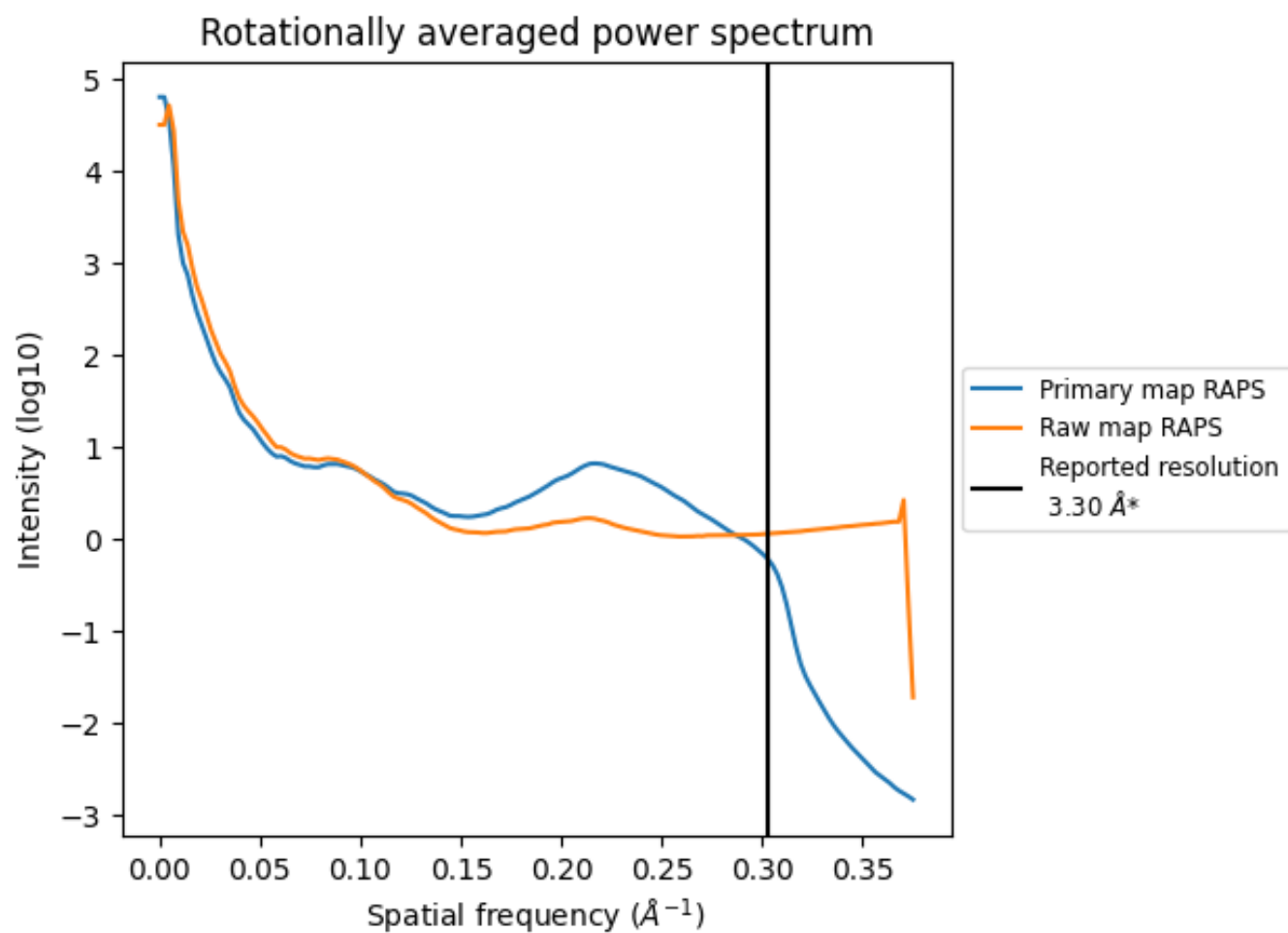
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 832  $\text{nm}^3$ ; this corresponds to an approximate mass of 752 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 ⓘ



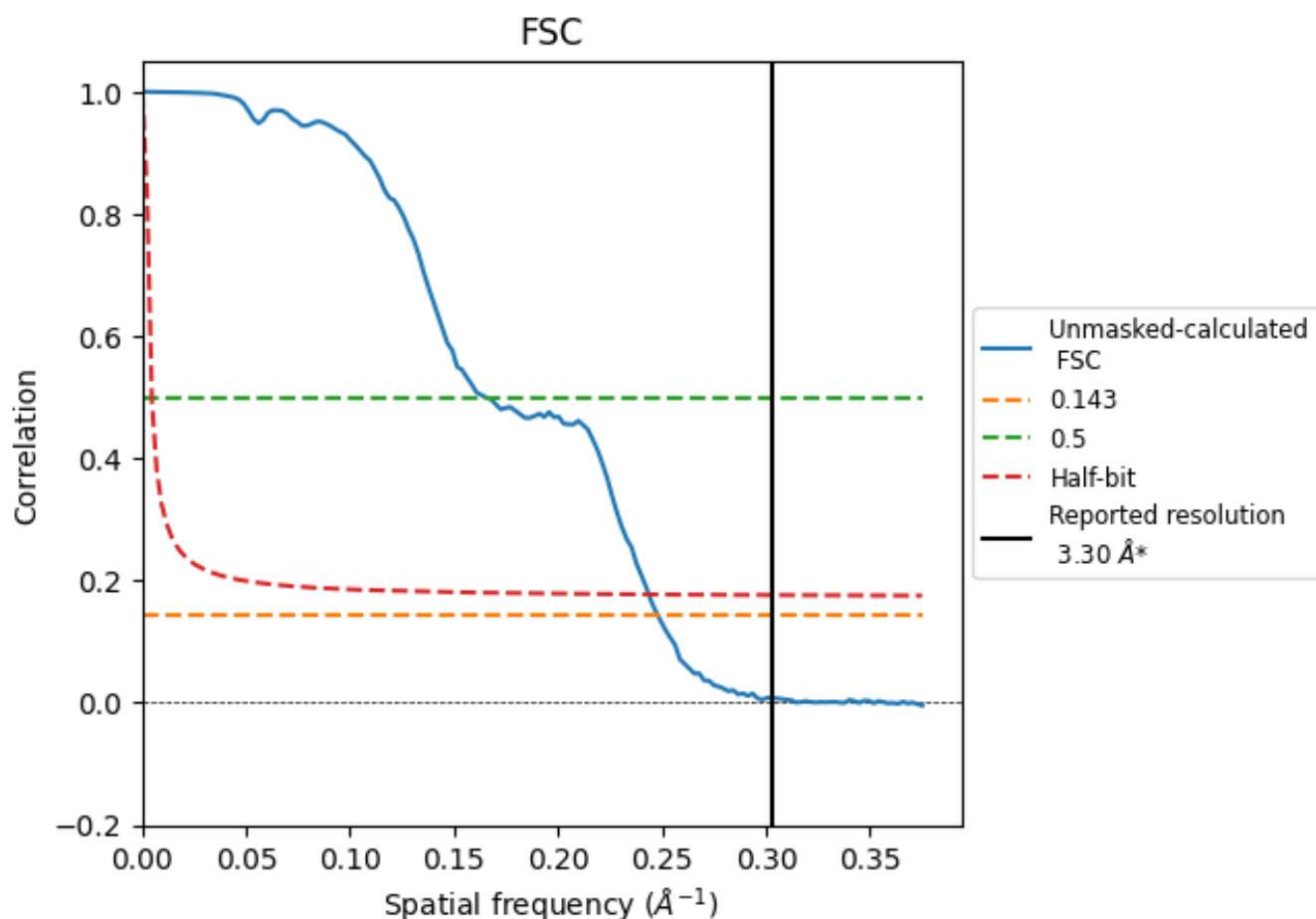
\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

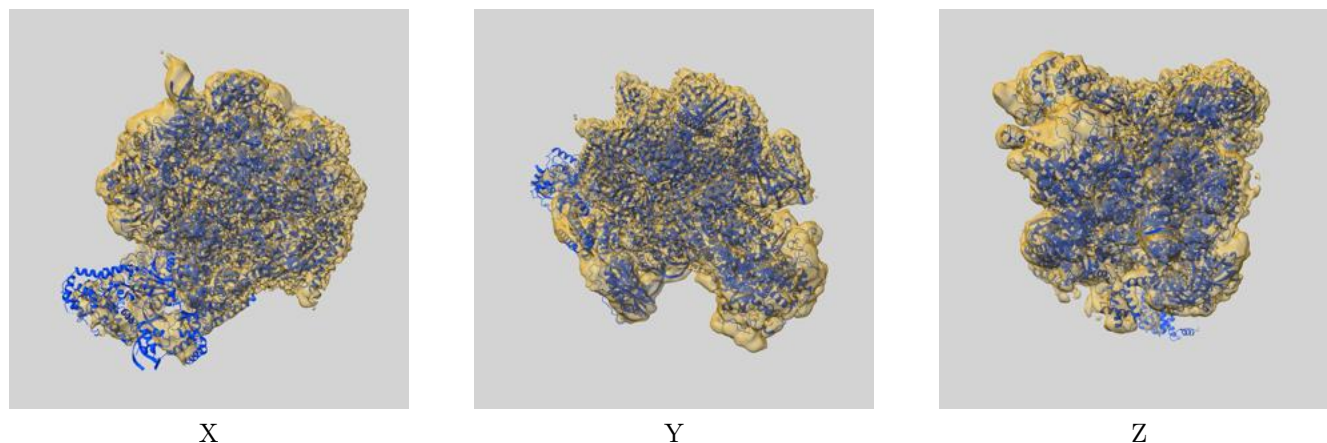
