WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Apr 10, 2025 – 01:11 PM JST

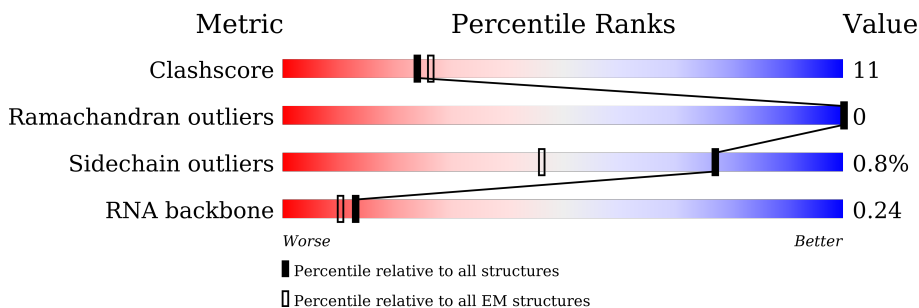|		
PDB ID	:	9K39 / pdb_00009k39
EMDB ID	:	EMD-62010
Title	:	Human RNA Polymerase III de novo transcribing complex 8 (TC8)
Authors	:	Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.
Deposited on	:	2024-10-18
Resolution	:	2.80 Å(reported)

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 2.80 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		0.8%
RNA backbone		0.24

Worse ────────────────────────── *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
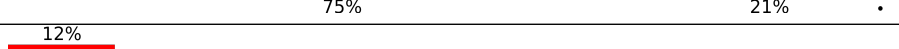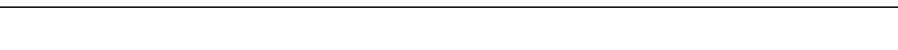
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 >=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	1390	79% ... 20%
2	B	1133	5% ... 77% ... 20%
3	C	346	77% ... 21%
4	D	148	14% ... 53% ... 29% ... 18%
5	E	210	88% ... 11%
6	F	127	50% ... 10% ... 40%
7	G	204	7% ... 59% ... 22% ... 19%

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Mol	Chain	Length	Quality of chain
8	H	150	81% 17%
9	I	108	39% 7% 50%
10	J	67	76% 21%
11	K	133	68% 10% 23%
12	L	58	57% 22% 21%
13	M	708	33% 50% 10% 40%
14	N	398	8% 29% 8% 63%
15	O	534	21% 77% 19%
16	P	316	62% 75% 21%
17	Q	223	12% 29% 10% 61%
18	V	419	7% 92%
19	X	50	68% 14% 76% 10%
20	Y	50	50% 26% 58% 16%
21	Z	7	86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	3AT	B	1202	-	-	X	-
25	SF4	P	401	-	-	X	-
26	GTP	Z	101	-	-	X	-

2 Entry composition ⓘ

There are 26 unique types of molecules in this entry. The entry contains 44526 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 III subunit RPC1.

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

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1105	Total 8736	C 5535	N 1529	O 1603	S 69	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			424	265	79	74	6		

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

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

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

- Molecule 18 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	34	Total 246	C 144	N 41	O 56	S 5	0	0

- Molecule 19 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	50	Total 1031	C 488	N 205	O 288	P 50	0	0

- Molecule 20 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	50	Total 1019	C 488	N 169	O 312	P 50	0	0

- Molecule 21 is a RNA chain called RNA (5'-R(P*UP*GP*CP*UP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	Z	7	146	65	23	51	7	0	0

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 24 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: $C_{10}H_{16}N_5O_{12}P_3$).
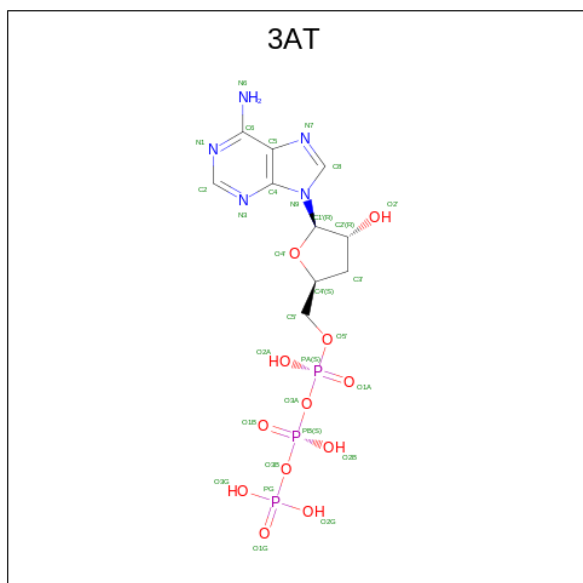
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	B	1	30	10	5	12	3	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).
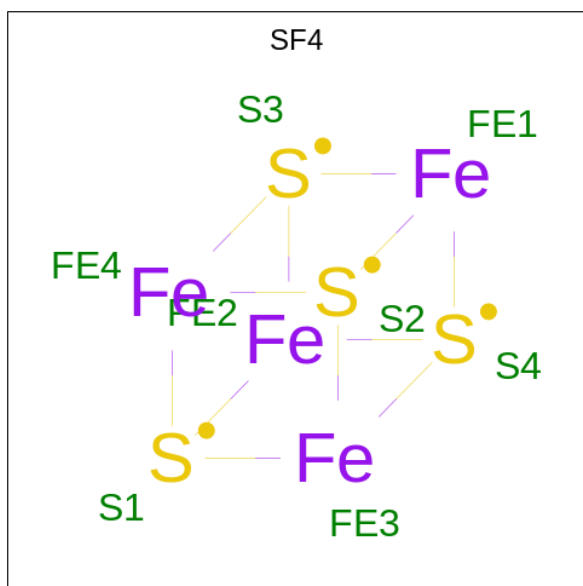
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
25	P	1	8	4	4	0

- Molecule 26 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).
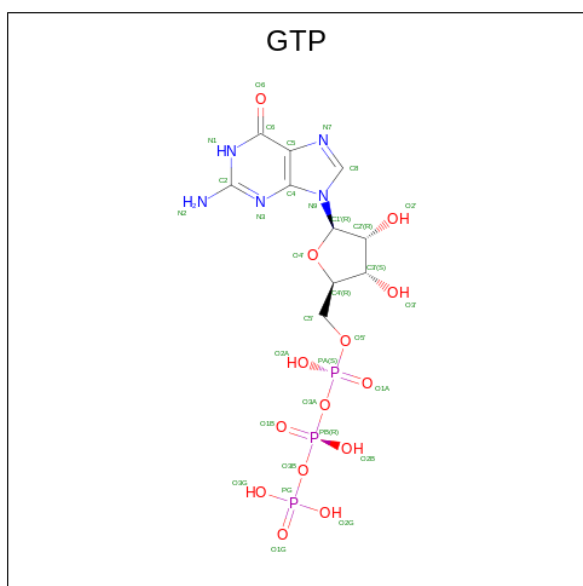
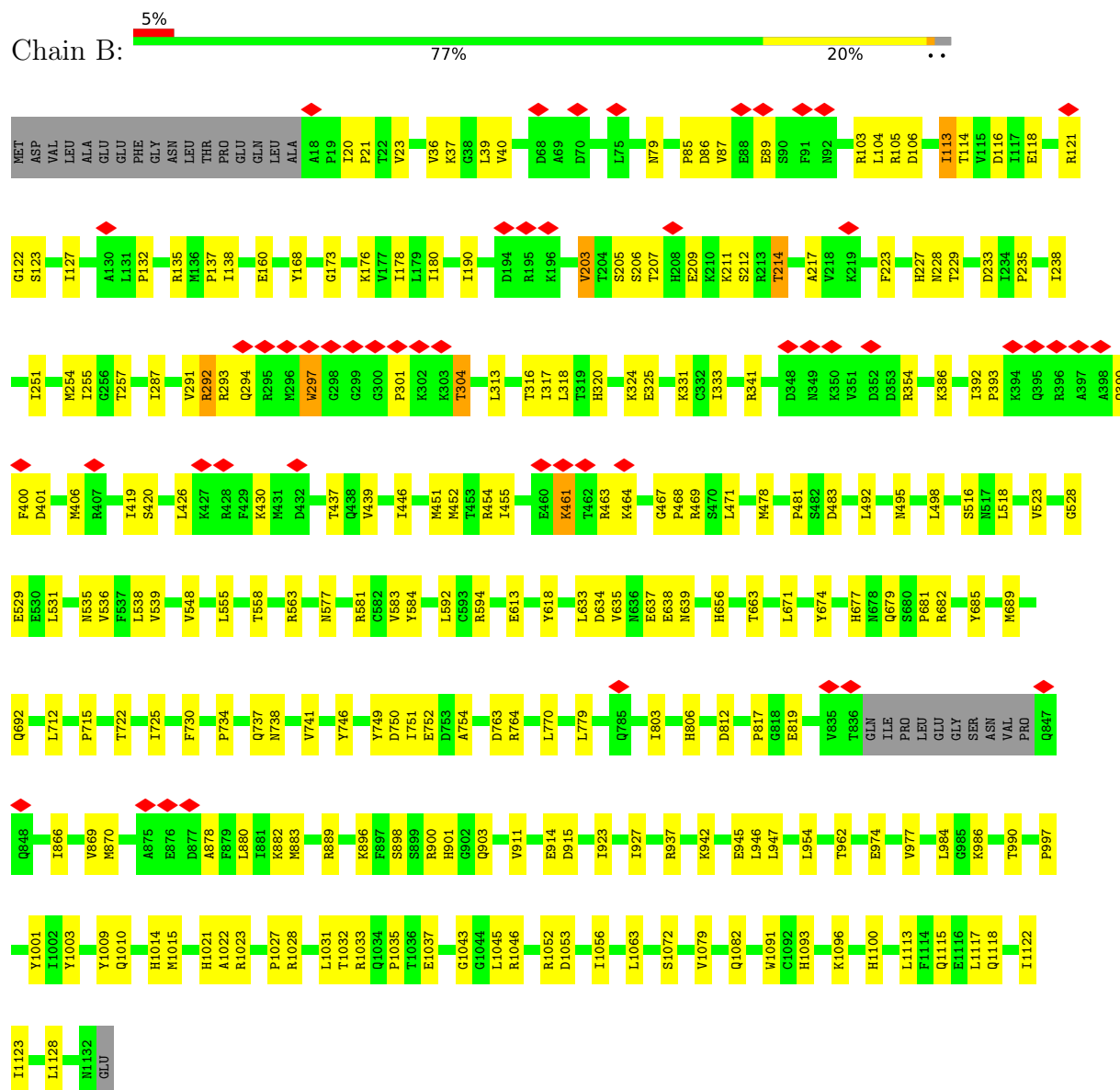| Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

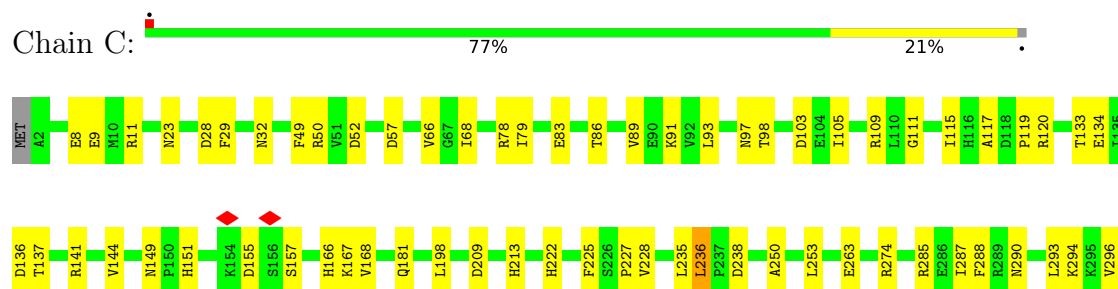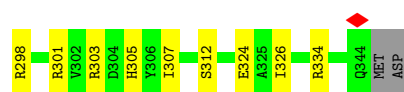• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

E1345 C1346 I1347 I1355 F1360 L1363 R1368 K1374 D1380 THR ASN GLU PHE HIS ILE PRO LEU VAL THR

• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:

5%

77%　　　　　　　　　　　　　　20%

MET ASP VAL LEU ALA GLU GLU PHE GLY ASN LEU THR PRO GLU GLN LEU ALA A18 P19 I20 P21 T22 V23 V36 K37 G38 L39 V40 D68 A69 D70 L75 N79 P85 D86 V87 E88 E89 S90 F91 N92 R103 L104 R105 D106 I113 T114 V115 D116 I117 E118 R121

G122 S123 I127 A130 L131 P132 R135 M136 P137 I138 E160 Y168 G173 K176 V177 I178 L179 I180 I190 D194 R195 K196 V203 T204 S205 S206 T207 H208 E209 K210 K211 S212 R213 T214 A217 V218 K219 F223 H227 N228 T229 D233 I234 P235 I238

I251 M254 I255 G256 T257 I287 V291 R292 R293 Q294 R295 M296 W297 G298 G299 G300 P301 K302 K303 T304 L313 T316 I317 L318 T319 H320 K324 E325 K331 C332 I333 R341 D348 N349 K350 V351 D352 D353 R354 K386 I392 P393 K394 Q395 R396 A397 A398 Q399

F400 D401 M406 R407 I419 S420 L426 K427 R428 F429 K430 M431 D432 T437 Q438 V439 I446 M451 M452 T453 R454 I455 E460 K461 T462 R463 K464 G467 P468 R469 S470 L471 M478 P481 S482 D483 L492 N495 L498 S516 N517 L518 V523 G528

E529 E530 L531 N535 V536 F537 L538 V539 V548 L555 T558 R563 N577 R581 C582 V583 Y584 L592 C593 R594 E613 Y618 L633 D634 V635 N636 E637 E638 N639 H656 T663 L671 Y674 H677 N678 Q679 S680 P681 R682 Y685 M689

Q692 L712 P715 T722 I725 F730 P734 Q737 N738 V741 Y746 Y749 D750 I751 E752 D753 A754 D763 R764 L770 L779 Q785 I803 H806 D812 P817 G818 E819 V835 T836 GLN ILE PRO LEU GLU GLY SER ASN VAL PRO Q847

Q848 I866 V869 M870 A875 E876 D877 A878 F879 L880 I881 K882 M883 R889 K896 F897 S898 S899 R900 H901 G902 Q903 V911 E914 D915 I923 I927 R937 K942 E945 L946 L947 L954 T962 E974 V977 L984 G985 K986 T990 P997

Y1001 I1002 Y1003 Y1009 Q1010 H1014 M1015 H1021 A1022 R1023 P1027 R1028 L1031 T1032 R1033 Q1034 P1035 T1036 E1037 G1043 G1044 L1045 R1046 R1052 D1053 I1056 L1063 S1072 V1079 Q1082 W1091 C1092 H1093 K1096 H1100 L1113 F1114 Q1115 E1116 L1117 Q1118 I1122

I1123 L1128 N1132 GLU

• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:

77%　　　　　　　　　　　　　　21%

MET A2 E8 E9 M10 R11 N23 D28 F29 N32 F49 R50 V51 D52 D57 V66 G67 I68 R78 I79 E83 T86 V89 E90 K91 V92 L93 N97 T98 D103 E104 I105 R109 L110 G111 I115 H116 A117 D118 P119 R120 T133 E134 I135

D136 T137 R141 V144 N149 P150 H151 K154 D155 S156 S157 H166 K167 V168 Q181 L198 D209 H213 H222 F225 S226 P227 V228 L235 L236 P237 D238 A250 L253 E263 R274 R285 E286 I287 F288 R289 N290 L293 K294 K295 V296 V297

R298 R301 V302 R303 D304 H305 Y306 I307 S312 E324 A325 I326 R334 Q344 MET ASP

• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:

14%
53% 29% 18%

M1 E2 V3 K4 D5 A6 N7 F17 D22 L23 K24 E25 Q26 R27 K28 E29 S30 G31 K32 N33 K34 H35 S36 S37 G38 N41 L42 N43 T44 E48 I53 S54 K55 T56 P57 C58 R59 L70 K74 T79 K80 A81 E82 K83 L84 Q85 L86 L87 N88 H89 R90 P91

V92 T93 A94 V95 Q98 L99 M100 E103 S104 E105 E106 R107 L108 T109 E110 E111 Q112 I113 E114 L117 V120 T121 S122 ILE LEU PRO ALA GLU PRO GLU ALA GLU GLN LYS LYS ASN THR ASN SER ASN VAL ALA MET ASP GLU GLU ASP PRO ALA

• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

88% 11%

MET D2 M18 Q19 L27 E32 Q35 E39 E50 P53 R54 R55 T56 T59 V60 H64 N65 D66 Q71 E78 V89 Q92 Q95 Y125 L136 I137 N138 L144 V145 P146 E147 H148 I193 T205 Q210

• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

50% 10% 40%

MET SER ASP ASN GLU ASP ASN PHE ASP ASP GLY ASP ASP PHE ASP ASP VAL GLU GLU GLU ASP GLU GLY LEU ASP ASP LEU GLU ASN ALA GLU GLU GLU GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO GLN ALA ASN GLN LYS R51 K59 A63 R64 R69 V81

E84 G85 E86 E96 R100 R107 L110 S114 L123 T126 ASP

• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:

7%
59% 22% 19%

MET F2 V5 E6 M7 N31 A35 N36 K37 V38 V39 V42 T52 K53 L54 E55 V59 D63 H71 V76 L81 D82 E83 I84 I89 S93 P94 E95 G96 L101 G102 F103 F104 D105 D106 I109 L114 Q115 Q116 P117 A118 K119 F120 D121 E122

A123 E124 Q125 V126 W127 V128 W129 E130 Y131 GLU THR GLU GLU GLY ALA HIS ASP LEU TYR MET ASP THR G145 I148 R149 F150 R151 V152 V153 D154 S161 P162 THR GLY PRO SER SER ALA ASP ALA THR THR SER SER GLU GLU LEU PRO LYS LYS GLU ALA PRO Y184 T185 L186 V187 G188

S189 I190 S191 E192 L195 L198 W201 THR SER ASN

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

Chain H:

81%   17%

MET A2 D8 I9 F10 K13 P17 K20 K21 F22 V25 S26 R27 L28 H29 C30 E31 I40 L58 L70 D71 D72 G73 E74 F88 V96 Y97 R98 D102 E107 L112 Y115 V116 G120 R124 A129 L143 A149 PHE

• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:

39%   7%   50%

M1 C5 C8 G9 N10 G11 L12 R19 C20 H21 P29 L46 K47 D51 V52 L53 G54 GLY ALA ALA ALA TRP GLU ASN VAL ASP SER THR ALA GLU SER CYS PRO LYS CYS GLU HIS PRO ARG ALA TYR PHE MET GLN LEU GLN THR ARG SER ALA ASP GLU PRO MET

THR THR PHE TYR LYS CYS CYS ASN ALA GLN CYS GLY HIS ARG TRP ARG ASP

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

Chain J:

76%   21%

M1 I2 I3 P4 V5 R6 W18 Y21 E28 Y29 T30 D36 L40 K41 R42 R46 R47 M48 L49 Y62 L65 GLU LYS

• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:

68%   10%   23%

MET GLU GLU ASP GLN GLU LEU GLU GLU ARG LYS ILE SER GLY LEU LYS THR SER MET ALA GLU GLY GLU ARG K24 L27 A33 G34 V43 T50 L51 R56 Y57 M58 K61 E66 F67 C68 R87 L103 M104 L111 A126 SER ARG ASN GLU SER THR PHE
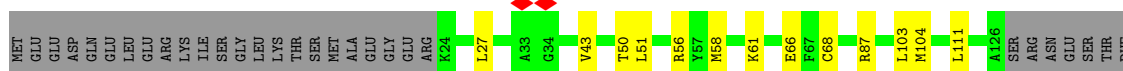
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

57%   22%   21%

MET ASP THR GLN LYS ASP VAL GLN PRO PRO LYS GLN Q13 I16 Y17 I18 C19 G20 E25 N26 K29 C36 R42 T43 M44 Y45 K46 T49 L52 R58
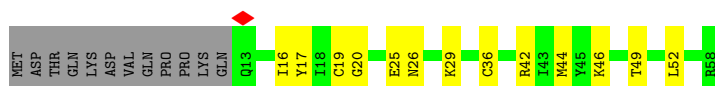
• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

33%

Chain M:

50%   10%   40%

MET ALA ASN GLU GLU D6 D7 P8 V9 V10 Q11 E12 I13 K50 Q53 V56 T64 L65 K73 D82 G83 A84 C85 A86 D87 E88 T89 Y92 L96 M97 S104 R113 A117 L118 Y119 R120 Q121 L124 L133 Q134 L135 R136 E151 R152 E153 A154

A155 N156 E157 A158 G159 D160 S161 S162 Q163 D164 E165 A166 E167 D168 D169 V170 K171 Q172 I173 T174 V175 R176 F177 S178 R179 P180 E181 S182 E183 Q184 A185 R186 Q187 R188 R189 V190 Q191 L196 Q197 K198 K199 H200 A201 R214 D215 S216 R217 S218 E221 L225 S230 S231 G232 L238
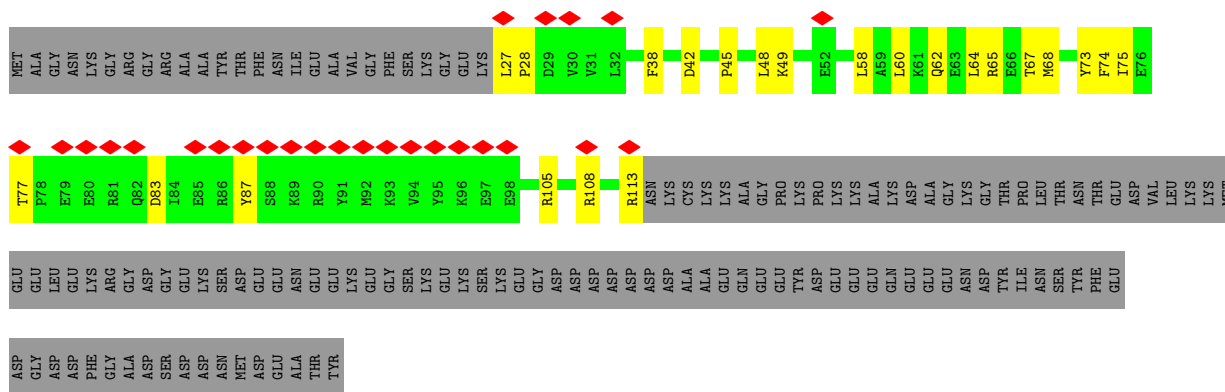
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4
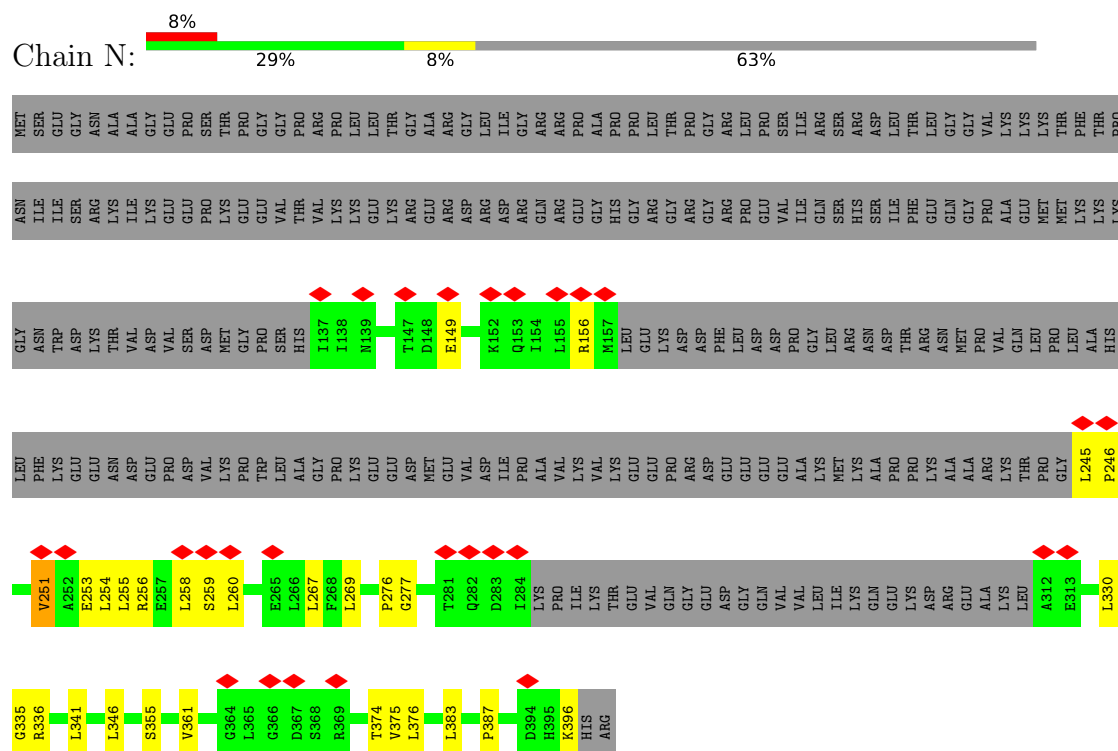
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:

21%

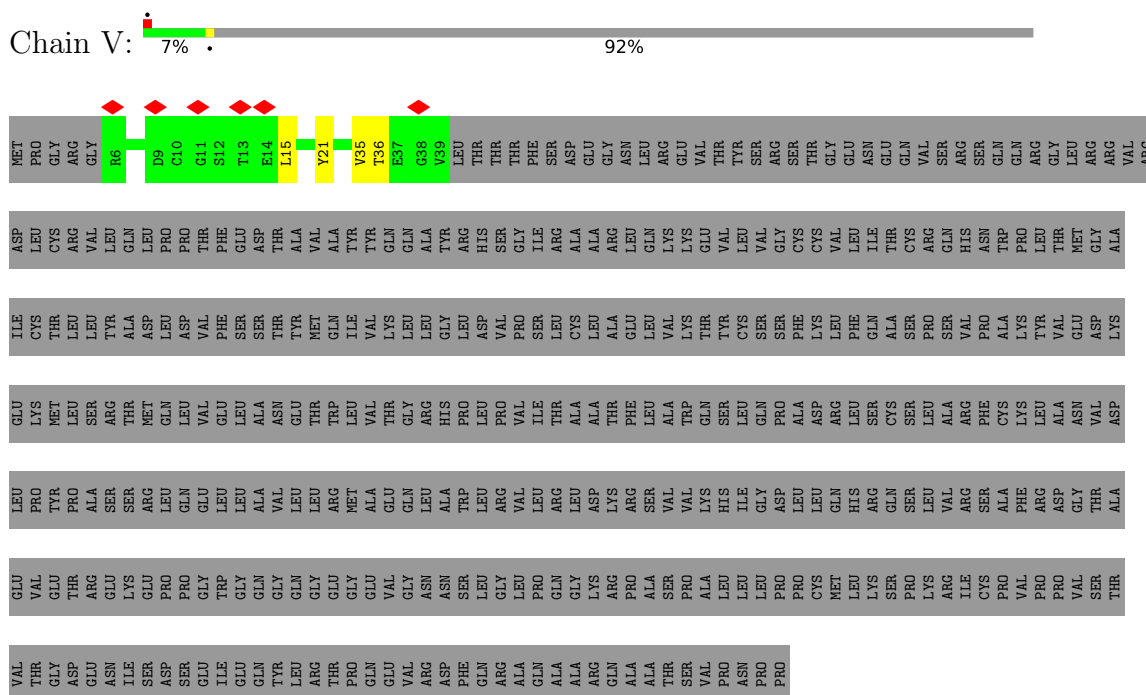77%
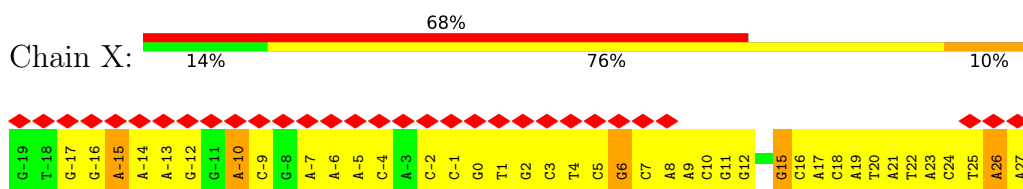
19%
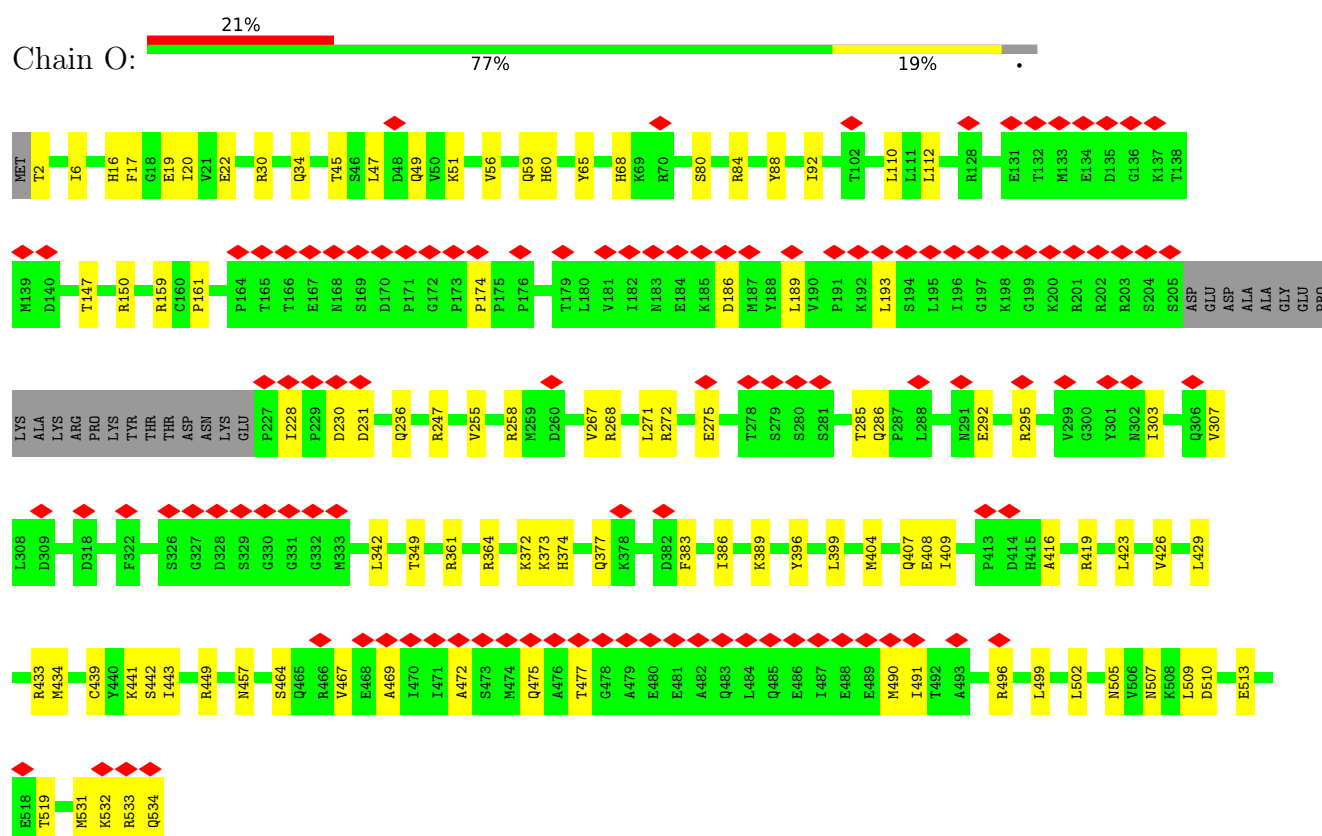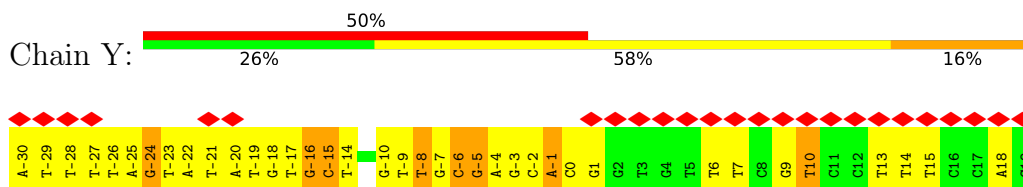
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:

62%

75%

21%
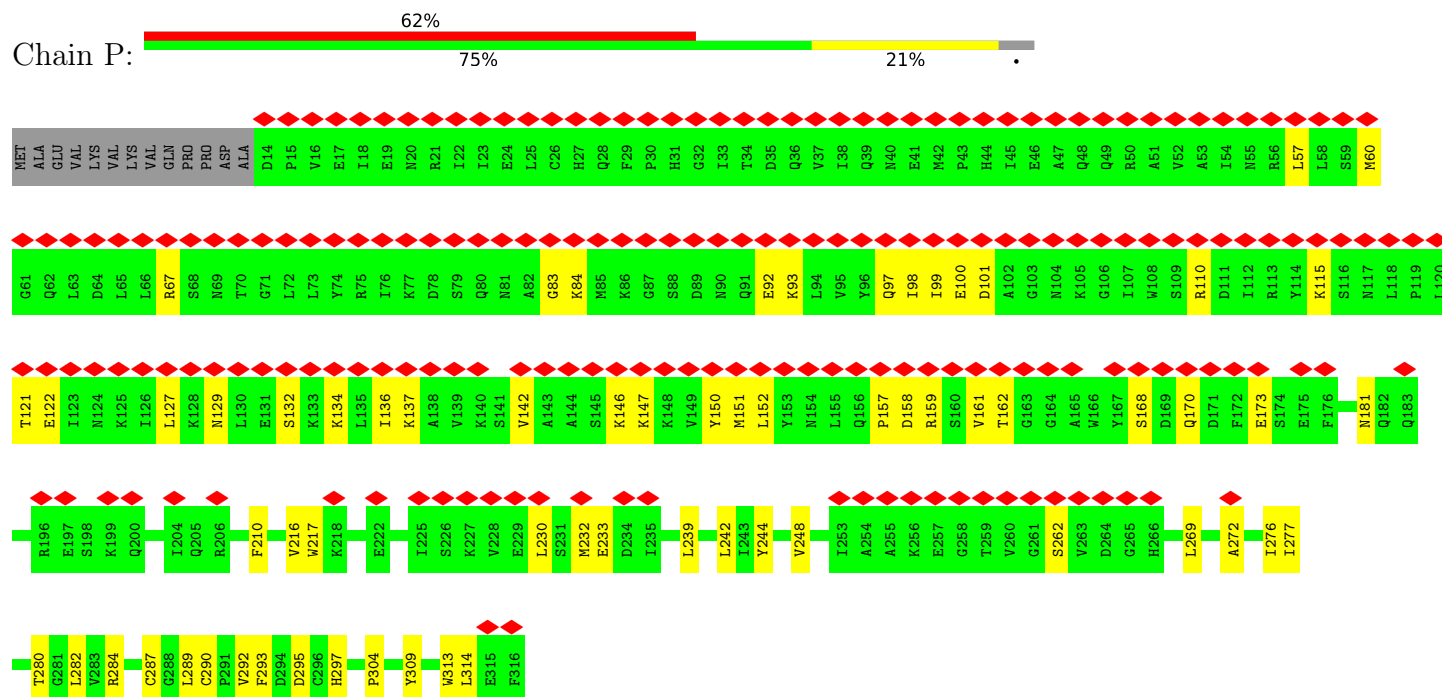
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q:

12%

29%

10%

61%

• Molecule 18: Transcription factor IIIB 50 kDa subunit

Chain V: 7% 92%

• Molecule 19: DNA (50-MER)

Chain X: 68% 14% 76% 10%

• Molecule 20: DNA (50-MER)

Chain Y: 50% 26% 58% 16%

• Molecule 21: RNA (5'-R(P*UP*GP*CP*UP*CP*GP*C)-3')

Chain Z:

86%

14%
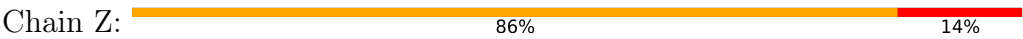
U2 G3 C4 U5 C6 G7 C8

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	633000	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.310	Depositor
Minimum map value	-0.176	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332538, 1.332538, 1.332538	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, GTP, MG, ZN, 3AT

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	0.24	0/11008	0.40	0/14842
2	B	0.24	0/8905	0.41	0/12011
3	C	0.24	0/2790	0.40	0/3782
4	D	0.23	0/997	0.39	0/1343
5	E	0.23	0/1745	0.39	0/2358
6	F	0.22	0/620	0.39	0/839
7	G	0.24	0/1374	0.42	0/1868
8	H	0.24	0/1207	0.42	0/1628
9	I	0.25	0/432	0.41	0/581
10	J	0.23	0/521	0.36	0/703
11	K	0.24	0/837	0.42	0/1129
12	L	0.23	0/394	0.42	0/524
13	M	0.23	0/3455	0.38	0/4673
14	N	0.23	0/1137	0.44	0/1530
15	O	0.23	0/4141	0.39	0/5592
16	P	0.23	0/2446	0.37	0/3301
17	Q	0.24	0/777	0.38	0/1050
18	V	0.23	0/248	0.43	0/336
19	X	0.97	5/1161 (0.4%)	0.97	0/1789
20	Y	1.52	22/1137 (1.9%)	1.47	23/1753 (1.3%)
21	Z	1.37	1/161 (0.6%)	1.69	7/248 (2.8%)
All	All	0.38	28/45493 (0.1%)	0.50	30/61880 (0.0%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	-9	DT	O3'-P	-15.25	1.42	1.61
20	Y	-8	DT	P-OP1	-12.76	1.27	1.49
20	Y	-7	DG	O3'-P	10.18	1.73	1.61
20	Y	-6	DC	P-OP1	-9.51	1.32	1.49
20	Y	-8	DT	O3'-P	-9.45	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	1	DG	C1'-N9	-9.26	1.34	1.47
20	Y	-6	DC	P-OP2	-8.67	1.34	1.49
21	Z	4	C	O3'-P	-8.66	1.50	1.61
20	Y	-6	DC	O3'-P	-8.10	1.51	1.61
20	Y	-8	DT	P-OP2	-7.79	1.35	1.49
20	Y	-7	DG	C2'-C1'	-6.22	1.46	1.52
20	Y	-7	DG	P-OP1	-6.08	1.38	1.49
20	Y	-24	DG	C1'-N9	-6.03	1.38	1.47
20	Y	-8	DT	C2'-C1'	-5.86	1.46	1.52
19	X	6	DG	C1'-N9	-5.47	1.39	1.47
20	Y	-16	DG	C1'-N9	-5.43	1.39	1.47
20	Y	-30	DA	C1'-N9	-5.40	1.39	1.47
19	X	15	DG	C1'-N9	-5.34	1.39	1.47
20	Y	-5	DG	P-O5'	-5.32	1.54	1.59
20	Y	-5	DG	P-OP2	-5.32	1.40	1.49
20	Y	-5	DG	O4'-C1'	-5.31	1.35	1.42
19	X	-10	DA	C1'-N9	-5.26	1.39	1.47
20	Y	-5	DG	P-OP1	-5.21	1.40	1.49
20	Y	10	DT	C1'-N1	5.11	1.55	1.49
20	Y	-15	DC	C1'-N1	5.11	1.55	1.49
20	Y	18	DA	C1'-N9	-5.11	1.40	1.47
19	X	-15	DA	C1'-N9	-5.03	1.40	1.47
19	X	26	DA	C1'-N9	-5.01	1.40	1.47

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Y	-8	DT	O5'-P-OP1	-14.40	92.74	105.70
20	Y	-6	DC	O4'-C4'-C3'	-14.32	97.41	106.00
20	Y	-7	DG	P-O3'-C3'	12.46	134.66	119.70
20	Y	-6	DC	O5'-P-OP1	-11.45	95.40	105.70
20	Y	-6	DC	P-O3'-C3'	-11.30	106.14	119.70
20	Y	-5	DG	O4'-C4'-C3'	-10.59	99.64	106.00
21	Z	6	C	O5'-P-OP1	10.10	122.82	110.70
20	Y	-6	DC	O3'-P-O5'	10.07	123.14	104.00
20	Y	-7	DG	C4'-C3'-C2'	-10.03	94.07	103.10
20	Y	-7	DG	O4'-C4'-C3'	-9.74	100.16	106.00
21	Z	4	C	C1'-C2'-O2'	-9.35	82.55	110.60
20	Y	-8	DT	O5'-P-OP2	8.95	121.44	110.70
21	Z	6	C	O5'-P-OP2	-7.99	98.51	105.70
20	Y	-6	DC	C4'-C3'-C2'	-7.49	96.36	103.10
20	Y	-7	DG	O5'-P-OP1	-7.38	99.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Y	1	DG	C3'-C2'-C1'	-7.33	93.70	102.50
20	Y	-1	DA	P-O3'-C3'	7.17	128.30	119.70
20	Y	-7	DG	C2'-C3'-O3'	-6.86	89.95	112.60
20	Y	-6	DC	OP1-P-O3'	-6.56	90.77	105.20
20	Y	1	DG	C1'-O4'-C4'	-6.55	103.55	110.10
20	Y	-7	DG	OP1-P-O3'	6.50	119.49	105.20
20	Y	-7	DG	O3'-P-O5'	-6.30	92.03	104.00
21	Z	6	C	O4'-C1'-N1	6.14	113.11	108.20
21	Z	5	U	P-O3'-C3'	-6.13	112.35	119.70
20	Y	-5	DG	C4'-C3'-C2'	-5.84	97.84	103.10
20	Y	-8	DT	C2'-C3'-O3'	-5.82	93.38	112.60
21	Z	6	C	C1'-C2'-O2'	-5.74	93.37	110.60
21	Z	2	U	O3'-P-O5'	-5.70	93.17	104.00
20	Y	-8	DT	C4'-C3'-C2'	-5.45	98.20	103.10
20	Y	-1	DA	O3'-P-O5'	-5.27	93.98	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11057	288	0
2	B	8736	0	8861	176	0
3	C	2736	0	2712	52	0
4	D	985	0	1006	30	0
5	E	1715	0	1733	14	0
6	F	610	0	642	10	0
7	G	1337	0	1306	30	0
8	H	1186	0	1147	16	0
9	I	424	0	422	18	0
10	J	512	0	525	12	0
11	K	822	0	810	10	0
12	L	388	0	393	9	0
13	M	3382	0	3376	71	0
14	N	1128	0	1181	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	4075	0	4149	147	0
16	P	2403	0	2408	75	0
17	Q	754	0	759	38	0
18	V	246	0	221	3	0
19	X	1031	0	558	70	0
20	Y	1019	0	570	105	0
21	Z	146	0	76	50	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
23	A	1	0	0	0	0
24	B	30	0	12	13	0
25	P	8	0	0	3	0
26	Z	32	0	11	11	0
All	All	44526	0	43935	932	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 11.