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	6.06	4.10

\*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 4.03 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

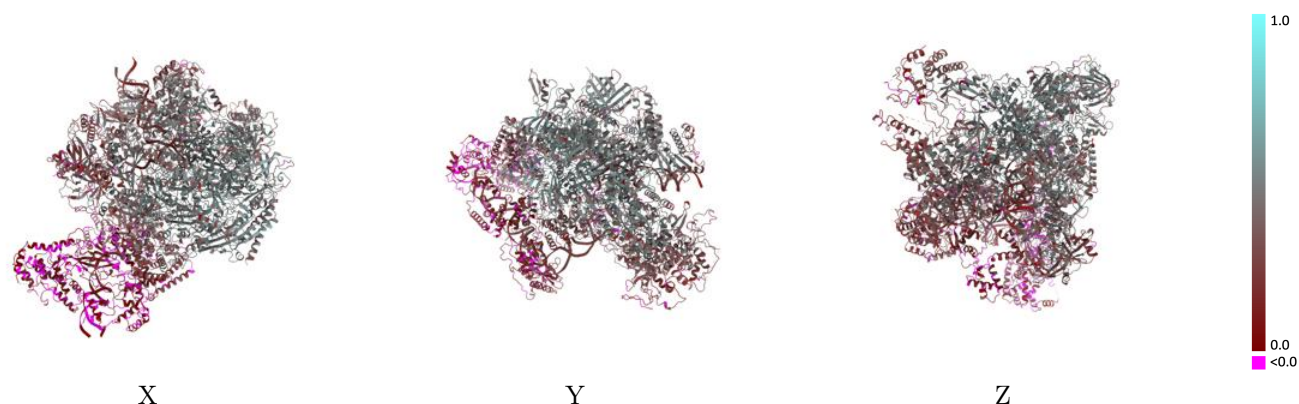
This section contains information regarding the fit between EMDB map EMD-63482 and PDB model 9LXN. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