All (932) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:OG1	15:O:377:GLN:NE2	1.68	1.26
20:Y:9:DG:H2"	20:Y:10:DT:C7	1.64	1.25
13:M:171:LYS:NZ	16:P:67:ARG:HB2	1.51	1.23
20:Y:9:DG:C2'	20:Y:10:DT:H71	1.70	1.20
1:A:196:SER:HB2	15:O:373:LYS:CB	1.72	1.19
1:A:199:THR:OG1	15:O:372:LYS:HD2	1.42	1.18
19:X:17:DA:C2	20:Y:-16:DG:N2	2.13	1.15
1:A:465:GLN:NE2	20:Y:-6:DC:H4'	1.60	1.14
20:Y:-27:DT:H2"	20:Y:-26:DT:H71	1.19	1.14
13:M:177:PHE:HE1	16:P:97:GLN:HB3	1.12	1.08
20:Y:-27:DT:C2'	20:Y:-26:DT:H71	1.82	1.08
13:M:171:LYS:HZ1	16:P:67:ARG:HB2	1.05	1.07
1:A:203:HIS:NE2	15:O:383:PHE:CZ	2.22	1.06
1:A:465:GLN:CD	20:Y:-6:DC:H4'	1.77	1.05
1:A:159:CYS:HB2	15:O:531:MET:HG2	1.33	1.05
2:B:689:MET:CE	21:Z:8:C:OP1	2.04	1.04
20:Y:-27:DT:H2"	20:Y:-26:DT:C7	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:9:DG:C2'	20:Y:10:DT:C7	2.34	1.02
21:Z:2:U:C6	26:Z:101:GTP:H2'	1.96	1.01
1:A:465:GLN:HG2	20:Y:-6:DC:C1'	1.90	1.00
20:Y:-18:DG:C2'	20:Y:-17:DT:H72	1.90	1.00
1:A:111:THR:HG23	15:O:429:LEU:CD2	1.91	1.00
1:A:465:GLN:HE21	20:Y:-6:DC:H5'	1.26	0.99
2:B:685:TYR:HE2	24:B:1202:3AT:O1G	1.45	0.99
1:A:1112:GLU:HB3	9:I:47:LYS:HG2	1.44	0.98
13:M:171:LYS:HZ3	16:P:67:ARG:CD	1.76	0.98
1:A:196:SER:O	15:O:373:LYS:HB2	1.63	0.97
1:A:196:SER:HB2	15:O:373:LYS:HB3	1.43	0.97
2:B:689:MET:HE3	21:Z:8:C:OP1	1.61	0.97
1:A:111:THR:HG23	15:O:429:LEU:HD22	1.44	0.96
13:M:171:LYS:NZ	16:P:67:ARG:CB	2.28	0.96
19:X:23:DA:H2"	19:X:24:DC:C5	2.00	0.96
1:A:197:PHE:CZ	15:O:374:HIS:CD2	2.55	0.94
2:B:685:TYR:CE2	24:B:1202:3AT:O1G	2.21	0.94
1:A:465:GLN:HG2	20:Y:-6:DC:H1'	1.48	0.94
16:P:284:ARG:HD3	17:Q:48:LEU:HA	1.49	0.94
19:X:25:DT:O2	20:Y:-24:DG:N2	2.02	0.93
21:Z:2:U:H6	26:Z:101:GTP:H2'	1.29	0.92
13:M:171:LYS:HZ3	16:P:67:ARG:HD2	1.33	0.92
13:M:177:PHE:CE1	16:P:97:GLN:HB3	2.03	0.92
20:Y:9:DG:H2"	20:Y:10:DT:H71	0.94	0.92
1:A:196:SER:HB2	15:O:373:LYS:CG	2.00	0.92
13:M:171:LYS:HZ3	16:P:67:ARG:CB	1.83	0.92
20:Y:-27:DT:C2'	20:Y:-26:DT:C7	2.48	0.90
2:B:692:GLN:NE2	21:Z:6:C:O3'	2.05	0.89
1:A:159:CYS:HA	15:O:531:MET:HB3	1.52	0.89
1:A:230:ILE:O	15:O:2:THR:N	2.05	0.89
13:M:171:LYS:HG3	16:P:67:ARG:HD3	1.52	0.89
20:Y:-18:DG:H2"	20:Y:-17:DT:C7	2.03	0.89
1:A:465:GLN:NE2	20:Y:-6:DC:C5'	2.36	0.89
1:A:203:HIS:HE2	15:O:383:PHE:HZ	0.96	0.88
1:A:465:GLN:HE21	20:Y:-6:DC:C5'	1.87	0.87
1:A:197:PHE:CE2	15:O:374:HIS:CD2	2.63	0.87
1:A:160:GLY:HA3	15:O:532:LYS:HE2	1.55	0.87
1:A:159:CYS:CB	15:O:531:MET:HG2	2.05	0.86
16:P:284:ARG:HB3	17:Q:48:LEU:HD13	1.55	0.86
19:X:17:DA:N1	20:Y:-16:DG:C2	2.44	0.85
2:B:689:MET:HE1	21:Z:8:C:OP1	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:17:DA:C2	20:Y:-16:DG:C2	2.64	0.85
1:A:217:ASN:OD1	15:O:408:GLU:HB3	1.77	0.85
1:A:197:PHE:CZ	15:O:374:HIS:NE2	2.45	0.84
1:A:231:PRO:HA	15:O:2:THR:OG1	1.78	0.84
1:A:465:GLN:NE2	20:Y:-6:DC:C4'	2.39	0.84
24:B:1202:3AT:O4'	21:Z:8:C:O2'	1.96	0.83
1:A:196:SER:CB	15:O:373:LYS:HG3	2.08	0.83
13:M:171:LYS:NZ	16:P:67:ARG:HD2	1.94	0.83
13:M:171:LYS:HZ3	16:P:67:ARG:HB2	1.42	0.82
1:A:465:GLN:NE2	20:Y:-6:DC:H5'	1.92	0.81
1:A:155:ILE:HD12	15:O:534:GLN:NE2	1.95	0.81
2:B:1014:HIS:CE1	21:Z:7:G:H4'	2.15	0.81
21:Z:6:C:H6	21:Z:6:C:H5"	1.44	0.80
1:A:159:CYS:O	15:O:531:MET:HA	1.81	0.80
13:M:177:PHE:CE2	16:P:98:ILE:HD12	2.15	0.80
1:A:196:SER:HB2	15:O:373:LYS:HG3	1.63	0.80
1:A:203:HIS:CE1	15:O:383:PHE:CZ	2.69	0.80
20:Y:-18:DG:H2"	20:Y:-17:DT:H72	1.62	0.80
11:K:66:GLU:HG2	11:K:87:ARG:HG2	1.65	0.79
1:A:111:THR:CG2	15:O:429:LEU:HD21	2.11	0.79
21:Z:2:U:O4'	26:Z:101:GTP:H2'	1.82	0.78
1:A:465:GLN:CG	20:Y:-6:DC:H4'	2.12	0.78
13:M:177:PHE:CD2	16:P:98:ILE:HD12	2.18	0.78
17:Q:27:LEU:HD23	19:X:-5:DA:H2'	1.65	0.78
19:X:-15:DA:C6	19:X:-14:DA:N6	2.52	0.78
13:M:177:PHE:CE1	16:P:98:ILE:HG13	2.19	0.77
21:Z:2:U:H1'	26:Z:101:GTP:N3	1.99	0.76
20:Y:9:DG:H2"	20:Y:10:DT:C5	2.19	0.76
15:O:349:THR:HG23	16:P:280:THR:HG21	1.68	0.76
1:A:1112:GLU:HB3	9:I:47:LYS:CG	2.16	0.75
20:Y:-27:DT:H2"	20:Y:-26:DT:C5	2.21	0.75
20:Y:-18:DG:C2'	20:Y:-17:DT:C7	2.63	0.75
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.68	0.75
1:A:465:GLN:HG2	20:Y:-6:DC:C2'	2.16	0.75
24:B:1202:3AT:H8	21:Z:8:C:H2'	1.67	0.75
1:A:203:HIS:NE2	15:O:383:PHE:HZ	1.69	0.74
1:A:111:THR:HG23	15:O:429:LEU:HD21	1.68	0.74
1:A:111:THR:CG2	15:O:429:LEU:CD2	2.65	0.74
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.70	0.74
2:B:1014:HIS:CE1	21:Z:7:G:C4'	2.71	0.73
1:A:155:ILE:HB	15:O:534:GLN:HE21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:CYS:HA	15:O:531:MET:CB	2.19	0.73
19:X:17:DA:N3	20:Y:-16:DG:N2	2.37	0.72
19:X:23:DA:C2	20:Y:-22:DA:C2	2.78	0.72
19:X:23:DA:H2"	19:X:24:DC:H5	1.52	0.72
20:Y:-1:DA:C6	21:Z:3:G:C2	2.78	0.71
2:B:715:PRO:HB2	2:B:734:PRO:HG2	1.71	0.71
13:M:221:GLU:HB3	14:N:374:THR:HG21	1.72	0.71
1:A:232:ALA:HB3	15:O:6:ILE:HD11	1.73	0.71
13:M:177:PHE:CZ	16:P:98:ILE:HB	2.25	0.71
1:A:464:ARG:NH1	24:B:1202:3AT:O2'	2.21	0.70
13:M:249:LEU:HD12	13:M:250:MET:HG2	1.73	0.70
1:A:199:THR:OG1	15:O:372:LYS:CD	2.32	0.69
21:Z:2:U:O4'	26:Z:101:GTP:C2'	2.40	0.69
4:D:41:ASN:HB2	7:G:36:ASN:HD22	1.58	0.69
1:A:197:PHE:CE1	15:O:374:HIS:CE1	2.80	0.69
19:X:11:DG:C2	20:Y:-10:DG:N2	2.61	0.69
3:C:49:PHE:HA	3:C:66:VAL:O	1.92	0.68
15:O:59:GLN:HG2	17:Q:73:TYR:CE1	2.29	0.68
16:P:216:VAL:HG21	16:P:239:LEU:HD11	1.75	0.68
15:O:20:ILE:HD11	17:Q:75:ILE:CG1	2.23	0.68
19:X:19:DA:C2	20:Y:-18:DG:C2	2.82	0.68
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.76	0.68
1:A:155:ILE:HB	15:O:534:GLN:NE2	2.08	0.68
1:A:344:ARG:HH21	1:A:351:ARG:HH21	1.39	0.68
1:A:485:THR:OG1	1:A:487:ARG:NH1	2.26	0.68
1:A:1215:ASP:O	1:A:1221:GLU:HA	1.93	0.68
19:X:29:DA:C2'	19:X:30:DT:H71	2.24	0.68
2:B:722:THR:HG23	2:B:962:THR:HA	1.76	0.68
1:A:1044:PRO:HG2	1:A:1282:ILE:HD11	1.77	0.67
3:C:91:LYS:HB2	3:C:213:HIS:HB2	1.76	0.67
1:A:300:GLY:HA3	15:O:389:LYS:HA	1.76	0.67
19:X:0:DG:N7	19:X:1:DT:O4	2.28	0.67
2:B:203:VAL:HG13	2:B:214:THR:HG23	1.77	0.67
13:M:11:GLN:HE22	14:N:258:LEU:HD23	1.60	0.67
1:A:471:LEU:HD22	1:A:538:LEU:HD12	1.76	0.67
7:G:115:GLN:NE2	7:G:192:GLU:O	2.27	0.67
16:P:313:TRP:HZ2	17:Q:48:LEU:HD21	1.60	0.67
20:Y:-28:DT:C2'	20:Y:-27:DT:H72	2.25	0.67
2:B:180:ILE:HB	2:B:455:ILE:HG12	1.77	0.67
2:B:1014:HIS:NE2	21:Z:7:G:H4'	2.09	0.67
2:B:914:GLU:HB2	3:C:78:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ASP:OD1	9:I:51:ASP:N	2.20	0.66
3:C:78:ARG:HE	11:K:50:THR:HG22	1.61	0.66
19:X:-10:DA:H2"	19:X:-9:DC:C6	2.30	0.66
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.78	0.66
2:B:679:GLN:HG2	2:B:681:PRO:HD2	1.76	0.66
1:A:874:ARG:HH22	1:A:1071:LYS:HG3	1.60	0.66
2:B:461:LYS:HB2	2:B:492:LEU:HD12	1.77	0.66
13:M:171:LYS:HZ3	16:P:67:ARG:CG	2.09	0.66
2:B:212:SER:HB2	2:B:227:HIS:HE2	1.61	0.66
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.78	0.65
24:B:1202:3AT:O4'	21:Z:8:C:C2'	2.43	0.65
1:A:159:CYS:HA	15:O:531:MET:CG	2.25	0.65
2:B:190:ILE:HG21	2:B:354:ARG:HE	1.61	0.65
2:B:178:ILE:HG12	2:B:437:THR:HG22	1.78	0.65
19:X:29:DA:H2"	19:X:30:DT:H71	1.78	0.65
1:A:196:SER:HB2	15:O:373:LYS:HB2	1.76	0.65
2:B:89:GLU:HG3	2:B:105:ARG:HH22	1.62	0.65
2:B:915:ASP:OD1	3:C:78:ARG:NH2	2.30	0.65
19:X:17:DA:N1	20:Y:-16:DG:N2	2.41	0.65
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.79	0.64
20:Y:-1:DA:N1	21:Z:3:G:C2	2.64	0.64
1:A:855:ARG:NH2	2:B:481:PRO:O	2.30	0.64
2:B:682:ARG:HD2	2:B:937:ARG:HB3	1.79	0.64
24:B:1202:3AT:C4'	21:Z:8:C:HO2'	2.08	0.64
20:Y:-19:DT:H2"	20:Y:-18:DG:C8	2.32	0.64
1:A:461:LEU:HD23	1:A:473:ILE:HD11	1.79	0.64
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.79	0.64
8:H:112:LEU:HD13	8:H:129:ALA:HB2	1.80	0.64
20:Y:-27:DT:H2'	20:Y:-26:DT:C7	2.27	0.64
1:A:159:CYS:CB	15:O:531:MET:CG	2.75	0.64
15:O:374:HIS:HB3	15:O:423:LEU:HD23	1.79	0.64
1:A:360:ARG:HG2	2:B:1046:ARG:HB2	1.80	0.64
16:P:83:GLY:N	16:P:92:GLU:OE2	2.30	0.64
16:P:142:VAL:HG23	16:P:170:GLN:HA	1.79	0.64
20:Y:-28:DT:C6	20:Y:-27:DT:H72	2.32	0.64
16:P:84:LYS:N	16:P:92:GLU:OE2	2.28	0.64
25:P:401:SF4:S3	17:Q:38:PHE:HE2	2.21	0.63
20:Y:-18:DG:C8	20:Y:-17:DT:H72	2.34	0.63
1:A:465:GLN:CG	20:Y:-6:DC:C4'	2.76	0.63
2:B:535:ASN:HD21	14:N:247:LYS:HE2	1.63	0.63
16:P:159:ARG:NH1	16:P:233:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-1:DA:C6	21:Z:3:G:N1	2.66	0.63
1:A:465:GLN:HG2	20:Y:-6:DC:C4'	2.29	0.63
1:A:1069:ARG:HH12	1:A:1080:ILE:HD12	1.64	0.63
2:B:228:ASN:O	2:B:292:ARG:NH2	2.29	0.63
15:O:112:LEU:HD11	17:Q:64:LEU:HD22	1.80	0.63
1:A:221:LEU:HD13	15:O:399:LEU:O	1.98	0.63
24:B:1202:3AT:O4'	21:Z:8:C:H2'	1.98	0.63
1:A:1194:GLU:O	1:A:1198:LYS:NZ	2.32	0.63
1:A:1273:TYR:O	1:A:1277:ASN:ND2	2.30	0.63
15:O:20:ILE:HD11	17:Q:75:ILE:HG13	1.80	0.62
16:P:290:CYS:SG	25:P:401:SF4:S4	2.98	0.62
20:Y:-27:DT:H2'	20:Y:-26:DT:H71	1.77	0.62
2:B:685:TYR:HE2	24:B:1202:3AT:PG	2.21	0.62
1:A:1112:GLU:HB3	9:I:47:LYS:HD2	1.82	0.62
1:A:740:PRO:HA	9:I:51:ASP:OD2	1.99	0.62
15:O:258:ARG:HD3	16:P:276:ILE:HG12	1.81	0.62
20:Y:-1:DA:N6	21:Z:3:G:N1	2.46	0.62
1:A:130:LYS:CE	15:O:34:GLN:NE2	2.62	0.61
1:A:465:GLN:CG	20:Y:-6:DC:H1'	2.25	0.61
19:X:-13:DA:H2"	19:X:-12:DG:C8	2.35	0.61
1:A:465:GLN:HE21	20:Y:-6:DC:C4'	2.09	0.61
20:Y:-28:DT:H2'	20:Y:-27:DT:H72	1.82	0.61
16:P:137:LYS:NZ	16:P:152:LEU:O	2.34	0.61
1:A:214:ALA:HB2	15:O:409:ILE:HG22	1.82	0.61
1:A:481:LYS:HB2	1:A:487:ARG:HH21	1.66	0.61
1:A:640:ILE:HG12	1:A:645:LEU:HA	1.82	0.61
1:A:5:GLN:HB2	7:G:185:THR:HG21	1.82	0.61
1:A:1340:VAL:HA	1:A:1345:GLU:HG3	1.82	0.61
1:A:130:LYS:HE2	15:O:34:GLN:NE2	2.16	0.60
2:B:750:ASP:HA	2:B:754:ALA:HB3	1.82	0.60
20:Y:-27:DT:H2"	20:Y:-26:DT:C6	2.36	0.60
21:Z:2:U:C1'	26:Z:101:GTP:H2'	2.30	0.60
1:A:125:PHE:HZ	1:A:149:LYS:HD2	1.66	0.60
21:Z:6:C:H5"	21:Z:6:C:C6	2.32	0.60
1:A:1119:GLU:HG3	1:A:1128:ILE:HG12	1.83	0.60
1:A:461:LEU:HD21	2:B:1063:LEU:HD21	1.84	0.60
1:A:465:GLN:HG2	20:Y:-6:DC:H2"	1.83	0.60
13:M:311:LEU:HD21	13:M:415:VAL:HG21	1.84	0.60
19:X:0:DG:N7	19:X:1:DT:C4	2.69	0.60
19:X:3:DC:H2"	19:X:4:DT:H3'	1.84	0.60
20:Y:-1:DA:H1'	20:Y:0:DC:H5'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:HIS:NE2	15:O:383:PHE:CE2	2.68	0.60
4:D:3:VAL:HG12	7:G:7:MET:HG2	1.84	0.60
15:O:507:ASN:OD1	17:Q:62:GLN:NE2	2.31	0.60
1:A:199:THR:CB	15:O:372:LYS:HD2	2.31	0.60
10:J:28:GLU:OE2	13:M:397:GLY:N	2.35	0.60
1:A:232:ALA:HB3	15:O:6:ILE:CD1	2.31	0.60
2:B:986:LYS:O	3:C:285:ARG:NH2	2.34	0.59
19:X:17:DA:C4	20:Y:-16:DG:N2	2.70	0.59
20:Y:-5:DG:H2'	20:Y:-4:DA:H8	1.67	0.59
1:A:159:CYS:HB3	15:O:531:MET:SD	2.42	0.59
1:A:942:LYS:HG3	1:A:977:SER:HB2	1.84	0.59
3:C:236:LEU:HD12	3:C:307:ILE:HD11	1.83	0.59
2:B:313:LEU:O	2:B:331:LYS:NZ	2.32	0.59
4:D:4:LYS:HB2	7:G:6:GLU:HB2	1.83	0.59
1:A:6:PHE:HB2	7:G:37:LYS:HB3	1.83	0.59
1:A:197:PHE:CE2	15:O:374:HIS:CG	2.90	0.59
1:A:891:ARG:HG2	1:A:897:ILE:HG12	1.85	0.59
3:C:326:ILE:HG21	11:K:111:LEU:HB2	1.85	0.59
20:Y:-5:DG:C6	21:Z:7:G:C6	2.91	0.59
1:A:111:THR:HG22	15:O:429:LEU:HD21	1.83	0.59
1:A:266:VAL:HB	1:A:275:ASN:HB2	1.84	0.59
1:A:303:THR:OG1	15:O:377:GLN:CD	2.39	0.59
2:B:85:PRO:HG3	2:B:138:ILE:HG13	1.85	0.59
3:C:235:LEU:HB2	3:C:301:ARG:HH11	1.68	0.59
20:Y:9:DG:H2'	20:Y:10:DT:C7	2.30	0.59
3:C:141:ARG:NH1	3:C:209:ASP:OD1	2.36	0.59
2:B:313:LEU:HD23	2:B:317:ILE:HD12	1.85	0.58
3:C:89:VAL:HB	3:C:111:GLY:HA2	1.85	0.58
15:O:159:ARG:NH2	15:O:189:LEU:O	2.35	0.58
5:E:95:GLN:OE1	5:E:125:TYR:OH	2.21	0.58
1:A:23:LYS:HG3	2:B:1123:ILE:HG13	1.84	0.58
6:F:100:ARG:NH2	6:F:123:LEU:O	2.35	0.58
1:A:937:GLU:OE1	1:A:1007:THR:OG1	2.22	0.58
15:O:147:THR:HG22	15:O:150:ARG:HH22	1.68	0.58
1:A:470:LYS:HB3	1:A:1039:GLN:HE22	1.68	0.58
1:A:1360:PHE:O	6:F:64:ARG:NH1	2.36	0.58
19:X:-7:DA:H2"	19:X:-6:DA:N7	2.18	0.58
9:I:52:VAL:HG22	9:I:52:VAL:O	2.03	0.58
15:O:20:ILE:HD11	17:Q:75:ILE:HG12	1.85	0.58
1:A:159:CYS:CB	15:O:531:MET:SD	2.91	0.58
2:B:539:VAL:HG12	2:B:583:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:ARG:NH2	2:B:1027:PRO:O	2.36	0.58
7:G:2:PHE:HA	7:G:76:VAL:O	2.03	0.58
19:X:23:DA:C2'	19:X:24:DC:C5	2.81	0.58
21:Z:2:U:O4'	26:Z:101:GTP:O2'	2.21	0.58
1:A:168:LYS:NZ	1:A:170:GLY:O	2.37	0.58
2:B:741:VAL:HG22	2:B:927:ILE:HB	1.86	0.58
16:P:146:LYS:HG3	16:P:147:LYS:HD3	1.84	0.58
1:A:159:CYS:HA	15:O:531:MET:SD	2.44	0.57
1:A:855:ARG:HD2	2:B:471:LEU:HB2	1.84	0.57
1:A:899:GLN:NE2	1:A:1292:ASP:OD2	2.28	0.57
1:A:1332:ALA:HB2	2:B:1122:ILE:HG23	1.84	0.57
2:B:738:ASN:HB2	10:J:47:ARG:HD3	1.86	0.57
15:O:56:VAL:HG23	17:Q:73:TYR:HD1	1.69	0.57
20:Y:14:DT:H2"	20:Y:15:DT:C6	2.39	0.57
20:Y:-18:DG:H2'	20:Y:-17:DT:H72	1.80	0.57
1:A:160:GLY:CA	15:O:532:LYS:HE2	2.33	0.57
1:A:199:THR:HG1	15:O:372:LYS:HD2	1.65	0.57
1:A:1112:GLU:HB3	9:I:47:LYS:CD	2.34	0.57
2:B:594:ARG:NH2	2:B:663:THR:OG1	2.30	0.57
2:B:692:GLN:HE22	21:Z:7:G:C5'	2.18	0.57
3:C:93:LEU:HD23	12:L:52:LEU:HD11	1.86	0.57
13:M:50:LYS:NZ	13:M:200:HIS:O	2.36	0.57
1:A:155:ILE:HD12	15:O:534:GLN:CD	2.25	0.57
2:B:301:PRO:O	2:B:304:THR:OG1	2.22	0.57
2:B:674:TYR:HB3	2:B:677:HIS:HD2	1.69	0.57
19:X:15:DG:H2"	19:X:16:DC:O5'	2.04	0.57
21:Z:3:G:OP1	21:Z:3:G:H4'	2.04	0.57
1:A:542:ILE:HG13	1:A:543:GLN:H	1.70	0.57
13:M:218:SER:HA	14:N:374:THR:HG23	1.86	0.57
15:O:292:GLU:HA	15:O:295:ARG:HG2	1.87	0.57
1:A:1132:LEU:HB2	1:A:1171:ALA:HB1	1.85	0.57
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.38	0.57
1:A:459:VAL:HB	1:A:516:LYS:HG3	1.87	0.57
4:D:87:LEU:O	4:D:90:ARG:NH1	2.37	0.57
15:O:472:ALA:HA	15:O:475:GLN:HE21	1.70	0.57
1:A:940:LEU:HB2	1:A:1006:ILE:HG23	1.87	0.56
1:A:231:PRO:CA	15:O:2:THR:HG23	2.35	0.56
1:A:306:ILE:HG13	15:O:396:TYR:CE2	2.40	0.56
2:B:254:MET:HA	2:B:528:GLY:HA3	1.85	0.56
13:M:409:ILE:HG23	13:M:416:VAL:HG21	1.87	0.56
2:B:903:GLN:OE1	2:B:937:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:332:ARG:HB2	14:N:336:ARG:HB2	1.87	0.56
13:M:171:LYS:HB2	16:P:67:ARG:HB3	1.88	0.56
1:A:159:CYS:O	15:O:531:MET:CA	2.50	0.56
20:Y:-18:DG:N9	20:Y:-17:DT:H72	2.19	0.56
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.87	0.56
1:A:26:GLU:HG2	16:P:297:HIS:HB2	1.87	0.56
2:B:764:ARG:HD3	10:J:6:ARG:HB3	1.88	0.56
3:C:9:GLU:OE2	3:C:298:ARG:NH1	2.38	0.56
19:X:21:DA:C8	19:X:21:DA:H5'	2.41	0.56
21:Z:2:U:H2'	21:Z:2:U:O2	2.04	0.56
1:A:598:LYS:HD2	8:H:120:GLY:HA3	1.88	0.56
3:C:28:ASP:O	11:K:61:LYS:NZ	2.38	0.56
15:O:505:ASN:HB3	16:P:314:LEU:HD13	1.87	0.56
20:Y:-19:DT:H2"	20:Y:-18:DG:H8	1.71	0.56
2:B:563:ARG:NH2	2:B:637:GLU:OE2	2.37	0.56
1:A:196:SER:CB	15:O:373:LYS:CB	2.66	0.56
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.37	0.56
9:I:8:CYS:SG	9:I:10:ASN:ND2	2.71	0.56
12:L:26:ASN:ND2	12:L:36:CYS:SG	2.78	0.56
13:M:177:PHE:CZ	16:P:98:ILE:CB	2.89	0.56
16:P:210:PHE:HB3	16:P:269:LEU:HB3	1.88	0.56
1:A:214:ALA:CB	15:O:409:ILE:HG22	2.35	0.55
1:A:866:ALA:HB2	20:Y:-8:DT:H72	1.87	0.55
1:A:903:GLY:HA3	1:A:1285:ARG:HG2	1.88	0.55
13:M:117:ALA:HB1	13:M:124:LEU:HD11	1.89	0.55
15:O:255:VAL:HG21	15:O:267:VAL:HG11	1.88	0.55
19:X:17:DA:H2"	19:X:18:DC:C6	2.42	0.55
1:A:499:ASP:OD1	1:A:499:ASP:N	2.39	0.55
3:C:109:ARG:NH2	3:C:198:LEU:O	2.39	0.55
15:O:59:GLN:HG2	17:Q:73:TYR:HE1	1.69	0.55
1:A:159:CYS:CA	15:O:531:MET:CG	2.84	0.55
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.89	0.55
7:G:81:LEU:HD22	7:G:152:VAL:HA	1.88	0.55
3:C:157:SER:HB3	13:M:377:LEU:HA	1.87	0.55
19:X:7:DC:H2"	19:X:8:DA:H4'	1.89	0.55
1:A:231:PRO:HA	15:O:2:THR:CB	2.37	0.55
2:B:392:ILE:HD13	2:B:400:PHE:HB3	1.88	0.55
3:C:149:ASN:ND2	3:C:151:HIS:O	2.40	0.55
8:H:20:LYS:NZ	8:H:22:PHE:O	2.39	0.55
11:K:50:THR:OG1	11:K:51:LEU:N	2.39	0.55
19:X:-2:DC:H5"	19:X:-2:DC:H6	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:-10:DA:H2"	19:X:-9:DC:C5	2.42	0.55
19:X:29:DA:H2'	19:X:30:DT:H71	1.89	0.55
2:B:712:LEU:HD21	2:B:737:GLN:HG3	1.89	0.54
1:A:29:ARG:HH21	1:A:254:ARG:HH21	1.53	0.54
1:A:1105:ILE:HG22	1:A:1238:THR:HG21	1.90	0.54
1:A:1185:MET:SD	1:A:1185:MET:N	2.80	0.54
2:B:206:SER:HB2	2:B:211:LYS:HG2	1.89	0.54
2:B:518:LEU:HD21	2:B:558:THR:HG21	1.89	0.54
10:J:28:GLU:OE2	13:M:396:LYS:N	2.40	0.54
21:Z:6:C:H2'	21:Z:7:G:H8	1.73	0.54
1:A:760:ARG:NH2	1:A:794:GLN:OE1	2.40	0.54
13:M:64:THR:HG21	13:M:96:LEU:HD13	1.89	0.54
1:A:590:LYS:NZ	8:H:88:PHE:O	2.40	0.54
2:B:483:ASP:OD2	2:B:495:ASN:ND2	2.41	0.54
10:J:36:ASP:OD1	10:J:46:ARG:NH1	2.39	0.54
20:Y:-21:DT:H2"	20:Y:-20:DA:C8	2.43	0.54
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.90	0.54
6:F:110:LEU:HD12	6:F:114:SER:HB3	1.90	0.54
1:A:56:LEU:HA	1:A:260:LEU:HD21	1.89	0.54
20:Y:-29:DT:H2"	20:Y:-28:DT:C7	2.38	0.54
20:Y:-5:DG:H2'	20:Y:-4:DA:C8	2.42	0.54
11:K:66:GLU:OE2	11:K:87:ARG:NH1	2.41	0.54
2:B:207:THR:HG23	2:B:209:GLU:H	1.73	0.53
3:C:263:GLU:OE2	3:C:274:ARG:NH1	2.41	0.53
20:Y:-18:DG:C1'	20:Y:-17:DT:H72	2.37	0.53
1:A:465:GLN:CG	20:Y:-6:DC:C1'	2.78	0.53
1:A:1087:ALA:HA	1:A:1246:THR:HG22	1.91	0.53
2:B:634:ASP:OD1	2:B:635:VAL:N	2.40	0.53
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.89	0.53
2:B:87:VAL:HG22	2:B:89:GLU:H	1.73	0.53
13:M:173:ILE:HG22	13:M:175:VAL:HG22	1.89	0.53
15:O:60:HIS:HE1	17:Q:73:TYR:CD1	2.27	0.53
16:P:217:TRP:NE1	16:P:230:LEU:O	2.35	0.53
1:A:36:VAL:HB	1:A:86:ILE:HG12	1.89	0.53
1:A:1105:ILE:HD13	1:A:1225:LEU:HD13	1.91	0.53
4:D:88:ASN:O	4:D:90:ARG:NH2	2.42	0.53
14:N:251:VAL:HG11	14:N:335:GLY:HA2	1.91	0.53
1:A:1087:ALA:HB3	1:A:1225:LEU:HB2	1.90	0.53
3:C:134:GLU:O	3:C:181:GLN:NE2	2.41	0.53
1:A:282:LYS:NZ	1:A:316:GLN:OE1	2.30	0.53
1:A:361:VAL:HG12	2:B:1072:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1079:VAL:HB	2:B:1128:LEU:HD11	1.91	0.53
13:M:364:ARG:HH22	13:M:403:PRO:HA	1.72	0.53
19:X:19:DA:C2	20:Y:-18:DG:N1	2.76	0.53
2:B:137:PRO:HG2	2:B:419:ILE:HD12	1.90	0.52
13:M:177:PHE:CZ	16:P:98:ILE:CG1	2.92	0.52
14:N:245:LEU:HD12	14:N:246:PRO:HD2	1.91	0.52
15:O:60:HIS:HE1	17:Q:73:TYR:CG	2.27	0.52
1:A:465:GLN:OE1	1:A:506:ASN:ND2	2.42	0.52
1:A:529:LEU:HA	1:A:539:ILE:HD13	1.90	0.52
13:M:177:PHE:CZ	16:P:98:ILE:HG13	2.44	0.52
20:Y:9:DG:C4	20:Y:10:DT:C4	2.96	0.52
1:A:196:SER:CA	15:O:373:LYS:HG3	2.39	0.52
1:A:470:LYS:HE3	1:A:532:PRO:HG3	1.92	0.52
1:A:130:LYS:CE	15:O:34:GLN:HE21	2.23	0.52
1:A:558:PHE:HB3	1:A:594:LEU:HD13	1.91	0.52
2:B:898:SER:HB3	2:B:1010:GLN:HG3	1.92	0.52
3:C:115:ILE:HG22	3:C:117:ALA:H	1.74	0.52
1:A:159:CYS:CA	15:O:531:MET:HB3	2.33	0.52
4:D:41:ASN:ND2	7:G:35:ALA:O	2.42	0.52
14:N:253:GLU:OE2	14:N:256:ARG:NH2	2.42	0.52
1:A:295:LYS:HB2	17:Q:28:PRO:HB3	1.91	0.52
1:A:339:ARG:HH22	1:A:351:ARG:HH22	1.56	0.52
1:A:656:GLY:O	1:A:662:ASN:ND2	2.41	0.52
1:A:1069:ARG:HH21	1:A:1270:GLU:HG2	1.73	0.52
15:O:65:TYR:OH	17:Q:105:ARG:O	2.24	0.52
19:X:19:DA:C2	20:Y:-18:DG:N2	2.78	0.52
1:A:555:LYS:HG2	8:H:25:VAL:HG21	1.92	0.52
2:B:318:LEU:HD12	2:B:331:LYS:HG3	1.91	0.52
2:B:869:VAL:HG22	2:B:883:MET:HG3	1.91	0.52
13:M:327:VAL:O	13:M:353:ARG:NH1	2.34	0.52
1:A:197:PHE:CZ	15:O:374:HIS:CE1	2.98	0.52
1:A:631:LEU:HD11	8:H:124:ARG:HD3	1.91	0.52
1:A:1347:ILE:HD13	2:B:1052:ARG:HD2	1.92	0.52
15:O:510:ASP:HB2	17:Q:58:LEU:HD13	1.91	0.52
2:B:531:LEU:HD22	2:B:538:LEU:HD21	1.92	0.52
2:B:205:SER:OG	2:B:320:HIS:N	2.34	0.51
4:D:25:GLU:HA	4:D:28:LYS:HG2	1.92	0.51
13:M:53:GLN:OE1	13:M:200:HIS:ND1	2.38	0.51
21:Z:2:U:C4'	26:Z:101:GTP:O2'	2.57	0.51
2:B:293:ARG:NH1	2:B:301:PRO:HG3	2.25	0.51
14:N:254:LEU:HD12	14:N:331:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:9:DG:C2'	20:Y:10:DT:H73	2.34	0.51
2:B:176:LYS:HE2	2:B:439:VAL:HG22	1.93	0.51
16:P:98:ILE:HD13	16:P:115:LYS:HD3	1.91	0.51
2:B:990:THR:HA	2:B:997:PRO:HA	1.92	0.51
13:M:347:GLU:OE2	13:M:351:ARG:NH2	2.43	0.51
1:A:231:PRO:HA	15:O:2:THR:HG23	1.92	0.51
20:Y:-29:DT:H2"	20:Y:-28:DT:C5	2.45	0.51
3:C:50:ARG:NH1	3:C:52:ASP:OD2	2.43	0.51
1:A:700:ILE:HG21	2:B:947:LEU:HD22	1.92	0.51
1:A:1313:GLU:OE2	1:A:1336:GLN:NE2	2.43	0.51
1:A:604:ILE:HG23	1:A:682:ARG:HB2	1.93	0.51
2:B:103:ARG:NH2	2:B:168:TYR:OH	2.44	0.51
1:A:987:TYR:OH	8:H:102:ASP:N	2.44	0.51
2:B:401:ASP:OD1	2:B:401:ASP:N	2.44	0.51
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.43	0.51
7:G:53:LYS:HB3	7:G:71:HIS:HB2	1.92	0.51
7:G:94:PRO:HA	7:G:121:ASP:HB2	1.92	0.50
15:O:469:ALA:HA	15:O:472:ALA:HB3	1.92	0.50
1:A:593:THR:HB	3:C:32:ASN:HA	1.93	0.50
9:I:20:CYS:SG	9:I:21:HIS:N	2.84	0.50
13:M:171:LYS:HG3	16:P:67:ARG:HB3	1.93	0.50
19:X:4:DT:H4'	19:X:5:DC:OP1	2.11	0.50
8:H:70:LEU:HD23	8:H:70:LEU:H	1.76	0.50
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.92	0.50
2:B:217:ALA:O	2:B:223:PHE:HA	2.12	0.50
2:B:235:PRO:HD2	2:B:238:ILE:HD12	1.93	0.50
1:A:799:VAL:HG23	1:A:837:SER:HA	1.92	0.50
3:C:144:VAL:HG21	3:C:168:VAL:HG13	1.93	0.50
19:X:21:DA:H2'	19:X:22:DT:H71	1.93	0.50
1:A:1185:MET:HG2	1:A:1187:TYR:H	1.76	0.50
3:C:228:VAL:HA	3:C:312:SER:HA	1.94	0.50
19:X:0:DG:C8	19:X:1:DT:C4	3.00	0.50
1:A:323:SER:OG	1:A:338:THR:OG1	2.27	0.50
1:A:701:GLY:HA3	2:B:984:LEU:HD13	1.92	0.50
1:A:553:THR:HG21	1:A:650:MET:HG2	1.92	0.50
1:A:1152:SER:OG	1:A:1200:VAL:O	2.28	0.50
2:B:471:LEU:HD21	2:B:481:PRO:HB3	1.94	0.50
24:B:1202:3AT:C8	21:Z:8:C:H2'	2.41	0.50
1:A:108:ILE:HA	1:A:115:ILE:HA	1.93	0.49
1:A:743:THR:HG23	1:A:746:GLU:H	1.77	0.49
2:B:121:ARG:HG2	2:B:399:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:322:GLN:HE22	13:M:364:ARG:HA	1.77	0.49
15:O:509:LEU:HD23	16:P:313:TRP:HZ3	1.76	0.49
4:D:32:LYS:HB2	4:D:35:HIS:HB2	1.93	0.49
8:H:96:VAL:HA	8:H:116:VAL:HG22	1.94	0.49
15:O:361:ARG:HH21	15:O:386:ILE:HG23	1.76	0.49
19:X:23:DA:H2"	19:X:24:DC:C6	2.45	0.49
1:A:523:MET:HA	1:A:528:ASN:HD21	1.76	0.49
2:B:451:MET:HA	2:B:454:ARG:HG3	1.94	0.49
15:O:228:ILE:HB	15:O:231:ASP:HB2	1.95	0.49
2:B:214:THR:HB	2:B:227:HIS:HD2	1.78	0.49
15:O:47:LEU:HG	15:O:51:LYS:HE3	1.93	0.49
15:O:161:PRO:O	17:Q:105:ARG:NH2	2.45	0.49
15:O:510:ASP:HB2	17:Q:58:LEU:CD1	2.42	0.49
20:Y:-27:DT:C2'	20:Y:-26:DT:C5	2.93	0.49
1:A:731:LEU:HB2	1:A:736:LEU:HD22	1.95	0.49
2:B:89:GLU:OE2	12:L:42:ARG:NE	2.45	0.49
2:B:803:ILE:HG13	2:B:806:HIS:H	1.78	0.49
15:O:174:PRO:O	17:Q:108:ARG:NH2	2.45	0.49
11:K:27:LEU:HG	11:K:43:VAL:HB	1.94	0.49
2:B:229:THR:HG21	2:B:316:THR:HG21	1.94	0.49
1:A:76:LEU:O	2:B:1033:ARG:NH2	2.46	0.49
1:A:231:PRO:HA	15:O:2:THR:CG2	2.42	0.49
1:A:669:ARG:NH2	1:A:910:ALA:O	2.46	0.49
2:B:478:MET:HB3	2:B:592:LEU:HD13	1.95	0.49
19:X:22:DT:H2"	19:X:23:DA:C8	2.47	0.49
20:Y:-15:DC:H2"	20:Y:-14:DT:C7	2.43	0.49
1:A:1112:GLU:OE1	9:I:47:LYS:HE3	2.13	0.49
21:Z:2:U:H6	26:Z:101:GTP:C2'	2.14	0.49
1:A:1102:LYS:HB2	1:A:1212:ILE:HD11	1.95	0.48
2:B:86:ASP:O	2:B:135:ARG:NH2	2.46	0.48
3:C:120:ARG:NH1	3:C:324:GLU:OE2	2.43	0.48
3:C:155:ASP:HB3	13:M:348:VAL:HG21	1.95	0.48
12:L:17:TYR:HB3	12:L:44:MET:HG3	1.94	0.48
19:X:28:DA:H2"	19:X:29:DA:C8	2.48	0.48
20:Y:-29:DT:H2"	20:Y:-28:DT:H71	1.95	0.48
1:A:996:GLU:HB3	1:A:997:PRO:HD3	1.95	0.48
1:A:1044:PRO:HA	1:A:1047:GLN:HB2	1.95	0.48
1:A:1117:ILE:HG12	1:A:1130:VAL:HG13	1.95	0.48
4:D:89:HIS:CE1	7:G:84:ILE:HB	2.48	0.48
15:O:496:ARG:HA	15:O:499:LEU:HD12	1.95	0.48
19:X:10:DC:H5'	19:X:10:DC:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:17:DA:H2"	19:X:18:DC:H6	1.78	0.48
2:B:430:LYS:HG3	19:X:5:DC:H1'	1.96	0.48
13:M:171:LYS:HG3	16:P:67:ARG:CD	2.34	0.48
21:Z:6:C:H2'	21:Z:7:G:C8	2.48	0.48
1:A:192:ASN:HA	1:A:195:GLN:HG2	1.95	0.48
1:A:405:ARG:NH1	1:A:441:ALA:O	2.46	0.48
1:A:772:ASP:OD1	1:A:773:LYS:N	2.46	0.48
1:A:217:ASN:OD1	15:O:407:GLN:O	2.32	0.48
1:A:389:ILE:HD12	2:B:1022:ALA:HB3	1.96	0.48
16:P:100:GLU:HG3	16:P:152:LEU:HD11	1.94	0.48
19:X:17:DA:C6	20:Y:-16:DG:N2	2.81	0.48
1:A:360:ARG:HA	2:B:1046:ARG:HA	1.96	0.48
1:A:602:SER:HB2	1:A:644:GLU:HA	1.96	0.48
1:A:1159:ARG:NH2	19:X:22:DT:OP2	2.47	0.48
2:B:1014:HIS:HE2	21:Z:7:G:H5"	1.78	0.48
3:C:86:THR:OG1	3:C:225:PHE:O	2.32	0.48
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.94	0.48
13:M:243:SER:HB2	14:N:396:LYS:HD2	1.94	0.48
15:O:247:ARG:HG3	15:O:342:LEU:HD21	1.94	0.48
1:A:306:ILE:HG13	15:O:396:TYR:CZ	2.48	0.48
1:A:868:THR:HG21	1:A:1046:THR:N	2.29	0.48
1:A:1214:ILE:HG23	9:I:52:VAL:HG23	1.95	0.48
2:B:468:PRO:HG2	2:B:492:LEU:HD21	1.95	0.48
8:H:13:LYS:NZ	8:H:31:GLU:OE1	2.47	0.48
19:X:29:DA:H2"	19:X:30:DT:C6	2.49	0.48
20:Y:0:DC:N4	26:Z:101:GTP:O6	2.35	0.48
2:B:176:LYS:NZ	2:B:420:SER:O	2.47	0.48
3:C:23:ASN:O	3:C:303:ARG:NH2	2.47	0.48
1:A:1237:ALA:HB1	5:E:136:LEU:HD12	1.96	0.48
2:B:467:GLY:H	2:B:468:PRO:HD2	1.79	0.48
2:B:516:SER:HB2	13:M:113:ARG:HH12	1.78	0.48
4:D:91:PRO:HD2	4:D:120:VAL:HG21	1.96	0.48
2:B:426:LEU:O	2:B:430:LYS:N	2.47	0.48
2:B:536:VAL:O	2:B:581:ARG:NH1	2.47	0.48
5:E:59:THR:OG1	5:E:71:GLN:OE1	2.32	0.48
16:P:168:SER:OG	16:P:173:GLU:OE2	2.32	0.48
2:B:518:LEU:HD13	2:B:555:LEU:HD12	1.95	0.47
14:N:269:LEU:HB3	14:N:383:LEU:HB2	1.96	0.47
15:O:443:ILE:HG23	15:O:513:GLU:HG3	1.94	0.47
2:B:779:LEU:O	2:B:878:ALA:HA	2.14	0.47
2:B:880:LEU:HD21	2:B:882:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:VAL:HG23	3:C:297:VAL:HG13	1.96	0.47
14:N:256:ARG:HA	14:N:260:LEU:HD23	1.95	0.47
15:O:17:PHE:C	17:Q:74:PHE:CD1	2.88	0.47
1:A:112:CYS:HA	15:O:433:ARG:CZ	2.44	0.47
2:B:20:ILE:HD12	2:B:21:PRO:HD2	1.96	0.47
14:N:361:VAL:HG12	14:N:375:VAL:HA	1.97	0.47
15:O:464:SER:HA	15:O:467:VAL:HG22	1.95	0.47
19:X:17:DA:C6	20:Y:-16:DG:N1	2.82	0.47
1:A:1112:GLU:CB	9:I:47:LYS:HD2	2.43	0.47
4:D:54:SER:HA	4:D:59:ARG:HD2	1.96	0.47
16:P:158:ASP:HB3	16:P:161:VAL:HG22	1.96	0.47
20:Y:-26:DT:H2"	20:Y:-25:DA:C8	2.48	0.47
1:A:1328:LEU:HD13	2:B:1117:LEU:HD21	1.96	0.47
3:C:8:GLU:HA	3:C:11:ARG:HG2	1.97	0.47
4:D:85:GLN:HE21	7:G:83:GLU:HA	1.80	0.47
7:G:116:GLN:HE22	7:G:118:ALA:HB3	1.80	0.47
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.97	0.47
19:X:8:DA:H5'	19:X:9:DA:H5"	1.96	0.47
13:M:273:LEU:HD11	13:M:281:GLN:HA	1.96	0.47
1:A:159:CYS:CA	15:O:531:MET:HG2	2.44	0.47
1:A:1044:PRO:O	1:A:1048:MET:N	2.46	0.47
2:B:901:HIS:NE2	2:B:945:GLU:OE1	2.43	0.47
2:B:974:GLU:HA	2:B:977:VAL:HG12	1.95	0.47
13:M:225:LEU:HD11	14:N:376:LEU:HD13	1.96	0.47
16:P:129:ASN:O	16:P:132:SER:OG	2.28	0.47
20:Y:-28:DT:C2'	20:Y:-27:DT:C7	2.92	0.47
2:B:461:LYS:HE3	2:B:461:LYS:HB3	1.72	0.47
2:B:923:ILE:HD11	10:J:42:ARG:HB2	1.95	0.47
8:H:8:ASP:OD1	8:H:9:ILE:N	2.47	0.47
13:M:13:ILE:HD13	13:M:119:TYR:HE1	1.80	0.47
2:B:896:LYS:NZ	21:Z:8:C:OP1	2.48	0.47
24:B:1202:3AT:H2'1	24:B:1202:3AT:N3	2.27	0.47
1:A:741:GLY:HA3	9:I:53:LEU:HD22	1.97	0.47
2:B:461:LYS:HG3	2:B:469:ARG:NH2	2.30	0.47
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.48	0.47
19:X:10:DC:H5'	19:X:10:DC:H6	1.80	0.47
21:Z:2:U:C6	26:Z:101:GTP:C4	3.03	0.47
1:A:225:ASN:HD21	15:O:434:MET:HB2	1.80	0.46
1:A:739:GLN:HG3	1:A:747:THR:HG23	1.96	0.46
1:A:811:ASP:OD1	1:A:811:ASP:N	2.46	0.46
2:B:674:TYR:HB3	2:B:677:HIS:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:PRO:O	16:P:121:THR:CG2	2.63	0.46
5:E:89:VAL:O	5:E:92:GLN:HG3	2.15	0.46
15:O:92:ILE:HG21	17:Q:60:LEU:HD11	1.97	0.46
15:O:110:LEU:HD12	15:O:236:GLN:HA	1.98	0.46
15:O:404:MET:HB3	15:O:426:VAL:HG22	1.98	0.46
1:A:123:LYS:HD2	15:O:68:HIS:CD2	2.51	0.46
1:A:754:LYS:NZ	1:A:755:GLU:OE2	2.34	0.46
2:B:251:ILE:O	2:B:255:ILE:HG12	2.15	0.46
4:D:79:THR:HG23	4:D:82:GLU:H	1.80	0.46
5:E:193:ILE:HB	5:E:205:THR:HG23	1.97	0.46
19:X:17:DA:C5	19:X:18:DC:C4	3.04	0.46
20:Y:-18:DG:H2"	20:Y:-17:DT:H73	1.93	0.46
1:A:262:ILE:HD11	2:B:1115:GLN:HB3	1.96	0.46
2:B:160:GLU:O	10:J:62:TYR:OH	2.27	0.46
7:G:148:ILE:HG23	7:G:190:ILE:HG23	1.97	0.46
12:L:17:TYR:HE1	12:L:46:LYS:HZ3	1.62	0.46
2:B:819:GLU:HG3	12:L:49:THR:HG21	1.97	0.46
13:M:117:ALA:HB3	14:N:267:LEU:HB2	1.98	0.46
13:M:171:LYS:NZ	16:P:67:ARG:CD	2.58	0.46
1:A:529:LEU:HD12	1:A:668:LEU:HD13	1.96	0.46
1:A:918:PRO:HB2	1:A:919:LEU:HD12	1.98	0.46
2:B:294:GLN:OE1	2:B:294:GLN:N	2.44	0.46
3:C:238:ASP:OD1	3:C:238:ASP:N	2.49	0.46
13:M:104:SER:HB2	13:M:133:LEU:HB3	1.98	0.46
13:M:238:LEU:HD13	14:N:341:LEU:HG	1.98	0.46
16:P:284:ARG:HB3	17:Q:48:LEU:CD1	2.36	0.46
20:Y:-24:DG:H2"	20:Y:-23:DT:C6	2.51	0.46
1:A:197:PHE:HE2	15:O:423:LEU:HD22	1.80	0.46
7:G:154:ASP:OD1	7:G:154:ASP:N	2.49	0.46
20:Y:-1:DA:N6	21:Z:3:G:C6	2.84	0.46
1:A:1355:ILE:HD11	2:B:1056:ILE:HG23	1.97	0.46
2:B:1028:ARG:NH1	2:B:1072:SER:O	2.49	0.46
15:O:449:ARG:HD3	16:P:304:PRO:O	2.15	0.46
1:A:1092:ASP:HB2	1:A:1222:LYS:HB2	1.97	0.45
2:B:333:ILE:HG21	2:B:523:VAL:HG21	1.98	0.45
2:B:946:LEU:HD22	2:B:1003:TYR:CZ	2.51	0.45
4:D:94:ALA:O	4:D:98:GLN:HG2	2.16	0.45
7:G:89:ILE:HG21	7:G:127:TRP:HE1	1.80	0.45
15:O:17:PHE:O	17:Q:74:PHE:HA	2.16	0.45
16:P:122:GLU:OE1	16:P:122:GLU:N	2.47	0.45
16:P:232:MET:SD	16:P:262:SER:OG	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-5:DG:C2	21:Z:7:G:C4	3.04	0.45
1:A:339:ARG:CZ	1:A:344:ARG:HG2	2.46	0.45
1:A:864:LYS:NZ	1:A:1048:MET:O	2.45	0.45
2:B:294:GLN:HB2	2:B:297:TRP:CD1	2.51	0.45
7:G:105:ASP:OD1	7:G:105:ASP:N	2.50	0.45
16:P:289:LEU:CD1	17:Q:45:PRO:HA	2.46	0.45
19:X:-7:DA:N6	20:Y:6:DT:O4	2.50	0.45
2:B:538:LEU:HD23	2:B:548:VAL:HG12	1.99	0.45
4:D:33:ASN:OD1	4:D:34:LYS:N	2.49	0.45
4:D:42:LEU:HD11	7:G:31:ASN:HB3	1.98	0.45
14:N:255:LEU:O	14:N:259:SER:OG	2.27	0.45
15:O:88:TYR:O	15:O:92:ILE:HG12	2.16	0.45
16:P:289:LEU:HD12	17:Q:45:PRO:HA	1.98	0.45