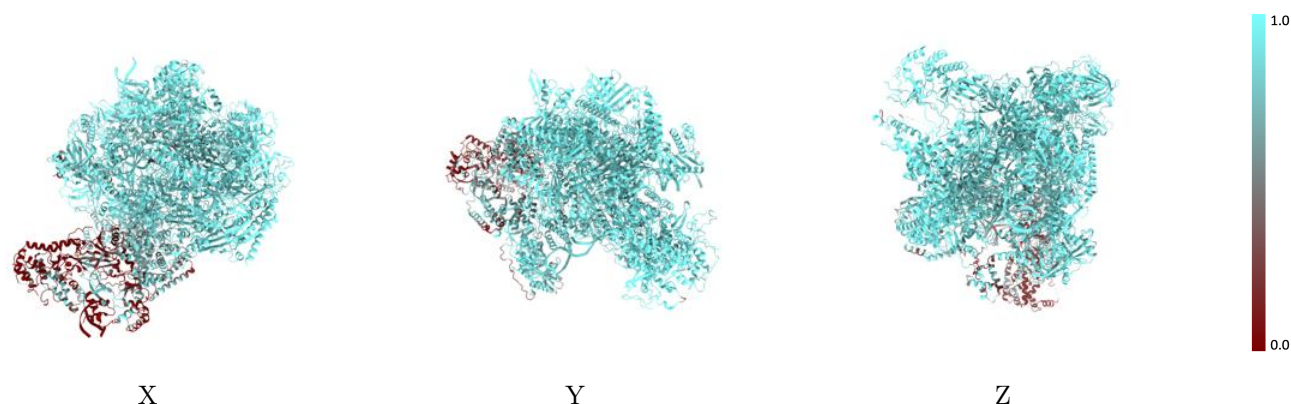
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



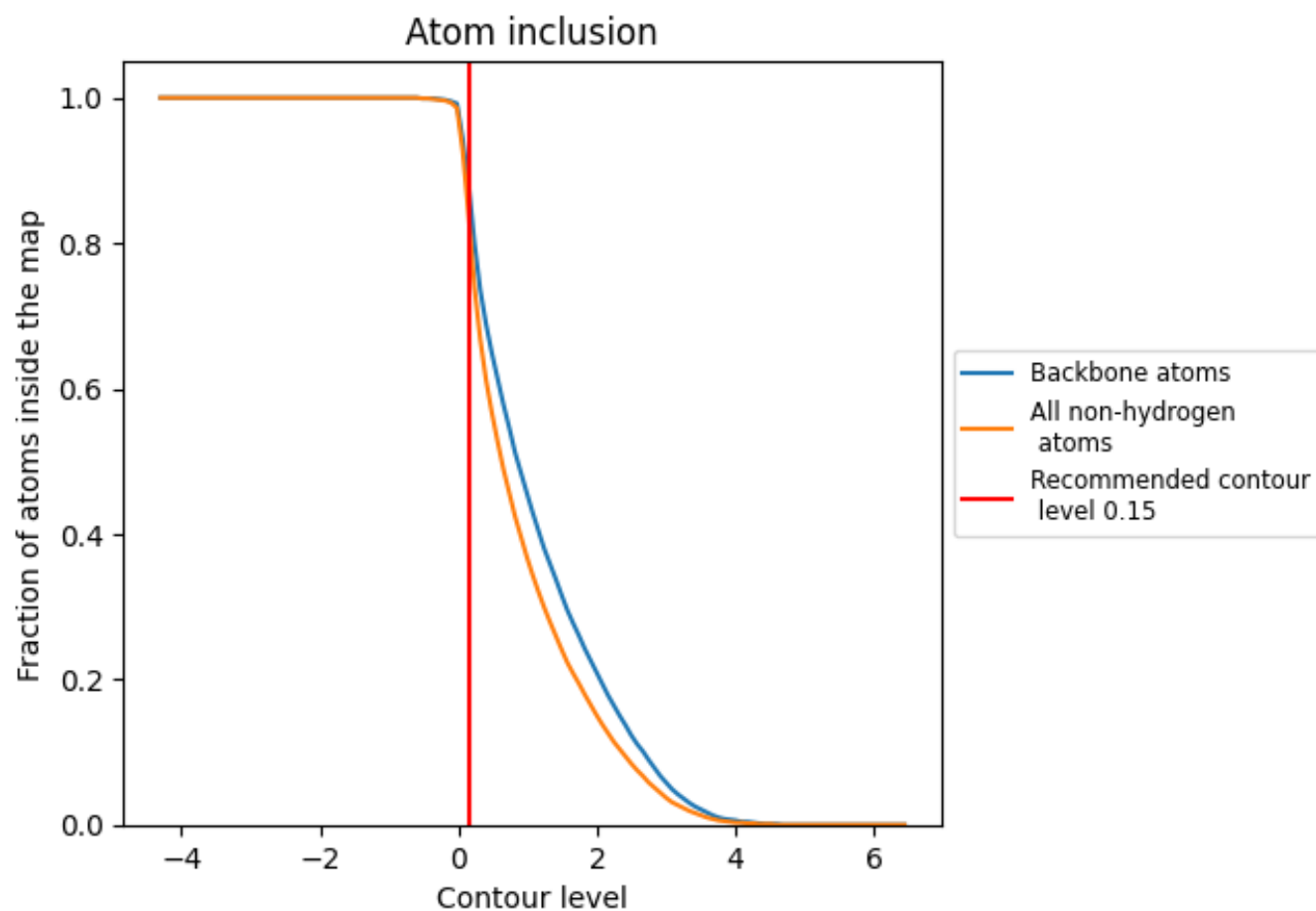
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.15).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.3330
1	 0.2130	 0.0320
3	 0.1840	 0.0240
4	 0.3230	 0.0500
A	 0.9410	 0.4520
B	 0.9460	 0.4670
C	 0.9530	 0.4790
D	 0.9740	 0.2800
E	 0.9480	 0.3880
F	 0.9510	 0.4870
G	 0.9510	 0.3430
H	 0.9490	 0.4580
I	 0.9450	 0.4040
J	 0.9500	 0.4740
K	 0.9480	 0.4620
L	 0.9440	 0.4050
M	 0.7890	 0.3070
N	 0.9180	 0.2890
O	 0.9450	 0.3570
P	 0.8700	 0.2310
Q	 0.9260	 0.3030
U	 0.8920	 0.1360
V	 0.7890	 0.2290
W	 0.7780	 0.1250
X	 0.8300	 0.1670
Y	 0.8190	 0.2160
Z	 0.9650	 0.4920