1:A:159:CYS:CA	15:O:531:MET:SD	3.05	0.45
1:A:233:GLU:HA	15:O:30:ARG:O	2.17	0.45
1:A:997:PRO:HB2	1:A:1000:LEU:HG	1.98	0.45
1:A:1054:HIS:CD2	1:A:1065:LEU:HD12	2.52	0.45
2:B:393:PRO:O	16:P:121:THR:HG21	2.17	0.45
20:Y:6:DT:C5	20:Y:7:DT:C4	3.05	0.45
21:Z:4:C:H2'	21:Z:5:U:H6	1.81	0.45
1:A:258:PRO:HB2	1:A:262:ILE:HD12	1.98	0.45
1:A:459:VAL:HG21	1:A:520:LEU:HB2	1.98	0.45
1:A:1374:LYS:HE3	7:G:52:THR:HG22	1.98	0.45
2:B:692:GLN:HE22	21:Z:7:G:P	2.38	0.45
2:B:817:PRO:HG3	2:B:869:VAL:HG23	1.98	0.45
4:D:80:LYS:HD2	4:D:83:LYS:HD2	1.99	0.45
16:P:284:ARG:CB	17:Q:48:LEU:HD13	2.35	0.45
19:X:29:DA:C2'	19:X:30:DT:C7	2.94	0.45
1:A:1149:VAL:O	1:A:1153:ILE:HG13	2.17	0.45
2:B:1118:GLN:HA	2:B:1123:ILE:HD13	1.99	0.45
9:I:5:CYS:HB2	9:I:12:LEU:HD21	1.98	0.45
15:O:159:ARG:NH1	15:O:186:ASP:OD2	2.49	0.45
15:O:490:MET:SD	15:O:491:ILE:N	2.81	0.45
1:A:546:LEU:HD12	1:A:785:SER:HA	1.99	0.45
2:B:114:THR:HA	2:B:132:PRO:HA	1.99	0.45
1:A:1186:TYR:C	1:A:1188:VAL:H	2.20	0.45
3:C:287:ILE:HD11	3:C:293:LEU:HB3	1.99	0.45
7:G:101:LEU:HB3	7:G:104:PHE:HB3	1.98	0.45
13:M:6:ASP:OD1	13:M:6:ASP:N	2.50	0.45
19:X:15:DG:H4'	19:X:16:DC:OP1	2.17	0.45
1:A:130:LYS:HE2	15:O:34:GLN:HE21	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:CD1	15:O:534:GLN:NE2	2.74	0.44
1:A:1007:THR:HG23	1:A:1010:GLN:H	1.81	0.44
2:B:817:PRO:HA	2:B:866:ILE:HB	1.99	0.44
4:D:95:VAL:HG11	7:G:198:LEU:HD22	1.98	0.44
9:I:29:PRO:HA	13:M:73:LYS:HD3	1.99	0.44
15:O:303:ILE:HG13	15:O:307:VAL:HB	1.99	0.44
1:A:325:LEU:HB2	1:A:328:ILE:HD11	2.00	0.44
1:A:389:ILE:HG12	18:V:21:TYR:CD2	2.53	0.44
2:B:287:ILE:O	2:B:291:VAL:HG23	2.18	0.44
10:J:18:TRP:O	10:J:21:TYR:HB3	2.17	0.44
17:Q:42:ASP:OD1	17:Q:42:ASP:N	2.50	0.44
1:A:289:LEU:HD11	1:A:316:GLN:HG3	2.00	0.44
1:A:623:GLN:HG2	1:A:636:SER:HB2	1.98	0.44
2:B:741:VAL:HG21	2:B:1009:TYR:CE1	2.53	0.44
3:C:79:ILE:HD13	3:C:83:GLU:HG3	1.98	0.44
3:C:155:ASP:N	3:C:155:ASP:OD1	2.46	0.44
3:C:166:HIS:CD2	3:C:167:LYS:HG3	2.51	0.44
13:M:56:VAL:N	13:M:104:SER:OG	2.50	0.44
6:F:81:VAL:HG11	6:F:96:GLU:HA	2.00	0.44
16:P:276:ILE:HG22	16:P:277:ILE:HG23	2.00	0.44
16:P:292:VAL:HG22	16:P:295:ASP:HB2	1.99	0.44
19:X:5:DC:H2"	19:X:6:DG:H5"	1.99	0.44
20:Y:-18:DG:C4	20:Y:-17:DT:C4	3.05	0.44
2:B:770:LEU:HD21	3:C:105:ILE:HD11	1.99	0.44
7:G:115:GLN:O	7:G:119:LYS:NZ	2.35	0.44
16:P:284:ARG:CZ	17:Q:49:LYS:HG3	2.47	0.44
1:A:197:PHE:HE2	15:O:423:LEU:CD2	2.31	0.44
1:A:415:HIS:CE1	1:A:480:VAL:HG11	2.53	0.44
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.99	0.44
16:P:57:LEU:HD23	16:P:60:MET:HE1	2.00	0.44
19:X:3:DC:H4'	19:X:4:DT:OP1	2.16	0.44
1:A:344:ARG:HH22	2:B:1031:LEU:HD11	1.83	0.44
1:A:464:ARG:HH22	24:B:1202:3AT:H1'	1.81	0.44
1:A:1214:ILE:CG2	9:I:52:VAL:CG2	2.96	0.44
4:D:24:LYS:HG3	4:D:27:ARG:HH21	1.82	0.44
13:M:418:ARG:O	13:M:421:MET:HG2	2.17	0.44
19:X:-17:DG:H2"	19:X:-16:DG:N7	2.33	0.44
1:A:384:VAL:HG13	1:A:415:HIS:CD2	2.53	0.44
2:B:113:ILE:H	2:B:113:ILE:HG13	1.57	0.44
3:C:49:PHE:HE1	3:C:68:ILE:HB	1.82	0.44
4:D:22:ASP:O	4:D:25:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:THR:O	4:D:48:GLU:HG2	2.18	0.44
4:D:94:ALA:HB2	4:D:117:LEU:HD11	2.00	0.44
15:O:80:SER:O	15:O:84:ARG:HG2	2.18	0.44
15:O:285:THR:OG1	15:O:286:GLN:N	2.50	0.44
20:Y:-16:DG:H2"	20:Y:-15:DC:C6	2.52	0.44
3:C:288:PHE:HA	3:C:294:LYS:HG2	1.99	0.44
4:D:99:LEU:HD22	7:G:195:LEU:HA	2.00	0.44
15:O:442:SER:OG	16:P:287:CYS:HB2	2.18	0.44
21:Z:5:U:H2'	21:Z:6:C:H5"	1.99	0.44
1:A:196:SER:HA	15:O:373:LYS:HG3	1.99	0.43
2:B:40:VAL:HG13	2:B:452:MET:HG2	1.99	0.43
11:K:56:ARG:HG2	11:K:68:CYS:SG	2.57	0.43
1:A:104:ILE:HD11	1:A:1333:TYR:HE1	1.83	0.43
2:B:233:ASP:N	2:B:233:ASP:OD1	2.52	0.43
2:B:751:ILE:HG22	2:B:752:GLU:HG3	2.00	0.43
5:E:35:GLN:NE2	5:E:39:GLU:OE1	2.51	0.43
7:G:93:SER:OG	7:G:96:GLY:O	2.24	0.43
20:Y:-2:DC:H2"	20:Y:-1:DA:H8	1.83	0.43
1:A:676:ALA:O	1:A:680:MET:HG3	2.18	0.43
1:A:876:VAL:HG11	2:B:1053:ASP:CG	2.38	0.43
2:B:1093:HIS:O	2:B:1096:LYS:NZ	2.46	0.43
16:P:127:LEU:HD13	16:P:150:TYR:CZ	2.53	0.43
1:A:360:ARG:CZ	2:B:1037:GLU:HA	2.48	0.43
1:A:1235:VAL:O	1:A:1238:THR:OG1	2.35	0.43
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.52	0.43
19:X:-14:DA:H2"	19:X:-13:DA:C8	2.53	0.43
1:A:303:THR:HG1	15:O:377:GLN:NE2	2.05	0.43
1:A:870:TYR:CZ	1:A:874:ARG:HD3	2.53	0.43
2:B:106:ASP:HA	2:B:173:GLY:HA3	2.00	0.43
2:B:122:GLY:O	2:B:123:SER:OG	2.32	0.43
3:C:109:ARG:NH1	10:J:3:ILE:O	2.44	0.43
3:C:144:VAL:HG11	3:C:168:VAL:HG22	2.00	0.43
13:M:238:LEU:HD23	14:N:277:GLY:HA3	2.00	0.43
15:O:16:HIS:CG	17:Q:68:MET:HE1	2.53	0.43
25:P:401:SF4:S3	17:Q:38:PHE:CE2	3.06	0.43
1:A:756:LEU:HD21	1:A:828:PRO:HB3	1.99	0.43
2:B:118:GLU:HB3	2:B:127:ILE:HG22	2.01	0.43
2:B:903:GLN:HG3	2:B:942:LYS:HE3	1.99	0.43
2:B:1091:TRP:CG	7:G:162:PRO:HG3	2.54	0.43
4:D:6:ALA:HA	7:G:5:VAL:HG22	2.00	0.43
13:M:431:GLU:HG2	13:M:436:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:15:LEU:HD22	18:V:35:VAL:HG21	2.01	0.43
20:Y:-15:DC:H2”	20:Y:-14:DT:H71	2.00	0.43
1:A:579:ILE:HB	1:A:608:SER:HB3	1.99	0.43
4:D:53:ILE:O	4:D:56:THR:OG1	2.28	0.43
1:A:366:ARG:HD2	2:B:1045:LEU:HD11	2.00	0.43
1:A:1247:THR:HG22	5:E:144:LEU:HD11	2.01	0.43
2:B:341:ARG:NH2	2:B:584:TYR:OH	2.51	0.43
2:B:1021:HIS:NE2	2:B:1043:GLY:O	2.36	0.43
15:O:416:ALA:HB3	15:O:419:ARG:HG2	2.01	0.43
3:C:133:THR:O	3:C:137:THR:HG22	2.19	0.43
5:E:27:LEU:HB2	5:E:64:HIS:HB3	2.01	0.43
13:M:88:GLU:HG2	13:M:89:THR:N	2.34	0.43
19:X:-5:DA:H2”	19:X:-4:DC:C6	2.53	0.43
19:X:20:DT:H1’	19:X:21:DA:C8	2.54	0.43
1:A:74:LYS:HB3	1:A:78:ASP:HB2	2.00	0.43
1:A:352:PHE:HA	1:A:356:LEU:HB2	2.01	0.43
1:A:980:ILE:HG12	1:A:1004:ASP:HB3	2.01	0.43
6:F:84:GLU:N	6:F:86:GLU:OE1	2.51	0.43
19:X:17:DA:C6	20:Y:-16:DG:C2	3.06	0.43
19:X:21:DA:C2’	19:X:22:DT:H71	2.49	0.43
1:A:63:SER:HB3	1:A:260:LEU:HB3	2.01	0.42
7:G:39:VAL:HB	7:G:42:VAL:HB	1.99	0.42
13:M:10:VAL:HG23	13:M:11:GLN:HG2	2.01	0.42
14:N:253:GLU:O	14:N:256:ARG:HG3	2.18	0.42
15:O:271:LEU:O	15:O:275:GLU:HG3	2.19	0.42
15:O:510:ASP:CG	17:Q:65:ARG:HH12	2.22	0.42
4:D:108:LEU:HD22	4:D:113:ILE:HD11	2.00	0.42
15:O:193:LEU:HD21	15:O:230:ASP:HB3	2.00	0.42
15:O:457:ASN:HD22	15:O:502:LEU:HD13	1.84	0.42
16:P:99:ILE:HD13	16:P:136:ILE:HG21	2.00	0.42
19:X:-13:DA:H2”	19:X:-12:DG:H8	1.83	0.42
1:A:94:HIS:CE1	1:A:321:ILE:HD13	2.55	0.42
2:B:257:THR:HG21	2:B:529:GLU:HG3	2.01	0.42
2:B:986:LYS:HB3	2:B:1001:TYR:HB2	2.01	0.42
16:P:151:MET:HE1	16:P:157:PRO:HA	2.01	0.42
16:P:181:ASN:HB3	16:P:242:LEU:HD21	2.00	0.42
16:P:309:TYR:HE2	17:Q:38:PHE:HD2	1.67	0.42
19:X:-15:DA:N6	19:X:-14:DA:N6	2.67	0.42
20:Y:-2:DC:H2”	20:Y:-1:DA:C8	2.54	0.42
1:A:1153:ILE:HG22	1:A:1154:CYS:H	1.84	0.42
2:B:812:ASP:OD2	12:L:46:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:27:ARG:HD2	8:H:40:ILE:HG22	2.01	0.42
15:O:110:LEU:HD13	15:O:110:LEU:HA	1.92	0.42
16:P:151:MET:HB3	16:P:151:MET:HE3	1.85	0.42
1:A:282:LYS:HZ1	1:A:319:LEU:HB2	1.85	0.42
1:A:356:LEU:HD11	2:B:1113:LEU:HD22	2.00	0.42
1:A:863:VAL:HA	2:B:464:LYS:HG2	2.01	0.42
2:B:746:TYR:HE2	2:B:911:VAL:HG11	1.83	0.42
5:E:53:PRO:HD3	5:E:78:GLU:HB2	2.01	0.42
15:O:16:HIS:CG	17:Q:68:MET:CE	3.03	0.42
1:A:28:MET:HB3	1:A:256:LEU:HD21	2.01	0.42
1:A:60:MET:HA	1:A:82:HIS:HB2	2.02	0.42
1:A:518:GLU:HA	6:F:63:ALA:HB1	2.00	0.42
1:A:1028:GLU:OE1	6:F:59:LYS:NZ	2.47	0.42
2:B:254:MET:HB3	2:B:254:MET:HE2	1.90	0.42
2:B:613:GLU:HB3	2:B:618:TYR:HB2	2.01	0.42
19:X:1:DT:H2”	19:X:2:DG:H4’	2.02	0.42
1:A:533:ARG:NH1	1:A:1043:GLU:OE1	2.53	0.42
2:B:464:LYS:NZ	20:Y:-8:DT:H72	2.35	0.42
2:B:577:ASN:O	2:B:581:ARG:N	2.52	0.42
3:C:57:ASP:N	3:C:57:ASP:OD1	2.52	0.42
3:C:86:THR:HA	3:C:119:PRO:HB3	2.01	0.42
4:D:57:PRO:HB2	4:D:90:ARG:HE	1.84	0.42
20:Y:-28:DT:H2”	20:Y:-27:DT:C7	2.49	0.42
20:Y:13:DT:H2”	20:Y:14:DT:C6	2.55	0.42
1:A:907:LEU:HD13	1:A:918:PRO:HB3	2.01	0.42
3:C:334:ARG:NH2	11:K:104:MET:SD	2.93	0.42
4:D:70:LEU:HG	4:D:74:LYS:HE3	2.02	0.42
13:M:276:LEU:O	13:M:281:GLN:NE2	2.52	0.42
13:M:278:LEU:HD11	13:M:301:LEU:HD13	2.01	0.42
15:O:519:THR:OG1	16:P:280:THR:HB	2.20	0.42
16:P:110:ARG:HE	16:P:147:LYS:HZ2	1.66	0.42
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.53	0.42
19:X:17:DA:C8	19:X:18:DC:C5	3.08	0.42
1:A:208:GLU:HB3	1:A:209:PRO:HD3	2.02	0.42
1:A:464:ARG:HH22	24:B:1202:3AT:C1’	2.33	0.42
13:M:171:LYS:CG	16:P:67:ARG:HD3	2.36	0.42
17:Q:64:LEU:HA	17:Q:67:THR:HG22	2.01	0.42
2:B:613:GLU:HG2	2:B:618:TYR:HD2	1.85	0.42
2:B:900:ARG:NH2	2:B:945:GLU:OE2	2.37	0.42
3:C:133:THR:OG1	3:C:136:ASP:OD1	2.28	0.42
15:O:429:LEU:HD21	15:O:433:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-1:DA:C6	21:Z:3:G:N2	2.88	0.42
1:A:196:SER:C	15:O:373:LYS:HB2	2.38	0.41
2:B:324:LYS:HD2	2:B:325:GLU:HG3	2.02	0.41
19:X:-2:DC:H4'	19:X:-1:DC:OP2	2.19	0.41
1:A:533:ARG:HH11	1:A:1044:PRO:HG3	1.85	0.41
1:A:902:TYR:CZ	1:A:1285:ARG:HB3	2.55	0.41
1:A:1368:ARG:NH1	7:G:55:GLU:O	2.53	0.41
2:B:36:VAL:HG23	2:B:37:LYS:HG3	2.01	0.41
1:A:1117:ILE:HG23	1:A:1130:VAL:HG22	2.02	0.41
2:B:633:LEU:HD11	2:B:656:HIS:CD2	2.55	0.41
12:L:19:CYS:SG	12:L:20:GLY:N	2.94	0.41
13:M:82:ASP:O	13:M:152:ARG:NH2	2.53	0.41
13:M:134:GLN:OE1	13:M:136:ARG:NH2	2.52	0.41
13:M:161:SER:OG	13:M:164:ASP:OD1	2.38	0.41
13:M:360:PHE:CZ	13:M:390:ALA:HB2	2.56	0.41
13:M:414:ASP:N	13:M:414:ASP:OD1	2.54	0.41
16:P:161:VAL:HG23	16:P:162:THR:HG22	2.03	0.41
19:X:17:DA:N1	20:Y:-16:DG:N1	2.66	0.41
19:X:23:DA:N1	20:Y:-22:DA:N1	2.68	0.41
1:A:366:ARG:CD	20:Y:-5:DG:H4'	2.50	0.41
2:B:889:ARG:NH1	2:B:1015:MET:SD	2.85	0.41
20:Y:9:DG:H2"	20:Y:10:DT:C6	2.54	0.41
15:O:45:THR:OG1	15:O:49:GLN:OE1	2.37	0.41
16:P:248:VAL:HG12	16:P:272:ALA:HA	2.03	0.41
19:X:11:DG:H2"	19:X:12:DG:H5'	2.02	0.41
1:A:570:SER:HB2	1:A:689:VAL:HG21	2.03	0.41
2:B:763:ASP:HB3	3:C:222:HIS:CE1	2.55	0.41
21:Z:8:C:H3'	21:Z:8:C:H6	1.86	0.41
1:A:731:LEU:HD23	1:A:748:LEU:HD22	2.01	0.41
1:A:792:ILE:HG23	1:A:796:ILE:HD12	2.02	0.41
1:A:875:LEU:HD23	1:A:1303:ILE:HG21	2.02	0.41
5:E:146:PRO:HD2	5:E:148:HIS:HE1	1.86	0.41
19:X:28:DA:H2"	19:X:29:DA:N7	2.36	0.41
20:Y:-5:DG:N1	21:Z:7:G:C6	2.89	0.41
20:Y:-4:DA:H2'	20:Y:-3:DG:H8	1.84	0.41
20:Y:14:DT:H2"	20:Y:15:DT:C5	2.55	0.41
21:Z:2:U:O2	21:Z:2:U:C2'	2.69	0.41
21:Z:6:C:C2'	21:Z:7:G:H5'	2.51	0.41
1:A:485:THR:H	1:A:487:ARG:HH12	1.68	0.41
1:A:1295:THR:HG22	1:A:1300:VAL:HG22	2.02	0.41
2:B:446:ILE:HG13	2:B:671:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:290:ASN:O	3:C:294:LYS:HG3	2.21	0.41
10:J:49:LEU:HD23	10:J:49:LEU:HA	1.87	0.41
1:A:230:ILE:C	15:O:2:THR:N	2.74	0.41
1:A:1363:LEU:HD11	6:F:107:ARG:HH11	1.85	0.41
2:B:79:ASN:N	2:B:116:ASP:OD1	2.53	0.41
2:B:386:LYS:HE3	2:B:386:LYS:HB3	1.91	0.41
2:B:633:LEU:HD11	2:B:656:HIS:CG	2.56	0.41
2:B:1014:HIS:CE1	21:Z:7:G:O4'	2.73	0.41
7:G:151:ARG:HB2	7:G:189:SER:OG	2.21	0.41
8:H:17:PRO:HG2	8:H:29:HIS:CE1	2.56	0.41
14:N:346:LEU:HD22	14:N:387:PRO:HA	2.02	0.41
15:O:268:ARG:HD3	15:O:272:ARG:HH22	1.84	0.41
15:O:439:CYS:SG	16:P:282:LEU:HD13	2.61	0.41
20:Y:-25:DA:C2	20:Y:-24:DG:C2	3.09	0.41
1:A:1193:LYS:HE3	1:A:1193:LYS:HB3	1.91	0.41
2:B:39:LEU:HD21	2:B:498:LEU:HD12	2.03	0.41
2:B:635:VAL:HA	2:B:638:GLU:HG2	2.03	0.41
18:V:35:VAL:HG12	18:V:36:THR:HG23	2.03	0.41
20:Y:13:DT:H2"	20:Y:14:DT:C5	2.56	0.41
3:C:29:PHE:HB2	3:C:32:ASN:ND2	2.35	0.40
5:E:18:MET:SD	5:E:32:GLU:HB3	2.61	0.40
19:X:4:DT:H1'	19:X:5:DC:H5"	2.04	0.40
1:A:169:CYS:O	1:A:173:LYS:HB2	2.21	0.40
1:A:814:GLU:HB2	2:B:639:ASN:HD21	1.86	0.40
1:A:1360:PHE:CE1	6:F:64:ARG:HD3	2.56	0.40
2:B:331:LYS:HE3	2:B:331:LYS:HB2	1.89	0.40
2:B:946:LEU:HD22	2:B:1003:TYR:CE2	2.56	0.40
9:I:53:LEU:H	9:I:53:LEU:HG	1.61	0.40
13:M:92:TYR:CZ	13:M:97:MET:HG3	2.57	0.40
14:N:149:GLU:OE2	14:N:355:SER:OG	2.35	0.40
1:A:1214:ILE:CG2	9:I:52:VAL:HG23	2.51	0.40
2:B:1023:ARG:NH1	2:B:1035:PRO:HB3	2.36	0.40
2:B:1082:GLN:HB2	2:B:1100:HIS:ND1	2.36	0.40
3:C:250:ALA:O	3:C:253:LEU:HB2	2.21	0.40
15:O:441:LYS:HD3	16:P:293:PHE:CZ	2.56	0.40
20:Y:-1:DA:C5	21:Z:3:G:N2	2.90	0.40
1:A:155:ILE:CB	15:O:534:GLN:NE2	2.83	0.40
2:B:104:LEU:HB3	2:B:870:MET:SD	2.61	0.40
2:B:954:LEU:HD23	2:B:954:LEU:HA	1.94	0.40
5:E:50:GLU:OE2	5:E:56:THR:OG1	2.39	0.40
5:E:50:GLU:HG2	5:E:55:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:PHE:HB3	8:H:30:CYS:HB3	2.03	0.40
15:O:19:GLU:O	15:O:22:GLU:HG3	2.21	0.40
15:O:364:ARG:HA	16:P:244:TYR:O	2.22	0.40
19:X:26:DA:H2"	19:X:27:DA:C8	2.56	0.40
1:A:551:LEU:HD21	1:A:779:THR:HG21	2.04	0.40
4:D:107:ARG:NH2	17:Q:87:TYR:HB2	2.36	0.40
11:K:58:MET:HG3	11:K:103:LEU:HB2	2.03	0.40
13:M:7:ASP:OD1	13:M:7:ASP:N	2.55	0.40
13:M:8:PRO:HG3	14:N:330:LEU:HD23	2.03	0.40
13:M:245:TYR:CD2	14:N:276:PRO:HB3	2.57	0.40
13:M:329:SER:HB3	13:M:350:CYS:HA	2.02	0.40
16:P:98:ILE:HA	16:P:101:ASP:HB2	2.03	0.40
21:Z:4:C:H2'	21:Z:5:U:C6	2.57	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	A	1376/1390 (99%)	1345 (98%)	31 (2%)	0	100	100
2	B	1101/1133 (97%)	1066 (97%)	35 (3%)	0	100	100
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
4	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
7	G	160/204 (78%)	146 (91%)	14 (9%)	0	100	100
8	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
9	I	52/108 (48%)	49 (94%)	3 (6%)	0	100	100
10	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	101/133 (76%)	98 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
13	M	418/708 (59%)	401 (96%)	17 (4%)	0	100	100
14	N	140/398 (35%)	139 (99%)	1 (1%)	0	100	100
15	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
16	P	301/316 (95%)	293 (97%)	8 (3%)	0	100	100
17	Q	85/223 (38%)	84 (99%)	1 (1%)	0	100	100
18	V	32/419 (8%)	31 (97%)	1 (3%)	0	100	100
All	All	5269/6672 (79%)	5124 (97%)	145 (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	A	1200/1212 (99%)	1194 (100%)	6 (0%)	86	95
2	B	963/988 (98%)	952 (99%)	11 (1%)	70	90
3	C	299/302 (99%)	297 (99%)	2 (1%)	81	94
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	190 (100%)	1 (0%)	86	95
6	F	66/111 (60%)	66 (100%)	0	100	100
7	G	149/181 (82%)	146 (98%)	3 (2%)	50	81
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	47/93 (50%)	42 (89%)	5 (11%)	5	18
10	J	53/56 (95%)	52 (98%)	1 (2%)	52	82
11	K	92/119 (77%)	92 (100%)	0	100	100
12	L	43/55 (78%)	42 (98%)	1 (2%)	45	78
13	M	377/622 (61%)	376 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	131/347 (38%)	129 (98%)	2 (2%)	60	86
15	O	458/476 (96%)	456 (100%)	2 (0%)	89	96
16	P	269/280 (96%)	267 (99%)	2 (1%)	81	94
17	Q	84/195 (43%)	82 (98%)	2 (2%)	44	77
18	V	31/365 (8%)	31 (100%)	0	100	100
All	All	4696/5861 (80%)	4657 (99%)	39 (1%)	77	93

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	VAL
1	A	362	ASP
1	A	431	PHE
1	A	494	THR
1	A	767	CYS
1	A	776	SER
2	B	23	VAL
2	B	113	ILE
2	B	203	VAL
2	B	214	THR
2	B	292	ARG
2	B	297	TRP
2	B	304	THR
2	B	406	MET
2	B	461	LYS
2	B	463	ARG
2	B	1032	THR
3	C	98	THR
3	C	236	LEU
5	E	56	THR
7	G	59	VAL
7	G	128	VAL
7	G	187	VAL
9	I	46	LEU
9	I	47	LYS
9	I	51	ASP
9	I	52	VAL
9	I	53	LEU
10	J	30	THR
12	L	29	LYS

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Mol	Chain	Res	Type
13	M	175	VAL
14	N	156	ARG
14	N	251	VAL
15	O	477	THR
15	O	533	ARG
16	P	93	LYS
16	P	134	LYS
17	Q	77	THR
17	Q	113	ARG

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	119	GLN
1	A	225	ASN
1	A	374	ASN
1	A	415	HIS
1	A	423	GLN
1	A	528	ASN
1	A	599	GLN
1	A	739	GLN
1	A	1039	GLN
1	A	1054	HIS
1	A	1213	HIS
1	A	1364	HIS
2	B	260	HIS
2	B	616	GLN
3	C	160	ASN
4	D	85	GLN
5	E	108	GLN
5	E	138	ASN
8	H	29	HIS
9	I	10	ASN
9	I	40	ASN
13	M	11	GLN
13	M	197	GLN
15	O	34	GLN
15	O	60	HIS
15	O	158	GLN
15	O	374	HIS
15	O	377	GLN

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Mol	Chain	Res	Type
15	O	402	ASN
15	O	407	GLN
15	O	457	ASN
15	O	475	GLN
15	O	497	GLN
15	O	534	GLN
16	P	182	GLN
16	P	201	ASN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	Z	6/7 (85%)	4 (66%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	Z	3	G
21	Z	6	C
21	Z	7	G
21	Z	8	C

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, 7 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
26	GTP	Z	101	-	26,34,34	0.91	1 (3%)	32,54,54	1.51	5 (15%)
25	SF4	P	401	16	0,12,12	-	-	-		
24	3AT	B	1202	-	25,32,32	1.01	1 (4%)	28,50,50	1.61	5 (17%)

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
26	GTP	Z	101	-	-	4/18/38/38	0/3/3/3
24	3AT	B	1202	-	-	6/18/34/34	0/3/3/3
25	SF4	P	401	16	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1202	3AT	C5-C4	2.51	1.47	1.40
26	Z	101	GTP	C6-N1	-2.30	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	101	GTP	PB-O3B-PG	-3.63	120.39	132.83
24	B	1202	3AT	PA-O3A-PB	-3.60	120.46	132.83
24	B	1202	3AT	PB-O3B-PG	-3.59	120.50	132.83
26	Z	101	GTP	PA-O3A-PB	-3.59	120.52	132.83
26	Z	101	GTP	C3'-C2'-C1'	3.37	106.05	100.98
24	B	1202	3AT	N3-C2-N1	-3.14	123.77	128.68
24	B	1202	3AT	C4-C5-N7	-2.60	106.69	109.40
26	Z	101	GTP	C8-N7-C5	2.33	107.43	102.99
26	Z	101	GTP	C5-C6-N1	2.24	117.91	113.95
24	B	1202	3AT	O4'-C4'-C3'	2.16	107.86	105.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	1202	3AT	C5'-O5'-PA-O3A
24	B	1202	3AT	O4'-C4'-C5'-O5'
24	B	1202	3AT	C3'-C4'-C5'-O5'
24	B	1202	3AT	C5'-O5'-PA-O2A
26	Z	101	GTP	C5'-O5'-PA-O2A
26	Z	101	GTP	C3'-C4'-C5'-O5'
26	Z	101	GTP	O4'-C4'-C5'-O5'
24	B	1202	3AT	PG-O3B-PB-O2B
26	Z	101	GTP	C5'-O5'-PA-O3A
24	B	1202	3AT	PG-O3B-PB-O1B

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Z	101	GTP	11	0
25	P	401	SF4	3	0
24	B	1202	3AT	13	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 then 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.

Ligand GTP Z 101

Bond lengths

Bond angles

Torsions

Rings

Ligand 3AT B 1202

Bond lengths

Bond angles

Torsions

Rings
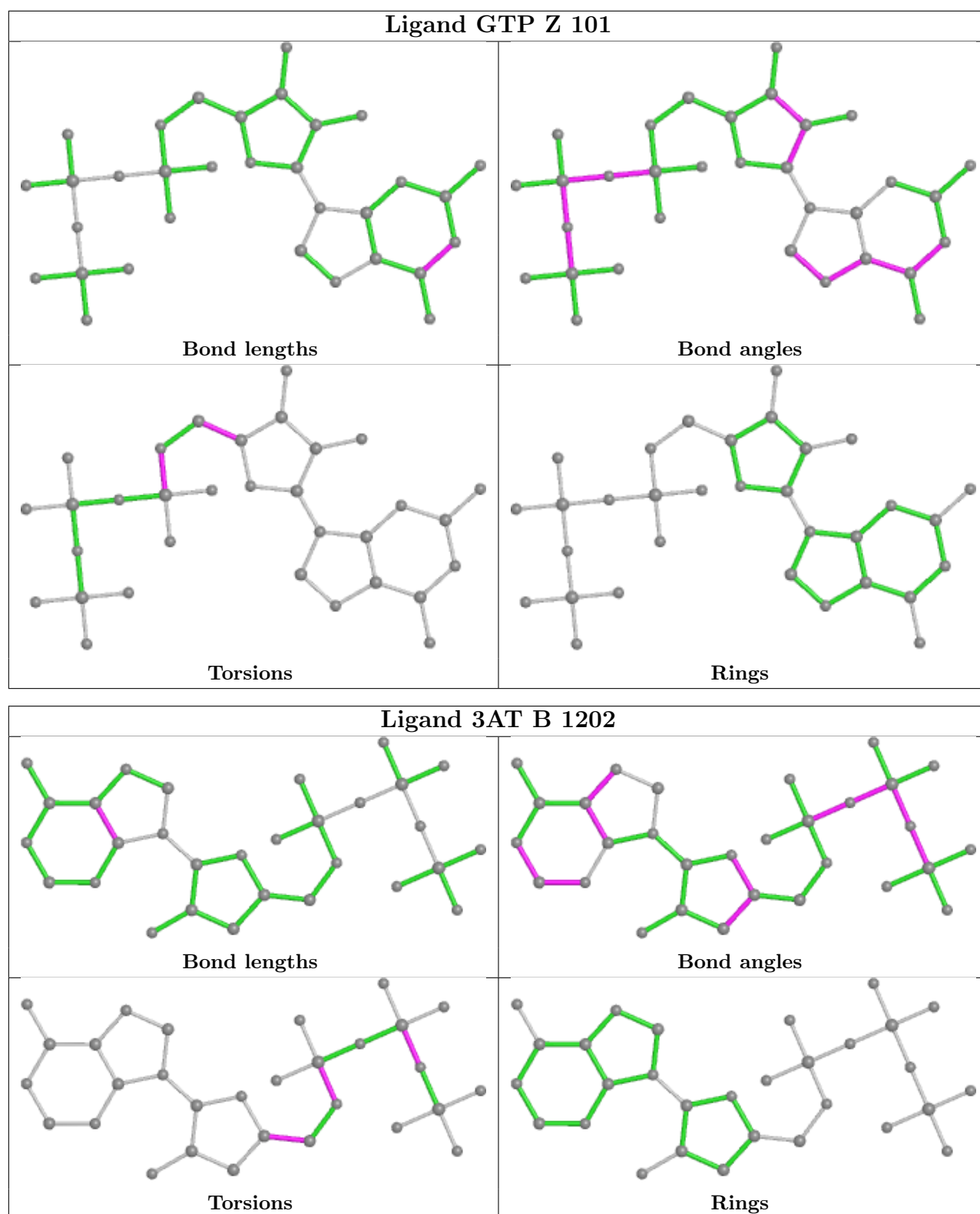
5.7 Other polymers ⓘ

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-62010. 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 ⓘ
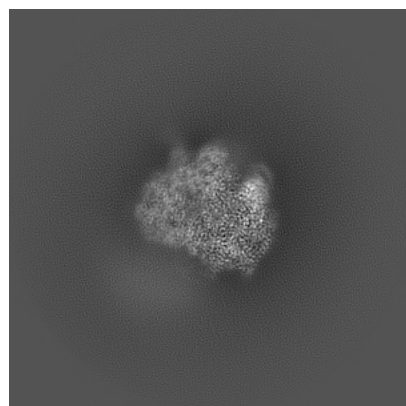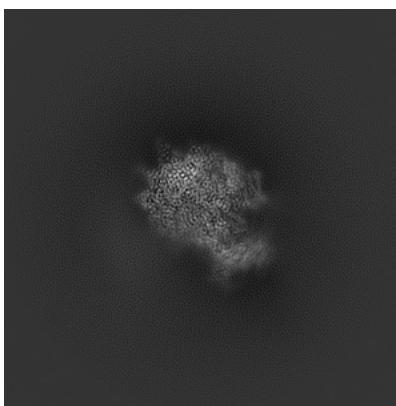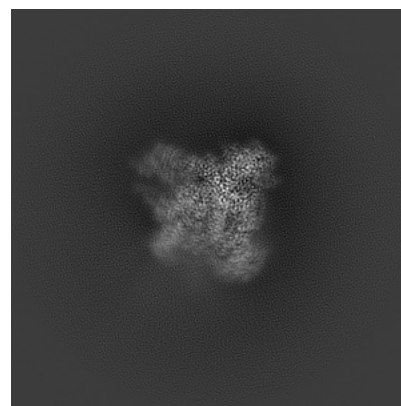
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
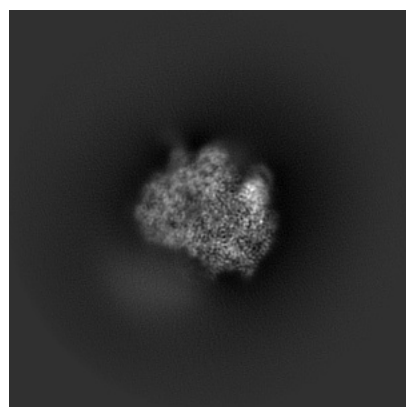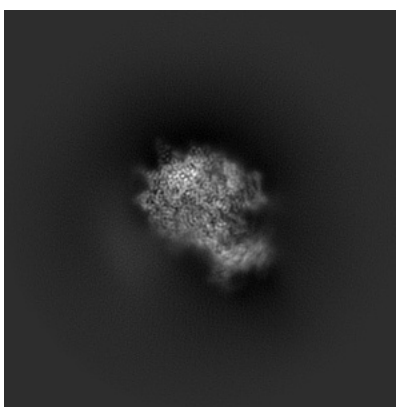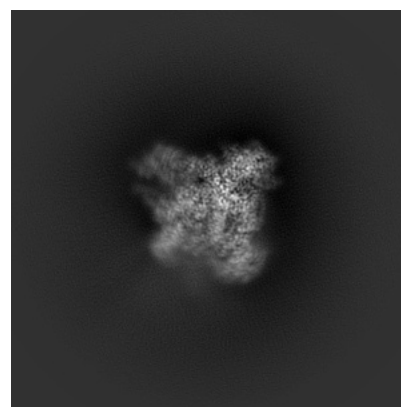
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
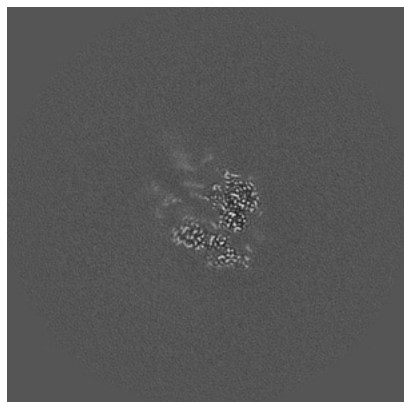
6.2.1 Primary map
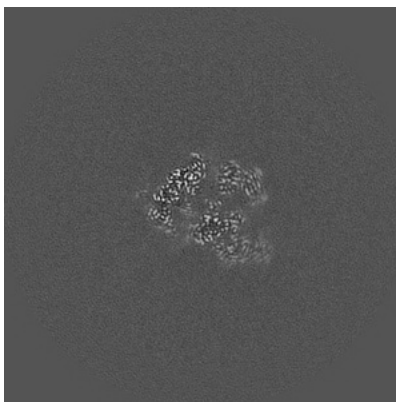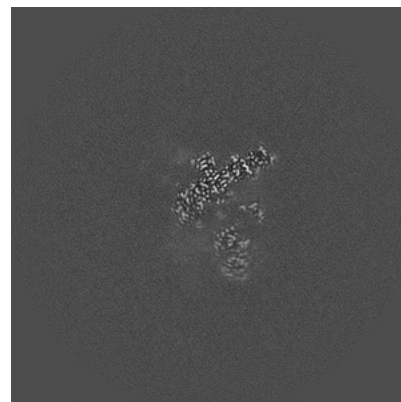
X Index: 161   Y Index: 161   Z Index: 161

6.2.2 Raw map
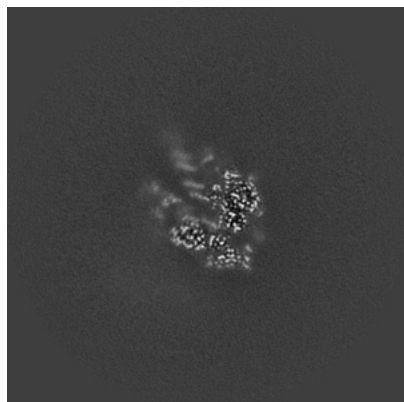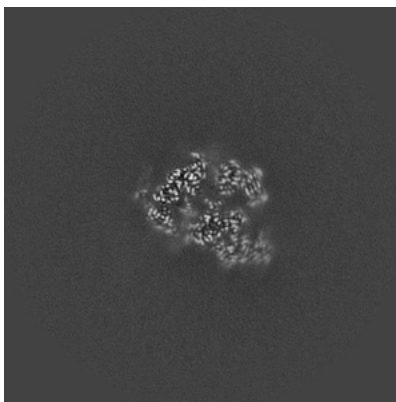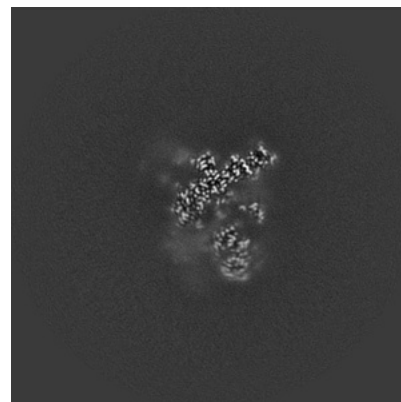
X Index: 161   Y Index: 161   Z Index: 161

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
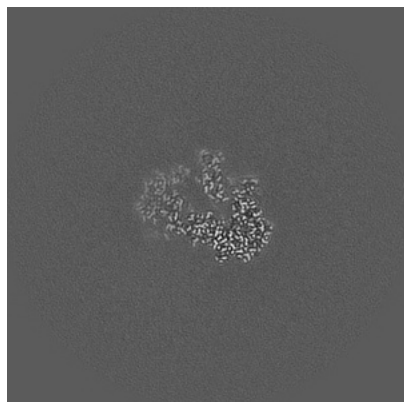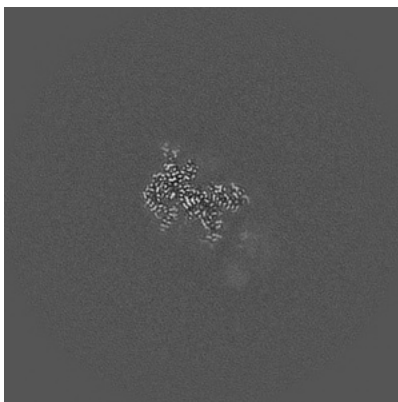
X Index: 180	Y Index: 178	Z Index: 145
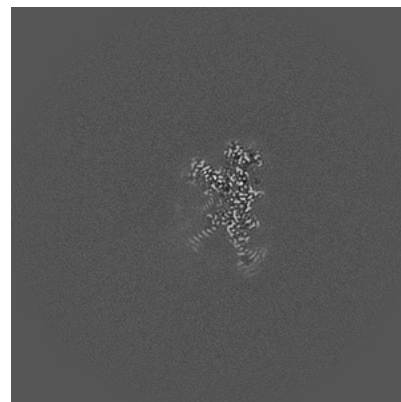
6.3.2 Raw map
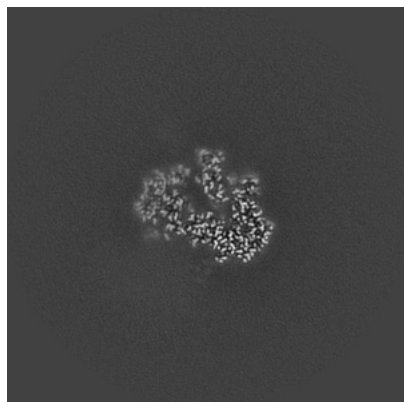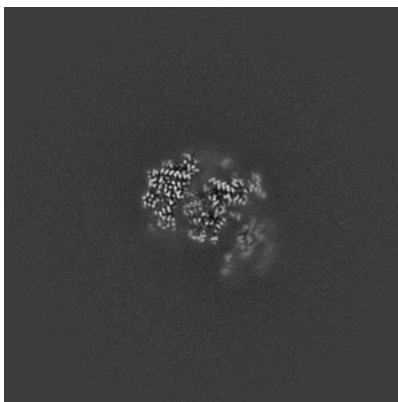
X Index: 180	Y Index: 171	Z Index: 146
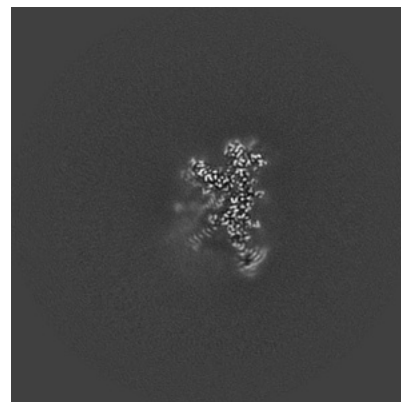
The images above show the largest variance slices of the map in three orthogonal directions.

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

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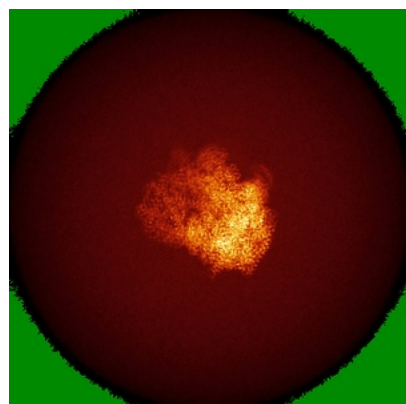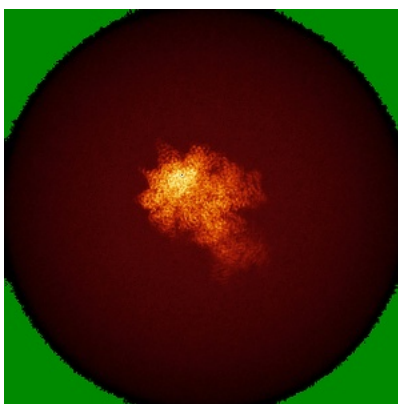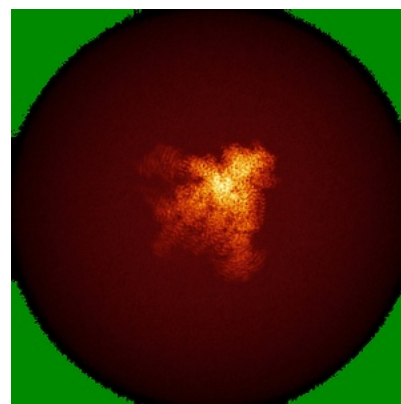
6.4.2 Raw map
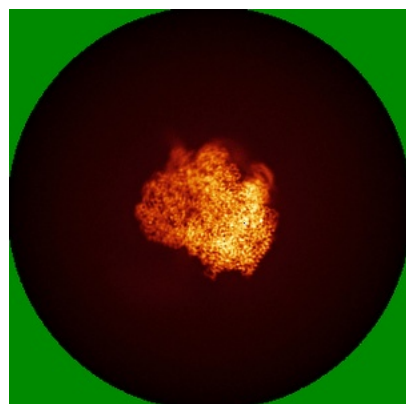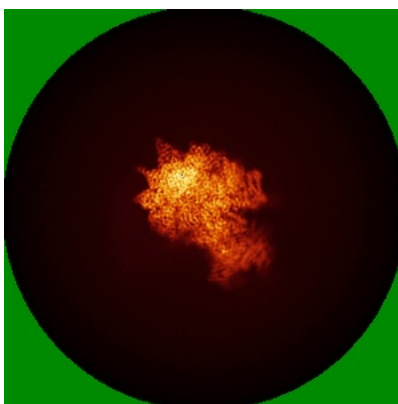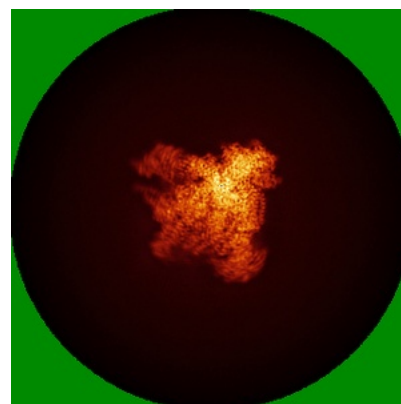
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
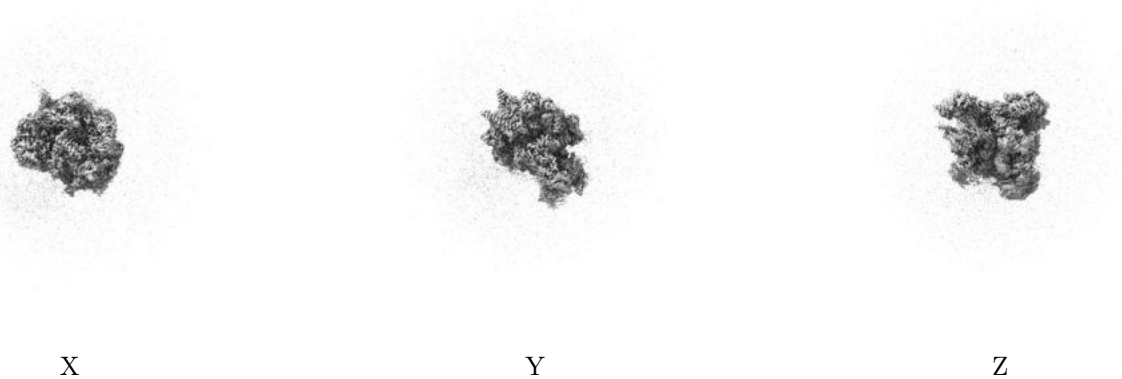
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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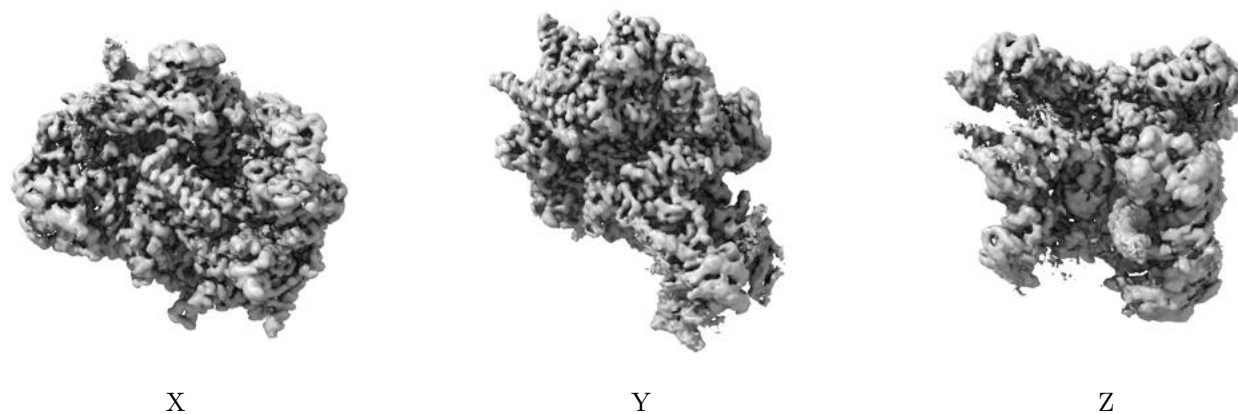
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7   Map analysis (i)

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

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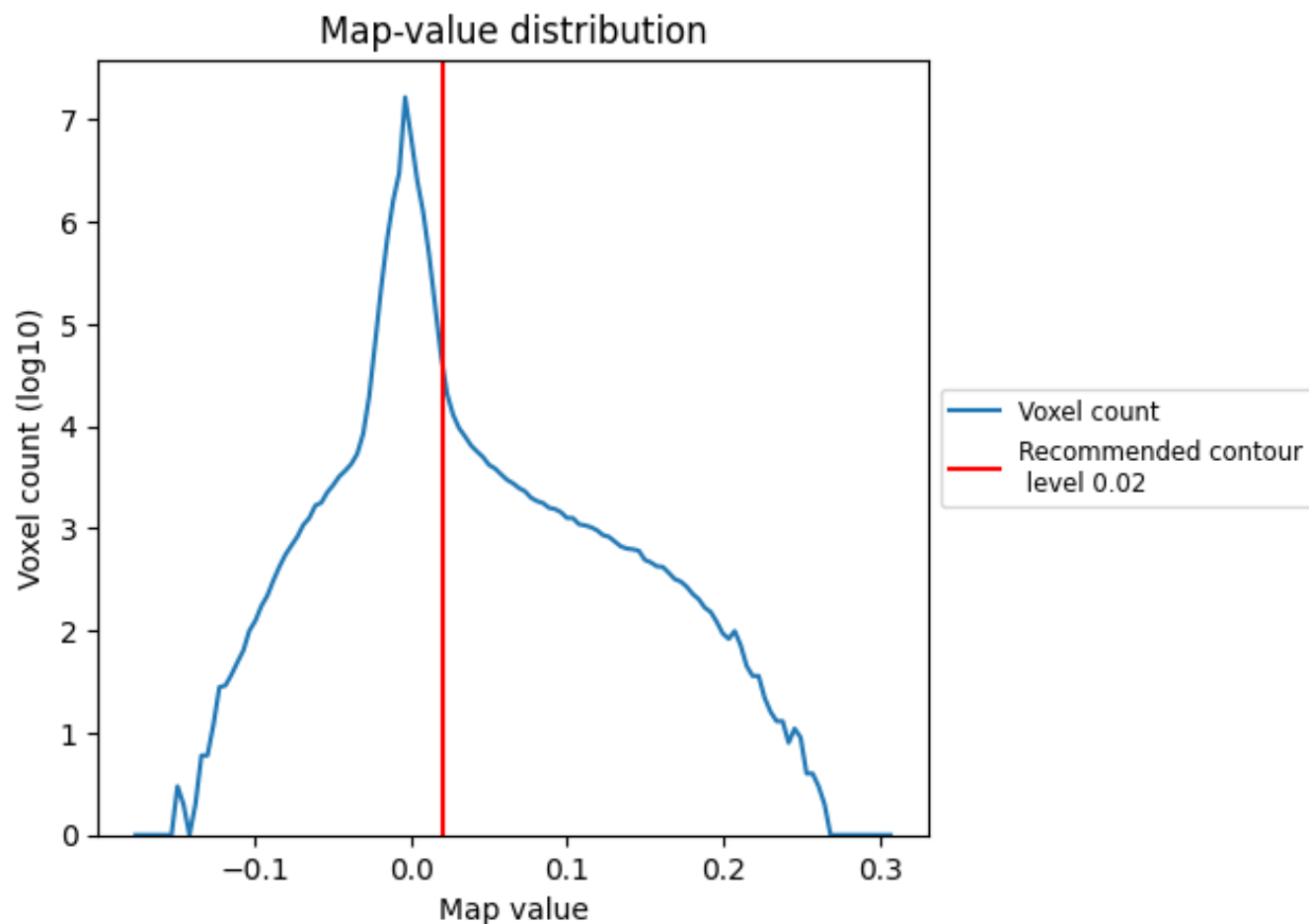
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
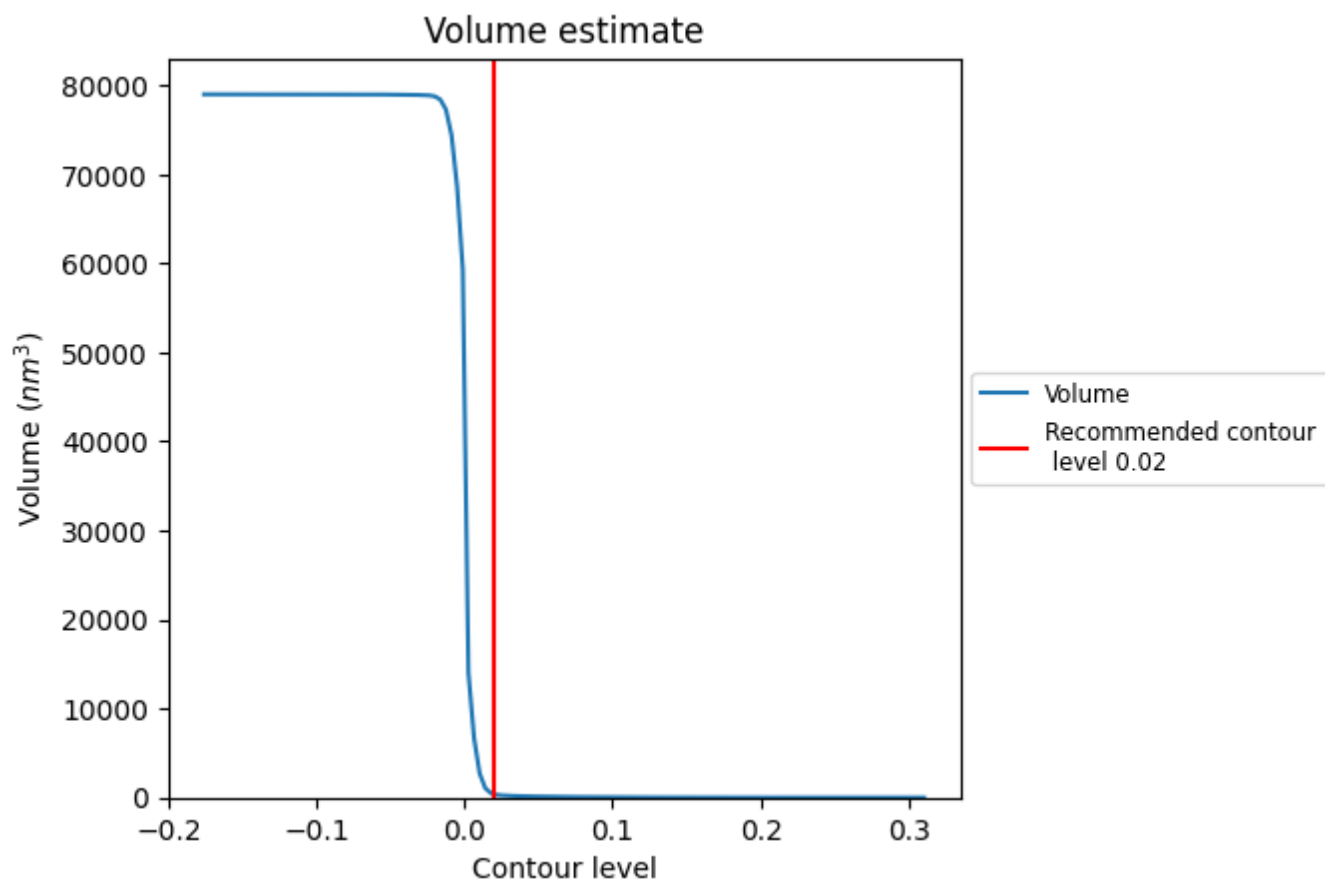
The volume at the recommended contour level is 387 nm^3; this corresponds to an approximate mass of 350 kDa.

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 ⓘ
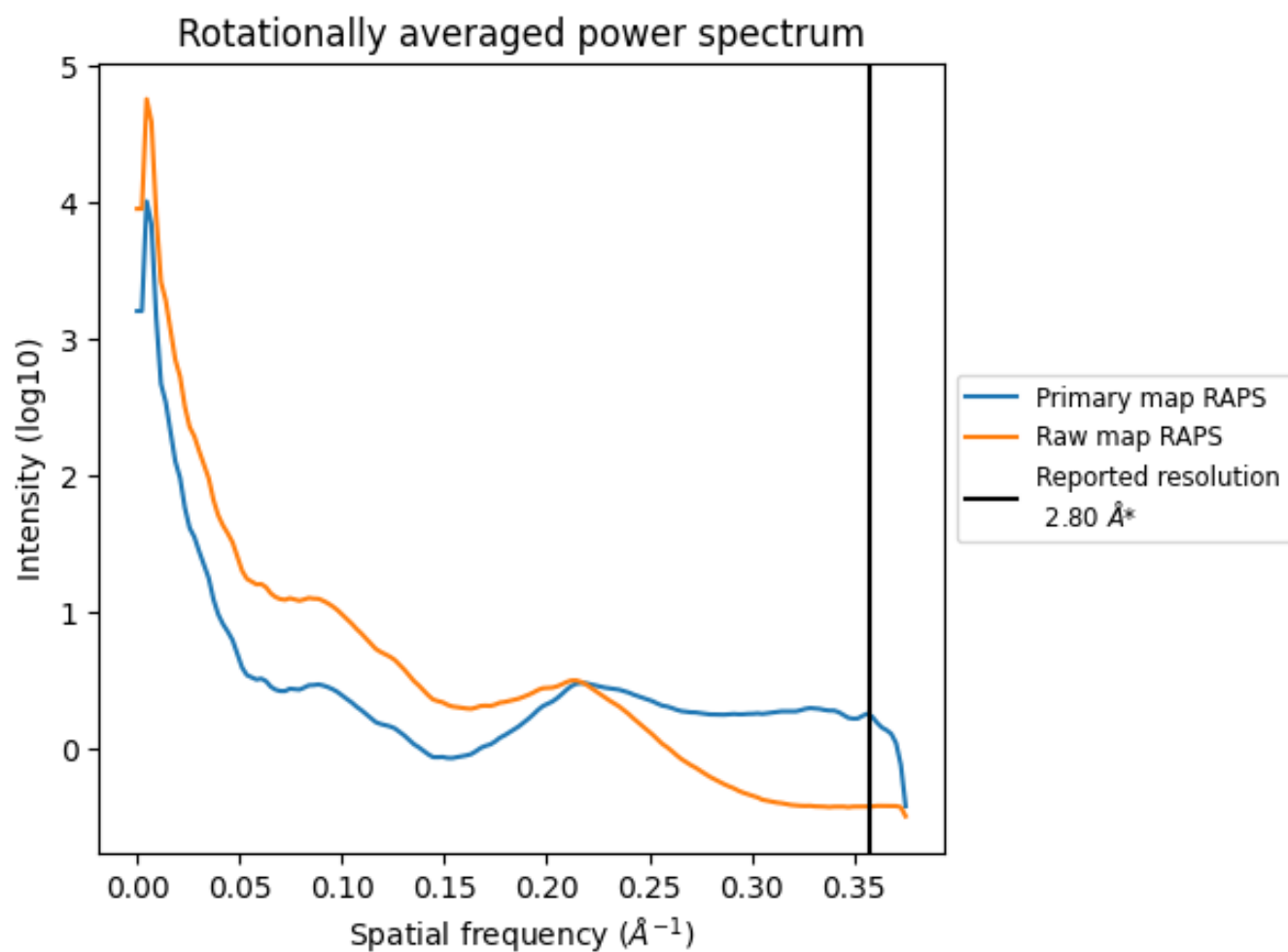
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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)
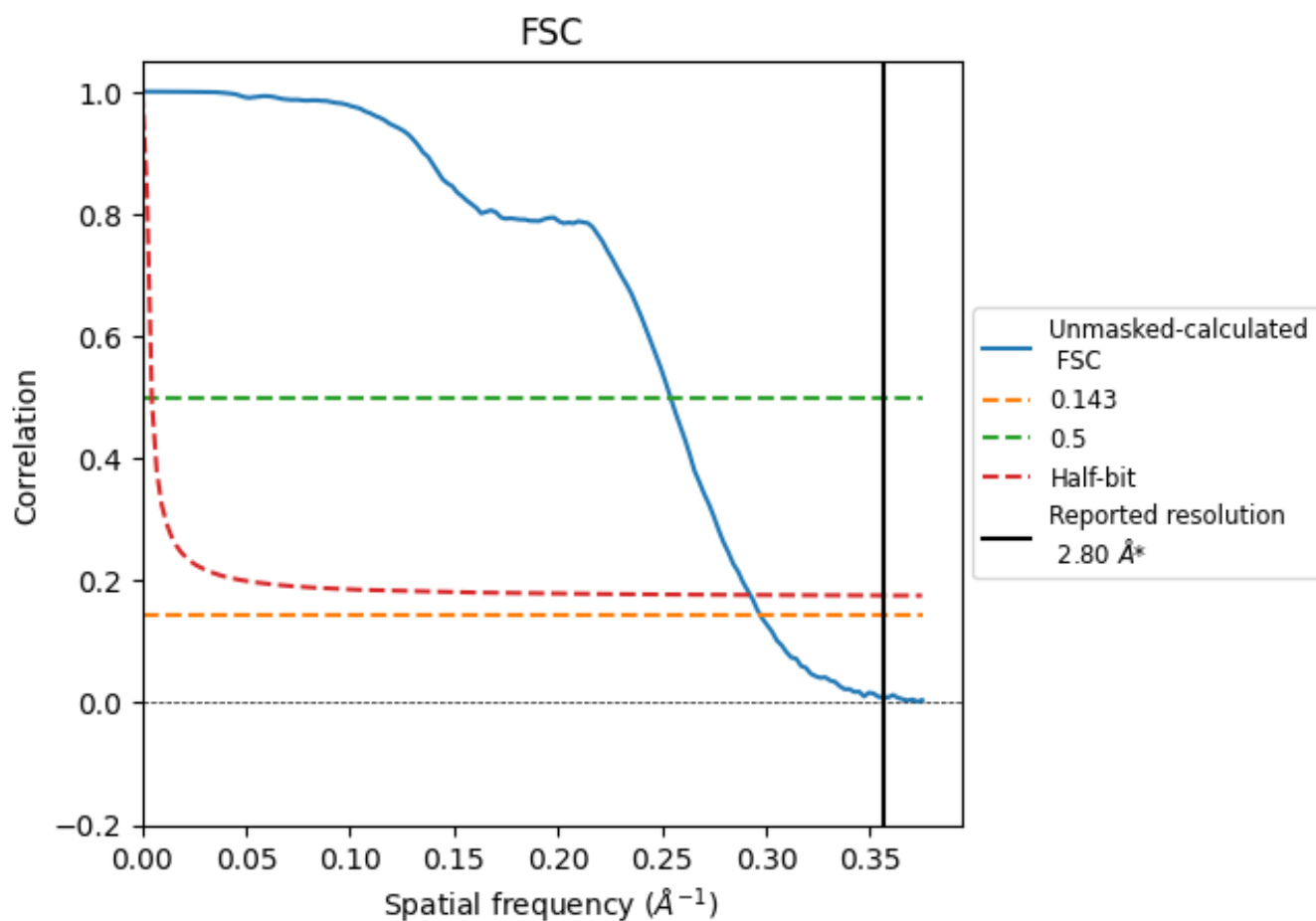
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.94	3.42

*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 3.36 differs from the reported value 2.8 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62010 and PDB model 9K39. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)

X	Y	Z
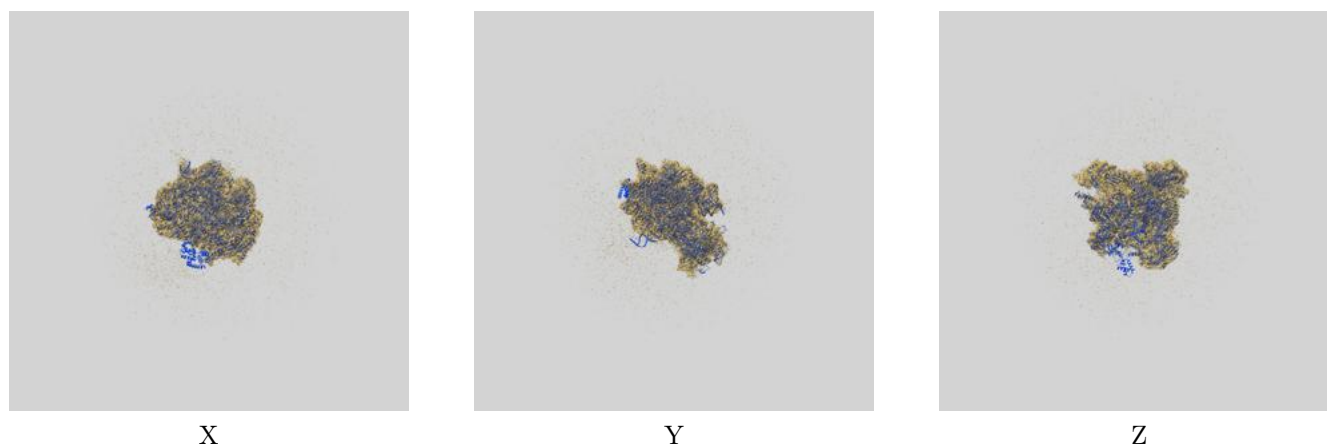
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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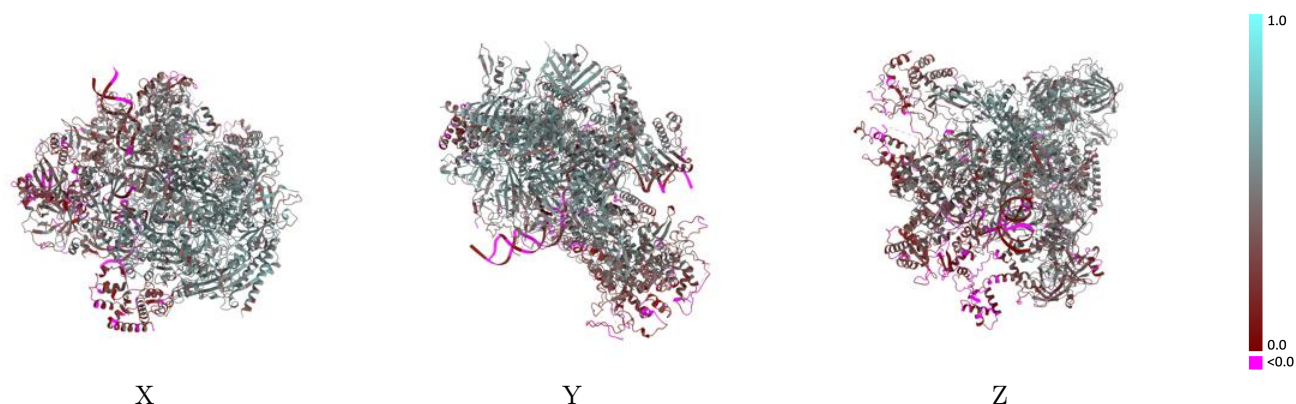
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ

X Y Z
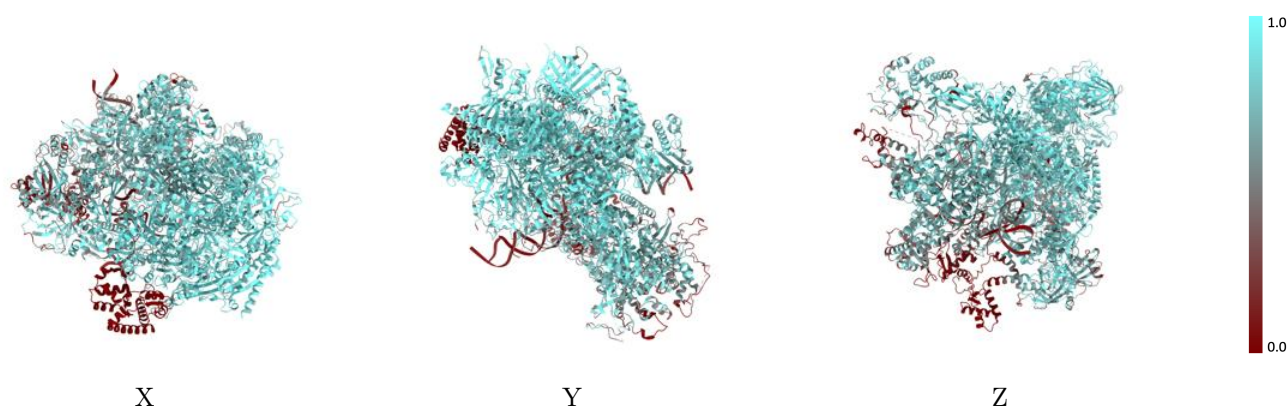
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)
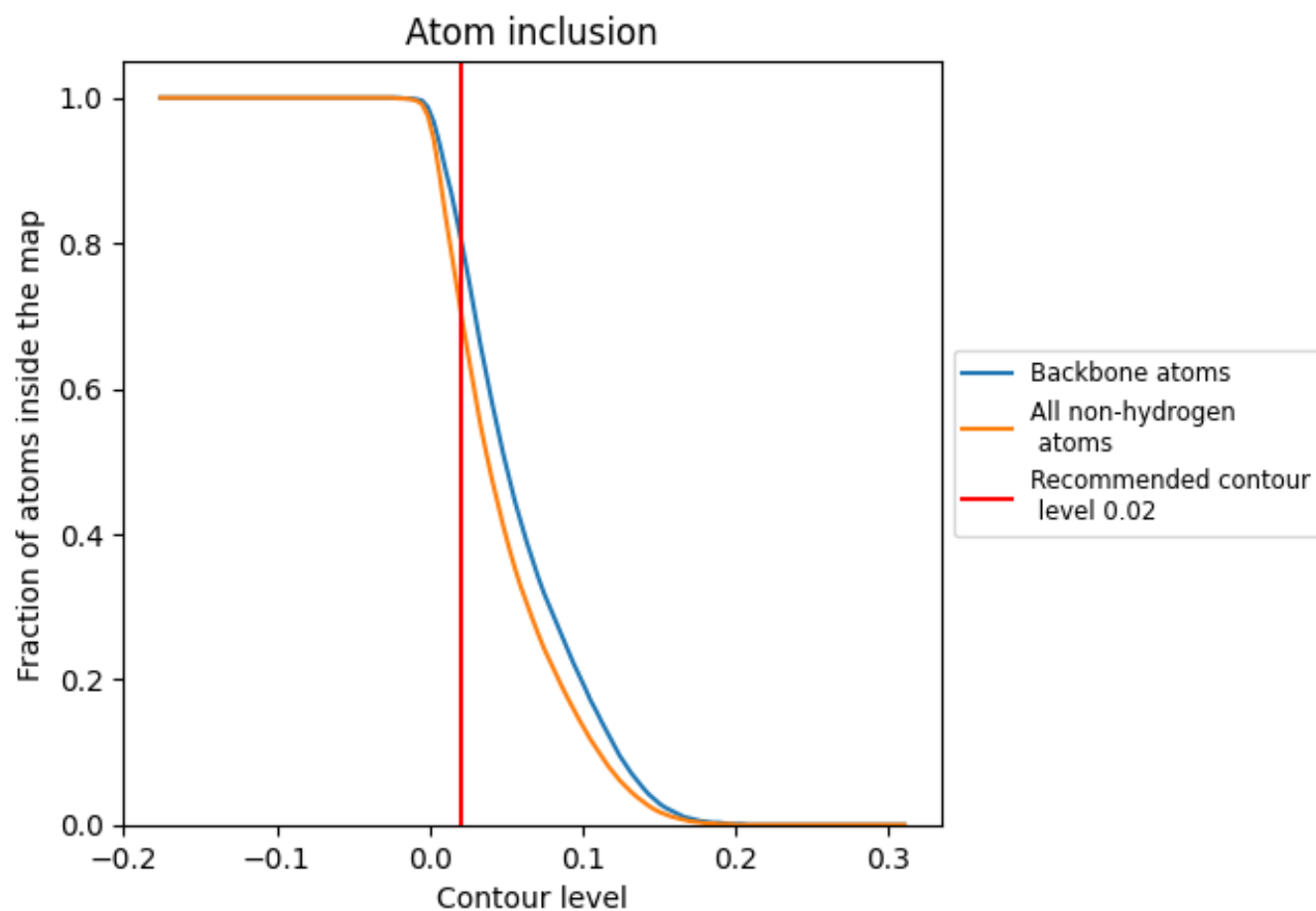
At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.4010
A	0.8280	0.4740
B	0.8370	0.4830
C	0.8910	0.5200
D	0.6430	0.2690
E	0.8040	0.4150
F	0.9090	0.5360
G	0.7500	0.3500
H	0.8490	0.4870
I	0.8050	0.4350
J	0.9000	0.5130
K	0.8850	0.5000
L	0.8230	0.4000
M	0.3600	0.2670
N	0.6080	0.2870
O	0.6090	0.3400
P	0.2860	0.1600
Q	0.5400	0.2920
V	0.5800	0.4280
X	0.2640	0.0890
Y	0.4150	0.1940
Z	0.7860	0.4450

1.0

0.0
<0.0